wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 07:59 AM EST

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

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

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

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

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

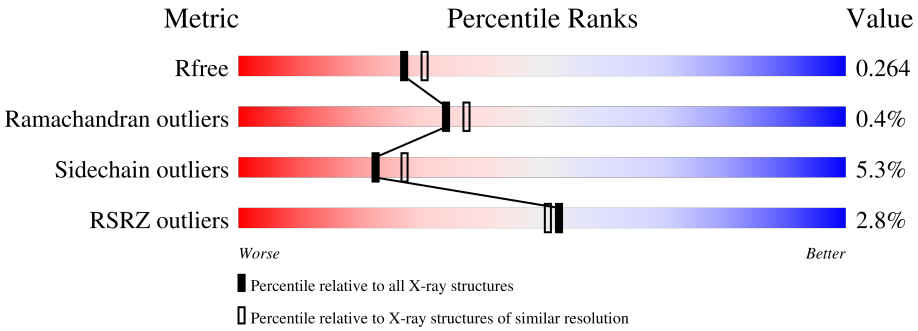
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	334	% 97% .
1	a	334	96% .

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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	96%
2	b	505	96%
3	C	451	95%
3	c	451	96%
4	D	341	97%
4	d	341	97%
5	E	82	89% 10%
5	e	82	90% 10%
6	F	34	97%
6	f	34	94% 6%
7	H	65	94% 6%
7	h	65	89% 8%
8	I	36	83% 17%
8	i	36	97%
9	J	36	100%
9	j	36	94% 6%
10	K	37	95% 5%
10	k	37	92% 8%
11	L	37	95% 5%
11	l	37	92% 5%
12	M	33	91% 9%
12	m	33	94%
13	O	244	91% 9%
13	o	244	92% 7%
14	T	30	87% 13%

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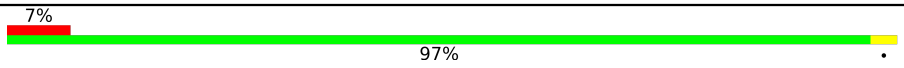
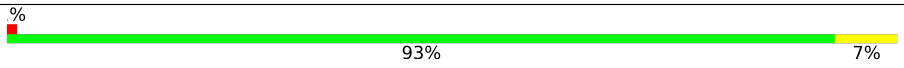
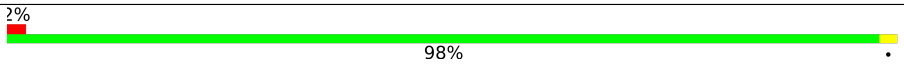
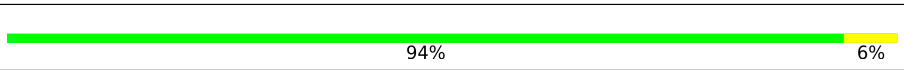
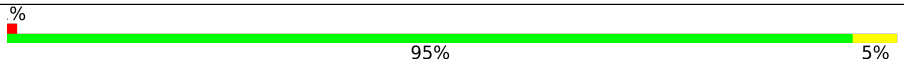
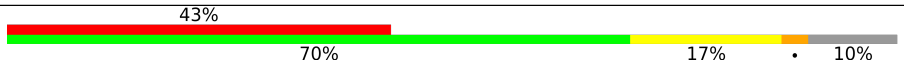
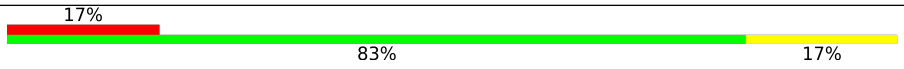
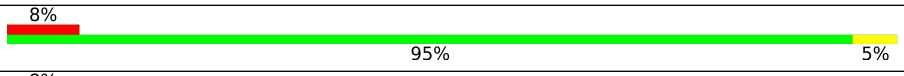
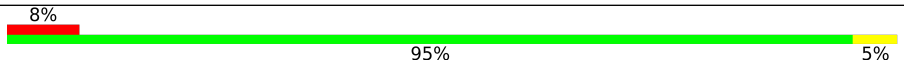
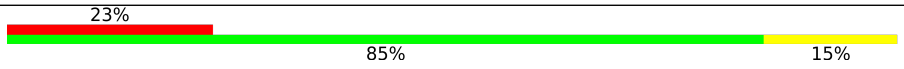
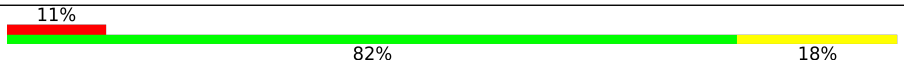
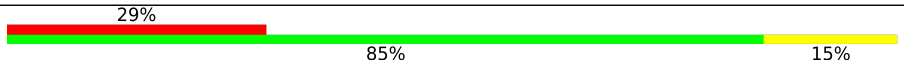
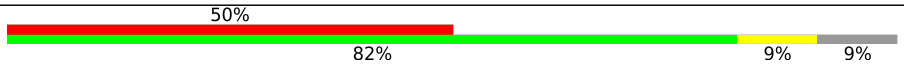
Mol	Chain	Length	Quality of chain
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	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	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	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	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	611	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	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 103673 atoms, of which 51476 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

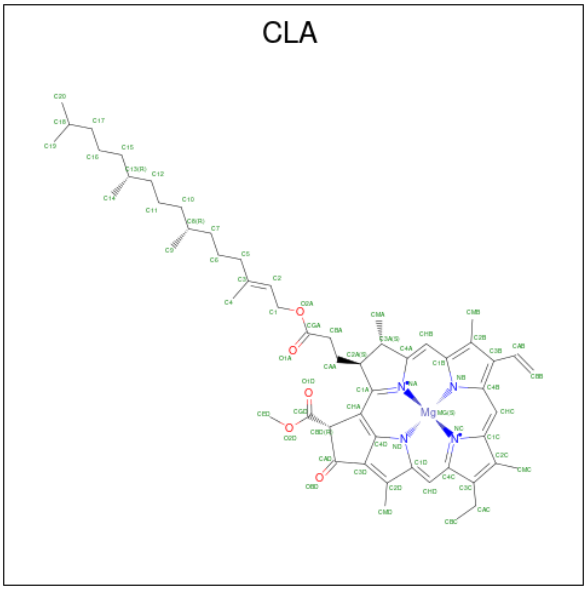
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0

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

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

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

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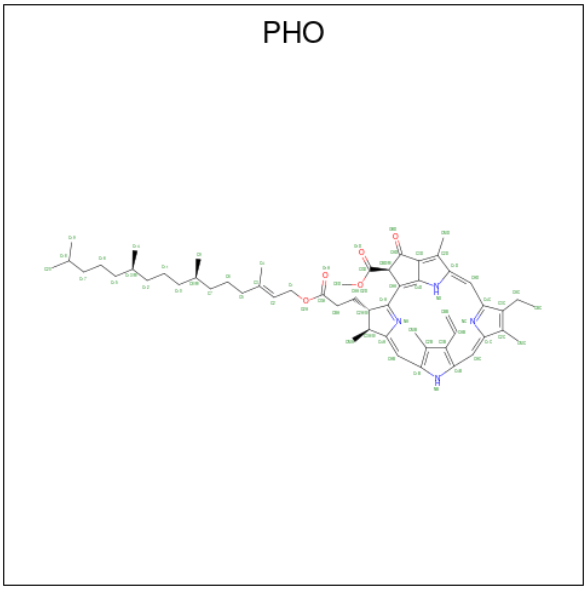
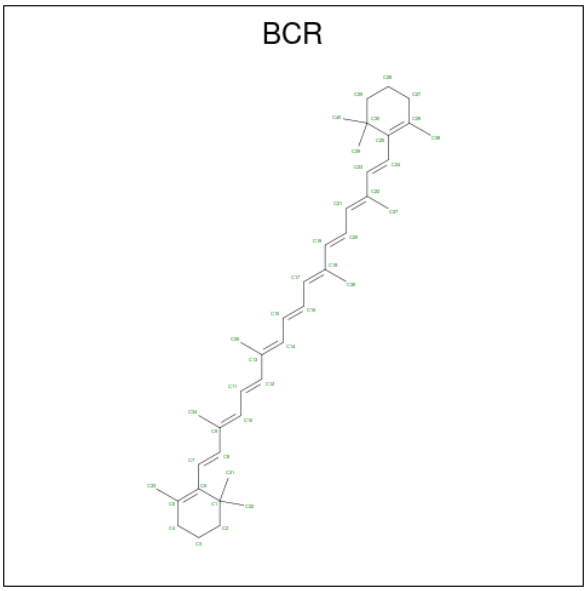
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 24 is PHEOPHYTIN A (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 BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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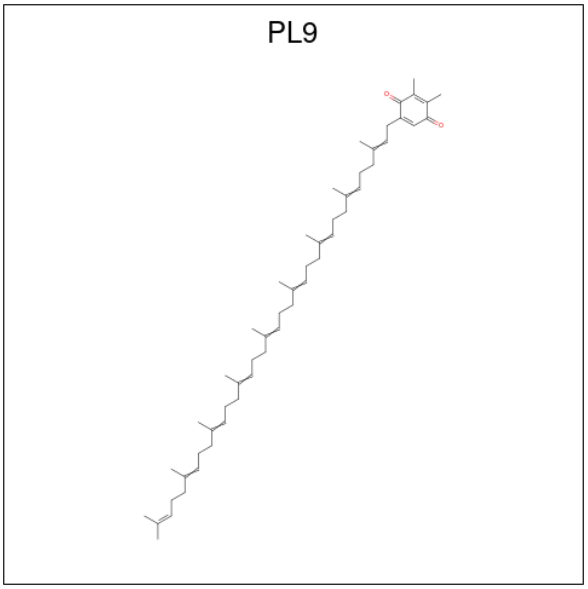
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	d	1	Total C H 96 40 56	0	0
25	h	1	Total C H 96 40 56	0	0
25	t	1	Total C H 96 40 56	0	0
25	y	1	Total C H 96 40 56	0	0

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



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

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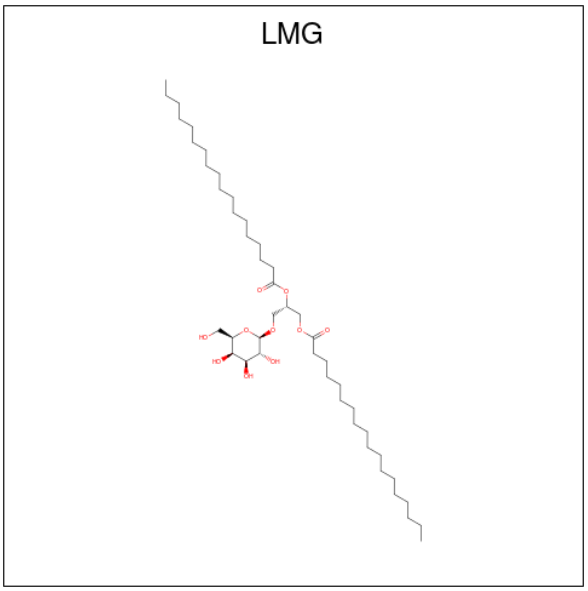
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total 135	C 53	H 80	O 2	0	0
26	d	1	Total 135	C 53	H 80	O 2	0	0

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

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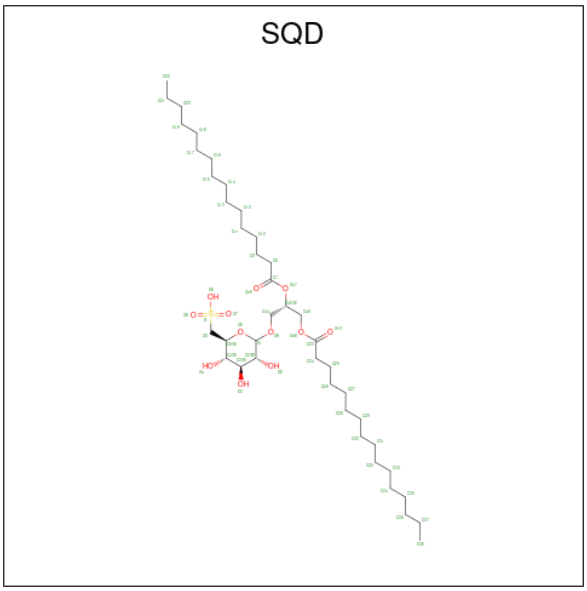
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C H O 81 27 44 10	0	0
27	c	1	Total C H O 117 38 69 10	0	0
27	d	1	Total C H O 102 34 58 10	0	0
27	m	1	Total C H O 123 41 72 10	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (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	F	1	Total C H O S 81 25 45 10 1	0	0
28	a	1	Total C H O S 132 41 78 12 1	0	0
28	a	1	Total C H O 92 31 56 5	0	0
28	b	1	Total C H O S 114 36 65 12 1	0	0

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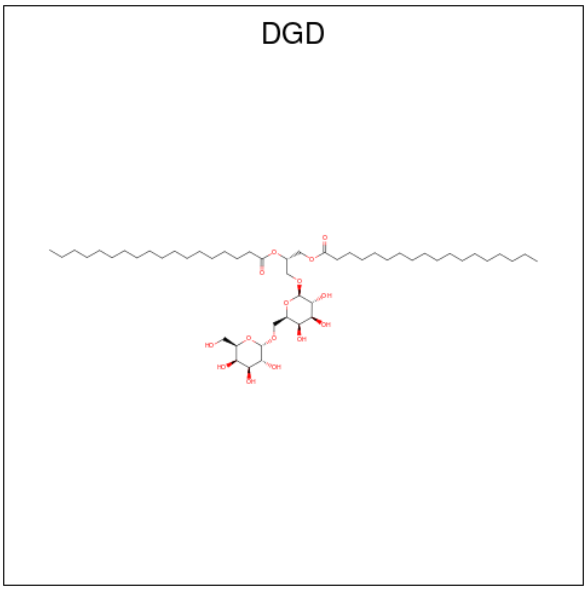
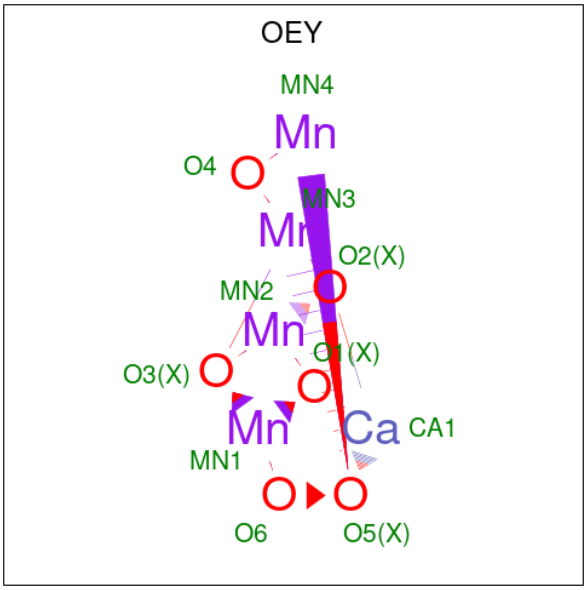
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

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



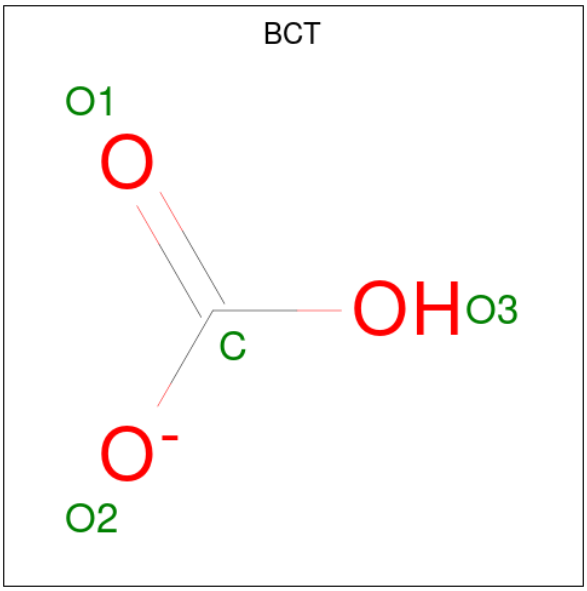
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	a	1	Total	C	H	O	0	0
			119	39	75	5		
29	c	1	Total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

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



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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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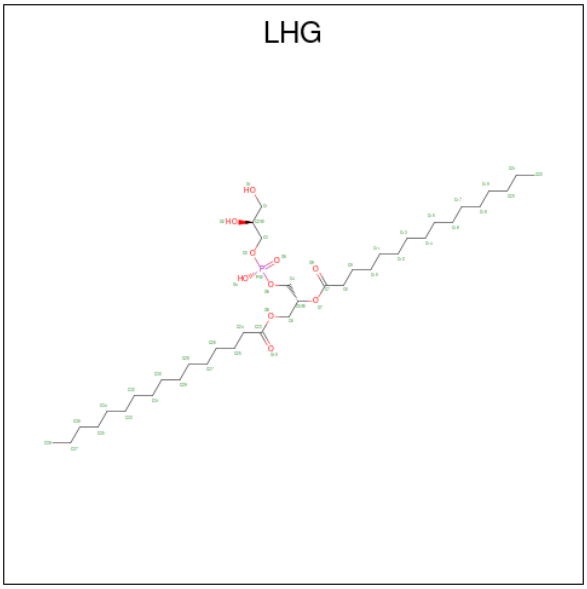
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	a	1	Total C H O 5 1 1 3	0	0

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

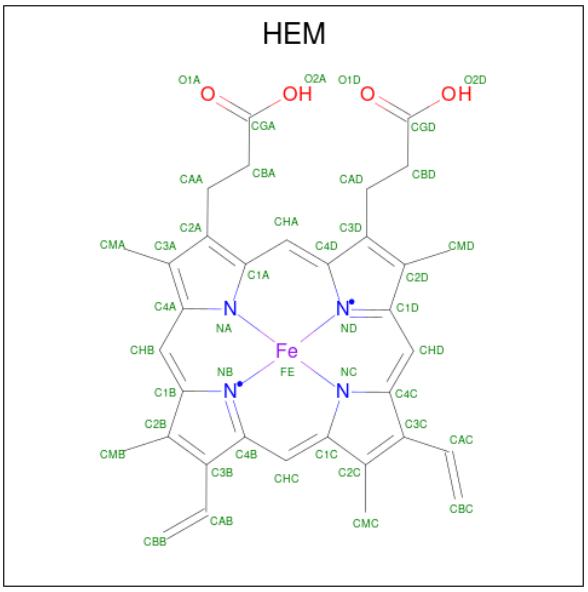
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	5	Total C H O 180 63 109 8	0	0
32	C	3	Total C H O 103 36 63 4	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	2	Total C H O 63 23 38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

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



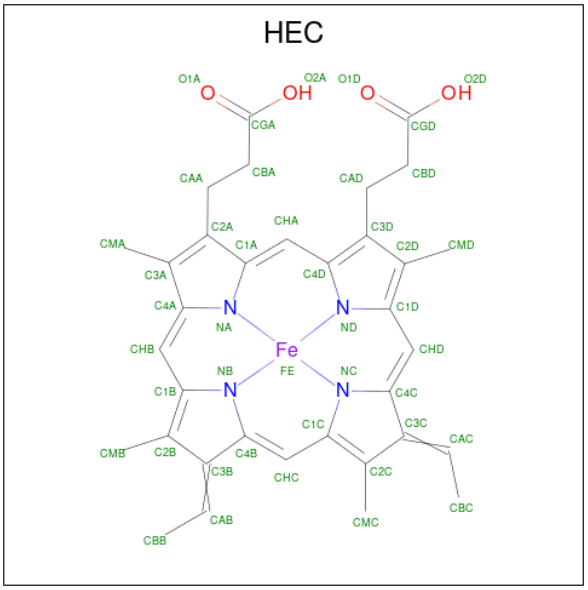
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	a	1	Total	C	H	O	P	0	0
			123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

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



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 36 is water.

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

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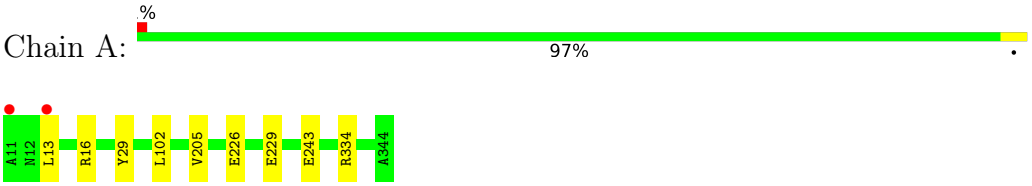
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	b	190	Total O 190 190	0	0
36	c	154	Total O 154 154	0	0
36	d	127	Total O 127 127	0	0
36	e	20	Total O 20 20	0	0
36	f	6	Total O 6 6	0	0
36	h	17	Total O 17 17	0	0
36	i	12	Total O 12 12	0	0
36	j	7	Total O 7 7	0	0
36	k	6	Total O 6 6	0	0
36	l	11	Total O 11 11	0	0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

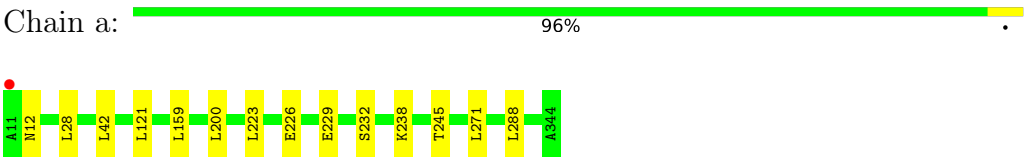
3 Residue-property plots (i)

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

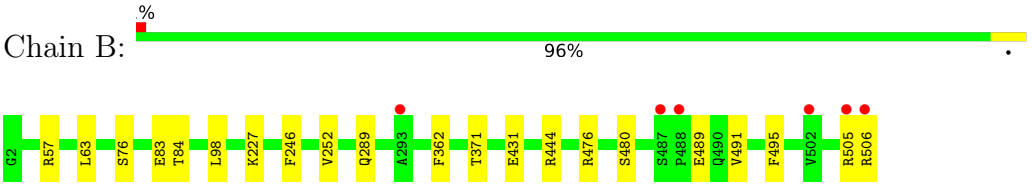
• Molecule 1: Photosystem II protein D1 1



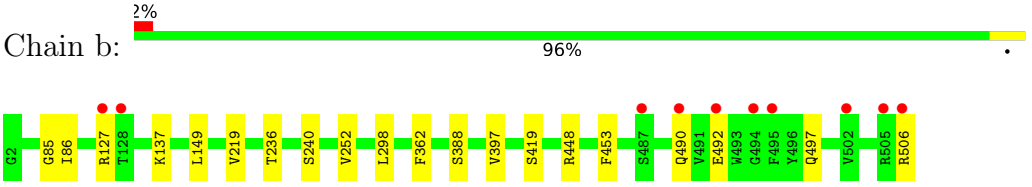
• Molecule 1: Photosystem II protein D1 1



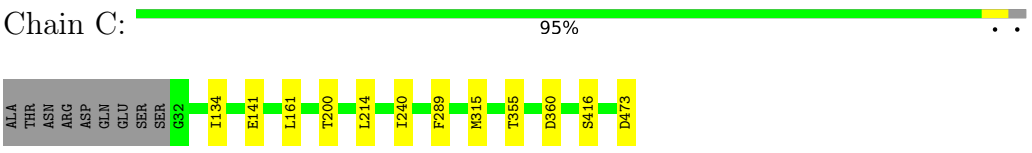
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

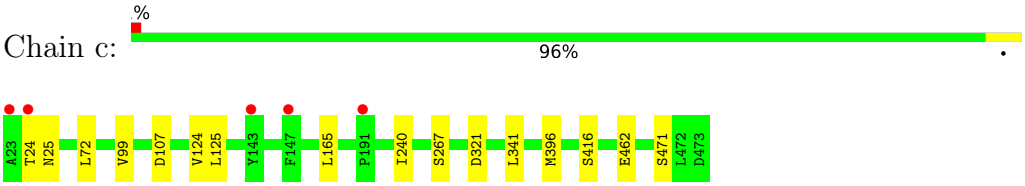


• Molecule 3: Photosystem II CP43 reaction center protein



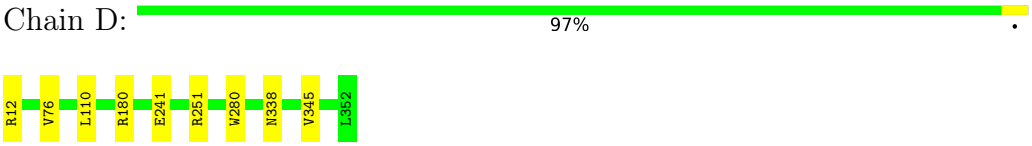
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



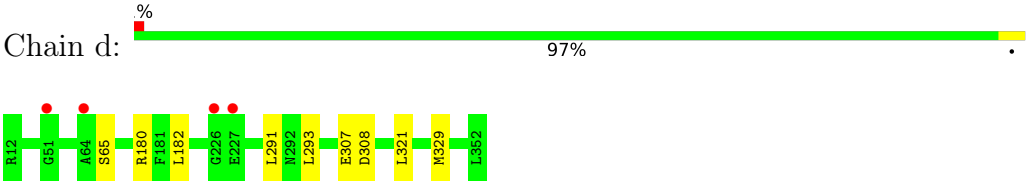
• Molecule 4: Photosystem II D2 protein

Chain D:



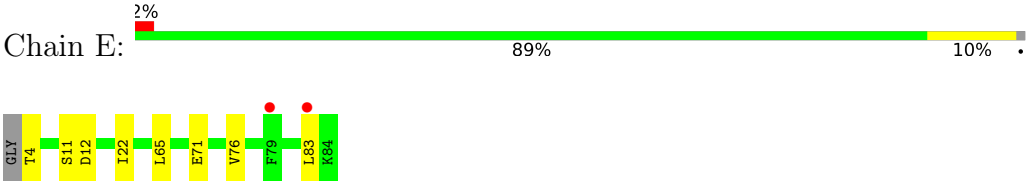
• Molecule 4: Photosystem II D2 protein

Chain d:



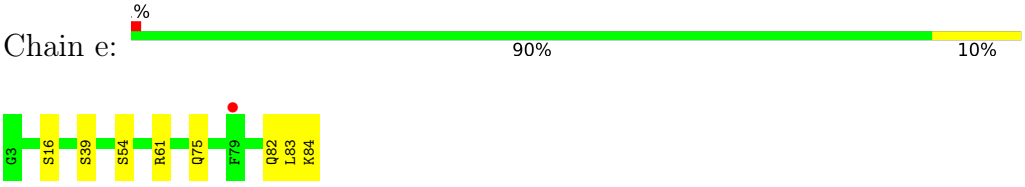
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



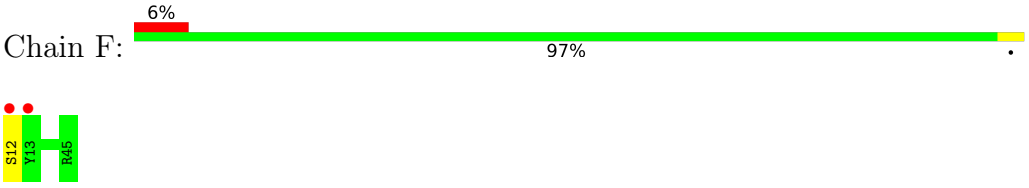
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



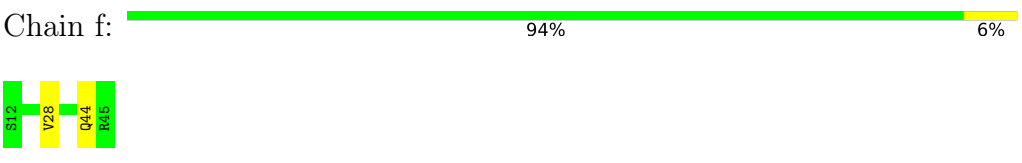
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



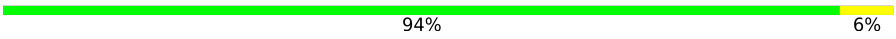
• Molecule 6: Cytochrome b559 subunit beta

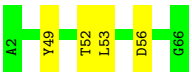
Chain f:



• Molecule 7: Photosystem II reaction center protein H

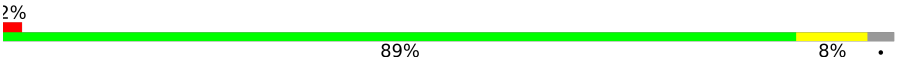
Chain H:





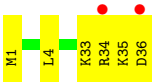
• Molecule 7: Photosystem II reaction center protein H

Chain h:



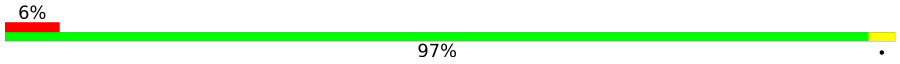
• Molecule 8: Photosystem II reaction center protein I

Chain I:



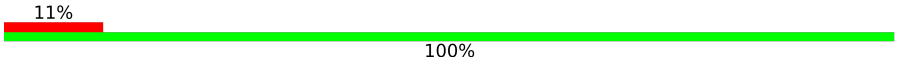
• Molecule 8: Photosystem II reaction center protein I

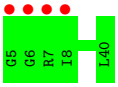
Chain i:



• Molecule 9: Photosystem II reaction center protein J

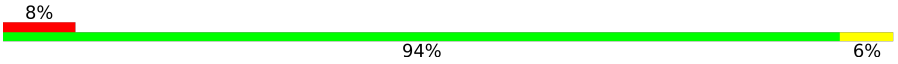
Chain J:





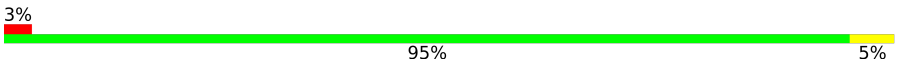
• Molecule 9: Photosystem II reaction center protein J

Chain j:



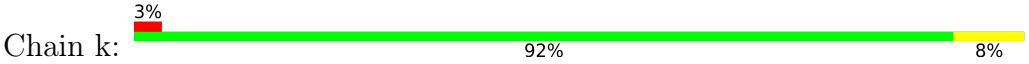
• Molecule 10: Photosystem II reaction center protein K

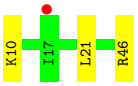
Chain K:



• Molecule 10: Photosystem II reaction center protein K

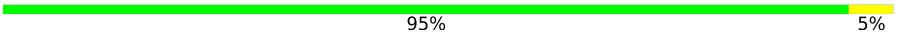
Chain k:





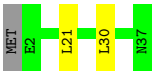
• Molecule 11: Photosystem II reaction center protein L

Chain L:



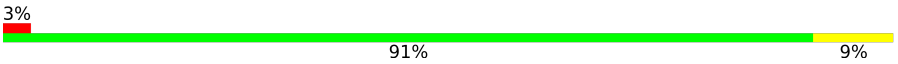
• Molecule 11: Photosystem II reaction center protein L

Chain l:



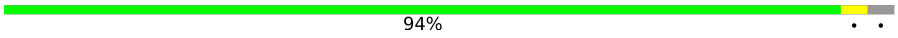
• Molecule 12: Photosystem II reaction center protein M

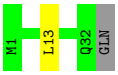
Chain M:



• Molecule 12: Photosystem II reaction center protein M

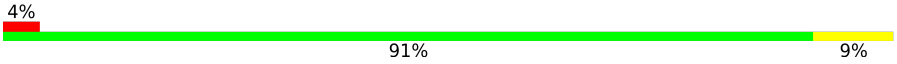
Chain m:





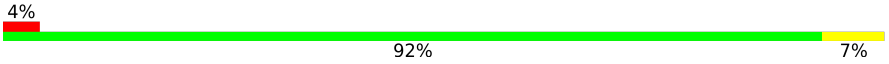
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

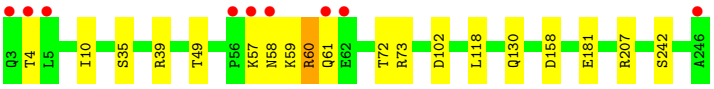
Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

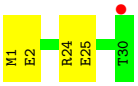
Chain o:





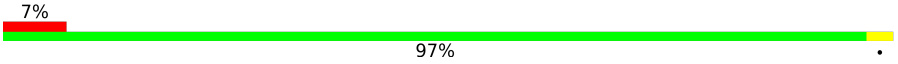
• Molecule 14: Photosystem II reaction center protein T

Chain T:



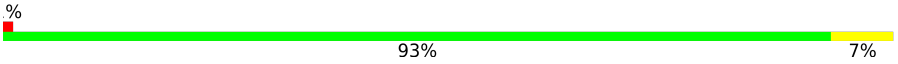
• Molecule 14: Photosystem II reaction center protein T

Chain t:



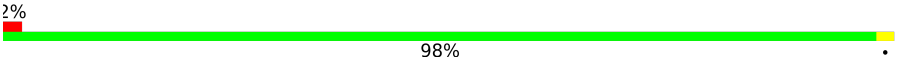
• Molecule 15: Photosystem II 12 kDa extrinsic protein

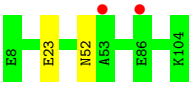
Chain U:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

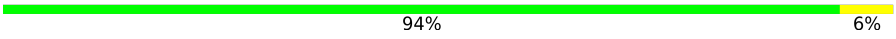
Chain u:





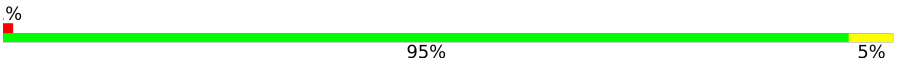
• Molecule 16: Cytochrome c-550

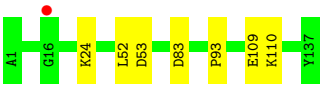
Chain V:



• Molecule 16: Cytochrome c-550

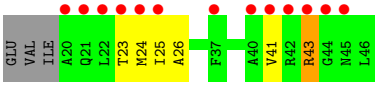
Chain v:



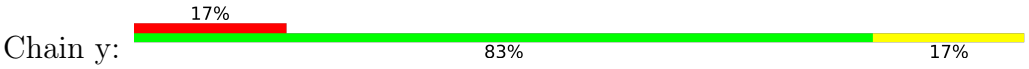


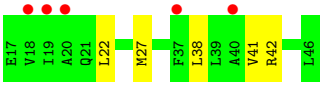
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

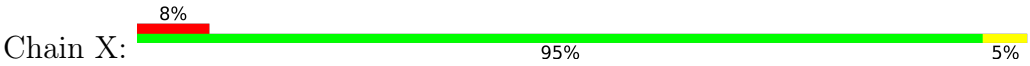


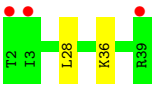
• Molecule 17: Photosystem II reaction center protein Ycf12





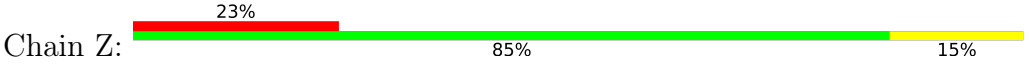
• Molecule 18: Photosystem II reaction center X protein

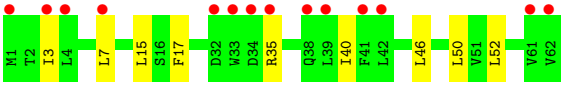




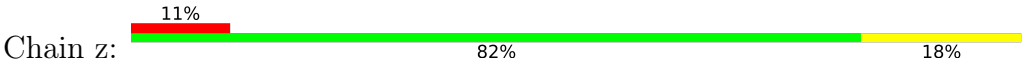
• Molecule 18: Photosystem II reaction center X protein

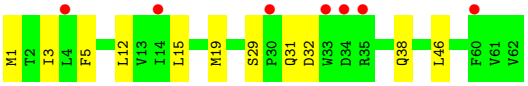
• Molecule 19: Photosystem II reaction center protein Z



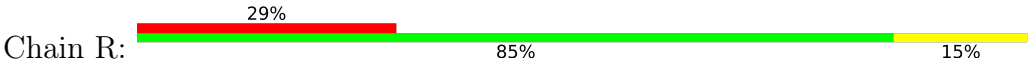


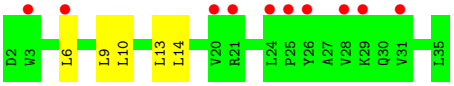
• Molecule 19: Photosystem II reaction center protein Z





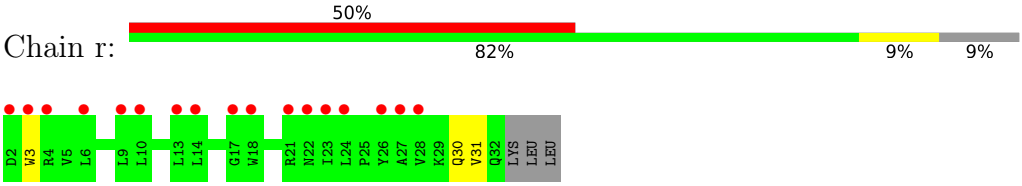
• Molecule 20: Photosystem II protein Y





• Molecule 20: Photosystem II protein Y

Chain r:


50%
82%
9%
9%
D2
W3
R4
V5
L6
L9
L10
L13
L14
G17
W18
R21
N22
I23
L24
P25
Y26
A27
V28
K29
Q30
V31
Q32
LYS
LEU
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.69Å 222.53Å 308.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.85 – 2.20 30.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.85-2.20) 83.7 (30.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.193 , 0.264 0.193 , 0.264	Depositor DCC
R_{free} test set	3620 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	103673	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	1/2707 (0.0%)	0.74	2/3692 (0.1%)
1	a	0.68	0/2704	0.71	1/3688 (0.0%)
2	B	0.69	1/4160 (0.0%)	0.71	1/5668 (0.0%)
2	b	0.67	1/4118 (0.0%)	0.69	1/5611 (0.0%)
3	C	0.65	0/3530	0.69	3/4807 (0.1%)
3	c	0.59	0/3610	0.70	3/4914 (0.1%)
4	D	0.72	1/2812 (0.0%)	0.71	1/3832 (0.0%)
4	d	0.66	0/2821	0.72	1/3844 (0.0%)
5	E	0.59	0/684	0.63	0/935
5	e	0.49	0/683	0.62	0/932
6	F	0.57	0/284	0.60	0/387
6	f	0.44	0/284	0.64	0/387
7	H	0.68	0/520	0.72	0/709
7	h	0.63	0/511	0.72	0/697
8	I	0.60	0/293	0.71	0/396
8	i	0.73	0/293	0.70	0/396
9	J	0.54	0/263	0.67	0/356
9	j	0.54	0/261	0.71	0/353
10	K	0.48	0/314	0.75	0/427
10	k	0.48	0/303	0.67	0/416
11	L	0.70	0/311	0.76	1/422 (0.2%)
11	l	0.64	0/303	0.70	0/412
12	M	0.63	0/249	0.75	0/341
12	m	0.71	0/244	0.70	0/334
13	O	0.62	0/1914	0.74	0/2596
13	o	0.62	0/1905	0.77	3/2583 (0.1%)
14	T	0.71	0/257	0.79	0/349
14	t	0.77	0/255	0.64	0/346
15	U	0.63	0/785	0.74	1/1064 (0.1%)
15	u	0.61	0/785	0.73	0/1064
16	V	0.58	0/1085	0.66	0/1473
16	v	0.55	0/1085	0.70	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.41	0/197	0.64	0/264
17	y	0.37	0/219	0.58	0/294
18	X	0.57	0/284	0.66	0/384
18	x	0.44	0/284	0.60	0/384
19	Z	0.51	0/490	0.62	0/669
19	z	0.46	0/488	0.57	0/666
20	R	0.45	0/277	0.62	0/380
20	r	0.37	0/233	0.54	0/323
All	All	0.64	4/42805 (0.0%)	0.70	19/58268 (0.0%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	TYR	CD1-CE1	-5.59	1.30	1.39
4	D	280	TRP	CB-CG	5.36	1.59	1.50
2	B	252	VAL	CB-CG1	5.24	1.63	1.52
2	b	453	PHE	CB-CG	-5.22	1.42	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	o	158	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	334	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	c	107	ASP	CB-CG-OD1	6.72	124.34	118.30
1	a	121	LEU	CB-CG-CD2	-6.53	99.89	111.00
3	C	360	ASP	CB-CG-OD1	-6.42	112.53	118.30

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
1	a	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
2	B	508/505 (101%)	490 (96%)	18 (4%)	0	100	100
2	b	503/505 (100%)	481 (96%)	20 (4%)	2 (0%)	34	37
3	C	440/451 (98%)	426 (97%)	13 (3%)	1 (0%)	47	55
3	c	450/451 (100%)	431 (96%)	18 (4%)	1 (0%)	47	55
4	D	339/341 (99%)	331 (98%)	7 (2%)	1 (0%)	41	46
4	d	340/341 (100%)	329 (97%)	10 (3%)	1 (0%)	41	46
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
7	H	63/65 (97%)	55 (87%)	8 (13%)	0	100	100
7	h	61/65 (94%)	56 (92%)	5 (8%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	28 (82%)	6 (18%)	0	100	100
9	j	34/36 (94%)	29 (85%)	5 (15%)	0	100	100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	4	2
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	222 (91%)	19 (8%)	2 (1%)	19	19
13	o	242/244 (99%)	225 (93%)	14 (6%)	3 (1%)	13	10
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	17 (68%)	5 (20%)	3 (12%)	0	0
17	y	28/30 (93%)	25 (89%)	1 (4%)	2 (7%)	1	0
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
19	z	60/62 (97%)	51 (85%)	6 (10%)	3 (5%)	2	0
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
20	r	29/34 (85%)	25 (86%)	2 (7%)	2 (7%)	1	0
All	All	5235/5326 (98%)	4988 (95%)	225 (4%)	22 (0%)	34	37

5 of 22 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/270 (100%)	263 (97%)	7 (3%)	46 58
1	a	269/270 (100%)	256 (95%)	13 (5%)	25 32
2	B	407/403 (101%)	387 (95%)	20 (5%)	25 31
2	b	402/403 (100%)	386 (96%)	16 (4%)	31 40
3	C	344/352 (98%)	336 (98%)	8 (2%)	50 63
3	c	353/352 (100%)	340 (96%)	13 (4%)	34 43
4	D	276/276 (100%)	270 (98%)	6 (2%)	52 65
4	d	277/276 (100%)	270 (98%)	7 (2%)	47 60
5	E	72/72 (100%)	63 (88%)	9 (12%)	4 4
5	e	71/72 (99%)	63 (89%)	8 (11%)	6 5
6	F	28/28 (100%)	27 (96%)	1 (4%)	35 45
6	f	28/28 (100%)	26 (93%)	2 (7%)	14 16
7	H	53/54 (98%)	49 (92%)	4 (8%)	13 14
7	h	53/54 (98%)	48 (91%)	5 (9%)	8 8
8	I	32/32 (100%)	27 (84%)	5 (16%)	2 2
8	i	32/32 (100%)	32 (100%)	0	100 100
9	J	24/24 (100%)	24 (100%)	0	100 100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10 10
10	K	31/30 (103%)	30 (97%)	1 (3%)	39 50
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 7
11	L	35/35 (100%)	34 (97%)	1 (3%)	42 54
11	l	34/35 (97%)	32 (94%)	2 (6%)	19 23
12	M	28/29 (97%)	26 (93%)	2 (7%)	14 16
12	m	28/29 (97%)	27 (96%)	1 (4%)	35 45
13	O	208/207 (100%)	188 (90%)	20 (10%)	8 8
13	o	207/207 (100%)	192 (93%)	15 (7%)	14 15
14	T	26/26 (100%)	23 (88%)	3 (12%)	5 5
14	t	25/26 (96%)	25 (100%)	0	100 100
15	U	84/84 (100%)	78 (93%)	6 (7%)	14 16
15	u	84/84 (100%)	83 (99%)	1 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	V	117/117 (100%)	109 (93%)	8 (7%)	16 17
16	v	117/117 (100%)	111 (95%)	6 (5%)	24 29
17	Y	19/23 (83%)	15 (79%)	4 (21%)	1 1
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 3
18	X	31/31 (100%)	29 (94%)	2 (6%)	17 19
18	x	31/31 (100%)	29 (94%)	2 (6%)	17 19
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2 1
19	z	51/52 (98%)	43 (84%)	8 (16%)	2 2
20	R	28/29 (97%)	23 (82%)	5 (18%)	2 1
20	r	19/29 (66%)	18 (95%)	1 (5%)	22 27
All	All	4321/4348 (99%)	4092 (95%)	229 (5%)	22 27

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	52	LEU
19	z	3	ILE
2	b	388	SER
18	x	15	LEU
13	o	58	ASN

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

Mol	Chain	Res	Type
13	o	58	ASN
15	u	78	ASN
15	U	73	GLN
17	Y	21	GLN
3	c	25	ASN

5.3.3 RNA

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	0.96	0	7,9,11	1.03	1 (14%)
14	FME	T	1	14	8,9,10	1.04	1 (12%)	7,9,11	2.02	2 (28%)
12	FME	M	1	12	8,9,10	1.14	1 (12%)	7,9,11	1.29	1 (14%)
12	FME	m	1	12	8,9,10	0.92	0	7,9,11	0.85	0
8	FME	i	1	8	8,9,10	0.96	0	7,9,11	1.10	1 (14%)
8	FME	I	1	8	8,9,10	0.98	0	7,9,11	1.49	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	-	4/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.55	1.42	1.46
14	T	1	FME	CA-N	-2.50	1.42	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	CA-N-CN	-3.99	116.68	122.82
8	I	1	FME	C-CA-N	3.13	115.38	109.73
12	M	1	FME	C-CA-N	-2.60	105.05	109.73
8	i	1	FME	C-CA-N	2.60	114.42	109.73
14	T	1	FME	O1-CN-N	-2.30	119.20	125.27

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

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

There are no ring outliers.

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	D	403	-	65,73,73	1.66	12 (18%)	76,113,113	1.61	10 (13%)
23	CLA	c	512	-	65,73,73	1.71	9 (13%)	76,113,113	1.54	10 (13%)
23	CLA	d	404	-	65,73,73	2.06	11 (16%)	76,113,113	1.29	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	b	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.41	11 (19%)
23	CLA	A	404	-	65,73,73	1.63	8 (12%)	76,113,113	1.65	13 (17%)
23	CLA	C	507	36	65,73,73	1.47	10 (15%)	76,113,113	1.33	9 (11%)
26	PL9	A	409	-	55,55,55	0.92	1 (1%)	68,69,69	1.66	13 (19%)
29	DGD	c	518	-	63,63,67	1.25	9 (14%)	77,77,81	1.47	14 (18%)
23	CLA	a	407	-	65,73,73	1.56	12 (18%)	76,113,113	1.41	16 (21%)
25	BCR	c	515	-	41,41,41	1.14	4 (9%)	56,56,56	1.47	11 (19%)
25	BCR	h	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.33	9 (16%)
25	BCR	C	520	-	41,41,41	1.01	1 (2%)	56,56,56	1.19	3 (5%)
23	CLA	A	407	-	54,62,73	1.95	15 (27%)	62,99,113	1.98	15 (24%)
31	BCT	A	415	21	2,3,3	1.35	0	2,3,3	2.85	1 (50%)
23	CLA	c	506	-	65,73,73	1.66	10 (15%)	76,113,113	1.66	18 (23%)
23	CLA	b	615	-	65,73,73	1.91	8 (12%)	76,113,113	1.67	11 (14%)
25	BCR	D	405	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	7 (12%)
23	CLA	c	509	-	65,73,73	1.89	9 (13%)	76,113,113	1.78	13 (17%)
23	CLA	b	604	-	65,73,73	1.80	12 (18%)	76,113,113	1.74	13 (17%)
23	CLA	c	507	36	65,73,73	1.45	9 (13%)	76,113,113	1.47	12 (15%)
23	CLA	B	609	-	65,73,73	1.86	12 (18%)	76,113,113	1.24	10 (13%)
23	CLA	b	605	-	65,73,73	1.61	10 (15%)	76,113,113	1.78	15 (19%)
30	OEY	a	416	1,3,36	0,16,16	-	-	-		
23	CLA	D	402	36	65,73,73	1.51	10 (15%)	76,113,113	1.60	13 (17%)
29	DGD	C	516	-	63,63,67	1.40	10 (15%)	77,77,81	1.39	9 (11%)
25	BCR	t	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	8 (14%)
25	BCR	a	408	-	41,41,41	1.15	4 (9%)	56,56,56	1.45	8 (14%)
25	BCR	B	619	-	41,41,41	1.23	3 (7%)	56,56,56	1.36	11 (19%)
23	CLA	b	614	-	65,73,73	1.52	11 (16%)	76,113,113	1.43	14 (18%)
23	CLA	C	501	-	65,73,73	2.26	10 (15%)	76,113,113	1.57	7 (9%)
23	CLA	b	608	36	65,73,73	1.39	8 (12%)	76,113,113	1.35	6 (7%)
23	CLA	C	508	-	65,73,73	1.63	8 (12%)	76,113,113	1.63	11 (14%)
23	CLA	b	611	36	65,73,73	1.41	10 (15%)	76,113,113	1.61	11 (14%)
23	CLA	C	513	-	65,73,73	1.51	9 (13%)	76,113,113	1.66	10 (13%)
23	CLA	c	510	-	65,73,73	1.42	7 (10%)	76,113,113	1.58	14 (18%)
23	CLA	B	604	-	65,73,73	1.52	8 (12%)	76,113,113	1.85	9 (11%)
23	CLA	C	502	-	65,73,73	1.69	8 (12%)	76,113,113	1.37	8 (10%)
23	CLA	h	101	36	65,73,73	1.65	13 (20%)	76,113,113	1.47	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	d	403	-	65,73,73	1.56	12 (18%)	76,113,113	1.22	7 (9%)
28	SQD	F	101	-	35,36,54	1.07	3 (8%)	42,45,65	1.88	9 (21%)
31	BCT	a	417	21	2,3,3	1.44	0	2,3,3	2.79	2 (100%)
23	CLA	B	602	-	65,73,73	1.71	8 (12%)	76,113,113	1.78	16 (21%)
25	BCR	d	405	-	41,41,41	1.12	2 (4%)	56,56,56	1.31	7 (12%)
23	CLA	C	509	-	65,73,73	1.55	8 (12%)	76,113,113	1.49	9 (11%)
23	CLA	b	617	-	60,68,73	1.67	12 (20%)	70,107,113	1.74	10 (14%)
28	SQD	f	101	-	40,41,54	1.09	4 (10%)	49,52,65	1.92	9 (18%)
33	LHG	l	101	-	48,48,48	0.83	3 (6%)	51,54,54	1.19	4 (7%)
23	CLA	c	503	-	65,73,73	1.47	7 (10%)	76,113,113	1.57	11 (14%)
27	LMG	A	410	-	48,48,55	1.03	3 (6%)	56,56,63	1.23	5 (8%)
29	DGD	c	517	-	63,63,67	1.28	11 (17%)	77,77,81	1.54	10 (12%)
23	CLA	b	613	-	65,73,73	1.65	12 (18%)	76,113,113	1.61	9 (11%)
23	CLA	b	607	-	65,73,73	1.71	11 (16%)	76,113,113	1.72	9 (11%)
23	CLA	b	609	-	65,73,73	1.43	6 (9%)	76,113,113	1.56	12 (15%)
23	CLA	C	506	-	65,73,73	1.78	11 (16%)	76,113,113	1.29	7 (9%)
23	CLA	b	603	-	65,73,73	1.61	9 (13%)	76,113,113	1.56	15 (19%)
23	CLA	c	501	-	65,73,73	1.61	10 (15%)	76,113,113	1.66	10 (13%)
23	CLA	c	508	-	64,72,73	1.47	8 (12%)	74,111,113	1.43	10 (13%)
23	CLA	B	610	36	65,73,73	1.90	11 (16%)	76,113,113	1.55	13 (17%)
33	LHG	d	408	-	38,38,48	0.89	1 (2%)	41,44,54	1.08	4 (9%)
23	CLA	c	513	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	8 (10%)
25	BCR	c	521	-	41,41,41	0.90	2 (4%)	56,56,56	1.12	4 (7%)
24	PHO	a	406	-	51,69,69	1.08	4 (7%)	47,99,99	1.29	6 (12%)
23	CLA	B	607	36	65,73,73	1.56	10 (15%)	76,113,113	1.30	8 (10%)
23	CLA	c	502	-	65,73,73	1.67	10 (15%)	76,113,113	1.50	10 (13%)
23	CLA	B	614	-	65,73,73	1.89	10 (15%)	76,113,113	1.33	7 (9%)
27	LMG	B	620	-	51,51,55	0.93	4 (7%)	59,59,63	1.54	12 (20%)
28	SQD	a	411	-	53,54,54	1.02	6 (11%)	62,65,65	1.86	13 (20%)
23	CLA	b	610	-	65,73,73	1.67	10 (15%)	76,113,113	1.41	8 (10%)
26	PL9	a	409	-	55,55,55	1.42	5 (9%)	68,69,69	1.41	10 (14%)
25	BCR	c	514	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
23	CLA	b	616	-	65,73,73	2.03	12 (18%)	76,113,113	1.56	13 (17%)
27	LMG	c	522	-	48,48,55	1.27	8 (16%)	56,56,63	1.45	7 (12%)
23	CLA	B	616	-	60,68,73	1.84	13 (21%)	70,107,113	1.54	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	b	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.35	7 (12%)
25	BCR	C	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.40	10 (17%)
34	HEM	E	102	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.38	6 (13%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.43	11 (19%)
23	CLA	a	405	36	65,73,73	1.63	10 (15%)	76,113,113	1.29	10 (13%)
23	CLA	b	612	-	65,73,73	1.75	9 (13%)	76,113,113	1.65	16 (21%)
29	DGD	a	413	-	43,43,67	1.15	3 (6%)	45,45,81	1.41	6 (13%)
33	LHG	d	407	-	48,48,48	0.87	3 (6%)	51,54,54	1.18	4 (7%)
25	BCR	C	515	-	41,41,41	1.23	4 (9%)	56,56,56	1.38	7 (12%)
23	CLA	B	603	-	65,73,73	1.49	11 (16%)	76,113,113	1.59	12 (15%)
23	CLA	B	612	-	65,73,73	1.32	7 (10%)	76,113,113	1.72	16 (21%)
23	CLA	B	605	-	65,73,73	1.38	11 (16%)	76,113,113	1.59	15 (19%)
25	BCR	B	617	-	41,41,41	1.15	3 (7%)	56,56,56	1.38	7 (12%)
27	LMG	d	409	-	44,44,55	1.14	4 (9%)	52,52,63	1.42	9 (17%)
33	LHG	e	101	-	41,41,48	0.81	2 (4%)	44,47,54	1.28	4 (9%)
25	BCR	A	408	-	41,41,41	1.00	2 (4%)	56,56,56	1.38	8 (14%)
28	SQD	A	411	-	51,52,54	1.06	4 (7%)	60,63,65	2.19	9 (15%)
27	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.56	13 (22%)
33	LHG	a	410	-	48,48,48	0.76	1 (2%)	51,54,54	1.35	6 (11%)
28	SQD	A	412	-	38,38,54	1.14	3 (7%)	40,40,65	1.06	1 (2%)
25	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.20	5 (8%)
23	CLA	B	608	-	65,73,73	1.61	10 (15%)	76,113,113	1.46	10 (13%)
23	CLA	C	512	-	65,73,73	1.70	12 (18%)	76,113,113	1.37	9 (11%)
23	CLA	B	615	-	65,73,73	1.79	10 (15%)	76,113,113	1.51	11 (14%)
24	PHO	d	401	-	51,69,69	1.05	4 (7%)	47,99,99	1.48	8 (17%)
33	LHG	D	408	-	48,48,48	1.12	5 (10%)	51,54,54	1.18	4 (7%)
33	LHG	B	622	-	48,48,48	0.88	2 (4%)	51,54,54	1.42	7 (13%)
23	CLA	c	505	-	65,73,73	1.58	8 (12%)	76,113,113	1.44	12 (15%)
28	SQD	a	412	-	35,35,54	1.11	2 (5%)	37,37,65	1.33	4 (10%)
23	CLA	B	611	-	65,73,73	1.39	9 (13%)	76,113,113	1.45	13 (17%)
26	PL9	D	406	-	55,55,55	1.36	5 (9%)	68,69,69	1.51	13 (19%)
27	LMG	c	519	-	37,37,55	1.11	4 (10%)	45,45,63	1.20	3 (6%)
23	CLA	A	405	36	65,73,73	1.41	8 (12%)	76,113,113	1.51	16 (21%)
35	HEC	v	201	16	32,50,50	2.09	4 (12%)	24,82,82	1.84	4 (16%)
23	CLA	D	404	-	65,73,73	1.65	10 (15%)	76,113,113	1.24	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	OEY	A	414	1,3,36	0,16,16	-	-	-		
27	LMG	b	623	-	21,21,55	0.97	1 (4%)	20,20,63	0.90	0
33	LHG	D	409	-	46,46,48	1.01	4 (8%)	49,52,54	1.32	4 (8%)
23	CLA	C	504	36	59,67,73	1.47	9 (15%)	68,105,113	1.51	11 (16%)
23	CLA	C	511	3	65,73,73	1.84	10 (15%)	76,113,113	1.53	9 (11%)
29	DGD	A	413	-	67,67,67	1.29	10 (14%)	81,81,81	1.36	7 (8%)
23	CLA	C	505	-	65,73,73	1.62	10 (15%)	76,113,113	1.38	9 (11%)
25	BCR	T	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.42	7 (12%)
25	BCR	b	620	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	7 (12%)
33	LHG	L	101	-	48,48,48	0.92	1 (2%)	51,54,54	1.17	3 (5%)
24	PHO	D	401	-	51,69,69	1.07	5 (9%)	47,99,99	1.39	7 (14%)
23	CLA	B	601	36	65,73,73	1.85	11 (16%)	76,113,113	1.70	10 (13%)
29	DGD	H	102	-	63,63,67	1.63	10 (15%)	77,77,81	1.64	15 (19%)
25	BCR	y	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.23	6 (10%)
23	CLA	a	404	-	65,73,73	1.36	8 (12%)	76,113,113	1.72	13 (17%)
23	CLA	b	606	-	65,73,73	1.62	5 (7%)	76,113,113	1.68	16 (21%)
23	CLA	c	511	3	65,73,73	1.81	10 (15%)	76,113,113	1.34	5 (6%)
29	DGD	C	518	-	63,63,67	1.12	6 (9%)	77,77,81	1.49	11 (14%)
27	LMG	D	407	-	51,51,55	1.04	2 (3%)	59,59,63	1.27	5 (8%)
28	SQD	B	623	-	53,54,54	0.91	3 (5%)	62,65,65	1.90	14 (22%)
35	HEC	V	201	16	32,50,50	2.27	4 (12%)	24,82,82	1.02	1 (4%)
28	SQD	b	601	-	48,49,54	1.00	3 (6%)	57,60,65	2.36	16 (28%)
23	CLA	C	503	-	65,73,73	1.52	10 (15%)	76,113,113	1.74	14 (18%)
29	DGD	c	516	-	63,63,67	1.28	10 (15%)	77,77,81	1.59	14 (18%)
29	DGD	h	103	-	63,63,67	0.98	4 (6%)	77,77,81	1.60	16 (20%)
27	LMG	a	414	-	49,49,55	0.86	2 (4%)	57,57,63	1.27	3 (5%)
24	PHO	A	406	-	51,69,69	1.19	5 (9%)	47,99,99	1.42	8 (17%)
27	LMG	b	622	-	55,55,55	1.09	4 (7%)	63,63,63	1.45	10 (15%)
29	DGD	C	517	-	63,63,67	1.27	7 (11%)	77,77,81	1.55	10 (12%)
23	CLA	B	606	-	65,73,73	1.92	10 (15%)	76,113,113	1.54	8 (10%)
25	BCR	B	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	7 (12%)
27	LMG	C	519	-	48,48,55	1.11	5 (10%)	56,56,63	1.34	6 (10%)
23	CLA	c	504	36	60,68,73	1.97	10 (16%)	70,107,113	1.64	10 (14%)
33	LHG	E	101	-	48,48,48	1.03	4 (8%)	51,54,54	1.14	3 (5%)
34	HEM	e	102	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.63	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	D	411	-	26,26,55	1.01	2 (7%)	26,26,63	1.24	3 (11%)
26	PL9	d	406	-	55,55,55	1.28	6 (10%)	68,69,69	1.68	20 (29%)
23	CLA	B	613	-	65,73,73	1.57	13 (20%)	76,113,113	1.50	14 (18%)
23	CLA	C	510	-	65,73,73	1.74	8 (12%)	76,113,113	1.63	8 (10%)
27	LMG	D	410	-	31,31,55	1.12	3 (9%)	33,33,63	1.12	2 (6%)
23	CLA	d	402	36	65,73,73	1.57	7 (10%)	76,113,113	1.62	8 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	403	-	1/1/20/20	12/37/115/115	-
23	CLA	c	512	-	1/1/20/20	21/37/115/115	-
23	CLA	d	404	-	1/1/20/20	9/37/115/115	-
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
23	CLA	A	404	-	1/1/20/20	5/37/115/115	-
23	CLA	C	507	36	1/1/20/20	12/37/115/115	-
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
29	DGD	c	518	-	-	20/51/91/95	0/2/2/2
23	CLA	a	407	-	1/1/20/20	10/37/115/115	-
25	BCR	c	515	-	-	9/29/63/63	0/2/2/2
25	BCR	h	102	-	-	6/29/63/63	0/2/2/2
25	BCR	C	520	-	-	12/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/17/20	2/24/102/115	-
23	CLA	c	506	-	1/1/20/20	21/37/115/115	-
23	CLA	b	615	-	1/1/20/20	16/37/115/115	-
25	BCR	D	405	-	-	13/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/20/20	10/37/115/115	-
23	CLA	b	604	-	1/1/20/20	11/37/115/115	-
23	CLA	c	507	36	1/1/20/20	12/37/115/115	-
23	CLA	B	609	-	-	8/37/115/115	-
23	CLA	b	605	-	1/1/20/20	12/37/115/115	-
23	CLA	D	402	36	1/1/20/20	4/37/115/115	-
29	DGD	C	516	-	-	20/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
25	BCR	a	408	-	-	2/29/63/63	0/2/2/2
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/20/20	7/37/115/115	-
23	CLA	C	501	-	1/1/20/20	3/37/115/115	-
23	CLA	b	608	36	1/1/20/20	14/37/115/115	-
23	CLA	C	508	-	-	9/37/115/115	-
23	CLA	b	611	36	1/1/20/20	7/37/115/115	-
23	CLA	C	513	-	1/1/20/20	13/37/115/115	-
23	CLA	c	510	-	1/1/20/20	19/37/115/115	-
23	CLA	B	604	-	1/1/20/20	11/37/115/115	-
23	CLA	C	502	-	-	10/37/115/115	-
23	CLA	h	101	36	1/1/20/20	16/37/115/115	-
23	CLA	d	403	-	1/1/20/20	8/37/115/115	-
28	SQD	F	101	-	-	14/28/48/69	0/1/1/1
23	CLA	B	602	-	1/1/20/20	6/37/115/115	-
25	BCR	d	405	-	-	14/29/63/63	0/2/2/2
23	CLA	C	509	-	1/1/20/20	10/37/115/115	-
23	CLA	b	617	-	1/1/19/20	9/31/109/115	-
28	SQD	f	101	-	-	12/36/56/69	0/1/1/1
33	LHG	l	101	-	-	19/53/53/53	-
23	CLA	c	503	-	-	13/37/115/115	-
27	LMG	A	410	-	-	20/43/63/70	0/1/1/1
29	DGD	c	517	-	-	20/51/91/95	0/2/2/2
23	CLA	b	613	-	1/1/20/20	13/37/115/115	-
23	CLA	b	607	-	1/1/20/20	9/37/115/115	-
23	CLA	b	609	-	-	7/37/115/115	-
23	CLA	C	506	-	1/1/20/20	16/37/115/115	-
23	CLA	b	603	-	1/1/20/20	8/37/115/115	-
23	CLA	c	501	-	1/1/20/20	8/37/115/115	-
23	CLA	c	508	-	-	11/36/114/115	-
23	CLA	B	610	36	1/1/20/20	7/37/115/115	-
33	LHG	d	408	-	-	14/43/43/53	-
23	CLA	c	513	-	1/1/20/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	c	521	-	-	4/29/63/63	0/2/2/2
24	PHO	a	406	-	-	7/37/103/103	0/5/6/6
23	CLA	B	607	36	1/1/20/20	12/37/115/115	-
23	CLA	c	502	-	-	7/37/115/115	-
23	CLA	B	614	-	1/1/20/20	13/37/115/115	-
27	LMG	B	620	-	-	21/46/66/70	0/1/1/1
28	SQD	a	411	-	-	18/49/69/69	0/1/1/1
23	CLA	b	610	-	-	7/37/115/115	-
26	PL9	a	409	-	-	27/53/73/73	0/1/1/1
25	BCR	c	514	-	-	11/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/20/20	8/37/115/115	-
27	LMG	c	522	-	-	21/43/63/70	0/1/1/1
23	CLA	B	616	-	1/1/19/20	9/31/109/115	-
25	BCR	b	619	-	-	5/29/63/63	0/2/2/2
25	BCR	C	514	-	-	15/29/63/63	0/2/2/2
34	HEM	E	102	6,5	-	1/12/54/54	-
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
23	CLA	a	405	36	1/1/20/20	10/37/115/115	-
23	CLA	b	612	-	-	11/37/115/115	-
29	DGD	a	413	-	-	21/45/45/95	-
33	LHG	d	407	-	-	24/53/53/53	-
25	BCR	C	515	-	-	4/29/63/63	0/2/2/2
23	CLA	B	603	-	-	16/37/115/115	-
23	CLA	B	612	-	1/1/20/20	11/37/115/115	-
23	CLA	B	605	-	1/1/20/20	8/37/115/115	-
25	BCR	B	617	-	-	4/29/63/63	0/2/2/2
27	LMG	d	409	-	-	11/39/59/70	0/1/1/1
33	LHG	e	101	-	-	23/46/46/53	-
25	BCR	A	408	-	-	7/29/63/63	0/2/2/2
28	SQD	A	411	-	-	19/47/67/69	0/1/1/1
27	LMG	m	101	-	-	19/46/66/70	0/1/1/1
33	LHG	a	410	-	-	19/53/53/53	-
28	SQD	A	412	-	-	17/39/39/69	-
25	BCR	K	101	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	608	-	-	3/37/115/115	-
23	CLA	C	512	-	1/1/20/20	10/37/115/115	-
23	CLA	B	615	-	1/1/20/20	9/37/115/115	-
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
33	LHG	D	408	-	-	25/53/53/53	-
33	LHG	B	622	-	-	11/53/53/53	-
23	CLA	c	505	-	1/1/20/20	15/37/115/115	-
28	SQD	a	412	-	-	22/37/37/69	-
23	CLA	B	611	-	1/1/20/20	10/37/115/115	-
26	PL9	D	406	-	-	10/53/73/73	0/1/1/1
27	LMG	c	519	-	-	10/31/51/70	0/1/1/1
23	CLA	A	405	36	-	4/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-
23	CLA	D	404	-	-	11/37/115/115	-
27	LMG	b	623	-	-	12/17/17/70	-
33	LHG	D	409	-	-	25/51/51/53	-
23	CLA	C	504	36	1/1/18/20	7/30/108/115	-
23	CLA	C	511	3	-	4/37/115/115	-
29	DGD	A	413	-	-	31/55/95/95	0/2/2/2
23	CLA	C	505	-	1/1/20/20	10/37/115/115	-
25	BCR	T	101	-	-	14/29/63/63	0/2/2/2
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
33	LHG	L	101	-	-	21/53/53/53	-
24	PHO	D	401	-	-	4/37/103/103	0/5/6/6
23	CLA	B	601	36	-	14/37/115/115	-
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
25	BCR	y	101	-	-	8/29/63/63	0/2/2/2
23	CLA	a	404	-	1/1/20/20	11/37/115/115	-
23	CLA	b	606	-	1/1/20/20	6/37/115/115	-
23	CLA	c	511	3	1/1/20/20	12/37/115/115	-
29	DGD	C	518	-	-	16/51/91/95	0/2/2/2
27	LMG	D	407	-	-	19/46/66/70	0/1/1/1
28	SQD	B	623	-	-	19/49/69/69	0/1/1/1
35	HEC	V	201	16	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	b	601	-	-	19/44/64/69	0/1/1/1
23	CLA	C	503	-	1/1/20/20	8/37/115/115	-
29	DGD	c	516	-	-	25/51/91/95	0/2/2/2
29	DGD	h	103	-	-	15/51/91/95	0/2/2/2
27	LMG	a	414	-	-	28/44/64/70	0/1/1/1
24	PHO	A	406	-	-	8/37/103/103	0/5/6/6
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
29	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	606	-	1/1/20/20	14/37/115/115	-
25	BCR	B	618	-	-	11/29/63/63	0/2/2/2
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
23	CLA	c	504	36	1/1/19/20	11/31/109/115	-
33	LHG	E	101	-	-	27/53/53/53	-
34	HEM	e	102	6,5	-	3/12/54/54	-
27	LMG	D	411	-	-	13/22/22/70	-
26	PL9	d	406	-	-	21/53/73/73	0/1/1/1
23	CLA	B	613	-	1/1/20/20	9/37/115/115	-
23	CLA	C	510	-	1/1/20/20	11/37/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
23	CLA	d	402	36	1/1/20/20	5/37/115/115	-

The worst 5 of 967 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	MG-ND	-11.02	1.83	2.05
23	B	614	CLA	C4B-NB	8.90	1.43	1.35
23	b	615	CLA	C4B-NB	8.81	1.43	1.35
23	C	511	CLA	MG-NA	8.53	2.26	2.06
23	C	501	CLA	MG-NA	8.49	2.26	2.06

The worst 5 of 1361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C4A-NA-C1A	10.58	111.46	106.71
23	d	402	CLA	C4A-NA-C1A	10.17	111.28	106.71
23	C	510	CLA	C4A-NA-C1A	9.94	111.18	106.71
23	b	607	CLA	C4A-NA-C1A	9.94	111.18	106.71
28	b	601	SQD	O6-C1-C2	9.77	123.55	108.30

5 of 55 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	602	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND

5 of 1775 torsion outliers are listed below:

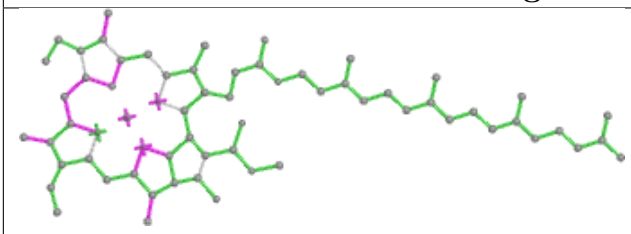
Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C2-C3-C5-C6
23	A	407	CLA	C4-C3-C5-C6
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6

There are no ring outliers.

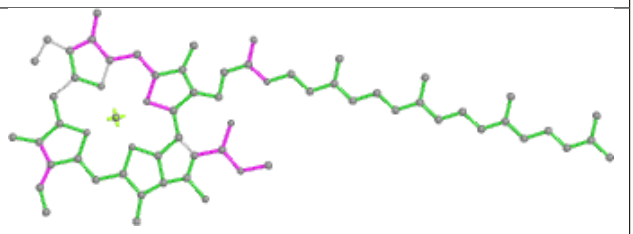
No monomer is involved in short contacts.

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.

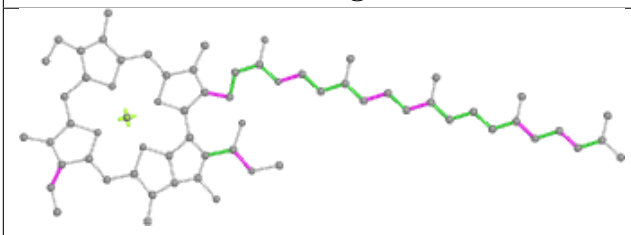
Ligand CLA D 403



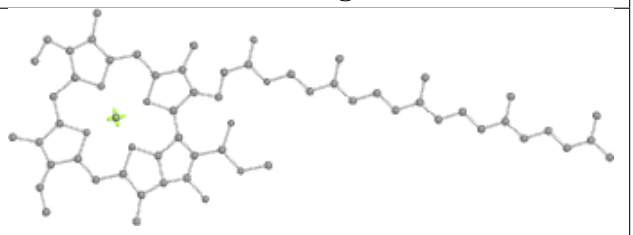
Bond lengths



Bond angles

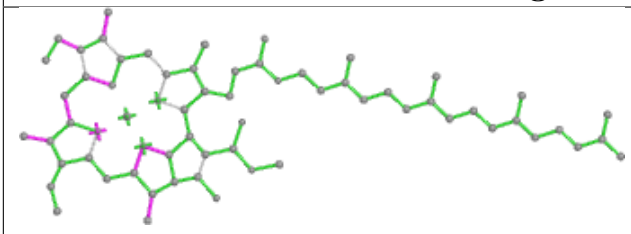


Torsions



Rings

Ligand CLA c 512



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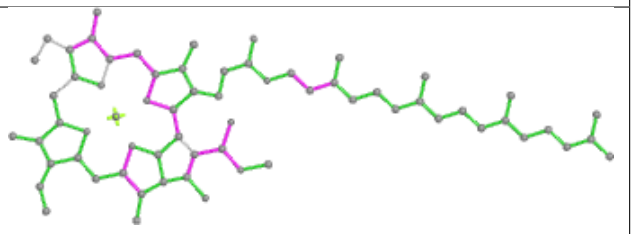

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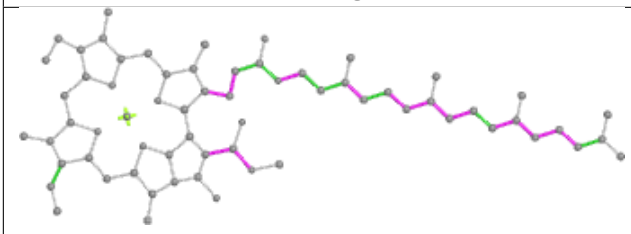

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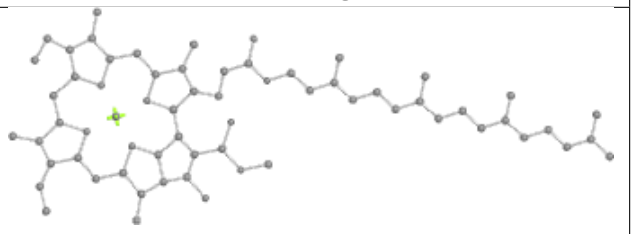
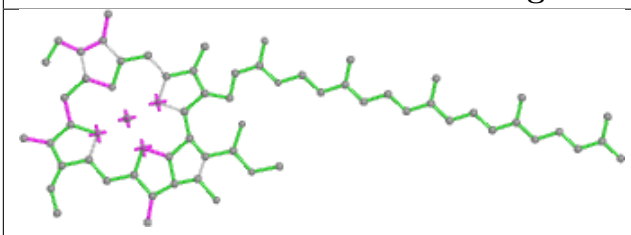


Rings

Ligand CLA d 404



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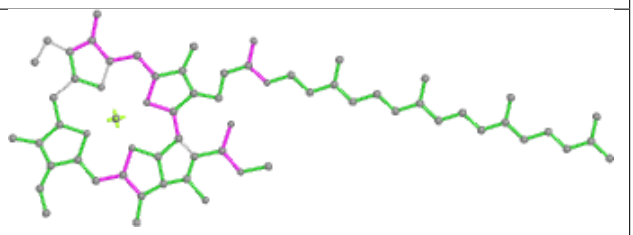

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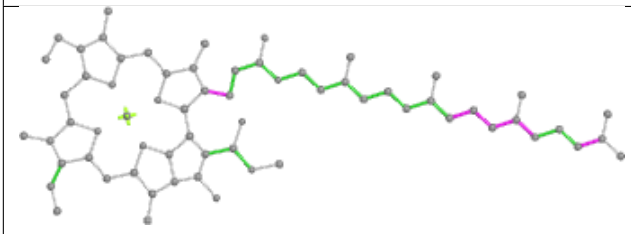

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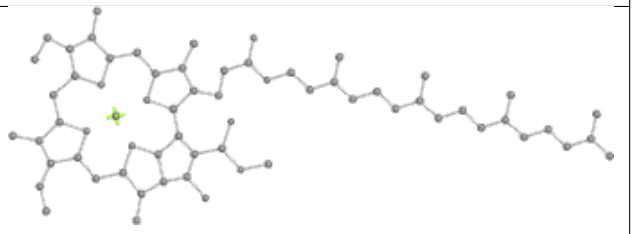
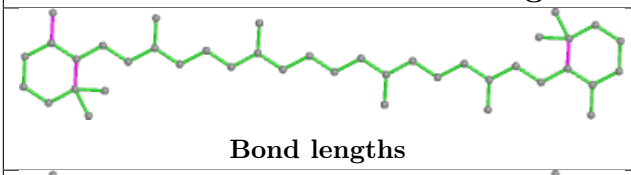


Rings

Ligand BCR b 618



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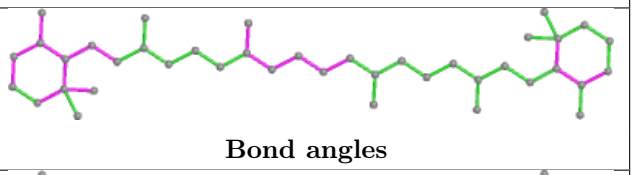

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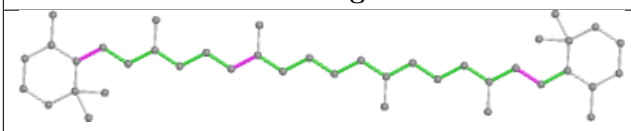

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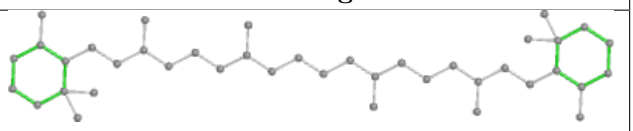
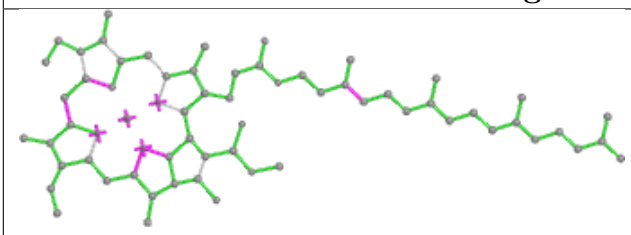


Rings

Ligand CLA A 404



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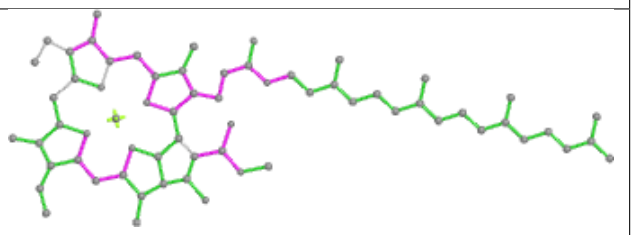

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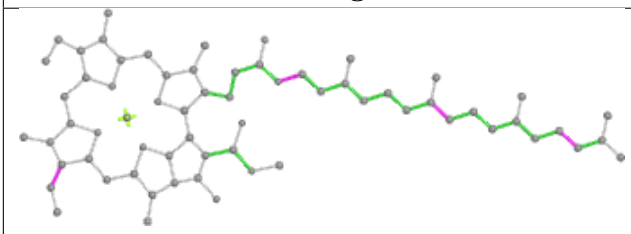

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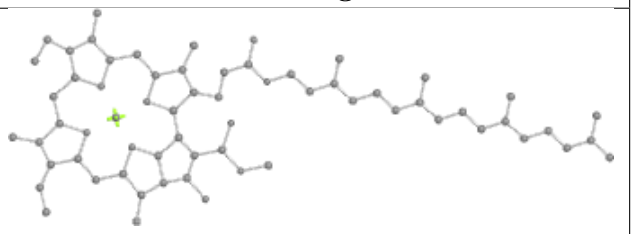
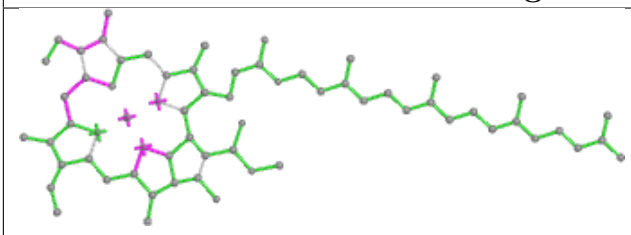


Rings

Ligand CLA C 507



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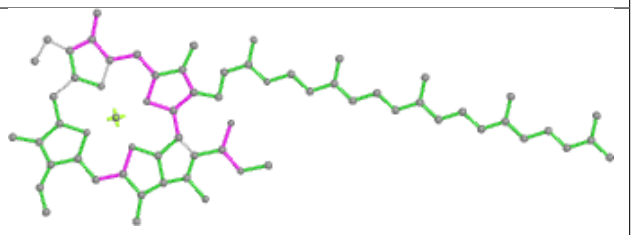

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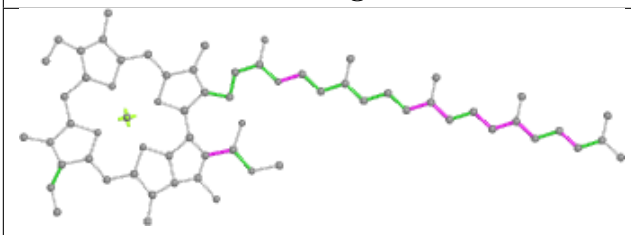

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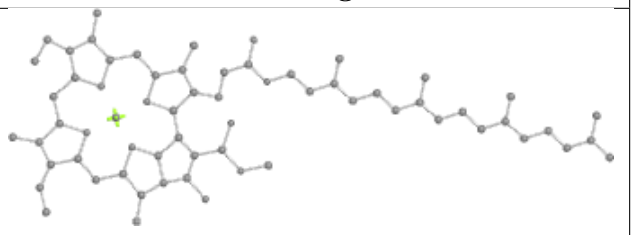
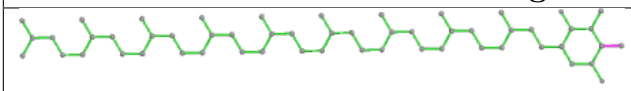


Rings

Ligand PL9 A 409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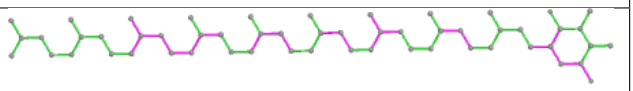
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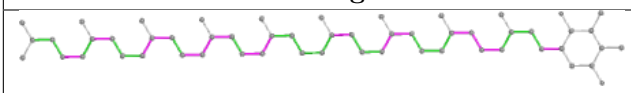
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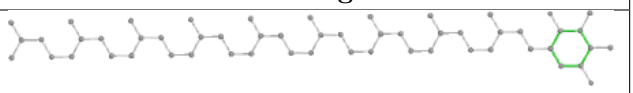
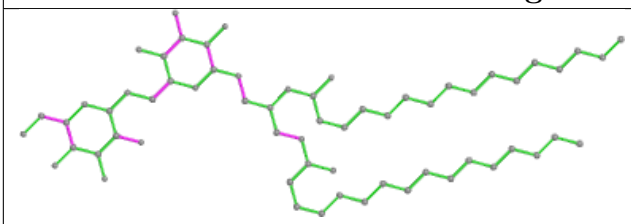

Rings

Ligand DGD c 518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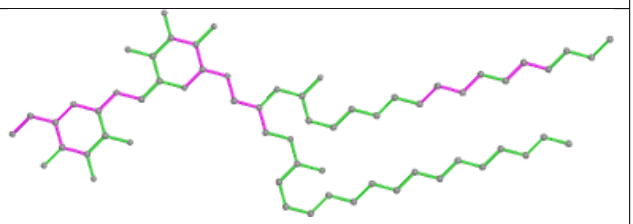
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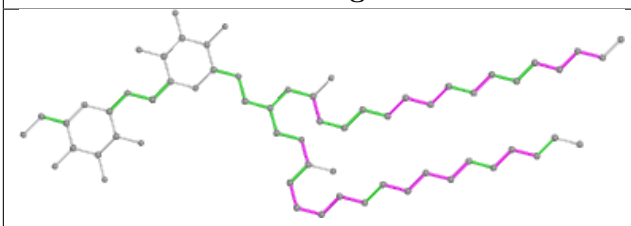
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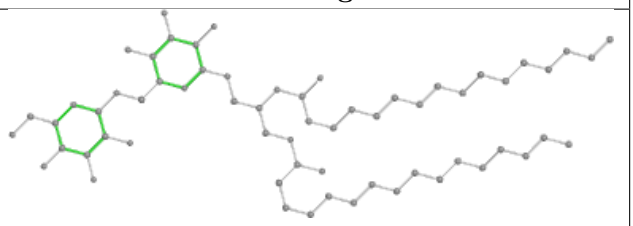
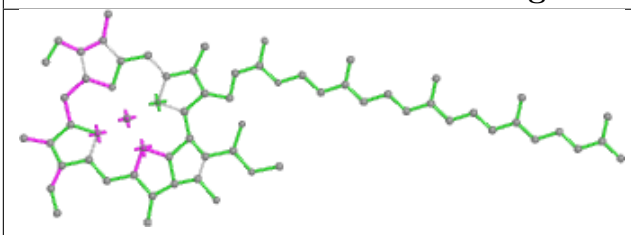

