wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 06:36 AM EST

PDB ID	:	6DHE
Title	:	RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.05 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	:	2.05 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:

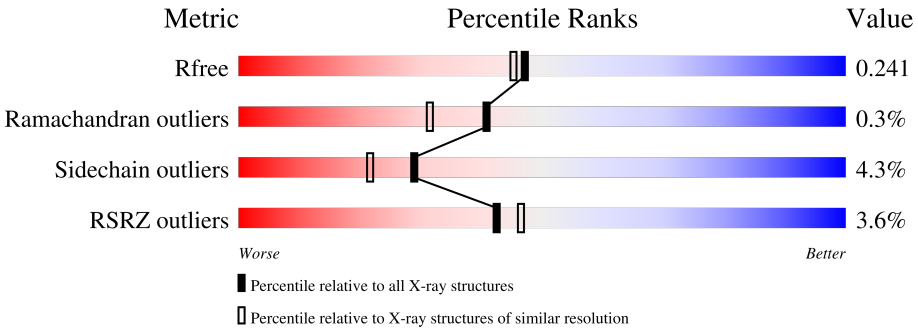
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

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 2.05 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}	130704	1692 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	% 99% .
1	a	334	% 97% .

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buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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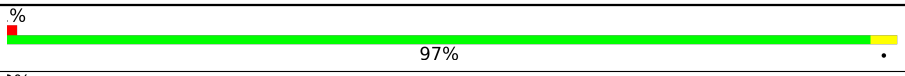
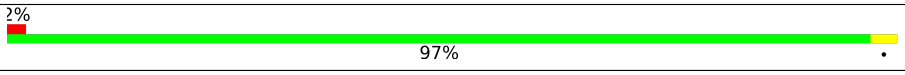
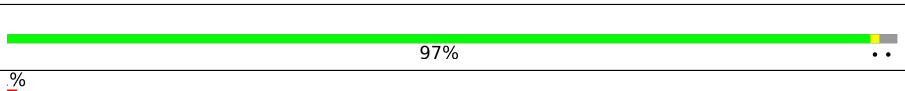
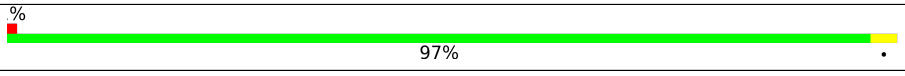
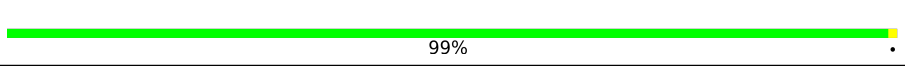
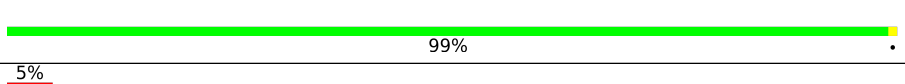
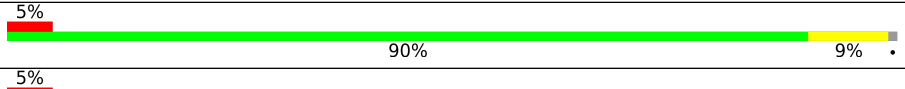
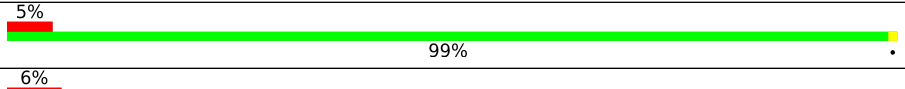
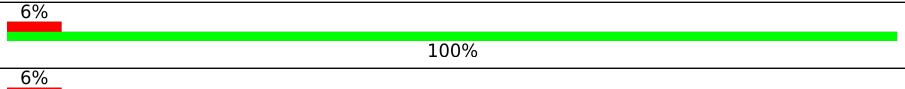
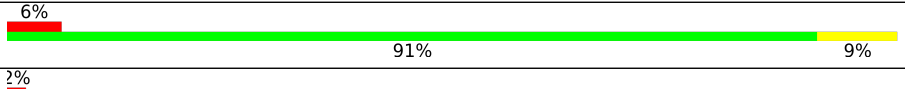
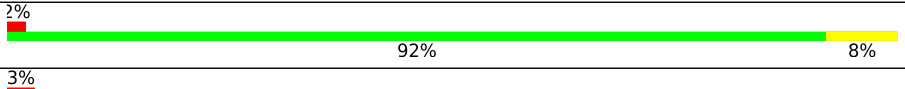
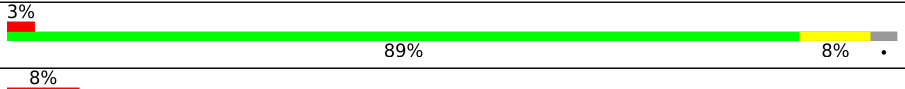
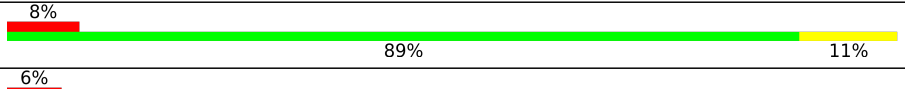
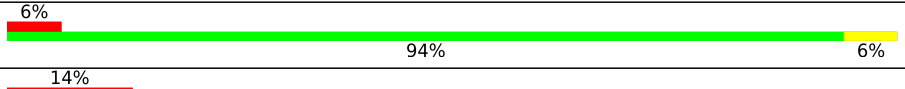
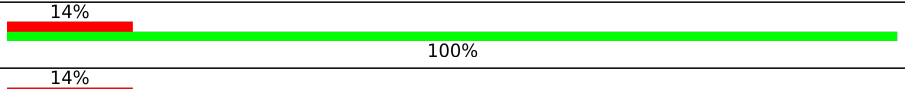
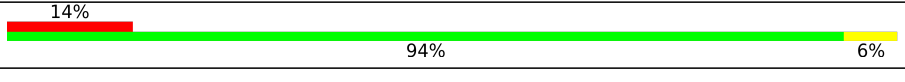
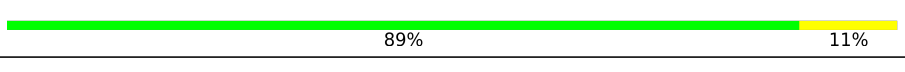
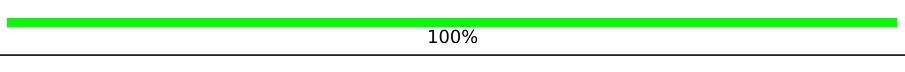
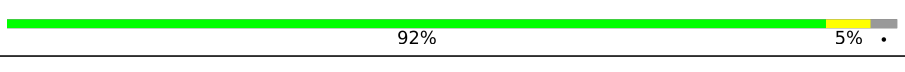
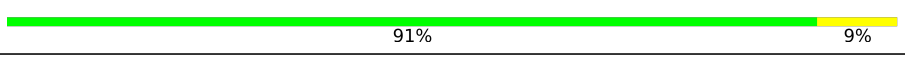
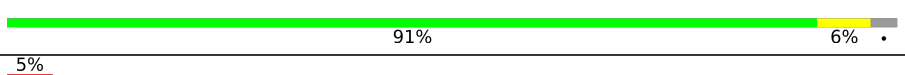
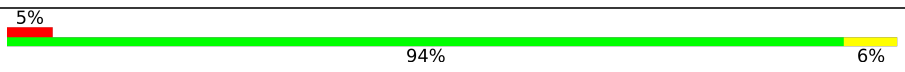
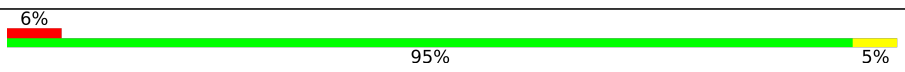
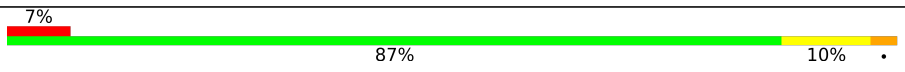
Mol	Chain	Length	Quality of chain
2	B	505	
2	b	505	
3	C	451	
3	c	451	
4	D	341	
4	d	341	
5	E	82	
5	e	82	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	36	
8	i	36	
9	J	36	
9	j	36	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	33	
12	m	33	
13	O	244	
13	o	244	
14	T	30	

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Mol	Chain	Length	Quality of chain
14	t	30	10% 97%
15	U	97	2% 96%
15	u	97	98%
16	V	137	96%
16	v	137	2% 96%
17	Y	30	37% 73% 13% 10%
17	y	30	30% 93% 7%
18	X	38	11% 97%
18	x	38	11% 95% 5%
19	Z	62	26% 89% 11%
19	z	62	21% 77% 23%
20	R	34	38% 85% 15%
20	r	34	59% 76% 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
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	404	X	-	-	-
25	8CT	A	408	X	-	-	-
25	8CT	B	617	X	-	-	-
25	8CT	B	619	X	-	-	-
25	8CT	C	514	X	-	-	-
25	8CT	C	515	X	-	-	-
25	8CT	C	520	X	-	-	-
25	8CT	D	405	X	-	-	-
25	8CT	b	620	X	-	-	-
25	8CT	c	514	X	-	-	-
25	8CT	d	405	X	-	-	-
25	8CT	k	101	X	-	-	-
25	8CT	t	101	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 103686 atoms, of which 51480 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	2	0
			6911	2290	3411	587	610	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 598 204 305 43 46	0	0	0

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

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

- 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 525 171 269 37 47 1	0	0	0
12	m	32	Total C H N O S 518 168 267 36 46 1	0	0	0

- 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 3730 1174 1850 317 385 4	0	1	0
13	o	244	Total C H N O S 3718 1170 1844 317 383 4	0	0	0

- 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 519 181 261 36 39 2	0	0	0
14	t	30	Total C H N O S 512 180 256 36 38 2	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

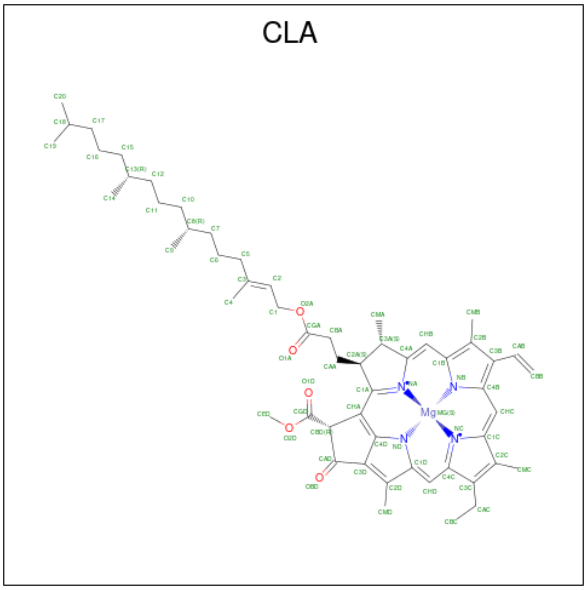
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: 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	A	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
			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		

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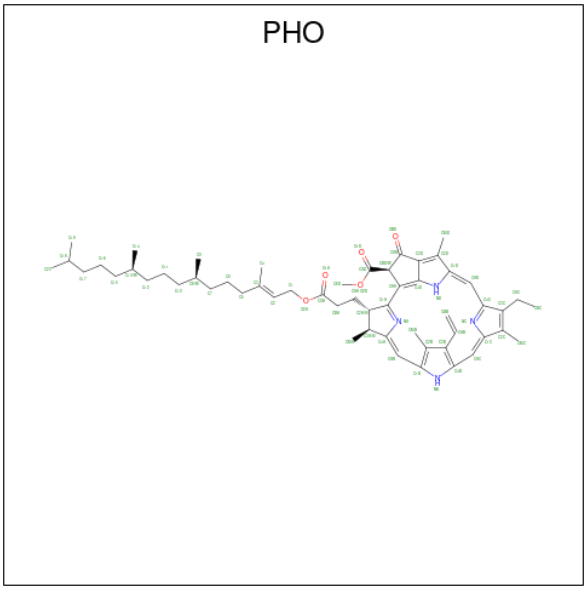
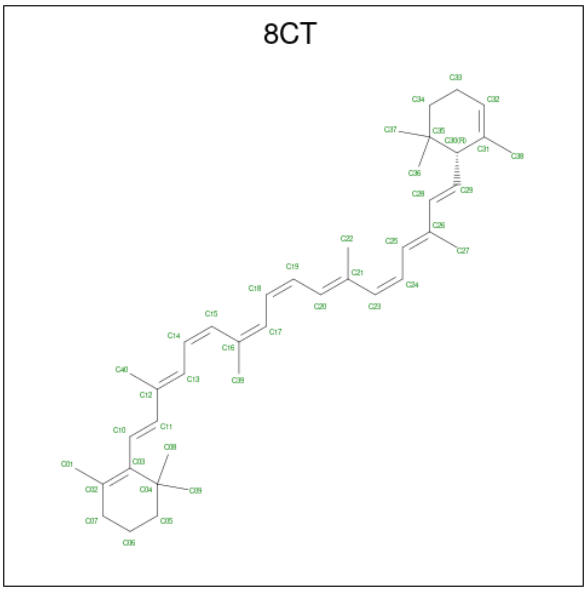
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: 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		

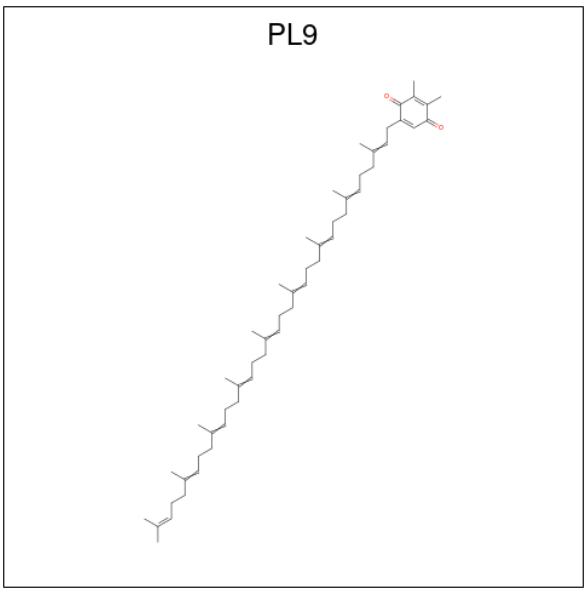
- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$).



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	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	b	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

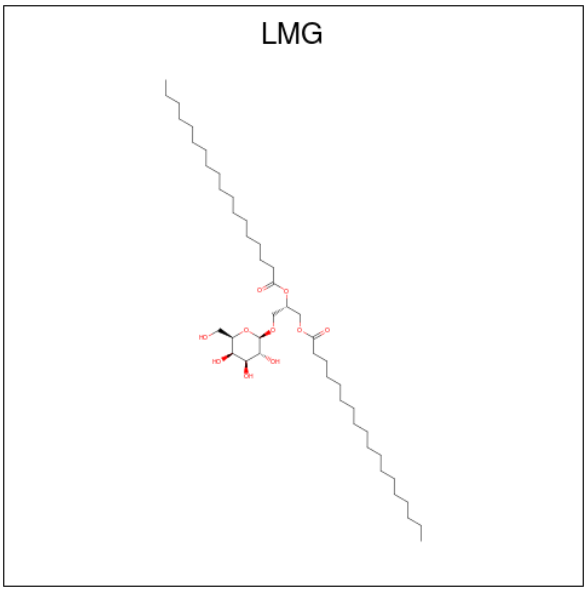
- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

$C_{53}H_{80}O_2$).



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

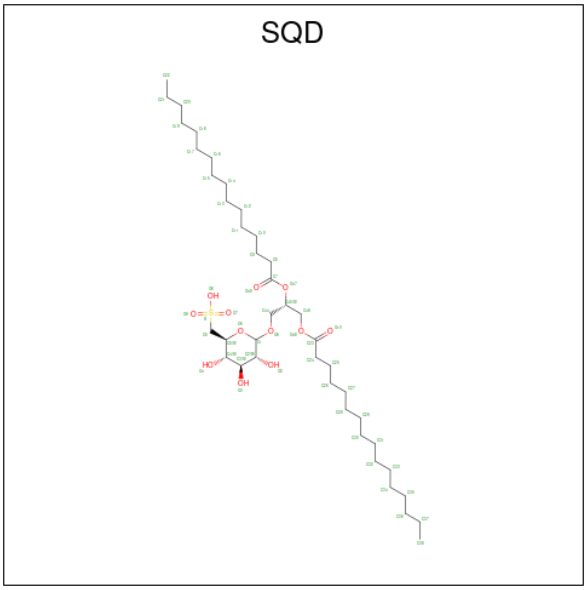
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

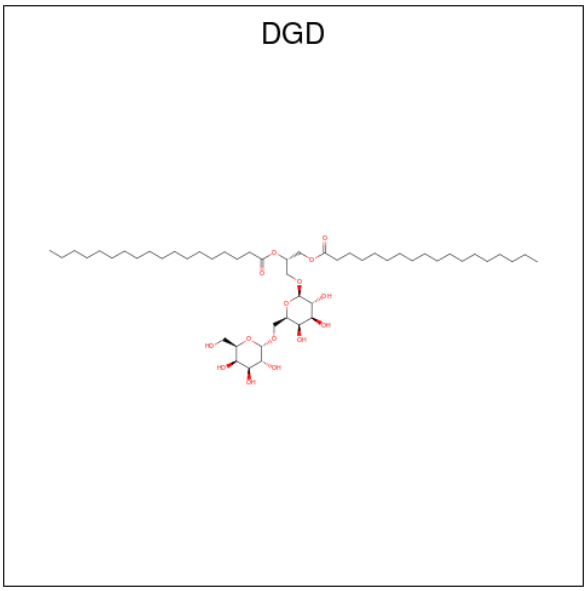
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



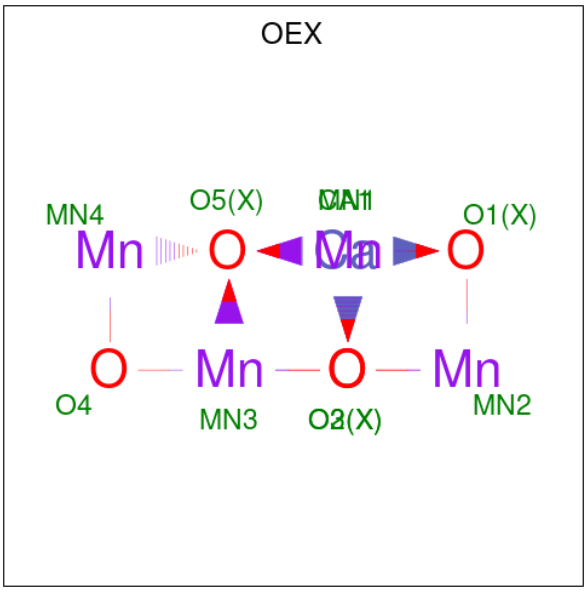
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H O S 122 39 70 12 1	0	0
28	A	1	Total C H O 104 35 65 4	0	0
28	B	1	Total C H O S 132 41 78 12 1	0	0
28	D	1	Total C H O S 81 25 45 10 1	0	0
28	a	1	Total C H O S 132 41 78 12 1	0	0
28	a	1	Total C H O 92 31 56 5	0	0
28	b	1	Total C H O S 114 36 65 12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

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



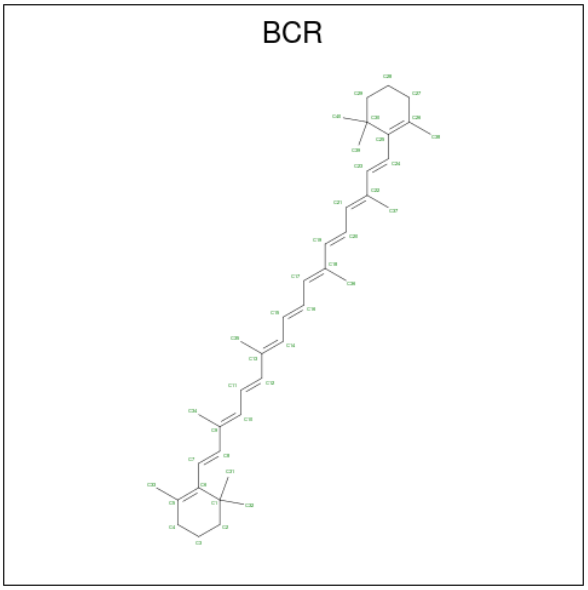
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total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

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: 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 BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	H	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	T	1	Total C H 96 40 56	0	0
31	Y	1	Total C H 96 40 56	0	0
31	a	1	Total C H 96 40 56	0	0
31	b	1	Total C H 96 40 56	0	0
31	b	1	Total C H 96 40 56	0	0
31	c	1	Total C H 96 40 56	0	0
31	c	1	Total C H 96 40 56	0	0
31	h	1	Total C H 96 40 56	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	5	Total C H O 192 67 117 8	0	0
32	C	3	Total C H O 103 36 63 4	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	2	Total C H 91 31 60	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	4	Total C H O 176 60 110 6	0	0

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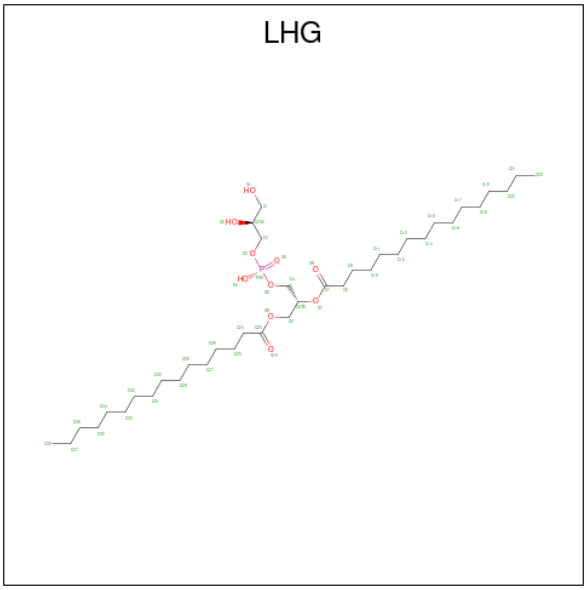
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	c	2	Total C H O 83 28 51 4	0	0
32	d	2	Total C H O 98 33 61 4	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	m	1	Total C H O 28 10 16 2	0	0
32	t	2	Total C H O 60 22 36 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C H O P 123 38 74 10 1	0	0
33	D	1	Total C H O P 123 38 74 10 1	0	0
33	D	1	Total C H O P 114 36 67 10 1	0	0
33	E	1	Total C H O P 123 38 74 10 1	0	0
33	L	1	Total C H O P 123 38 74 10 1	0	0

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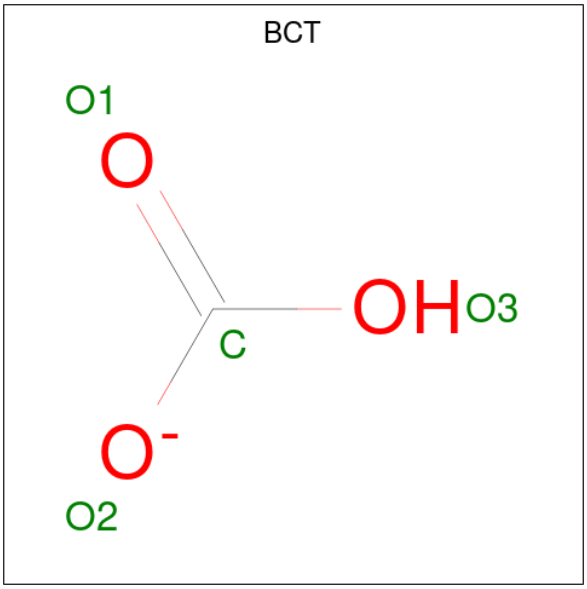
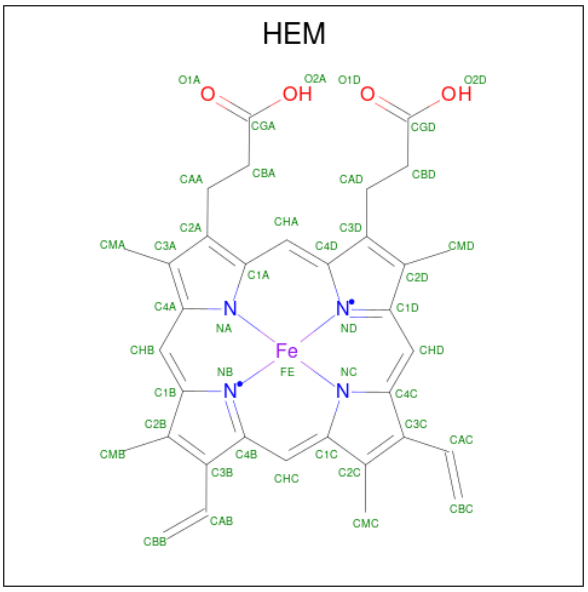
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



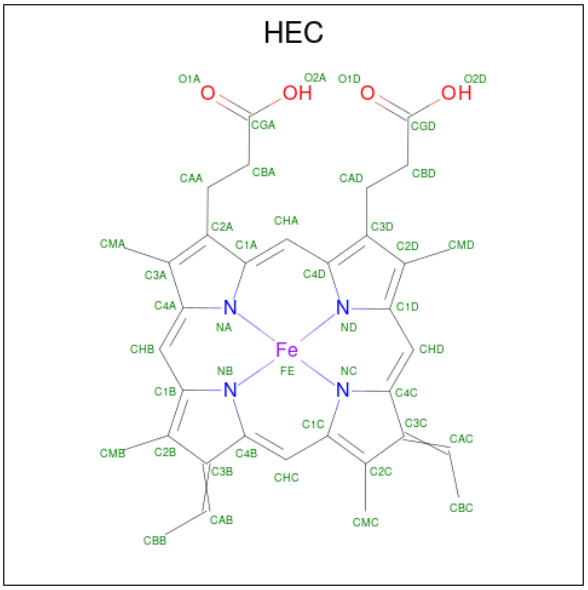
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 36 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	140	Total O 140 140	0	0
37	B	214	Total O 214 214	0	0
37	C	199	Total O 199 199	0	0
37	D	137	Total O 137 137	0	0
37	E	28	Total O 28 28	0	0
37	F	12	Total O 12 12	0	0
37	H	26	Total O 26 26	0	0
37	I	15	Total O 15 15	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	7	Total O 7 7	0	0
37	M	5	Total O 5 5	0	0
37	O	129	Total O 129 129	0	0
37	T	13	Total O 13 13	0	0
37	U	49	Total O 49 49	0	0
37	V	72	Total O 72 72	0	0
37	Y	5	Total O 5 5	0	0
37	X	9	Total O 9 9	0	0
37	Z	5	Total O 5 5	0	0
37	R	3	Total O 3 3	0	0
37	a	124	Total O 124 124	0	0

Continued on next page...

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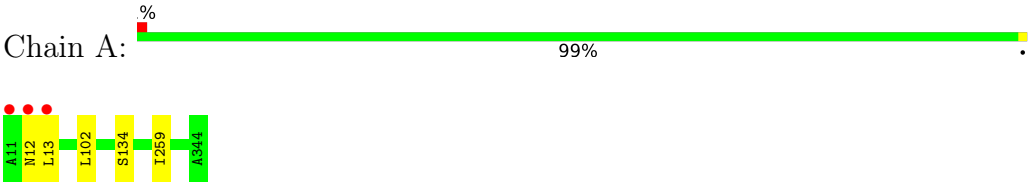
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	b	191	Total O 191 191	0	0
37	c	161	Total O 161 161	0	0
37	d	123	Total O 123 123	0	0
37	e	24	Total O 24 24	0	0
37	f	6	Total O 6 6	0	0
37	h	17	Total O 17 17	0	0
37	i	9	Total O 9 9	0	0
37	j	7	Total O 7 7	0	0
37	k	5	Total O 5 5	0	0
37	l	10	Total O 10 10	0	0
37	m	8	Total O 8 8	0	0
37	o	111	Total O 111 111	0	0
37	t	10	Total O 10 10	0	0
37	u	50	Total O 50 50	0	0
37	v	61	Total O 61 61	0	0
37	y	4	Total O 4 4	0	0
37	x	11	Total O 11 11	0	0
37	z	1	Total O 1 1	0	0
37	r	6	Total O 6 6	0	0

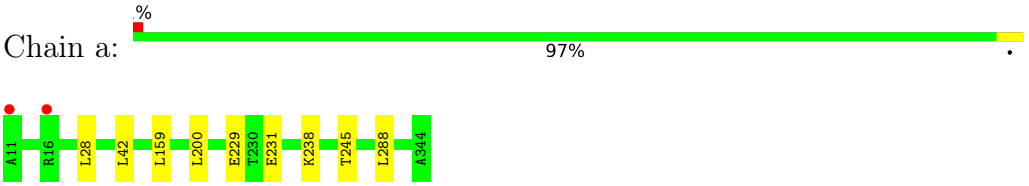
3 Residue-property plots (i)

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

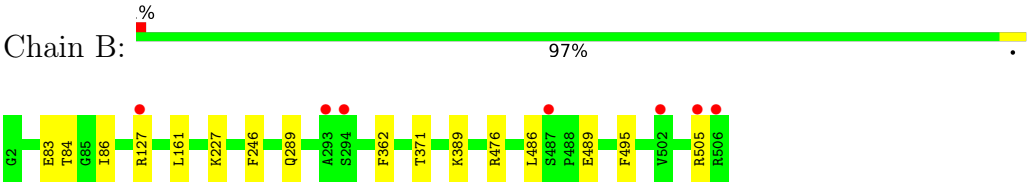
• Molecule 1: Photosystem II protein D1 1



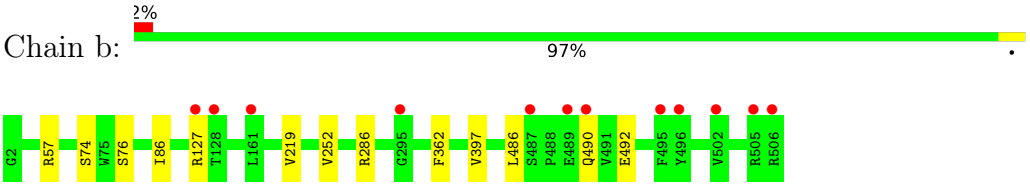
• Molecule 1: Photosystem II protein D1 1



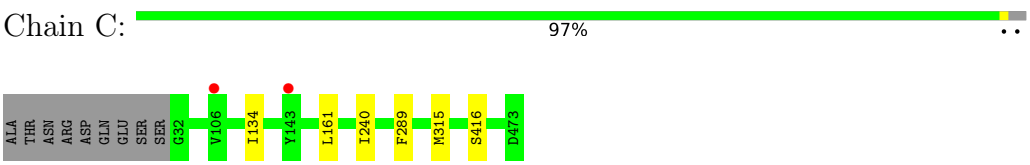
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

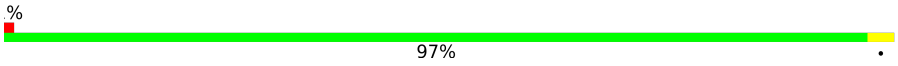


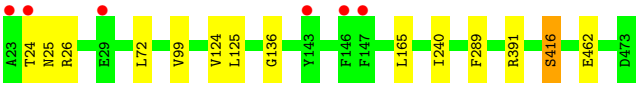
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

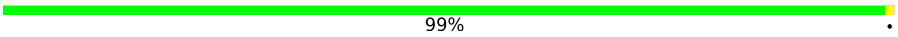
Chain c:





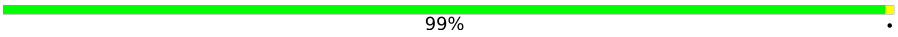
• Molecule 4: Photosystem II D2 protein

Chain D:



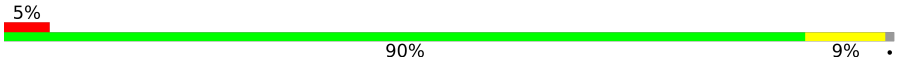
• Molecule 4: Photosystem II D2 protein

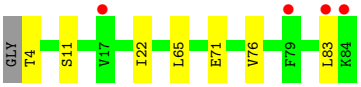
Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

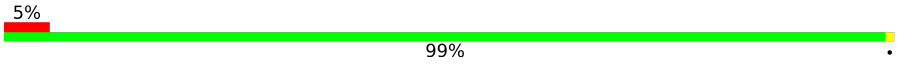
Chain E:

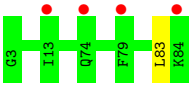




• Molecule 5: Cytochrome b559 subunit alpha

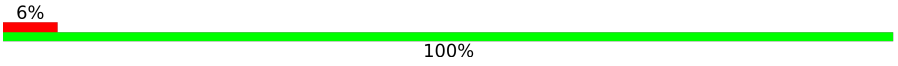
Chain e:





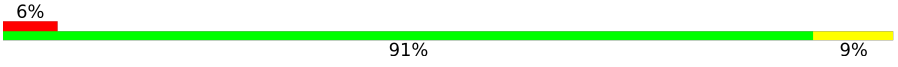
• Molecule 6: Cytochrome b559 subunit beta

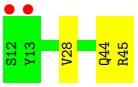
Chain F:



• Molecule 6: Cytochrome b559 subunit beta

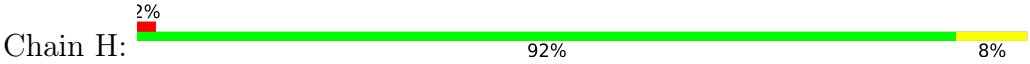
Chain f:





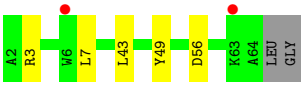
• Molecule 7: Photosystem II reaction center protein H

Chain H:



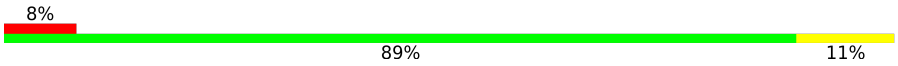
• Molecule 7: Photosystem II reaction center protein H

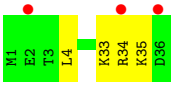
Chain h:



• Molecule 8: Photosystem II reaction center protein I

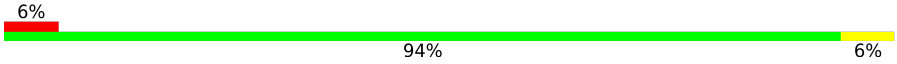
Chain I:

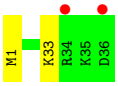




• Molecule 8: Photosystem II reaction center protein I

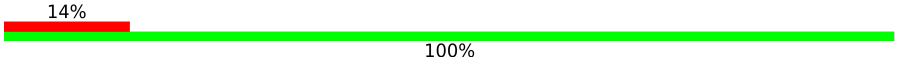
Chain i:

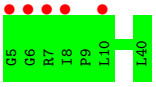




• Molecule 9: Photosystem II reaction center protein J

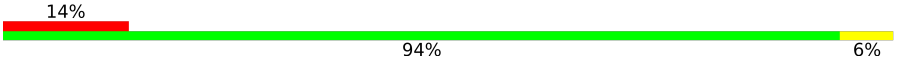
Chain J:

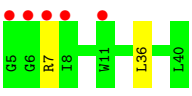




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

• Molecule 10: Photosystem II reaction center protein K

Chain k:

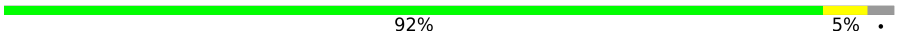
• Molecule 11: Photosystem II reaction center protein L

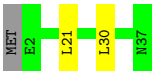
Chain L:

There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem II reaction center protein L

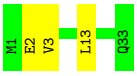
Chain l:





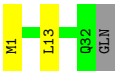
• Molecule 12: Photosystem II reaction center protein M

Chain M:



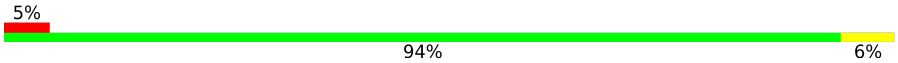
• Molecule 12: Photosystem II reaction center protein M

Chain m:



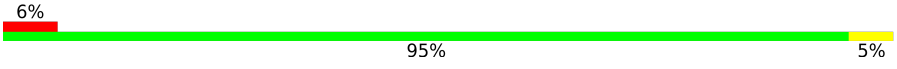
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

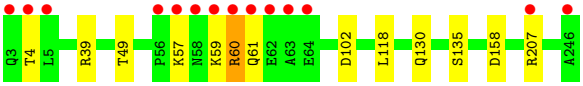
Chain O:



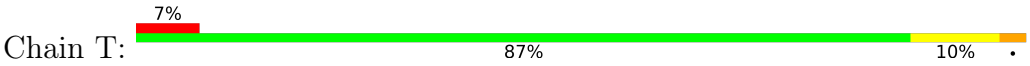
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

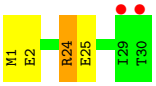
Chain o:



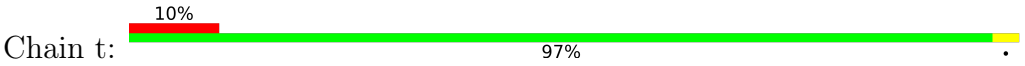


• Molecule 14: Photosystem II reaction center protein T

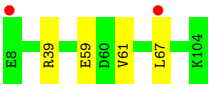




• Molecule 14: Photosystem II reaction center protein T



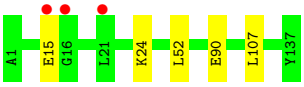
• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

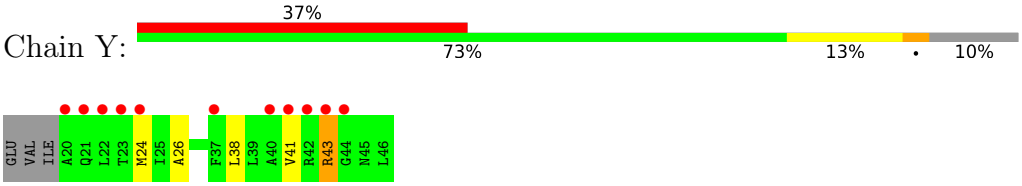
• Molecule 16: Cytochrome c-550

• Molecule 16: Cytochrome c-550



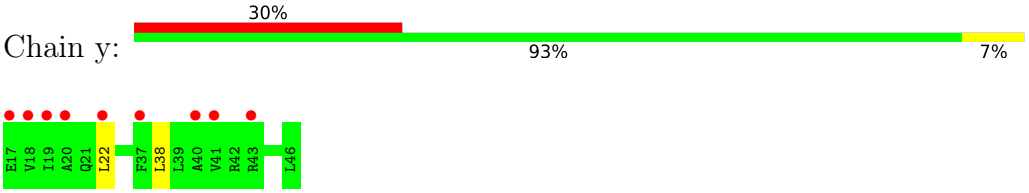
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



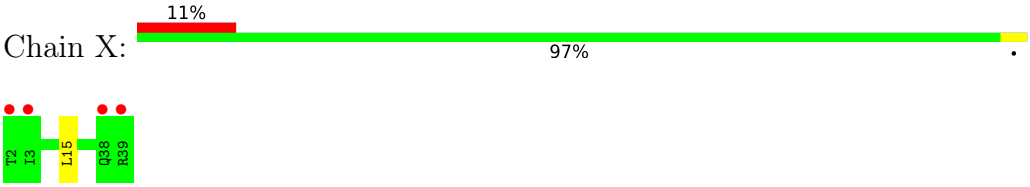
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



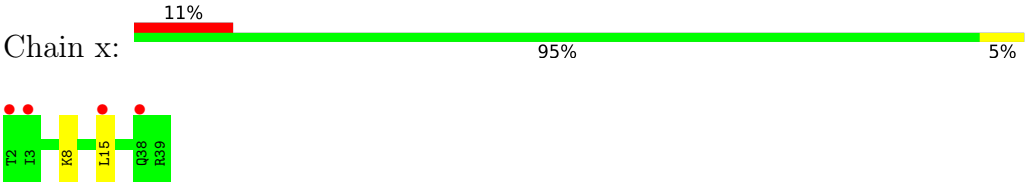
• Molecule 18: Photosystem II reaction center X protein

Chain X:



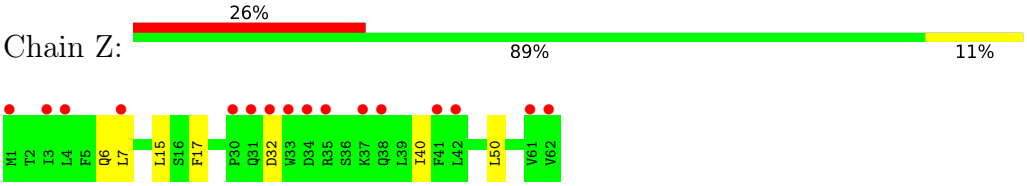
• Molecule 18: Photosystem II reaction center X protein

Chain x:



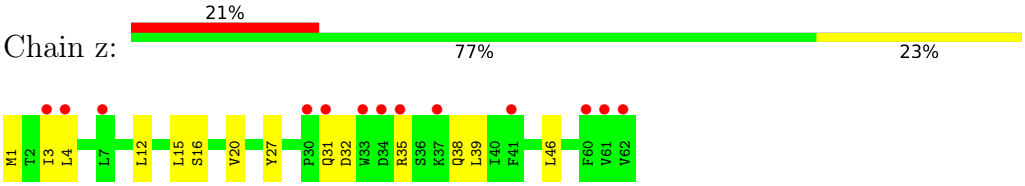
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



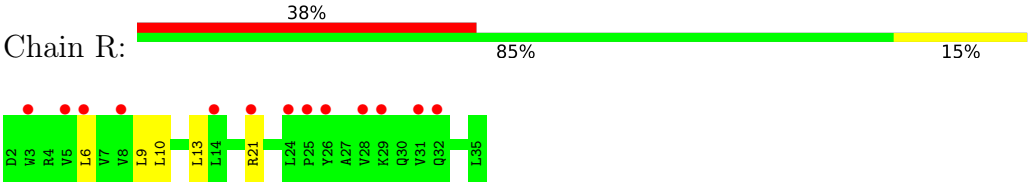
• Molecule 19: Photosystem II reaction center protein Z

Chain z:

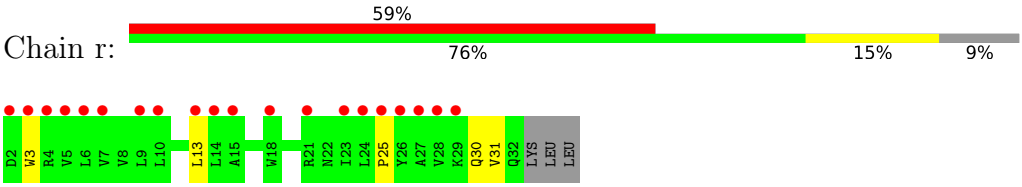


• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.91Å 221.41Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.55 – 2.05 30.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.55-2.05) 87.7 (30.55-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.185 , 0.241 0.185 , 0.241	Depositor DCC
R_{free} test set	4419 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	103686	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, OEX, CL, UNL, 8CT, FME, PHO, SQD, BCR, PL9, HEC, LMG, BCT, FE2, HEM, DGD, LHG

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	0.64	0/2707	0.70	0/3692
1	a	0.61	0/2704	0.67	0/3688
2	B	0.62	0/4160	0.68	0/5668
2	b	0.60	0/4118	0.66	1/5611 (0.0%)
3	C	0.63	0/3530	0.67	0/4807
3	c	0.54	0/3619	0.65	0/4926
4	D	0.63	0/2812	0.67	0/3832
4	d	0.60	0/2821	0.68	0/3844
5	E	0.51	0/684	0.65	0/935
5	e	0.49	0/683	0.57	0/932
6	F	0.51	0/284	0.59	0/387
6	f	0.51	0/284	0.57	0/387
7	H	0.60	0/520	0.67	0/709
7	h	0.54	0/511	0.68	0/697
8	I	0.61	0/293	0.63	0/396
8	i	0.67	0/293	0.72	0/396
9	J	0.52	0/263	0.70	0/356
9	j	0.49	0/261	0.63	0/353
10	K	0.44	0/314	0.67	0/427
10	k	0.44	0/303	0.65	0/416
11	L	0.62	0/311	0.65	0/422
11	l	0.64	0/303	0.70	0/412
12	M	0.57	0/249	0.70	0/341
12	m	0.61	0/244	0.63	0/334
13	O	0.56	0/1914	0.70	0/2596
13	o	0.57	0/1905	0.74	2/2583 (0.1%)
14	T	0.63	0/257	0.79	2/349 (0.6%)
14	t	0.66	0/255	0.58	0/346
15	U	0.54	0/785	0.65	0/1064
15	u	0.57	0/785	0.69	0/1064
16	V	0.56	0/1085	0.65	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.50	0/1085	0.64	0/1473
17	Y	0.39	0/197	0.59	0/264
17	y	0.36	0/219	0.56	0/294
18	X	0.51	0/284	0.63	0/384
18	x	0.37	0/284	0.54	0/384
19	Z	0.46	0/490	0.58	0/669
19	z	0.41	0/488	0.55	0/666
20	R	0.39	0/277	0.65	0/380
20	r	0.34	0/233	0.49	0/323
All	All	0.58	0/42814	0.67	5/58280 (0.0%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	24	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	b	57	ARG	NE-CZ-NH1	-6.30	117.15	120.30
13	o	158	ASP	CB-CG-OD1	5.42	123.18	118.30
13	o	102	ASP	CB-CG-OD1	5.20	122.98	118.30
14	T	24	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	52	ASN	Peptide

5.2 Too-close contacts (i)

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

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%)	324 (98%)	7 (2%)	1 (0%)	41 31
1	a	332/334 (99%)	325 (98%)	7 (2%)	0	100 100
2	B	508/505 (101%)	499 (98%)	9 (2%)	0	100 100
2	b	503/505 (100%)	493 (98%)	10 (2%)	0	100 100
3	C	440/451 (98%)	426 (97%)	13 (3%)	1 (0%)	47 39
3	c	451/451 (100%)	436 (97%)	13 (3%)	2 (0%)	34 24
4	D	339/341 (99%)	329 (97%)	10 (3%)	0	100 100
4	d	340/341 (100%)	330 (97%)	10 (3%)	0	100 100
5	E	80/82 (98%)	77 (96%)	3 (4%)	0	100 100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100 100
6	F	32/34 (94%)	32 (100%)	0	0	100 100
6	f	32/34 (94%)	32 (100%)	0	0	100 100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100 100
7	h	61/65 (94%)	57 (93%)	4 (7%)	0	100 100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
8	i	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
9	J	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
9	j	34/36 (94%)	31 (91%)	3 (9%)	0	100 100
10	K	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4 0
10	k	35/37 (95%)	35 (100%)	0	0	100 100
11	L	35/37 (95%)	35 (100%)	0	0	100 100
11	l	34/37 (92%)	34 (100%)	0	0	100 100
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100 100
12	m	30/33 (91%)	30 (100%)	0	0	100 100
13	O	243/244 (100%)	230 (95%)	11 (4%)	2 (1%)	19 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	19 10
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%)	92 (97%)	3 (3%)	0	100 100
15	u	95/97 (98%)	90 (95%)	5 (5%)	0	100 100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100 100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100 100
17	Y	25/30 (83%)	16 (64%)	6 (24%)	3 (12%)	0 0
17	y	28/30 (93%)	25 (89%)	3 (11%)	0	100 100
18	X	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	55 (92%)	4 (7%)	1 (2%)	9 2
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9 2
20	R	32/34 (94%)	30 (94%)	2 (6%)	0	100 100
20	r	29/34 (85%)	24 (83%)	2 (7%)	3 (10%)	0 0
All	All	5236/5326 (98%)	5051 (96%)	168 (3%)	17 (0%)	41 31

5 of 17 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
17	Y	43	ARG

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%)	266 (98%)	4 (2%)	65 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	269/270 (100%)	260 (97%)	9 (3%)	38 31
2	B	407/403 (101%)	391 (96%)	16 (4%)	32 25
2	b	402/403 (100%)	390 (97%)	12 (3%)	41 34
3	C	344/352 (98%)	339 (98%)	5 (2%)	65 62
3	c	354/352 (101%)	340 (96%)	14 (4%)	31 24
4	D	276/276 (100%)	273 (99%)	3 (1%)	73 73
4	d	277/276 (100%)	272 (98%)	5 (2%)	59 55
5	E	72/72 (100%)	64 (89%)	8 (11%)	6 1
5	e	71/72 (99%)	70 (99%)	1 (1%)	67 65
6	F	28/28 (100%)	28 (100%)	0	100 100
6	f	28/28 (100%)	25 (89%)	3 (11%)	6 2
7	H	53/54 (98%)	48 (91%)	5 (9%)	8 3
7	h	53/54 (98%)	48 (91%)	5 (9%)	8 3
8	I	32/32 (100%)	28 (88%)	4 (12%)	4 1
8	i	32/32 (100%)	31 (97%)	1 (3%)	40 33
9	J	24/24 (100%)	24 (100%)	0	100 100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10 4
10	K	31/30 (103%)	27 (87%)	4 (13%)	4 1
10	k	30/30 (100%)	26 (87%)	4 (13%)	4 1
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	34/35 (97%)	32 (94%)	2 (6%)	19 11
12	M	28/29 (97%)	25 (89%)	3 (11%)	6 2
12	m	28/29 (97%)	27 (96%)	1 (4%)	35 28
13	O	208/207 (100%)	195 (94%)	13 (6%)	18 9
13	o	207/207 (100%)	197 (95%)	10 (5%)	25 18
14	T	26/26 (100%)	23 (88%)	3 (12%)	5 1
14	t	25/26 (96%)	25 (100%)	0	100 100
15	U	84/84 (100%)	80 (95%)	4 (5%)	25 18
15	u	84/84 (100%)	83 (99%)	1 (1%)	71 70
16	V	117/117 (100%)	112 (96%)	5 (4%)	29 22
16	v	117/117 (100%)	112 (96%)	5 (4%)	29 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2 0
17	y	22/23 (96%)	20 (91%)	2 (9%)	9 3
18	X	31/31 (100%)	30 (97%)	1 (3%)	39 32
18	x	31/31 (100%)	29 (94%)	2 (6%)	17 9
19	Z	52/52 (100%)	46 (88%)	6 (12%)	5 1
19	z	51/52 (98%)	38 (74%)	13 (26%)	0 0
20	R	28/29 (97%)	23 (82%)	5 (18%)	2 0
20	r	19/29 (66%)	17 (90%)	2 (10%)	7 2
All	All	4322/4348 (99%)	4136 (96%)	186 (4%)	29 22

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	26	ARG
9	j	36	LEU
3	c	125	LEU
4	d	321	LEU
12	m	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
19	z	38	GLN
19	z	58	ASN
17	Y	21	GLN
2	b	497	GLN
3	c	25	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	0.97	0	7,9,11	1.61	2 (28%)
8	FME	I	1	8	8,9,10	0.96	0	7,9,11	0.95	0
8	FME	i	1	8	8,9,10	1.07	0	7,9,11	1.36	1 (14%)
12	FME	M	1	12	8,9,10	0.99	0	7,9,11	0.84	0
12	FME	m	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.97	1 (14%)
14	FME	t	1	14	8,9,10	0.93	0	7,9,11	1.15	1 (14%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	FME	CA-N	-2.18	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-2.57	118.87	122.82
14	T	1	FME	C-CA-N	2.23	113.76	109.73
14	t	1	FME	C-CA-N	2.17	113.65	109.73
14	T	1	FME	O1-CN-N	-2.13	119.66	125.27
12	m	1	FME	C-CA-N	-2.08	105.99	109.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 monosaccharides 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	$\#\|Z\| > 2$
23	CLA	c	511	3	65,73,73	1.81	8 (12%)	76,113,113	1.42	5 (6%)
25	8CT	b	620	-	40,41,41	1.70	4 (10%)	50,56,56	2.27	11 (22%)
23	CLA	C	506	-	65,73,73	1.83	8 (12%)	76,113,113	1.28	6 (7%)
27	LMG	D	411	-	31,31,55	1.38	5 (16%)	33,33,63	1.13	3 (9%)
33	LHG	D	410	-	46,46,48	1.05	3 (6%)	49,52,54	1.25	3 (6%)
23	CLA	a	406	37	65,73,73	1.62	11 (16%)	76,113,113	1.60	14 (18%)
33	LHG	D	409	-	48,48,48	1.01	4 (8%)	51,54,54	1.19	5 (9%)
24	PHO	d	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.44	5 (10%)
23	CLA	b	606	-	65,73,73	1.37	6 (9%)	76,113,113	1.64	11 (14%)
23	CLA	b	612	-	65,73,73	1.51	9 (13%)	76,113,113	1.60	14 (18%)
25	8CT	C	520	-	40,41,41	1.62	4 (10%)	50,56,56	2.44	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	c	521	-	41,41,41	0.98	1 (2%)	56,56,56	1.30	7 (12%)
34	BCT	a	404	21	2,3,3	1.45	0	2,3,3	3.11	2 (100%)
23	CLA	b	604	-	65,73,73	1.61	10 (15%)	76,113,113	1.64	12 (15%)
33	LHG	L	101	-	48,48,48	0.86	1 (2%)	51,54,54	1.19	3 (5%)
34	BCT	D	401	21	2,3,3	1.08	0	2,3,3	3.53	2 (100%)
27	LMG	B	622	-	26,26,55	0.82	1 (3%)	26,26,63	0.99	1 (3%)
31	BCR	c	515	-	41,41,41	1.22	3 (7%)	56,56,56	1.32	9 (16%)
23	CLA	B	607	37	65,73,73	1.49	7 (10%)	76,113,113	1.47	9 (11%)
23	CLA	B	615	-	65,73,73	1.60	11 (16%)	76,113,113	1.37	10 (13%)
24	PHO	a	407	-	51,69,69	1.13	6 (11%)	47,99,99	1.32	6 (12%)
25	8CT	C	514	-	40,41,41	1.67	4 (10%)	50,56,56	2.59	11 (22%)
23	CLA	C	502	-	65,73,73	1.55	7 (10%)	76,113,113	1.39	9 (11%)
23	CLA	C	504	37	59,67,73	1.57	8 (13%)	68,105,113	1.48	10 (14%)
28	SQD	a	412	-	35,35,54	1.12	2 (5%)	37,37,65	1.39	5 (13%)
23	CLA	C	503	-	65,73,73	1.65	7 (10%)	76,113,113	1.57	13 (17%)
31	BCR	a	409	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	4 (7%)
27	LMG	c	519	-	37,37,55	1.17	5 (13%)	45,45,63	1.28	4 (8%)
29	DGD	C	516	-	63,63,67	1.16	5 (7%)	77,77,81	1.38	11 (14%)
23	CLA	b	611	37	65,73,73	1.62	11 (16%)	76,113,113	1.37	13 (17%)
27	LMG	b	621	-	51,51,55	0.86	1 (1%)	59,59,63	1.53	7 (11%)
27	LMG	D	407	-	51,51,55	1.04	1 (1%)	59,59,63	1.25	5 (8%)
23	CLA	b	613	-	65,73,73	1.34	5 (7%)	76,113,113	1.55	13 (17%)
31	BCR	H	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.28	6 (10%)
23	CLA	B	601	37	65,73,73	1.98	9 (13%)	76,113,113	1.62	12 (15%)
23	CLA	A	405	37	65,73,73	1.55	10 (15%)	76,113,113	1.70	13 (17%)
33	LHG	d	409	-	38,38,48	0.95	2 (5%)	41,44,54	1.11	2 (4%)
25	8CT	A	408	-	40,41,41	1.72	4 (10%)	50,56,56	2.42	13 (26%)
33	LHG	E	101	-	48,48,48	0.90	3 (6%)	51,54,54	1.15	2 (3%)
28	SQD	A	413	-	38,38,54	1.05	3 (7%)	40,40,65	1.33	2 (5%)
23	CLA	c	505	-	65,73,73	1.67	10 (15%)	76,113,113	1.27	10 (13%)
29	DGD	c	517	-	63,63,67	1.14	7 (11%)	77,77,81	1.38	9 (11%)
23	CLA	B	613	-	65,73,73	1.61	10 (15%)	76,113,113	1.51	10 (13%)
23	CLA	c	503	-	65,73,73	1.62	9 (13%)	76,113,113	1.55	12 (15%)
23	CLA	b	616	-	65,73,73	1.73	11 (16%)	76,113,113	1.59	14 (18%)
23	CLA	d	403	-	65,73,73	1.52	9 (13%)	76,113,113	1.44	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	DGD	o	301	-	43,43,67	1.10	4 (9%)	45,45,81	1.26	3 (6%)
27	LMG	c	522	-	48,48,55	1.14	6 (12%)	56,56,63	1.26	6 (10%)
23	CLA	C	501	-	65,73,73	1.97	10 (15%)	76,113,113	1.45	5 (6%)
36	HEC	v	201	16	32,50,50	2.25	5 (15%)	24,82,82	1.61	4 (16%)
28	SQD	a	411	-	53,54,54	0.99	4 (7%)	62,65,65	1.96	14 (22%)
29	DGD	A	414	-	67,67,67	1.33	8 (11%)	81,81,81	1.39	11 (13%)
28	SQD	B	624	-	53,54,54	0.92	3 (5%)	62,65,65	1.76	12 (19%)
25	8CT	B	617	-	40,41,41	1.75	5 (12%)	50,56,56	2.56	11 (22%)
31	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	6 (10%)
28	SQD	D	408	-	35,36,54	1.02	3 (8%)	42,45,65	1.73	10 (23%)
27	LMG	b	623	-	55,55,55	0.92	3 (5%)	63,63,63	1.35	7 (11%)
23	CLA	B	609	-	65,73,73	1.56	12 (18%)	76,113,113	1.42	9 (11%)
23	CLA	c	509	-	65,73,73	1.56	7 (10%)	76,113,113	1.47	9 (11%)
29	DGD	c	516	-	63,63,67	1.05	6 (9%)	77,77,81	1.36	10 (12%)
23	CLA	C	508	-	65,73,73	1.62	9 (13%)	76,113,113	1.48	11 (14%)
25	8CT	B	619	-	40,41,41	1.77	5 (12%)	50,56,56	2.51	11 (22%)
33	LHG	d	408	-	48,48,48	0.72	0	51,54,54	1.22	4 (7%)
24	PHO	A	406	-	51,69,69	1.07	5 (9%)	47,99,99	1.34	6 (12%)
25	8CT	D	405	-	40,41,41	1.72	4 (10%)	50,56,56	2.65	8 (16%)
23	CLA	C	513	-	65,73,73	1.55	8 (12%)	76,113,113	1.56	11 (14%)
28	SQD	f	101	-	40,41,54	1.14	5 (12%)	49,52,65	1.59	10 (20%)
23	CLA	B	610	37	65,73,73	1.81	9 (13%)	76,113,113	1.60	13 (17%)
31	BCR	b	618	-	41,41,41	1.20	3 (7%)	56,56,56	1.35	6 (10%)
33	LHG	d	407	-	48,48,48	0.76	1 (2%)	51,54,54	1.25	5 (9%)
27	LMG	B	620	-	51,51,55	0.99	3 (5%)	59,59,63	1.51	12 (20%)
35	HEM	e	102	6,5	41,50,50	1.44	5 (12%)	45,82,82	1.66	8 (17%)
23	CLA	B	611	-	65,73,73	1.58	11 (16%)	76,113,113	1.45	13 (17%)
23	CLA	b	609	-	65,73,73	1.41	10 (15%)	76,113,113	1.41	12 (15%)
29	DGD	c	518	-	63,63,67	1.13	5 (7%)	77,77,81	1.43	15 (19%)
26	PL9	a	410	-	55,55,55	1.12	2 (3%)	68,69,69	1.62	13 (19%)
27	LMG	b	624	-	21,21,55	0.76	0	20,20,63	0.98	0
23	CLA	b	607	-	65,73,73	1.83	10 (15%)	76,113,113	1.65	17 (22%)
23	CLA	b	615	-	65,73,73	1.52	10 (15%)	76,113,113	1.52	11 (14%)
30	OEX	a	414	3,37,1	0,15,15	-	-	-		
23	CLA	C	505	-	65,73,73	1.52	7 (10%)	76,113,113	1.41	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LHG	e	101	-	41,41,48	0.80	1 (2%)	44,47,54	1.27	5 (11%)
23	CLA	a	405	-	65,73,73	1.55	9 (13%)	76,113,113	1.53	12 (15%)
23	CLA	B	608	-	65,73,73	1.56	11 (16%)	76,113,113	1.48	11 (14%)
23	CLA	c	508	-	64,72,73	1.52	9 (14%)	74,111,113	1.29	7 (9%)
27	LMG	d	410	-	44,44,55	0.99	3 (6%)	52,52,63	1.34	7 (13%)
23	CLA	C	511	3	65,73,73	1.75	11 (16%)	76,113,113	1.38	5 (6%)
23	CLA	C	512	-	65,73,73	1.52	8 (12%)	76,113,113	1.34	10 (13%)
23	CLA	b	610	-	65,73,73	1.53	9 (13%)	76,113,113	1.32	7 (9%)
23	CLA	D	403	-	65,73,73	1.29	7 (10%)	76,113,113	1.26	9 (11%)
26	PL9	D	406	-	55,55,55	1.51	10 (18%)	68,69,69	1.54	14 (20%)
23	CLA	c	506	-	65,73,73	1.86	9 (13%)	76,113,113	1.34	12 (15%)
23	CLA	c	512	-	65,73,73	1.57	9 (13%)	76,113,113	1.42	10 (13%)
30	OEX	A	415	3,37,1	0,15,15	-	-	-		
33	LHG	l	101	-	48,48,48	0.67	0	51,54,54	1.25	4 (7%)
23	CLA	c	501	-	65,73,73	1.38	7 (10%)	76,113,113	1.68	11 (14%)
23	CLA	d	404	-	65,73,73	1.76	10 (15%)	76,113,113	1.24	10 (13%)
23	CLA	B	604	-	65,73,73	1.74	11 (16%)	76,113,113	1.64	8 (10%)
23	CLA	c	502	-	65,73,73	1.63	9 (13%)	76,113,113	1.67	9 (11%)
28	SQD	A	412	-	51,52,54	1.05	5 (9%)	60,63,65	2.27	14 (23%)
23	CLA	B	605	-	65,73,73	1.22	7 (10%)	76,113,113	1.53	10 (13%)
29	DGD	h	102	-	63,63,67	1.17	9 (14%)	77,77,81	1.55	16 (20%)
35	HEM	F	101	6,5	41,50,50	1.56	3 (7%)	45,82,82	1.25	4 (8%)
23	CLA	b	614	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	13 (17%)
25	8CT	C	515	-	40,41,41	1.75	6 (15%)	50,56,56	2.36	14 (28%)
23	CLA	A	411	37	65,73,73	1.56	10 (15%)	76,113,113	1.24	7 (9%)
25	8CT	d	405	-	40,41,41	1.71	5 (12%)	50,56,56	2.45	9 (18%)
23	CLA	B	606	-	65,73,73	1.98	10 (15%)	76,113,113	1.39	9 (11%)
23	CLA	B	612	-	65,73,73	1.48	6 (9%)	76,113,113	1.65	10 (13%)
23	CLA	B	602	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	9 (11%)
23	CLA	B	603	-	65,73,73	1.38	8 (12%)	76,113,113	1.47	12 (15%)
23	CLA	b	617	-	60,68,73	1.56	9 (15%)	70,107,113	1.59	10 (14%)
23	CLA	c	507	37	65,73,73	1.54	11 (16%)	76,113,113	1.57	12 (15%)
29	DGD	C	517	-	63,63,67	1.23	8 (12%)	77,77,81	1.49	9 (11%)
23	CLA	C	507	37	65,73,73	1.65	10 (15%)	76,113,113	1.34	11 (14%)
33	LHG	B	623	-	48,48,48	0.83	1 (2%)	51,54,54	1.36	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
25	8CT	k	101	-	40,41,41	1.65	5 (12%)	50,56,56	2.33	7 (14%)
23	CLA	a	408	-	65,73,73	1.70	11 (16%)	76,113,113	1.41	12 (15%)
23	CLA	b	603	-	65,73,73	1.49	8 (12%)	76,113,113	1.69	10 (13%)
23	CLA	d	402	37	65,73,73	1.56	8 (12%)	76,113,113	1.46	7 (9%)
23	CLA	D	404	-	65,73,73	1.54	9 (13%)	76,113,113	1.17	5 (6%)
29	DGD	C	518	-	63,63,67	0.99	3 (4%)	77,77,81	1.46	12 (15%)
23	CLA	b	608	37	65,73,73	1.39	10 (15%)	76,113,113	1.19	7 (9%)
23	CLA	c	510	-	65,73,73	1.42	8 (12%)	76,113,113	1.69	7 (9%)
26	PL9	d	406	-	55,55,55	1.35	6 (10%)	68,69,69	1.85	22 (32%)
31	BCR	Y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	9 (16%)
23	CLA	B	614	-	65,73,73	1.50	7 (10%)	76,113,113	1.36	9 (11%)
26	PL9	A	409	-	55,55,55	1.10	3 (5%)	68,69,69	1.75	12 (17%)
23	CLA	A	407	-	54,62,73	1.85	10 (18%)	62,99,113	1.64	12 (19%)
25	8CT	c	514	-	40,41,41	1.69	3 (7%)	50,56,56	2.41	13 (26%)
24	PHO	D	402	-	51,69,69	1.13	3 (5%)	47,99,99	1.20	6 (12%)
23	CLA	B	616	-	60,68,73	1.80	11 (18%)	70,107,113	1.70	11 (15%)
23	CLA	c	513	-	65,73,73	1.51	6 (9%)	76,113,113	1.22	6 (7%)
27	LMG	c	524	-	49,49,55	1.02	4 (8%)	57,57,63	1.21	4 (7%)
31	BCR	h	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.33	7 (12%)
23	CLA	C	509	-	65,73,73	1.47	7 (10%)	76,113,113	1.49	11 (14%)
23	CLA	b	602	37	65,73,73	1.78	13 (20%)	76,113,113	1.44	10 (13%)
25	8CT	t	101	-	40,41,41	1.63	4 (10%)	50,56,56	2.67	17 (34%)
23	CLA	b	605	-	65,73,73	1.68	9 (13%)	76,113,113	1.61	13 (17%)
28	SQD	b	601	-	48,49,54	0.97	3 (6%)	57,60,65	2.02	13 (22%)
29	DGD	H	102	-	63,63,67	1.34	9 (14%)	77,77,81	1.48	13 (16%)
27	LMG	C	519	-	48,48,55	0.94	3 (6%)	56,56,63	1.27	7 (12%)
23	CLA	A	404	-	65,73,73	1.42	10 (15%)	76,113,113	1.40	7 (9%)
27	LMG	A	410	-	48,48,55	0.92	4 (8%)	56,56,63	1.34	8 (14%)
31	BCR	T	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.39	8 (14%)
31	BCR	b	619	-	41,41,41	1.28	3 (7%)	56,56,56	1.24	5 (8%)
23	CLA	c	504	37	60,68,73	1.55	7 (11%)	70,107,113	1.58	10 (14%)
36	HEC	V	201	16	32,50,50	2.13	5 (15%)	24,82,82	1.54	4 (16%)

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
23	CLA	c	511	3	1/1/20/20	7/37/115/115	-
25	8CT	b	620	-	1/1/25/25	9/29/63/63	0/2/2/2
23	CLA	C	506	-	1/1/20/20	14/37/115/115	-
27	LMG	D	411	-	-	18/33/33/70	-
33	LHG	D	410	-	-	20/51/51/53	-
23	CLA	a	406	37	-	11/37/115/115	-
33	LHG	D	409	-	-	18/53/53/53	-
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
23	CLA	b	606	-	1/1/20/20	9/37/115/115	-
23	CLA	b	612	-	1/1/20/20	5/37/115/115	-
25	8CT	C	520	-	1/1/25/25	8/29/63/63	0/2/2/2
31	BCR	c	521	-	-	9/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/20/20	9/37/115/115	-
33	LHG	L	101	-	-	22/53/53/53	-
27	LMG	B	622	-	-	10/22/22/70	-
31	BCR	c	515	-	-	7/29/63/63	0/2/2/2
23	CLA	B	607	37	1/1/20/20	12/37/115/115	-
23	CLA	B	615	-	1/1/20/20	11/37/115/115	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	8CT	C	514	-	1/1/25/25	8/29/63/63	0/2/2/2
23	CLA	C	502	-	1/1/20/20	10/37/115/115	-
23	CLA	C	504	37	1/1/18/20	9/30/108/115	-
28	SQD	a	412	-	-	19/37/37/69	-
23	CLA	C	503	-	1/1/20/20	5/37/115/115	-
31	BCR	a	409	-	-	1/29/63/63	0/2/2/2
27	LMG	c	519	-	-	13/31/51/70	0/1/1/1
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
23	CLA	b	611	37	1/1/20/20	5/37/115/115	-
27	LMG	b	621	-	-	18/46/66/70	0/1/1/1
27	LMG	D	407	-	-	14/46/66/70	0/1/1/1
23	CLA	b	613	-	1/1/20/20	9/37/115/115	-
31	BCR	H	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	601	37	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	405	37	-	6/37/115/115	-
33	LHG	d	409	-	-	12/43/43/53	-
25	8CT	A	408	-	1/1/25/25	6/29/63/63	0/2/2/2
33	LHG	E	101	-	-	27/53/53/53	-
28	SQD	A	413	-	-	11/39/39/69	-
23	CLA	c	505	-	1/1/20/20	11/37/115/115	-
29	DGD	c	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	613	-	1/1/20/20	5/37/115/115	-
23	CLA	c	503	-	-	5/37/115/115	-
23	CLA	b	616	-	1/1/20/20	9/37/115/115	-
23	CLA	d	403	-	-	9/37/115/115	-
29	DGD	o	301	-	-	23/45/45/95	-
27	LMG	c	522	-	-	22/43/63/70	0/1/1/1
23	CLA	C	501	-	1/1/20/20	2/37/115/115	-
36	HEC	v	201	16	-	2/10/54/54	-
28	SQD	a	411	-	-	19/49/69/69	0/1/1/1
29	DGD	A	414	-	-	26/55/95/95	0/2/2/2
28	SQD	B	624	-	-	22/49/69/69	0/1/1/1
25	8CT	B	617	-	1/1/25/25	10/29/63/63	0/2/2/2
31	BCR	B	618	-	-	4/29/63/63	0/2/2/2
28	SQD	D	408	-	-	17/28/48/69	0/1/1/1
27	LMG	b	623	-	-	19/50/70/70	0/1/1/1
23	CLA	B	609	-	-	5/37/115/115	-
23	CLA	c	509	-	1/1/20/20	12/37/115/115	-
29	DGD	c	516	-	-	26/51/91/95	0/2/2/2
23	CLA	C	508	-	-	7/37/115/115	-
25	8CT	B	619	-	1/1/25/25	7/29/63/63	0/2/2/2
33	LHG	d	408	-	-	24/53/53/53	-
24	PHO	A	406	-	-	7/37/103/103	0/5/6/6
25	8CT	D	405	-	1/1/25/25	6/29/63/63	0/2/2/2
23	CLA	C	513	-	1/1/20/20	11/37/115/115	-
28	SQD	f	101	-	-	17/36/56/69	0/1/1/1
23	CLA	B	610	37	1/1/20/20	4/37/115/115	-
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	d	407	-	-	22/53/53/53	-
27	LMG	B	620	-	-	19/46/66/70	0/1/1/1
35	HEM	e	102	6,5	-	3/12/54/54	-
23	CLA	B	611	-	-	6/37/115/115	-
23	CLA	b	609	-	-	6/37/115/115	-
29	DGD	c	518	-	-	17/51/91/95	0/2/2/2
26	PL9	a	410	-	-	19/53/73/73	0/1/1/1
27	LMG	b	624	-	-	10/17/17/70	-
23	CLA	b	607	-	1/1/20/20	9/37/115/115	-
23	CLA	b	615	-	1/1/20/20	14/37/115/115	-
23	CLA	C	505	-	1/1/20/20	12/37/115/115	-
33	LHG	e	101	-	-	28/46/46/53	-
23	CLA	a	405	-	1/1/20/20	7/37/115/115	-
23	CLA	B	608	-	-	6/37/115/115	-
23	CLA	c	508	-	-	9/36/114/115	-
27	LMG	d	410	-	-	11/39/59/70	0/1/1/1
23	CLA	C	511	3	1/1/20/20	8/37/115/115	-
23	CLA	C	512	-	1/1/20/20	9/37/115/115	-
23	CLA	b	610	-	1/1/20/20	9/37/115/115	-
23	CLA	D	403	-	1/1/20/20	8/37/115/115	-
26	PL9	D	406	-	-	13/53/73/73	0/1/1/1
23	CLA	c	506	-	1/1/20/20	18/37/115/115	-
23	CLA	c	512	-	1/1/20/20	19/37/115/115	-
33	LHG	l	101	-	-	16/53/53/53	-
23	CLA	c	501	-	1/1/20/20	6/37/115/115	-
23	CLA	d	404	-	1/1/20/20	8/37/115/115	-
23	CLA	B	604	-	1/1/20/20	11/37/115/115	-
23	CLA	c	502	-	-	3/37/115/115	-
28	SQD	A	412	-	-	22/47/67/69	0/1/1/1
23	CLA	B	605	-	1/1/20/20	13/37/115/115	-
29	DGD	h	102	-	-	20/51/91/95	0/2/2/2
35	HEM	F	101	6,5	-	2/12/54/54	-
23	CLA	b	614	-	1/1/20/20	5/37/115/115	-
25	8CT	C	515	-	1/1/25/25	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	411	37	-	2/37/115/115	-
25	8CT	d	405	-	1/1/25/25	11/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/20/20	11/37/115/115	-
23	CLA	B	612	-	1/1/20/20	12/37/115/115	-
23	CLA	B	602	-	1/1/20/20	5/37/115/115	-
23	CLA	B	603	-	1/1/20/20	7/37/115/115	-
23	CLA	b	617	-	1/1/19/20	9/31/109/115	-
23	CLA	c	507	37	1/1/20/20	9/37/115/115	-
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	CLA	C	507	37	1/1/20/20	6/37/115/115	-
33	LHG	B	623	-	-	17/53/53/53	-
23	CLA	C	510	-	1/1/20/20	13/37/115/115	-
25	8CT	k	101	-	1/1/25/25	13/29/63/63	0/2/2/2
23	CLA	a	408	-	1/1/20/20	8/37/115/115	-
23	CLA	b	603	-	1/1/20/20	10/37/115/115	-
23	CLA	d	402	37	1/1/20/20	8/37/115/115	-
23	CLA	D	404	-	1/1/20/20	11/37/115/115	-
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
23	CLA	b	608	37	1/1/20/20	14/37/115/115	-
23	CLA	c	510	-	1/1/20/20	15/37/115/115	-
26	PL9	d	406	-	-	18/53/73/73	0/1/1/1
31	BCR	Y	101	-	-	9/29/63/63	0/2/2/2
23	CLA	B	614	-	1/1/20/20	9/37/115/115	-
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
23	CLA	A	407	-	1/1/17/20	4/24/102/115	-
25	8CT	c	514	-	1/1/25/25	15/29/63/63	0/2/2/2
24	PHO	D	402	-	-	2/37/103/103	0/5/6/6
23	CLA	B	616	-	1/1/19/20	9/31/109/115	-
23	CLA	c	513	-	1/1/20/20	11/37/115/115	-
27	LMG	c	524	-	-	22/44/64/70	0/1/1/1
31	BCR	h	101	-	-	7/29/63/63	0/2/2/2
23	CLA	C	509	-	1/1/20/20	14/37/115/115	-
23	CLA	b	602	37	1/1/20/20	18/37/115/115	-
25	8CT	t	101	-	1/1/25/25	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	605	-	1/1/20/20	10/37/115/115	-
28	SQD	b	601	-	-	20/44/64/69	0/1/1/1
29	DGD	H	102	-	-	19/51/91/95	0/2/2/2
27	LMG	C	519	-	-	13/43/63/70	0/1/1/1
23	CLA	A	404	-	1/1/20/20	4/37/115/115	-
27	LMG	A	410	-	-	22/43/63/70	0/1/1/1
31	BCR	T	101	-	-	1/29/63/63	0/2/2/2
31	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	c	504	37	1/1/19/20	6/31/109/115	-
36	HEC	V	201	16	-	2/10/54/54	-

The worst 5 of 905 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	MG-NA	9.72	2.29	2.06
23	c	506	CLA	MG-ND	-9.38	1.87	2.05
23	B	601	CLA	C4B-NB	9.09	1.43	1.35
23	B	610	CLA	C4B-NB	8.81	1.43	1.35
23	b	605	CLA	C4B-NB	8.66	1.42	1.35

The worst 5 of 1320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	405	8CT	C33-C32-C31	-14.89	110.57	124.85
25	C	514	8CT	C33-C32-C31	-13.80	111.62	124.85
25	B	617	8CT	C33-C32-C31	-13.56	111.85	124.85
25	t	101	8CT	C33-C32-C31	-13.35	112.05	124.85
25	d	405	8CT	C33-C32-C31	-12.71	112.67	124.85

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 1646 torsion outliers are listed below:

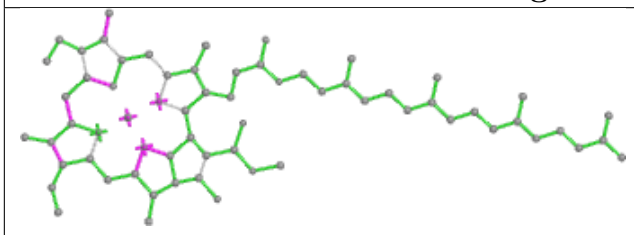
Mol	Chain	Res	Type	Atoms
23	A	411	CLA	CHA-CBD-CGD-O1D
23	A	411	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

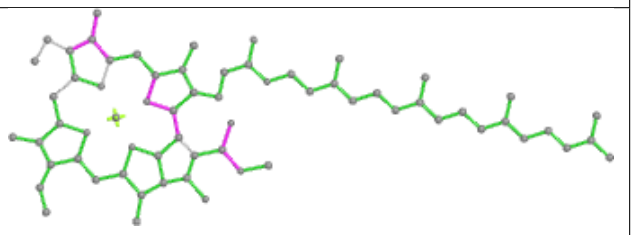
No monomer is involved in short contacts.

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

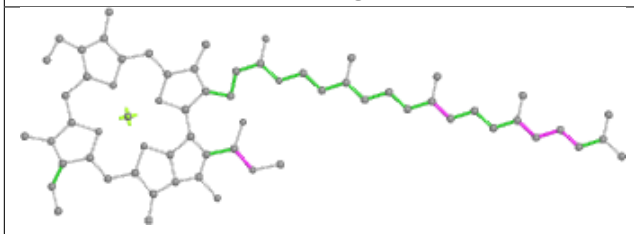
Ligand CLA c 511



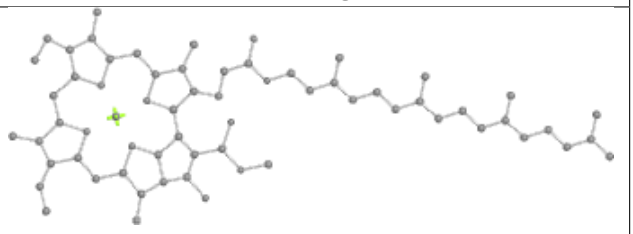
Bond lengths



Bond angles

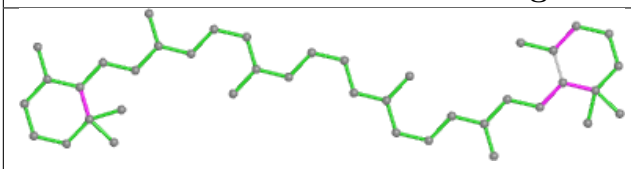


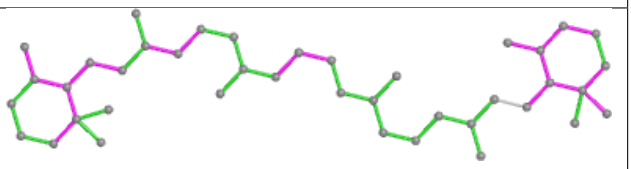
Torsions

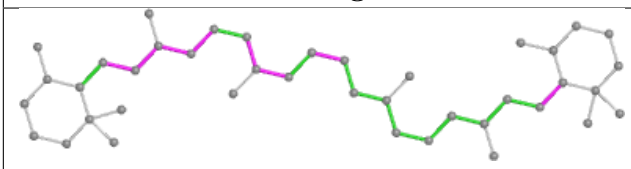


Rings

Ligand 8CT b 620


Bond lengths


Bond angles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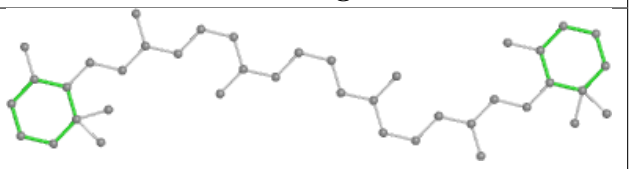
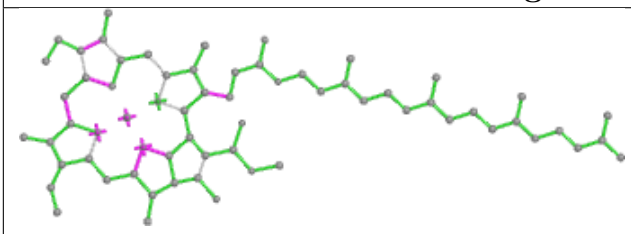

Rings

Ligand CLA C 506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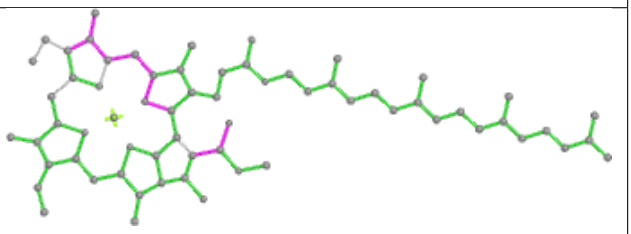
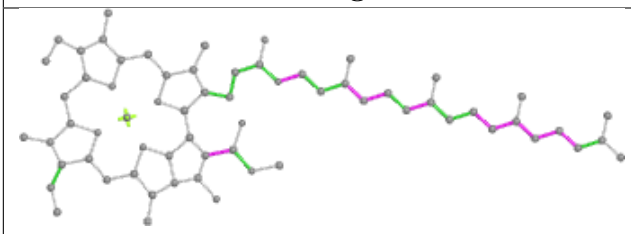
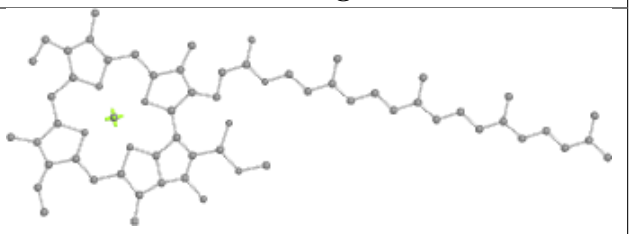
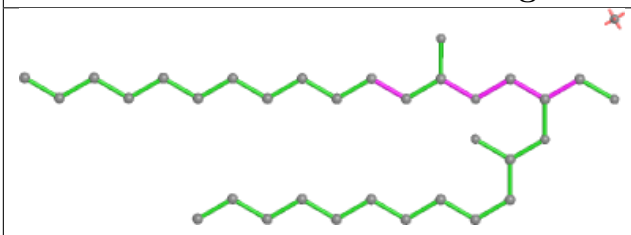
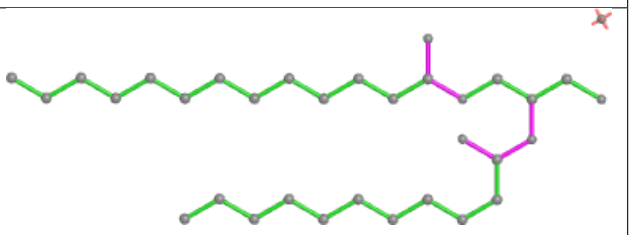

Bond angles

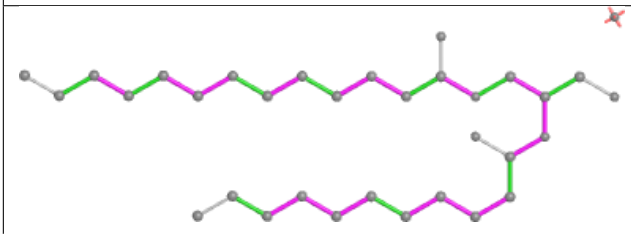

Torsions

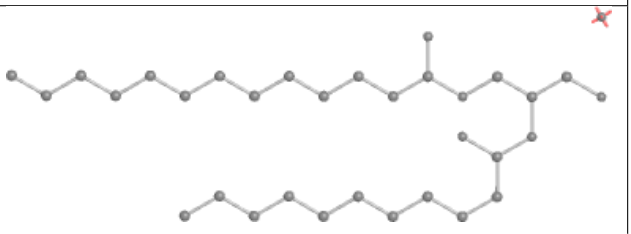

Rings

Ligand LMG D 411

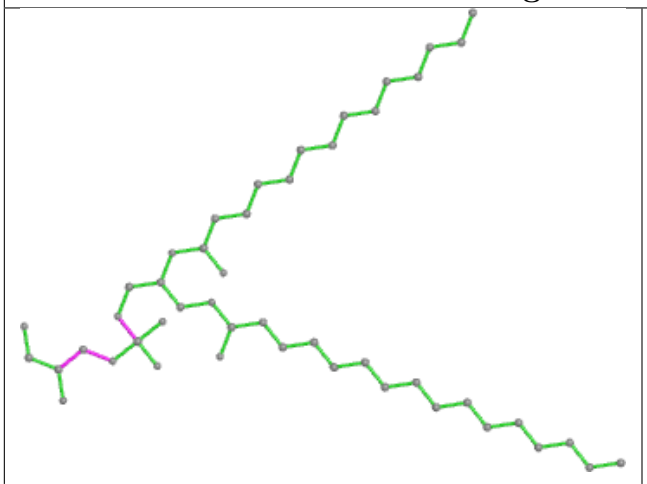

Bond lengths


Bond angles

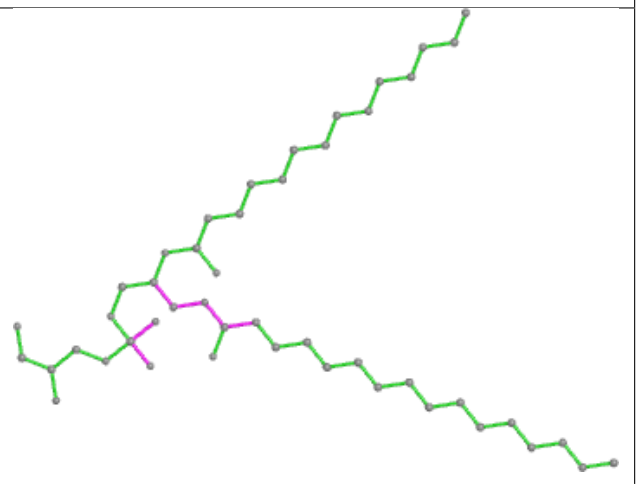

Torsions


Rings

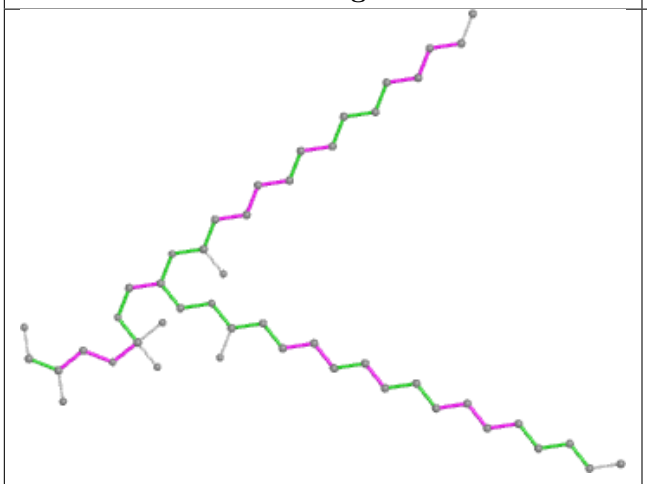
Ligand LHG D 410



Bond lengths



Bond angles



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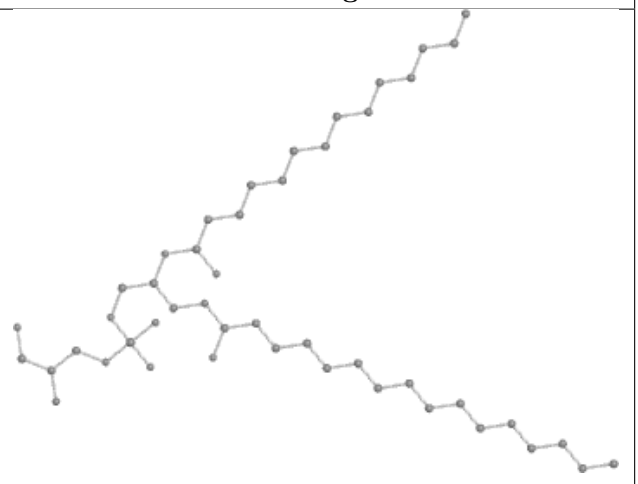
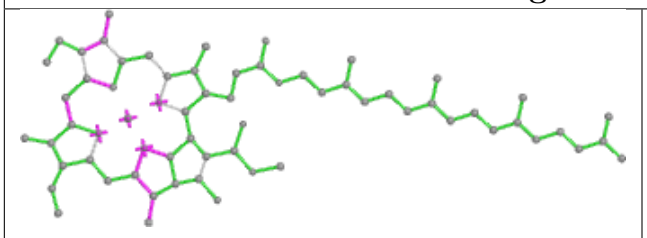


Rings

Ligand CLA a 406



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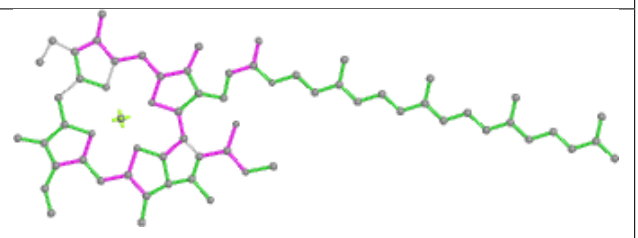
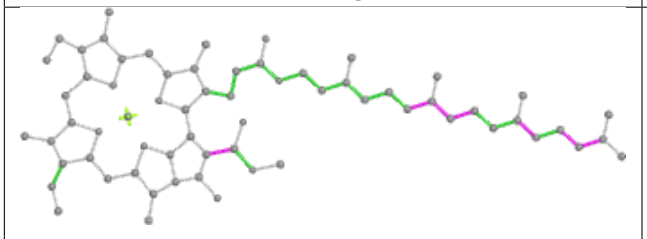
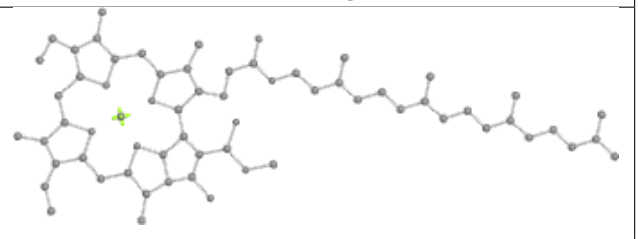


Bond angles

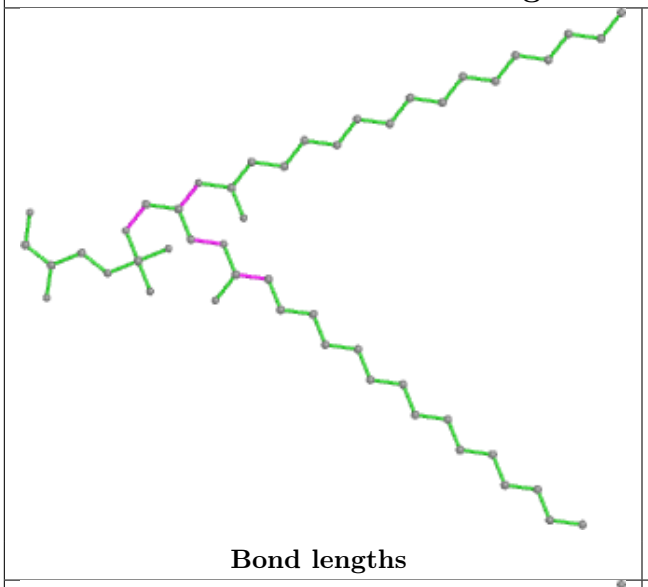


Torsions



Rings

Ligand LHG D 409



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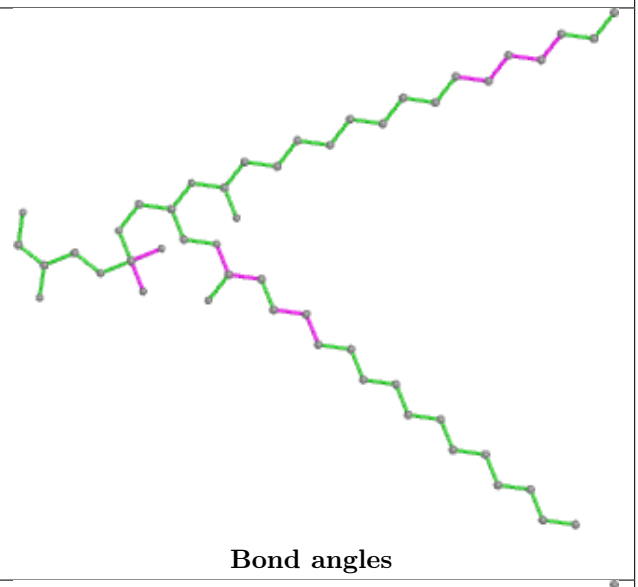
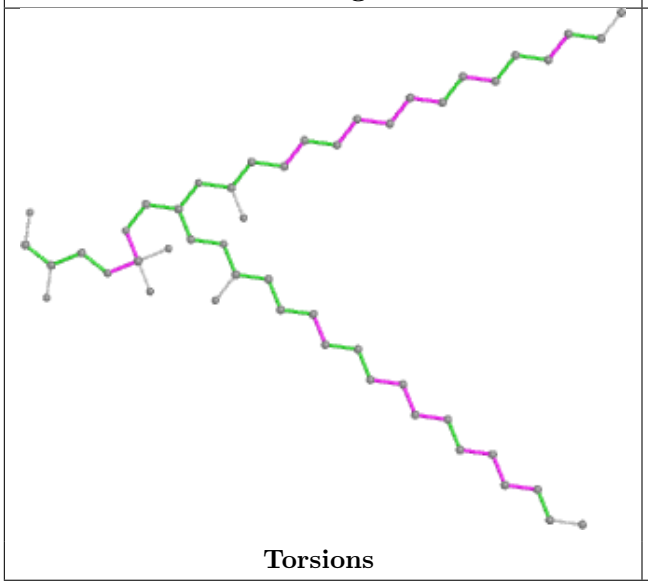


Bond angles



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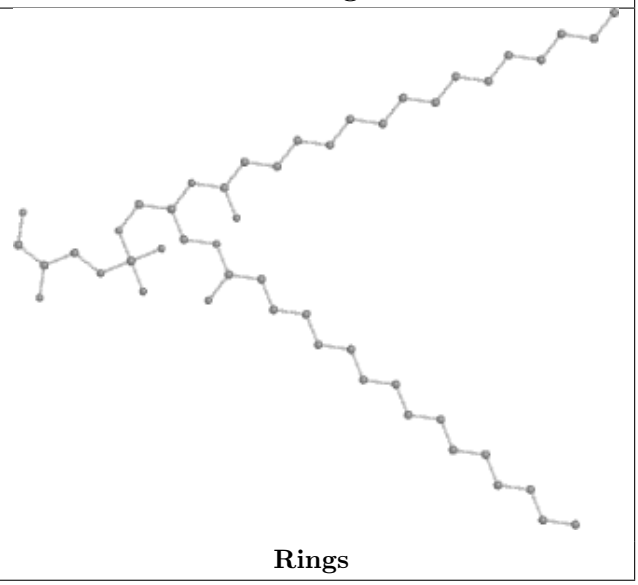
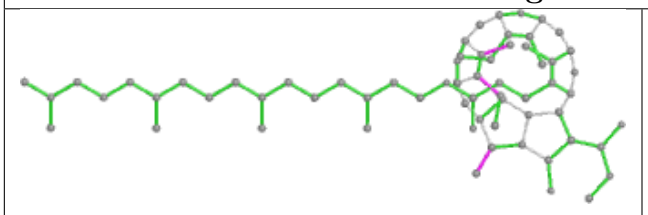


Rings

Ligand PHO d 401



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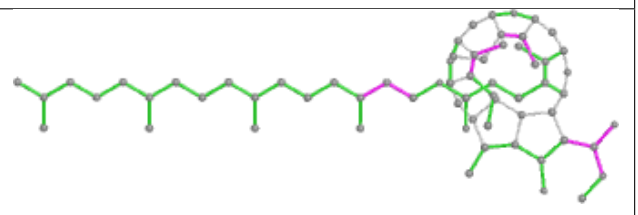
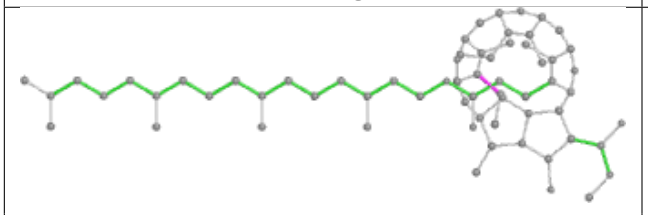
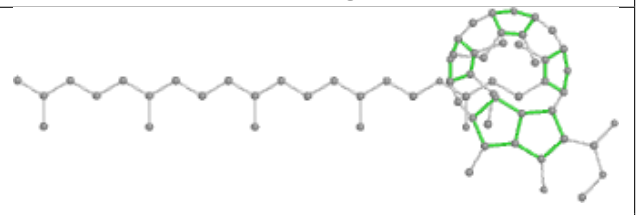