Rings

Ligand CLA a 407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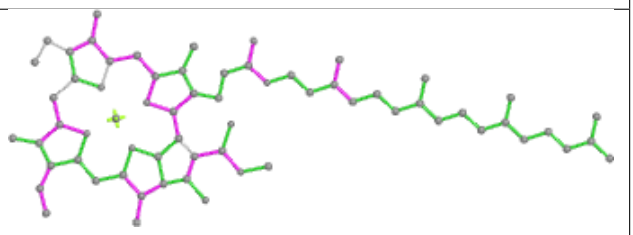
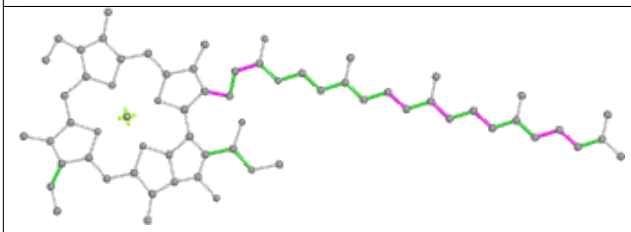

Bond angles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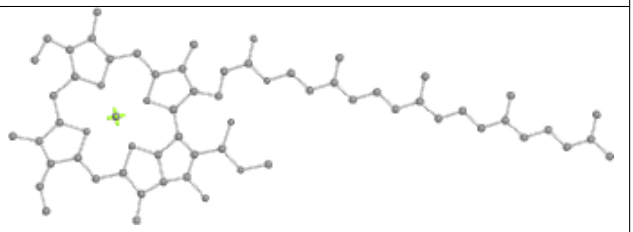
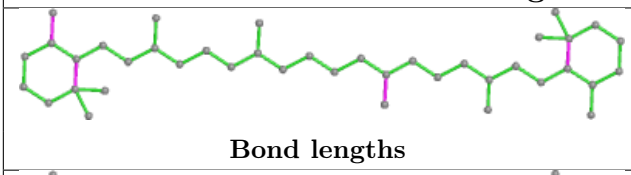

Rings

Ligand BCR c 515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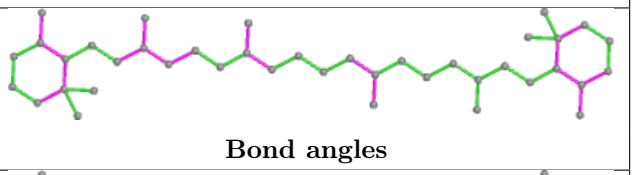
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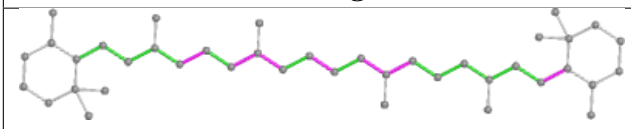
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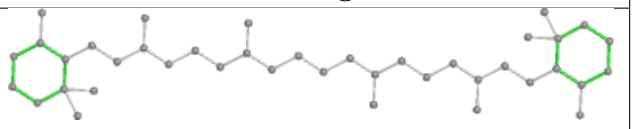
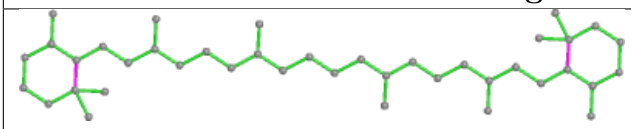

Rings

Ligand BCR h 102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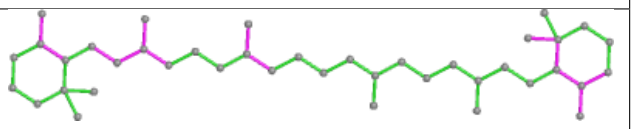
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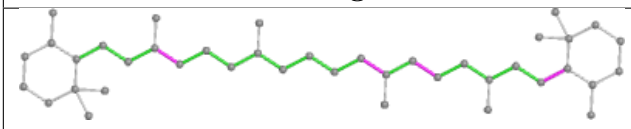
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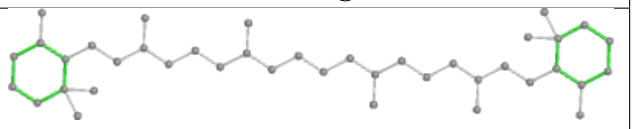
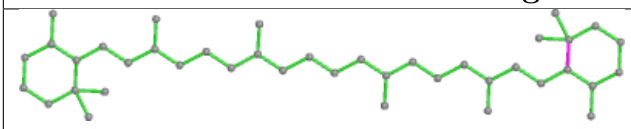

Rings

Ligand BCR C 520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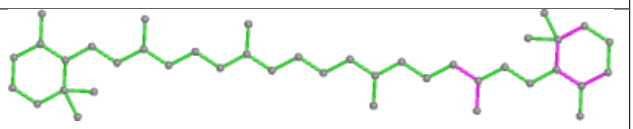
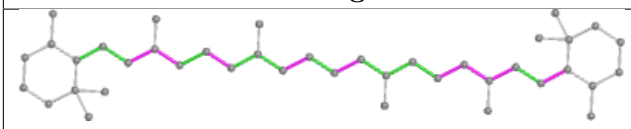

Bond angles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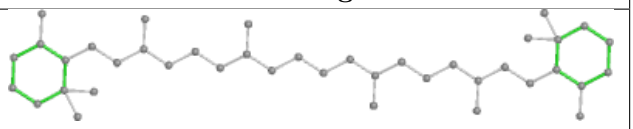
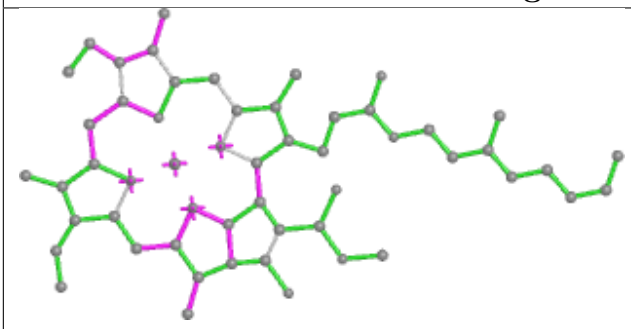
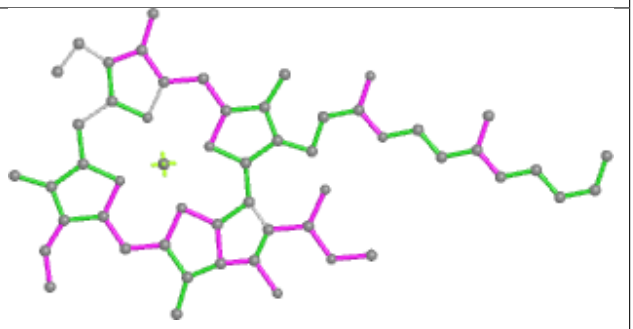

Rings

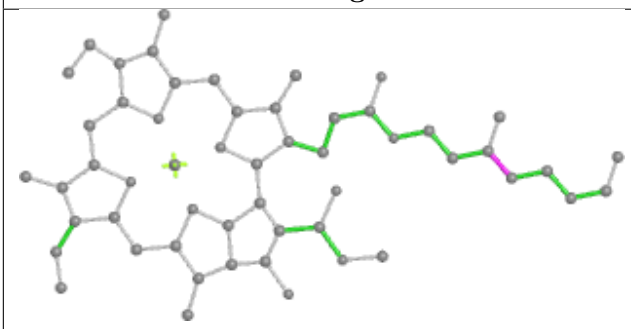
Ligand CLA A 407



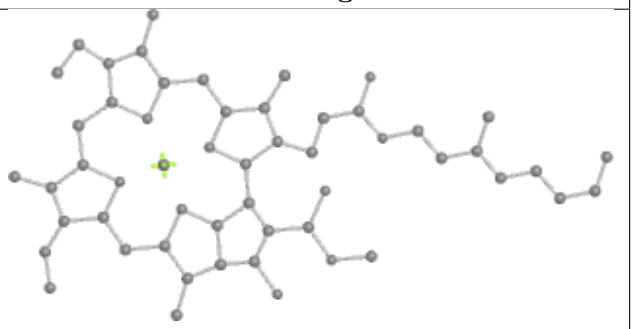
Bond lengths



Bond angles

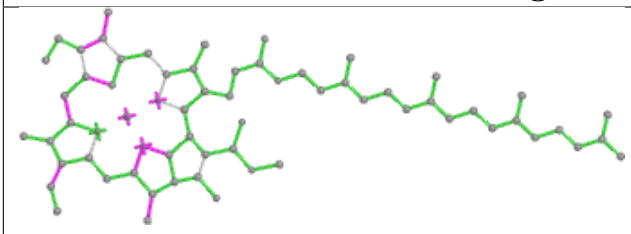


Torsions

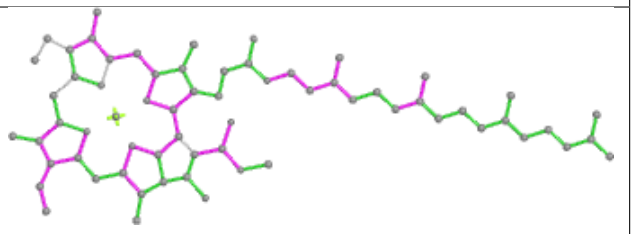


Rings

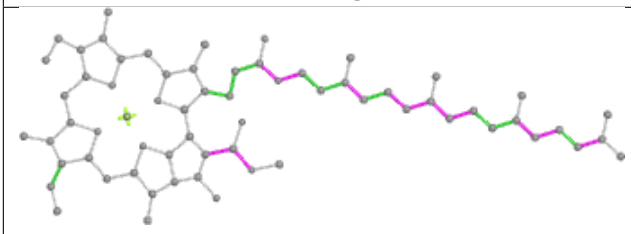
Ligand CLA c 506



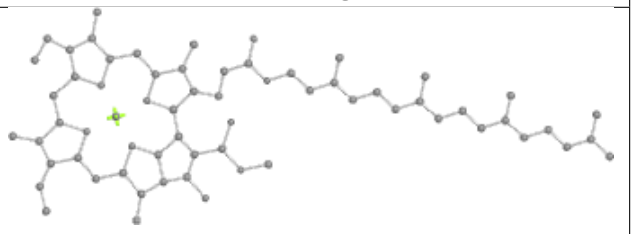
Bond lengths



Bond angles

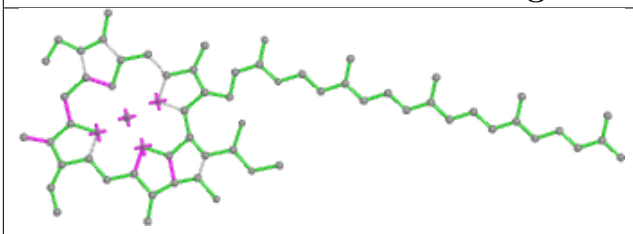


Torsions

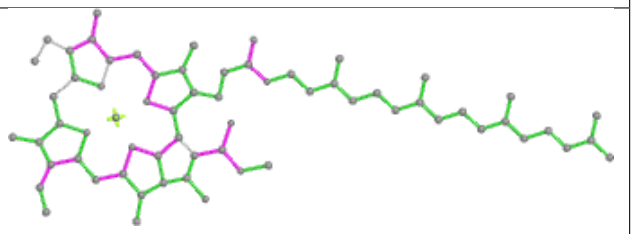


Rings

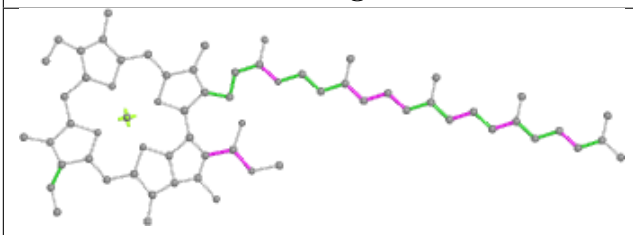
Ligand CLA b 615



Bond lengths



Bond angles



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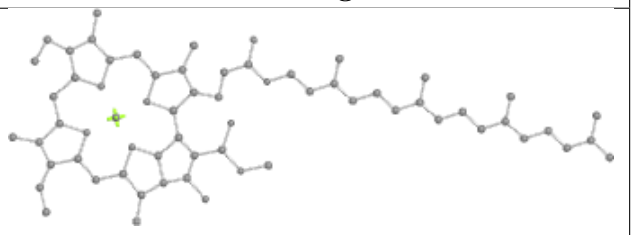
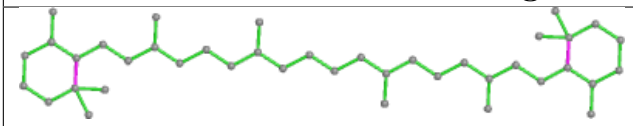


Rings

Ligand BCR D 405



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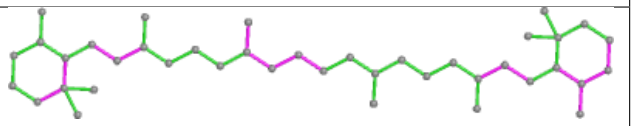
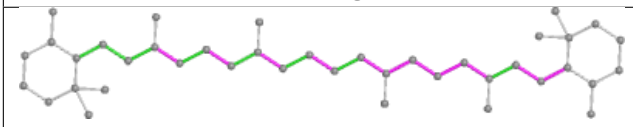


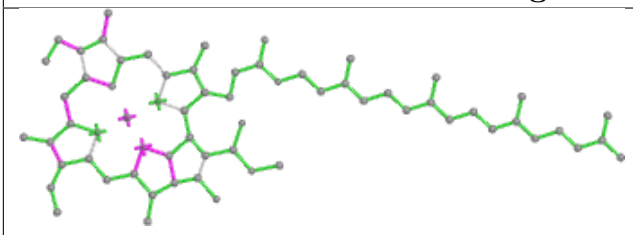
Bond angles



Torsions

Rings

Ligand CLA c 509



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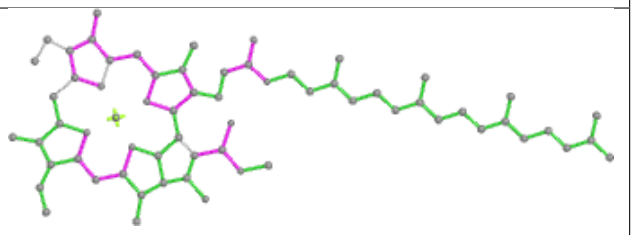
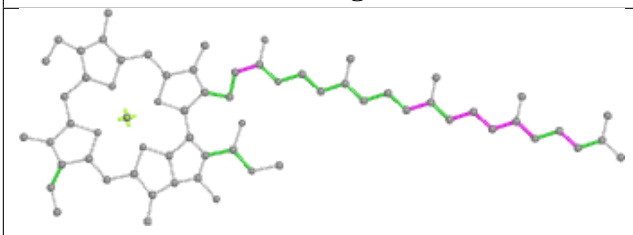
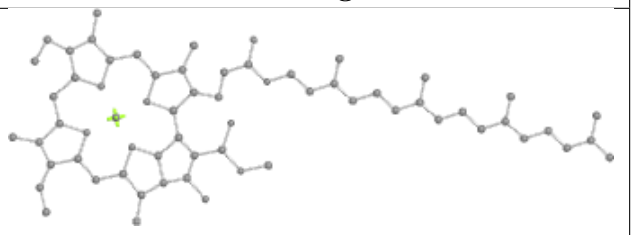


Bond angles

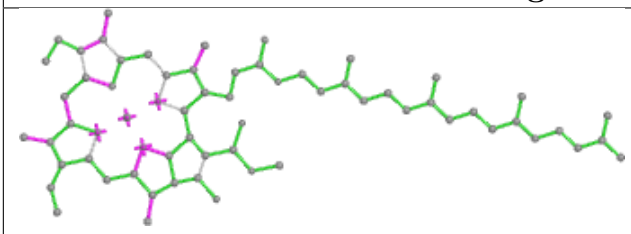


Torsions



Rings

Ligand CLA b 604



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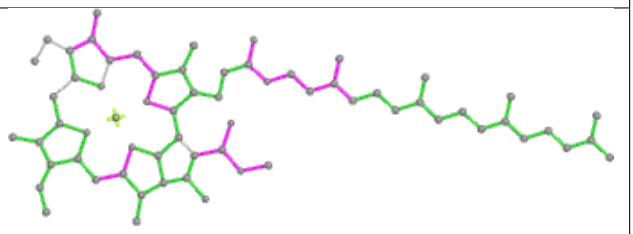
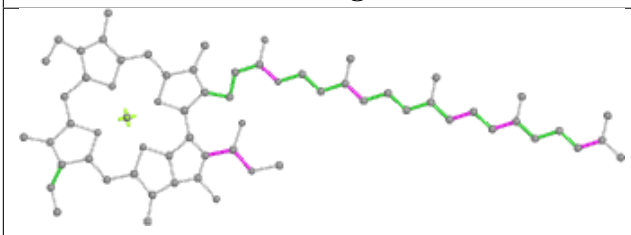


Bond angles



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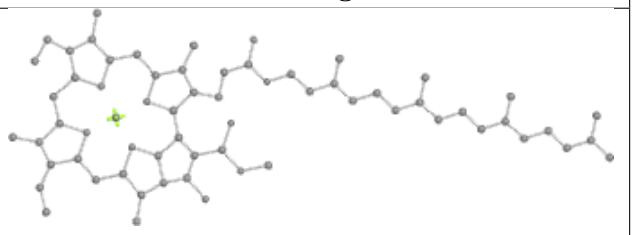
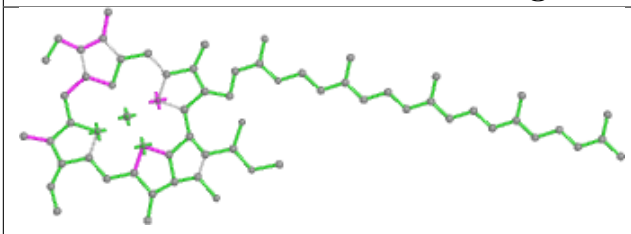


Rings

Ligand CLA c 507



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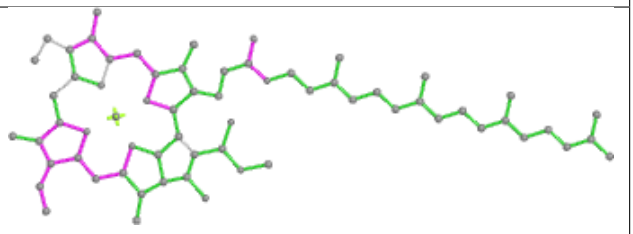
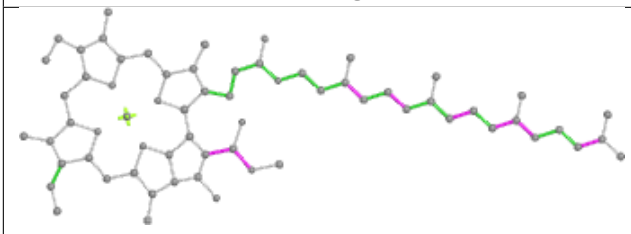


Bond angles



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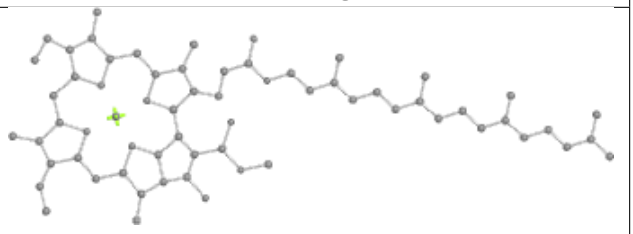
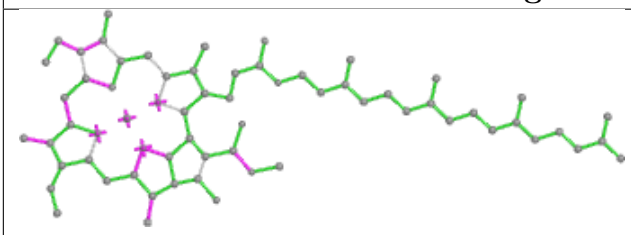


Rings

Ligand CLA B 609



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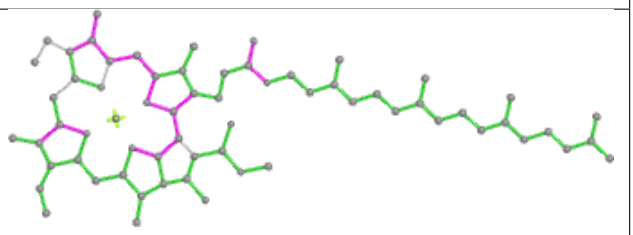
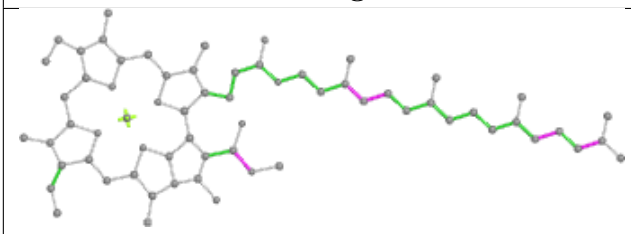


Bond angles



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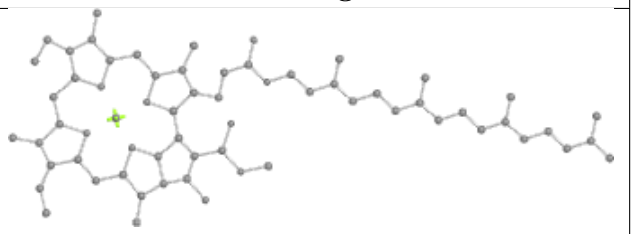
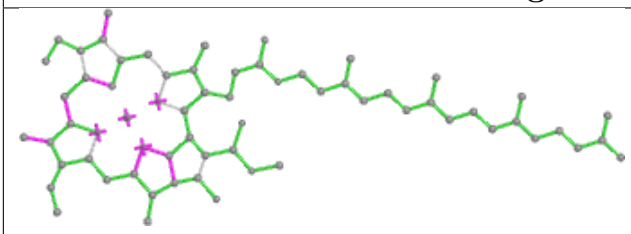
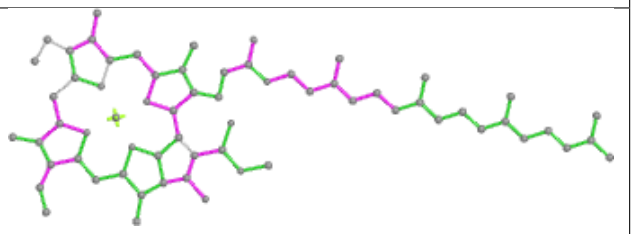


Rings

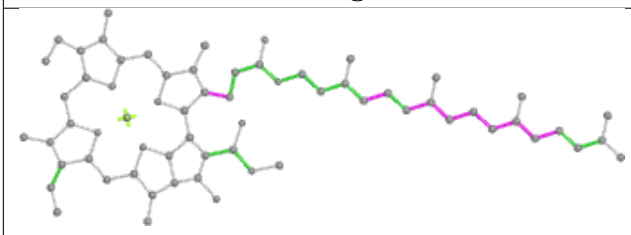
Ligand CLA b 605



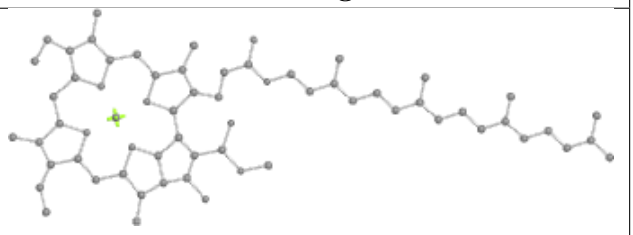
Bond lengths



Bond angles

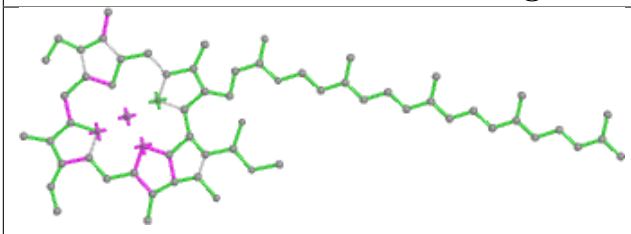


Torsions

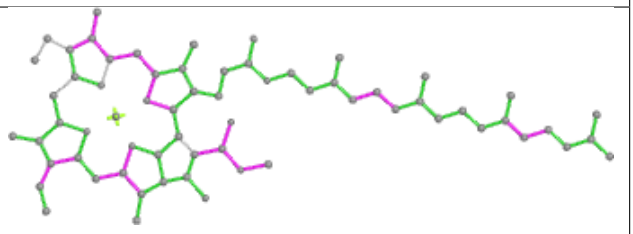


Rings

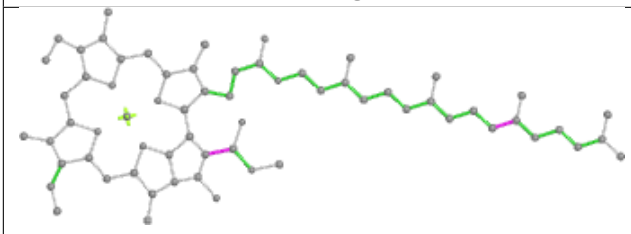
Ligand CLA D 402



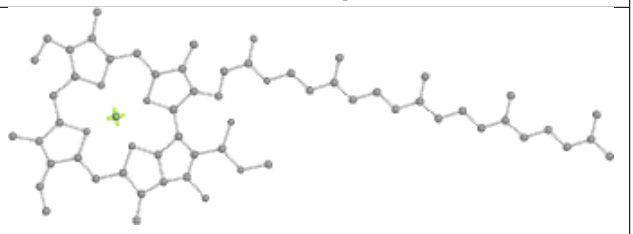
Bond lengths



Bond angles

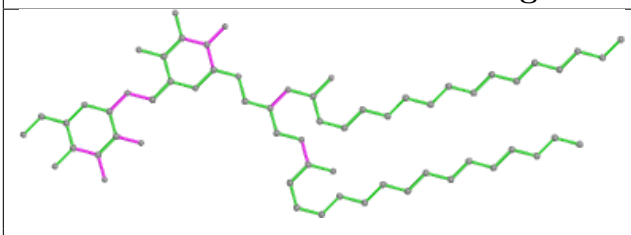


Torsions

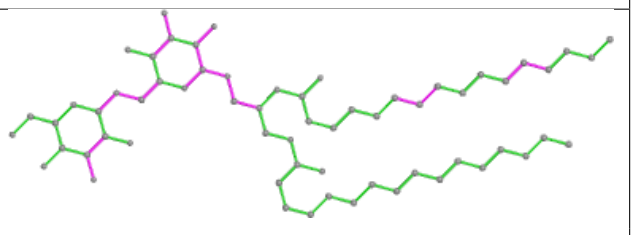


Rings

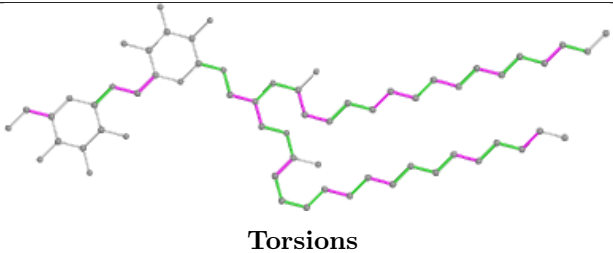
Ligand DGD C 516



Bond lengths



Bond angles



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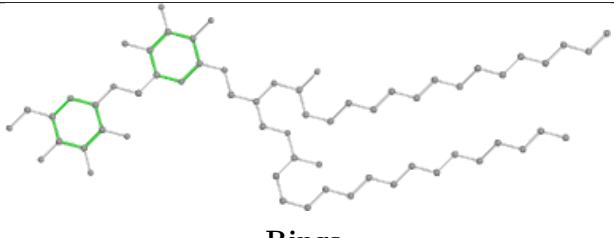
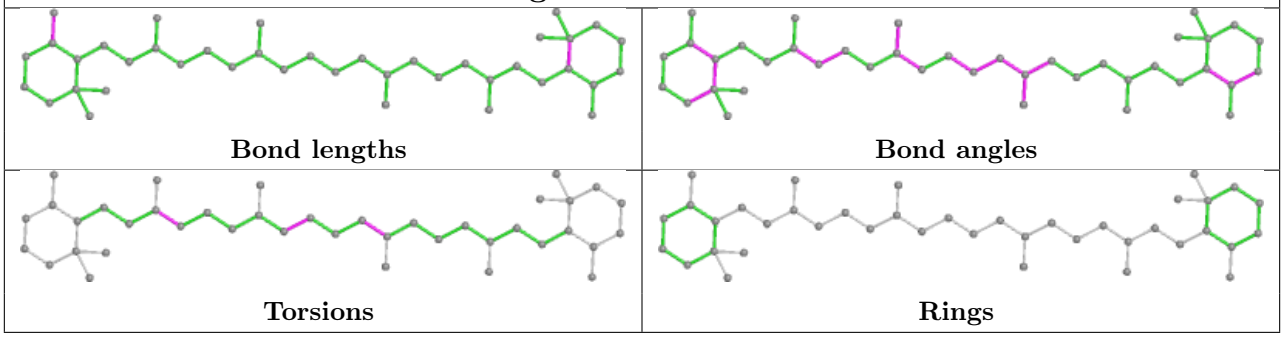
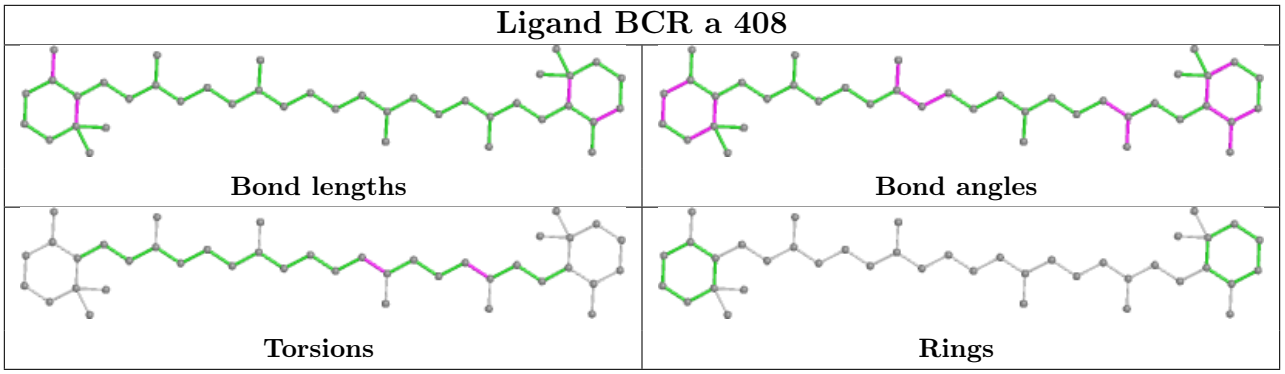


Rings

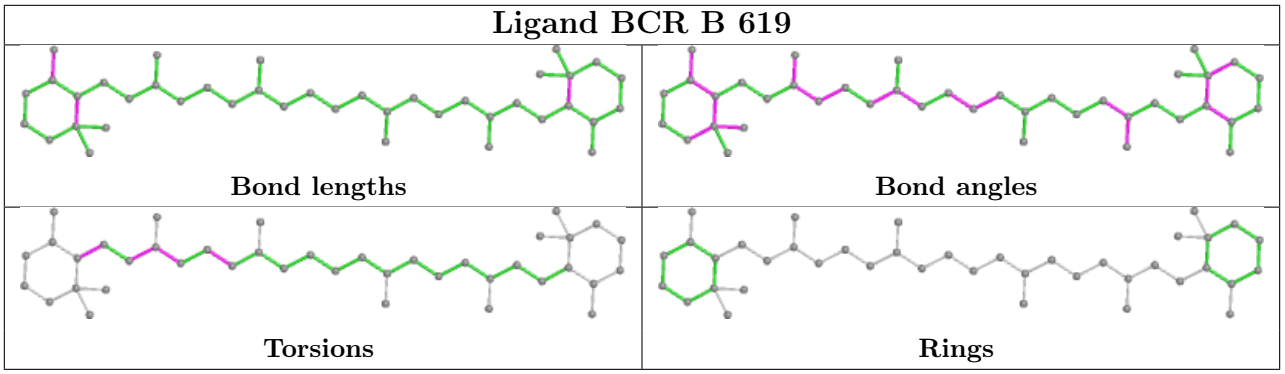
Ligand BCR t 101



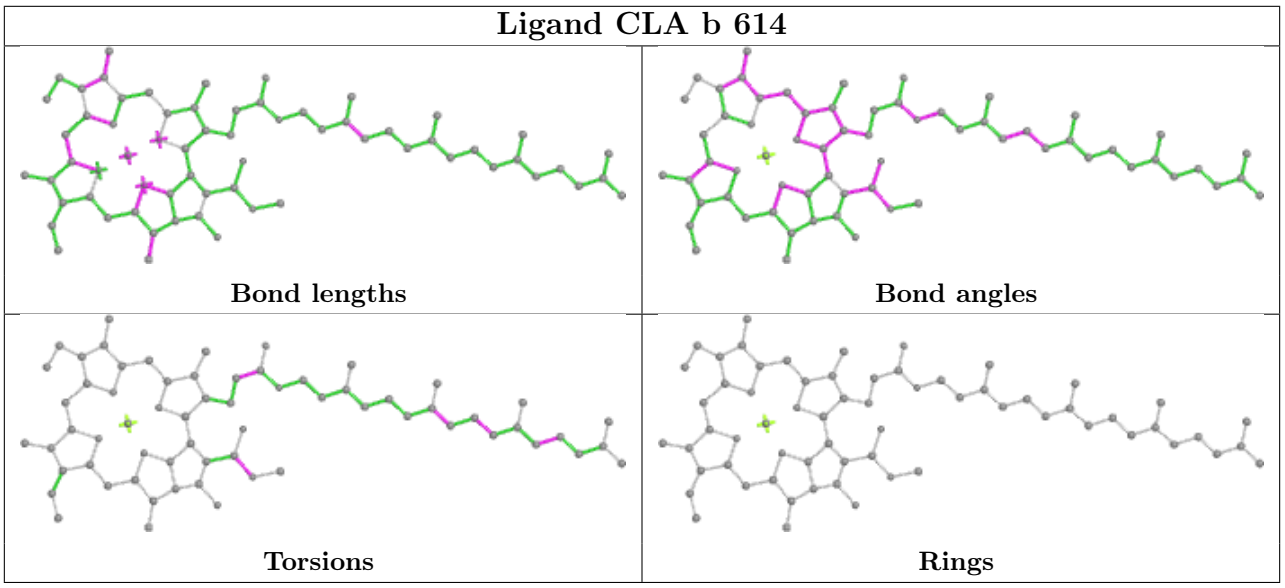
Ligand BCR a 408



Ligand BCR B 619



Ligand CLA b 614



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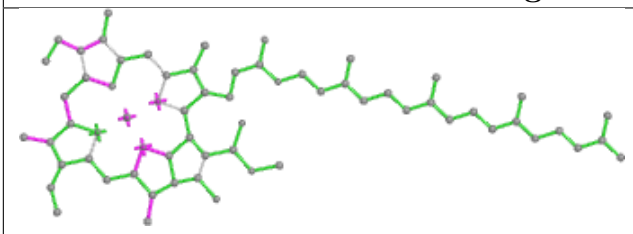
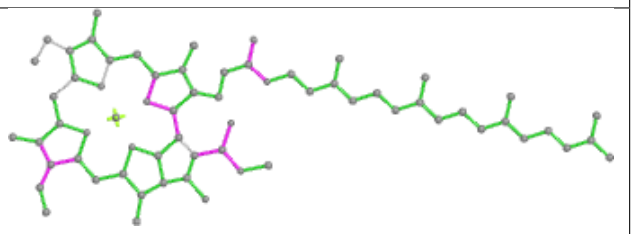
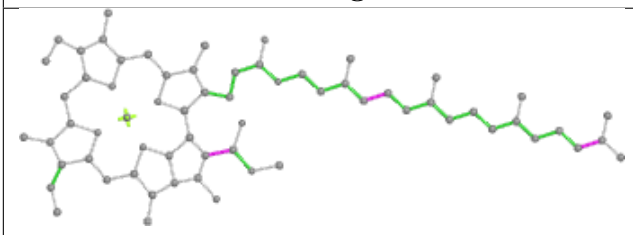


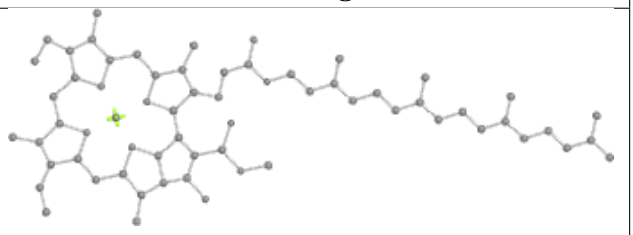
Bond lengths



Bond angles

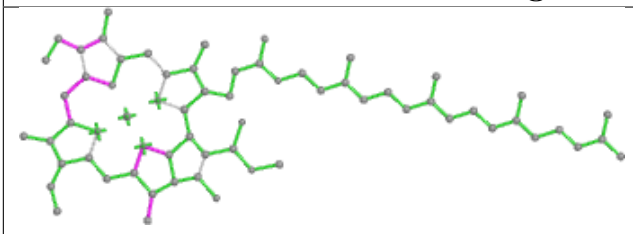


Torsions

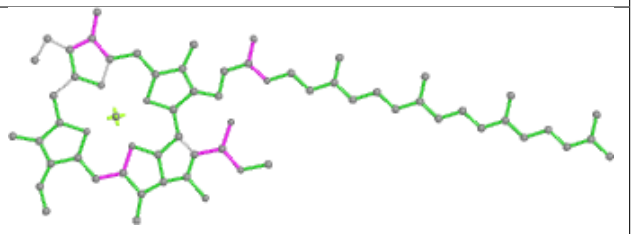


Rings

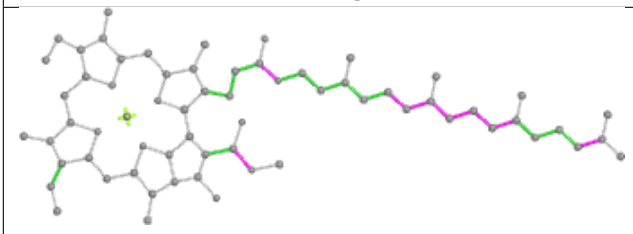
Ligand CLA b 608



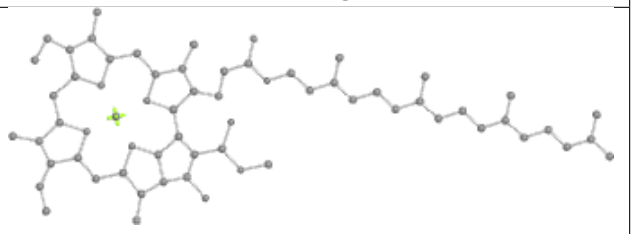
Bond lengths



Bond angles

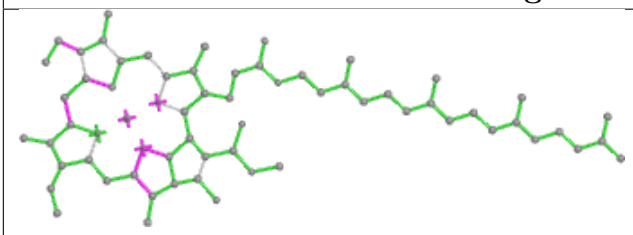


Torsions

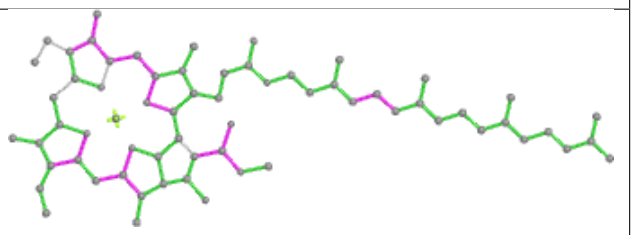


Rings

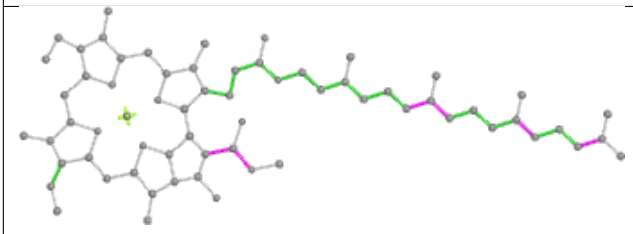
Ligand CLA C 508



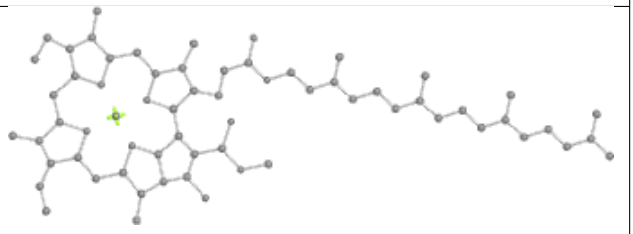
Bond lengths



Bond angles

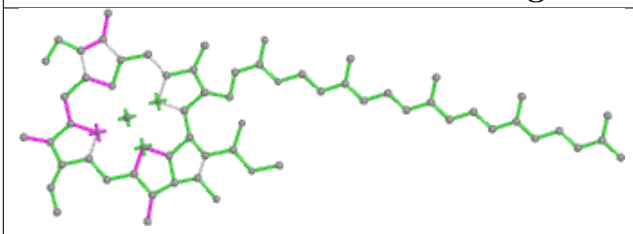


Torsions

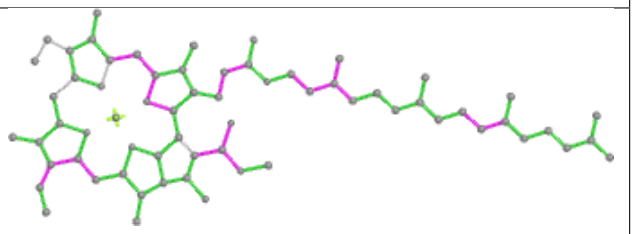


Rings

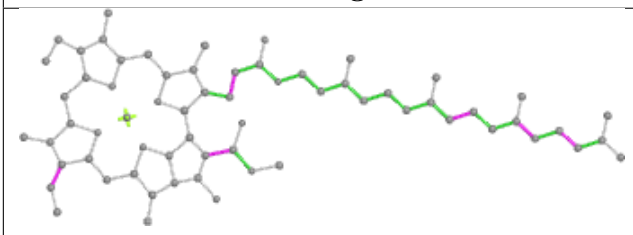
Ligand CLA b 611



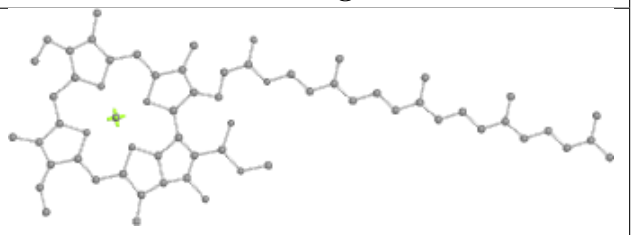
Bond lengths



Bond angles

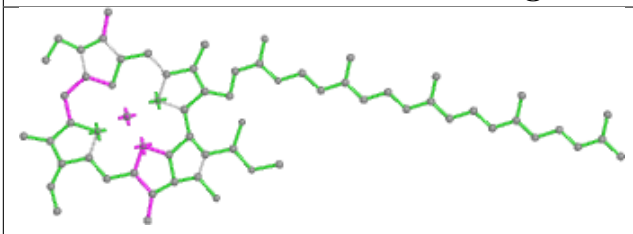


Torsions

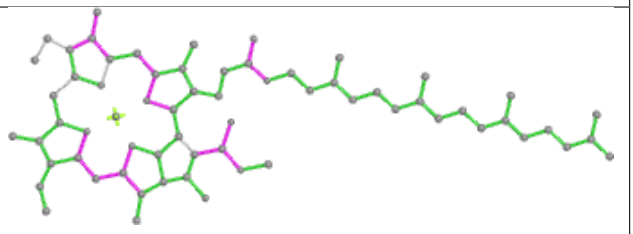


Rings

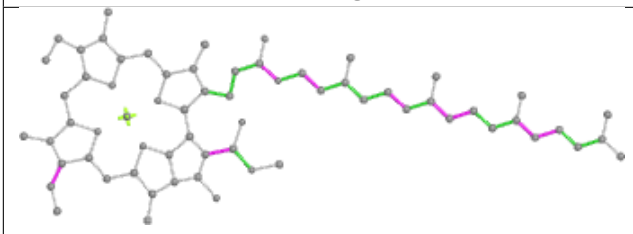
Ligand CLA C 513



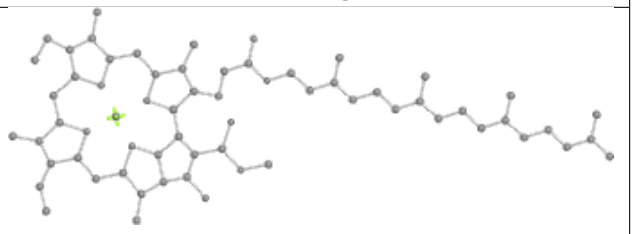
Bond lengths



Bond angles

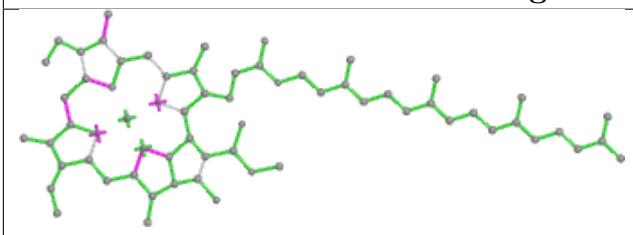


Torsions



Rings

Ligand CLA c 510



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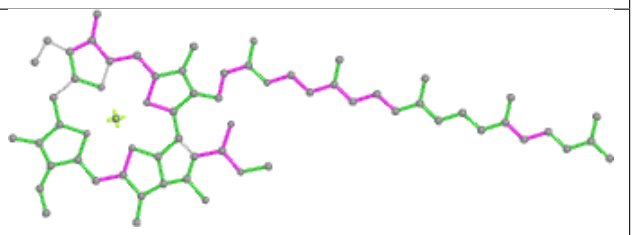

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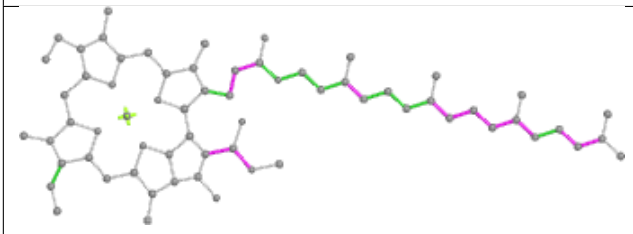

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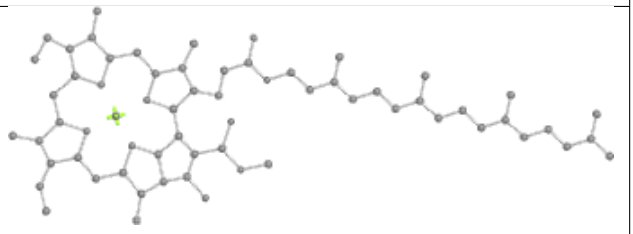
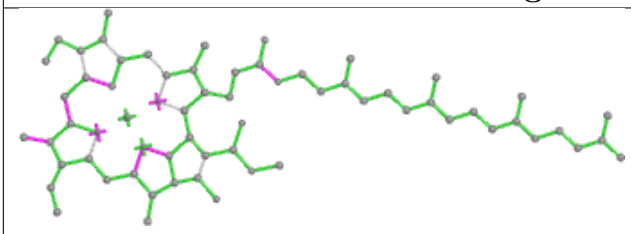


Rings

Ligand CLA B 604



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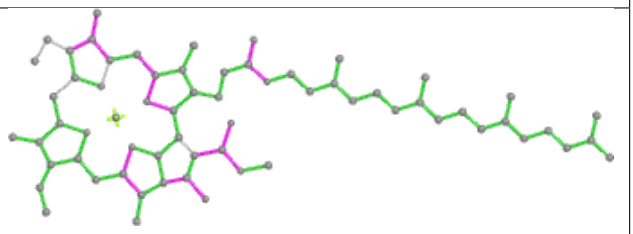
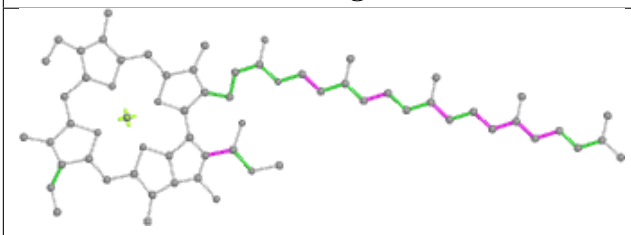


Bond angles



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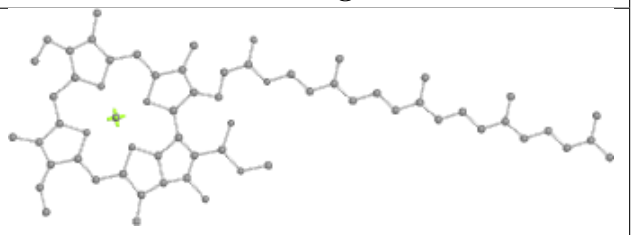
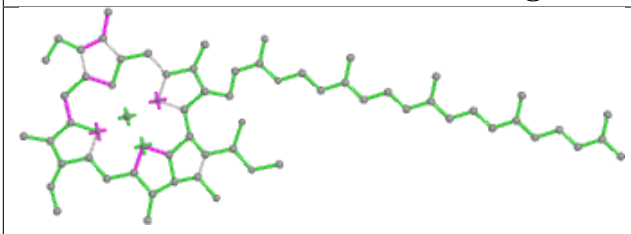


Rings

Ligand CLA C 502



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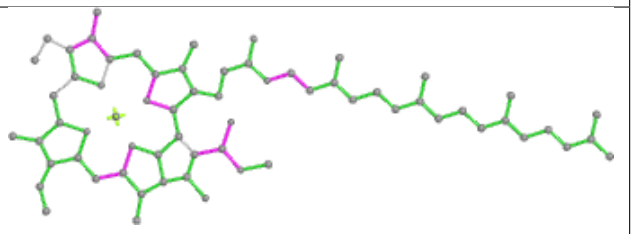
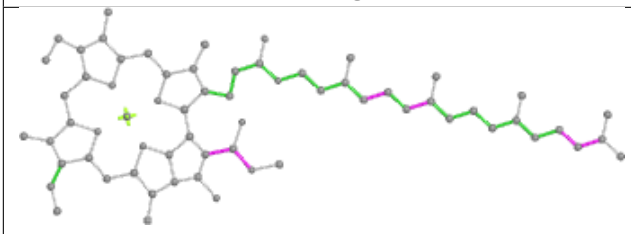


Bond angles



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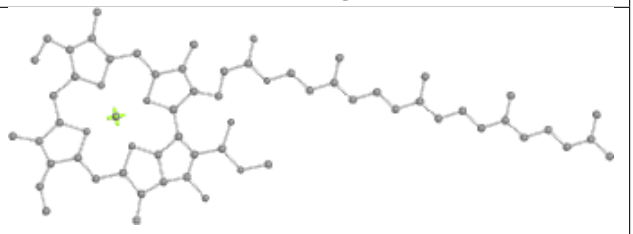
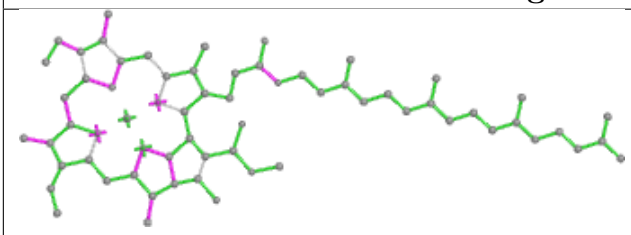


Rings

Ligand CLA h 101



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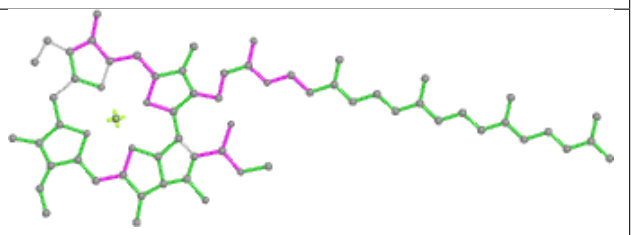
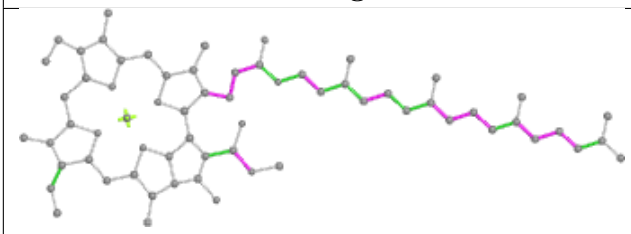


Bond angles



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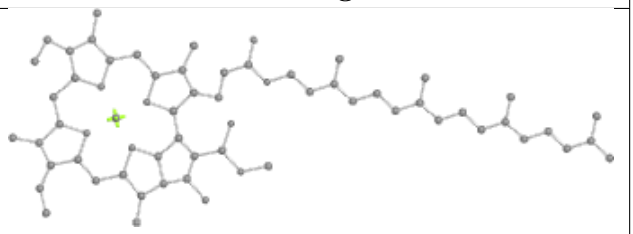
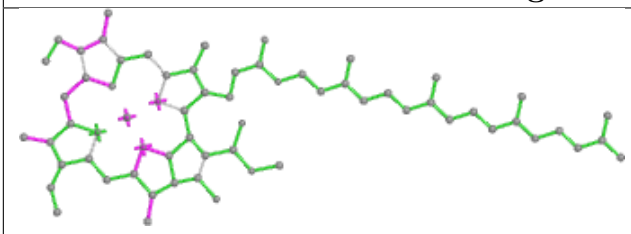


Rings

Ligand CLA d 403



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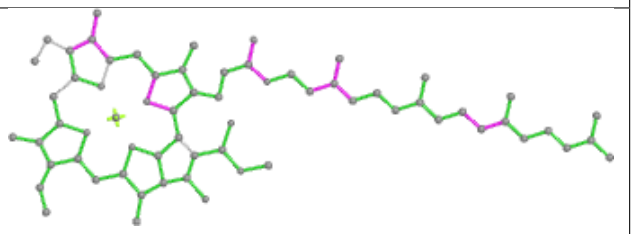
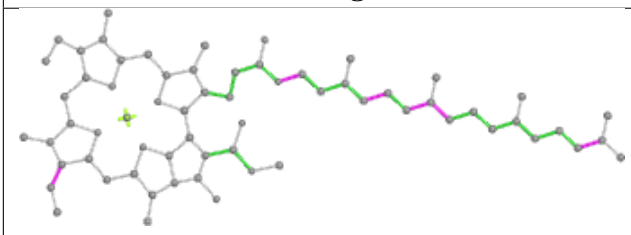


Bond angles



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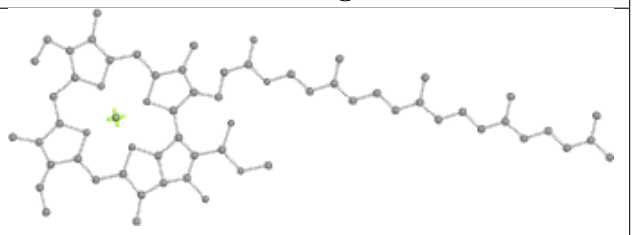
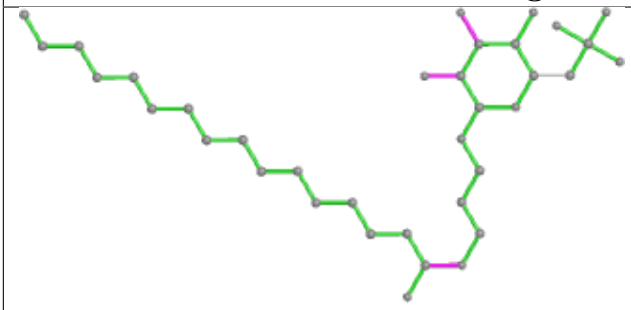


Rings

Ligand SQD F 101



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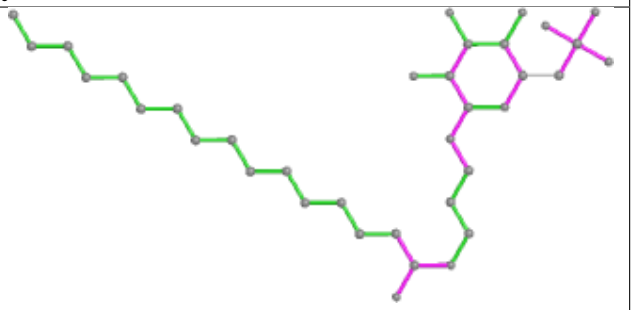
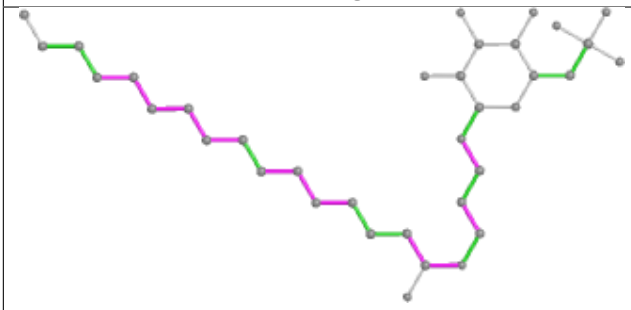


Bond angles



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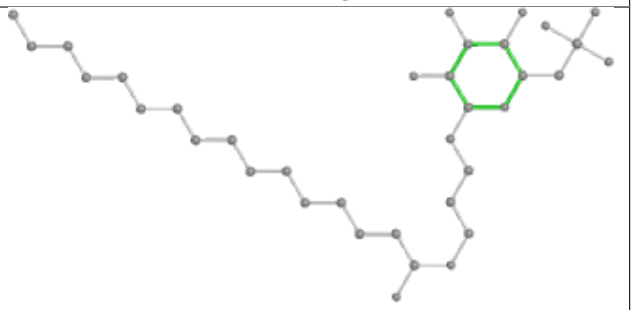
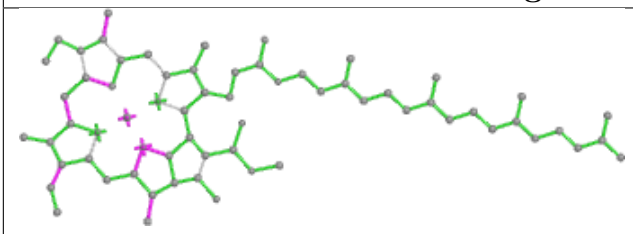


Rings

Ligand CLA B 602



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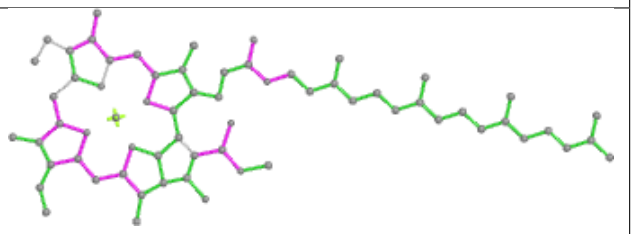
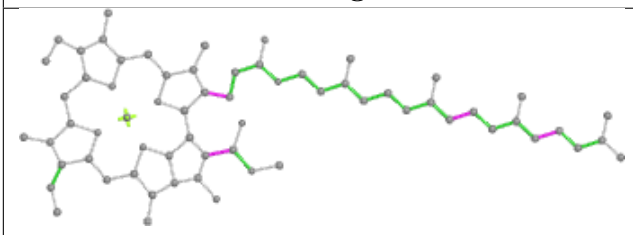


Bond angles



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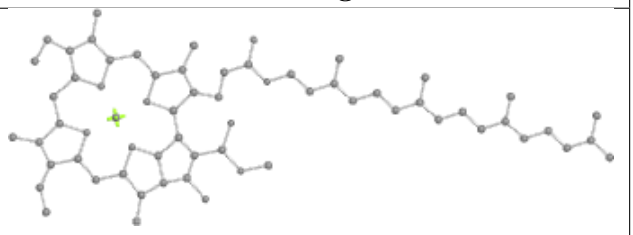
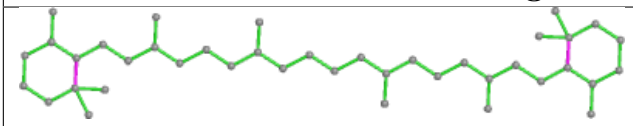


Rings

Ligand BCR d 405



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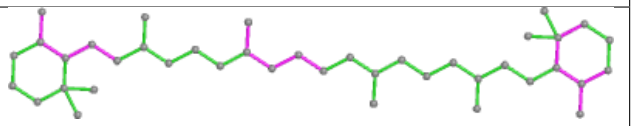
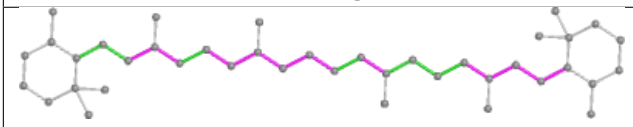


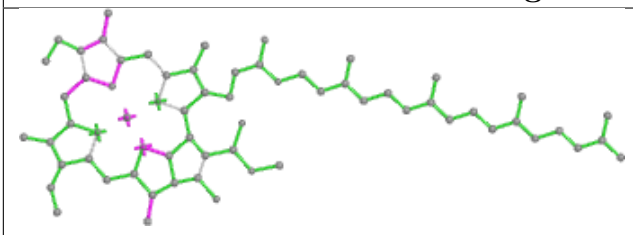
Bond angles



Torsions

Rings

Ligand CLA C 509



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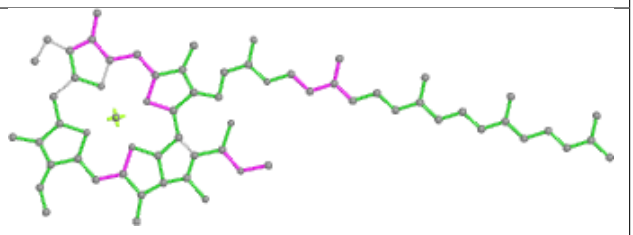

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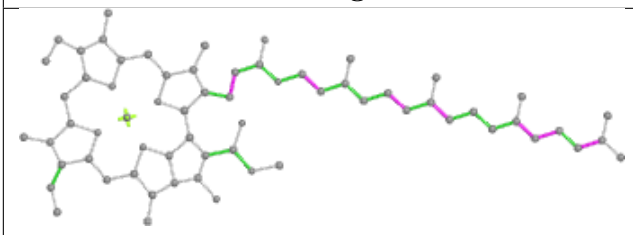

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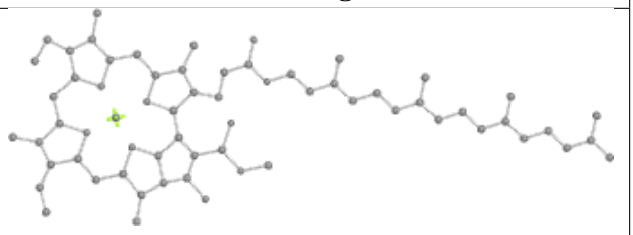
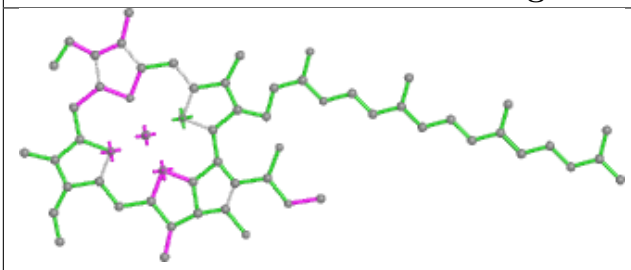


Rings

Ligand CLA b 617



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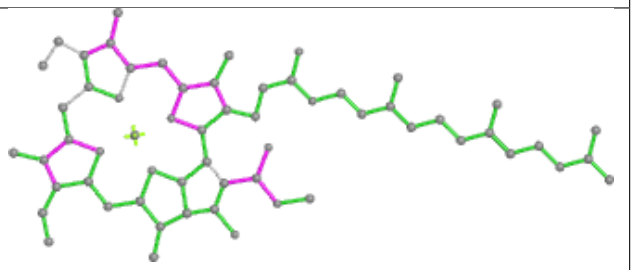

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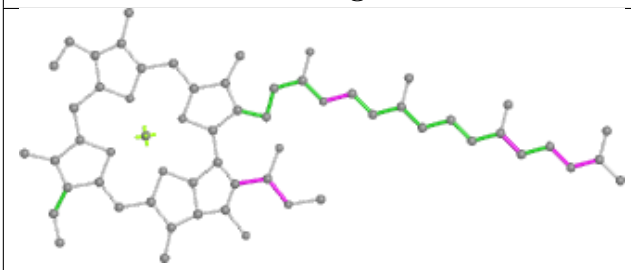

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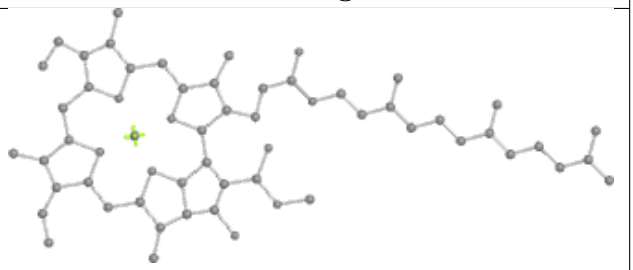
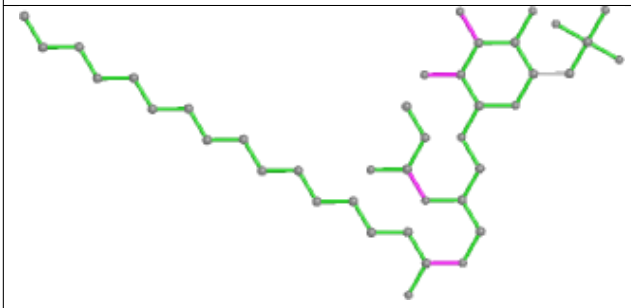


Rings

Ligand SQD f 101



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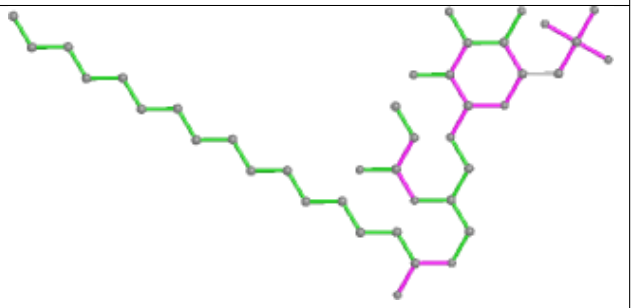
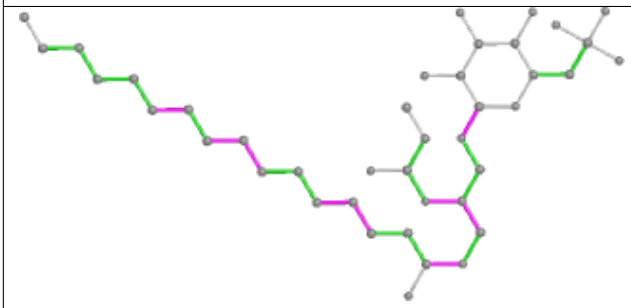


Bond angles



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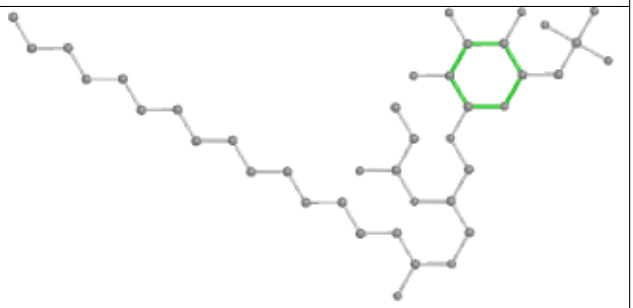
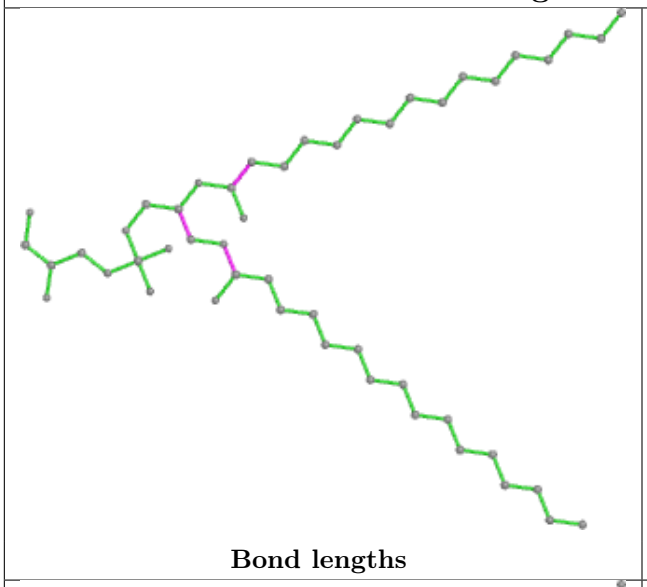
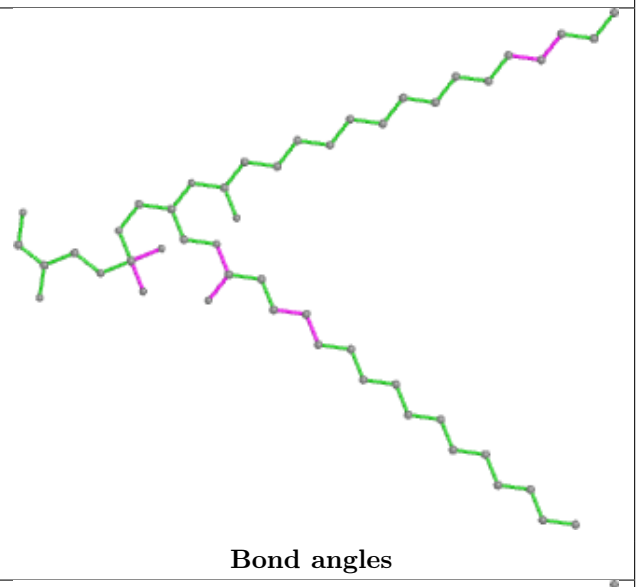


Rings

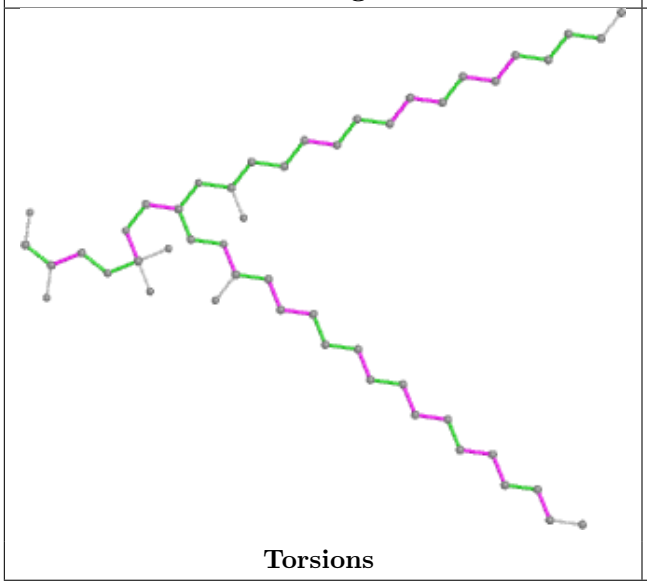
Ligand LHG l 101



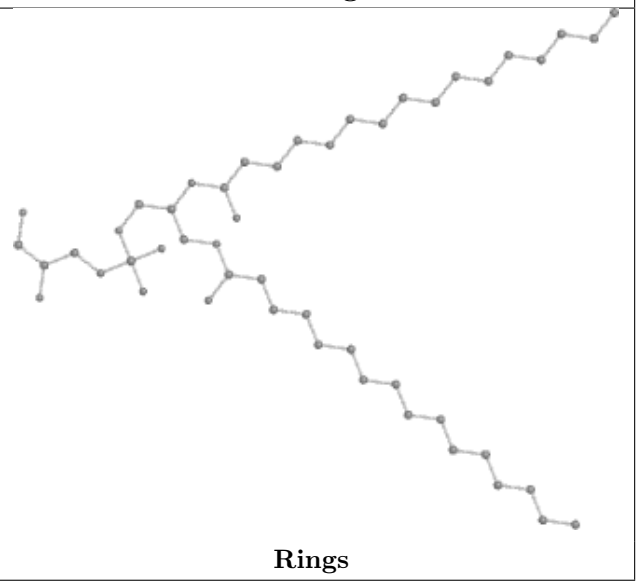
Bond lengths



Bond angles

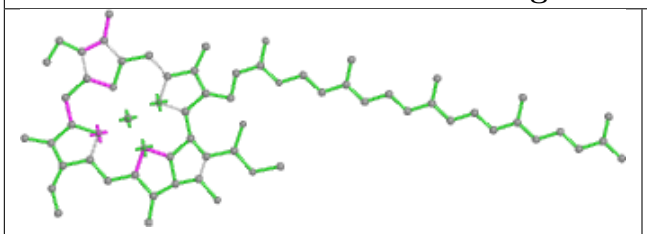


Torsions



Rings

Ligand CLA c 503



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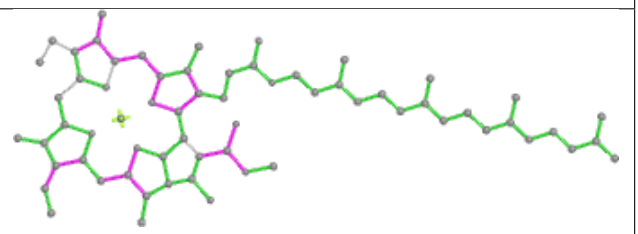
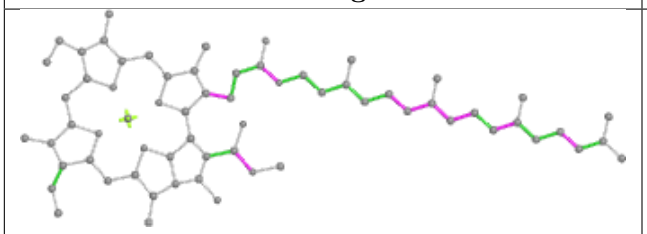


Bond angles



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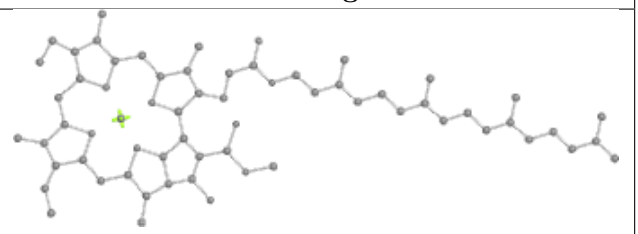
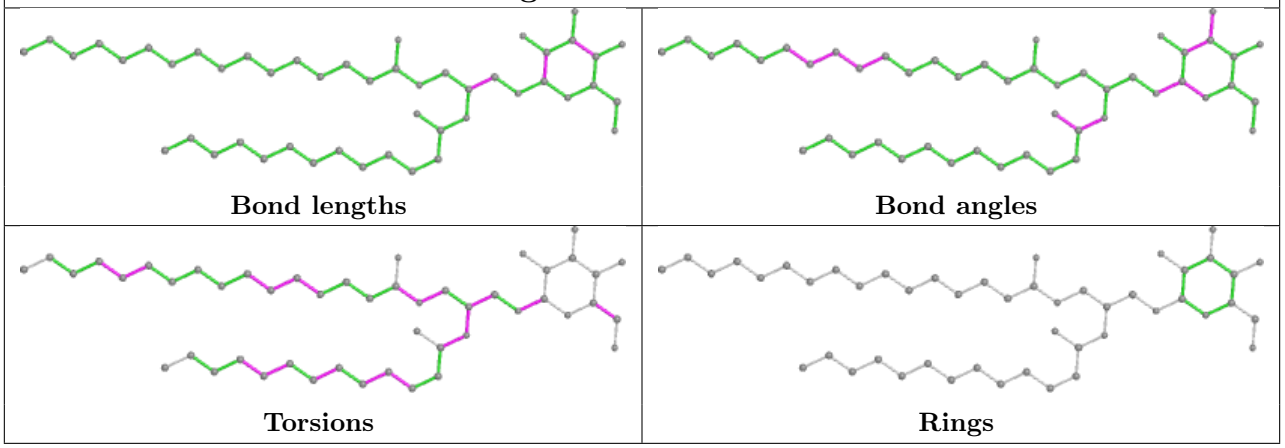
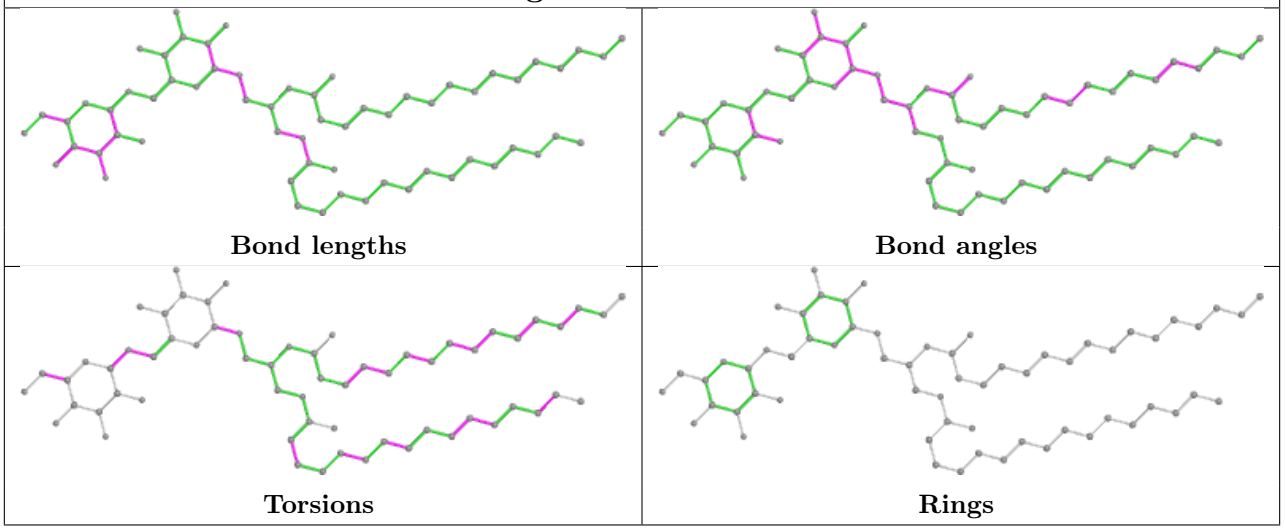


Rings

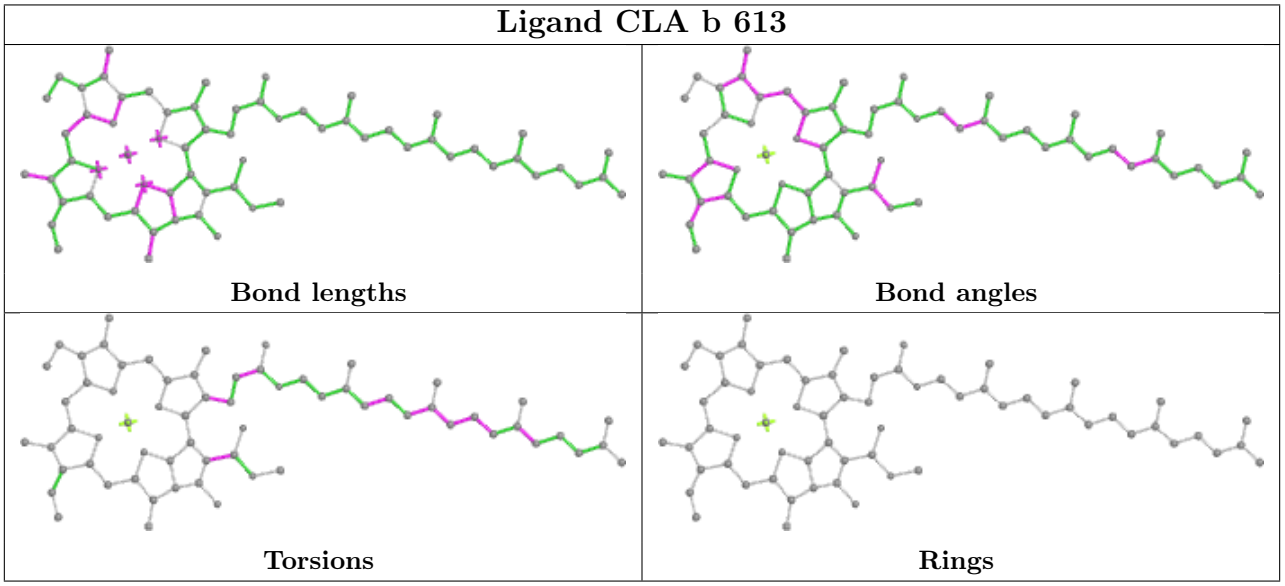
Ligand LMG A 410



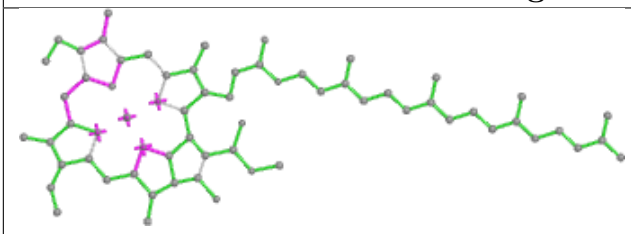
Ligand DGD c 517



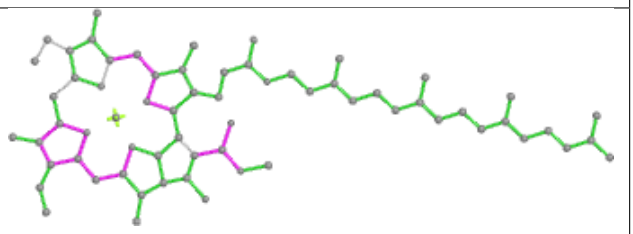
Ligand CLA b 613



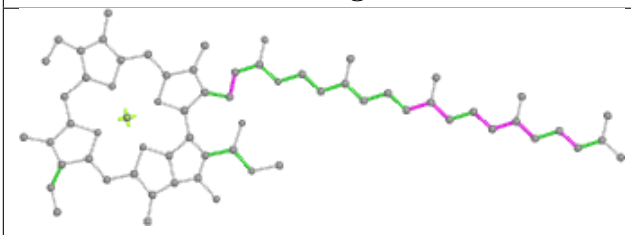
Ligand CLA b 607



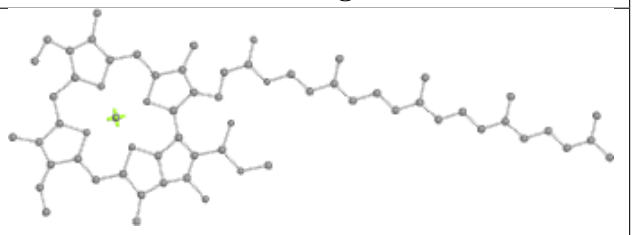
Bond lengths



Bond angles

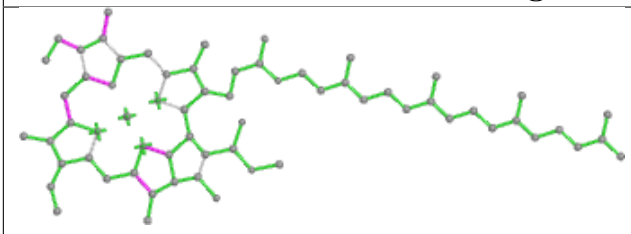


Torsions

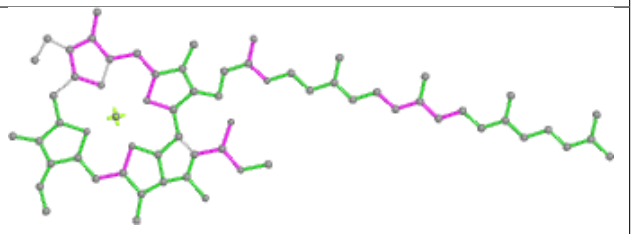


Rings

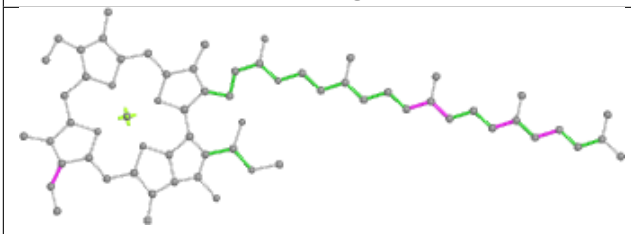
Ligand CLA b 609



Bond lengths



Bond angles



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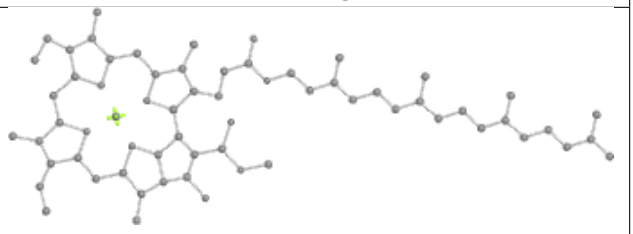
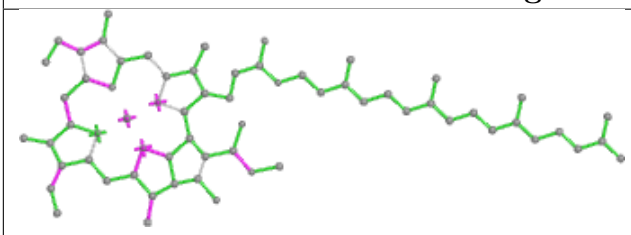
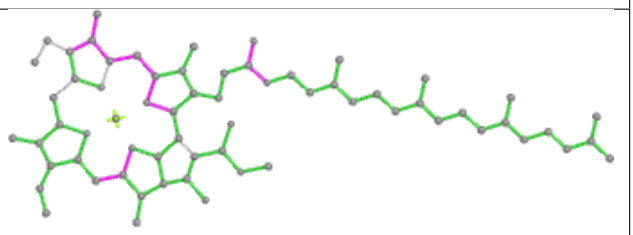


Rings

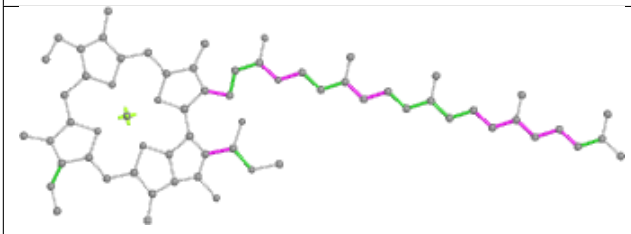
Ligand CLA C 506



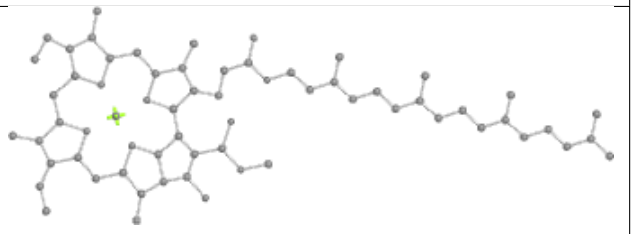
Bond lengths



Bond angles

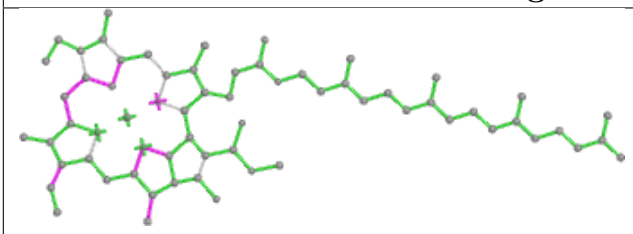


Torsions

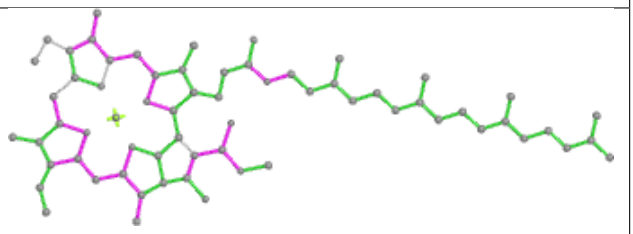


Rings

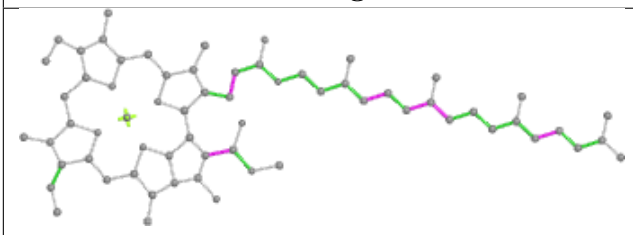
Ligand CLA b 603



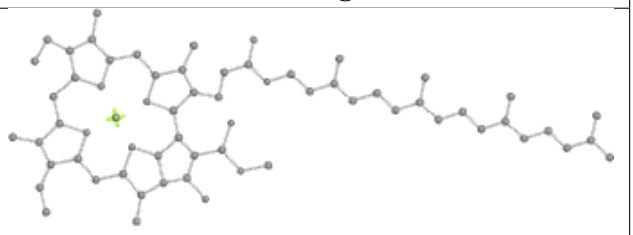
Bond lengths



Bond angles

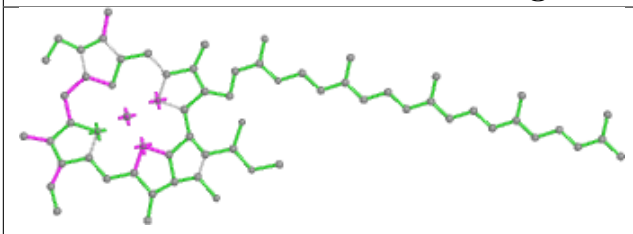


Torsions



Rings

Ligand CLA c 501



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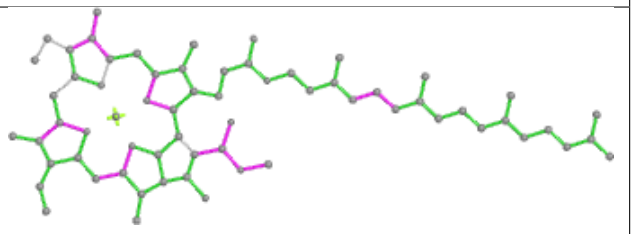
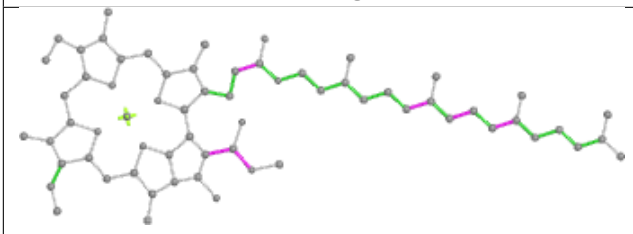


Bond angles



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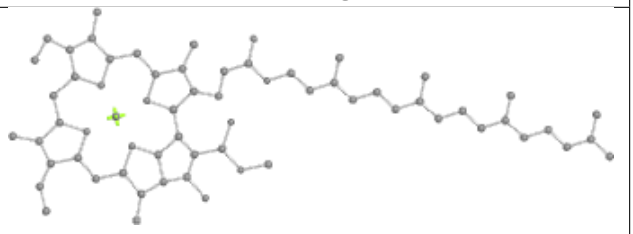
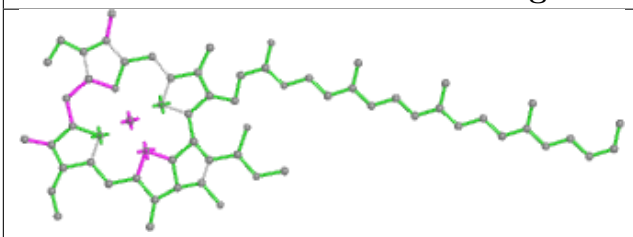
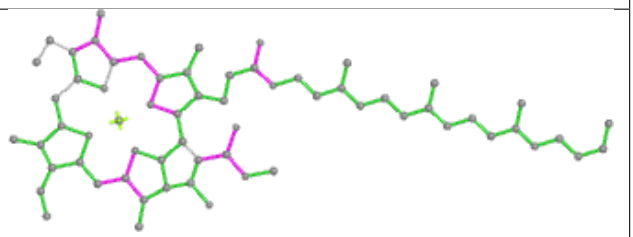


Rings

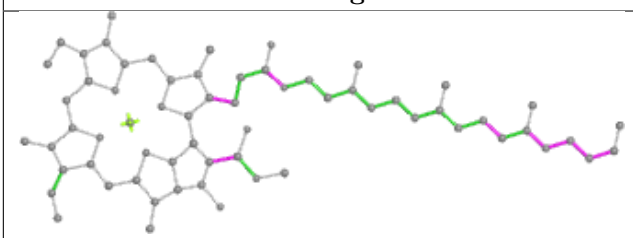
Ligand CLA c 508



Bond lengths



Bond angles



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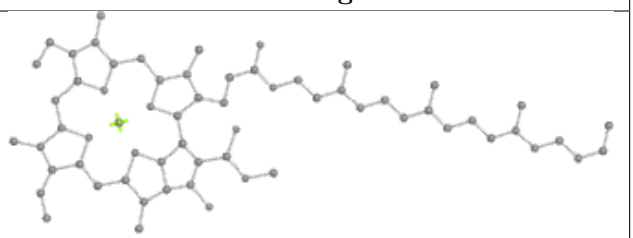
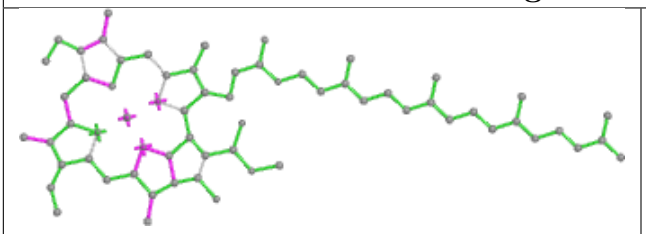
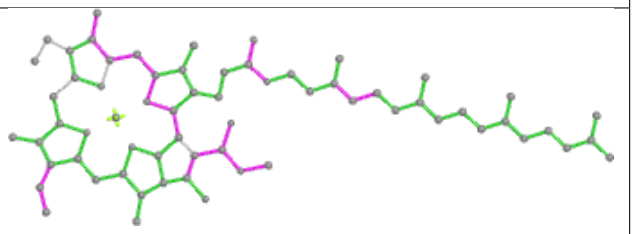


Rings

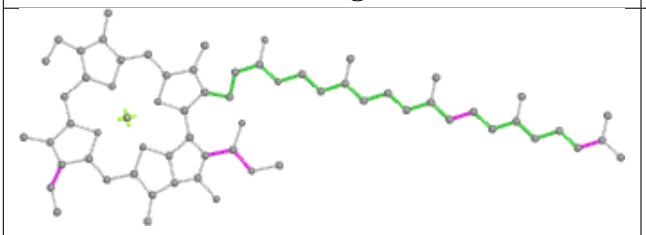
Ligand CLA B 610



Bond lengths



Bond angles



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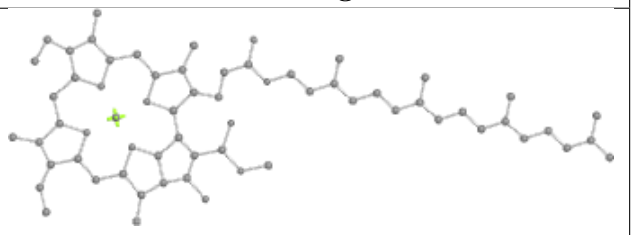
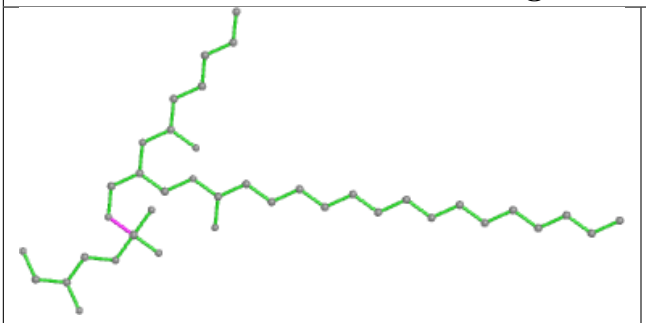


Rings

Ligand LHG d 408



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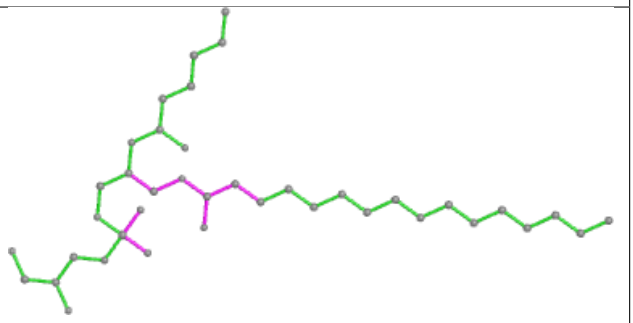
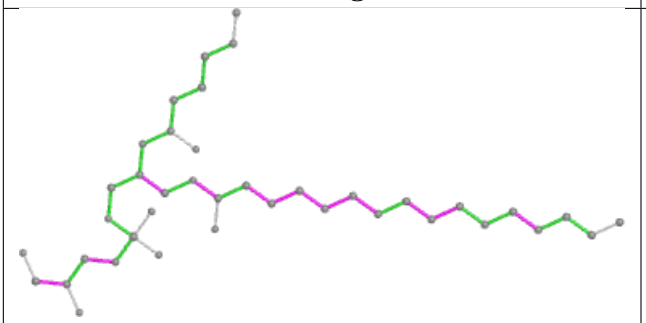


Bond angles



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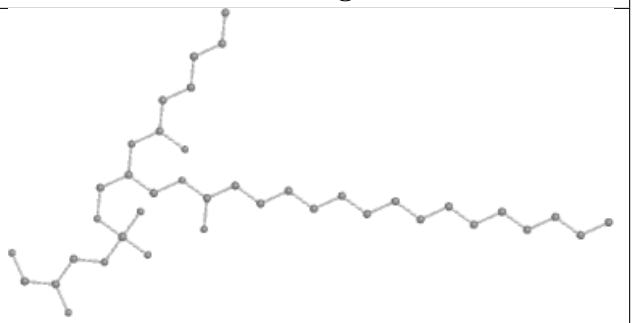
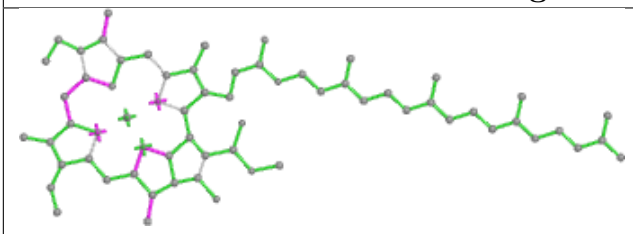


Rings

Ligand CLA c 513



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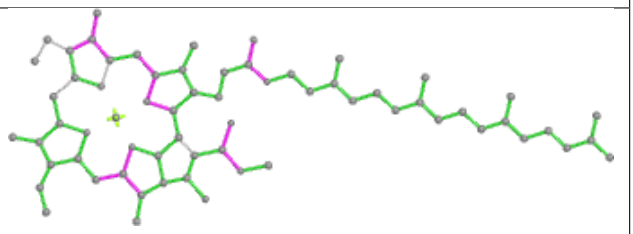
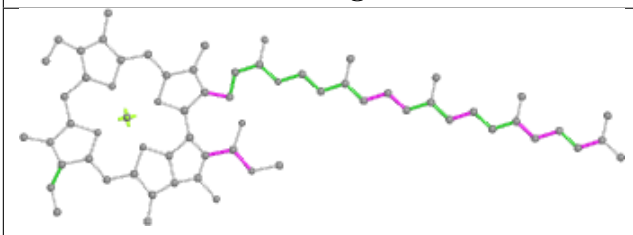


Bond angles



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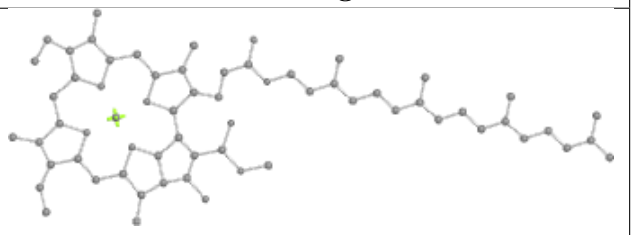
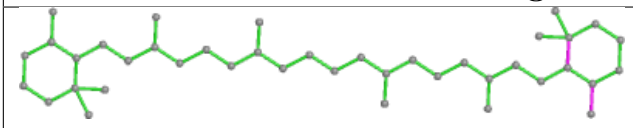
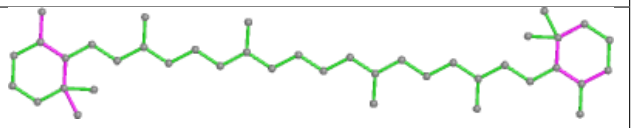


Rings

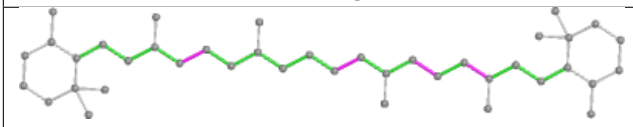
Ligand BCR c 521



Bond lengths



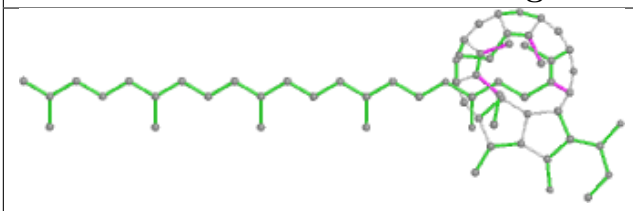
Bond angles



Torsions

Rings

Ligand PHO a 406



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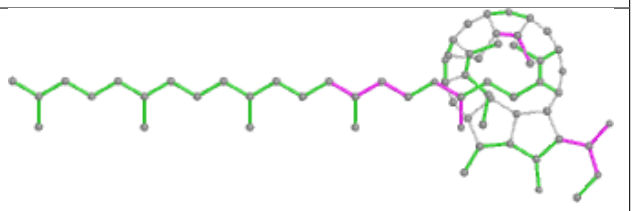
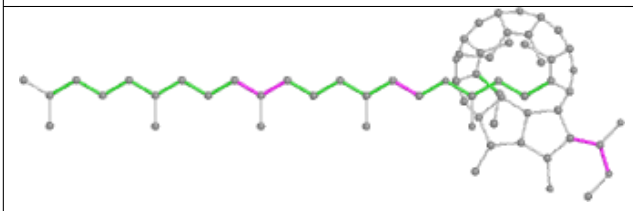


Bond angles



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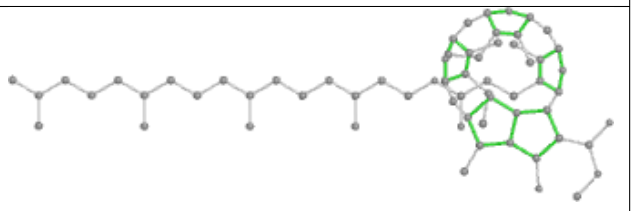
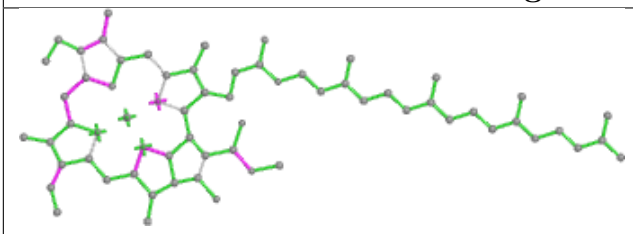


Rings

Ligand CLA B 607



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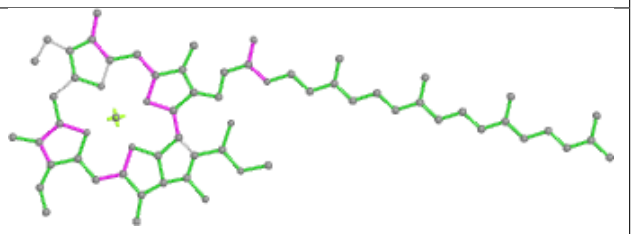
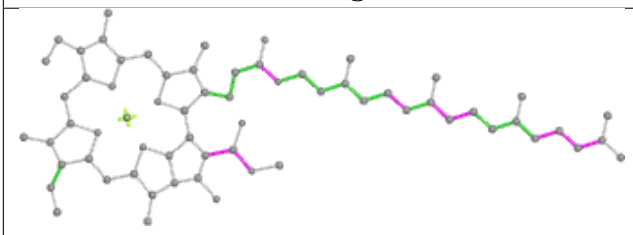


Bond angles



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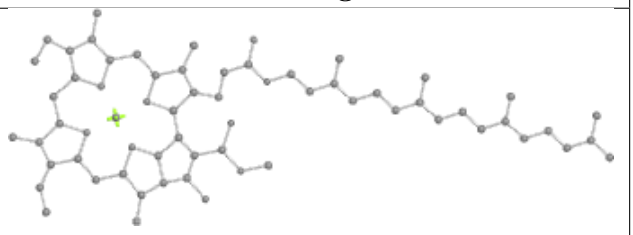
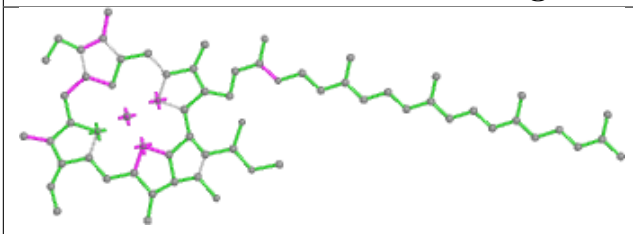
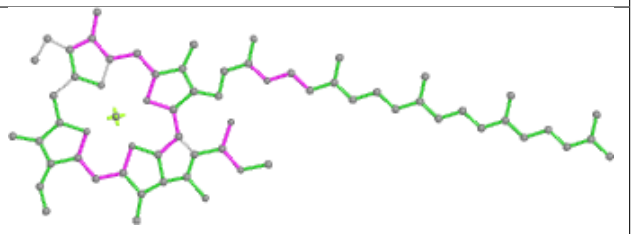


Rings

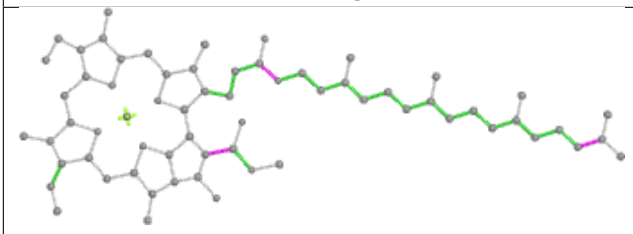
Ligand CLA c 502



Bond lengths



Bond angles



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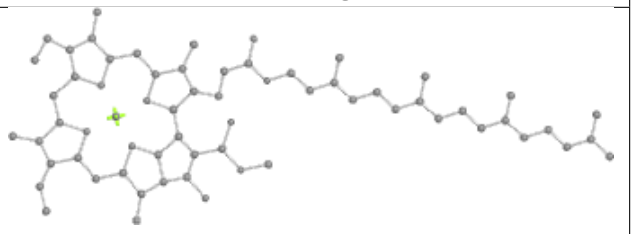
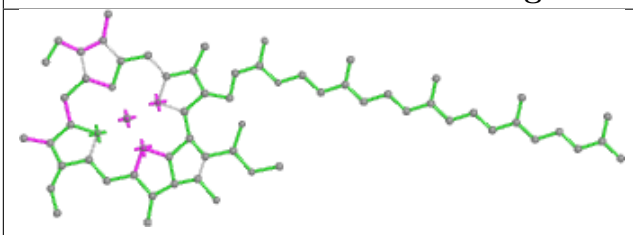
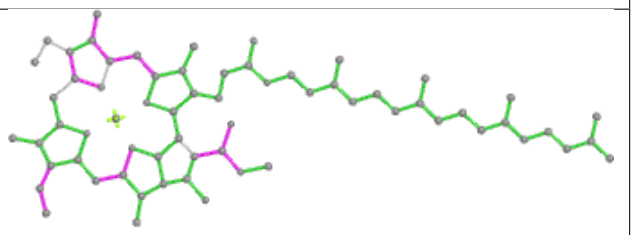


Rings

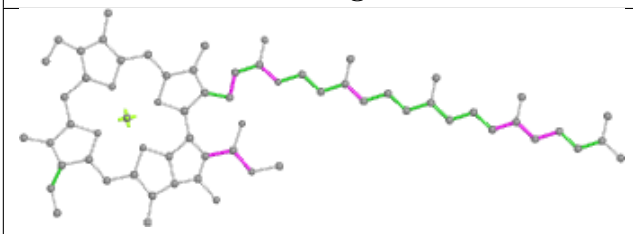
Ligand CLA B 614



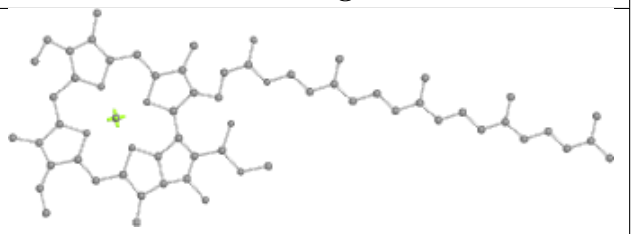
Bond lengths



Bond angles

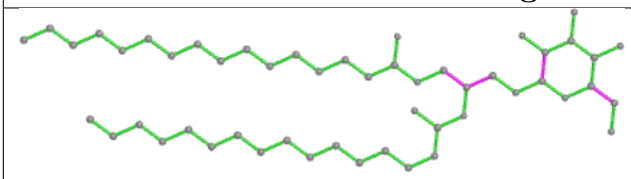


Torsions

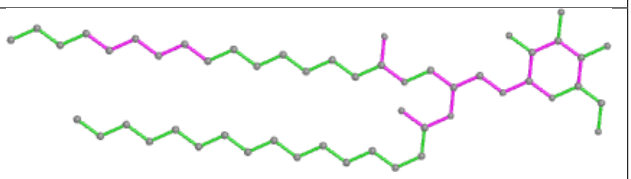


Rings

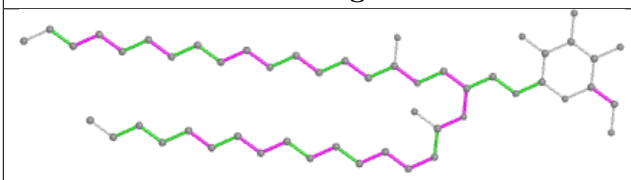
Ligand LMG B 620



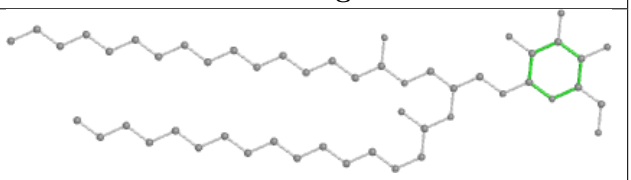
Bond lengths



Bond angles

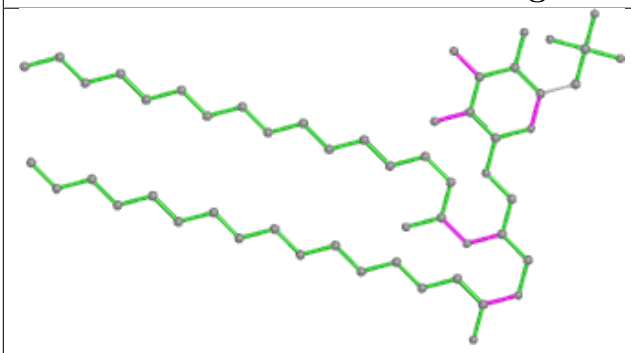


Torsions

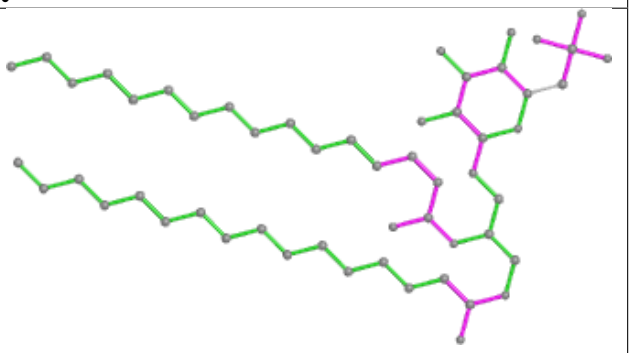


Rings

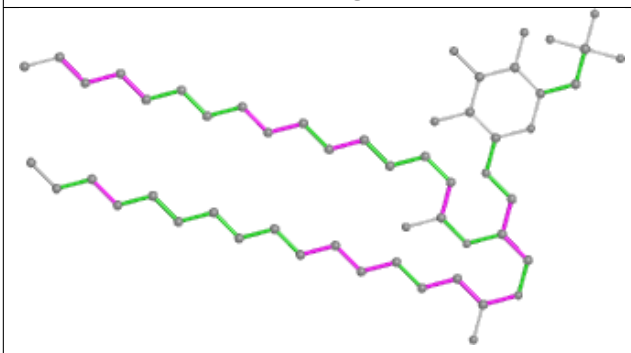
Ligand SQD a 411



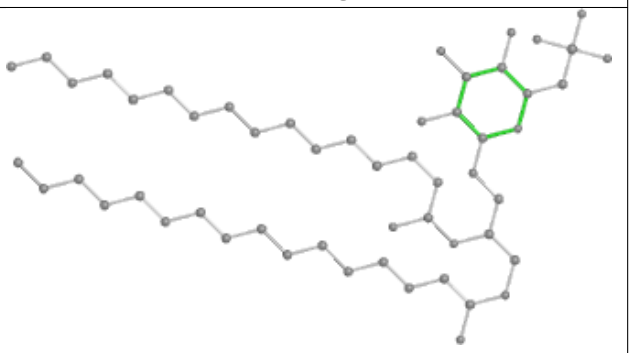
Bond lengths



Bond angles

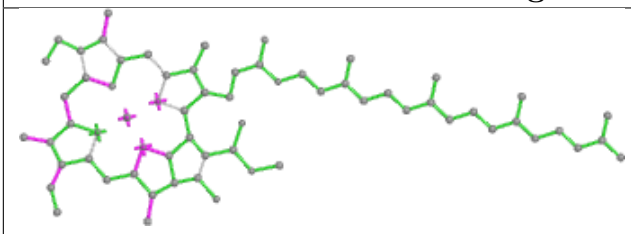


Torsions

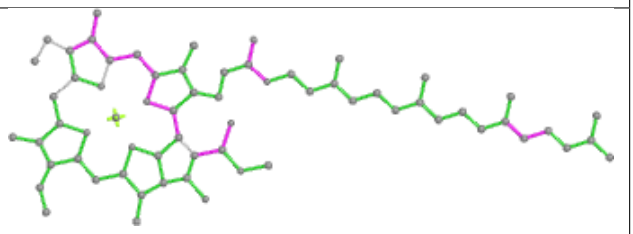


Rings

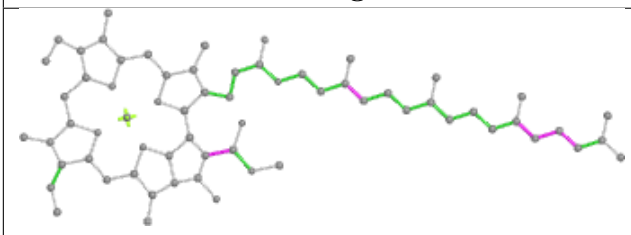
Ligand CLA b 610



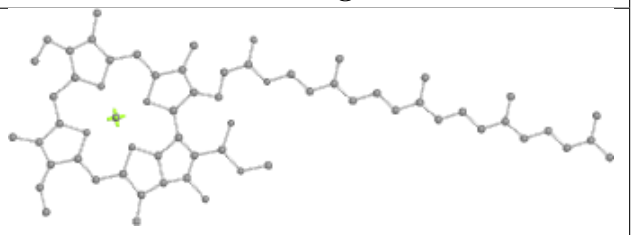
Bond lengths



Bond angles

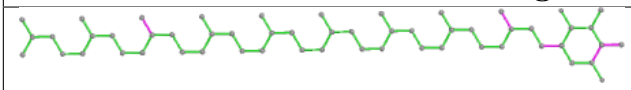


Torsions

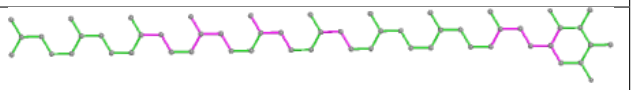


Rings

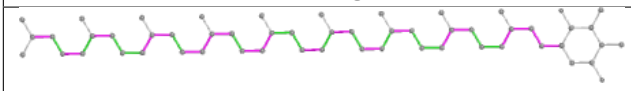
Ligand PL9 a 409



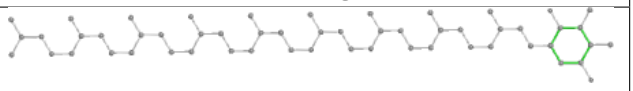
Bond lengths



Bond angles

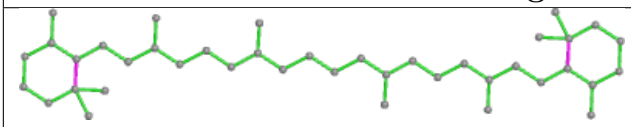


Torsions

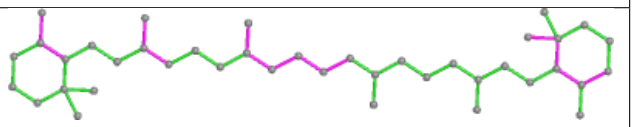


Rings

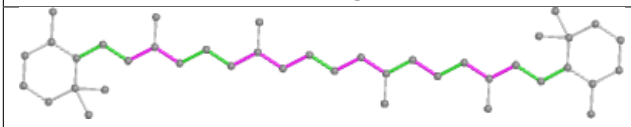
Ligand BCR c 514



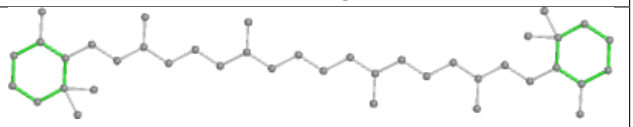
Bond lengths



Bond angles

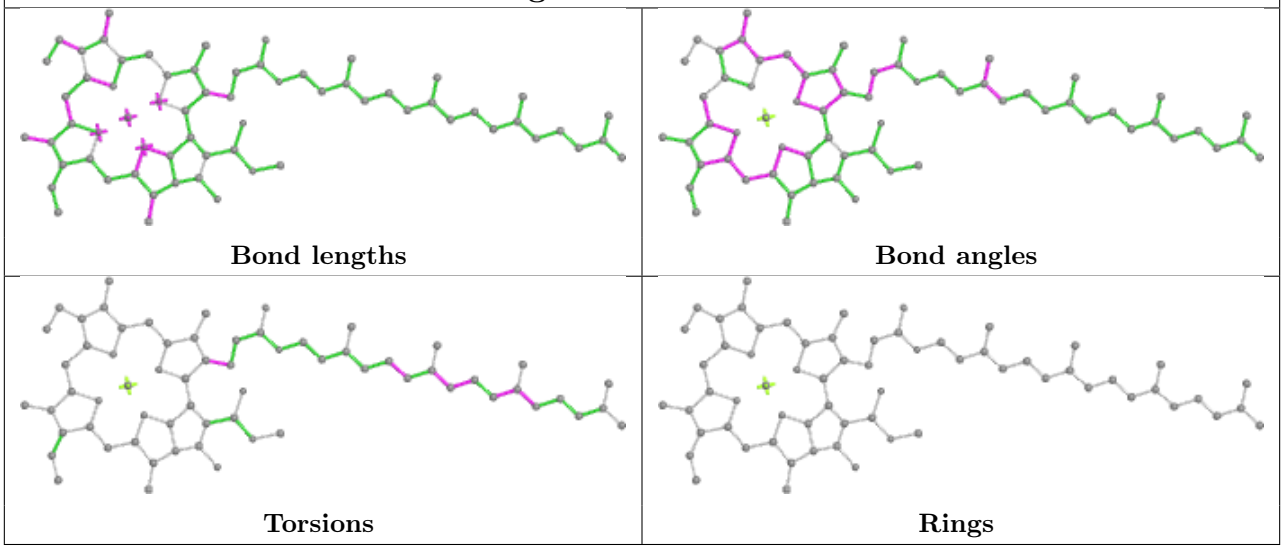


Torsions

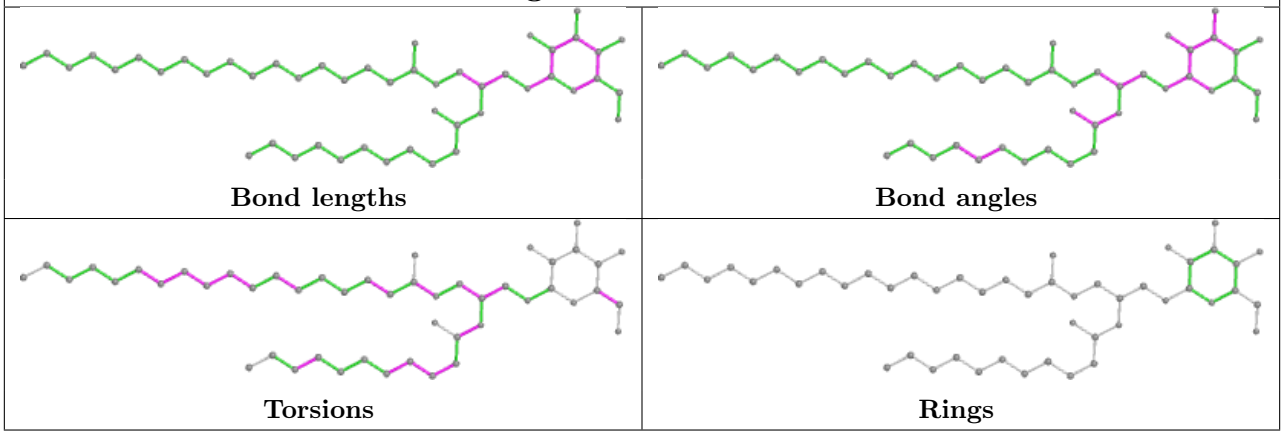


Rings

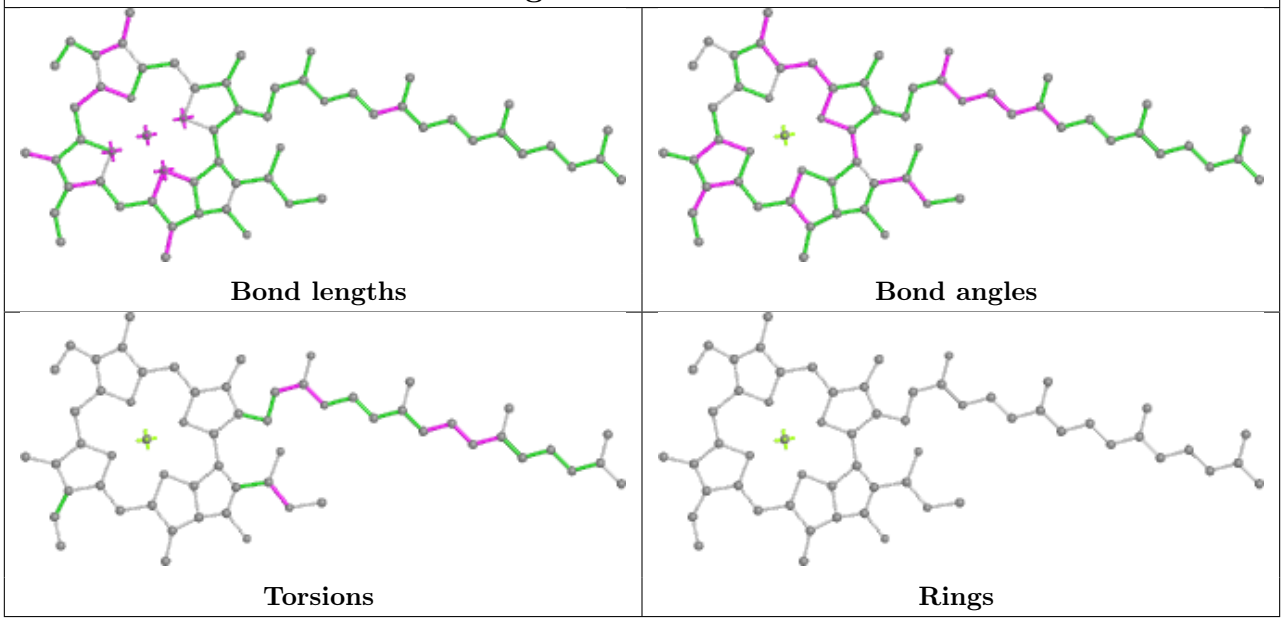
Ligand CLA b 616



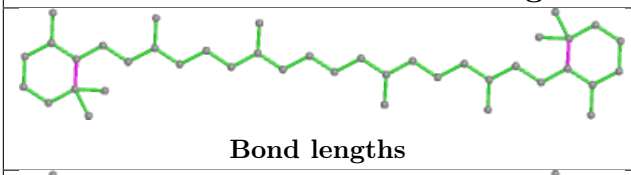
Ligand LMG c 522



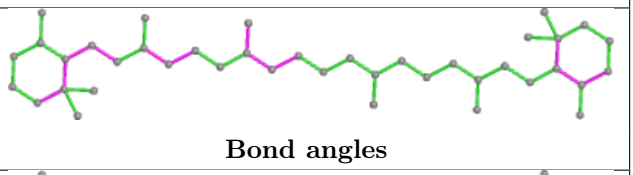
Ligand CLA B 616



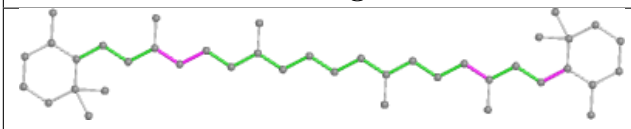
Ligand BCR b 619



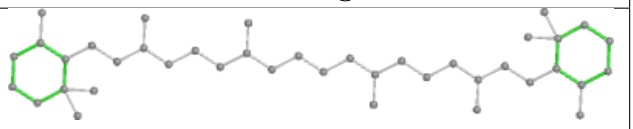
Bond lengths



Bond angles

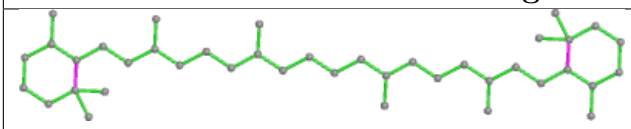


Torsions

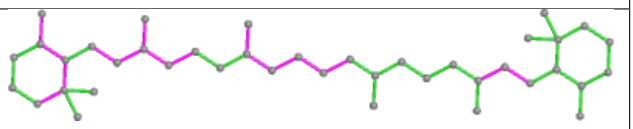


Rings

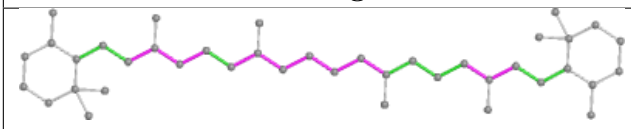
Ligand BCR C 514



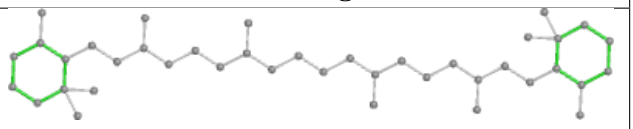
Bond lengths



Bond angles

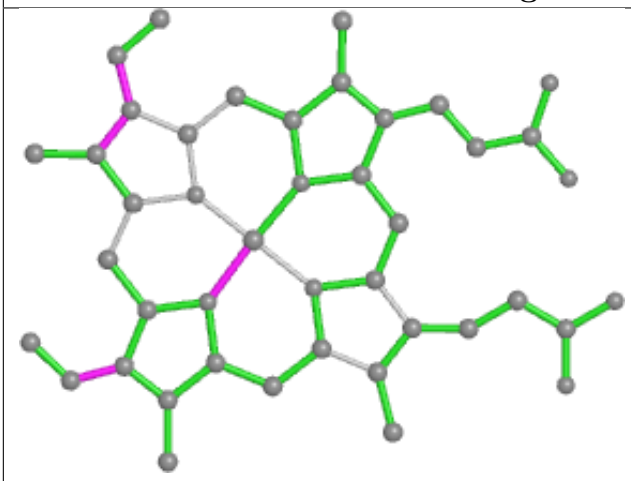


Torsions

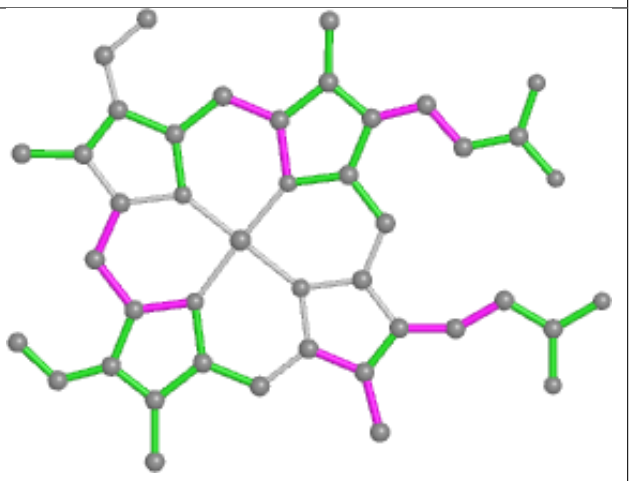


Rings

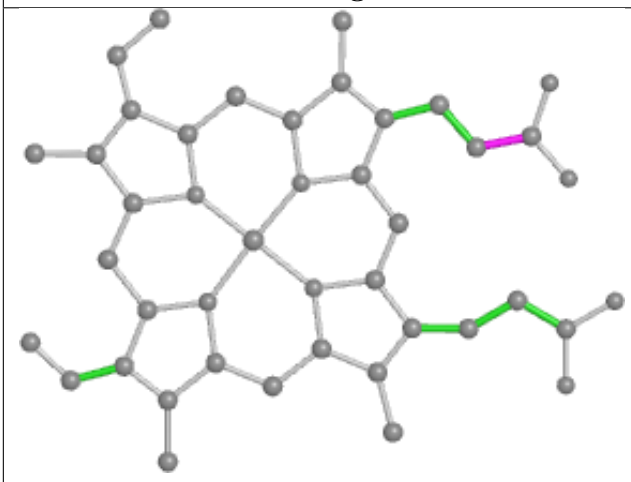
Ligand HEM E 102



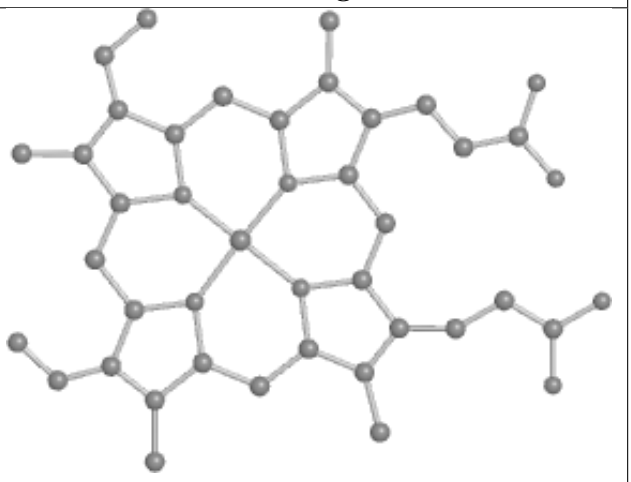
Bond lengths



Bond angles

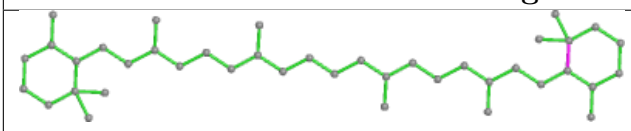


Torsions

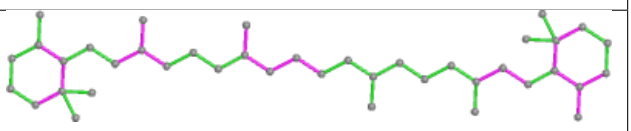


Rings

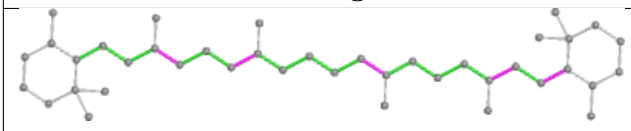
Ligand BCR H 101



Bond lengths



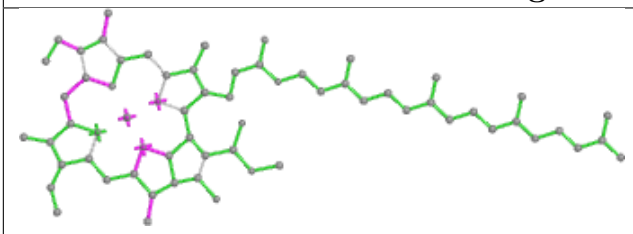
Bond angles



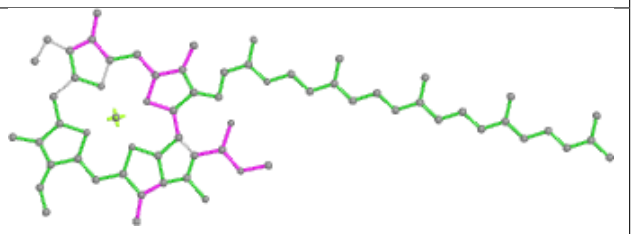
Torsions

Rings

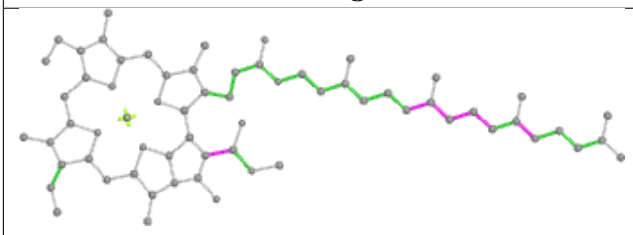
Ligand CLA a 405



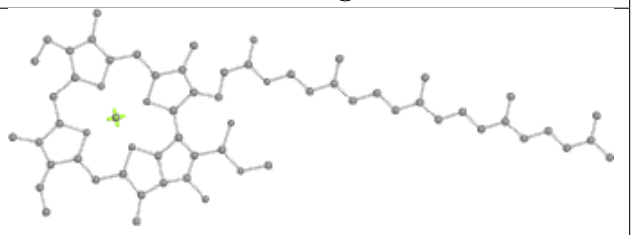
Bond lengths



Bond angles

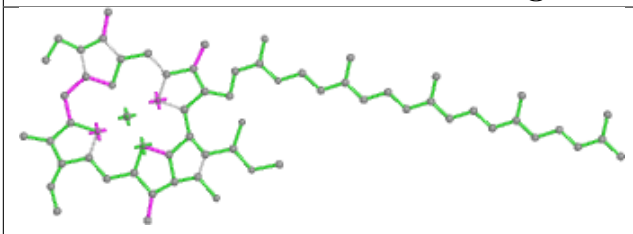


Torsions



Rings

Ligand CLA b 612



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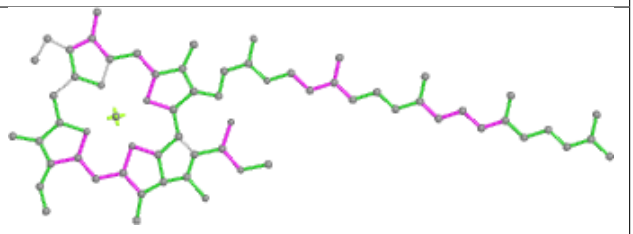
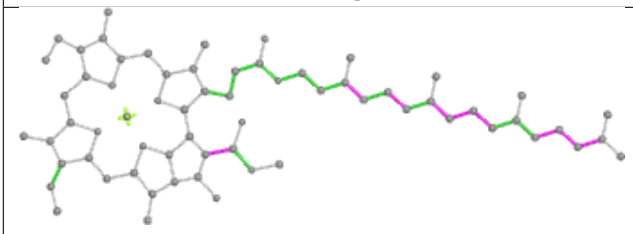


Bond angles



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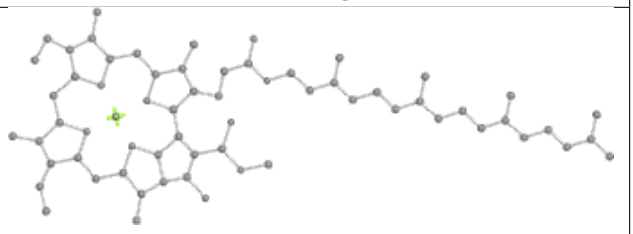
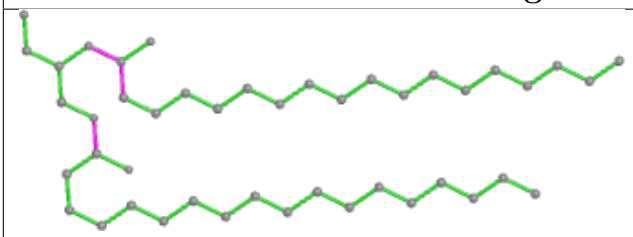
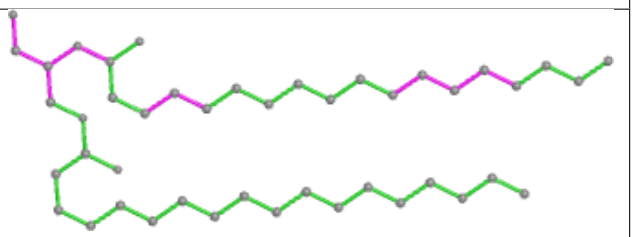


Rings

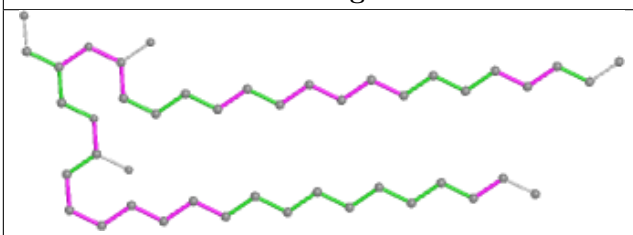
Ligand DGD a 413



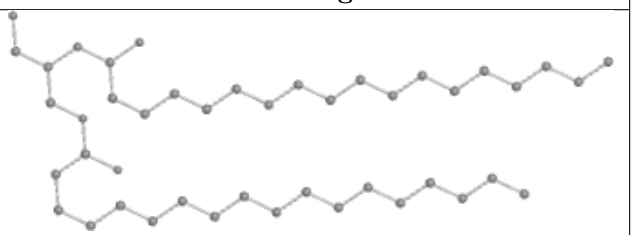
Bond lengths



Bond angles

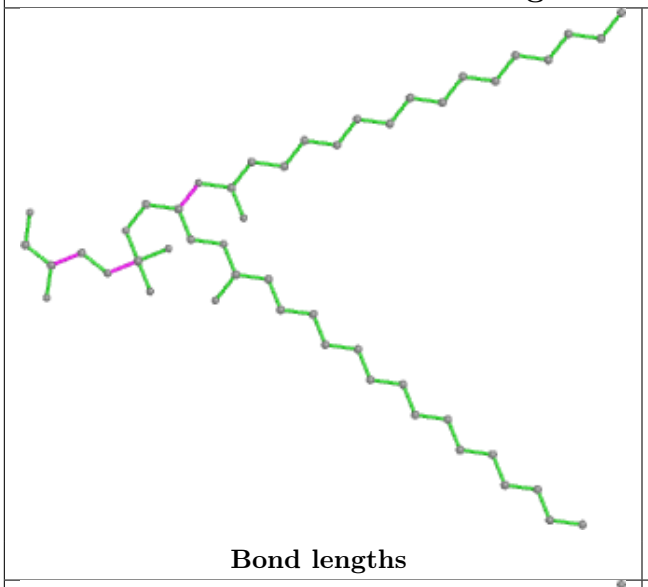


Torsions

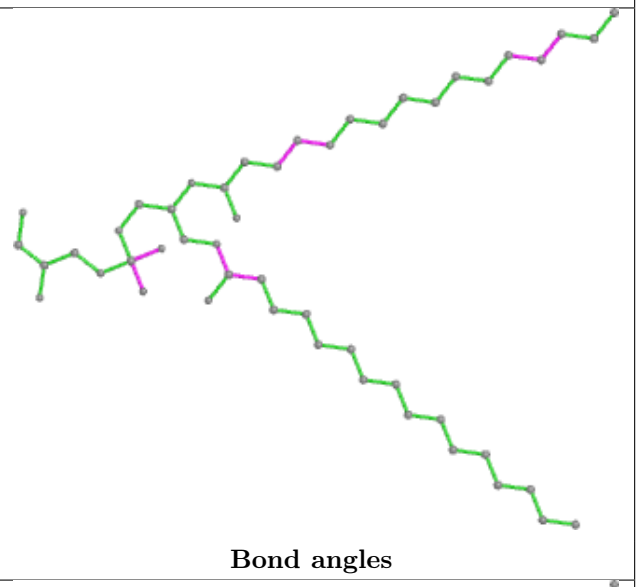


Rings

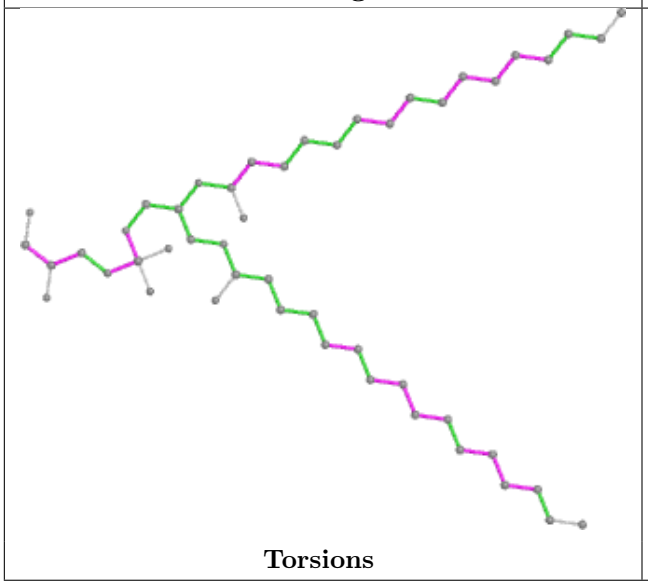
Ligand LHG d 407



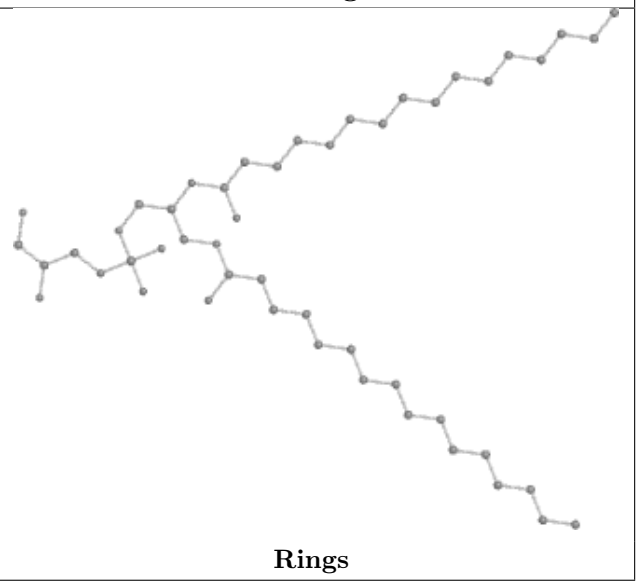
Bond lengths



Bond angles

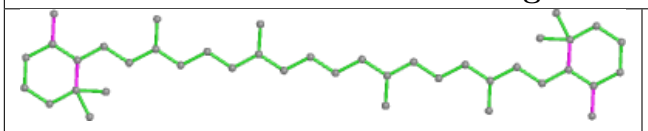


Torsions

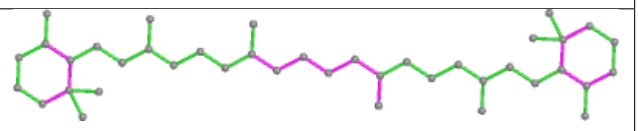


Rings

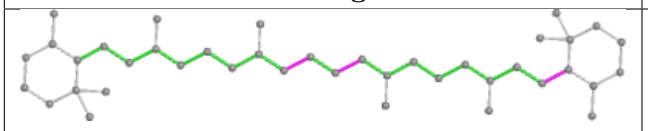
Ligand BCR C 515



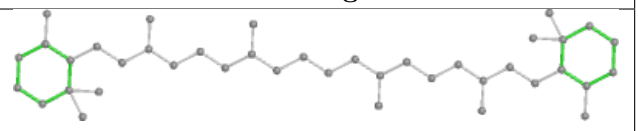
Bond lengths



Bond angles

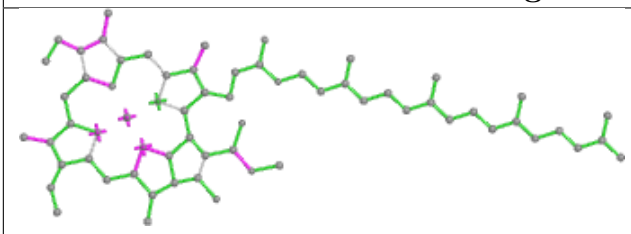


Torsions

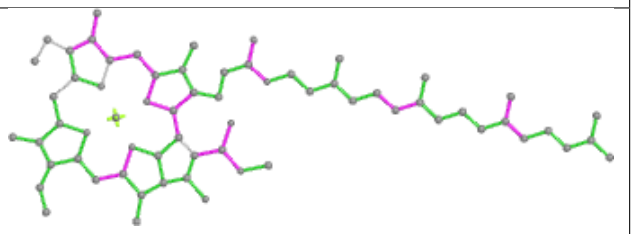


Rings

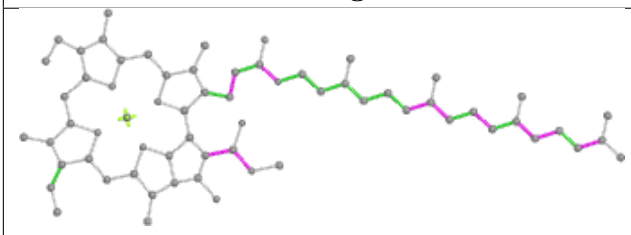
Ligand CLA B 603



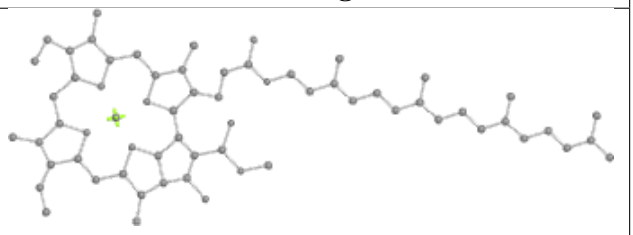
Bond lengths



Bond angles

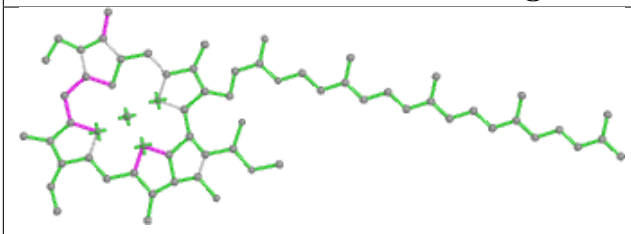


Torsions



Rings

Ligand CLA B 612



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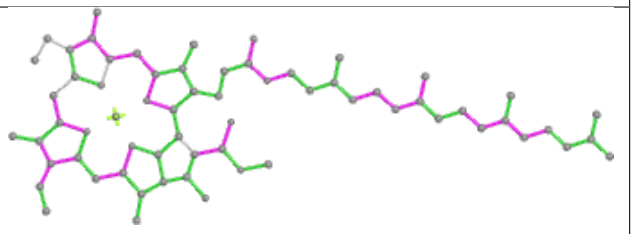
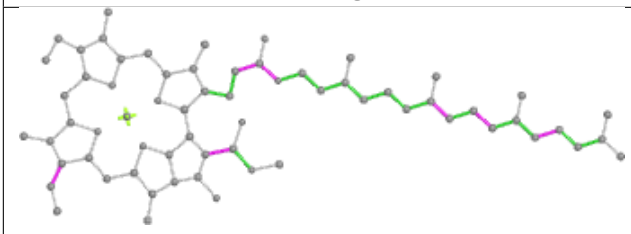
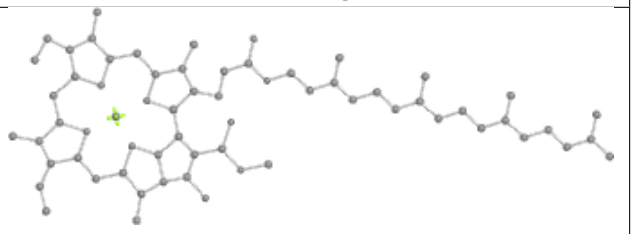


Bond angles

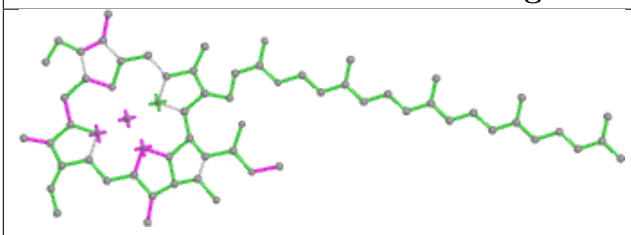


Torsions



Rings

Ligand CLA B 605



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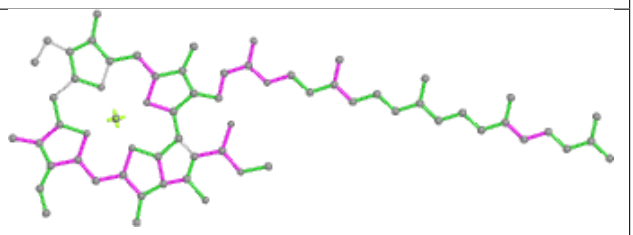
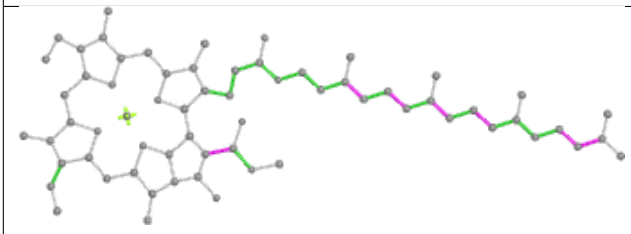


Bond angles



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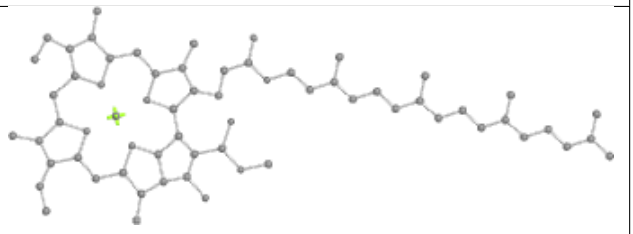
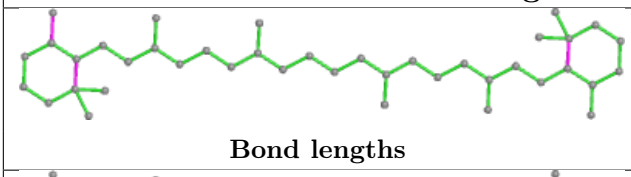


Rings

Ligand BCR B 617



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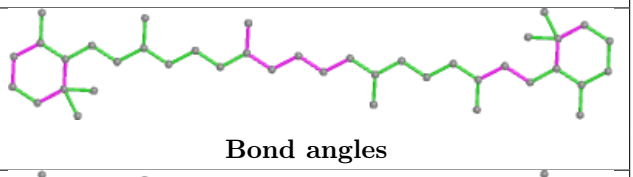
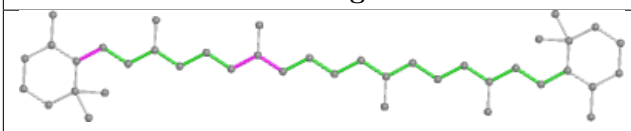


Bond angles



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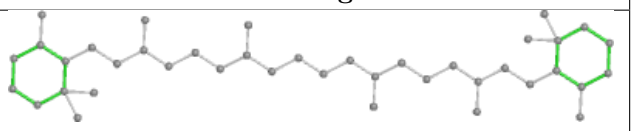
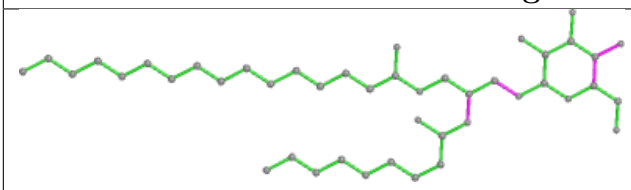


Rings

Ligand LMG d 409



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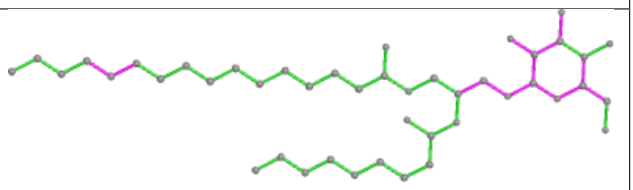
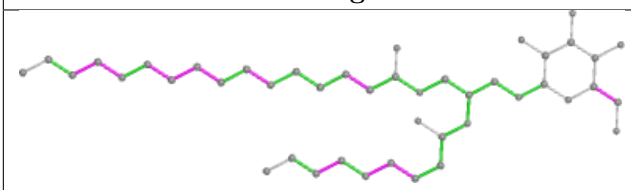


Bond angles



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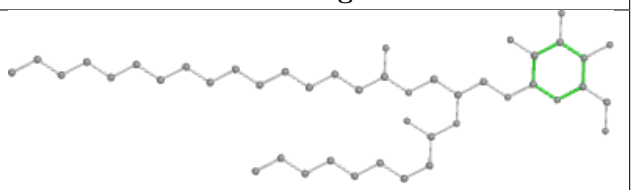
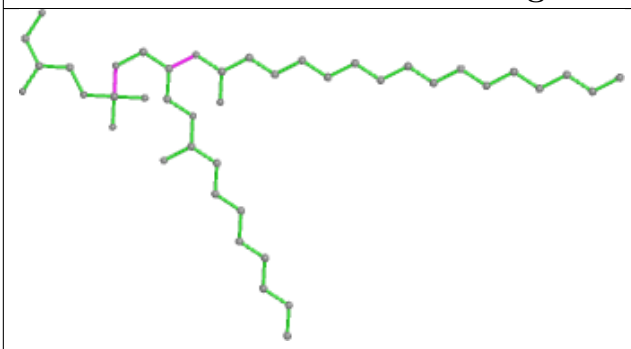


Rings

Ligand LHG e 101



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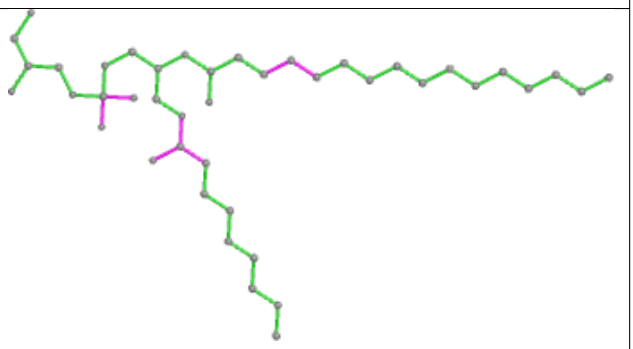
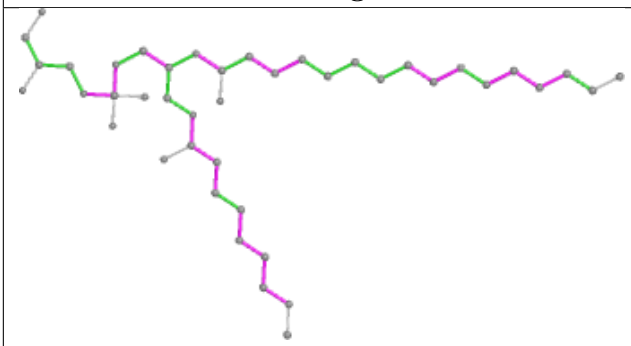


Bond angles



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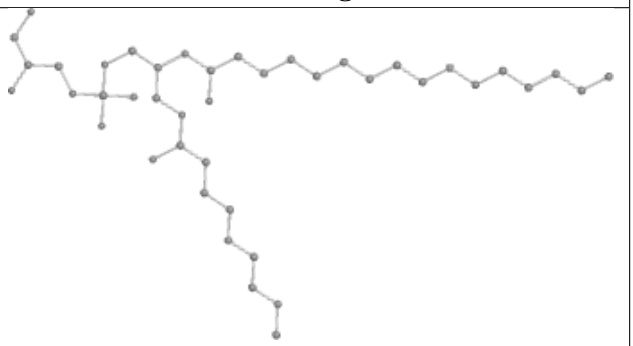
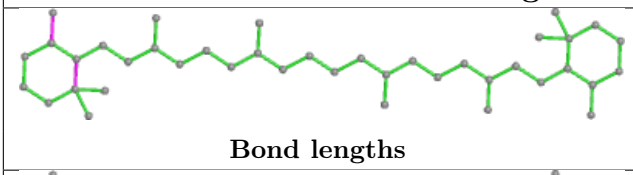


Rings

Ligand BCR A 408



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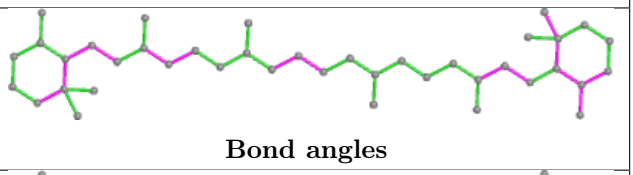
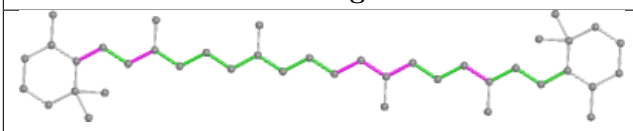


Bond angles



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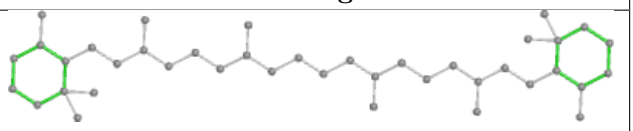
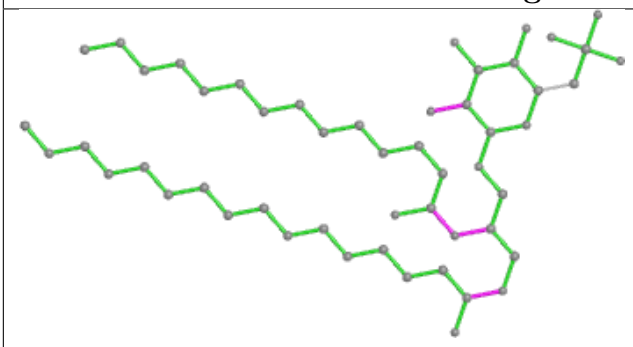


Rings

Ligand SQD A 411



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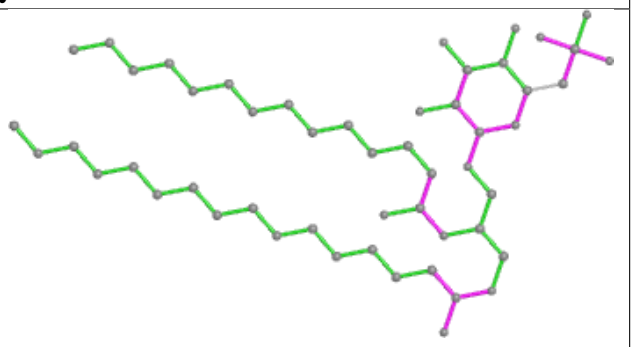
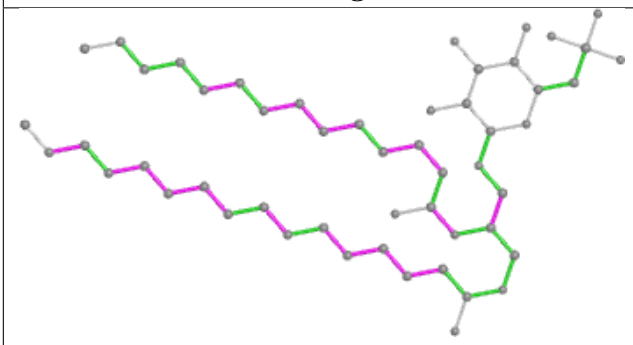


Bond angles



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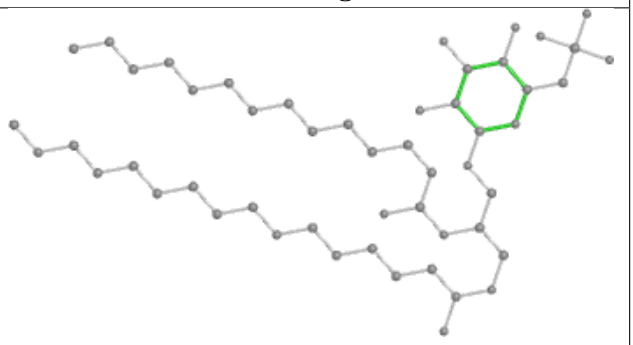
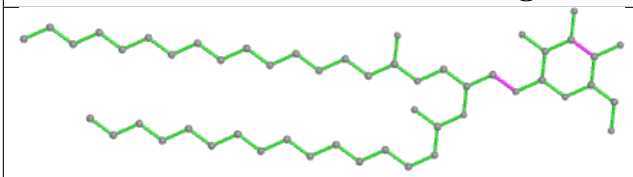


Rings

Ligand LMG m 101



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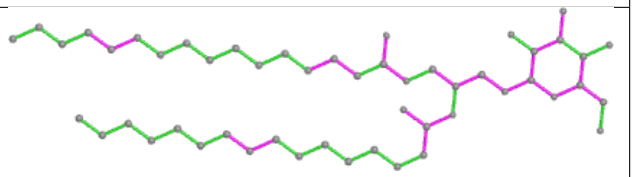
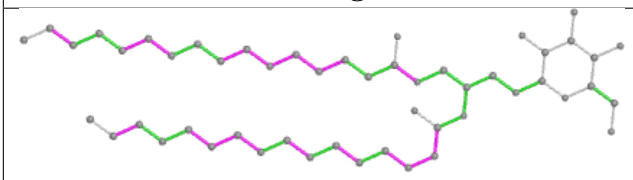


Bond angles



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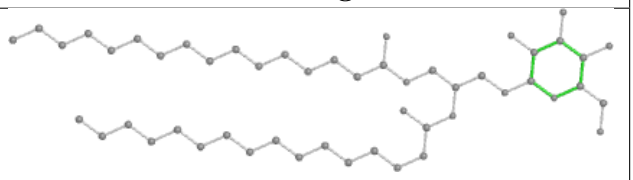
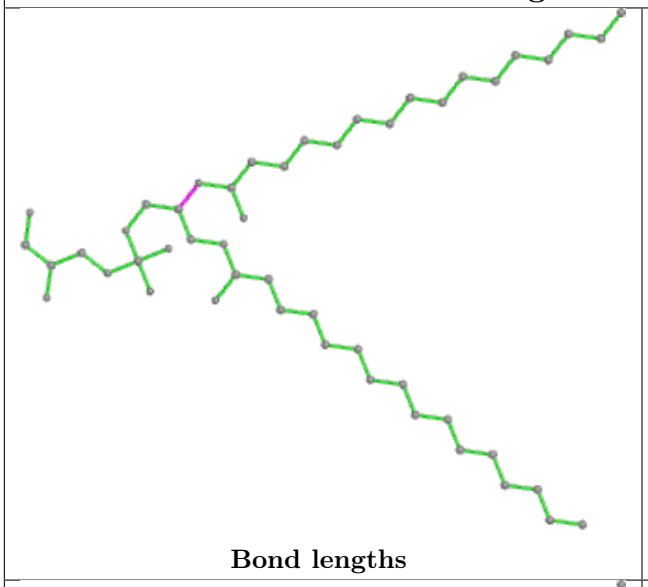
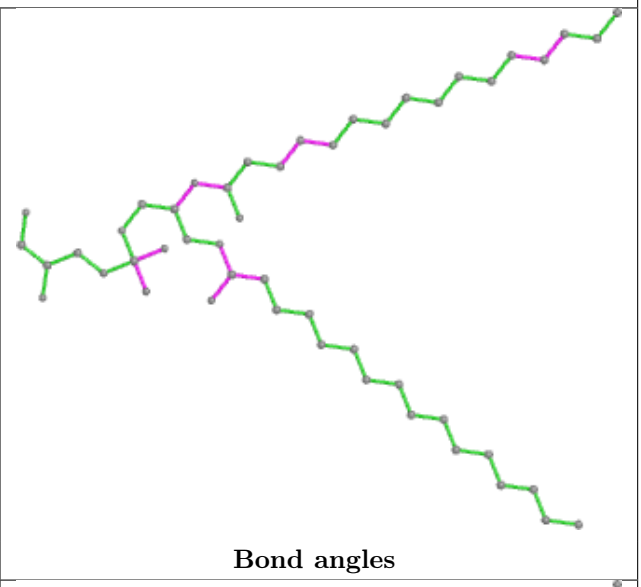


Rings

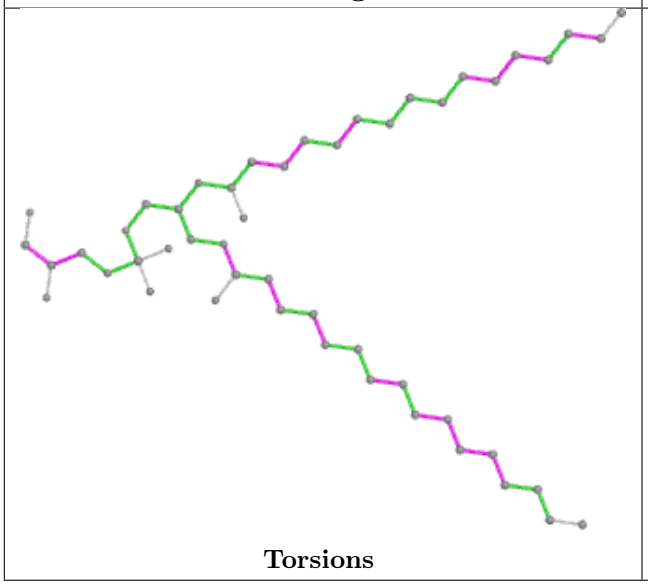
Ligand LHG a 410



Bond lengths



Bond angles



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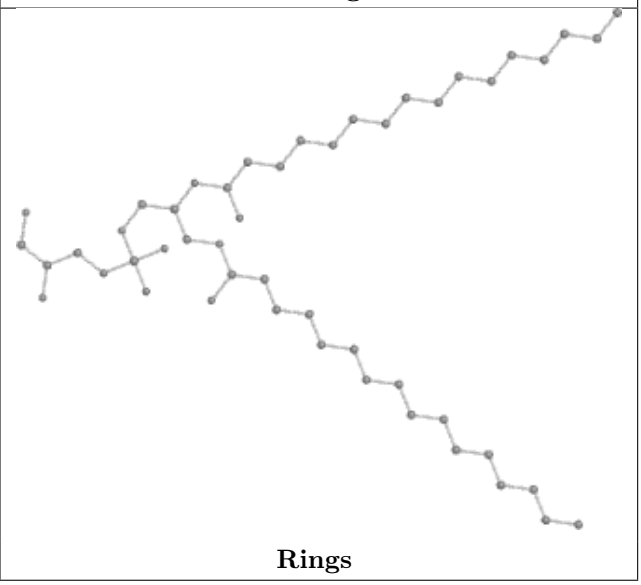
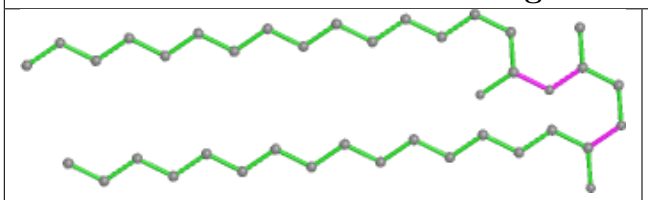


Rings

Ligand SQD A 412



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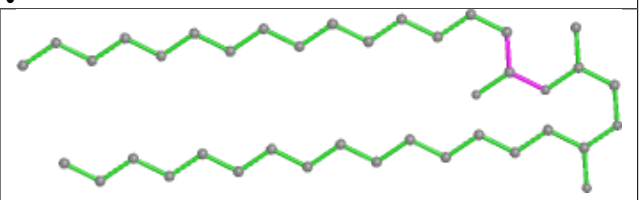
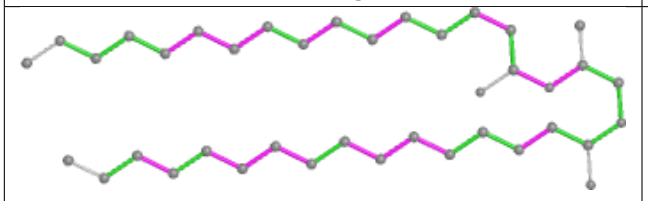