Bond angles

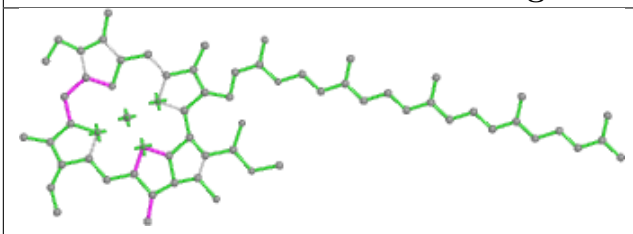


Torsions

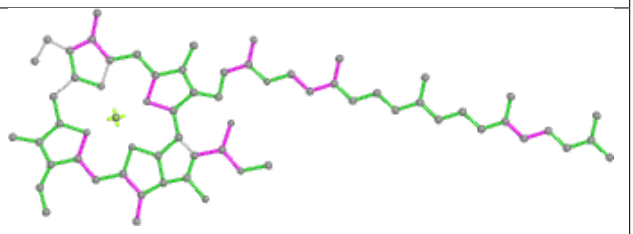


Rings

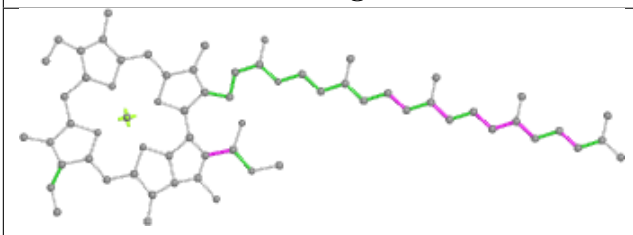
Ligand CLA b 606



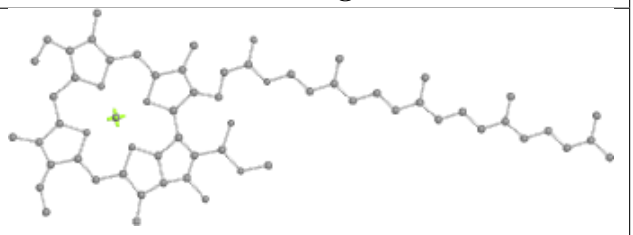
Bond lengths



Bond angles

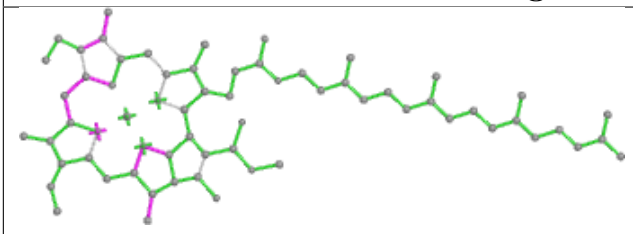


Torsions

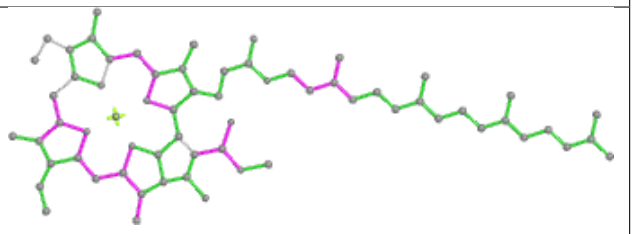


Rings

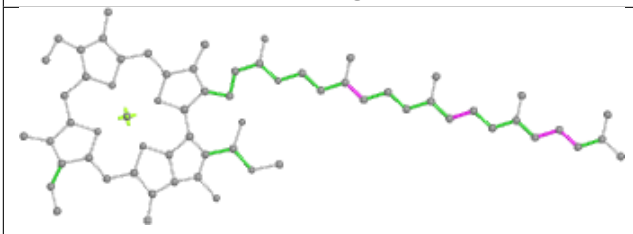
Ligand CLA b 612



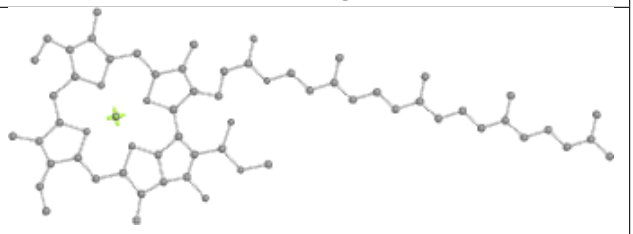
Bond lengths



Bond angles

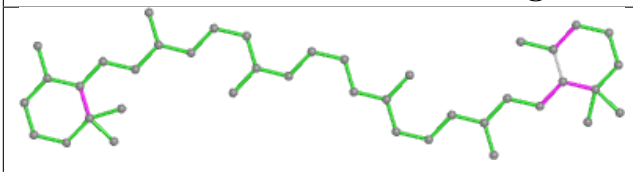


Torsions

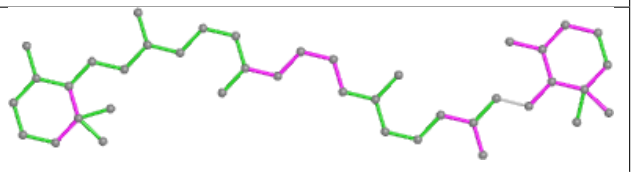


Rings

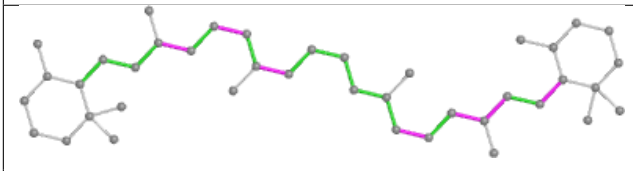
Ligand 8CT C 520



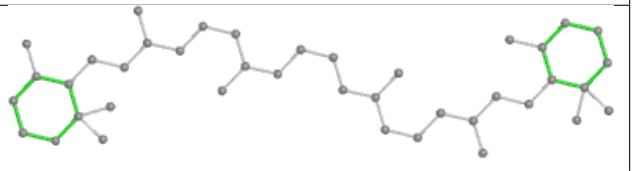
Bond lengths



Bond angles

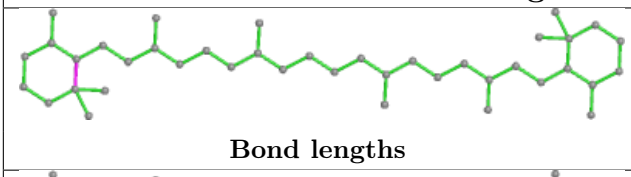


Torsions



Rings

Ligand BCR c 521



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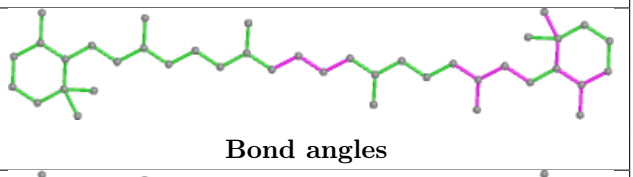
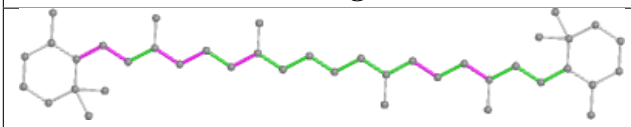
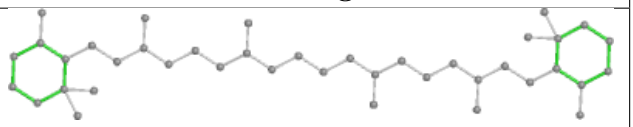


Bond angles

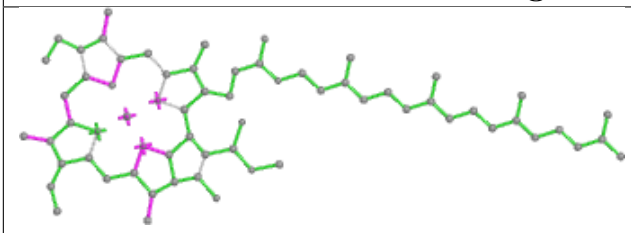


Torsions



Rings

Ligand CLA b 604



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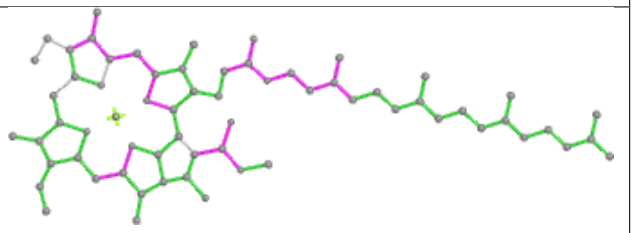
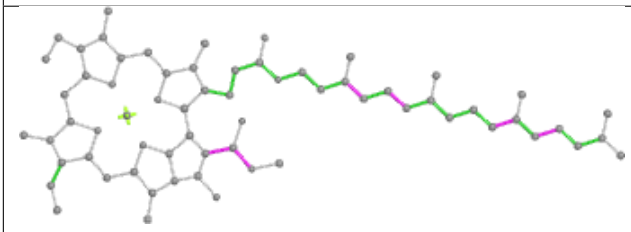
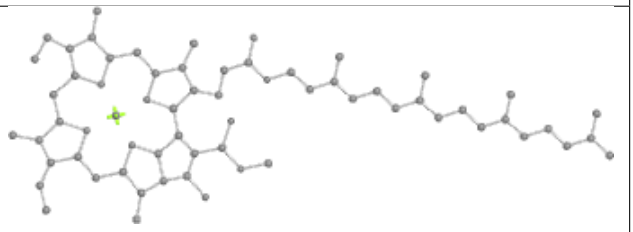


Bond angles

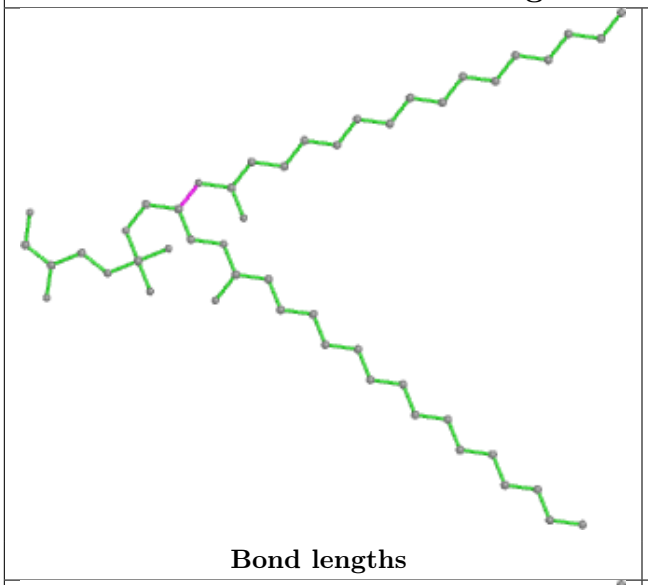


Torsions



Rings

Ligand LHG L 101



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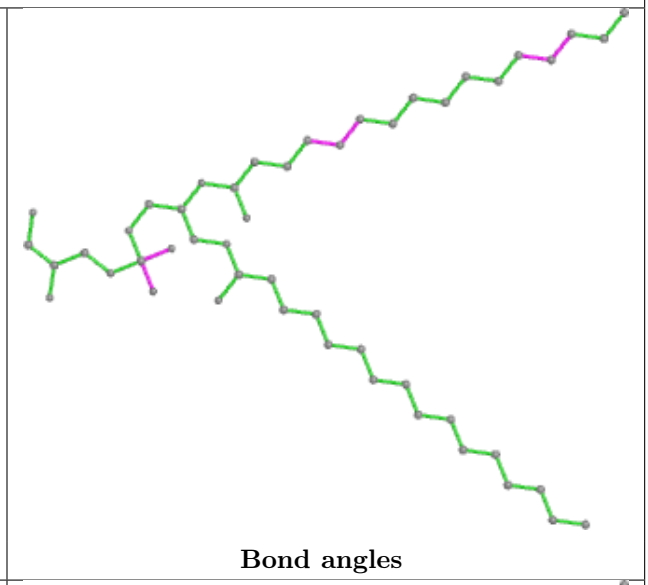
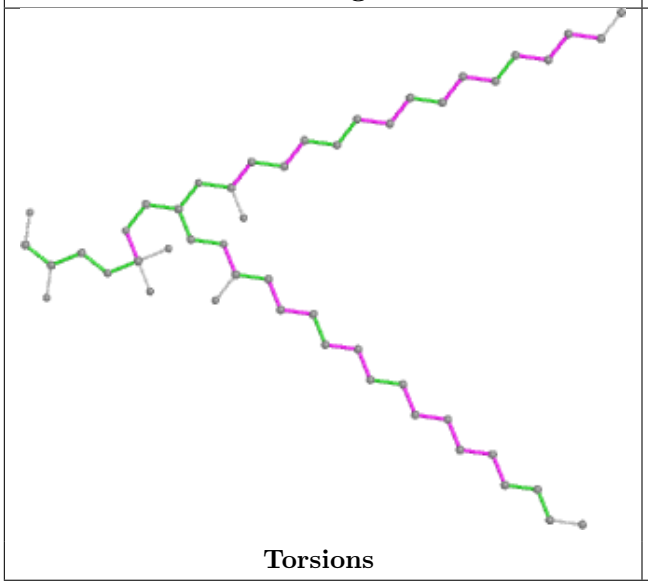
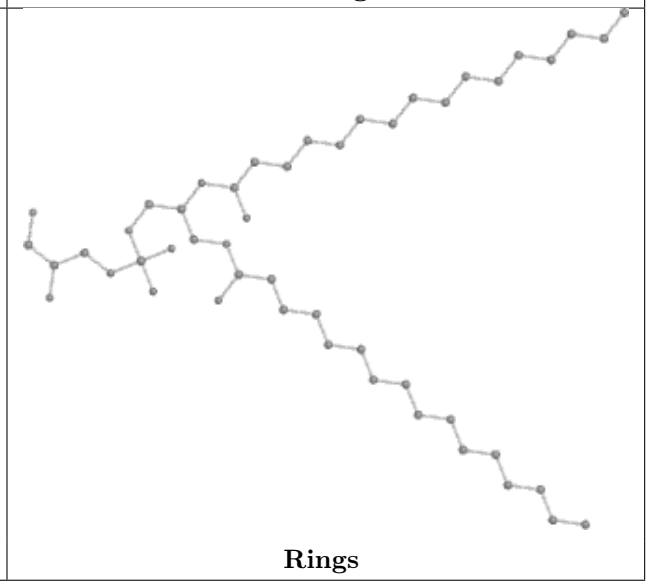


Bond angles

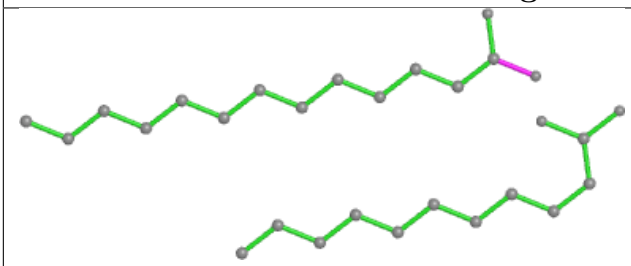


Torsions



Rings

Ligand LMG B 622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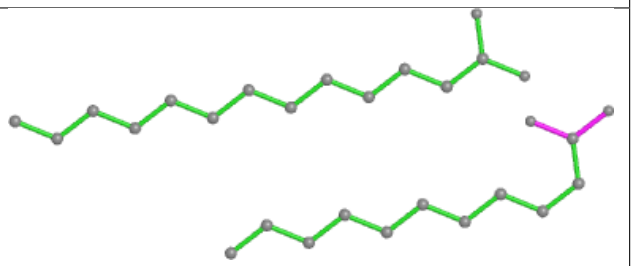
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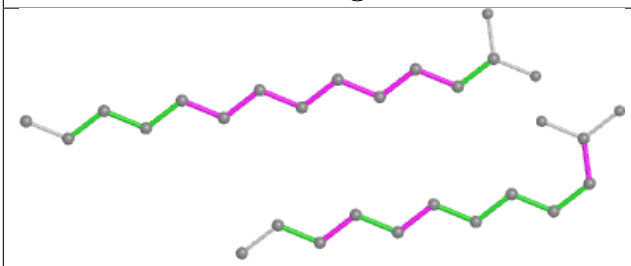
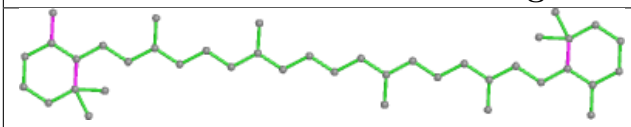

Torsions

Rings

Ligand BCR c 515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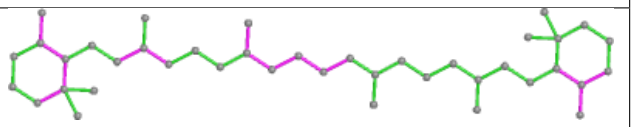
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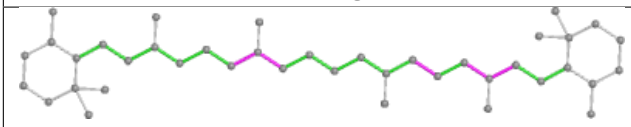
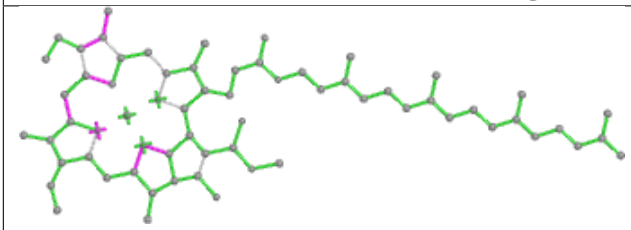

Torsions

Rings

Ligand CLA B 607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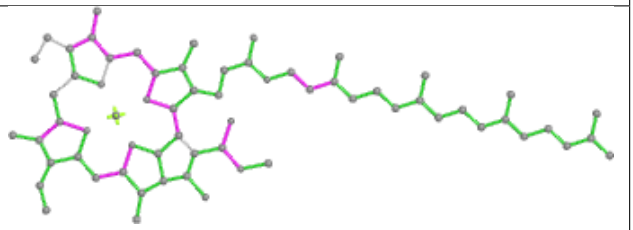
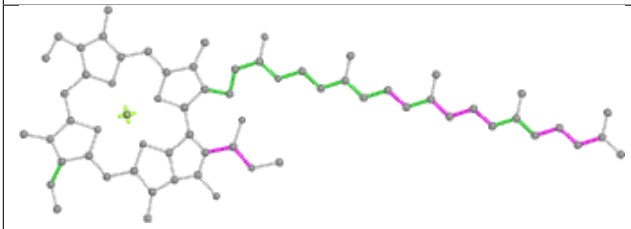

Bond angles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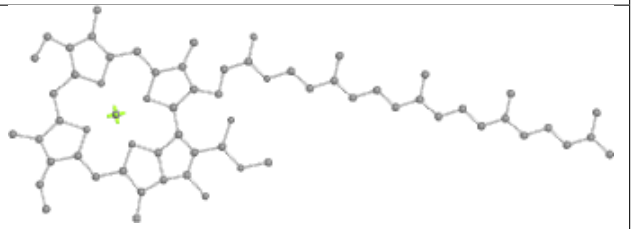
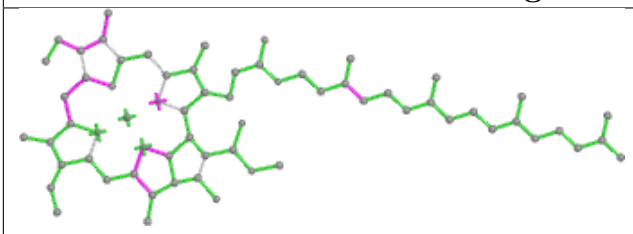

Rings

Ligand CLA B 615



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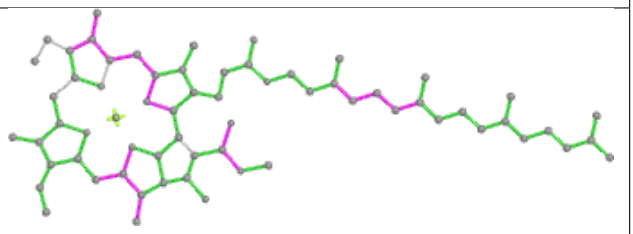
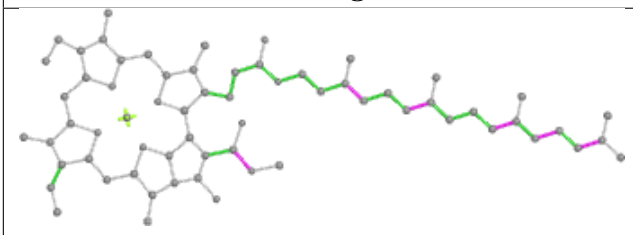


Bond angles



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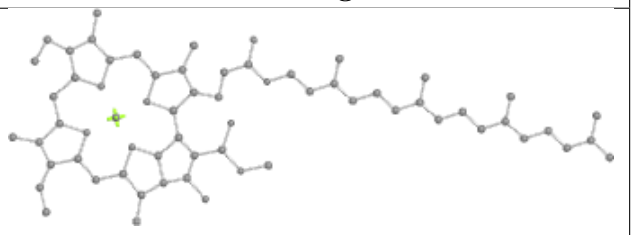
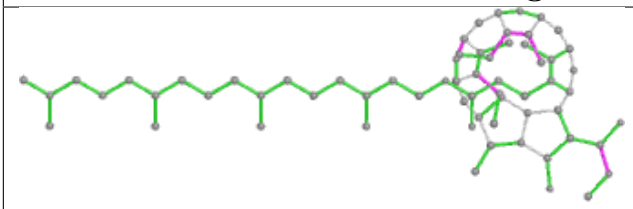


Rings

Ligand PHO a 407



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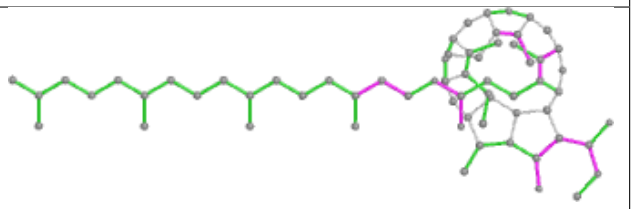
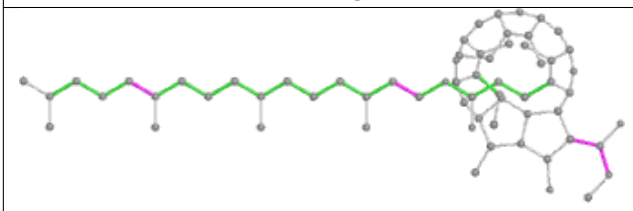
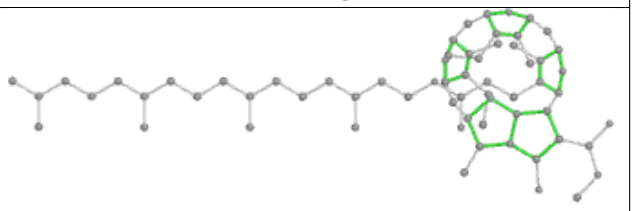


Bond angles

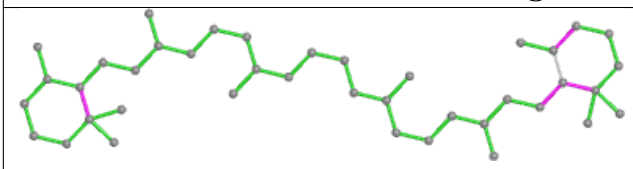


Torsions



Rings

Ligand 8CT C 514



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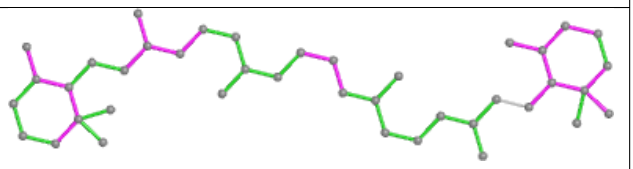
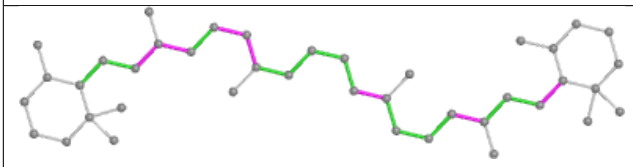
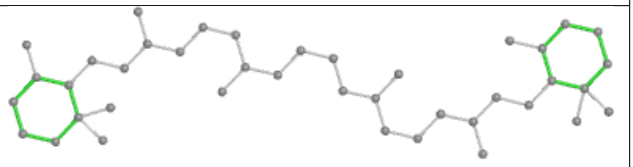


Bond angles

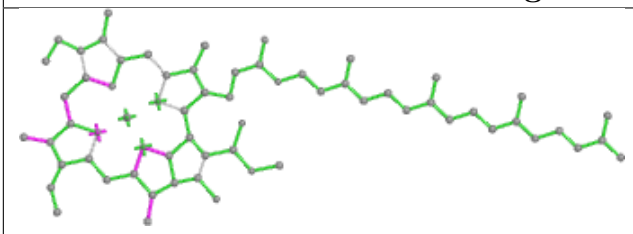


Torsions



Rings

Ligand CLA C 502



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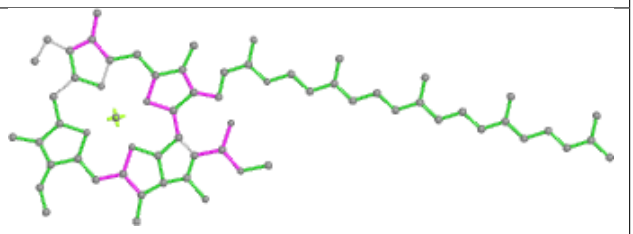
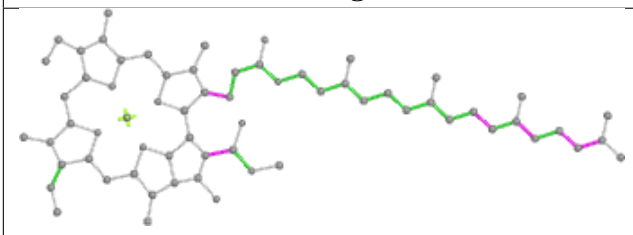
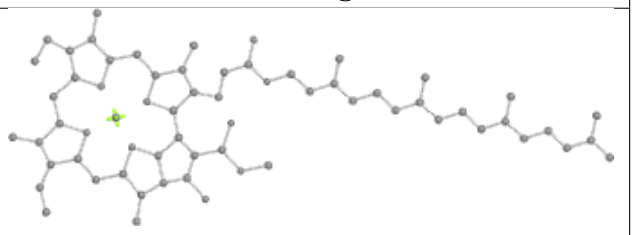


Bond angles

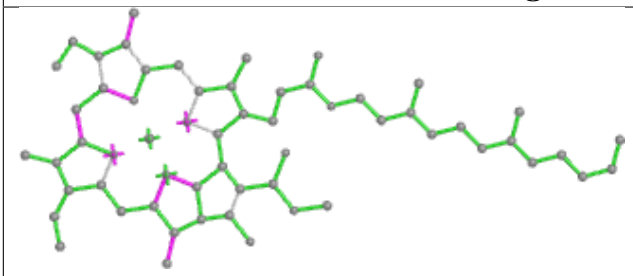


Torsions



Rings

Ligand CLA C 504



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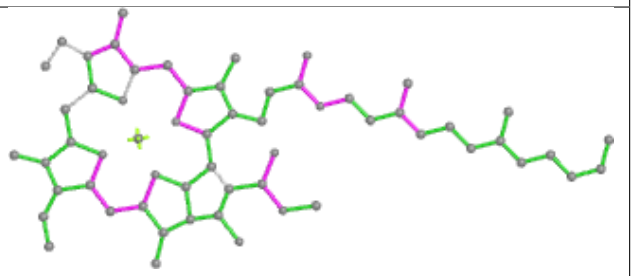
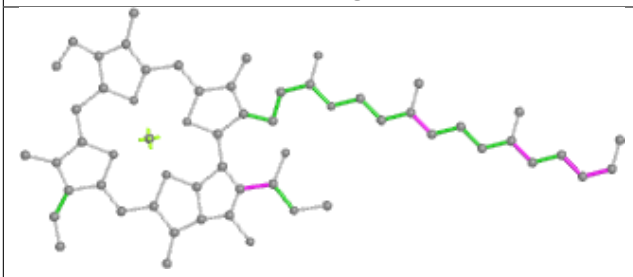
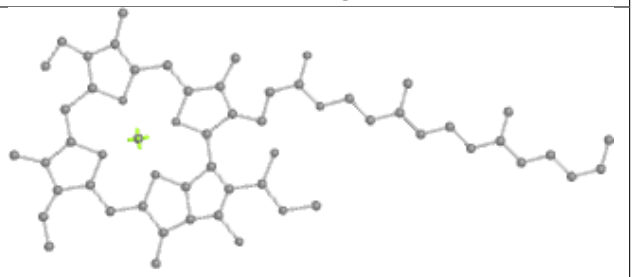


Bond angles

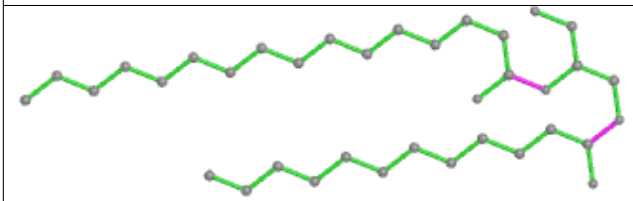


Torsions

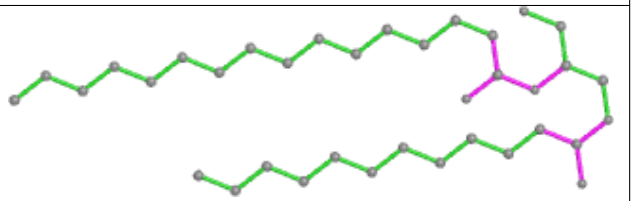


Rings

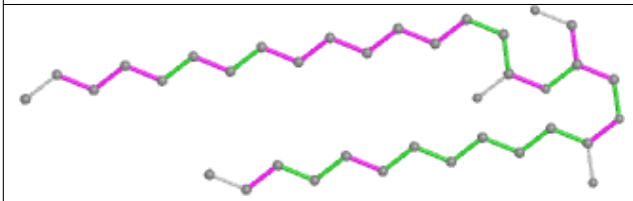
Ligand SQD a 412



Bond lengths



Bond angles



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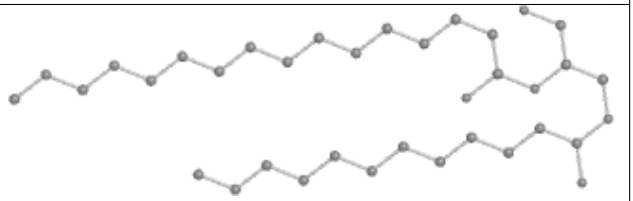
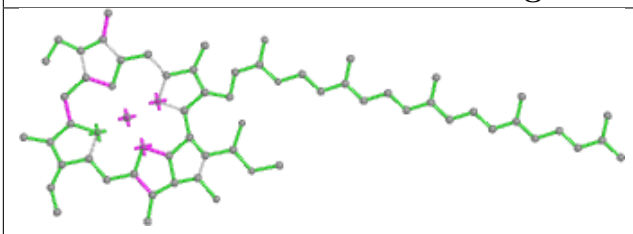
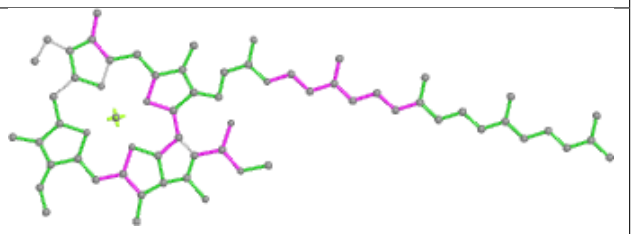


Rings

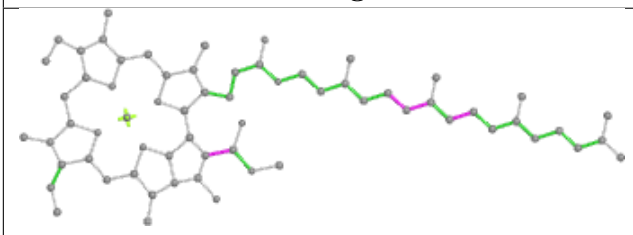
Ligand CLA C 503



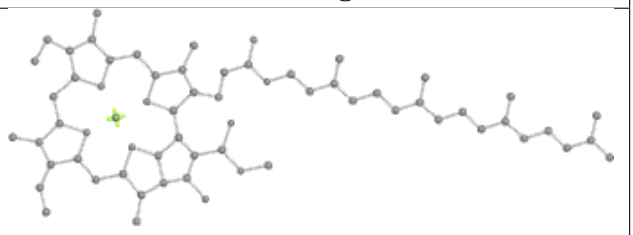
Bond lengths



Bond angles

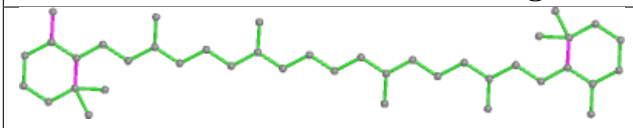


Torsions



Rings

Ligand BCR a 409



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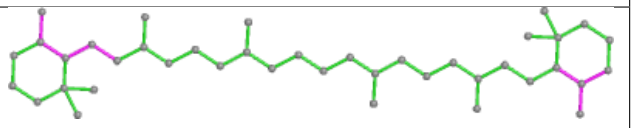
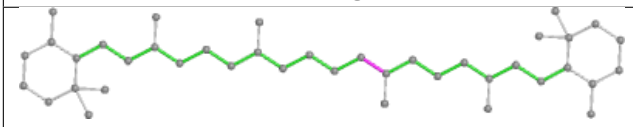


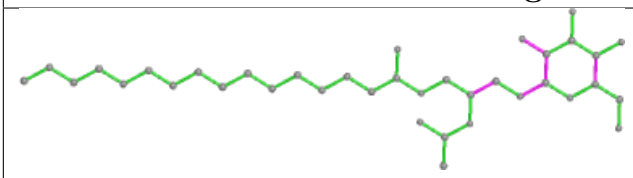
Bond angles



Torsions

Rings

Ligand LMG c 519



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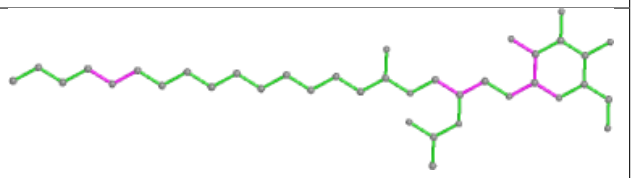
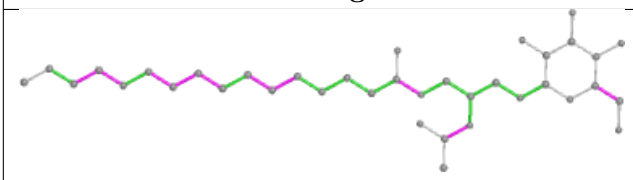
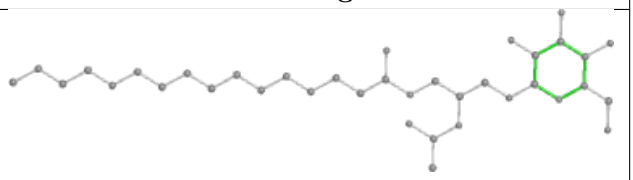


Bond angles

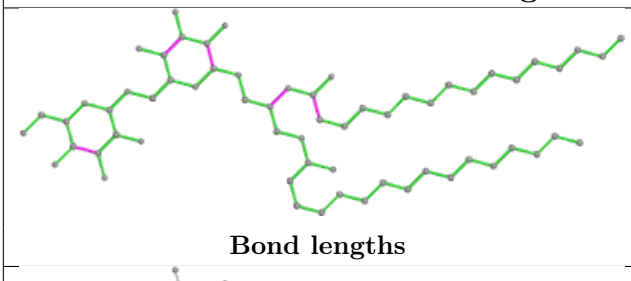


Torsions



Rings

Ligand DGD C 516



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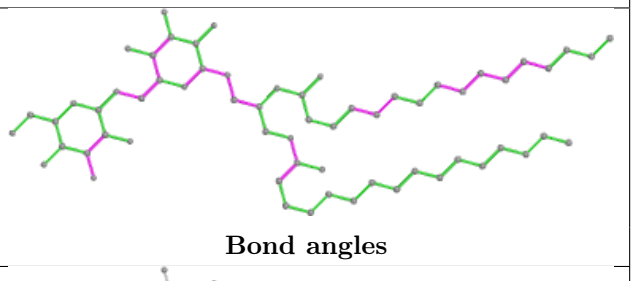
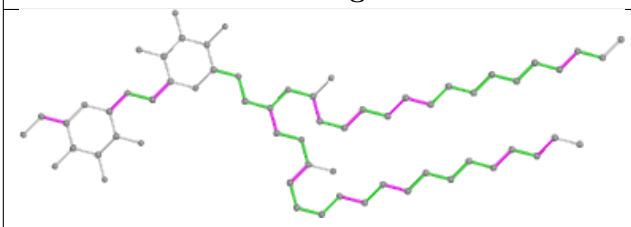


Bond angles



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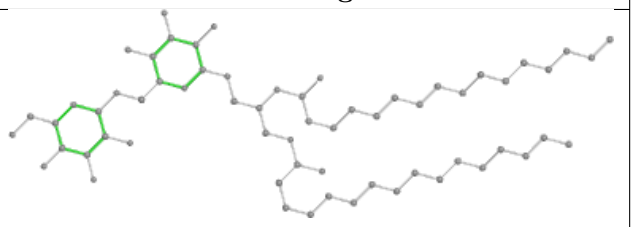
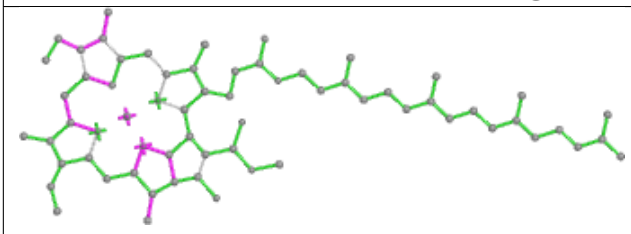


Rings

Ligand CLA b 611



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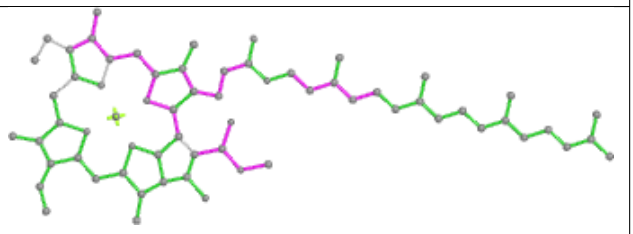
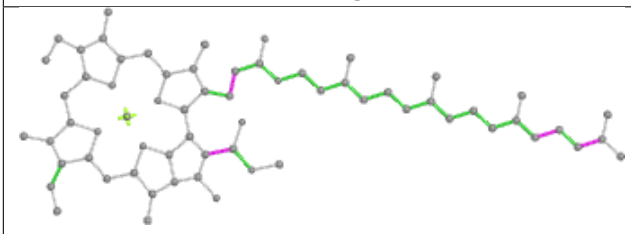


Bond angles



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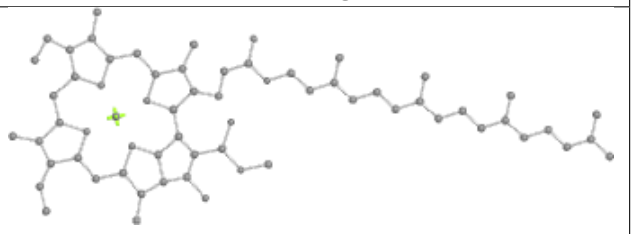
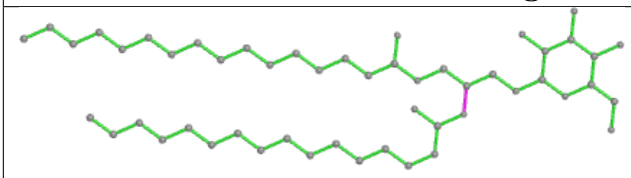


Rings

Ligand LMG b 621



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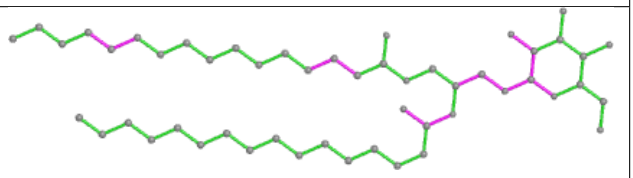

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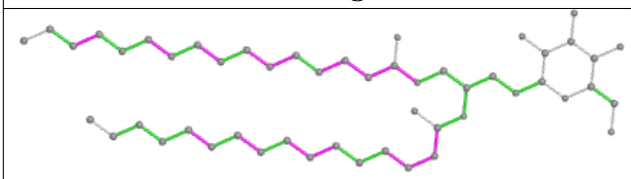

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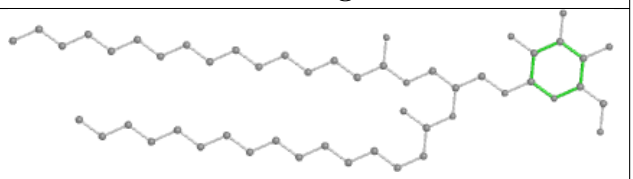
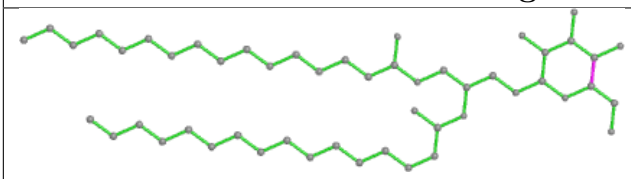


Rings

Ligand LMG D 407



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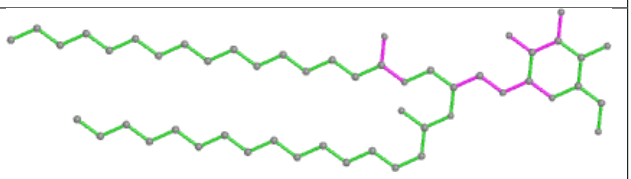
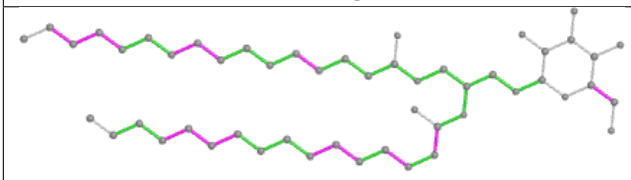


Bond angles



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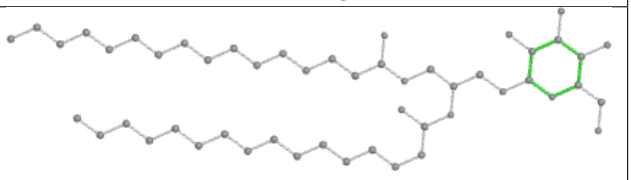
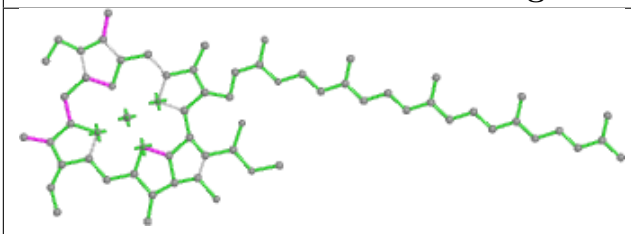


Rings

Ligand CLA b 613



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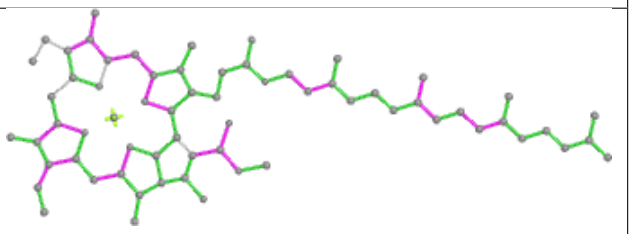
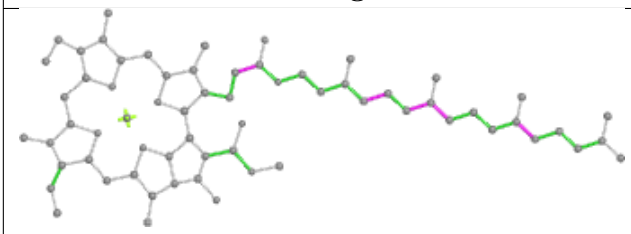


Bond angles



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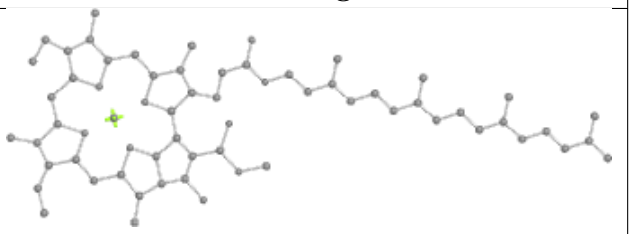
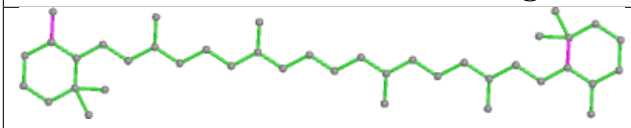


Rings

Ligand BCR H 101



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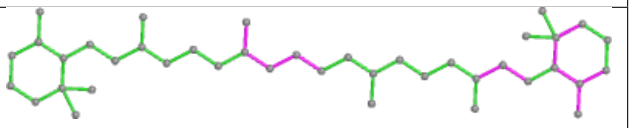
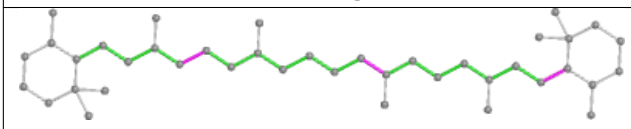


Bond angles



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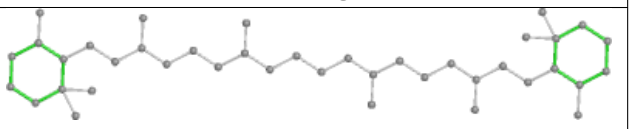
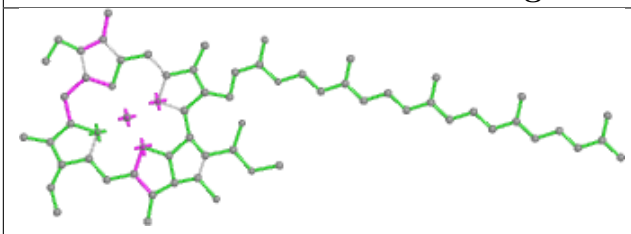


Rings

Ligand CLA B 601



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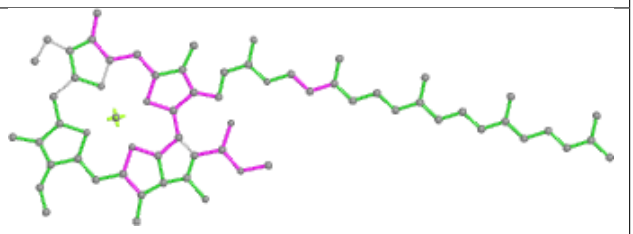

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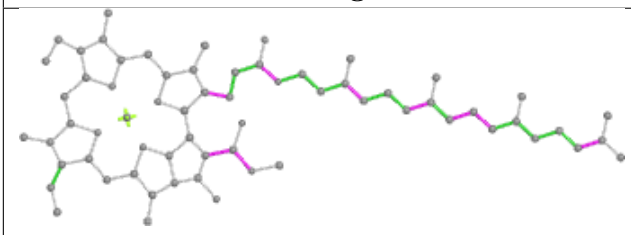

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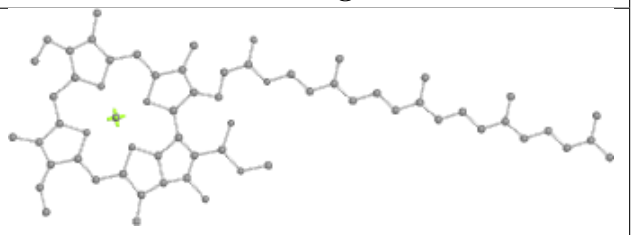
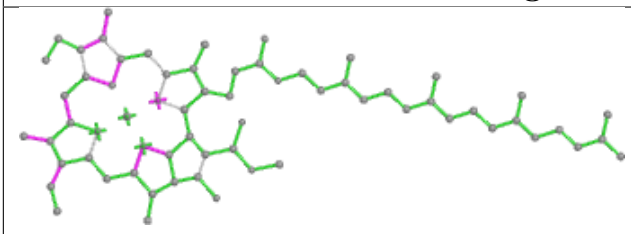


Rings

Ligand CLA A 405



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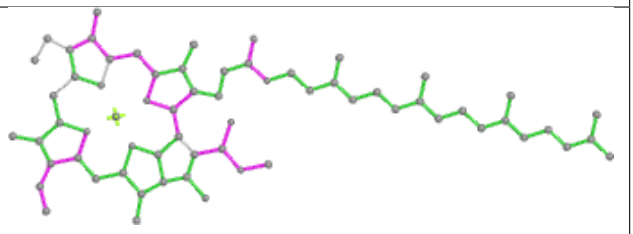
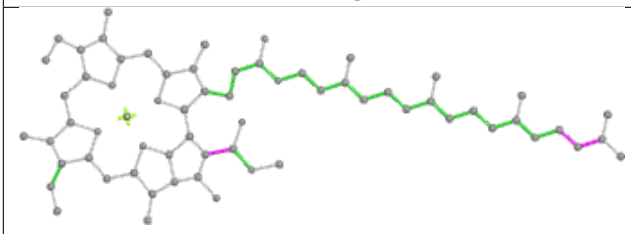


Bond angles



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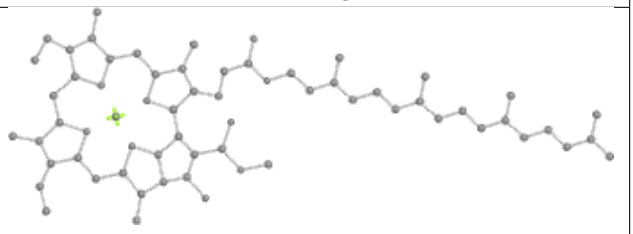
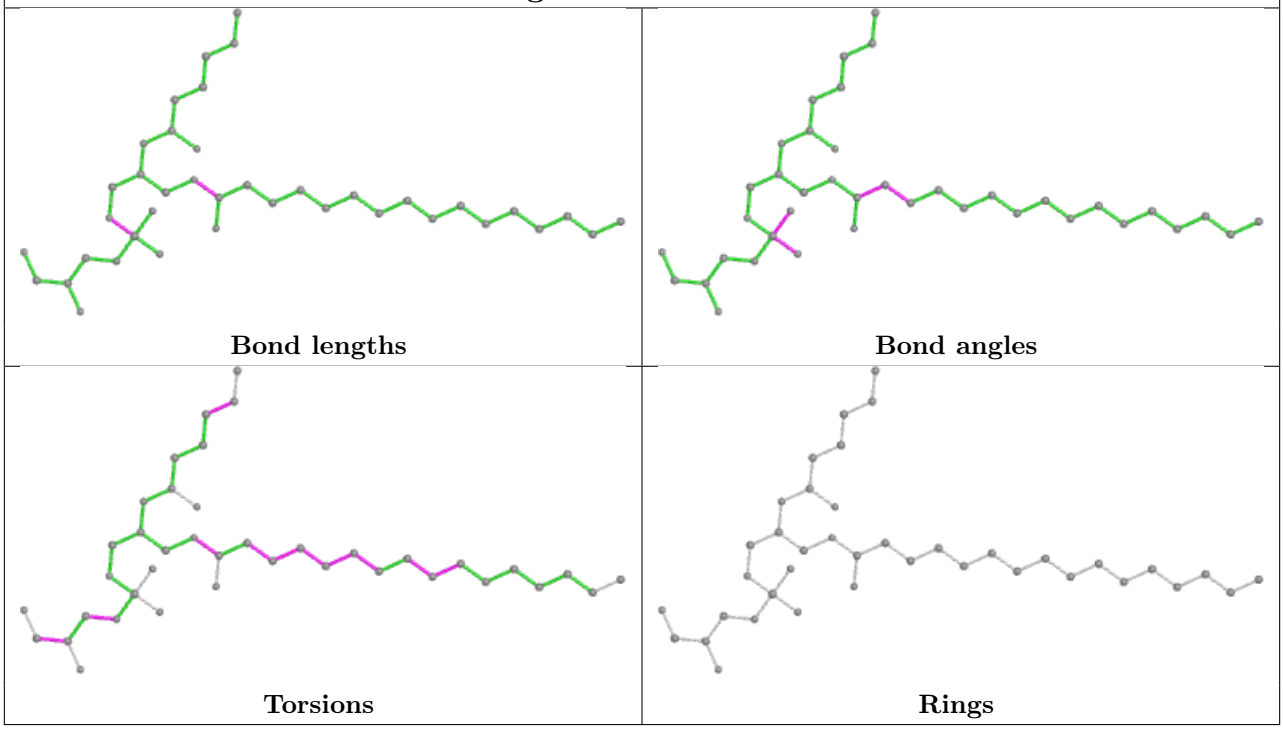
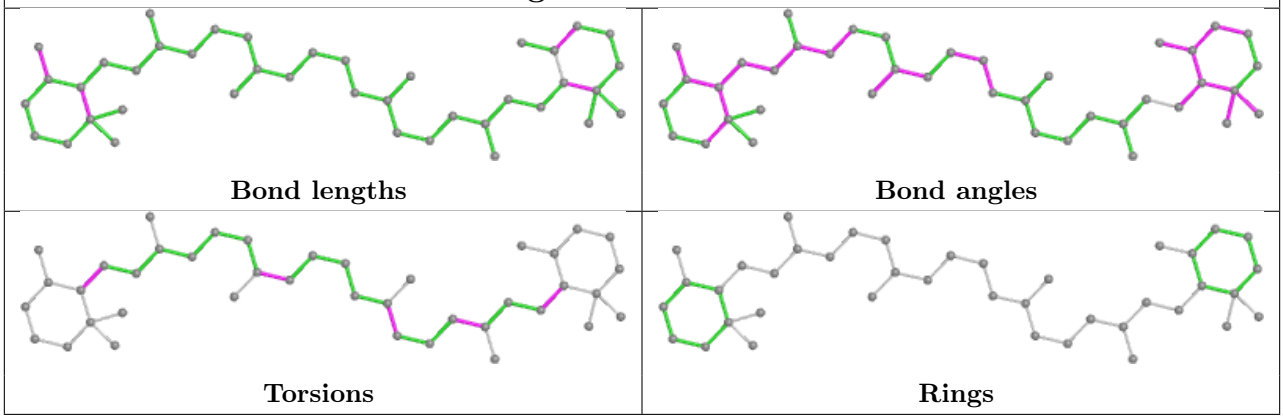


Rings

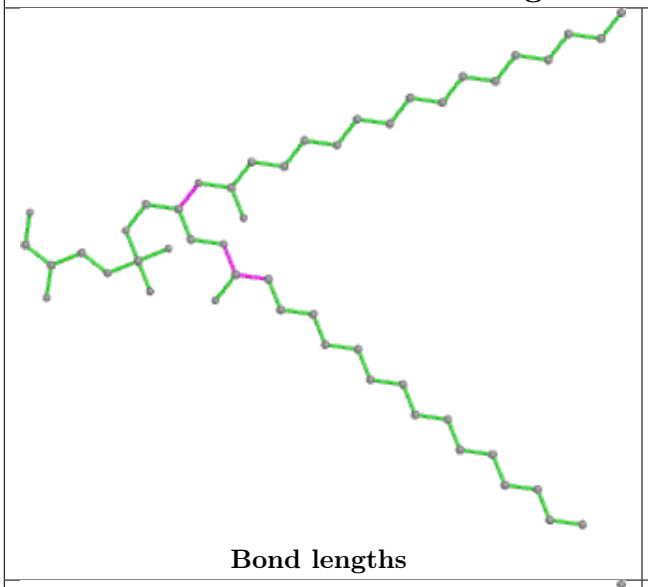
Ligand LHG d 409



Ligand 8CT A 408



Ligand LHG E 101



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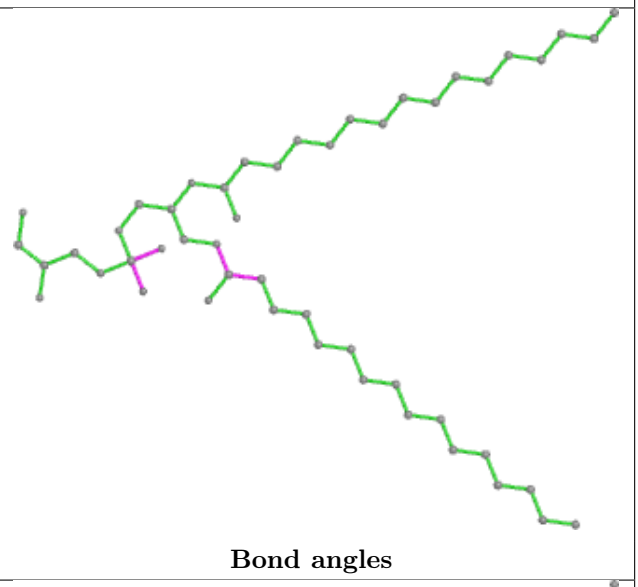
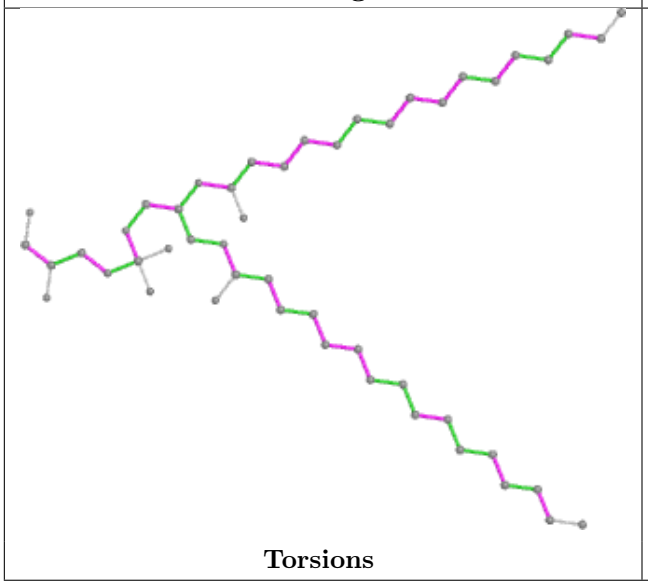


Bond angles



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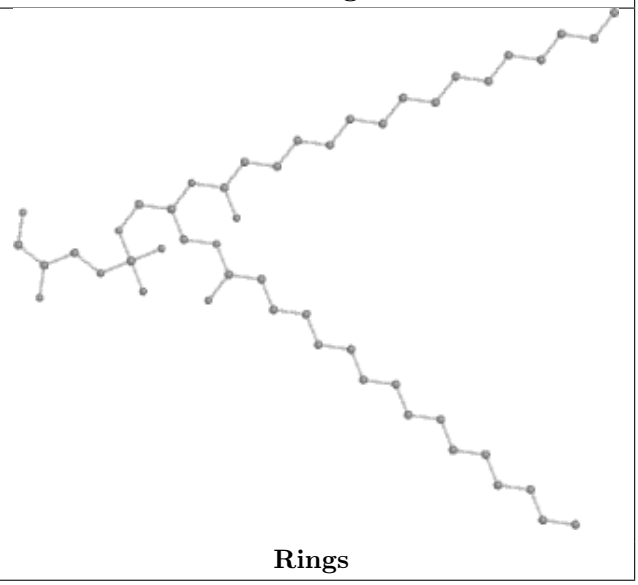
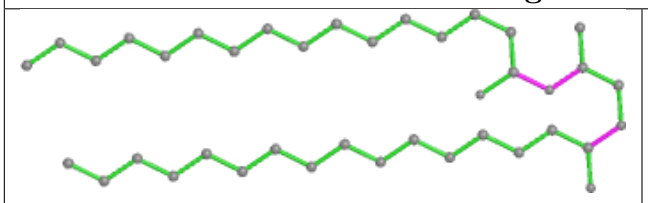


Rings

Ligand SQD A 413



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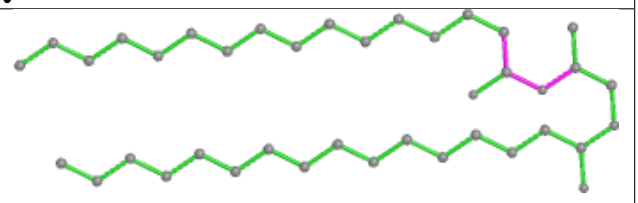
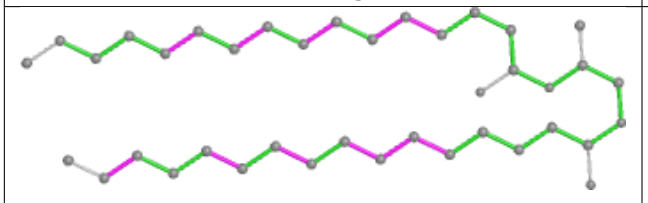
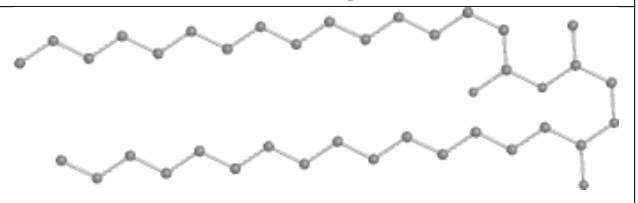


Bond angles

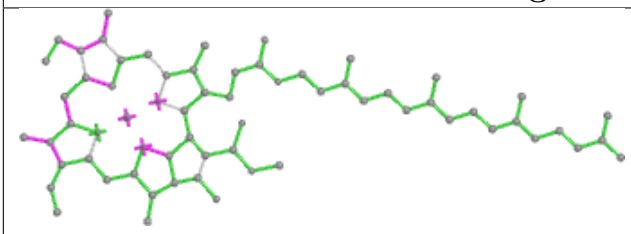


Torsions

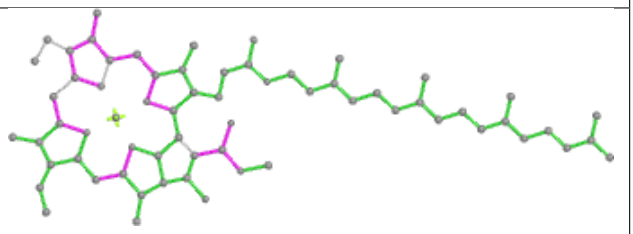


Rings

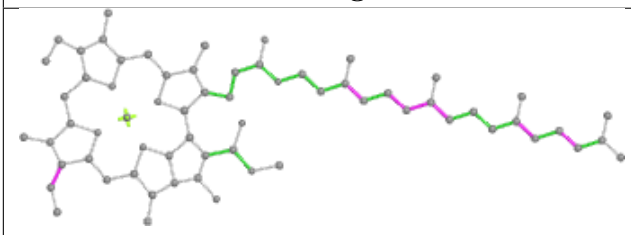
Ligand CLA c 505



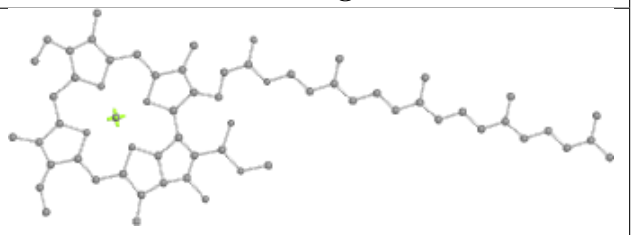
Bond lengths



Bond angles

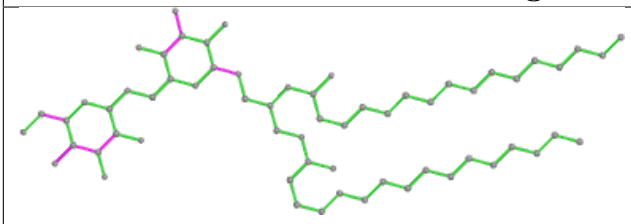


Torsions

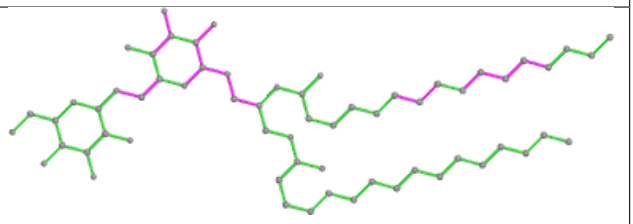


Rings

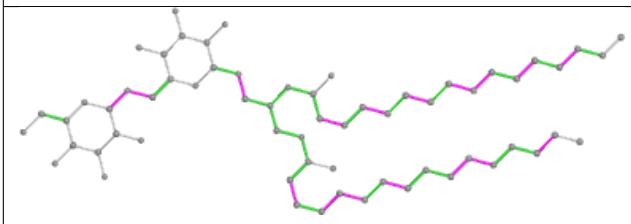
Ligand DGD c 517



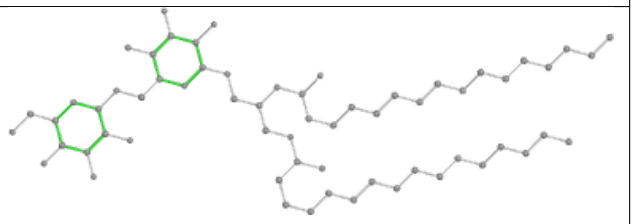
Bond lengths



Bond angles

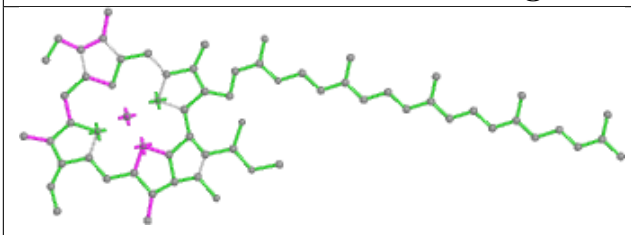


Torsions

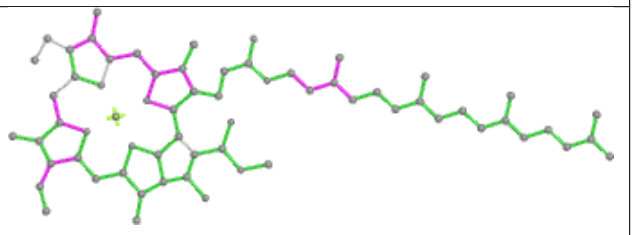


Rings

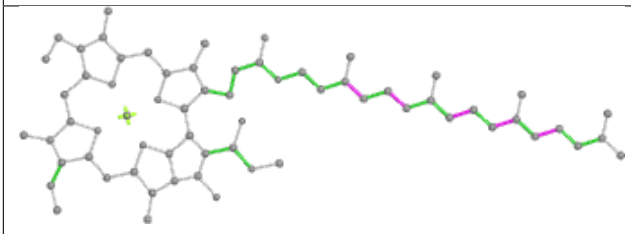
Ligand CLA B 613



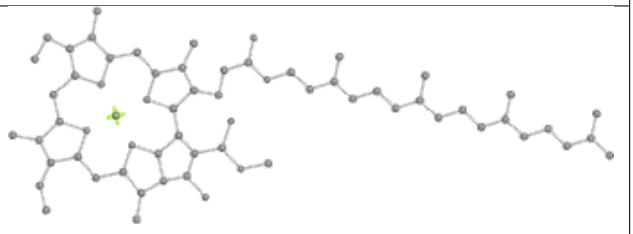
Bond lengths



Bond angles

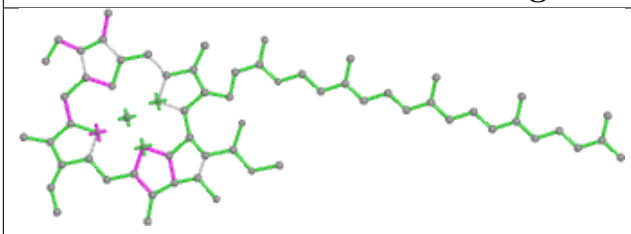


Torsions



Rings

Ligand CLA c 503



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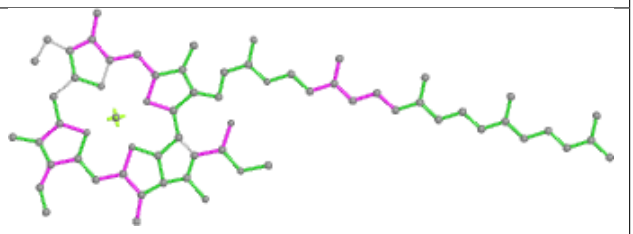
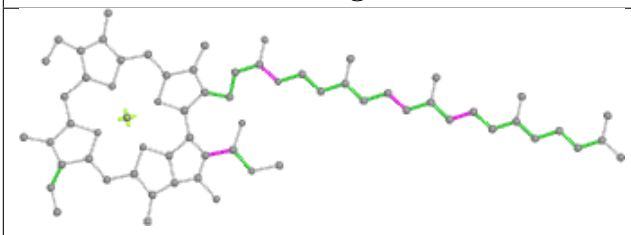


Bond angles



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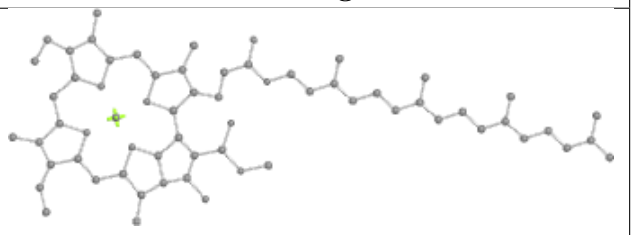
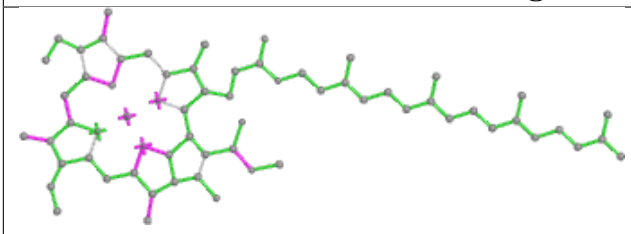


Rings

Ligand CLA b 616



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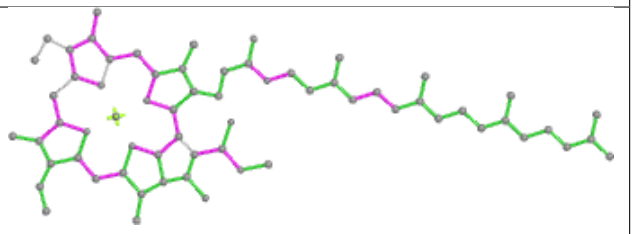
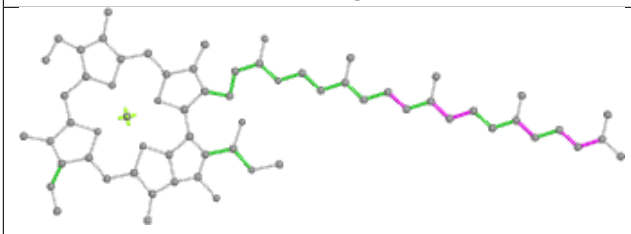
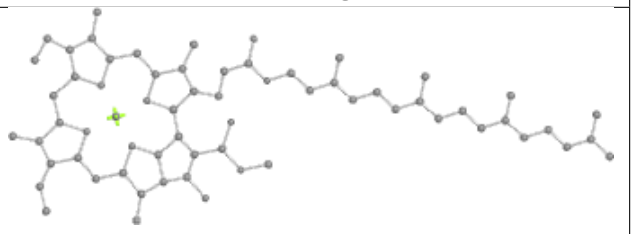


Bond angles

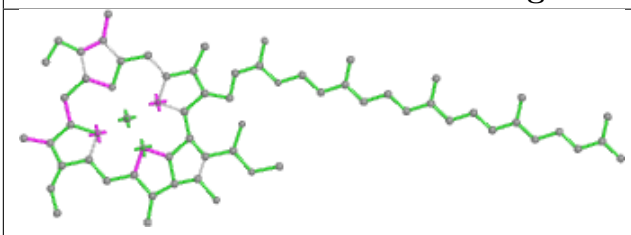


Torsions

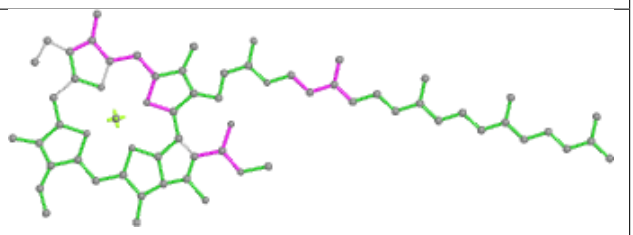


Rings

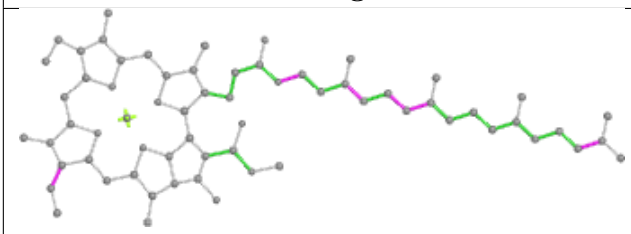
Ligand CLA d 403



Bond lengths



Bond angles



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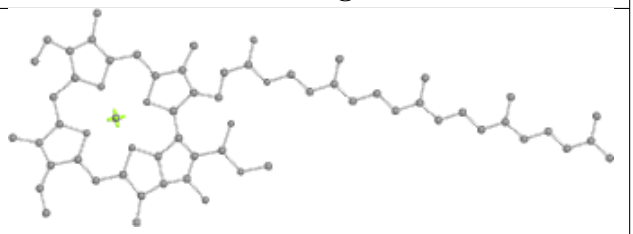
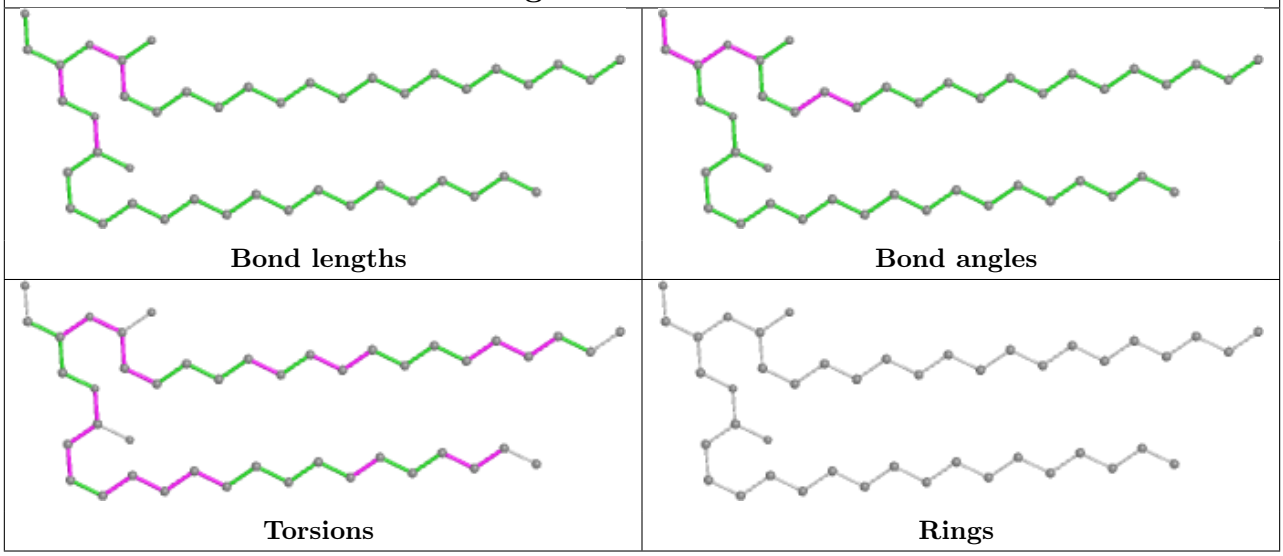
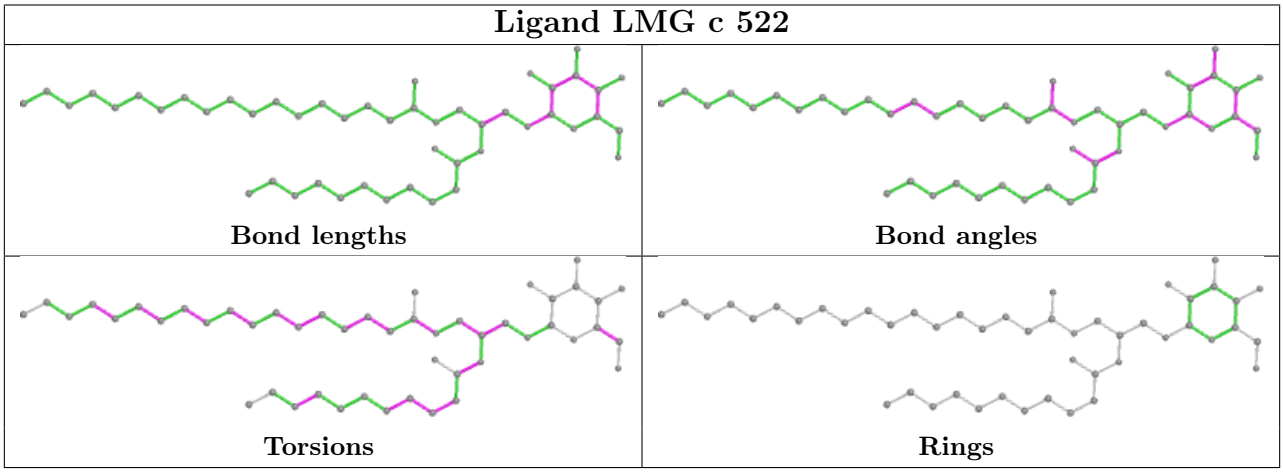


Rings

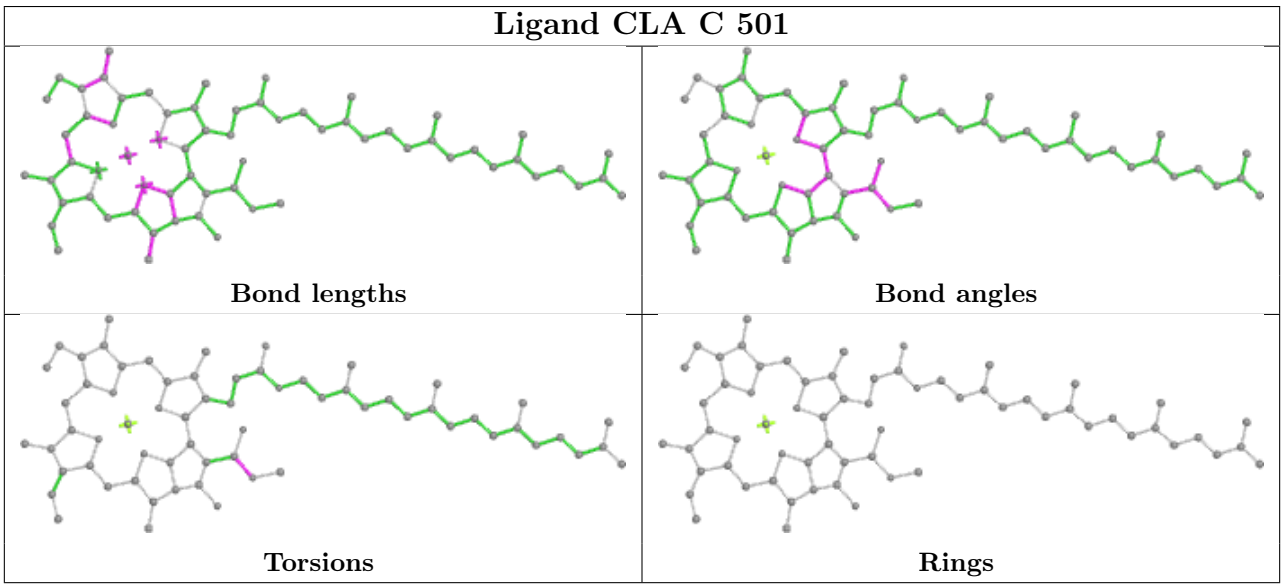
Ligand DGD o 301



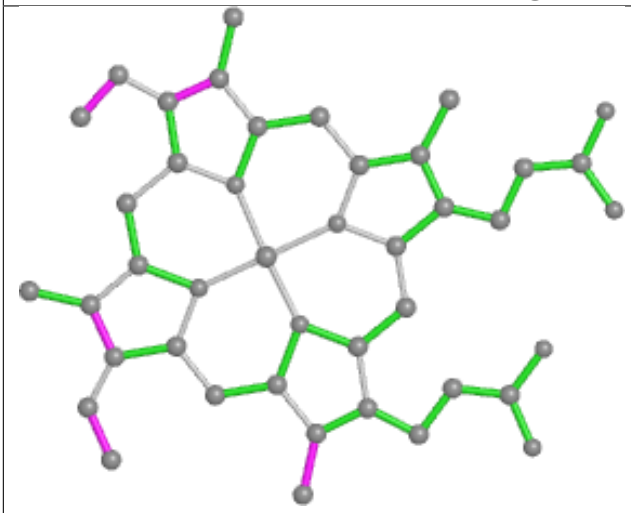
Ligand LMG c 522



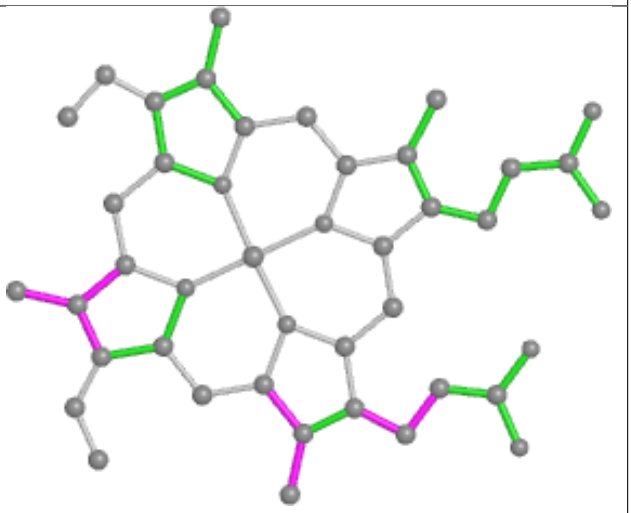
Ligand CLA C 501



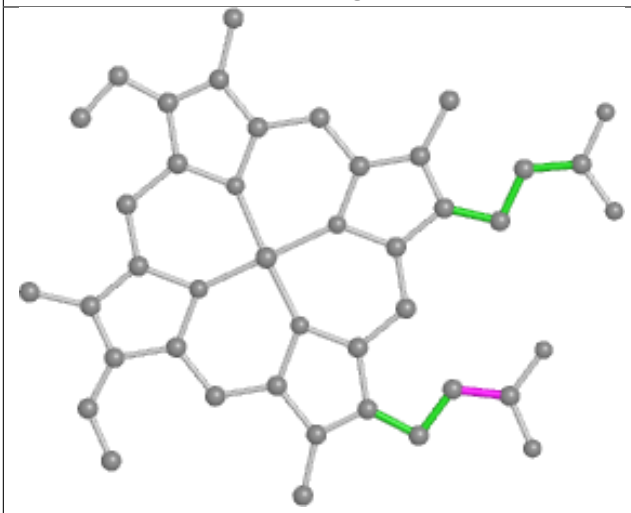
Ligand HEC v 201



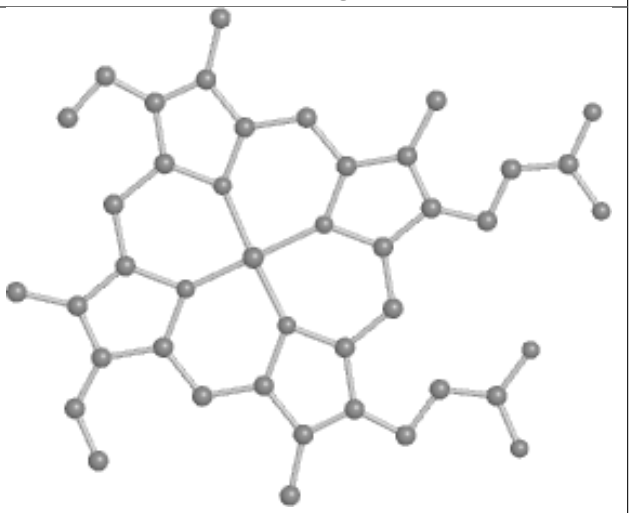
Bond lengths



Bond angles

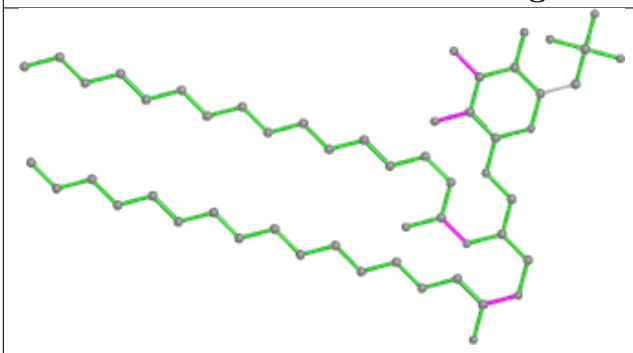


Torsions



Rings

Ligand SQD a 411



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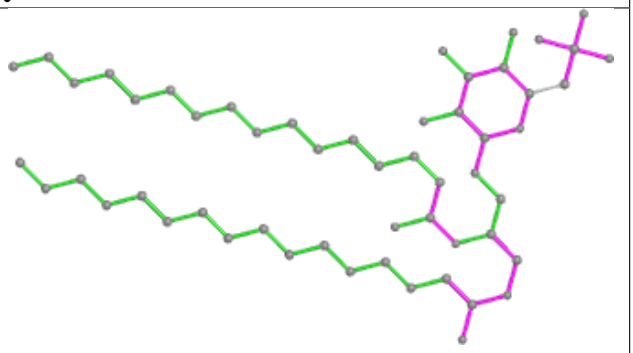
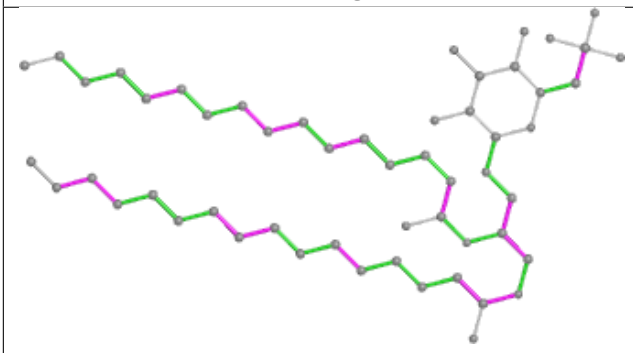


Bond angles



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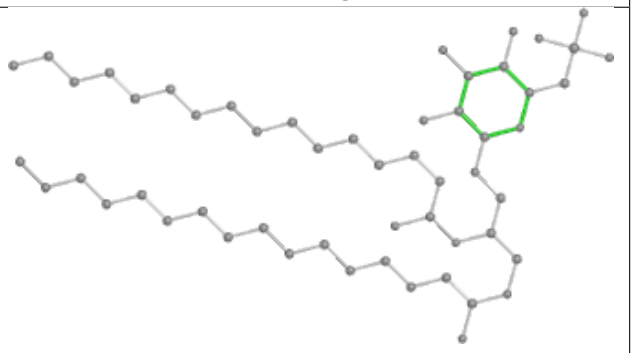
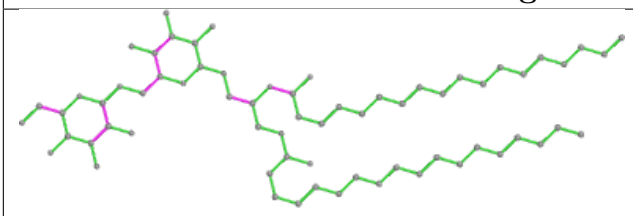


Rings

Ligand DGD A 414



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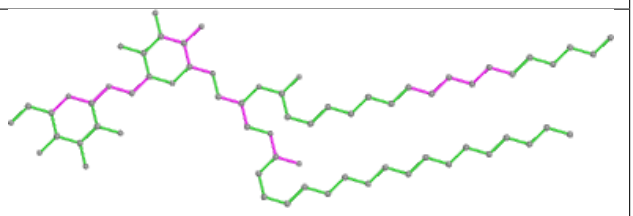
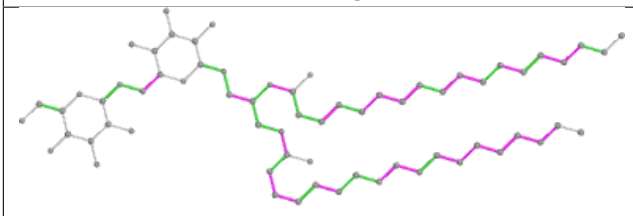


Bond angles



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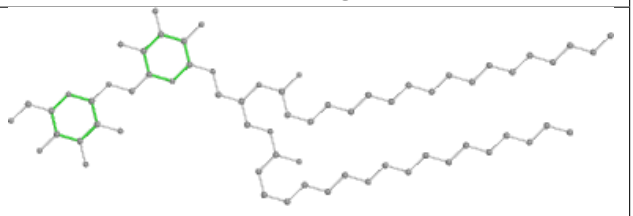
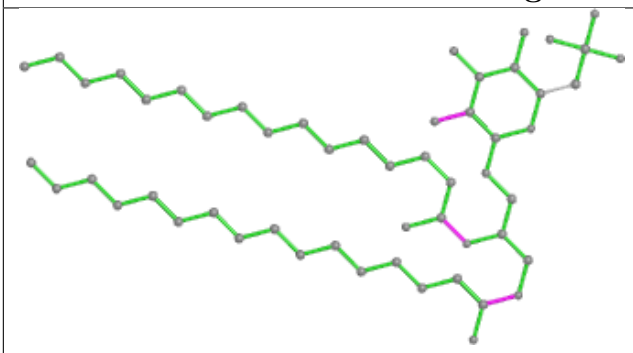


Rings

Ligand SQD B 624



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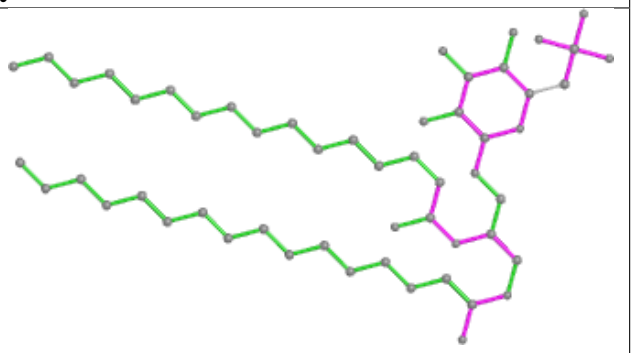
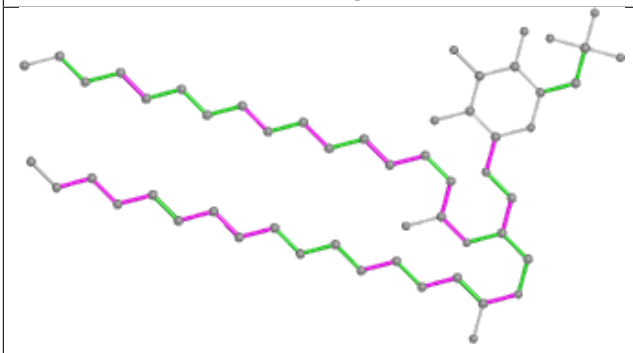


Bond angles



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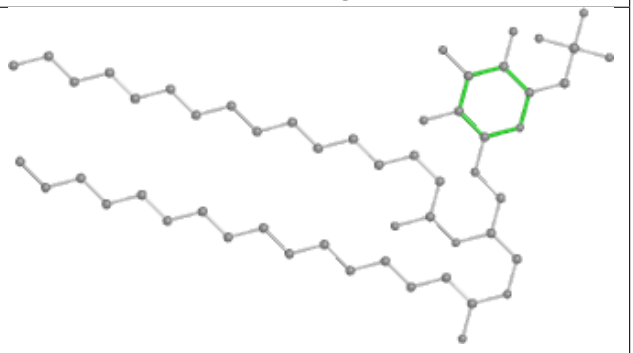
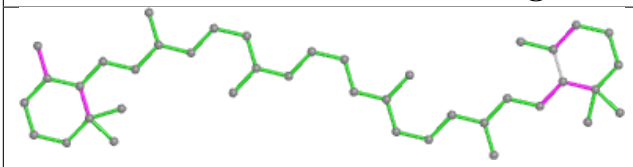


Rings

Ligand 8CT B 617



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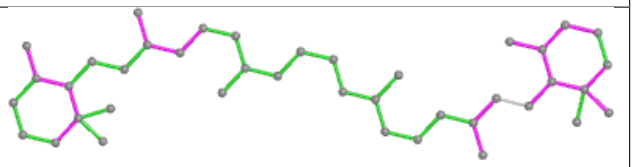
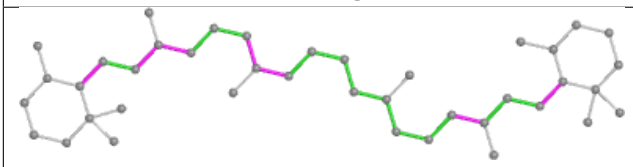
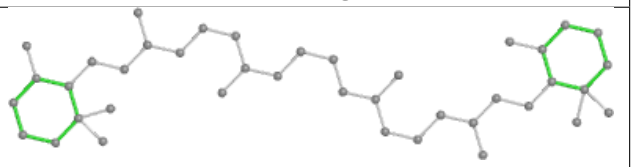


Bond angles

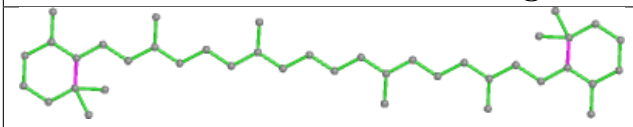


Torsions

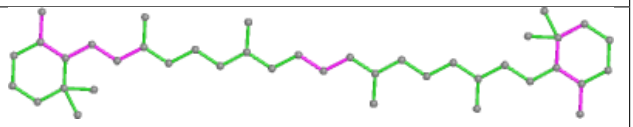


Rings

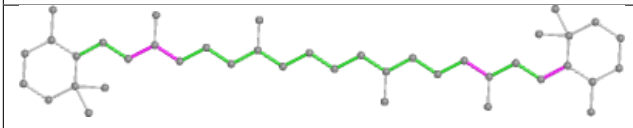
Ligand BCR B 618



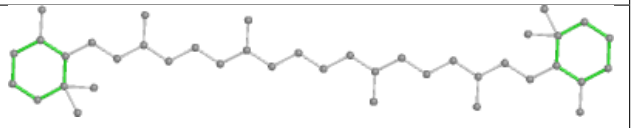
Bond lengths



Bond angles

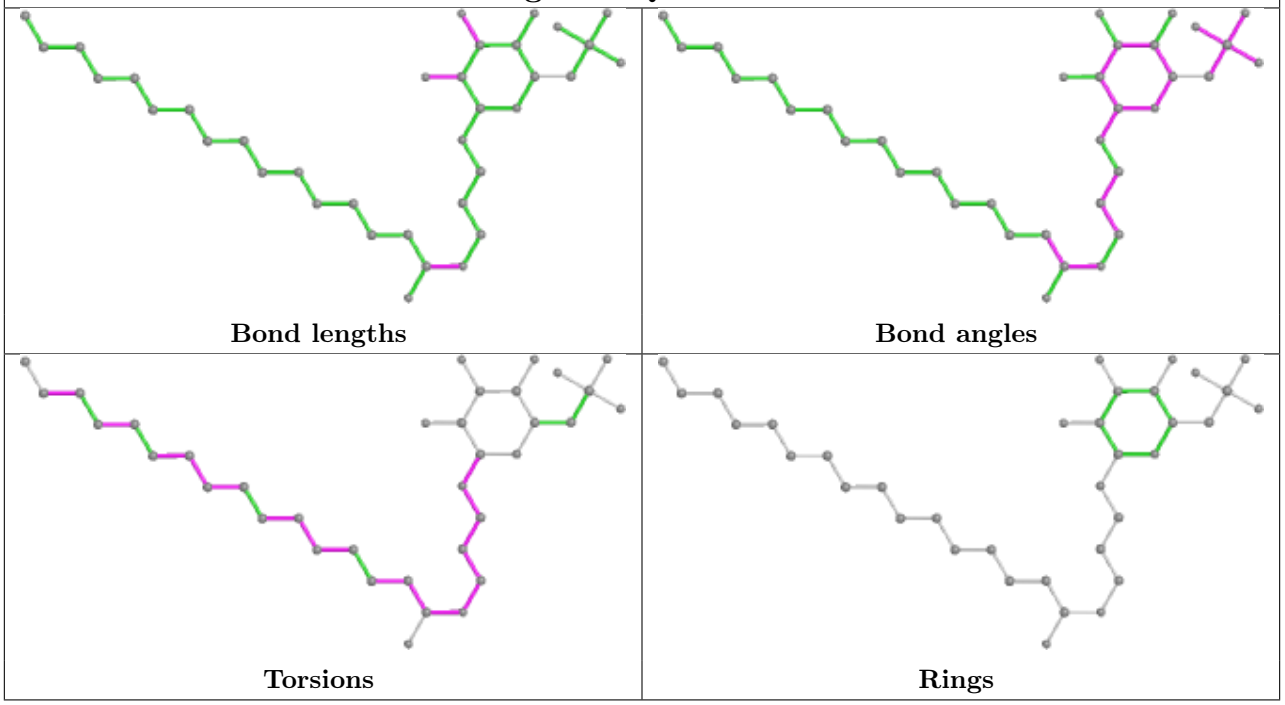


Torsions

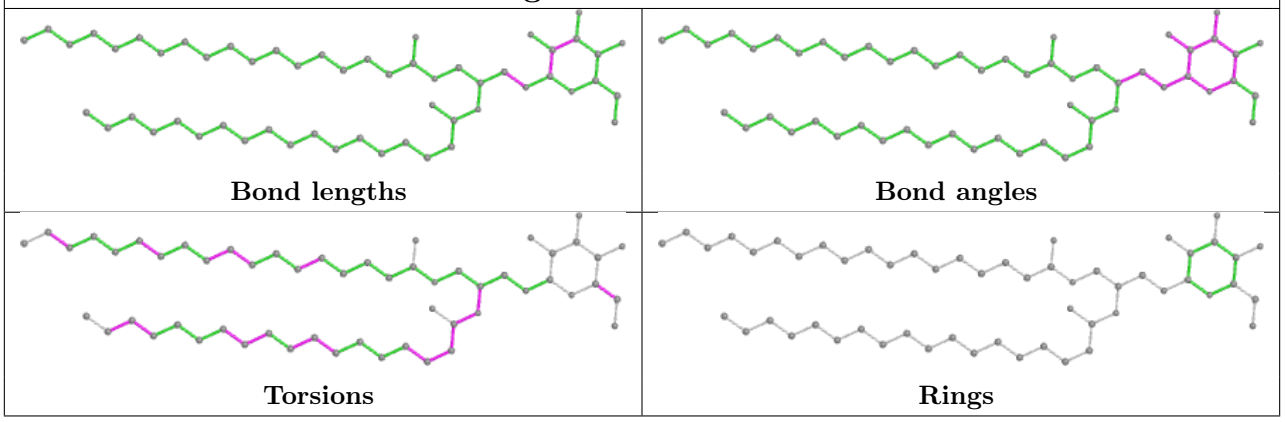


Rings

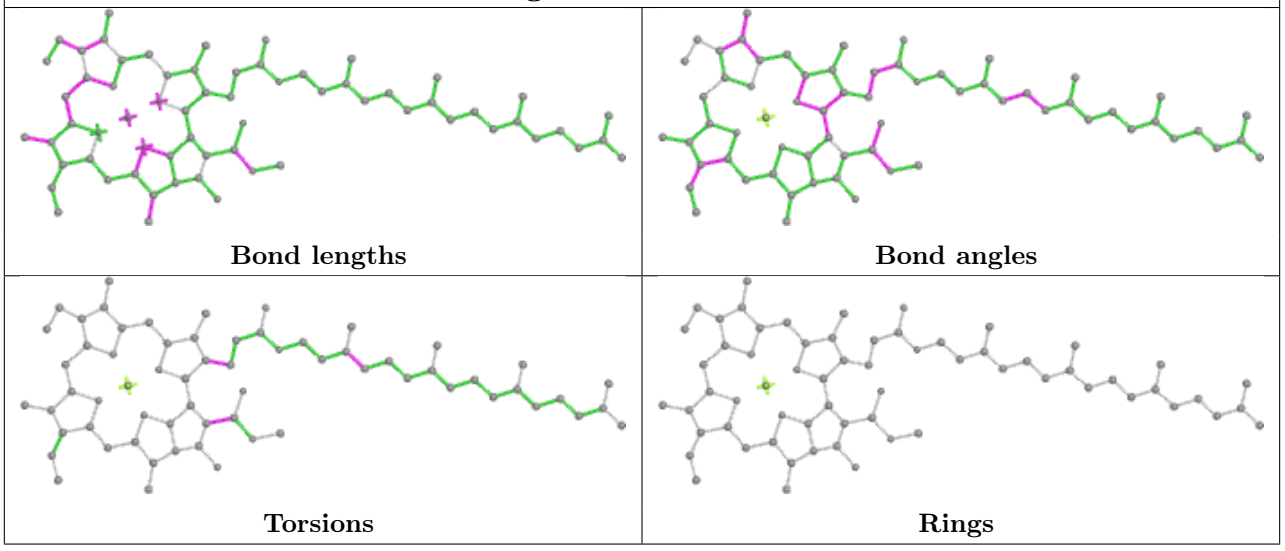
Ligand SQD D 408



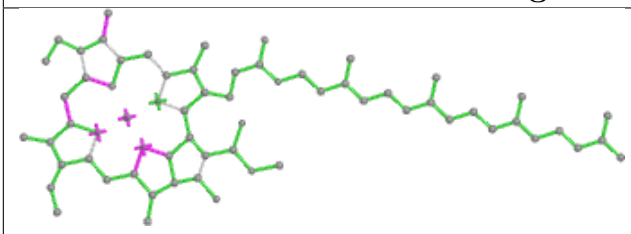
Ligand LMG b 623



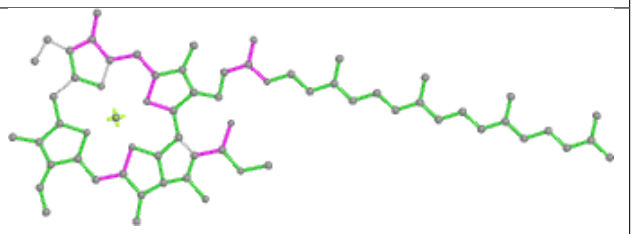
Ligand CLA B 609



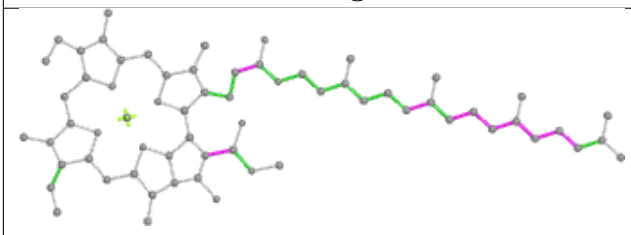
Ligand CLA c 509



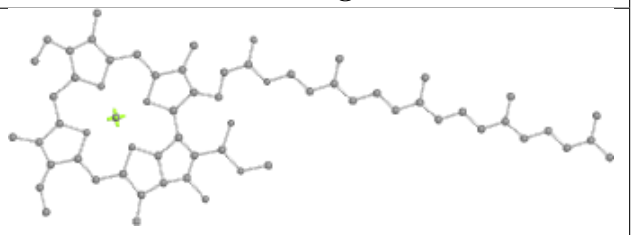
Bond lengths



Bond angles

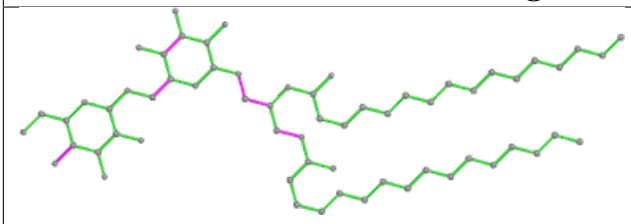


Torsions

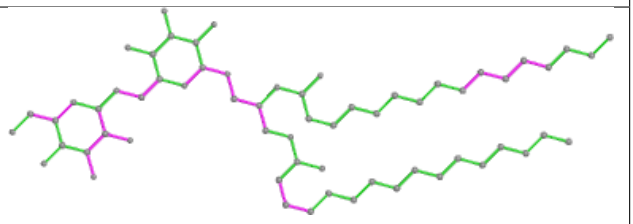


Rings

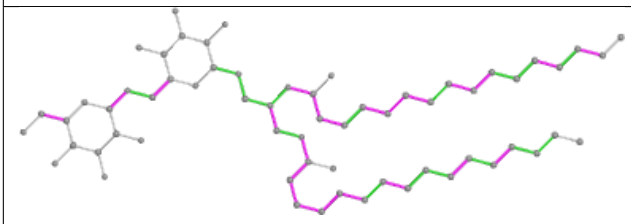
Ligand DGD c 516



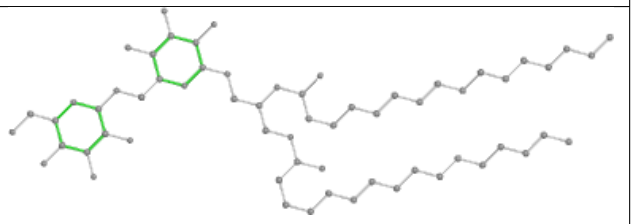
Bond lengths



Bond angles

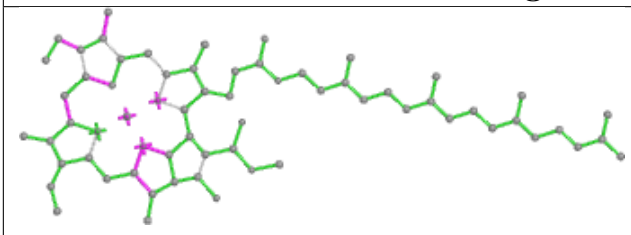


Torsions



Rings

Ligand CLA C 508



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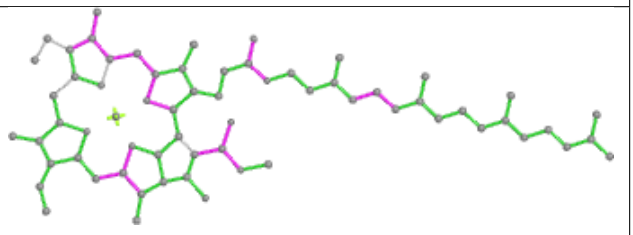
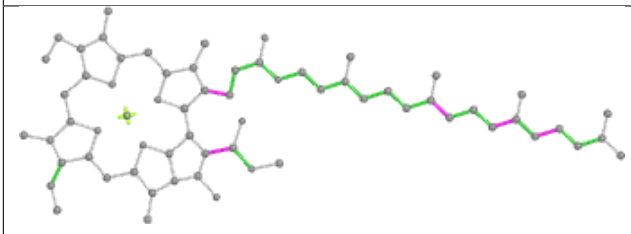
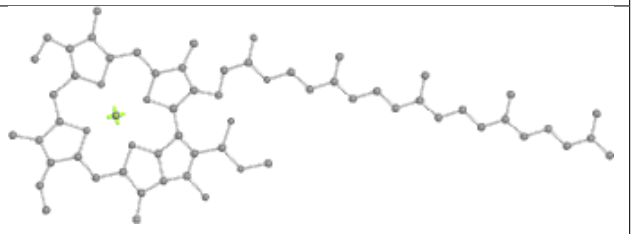


Bond angles

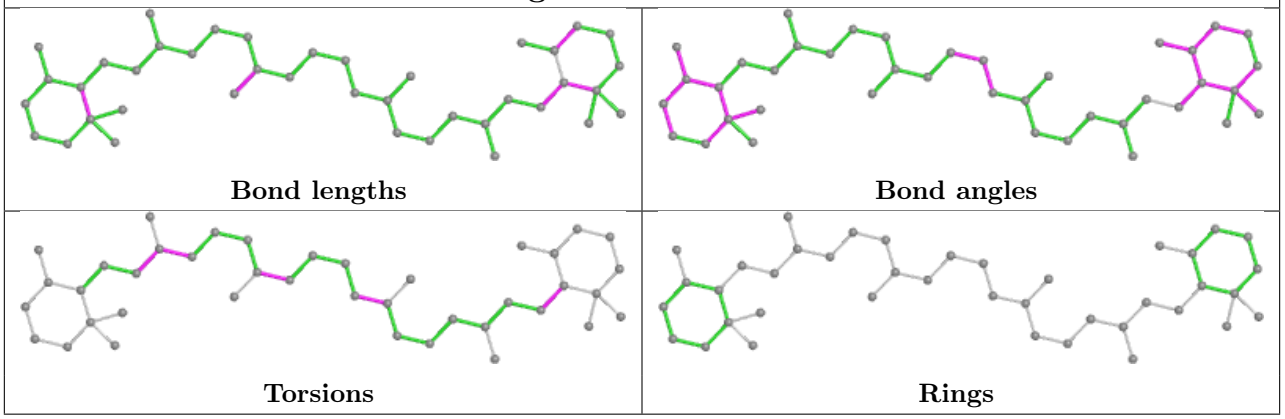


Torsions

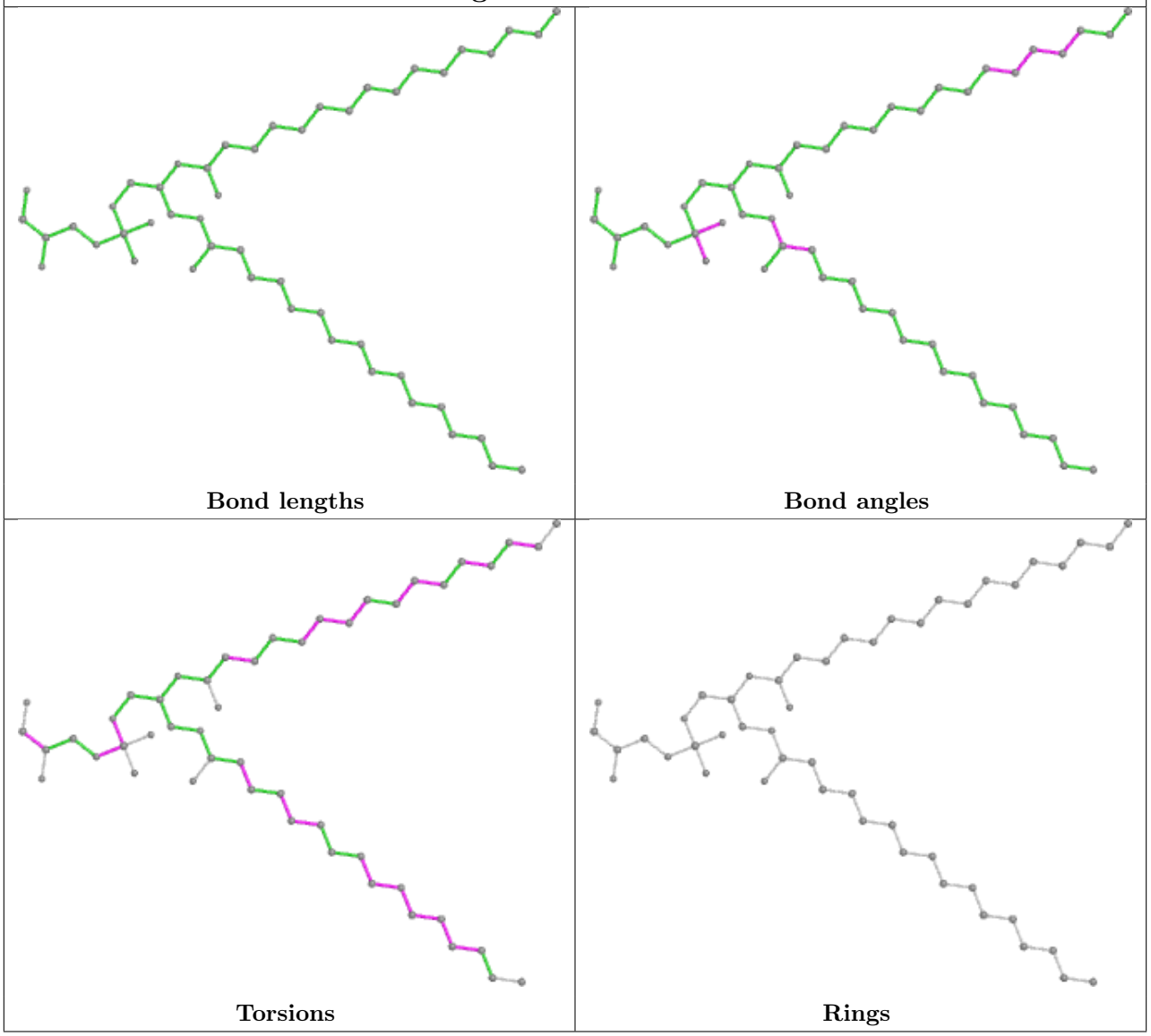


Rings

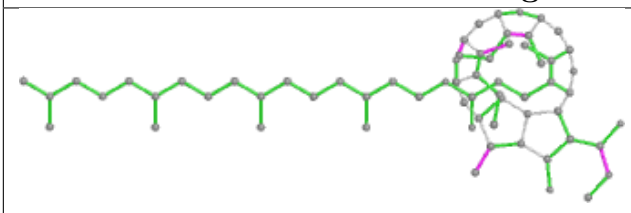
Ligand 8CT B 619



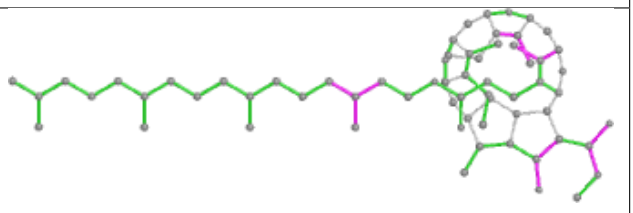
Ligand LHG d 408



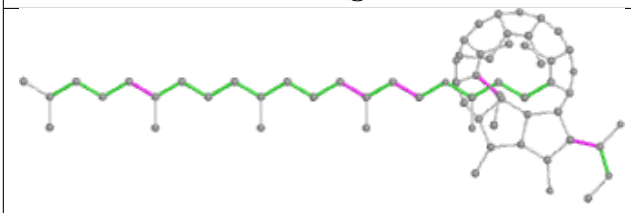
Ligand PHO A 406



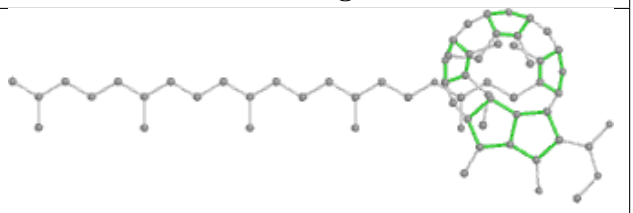
Bond lengths



Bond angles

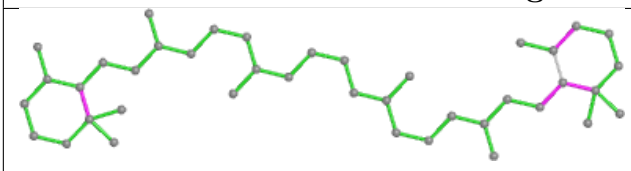


Torsions

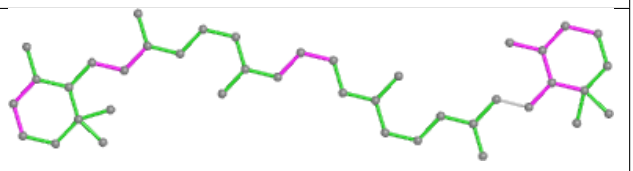


Rings

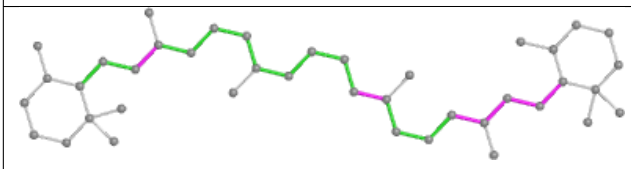
Ligand 8CT D 405



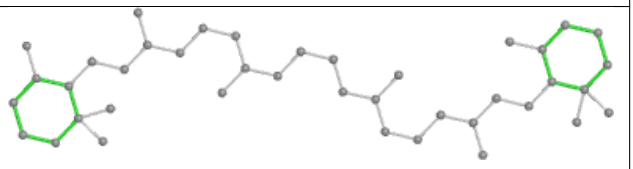
Bond lengths



Bond angles

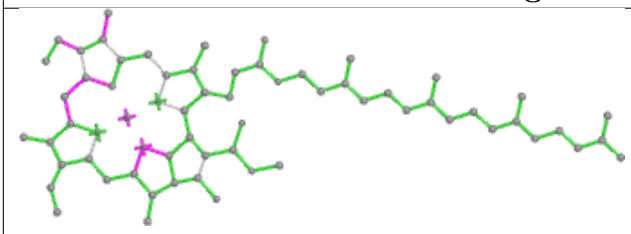


Torsions

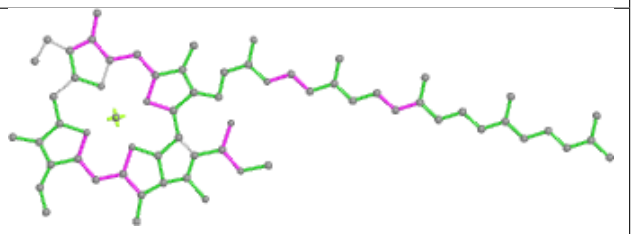


Rings

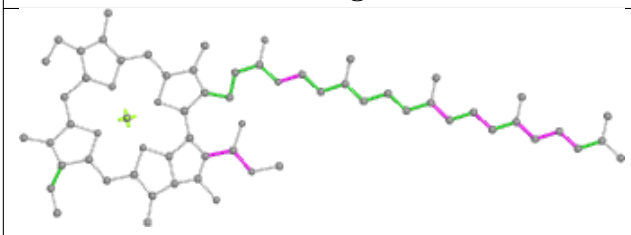
Ligand CLA C 513



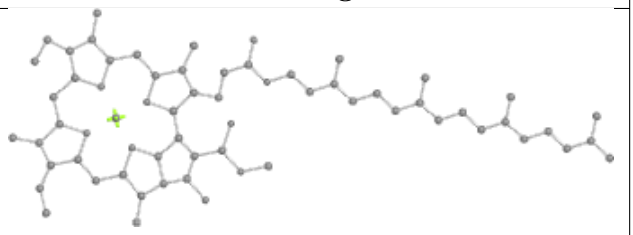
Bond lengths



Bond angles

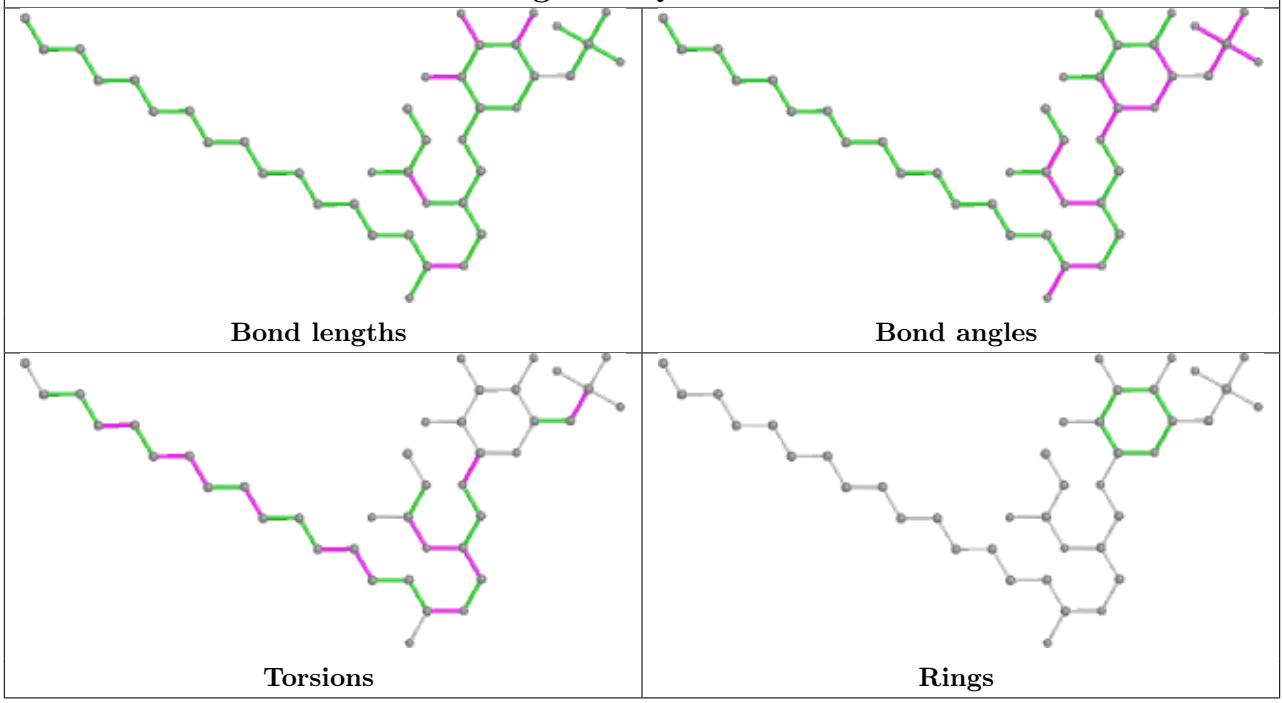


Torsions

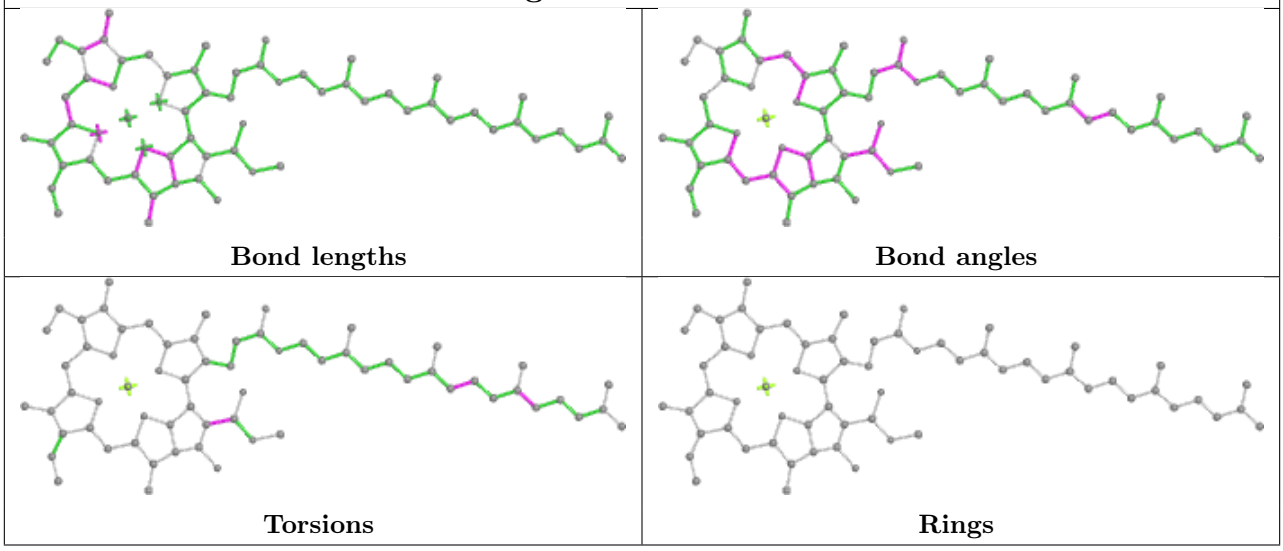


Rings

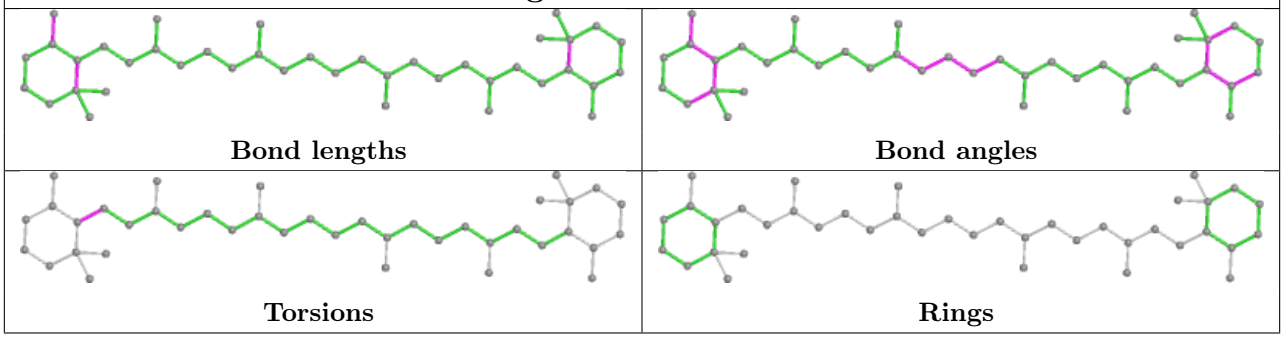
Ligand SQD f 101



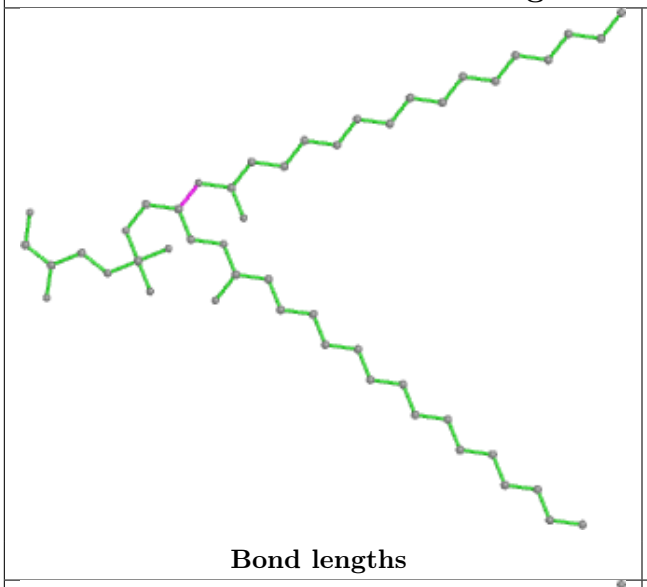
Ligand CLA B 610



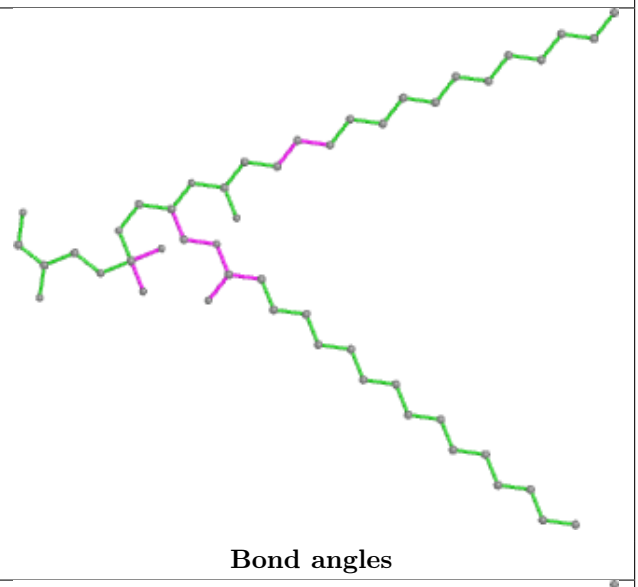
Ligand BCR b 618



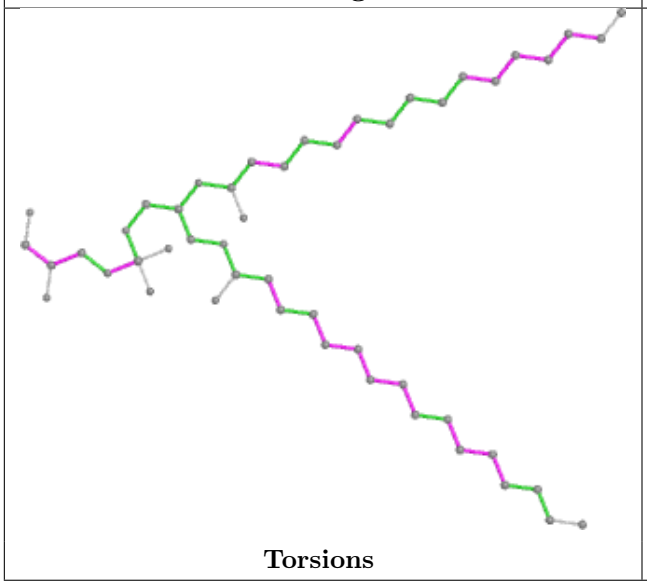
Ligand LHG d 407



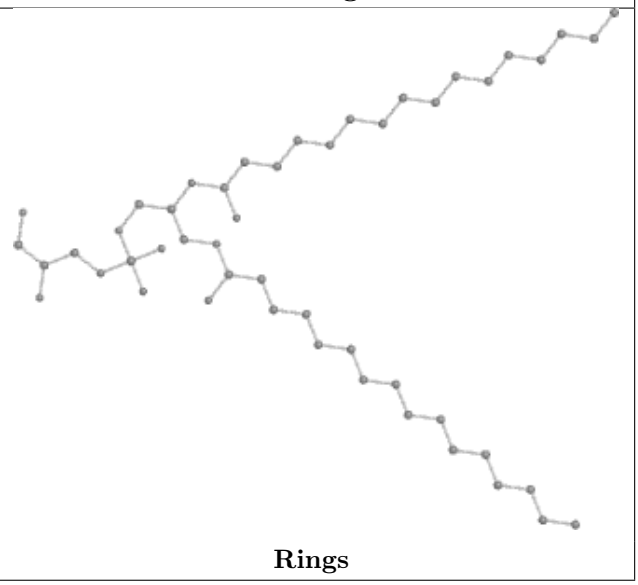
Bond lengths



Bond angles

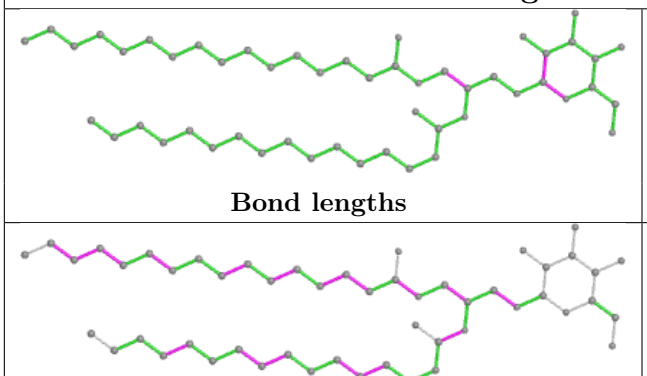


Torsions

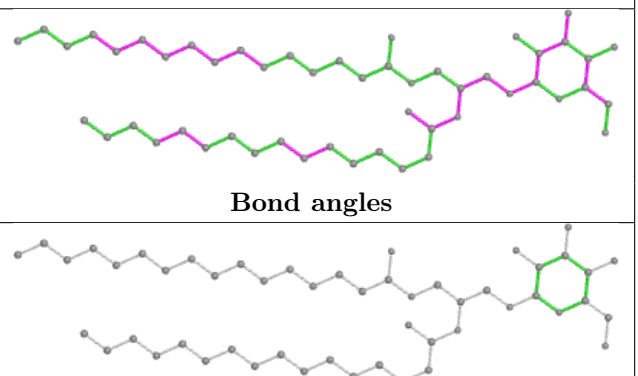


Rings

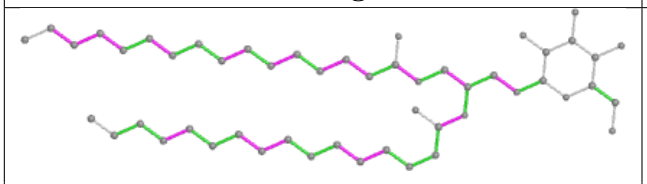
Ligand LMG B 620



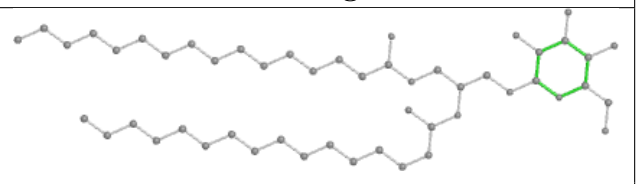
Bond lengths



Bond angles

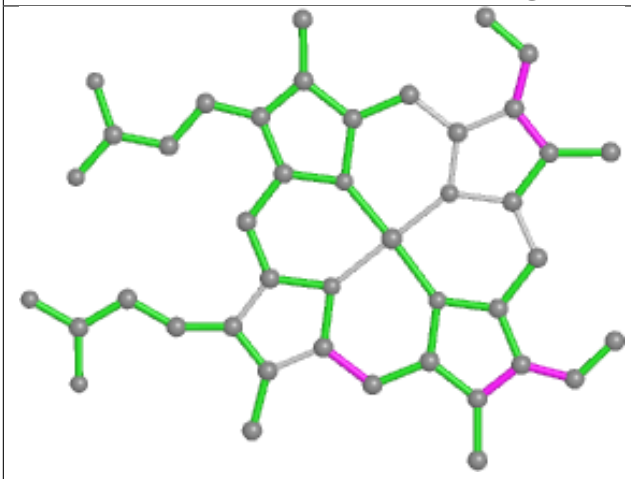


Torsions

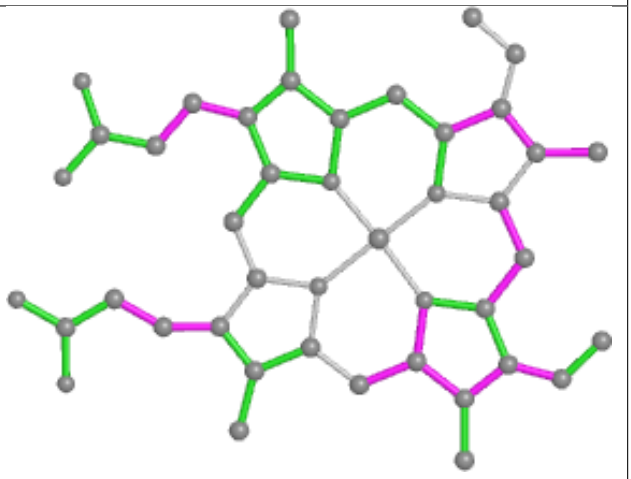


Rings

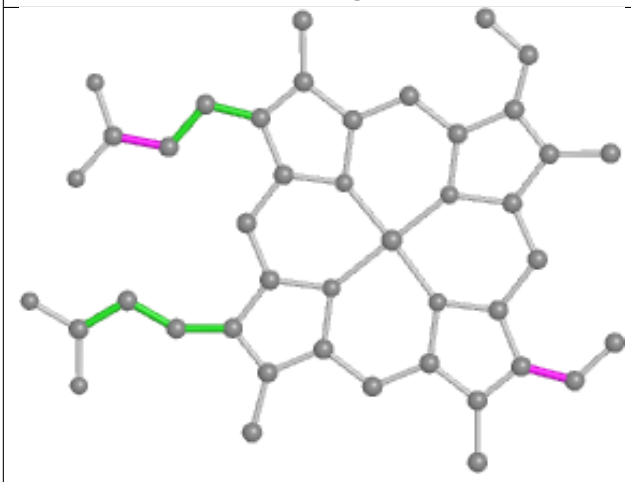
Ligand HEM e 102



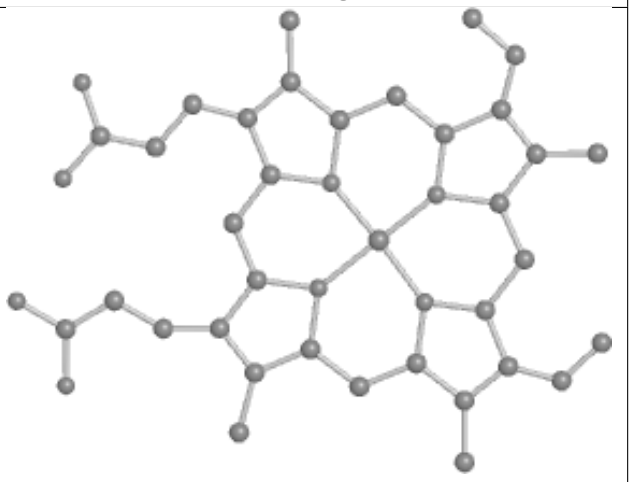
Bond lengths



Bond angles

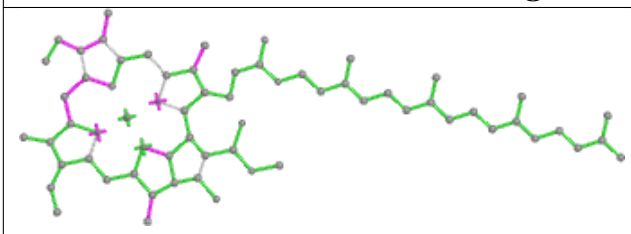


Torsions



Rings

Ligand CLA B 611



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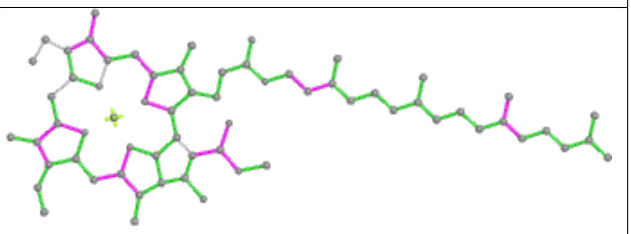
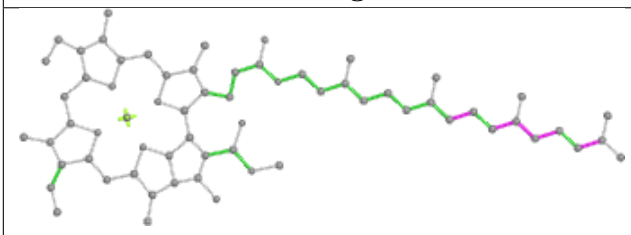


Bond angles



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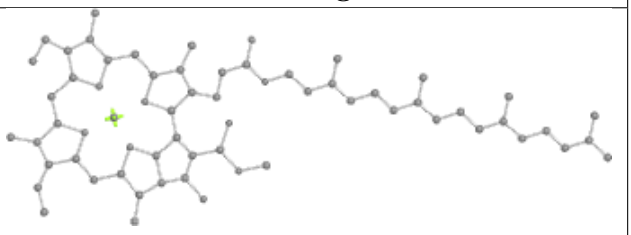
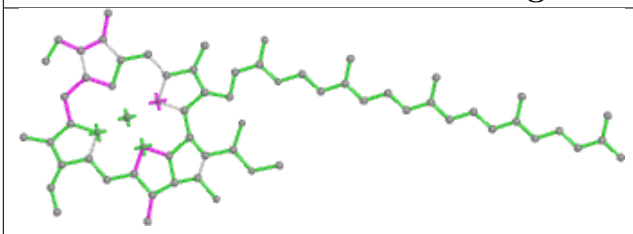


Rings

Ligand CLA b 609



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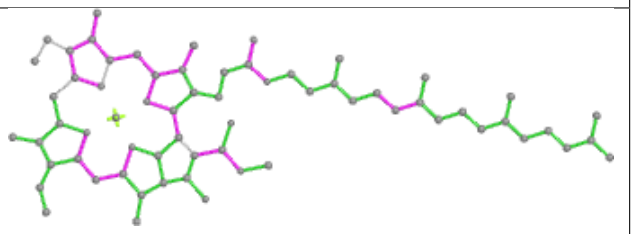
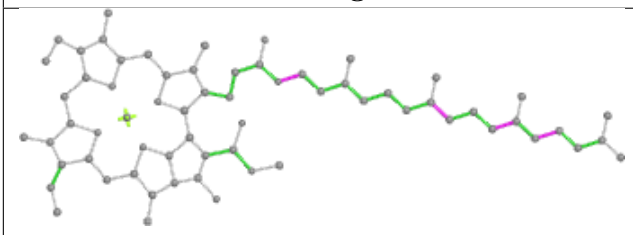
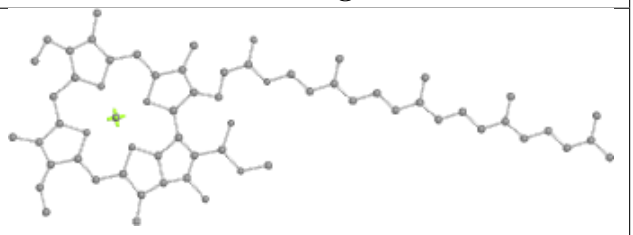


Bond angles

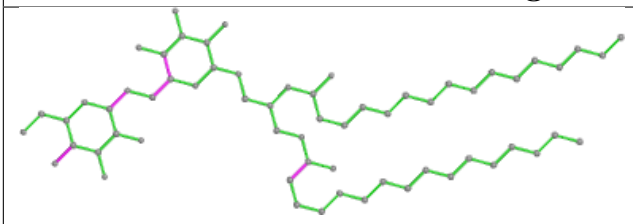


Torsions

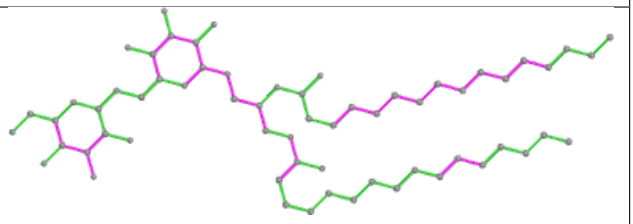


Rings

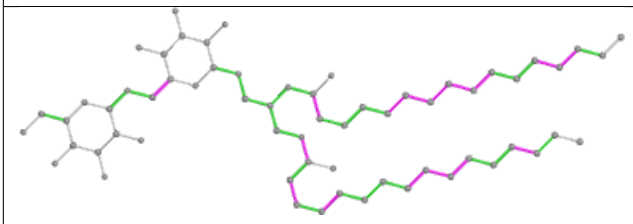
Ligand DGD c 518



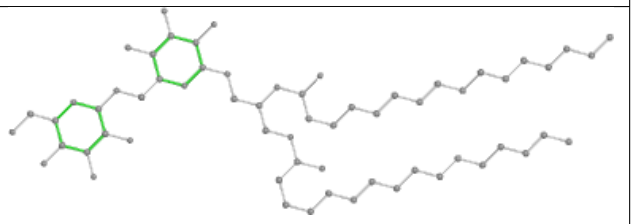
Bond lengths



Bond angles

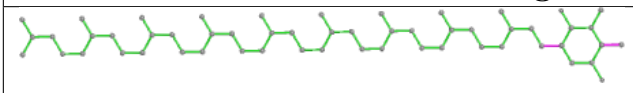


Torsions

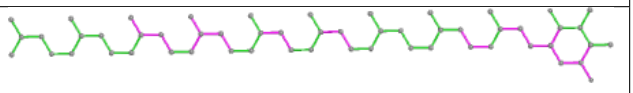


Rings

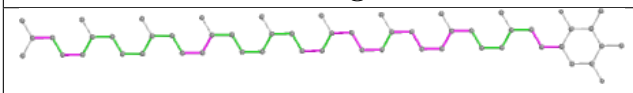
Ligand PL9 a 410



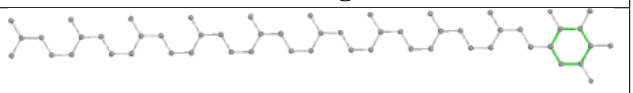
Bond lengths



Bond angles

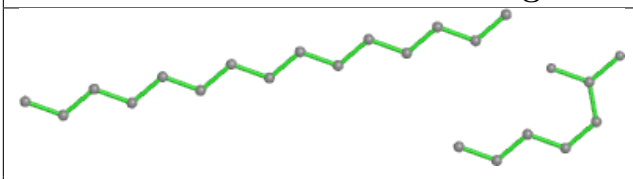


Torsions



Rings

Ligand LMG b 624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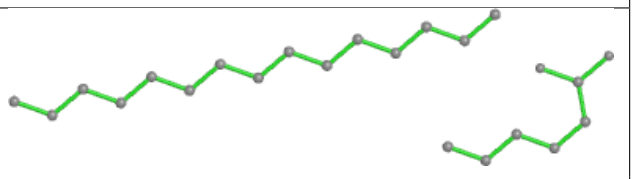
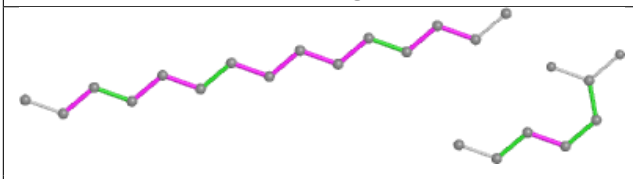
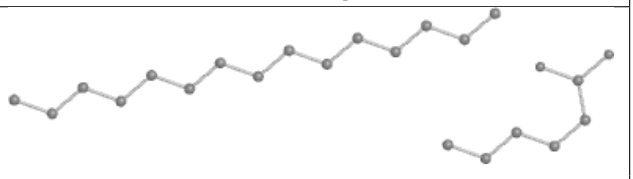
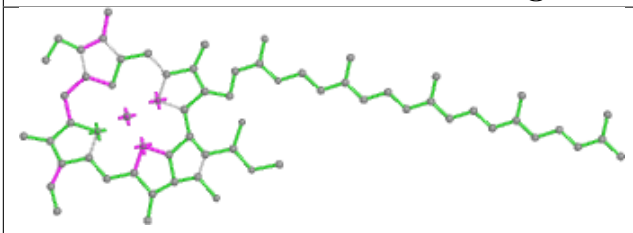
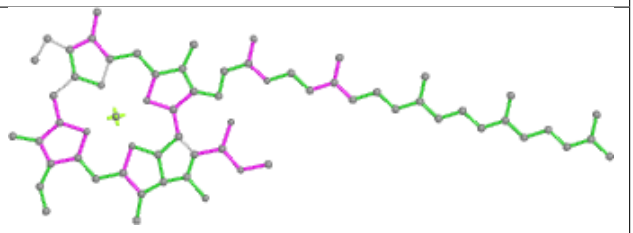

Bond angles

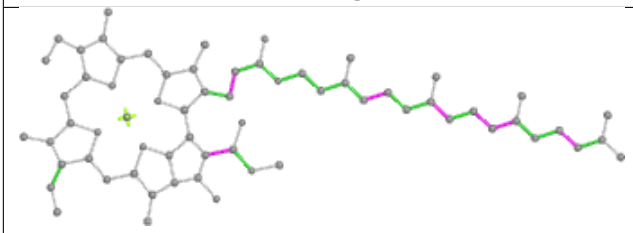

Torsions

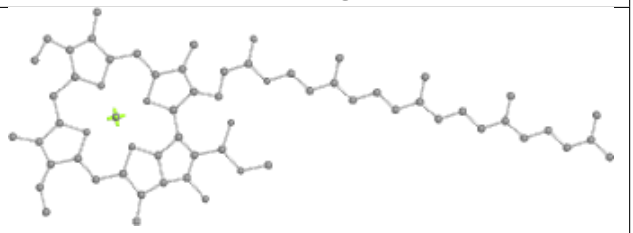

Rings

Ligand CLA b 607

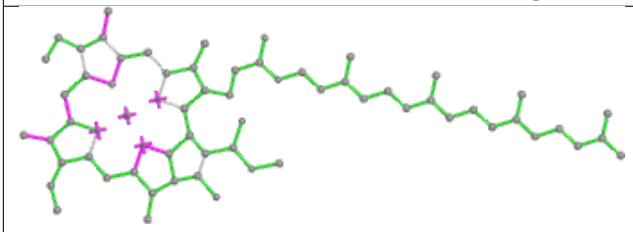

Bond lengths

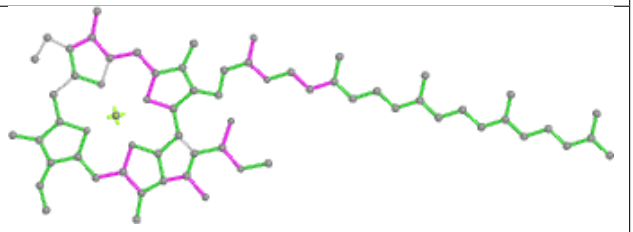

Bond angles

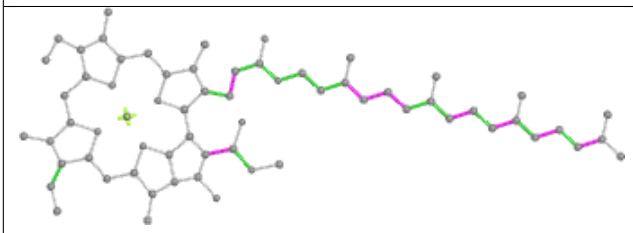

Torsions

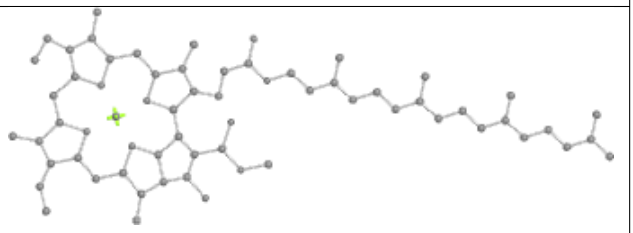

Rings

Ligand CLA b 615

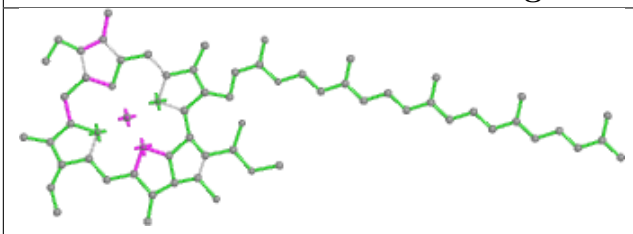

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA C 505



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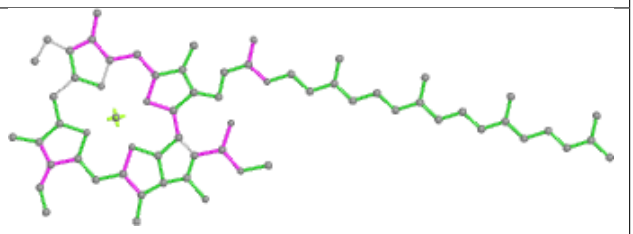
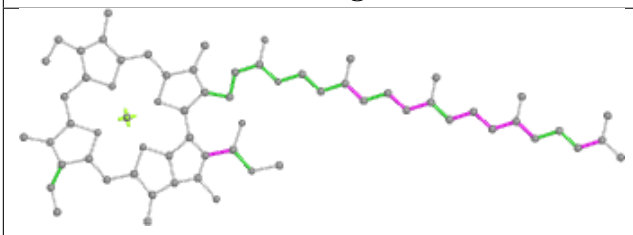


Bond angles



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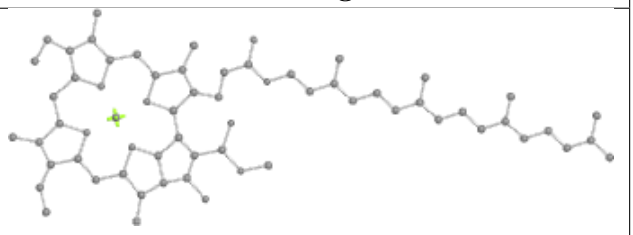
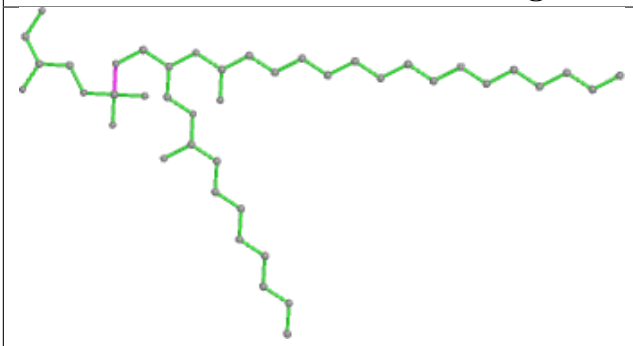


Rings

Ligand LHG e 101



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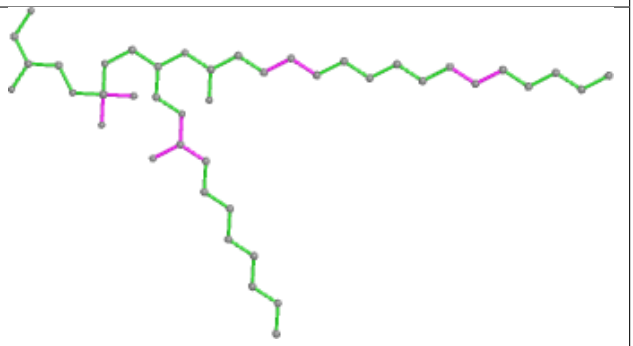
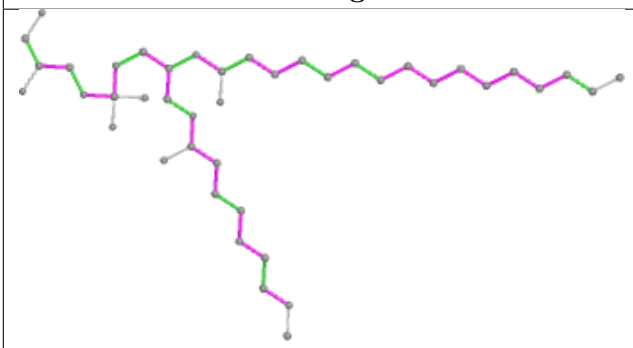


Bond angles



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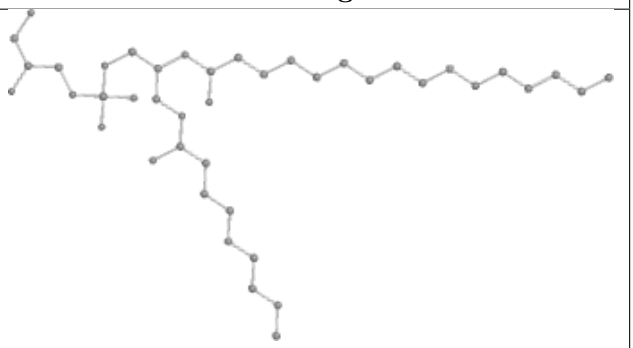
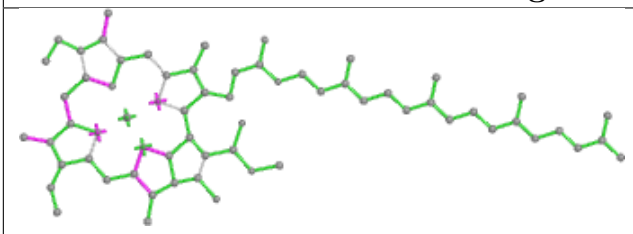


Rings

Ligand CLA a 405



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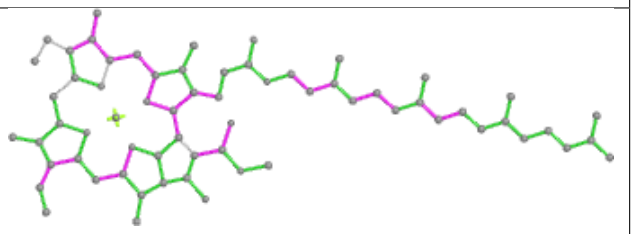
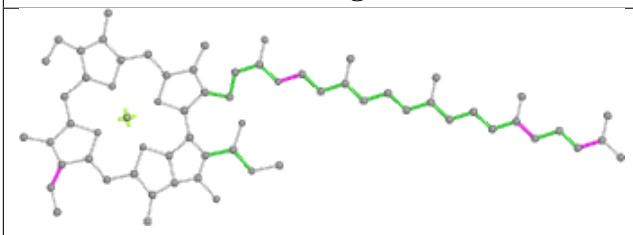


Bond angles



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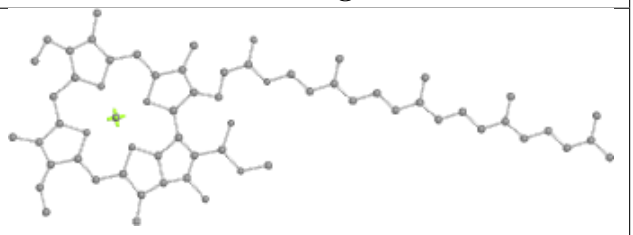
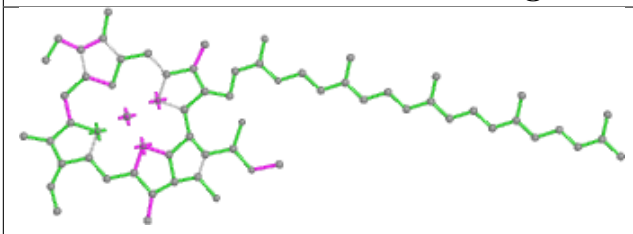


Rings

Ligand CLA B 608



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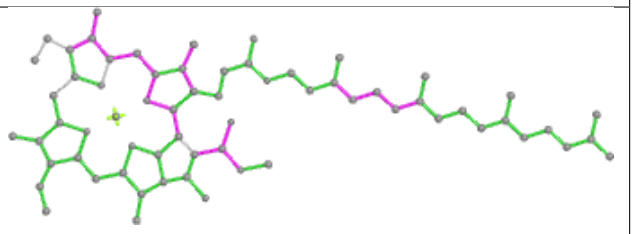
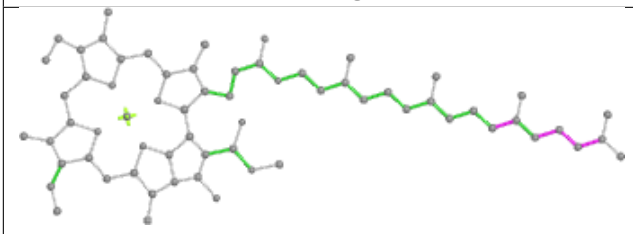


Bond angles



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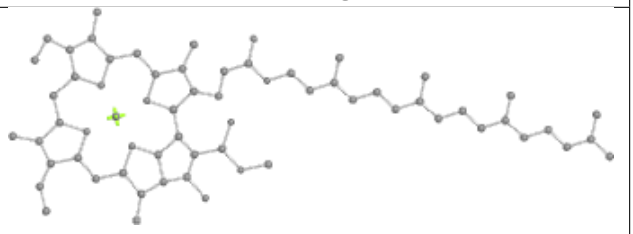
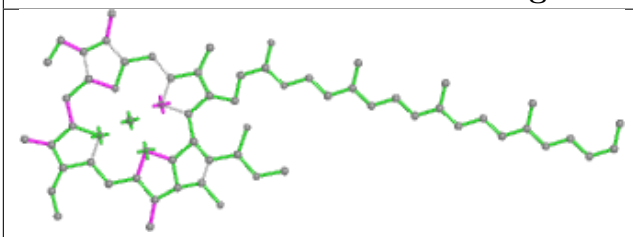


Rings

Ligand CLA c 508



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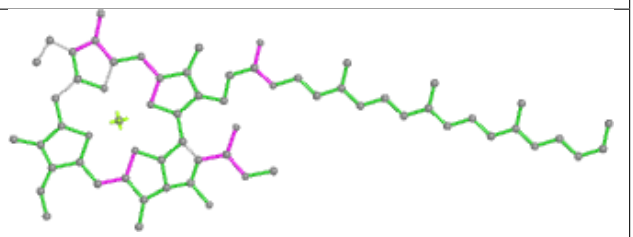
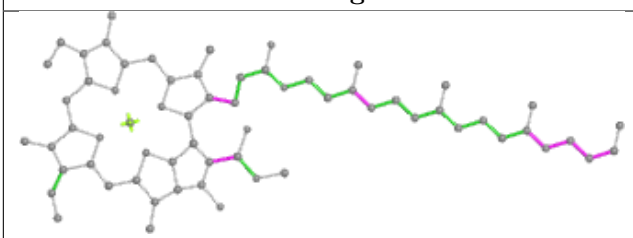


Bond angles



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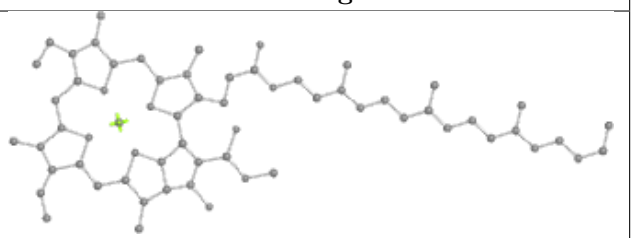
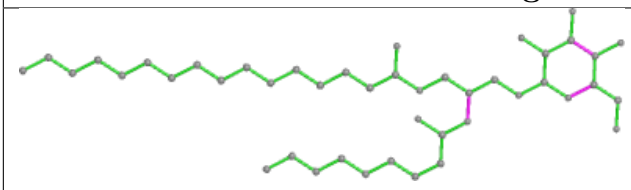


Rings

Ligand LMG d 410



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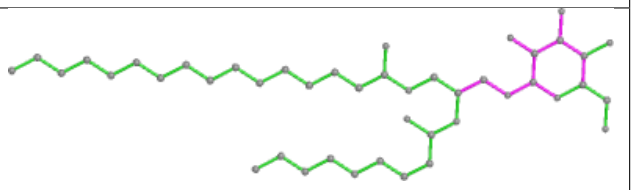
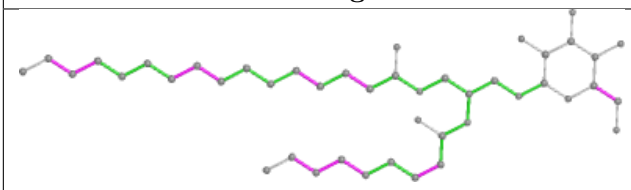
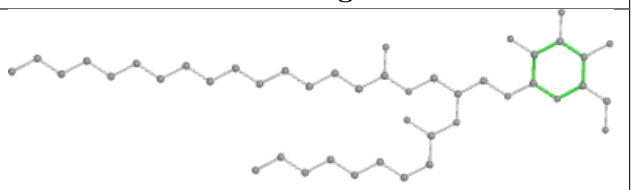


Bond angles

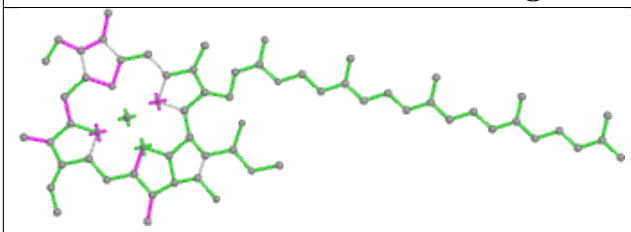


Torsions

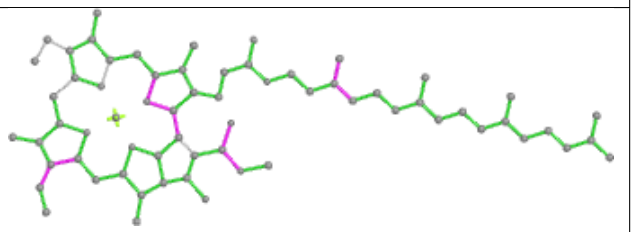


Rings

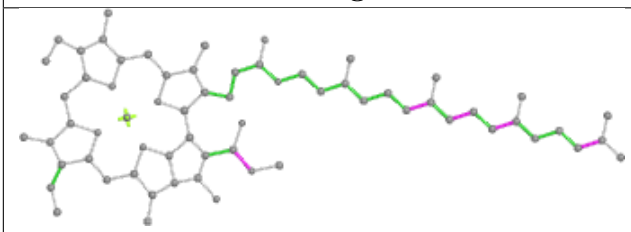
Ligand CLA C 511



Bond lengths



Bond angles



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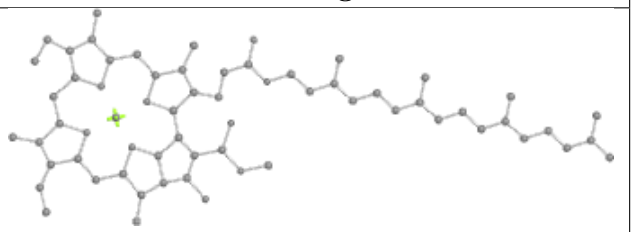
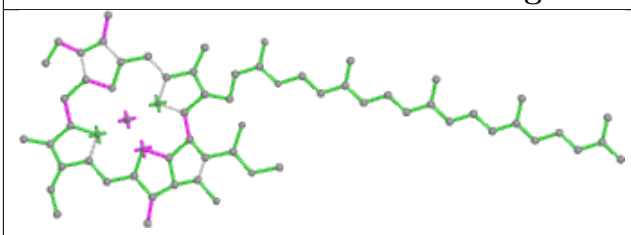


Rings

Ligand CLA C 512



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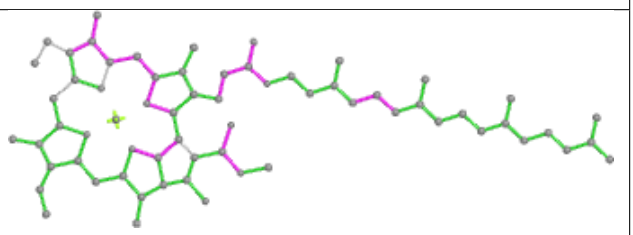
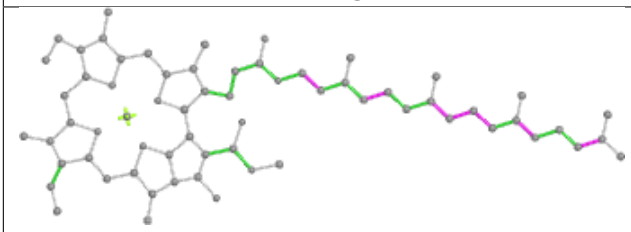


Bond angles



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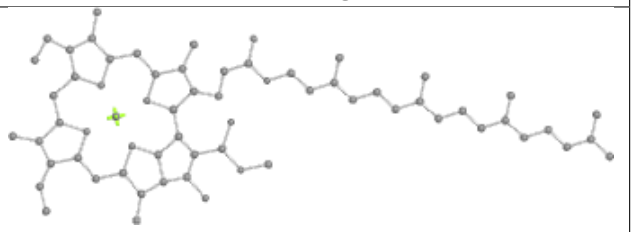
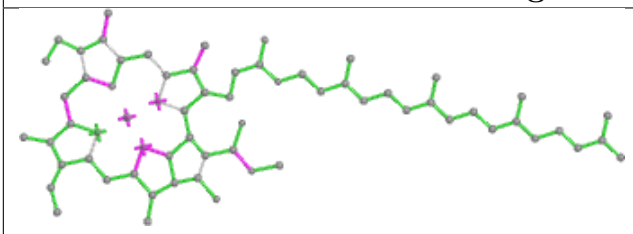


Rings

Ligand CLA b 610



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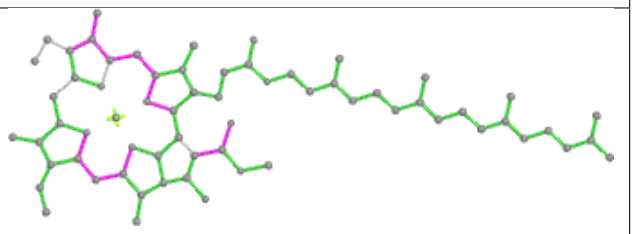
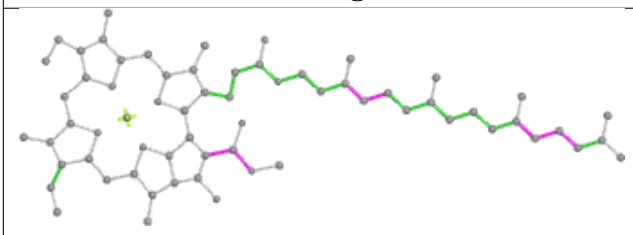


Bond angles



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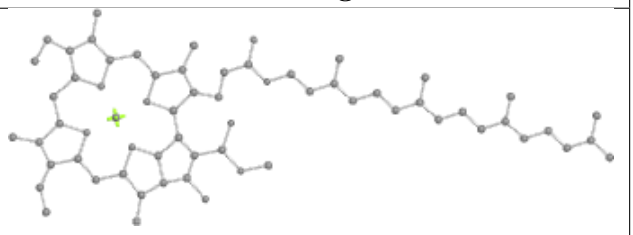
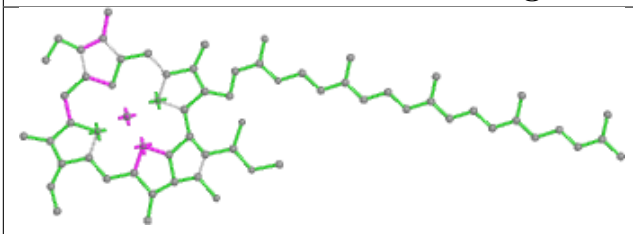


Rings

Ligand CLA D 403



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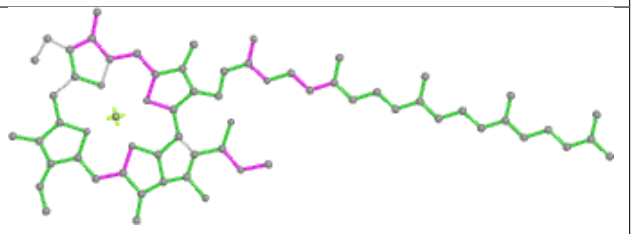
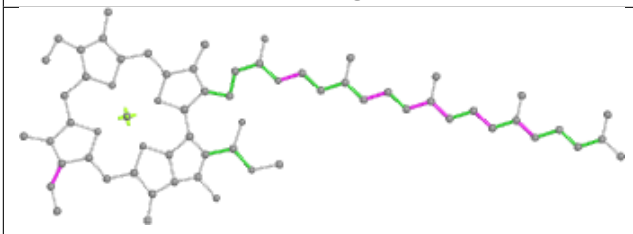
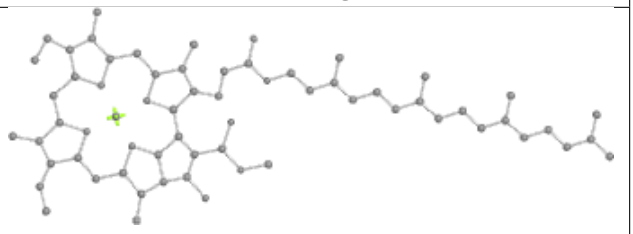


Bond angles

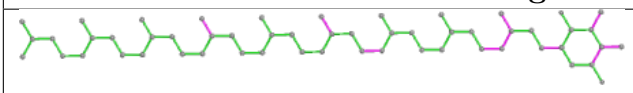


Torsions



Rings

Ligand PL9 D 406



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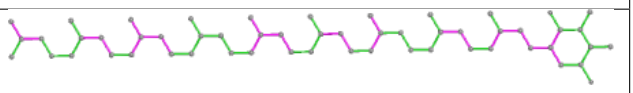
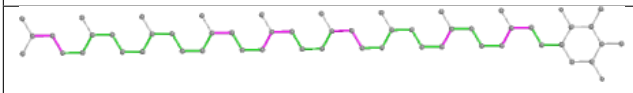
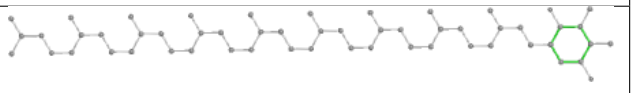


Bond angles

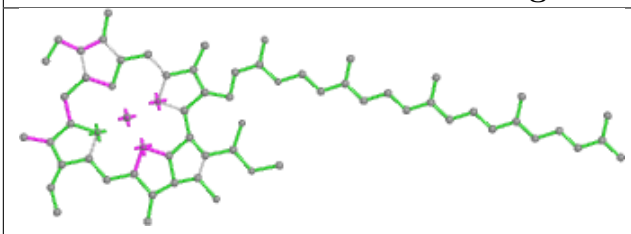


Torsions

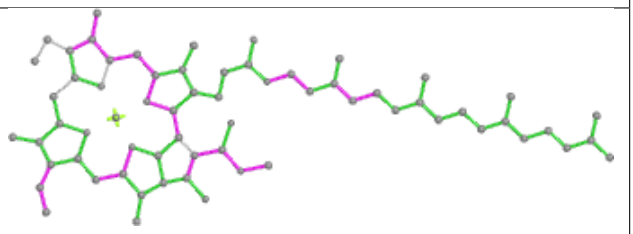


Rings

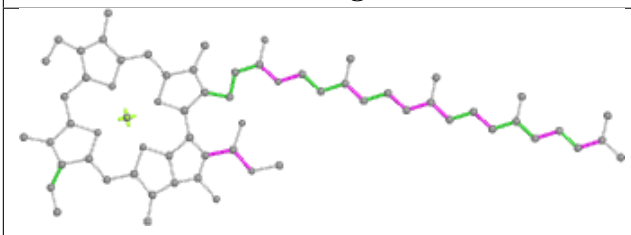
Ligand CLA c 506



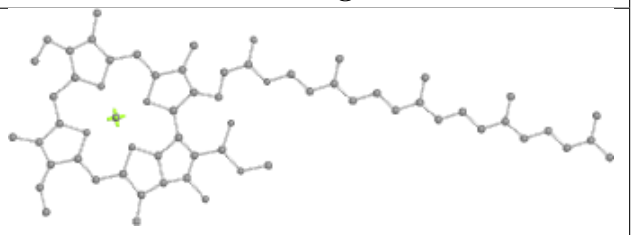
Bond lengths



Bond angles

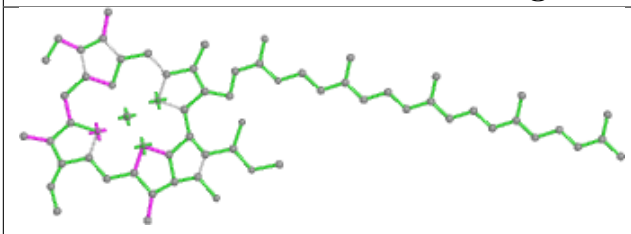


Torsions



Rings

Ligand CLA c 512



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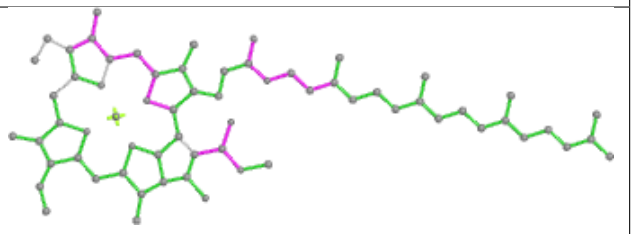
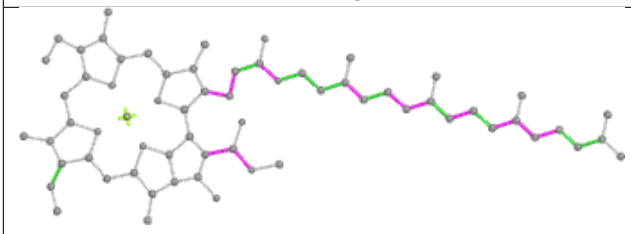


Bond angles



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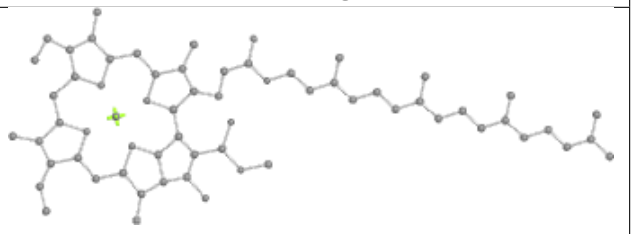
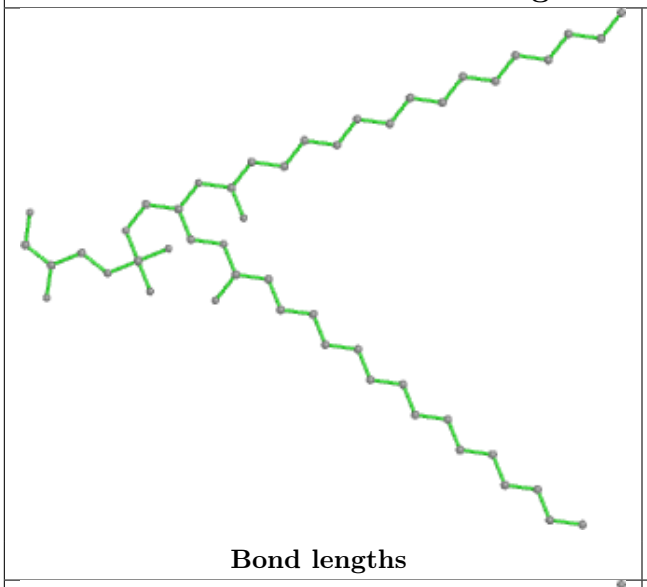


Rings

Ligand LHG l 101



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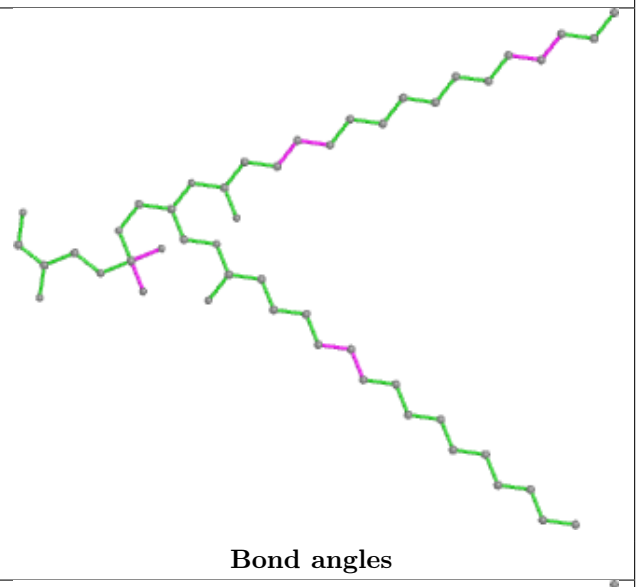
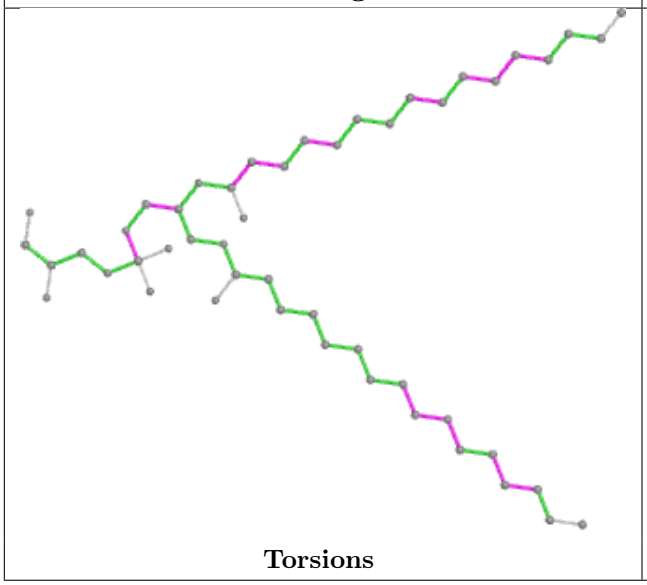


Bond angles



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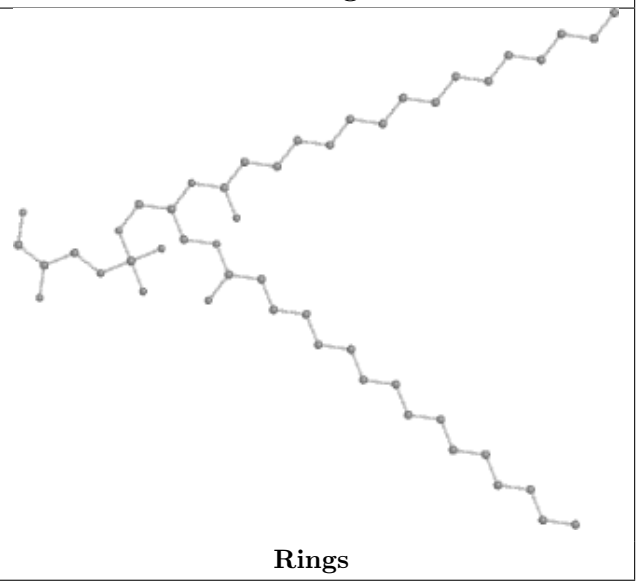
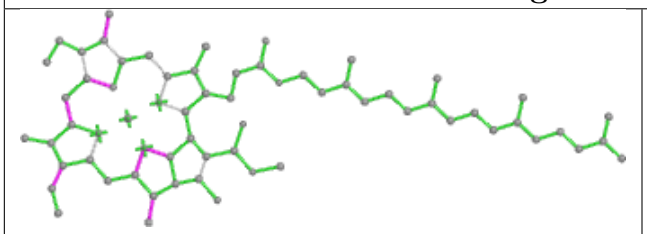


Rings

Ligand CLA c 501



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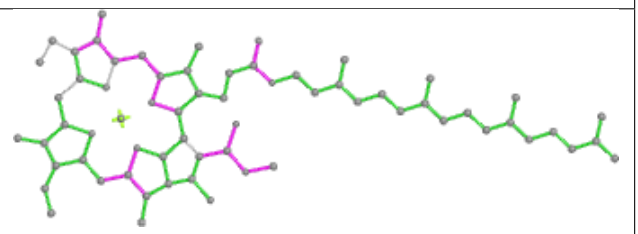
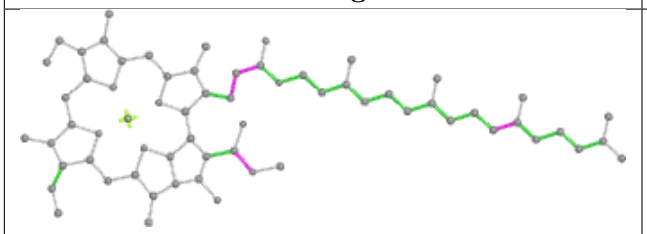


Bond angles



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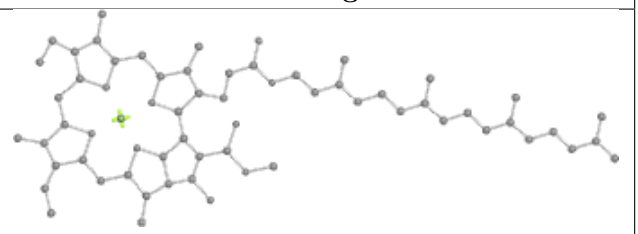
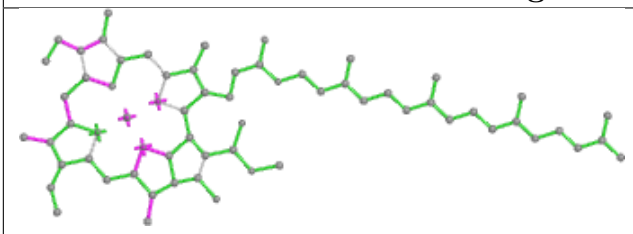


Rings

Ligand CLA d 404



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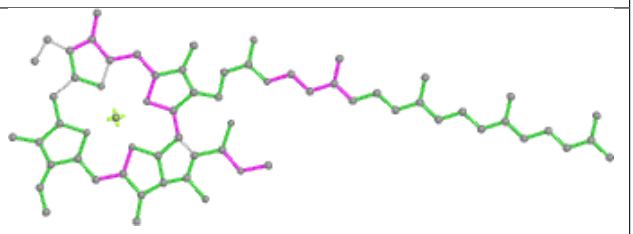
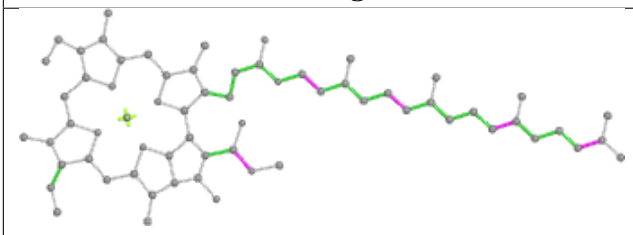


Bond angles



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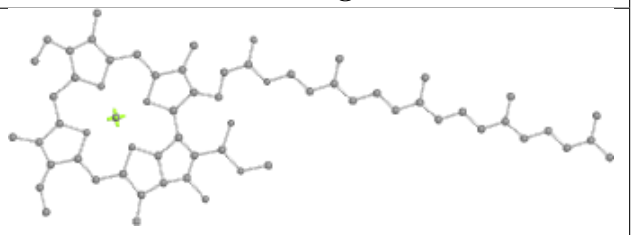
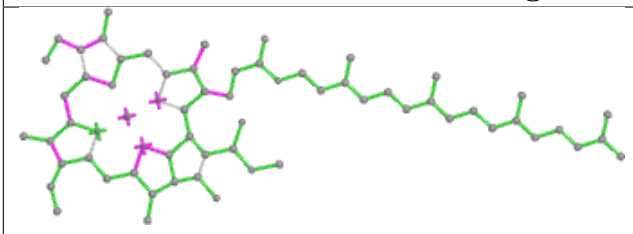


Rings

Ligand CLA B 604



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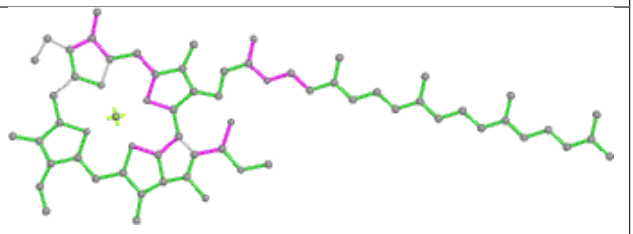
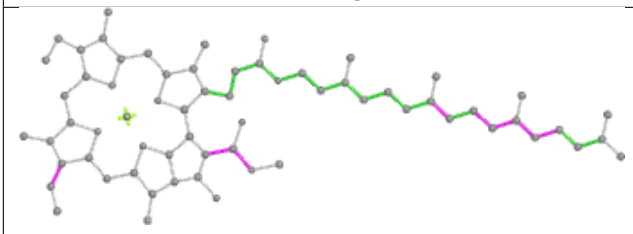


Bond angles



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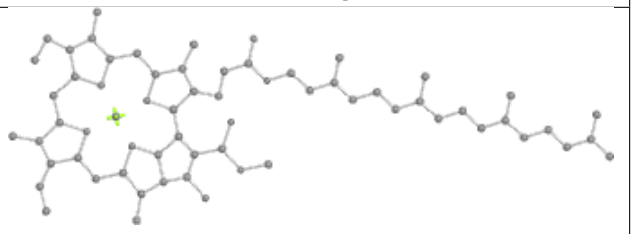
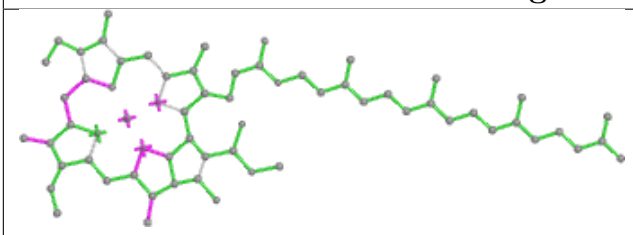


Rings

Ligand CLA c 502



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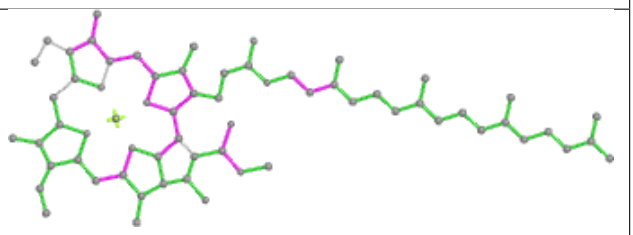
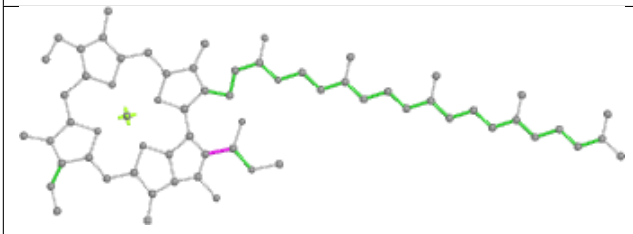


Bond angles



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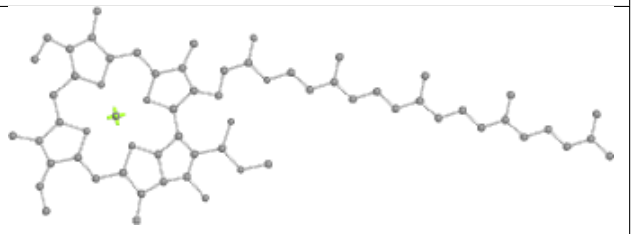
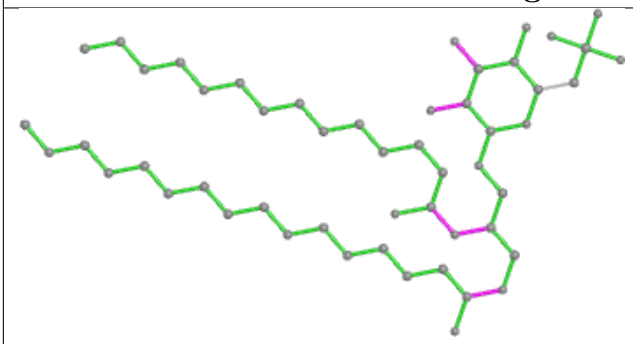


Rings

Ligand SQD A 412



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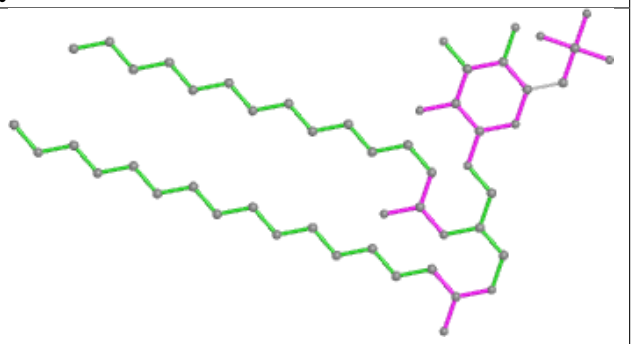
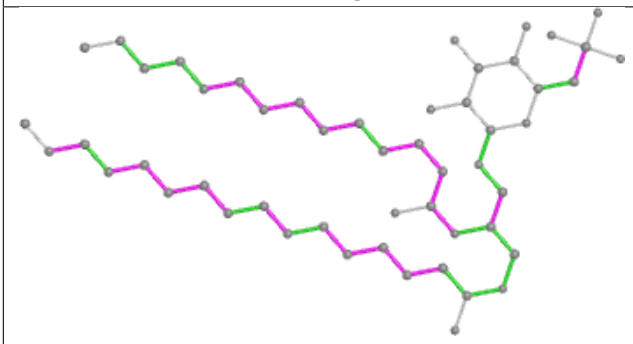


Bond angles



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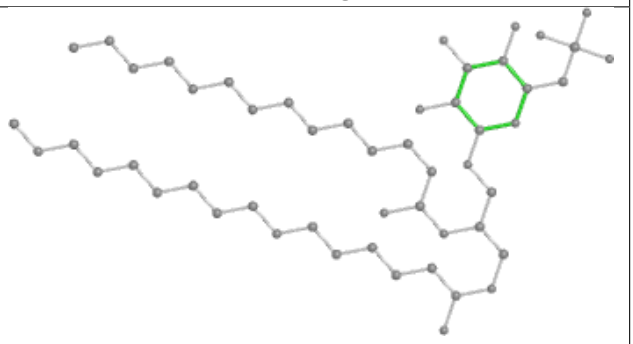
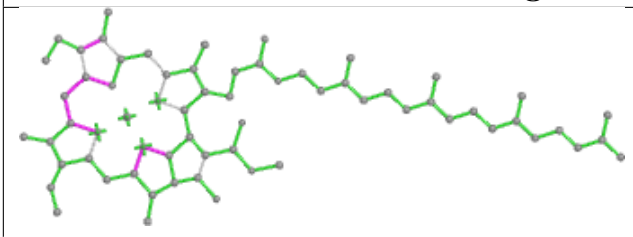


Rings

Ligand CLA B 605



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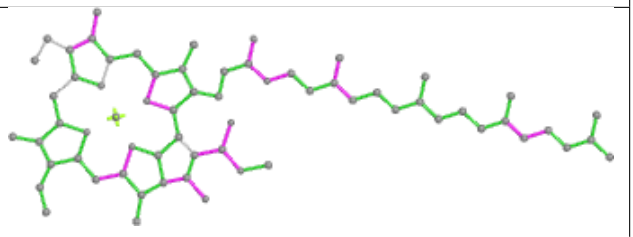
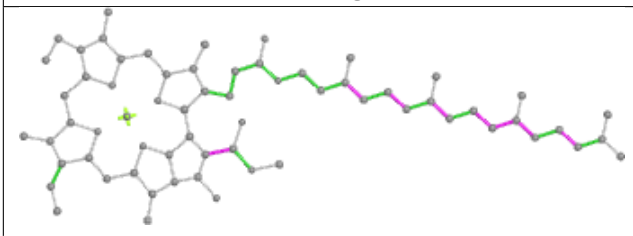


Bond angles



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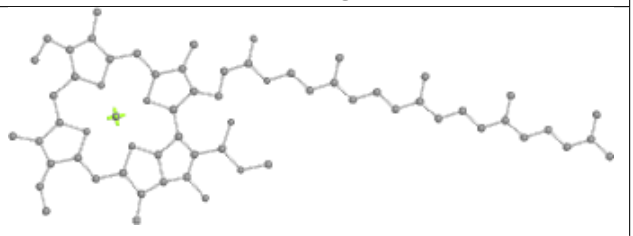
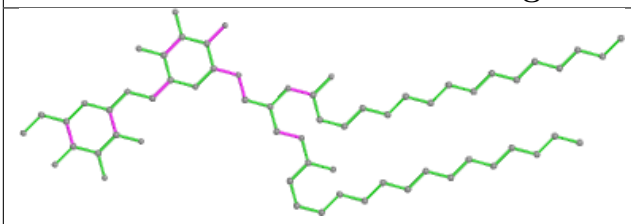


Rings

Ligand DGD h 102



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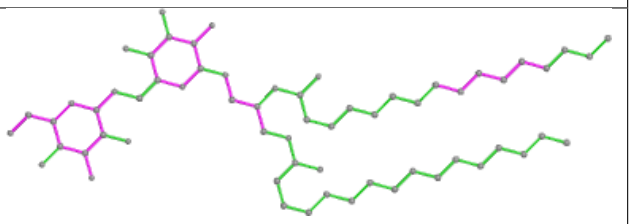

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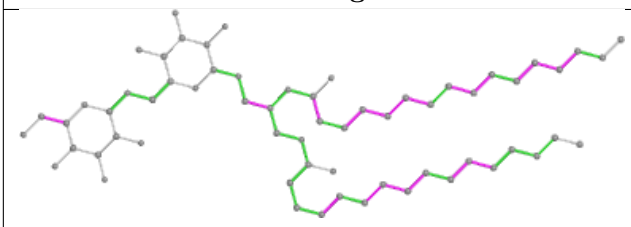

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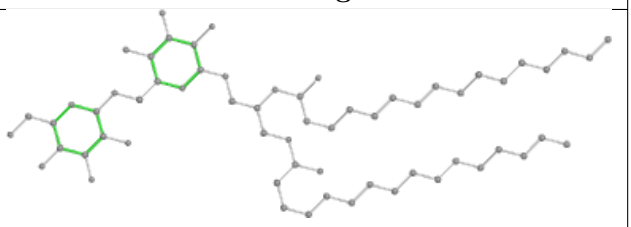
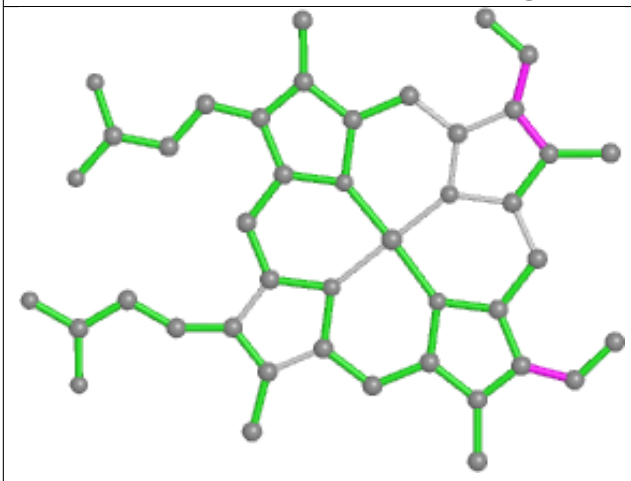


Rings

Ligand HEM F 101



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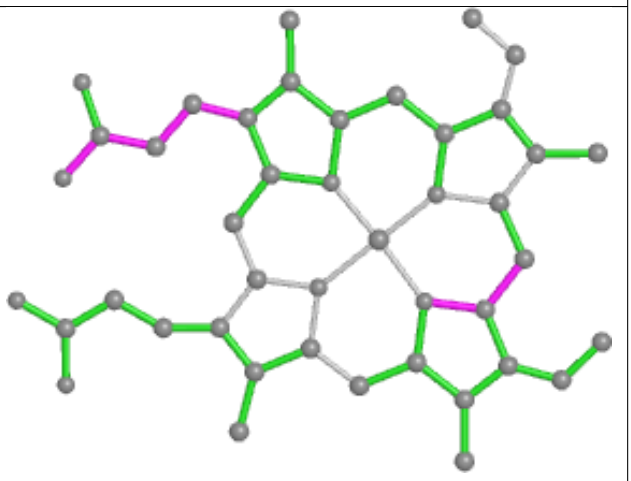
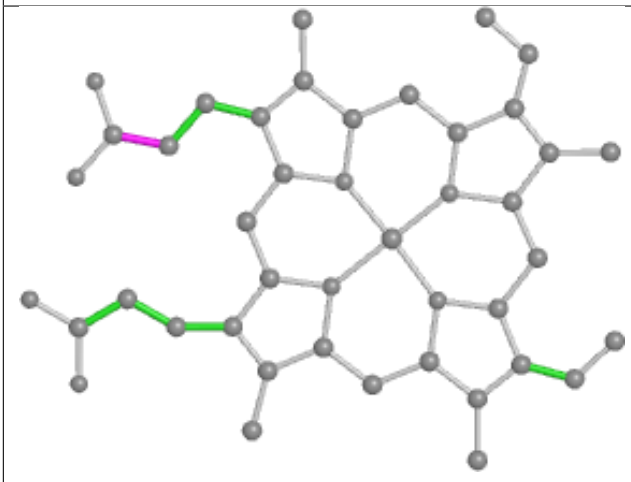


Bond angles



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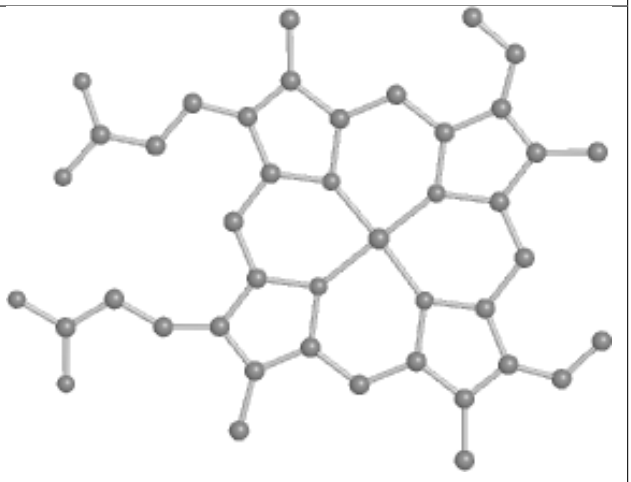
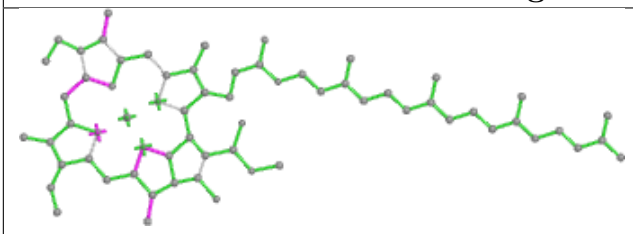


Rings

Ligand CLA b 614



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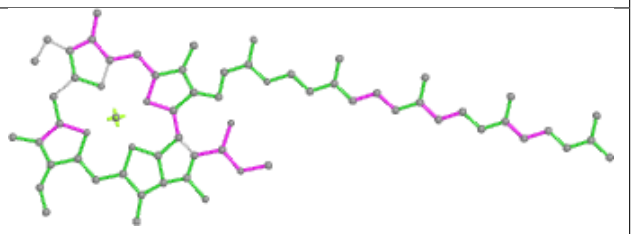
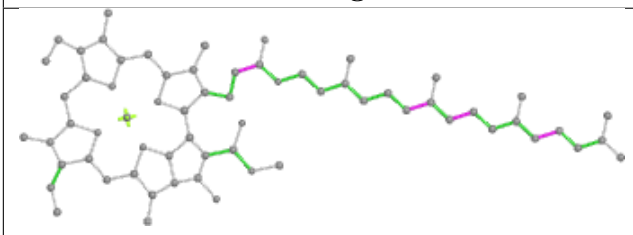
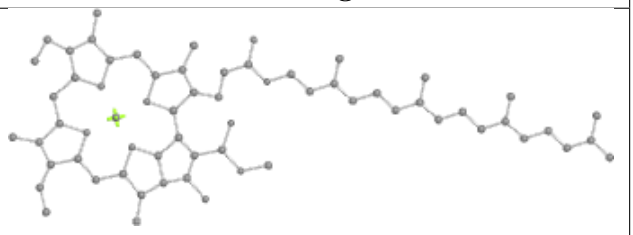