Bond angles



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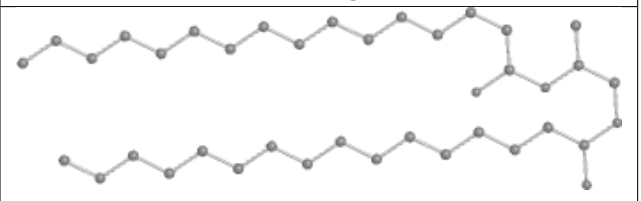
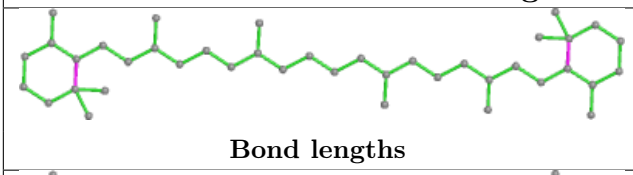


Rings

Ligand BCR K 101



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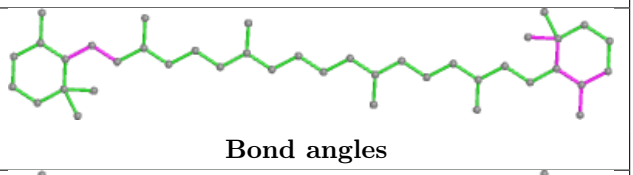
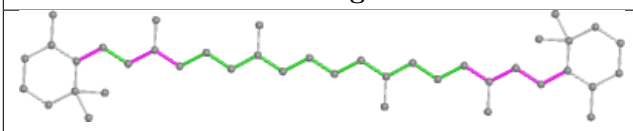


Bond angles



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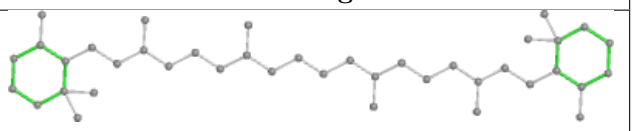
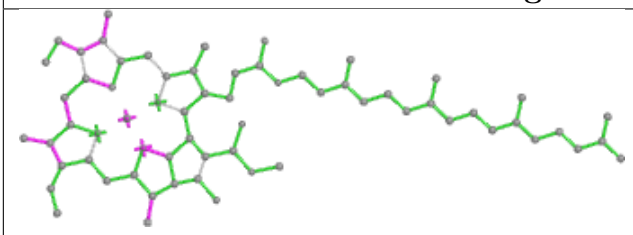
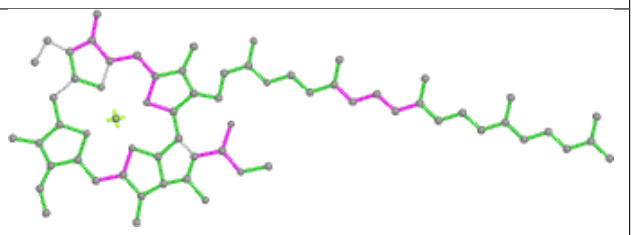


Rings

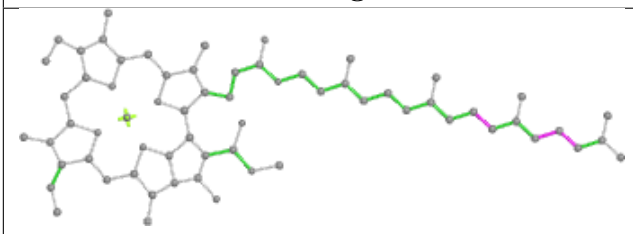
Ligand CLA B 608



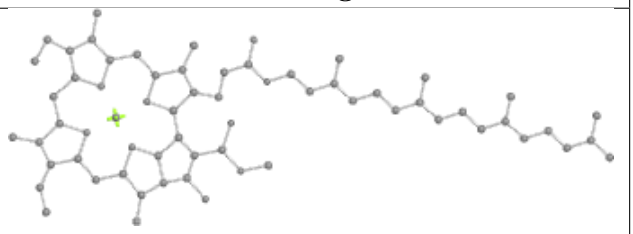
Bond lengths



Bond angles

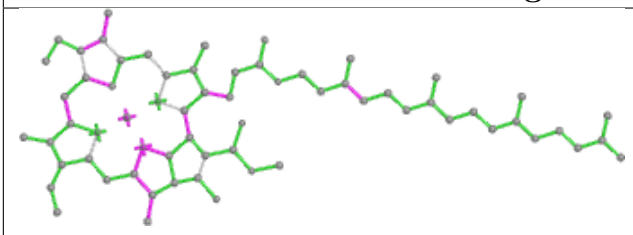


Torsions

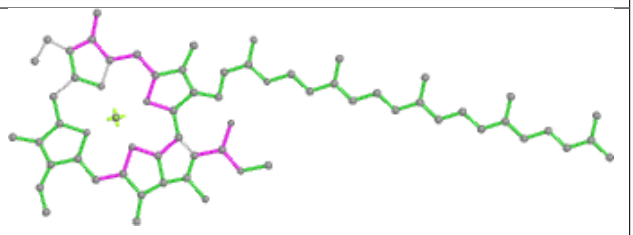


Rings

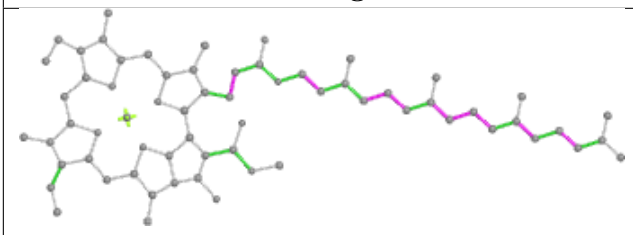
Ligand CLA C 512



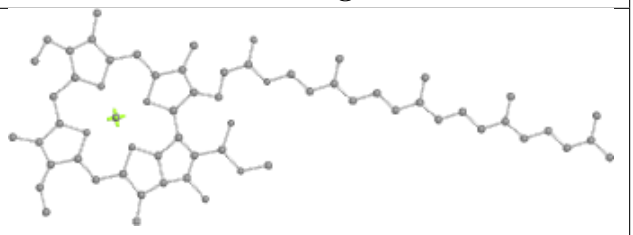
Bond lengths



Bond angles

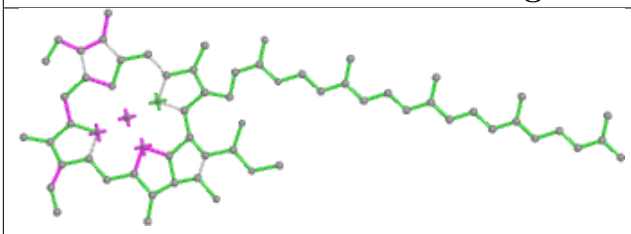


Torsions

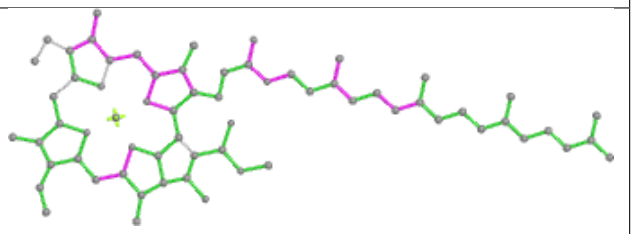


Rings

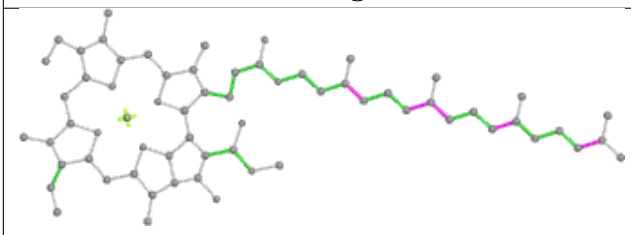
Ligand CLA B 615



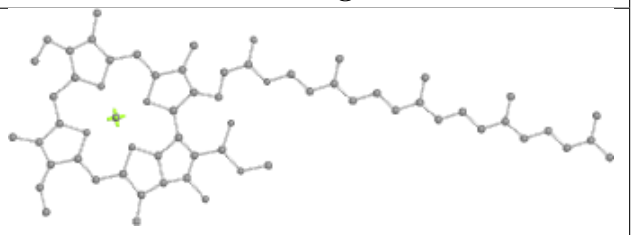
Bond lengths



Bond angles

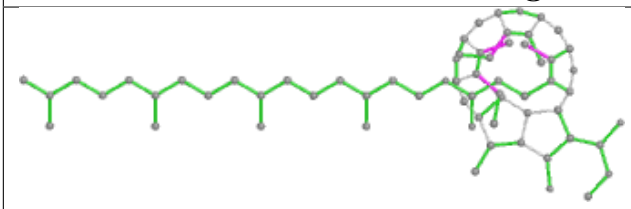


Torsions



Rings

Ligand PHO d 401



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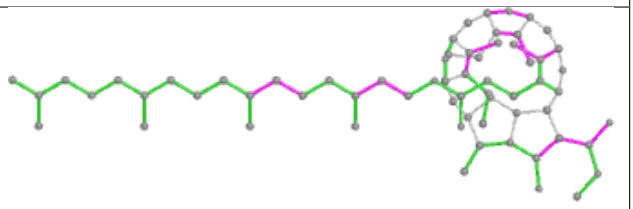
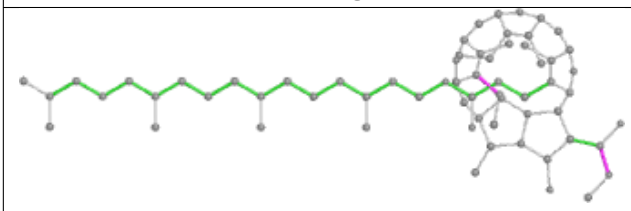
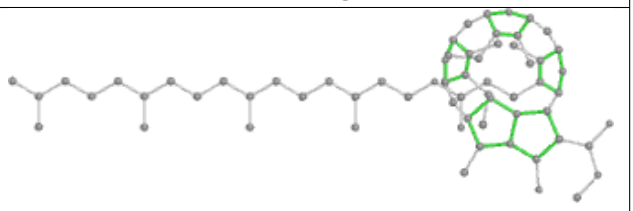


Bond angles

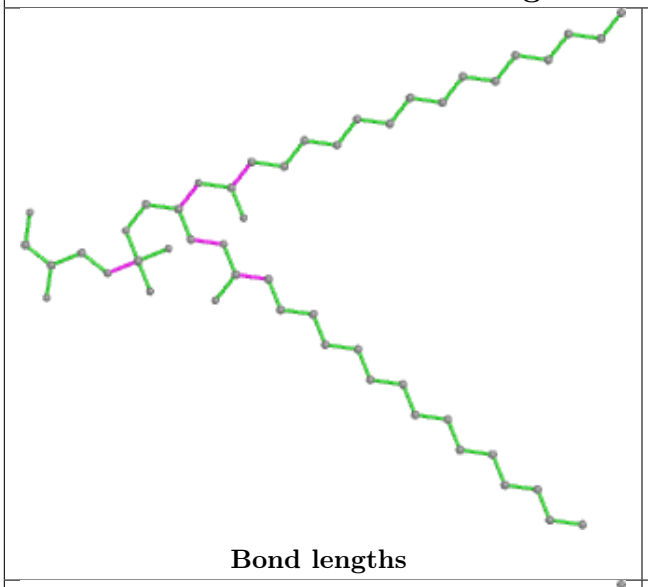


Torsions

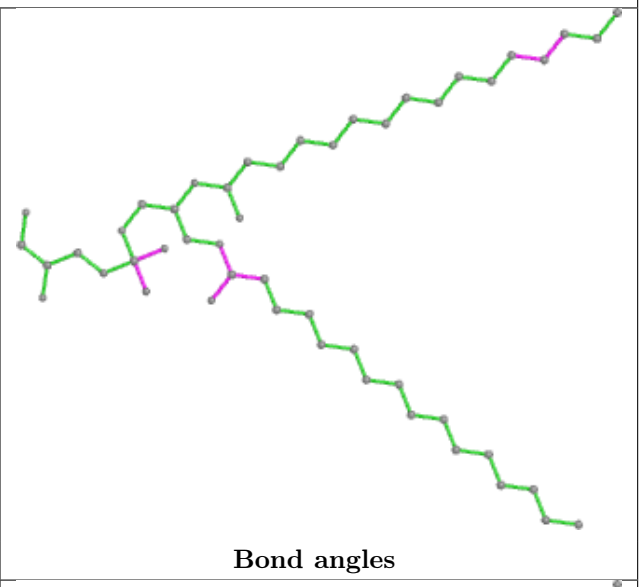


Rings

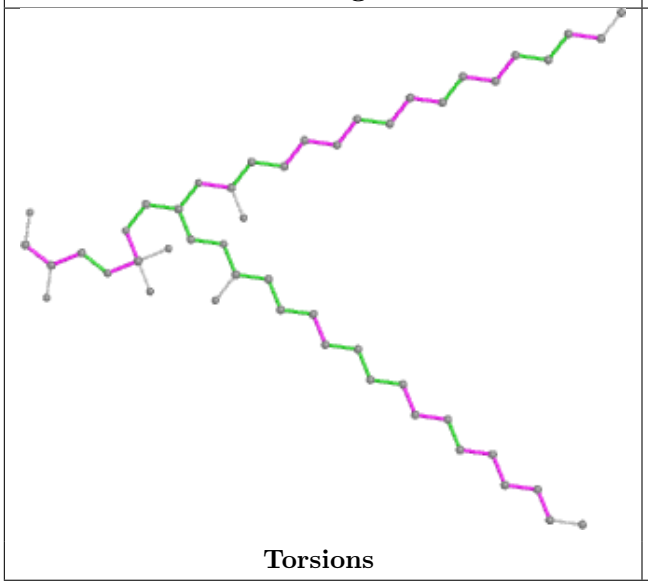
Ligand LHG D 408



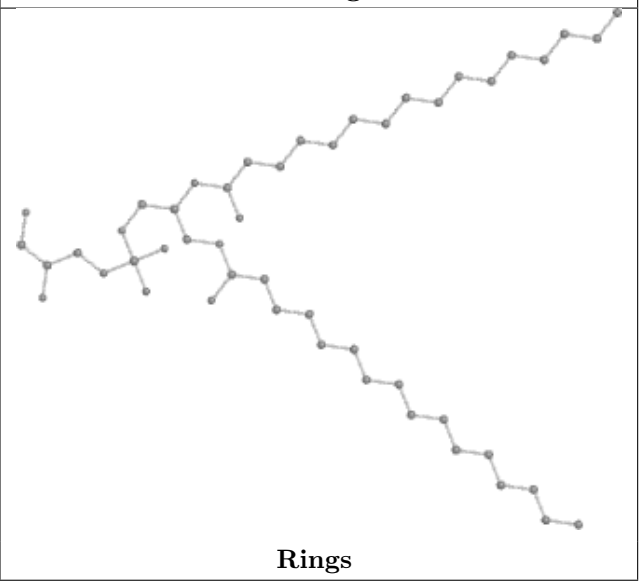
Bond lengths



Bond angles

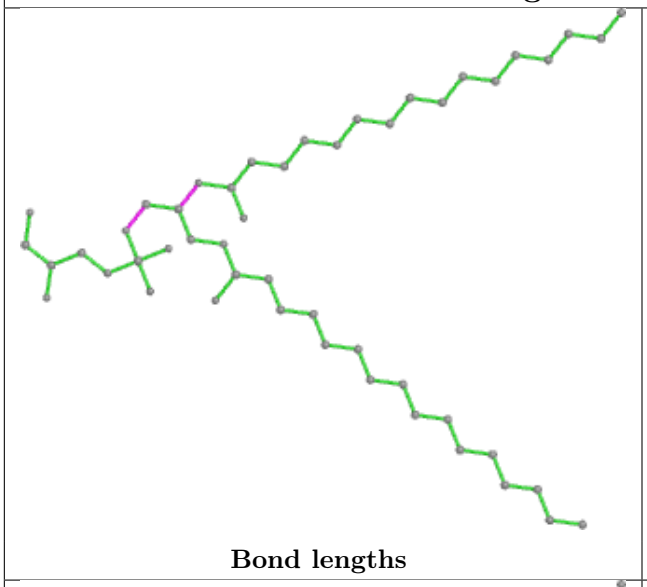


Torsions



Rings

Ligand LHG B 622



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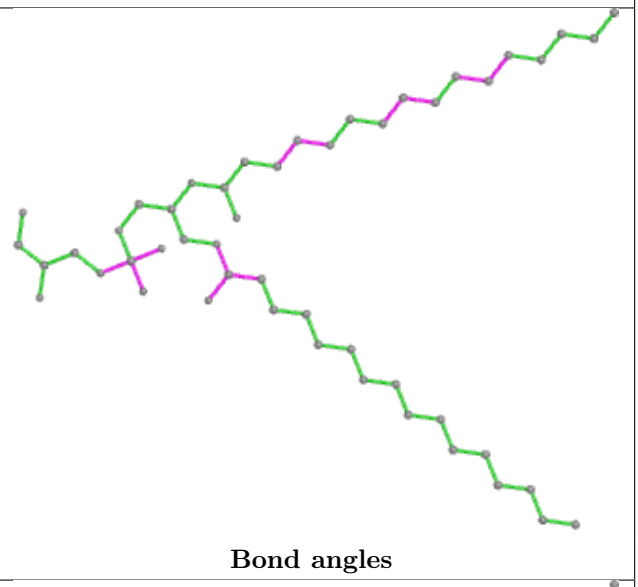
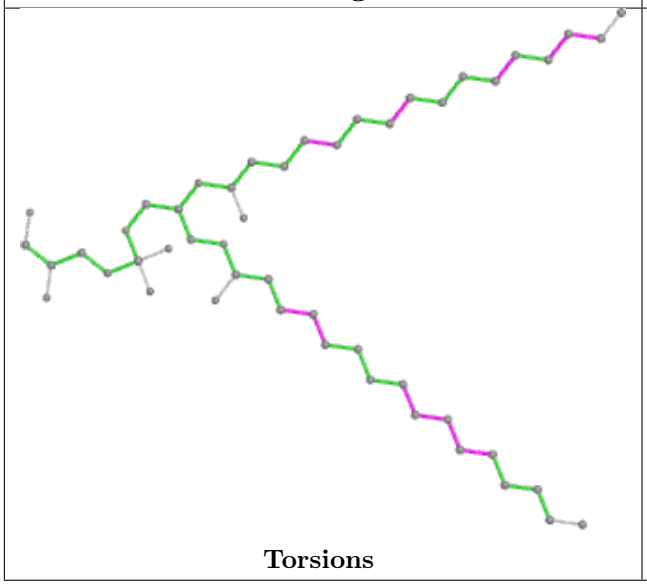
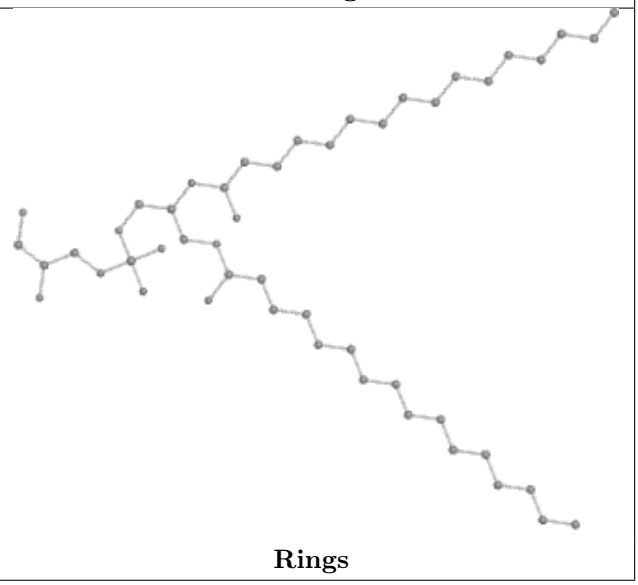


Bond angles

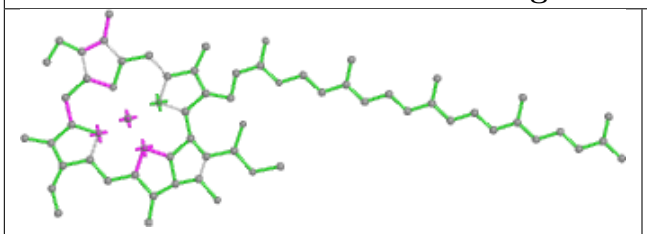


Torsions

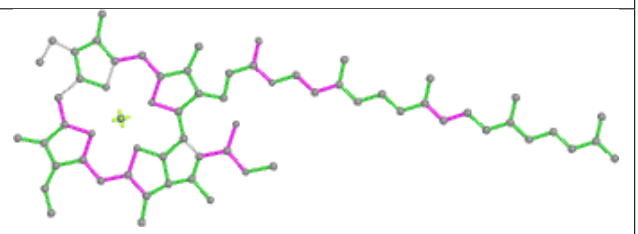


Rings

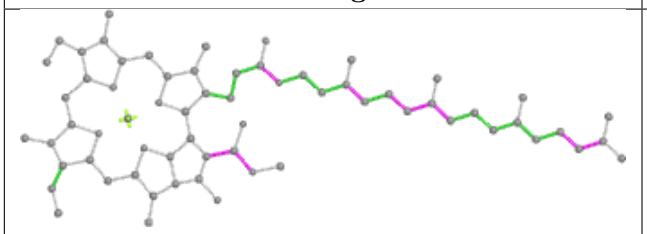
Ligand CLA c 505



Bond lengths



Bond angles



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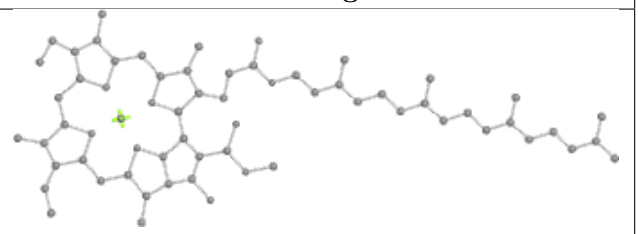
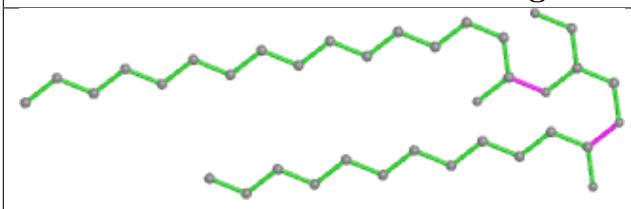


Rings

Ligand SQD a 412



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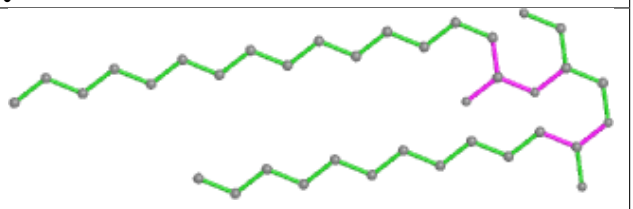
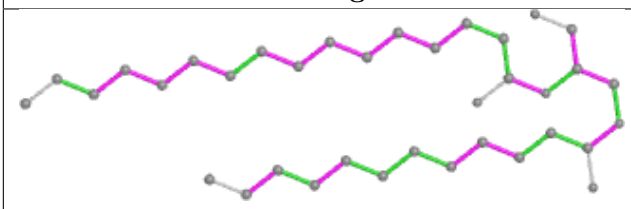


Bond angles



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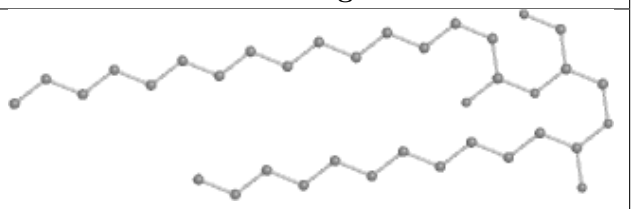
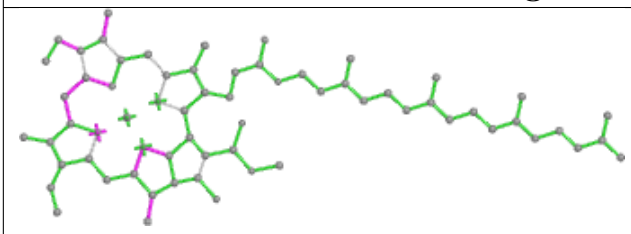


Rings

Ligand CLA B 611



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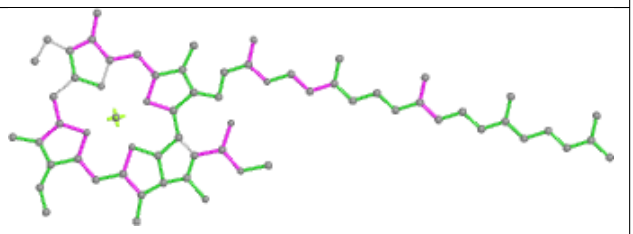
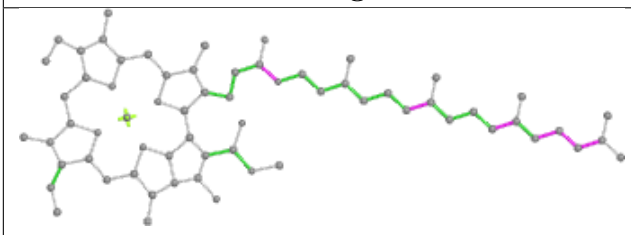


Bond angles



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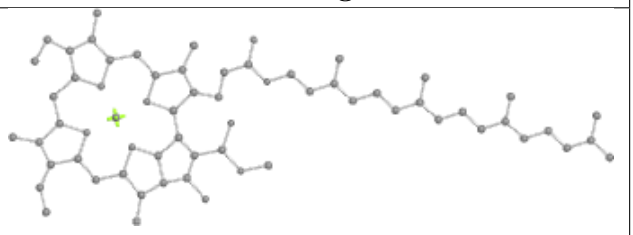
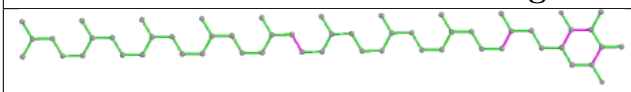
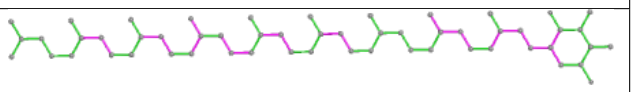


Rings

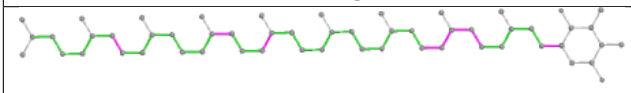
Ligand PL9 D 406



Bond lengths



Bond angles



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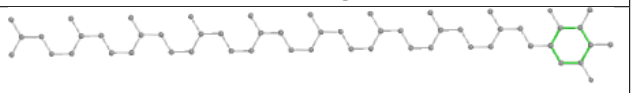
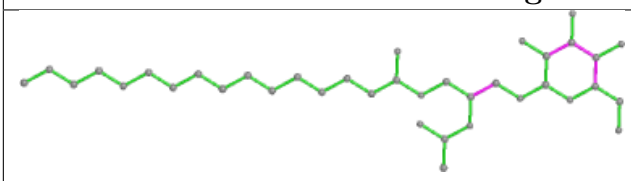


Rings

Ligand LMG c 519



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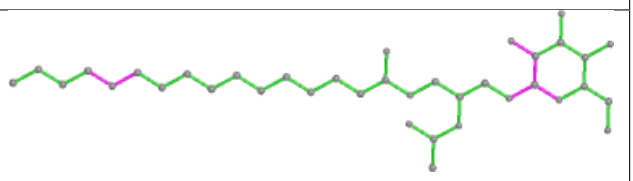
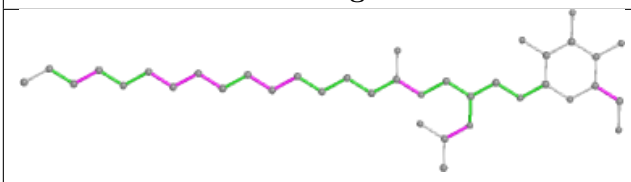
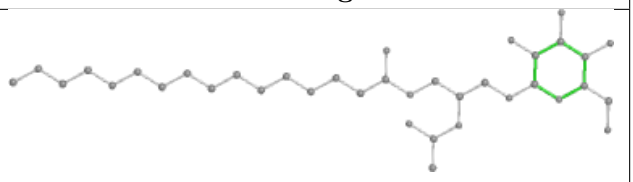


Bond angles

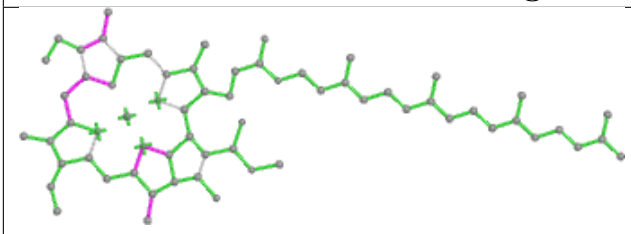


Torsions

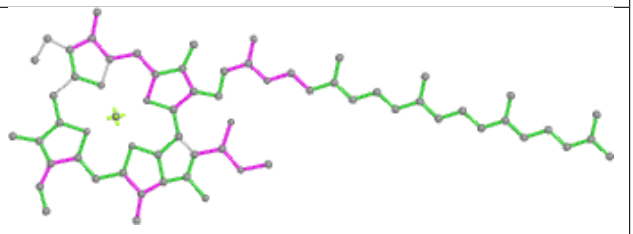


Rings

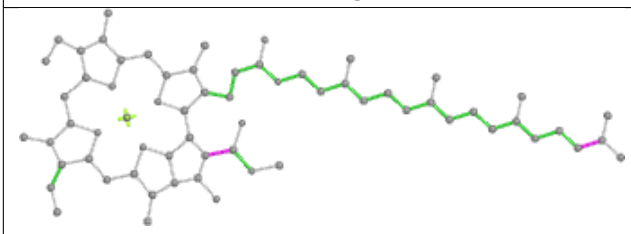
Ligand CLA A 405



Bond lengths



Bond angles



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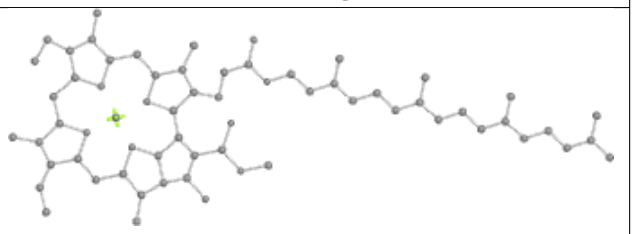
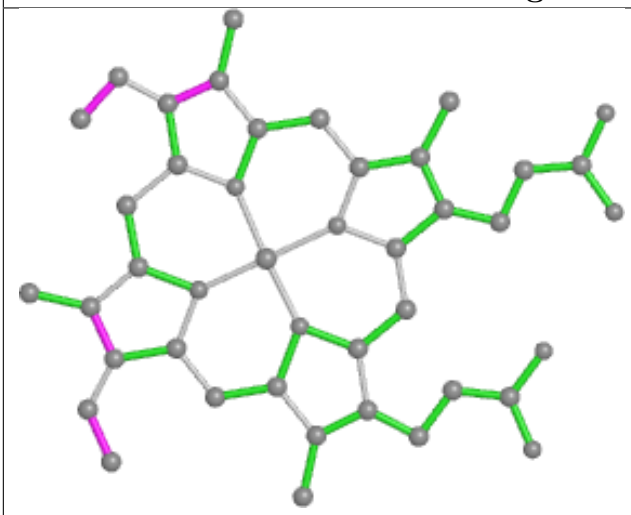


Rings

Ligand HEC v 201



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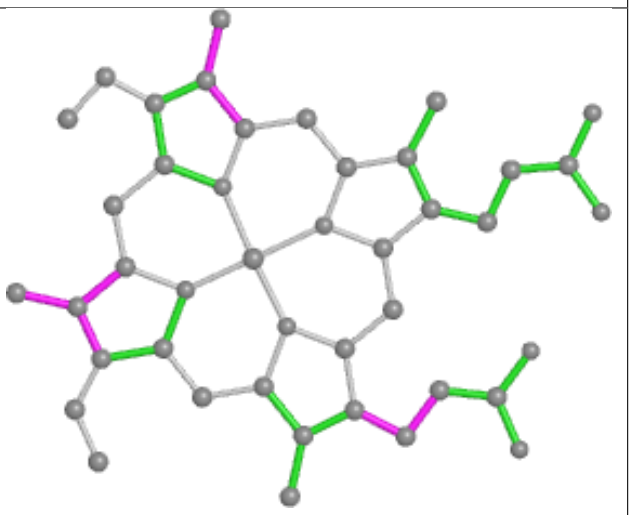
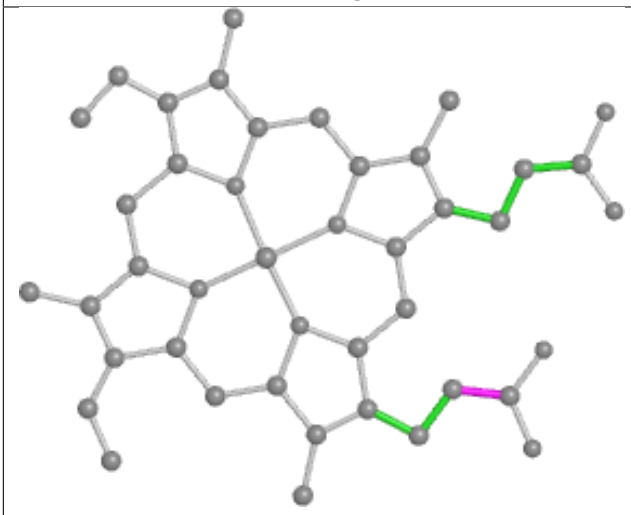
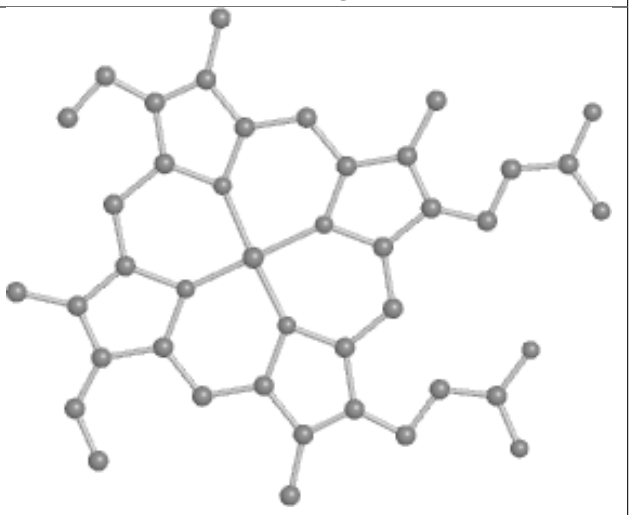


Bond angles

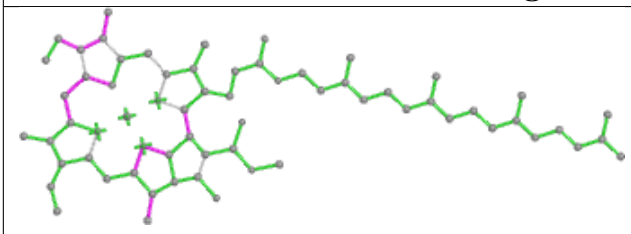


Torsions



Rings

Ligand CLA D 404



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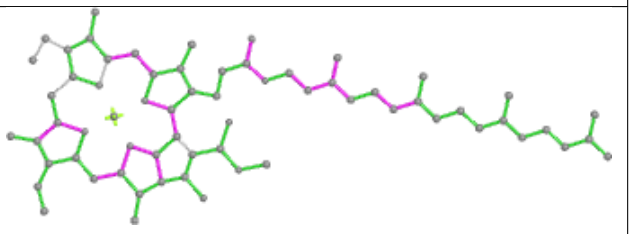
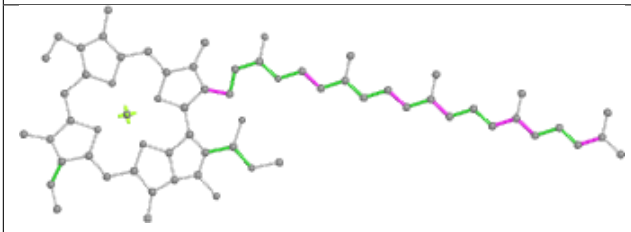


Bond angles



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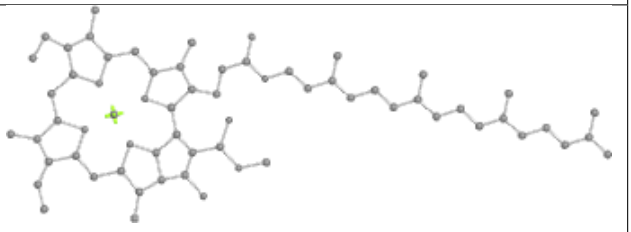
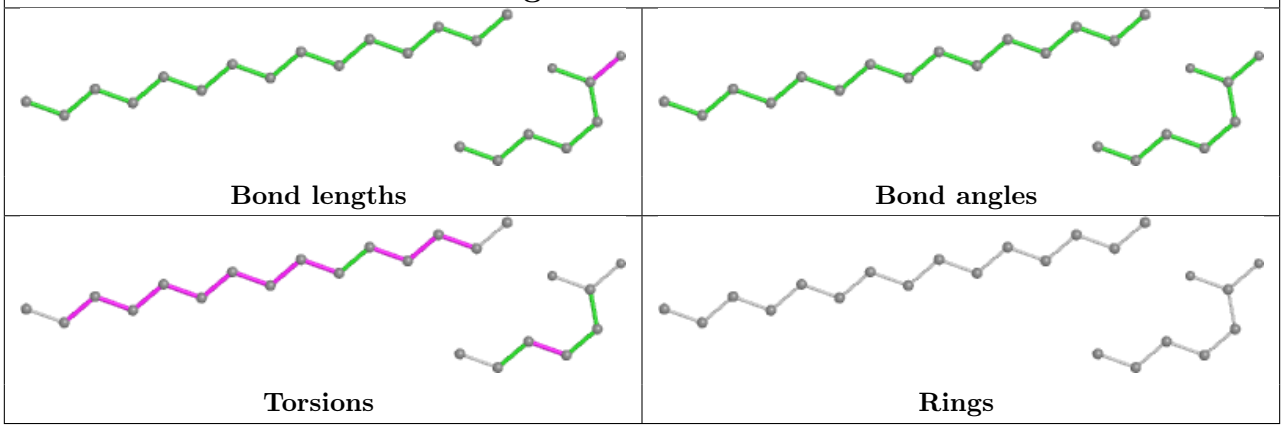
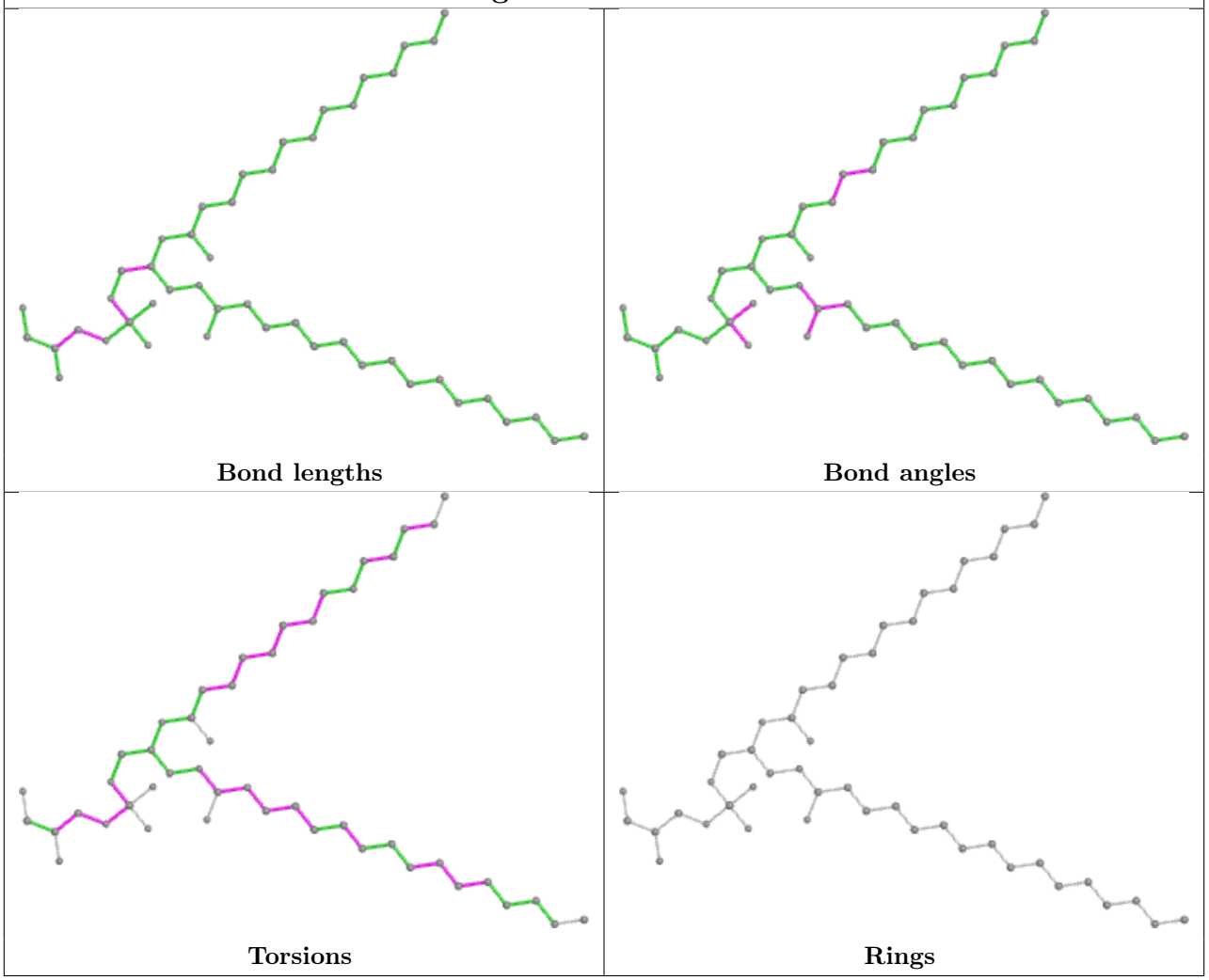


Rings

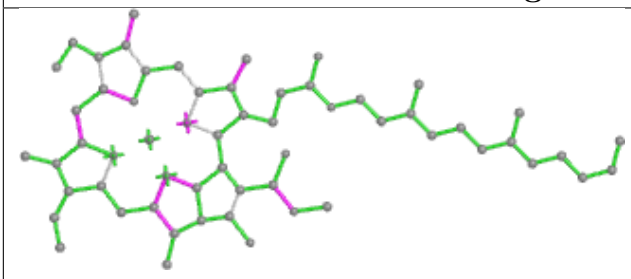
Ligand LMG b 623



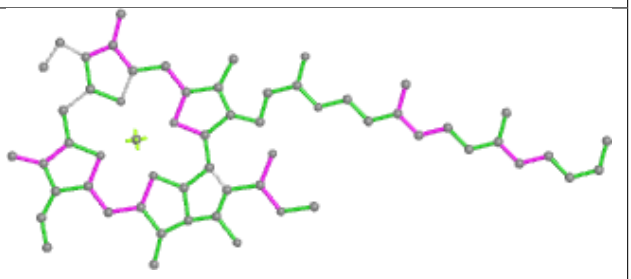
Ligand LHG D 409



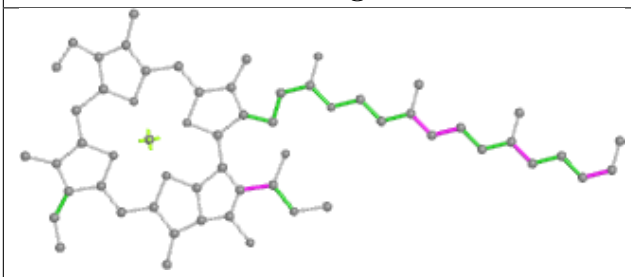
Ligand CLA C 504



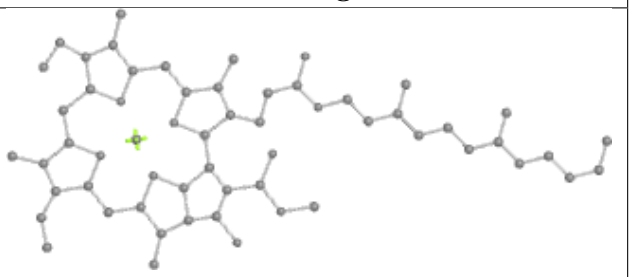
Bond lengths



Bond angles

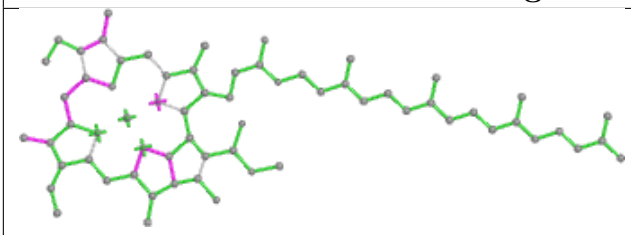


Torsions

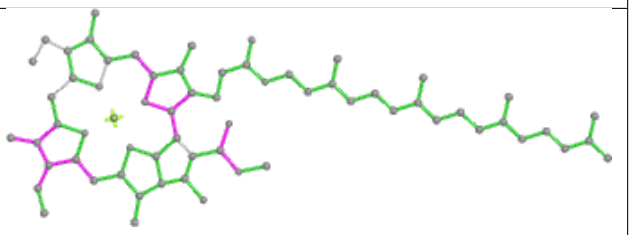


Rings

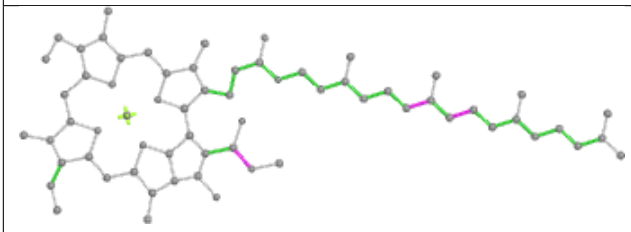
Ligand CLA C 511



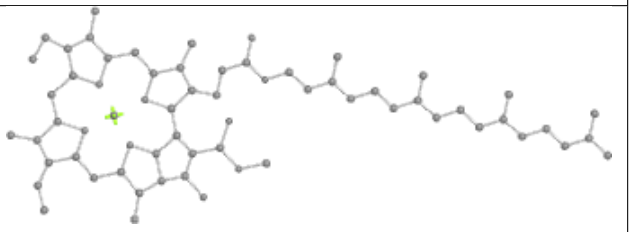
Bond lengths



Bond angles

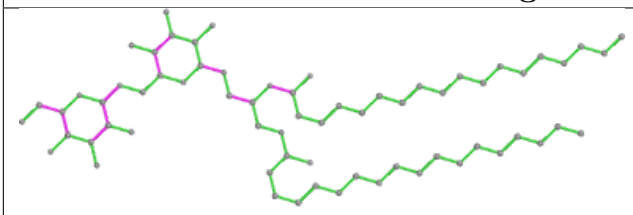


Torsions

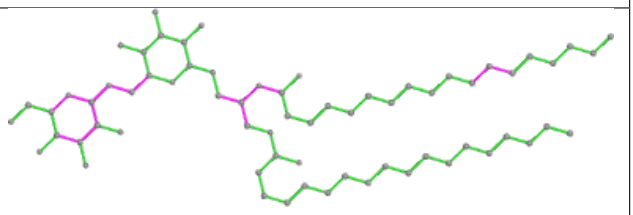


Rings

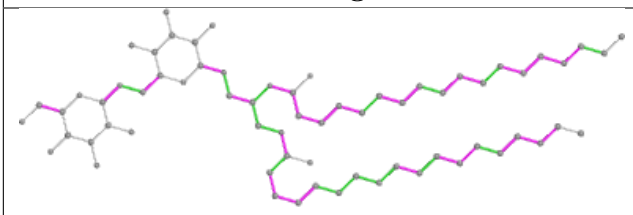
Ligand DGD A 413



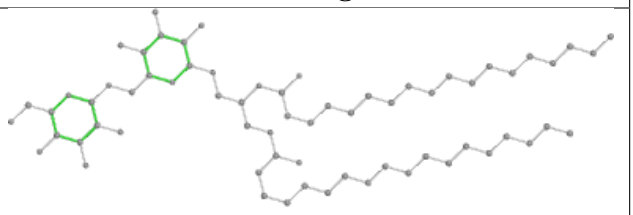
Bond lengths



Bond angles

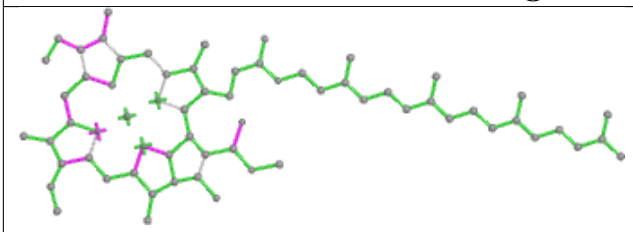


Torsions

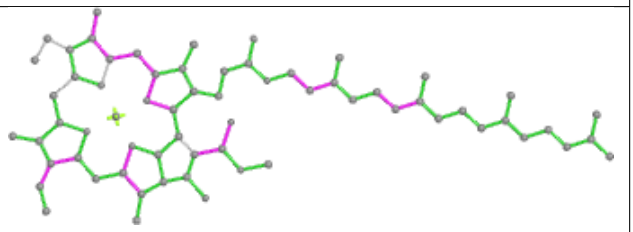


Rings

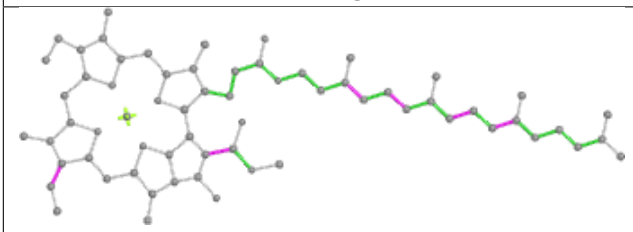
Ligand CLA C 505



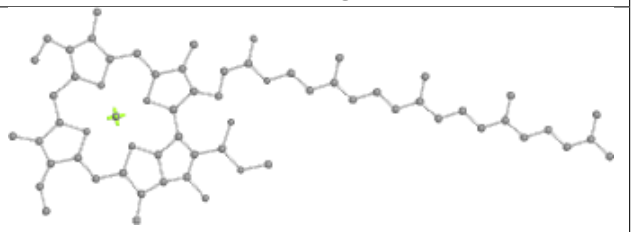
Bond lengths



Bond angles

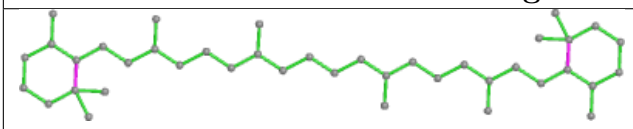


Torsions

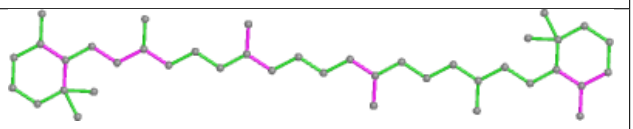


Rings

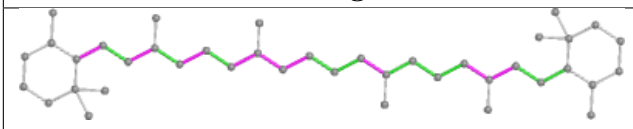
Ligand BCR T 101



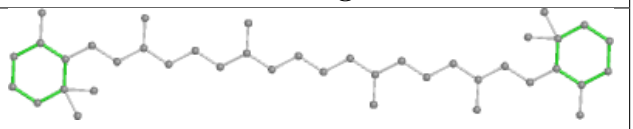
Bond lengths



Bond angles

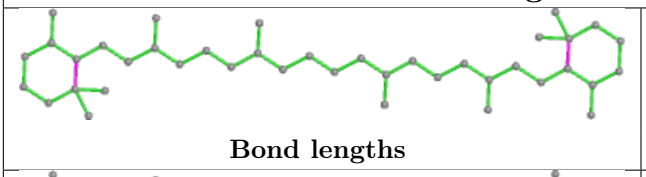


Torsions

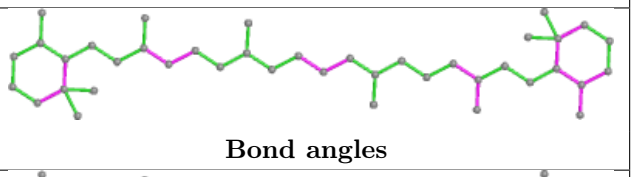


Rings

Ligand BCR b 620

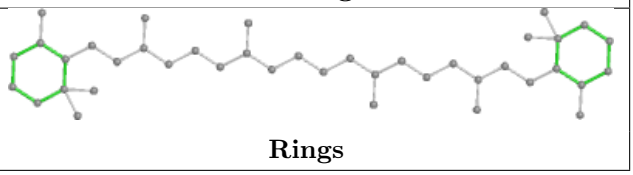


Bond lengths



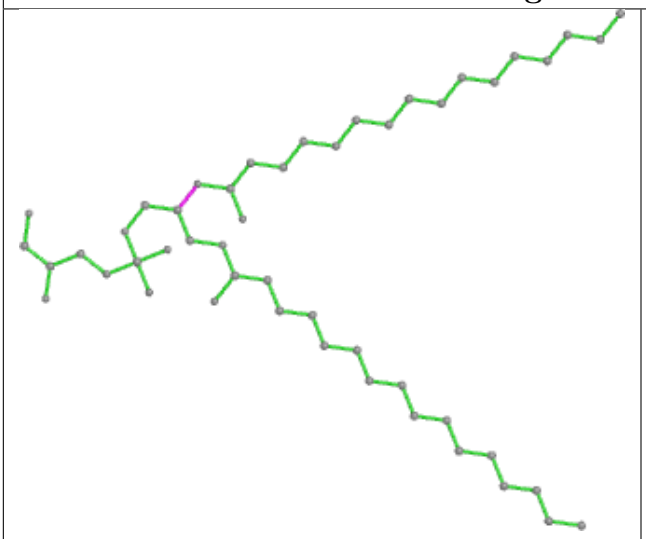
Bond angles

Torsions

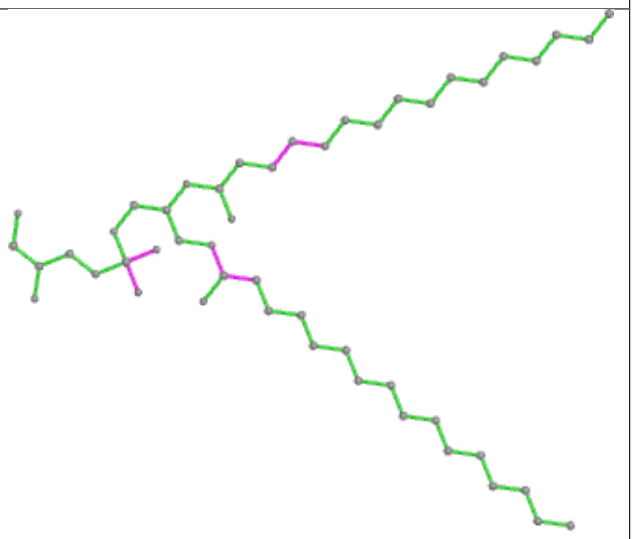


Rings

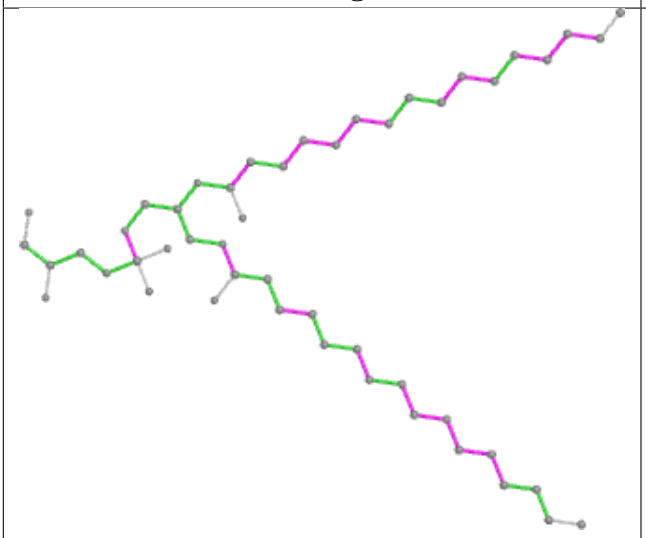
Ligand LHG L 101



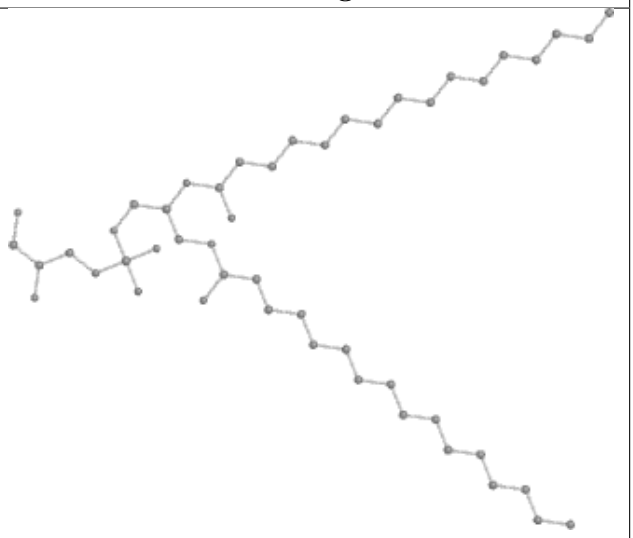
Bond lengths



Bond angles

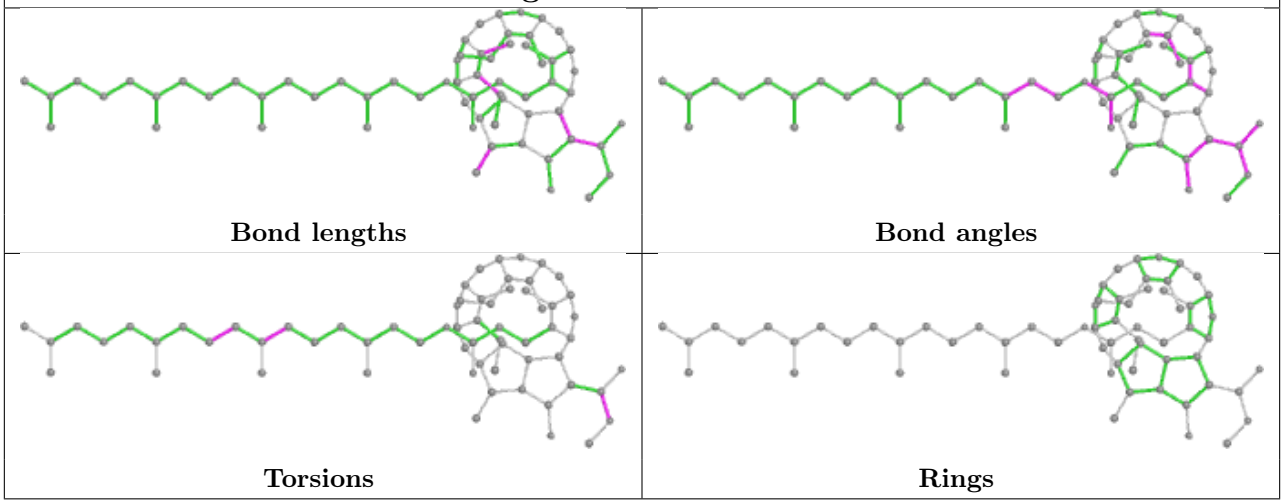


Torsions

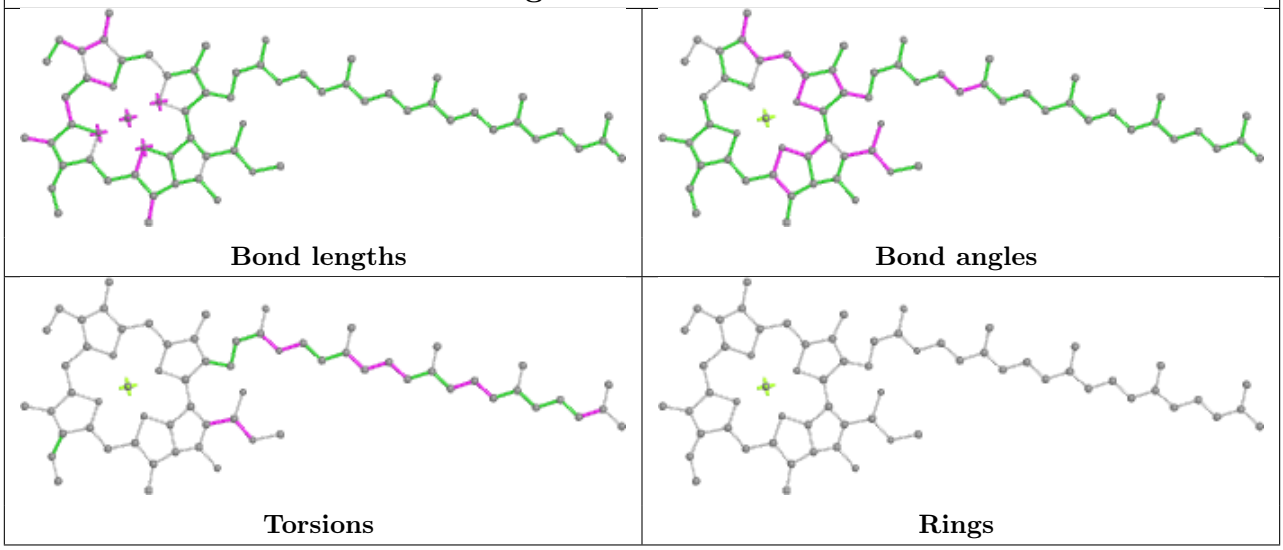


Rings

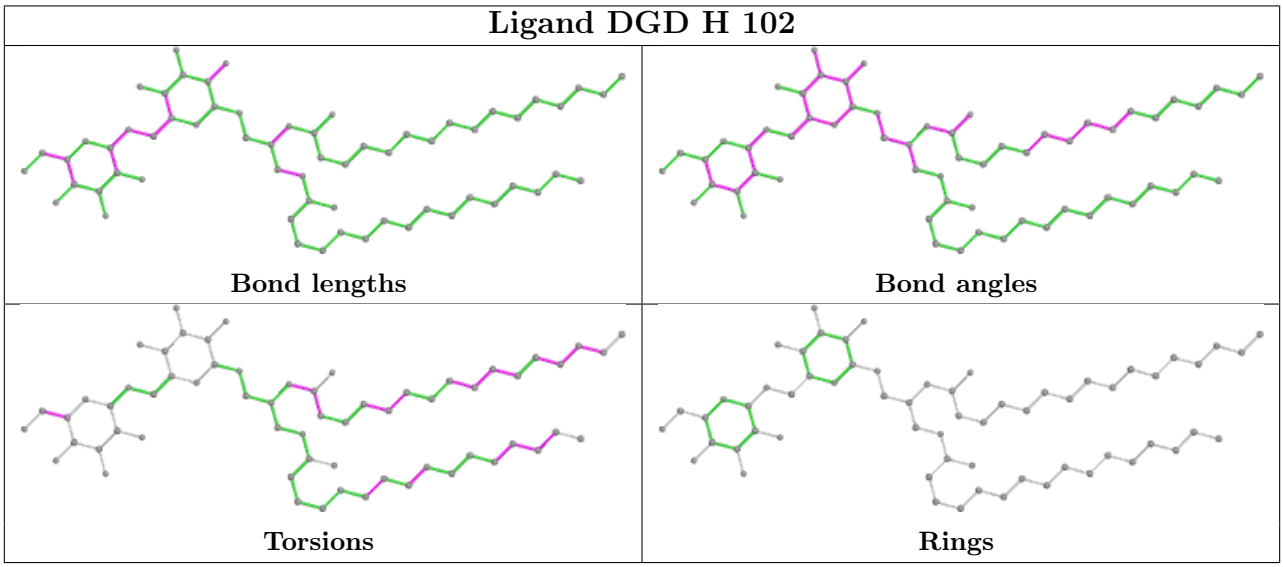
Ligand PHO D 401



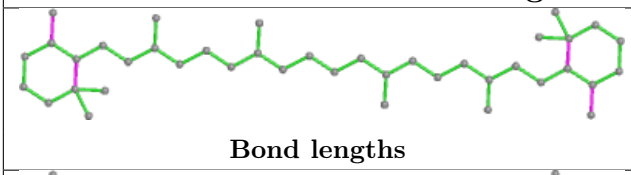
Ligand CLA B 601



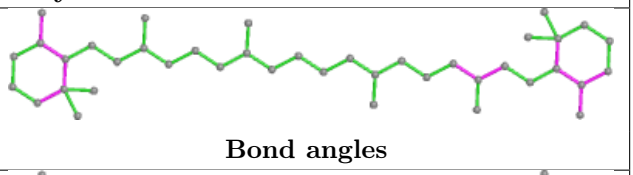
Ligand DGD H 102



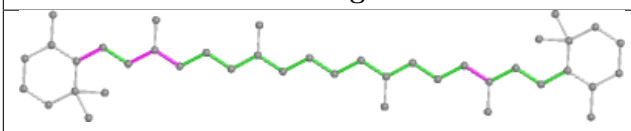
Ligand BCR y 101



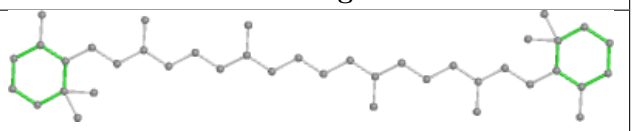
Bond lengths



Bond angles

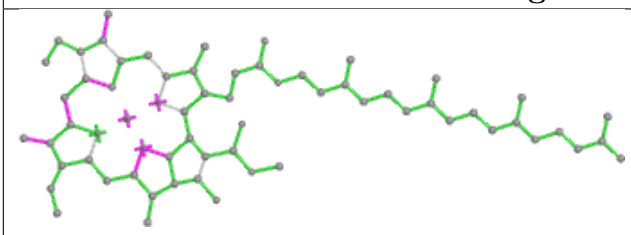


Torsions

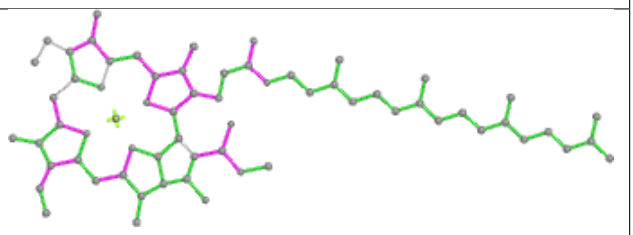


Rings

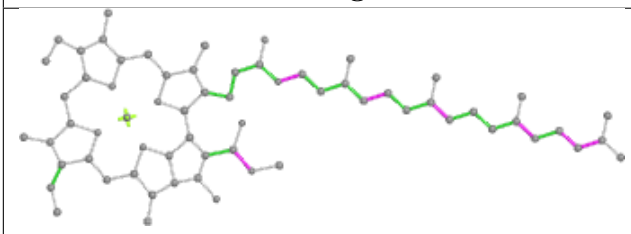
Ligand CLA a 404



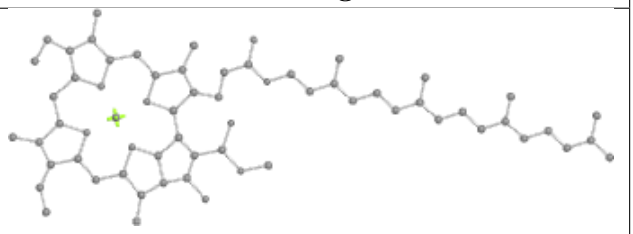
Bond lengths



Bond angles

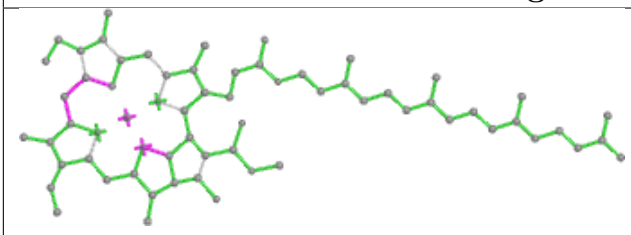


Torsions

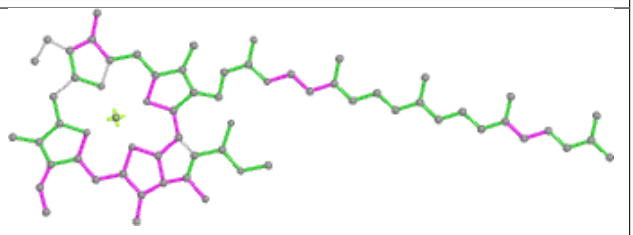


Rings

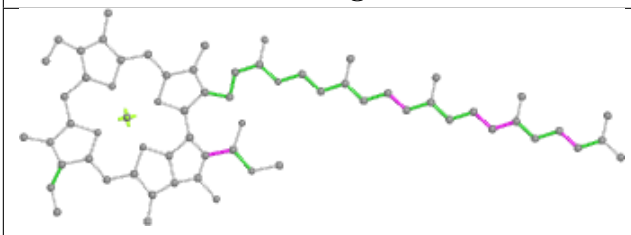
Ligand CLA b 606



Bond lengths



Bond angles



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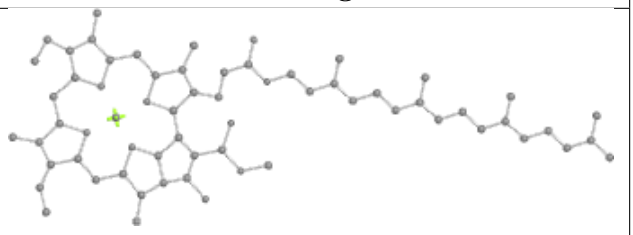
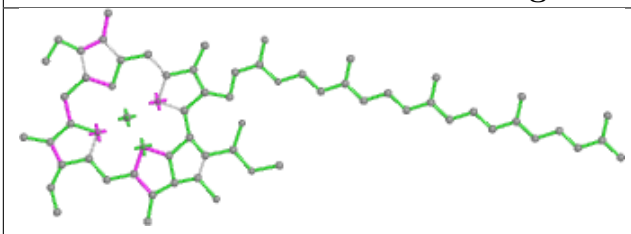
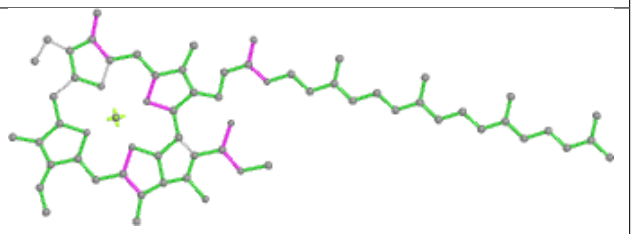


Rings

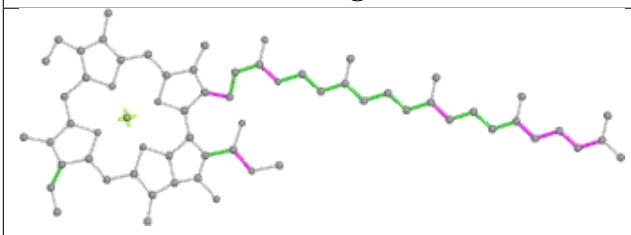
Ligand CLA c 511



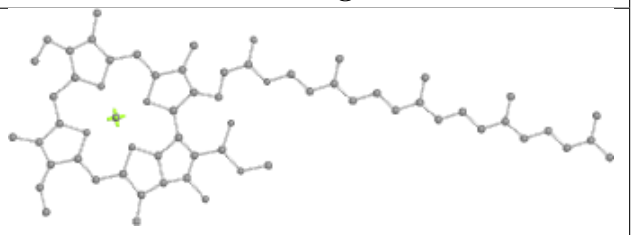
Bond lengths



Bond angles

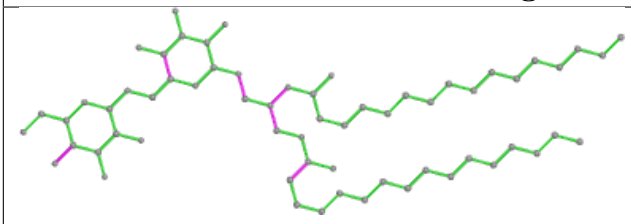


Torsions

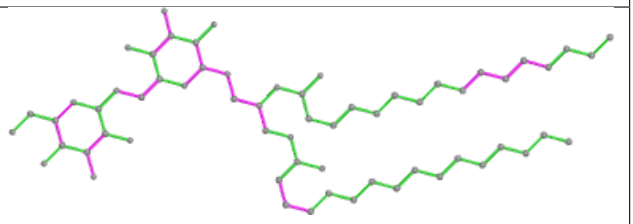


Rings

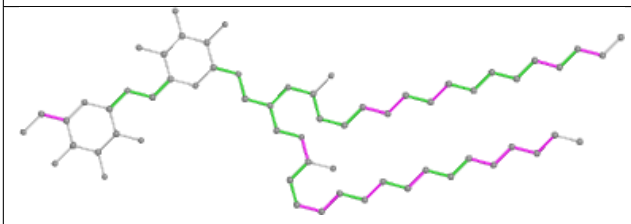
Ligand DGD C 518



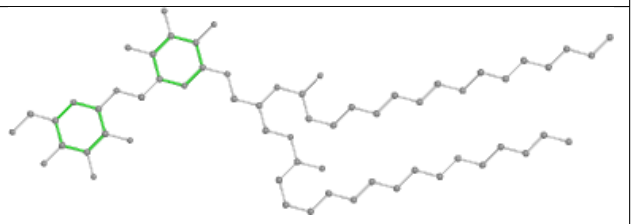
Bond lengths



Bond angles

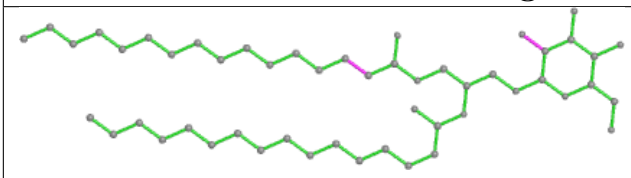


Torsions

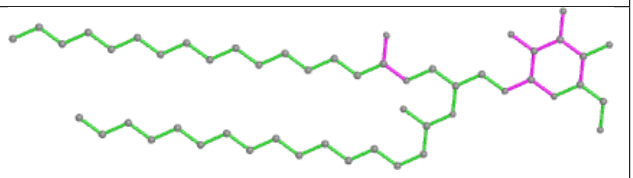


Rings

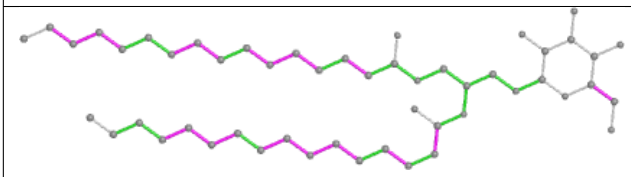
Ligand LMG D 407



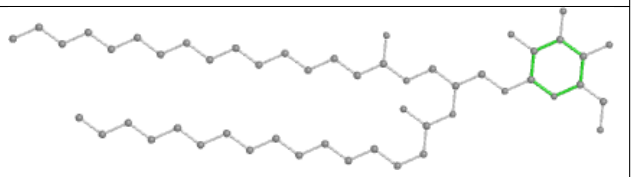
Bond lengths



Bond angles

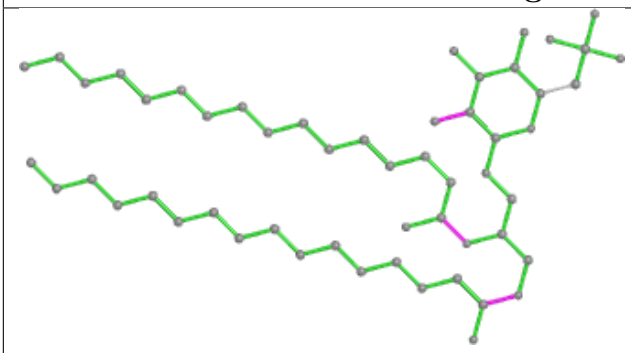


Torsions



Rings

Ligand SQD B 623



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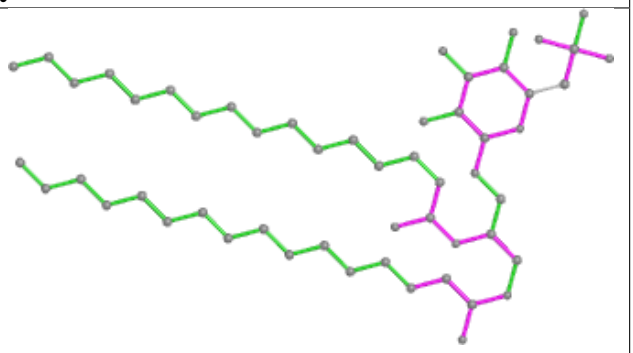
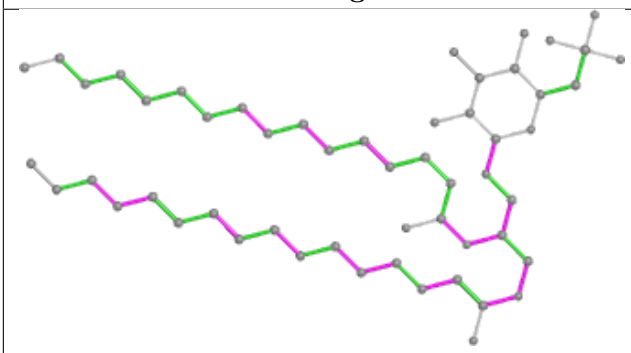
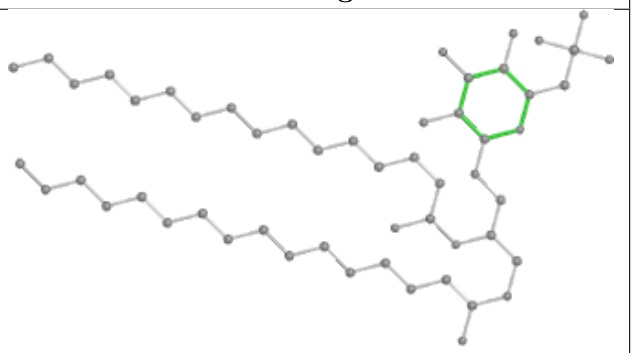