Bond angles

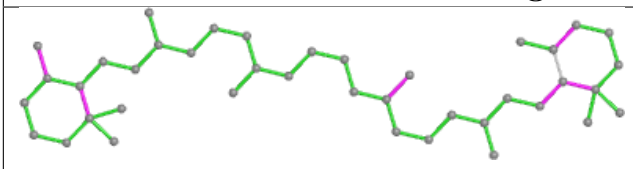


Torsions



Rings

Ligand 8CT C 515



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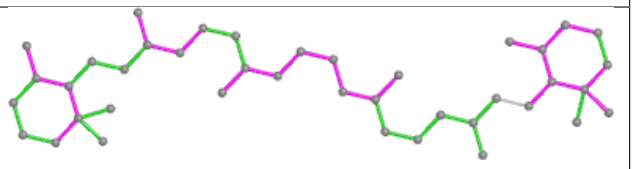
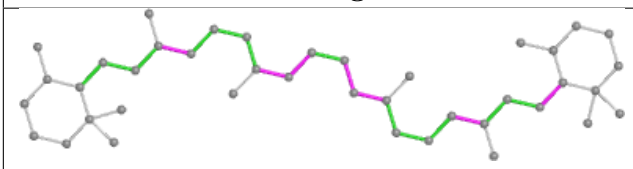
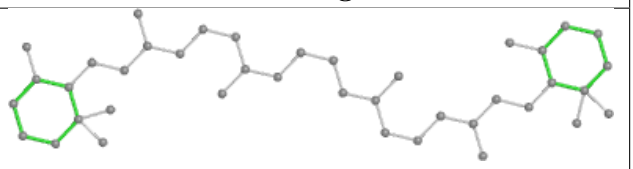


Bond angles

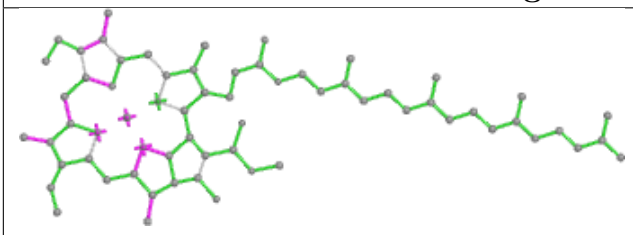


Torsions

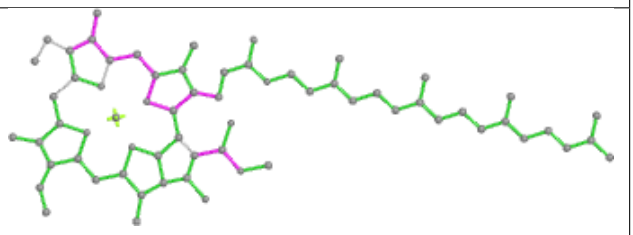


Rings

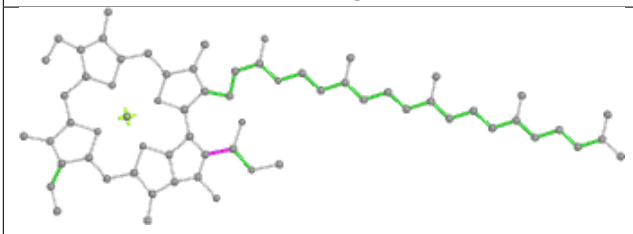
Ligand CLA A 411



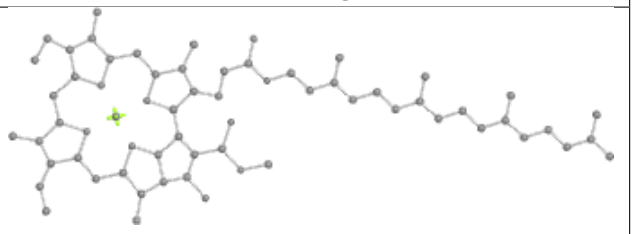
Bond lengths



Bond angles

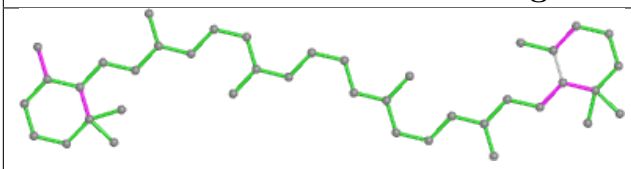


Torsions

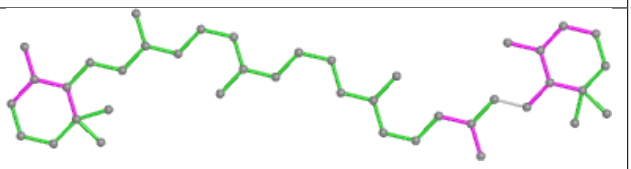


Rings

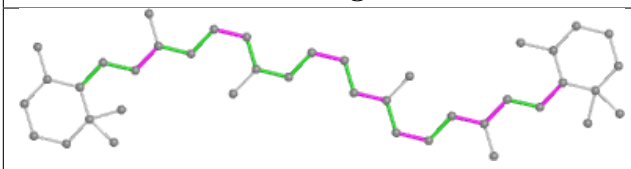
Ligand 8CT d 405



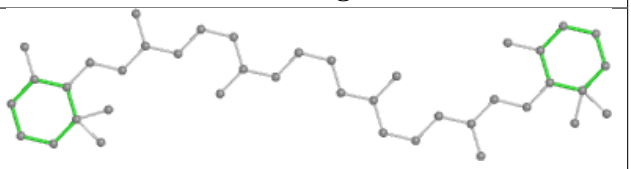
Bond lengths



Bond angles

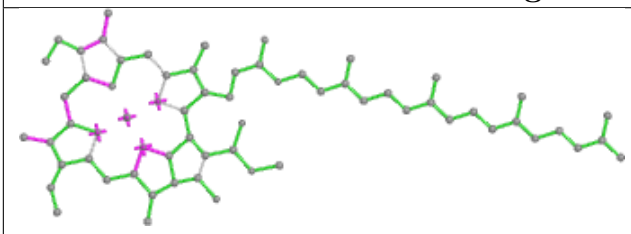


Torsions



Rings

Ligand CLA B 606



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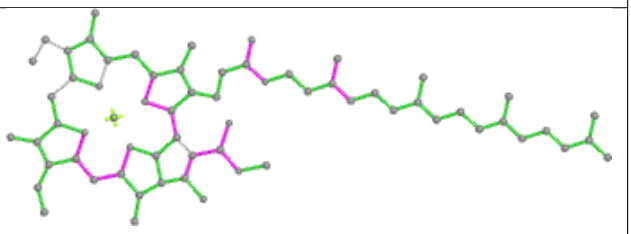
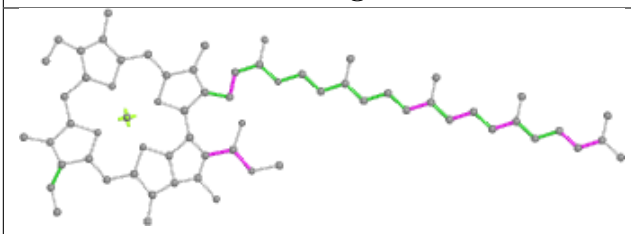
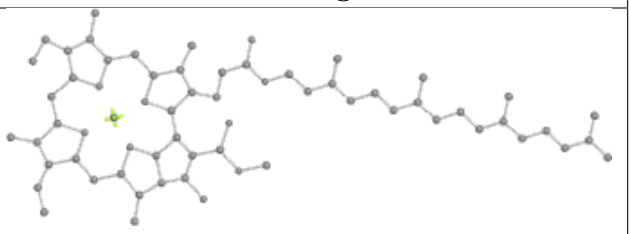


Bond angles

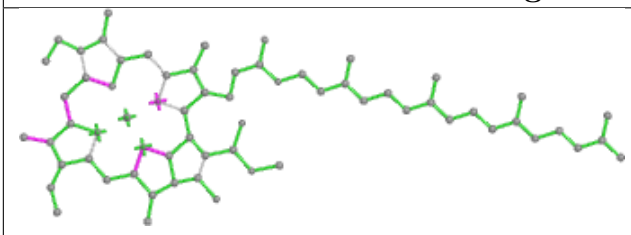


Torsions



Rings

Ligand CLA B 612



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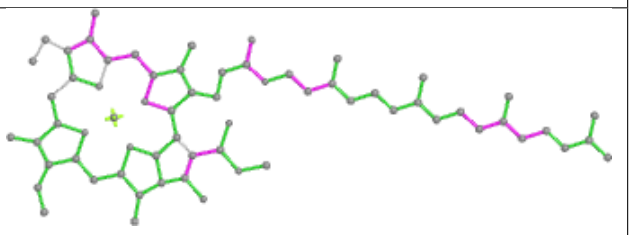
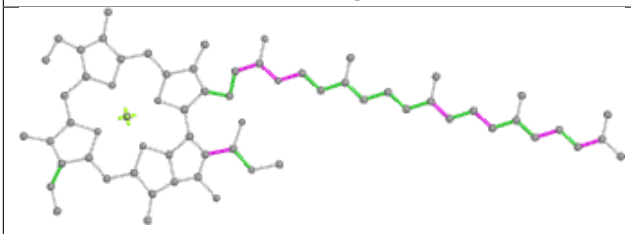


Bond angles



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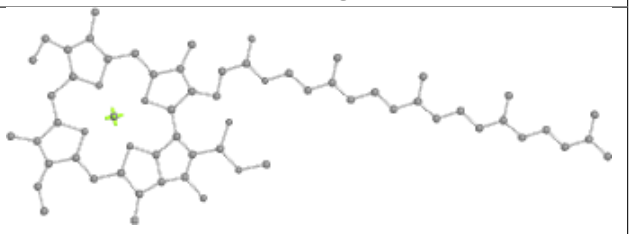
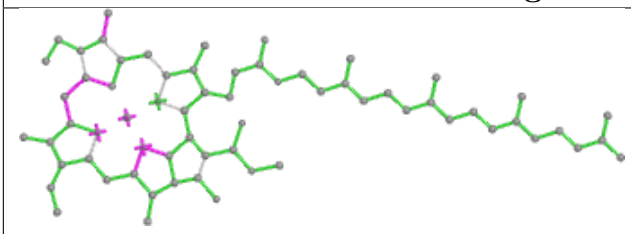


Rings

Ligand CLA B 602



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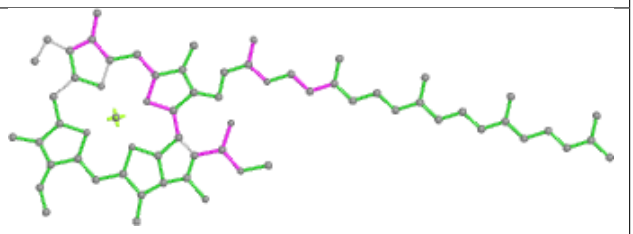
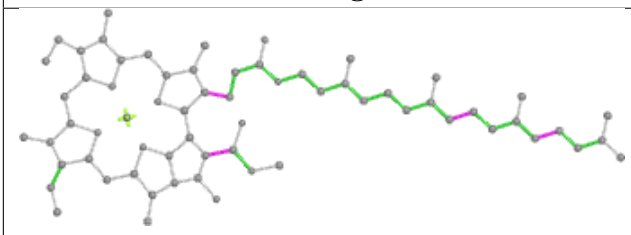


Bond angles



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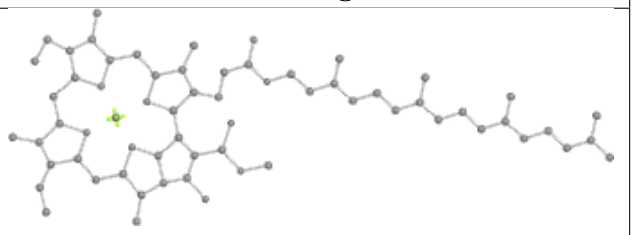
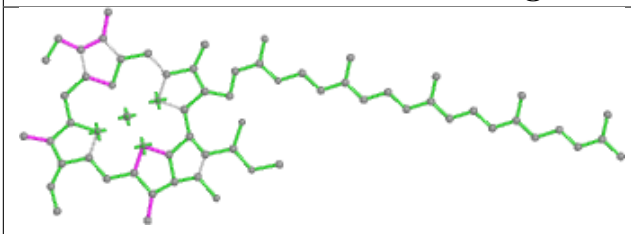


Rings

Ligand CLA B 603



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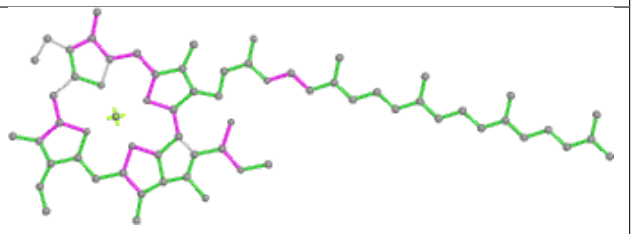
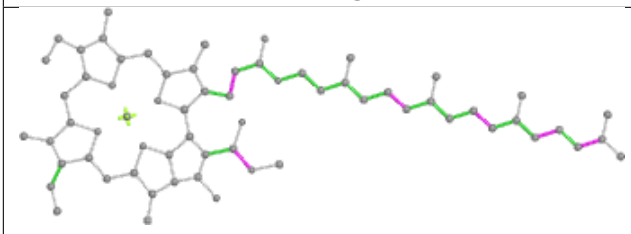


Bond angles



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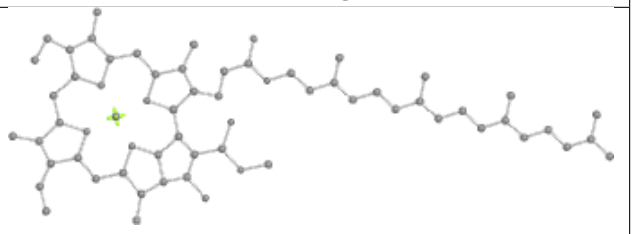
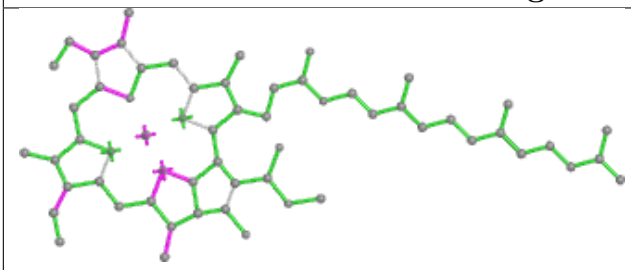


Rings

Ligand CLA b 617



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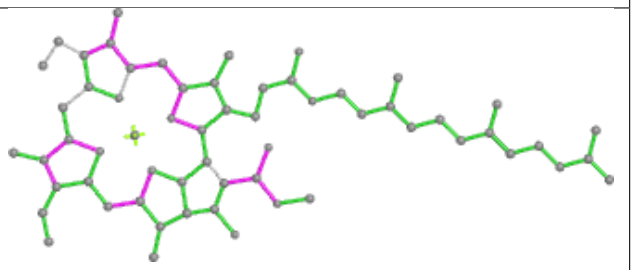
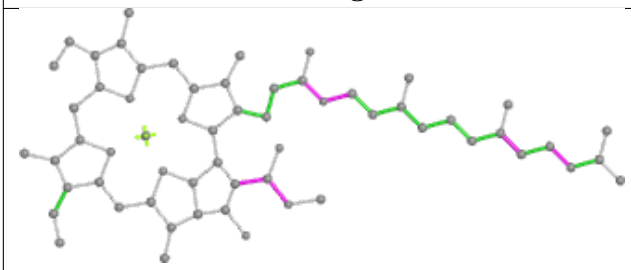


Bond angles



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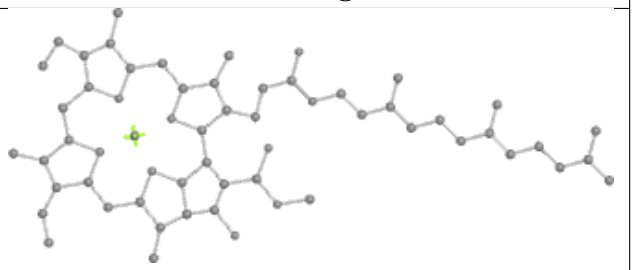
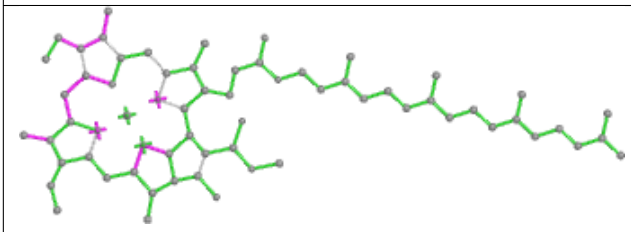


Rings

Ligand CLA c 507



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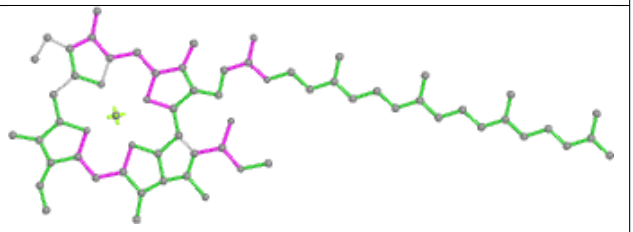
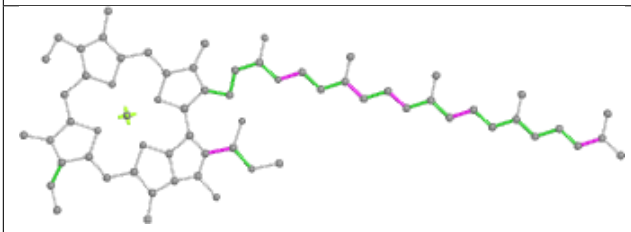


Bond angles



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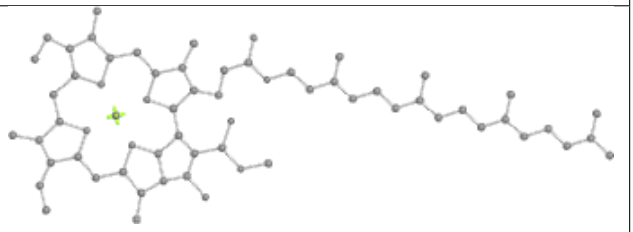
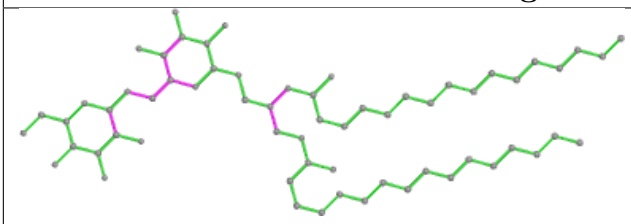
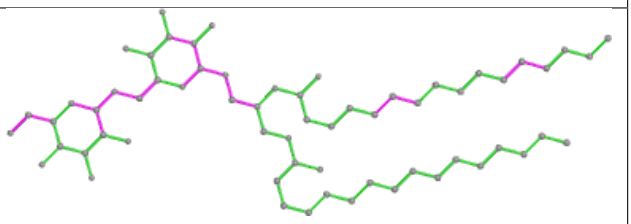


Rings

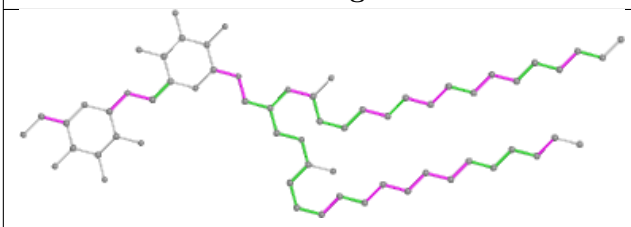
Ligand DGD C 517



Bond lengths



Bond angles



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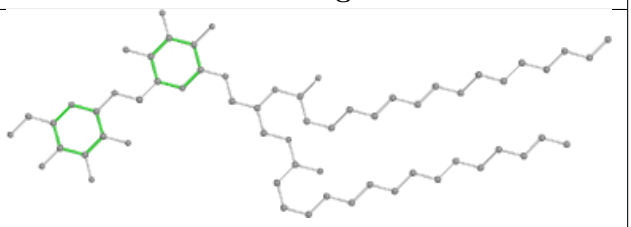
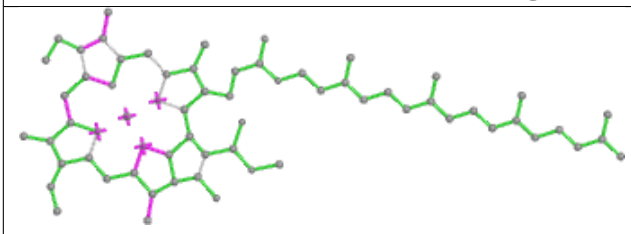


Rings

Ligand CLA C 507



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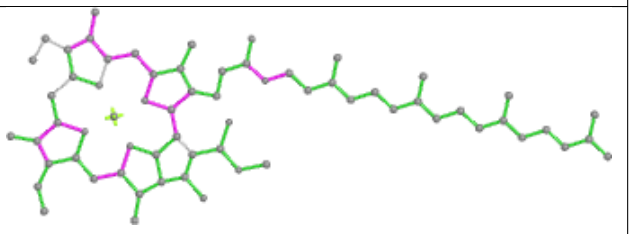
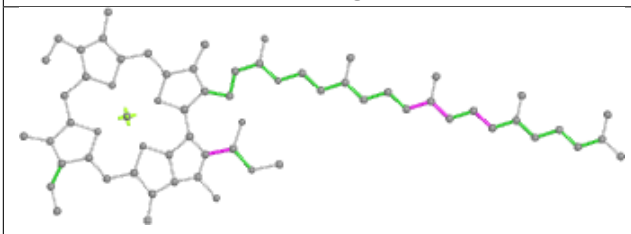
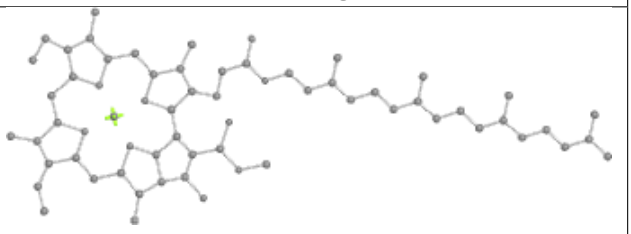


Bond angles

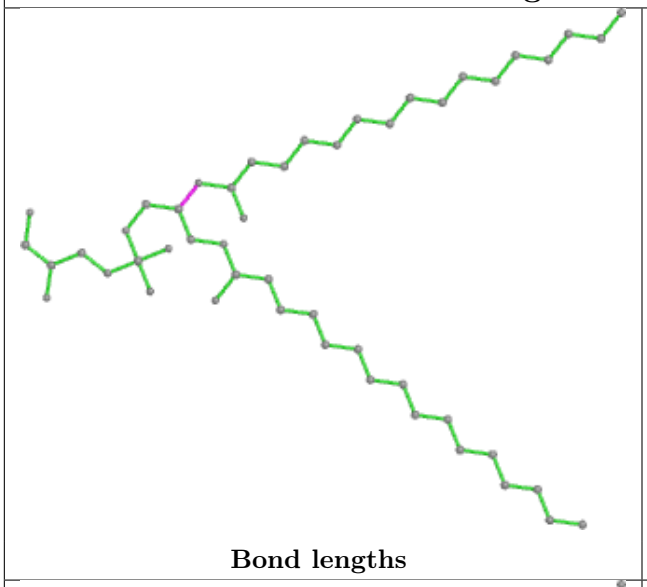


Torsions



Rings

Ligand LHG B 623



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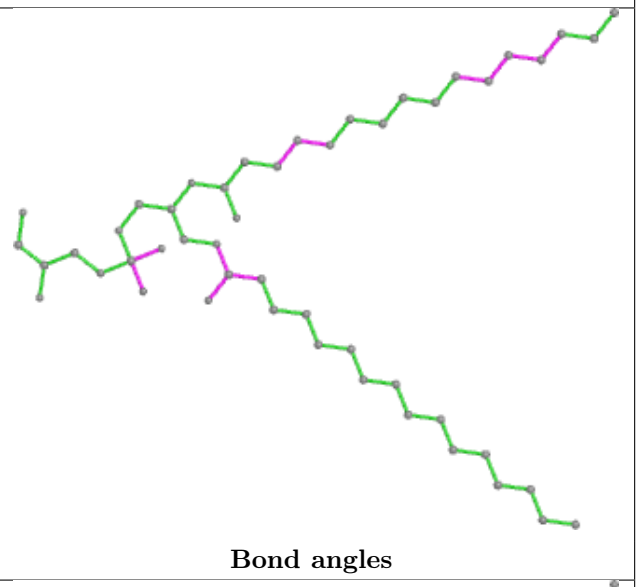
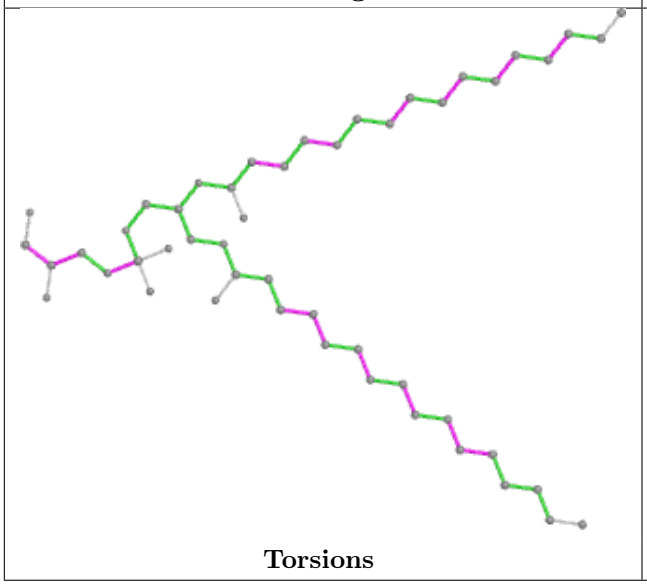


Bond angles



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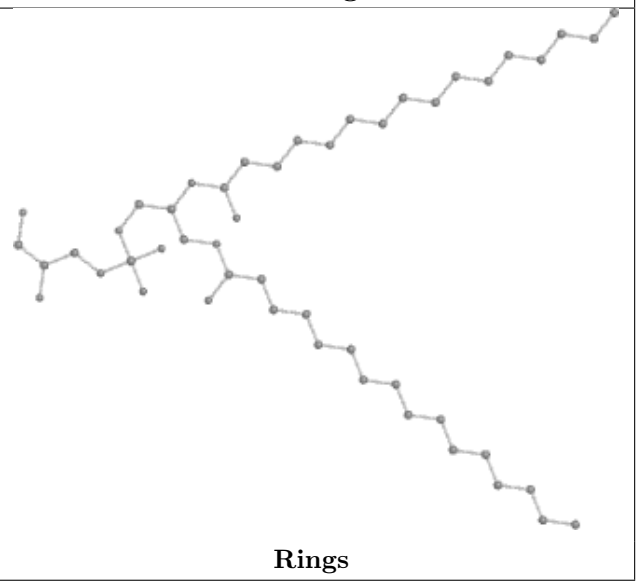
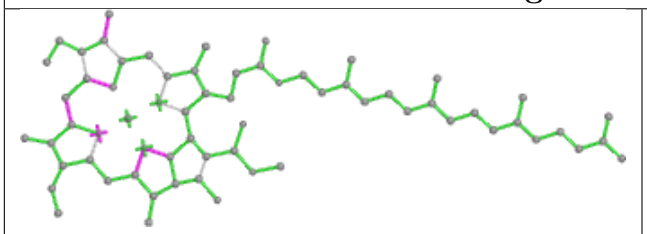


Rings

Ligand CLA C 510



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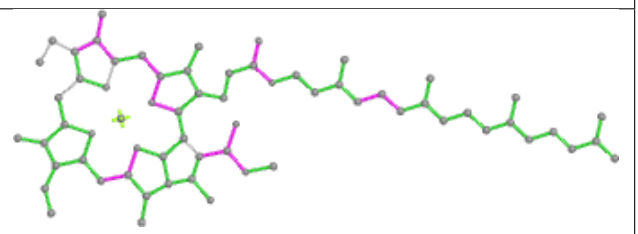
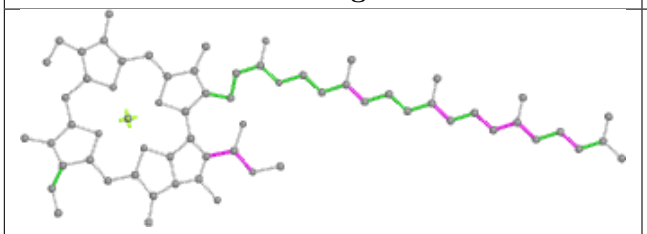


Bond angles



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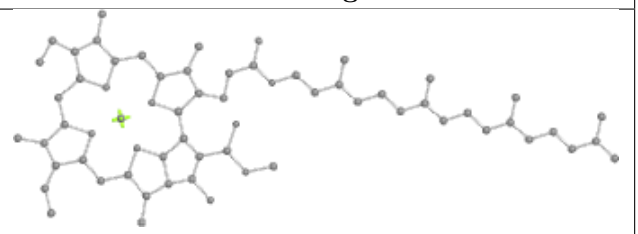
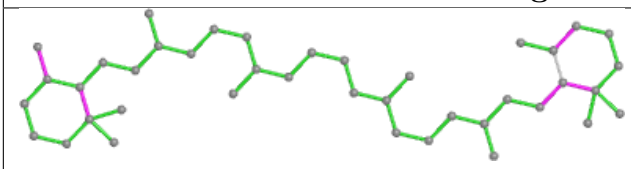


Rings

Ligand 8CT k 101



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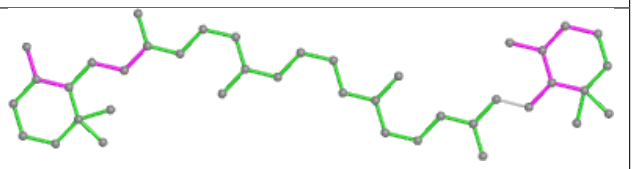
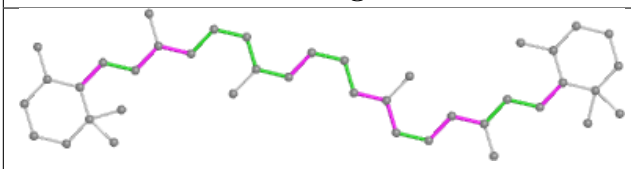
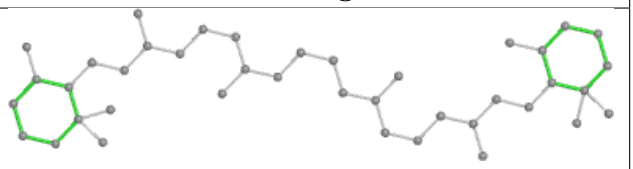


Bond angles

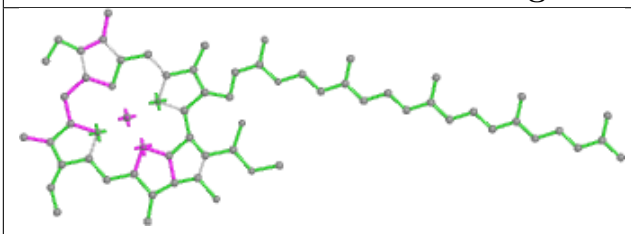


Torsions

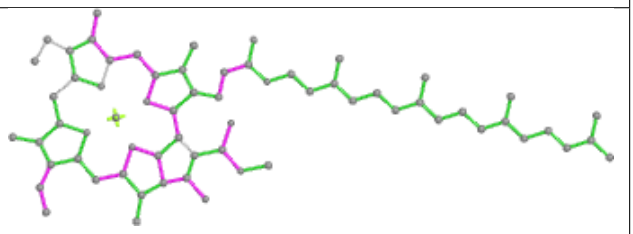


Rings

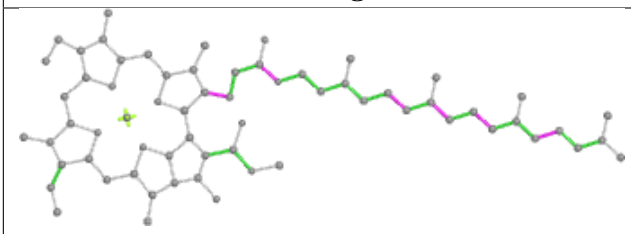
Ligand CLA a 408



Bond lengths



Bond angles



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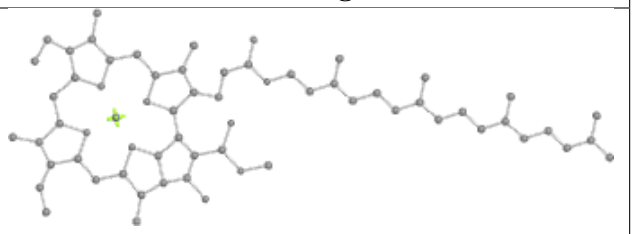
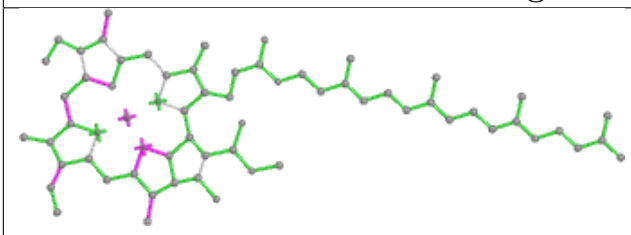
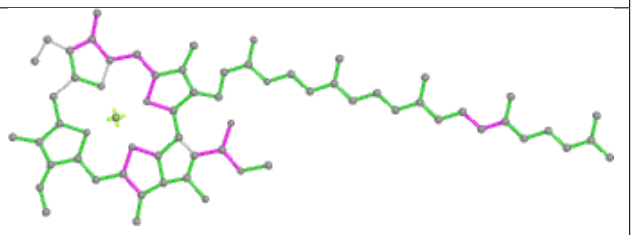


Rings

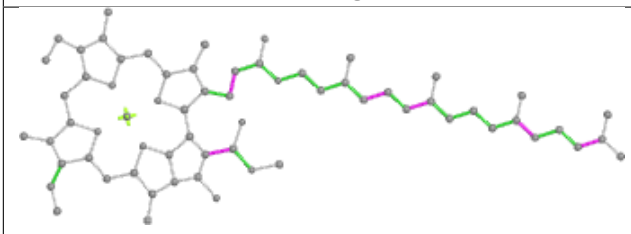
Ligand CLA b 603



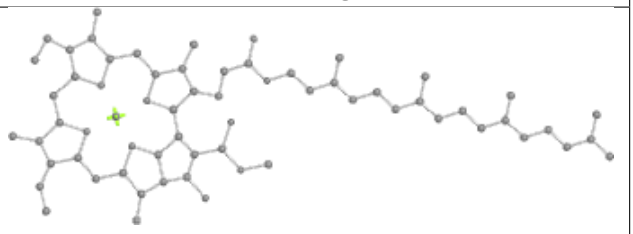
Bond lengths



Bond angles

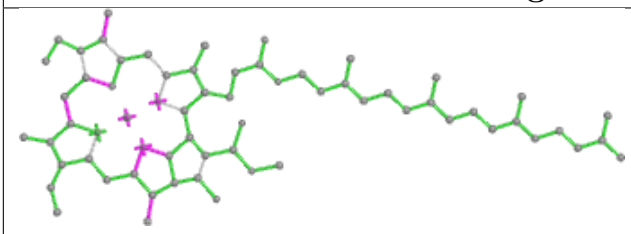


Torsions



Rings

Ligand CLA d 402



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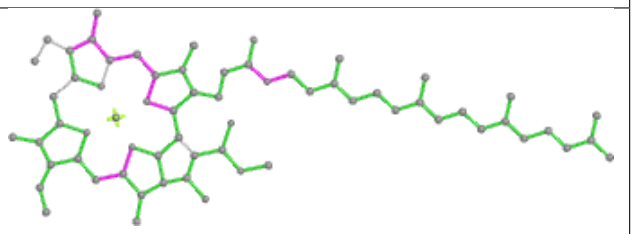
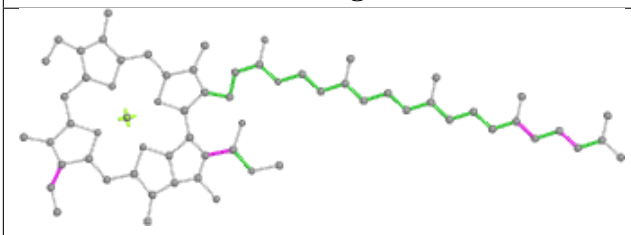


Bond angles



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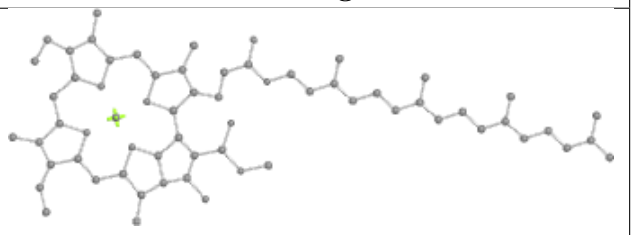
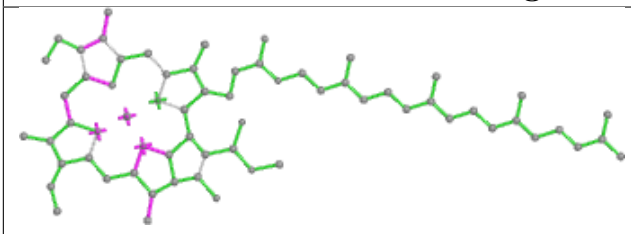


Rings

Ligand CLA D 404



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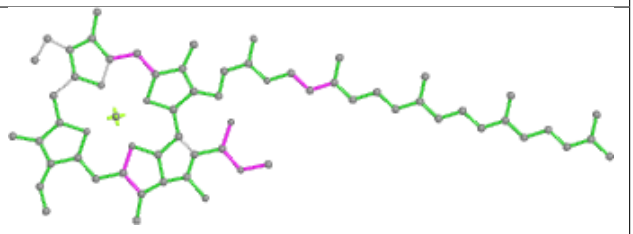
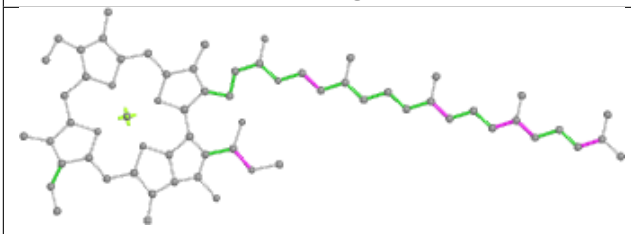


Bond angles



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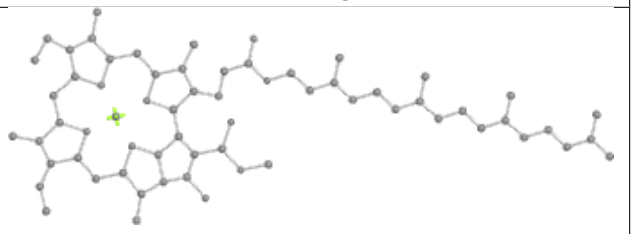
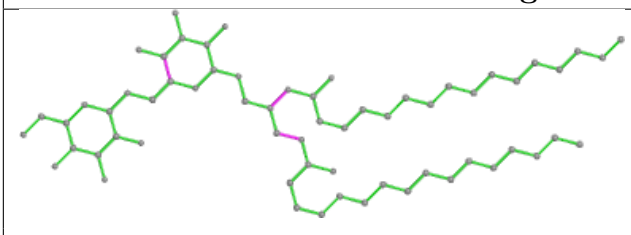


Rings

Ligand DGD C 518



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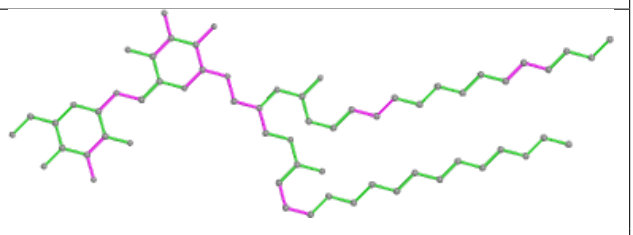
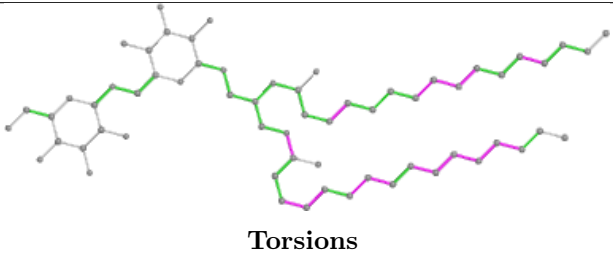


Bond angles



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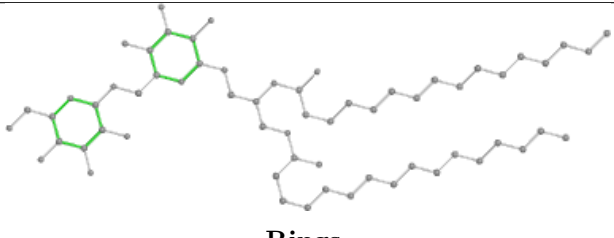
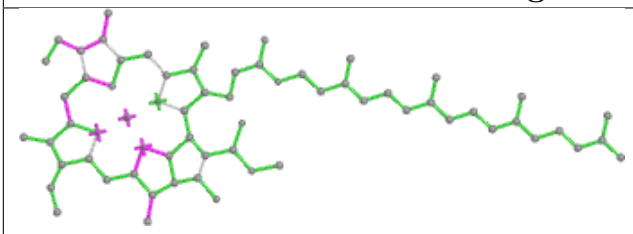


Rings

Ligand CLA b 608



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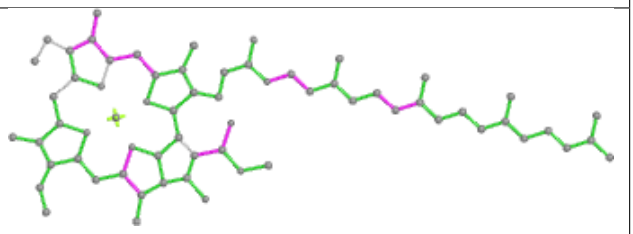
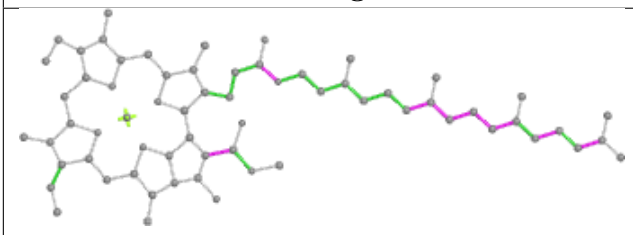


Bond angles



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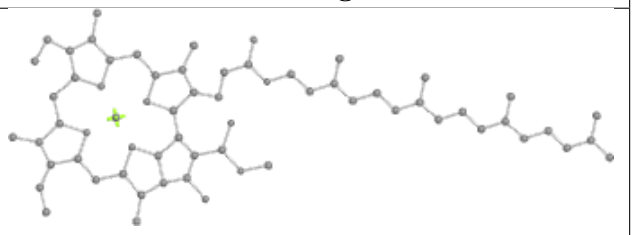
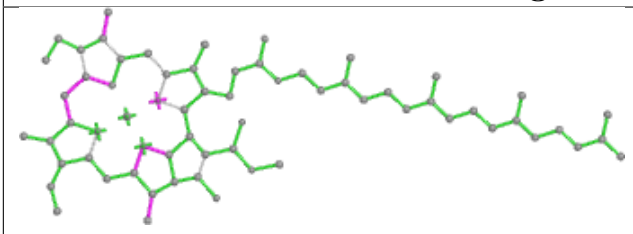


Rings

Ligand CLA c 510



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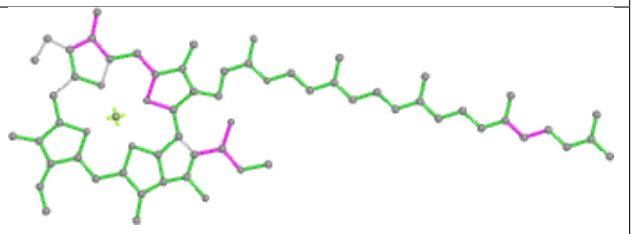
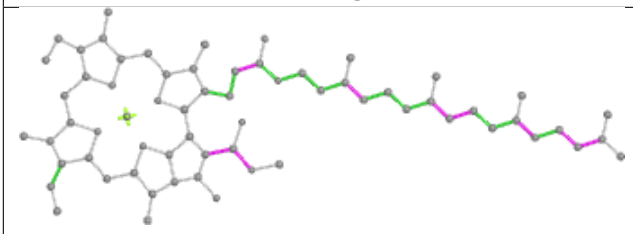


Bond angles



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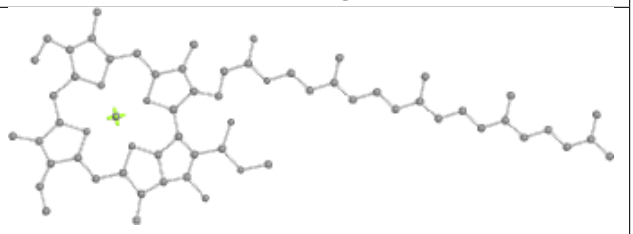
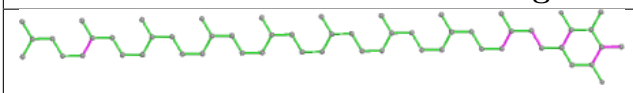


Rings

Ligand PL9 d 406



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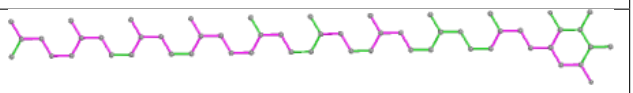
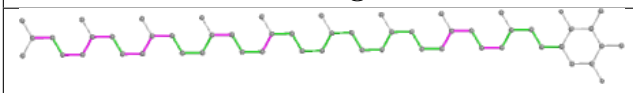


Bond angles



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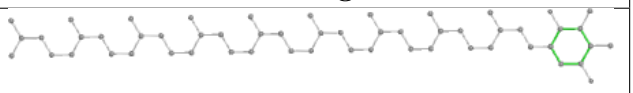
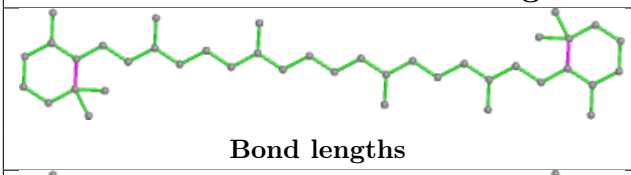


Rings

Ligand BCR Y 101



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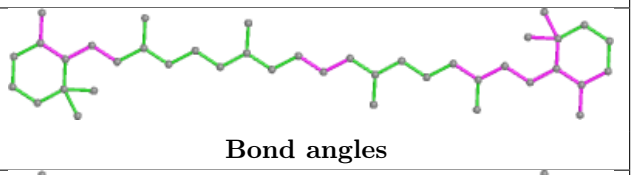

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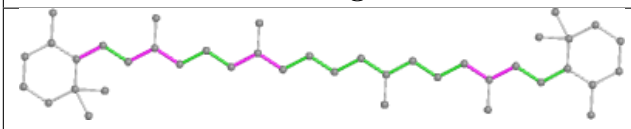

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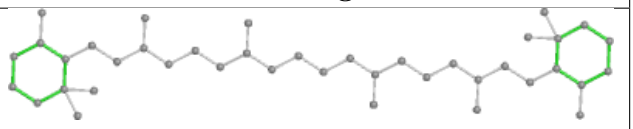
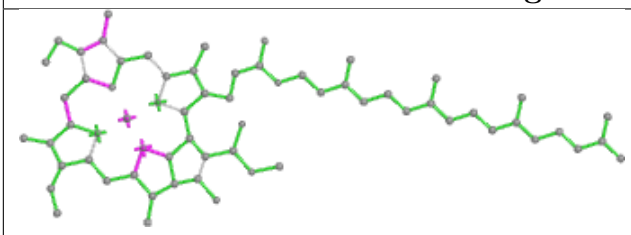


Rings

Ligand CLA B 614



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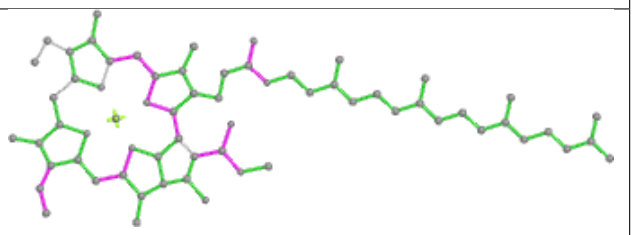
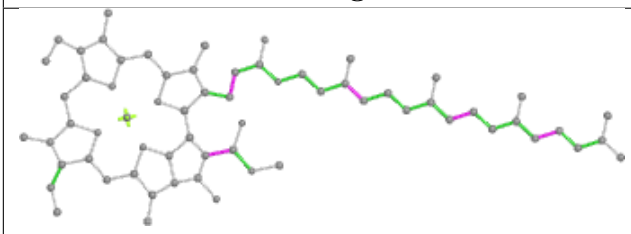
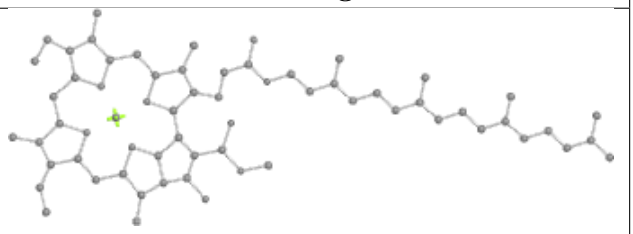


Bond angles

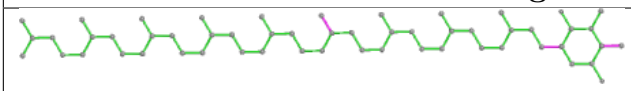


Torsions



Rings

Ligand PL9 A 409



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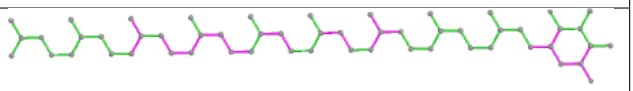
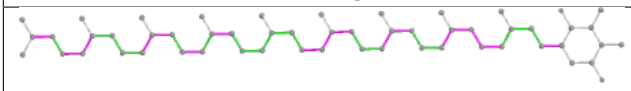


Bond angles



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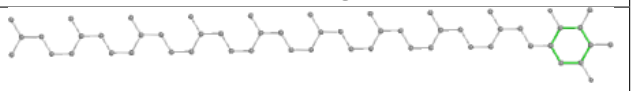
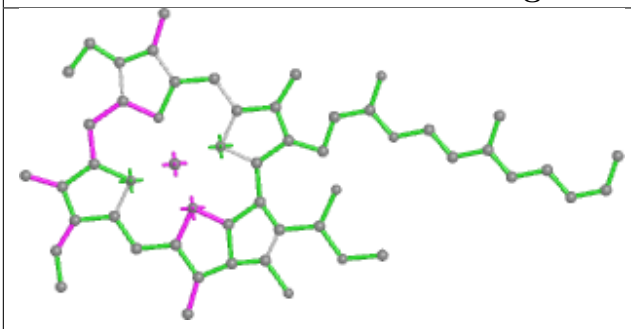


Rings

Ligand CLA A 407



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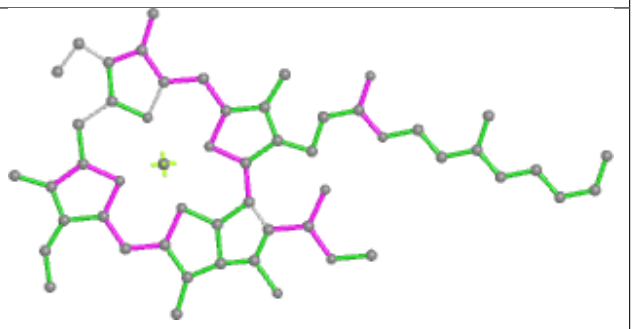
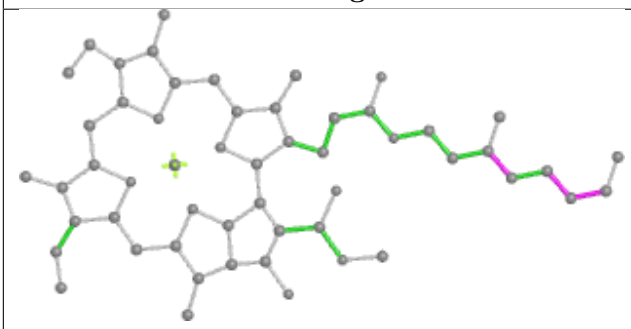


Bond angles



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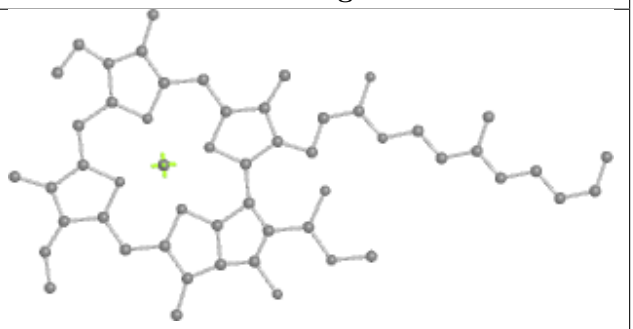
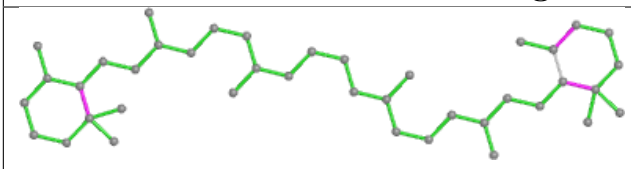


Rings

Ligand 8CT c 514



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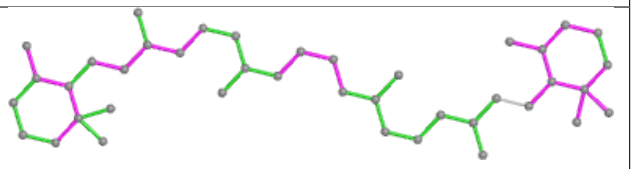
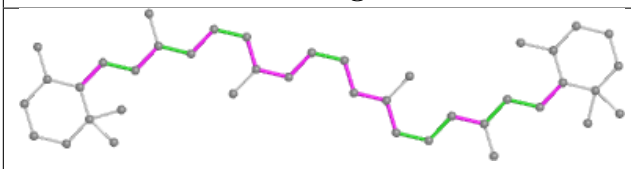


Bond angles



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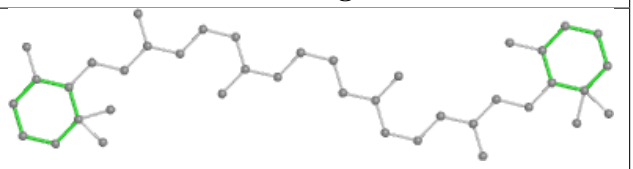
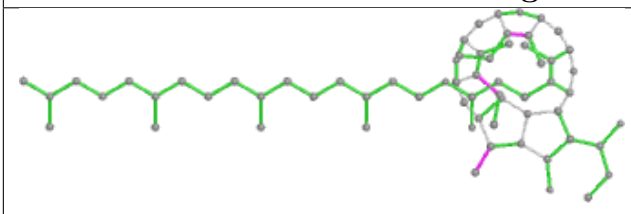
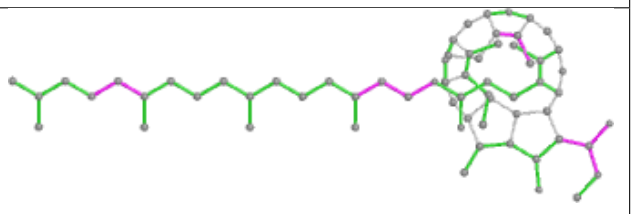


Rings

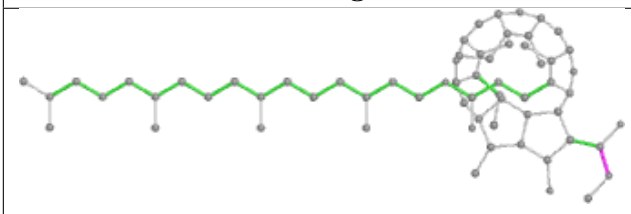
Ligand PHO D 402



Bond lengths



Bond angles



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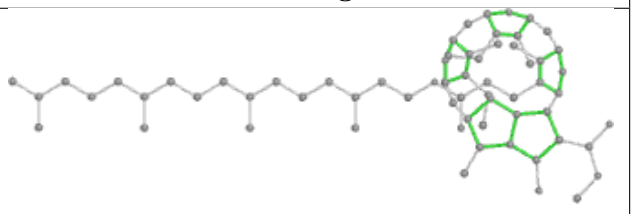
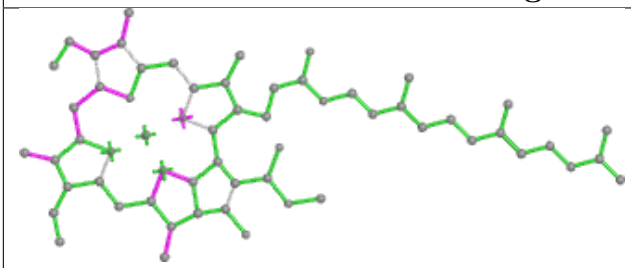
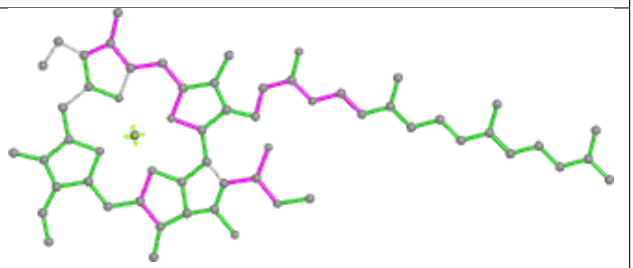


Rings

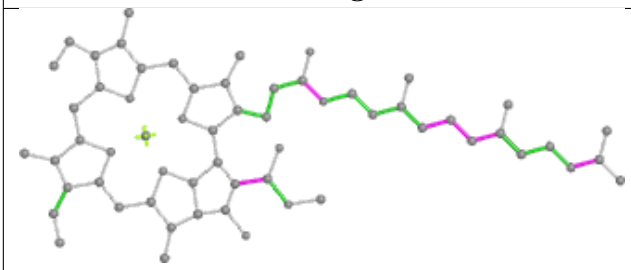
Ligand CLA B 616



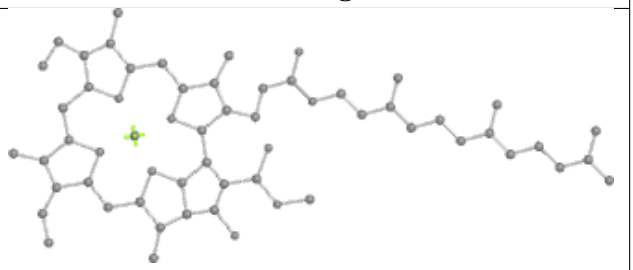
Bond lengths



Bond angles

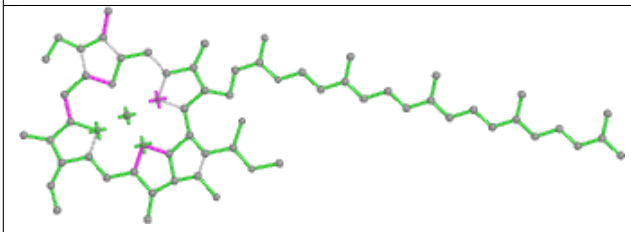


Torsions

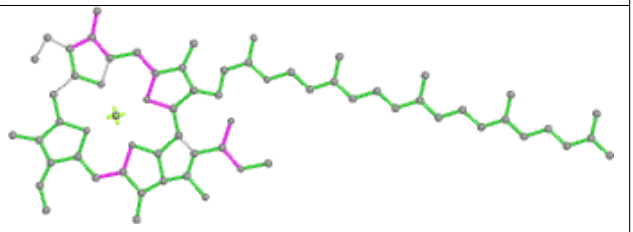


Rings

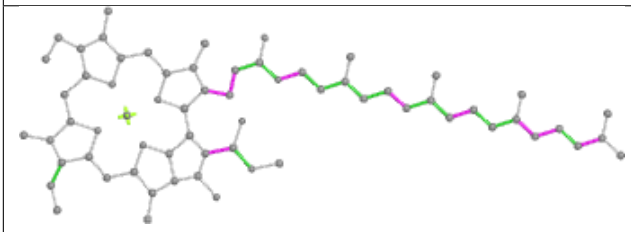
Ligand CLA c 513



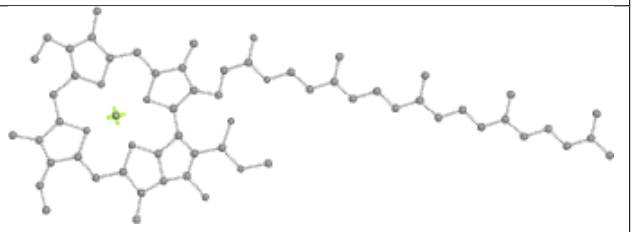
Bond lengths



Bond angles

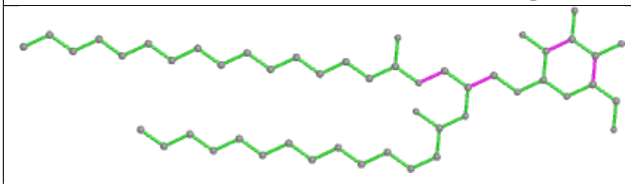


Torsions



Rings

Ligand LMG c 524



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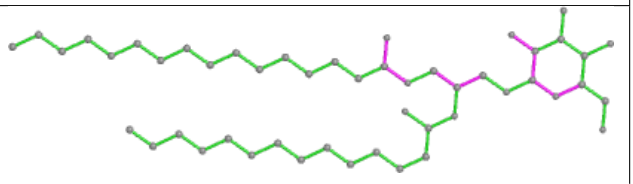
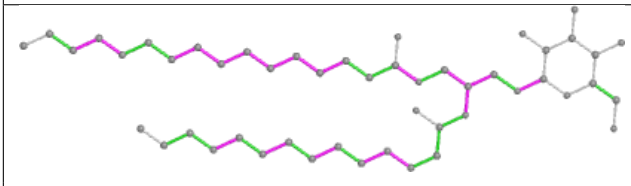
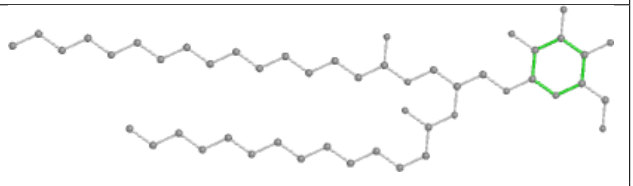


Bond angles

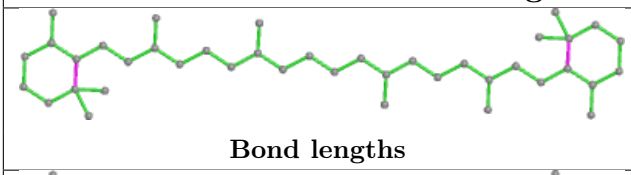


Torsions



Rings

Ligand BCR h 101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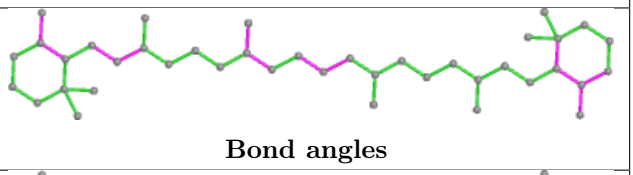
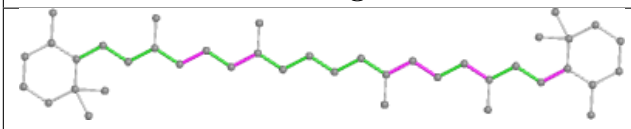

Bond angles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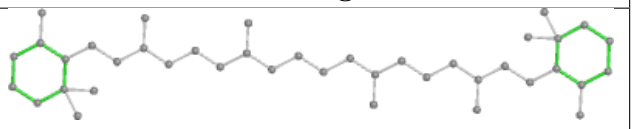
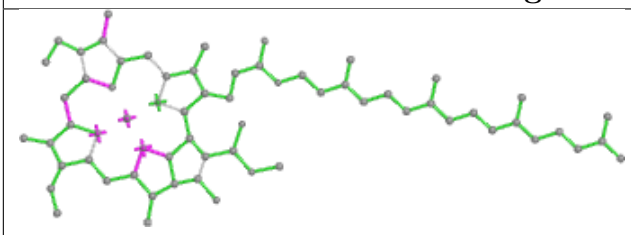

Rings

Ligand CLA C 509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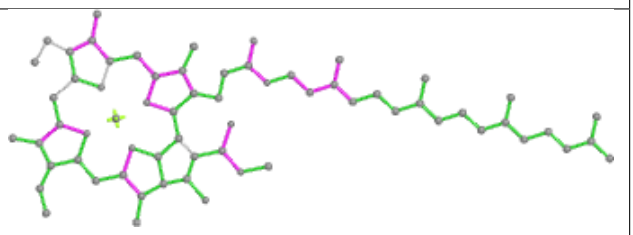
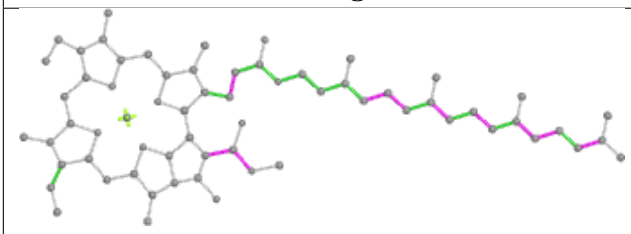

Bond angles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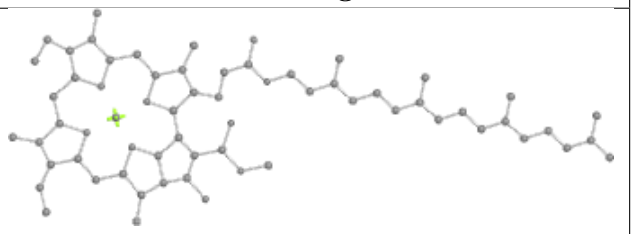
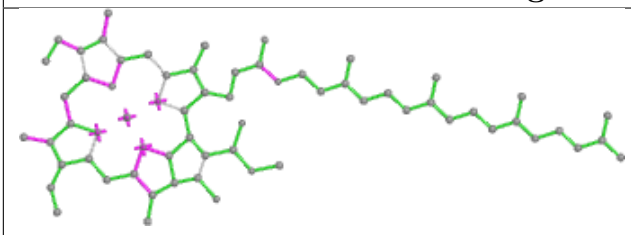

Rings

Ligand CLA b 602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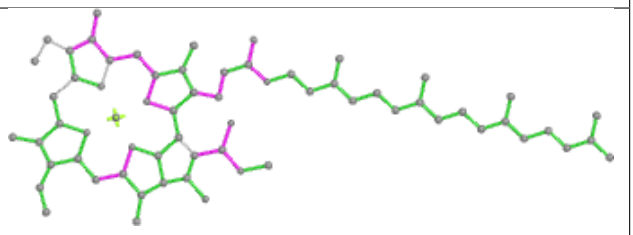
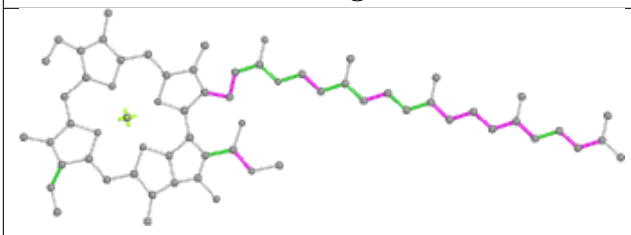

Bond angles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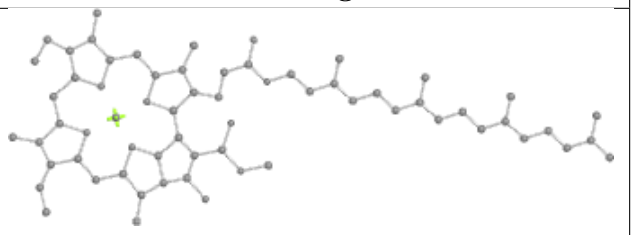
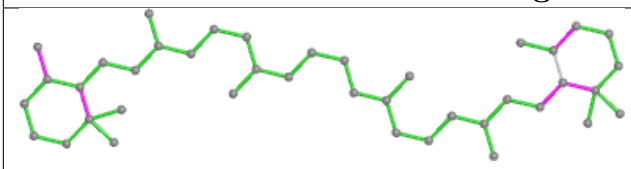
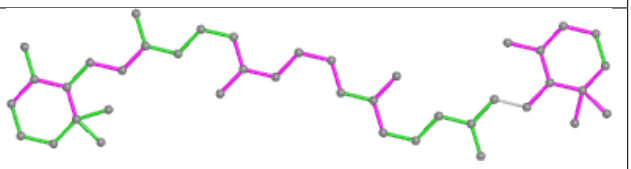
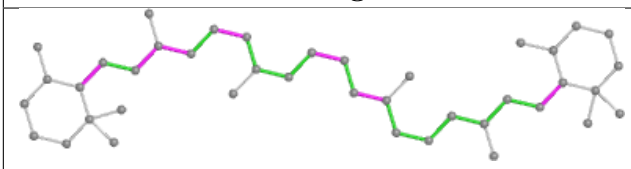
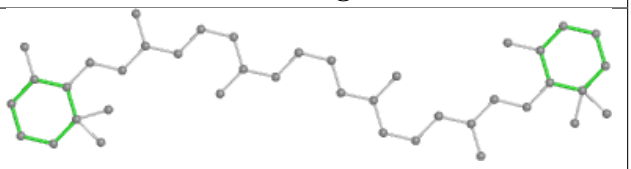
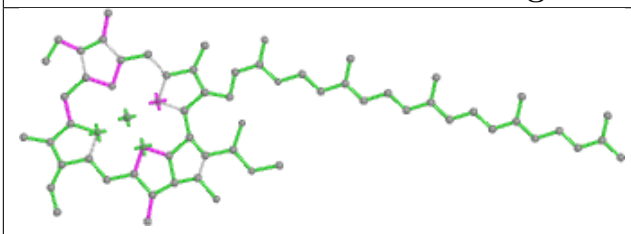
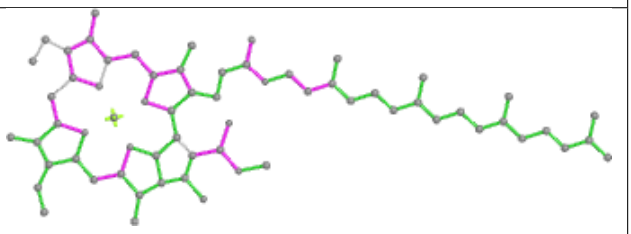
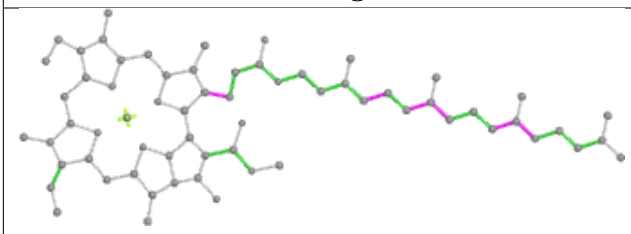
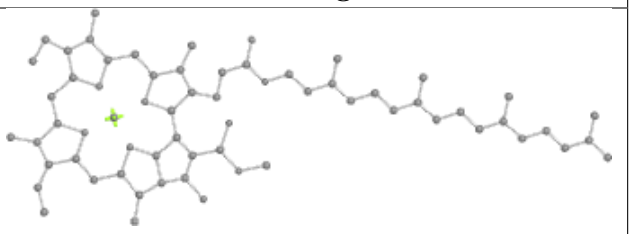
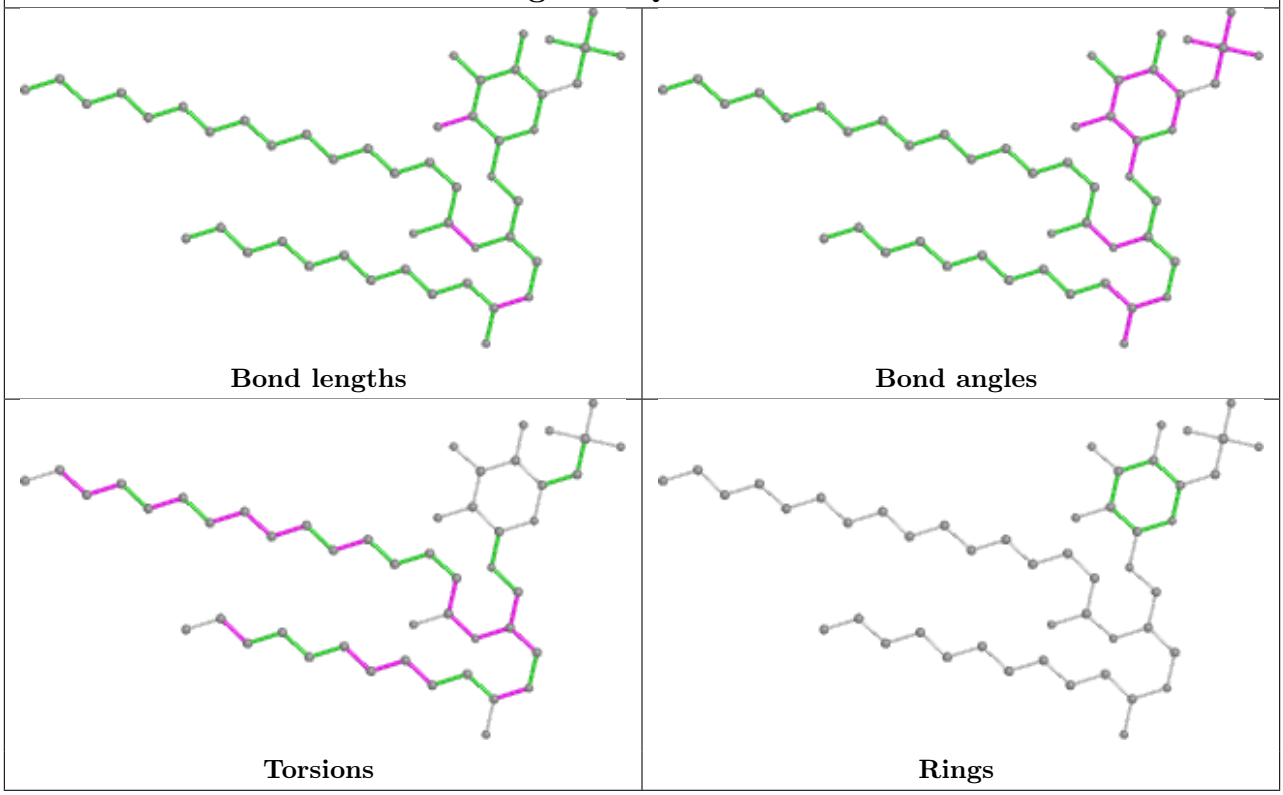

Rings

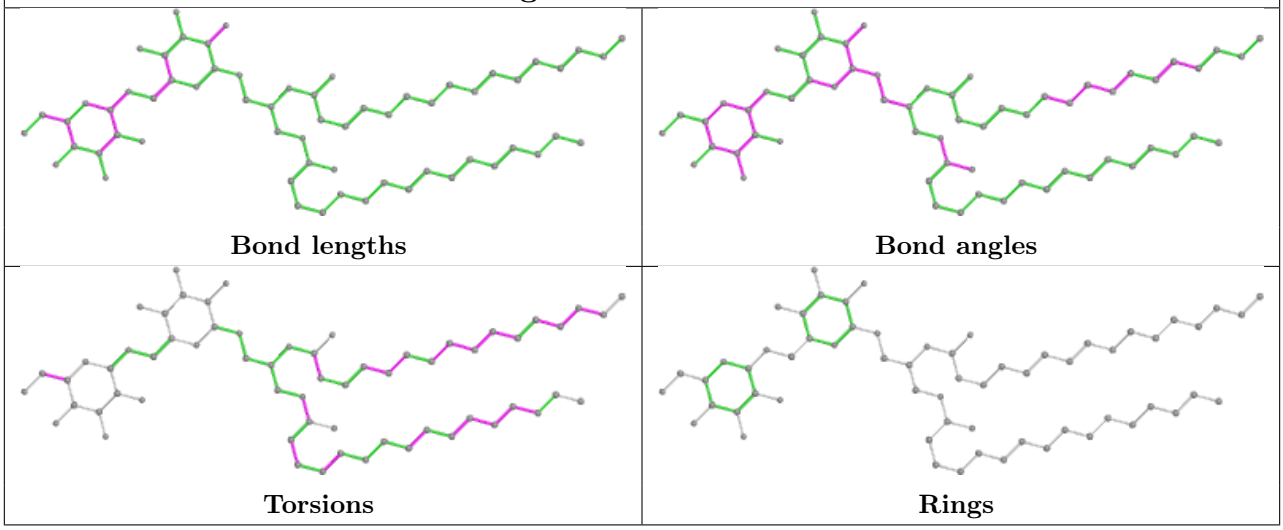
Ligand 8CT t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

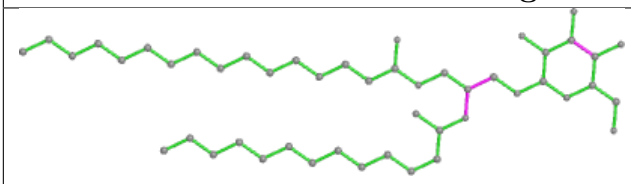
Ligand SQD b 601

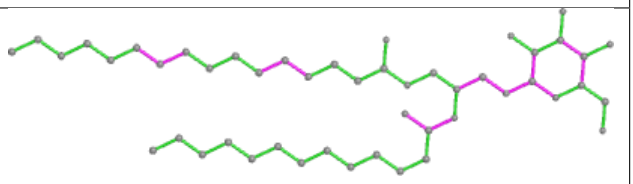


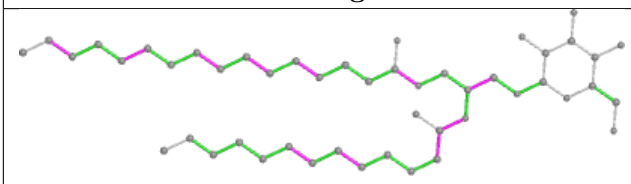
Ligand DGD H 102

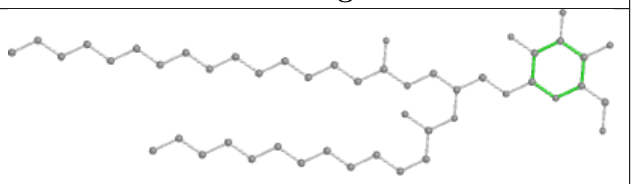


Ligand LMG C 519

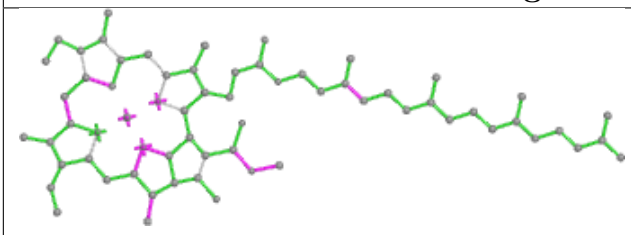

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA A 404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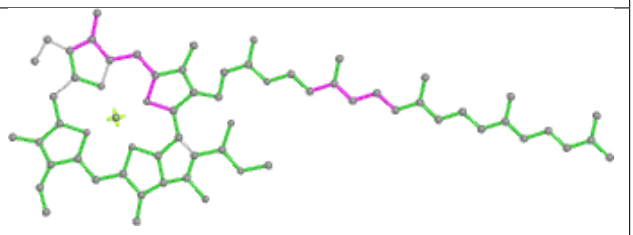
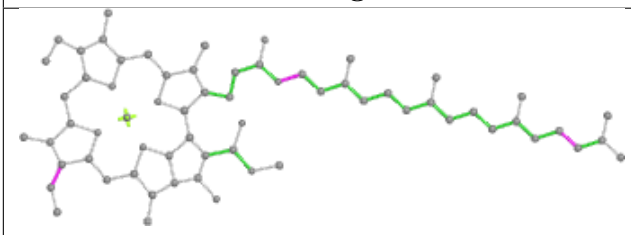

Bond angles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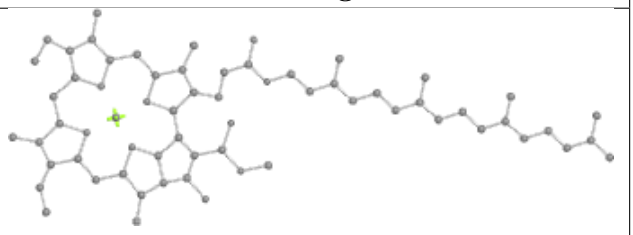
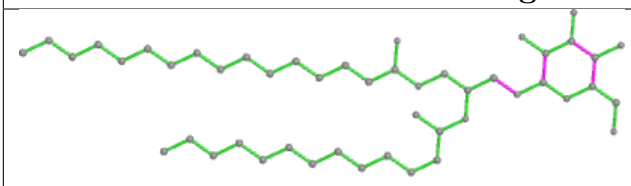

Rings

Ligand LMG A 410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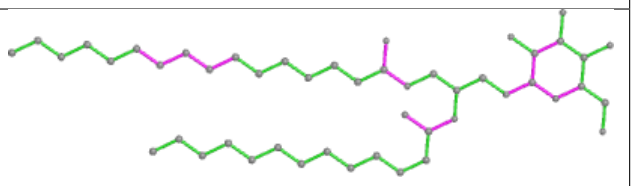
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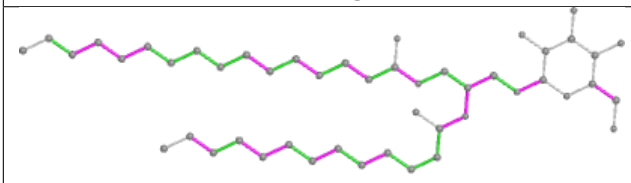
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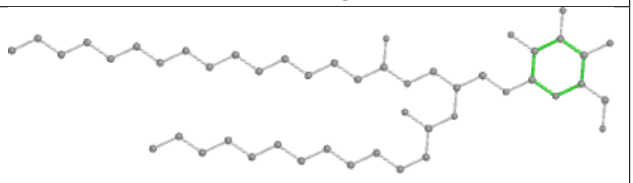
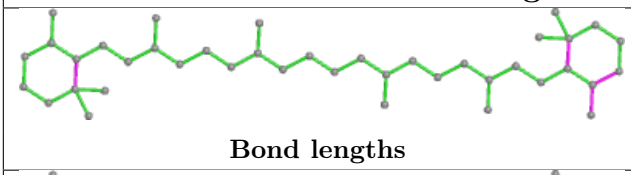

Rings

Ligand BCR T 101



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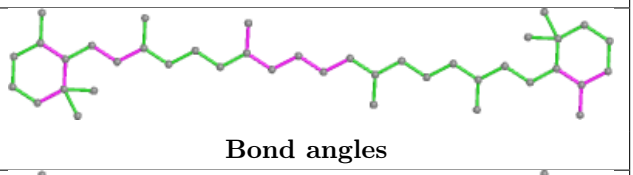
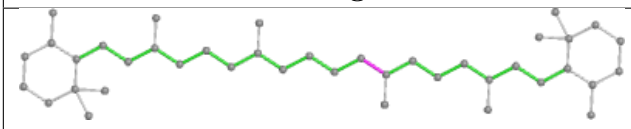


Bond angles



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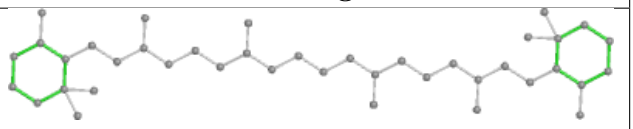
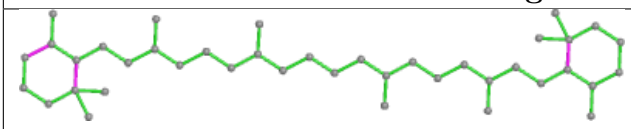


Rings

Ligand BCR b 619



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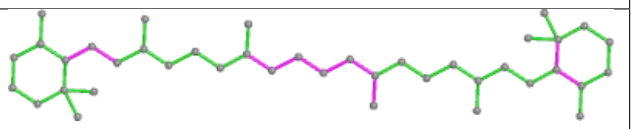
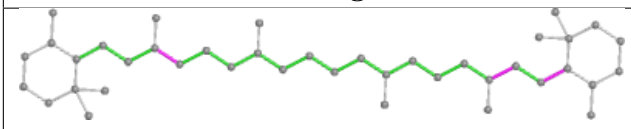


Bond angles



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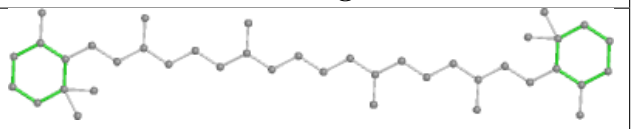
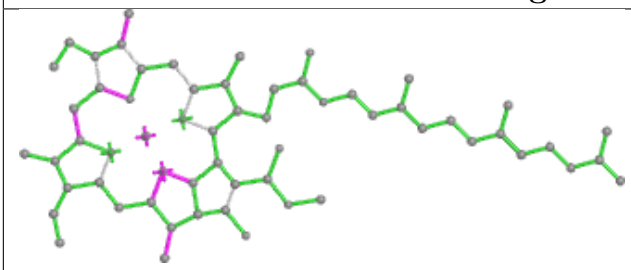
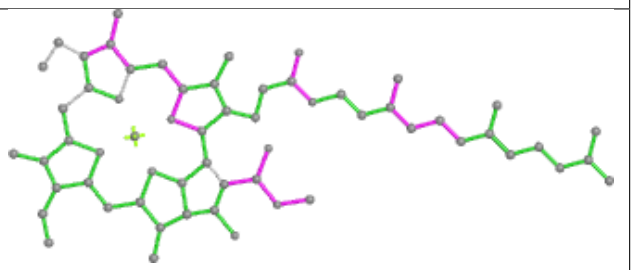


Rings

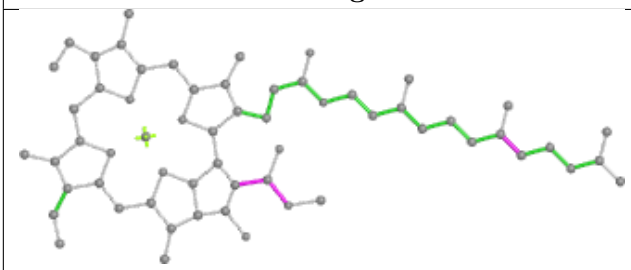
Ligand CLA c 504



Bond lengths



Bond angles



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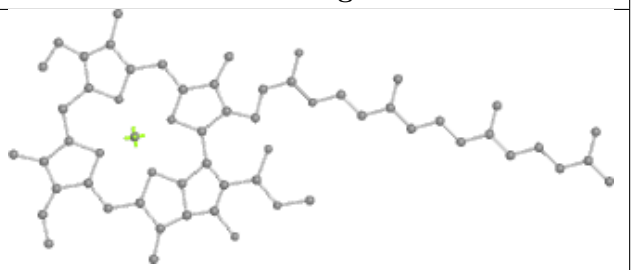
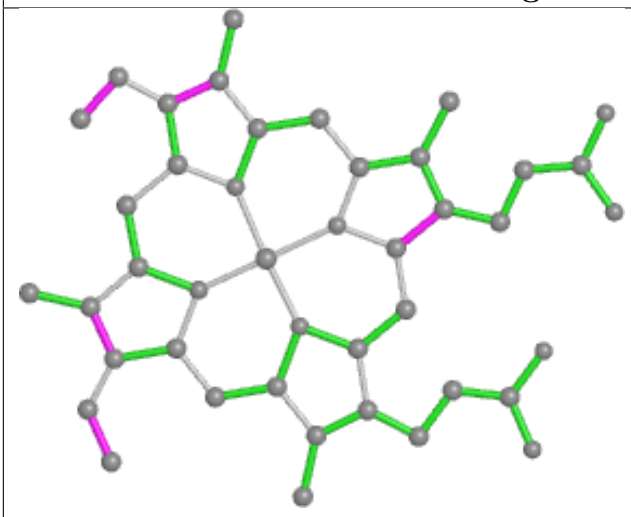
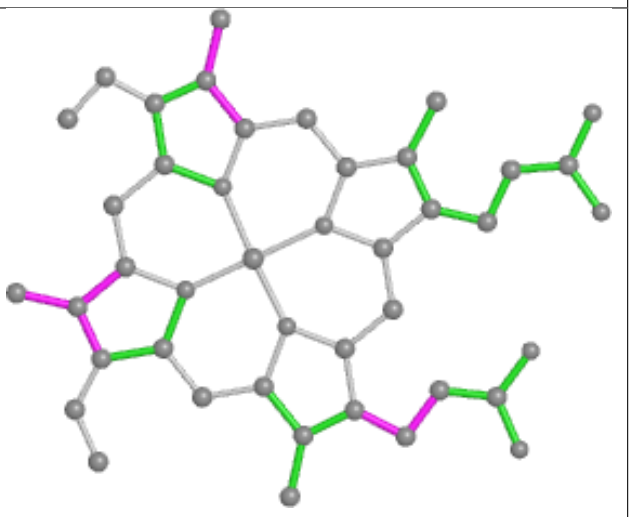


Rings

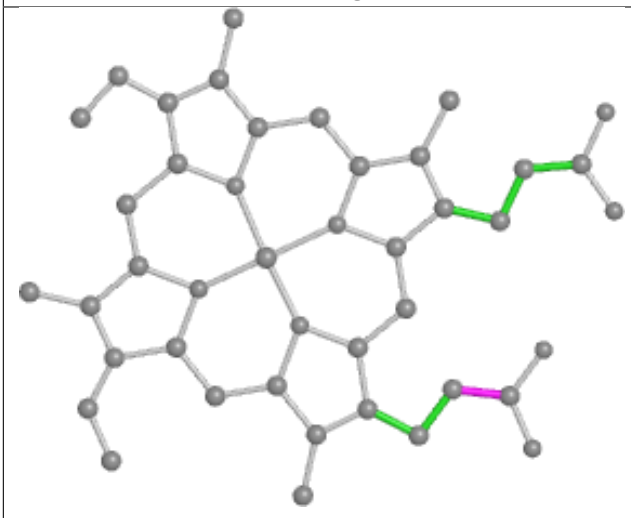
Ligand HEC V 201



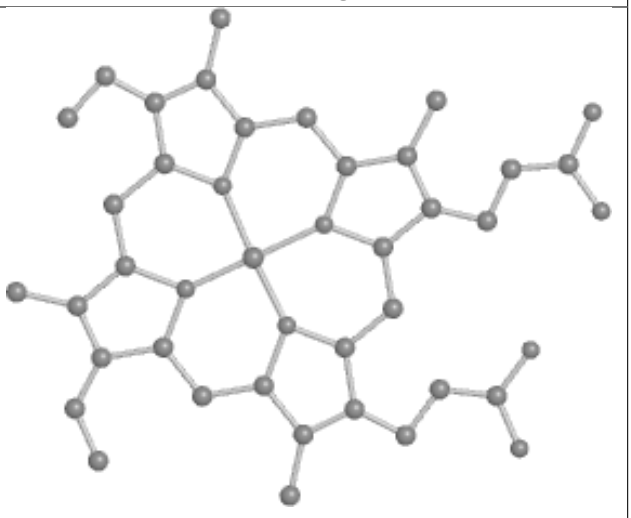
Bond lengths



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%)	-0.50	3 (0%) 84 86	19, 27, 46, 75	0
1	a	334/334 (100%)	-0.47	2 (0%) 89 91	21, 29, 55, 82	0
2	B	505/505 (100%)	-0.43	7 (1%) 75 78	19, 30, 60, 91	0
2	b	505/505 (100%)	-0.31	12 (2%) 59 63	22, 34, 67, 101	0
3	C	442/451 (98%)	-0.37	2 (0%) 91 92	22, 34, 51, 74	0
3	c	451/451 (100%)	-0.34	6 (1%) 77 79	23, 37, 58, 95	0
4	D	341/341 (100%)	-0.37	0 100 100	21, 28, 46, 80	0
4	d	341/341 (100%)	-0.39	1 (0%) 94 94	20, 32, 55, 75	0
5	E	81/82 (98%)	0.07	4 (4%) 29 31	31, 48, 65, 76	0
5	e	82/82 (100%)	0.27	4 (4%) 29 31	37, 57, 79, 87	0
6	F	34/34 (100%)	-0.33	2 (5%) 22 24	34, 40, 59, 79	0
6	f	34/34 (100%)	-0.12	2 (5%) 22 24	38, 48, 71, 82	0
7	H	65/65 (100%)	-0.08	1 (1%) 73 76	32, 37, 57, 69	0
7	h	63/65 (96%)	0.05	2 (3%) 47 52	38, 47, 60, 64	0
8	I	35/36 (97%)	-0.21	3 (8%) 10 11	28, 36, 67, 74	0
8	i	35/36 (97%)	-0.17	2 (5%) 23 25	30, 37, 68, 79	0
9	J	36/36 (100%)	0.24	5 (13%) 2 2	31, 47, 71, 86	0
9	j	36/36 (100%)	0.22	5 (13%) 2 2	35, 49, 83, 85	0
10	K	37/37 (100%)	-0.12	0 100 100	41, 49, 64, 72	0
10	k	37/37 (100%)	0.06	0 100 100	46, 56, 70, 77	0
11	L	37/37 (100%)	-0.33	0 100 100	23, 27, 60, 66	0
11	l	36/37 (97%)	-0.34	0 100 100	24, 29, 66, 77	0
12	M	32/33 (96%)	-0.31	0 100 100	25, 31, 60, 67	0
12	m	31/33 (93%)	-0.37	0 100 100	24, 32, 45, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.08	12 (4%) 29 31	21, 39, 80, 130	0
13	o	244/244 (100%)	-0.18	14 (5%) 23 25	21, 38, 74, 128	0
14	T	29/30 (96%)	-0.60	2 (6%) 16 18	25, 29, 56, 72	0
14	t	29/30 (96%)	-0.31	3 (10%) 6 6	23, 29, 76, 92	0
15	U	97/97 (100%)	-0.30	2 (2%) 63 67	30, 40, 67, 93	0
15	u	97/97 (100%)	-0.48	0 100 100	30, 37, 56, 81	0
16	V	137/137 (100%)	-0.56	0 100 100	25, 37, 53, 78	0
16	v	137/137 (100%)	-0.26	3 (2%) 62 66	31, 44, 64, 83	0
17	Y	27/30 (90%)	1.84	11 (40%) 0 0	50, 69, 108, 115	0
17	y	30/30 (100%)	0.98	9 (30%) 0 0	58, 72, 94, 97	0
18	X	38/38 (100%)	0.12	4 (10%) 6 6	34, 47, 71, 80	0
18	x	38/38 (100%)	0.45	4 (10%) 6 6	47, 56, 80, 94	0
19	Z	62/62 (100%)	0.78	16 (25%) 0 0	48, 61, 108, 116	0
19	z	62/62 (100%)	1.11	13 (20%) 1 0	54, 69, 108, 119	0
20	R	34/34 (100%)	1.82	13 (38%) 0 0	56, 65, 82, 90	0
20	r	31/34 (91%)	2.43	20 (64%) 0 0	66, 81, 90, 95	0
All	All	5300/5326 (99%)	-0.23	189 (3%) 42 46	19, 35, 70, 130	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	9.7
17	Y	20	ALA	8.3
13	O	59	LYS	7.7
13	O	60	ARG	7.7
13	o	3	GLN	7.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.94	0.09	28,37,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.95	0.10	28,45,62,68	0
8	FME	I	1	10/11	0.96	0.14	36,54,63,65	0
8	FME	i	1	10/11	0.96	0.12	37,48,59,59	0
12	FME	m	1	10/11	0.96	0.14	32,46,70,77	0
12	FME	M	1	10/11	0.96	0.16	34,42,70,81	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	E	102	28/-	0.51	0.37	63,78,89,91	0
32	UNL	H	103	53/-	0.71	0.28	53,76,91,91	0
32	UNL	a	413	28/-	0.72	0.29	35,63,70,73	0
32	UNL	b	626	55/-	0.76	0.20	41,62,82,85	0
26	PL9	A	409	55/55	0.77	0.26	38,60,83,97	135
32	UNL	c	523	28/-	0.77	0.18	47,68,82,85	0
33	LHG	E	101	49/49	0.77	0.25	44,85,112,121	0
32	UNL	b	625	40/-	0.78	0.18	52,69,87,92	0
26	PL9	a	410	55/55	0.79	0.22	40,68,89,93	0
32	UNL	c	520	55/-	0.80	0.18	41,56,75,82	0
32	UNL	B	628	47/-	0.80	0.30	44,67,86,86	0
27	LMG	D	411	33/55	0.80	0.16	35,56,88,94	0
29	DGD	A	414	66/66	0.81	0.19	41,64,84,113	0
27	LMG	b	624	23/55	0.81	0.23	34,70,96,100	0
27	LMG	c	522	48/55	0.82	0.21	42,73,112,117	0
27	LMG	b	623	55/55	0.82	0.26	44,75,99,109	0
32	UNL	j	101	28/-	0.82	0.14	46,59,70,74	0
32	UNL	t	103	26/-	0.82	0.20	47,65,79,84	0
32	UNL	B	627	28/-	0.82	0.33	47,68,85,91	0
32	UNL	d	411	43/-	0.83	0.18	48,60,70,78	0
29	DGD	o	301	44/66	0.83	0.15	31,56,79,85	0
23	CLA	c	512	65/65	0.84	0.16	43,60,98,114	0
32	UNL	C	523	47/-	0.84	0.12	41,54,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	J	101	28/-	0.84	0.19	49,62,75,83	0
28	SQD	a	412	36/54	0.85	0.15	29,62,85,87	0
28	SQD	f	101	41/54	0.86	0.22	58,84,117,131	0
23	CLA	b	602	65/65	0.86	0.14	39,63,87,98	0
28	SQD	b	601	49/54	0.86	0.14	40,62,98,102	0
31	BCR	Y	101	40/40	0.86	0.13	36,50,68,75	0
31	BCR	h	101	40/40	0.86	0.14	32,54,79,80	0
32	UNL	t	102	34/-	0.87	0.12	40,52,65,65	0
32	UNL	T	102	47/-	0.87	0.20	38,50,66,69	0
27	LMG	c	524	49/55	0.87	0.15	35,57,86,104	0
33	LHG	e	101	42/49	0.87	0.29	62,88,118,134	0
28	SQD	B	624	54/54	0.88	0.12	35,59,93,104	0
32	UNL	b	622	55/-	0.88	0.18	36,53,74,82	0
32	UNL	B	621	43/-	0.88	0.13	36,52,69,73	0
23	CLA	C	512	65/65	0.88	0.15	30,54,103,114	0
23	CLA	c	513	65/65	0.88	0.20	39,68,105,107	0
23	CLA	C	513	65/65	0.88	0.18	41,61,97,101	0
23	CLA	B	616	60/65	0.88	0.16	23,38,87,90	0
27	LMG	C	519	48/55	0.88	0.14	45,70,89,96	0
32	UNL	I	101	41/-	0.88	0.13	38,53,76,79	0
31	BCR	H	101	40/40	0.88	0.11	29,45,58,62	0
28	SQD	A	413	39/54	0.88	0.19	36,65,86,94	0
32	UNL	X	101	55/-	0.88	0.21	33,51,72,77	0
32	UNL	B	625	28/-	0.89	0.10	26,47,70,72	0
32	UNL	M	102	26/-	0.89	0.15	34,47,56,61	0
25	8CT	k	101	40/40	0.89	0.11	40,60,75,77	0
32	UNL	d	412	55/-	0.89	0.18	40,60,77,78	0
23	CLA	B	601	65/65	0.89	0.14	31,62,100,113	0
32	UNL	m	101	28/-	0.89	0.15	39,59,78,81	0
23	CLA	b	617	60/65	0.89	0.14	25,42,79,91	0
27	LMG	A	410	48/55	0.89	0.14	35,54,70,94	0
27	LMG	c	519	37/55	0.89	0.16	39,68,83,90	0
27	LMG	B	622	28/55	0.89	0.15	29,46,64,69	0
32	UNL	B	626	46/-	0.90	0.11	44,59,74,76	0
32	UNL	l	102	53/-	0.90	0.14	31,46,90,92	0
32	UNL	b	627	26/-	0.90	0.21	39,56,67,73	0
27	LMG	b	621	51/55	0.90	0.11	34,51,75,90	0
23	CLA	D	404	65/65	0.90	0.16	19,42,124,131	0
32	UNL	C	522	28/-	0.90	0.12	42,53,59,61	0
23	CLA	b	616	65/65	0.90	0.14	25,39,58,70	0
23	CLA	a	408	65/65	0.91	0.15	16,37,90,97	0
25	8CT	D	405	40/40	0.91	0.12	26,42,100,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	T	103	44/-	0.91	0.18	36,57,75,81	0
27	LMG	B	620	51/55	0.91	0.11	28,47,71,86	0
23	CLA	d	404	65/65	0.92	0.14	27,49,94,106	0
29	DGD	H	102	62/66	0.92	0.11	31,46,63,71	0
29	DGD	h	102	62/66	0.92	0.11	27,52,67,71	0
25	8CT	C	514	40/40	0.92	0.11	36,53,67,73	0
27	LMG	D	407	51/55	0.92	0.15	25,57,88,98	0
32	UNL	C	521	28/-	0.92	0.10	31,47,55,68	0
23	CLA	C	505	65/65	0.92	0.17	23,39,69,90	0
23	CLA	c	508	64/65	0.92	0.12	24,43,79,112	0
25	8CT	C	515	40/40	0.93	0.11	26,38,52,53	0
28	SQD	D	408	36/54	0.93	0.15	44,69,85,92	0
28	SQD	a	411	54/54	0.93	0.13	42,66,89,96	0
23	CLA	B	615	65/65	0.93	0.12	21,35,67,73	0
25	8CT	c	514	40/40	0.93	0.15	39,56,69,69	0
25	8CT	d	405	40/40	0.93	0.11	30,55,92,108	0
23	CLA	c	511	65/65	0.93	0.13	39,53,71,77	0
29	DGD	C	516	62/66	0.93	0.12	19,38,73,96	0
29	DGD	C	517	62/66	0.93	0.12	27,52,95,110	0
23	CLA	c	502	65/65	0.93	0.12	24,42,60,63	0
23	CLA	c	503	65/65	0.93	0.13	31,43,55,58	0
23	CLA	c	506	65/65	0.93	0.13	26,50,108,115	0
25	8CT	B	619	40/40	0.93	0.09	24,38,62,69	0
32	UNL	M	101	37/-	0.93	0.12	31,48,69,71	0
23	CLA	c	507	65/65	0.93	0.14	22,43,60,68	0
31	BCR	b	618	40/40	0.93	0.11	27,41,54,58	0
31	BCR	c	521	40/40	0.93	0.15	34,52,71,74	0
23	CLA	c	504	60/65	0.94	0.11	27,46,83,86	0
23	CLA	c	505	65/65	0.94	0.14	22,39,63,76	0
23	CLA	A	405	65/65	0.94	0.12	19,34,103,112	0
23	CLA	a	406	65/65	0.94	0.12	25,39,100,106	0
23	CLA	C	502	65/65	0.94	0.10	23,40,55,60	0
29	DGD	c	517	62/66	0.94	0.10	30,51,86,100	0
23	CLA	c	510	65/65	0.94	0.12	29,47,68,77	0
23	CLA	B	606	65/65	0.94	0.09	22,34,72,80	0
23	CLA	b	605	65/65	0.94	0.14	18,32,76,91	0
31	BCR	T	101	40/40	0.94	0.10	23,39,59,61	0
23	CLA	b	607	65/65	0.94	0.10	25,40,68,80	0
23	CLA	b	610	65/65	0.94	0.11	29,45,64,71	0
31	BCR	b	619	40/40	0.94	0.09	25,38,51,62	0
25	8CT	B	617	40/40	0.94	0.10	22,41,53,56	0
23	CLA	b	613	65/65	0.94	0.16	18,33,48,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	614	65/65	0.94	0.12	14,32,69,85	0
23	CLA	b	615	65/65	0.94	0.14	19,38,77,89	0
27	LMG	d	410	44/55	0.94	0.12	30,52,94,108	0
25	8CT	C	520	40/40	0.94	0.14	35,51,66,70	0
23	CLA	C	506	65/65	0.94	0.12	22,40,95,110	0
25	8CT	b	620	40/40	0.94	0.10	22,45,59,68	0
23	CLA	C	507	65/65	0.94	0.13	17,38,55,65	0
23	CLA	B	614	65/65	0.94	0.13	20,39,81,96	0
33	LHG	d	409	39/49	0.94	0.11	28,47,73,77	0
23	CLA	A	407	54/65	0.94	0.13	15,28,65,73	0
26	PL9	d	406	55/55	0.95	0.10	21,36,48,53	0
23	CLA	C	511	65/65	0.95	0.10	27,50,65,69	0
23	CLA	C	501	65/65	0.95	0.12	24,36,50,61	0
23	CLA	d	403	65/65	0.95	0.10	18,32,63,76	0
29	DGD	c	518	62/66	0.95	0.10	26,50,75,90	0
23	CLA	B	612	65/65	0.95	0.15	18,29,46,53	0
24	PHO	a	407	64/64	0.95	0.10	18,30,37,43	0
31	BCR	B	618	40/40	0.95	0.08	21,37,51,51	0
24	PHO	d	401	64/64	0.95	0.10	25,39,48,71	0
25	8CT	A	408	40/40	0.95	0.09	22,31,43,46	0
23	CLA	D	403	65/65	0.95	0.10	15,27,55,72	0
23	CLA	C	503	65/65	0.95	0.10	28,40,52,54	0
23	CLA	B	604	65/65	0.95	0.10	17,29,80,90	0
31	BCR	c	515	40/40	0.95	0.10	28,41,58,72	0
23	CLA	B	609	65/65	0.95	0.09	23,35,53,62	0
23	CLA	B	610	65/65	0.95	0.14	17,31,42,46	0
23	CLA	b	603	65/65	0.95	0.14	24,42,72,80	0
23	CLA	C	508	65/65	0.95	0.11	25,40,100,116	0
23	CLA	b	606	65/65	0.95	0.12	16,34,47,56	0
23	CLA	C	509	65/65	0.95	0.14	23,43,63,70	0
23	CLA	c	509	65/65	0.95	0.15	28,47,65,68	0
25	8CT	t	101	40/40	0.95	0.08	24,37,58,61	0
33	LHG	D	410	47/49	0.95	0.11	23,48,82,99	0
23	CLA	b	609	65/65	0.95	0.11	20,41,62,74	0
33	LHG	d	407	49/49	0.95	0.12	30,52,78,89	0
26	PL9	D	406	55/55	0.95	0.10	17,32,45,47	0
23	CLA	C	510	65/65	0.95	0.12	29,46,74,78	0
23	CLA	B	605	65/65	0.96	0.14	19,31,45,51	0
23	CLA	b	608	65/65	0.96	0.11	19,37,65,72	0
23	CLA	A	404	65/65	0.96	0.10	17,26,44,51	0
23	CLA	a	405	65/65	0.96	0.09	17,28,46,61	0
23	CLA	b	611	65/65	0.96	0.13	21,36,52,57	0

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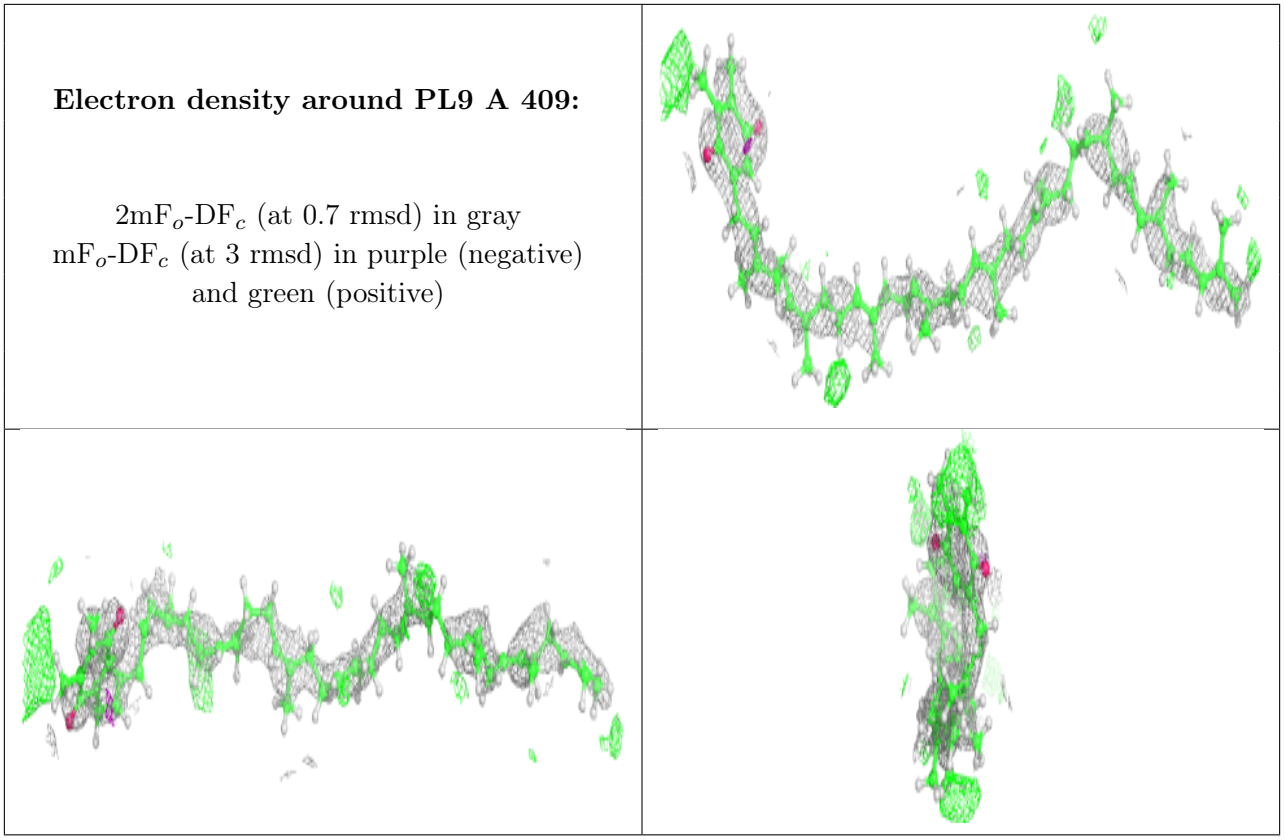
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	612	65/65	0.96	0.10	18,32,49,55	0
23	CLA	B	602	65/65	0.96	0.11	21,36,60,65	0
29	DGD	C	518	62/66	0.96	0.09	23,46,76,86	0
23	CLA	B	603	65/65	0.96	0.14	17,31,64,72	0
29	DGD	c	516	62/66	0.96	0.10	19,40,69,78	0
23	CLA	B	611	65/65	0.96	0.12	16,29,47,51	0
23	CLA	A	411	65/65	0.96	0.11	16,27,53,61	0
23	CLA	d	402	65/65	0.96	0.10	18,29,46,49	0
23	CLA	b	604	65/65	0.96	0.12	18,36,64,68	0
23	CLA	c	501	65/65	0.96	0.12	26,38,49,52	0
33	LHG	B	623	49/49	0.96	0.12	26,45,68,78	0
33	LHG	D	409	49/49	0.96	0.11	21,39,54,66	0
28	SQD	A	412	52/54	0.96	0.11	30,58,89,95	0
24	PHO	A	406	64/64	0.96	0.09	15,27,36,39	0
33	LHG	L	101	49/49	0.96	0.11	24,39,56,65	0
23	CLA	C	504	59/65	0.96	0.12	20,41,87,92	0
33	LHG	d	408	49/49	0.96	0.12	22,41,60,72	0
31	BCR	a	409	40/40	0.96	0.08	19,31,44,46	0
23	CLA	B	613	65/65	0.96	0.12	13,30,67,73	0
33	LHG	l	101	49/49	0.96	0.10	29,44,54,61	0
35	HEM	F	101	43/43	0.96	0.12	34,48,58,68	0
35	HEM	e	102	43/43	0.96	0.11	42,54,73,75	0
23	CLA	B	608	65/65	0.97	0.10	17,32,57,57	0
34	BCT	a	404	4/4	0.97	0.17	23,28,41,50	0
23	CLA	B	607	65/65	0.97	0.10	15,31,65,73	0
24	PHO	D	402	64/64	0.97	0.08	17,31,43,49	0
36	HEC	v	201	43/43	0.97	0.12	27,35,46,55	0
30	OEX	A	415	10/10	0.98	0.11	22,25,27,28	0
36	HEC	V	201	43/43	0.98	0.11	20,32,42,44	0
34	BCT	D	401	4/4	0.98	0.22	28,28,35,42	0
21	FE2	a	401	1/1	0.99	0.06	31,31,31,31	0
22	CL	A	402	1/1	0.99	0.03	25,25,25,25	0
30	OEX	a	414	10/10	0.99	0.11	16,25,28,29	0
22	CL	a	402	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	1.00	0.05	25,25,25,25	0
21	FE2	A	401	1/1	1.00	0.09	28,28,28,28	0
22	CL	a	403	1/1	1.00	0.02	27,27,27,27	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.

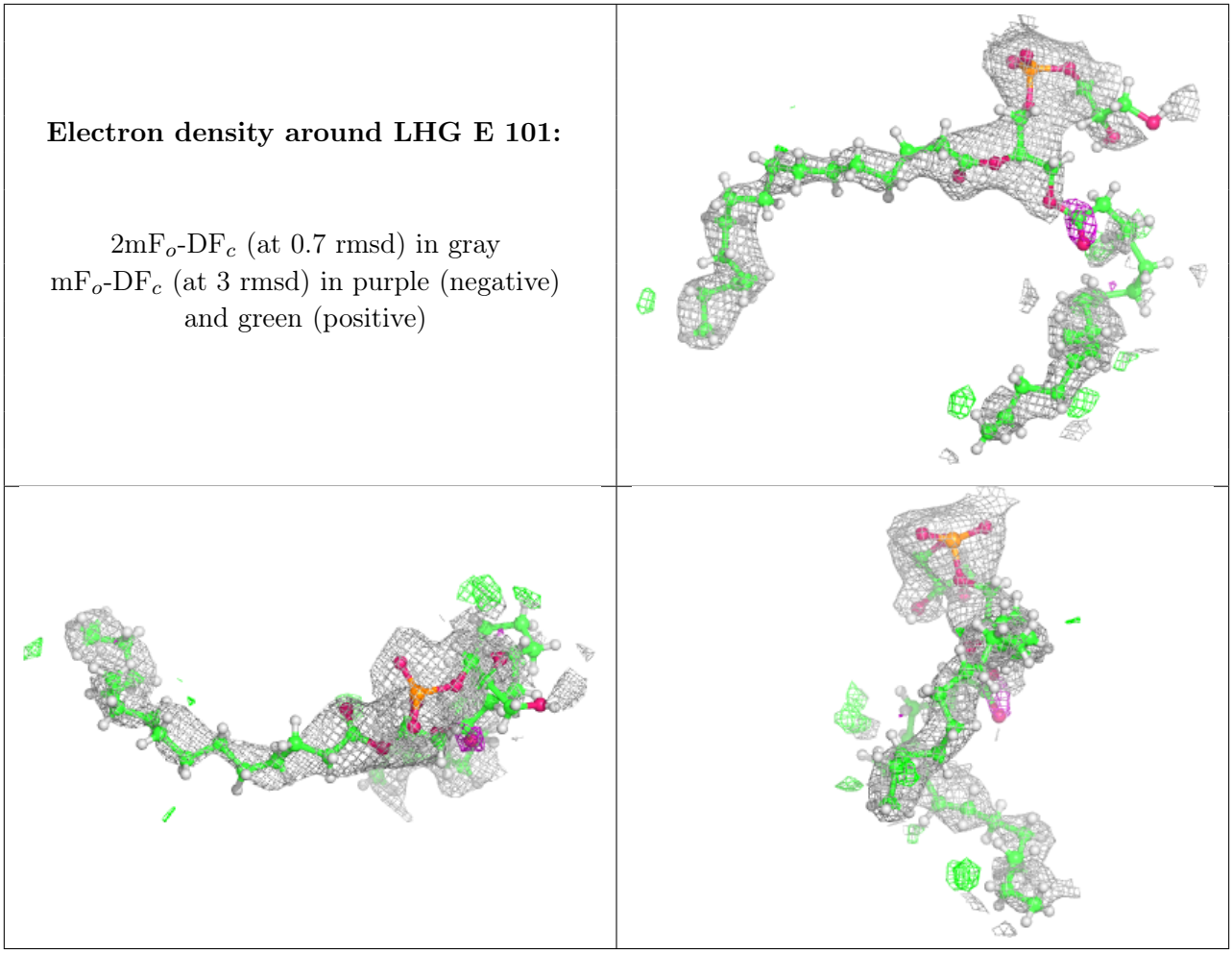
Electron density around PL9 A 409:

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



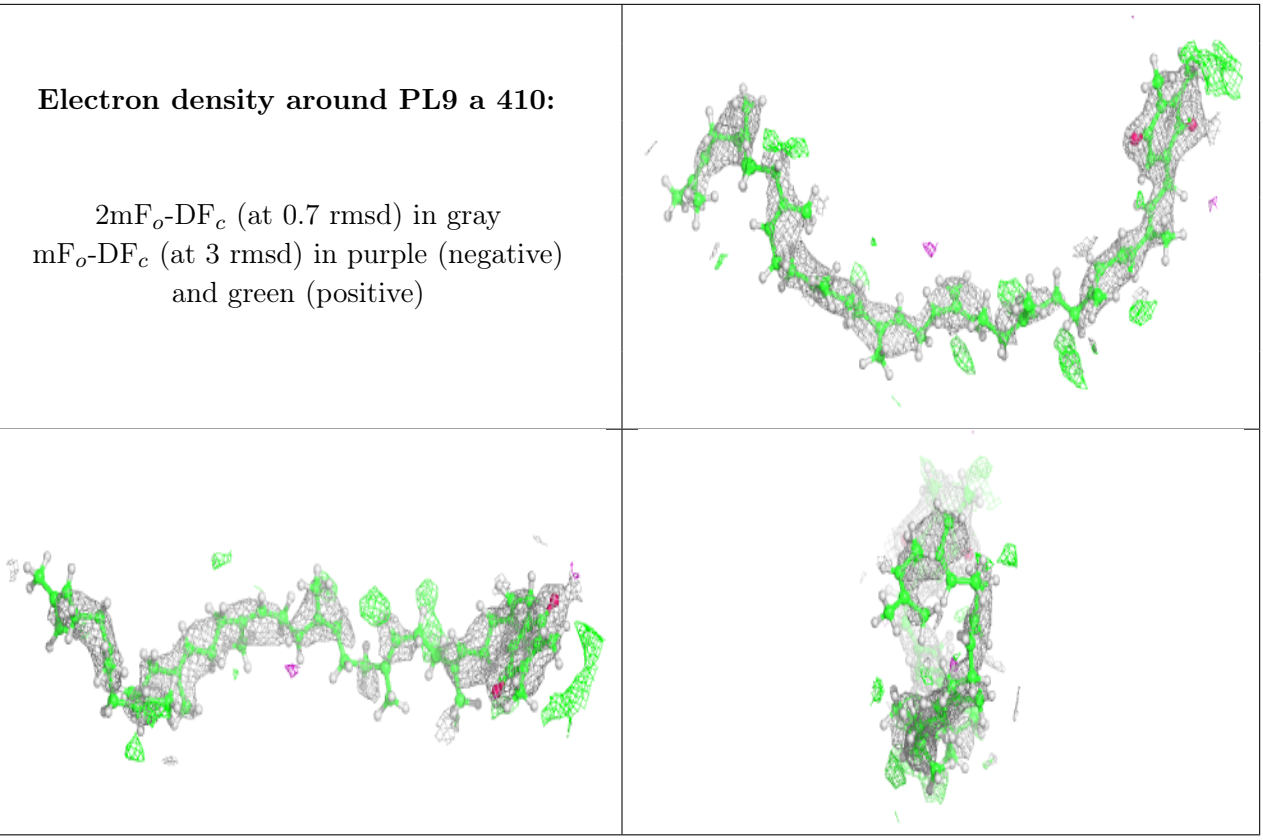
Electron density around LHG E 101:

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



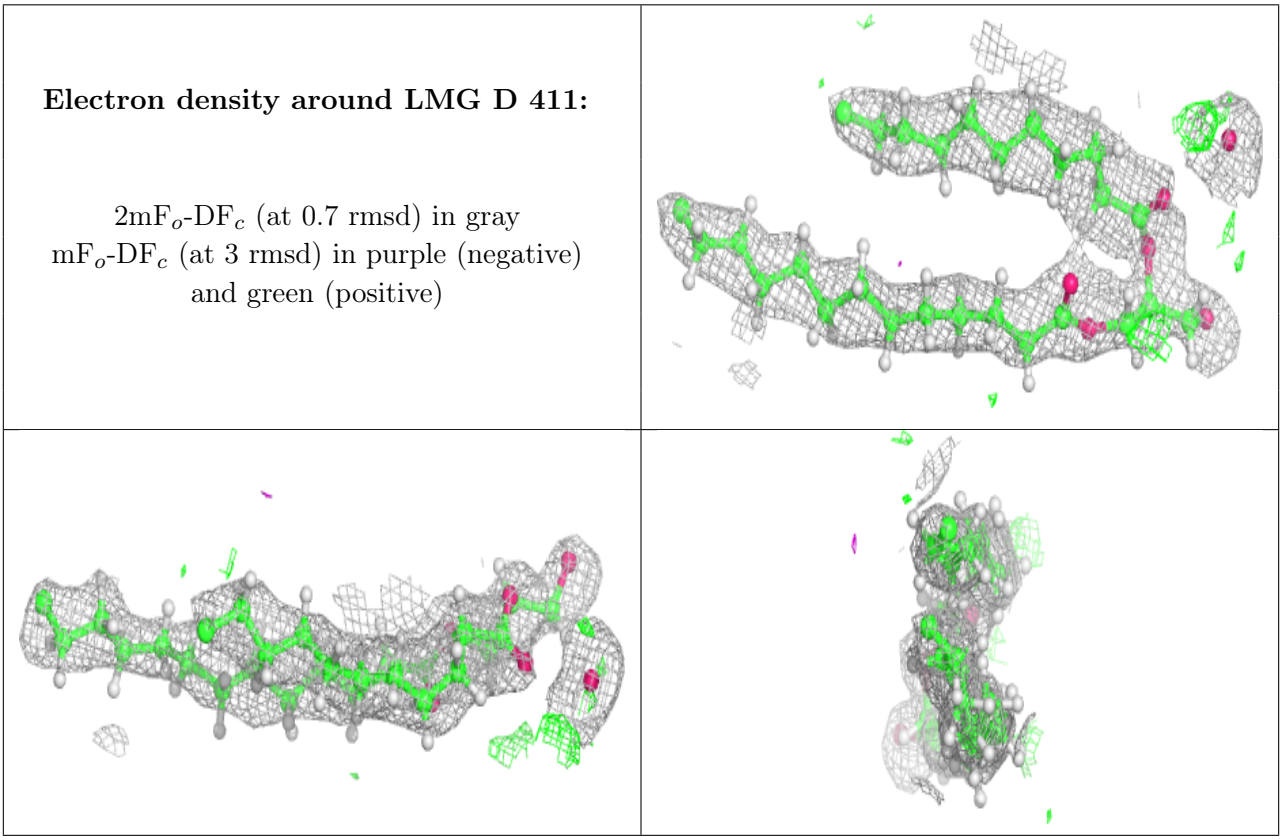
Electron density around PL9 a 410:

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



Electron density around 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 DGD A 414:

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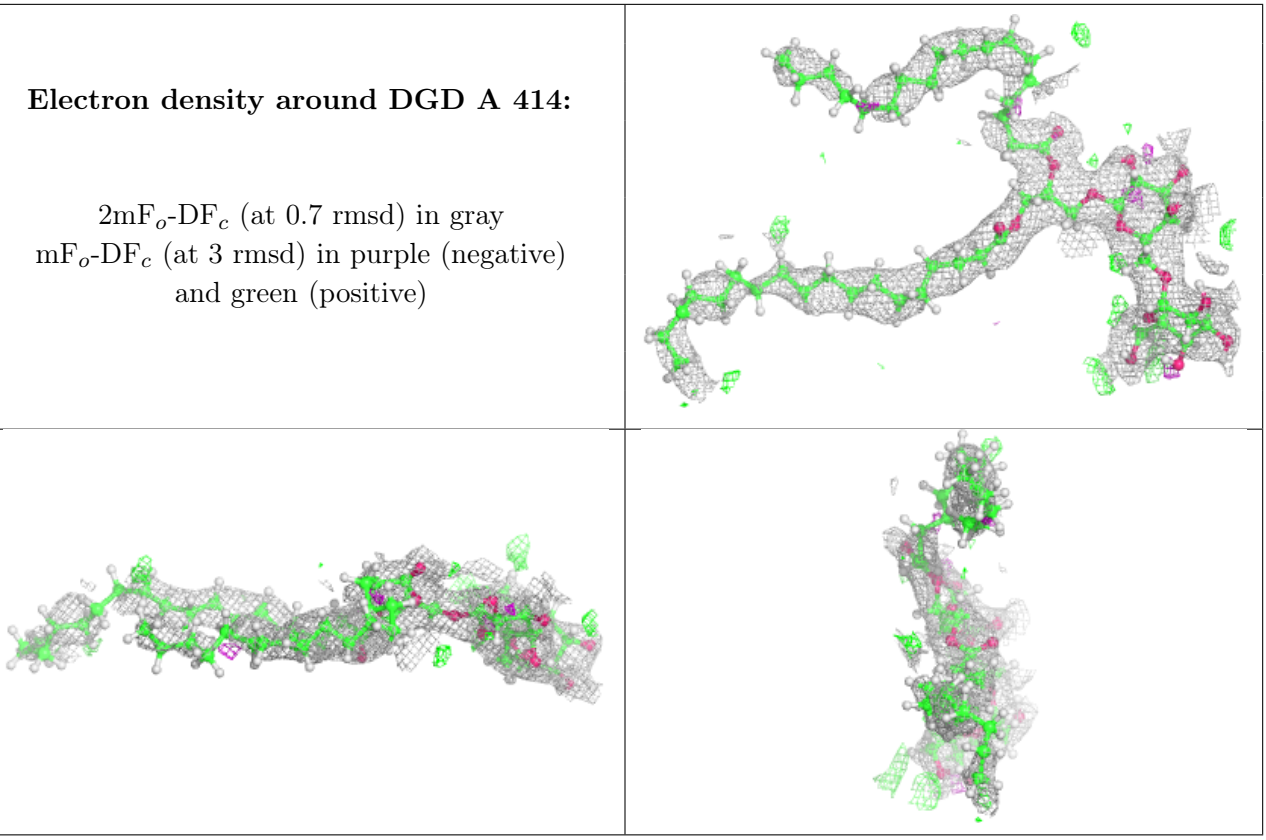
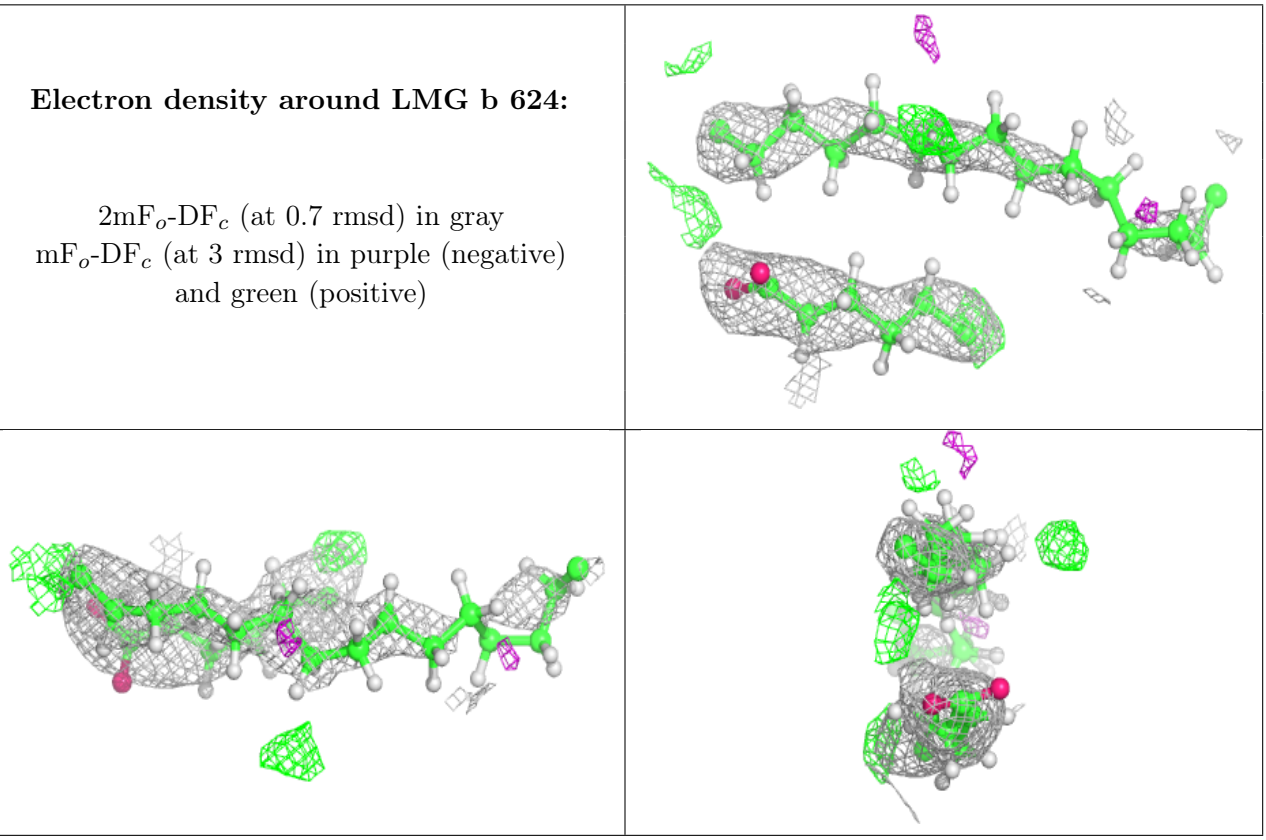
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



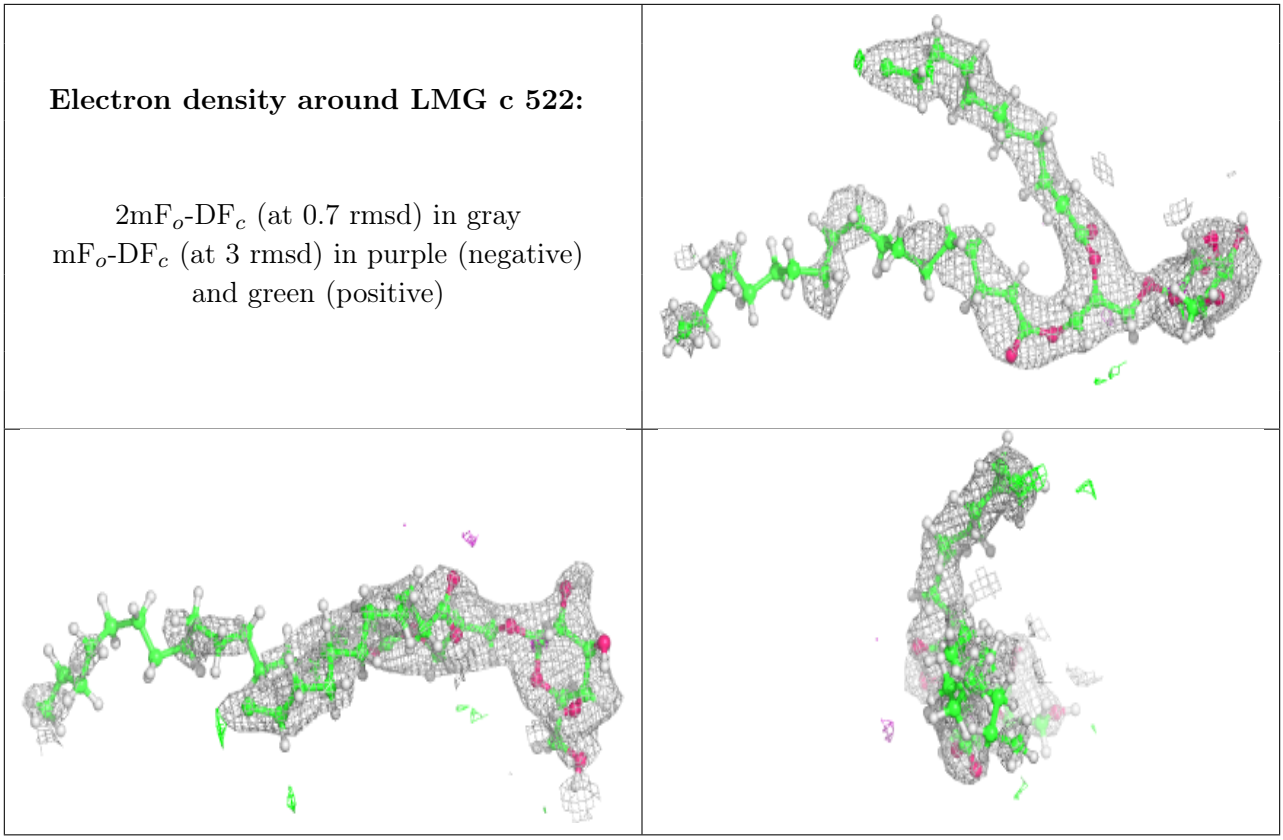
Electron density around LMG b 624:

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



Electron density around LMG c 522:

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



Electron density around LMG b 623:

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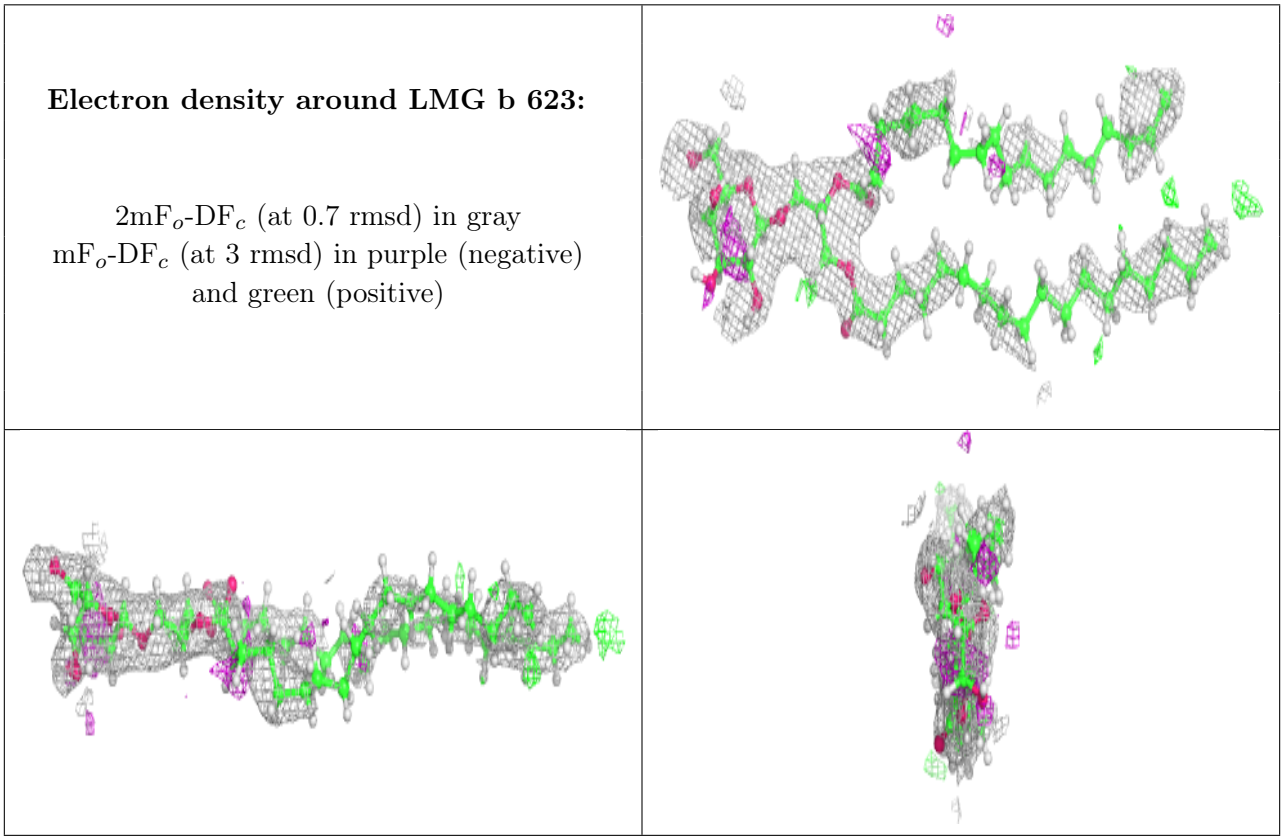
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD o 301:

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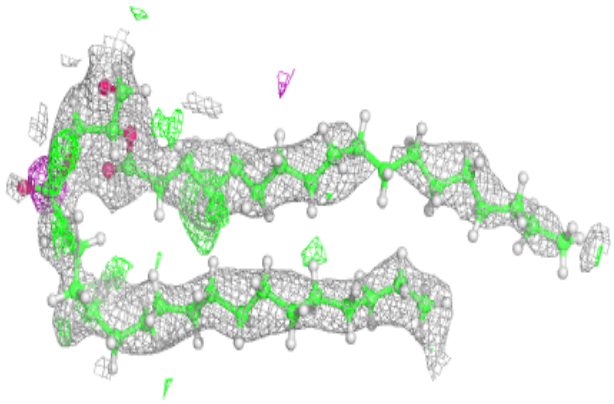
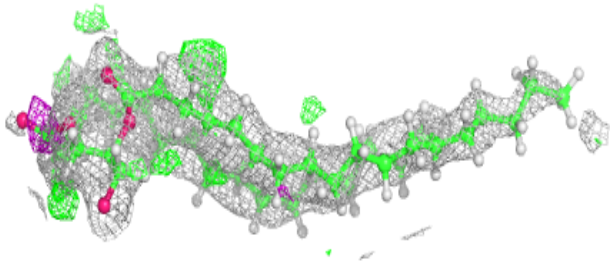
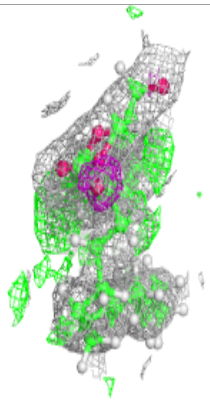
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

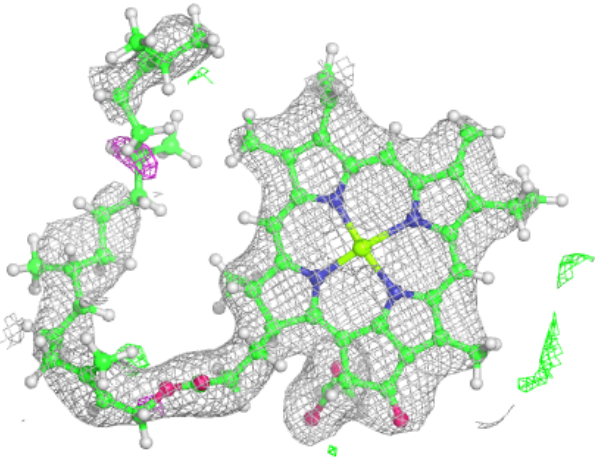


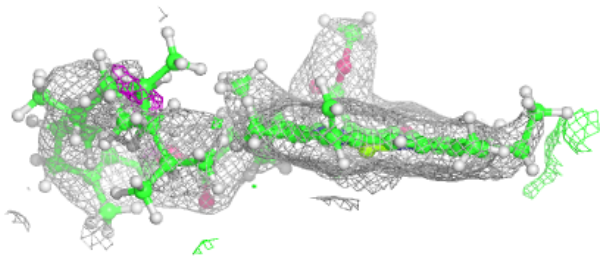


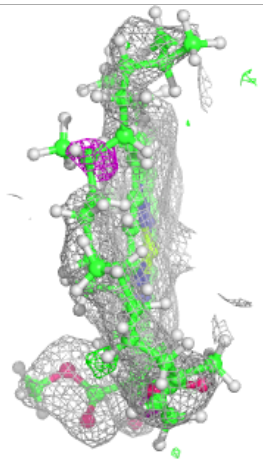


Electron density around CLA c 512:

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

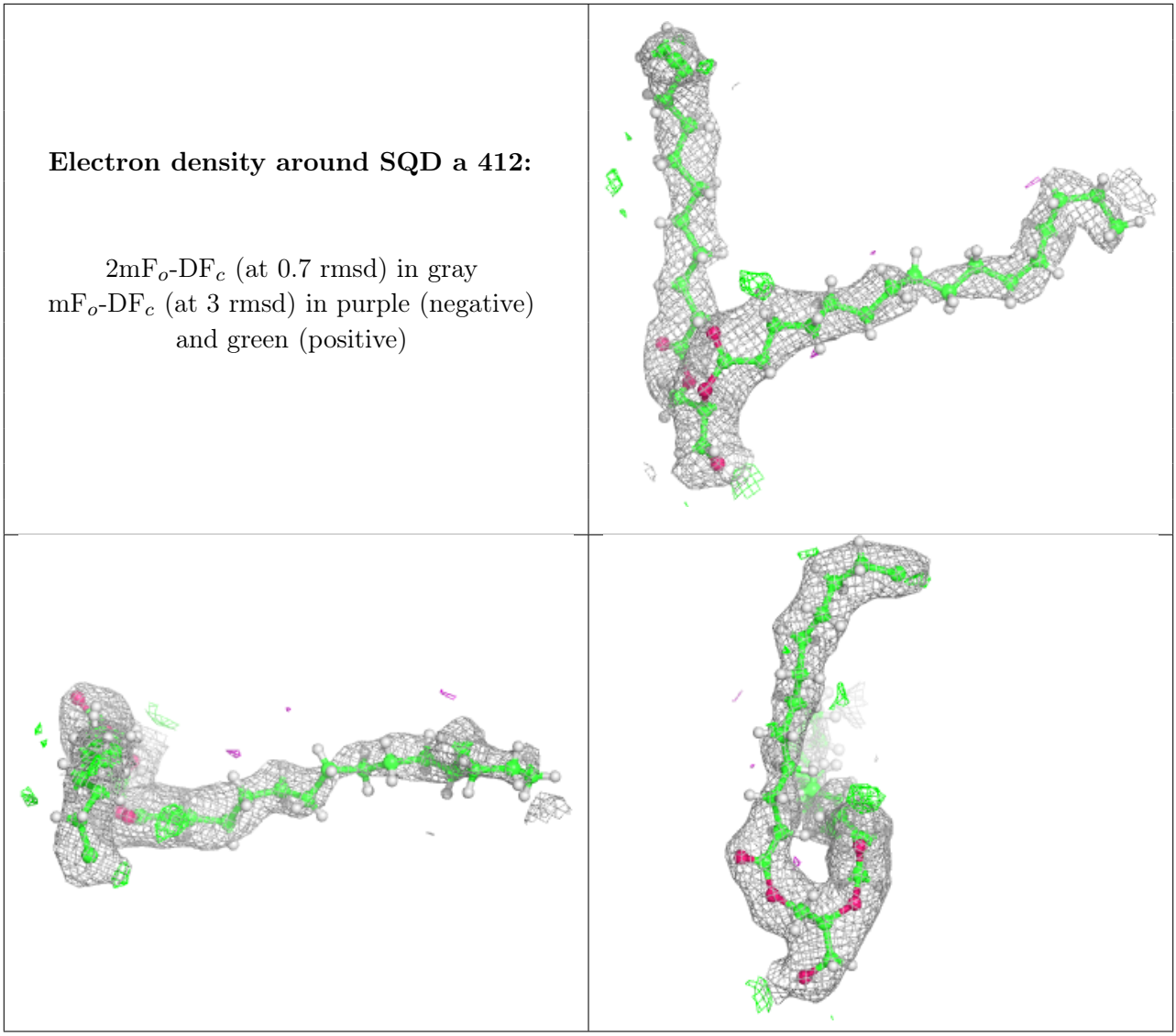






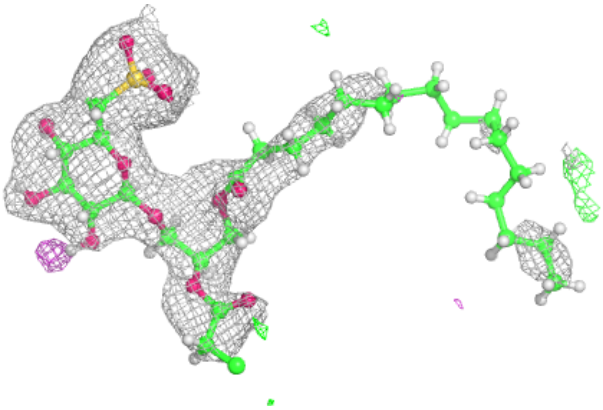
Electron density around SQD a 412:

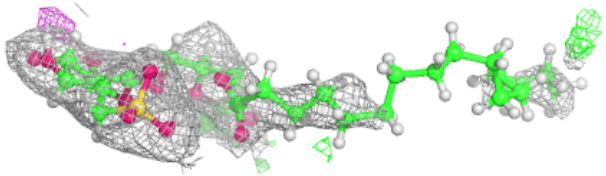
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

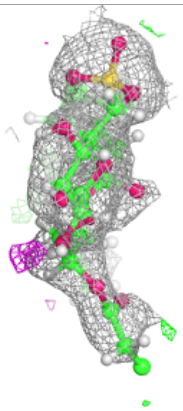


Electron density around SQD f 101:

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

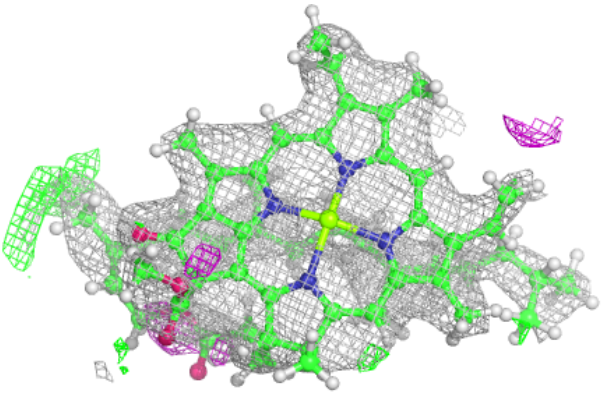


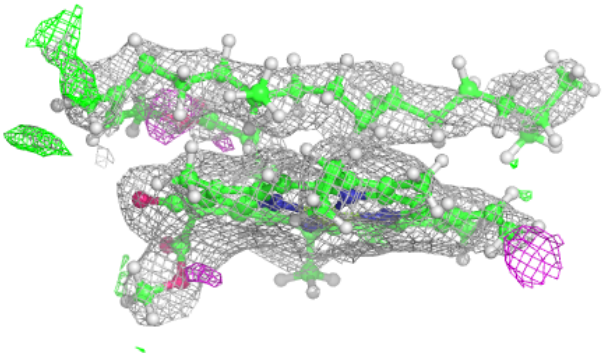




Electron density around CLA b 602:

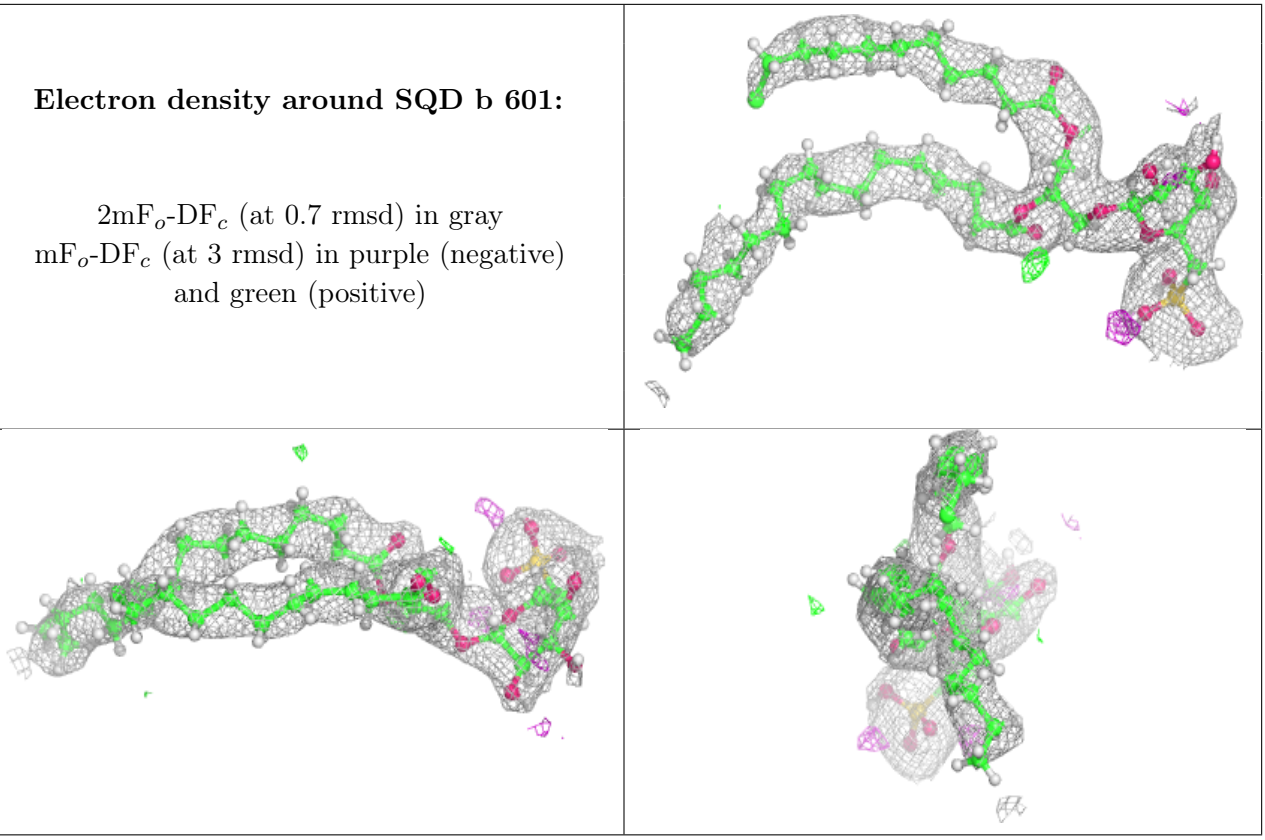
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





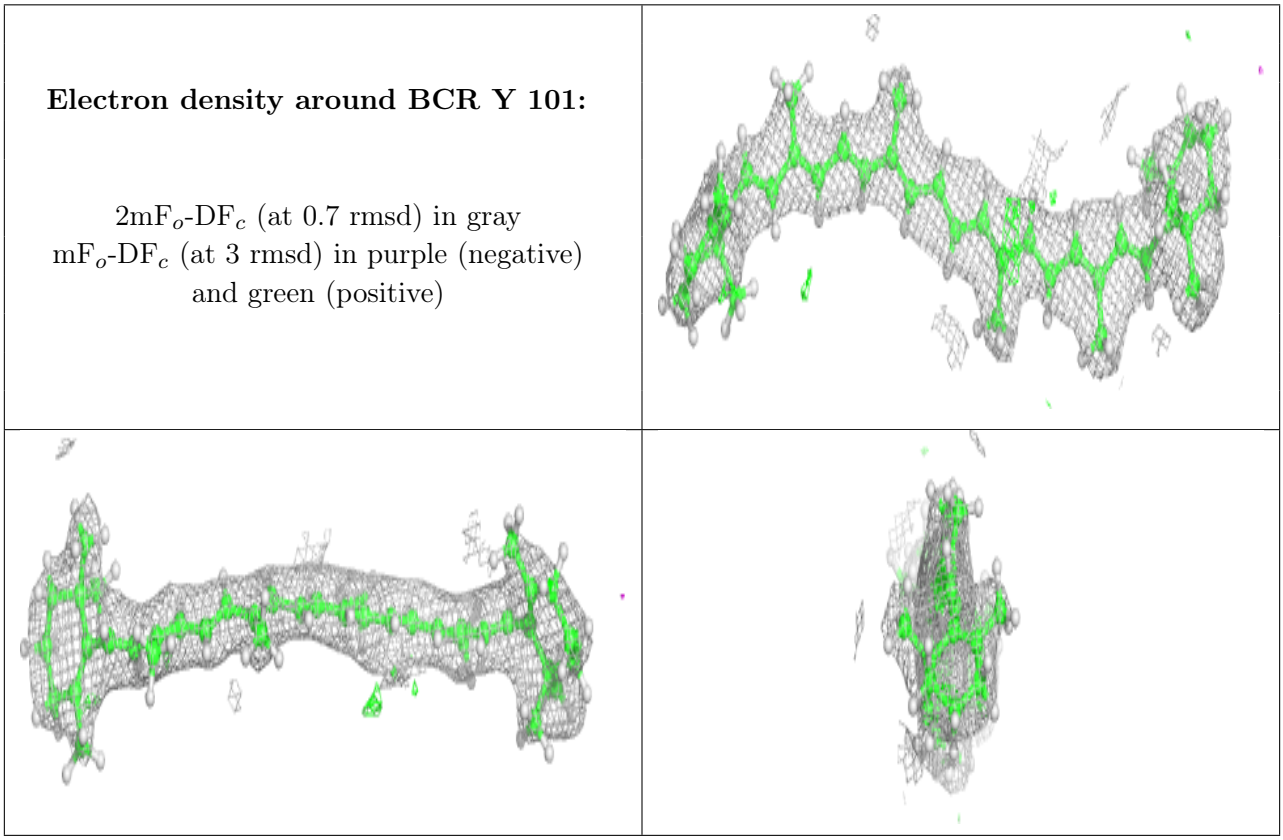
Electron density around SQD b 601:

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



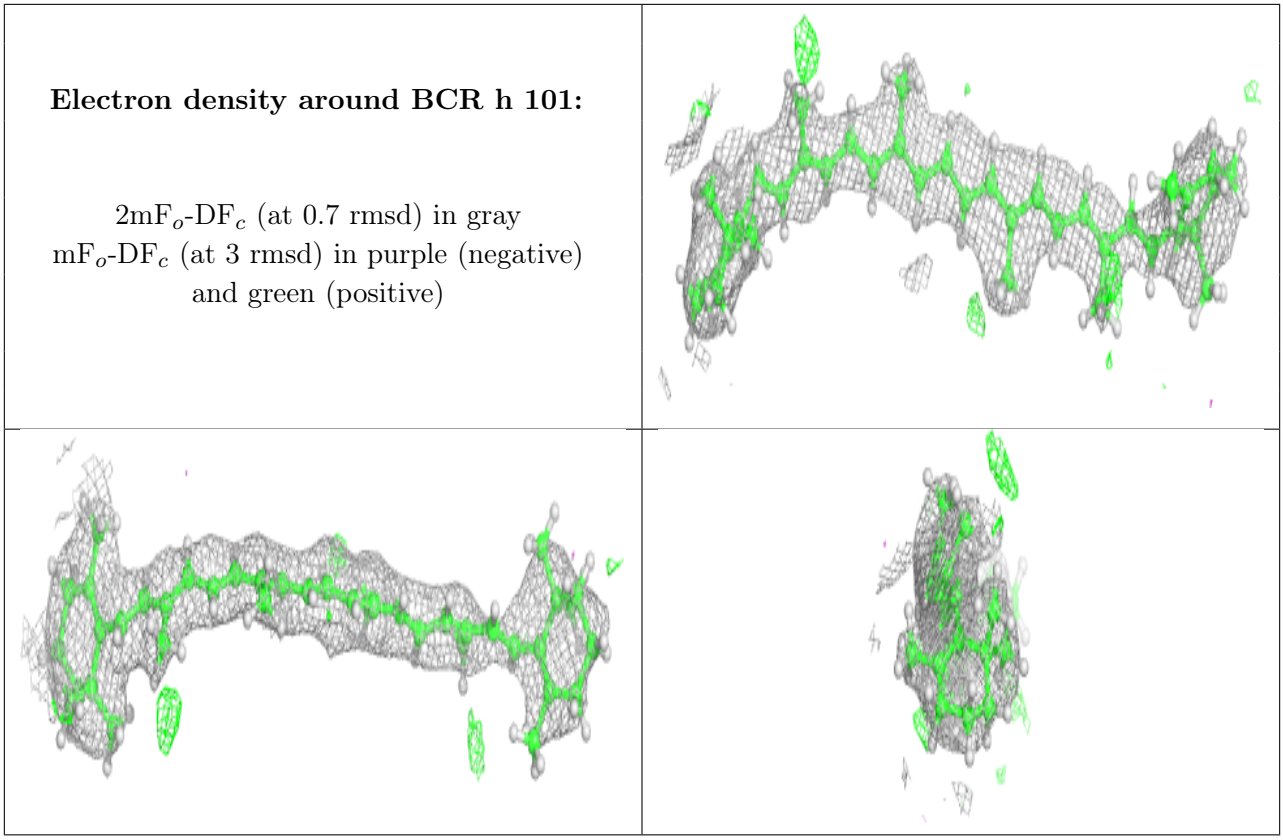
Electron density around BCR Y 101:

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



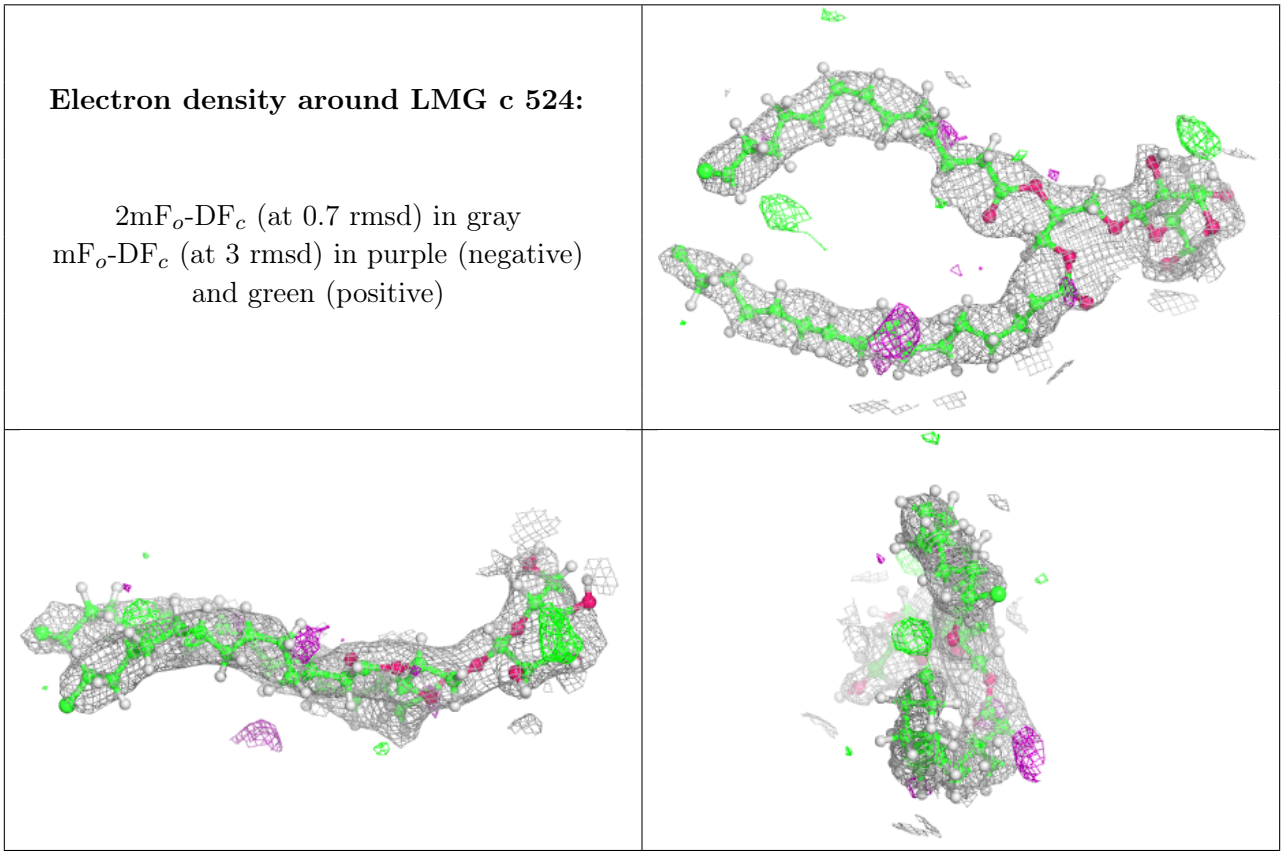
Electron density around BCR h 101:

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



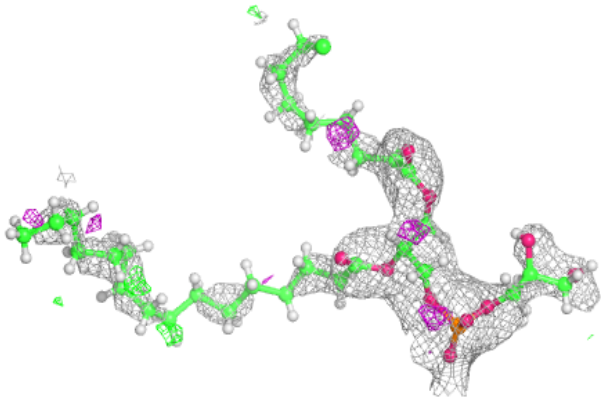
Electron density around LMG c 524:

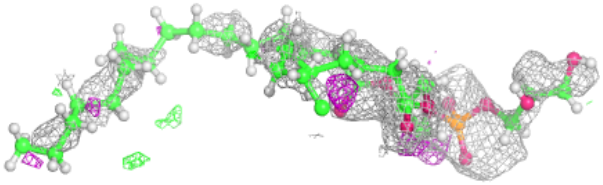
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

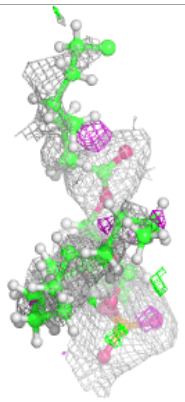


Electron density around LHG e 101:

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

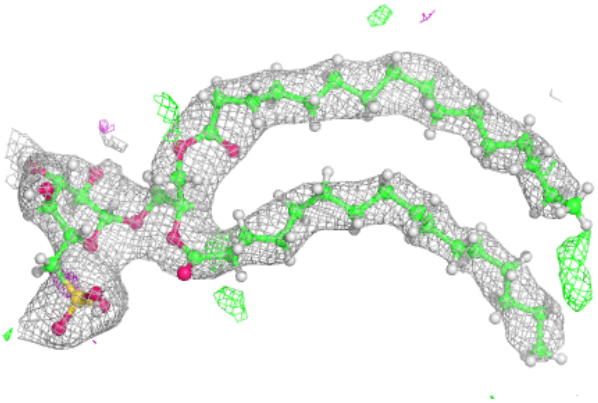


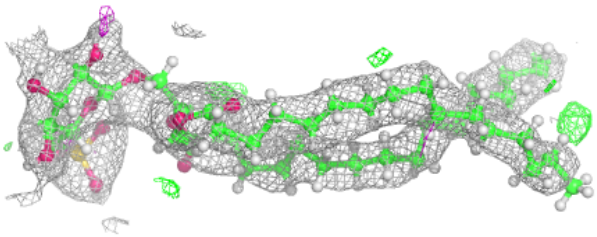


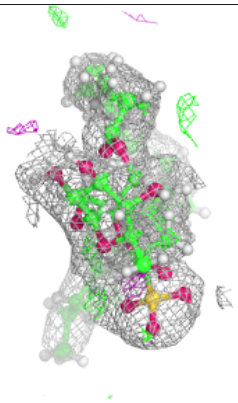


Electron density around SQD B 624:

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

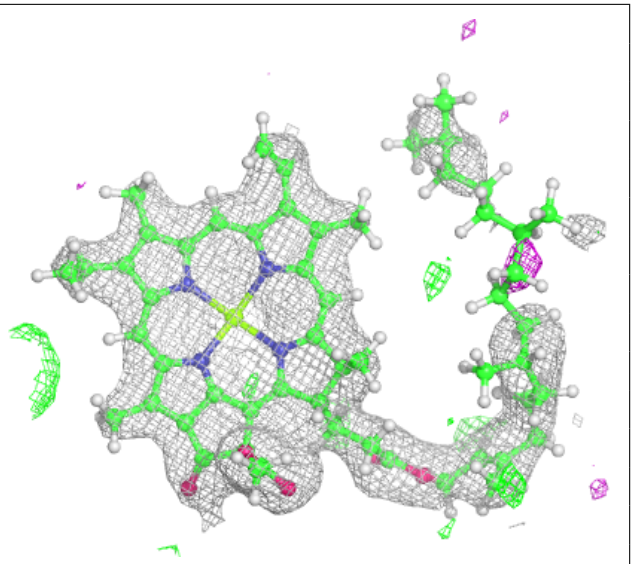


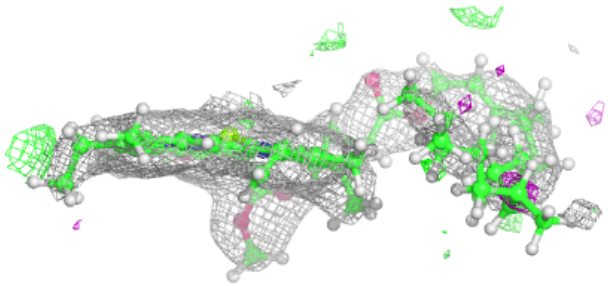


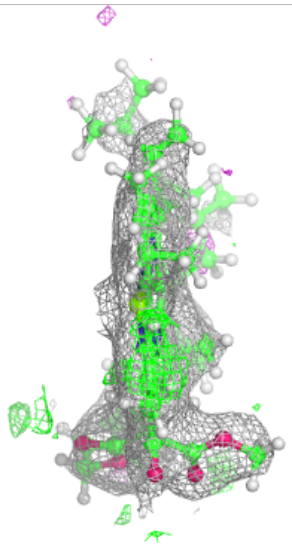


Electron density around CLA C 512:

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

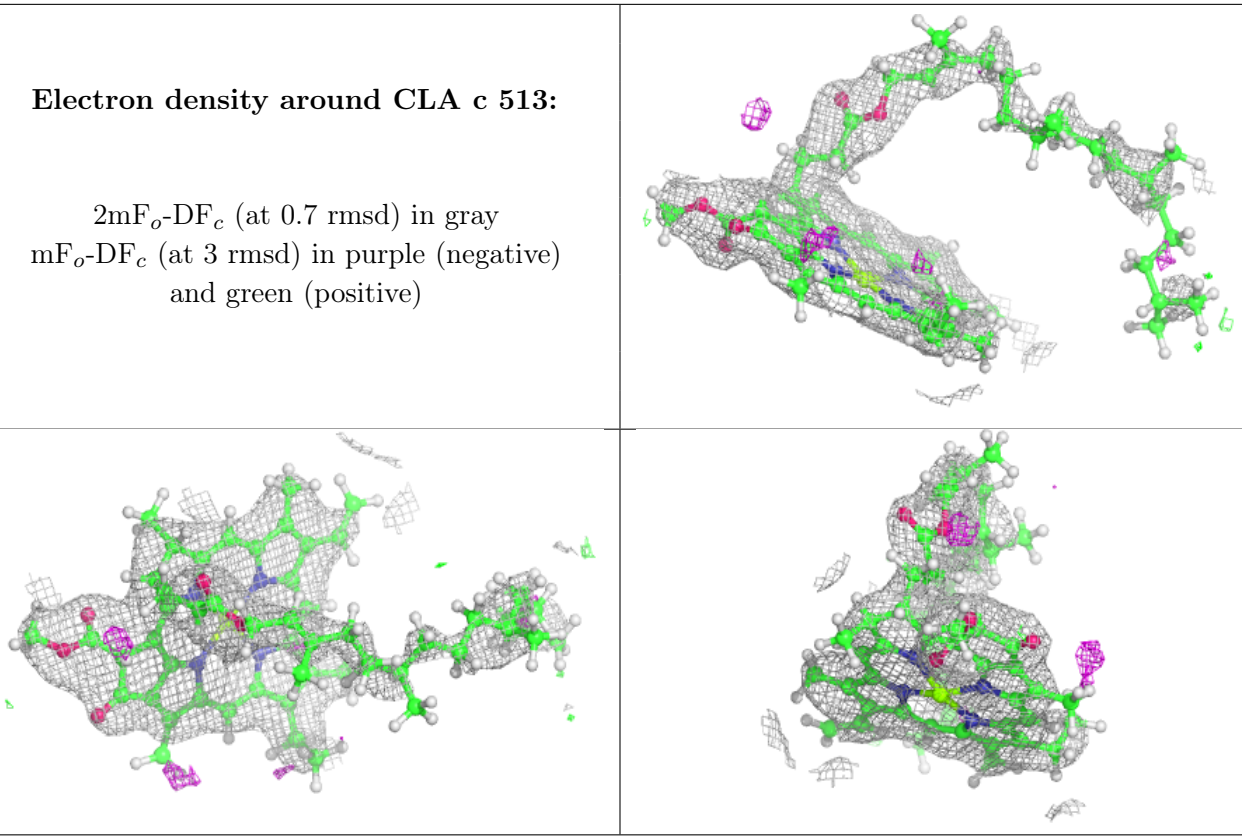






Electron density around CLA c 513:

$2mF_o$-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 C 513:

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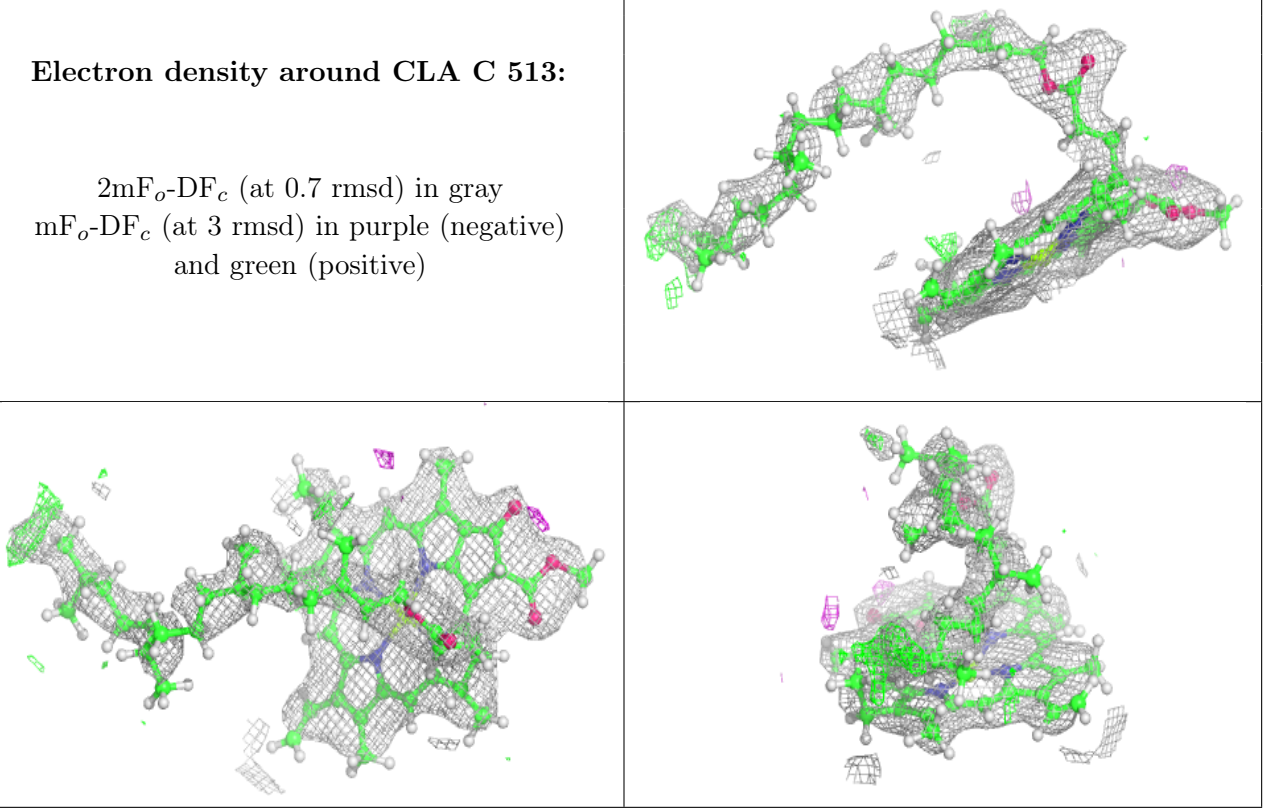
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 616:

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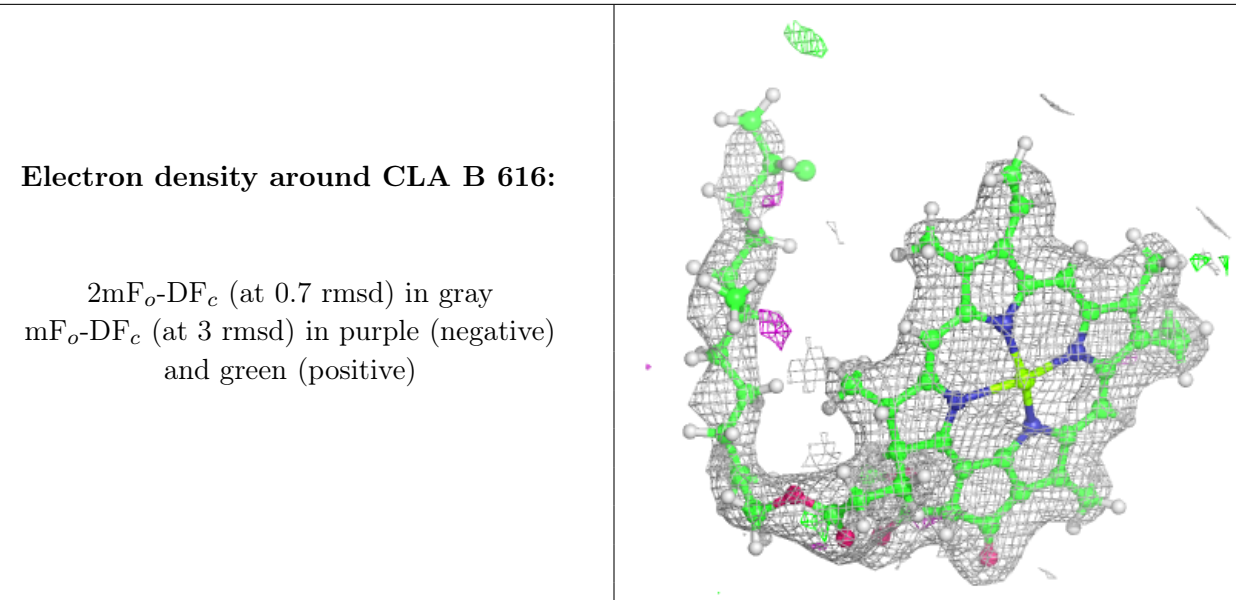
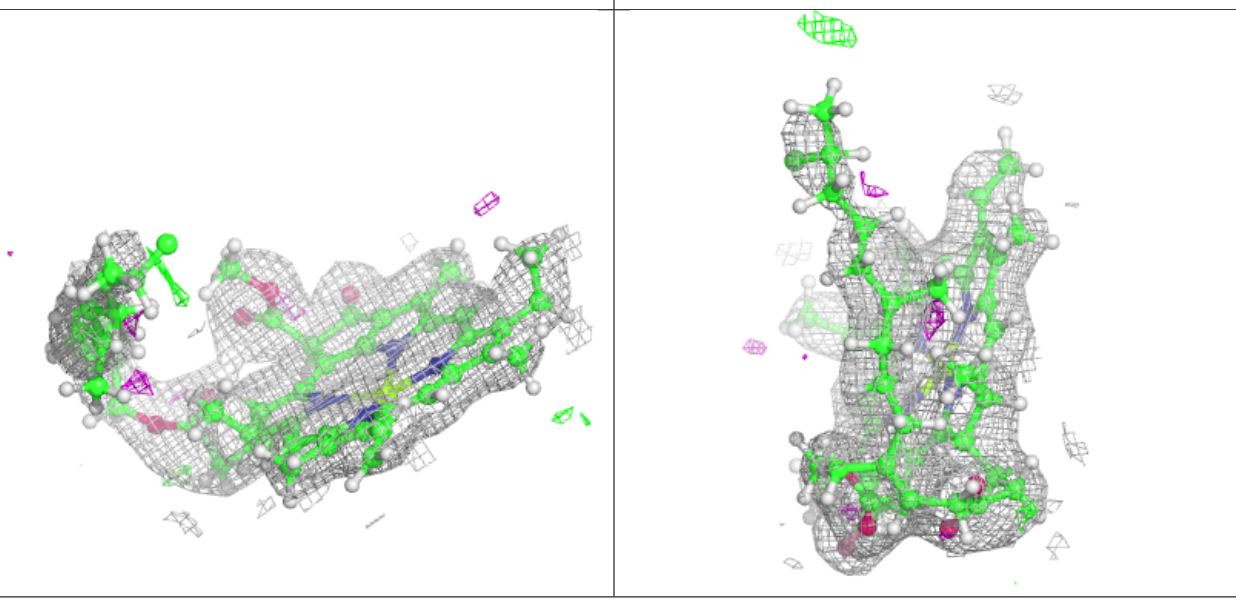
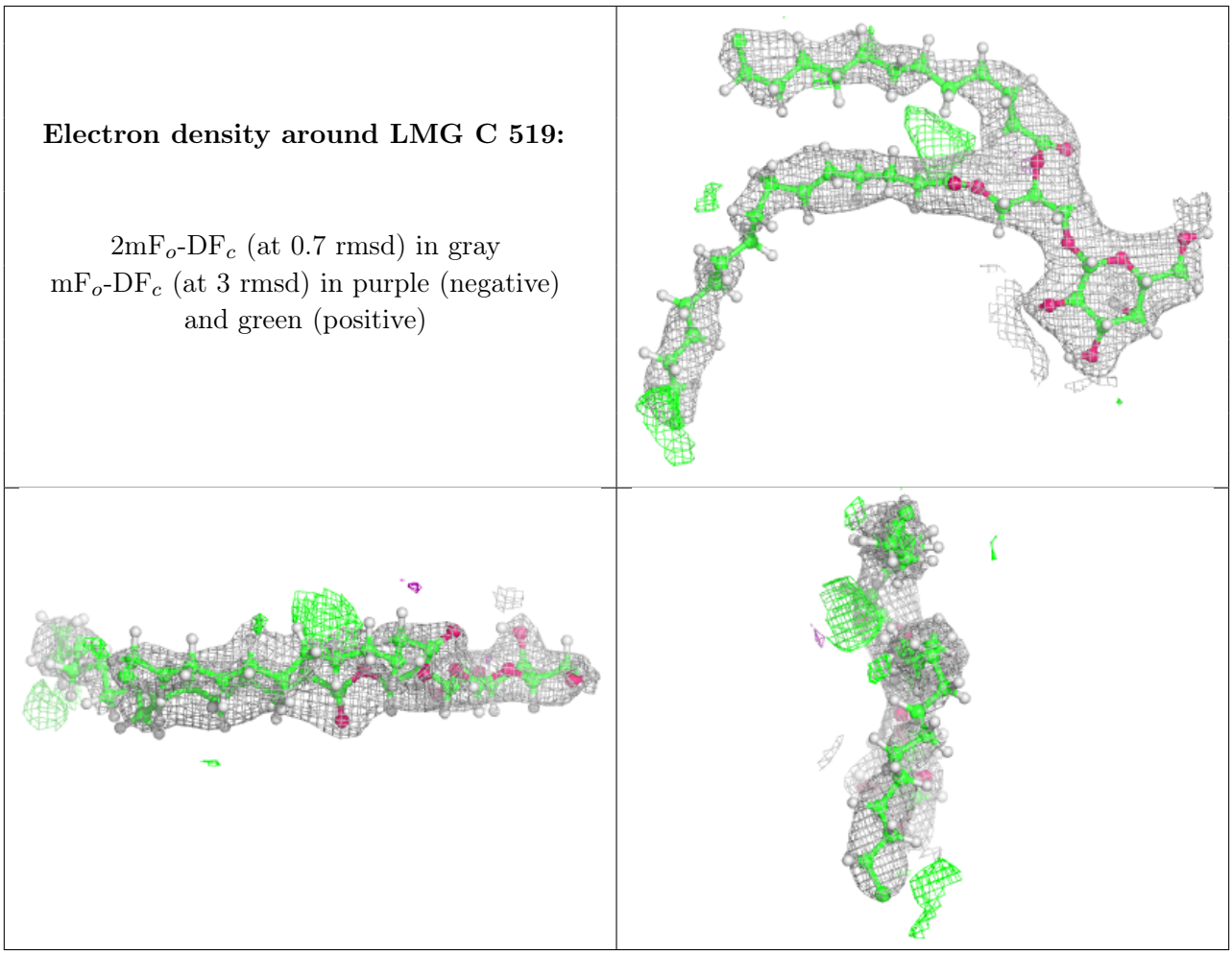
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





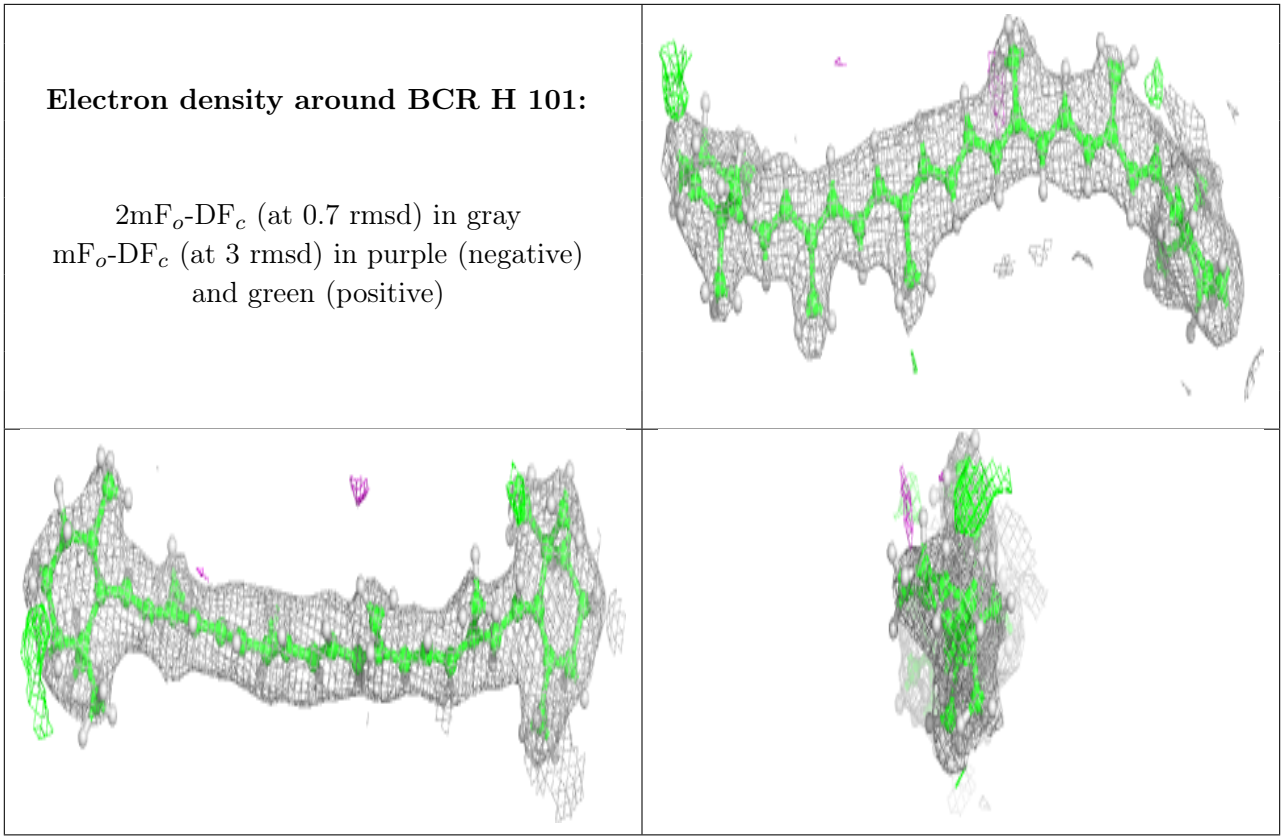
Electron density around LMG C 519:

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



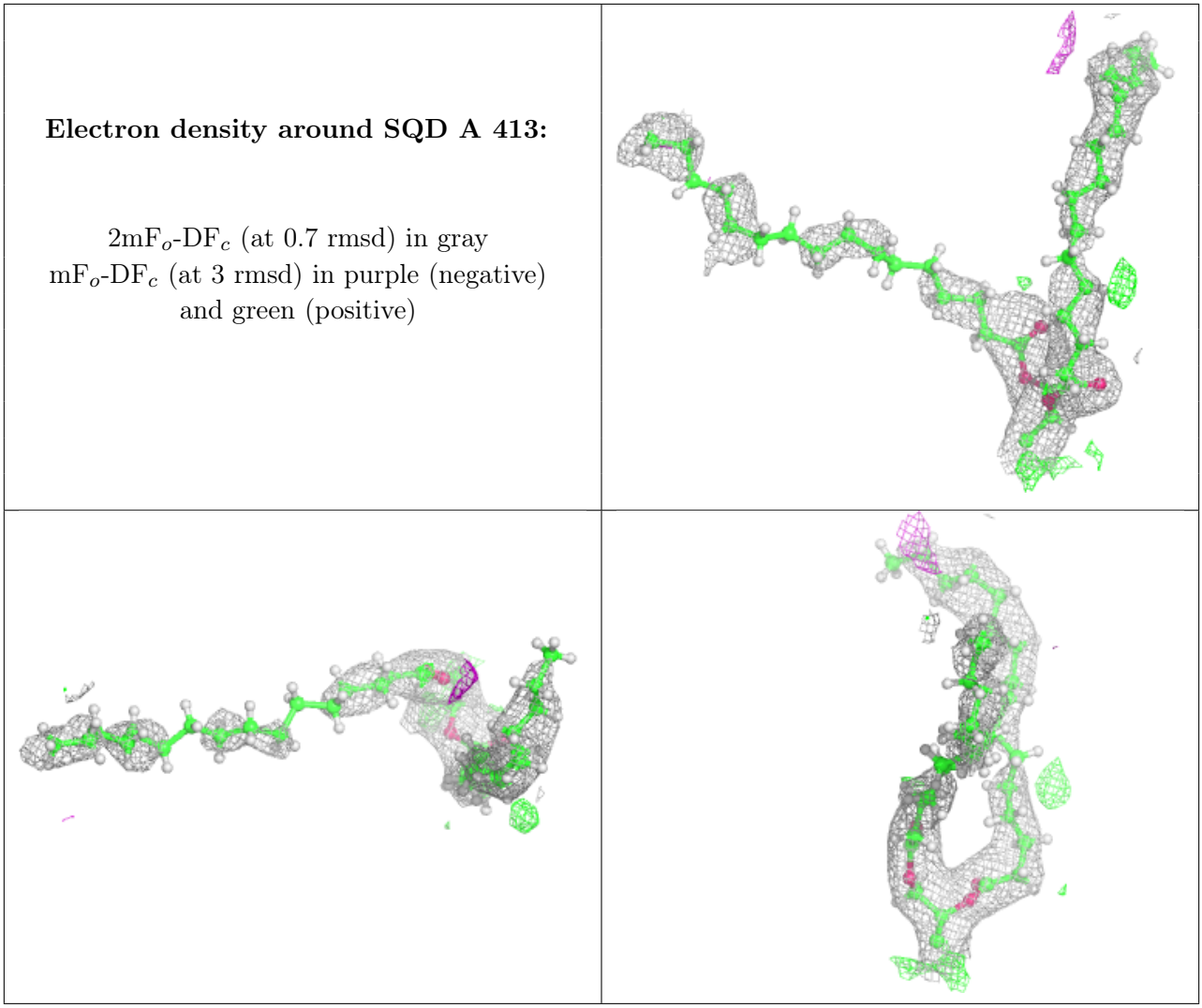
Electron density around BCR H 101:

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



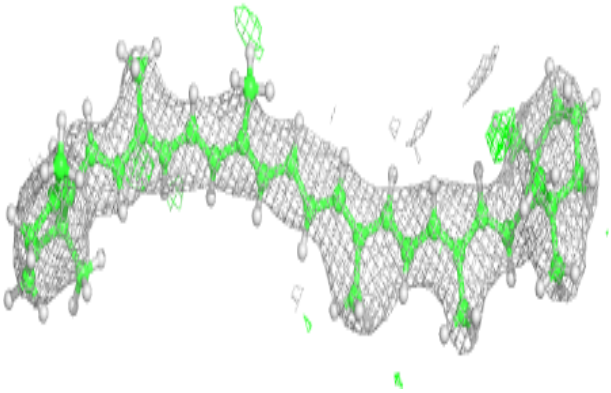
Electron density around SQD A 413:

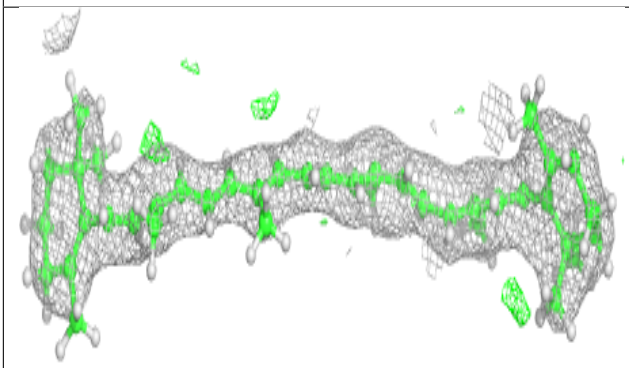
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

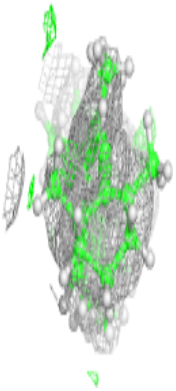


Electron density around 8CT k 101:

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

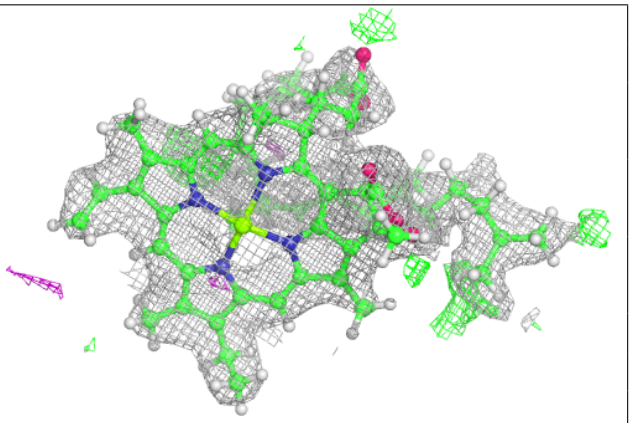


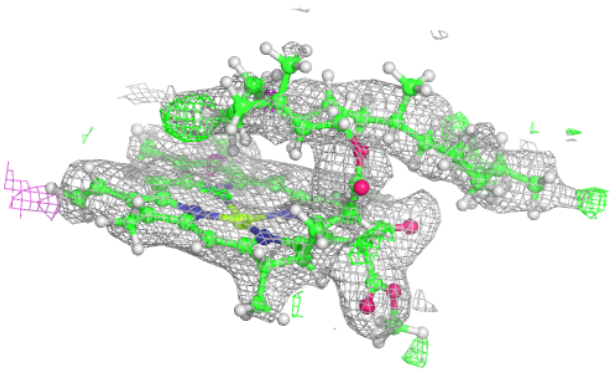


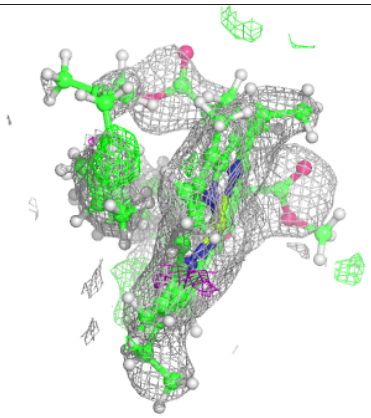


Electron density around CLA B 601:

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

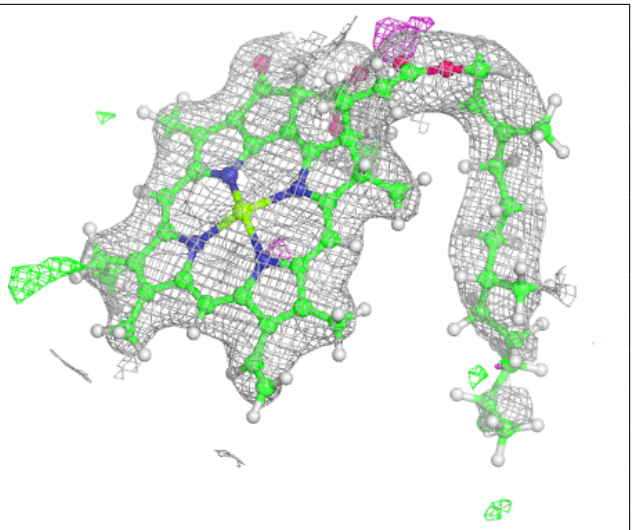


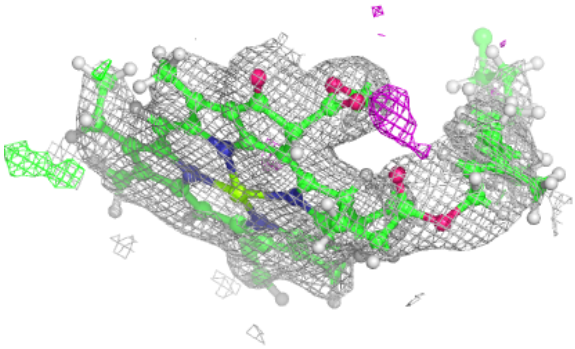


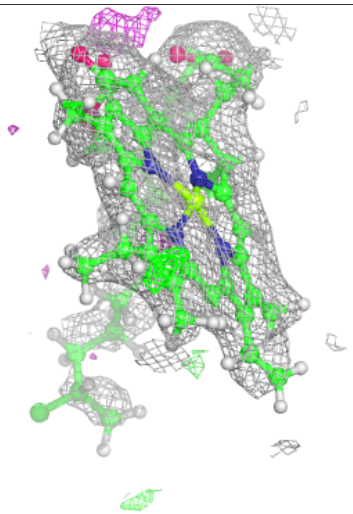


Electron density around CLA b 617:

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

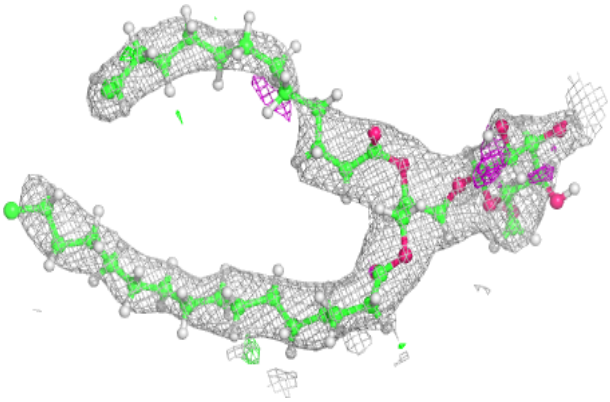


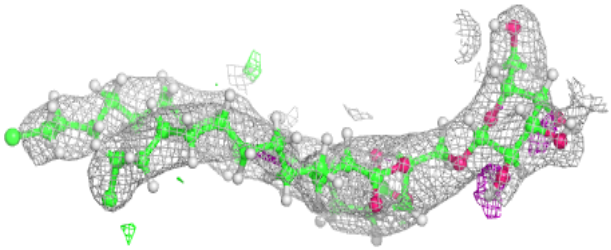


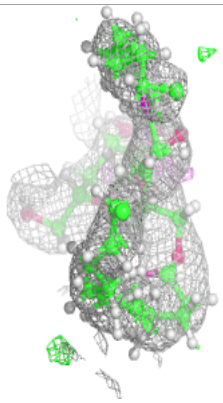


Electron density around LMG A 410:

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

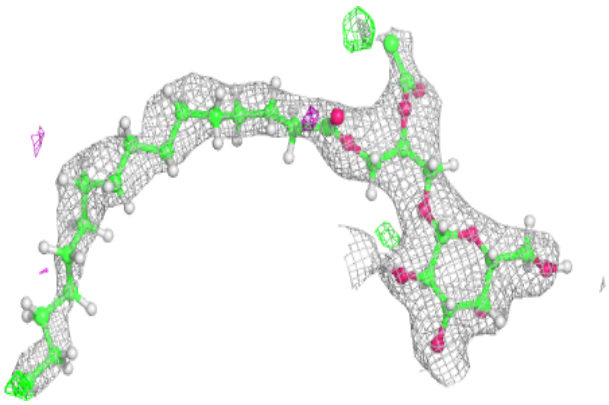


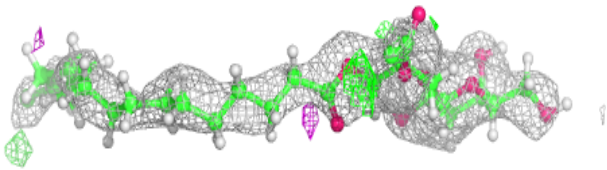


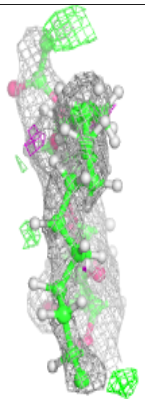


Electron density around LMG c 519:

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

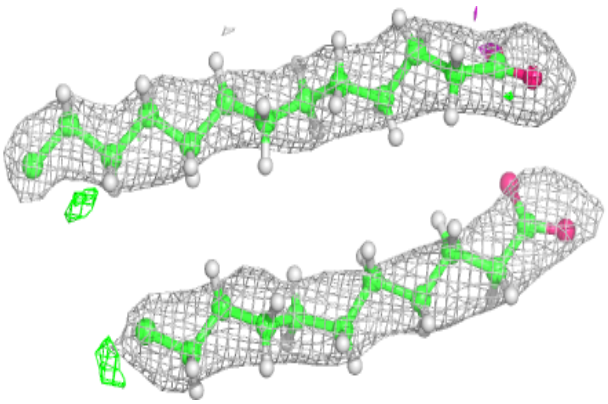


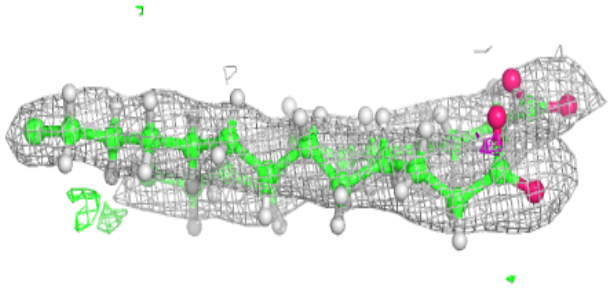


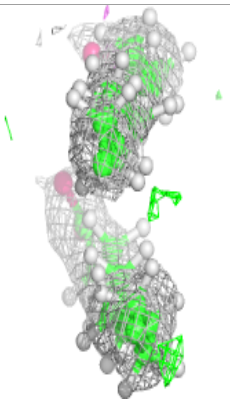


Electron density around LMG B 622:

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

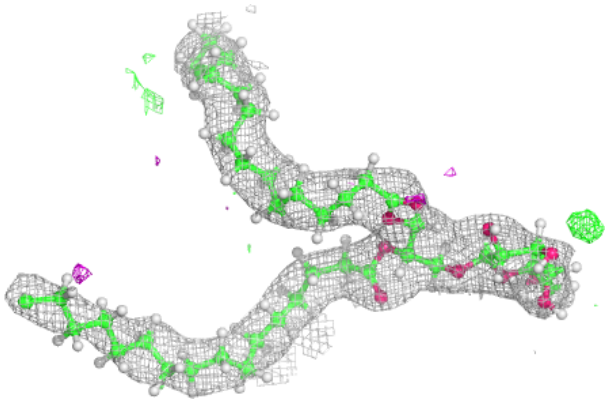


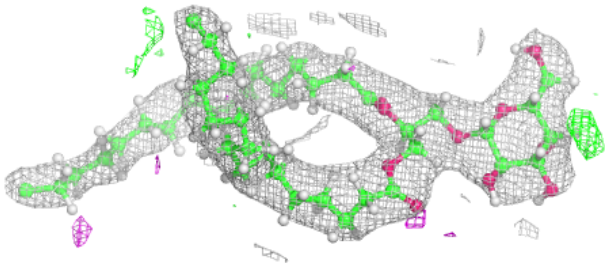


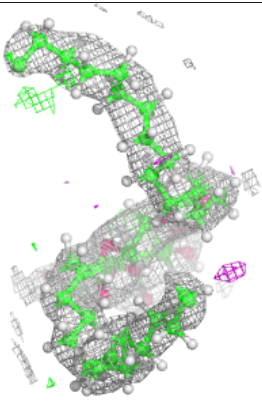


Electron density around LMG b 621:

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

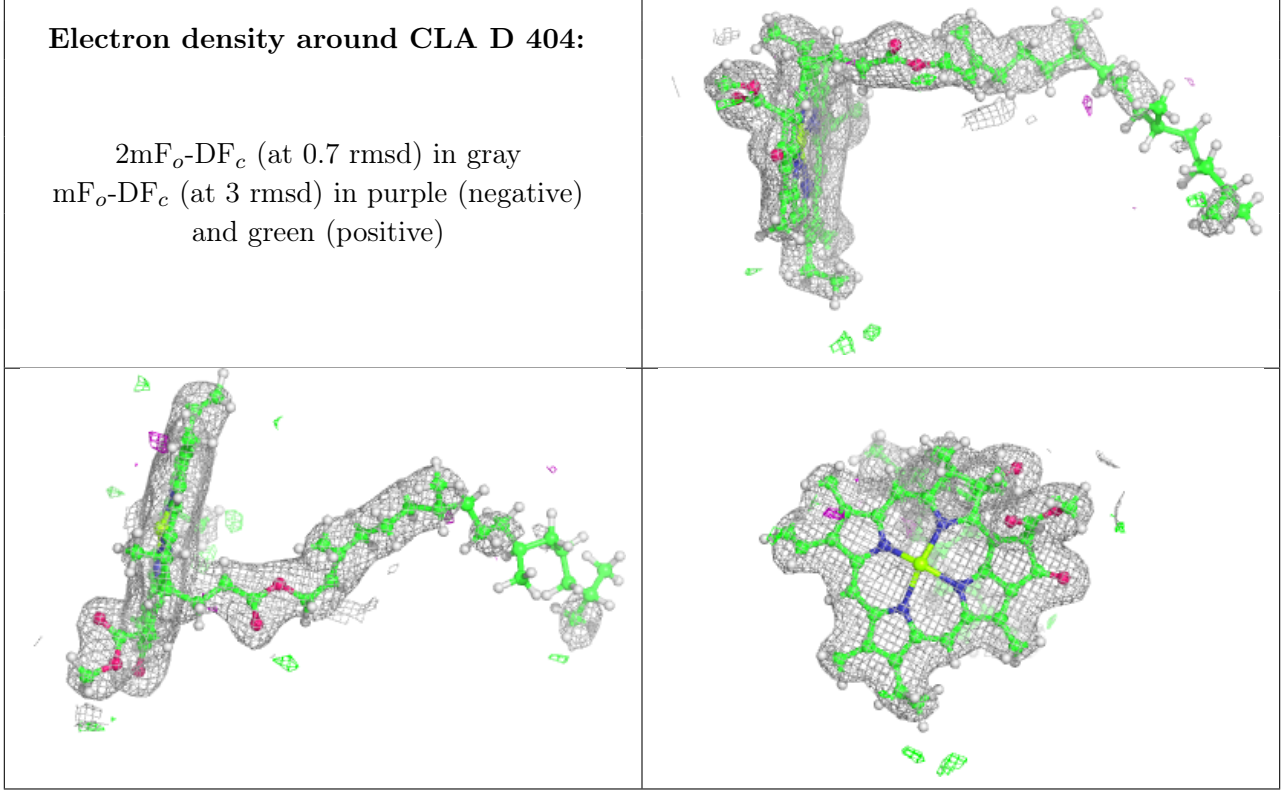






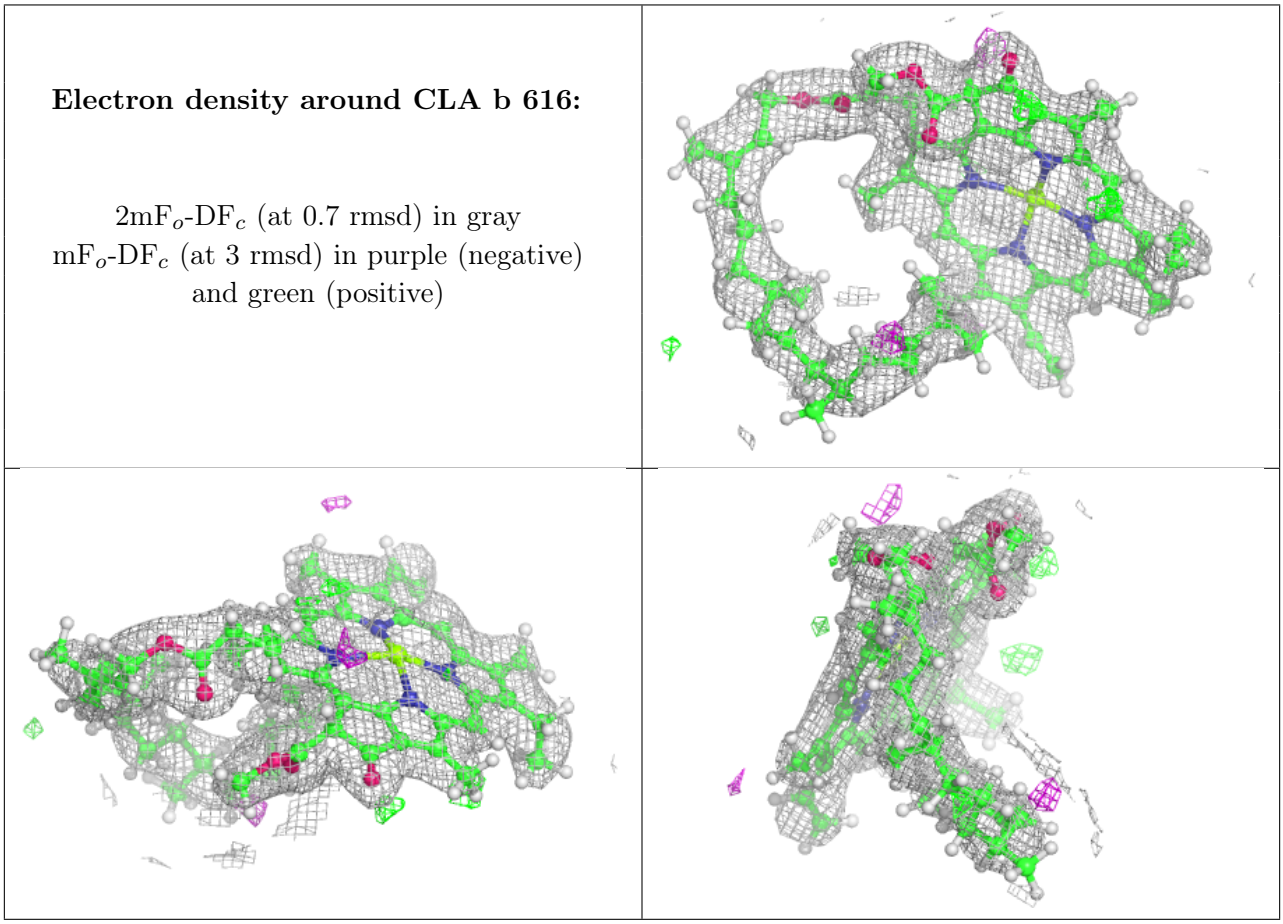
Electron density around CLA D 404:

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



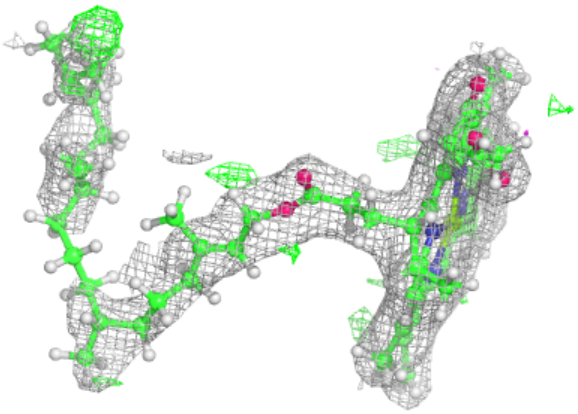
Electron density around CLA b 616:

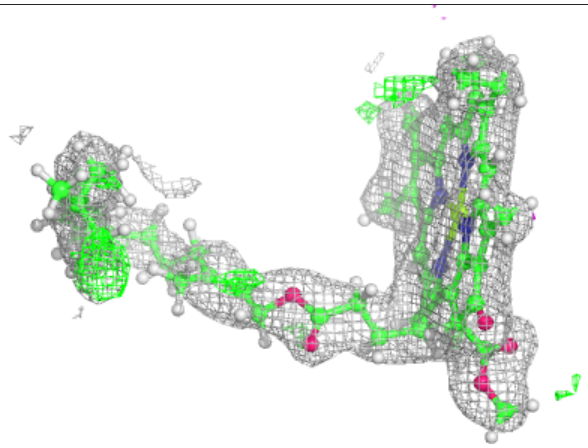
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

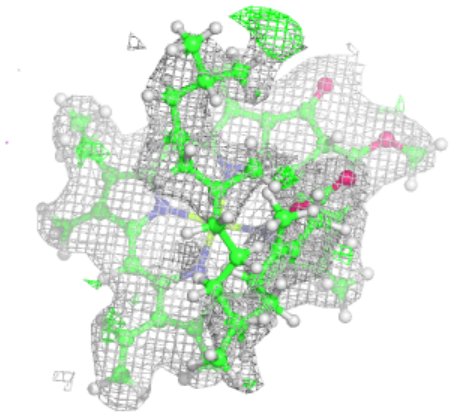


Electron density around CLA a 408:

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

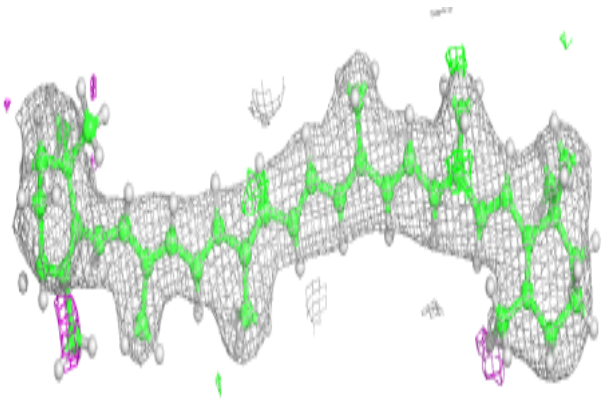


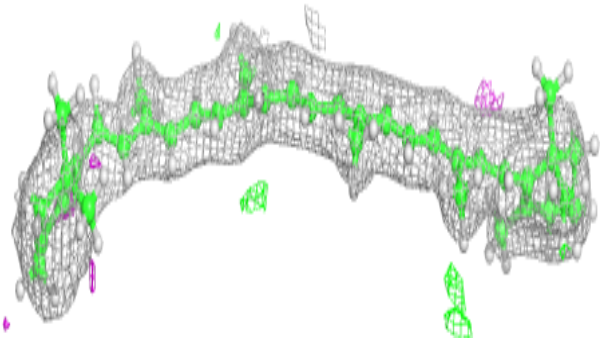


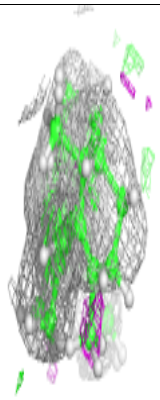


Electron density around 8CT D 405:

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

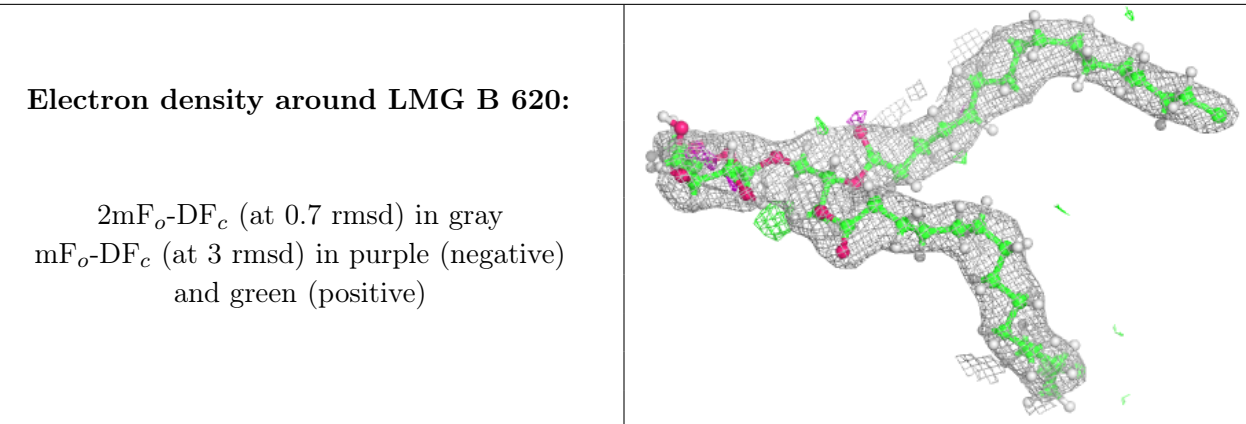






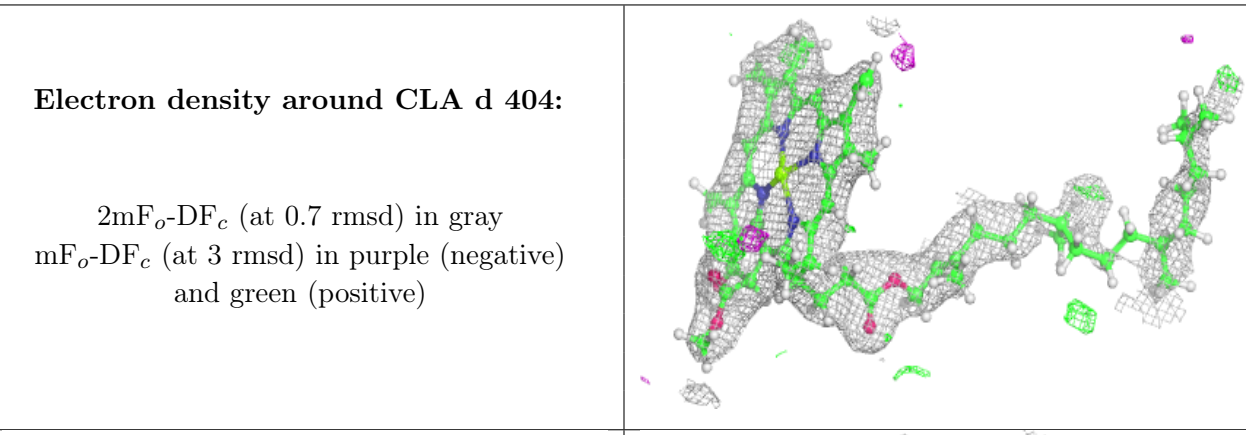
Electron density around LMG B 620:

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



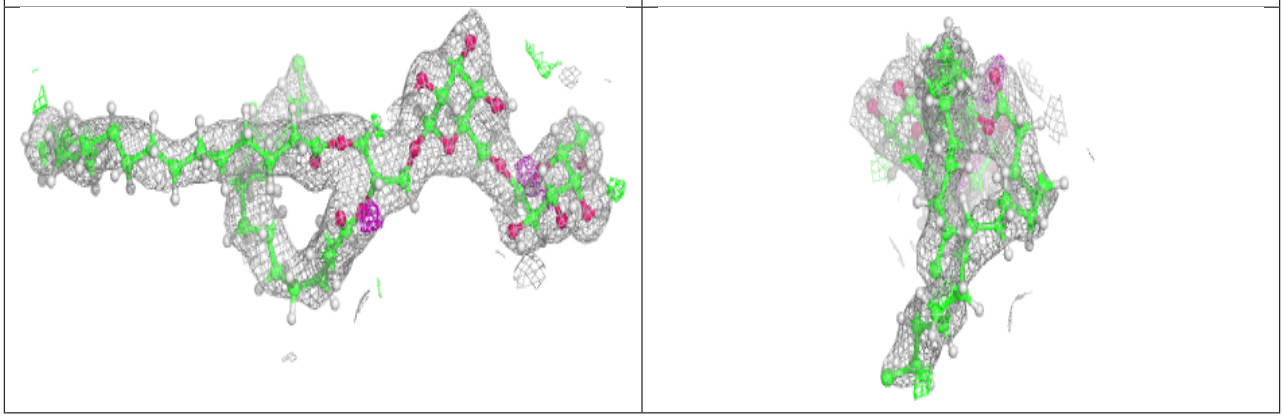
Electron density around CLA d 404:

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



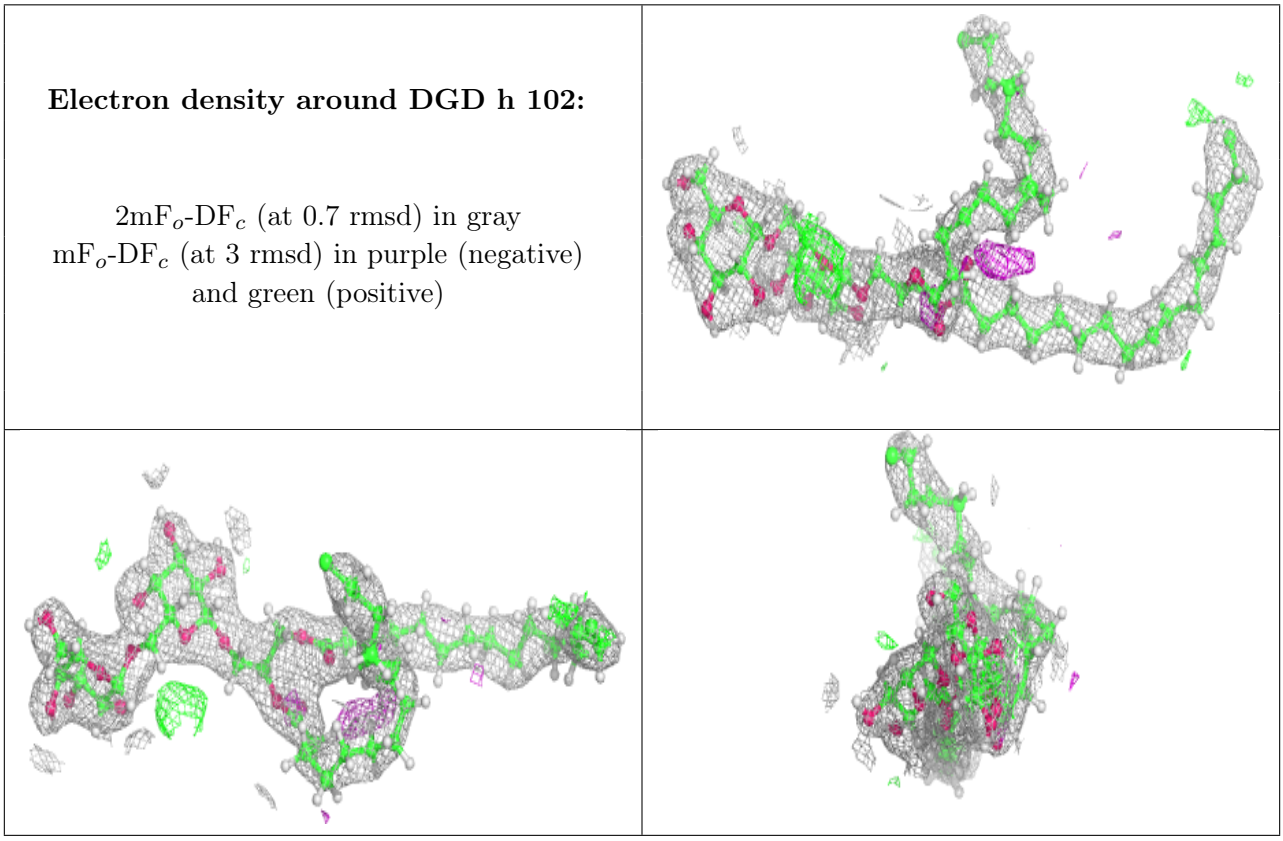
Electron density around DGD H 102:

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



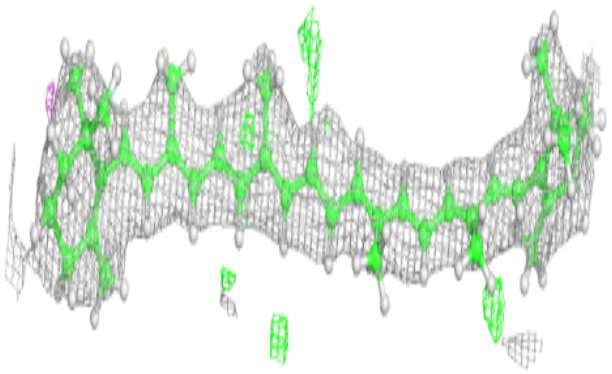
Electron density around DGD h 102:

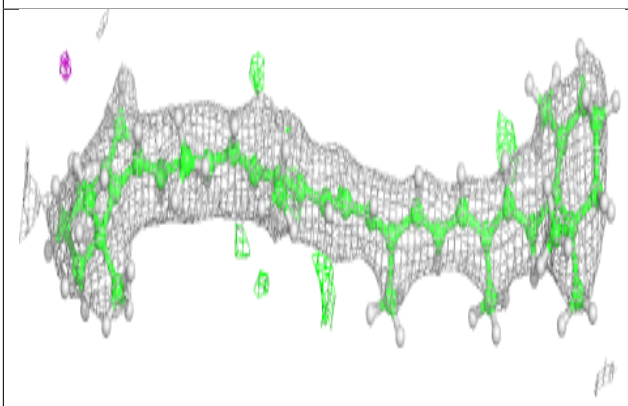
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

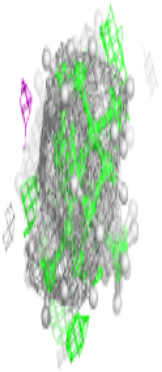


Electron density around 8CT C 514:

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

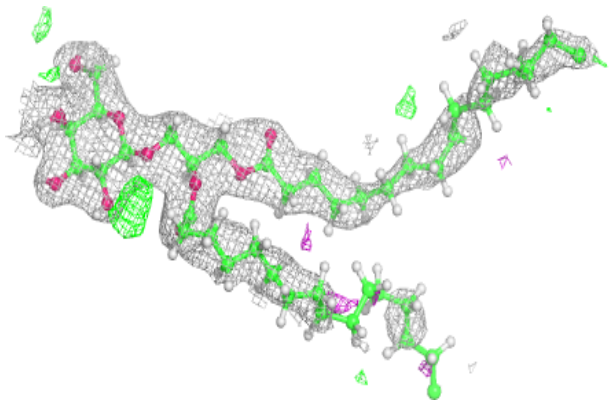


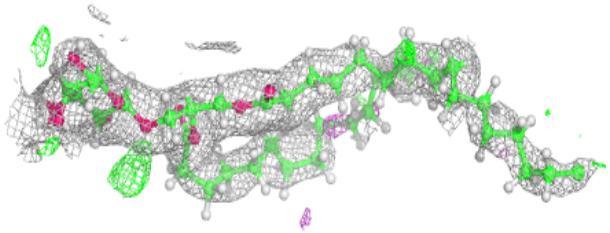




Electron density around LMG D 407:

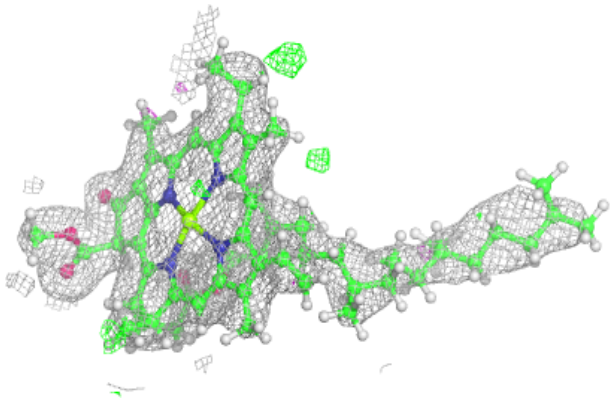
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

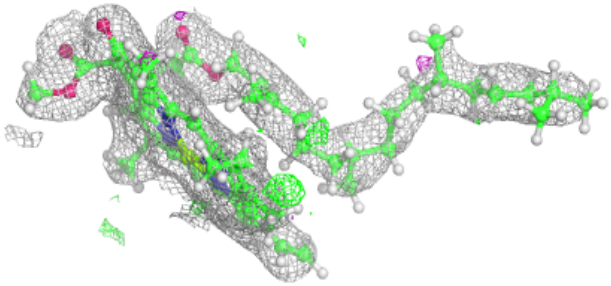


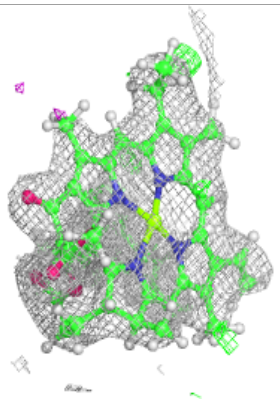


Electron density around CLA C 505:

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

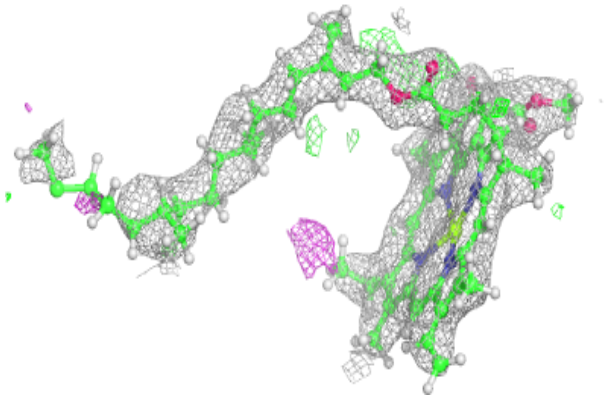


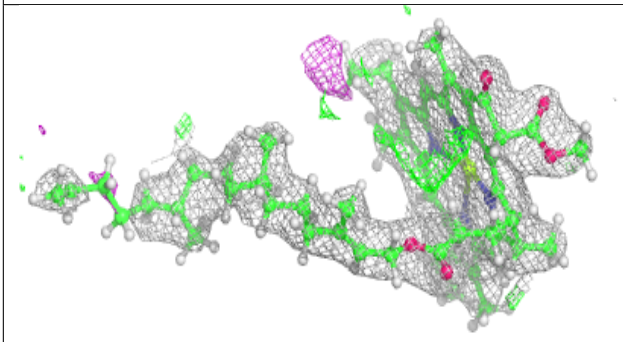


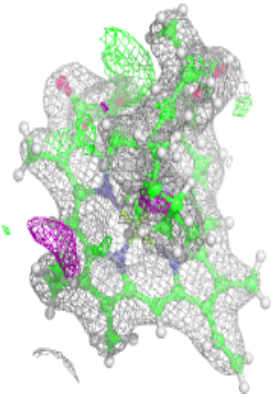


Electron density around CLA c 508:

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

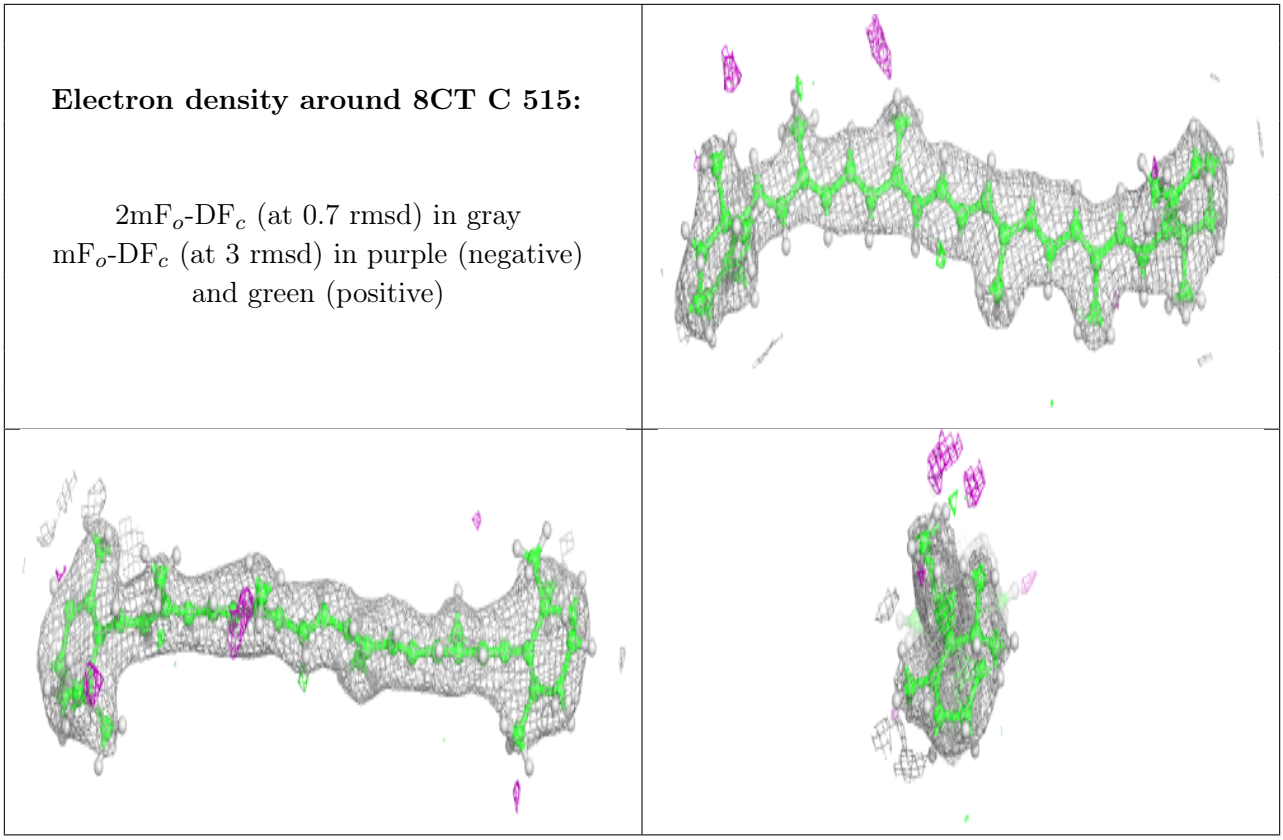






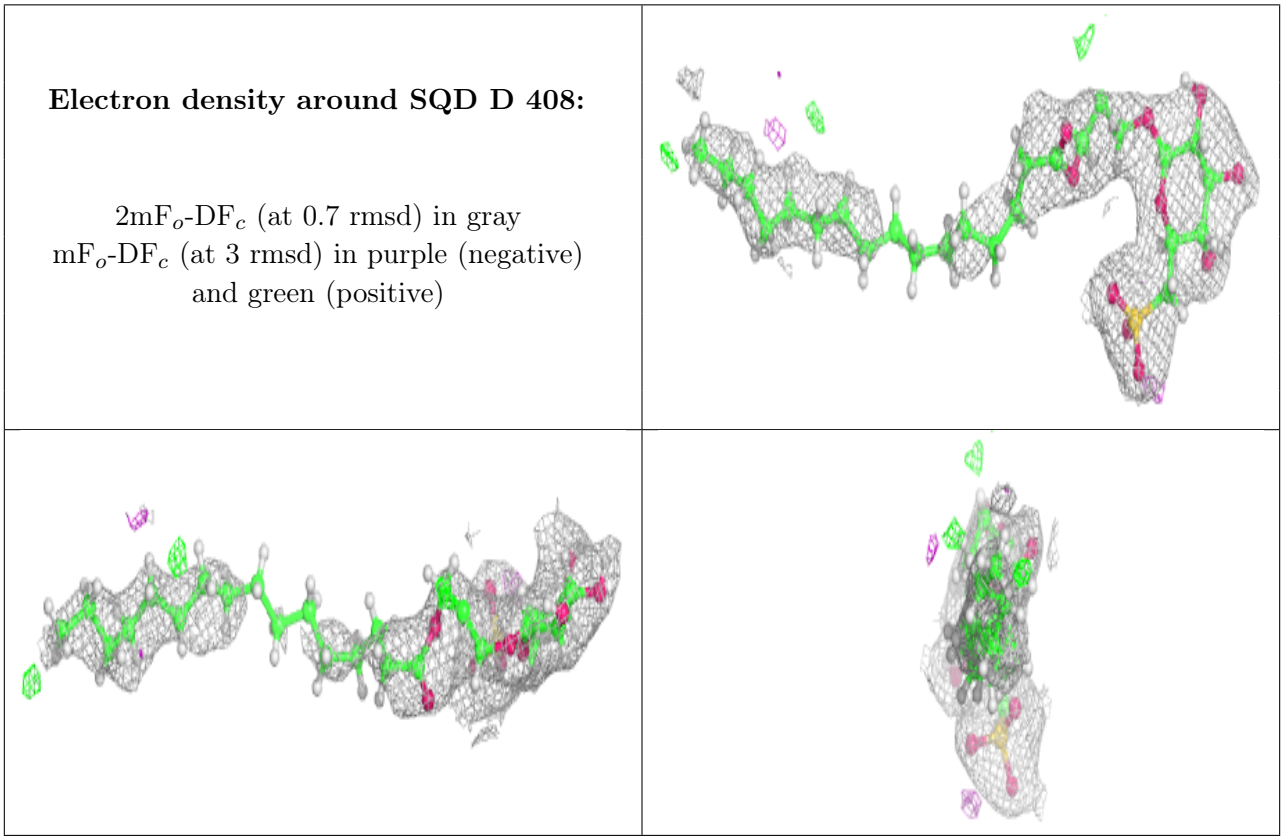
Electron density around 8CT C 515:

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



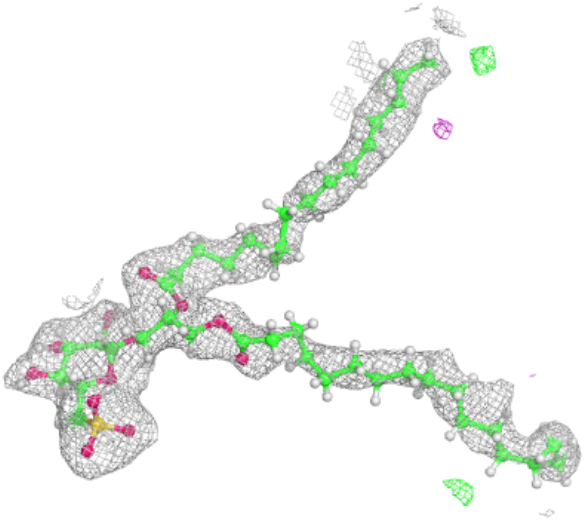
Electron density around SQD D 408:

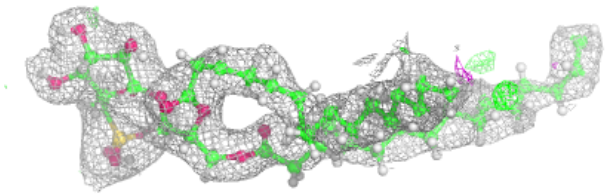
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD a 411:

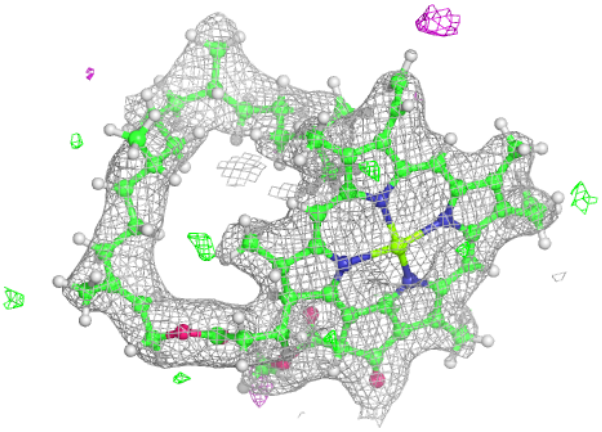
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

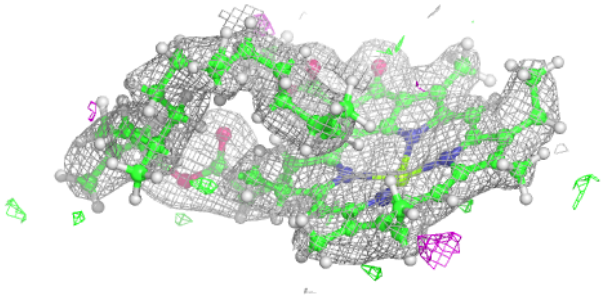


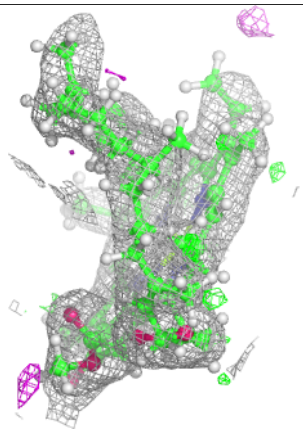


Electron density around CLA B 615:

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

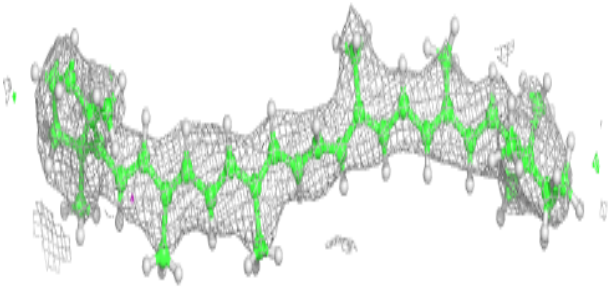


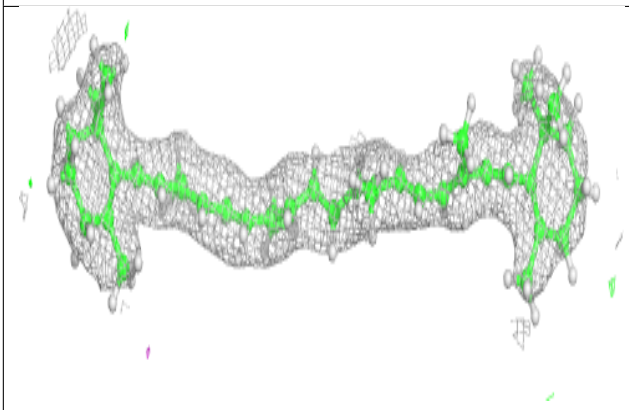


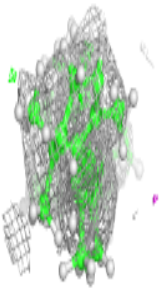


Electron density around 8CT c 514:

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

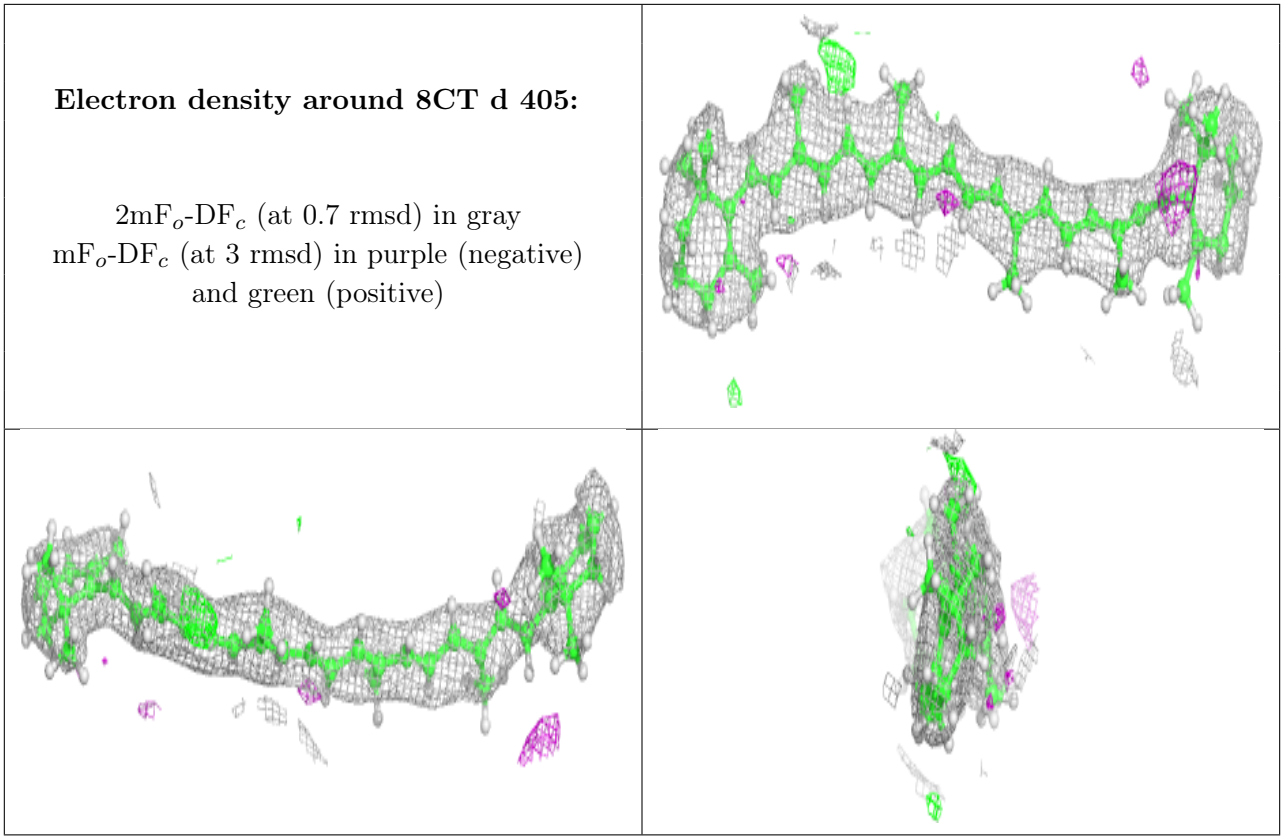






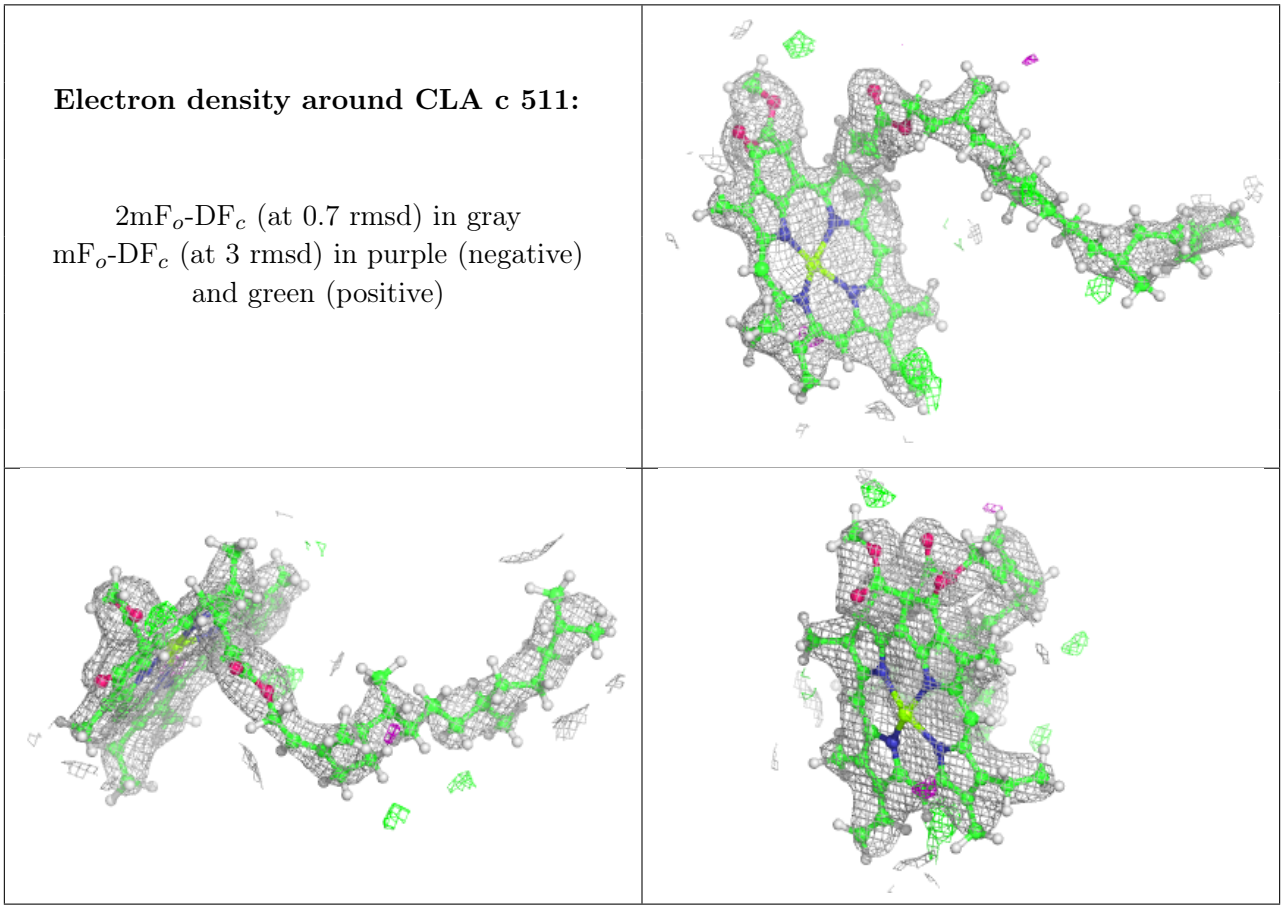
Electron density around 8CT d 405:

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



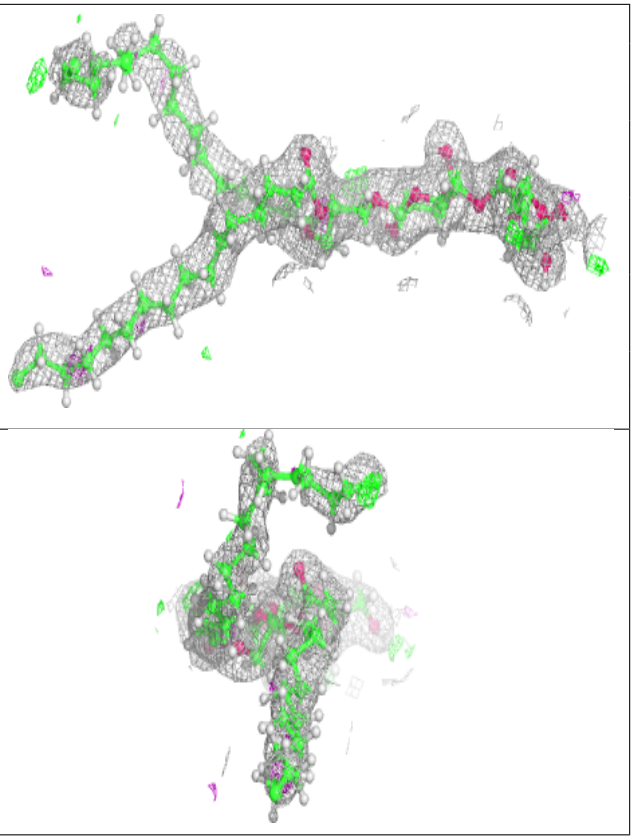
Electron density around CLA c 511:

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



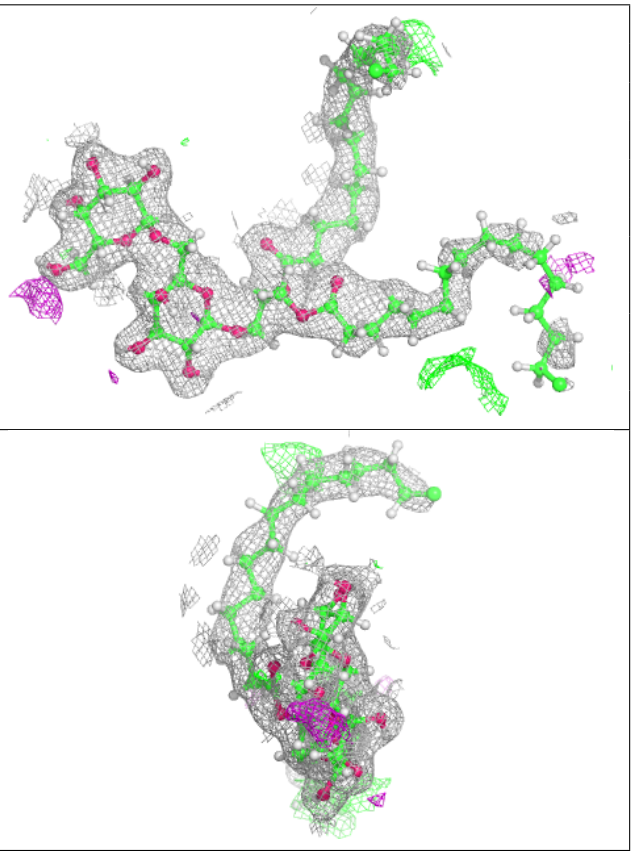
Electron density around DGD C 516:

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



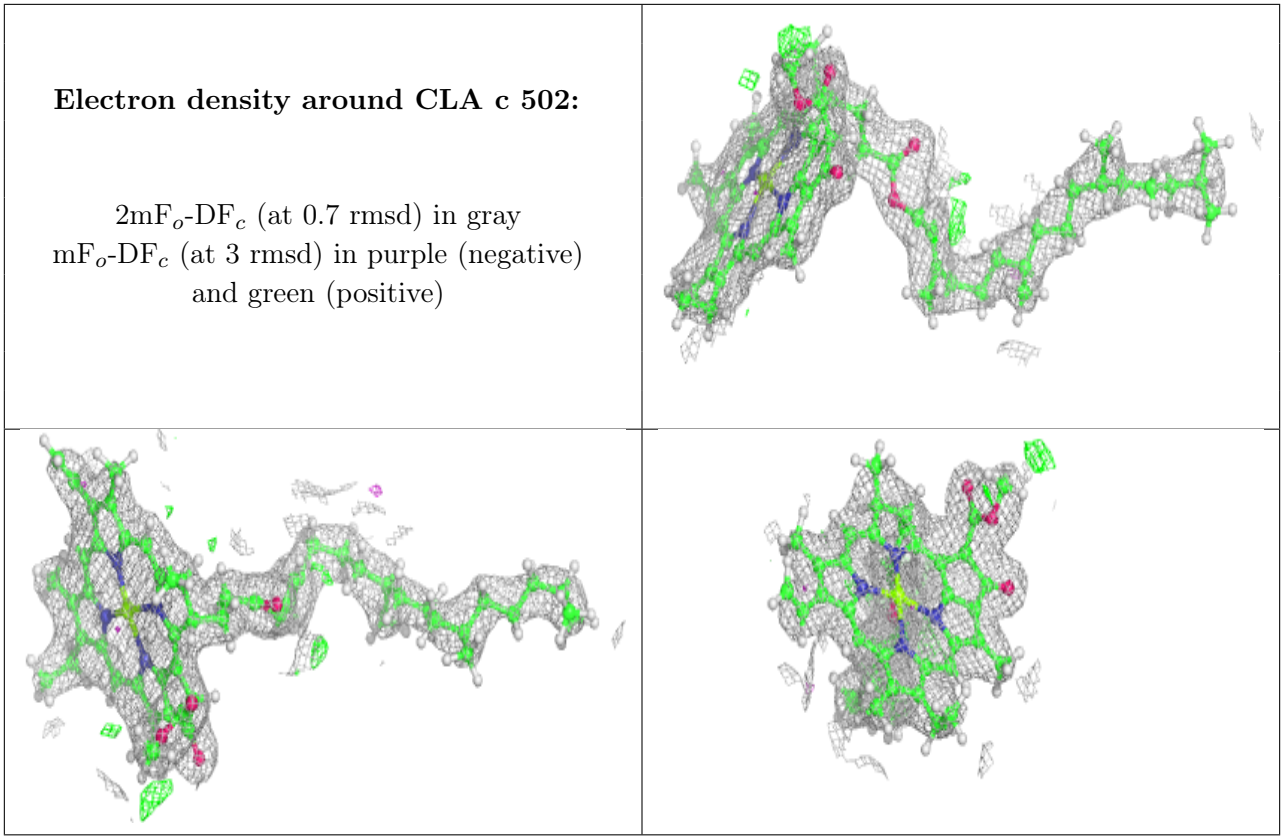
Electron density around DGD C 517:

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



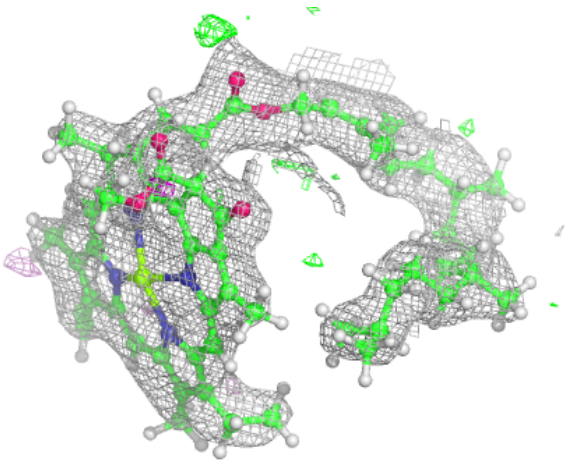
Electron density around CLA c 502:

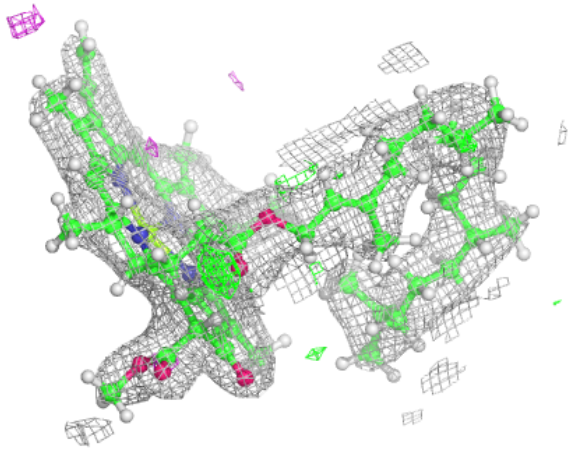
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

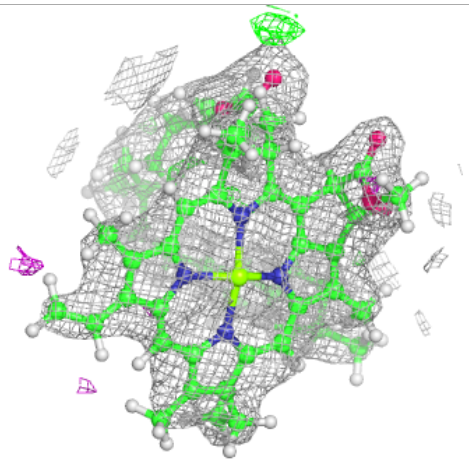


Electron density around CLA c 503:

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

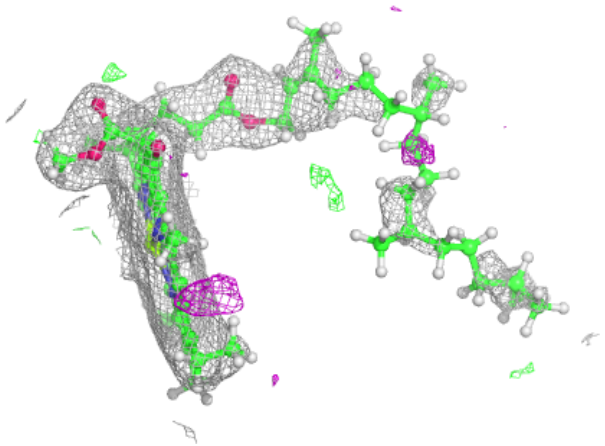


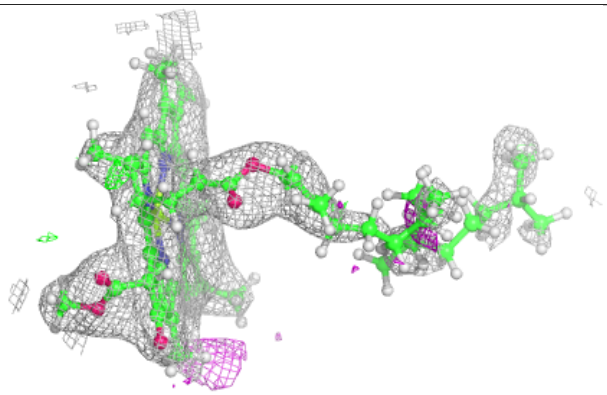


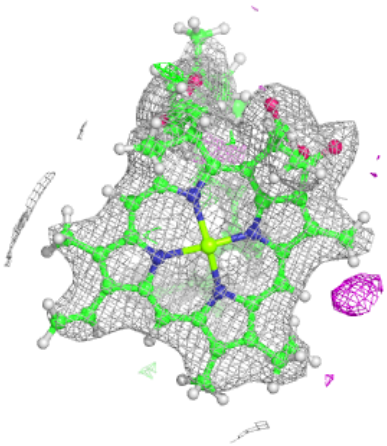


Electron density around CLA c 506:

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

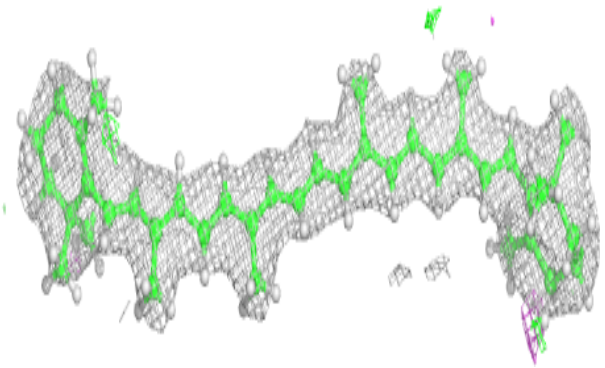


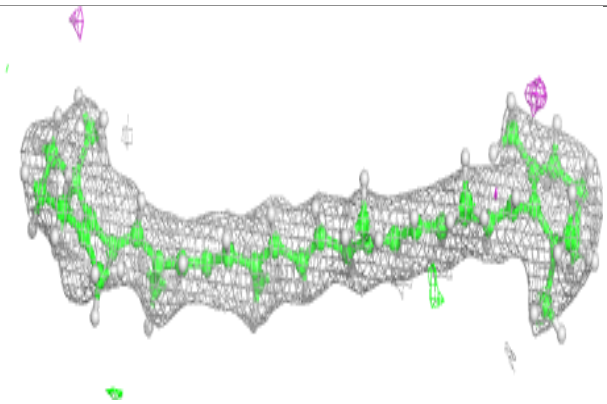


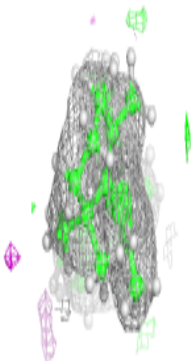


Electron density around 8CT B 619:

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

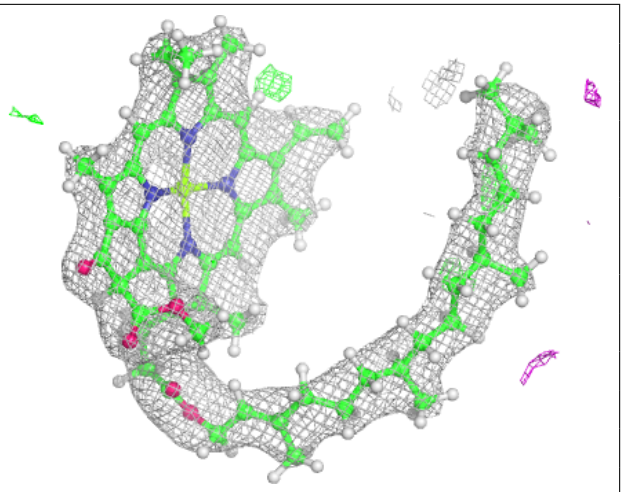


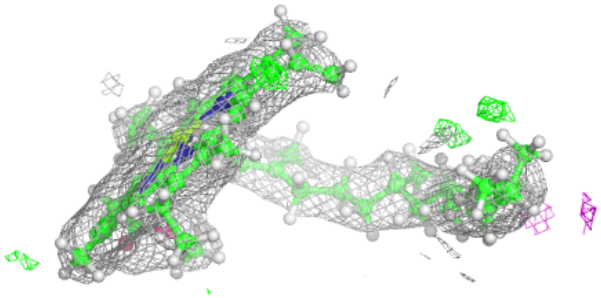


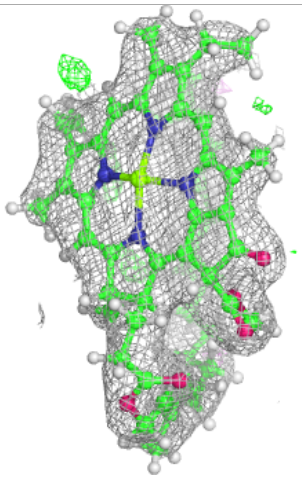


Electron density around CLA c 507:

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

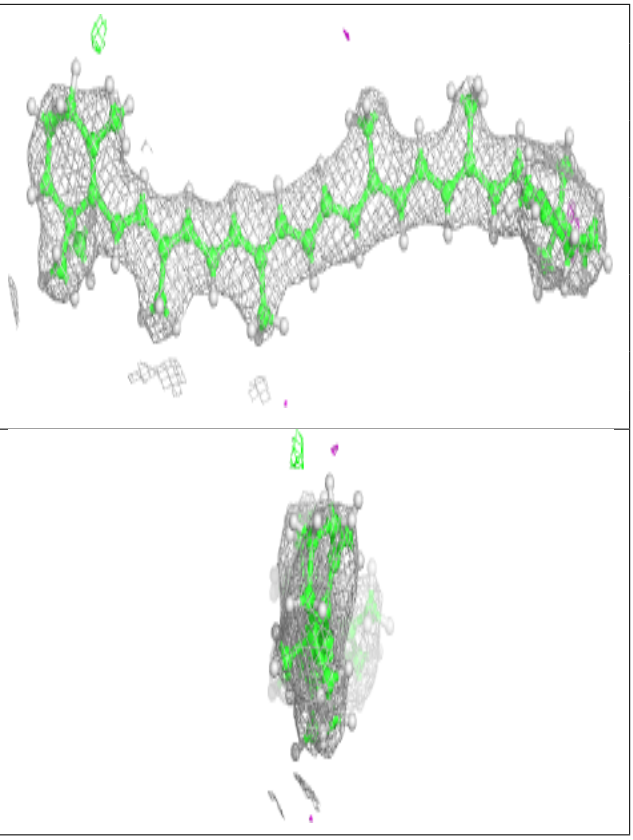






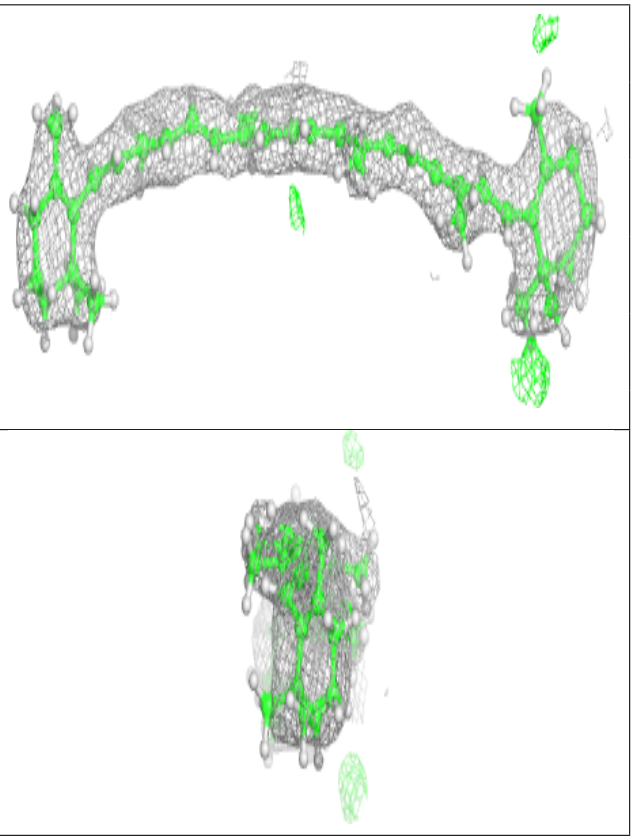
Electron density around BCR b 618:

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



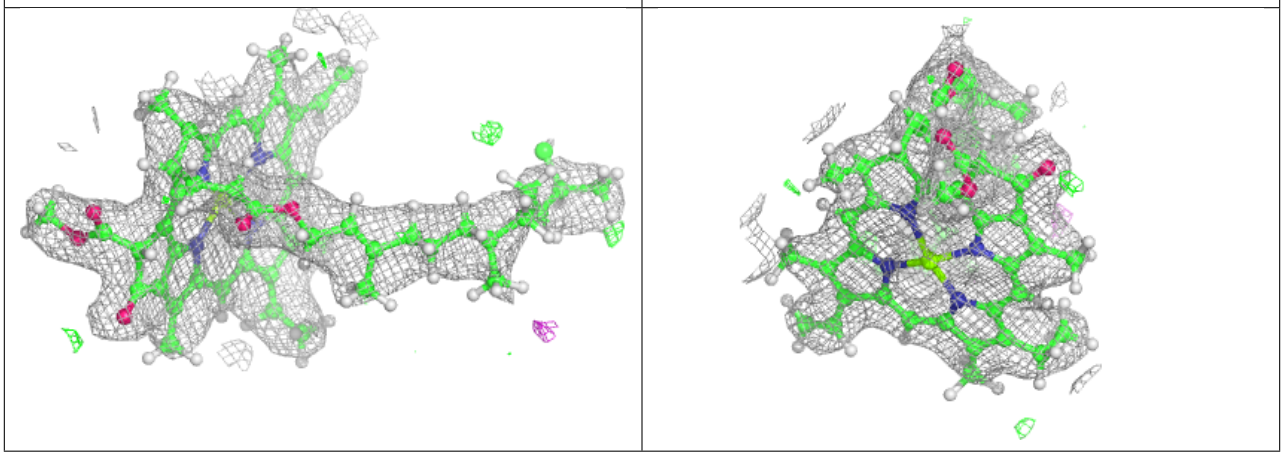
Electron density around BCR c 521:

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



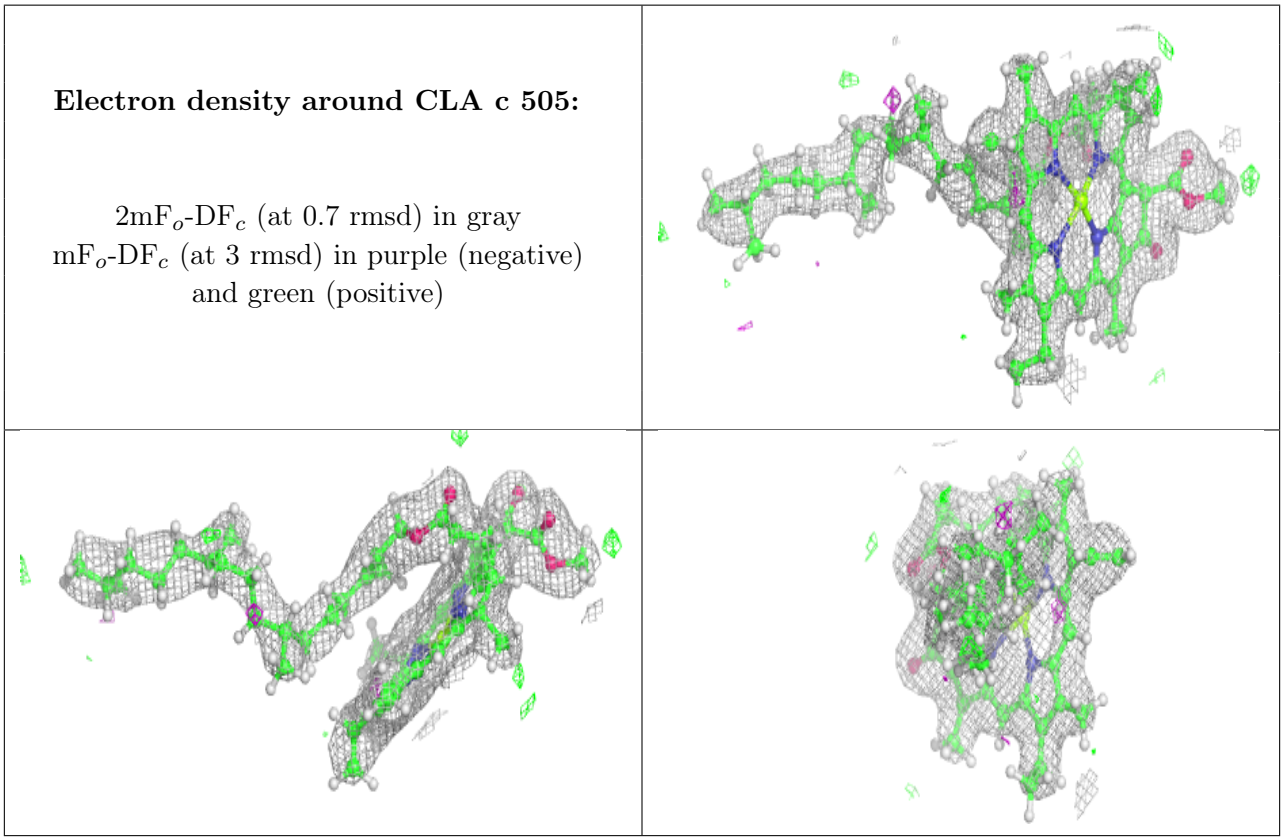
Electron density around CLA c 504:

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



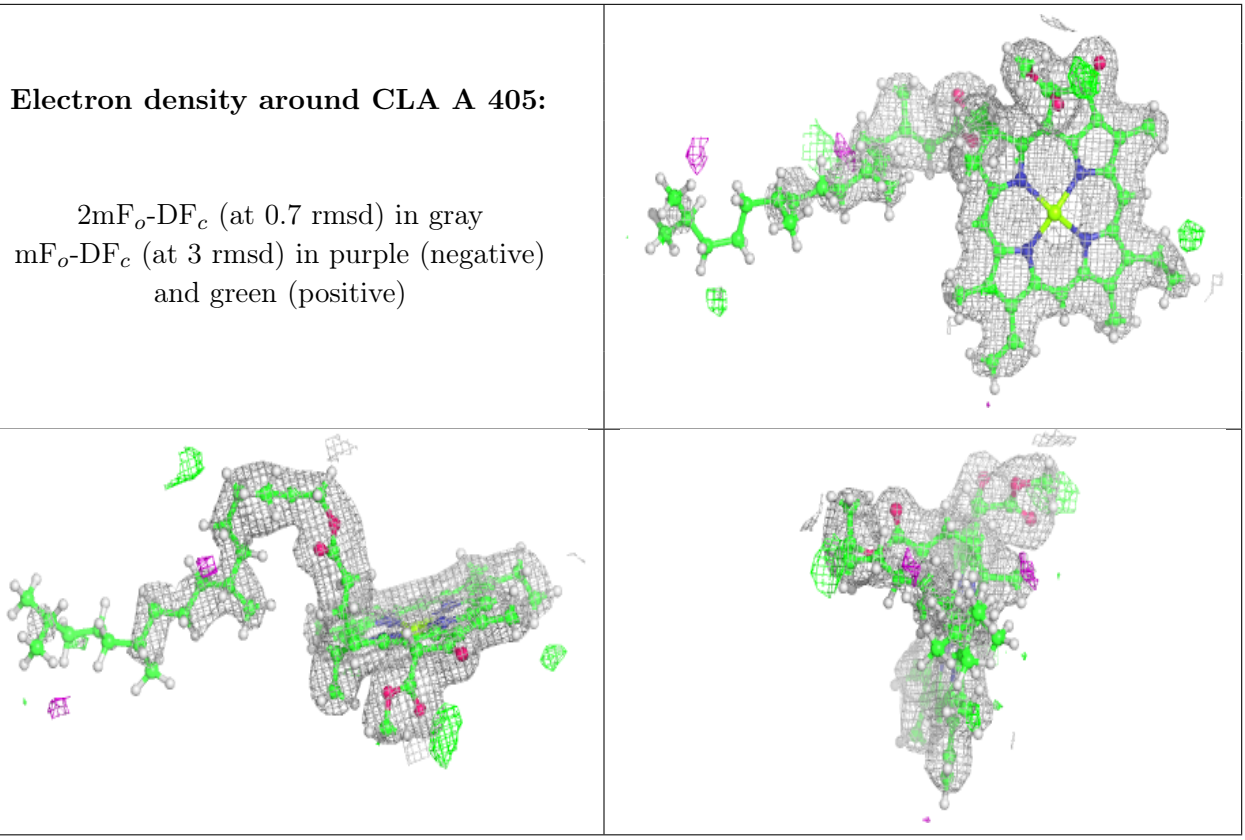
Electron density around CLA c 505:

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



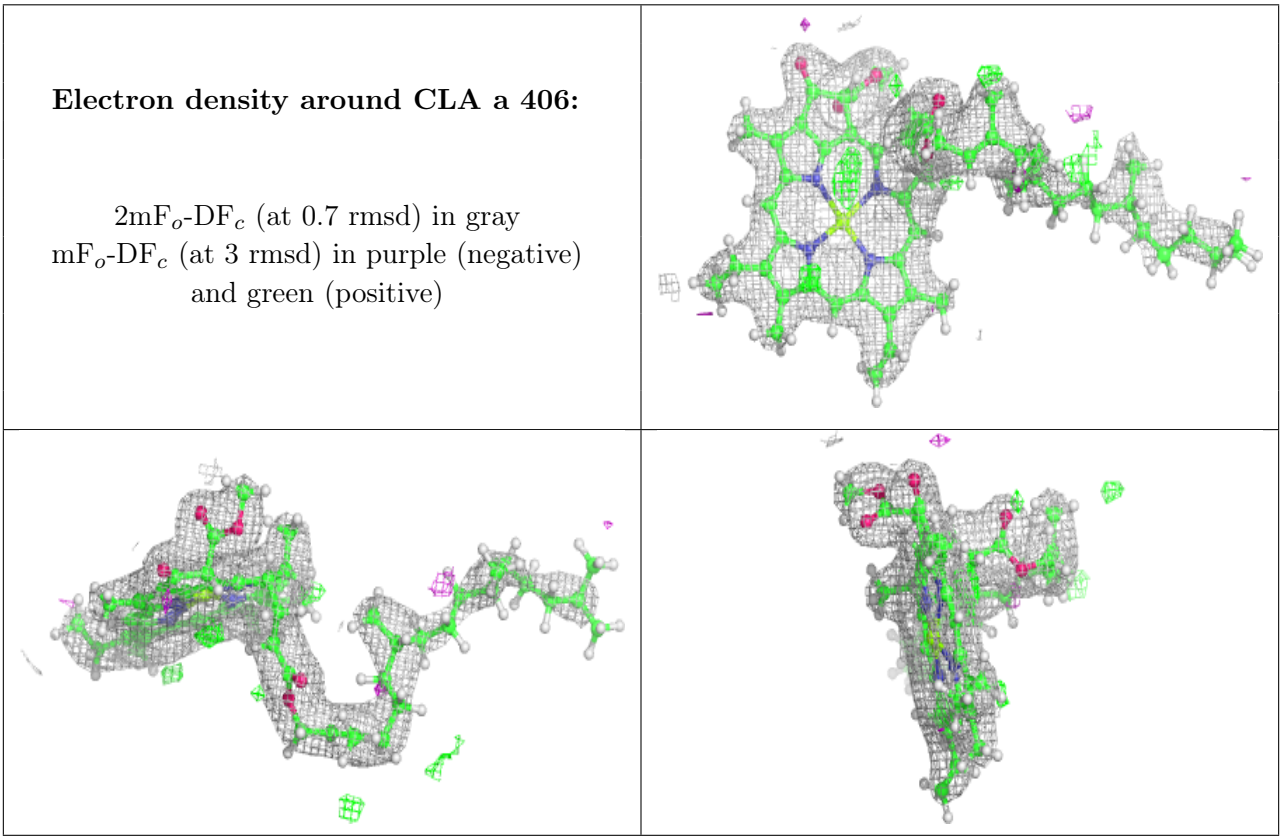
Electron density around CLA A 405:

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



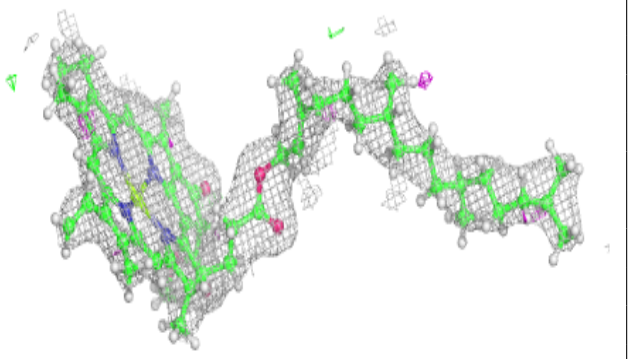
Electron density around CLA a 406:

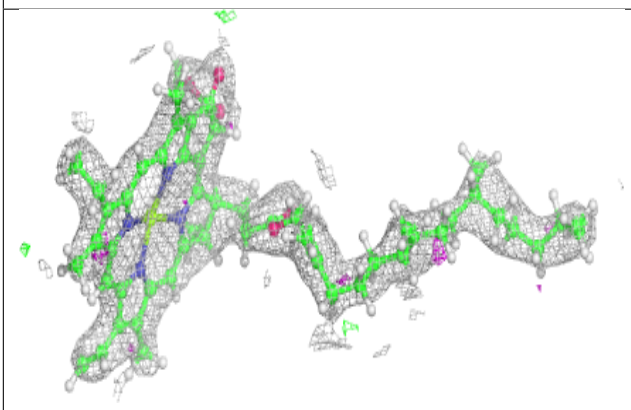
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

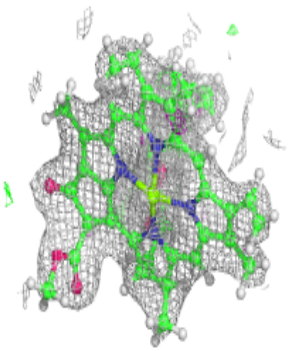


Electron density around CLA C 502:

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

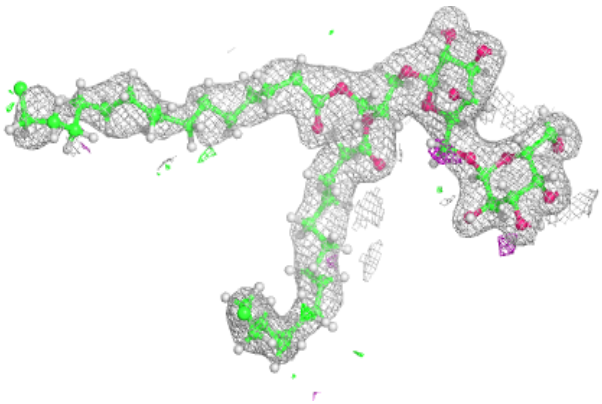


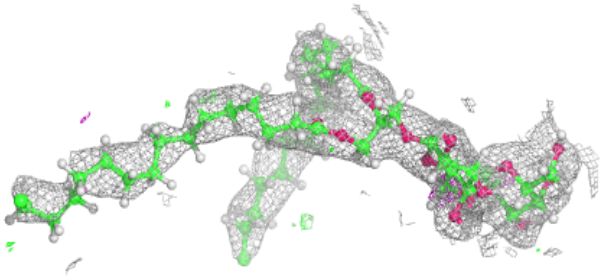


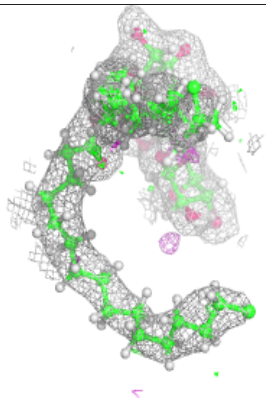


Electron density around DGD c 517:

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

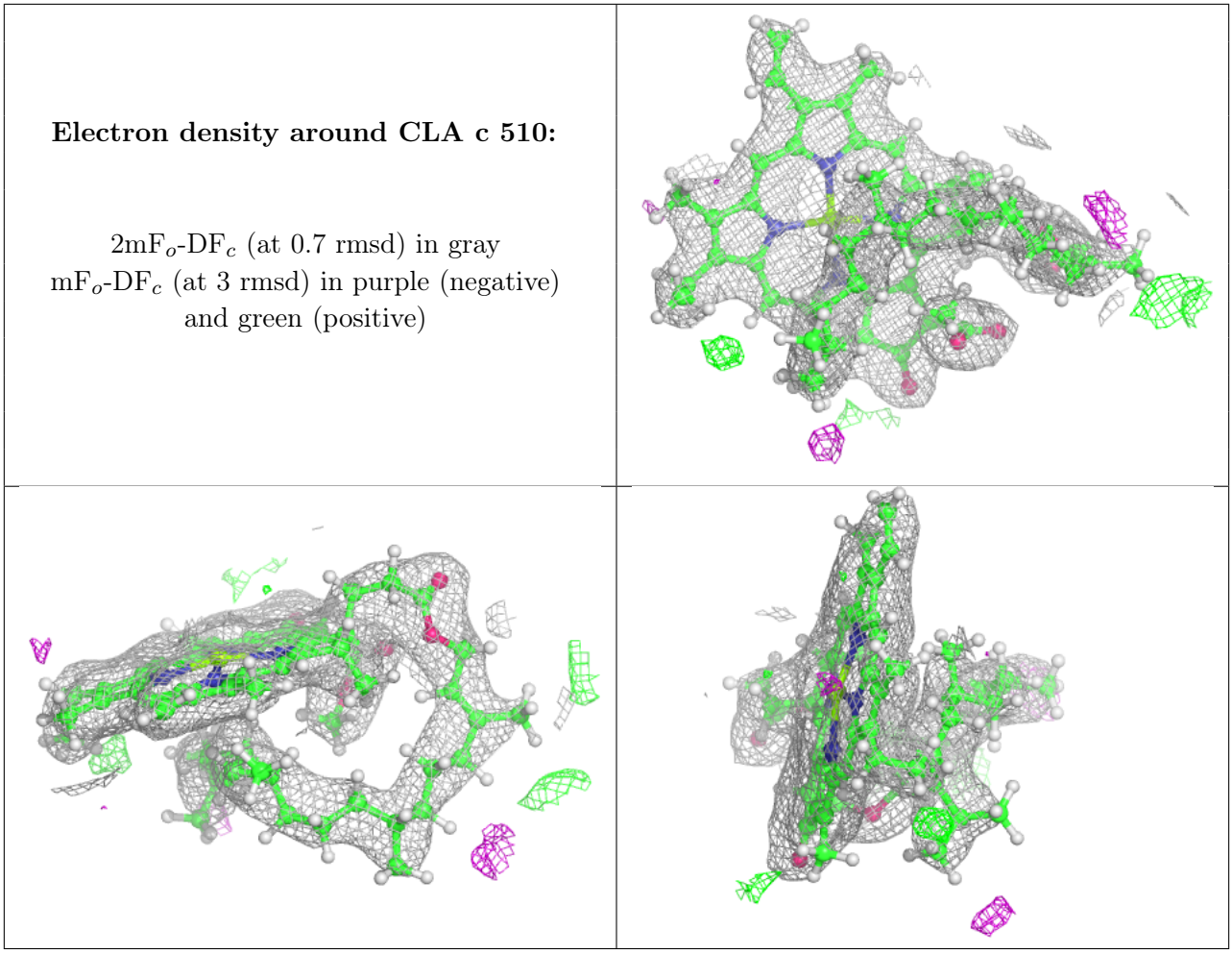






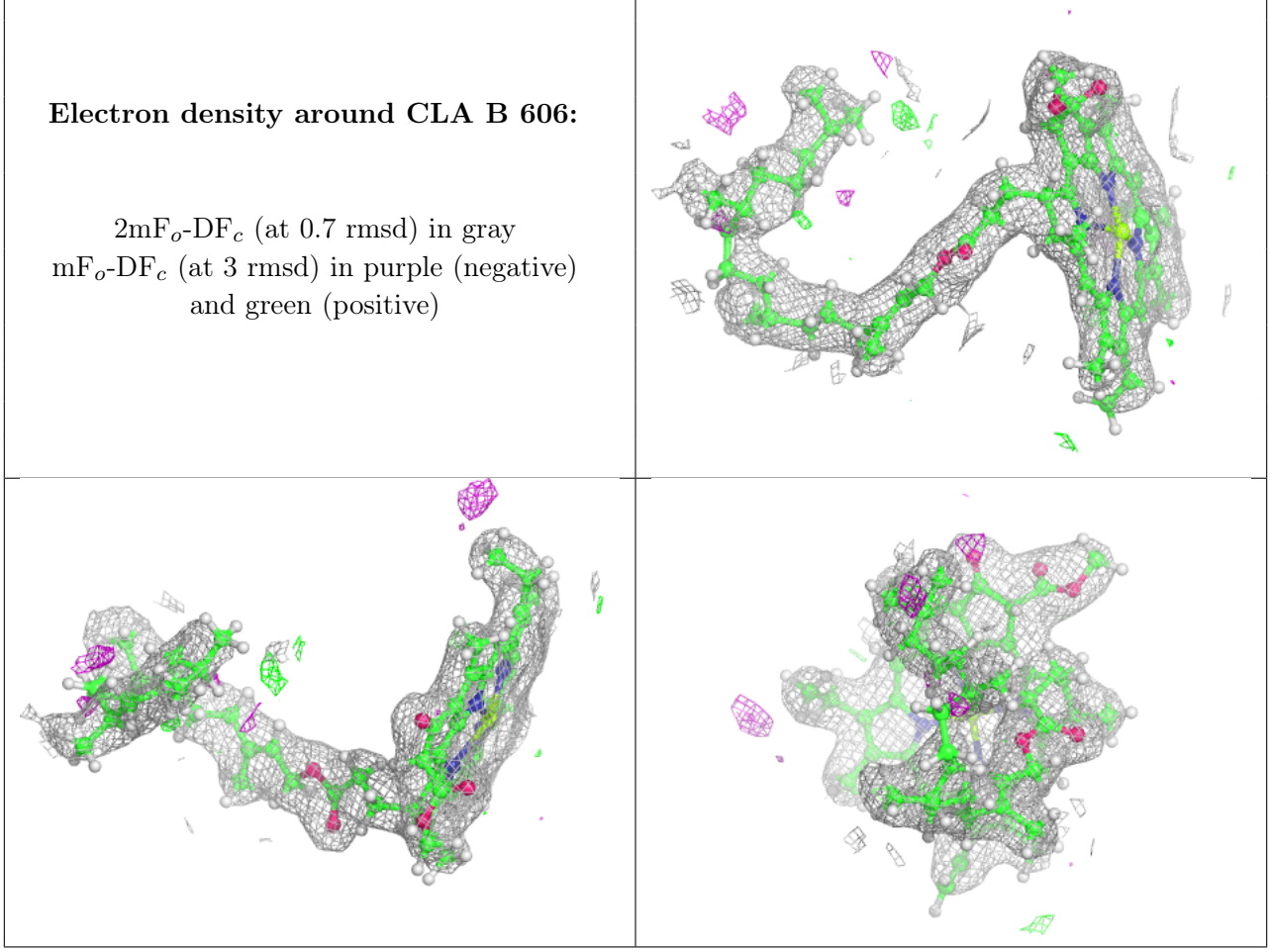
Electron density around CLA c 510:

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



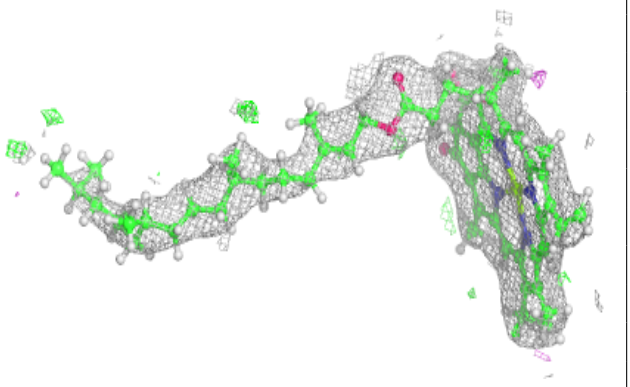
Electron density around CLA B 606:

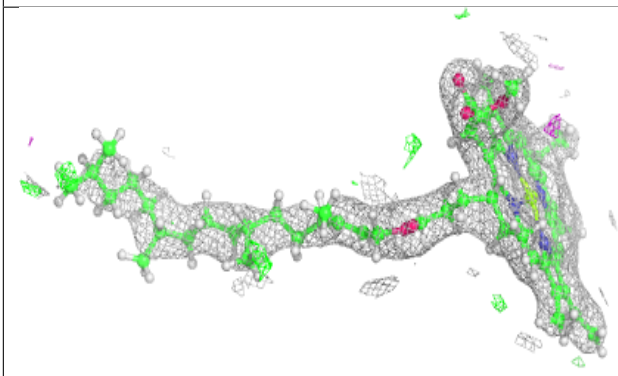
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

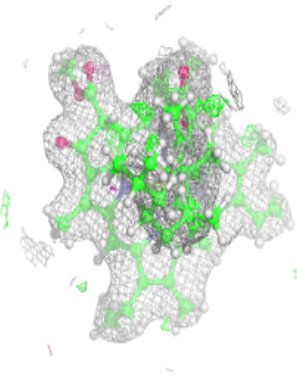


Electron density around CLA b 605:

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

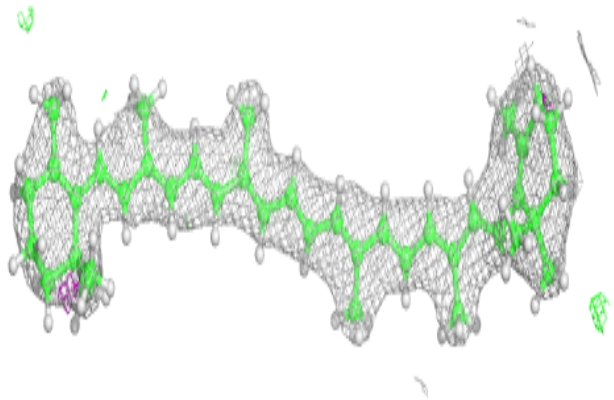


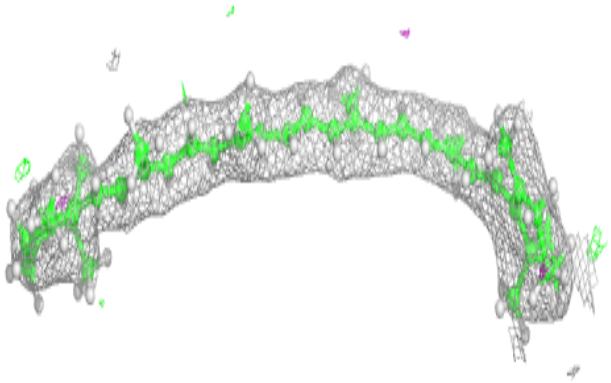


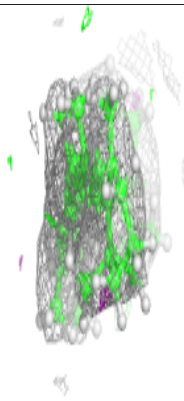


Electron density around BCR T 101:

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

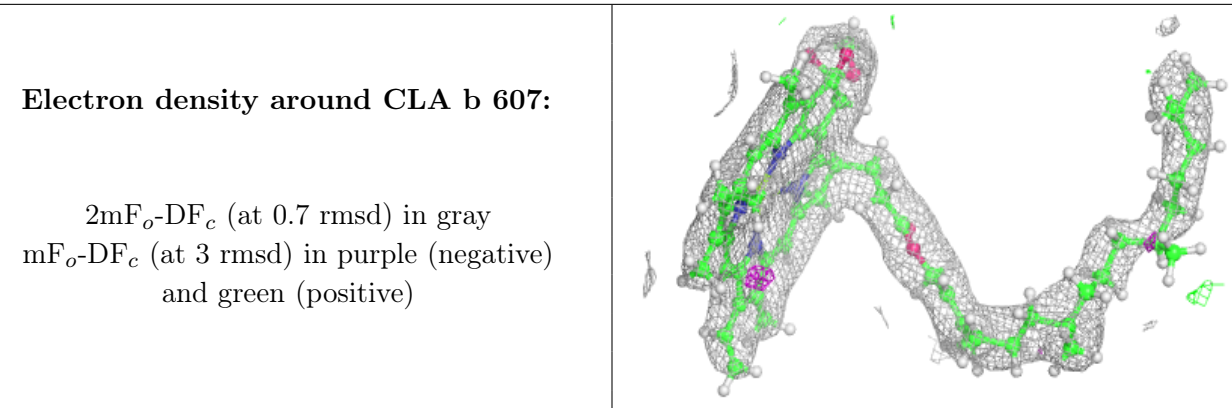






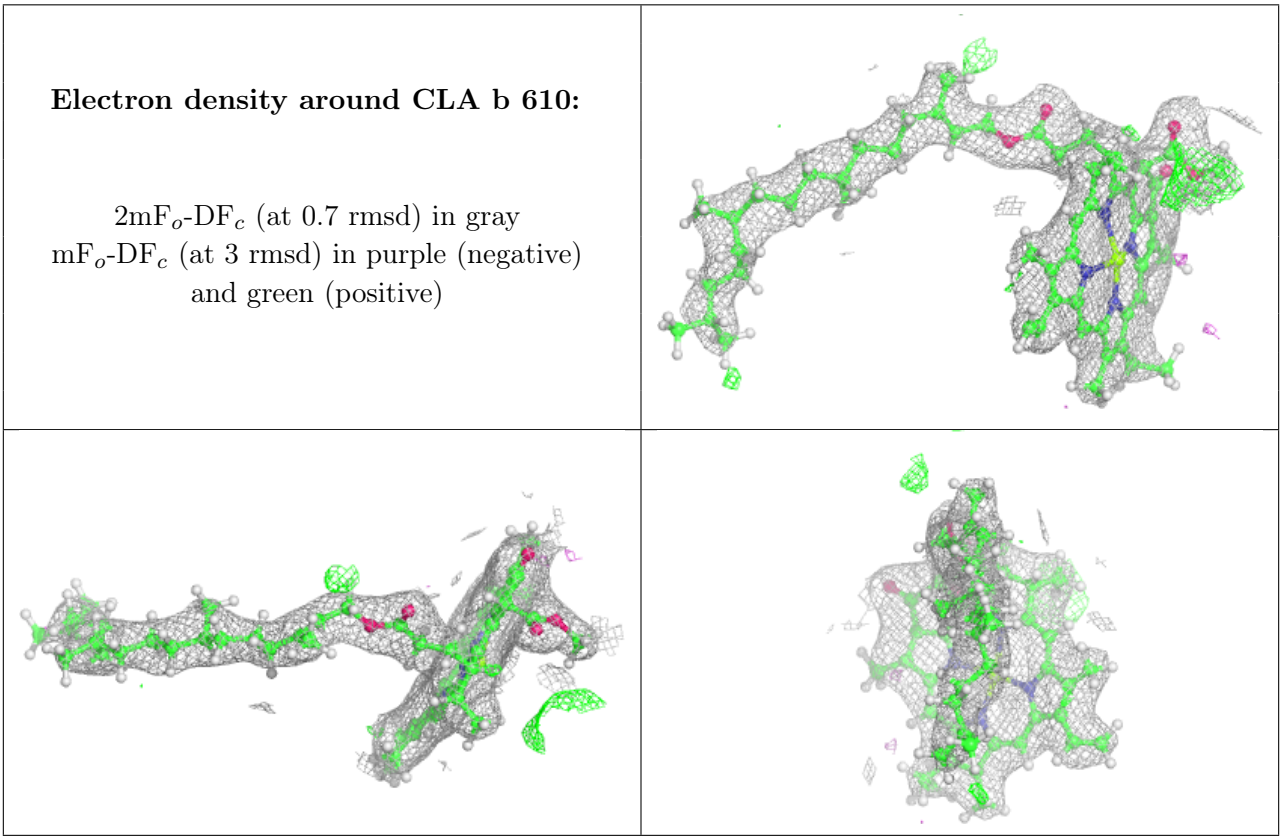
Electron density around CLA b 607:

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



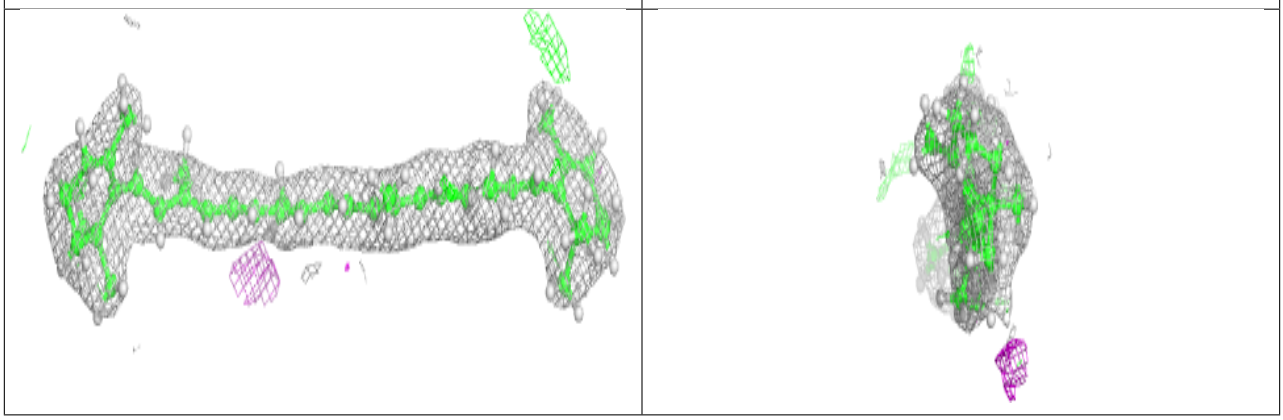
Electron density around CLA b 610:

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



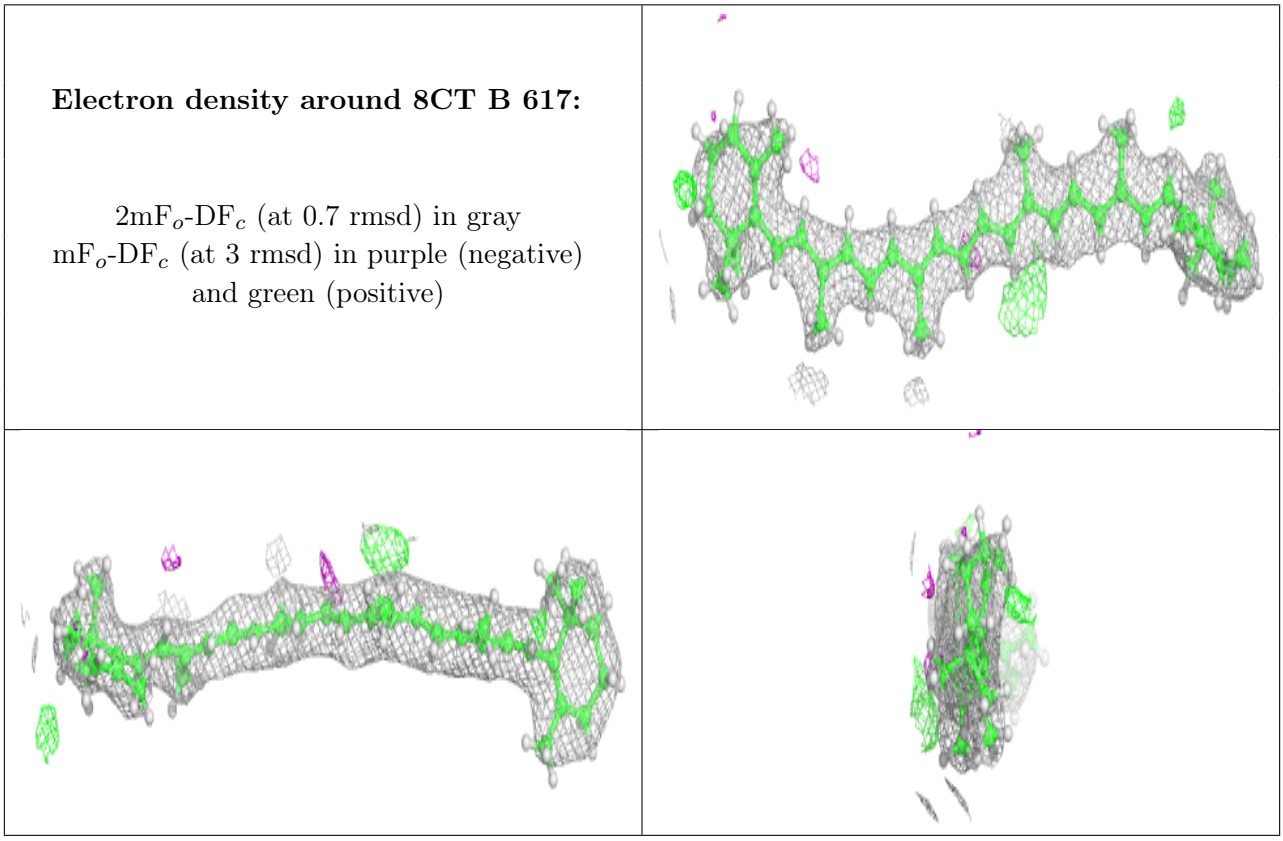
Electron density around BCR b 619:

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



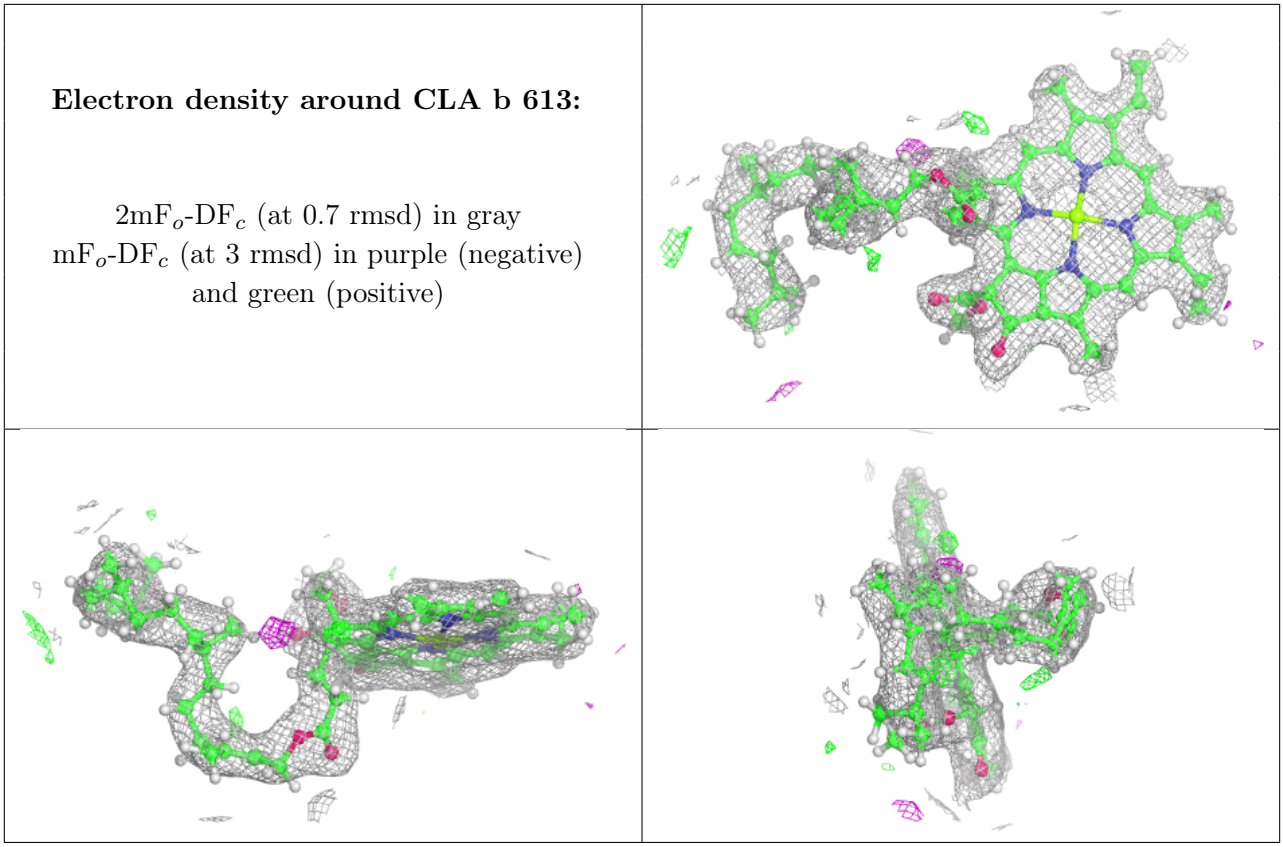
Electron density around 8CT B 617:

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



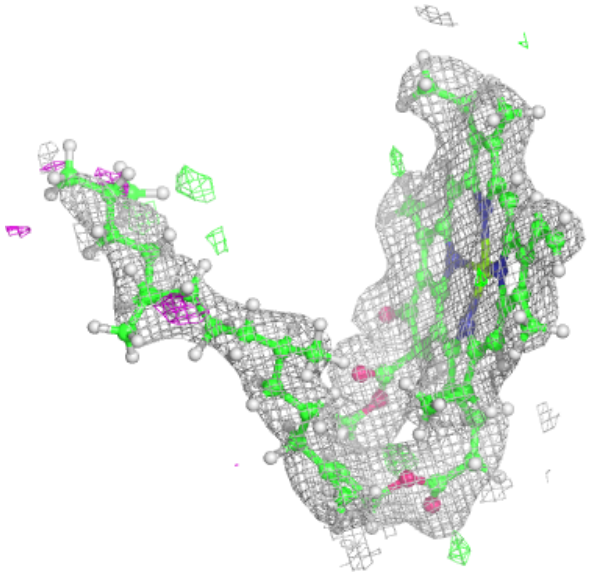
Electron density around CLA b 613:

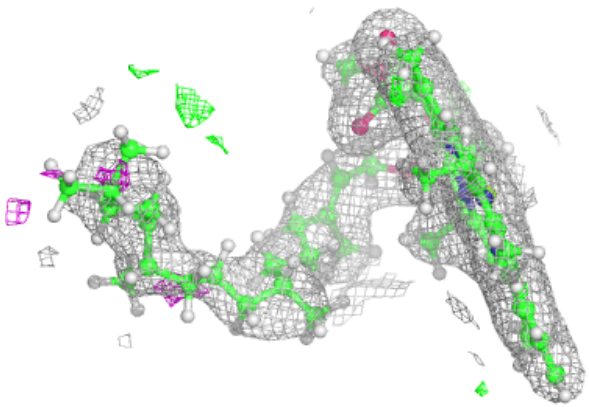
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

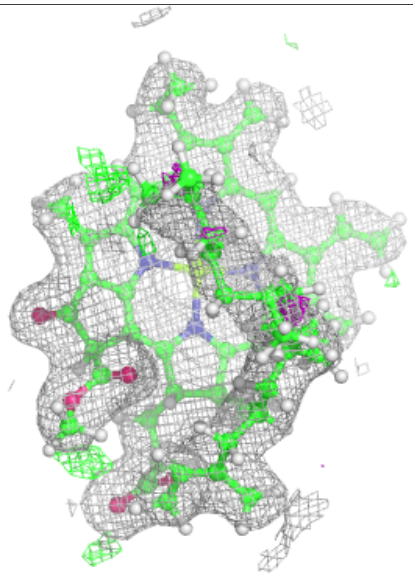


Electron density around CLA b 614:

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

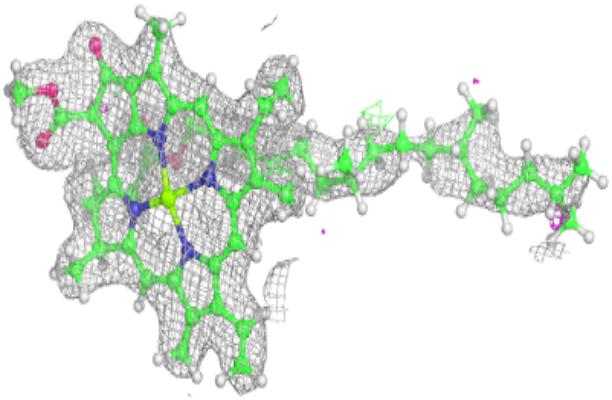


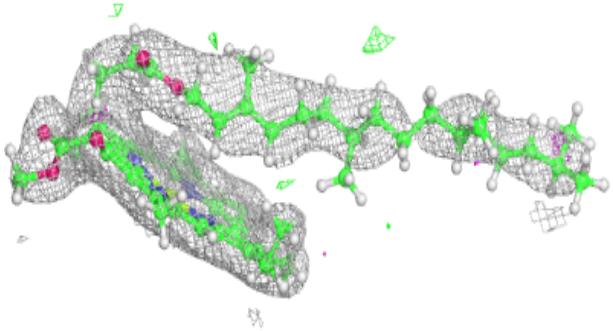


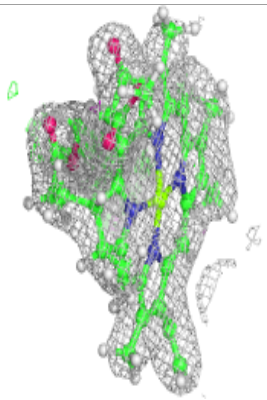


Electron density around CLA b 615:

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

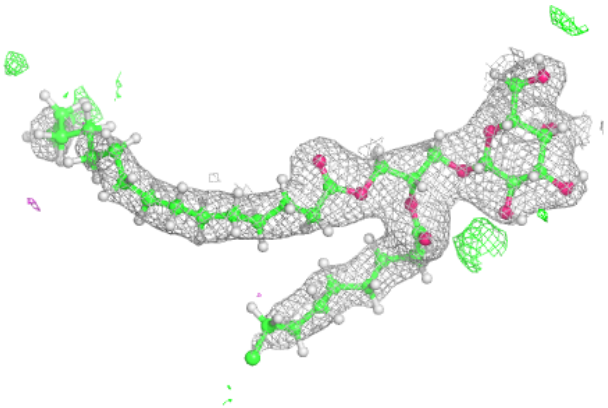


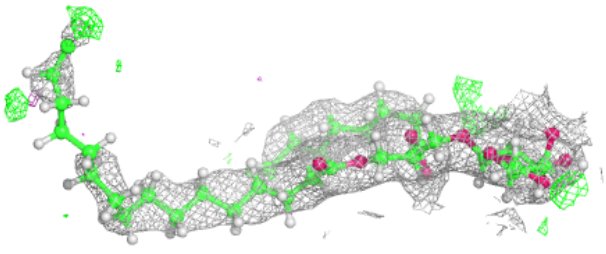


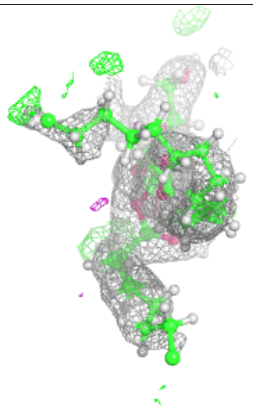


Electron density around LMG d 410:

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

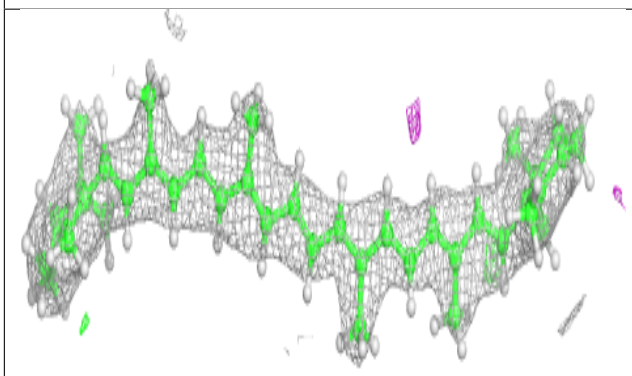


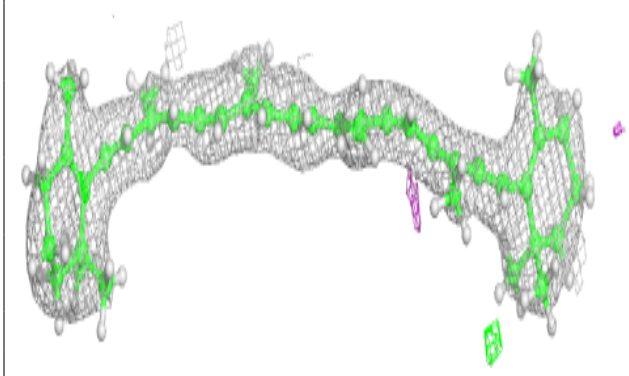


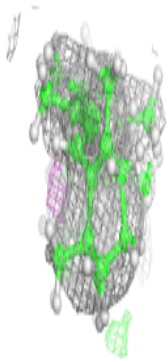


Electron density around 8CT C 520:

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

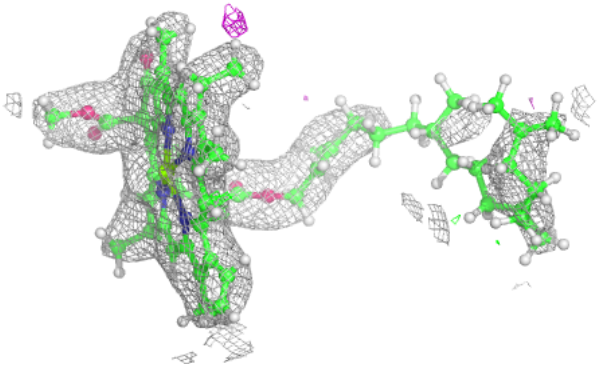


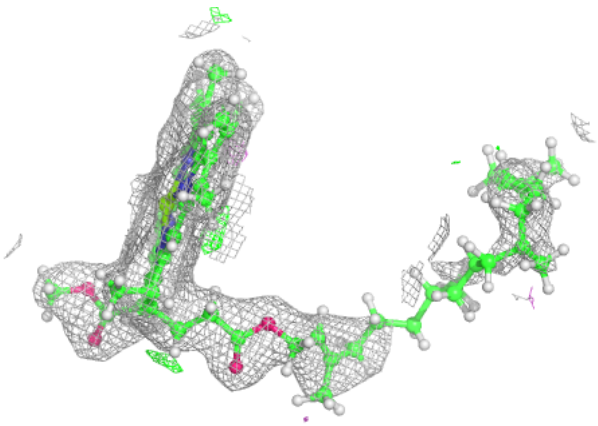


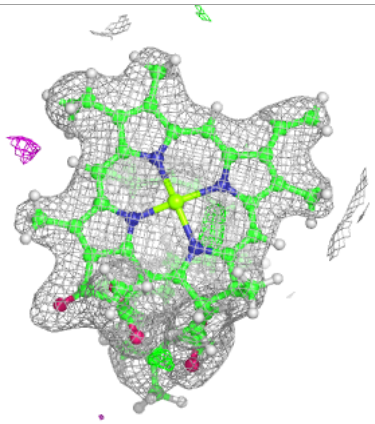


Electron density around CLA C 506:

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

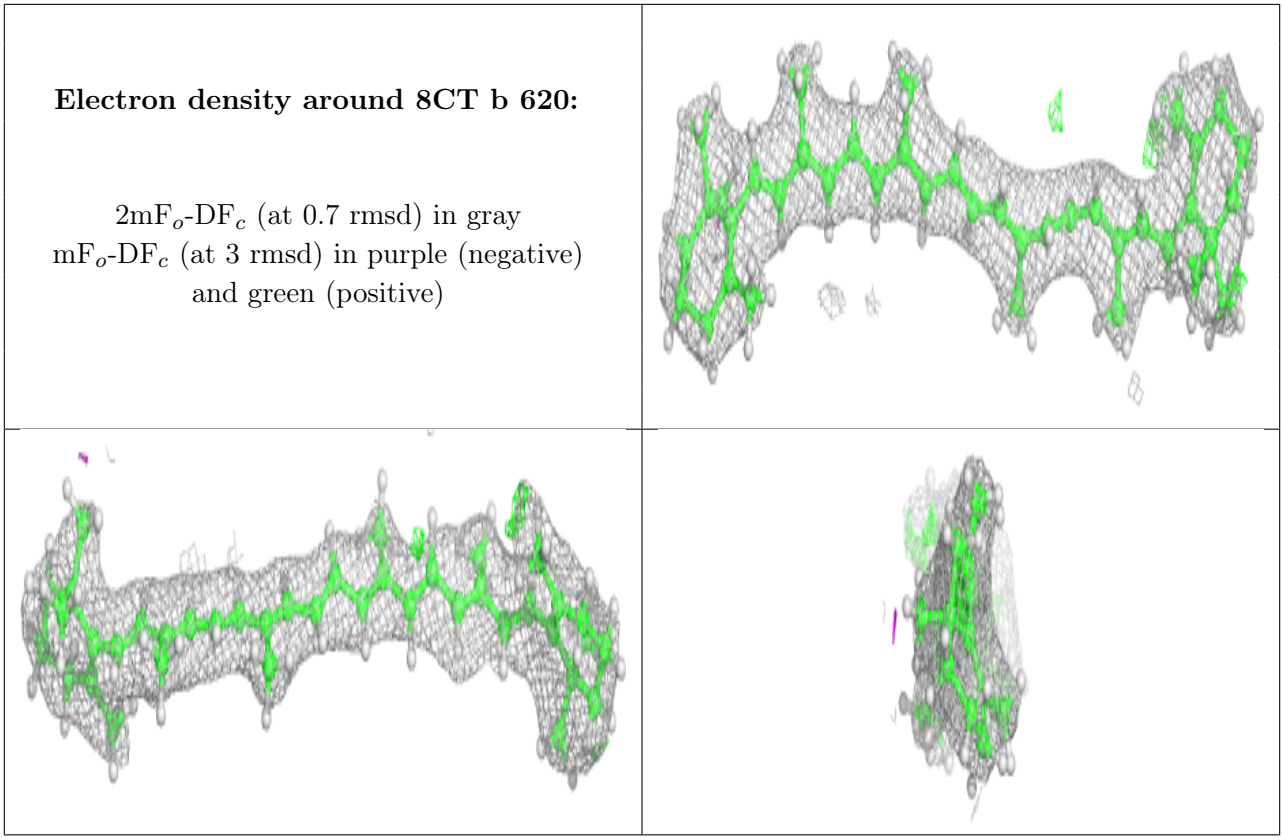






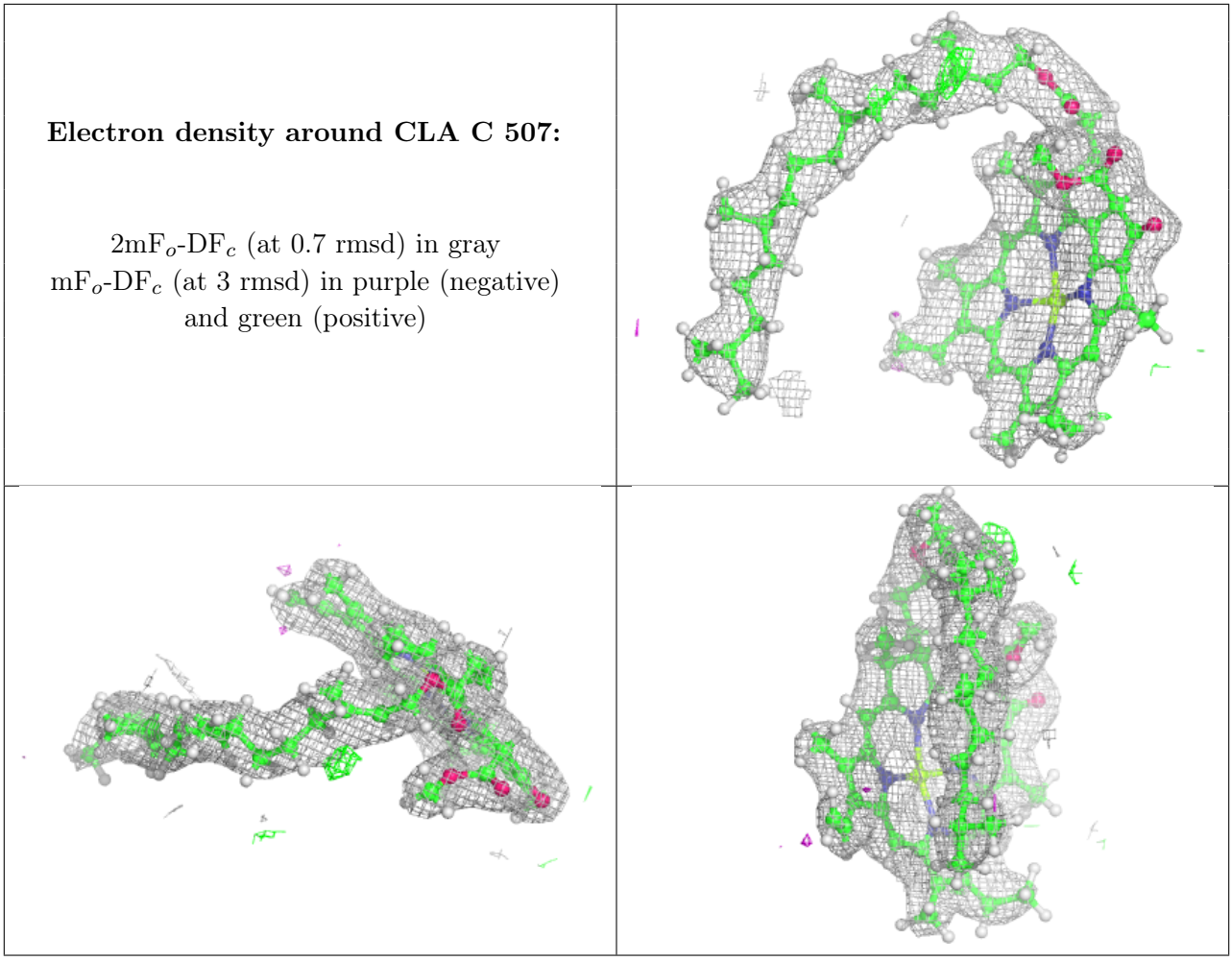
Electron density around 8CT b 620:

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



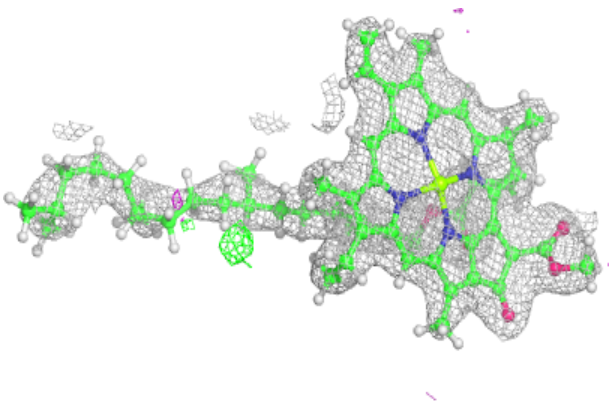
Electron density around CLA C 507:

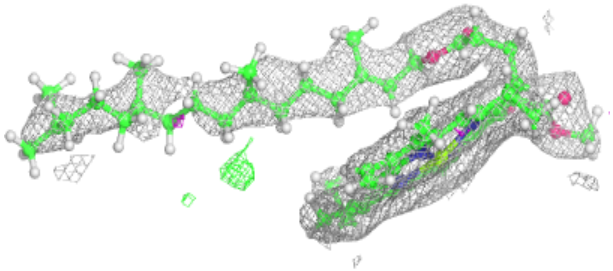
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 614:

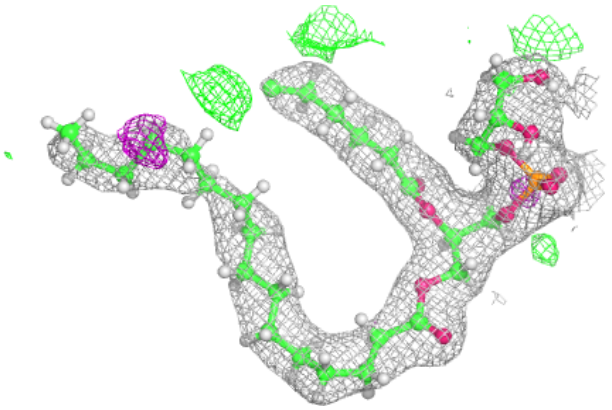
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

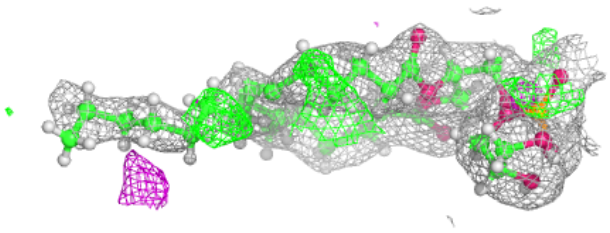


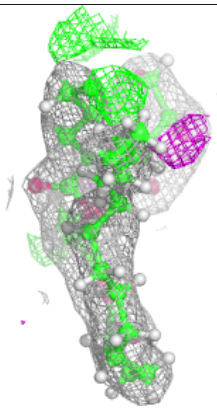


Electron density around LHG d 409:

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

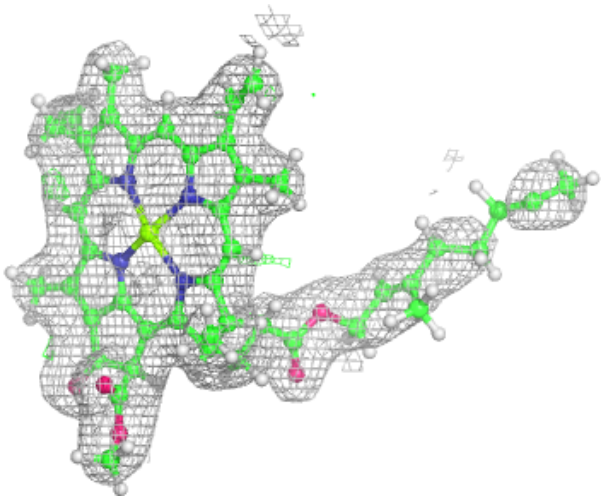


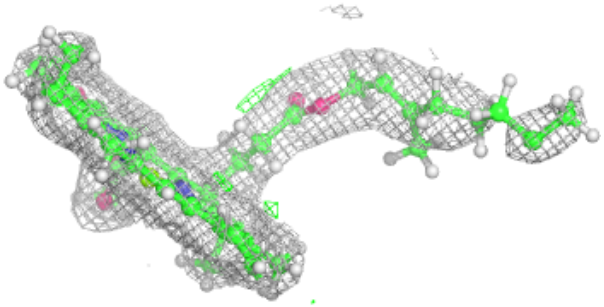


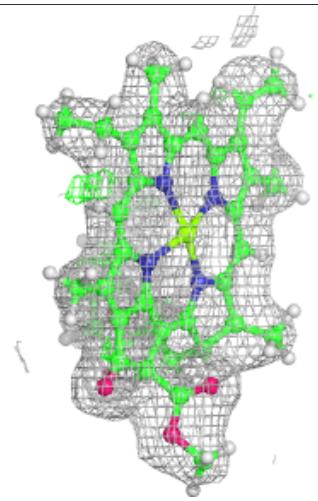


Electron density around CLA A 407:

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

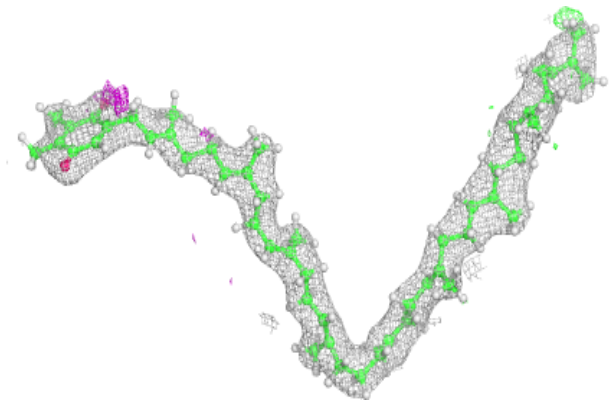


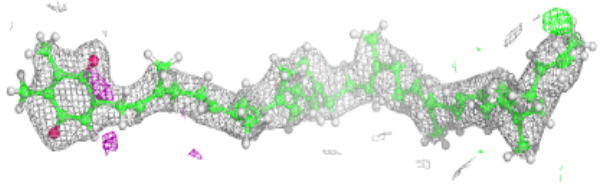




Electron density around PL9 d 406:

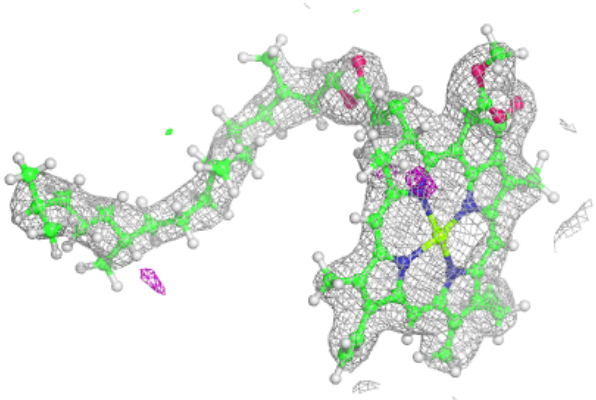
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

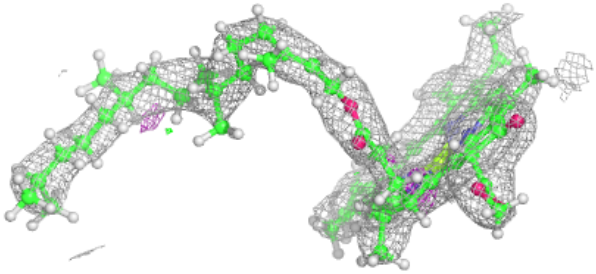


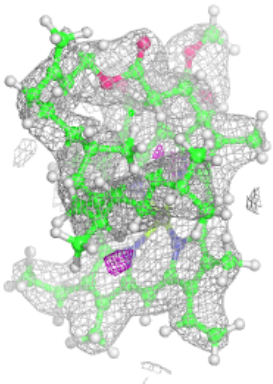


Electron density around CLA C 511:

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

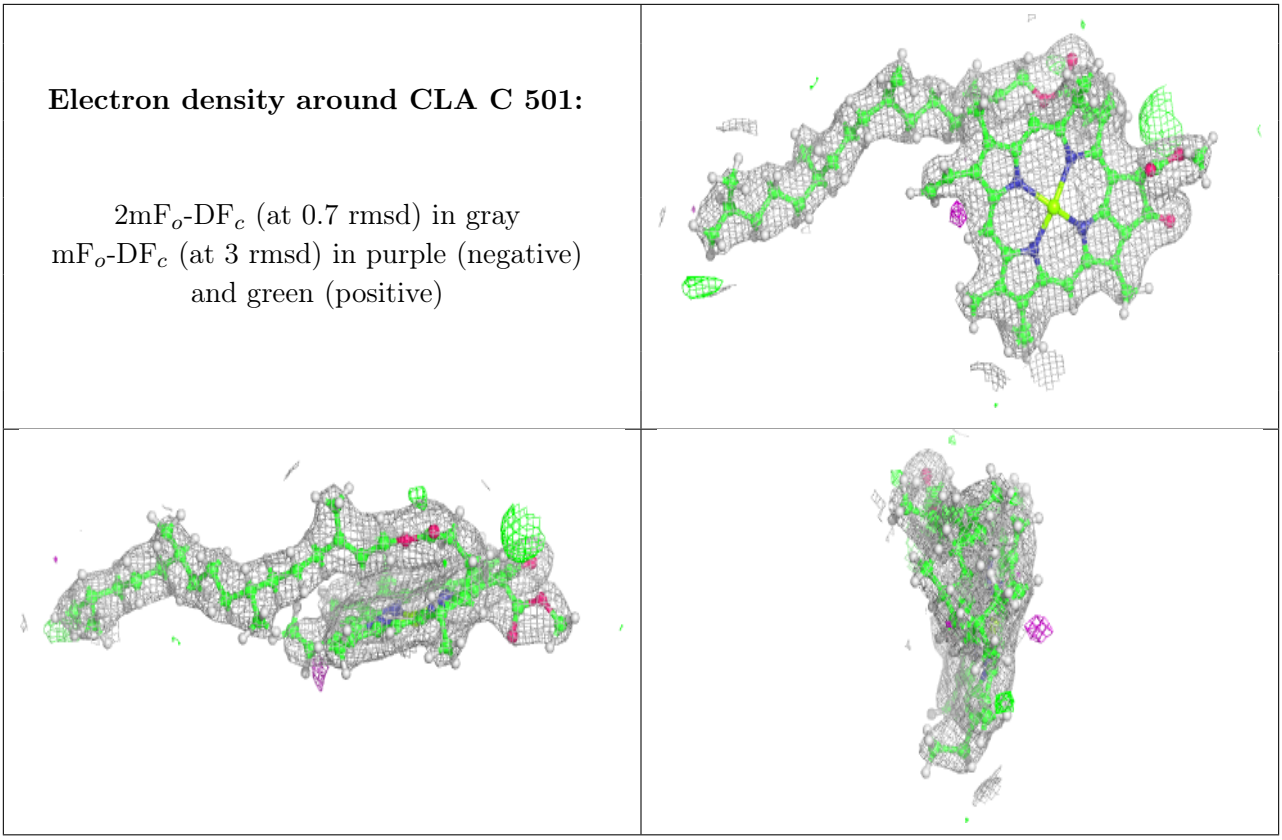






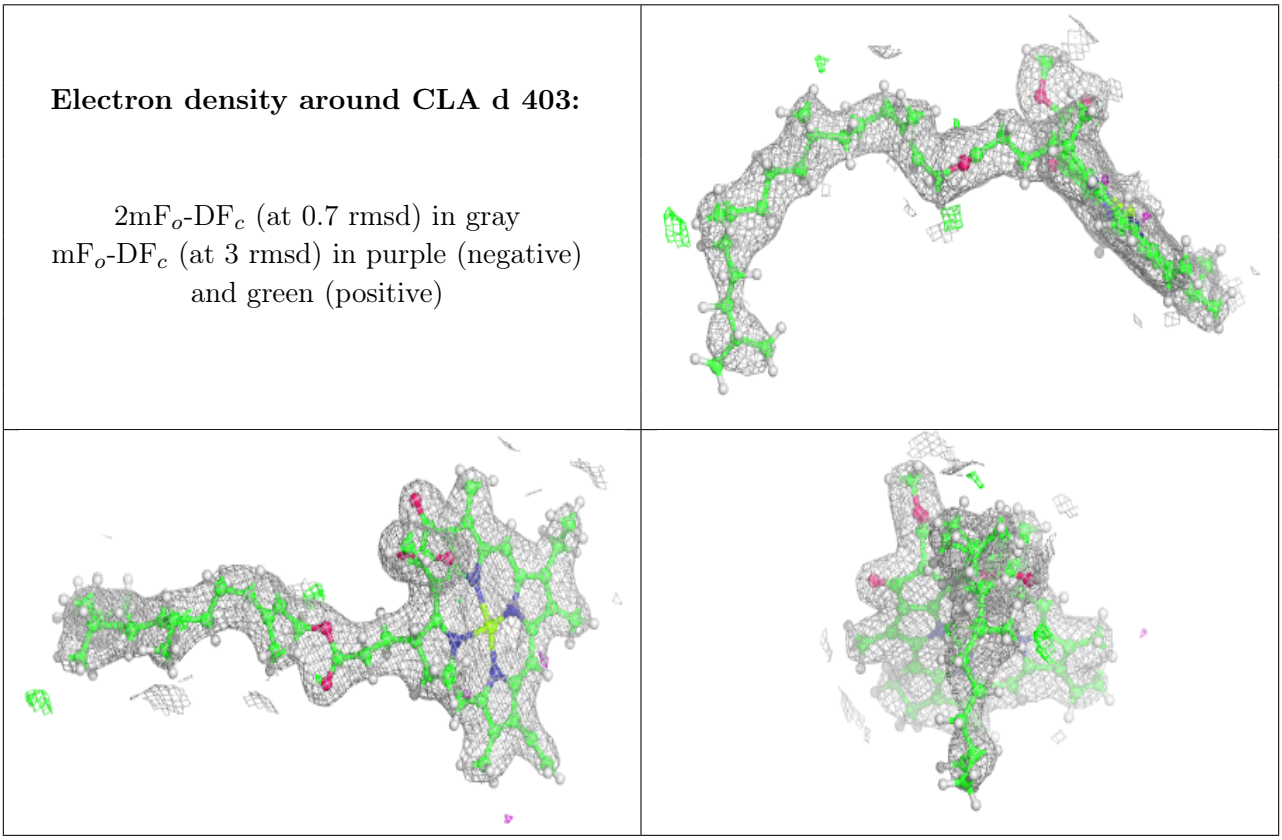
Electron density around CLA C 501:

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



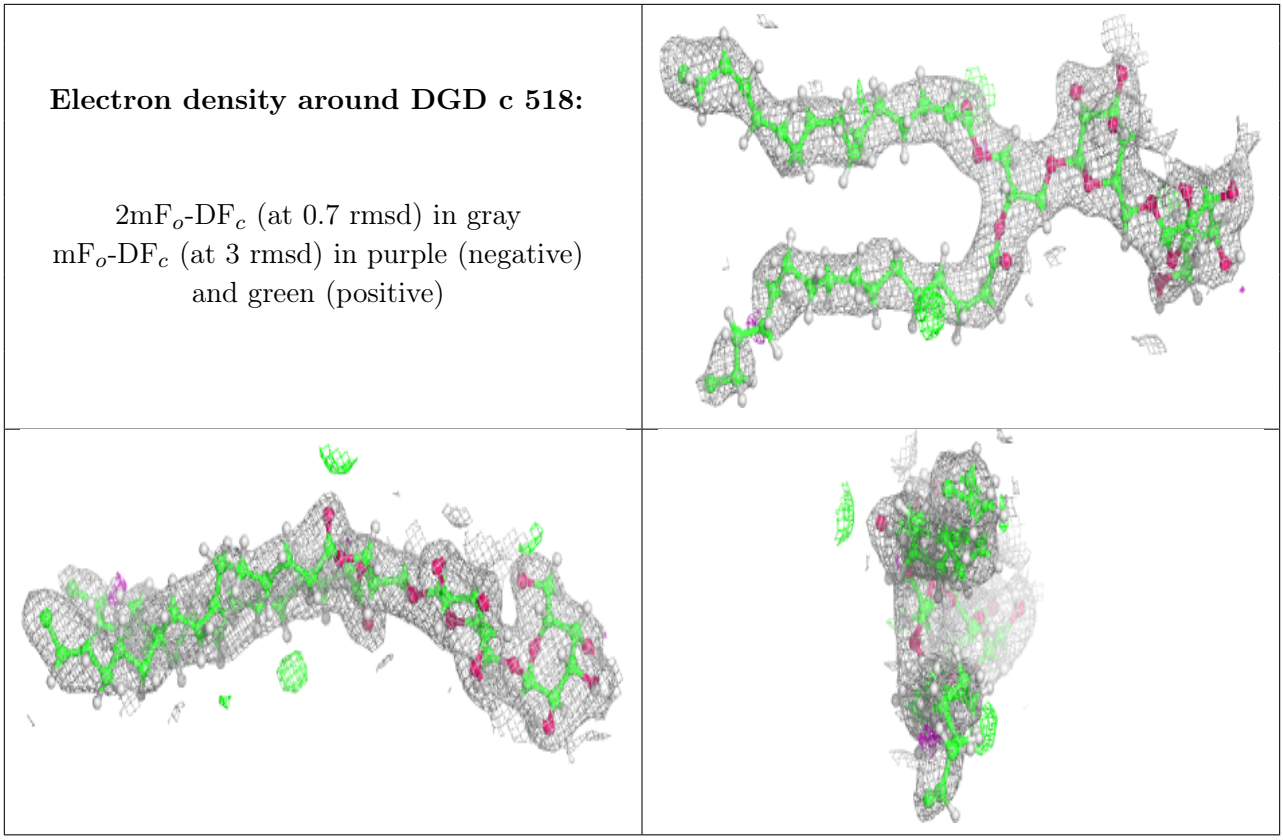
Electron density around CLA d 403:

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



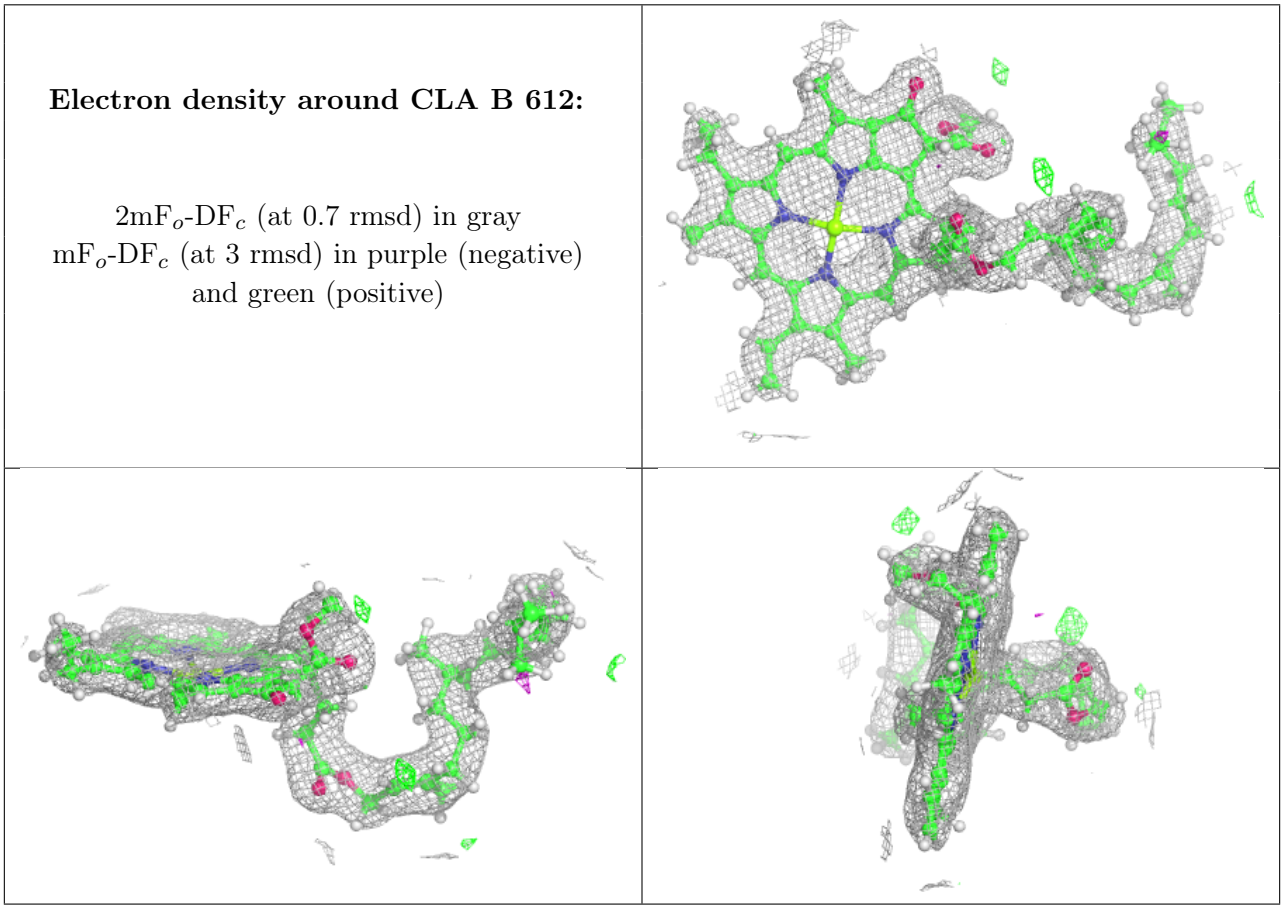
Electron density around DGD c 518:

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



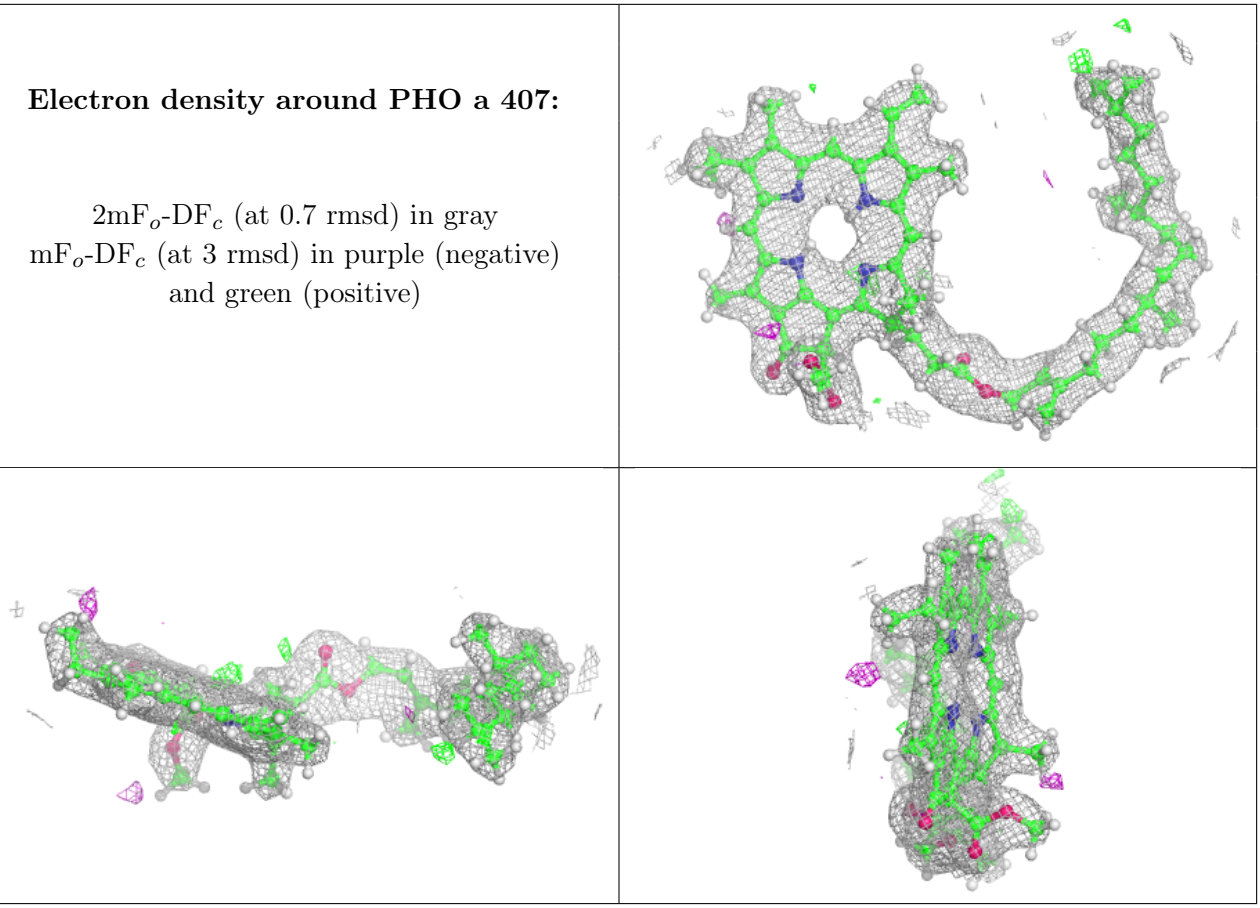
Electron density around CLA B 612:

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



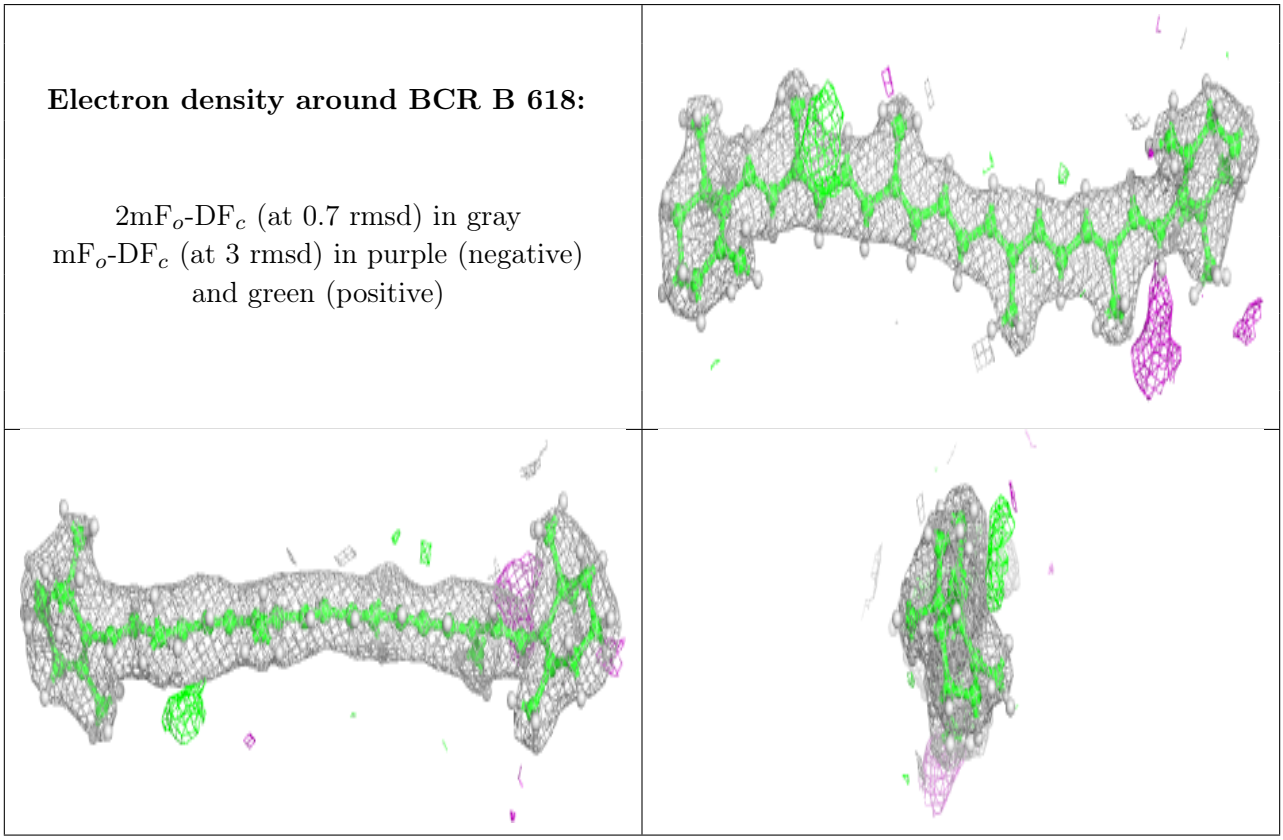
Electron density around PHO a 407:

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



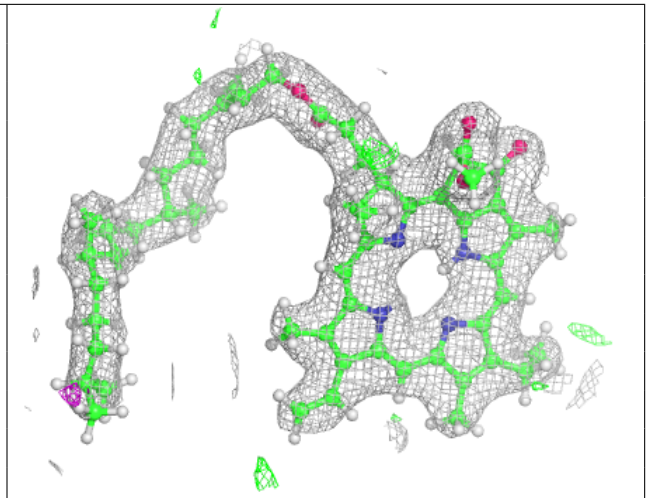
Electron density around BCR B 618:

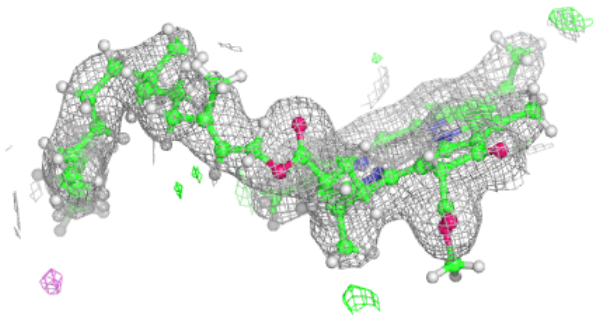
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

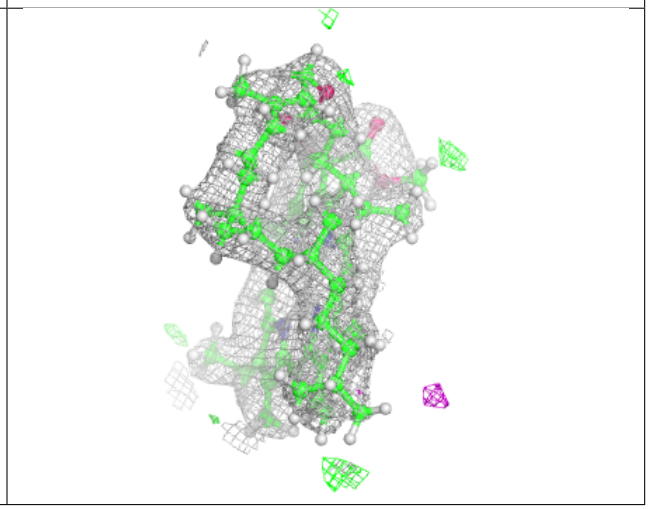


Electron density around PHO d 401:

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

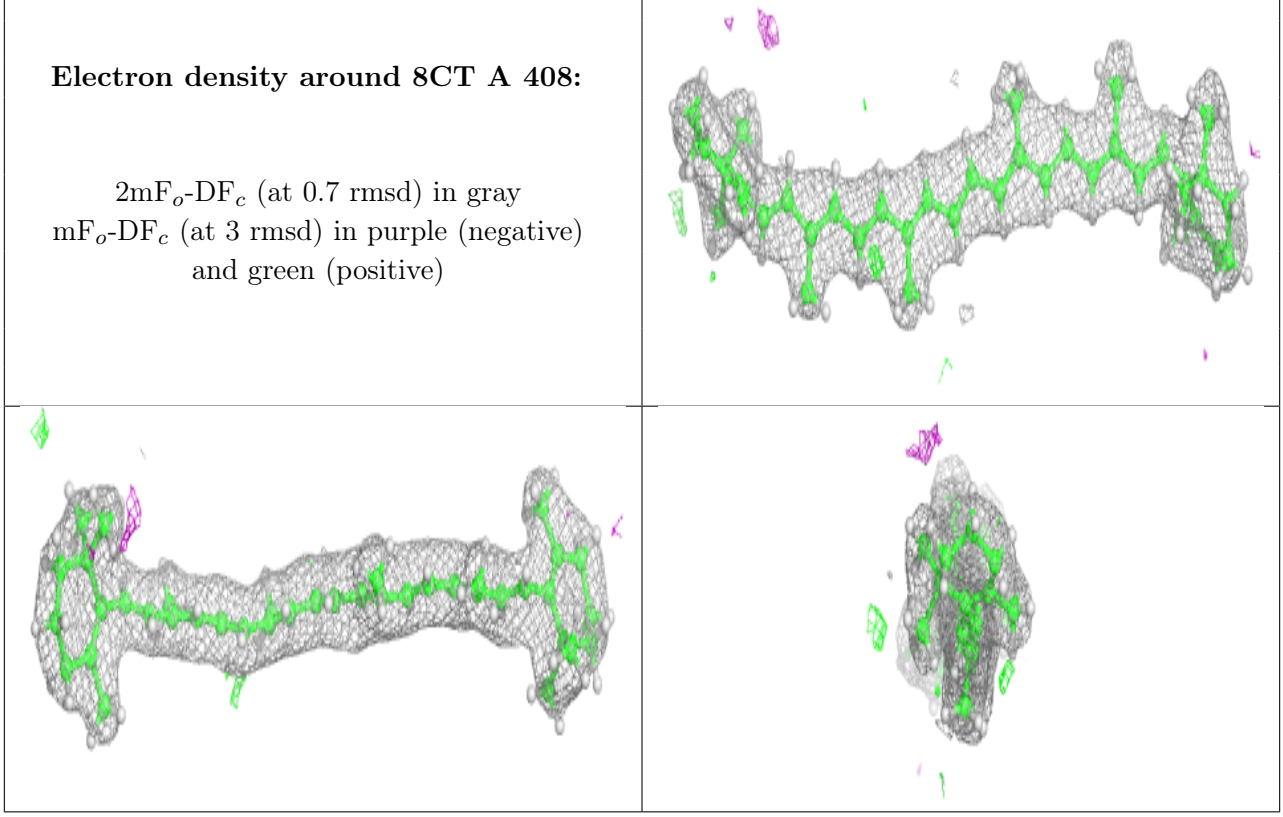






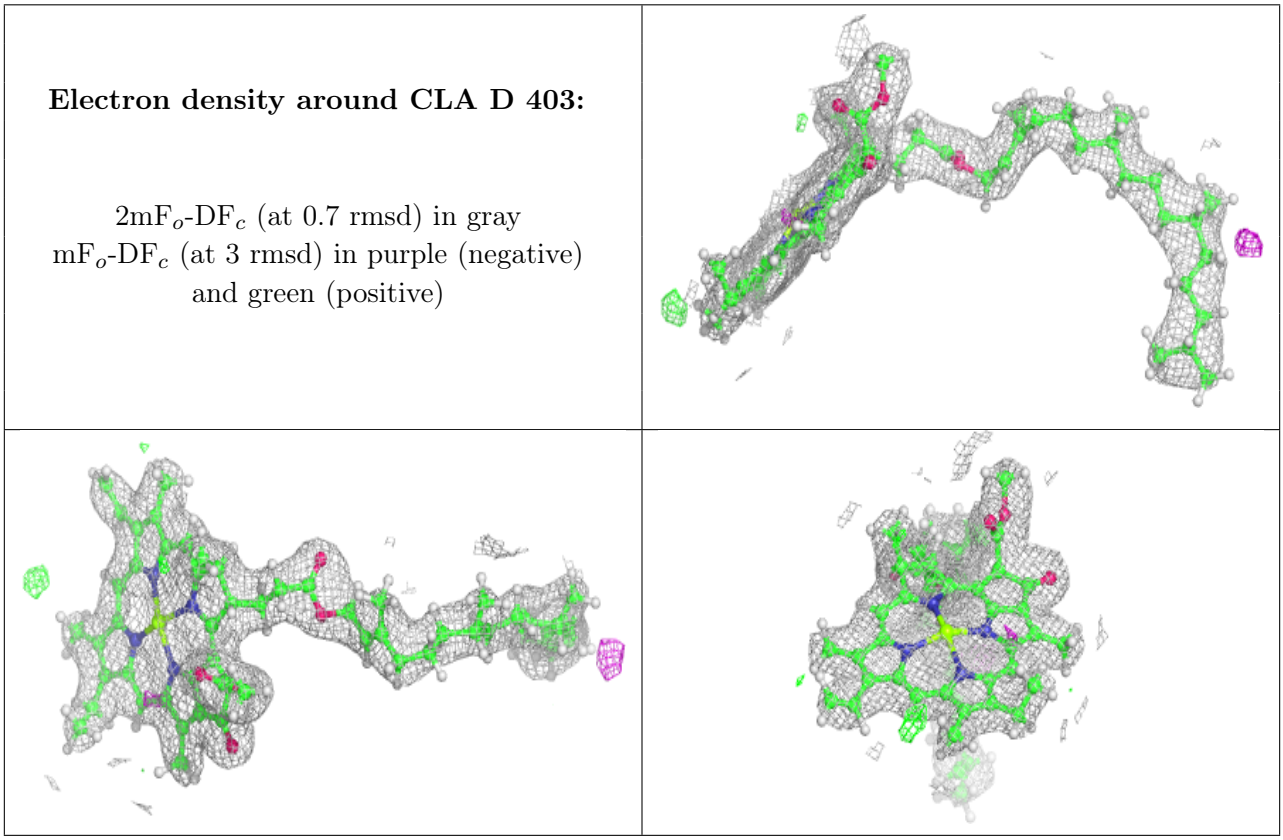
Electron density around 8CT A 408:

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



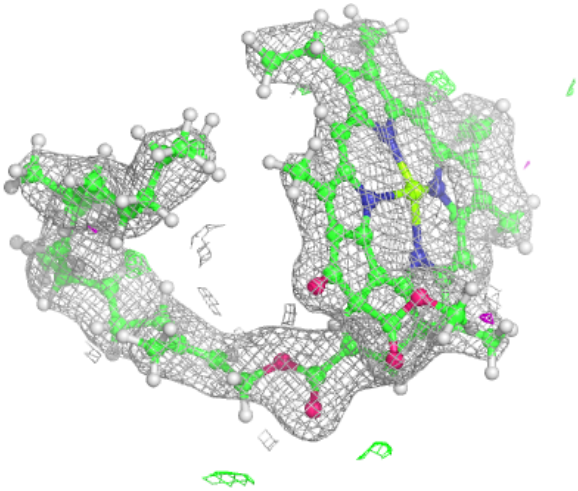
Electron density around CLA D 403:

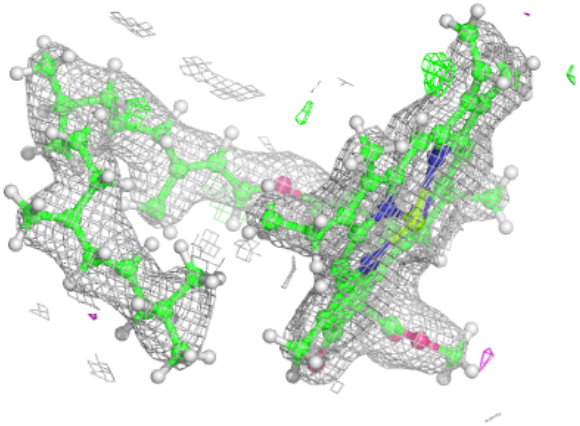
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

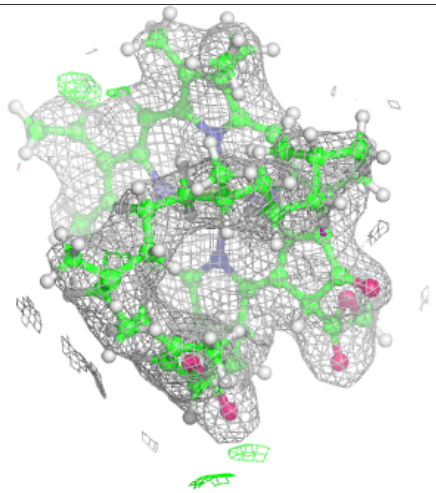


Electron density around CLA C 503:

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

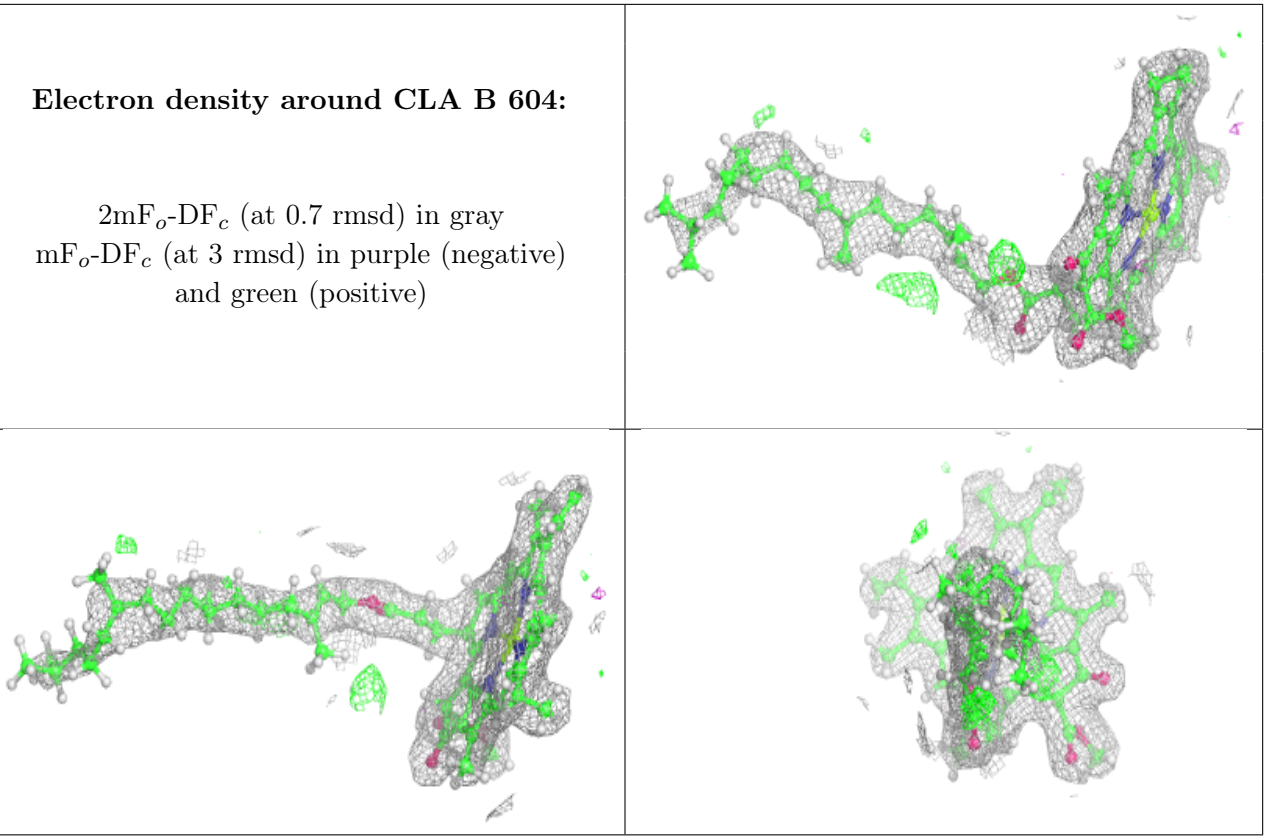






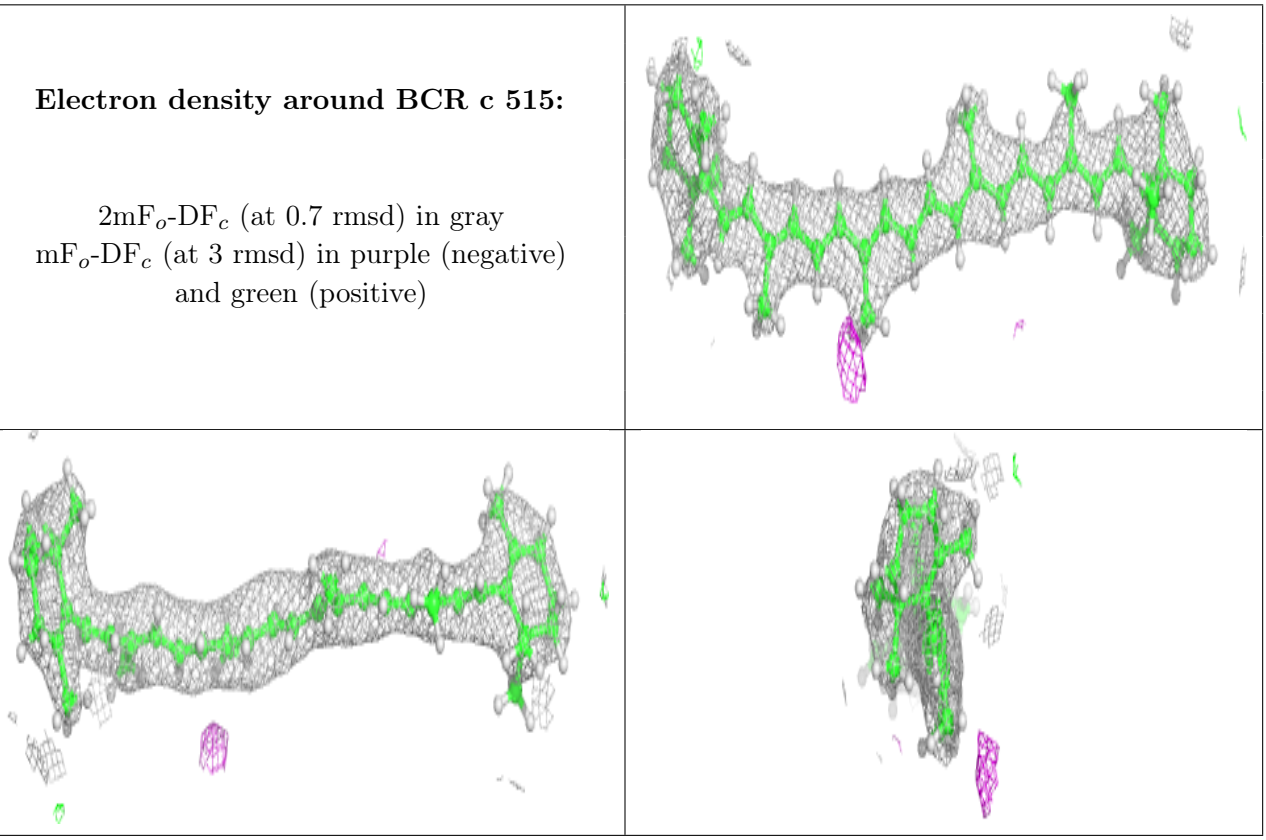
Electron density around CLA B 604:

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



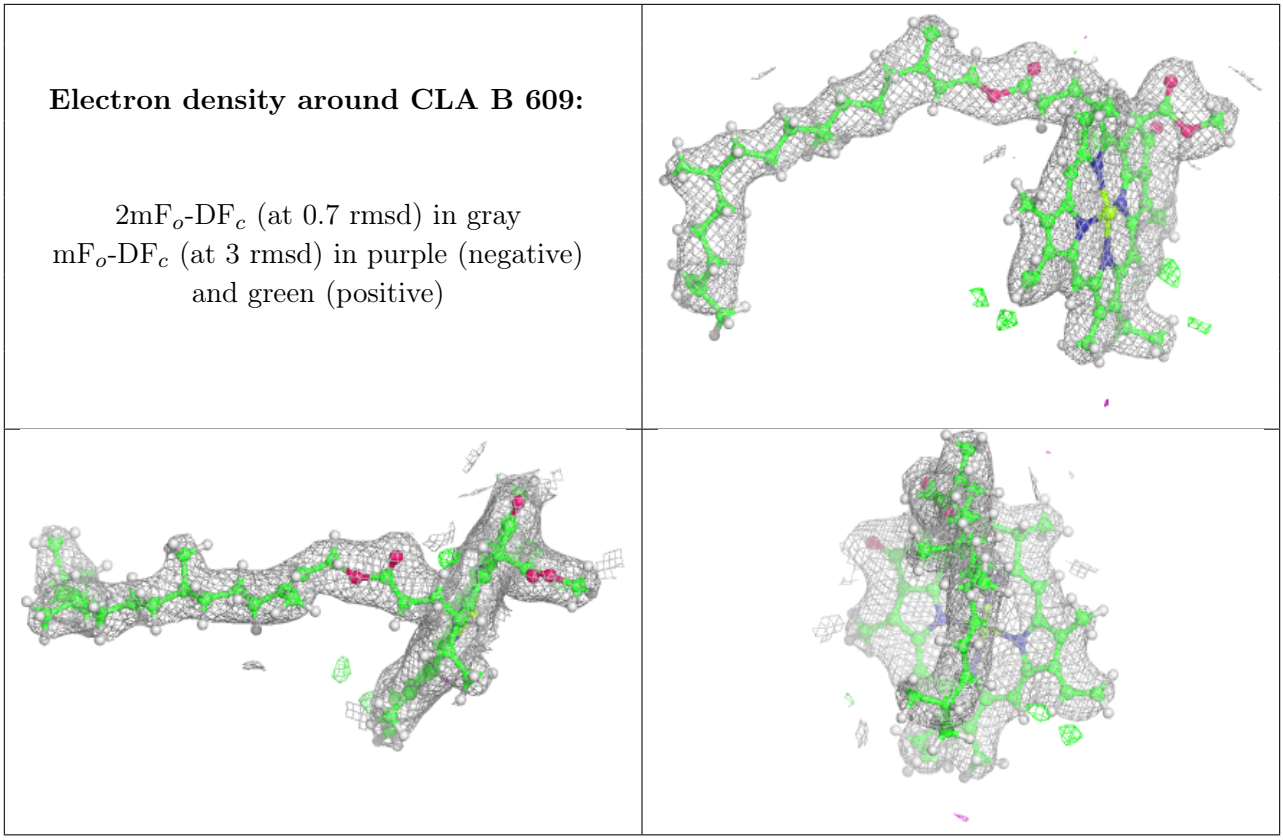
Electron density around BCR c 515:

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



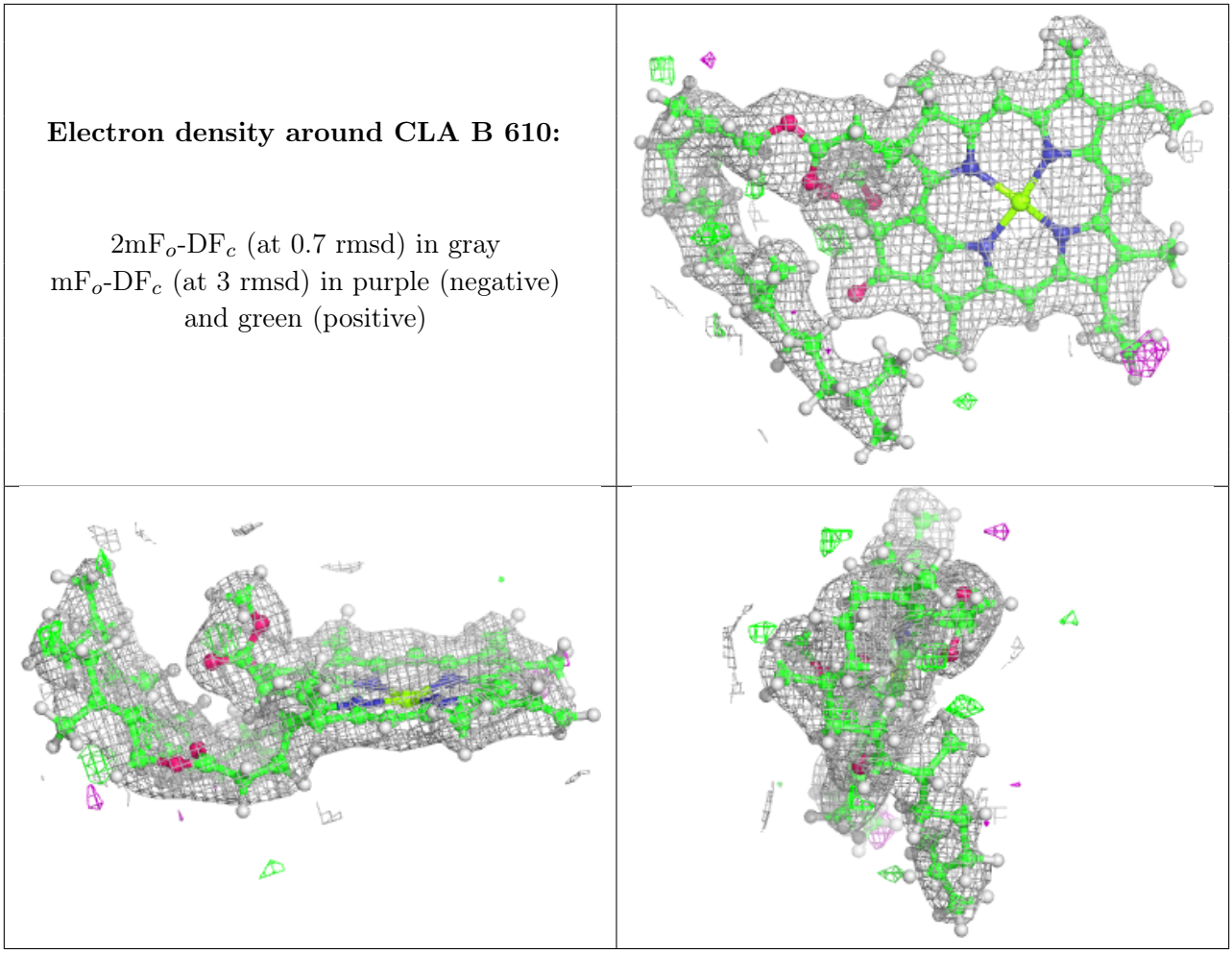
Electron density around CLA B 609:

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



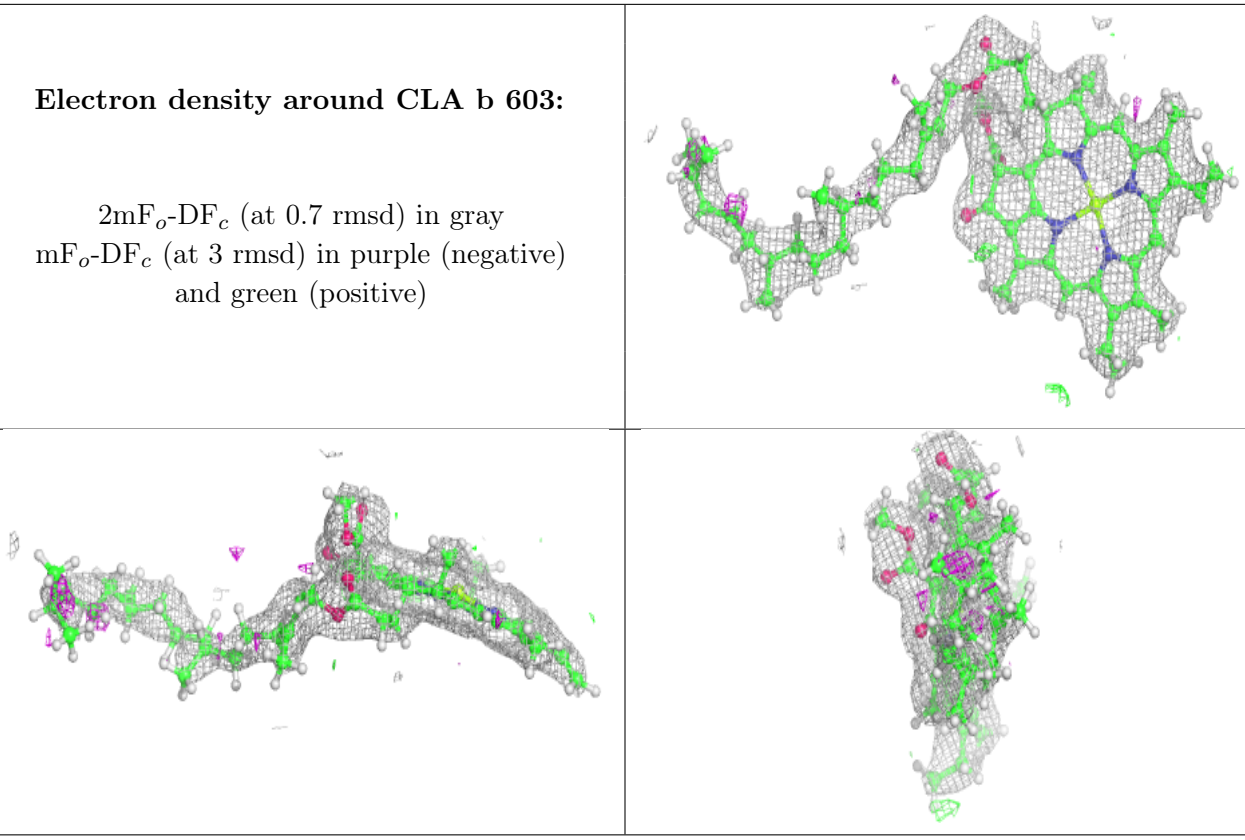
Electron density around CLA B 610:

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



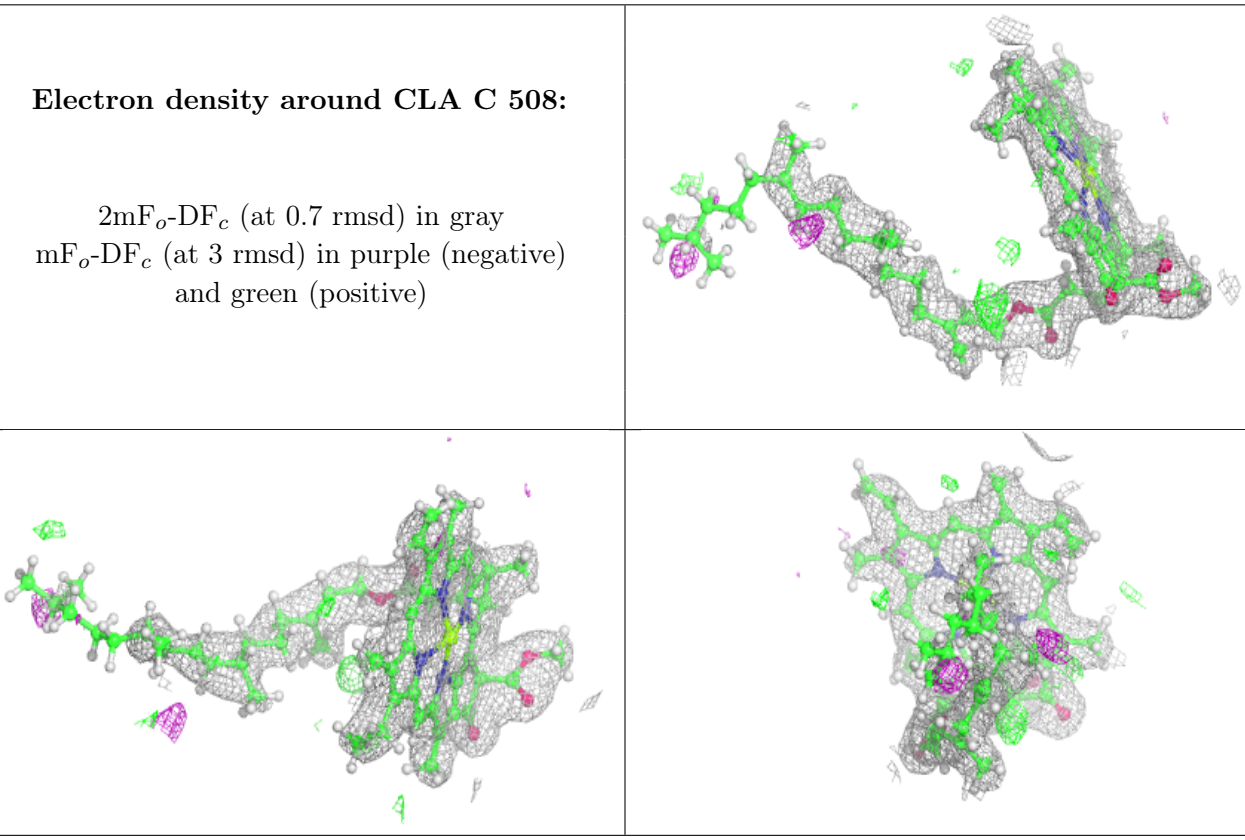
Electron density around CLA b 603:

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



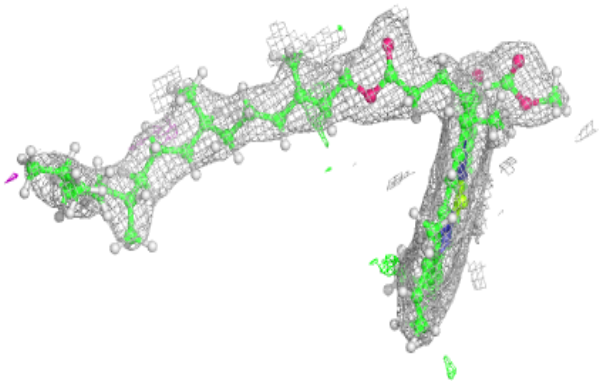
Electron density around CLA C 508:

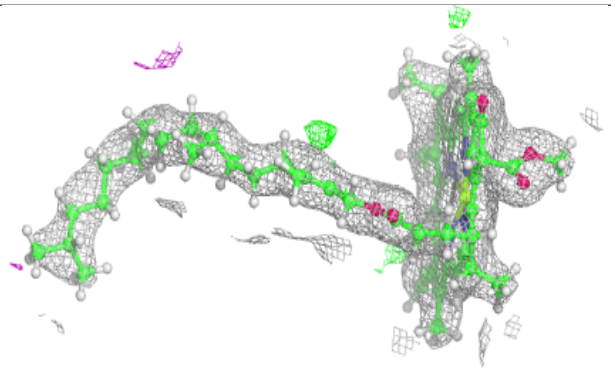
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

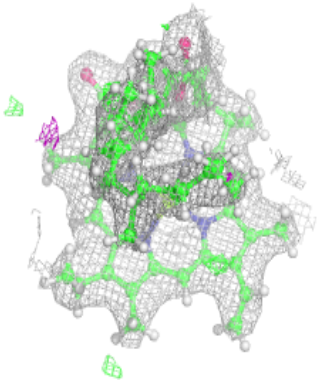


Electron density around CLA b 606:

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

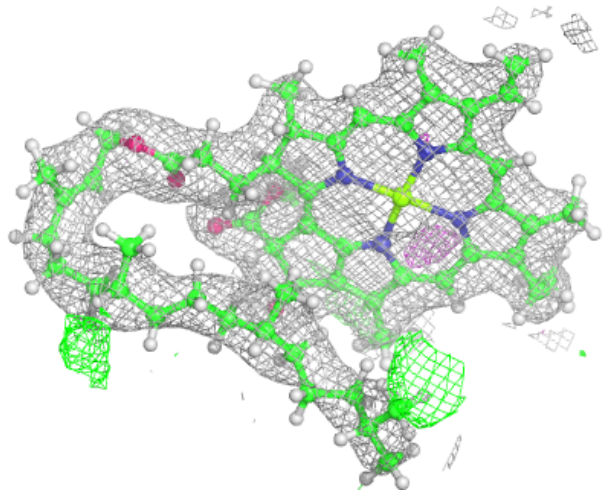


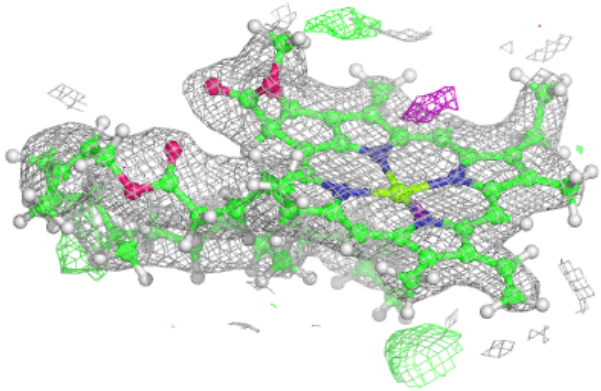


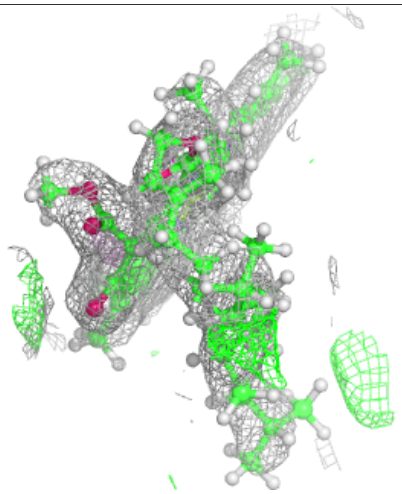


Electron density around CLA C 509:

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

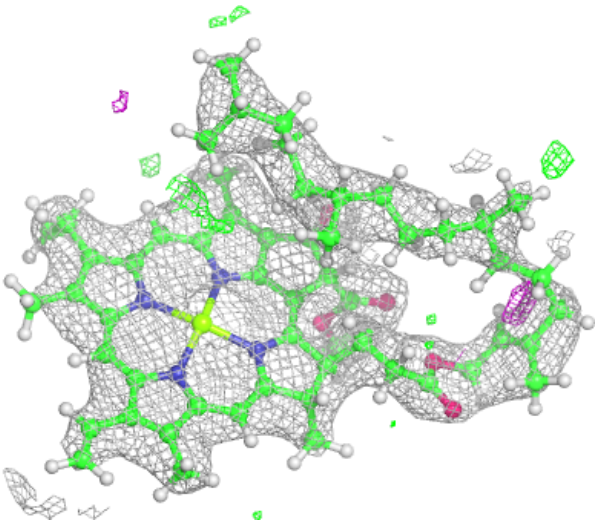


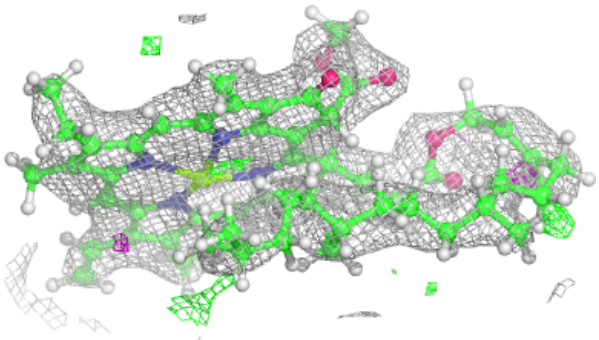


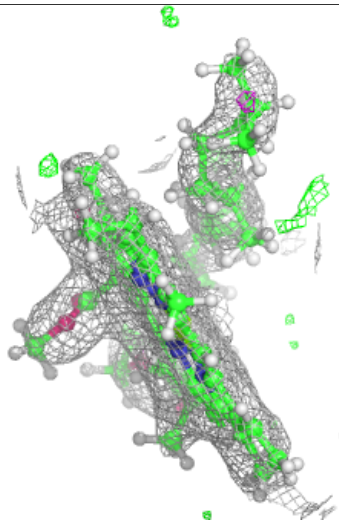


Electron density around CLA c 509:

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

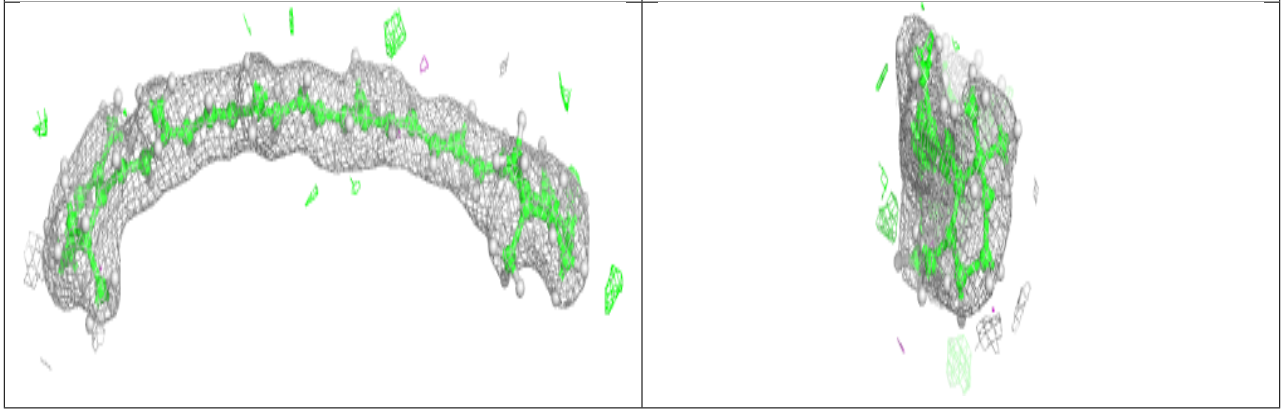






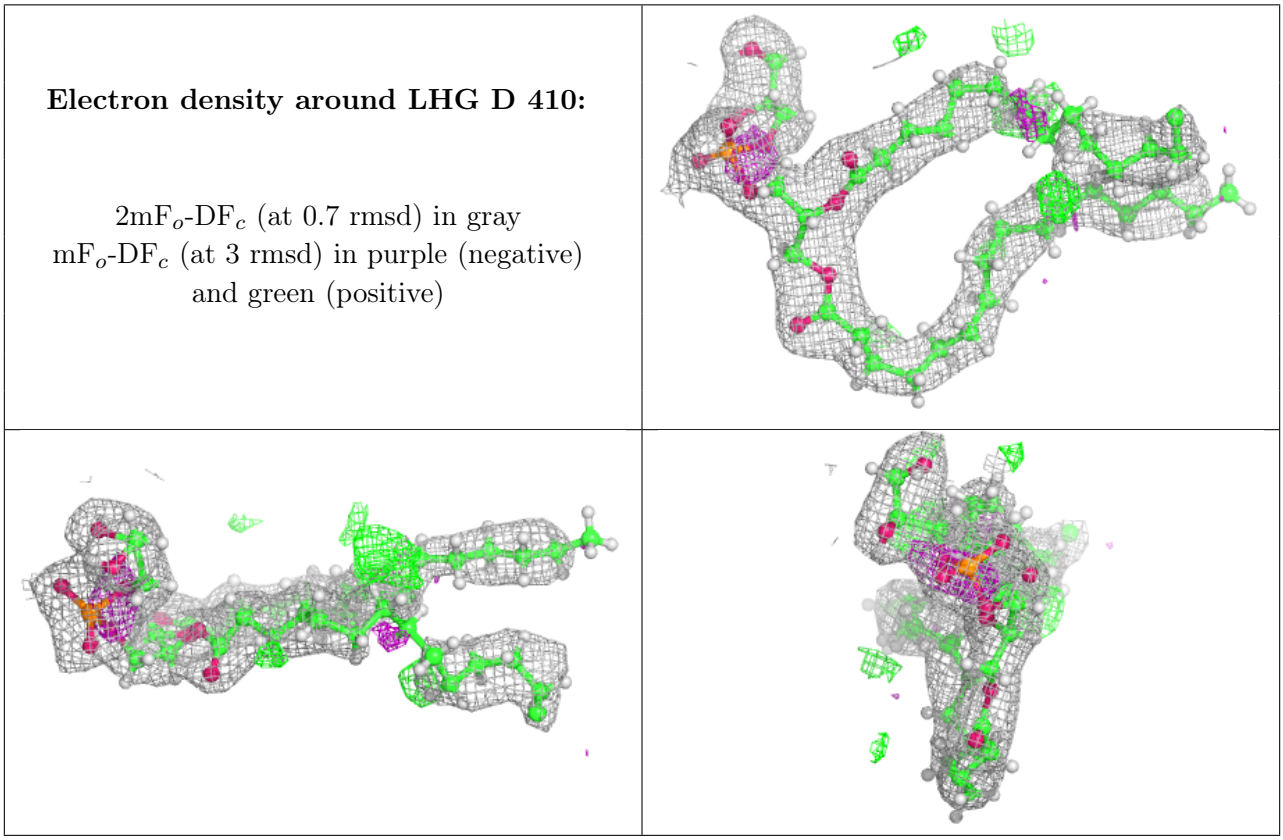
Electron density around 8CT t 101:

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



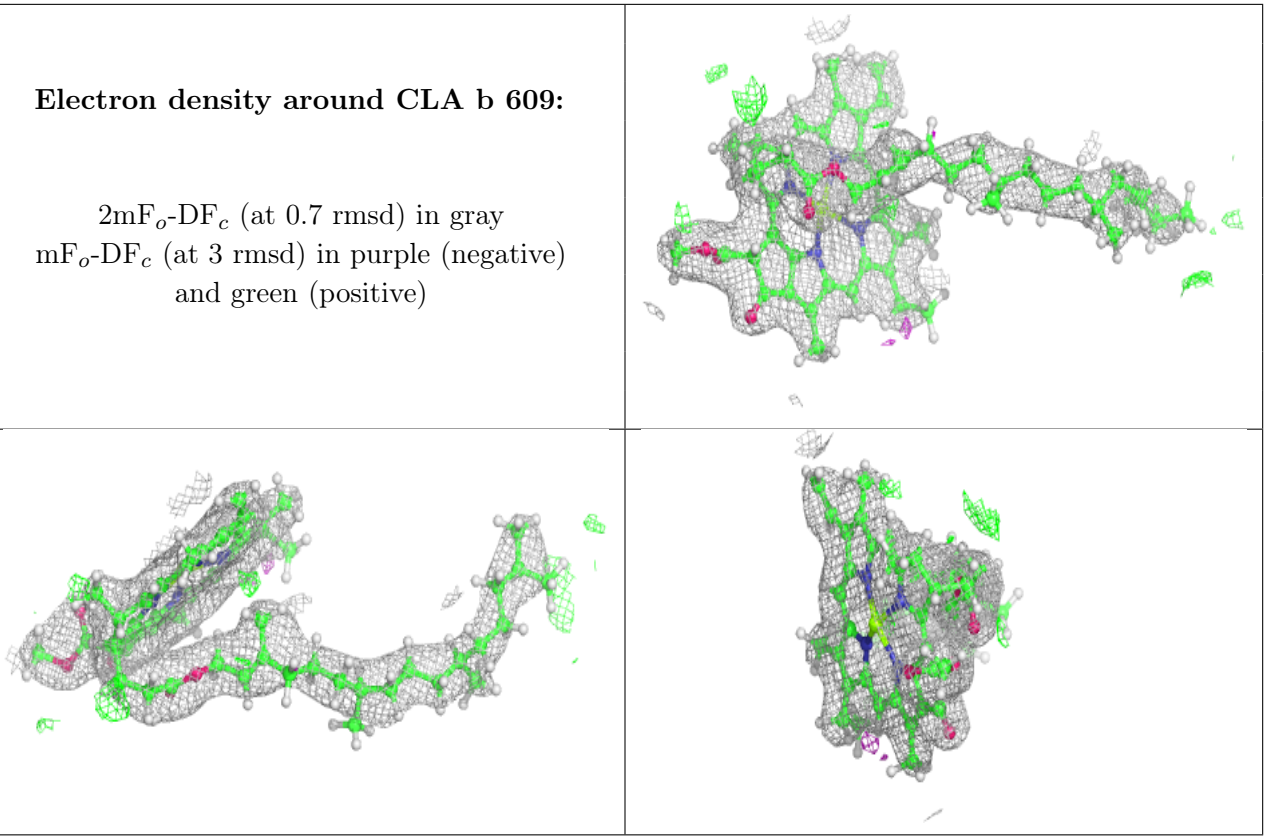
Electron density around LHG D 410:

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



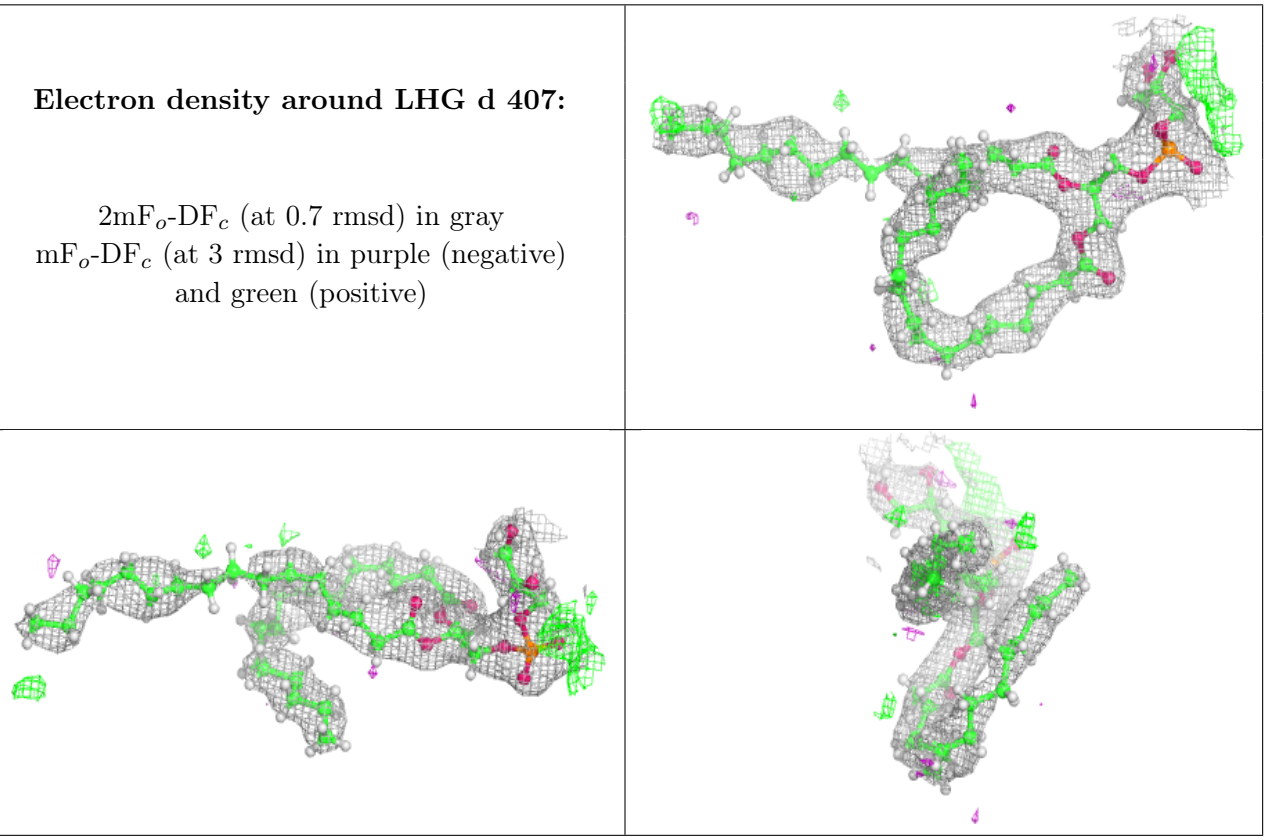
Electron density around CLA b 609:

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



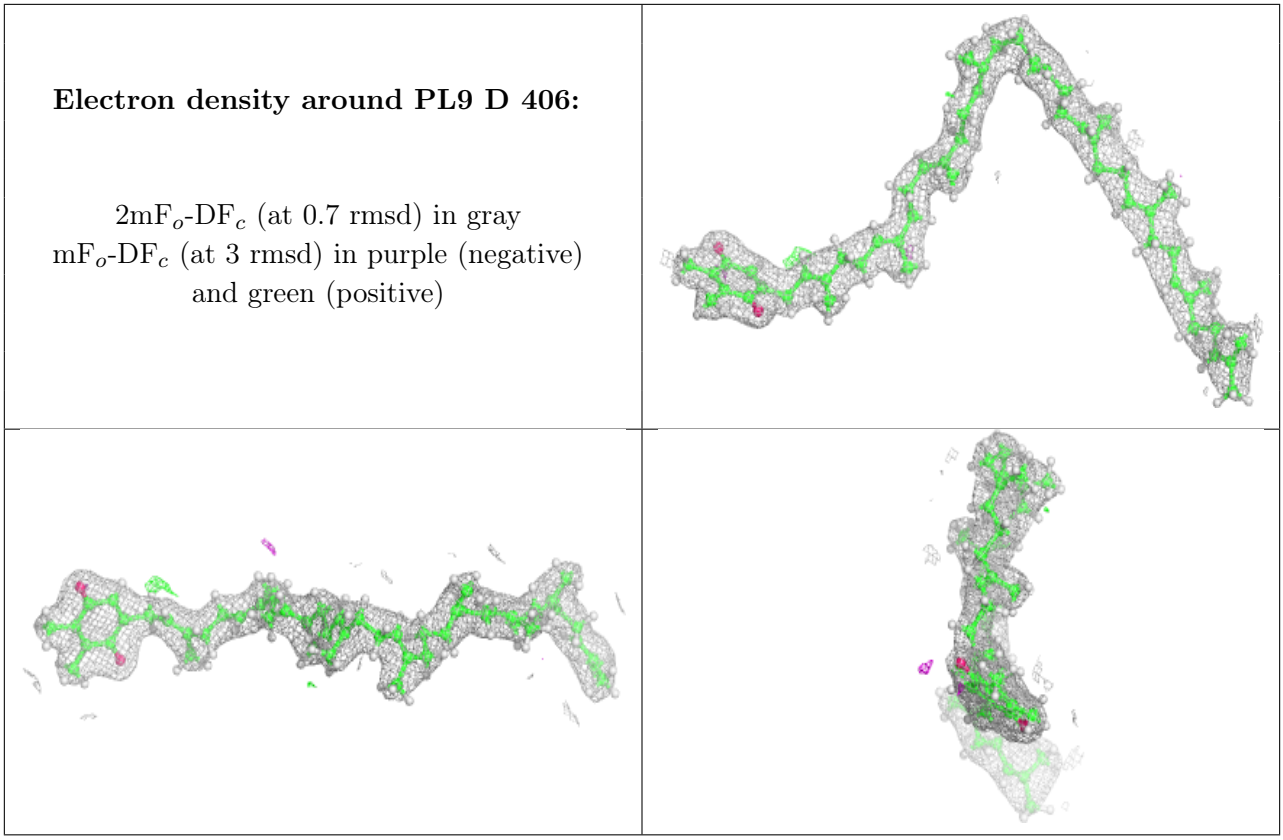
Electron density around LHG d 407:

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



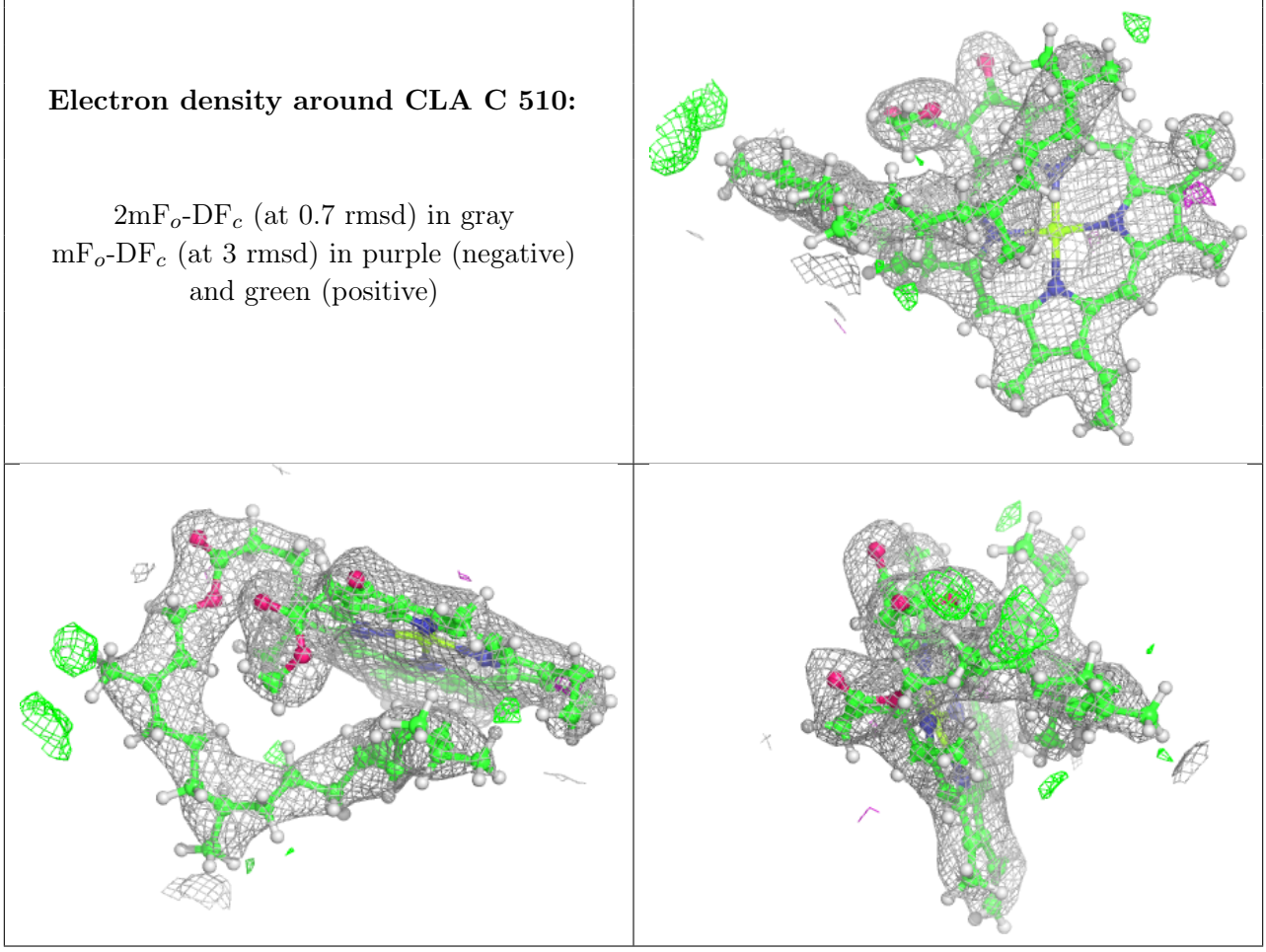
Electron density around PL9 D 406:

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



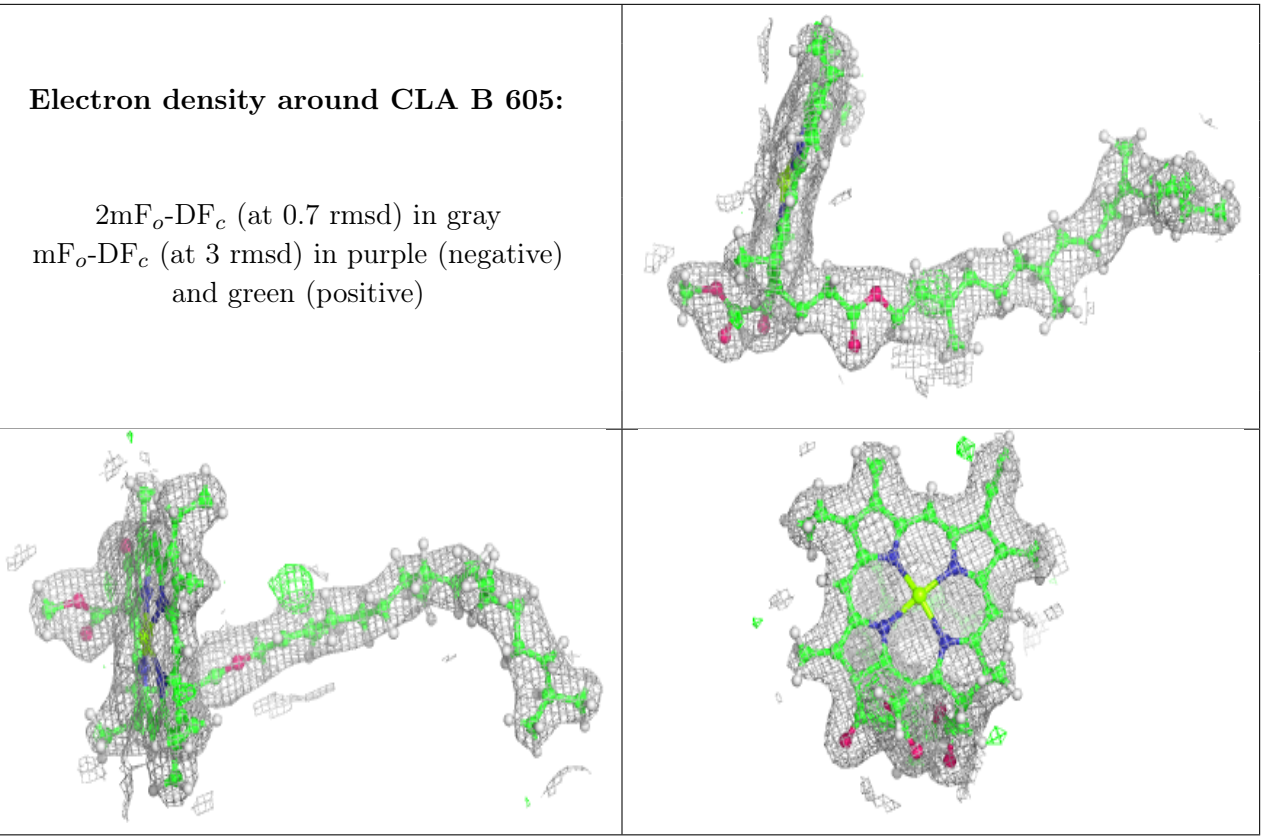
Electron density around CLA C 510:

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



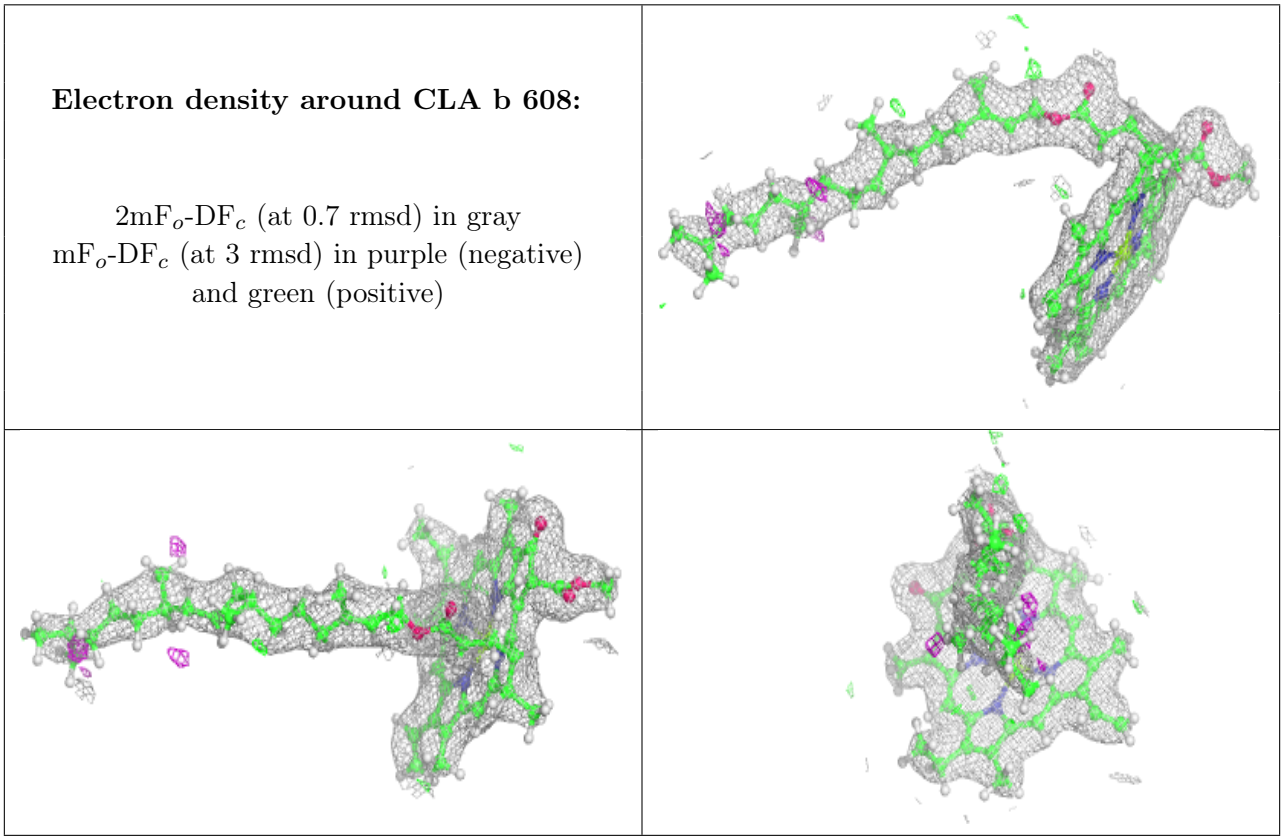
Electron density around CLA B 605:

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



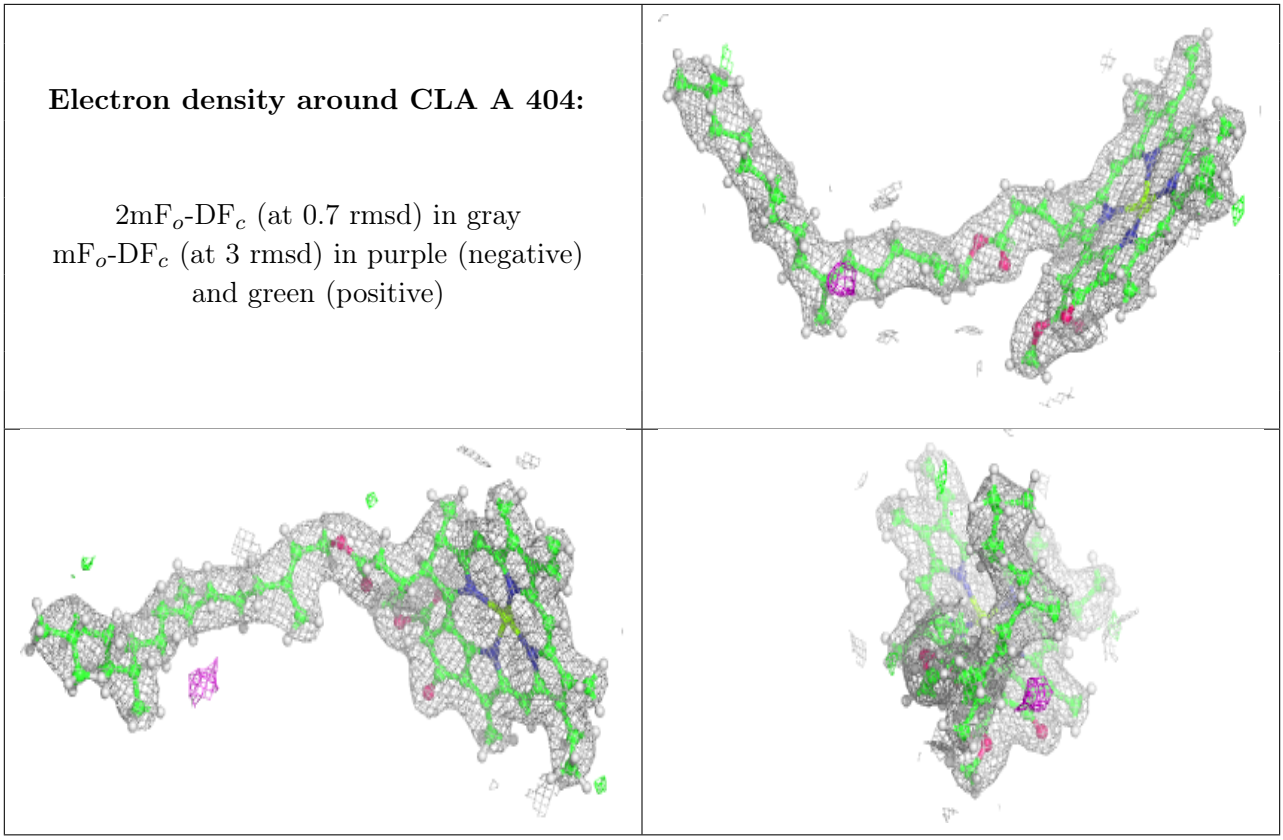
Electron density around CLA b 608:

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



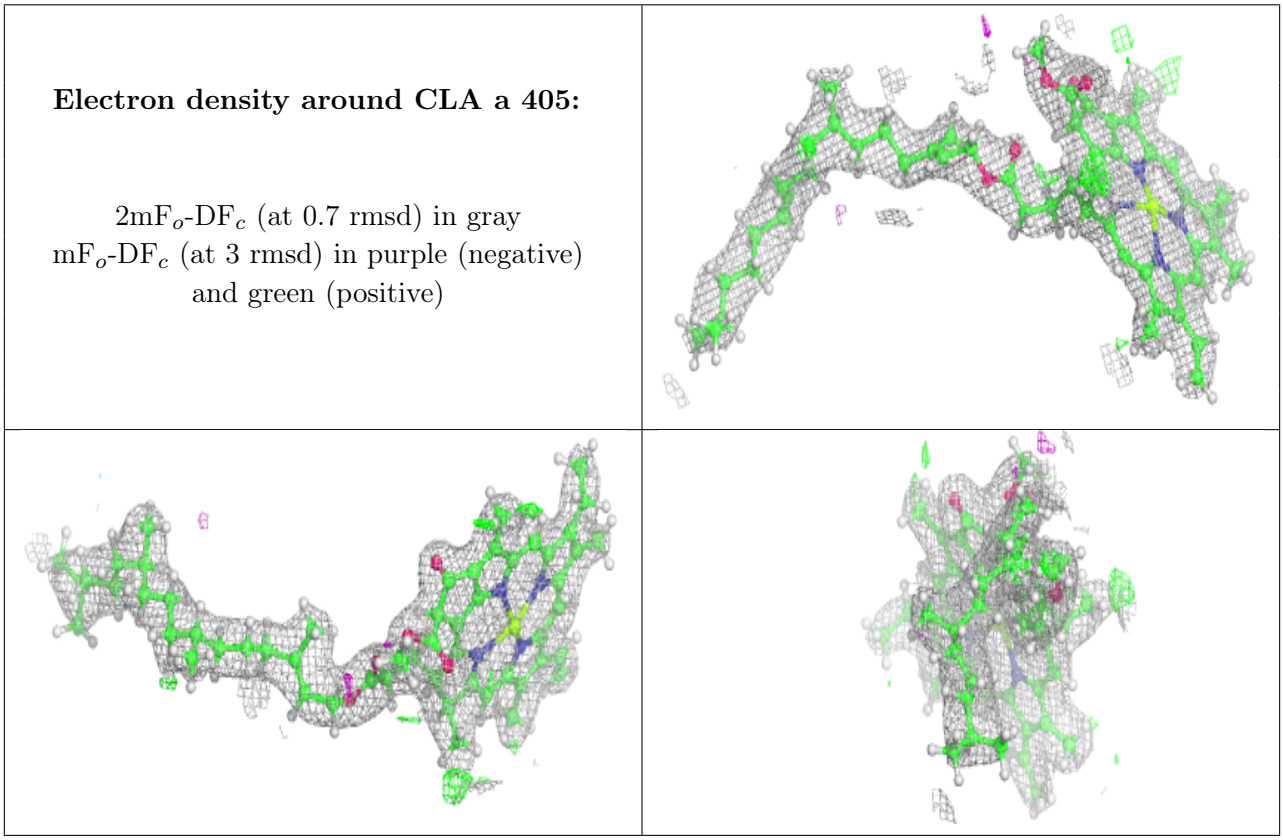
Electron density around CLA A 404:

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



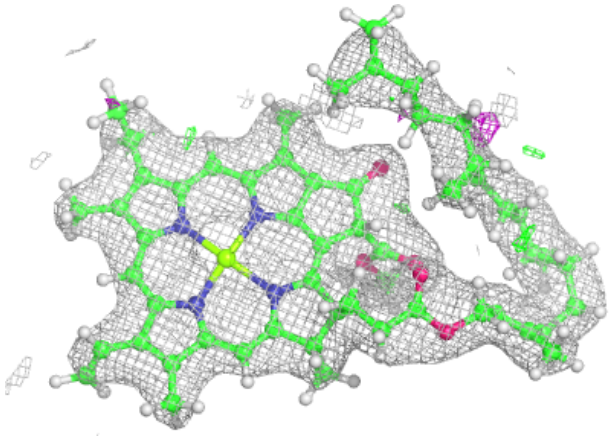
Electron density around CLA a 405:

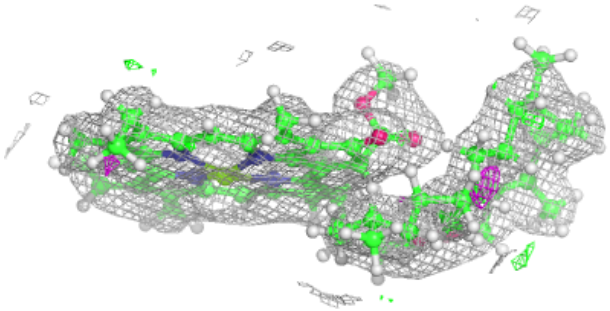
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

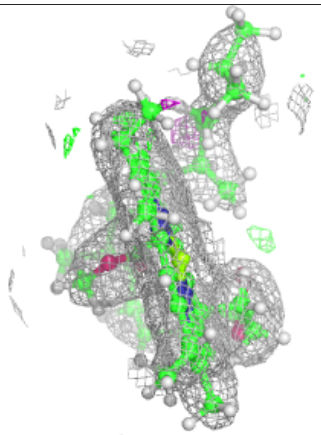


Electron density around CLA b 611:

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

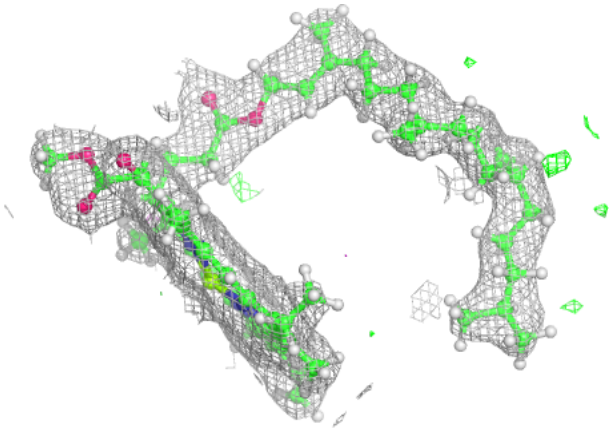


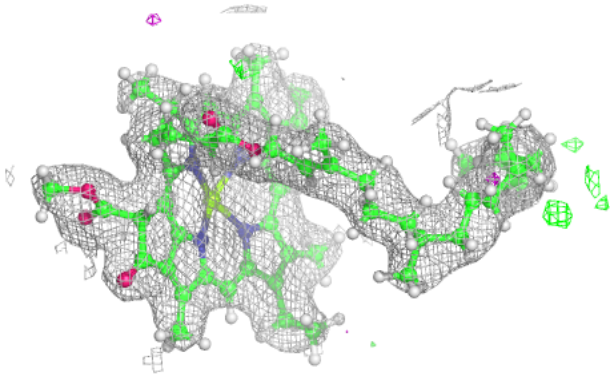


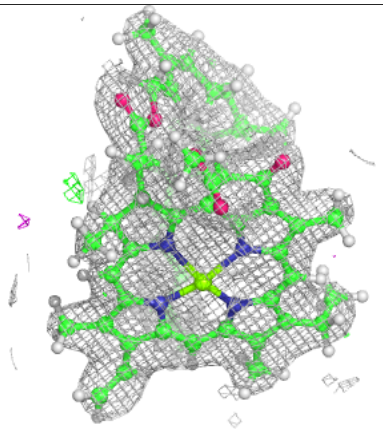


Electron density around CLA b 612:

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

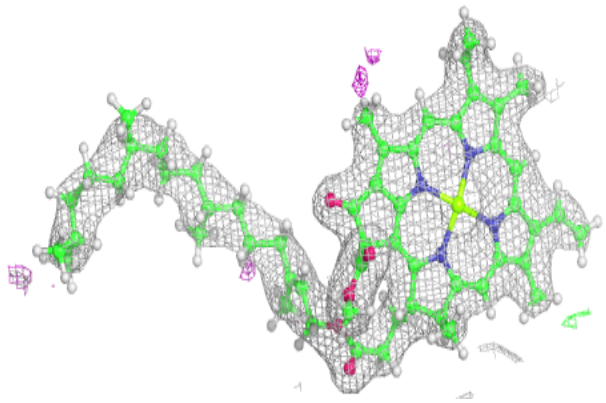


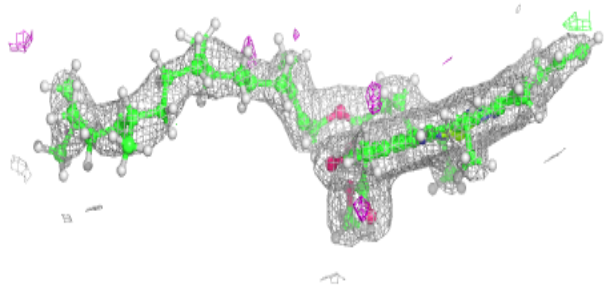


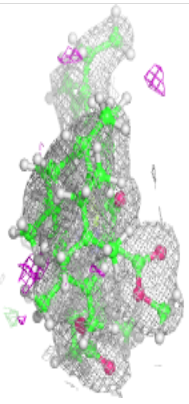


Electron density around CLA B 602:

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

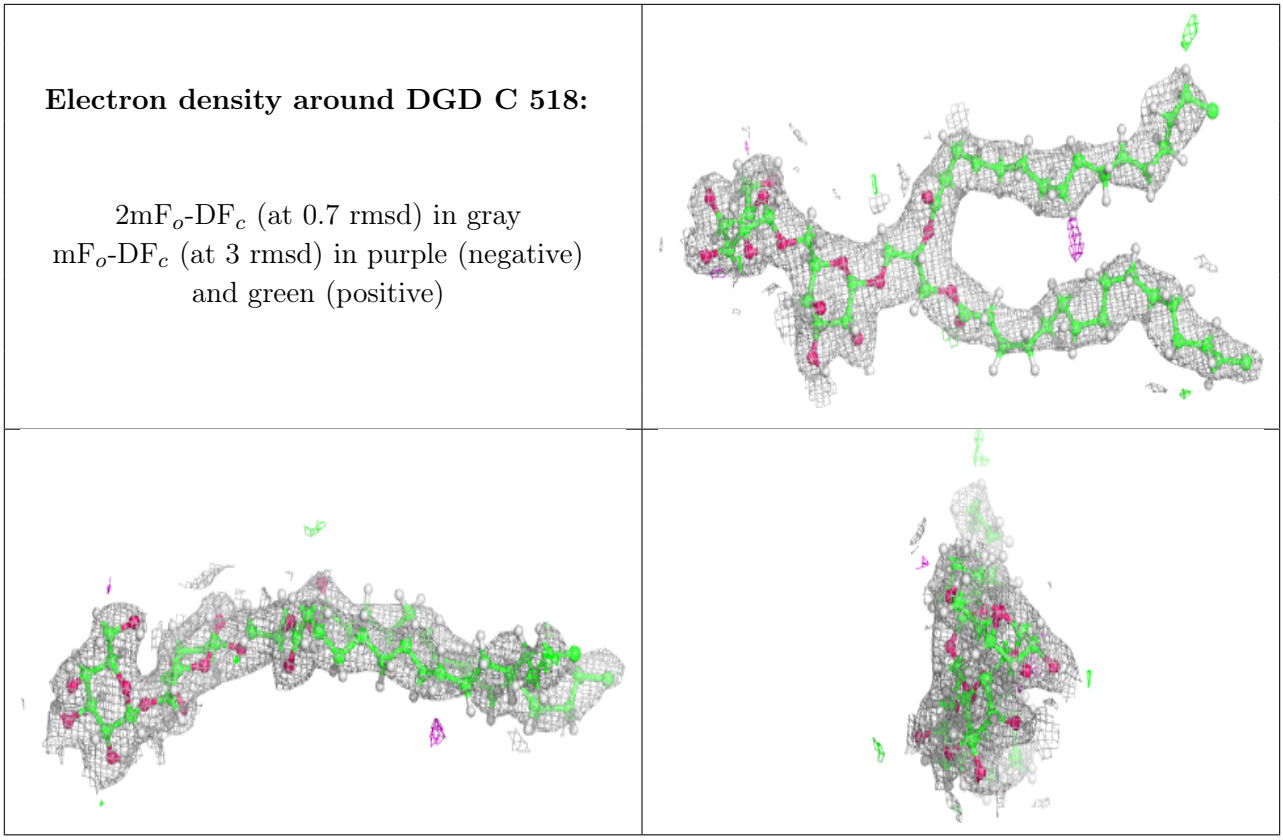






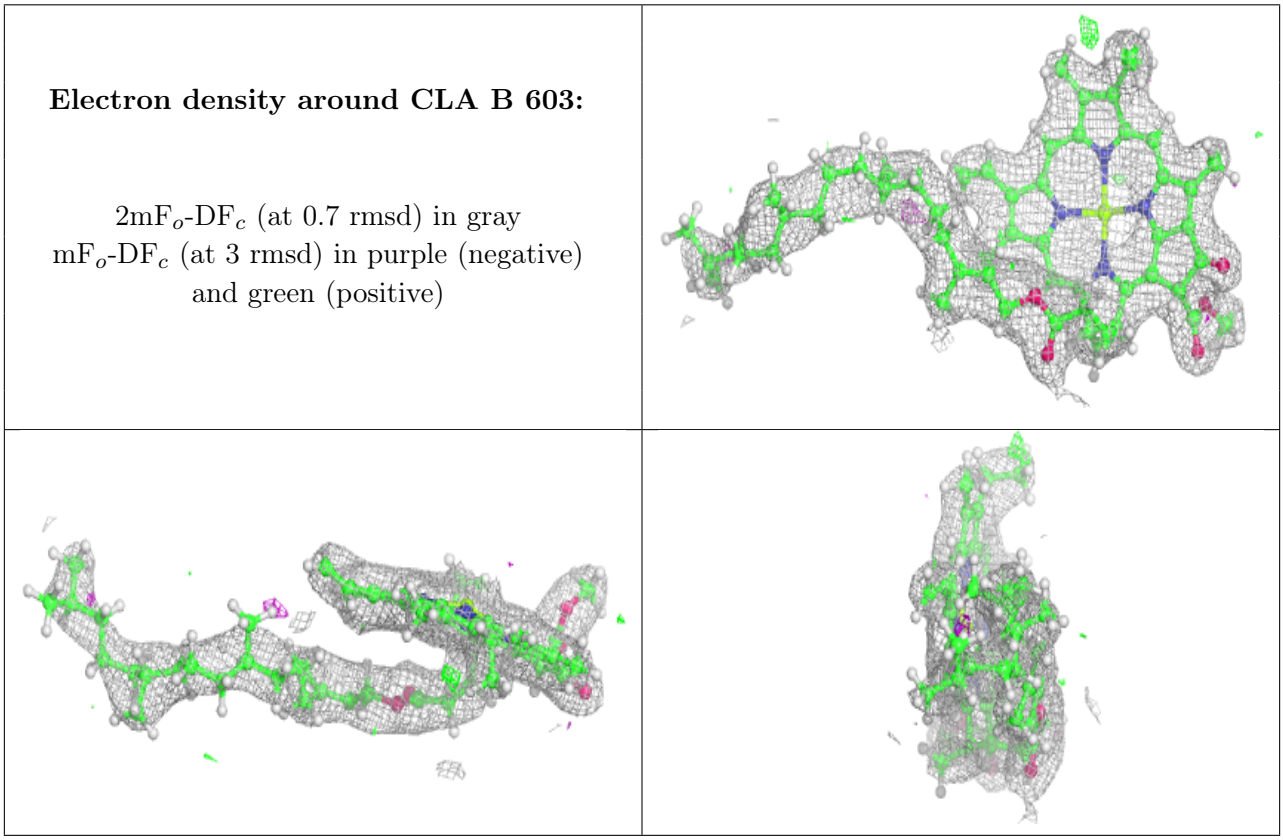
Electron density around DGD C 518:

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



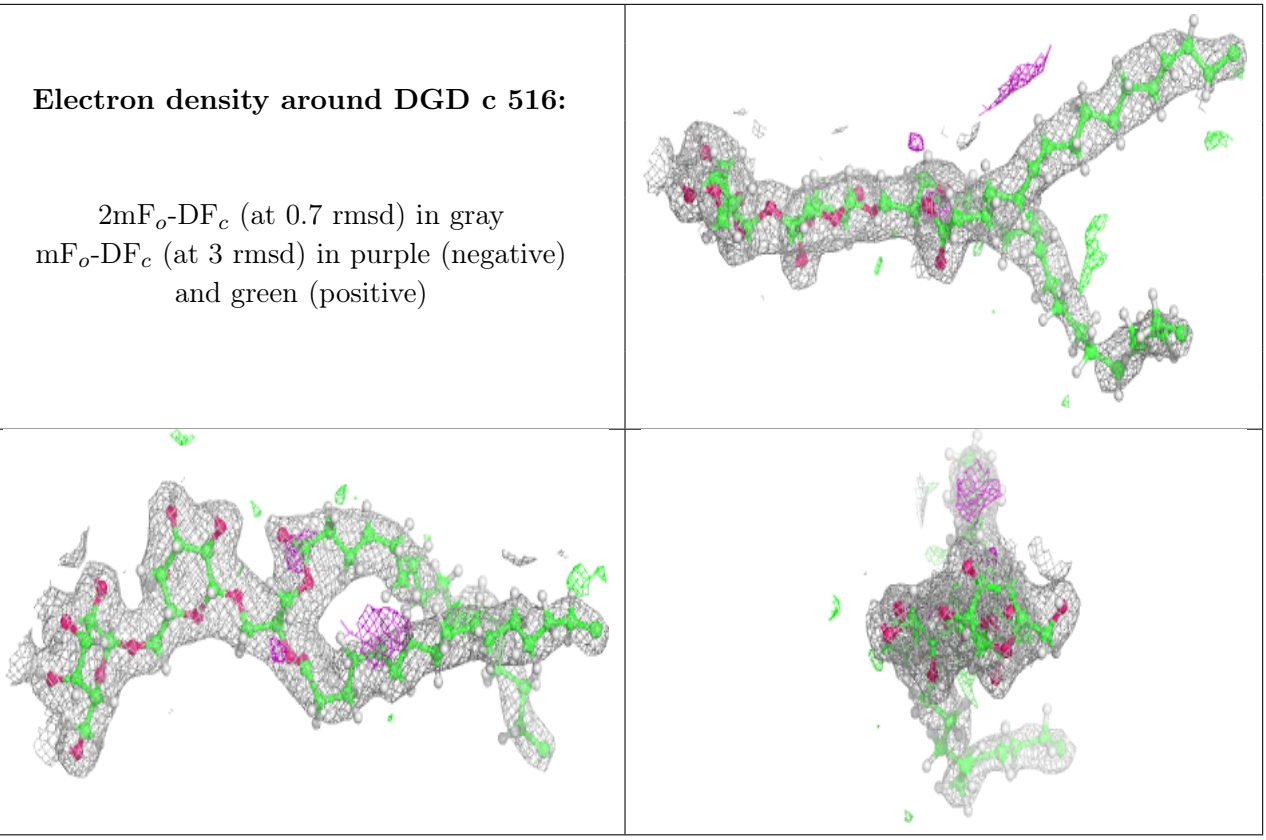
Electron density around CLA B 603:

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



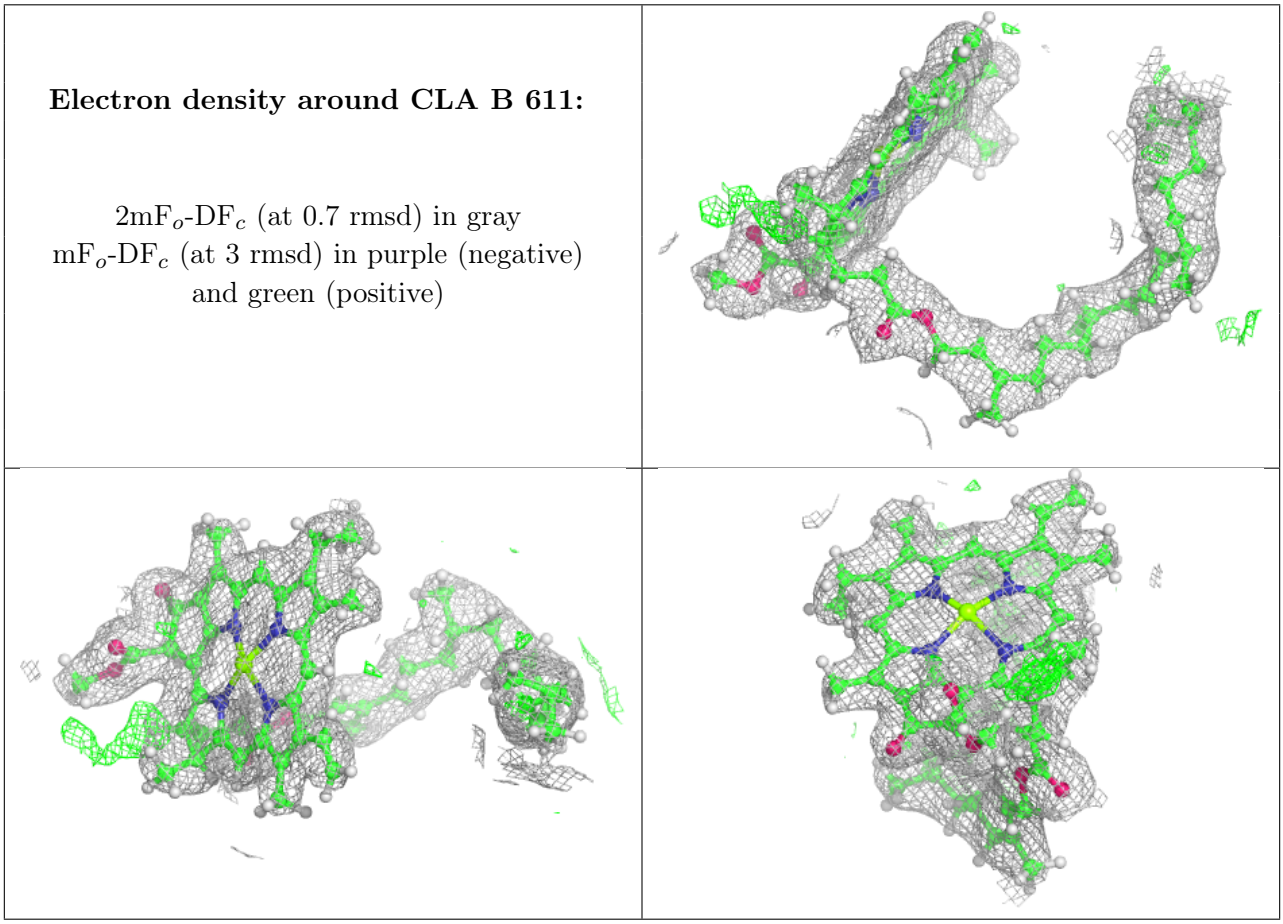
Electron density around DGD c 516:

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



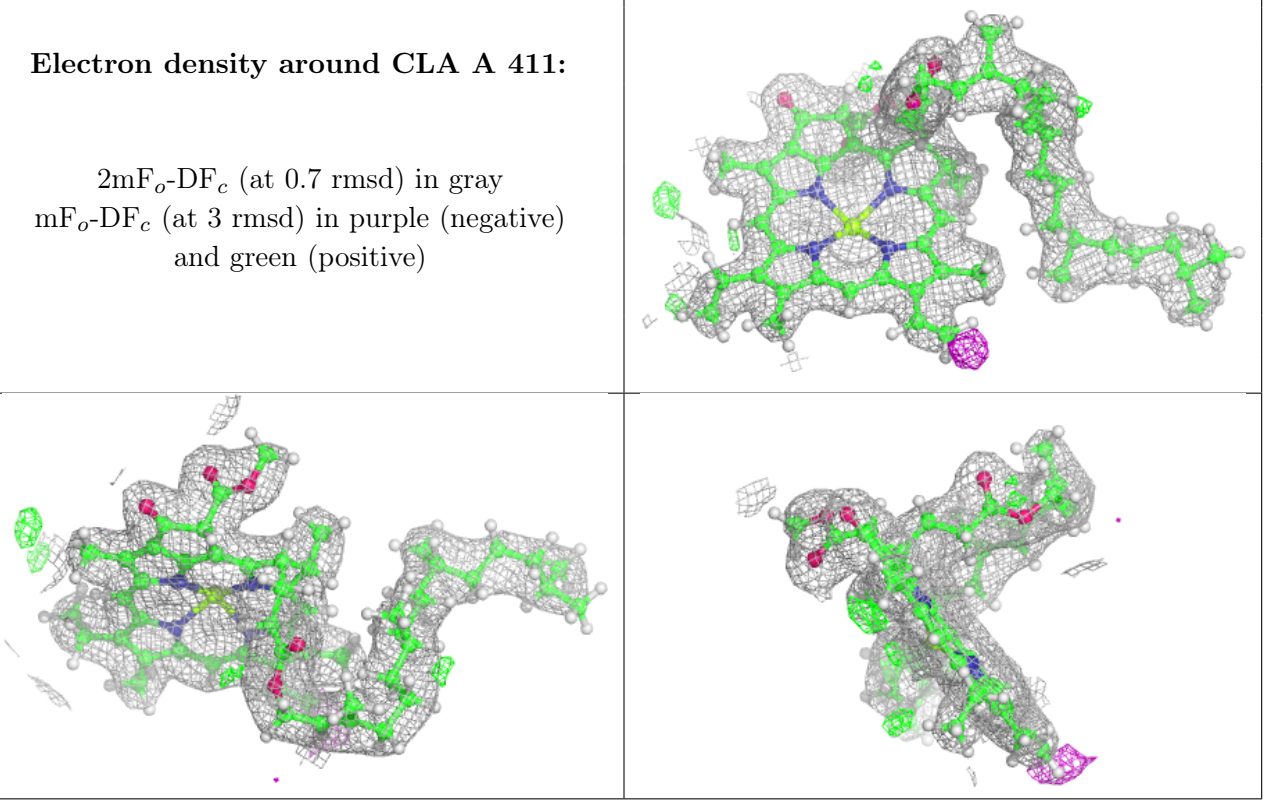
Electron density around CLA B 611:

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



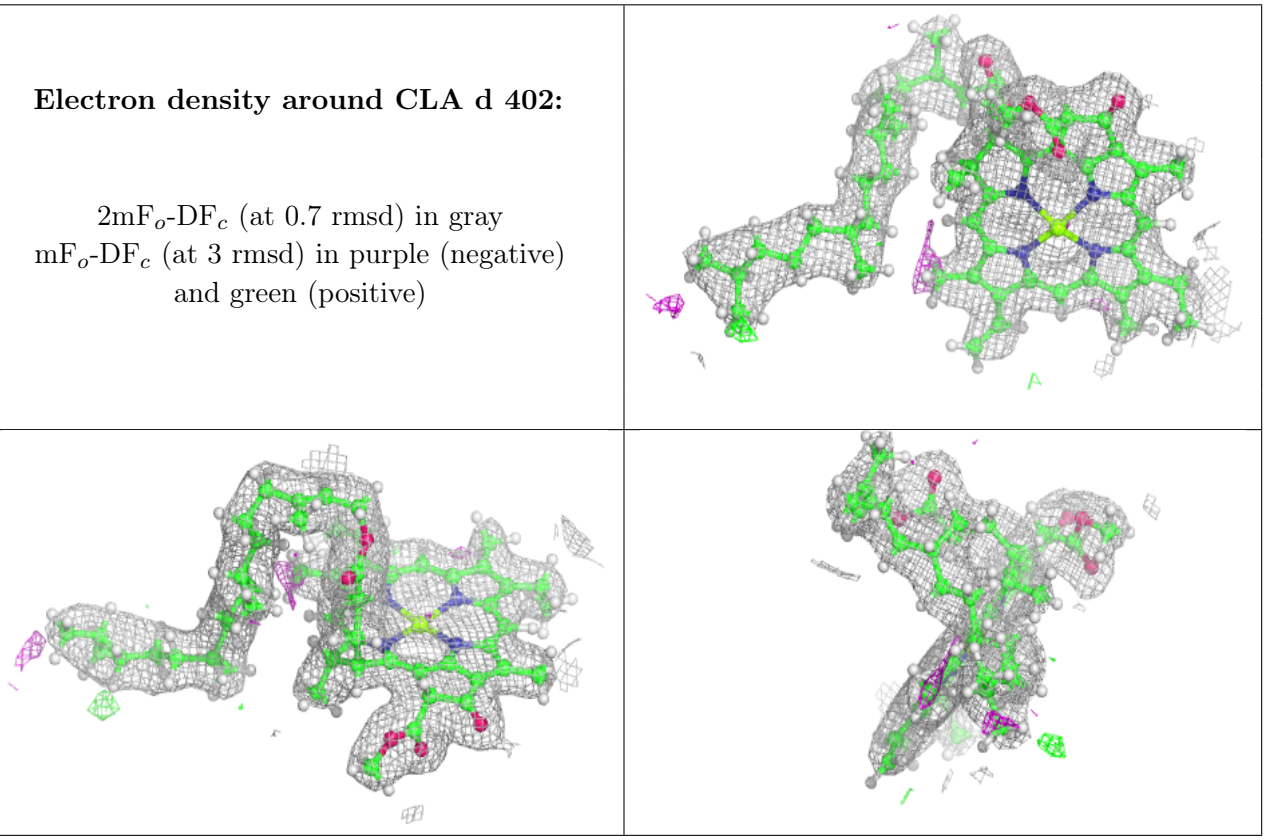
Electron density around CLA A 411:

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



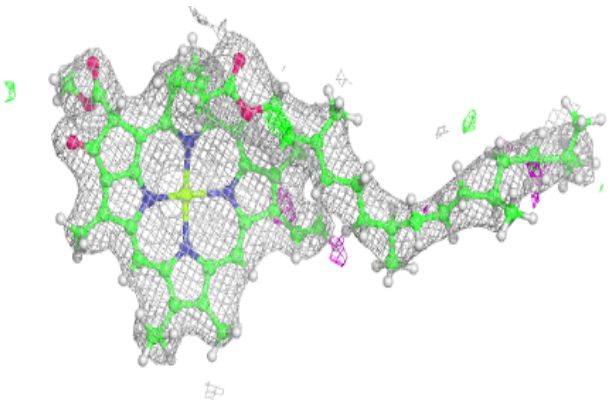
Electron density around CLA d 402:

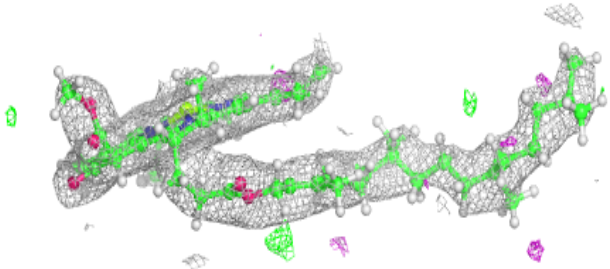
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

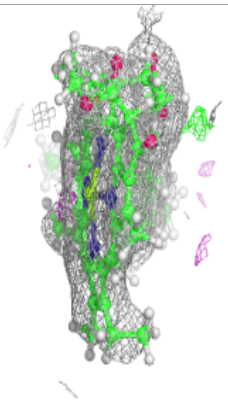


Electron density around CLA b 604:

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

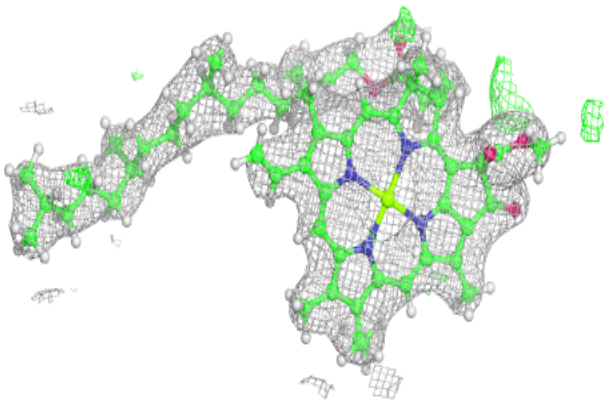


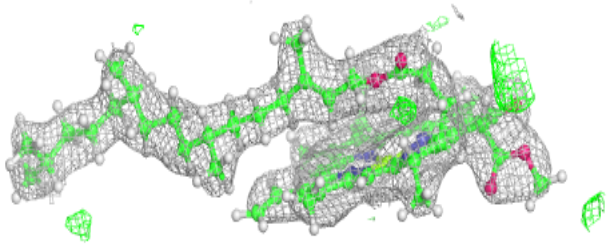


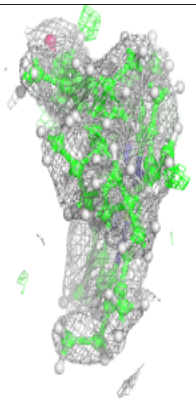


Electron density around CLA c 501:

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

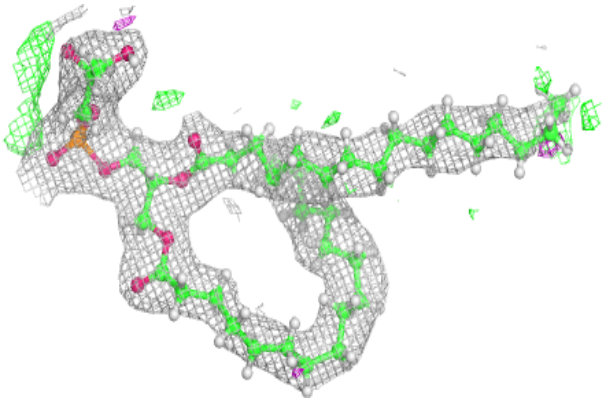


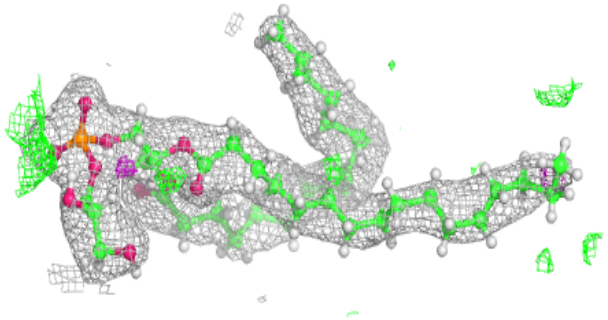


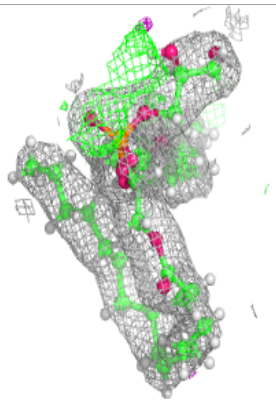


Electron density around LHG B 623:

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

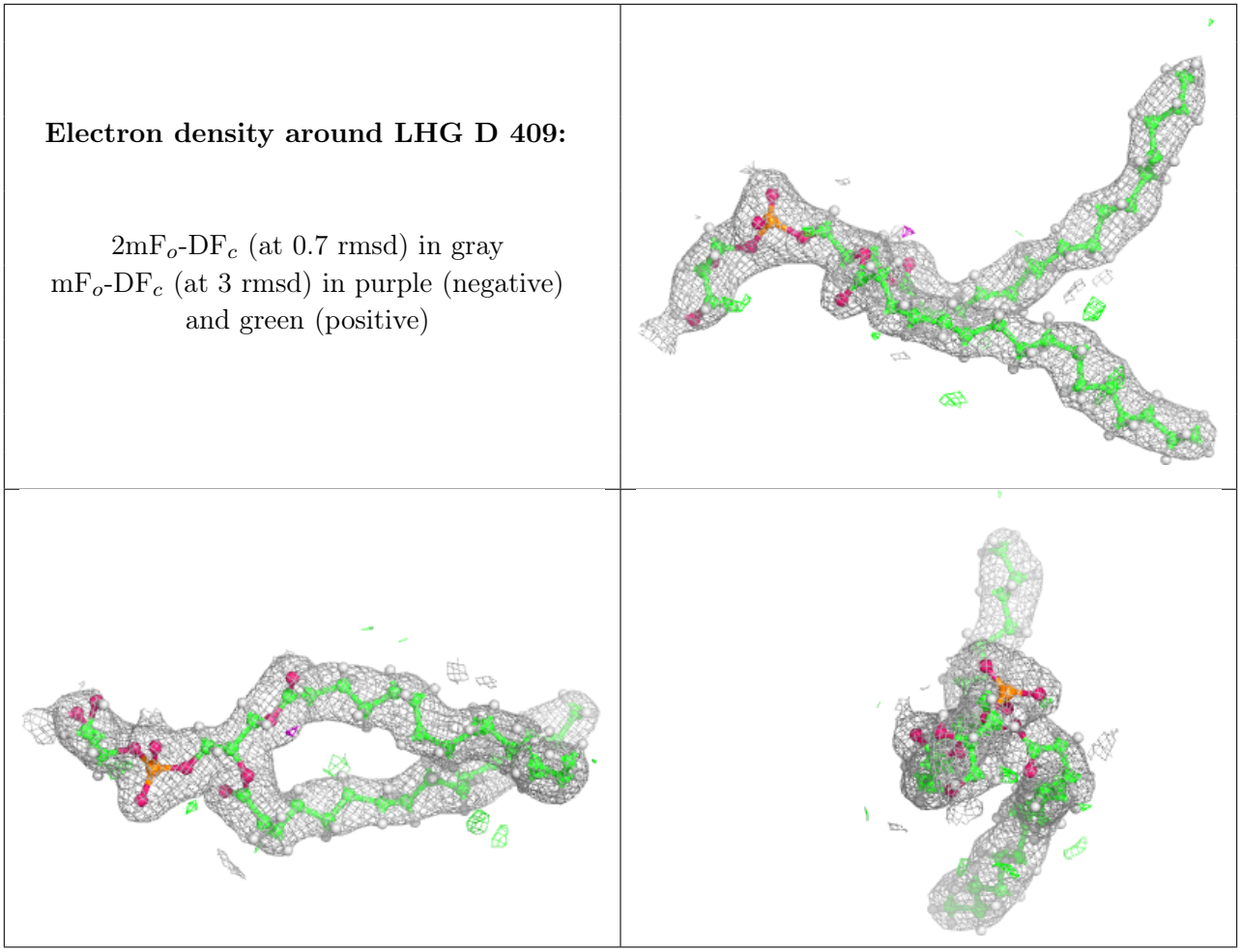






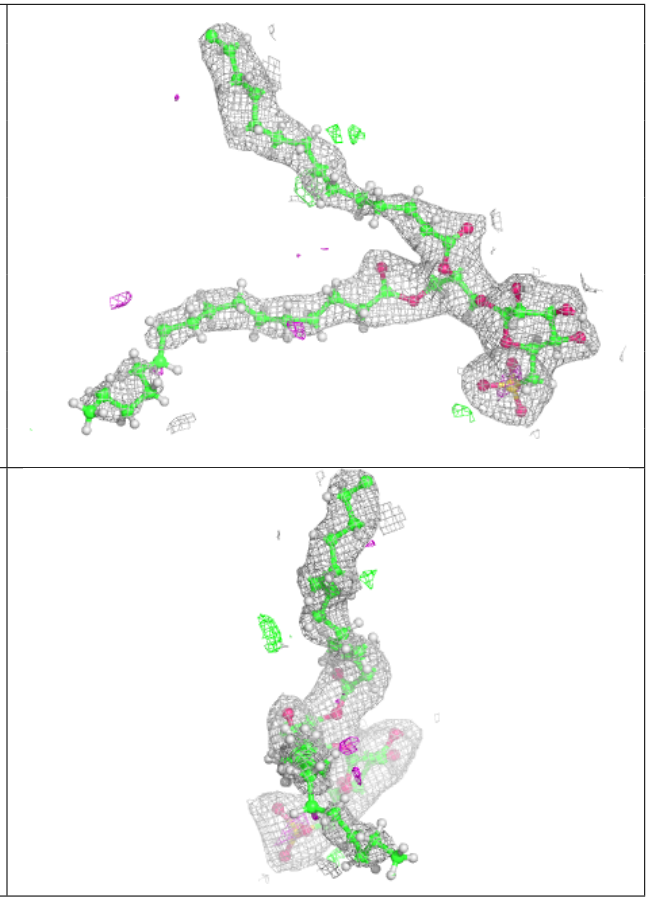
Electron density around LHG D 409:

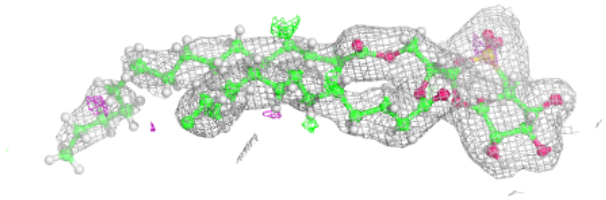
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD A 412:

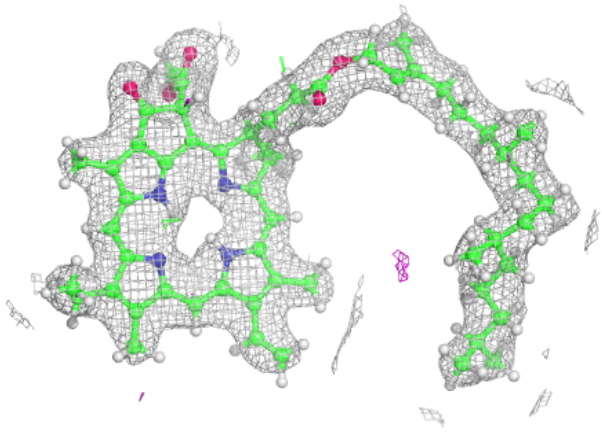
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

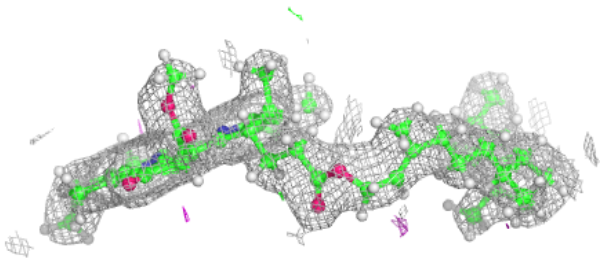


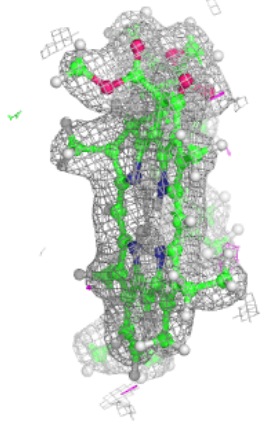


Electron density around PHO A 406:

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

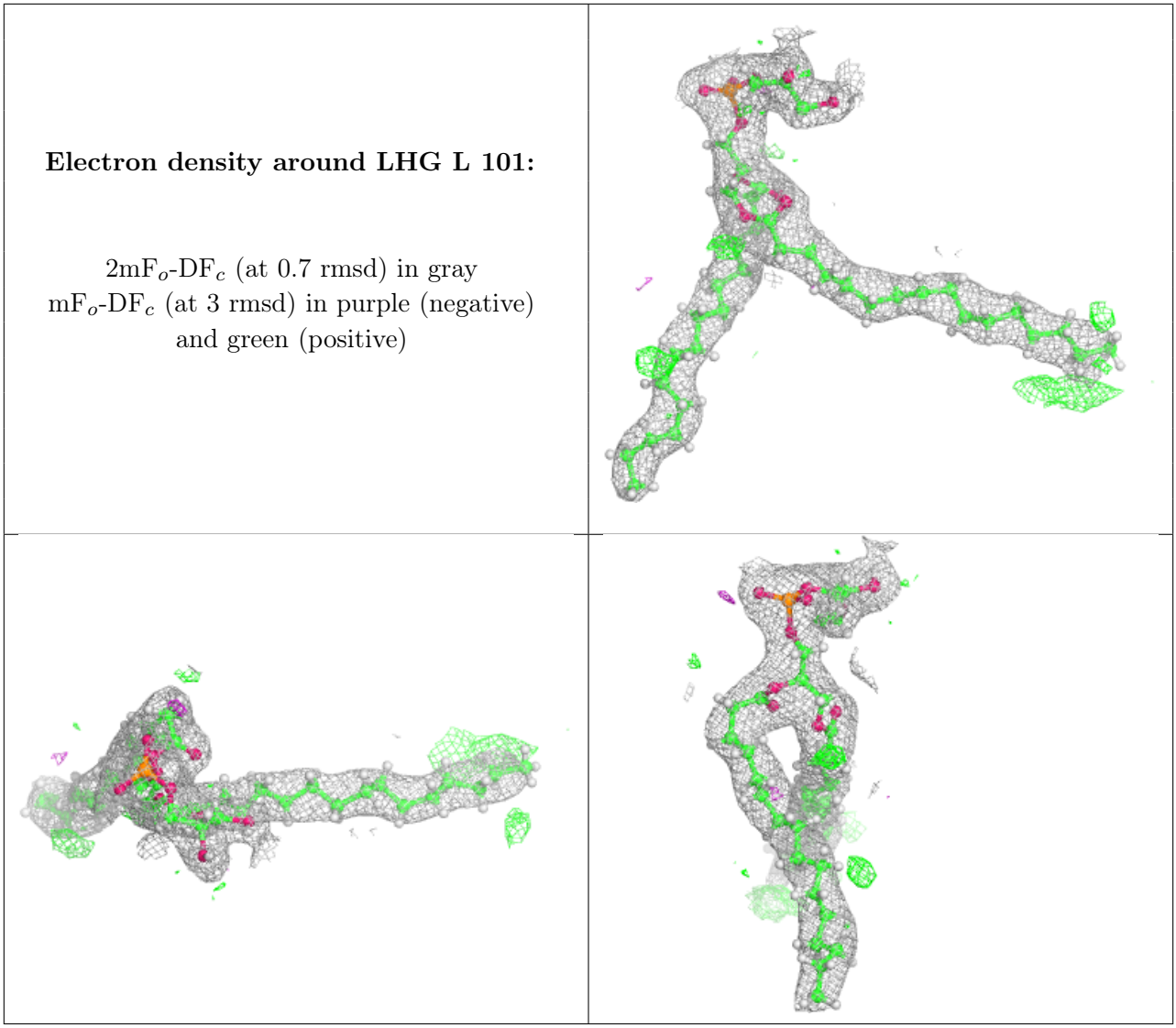






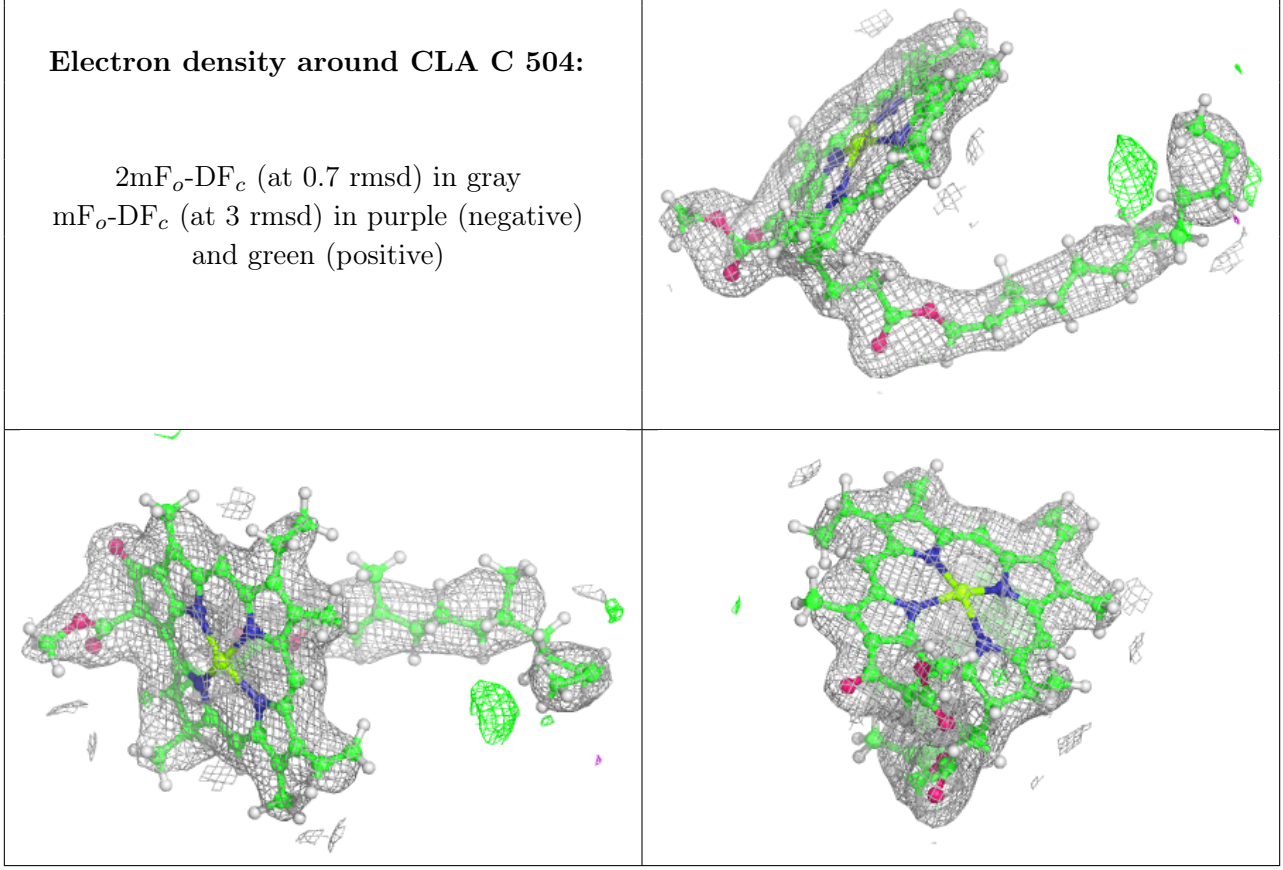
Electron density around LHG L 101:

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



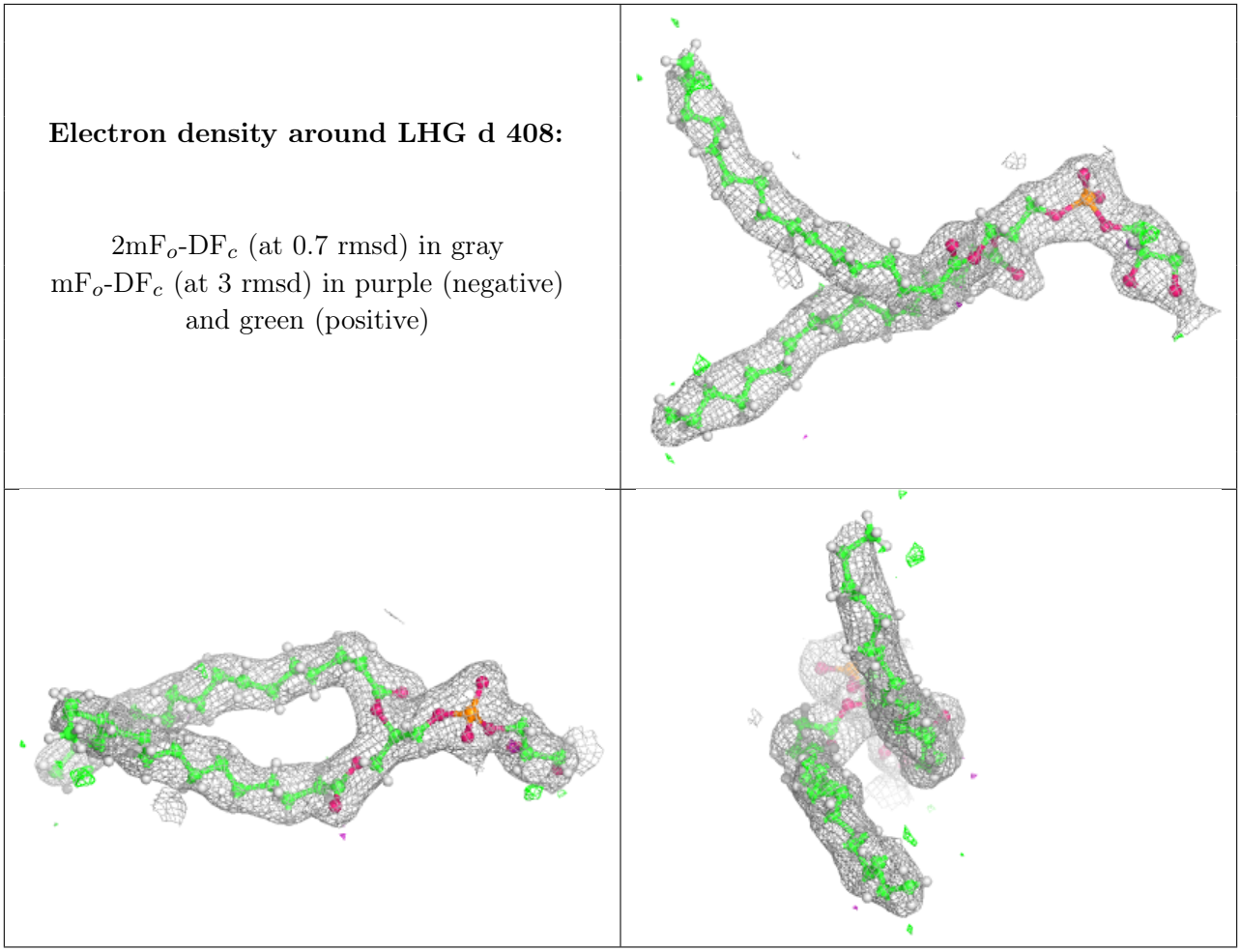
Electron density around CLA C 504:

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



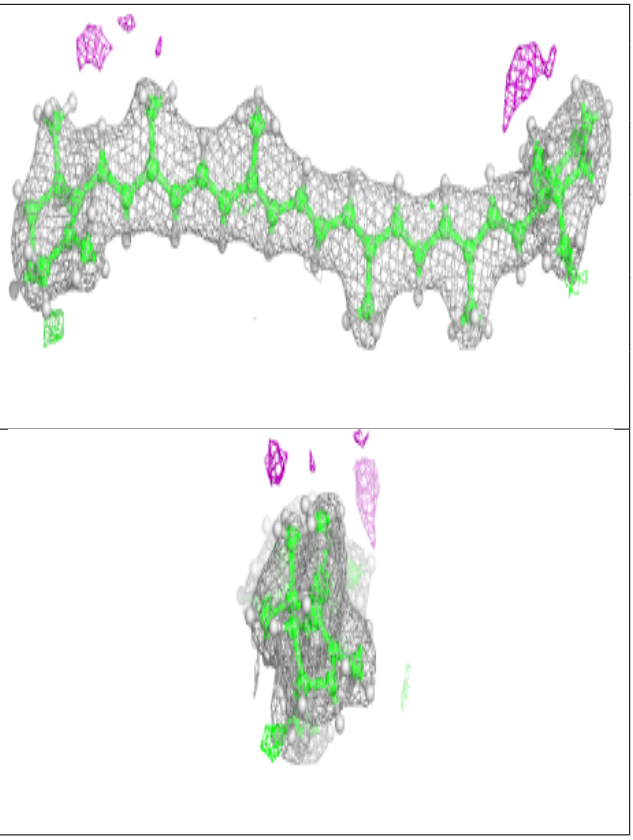
Electron density around LHG d 408:

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



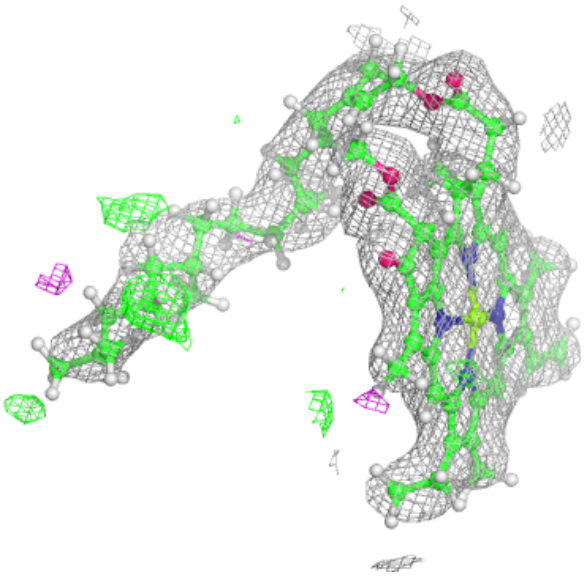
Electron density around BCR a 409:

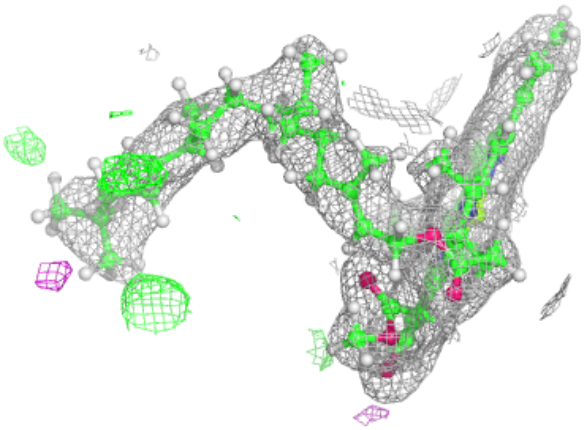
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

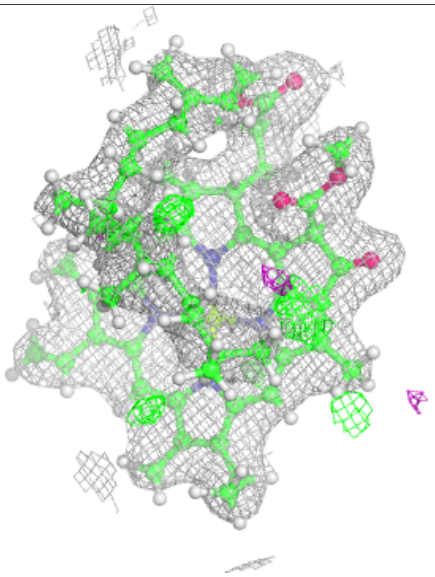


Electron density around CLA B 613:

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

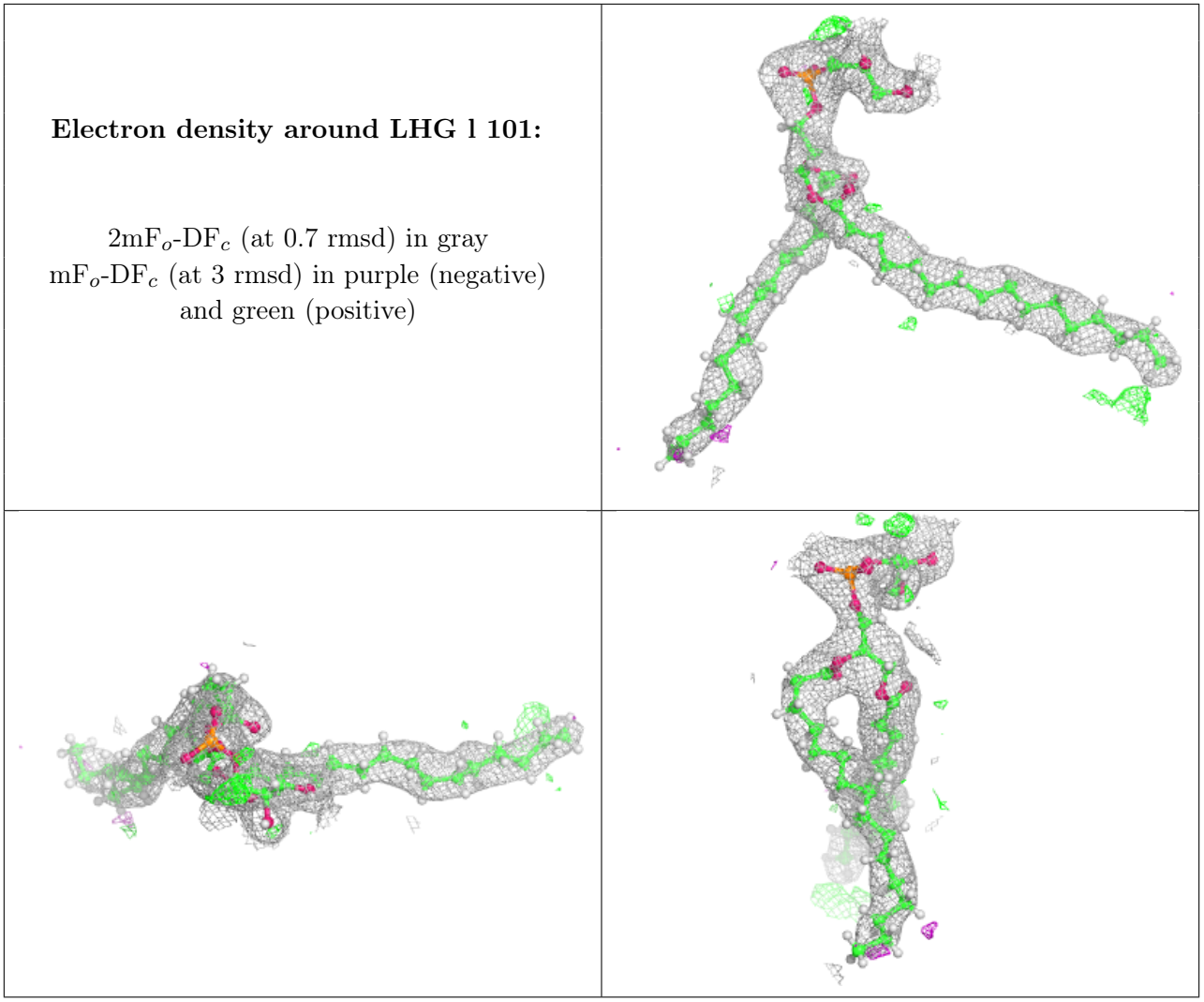






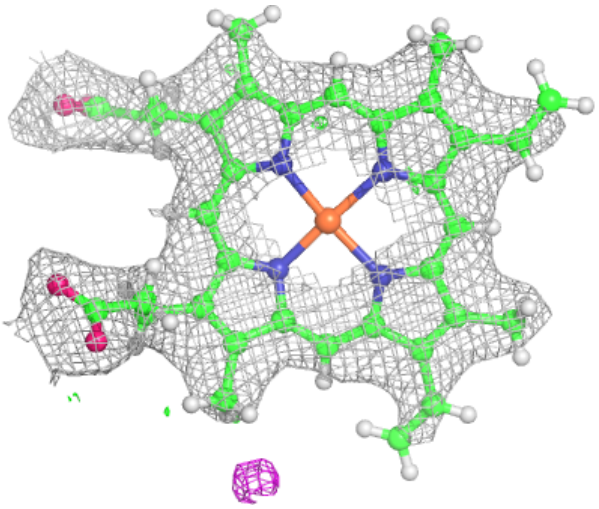
Electron density around LHG l 101:

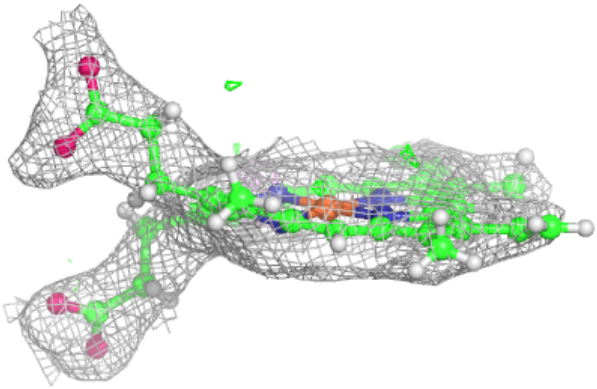
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

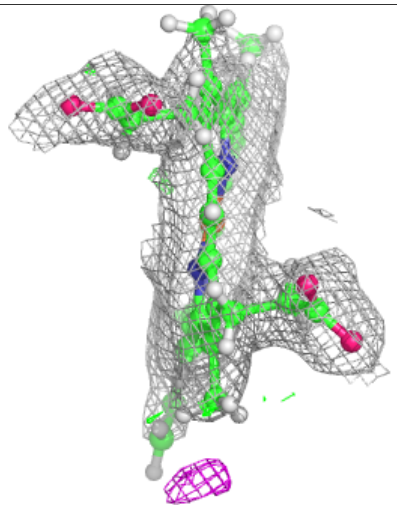


Electron density around HEM F 101:

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

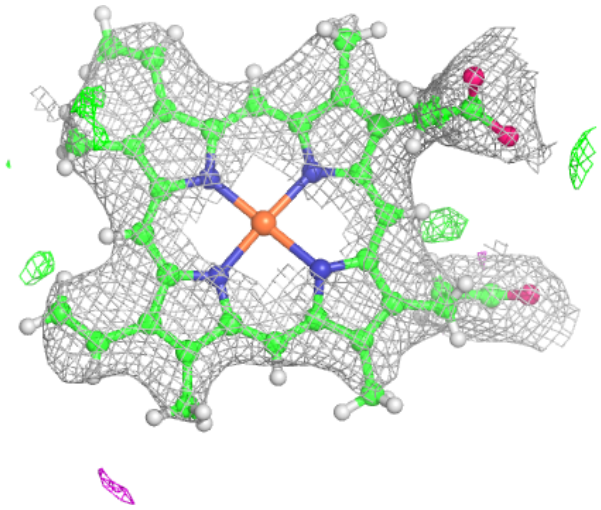


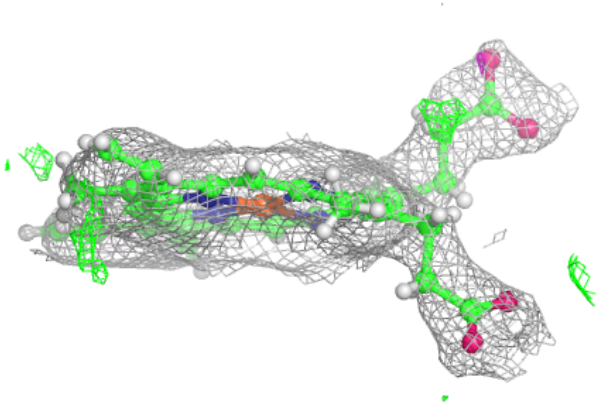


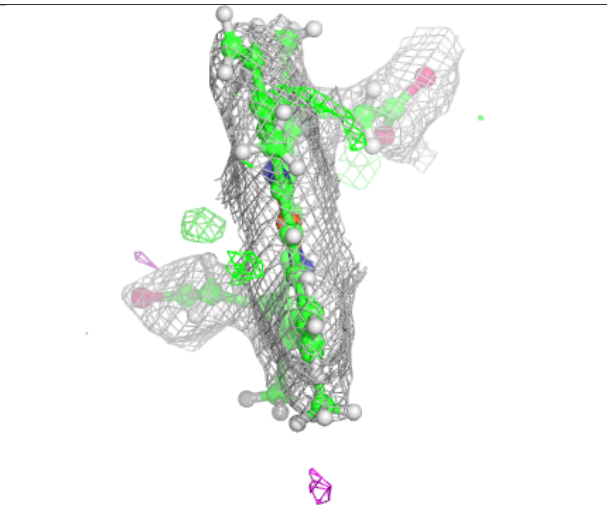


Electron density around HEM e 102:

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

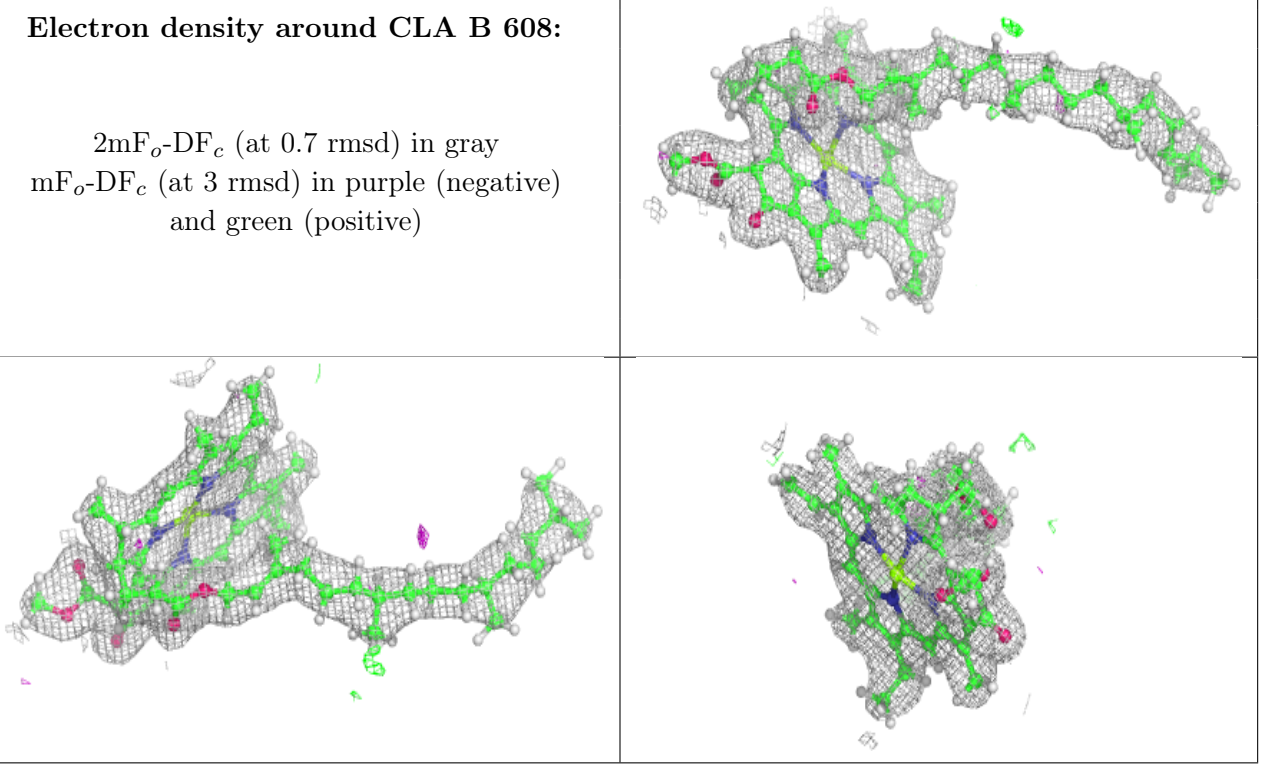






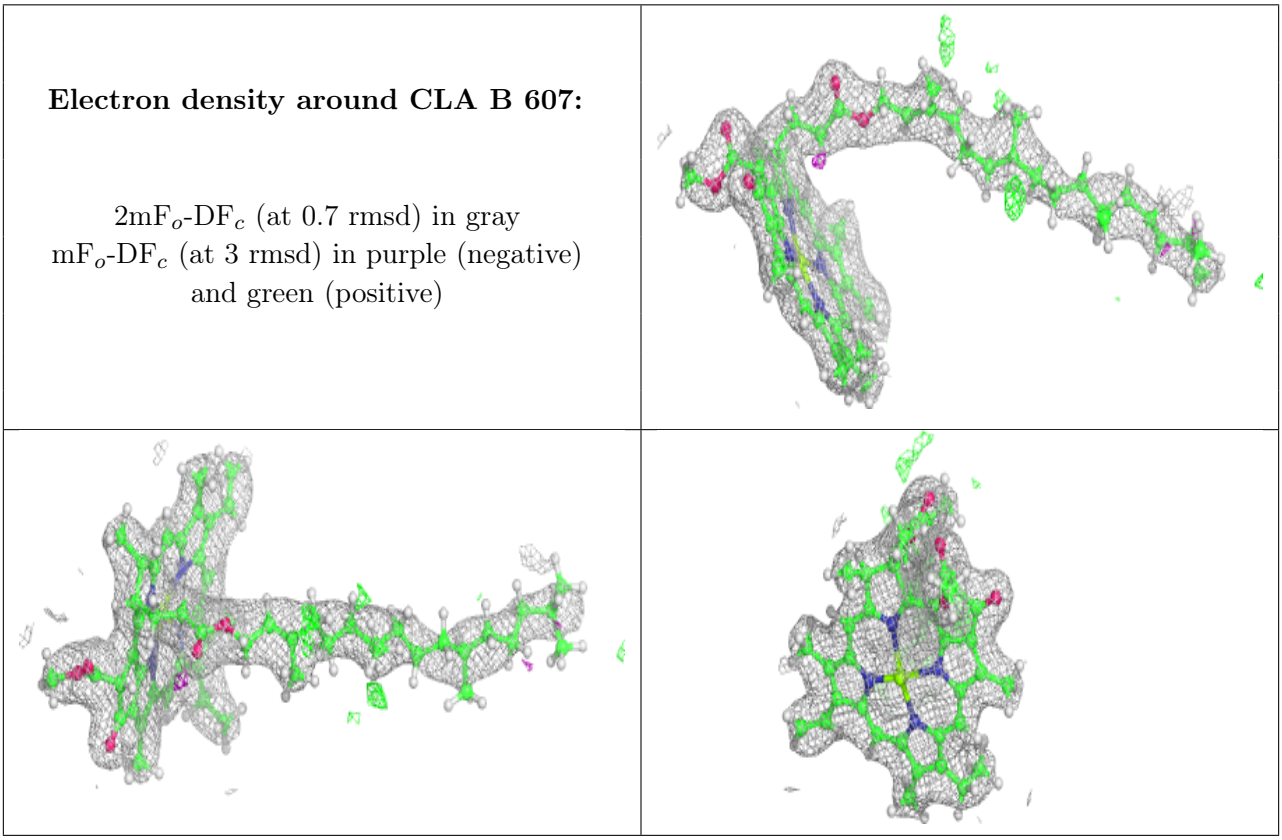
Electron density around CLA B 608:

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



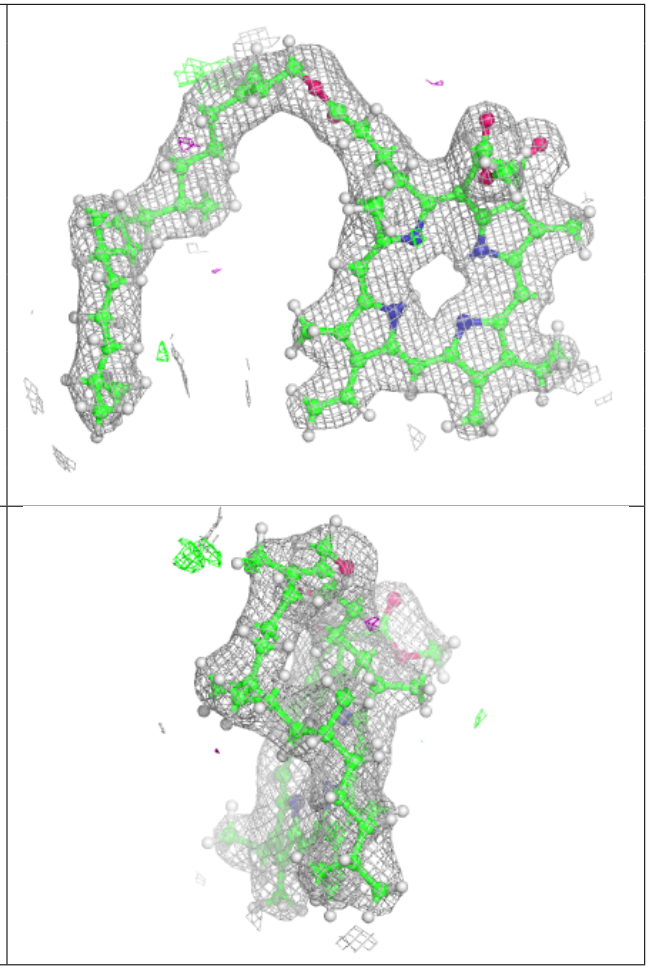
Electron density around CLA B 607:

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



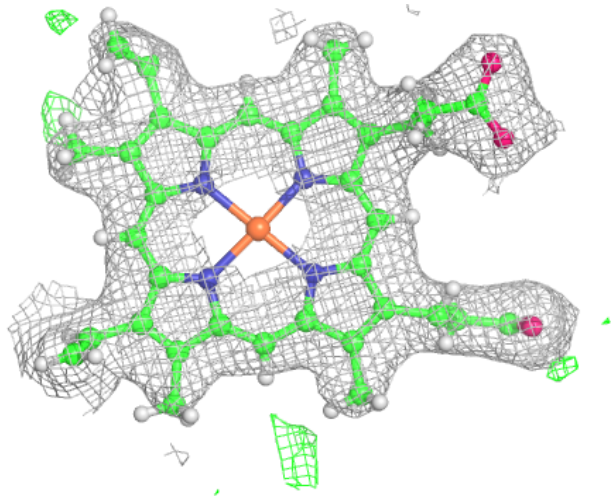
Electron density around PHO D 402:

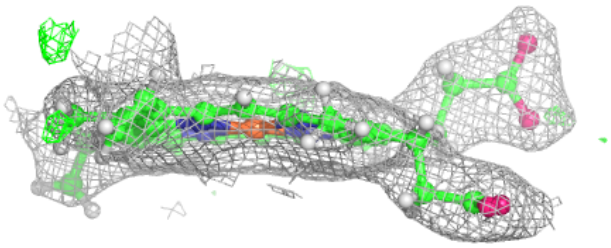
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC v 201:

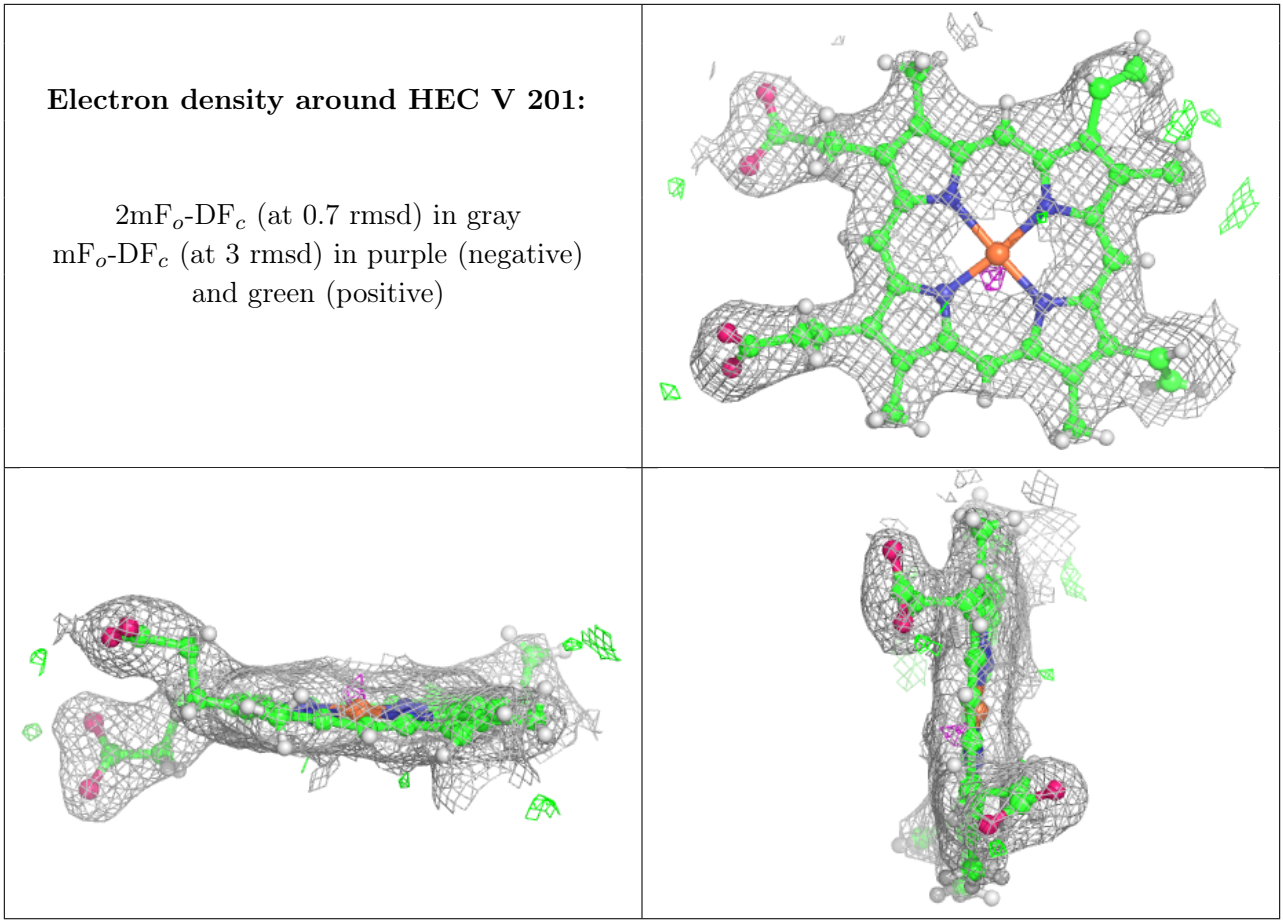
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.