Bond angles

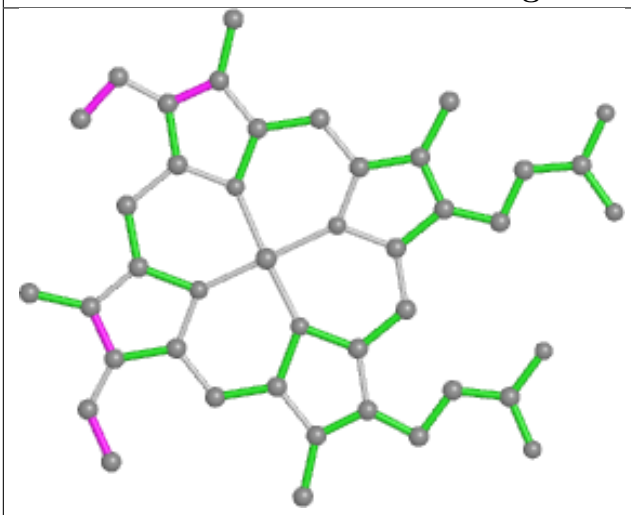


Torsions

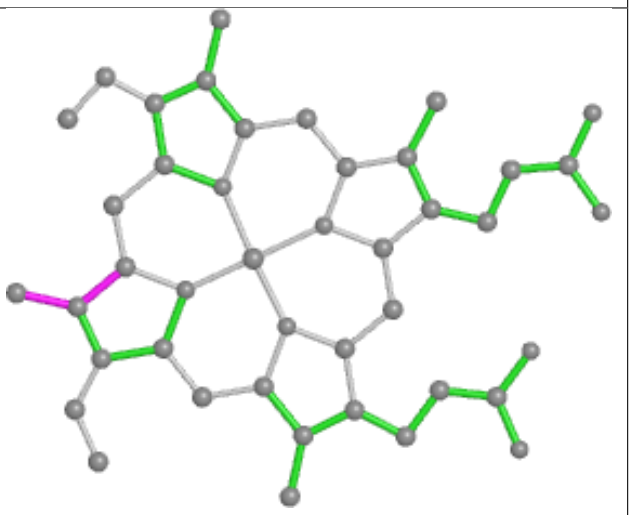


Rings

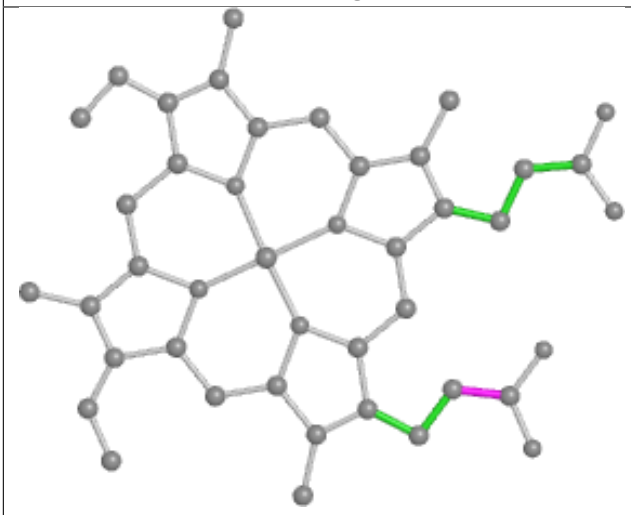
Ligand HEC V 201



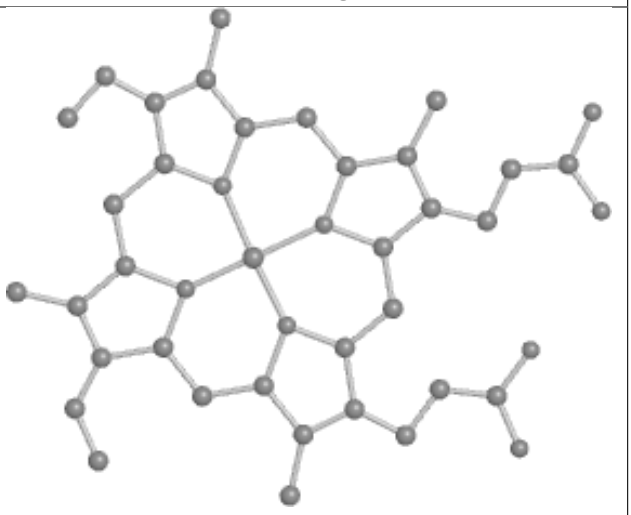
Bond lengths



Bond angles

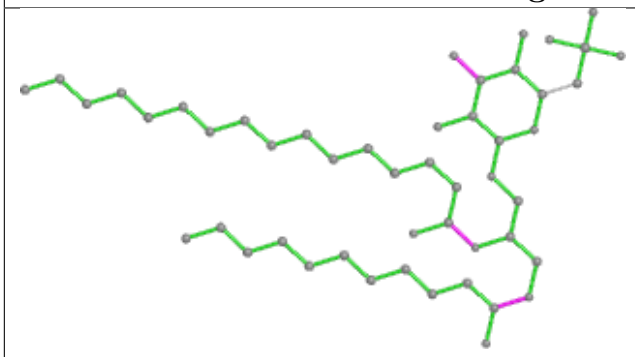


Torsions

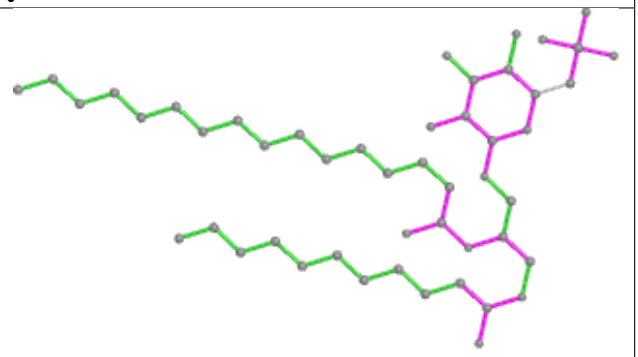


Rings

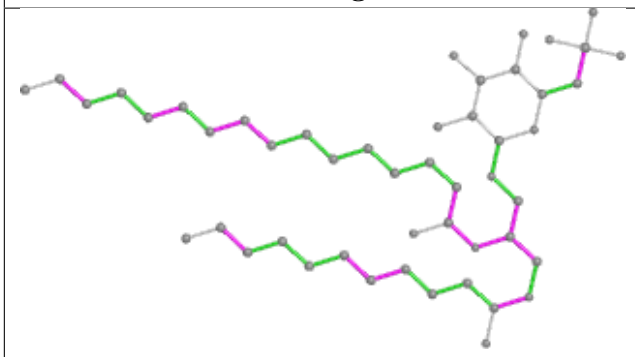
Ligand SQD b 601



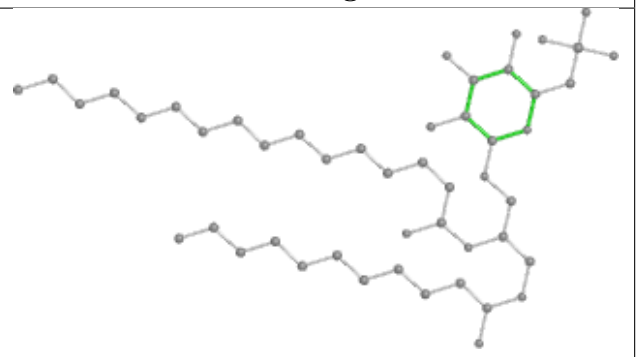
Bond lengths



Bond angles

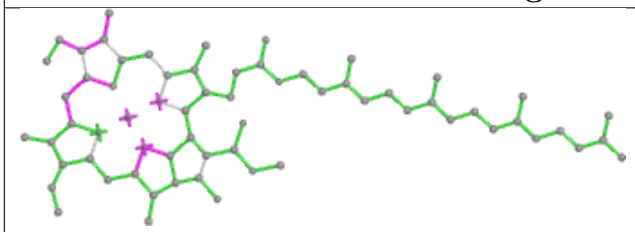


Torsions

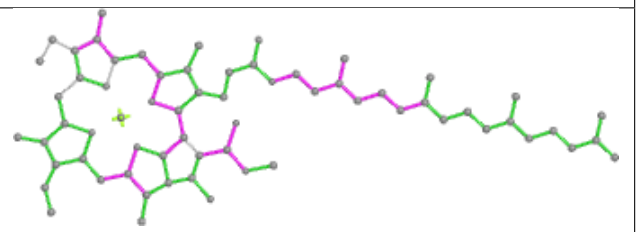


Rings

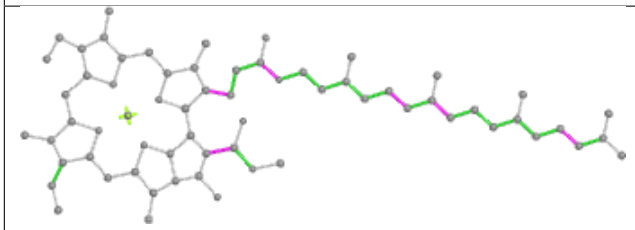
Ligand CLA C 503



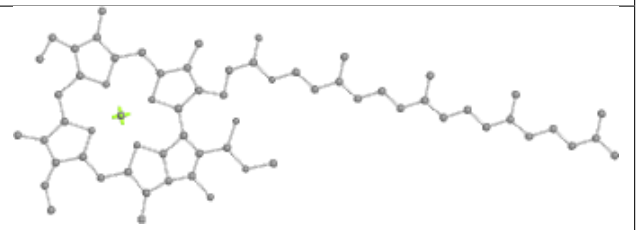
Bond lengths



Bond angles

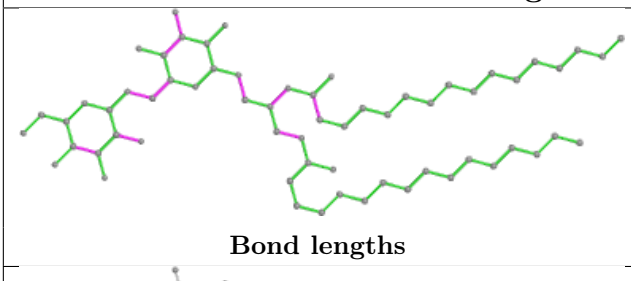


Torsions

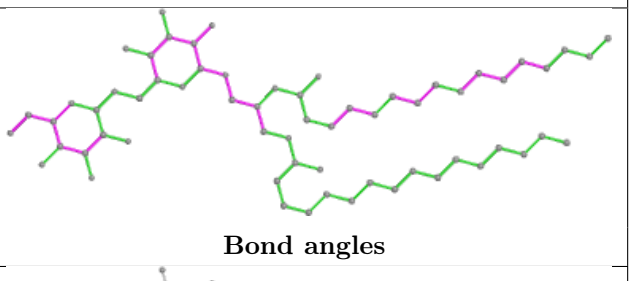


Rings

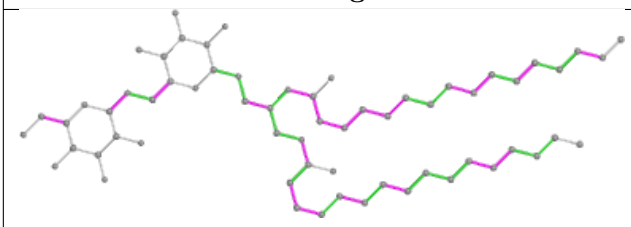
Ligand DGD c 516



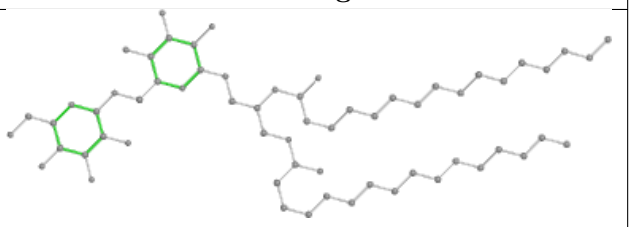
Bond lengths



Bond angles

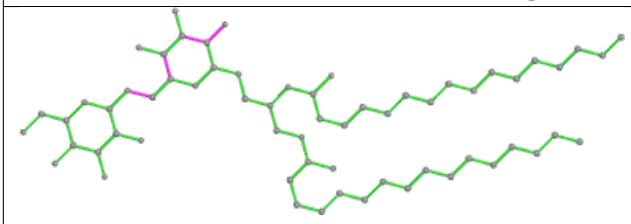


Torsions

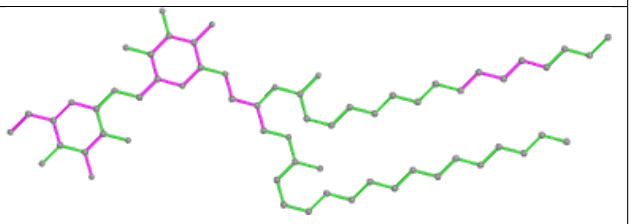


Rings

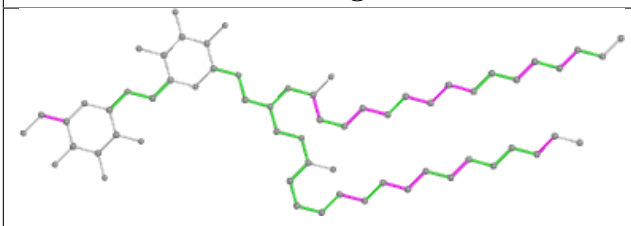
Ligand DGD h 103



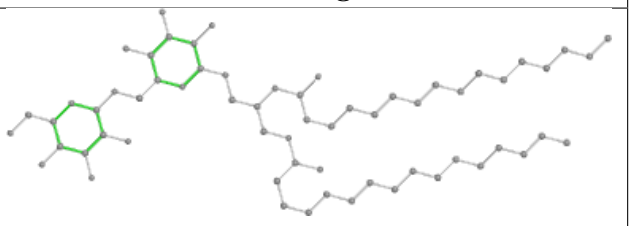
Bond lengths



Bond angles

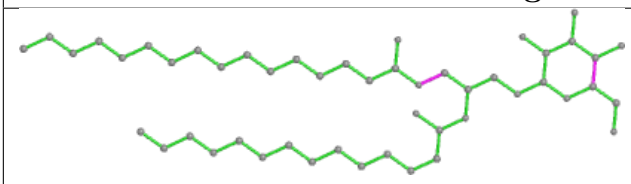


Torsions

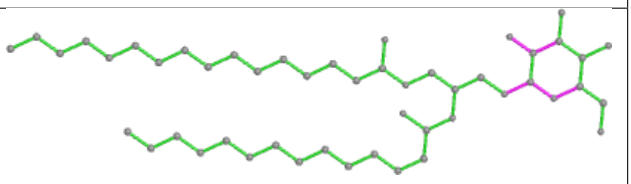


Rings

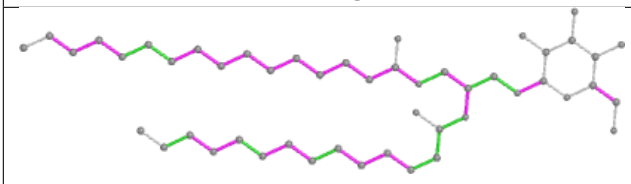
Ligand LMG a 414



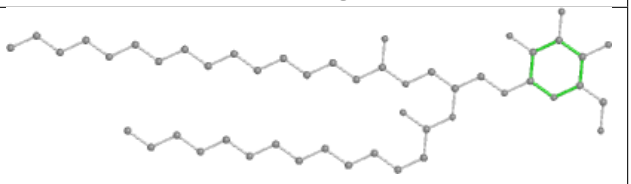
Bond lengths



Bond angles

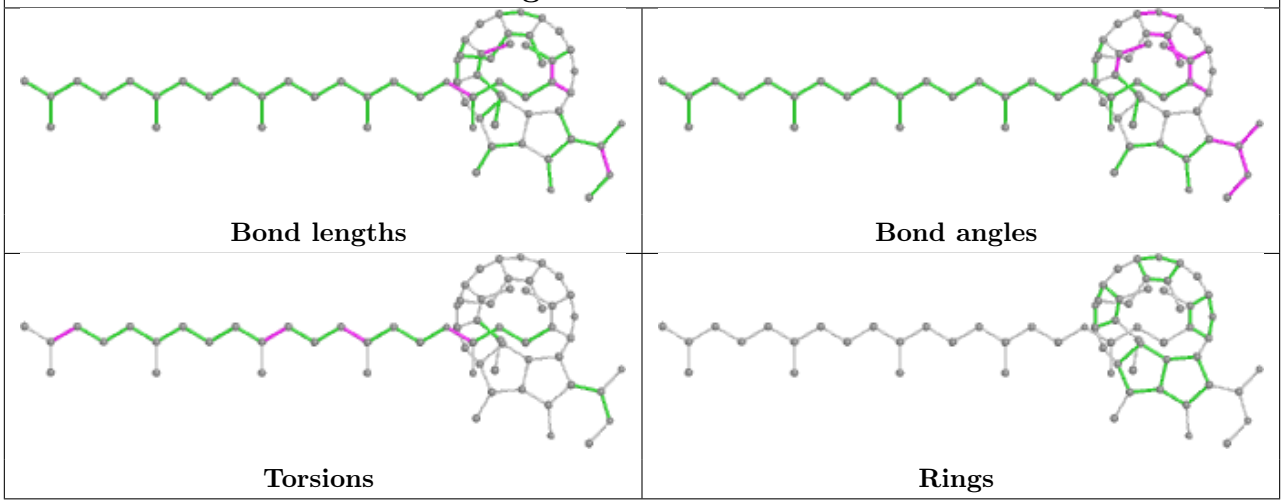


Torsions

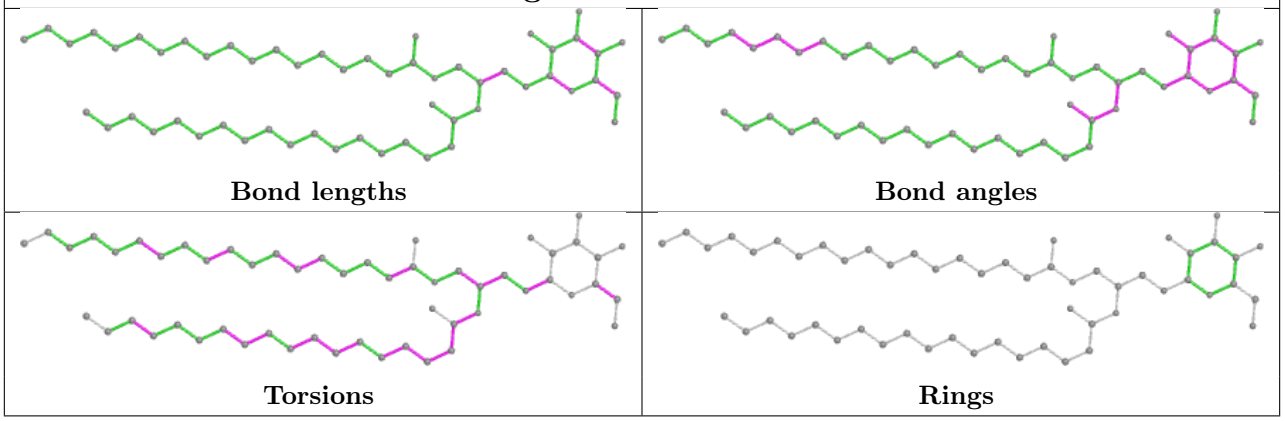


Rings

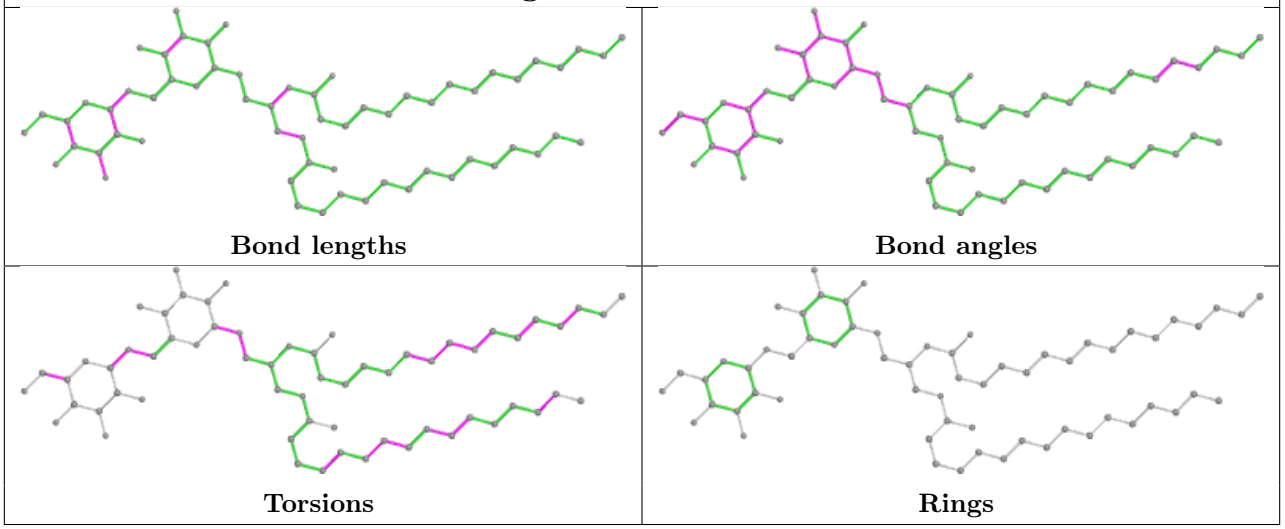
Ligand PHO A 406



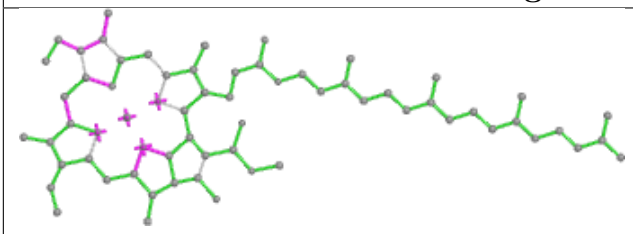
Ligand LMG b 622



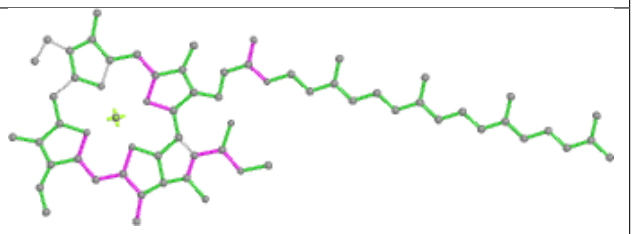
Ligand DGD C 517



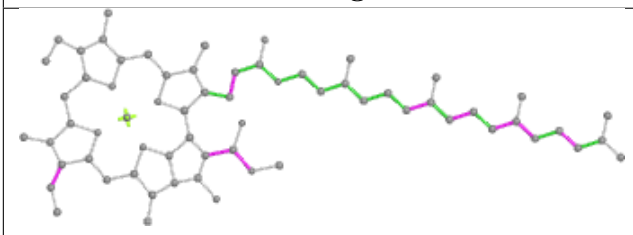
Ligand CLA B 606



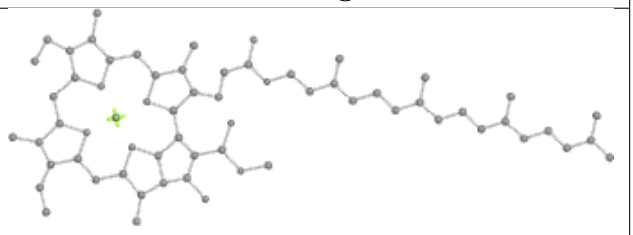
Bond lengths



Bond angles

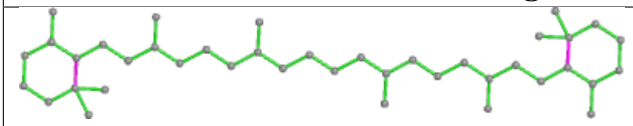


Torsions

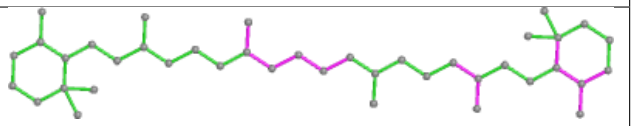


Rings

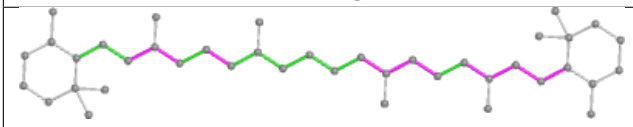
Ligand BCR B 618



Bond lengths



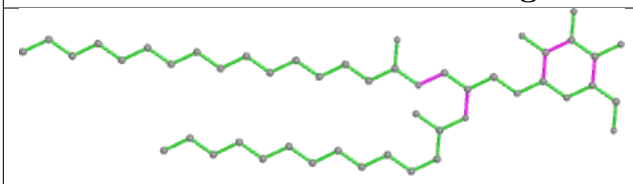
Bond angles



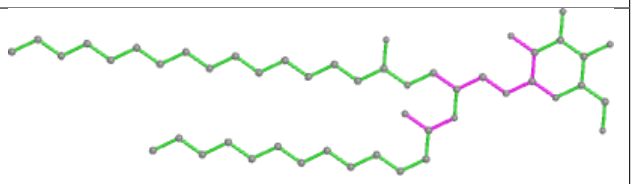
Torsions

Rings

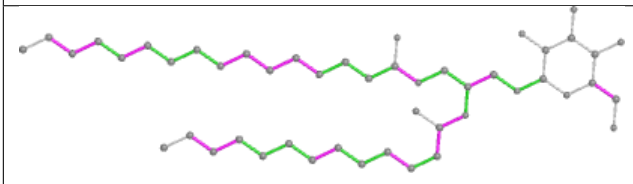
Ligand LMG C 519



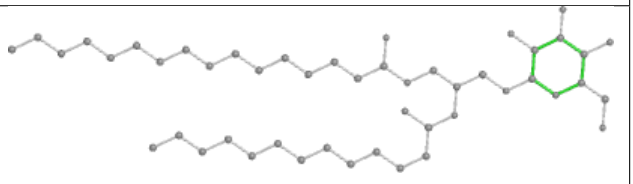
Bond lengths



Bond angles

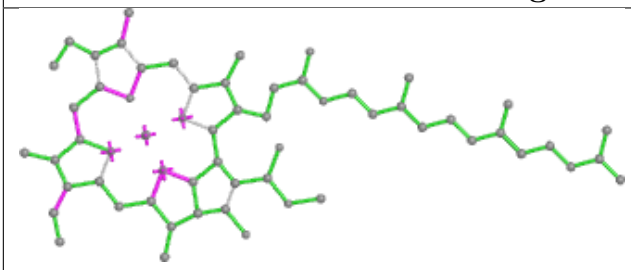


Torsions



Rings

Ligand CLA c 504



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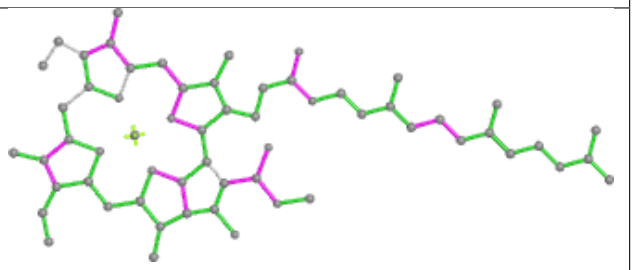
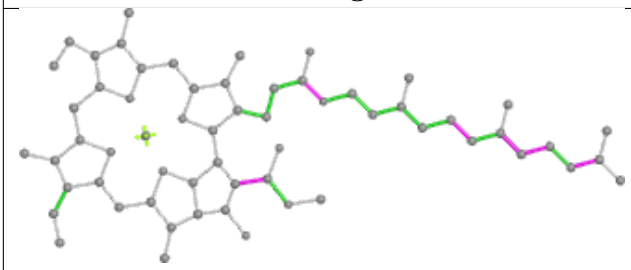
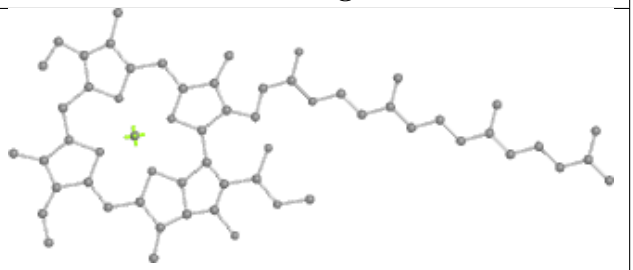


Bond angles

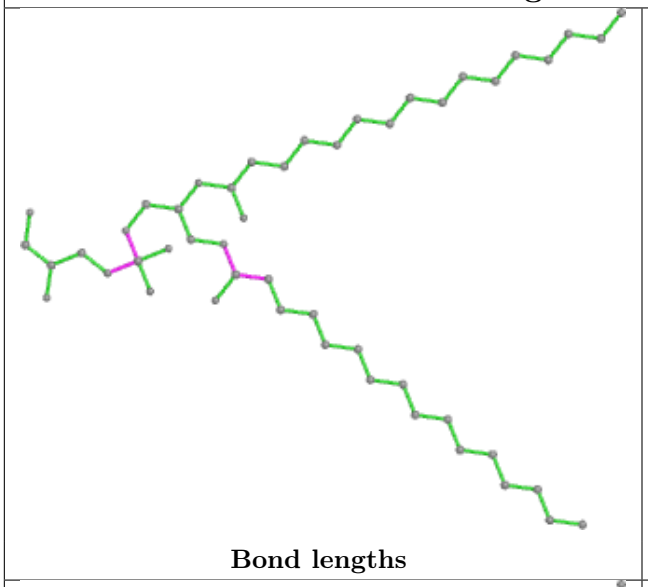


Torsions

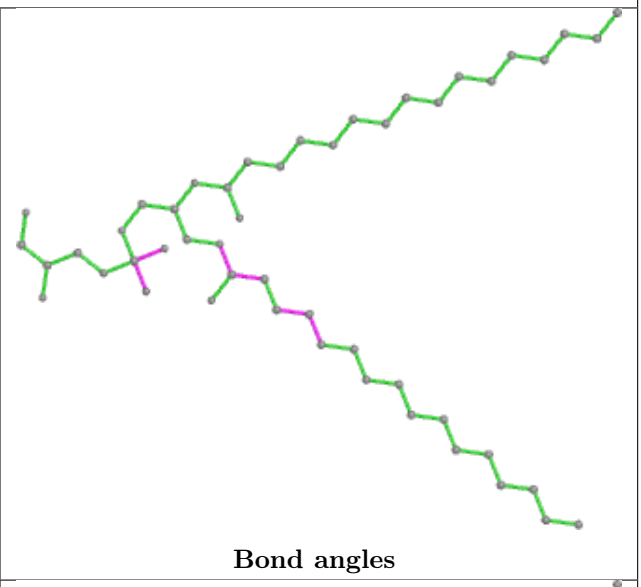


Rings

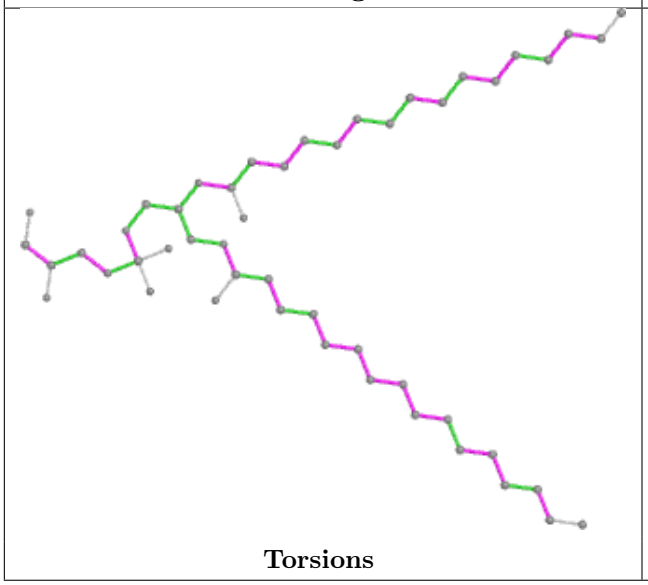
Ligand LHG E 101



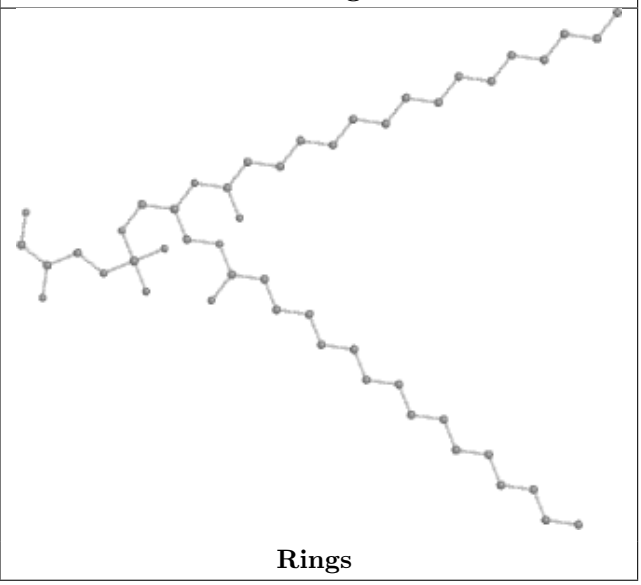
Bond lengths



Bond angles

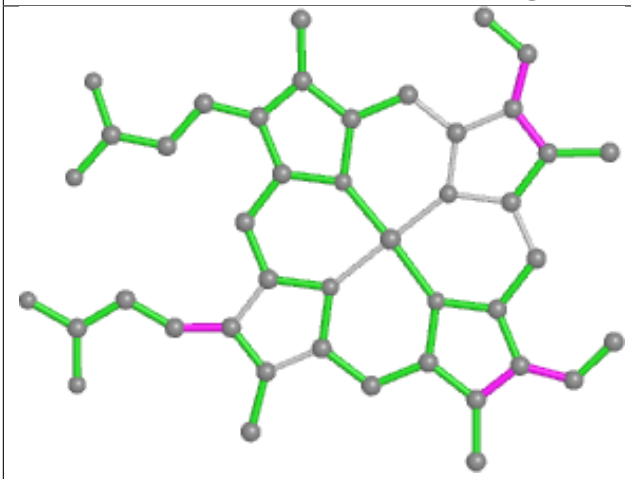


Torsions

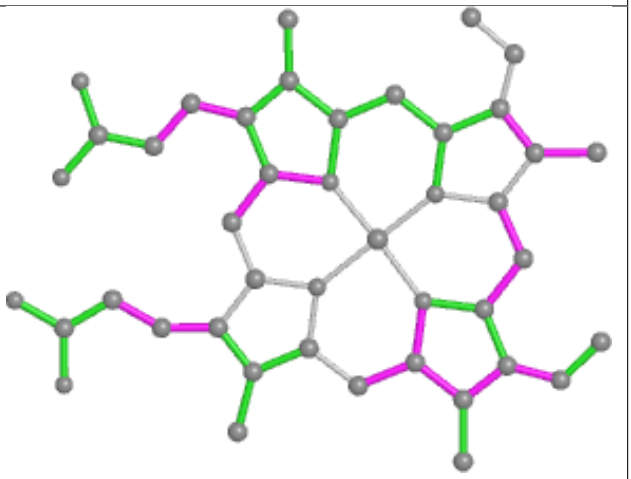


Rings

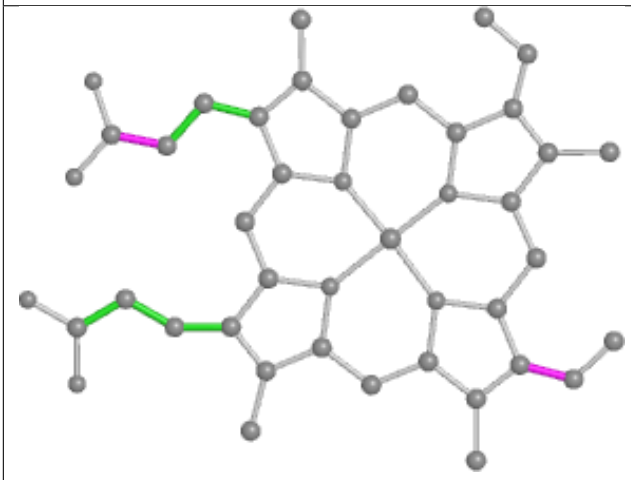
Ligand HEM e 102



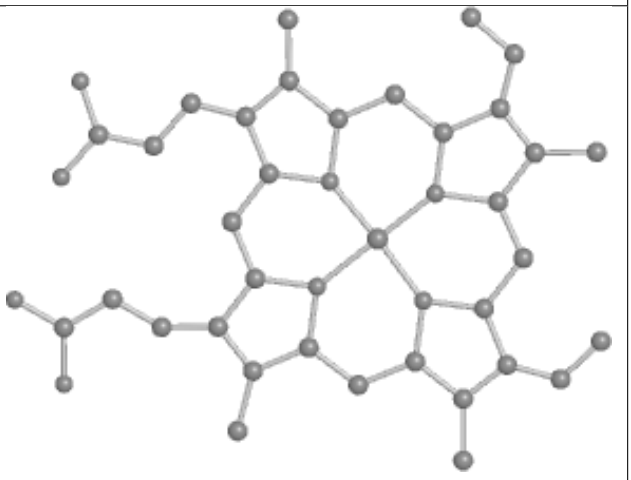
Bond lengths



Bond angles

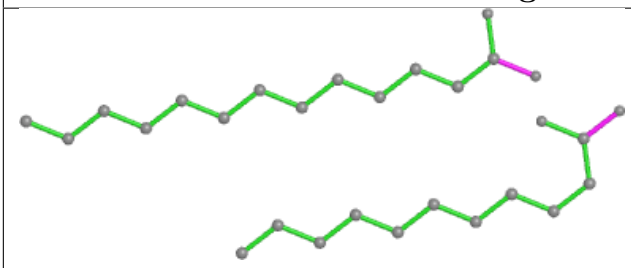


Torsions



Rings

Ligand LMG D 411



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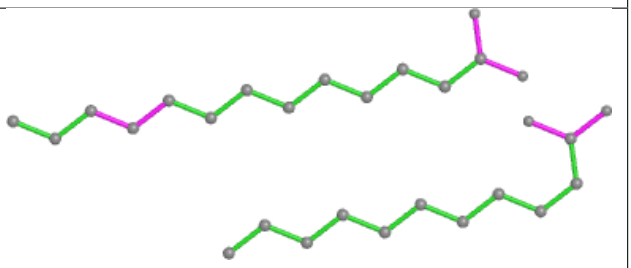
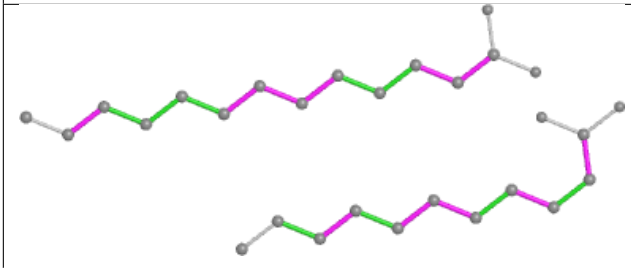
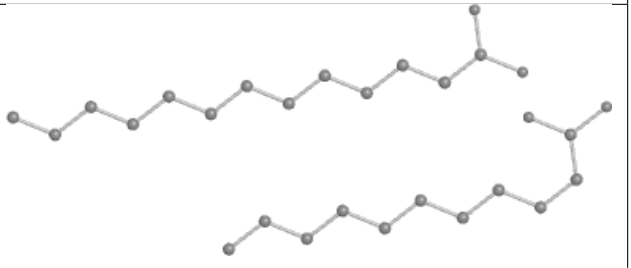


Bond angles

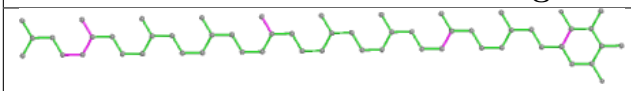


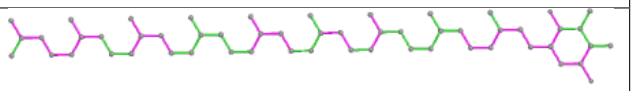
Torsions

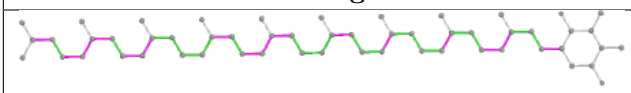


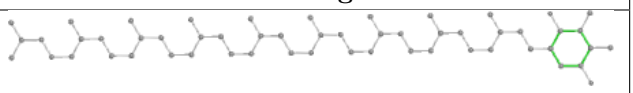
Rings

Ligand PL9 d 406

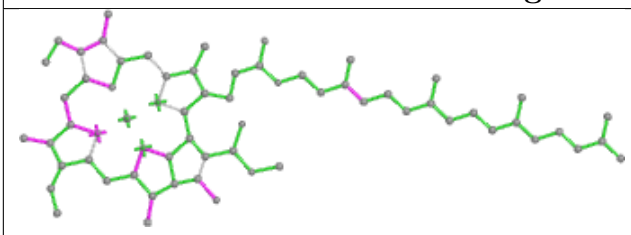

Bond lengths

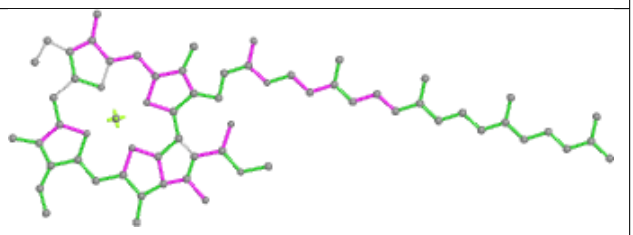

Bond angles

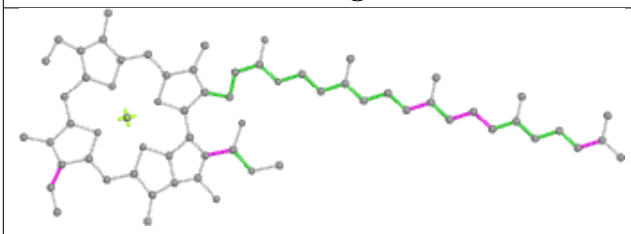

Torsions

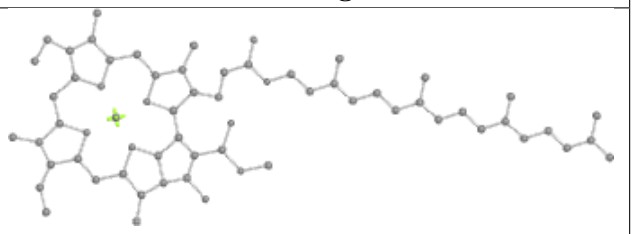

Rings

Ligand CLA B 613

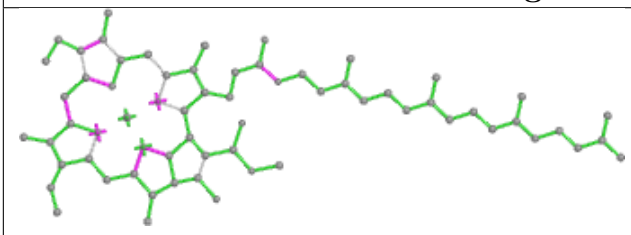

Bond lengths

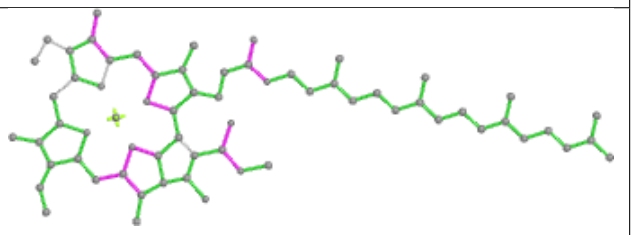

Bond angles

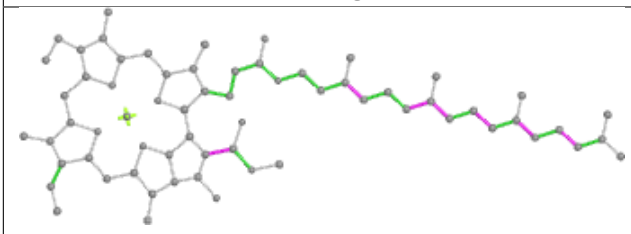

Torsions

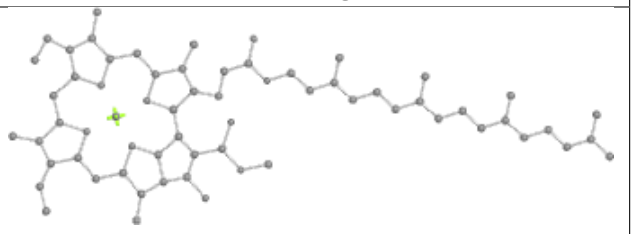

Rings

Ligand CLA C 510

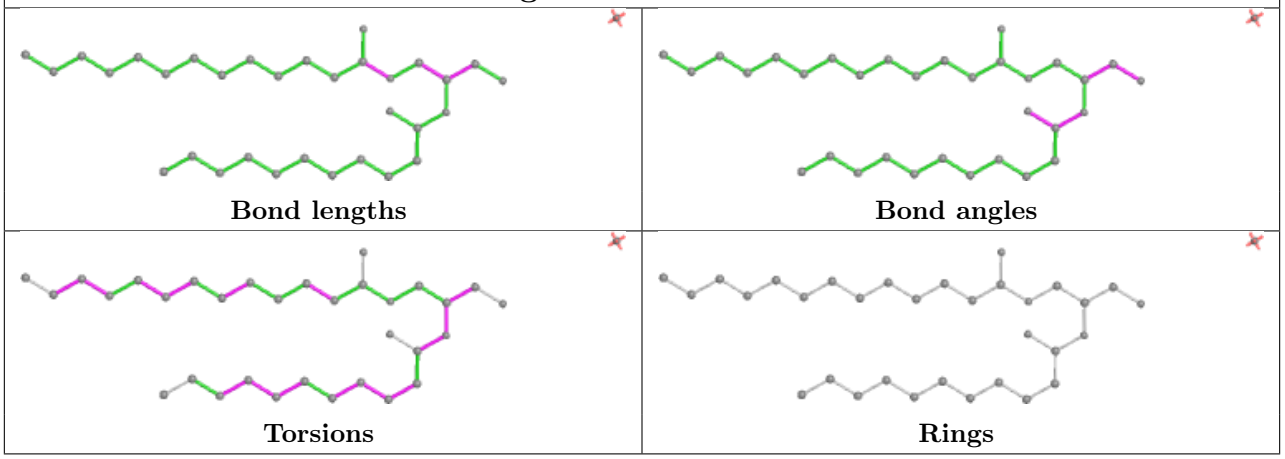

Bond lengths


Bond angles

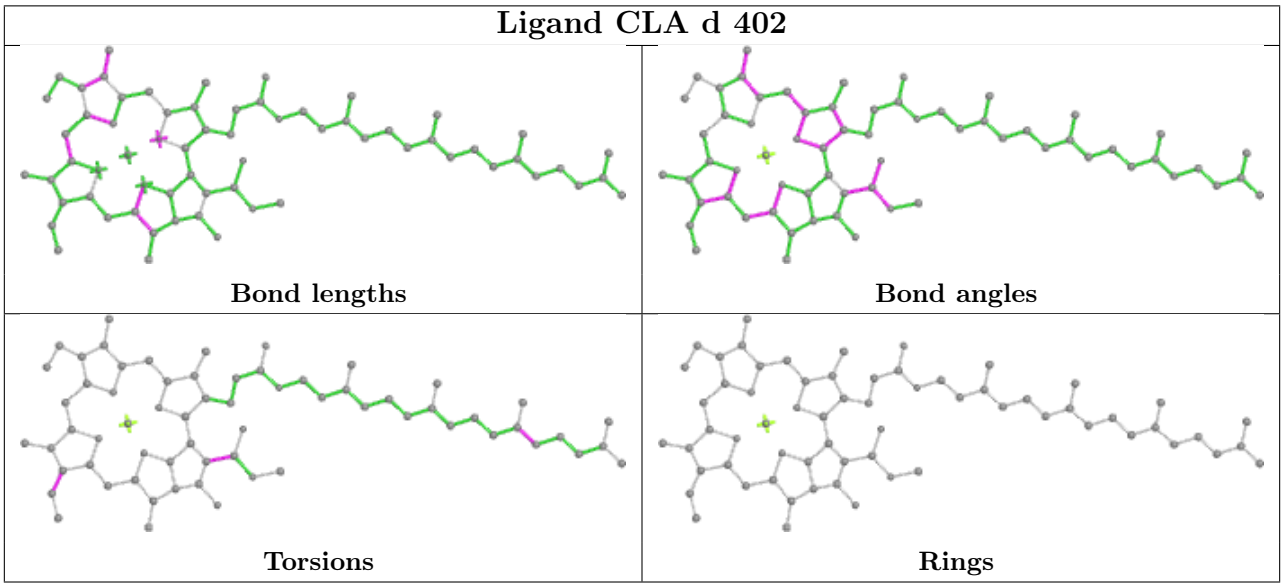

Torsions


Rings

Ligand LMG D 410



Ligand CLA d 402



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%)	-0.53	2 (0%) 89 88	22, 30, 52, 77	0
1	a	334/334 (100%)	-0.49	1 (0%) 94 93	22, 32, 61, 86	0
2	B	505/505 (100%)	-0.45	6 (1%) 79 77	22, 34, 64, 101	0
2	b	505/505 (100%)	-0.34	10 (1%) 65 63	24, 38, 74, 107	0
3	C	442/451 (98%)	-0.40	0 100 100	24, 38, 56, 78	0
3	c	451/451 (100%)	-0.30	5 (1%) 80 79	26, 42, 62, 108	0
4	D	341/341 (100%)	-0.46	0 100 100	23, 32, 51, 87	0
4	d	341/341 (100%)	-0.39	4 (1%) 79 77	23, 36, 60, 85	0
5	E	81/82 (98%)	-0.06	2 (2%) 57 55	32, 50, 70, 76	0
5	e	82/82 (100%)	0.06	1 (1%) 79 77	40, 60, 79, 90	0
6	F	34/34 (100%)	-0.30	2 (5%) 22 21	36, 45, 67, 93	0
6	f	34/34 (100%)	-0.20	0 100 100	42, 51, 81, 88	0
7	H	65/65 (100%)	-0.13	0 100 100	33, 42, 60, 67	0
7	h	63/65 (96%)	0.05	1 (1%) 72 70	39, 51, 62, 74	0
8	I	35/36 (97%)	-0.29	2 (5%) 23 22	32, 39, 71, 79	0
8	i	35/36 (97%)	-0.22	2 (5%) 23 22	33, 42, 72, 86	0
9	J	36/36 (100%)	0.00	4 (11%) 5 4	35, 51, 75, 96	0
9	j	36/36 (100%)	0.05	3 (8%) 11 10	38, 55, 79, 88	0
10	K	37/37 (100%)	-0.20	1 (2%) 54 52	41, 54, 68, 74	0
10	k	37/37 (100%)	0.02	1 (2%) 54 52	45, 59, 72, 85	0
11	L	37/37 (100%)	-0.31	0 100 100	25, 32, 67, 78	0
11	l	36/37 (97%)	-0.43	0 100 100	26, 33, 74, 77	0
12	M	32/33 (96%)	-0.36	1 (3%) 49 47	28, 35, 62, 76	0
12	m	31/33 (93%)	-0.27	0 100 100	26, 35, 52, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.14	10 (4%) 37 35	23, 43, 79, 137	0
13	o	244/244 (100%)	-0.24	9 (3%) 41 39	24, 42, 82, 122	0
14	T	29/30 (96%)	-0.69	1 (3%) 45 43	26, 32, 62, 79	0
14	t	29/30 (96%)	-0.37	2 (6%) 16 15	28, 33, 81, 93	0
15	U	97/97 (100%)	-0.39	1 (1%) 82 81	29, 44, 68, 93	0
15	u	97/97 (100%)	-0.48	2 (2%) 63 61	30, 42, 61, 83	0
16	V	137/137 (100%)	-0.62	0 100 100	29, 41, 56, 84	0
16	v	137/137 (100%)	-0.28	1 (0%) 87 86	33, 49, 70, 81	0
17	Y	27/30 (90%)	1.70	13 (48%) 0 0	55, 78, 107, 116	0
17	y	30/30 (100%)	0.40	5 (16%) 1 1	58, 70, 87, 102	0
18	X	38/38 (100%)	-0.13	3 (7%) 12 11	35, 49, 79, 87	0
18	x	38/38 (100%)	0.00	3 (7%) 12 11	46, 57, 75, 103	0
19	Z	62/62 (100%)	0.64	14 (22%) 0 0	47, 64, 110, 120	0
19	z	62/62 (100%)	0.70	7 (11%) 5 4	55, 71, 110, 125	0
20	R	34/34 (100%)	1.28	10 (29%) 0 0	56, 70, 89, 97	0
20	r	31/34 (91%)	2.02	17 (54%) 0 0	65, 84, 101, 108	0
All	All	5300/5326 (99%)	-0.29	146 (2%) 53 51	22, 39, 75, 137	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	59	LYS	8.3
19	z	33	TRP	7.8
13	o	3	GLN	7.3
1	A	13	LEU	6.4
13	O	60	ARG	5.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.90	0.18	40,50,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.90	0.12	33,48,73,78	0
14	FME	T	1	10/11	0.91	0.14	32,46,75,75	0
8	FME	i	1	10/11	0.94	0.12	37,52,72,72	0
8	FME	I	1	10/11	0.94	0.16	39,53,74,74	0
12	FME	m	1	10/11	0.96	0.14	34,58,78,84	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	a	415	28/-	0.70	0.37	43,71,87,94	0
27	LMG	b	623	23/55	0.76	0.22	35,66,90,91	0
32	UNL	E	103	28/-	0.78	0.31	58,81,95,97	0
27	LMG	b	622	55/55	0.79	0.26	41,78,99,111	0
33	LHG	E	101	49/49	0.80	0.23	51,82,112,120	0
32	UNL	H	103	53/-	0.81	0.23	35,77,97,101	0
32	UNL	B	626	28/-	0.81	0.36	50,75,87,89	0
32	UNL	b	621	55/-	0.81	0.19	40,62,91,109	0
28	SQD	a	412	36/54	0.81	0.18	29,68,100,110	0
32	UNL	I	101	41/-	0.82	0.16	40,55,77,82	0
32	UNL	b	625	55/-	0.82	0.21	44,66,86,91	0
32	UNL	c	523	28/-	0.82	0.20	43,69,80,82	0
27	LMG	c	522	48/55	0.82	0.26	50,82,110,114	0
32	UNL	b	626	26/-	0.83	0.24	33,59,66,67	0
26	PL9	a	409	55/55	0.83	0.27	34,67,89,101	0
32	UNL	B	627	47/-	0.83	0.27	41,65,89,89	0
29	DGD	a	413	44/66	0.84	0.16	33,59,88,94	0
32	UNL	C	521	28/-	0.84	0.13	36,50,61,62	0
32	UNL	J	101	28/-	0.84	0.12	49,62,72,75	0
32	UNL	T	102	44/-	0.84	0.19	41,55,68,72	0
32	UNL	x	101	55/-	0.84	0.20	47,62,78,78	0
27	LMG	D	410	33/55	0.84	0.16	29,57,87,90	0
25	BCR	h	102	40/40	0.85	0.15	33,56,73,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	d	410	43/-	0.85	0.20	33,57,72,73	0
23	CLA	h	101	65/65	0.85	0.17	44,72,93,100	0
32	UNL	c	520	55/-	0.85	0.20	42,61,79,90	0
26	PL9	A	409	55/55	0.86	0.26	37,62,89,101	0
32	UNL	b	624	40/-	0.86	0.16	38,64,80,83	0
32	UNL	C	522	28/-	0.86	0.14	42,59,72,78	0
28	SQD	b	601	49/54	0.86	0.15	44,64,103,114	0
29	DGD	A	413	66/66	0.86	0.19	43,68,93,121	0
23	CLA	c	512	65/65	0.86	0.14	39,60,93,109	0
32	UNL	B	624	34/-	0.86	0.20	39,55,71,72	0
23	CLA	c	513	65/65	0.86	0.22	42,75,107,123	0
28	SQD	A	412	39/54	0.86	0.23	40,69,102,121	0
25	BCR	y	101	40/40	0.87	0.14	41,63,77,84	0
23	CLA	C	512	65/65	0.87	0.18	36,61,111,127	0
32	UNL	l	102	53/-	0.87	0.16	30,48,99,103	0
32	UNL	t	103	46/-	0.87	0.13	38,61,81,82	0
23	CLA	C	513	65/65	0.87	0.17	40,70,102,114	0
23	CLA	B	616	60/65	0.87	0.16	27,44,87,103	0
33	LHG	e	101	42/49	0.87	0.27	63,88,113,120	0
27	LMG	D	411	28/55	0.88	0.16	30,51,68,74	0
28	SQD	f	101	41/54	0.88	0.22	49,85,120,123	0
25	BCR	D	405	40/40	0.88	0.14	29,46,100,116	0
25	BCR	H	101	40/40	0.88	0.12	32,46,59,66	0
32	UNL	B	621	43/-	0.88	0.14	38,54,69,73	0
32	UNL	M	102	26/-	0.88	0.19	30,53,63,67	0
32	UNL	m	102	28/-	0.88	0.15	40,55,69,77	0
27	LMG	c	519	37/55	0.88	0.18	34,70,93,96	0
25	BCR	d	405	40/40	0.88	0.14	36,57,95,108	0
27	LMG	C	519	48/55	0.88	0.15	43,68,88,96	0
23	CLA	B	601	65/65	0.88	0.15	31,63,100,113	0
32	UNL	j	101	28/-	0.89	0.10	42,60,71,74	0
27	LMG	a	414	49/55	0.89	0.16	36,60,94,101	0
32	UNL	D	412	55/-	0.89	0.20	32,51,79,101	0
32	UNL	t	102	26/-	0.89	0.21	42,56,67,68	0
25	BCR	K	101	40/40	0.89	0.13	41,56,68,75	0
27	LMG	A	410	48/55	0.89	0.18	30,61,81,105	0
32	UNL	b	602	47/-	0.89	0.21	36,59,74,79	0
27	LMG	B	620	51/55	0.89	0.12	29,51,72,81	0
23	CLA	b	617	60/65	0.90	0.15	26,49,99,106	0
32	UNL	B	625	28/-	0.90	0.11	29,46,67,72	0
28	SQD	B	623	54/54	0.90	0.13	37,62,88,98	0
23	CLA	D	404	65/65	0.90	0.15	19,42,114,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	LMG	m	101	51/55	0.90	0.13	29,52,83,98	0
23	CLA	c	508	64/65	0.91	0.14	32,51,98,118	0
23	CLA	b	616	65/65	0.91	0.13	20,40,63,68	0
27	LMG	D	407	51/55	0.91	0.16	27,59,79,87	0
29	DGD	C	517	62/66	0.91	0.14	31,56,95,117	0
23	CLA	a	407	65/65	0.91	0.14	15,37,99,110	0
23	CLA	d	404	65/65	0.91	0.15	25,53,100,107	0
25	BCR	c	514	40/40	0.91	0.16	37,58,73,75	0
28	SQD	a	411	54/54	0.91	0.13	36,71,94,110	0
25	BCR	c	521	40/40	0.91	0.17	34,57,70,77	0
25	BCR	B	617	40/40	0.92	0.12	26,43,57,60	0
29	DGD	c	518	62/66	0.92	0.12	26,54,77,93	0
29	DGD	h	103	62/66	0.92	0.13	35,54,73,79	0
25	BCR	C	514	40/40	0.92	0.14	34,59,76,77	0
25	BCR	C	515	40/40	0.92	0.12	21,38,53,67	0
25	BCR	C	520	40/40	0.92	0.18	38,55,67,74	0
23	CLA	c	506	65/65	0.92	0.14	32,53,112,129	0
23	CLA	B	615	65/65	0.92	0.14	20,41,67,95	0
23	CLA	b	605	65/65	0.92	0.15	20,39,87,103	0
25	BCR	b	619	40/40	0.92	0.10	25,42,59,66	0
32	UNL	C	523	47/-	0.92	0.10	39,52,63,69	0
25	BCR	b	620	40/40	0.92	0.12	30,50,66,69	0
23	CLA	B	606	65/65	0.92	0.13	21,41,75,98	0
23	CLA	C	505	65/65	0.92	0.18	24,42,75,88	0
29	DGD	C	516	62/66	0.92	0.14	21,40,76,98	0
23	CLA	c	503	65/65	0.92	0.16	31,48,61,68	0
32	UNL	M	101	37/-	0.92	0.13	30,49,71,75	0
29	DGD	H	102	62/66	0.92	0.13	28,49,67,77	0
29	DGD	c	517	62/66	0.93	0.12	32,52,81,95	0
23	CLA	B	604	65/65	0.93	0.13	21,36,84,94	0
23	CLA	c	502	65/65	0.93	0.13	24,46,76,85	0
25	BCR	A	408	40/40	0.93	0.10	24,34,42,56	0
27	LMG	d	409	44/55	0.93	0.13	31,53,84,107	0
23	CLA	a	405	65/65	0.93	0.13	25,42,98,111	0
25	BCR	B	618	40/40	0.93	0.11	25,43,58,64	0
25	BCR	B	619	40/40	0.93	0.12	33,47,58,62	0
28	SQD	F	101	36/54	0.93	0.14	43,66,89,96	0
23	CLA	c	504	60/65	0.93	0.13	24,47,79,81	0
23	CLA	C	506	65/65	0.93	0.13	28,45,95,114	0
23	CLA	c	507	65/65	0.93	0.14	28,45,63,74	0
23	CLA	A	405	65/65	0.93	0.13	23,36,106,121	0
23	CLA	c	510	65/65	0.93	0.14	30,51,72,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	511	65/65	0.93	0.15	34,62,79,87	0
25	BCR	T	101	40/40	0.93	0.10	29,43,58,68	0
23	CLA	b	607	65/65	0.93	0.11	25,46,80,86	0
33	LHG	d	408	39/49	0.93	0.12	36,50,75,78	0
23	CLA	C	502	65/65	0.93	0.12	25,42,62,68	0
23	CLA	B	613	65/65	0.94	0.13	17,34,63,74	0
23	CLA	C	507	65/65	0.94	0.13	22,39,51,59	0
23	CLA	b	603	65/65	0.94	0.16	29,47,74,80	0
23	CLA	c	509	65/65	0.94	0.16	28,49,74,79	0
23	CLA	C	508	65/65	0.94	0.12	27,46,102,120	0
23	CLA	C	509	65/65	0.94	0.15	27,46,61,74	0
25	BCR	a	408	40/40	0.94	0.09	25,35,50,55	0
25	BCR	b	618	40/40	0.94	0.11	25,46,57,65	0
23	CLA	b	610	65/65	0.94	0.12	28,46,65,77	0
23	CLA	b	613	65/65	0.94	0.15	17,35,49,56	0
23	CLA	b	615	65/65	0.94	0.15	23,44,73,79	0
23	CLA	C	510	65/65	0.94	0.13	31,51,78,88	0
24	PHO	a	406	64/64	0.94	0.12	22,34,46,48	0
24	PHO	d	401	64/64	0.94	0.11	27,42,52,57	0
23	CLA	C	511	65/65	0.94	0.12	33,57,78,85	0
23	CLA	B	614	65/65	0.94	0.13	22,41,85,96	0
26	PL9	D	406	55/55	0.94	0.12	22,36,51,54	0
23	CLA	C	504	59/65	0.94	0.14	22,44,81,96	0
33	LHG	a	410	49/49	0.94	0.13	38,53,87,104	0
23	CLA	B	609	65/65	0.94	0.11	23,37,52,63	0
23	CLA	c	505	65/65	0.94	0.14	26,44,62,69	0
33	LHG	l	101	49/49	0.94	0.14	31,49,66,78	0
28	SQD	A	411	52/54	0.95	0.14	30,64,88,97	0
23	CLA	d	403	65/65	0.95	0.11	20,38,63,75	0
25	BCR	c	515	40/40	0.95	0.12	32,49,69,77	0
23	CLA	b	612	65/65	0.95	0.11	18,36,51,56	0
23	CLA	C	501	65/65	0.95	0.12	24,37,54,64	0
24	PHO	A	406	64/64	0.95	0.11	17,30,42,53	0
25	BCR	t	101	40/40	0.95	0.09	27,42,57,61	0
23	CLA	b	614	65/65	0.95	0.14	19,33,86,94	0
23	CLA	B	607	65/65	0.95	0.12	18,35,71,85	0
23	CLA	C	503	65/65	0.95	0.11	27,44,56,69	0
23	CLA	D	402	65/65	0.95	0.11	17,29,54,61	0
29	DGD	C	518	62/66	0.95	0.10	28,47,84,98	0
26	PL9	d	406	55/55	0.95	0.11	23,37,48,48	0
23	CLA	c	501	65/65	0.95	0.13	25,42,59,68	0
29	DGD	c	516	62/66	0.95	0.12	20,45,71,80	0

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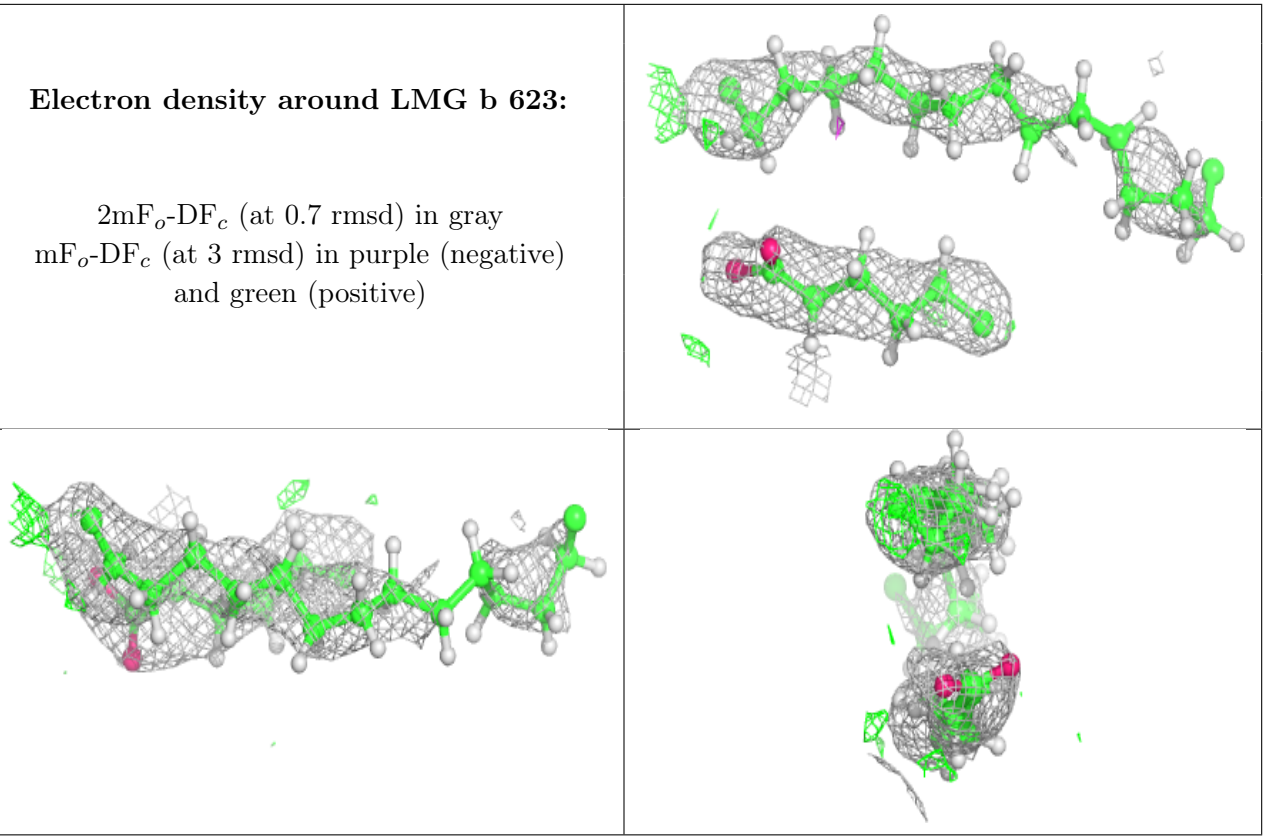
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	D	403	65/65	0.95	0.11	15,34,60,62	0
23	CLA	B	602	65/65	0.95	0.12	24,39,68,80	0
23	CLA	a	404	65/65	0.95	0.11	20,32,45,53	0
23	CLA	B	610	65/65	0.95	0.15	18,33,48,50	0
23	CLA	B	611	65/65	0.95	0.10	19,32,49,53	0
23	CLA	B	603	65/65	0.95	0.14	18,34,60,70	0
23	CLA	b	604	65/65	0.95	0.14	24,41,67,69	0
33	LHG	B	622	49/49	0.95	0.12	26,46,73,77	0
33	LHG	D	409	47/49	0.95	0.11	25,51,82,101	0
23	CLA	A	407	54/65	0.95	0.13	12,31,68,79	0
23	CLA	B	605	65/65	0.95	0.14	18,33,47,57	0
33	LHG	d	407	49/49	0.95	0.11	26,45,64,80	0
23	CLA	b	609	65/65	0.95	0.12	26,43,65,70	0
23	CLA	A	404	65/65	0.95	0.10	16,29,43,51	0
23	CLA	b	611	65/65	0.95	0.14	25,39,59,60	0
34	HEM	E	102	43/43	0.95	0.13	33,52,67,72	0
23	CLA	b	608	65/65	0.96	0.11	19,37,78,96	0
33	LHG	L	101	49/49	0.96	0.12	28,45,61,67	0
23	CLA	B	612	65/65	0.96	0.14	17,32,57,69	0
23	CLA	b	606	65/65	0.96	0.12	21,36,53,59	0
24	PHO	D	401	64/64	0.96	0.09	23,35,46,51	0
23	CLA	d	402	65/65	0.96	0.10	22,34,43,51	0
33	LHG	D	408	49/49	0.96	0.11	22,43,59,74	0
23	CLA	B	608	65/65	0.96	0.10	19,37,56,61	0
34	HEM	e	102	43/43	0.96	0.13	39,56,79,91	0
31	BCT	A	415	4/4	0.97	0.16	31,36,37,44	0
35	HEC	V	201	43/43	0.97	0.13	25,34,45,49	0
35	HEC	v	201	43/43	0.97	0.14	26,38,52,54	0
31	BCT	a	417	4/4	0.98	0.15	30,37,42,45	0
22	CL	a	403	1/1	0.98	0.05	29,29,29,29	0
30	OEY	A	414	11/11	0.99	0.10	28,31,39,43	1
30	OEY	a	416	11/11	0.99	0.11	24,30,34,35	0
22	CL	A	402	1/1	0.99	0.08	26,26,26,26	0
22	CL	A	403	1/1	0.99	0.02	25,25,25,25	0
22	CL	a	402	1/1	0.99	0.02	31,31,31,31	0
21	FE2	A	401	1/1	0.99	0.08	33,33,33,33	0
21	FE2	a	401	1/1	0.99	0.06	37,37,37,37	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.

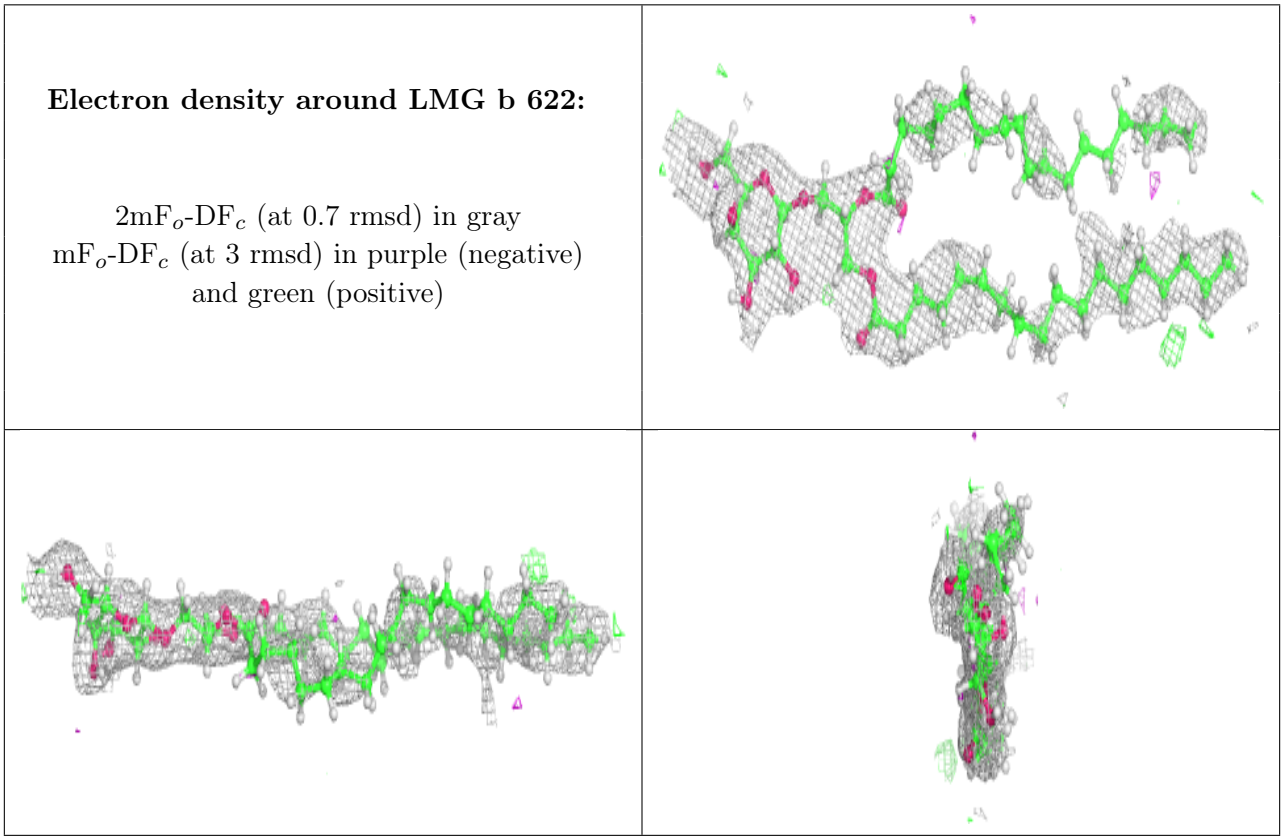
Electron density around LMG b 623:

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



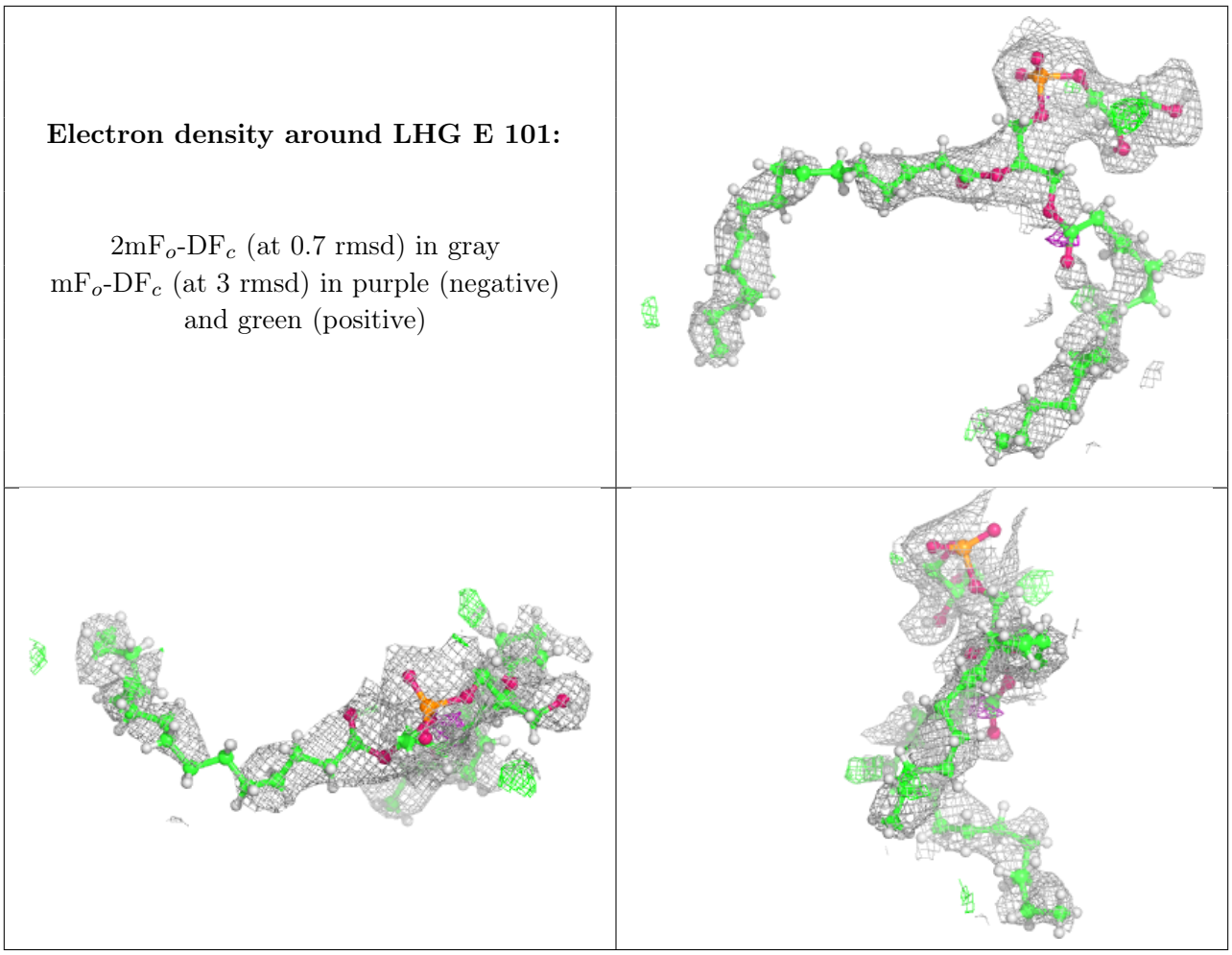
Electron density around LMG b 622:

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



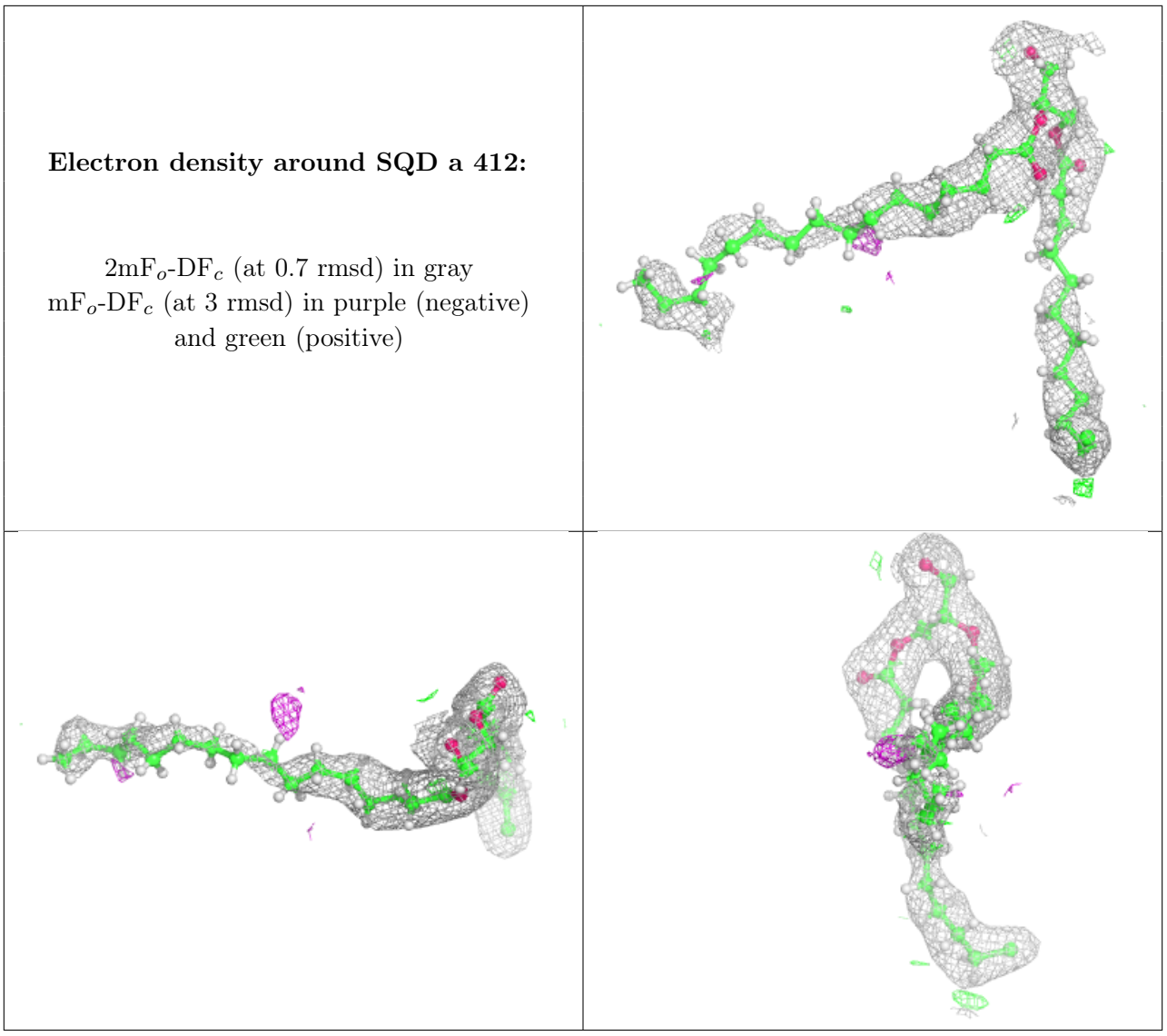
Electron density around LHG E 101:

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



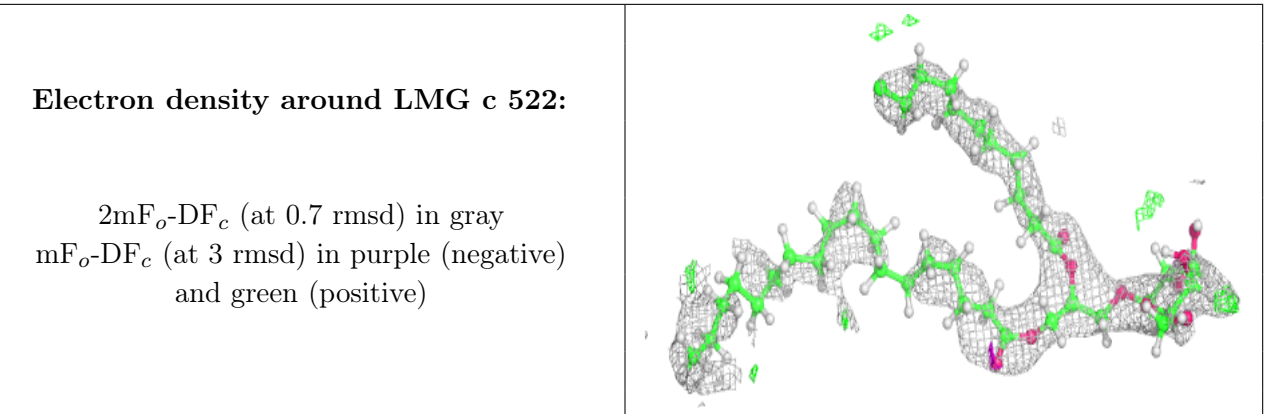
Electron density around SQD a 412:

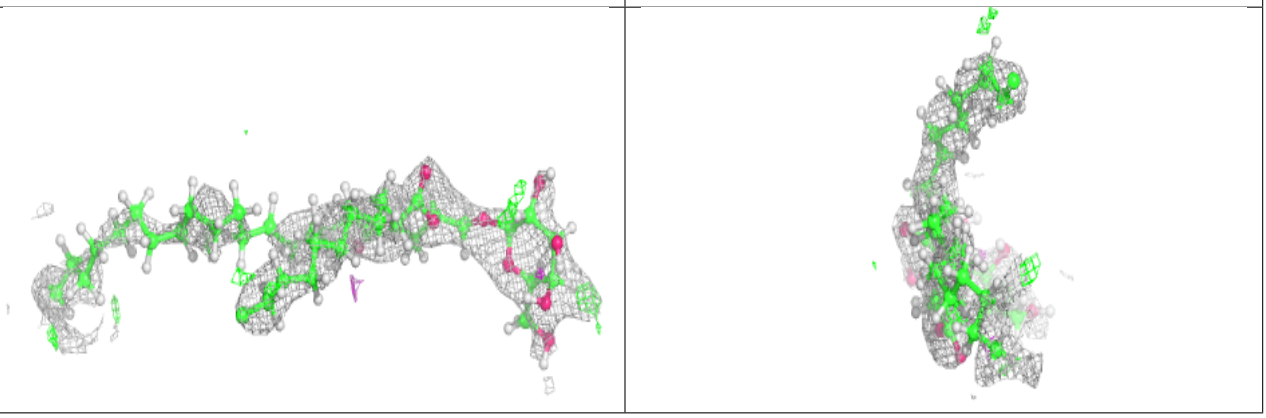
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG c 522:

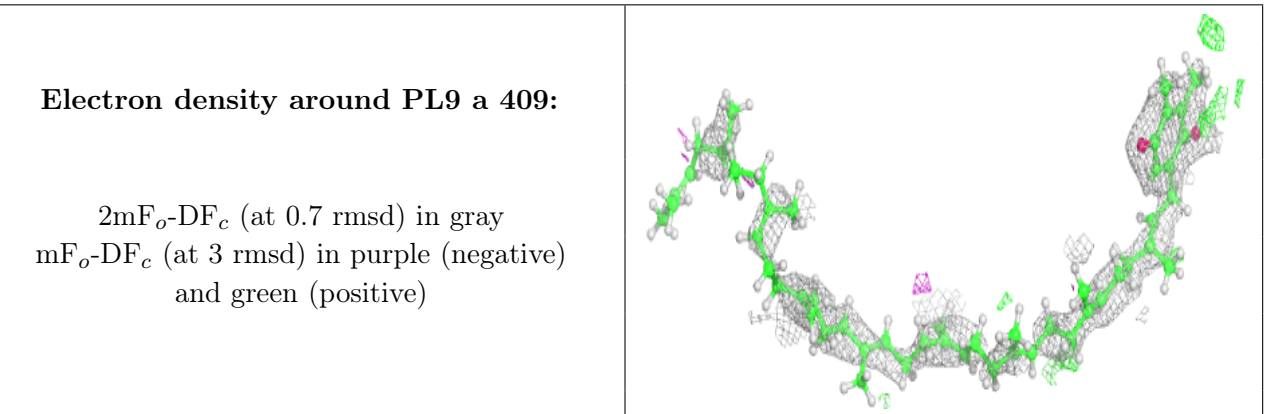
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

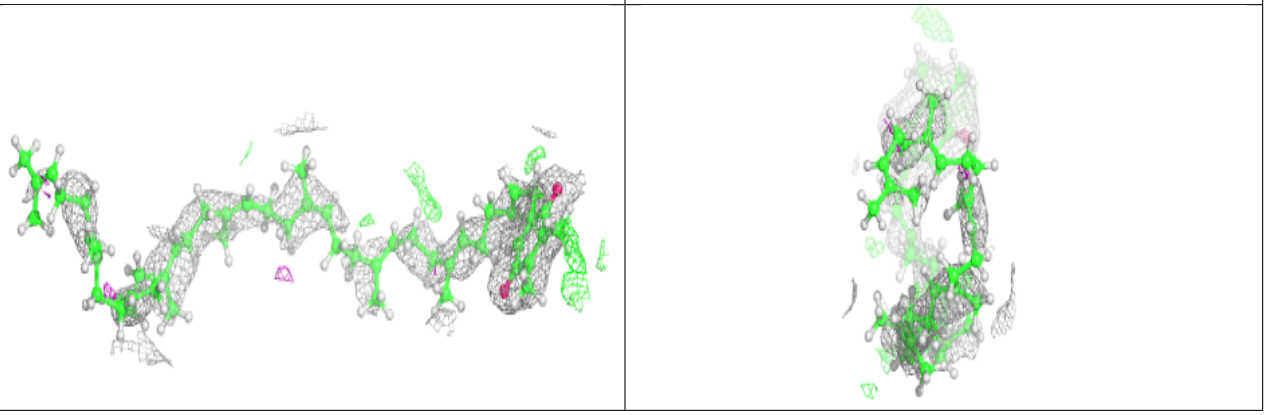




Electron density around PL9 a 409:

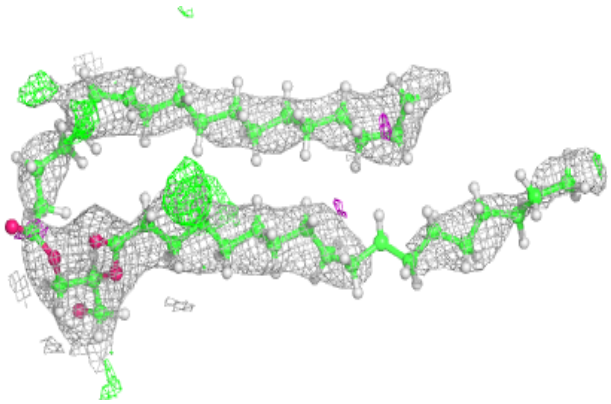
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

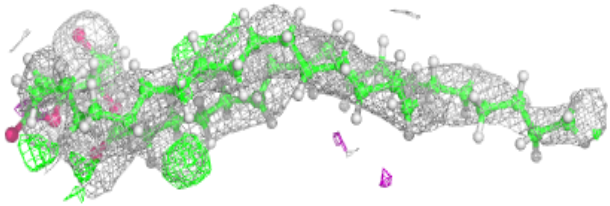


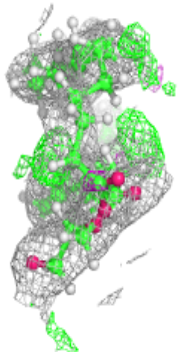


Electron density around DGD a 413:

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

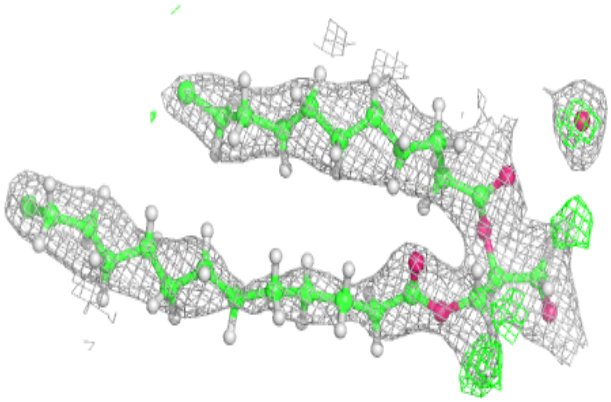


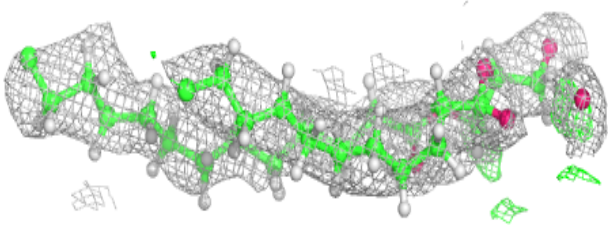


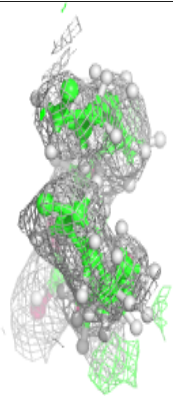


Electron density around LMG D 410:

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

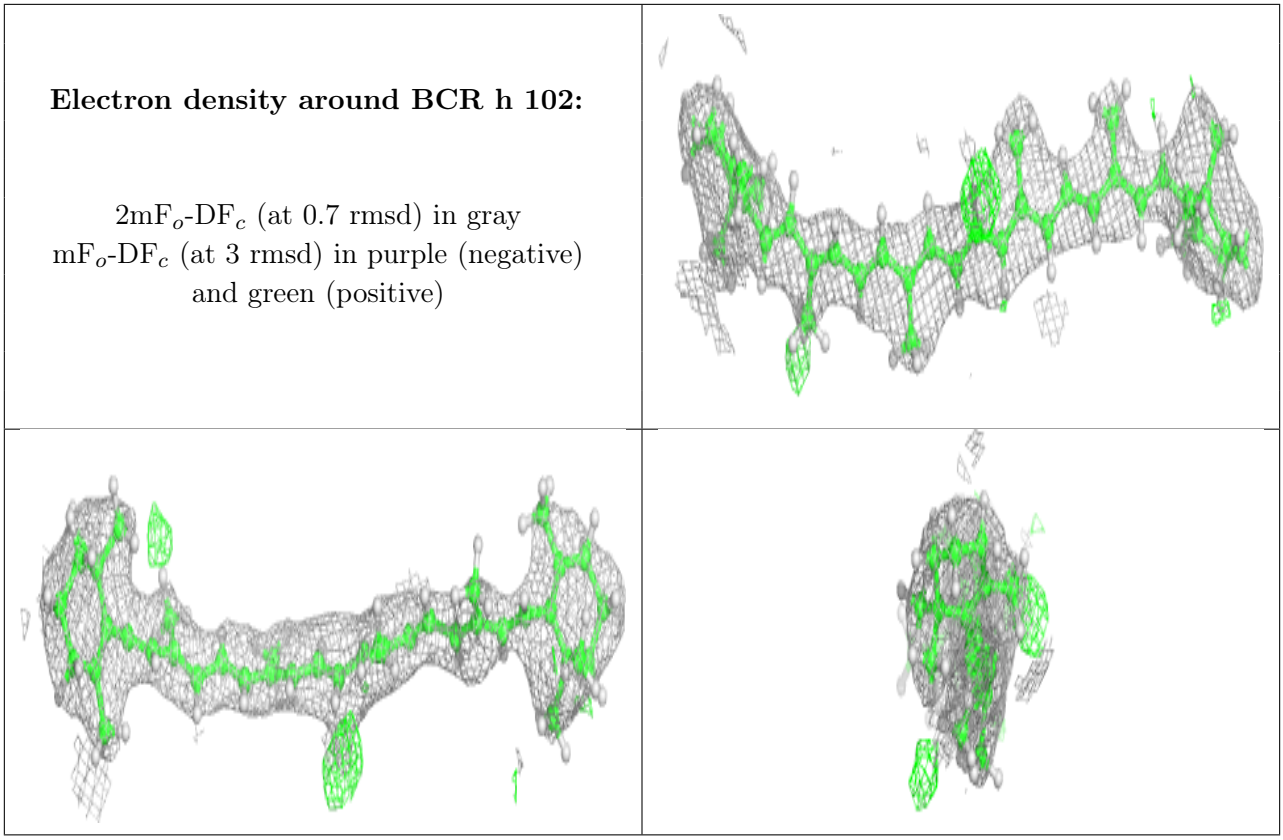






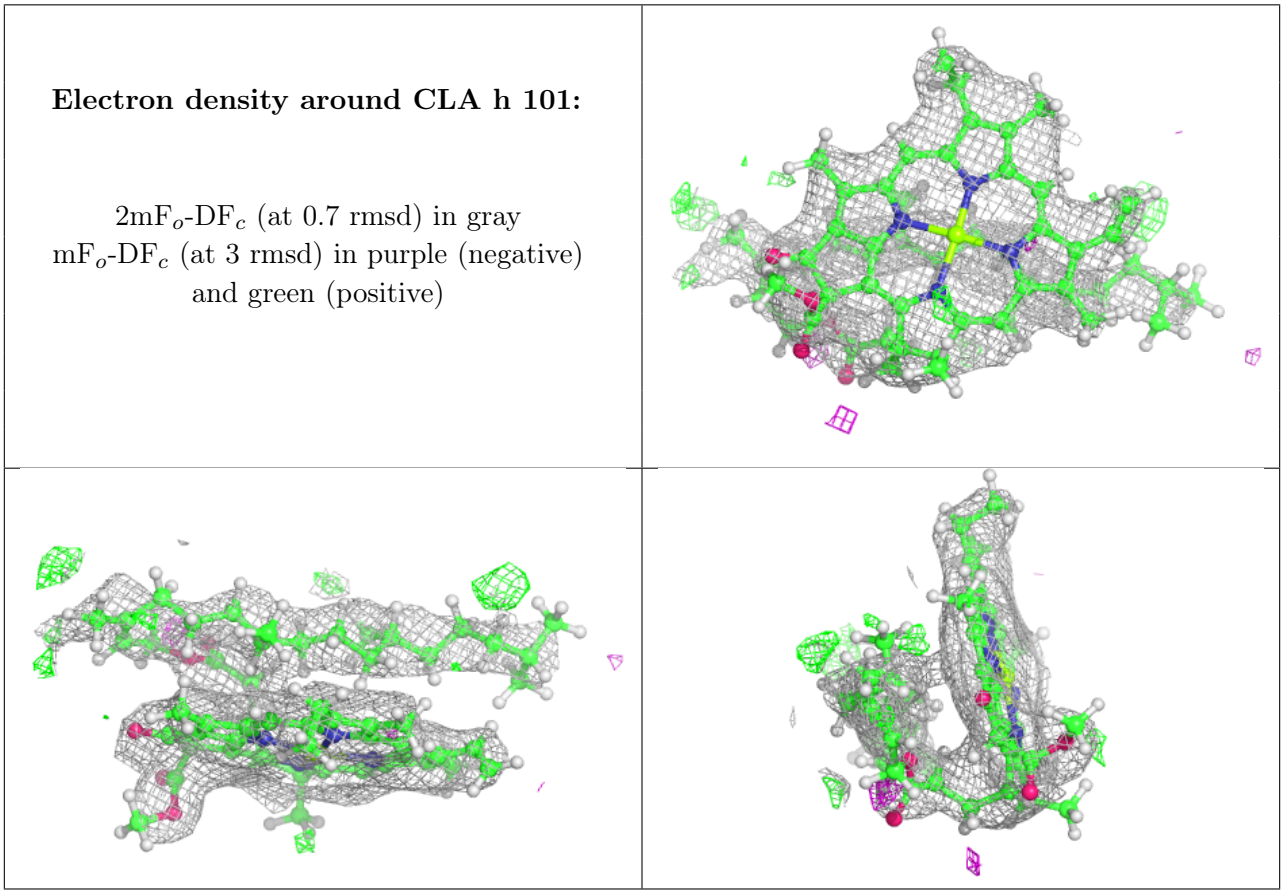
Electron density around BCR h 102:

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



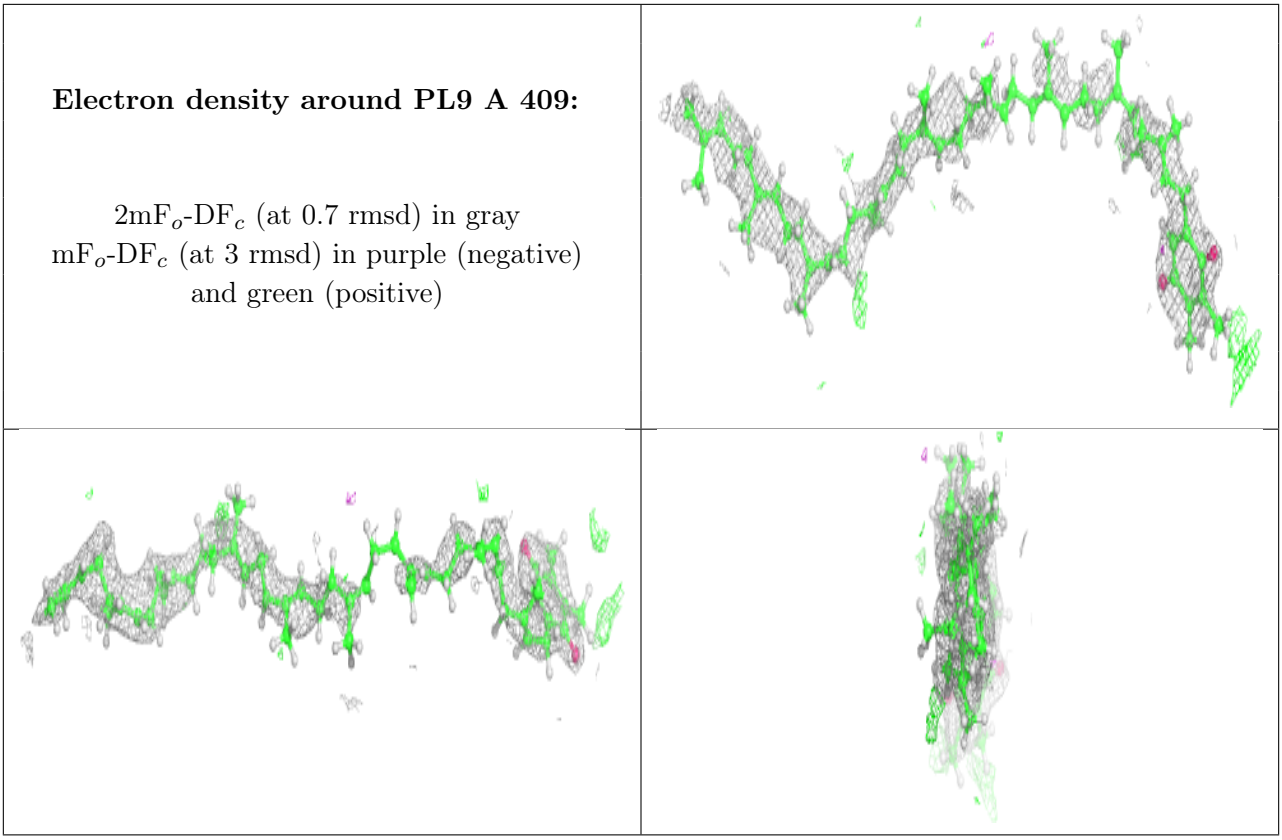
Electron density around CLA h 101:

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



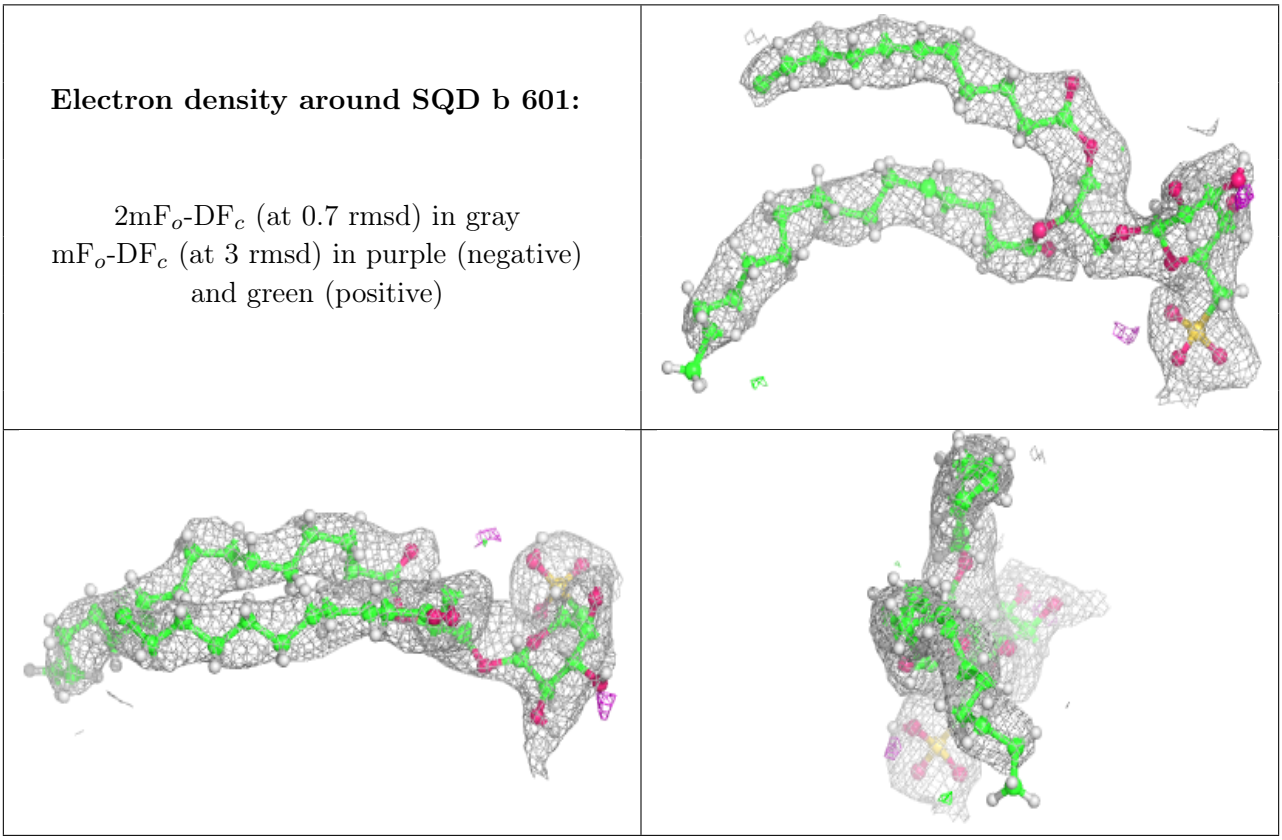
Electron density around PL9 A 409:

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



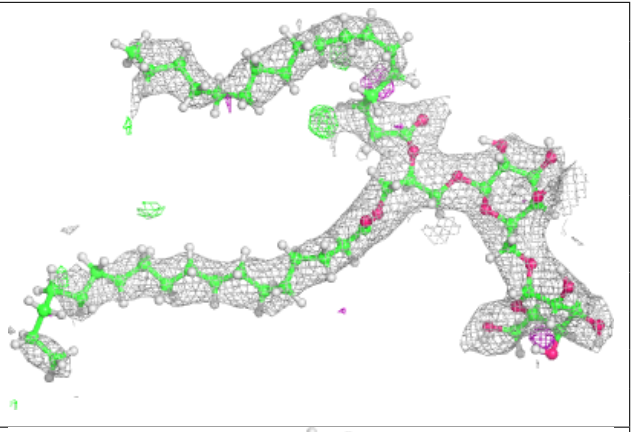
Electron density around SQD b 601:

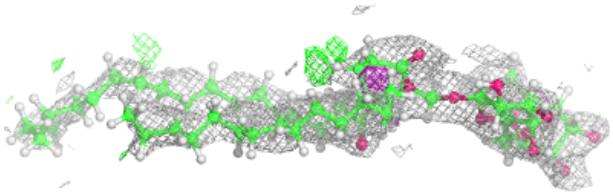
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

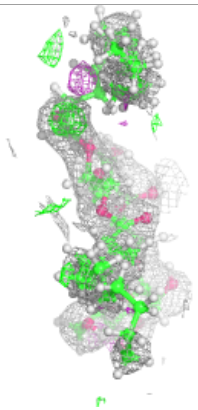


Electron density around DGD A 413:

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

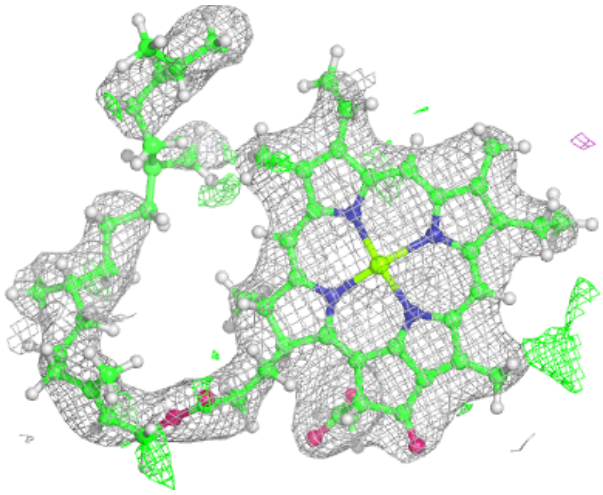


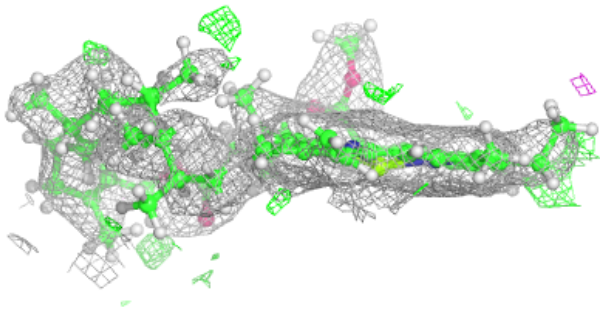


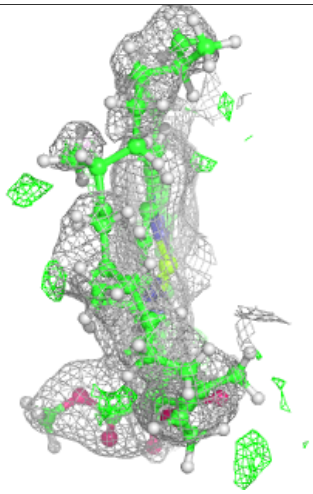


Electron density around CLA c 512:

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

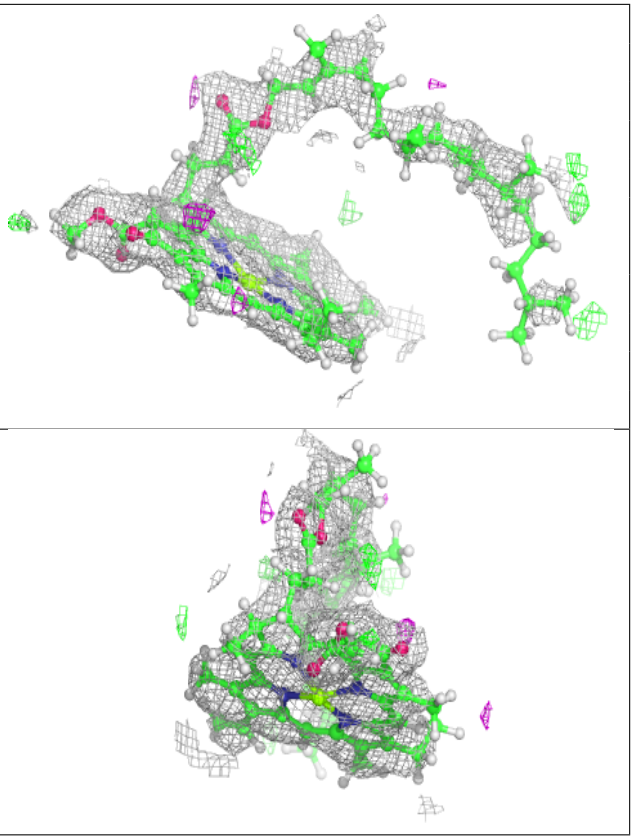


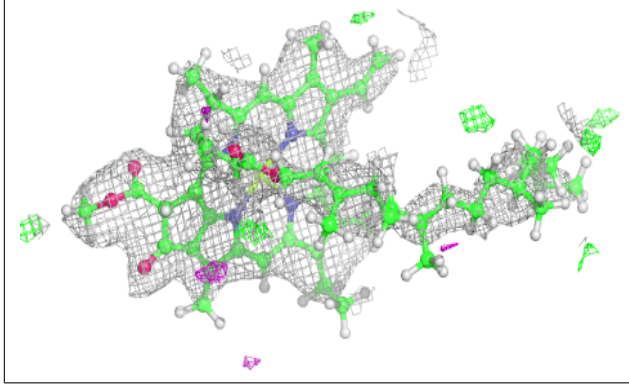




Electron density around CLA c 513:

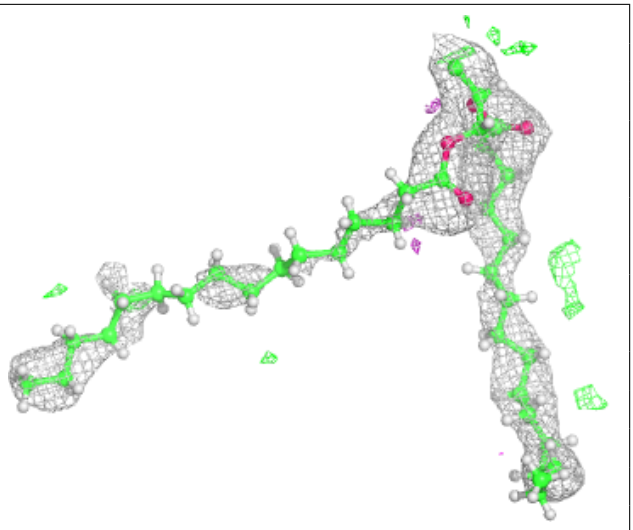
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

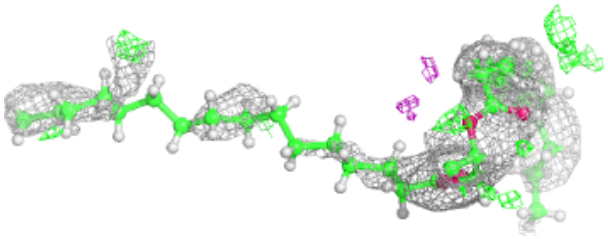


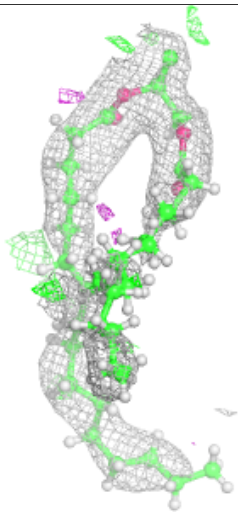


Electron density around SQD A 412:

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

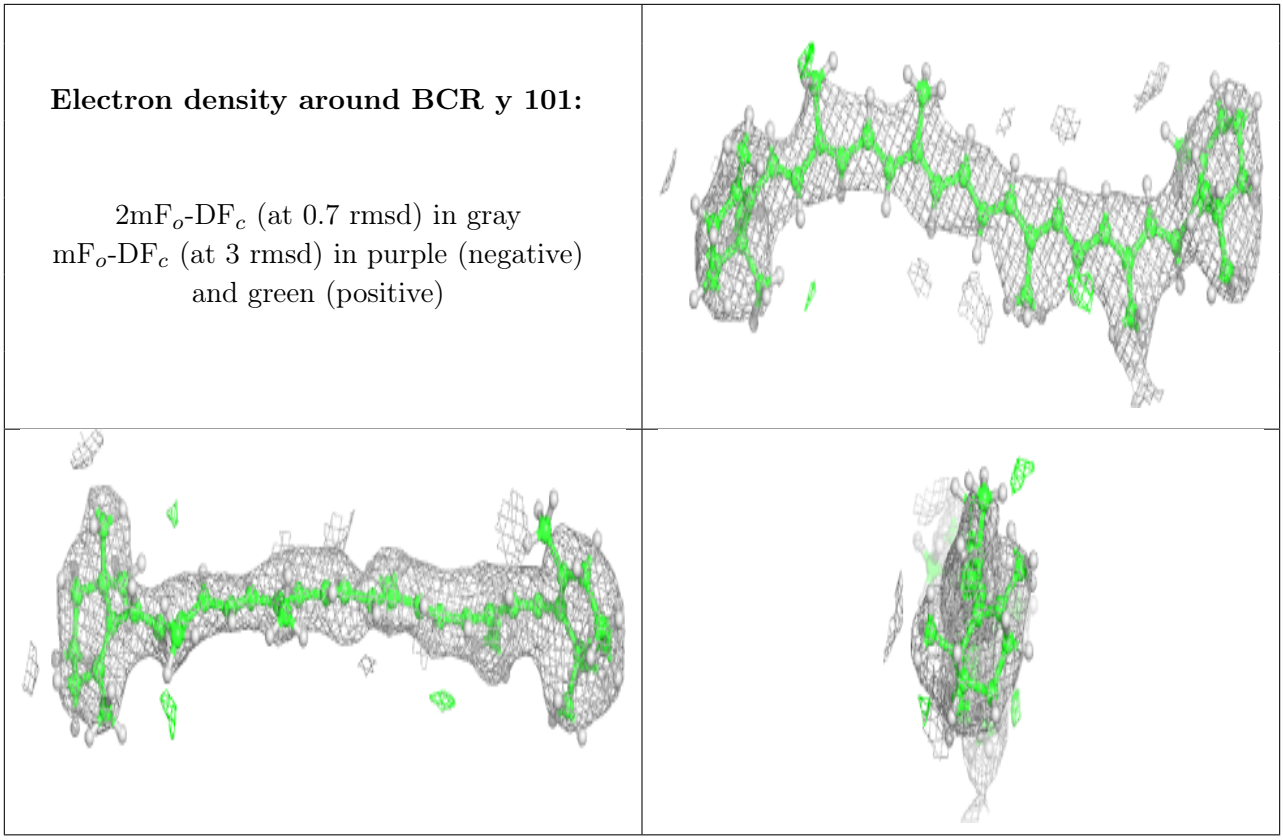






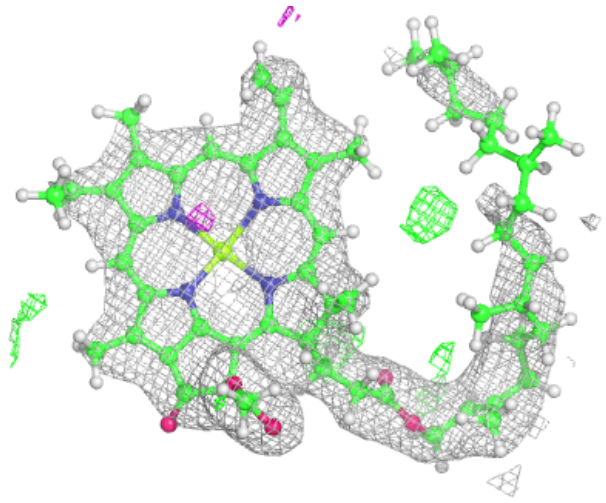
Electron density around BCR y 101:

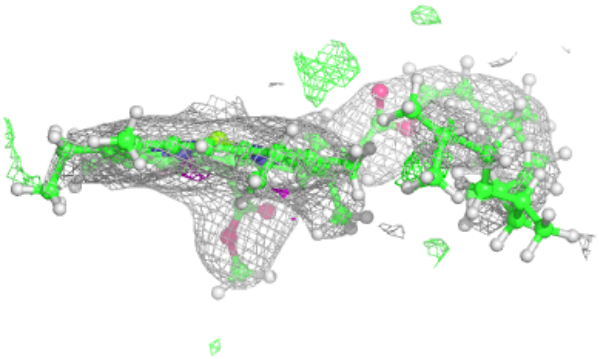
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

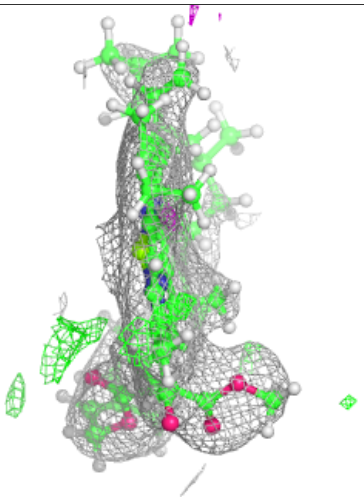


Electron density around CLA C 512:

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

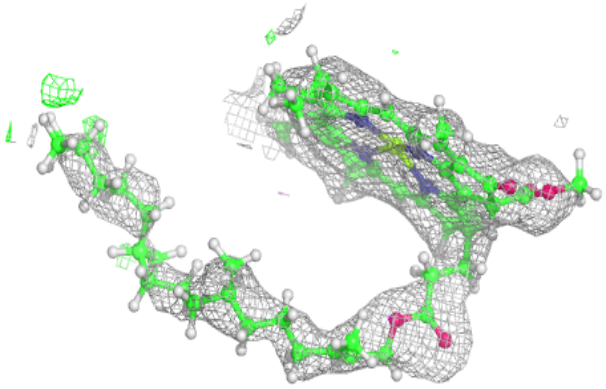


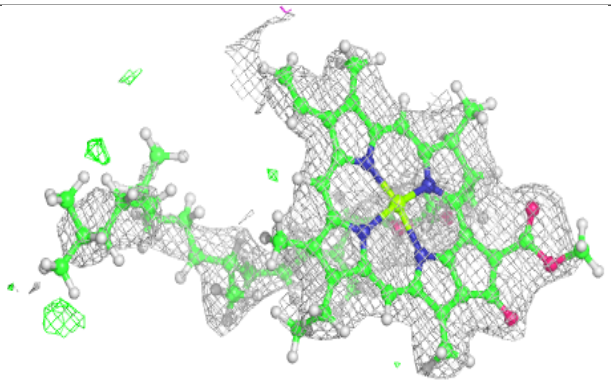


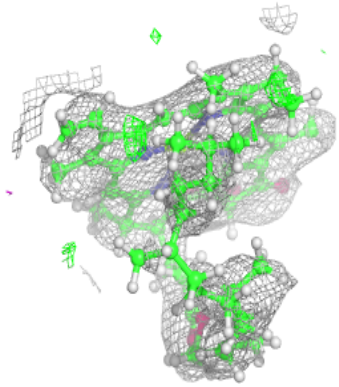


Electron density around CLA C 513:

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

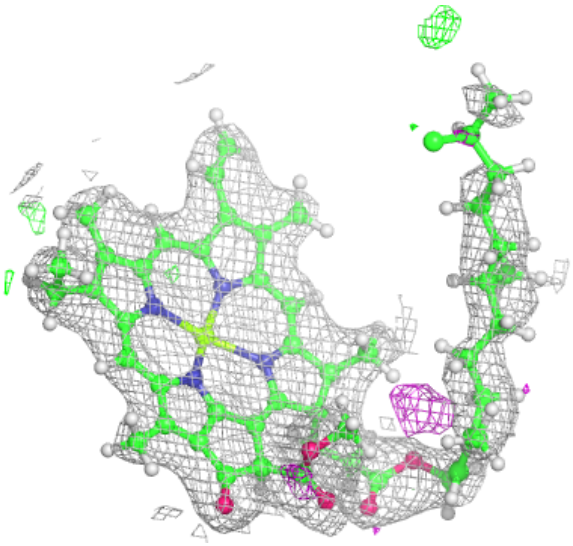


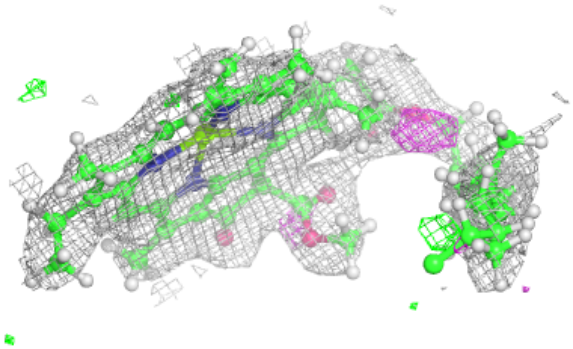


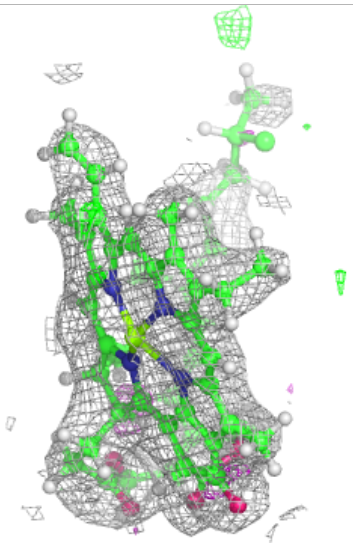


Electron density around CLA B 616:

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

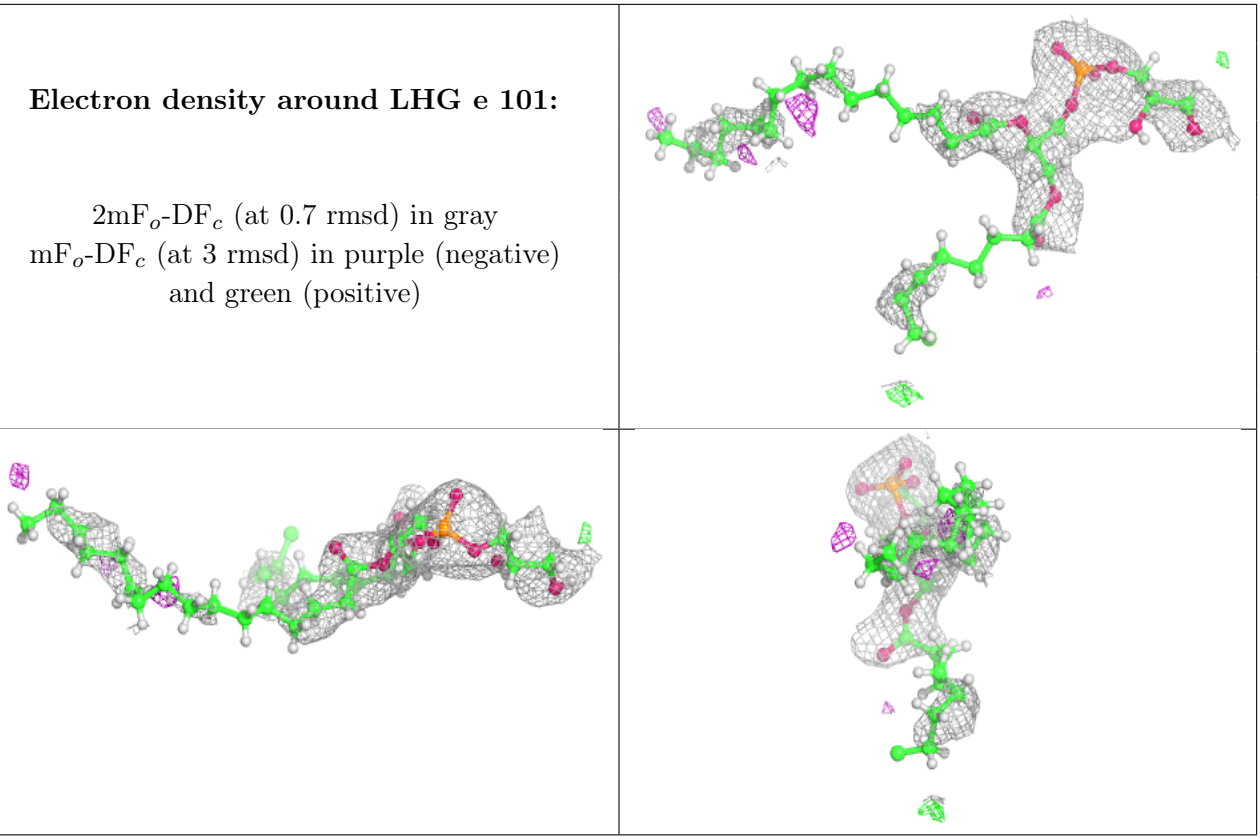






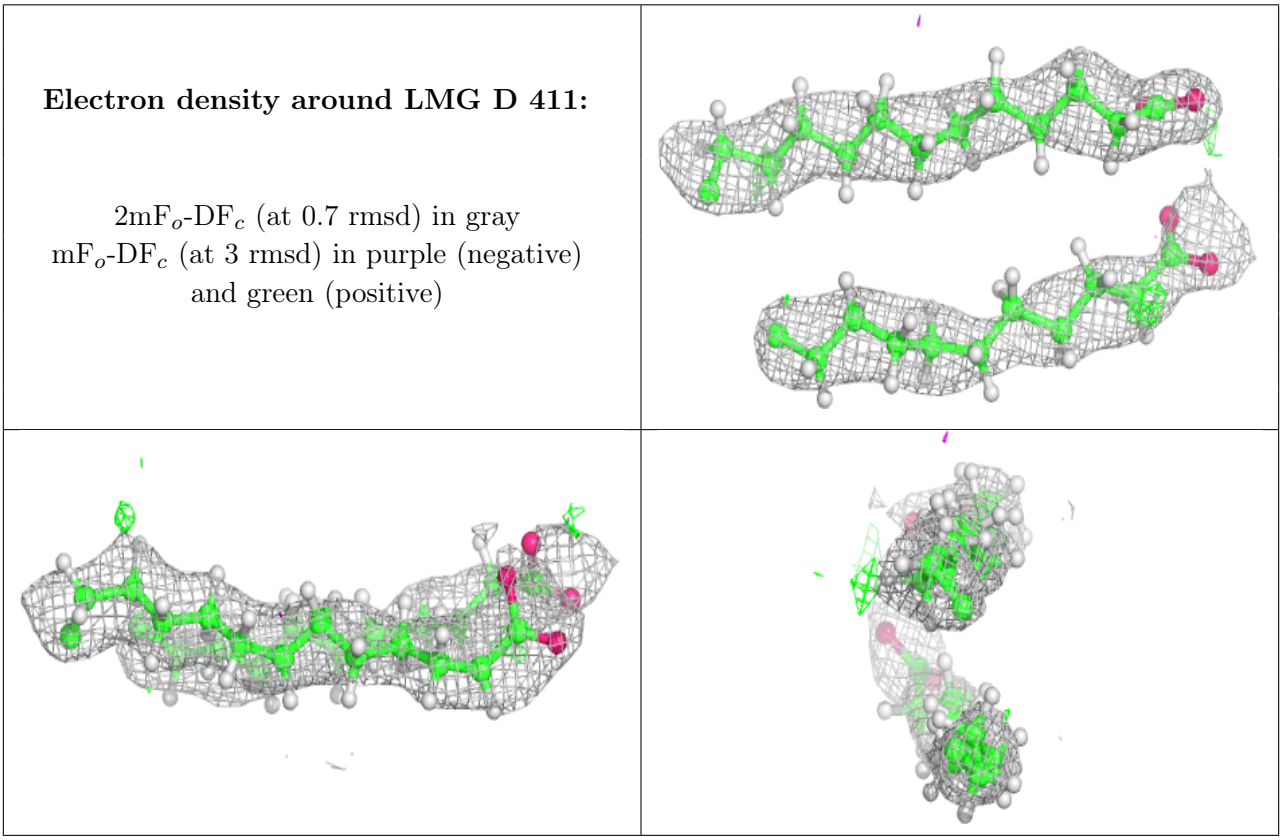
Electron density around LHG e 101:

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



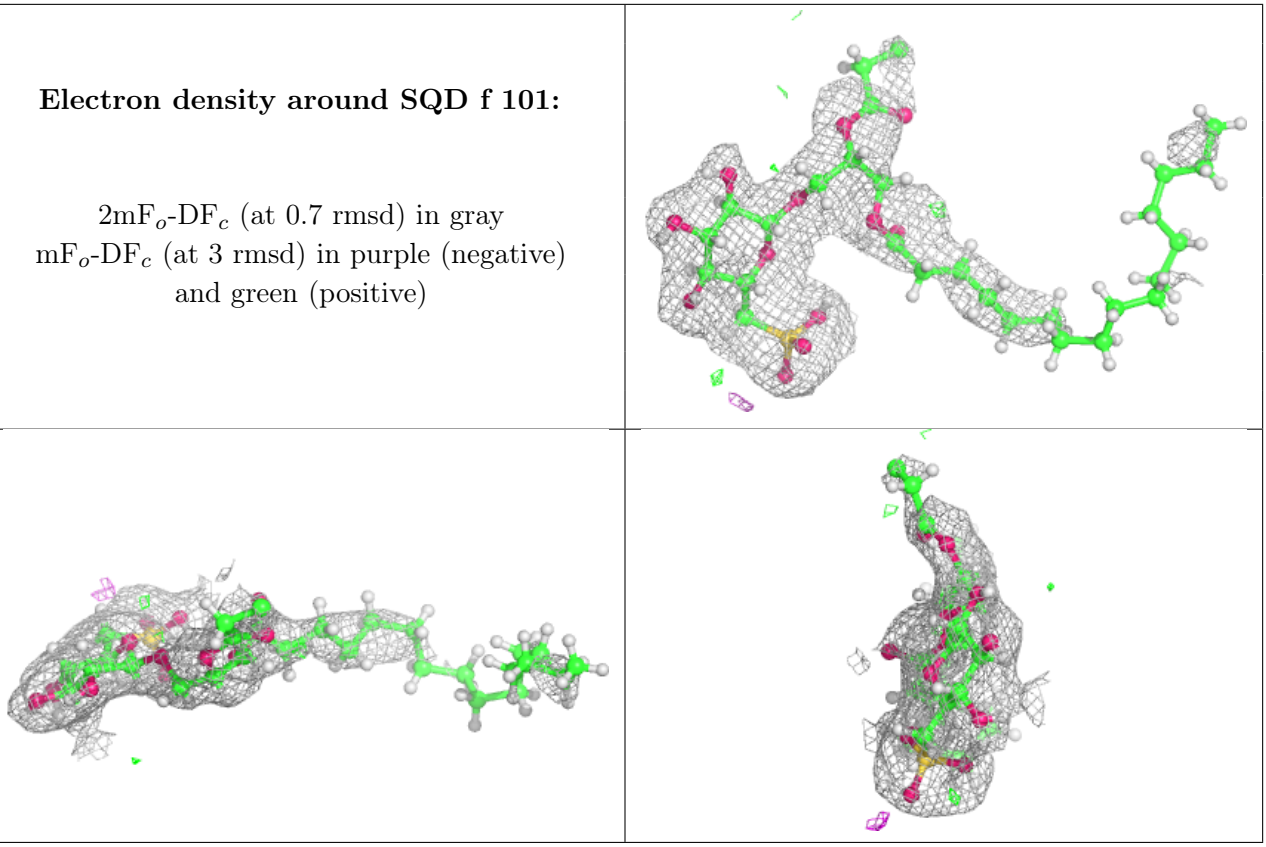
Electron density around LMG D 411:

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



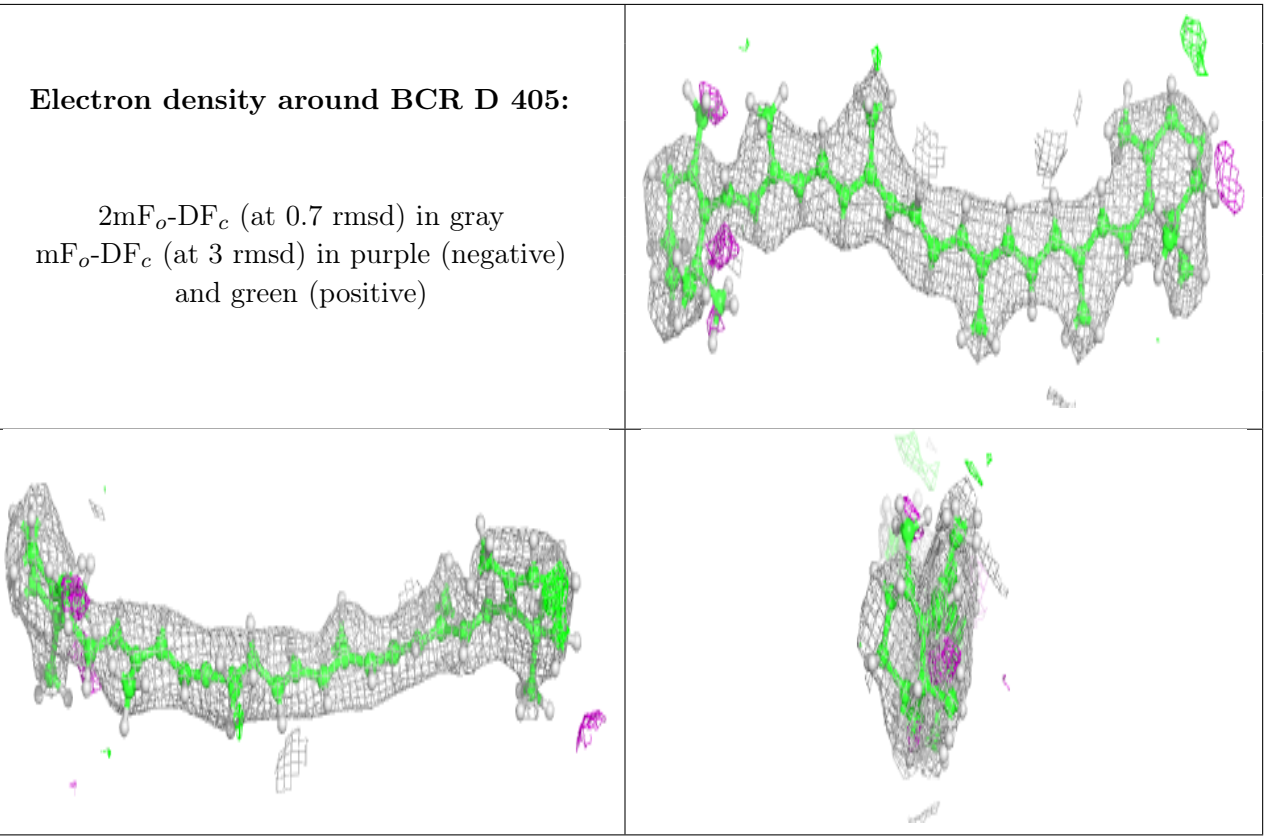
Electron density around SQD f 101:

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



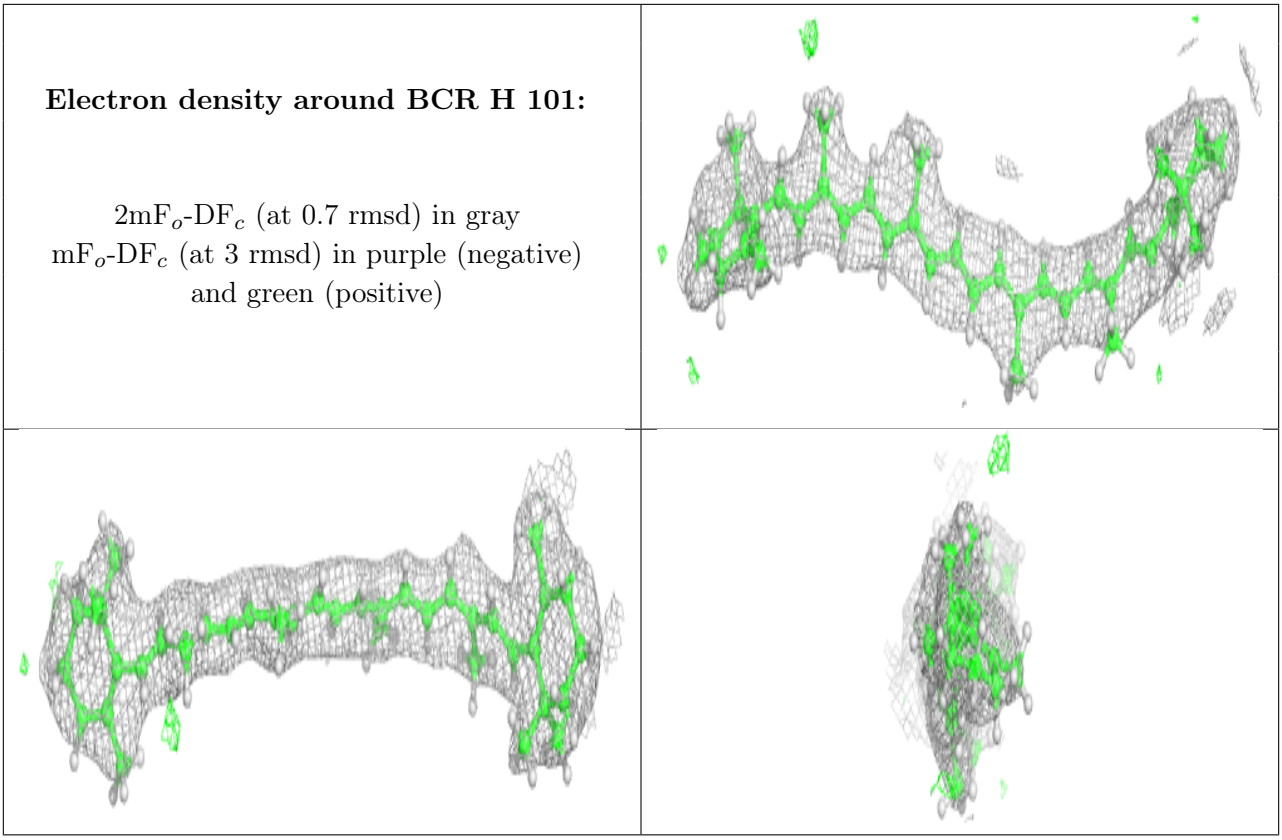
Electron density around BCR D 405:

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



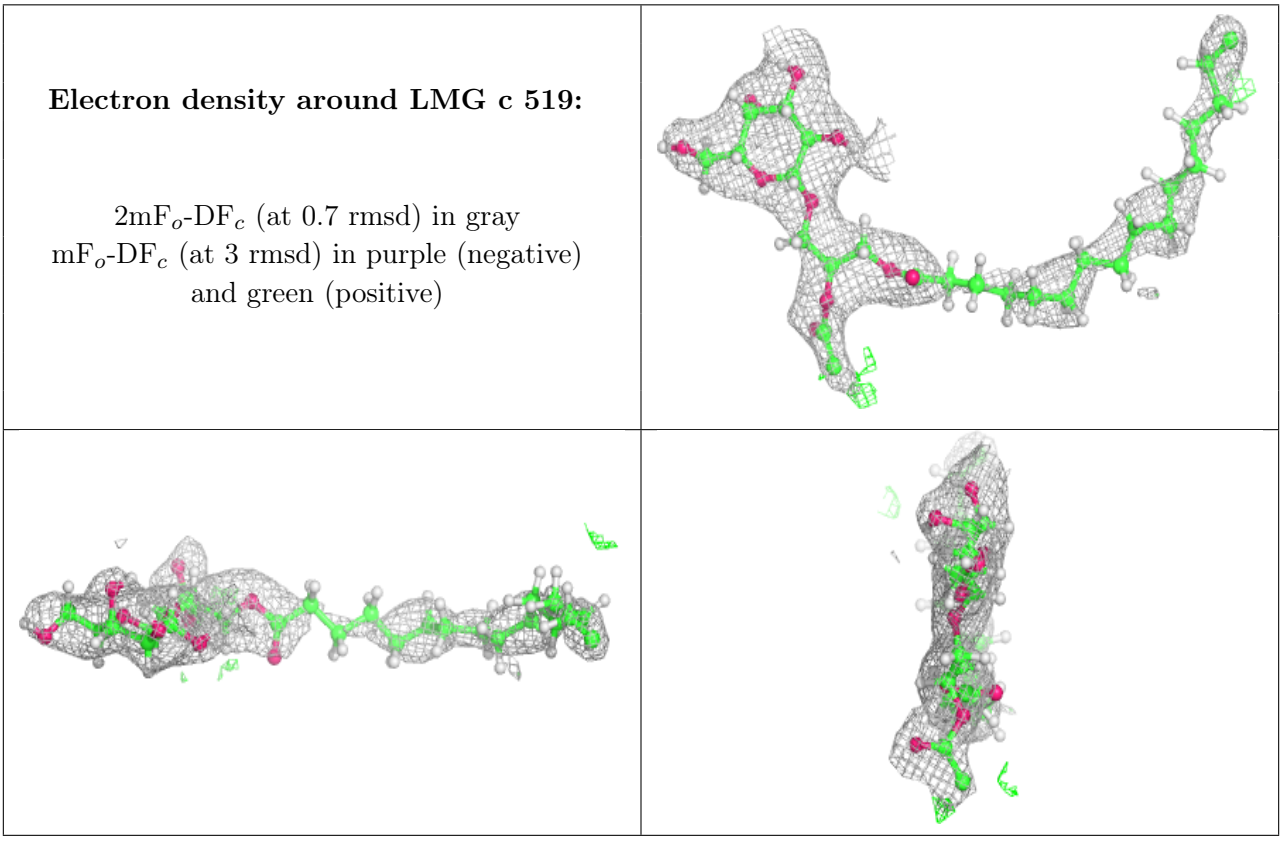
Electron density around BCR H 101:

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



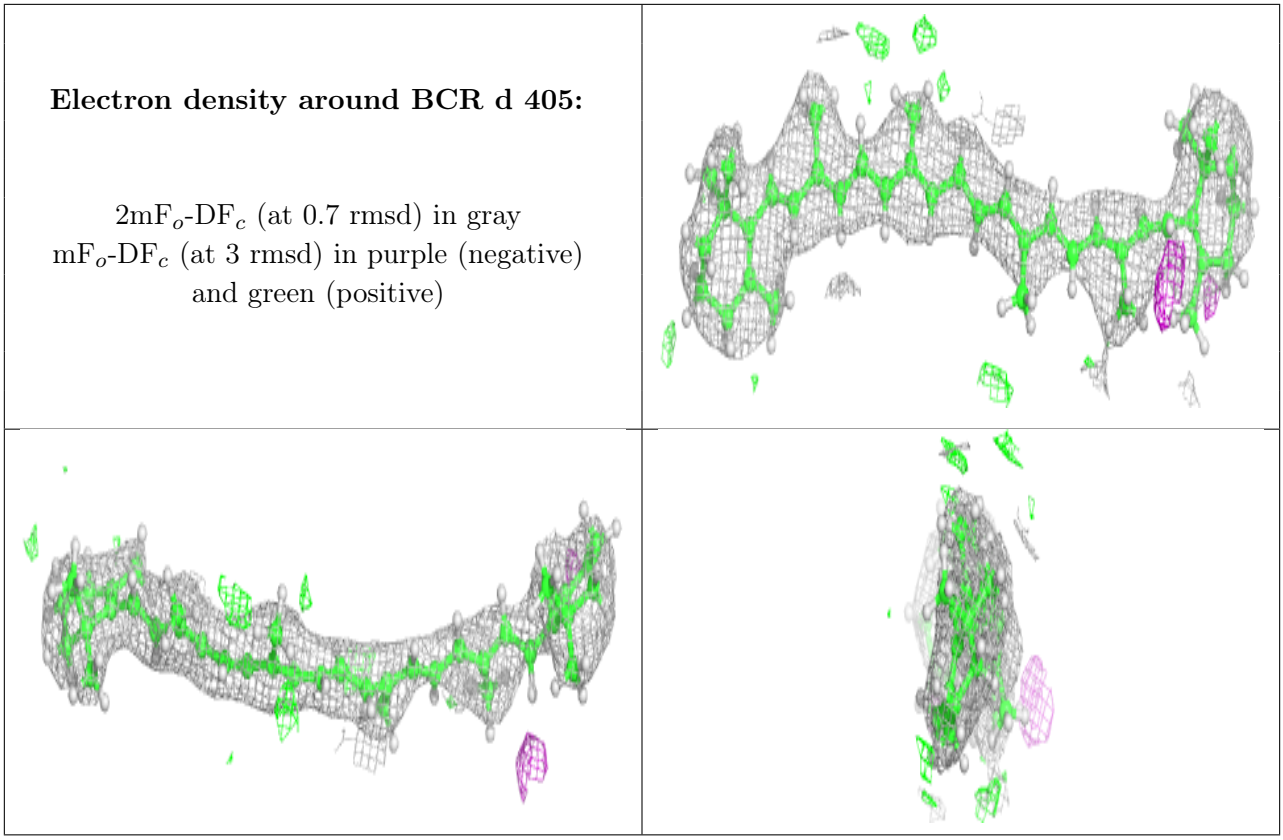
Electron density around LMG c 519:

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



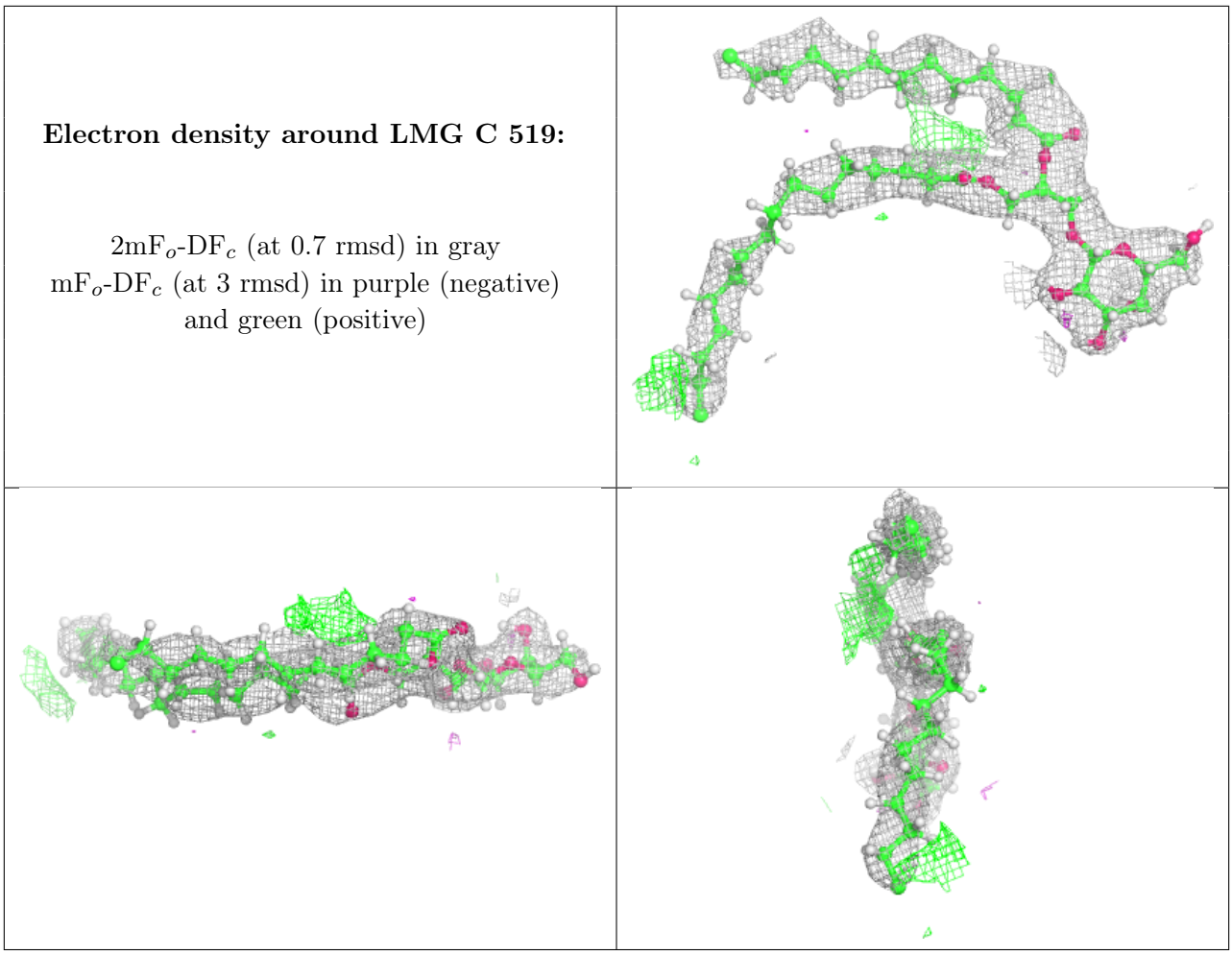
Electron density around BCR d 405:

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



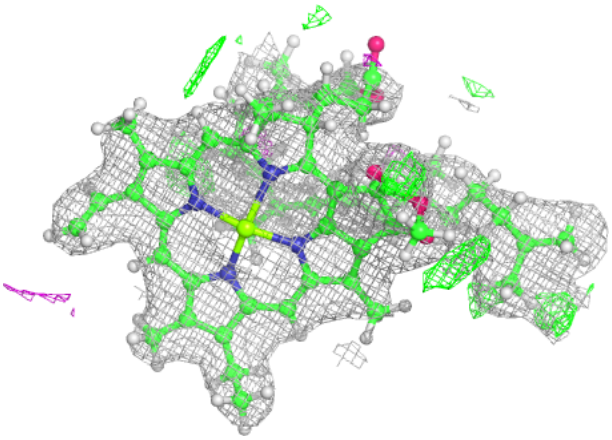
Electron density around LMG C 519:

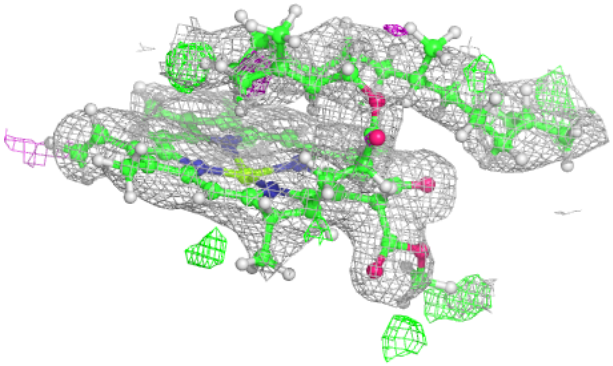
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

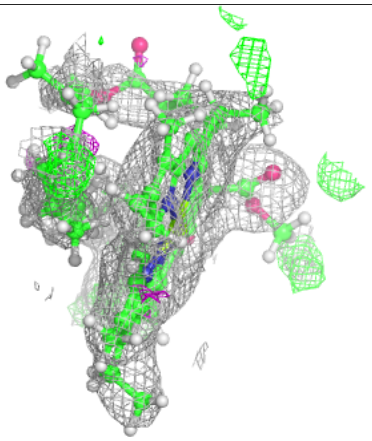


Electron density around CLA B 601:

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

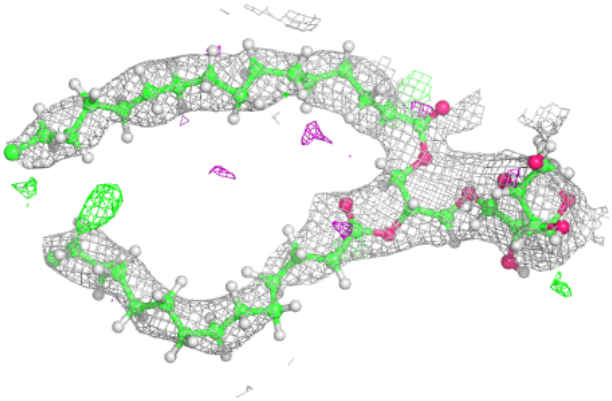


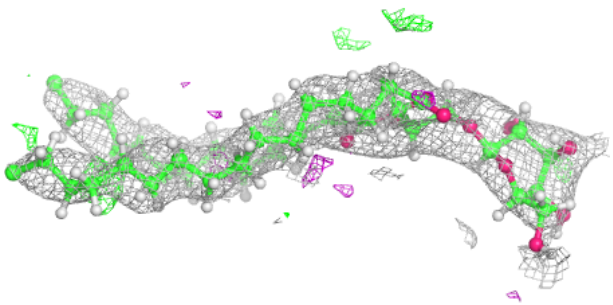


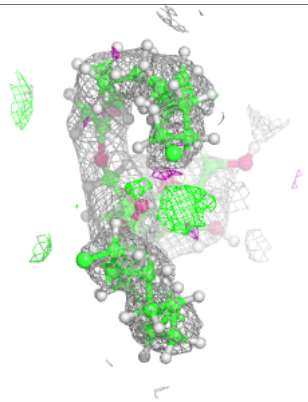


Electron density around LMG a 414:

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

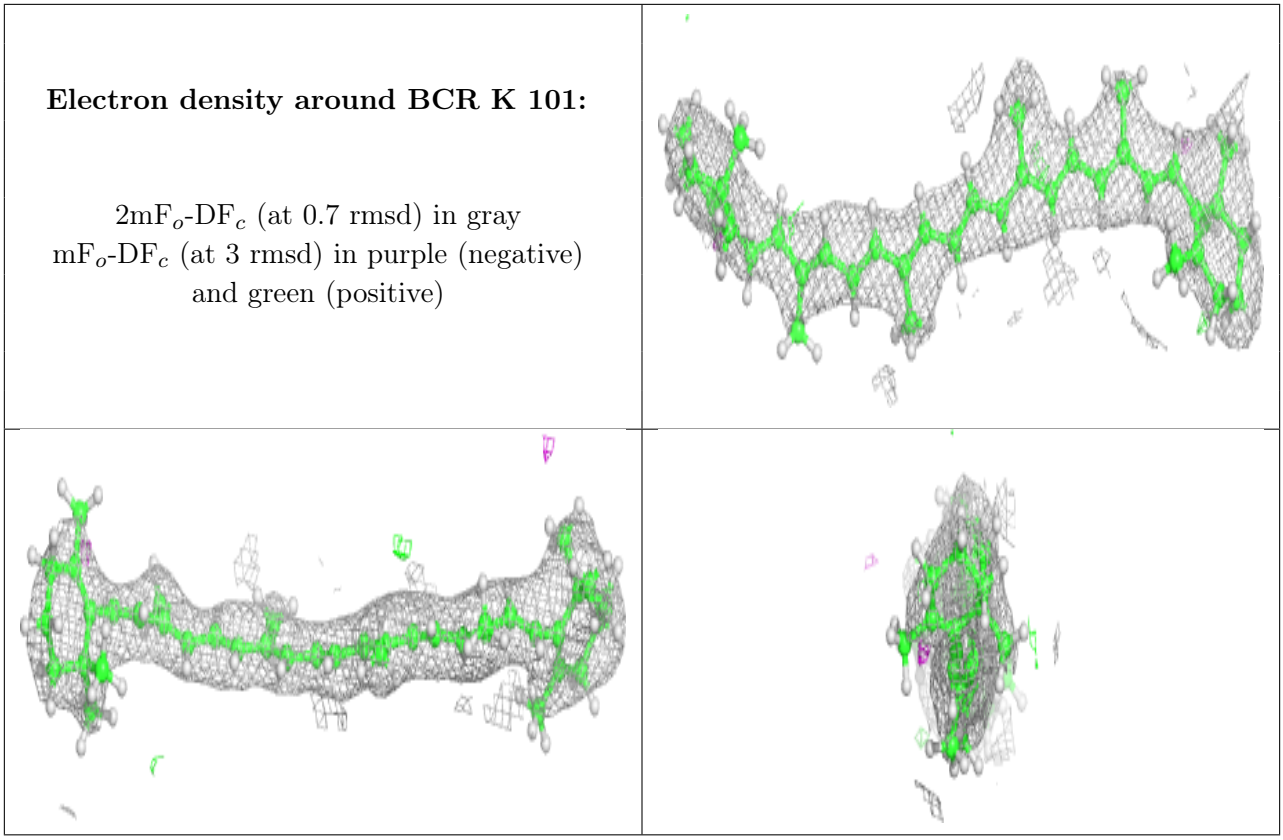






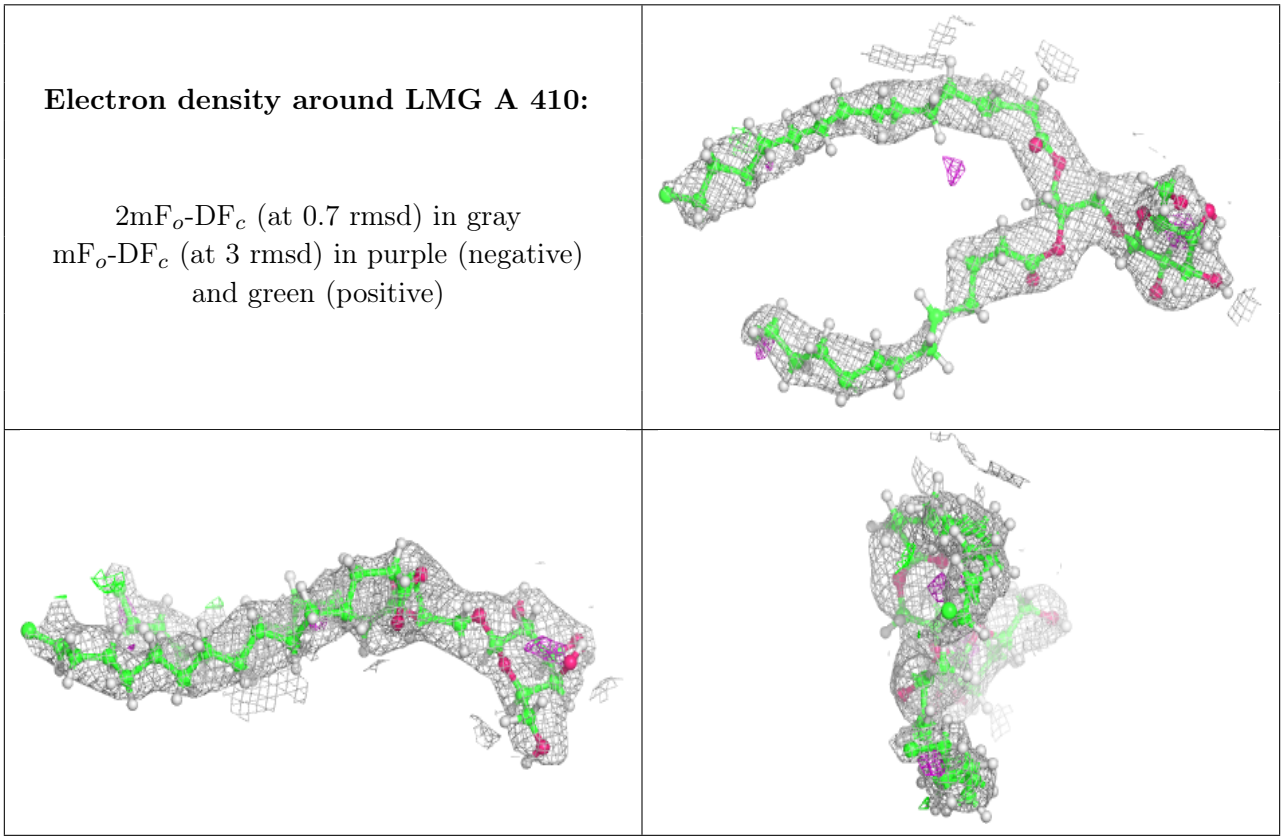
Electron density around BCR K 101:

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



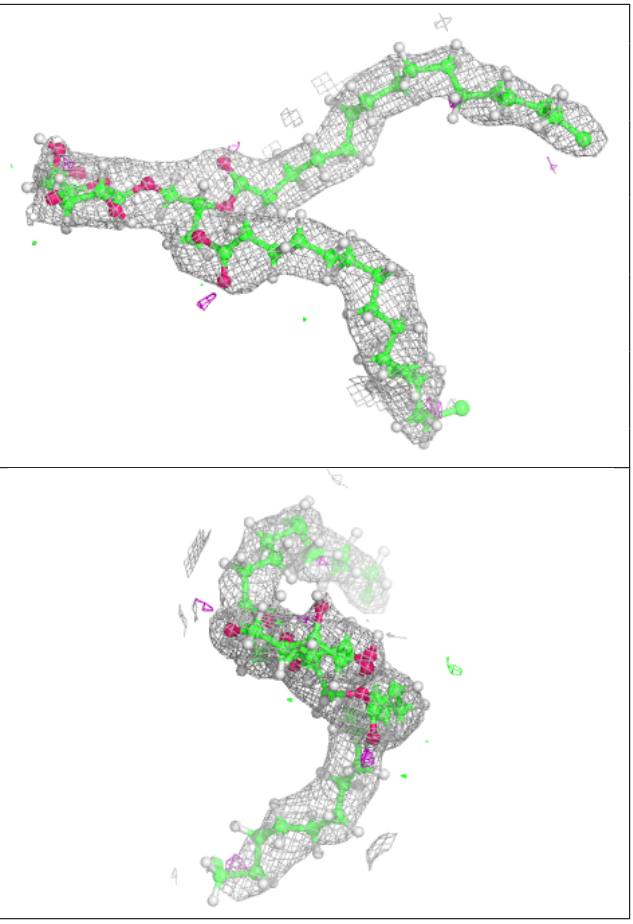
Electron density around LMG A 410:

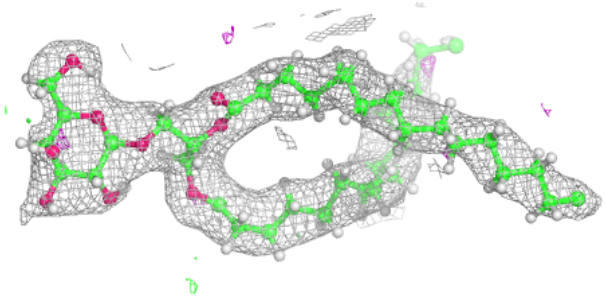
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG B 620:

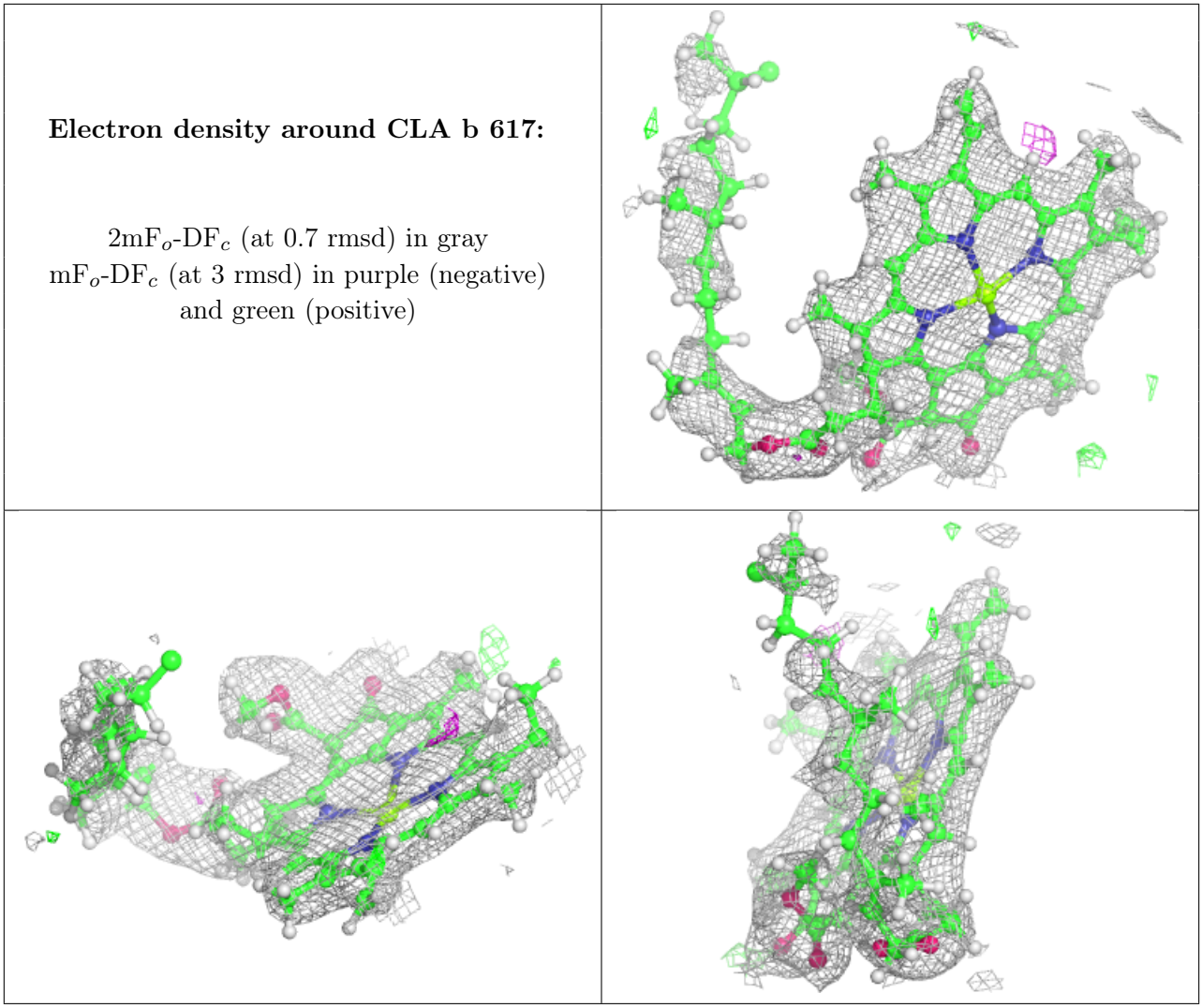
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





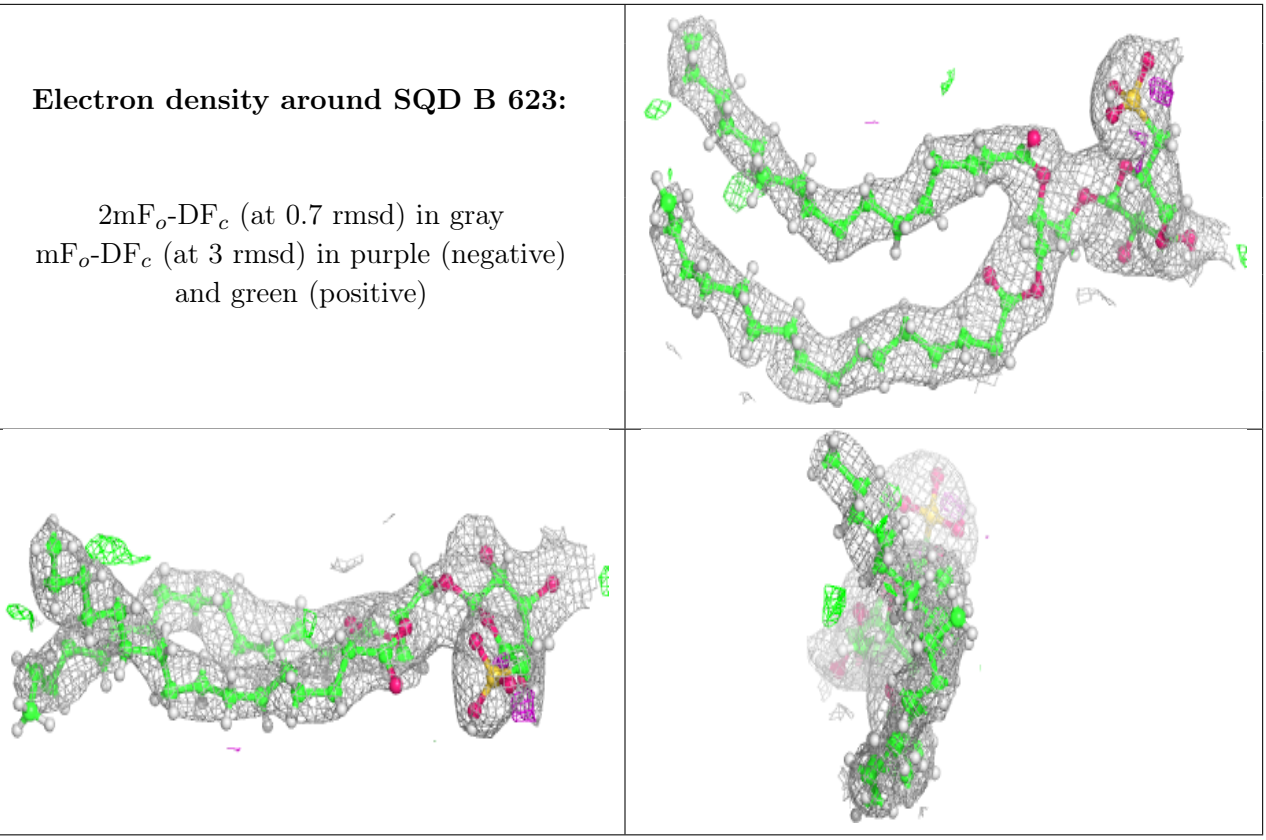
Electron density around CLA b 617:

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



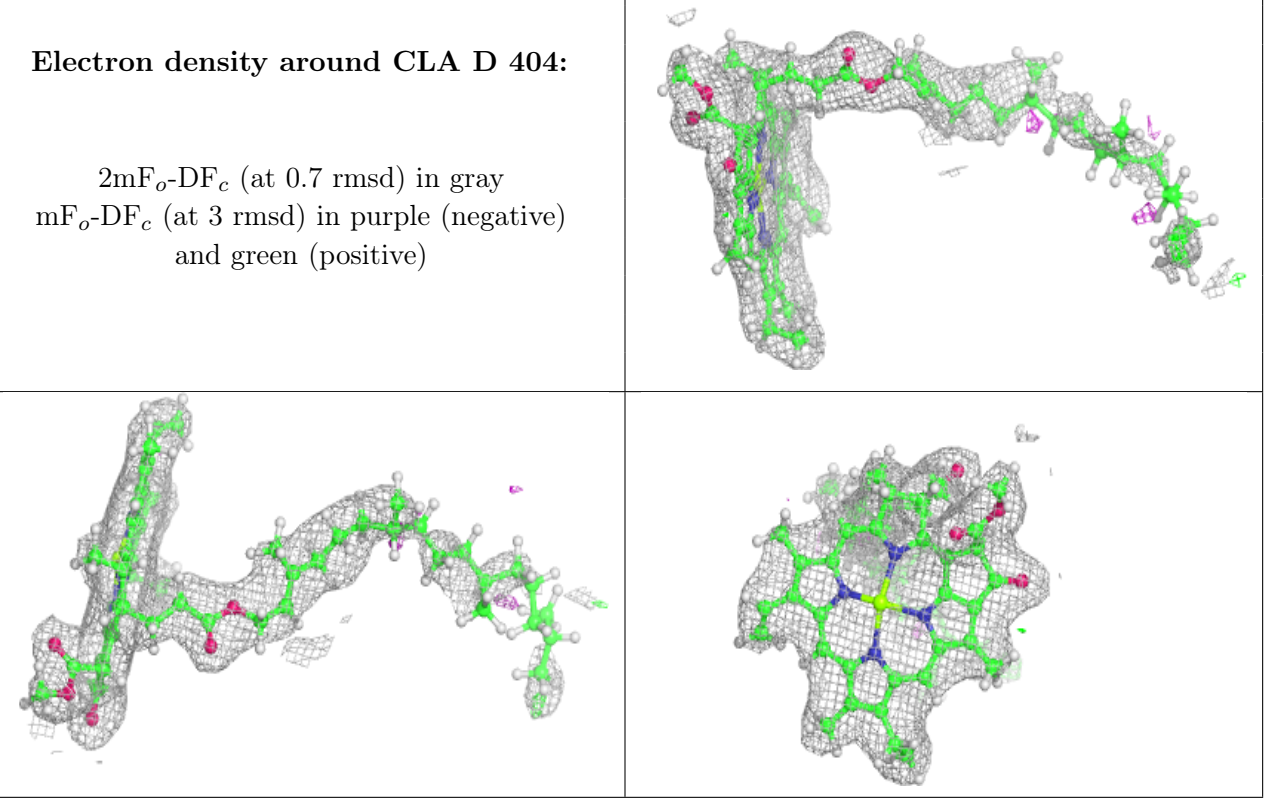
Electron density around SQD B 623:

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



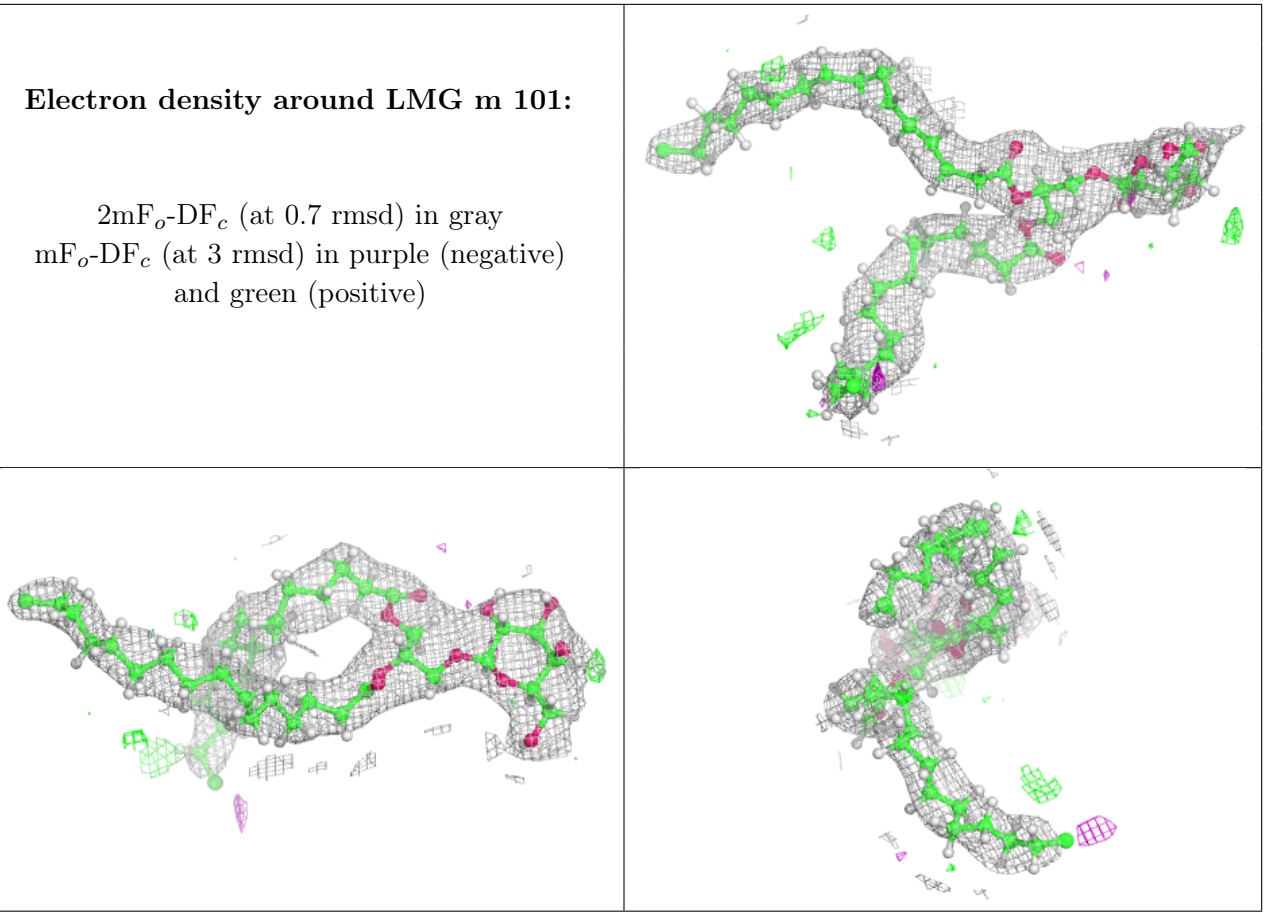
Electron density around CLA D 404:

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



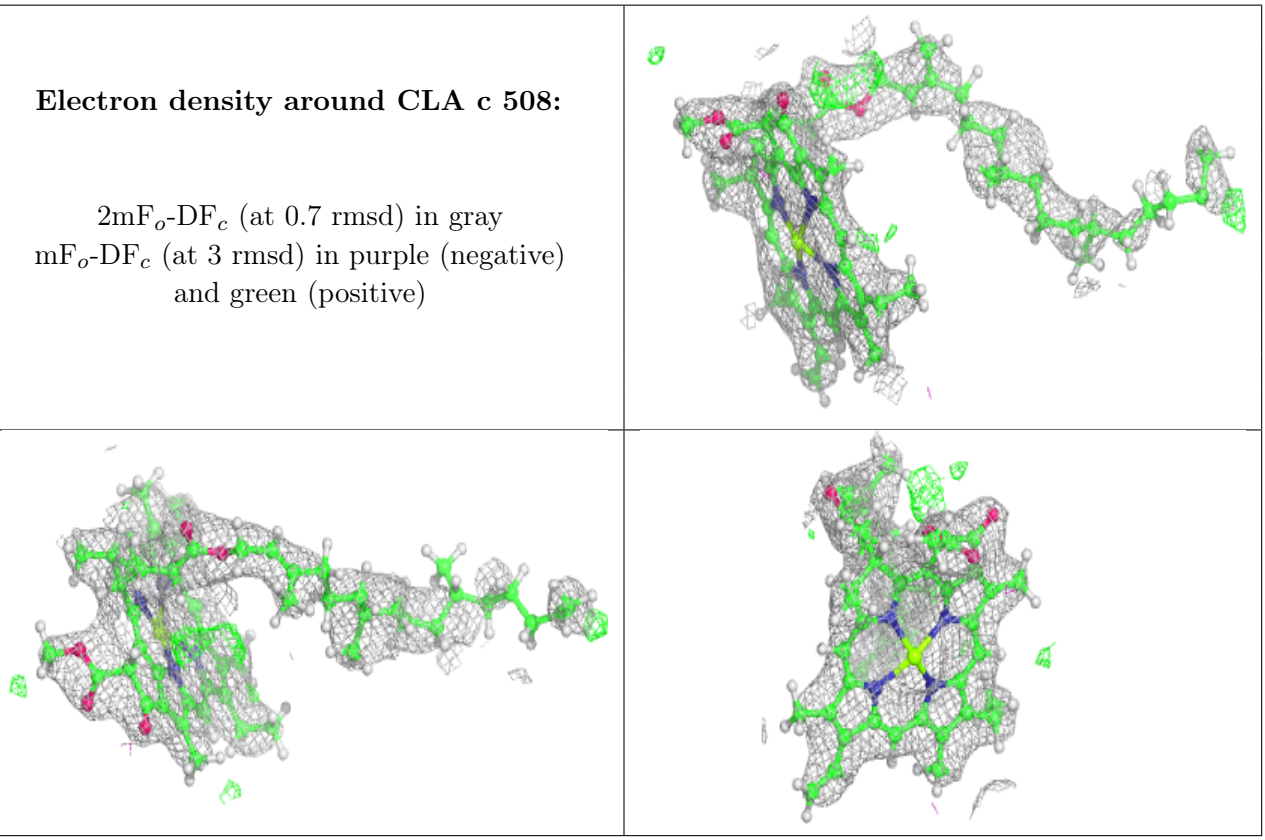
Electron density around LMG m 101:

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



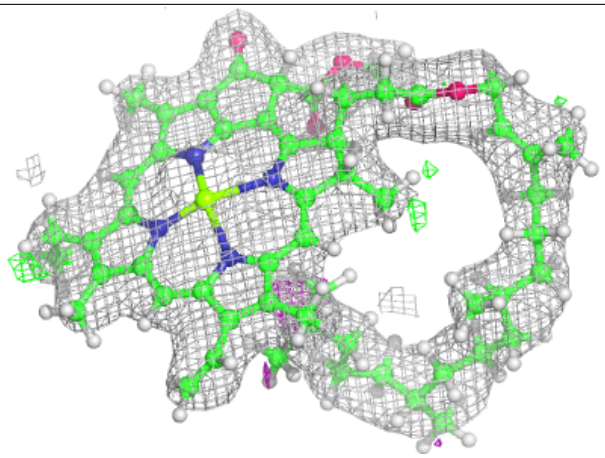
Electron density around CLA c 508:

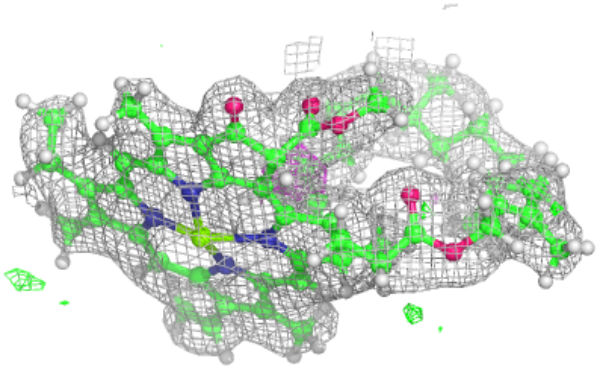
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

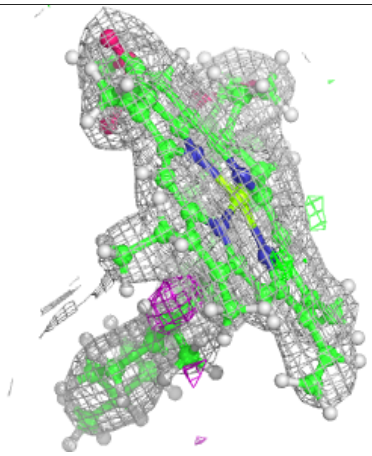


Electron density around CLA b 616:

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

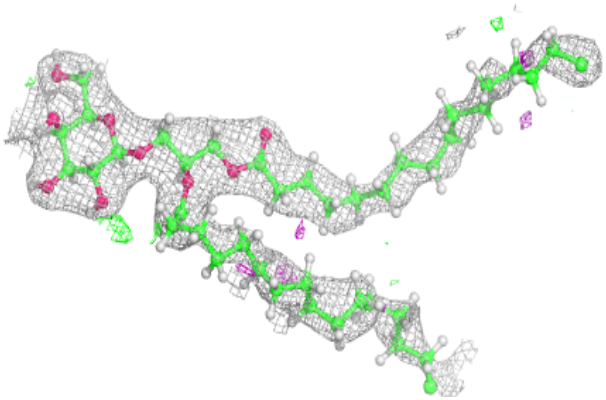


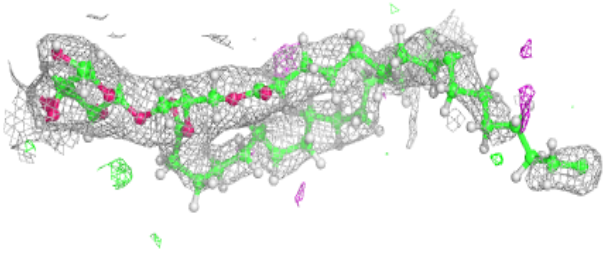


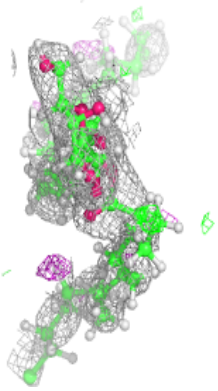


Electron density around LMG D 407:

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

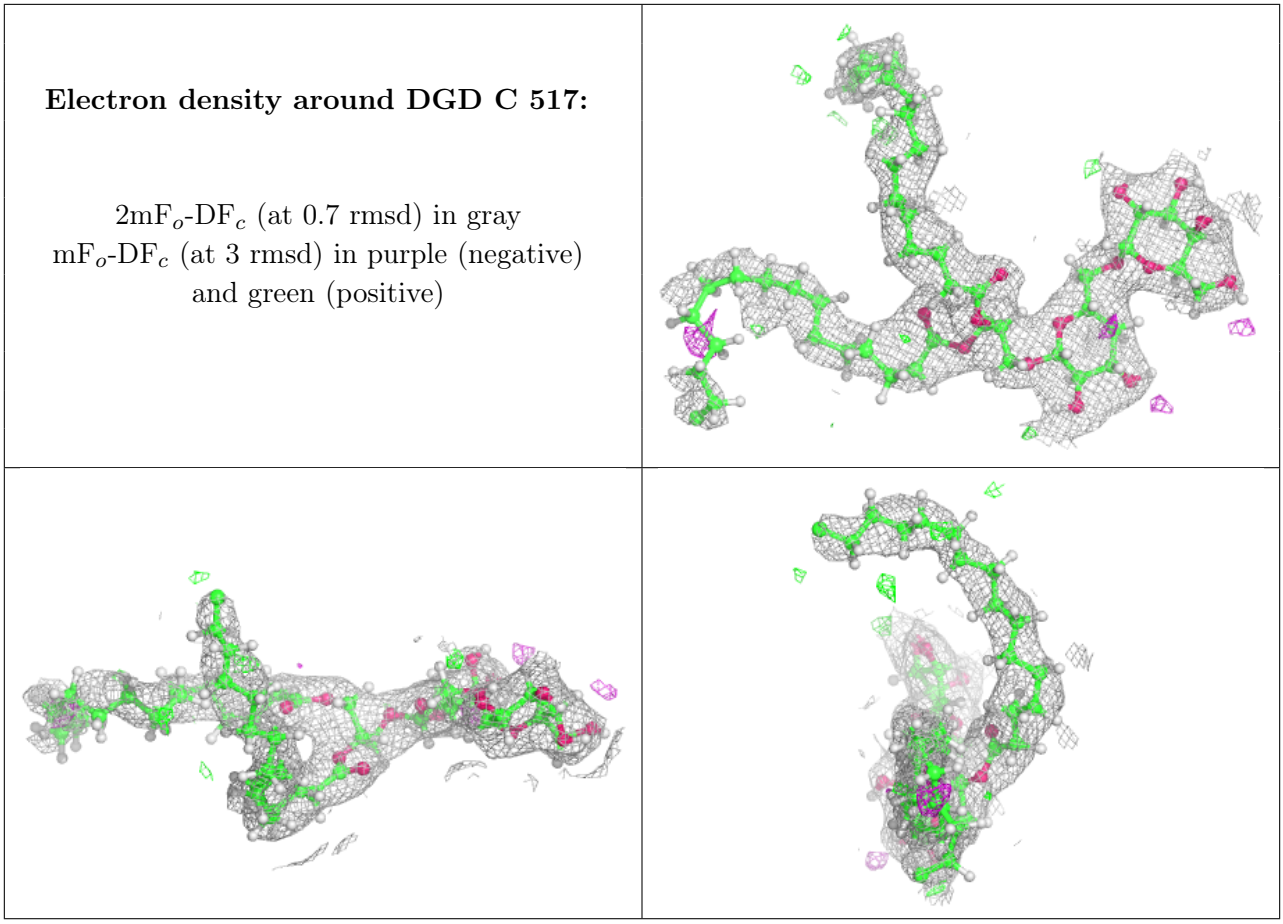






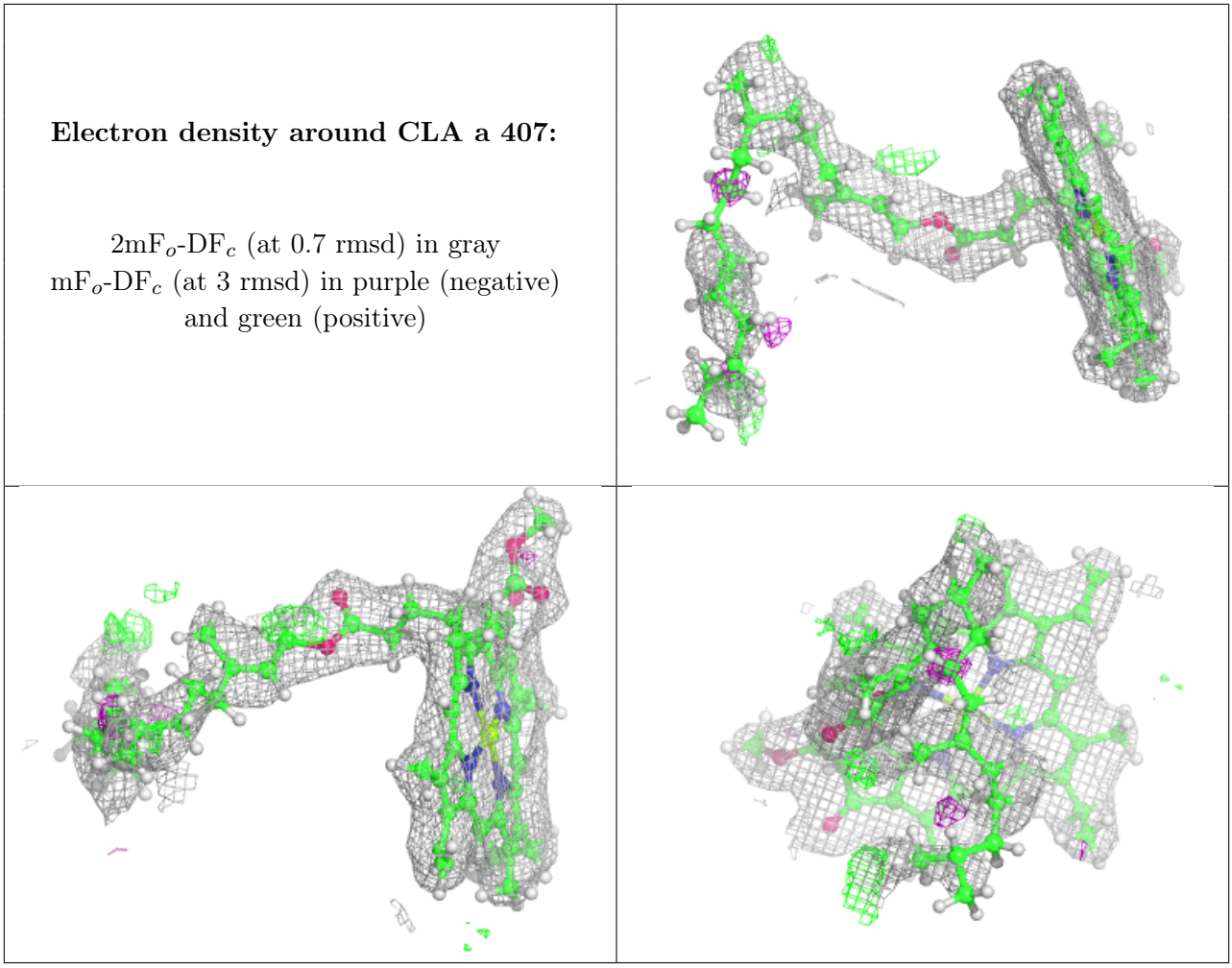
Electron density around DGD C 517:

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



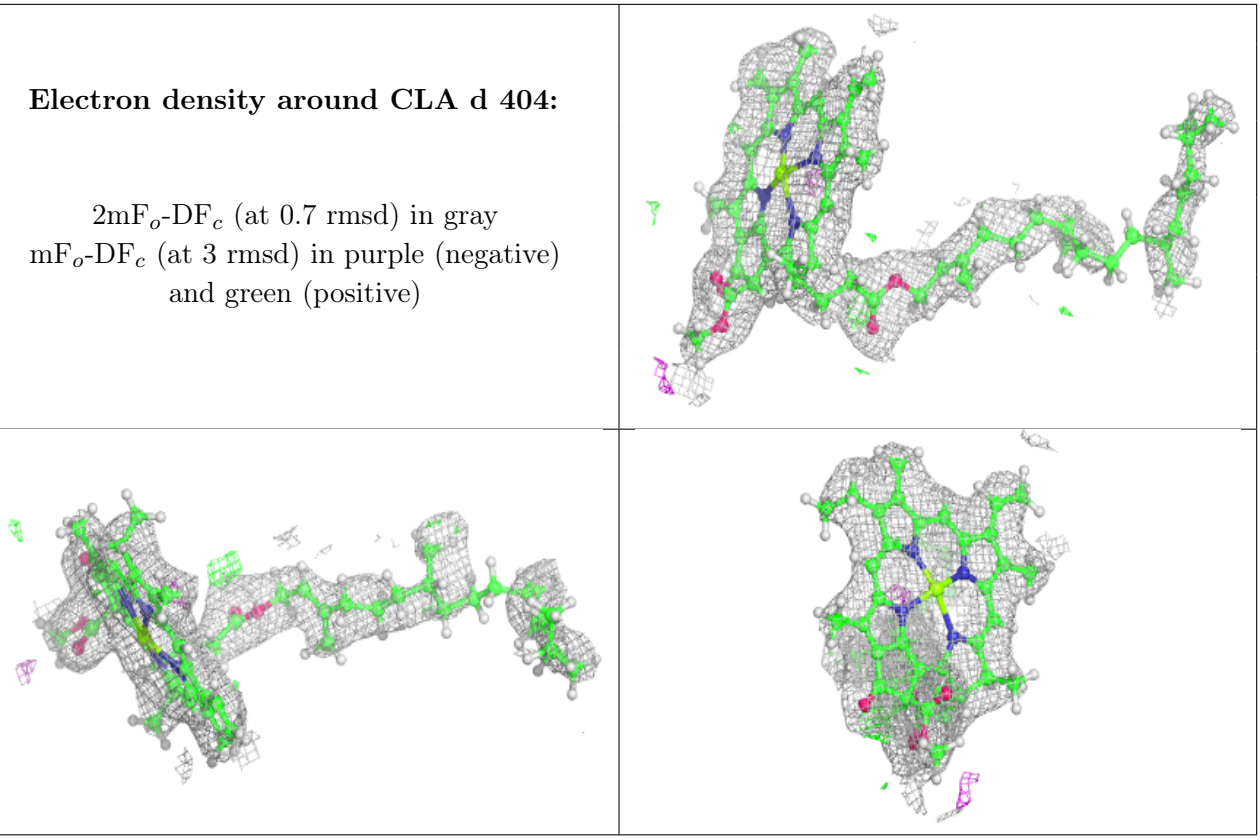
Electron density around CLA a 407:

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



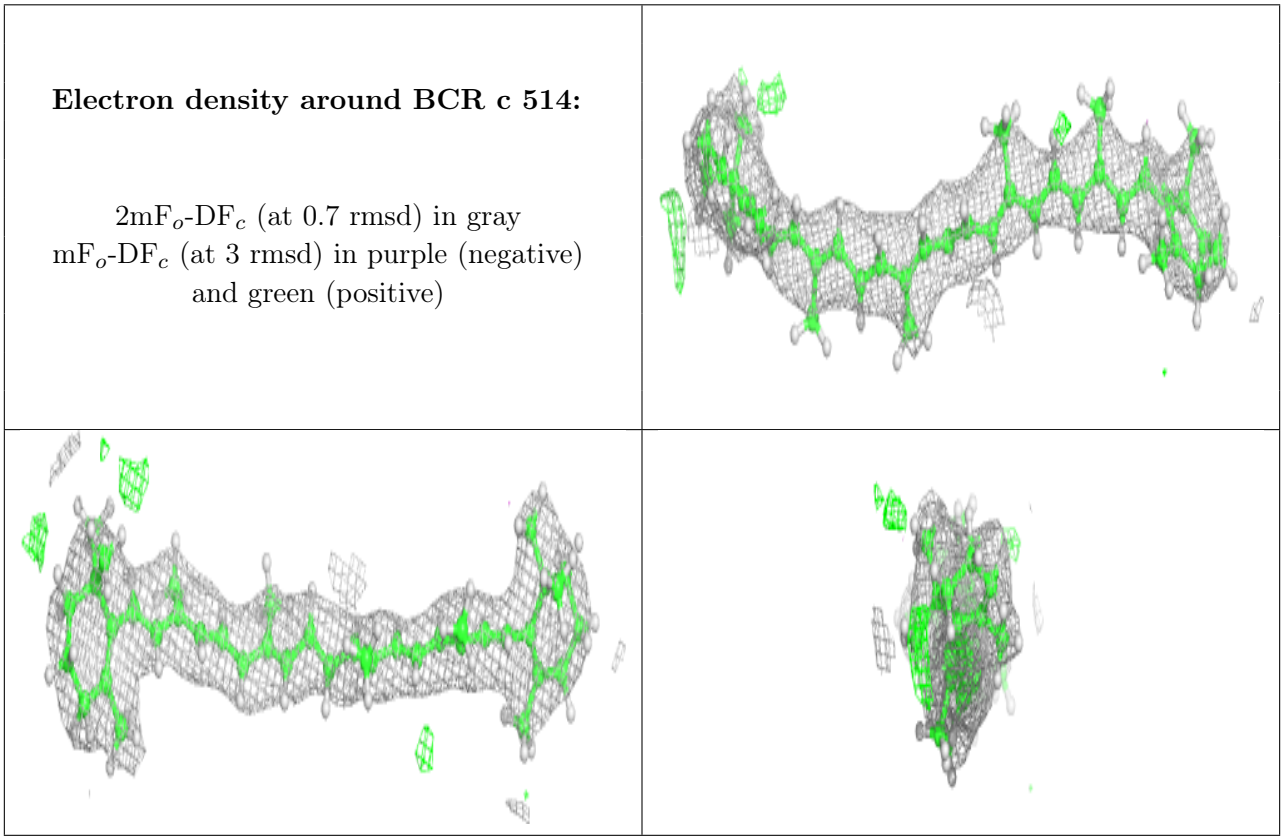
Electron density around CLA d 404:

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



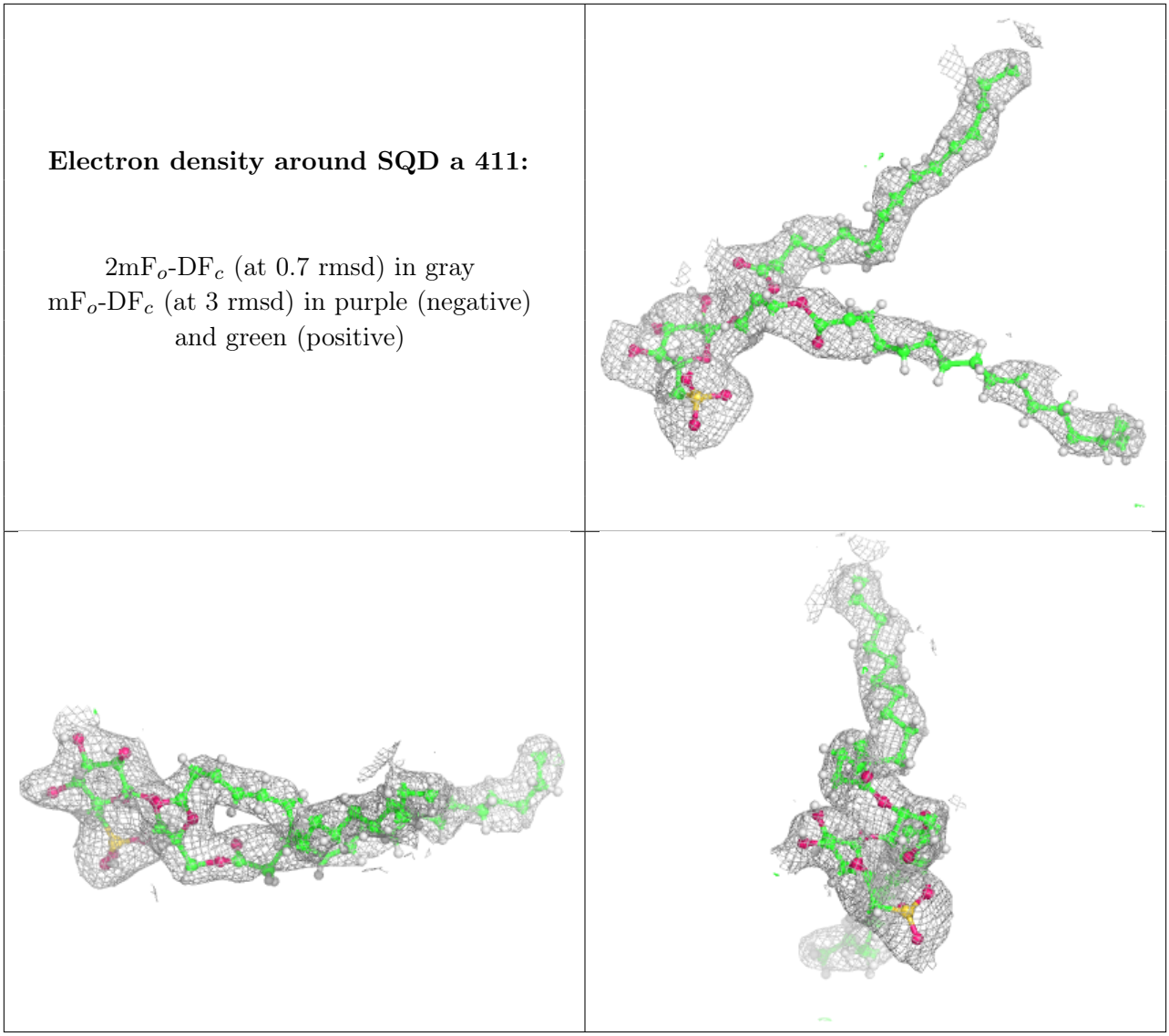
Electron density around BCR c 514:

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



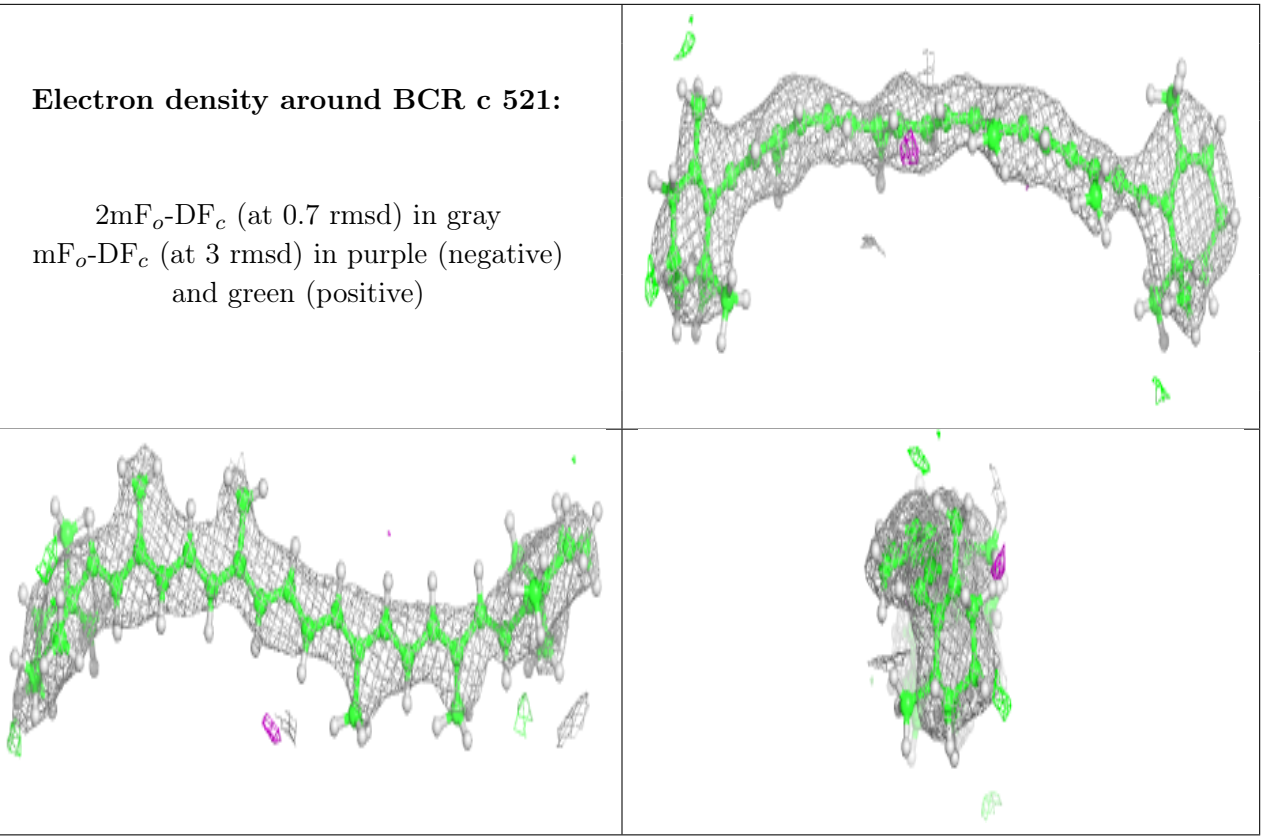
Electron density around SQD a 411:

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



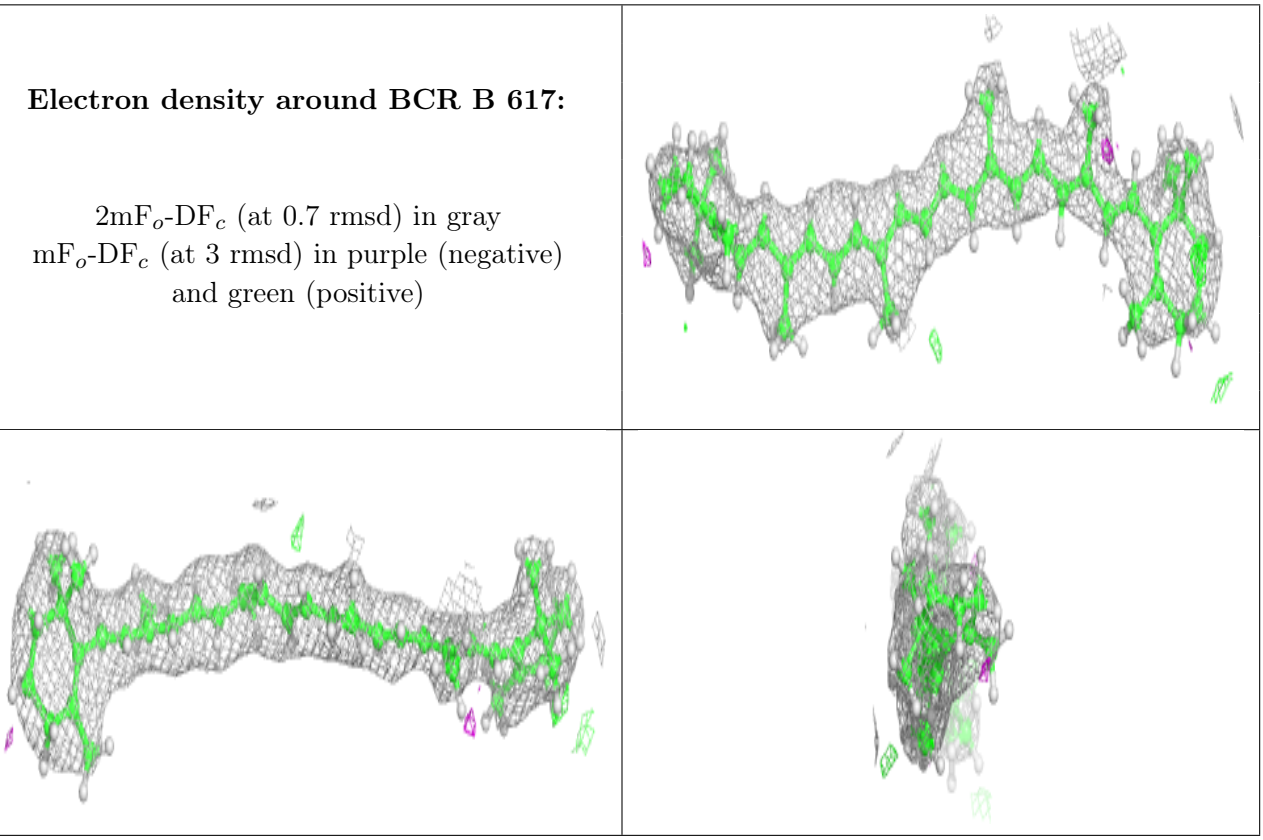
Electron density around BCR c 521:

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



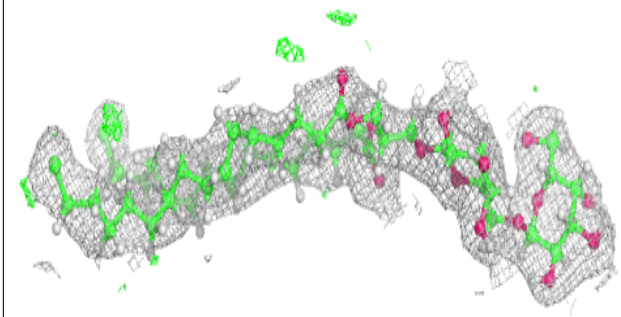
Electron density around BCR B 617:

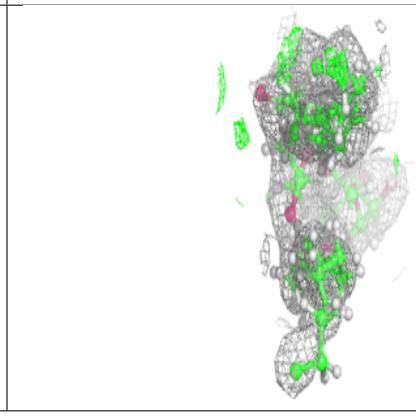
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD c 518:

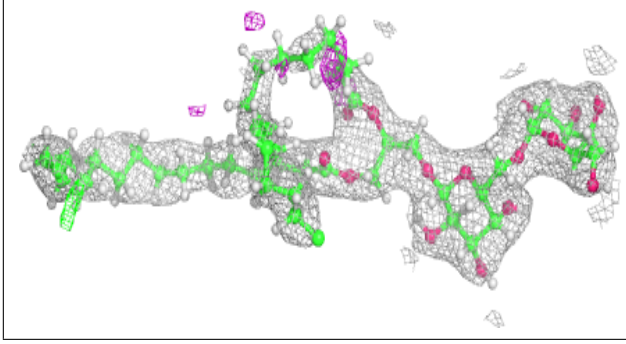
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

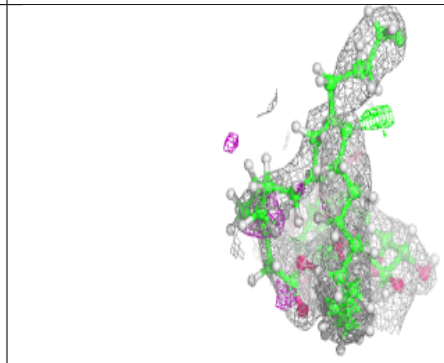




Electron density around DGD h 103:

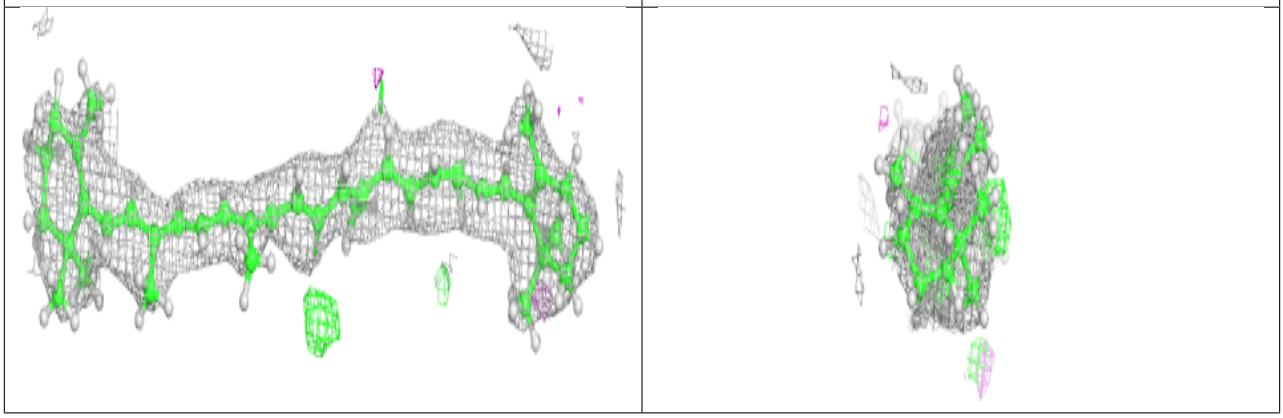
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





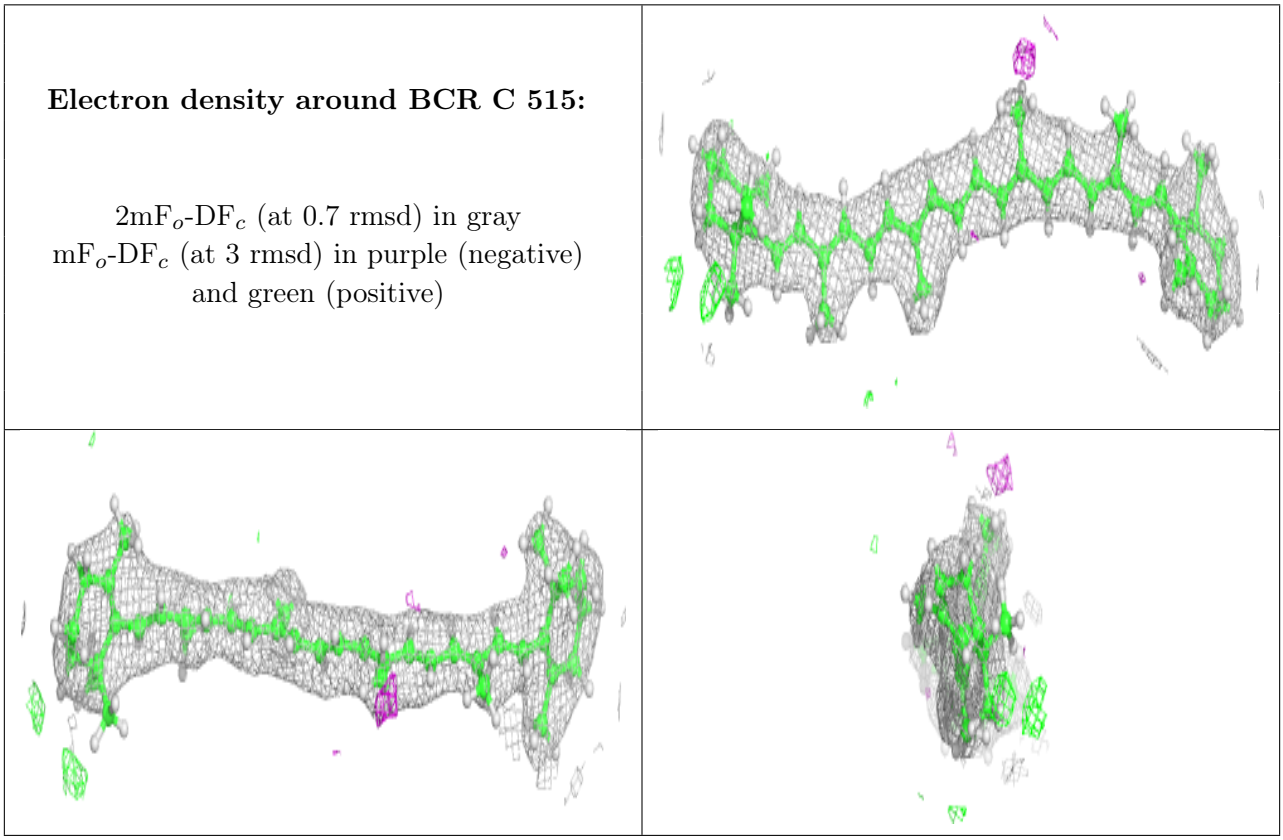
Electron density around BCR C 514:

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



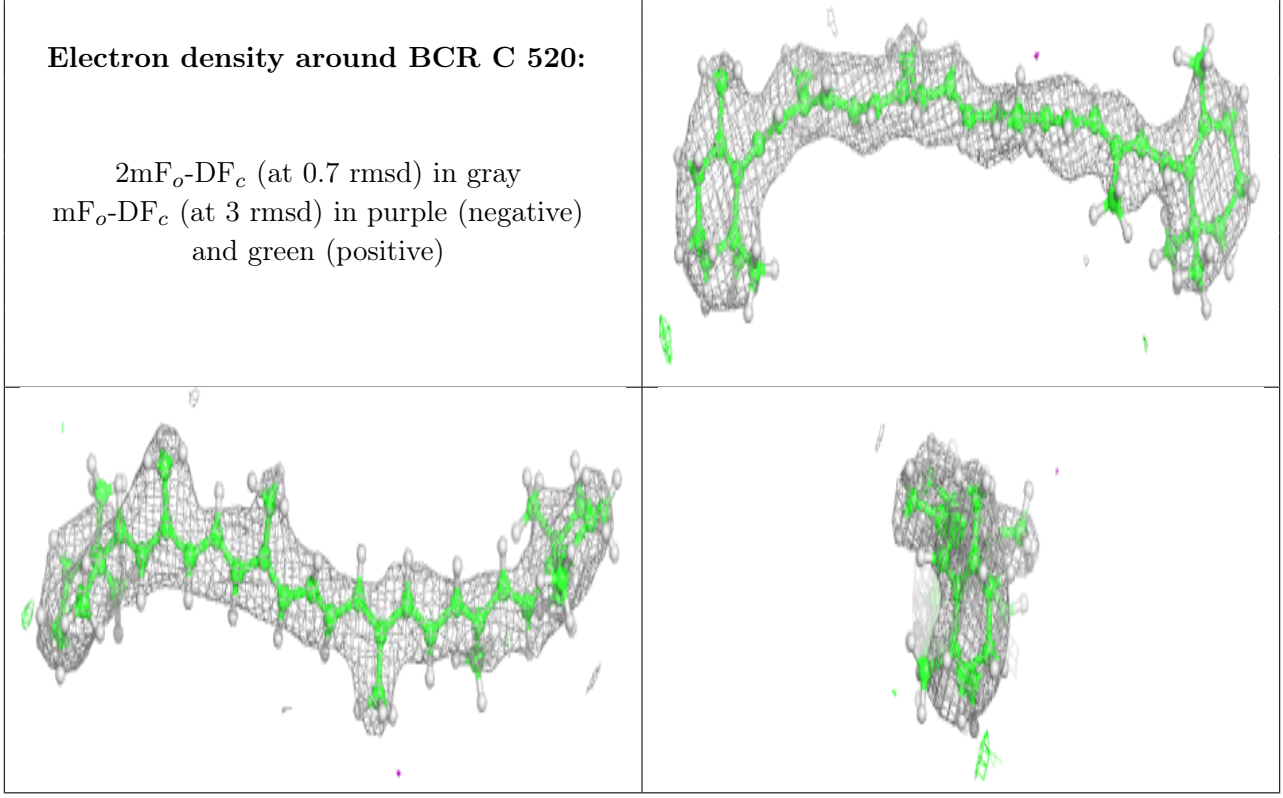
Electron density around BCR C 515:

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



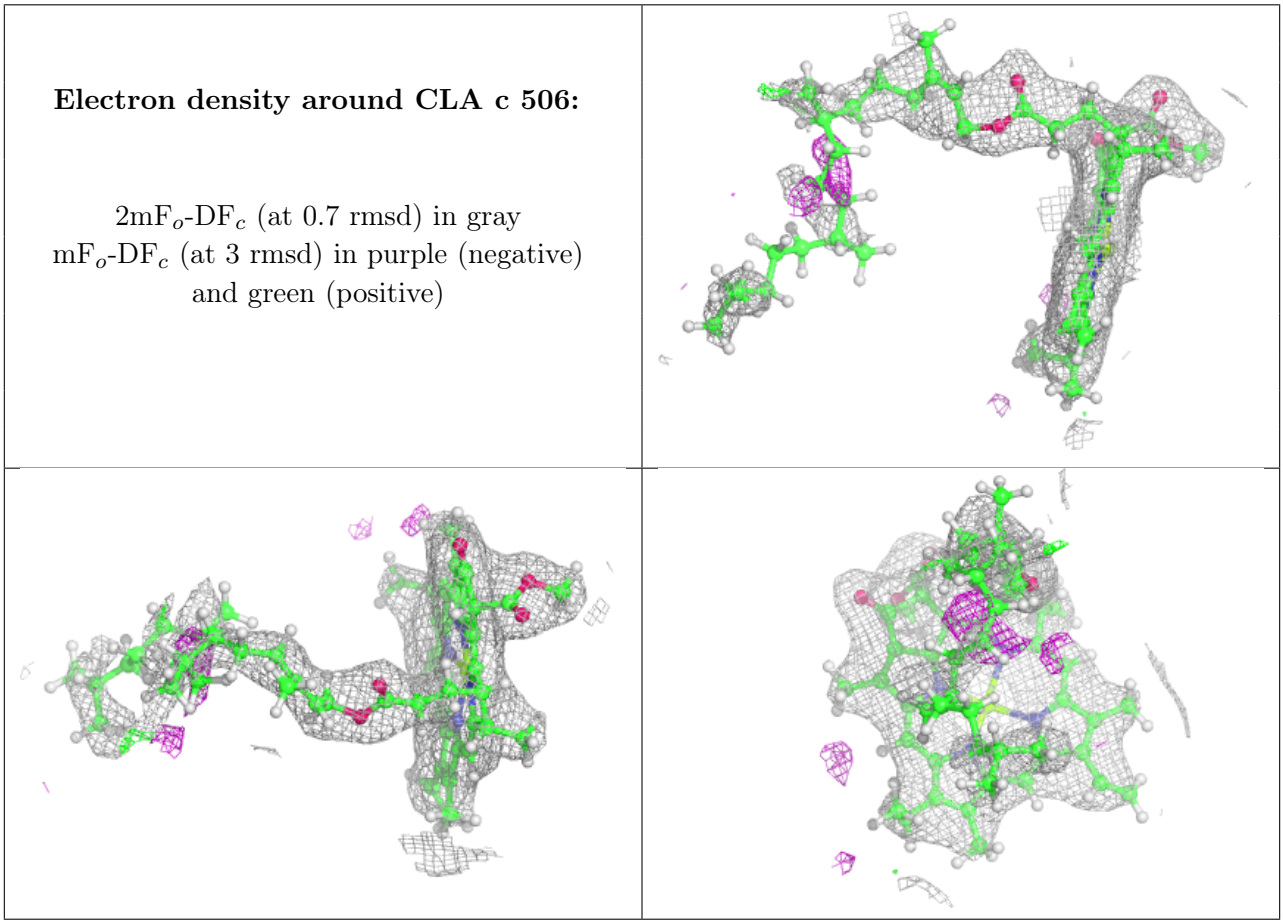
Electron density around BCR C 520:

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



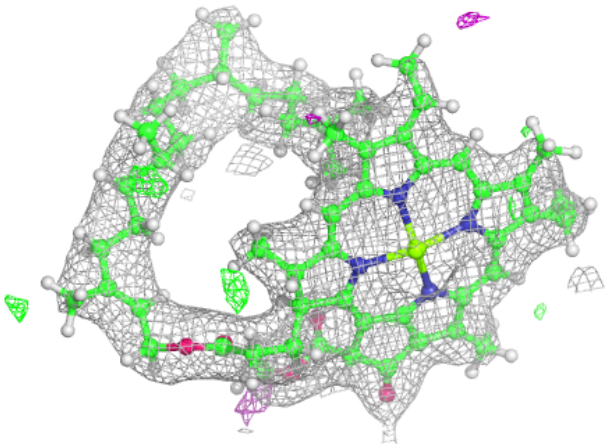
Electron density around CLA c 506:

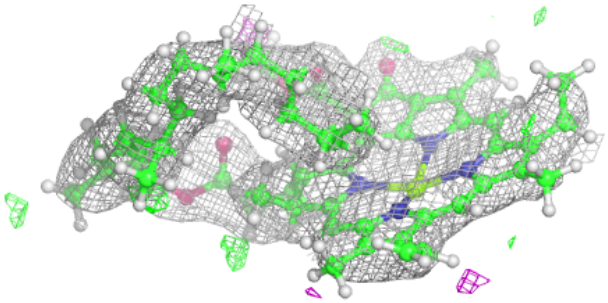
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

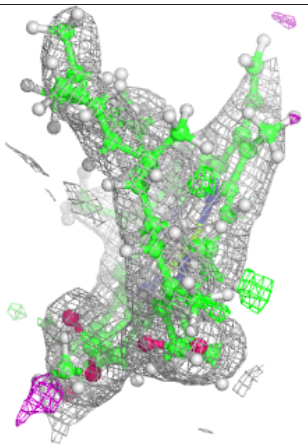


Electron density around CLA B 615:

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

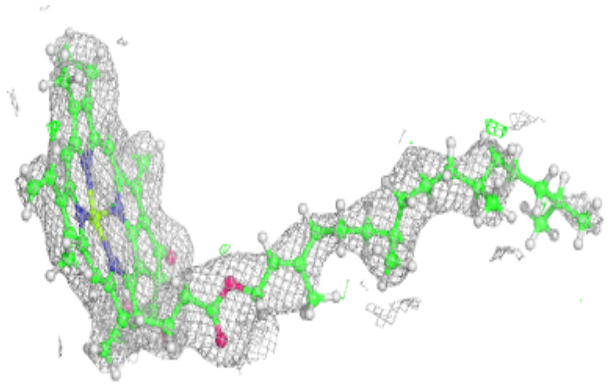


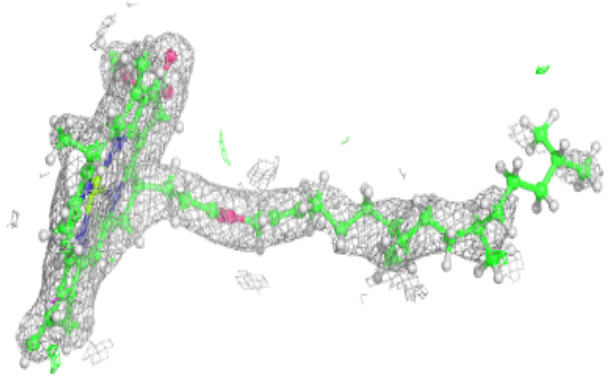


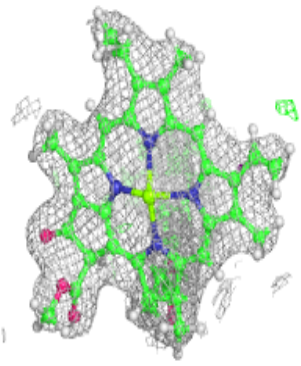


Electron density around CLA b 605:

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

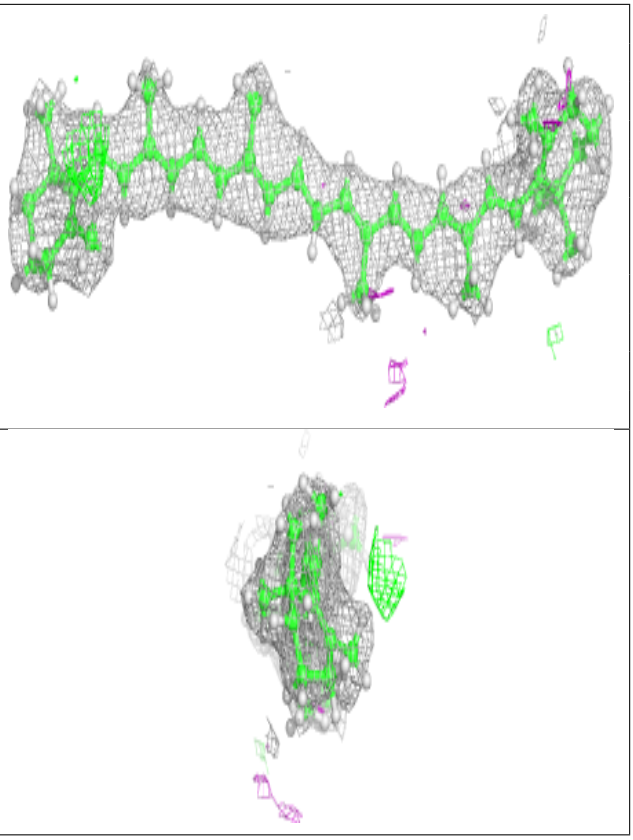






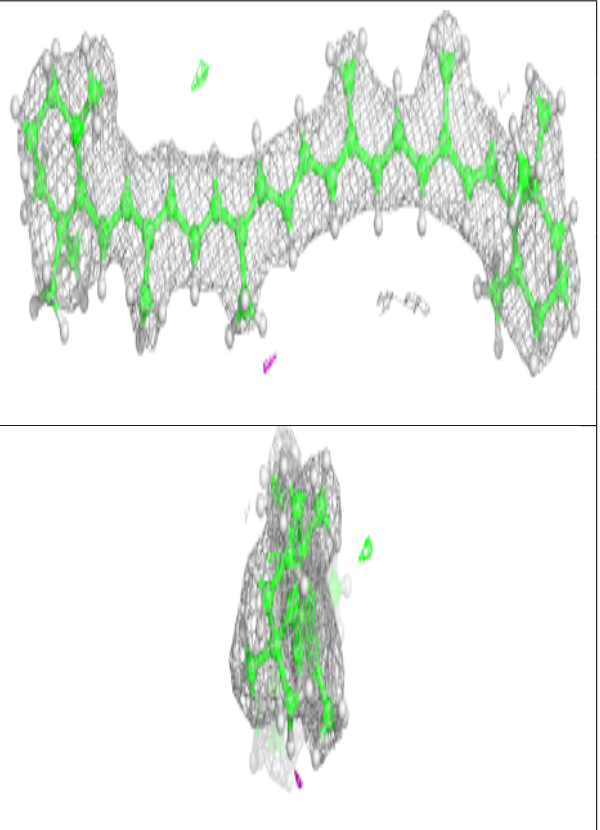
Electron density around BCR b 619:

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



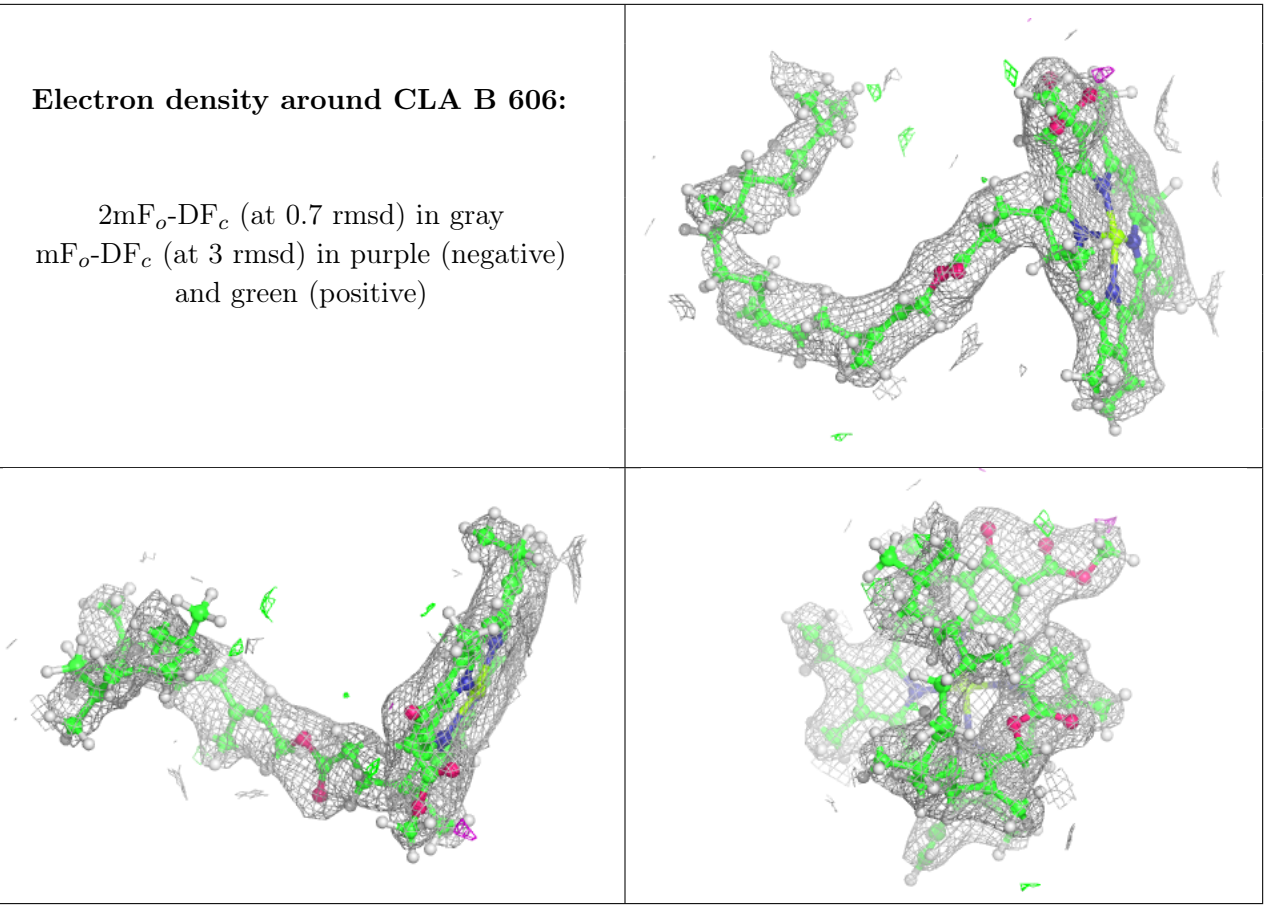
Electron density around BCR b 620:

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



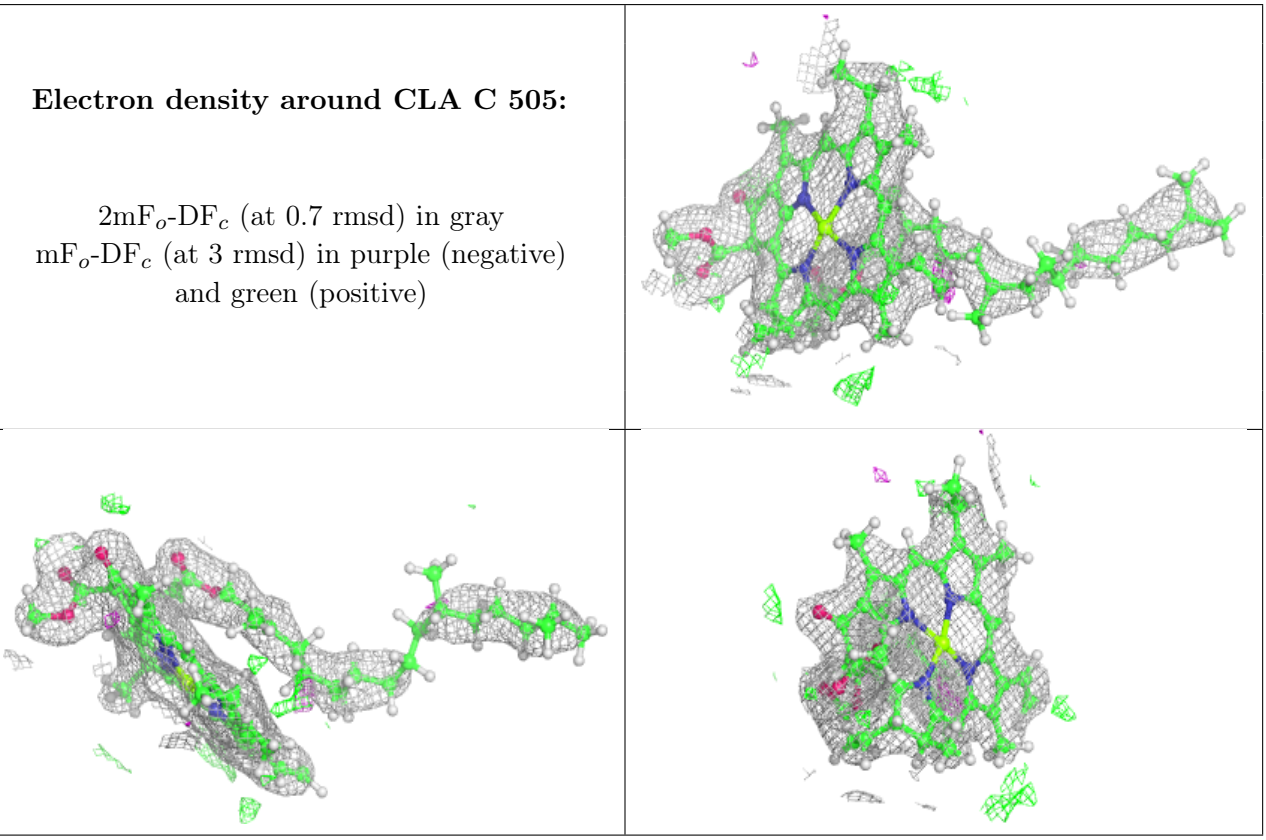
Electron density around CLA B 606:

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



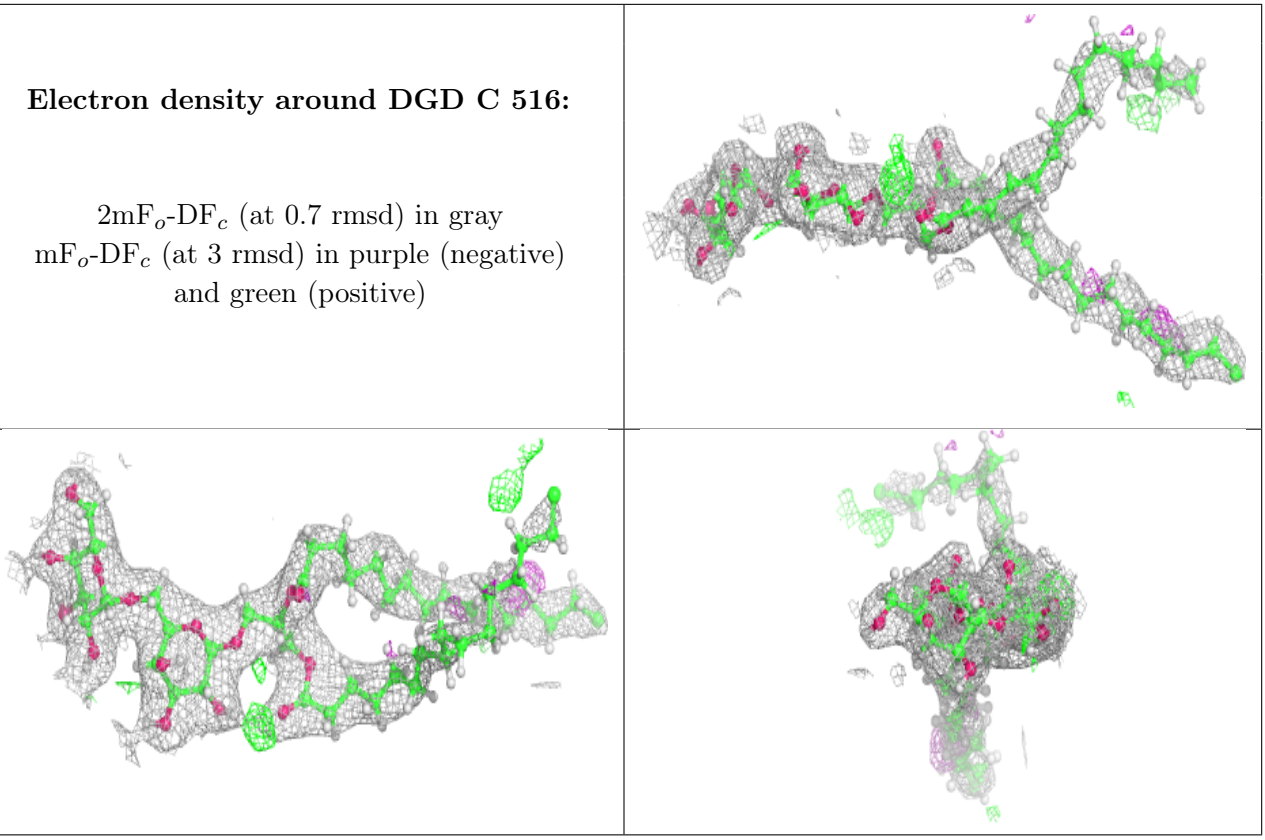
Electron density around CLA C 505:

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



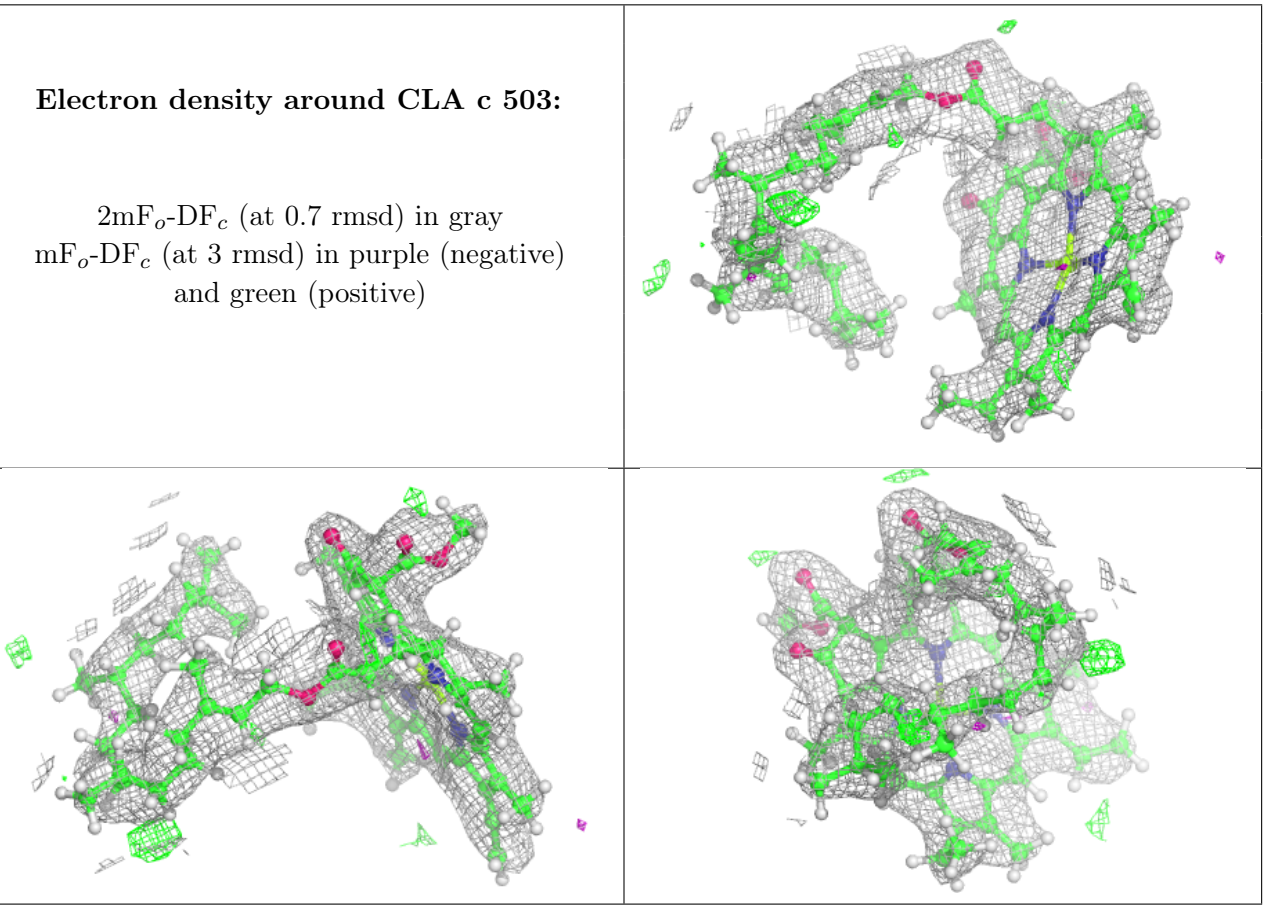
Electron density around DGD C 516:

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



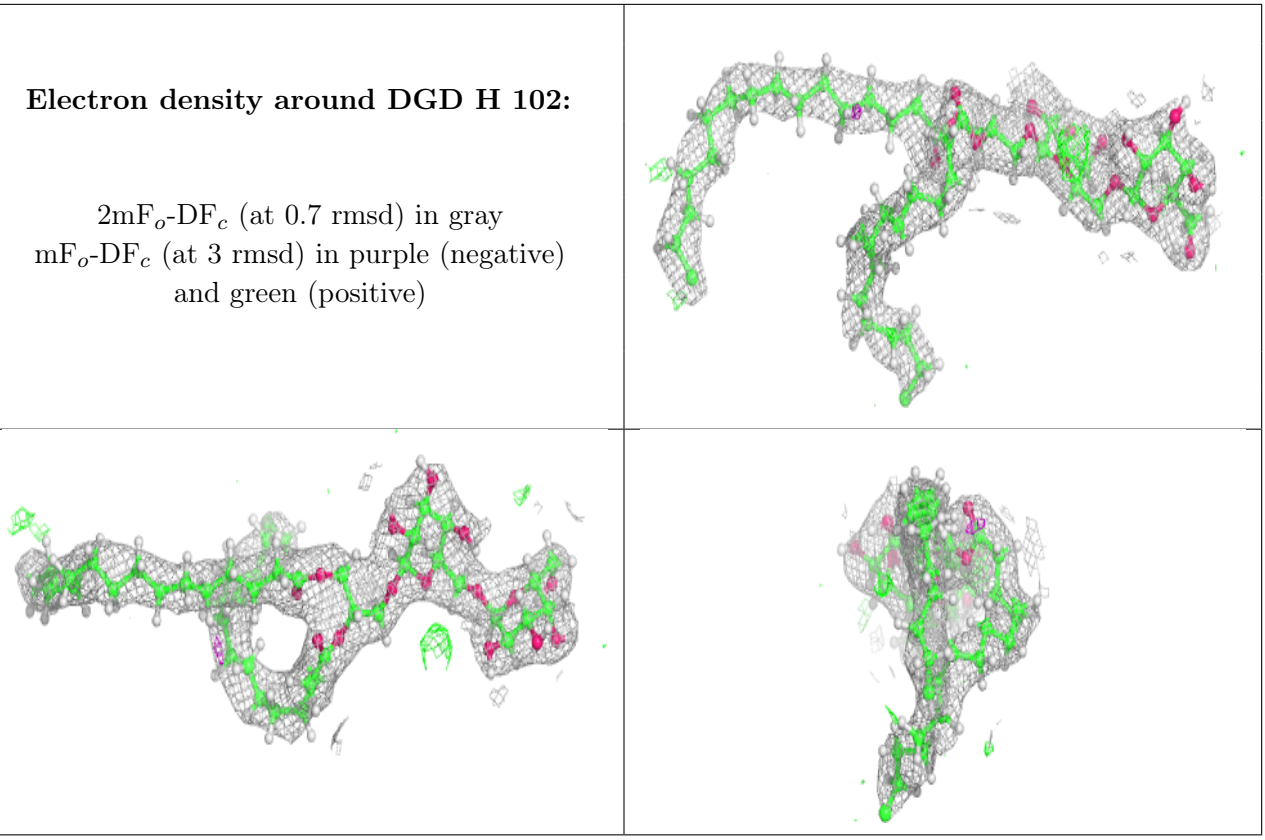
Electron density around CLA c 503:

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



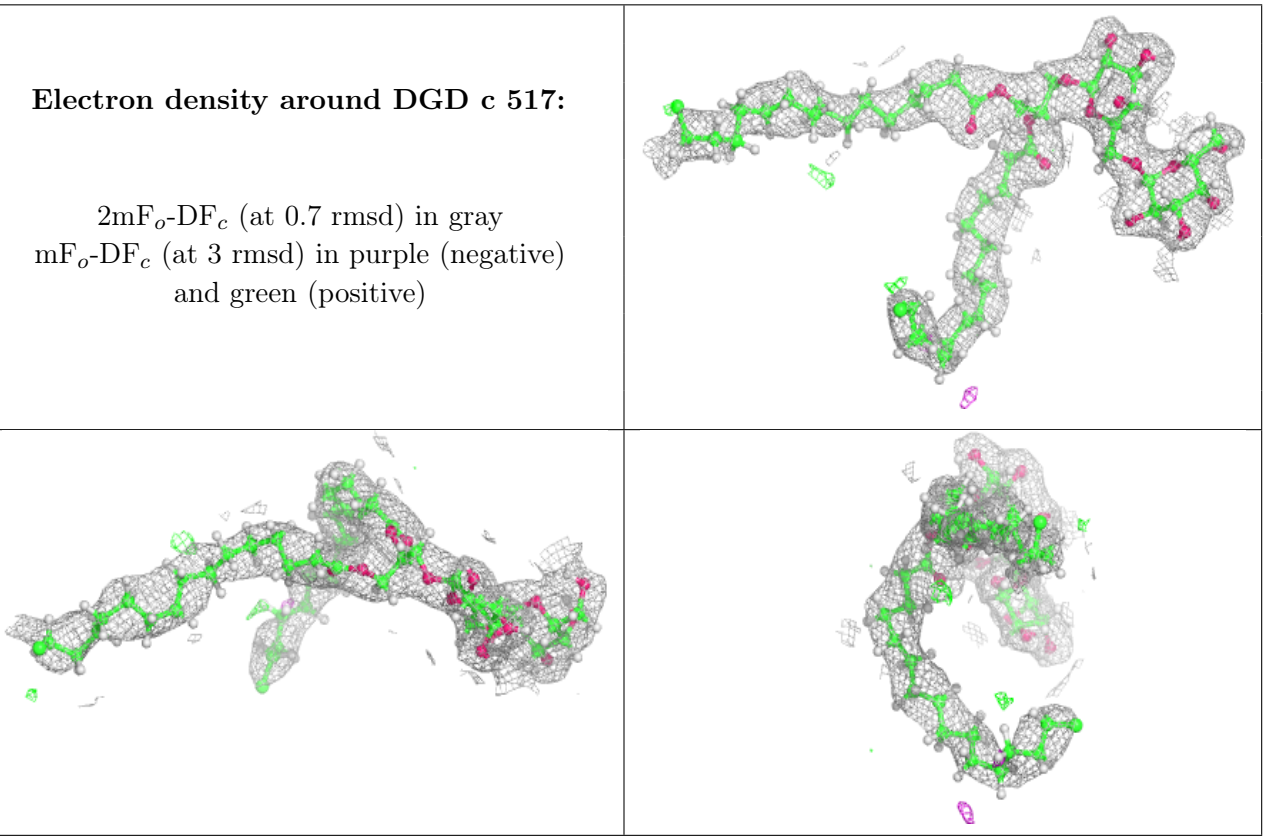
Electron density around DGD H 102:

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



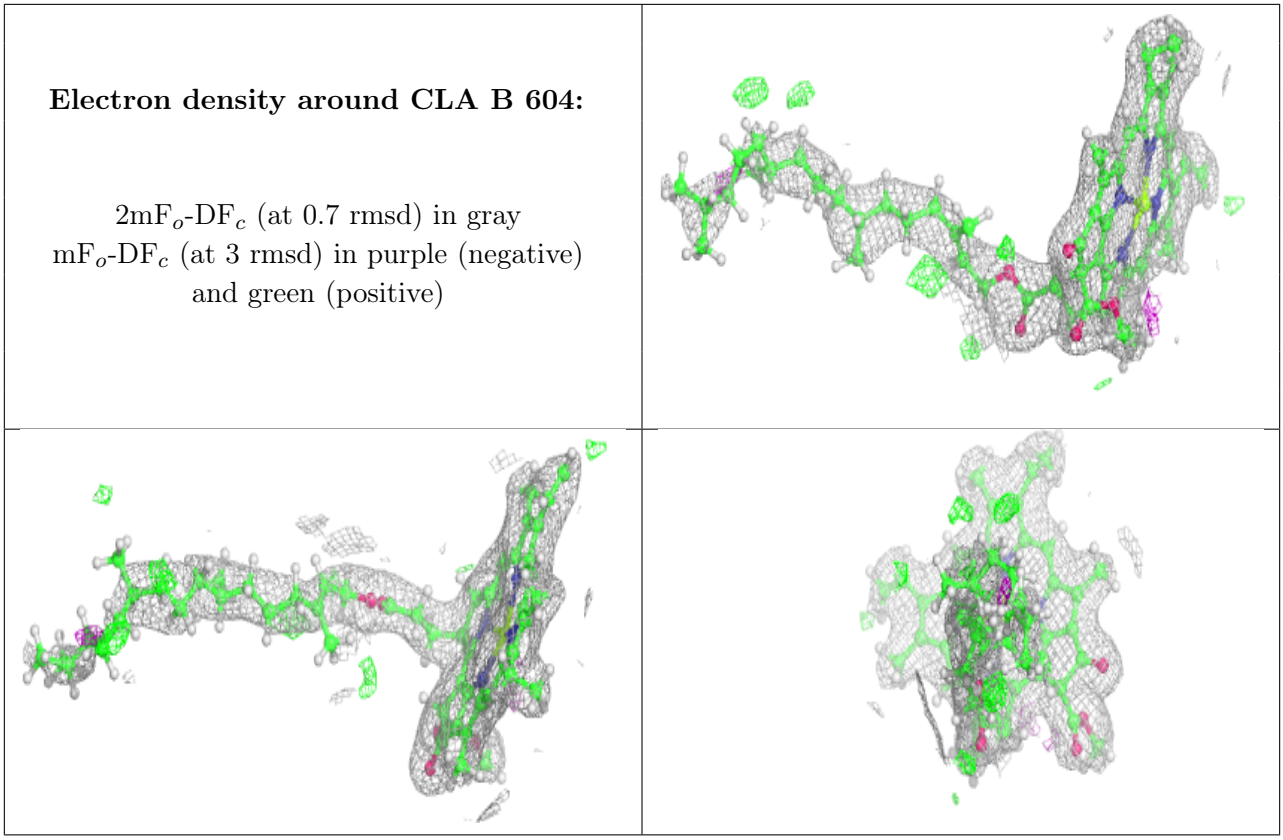
Electron density around DGD c 517:

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



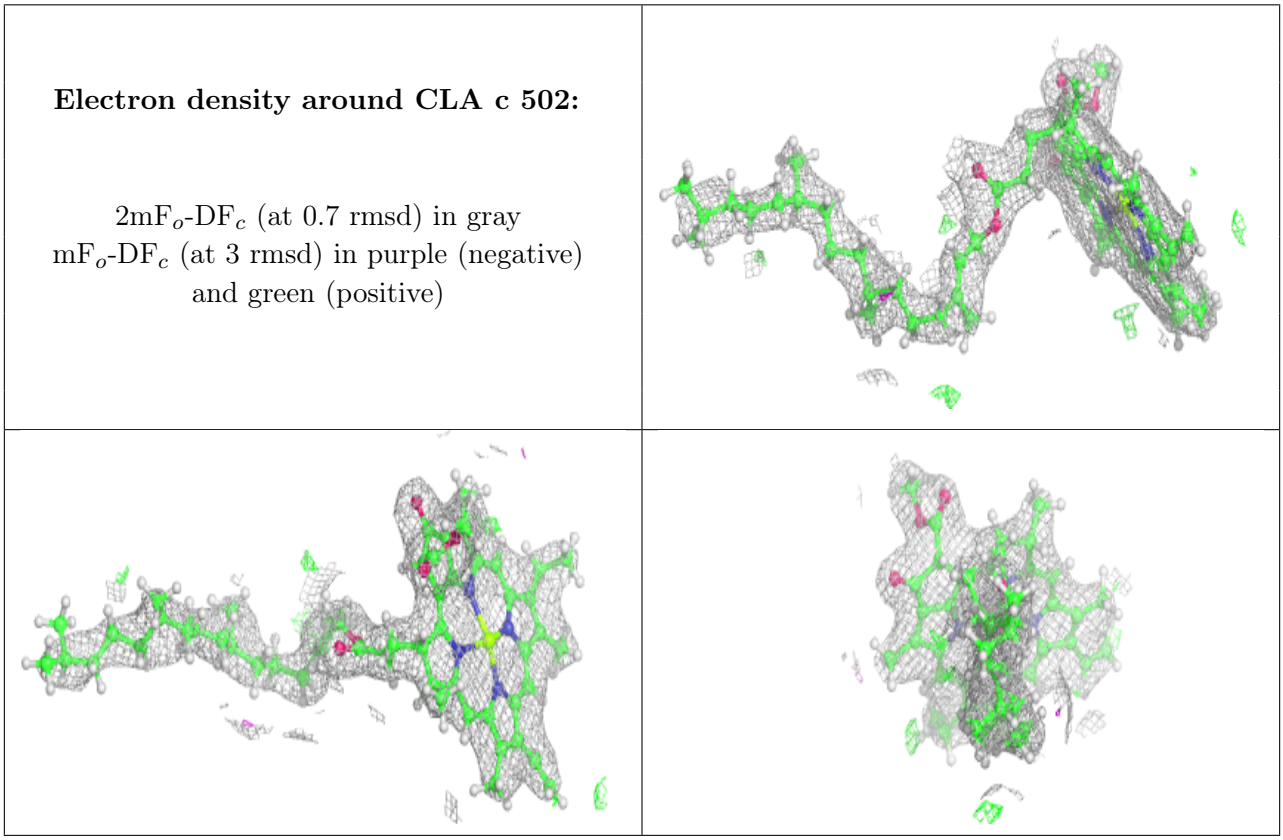
Electron density around CLA B 604:

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



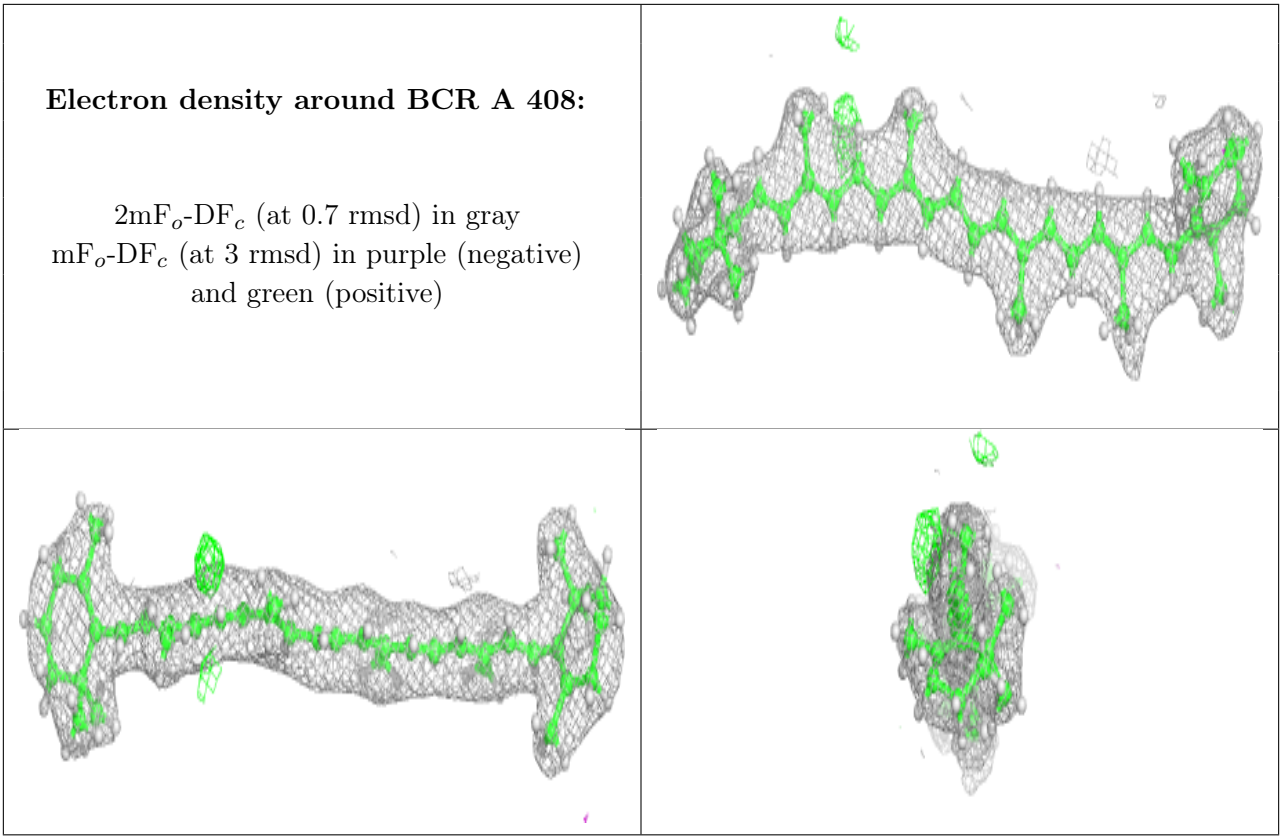
Electron density around CLA c 502:

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



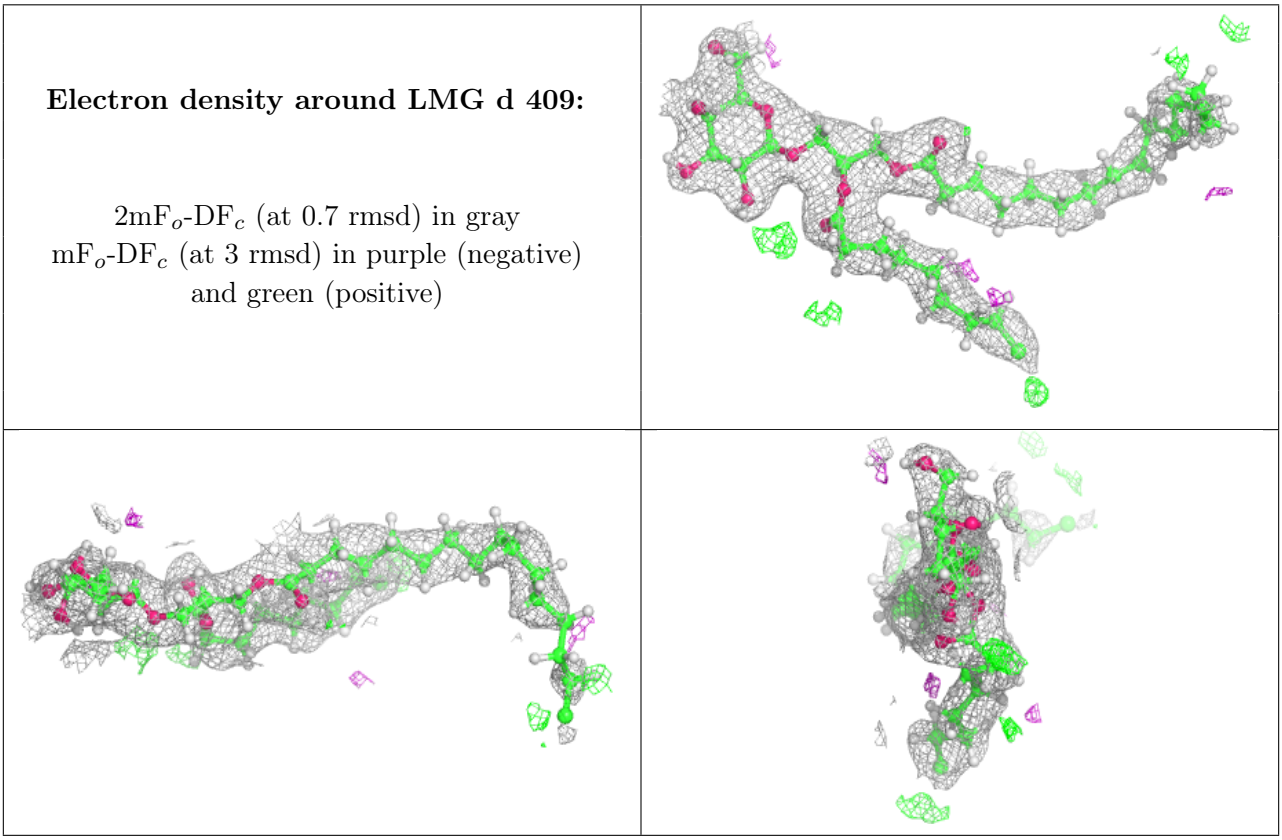
Electron density around BCR A 408:

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



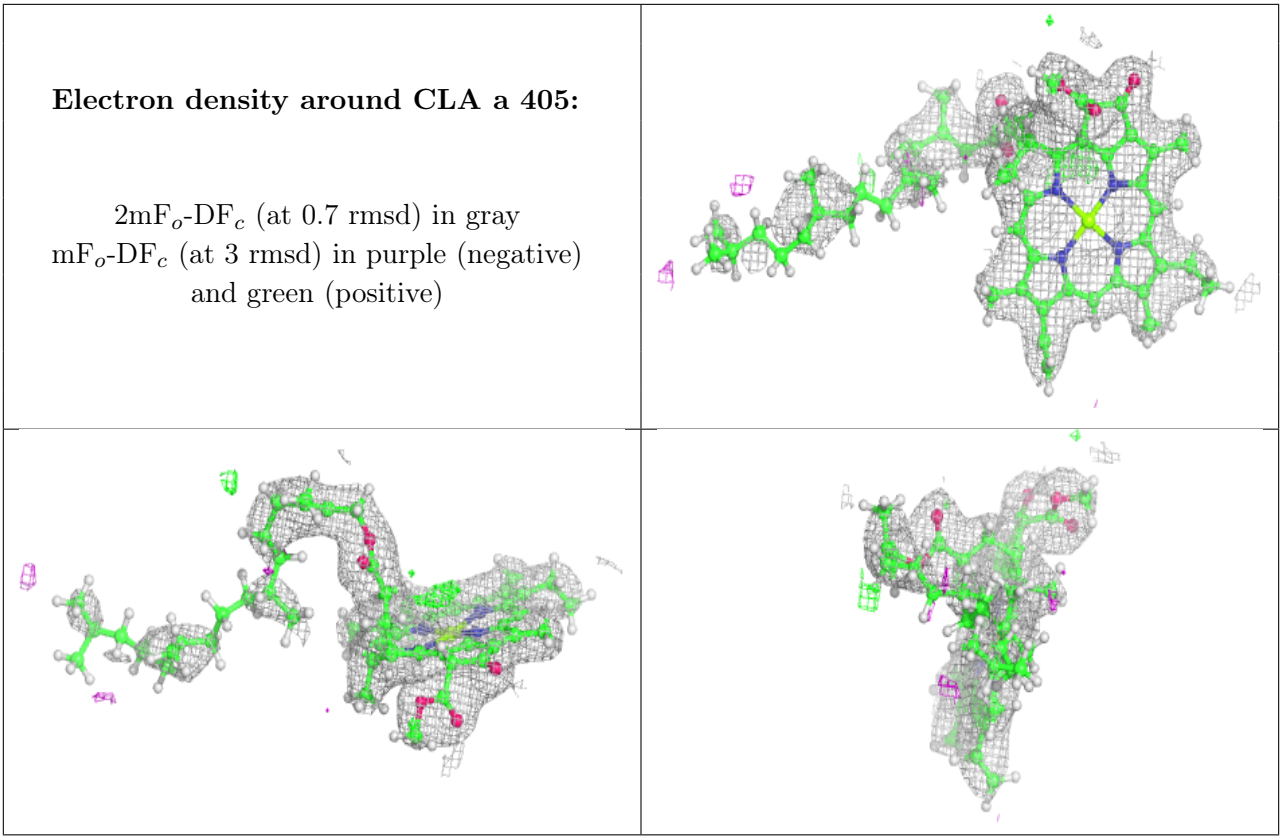
Electron density around LMG d 409:

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



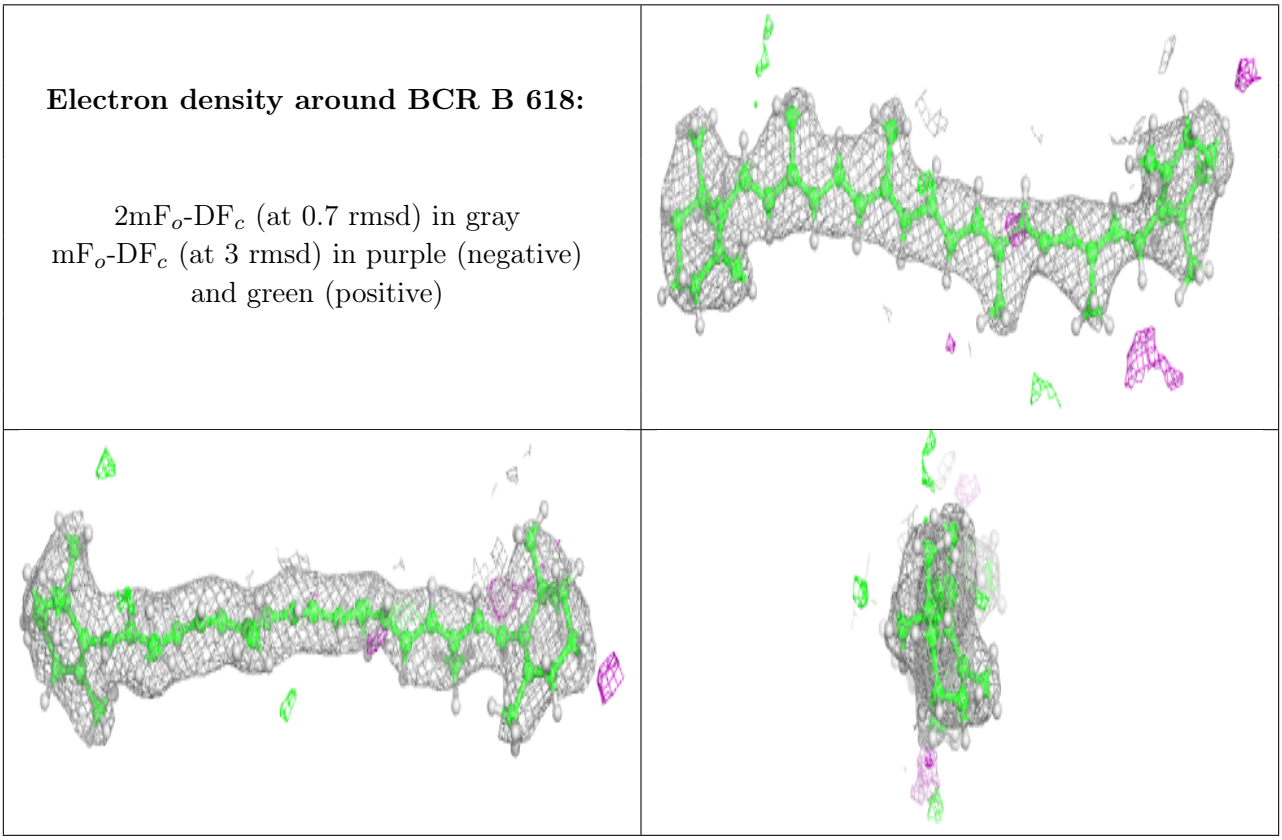
Electron density around CLA a 405:

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



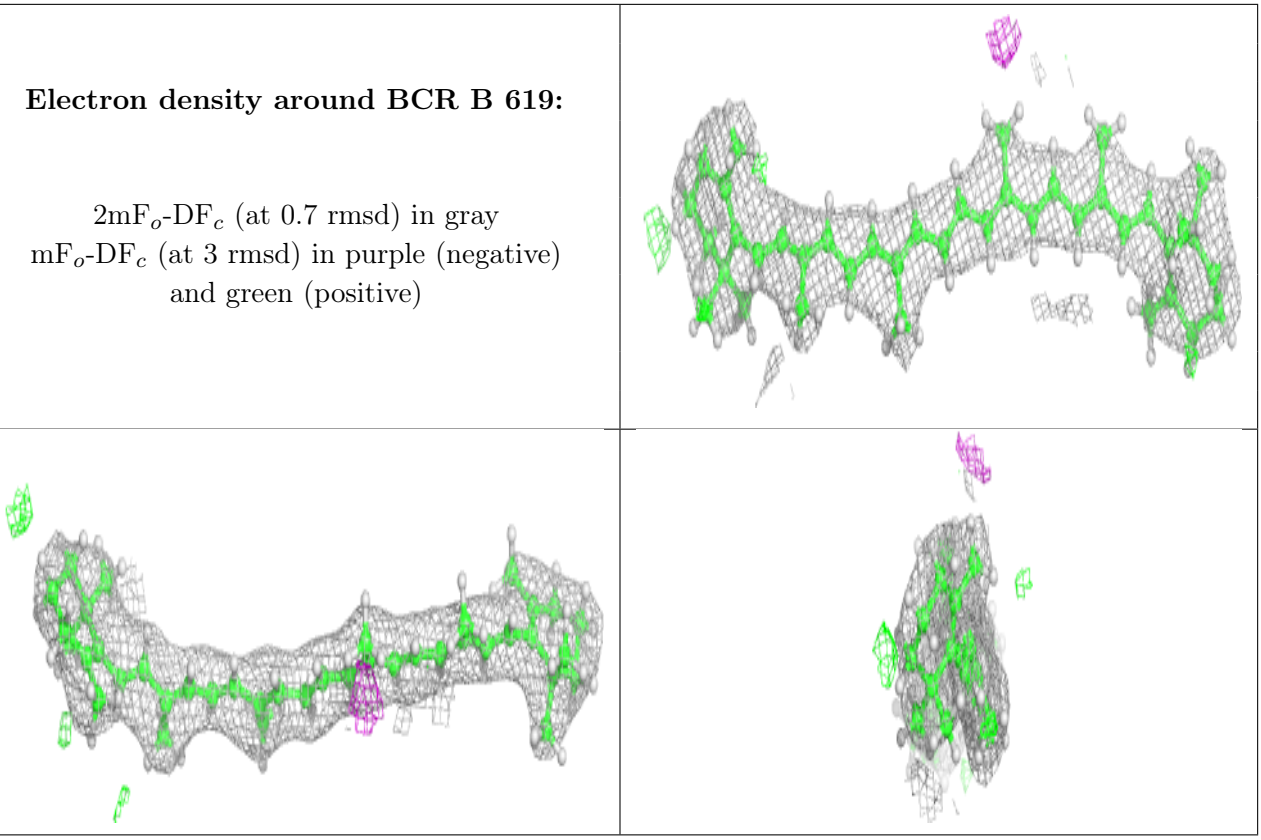
Electron density around BCR B 618:

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



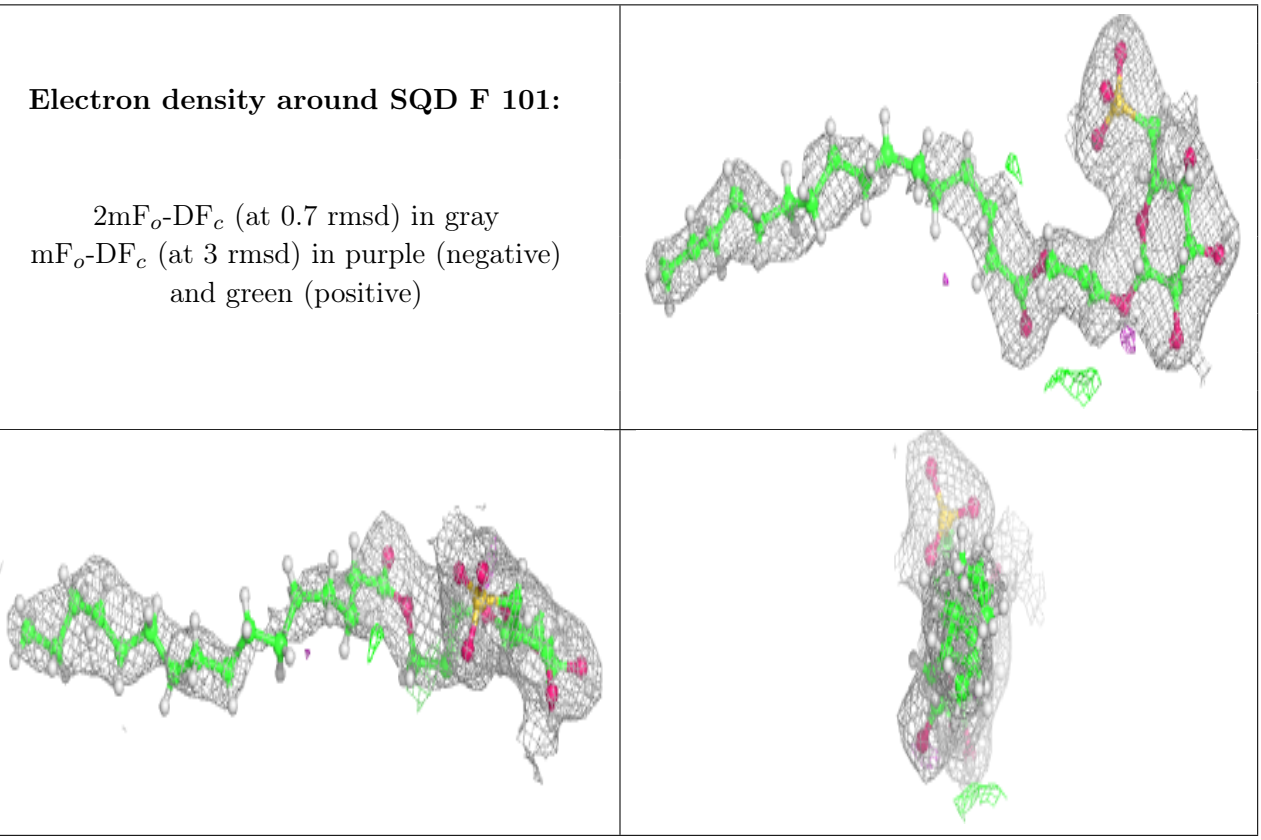
Electron density around BCR B 619:

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



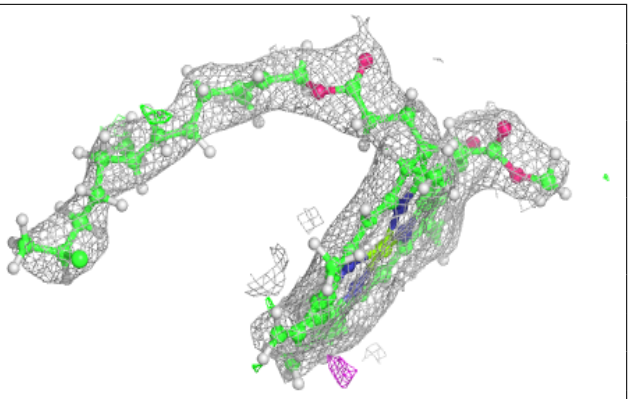
Electron density around SQD F 101:

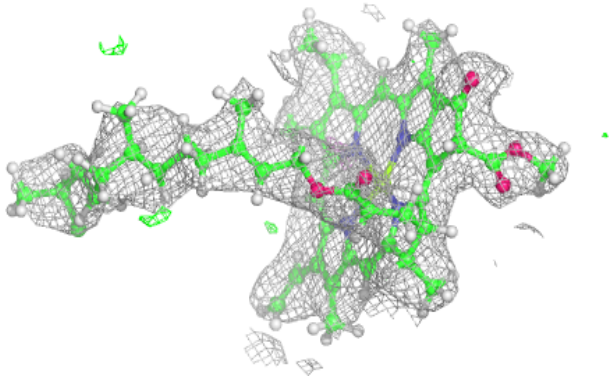
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

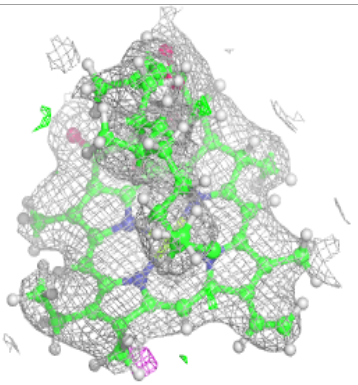


Electron density around CLA c 504:

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

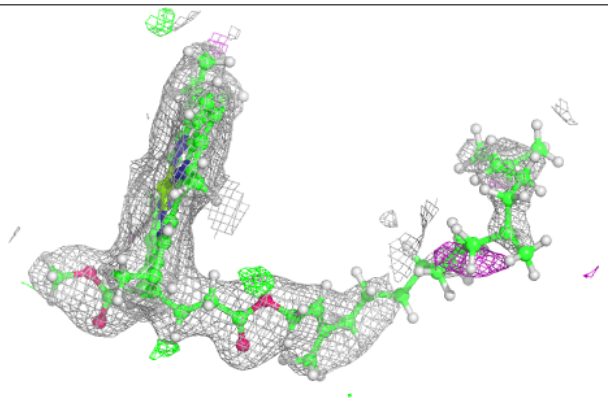


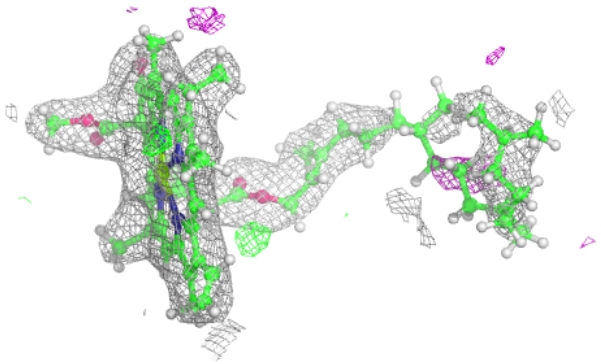


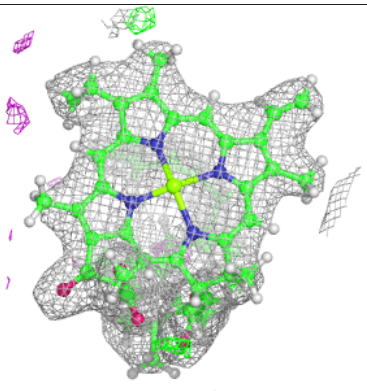


Electron density around CLA C 506:

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

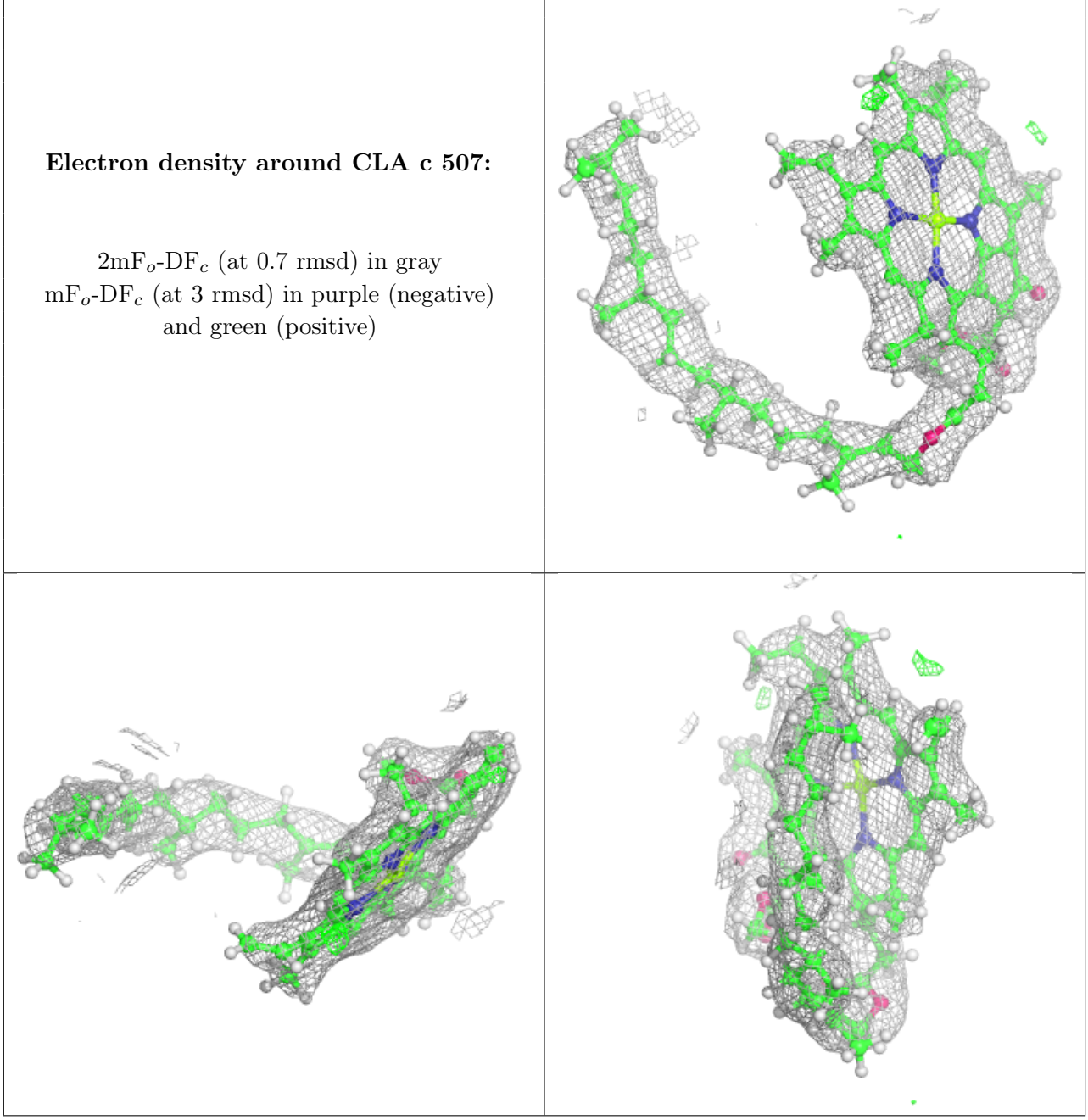






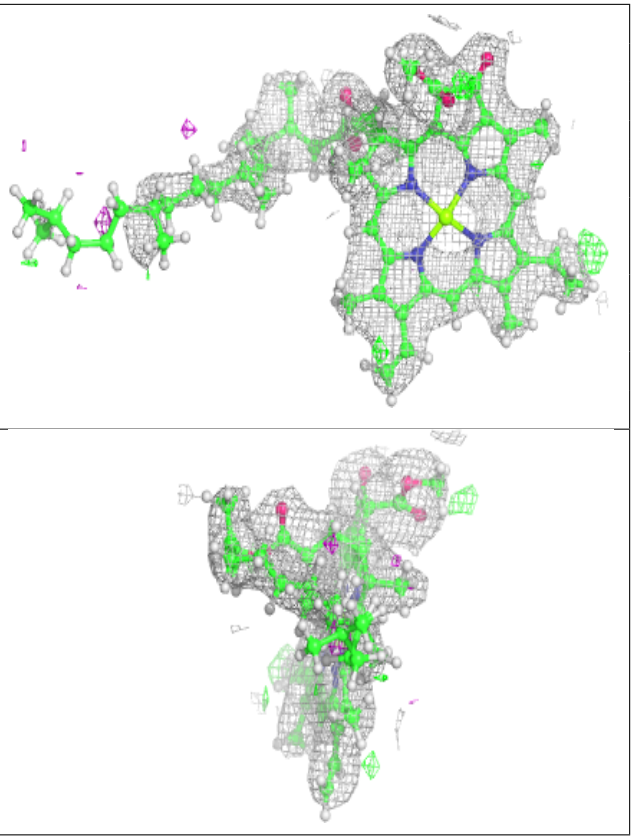
Electron density around CLA c 507:

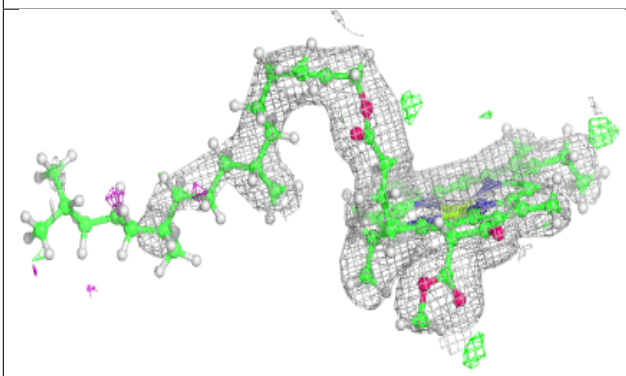
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 405:

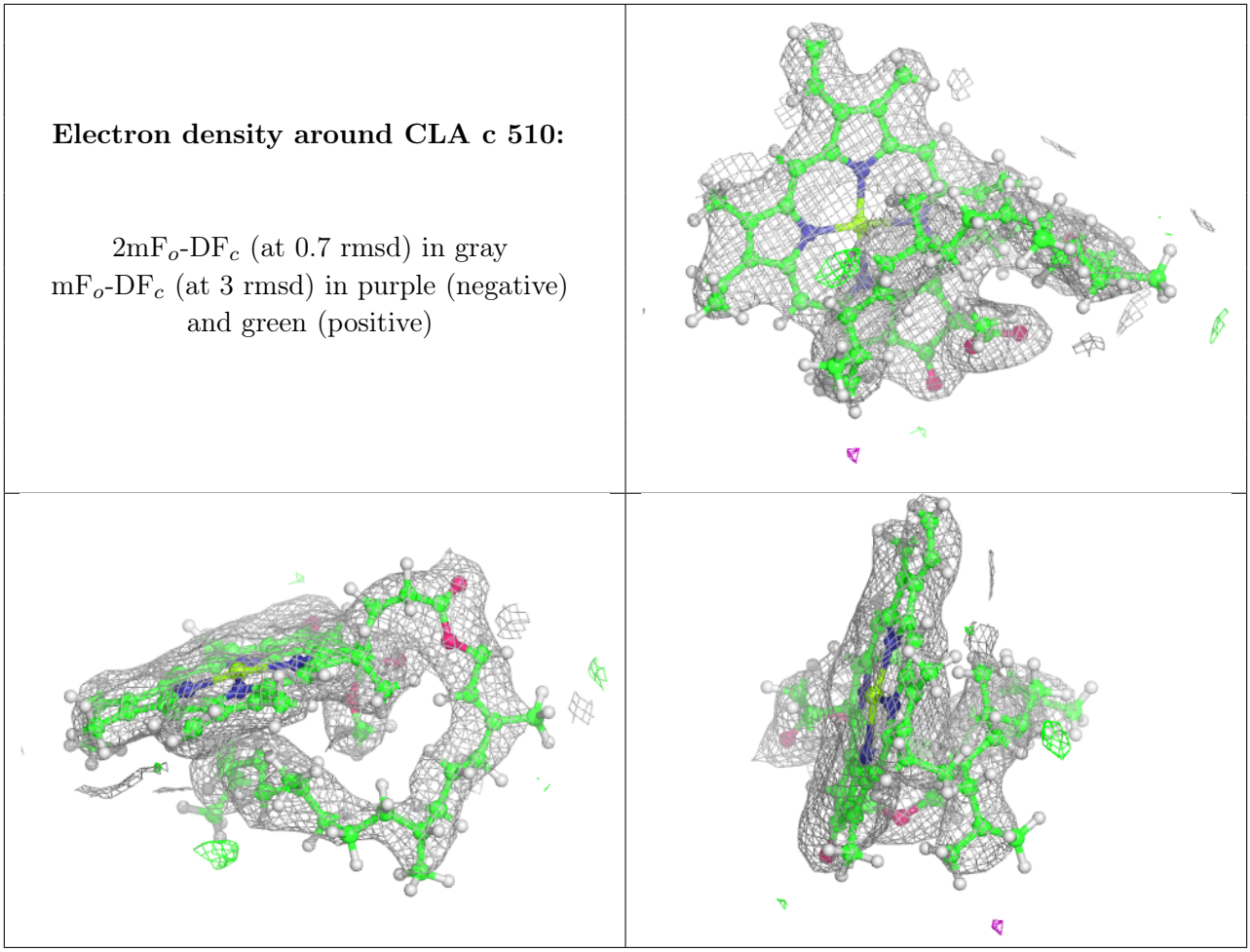
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





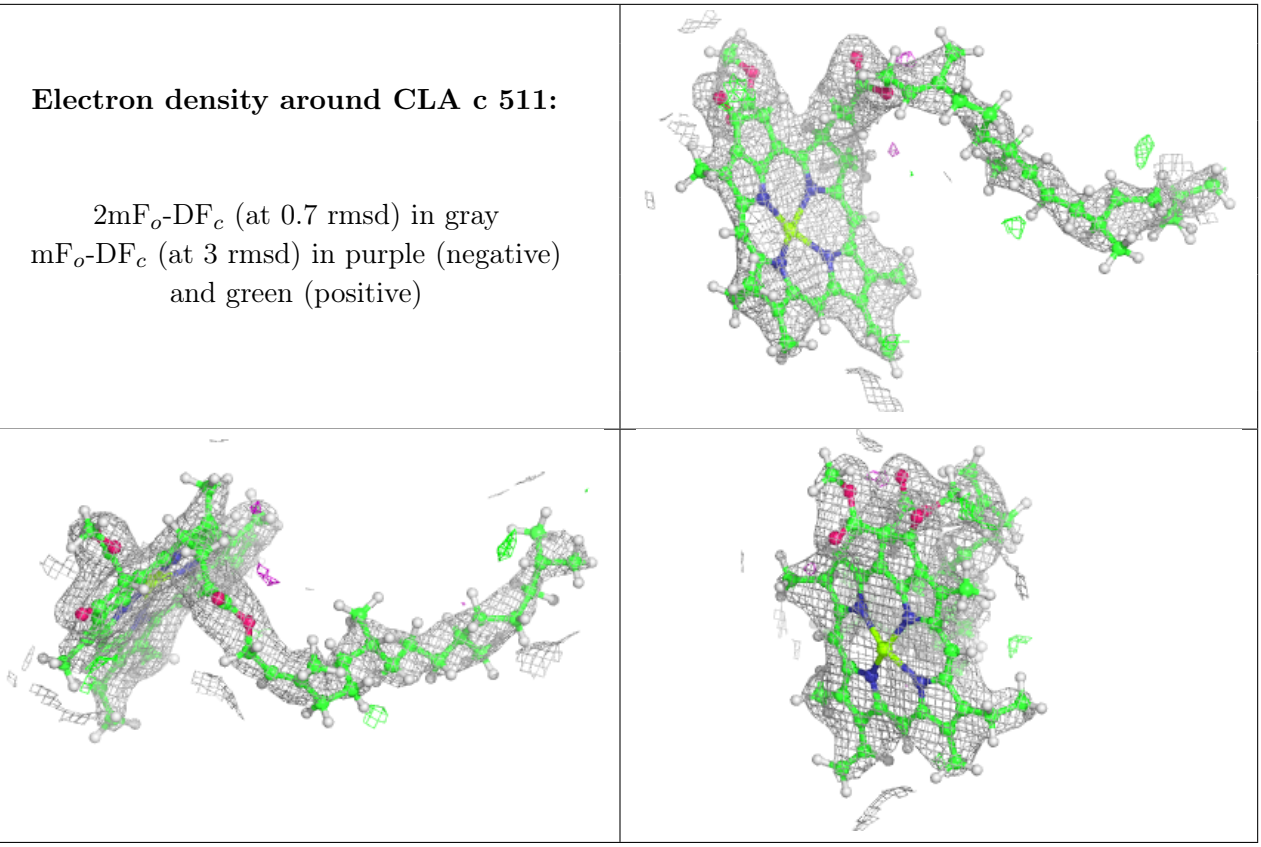
Electron density around CLA c 510:

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



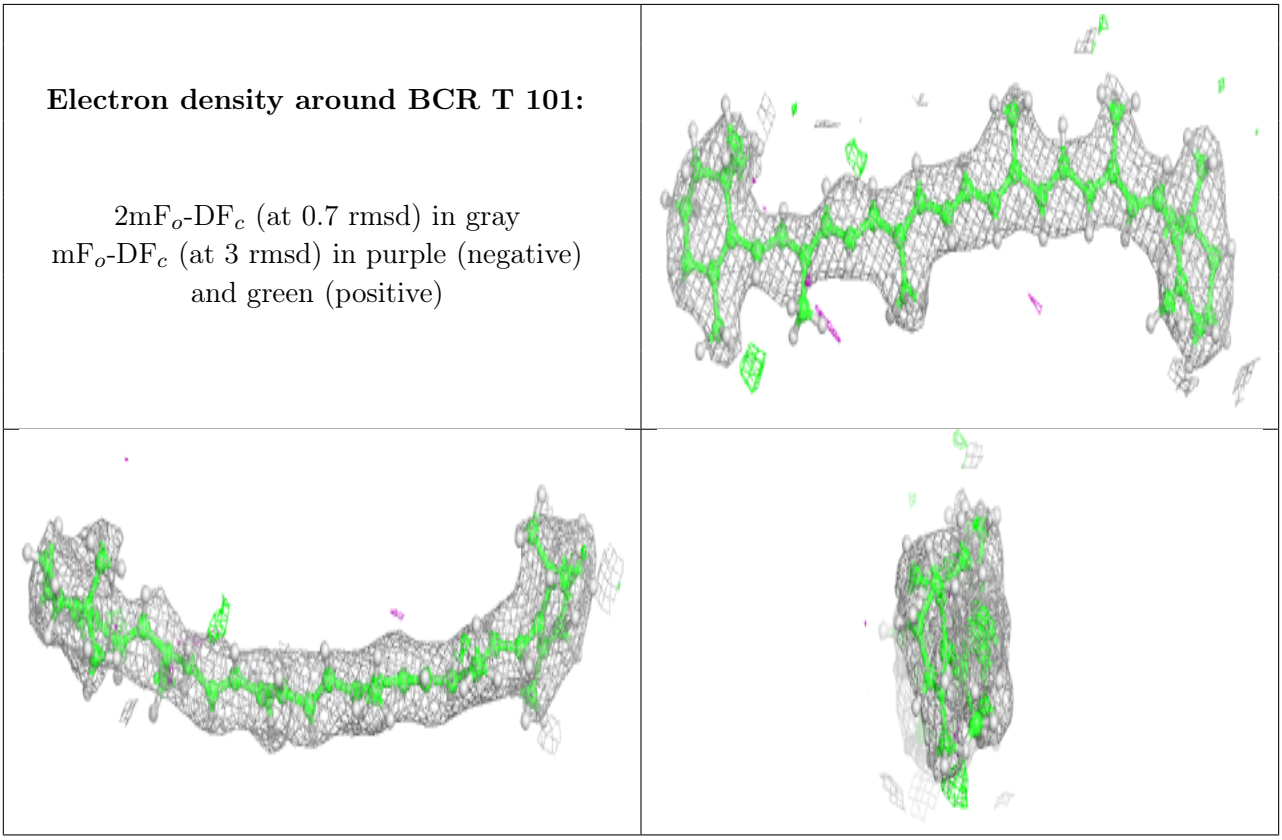
Electron density around CLA c 511:

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



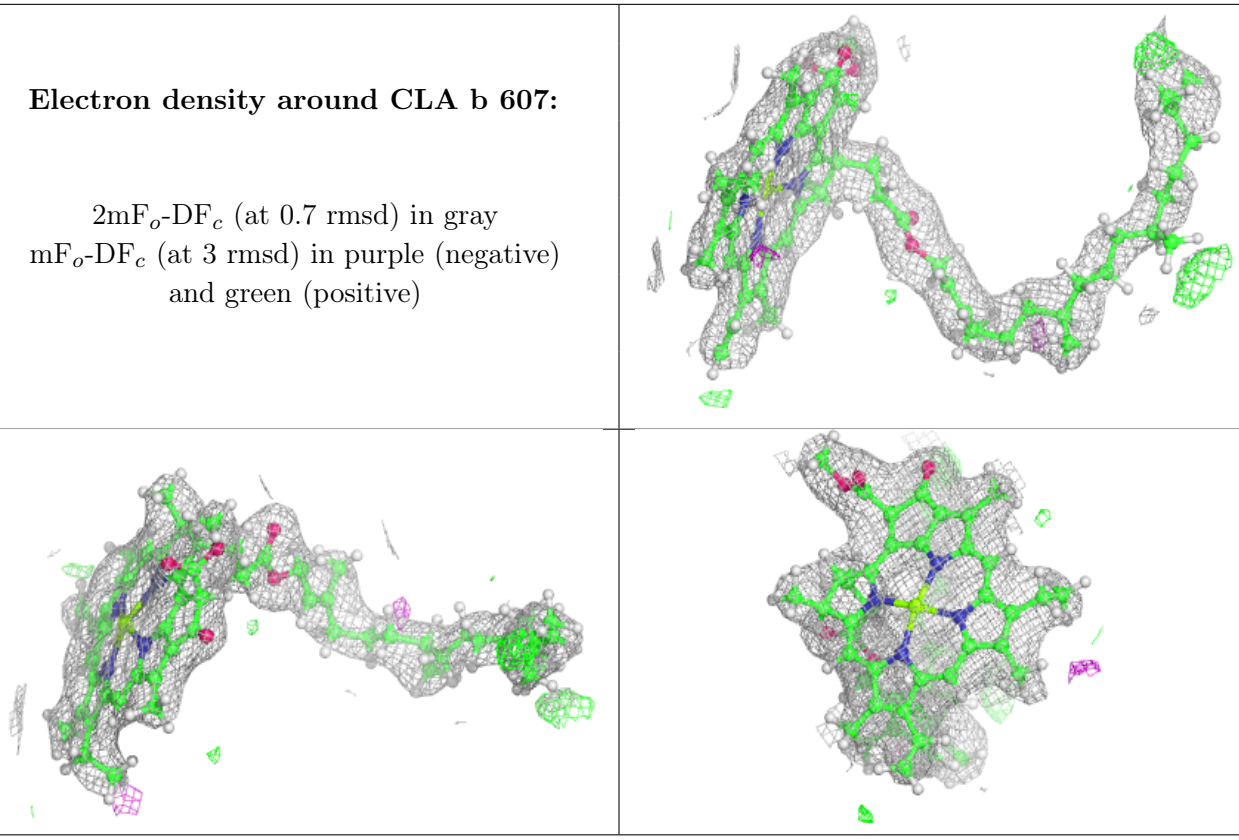
Electron density around BCR T 101:

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



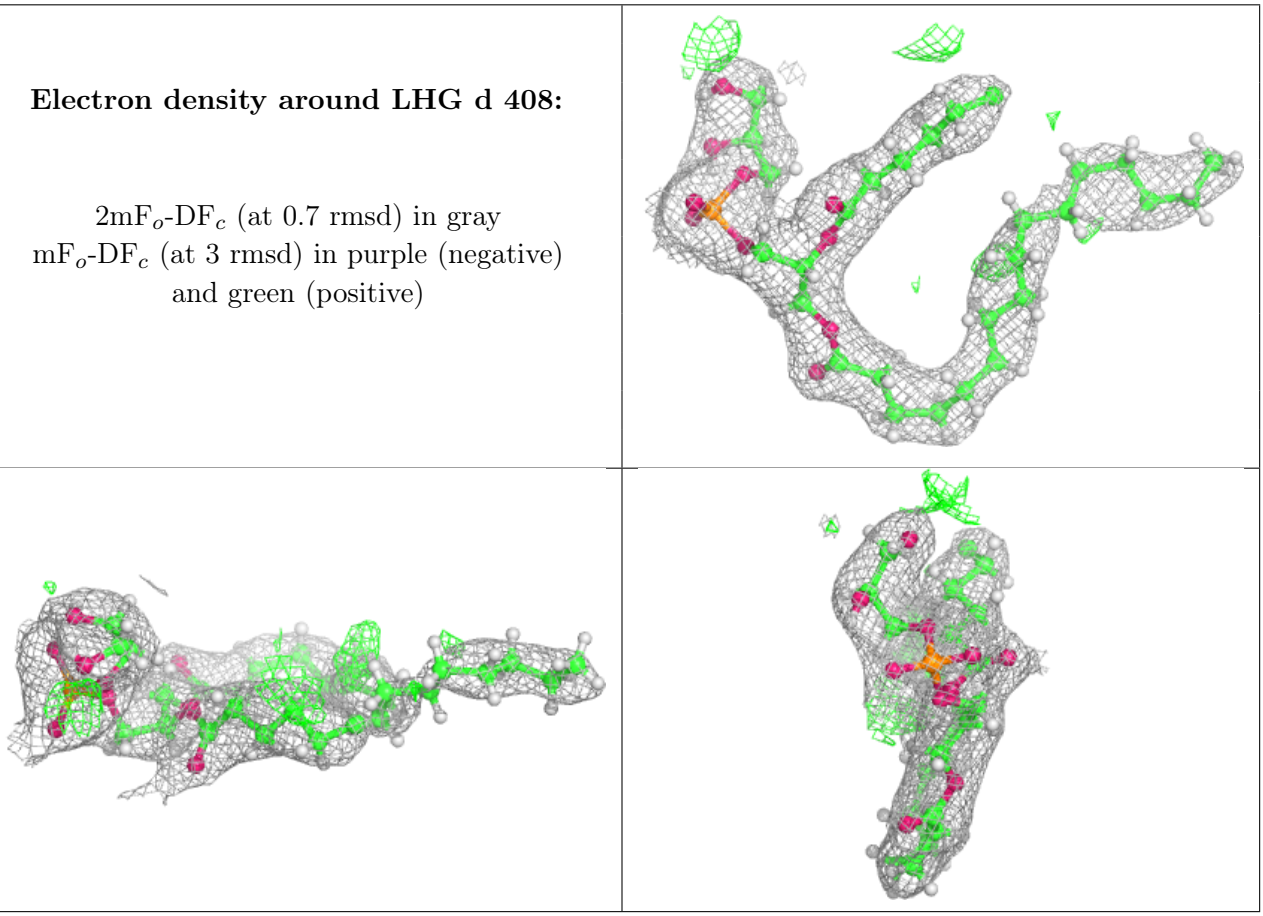
Electron density around CLA b 607:

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



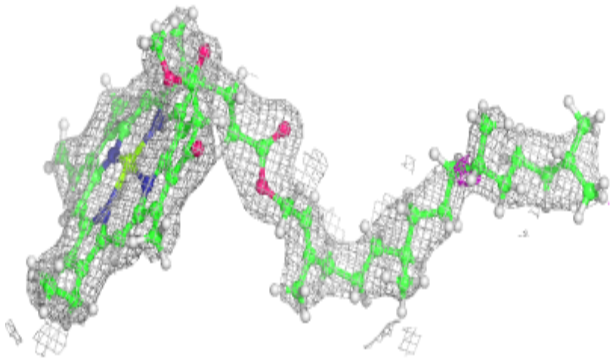
Electron density around LHG d 408:

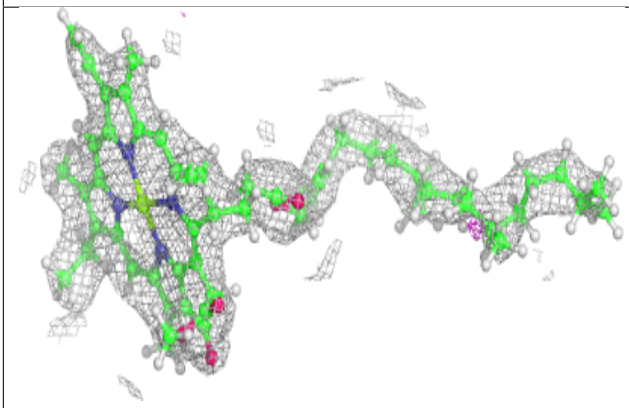
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

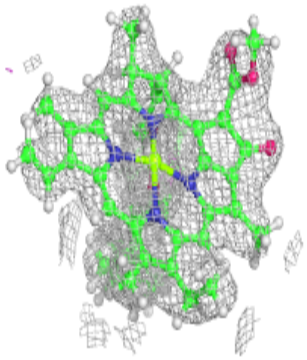


Electron density around CLA C 502:

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

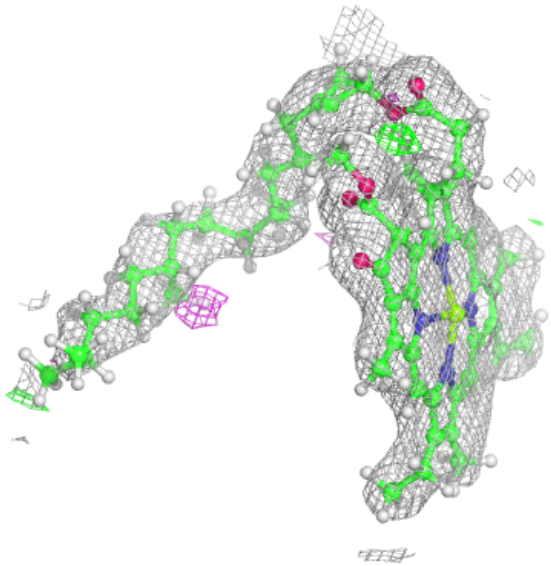


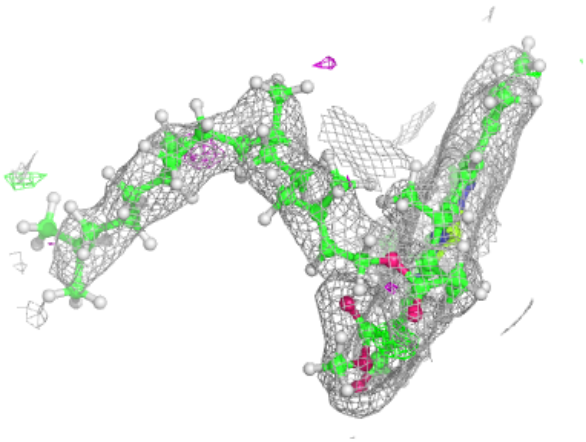


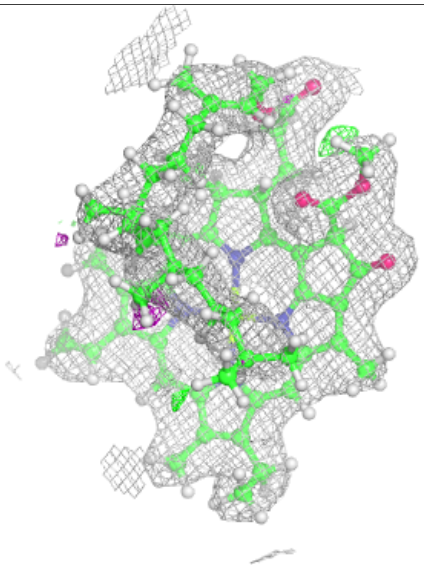


Electron density around CLA B 613:

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

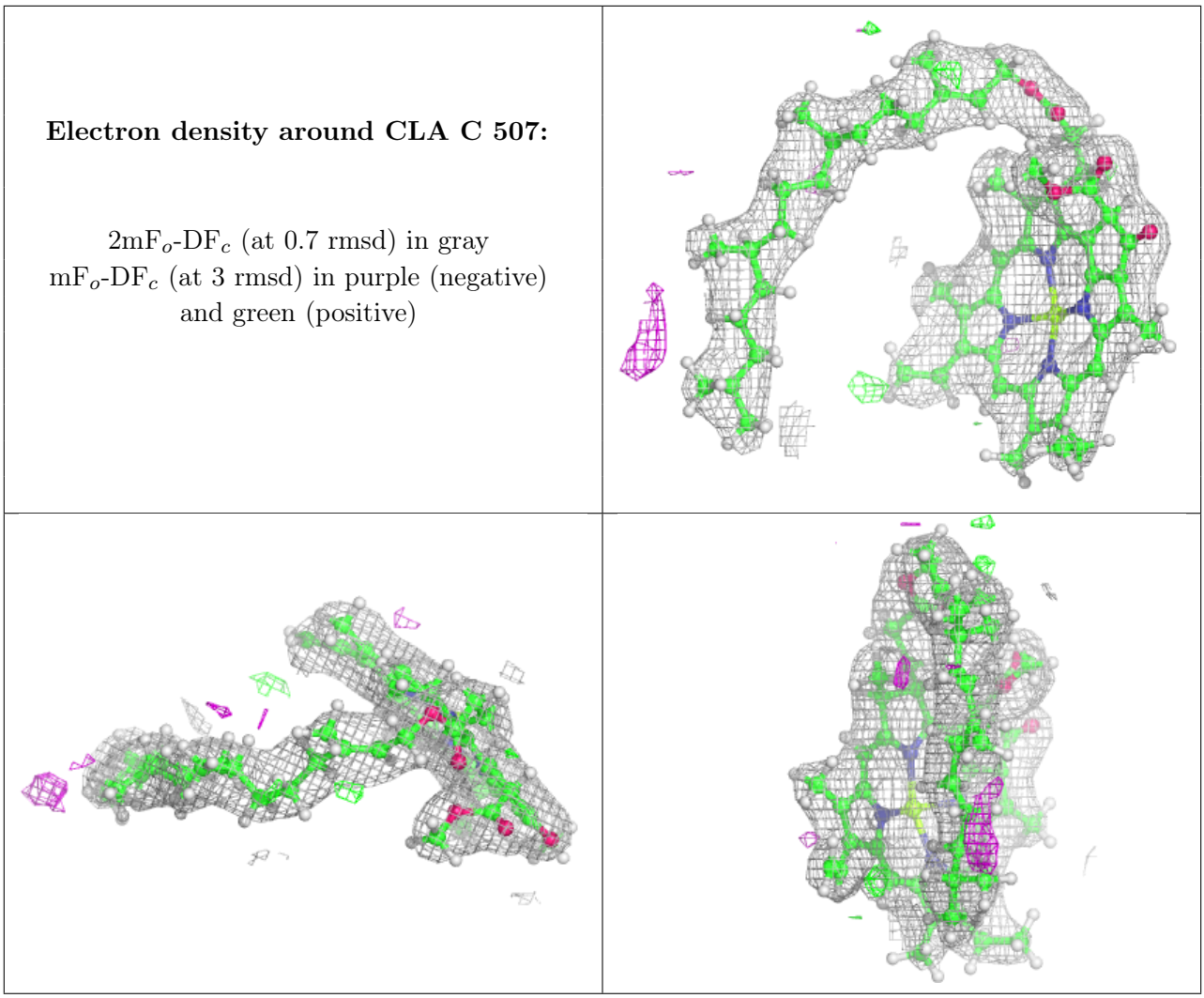






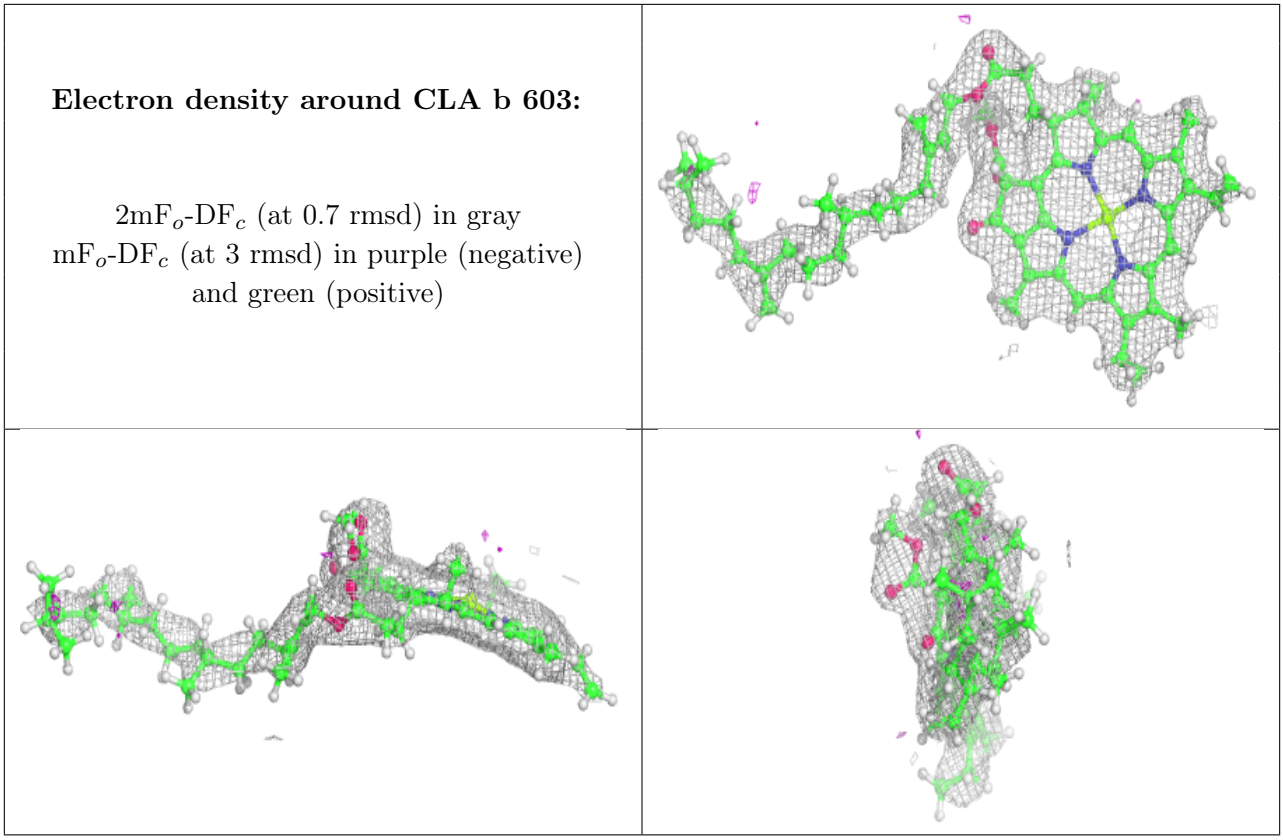
Electron density around CLA C 507:

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



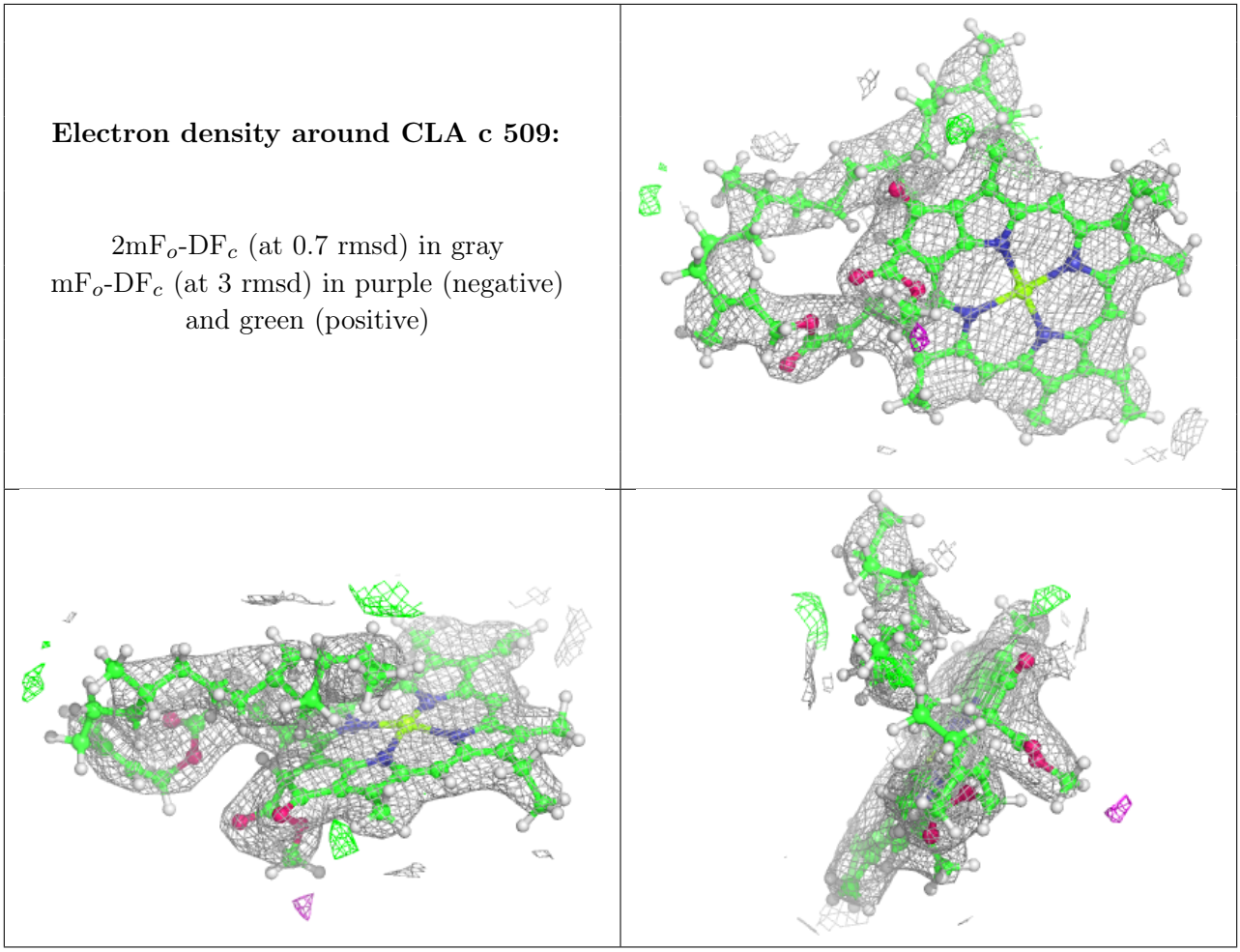
Electron density around CLA b 603:

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



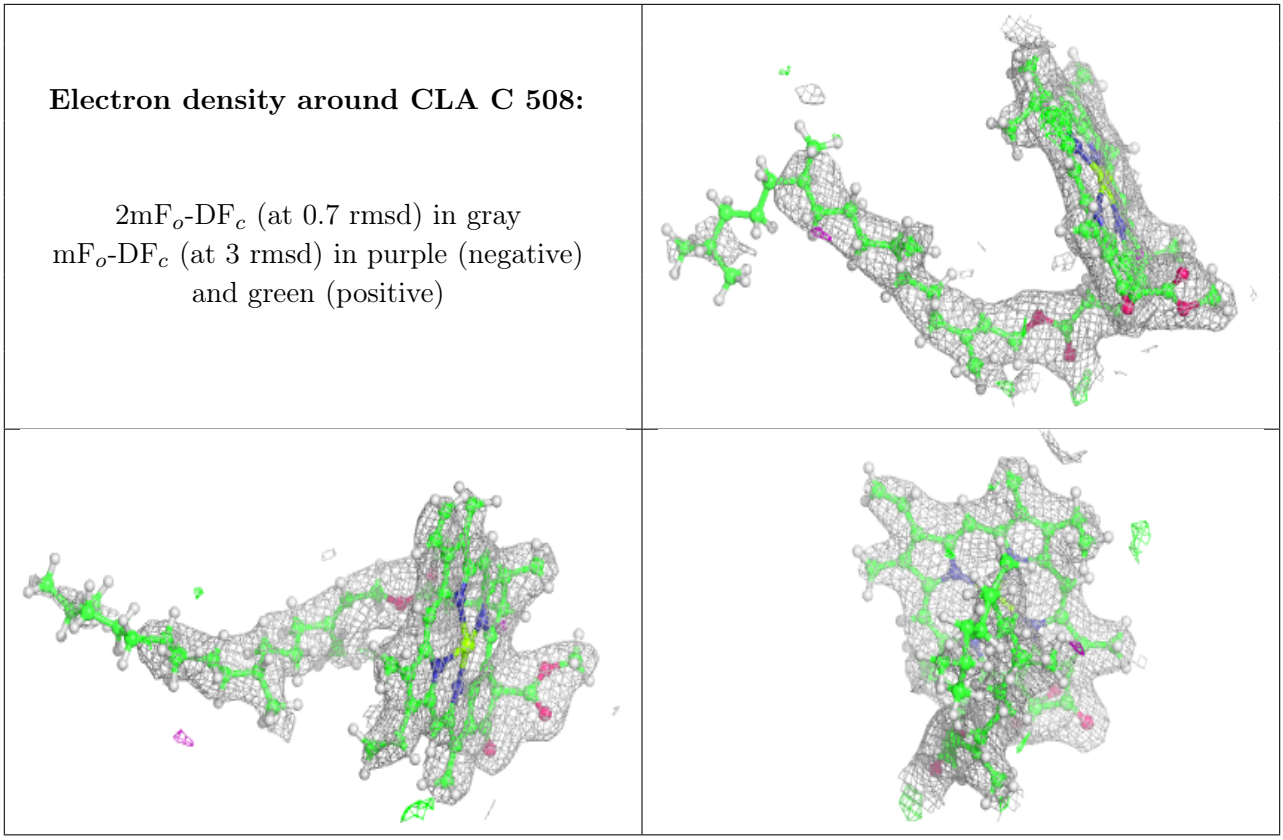
Electron density around CLA c 509:

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



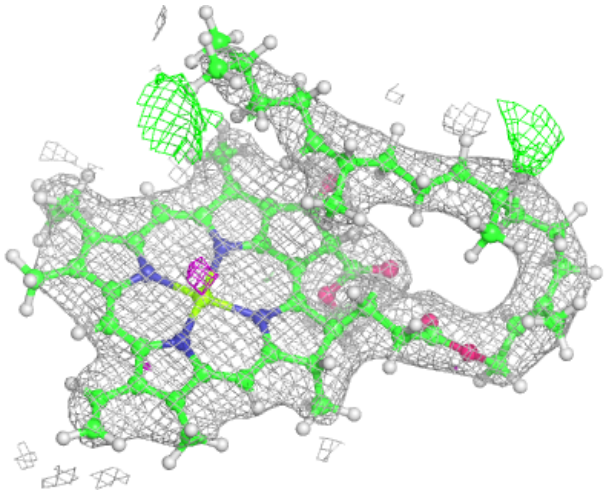
Electron density around CLA C 508:

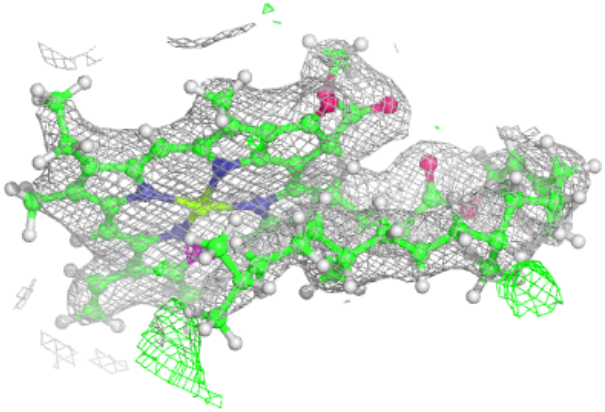
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

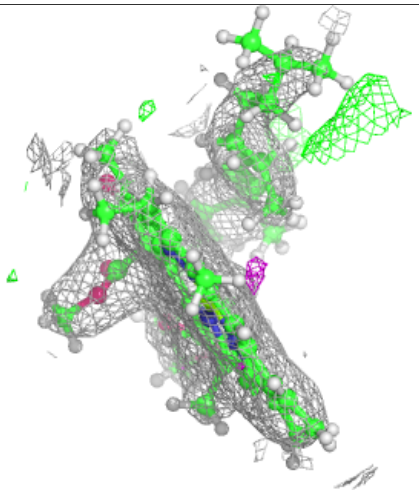


Electron density around CLA C 509:

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

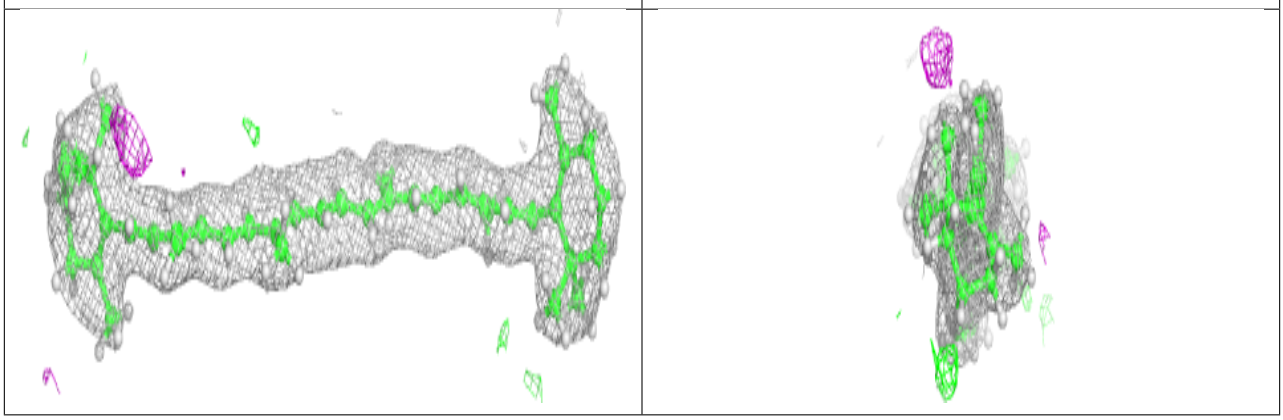






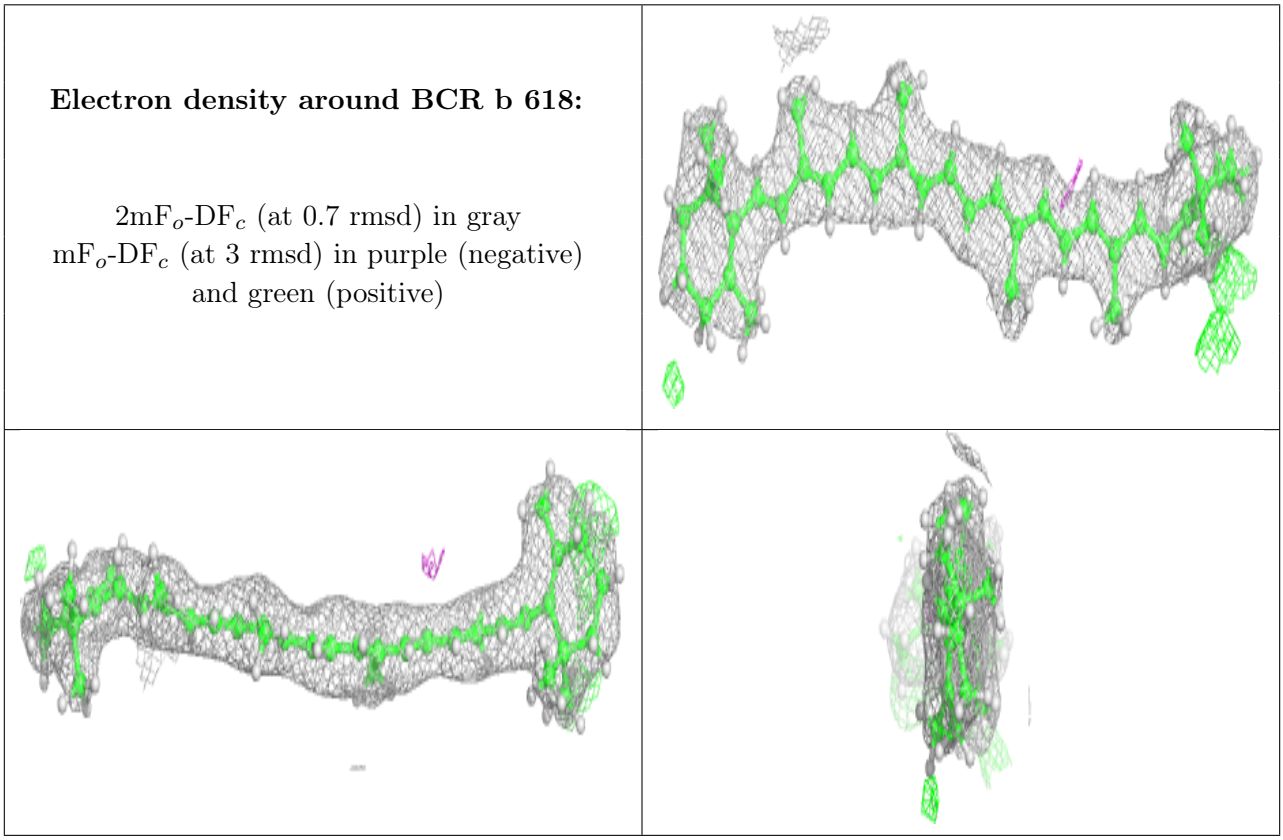
Electron density around BCR a 408:

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



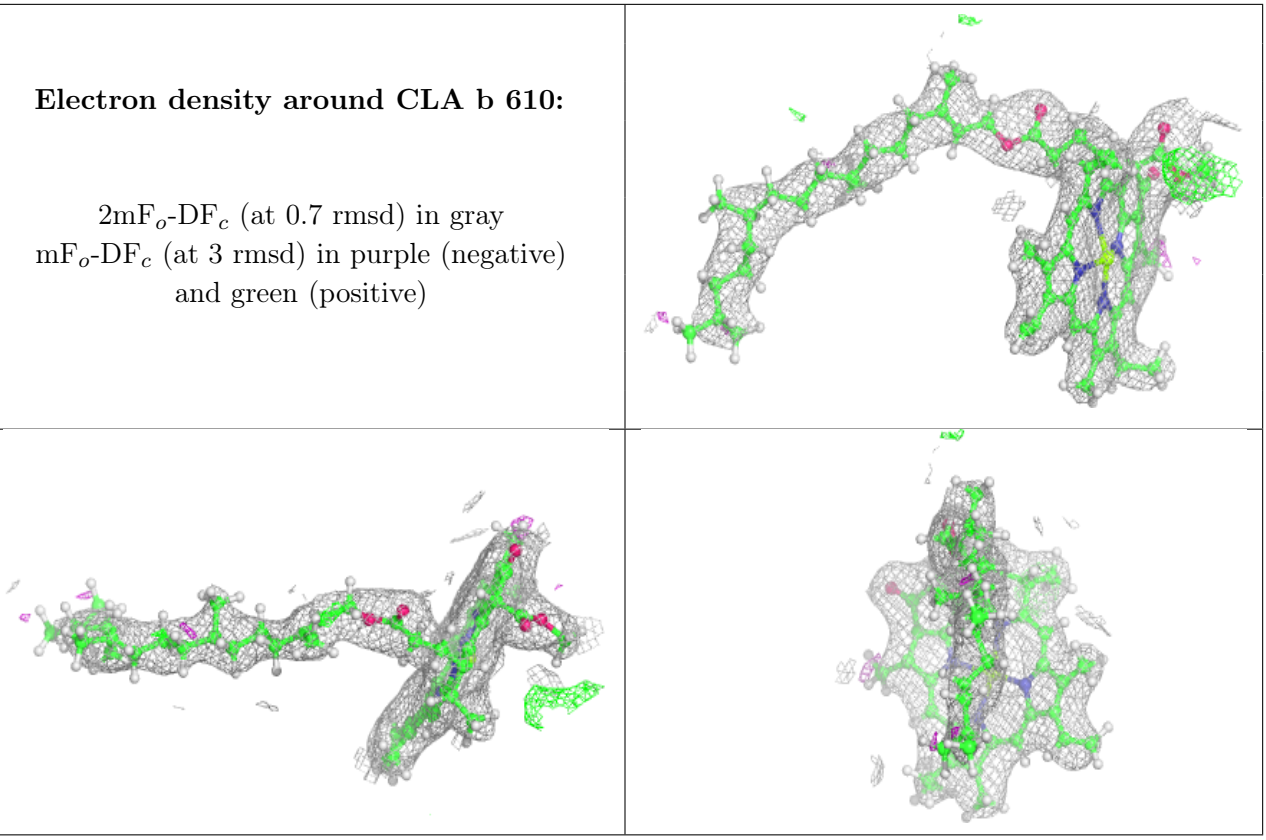
Electron density around BCR b 618:

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



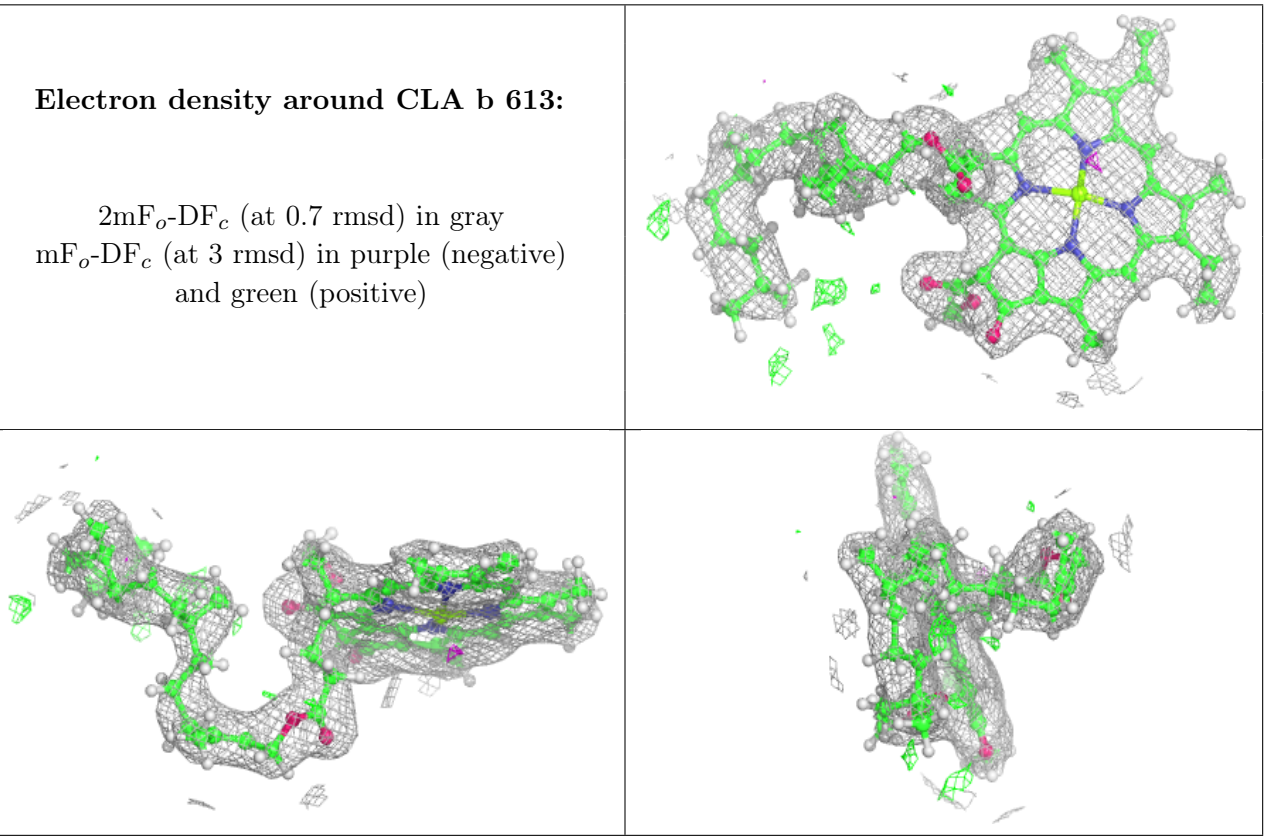
Electron density around CLA b 610:

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



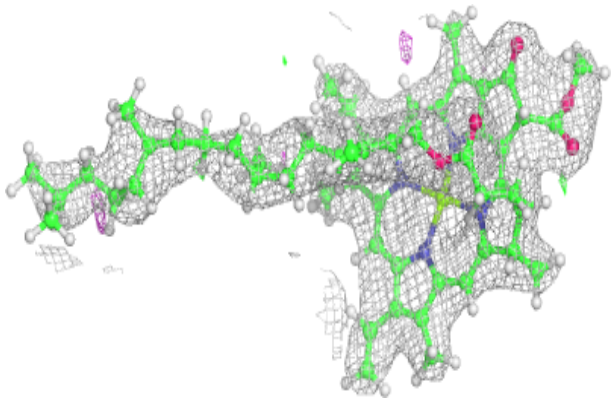
Electron density around CLA b 613:

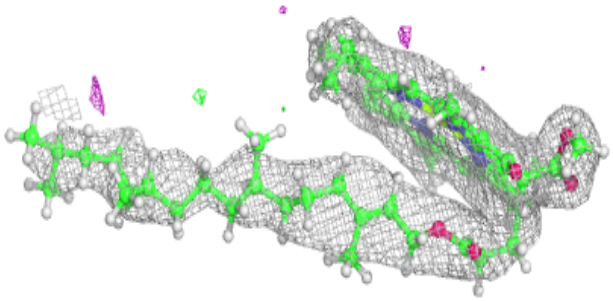
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

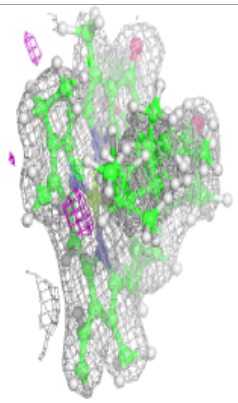


Electron density around CLA b 615:

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

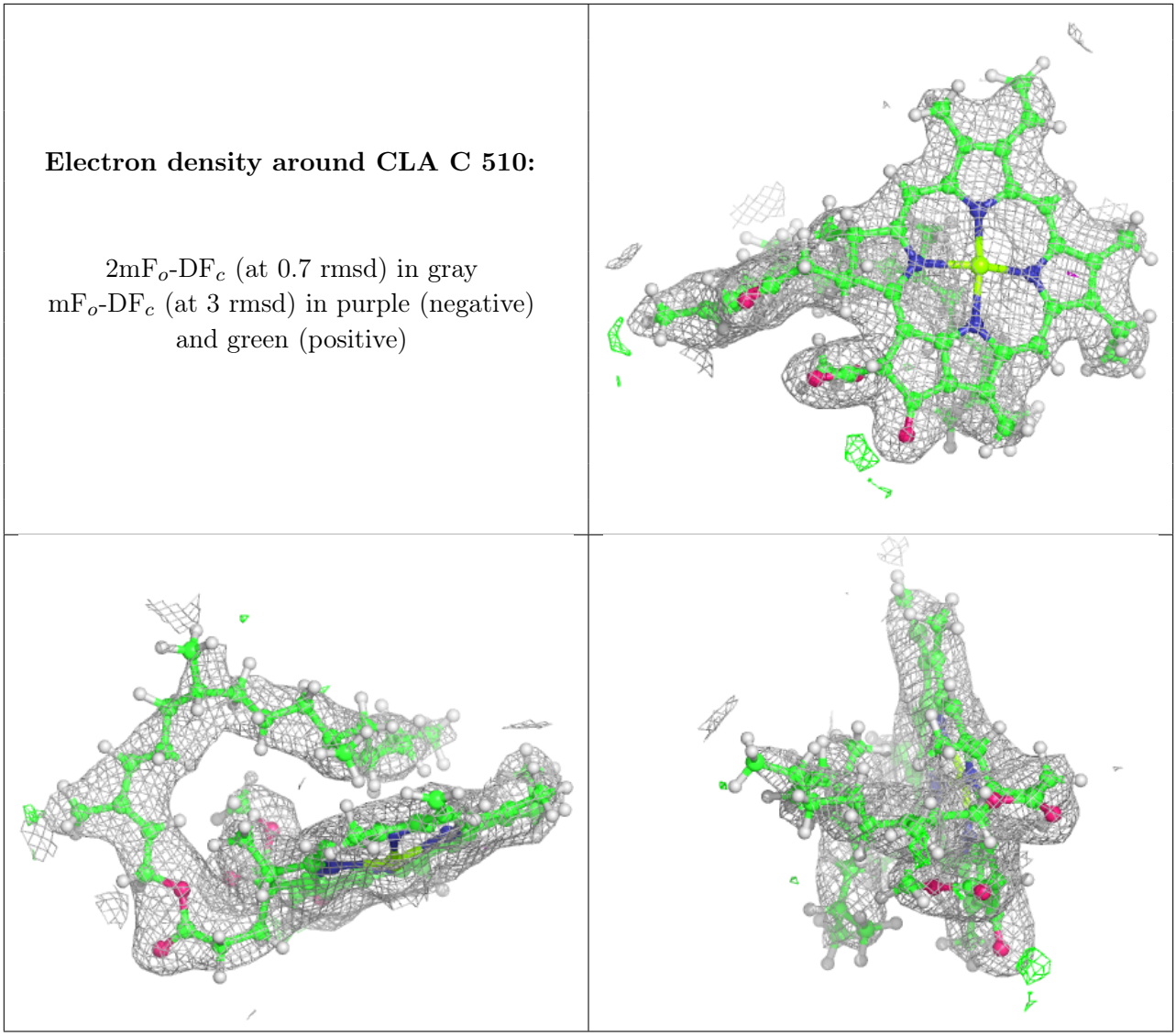






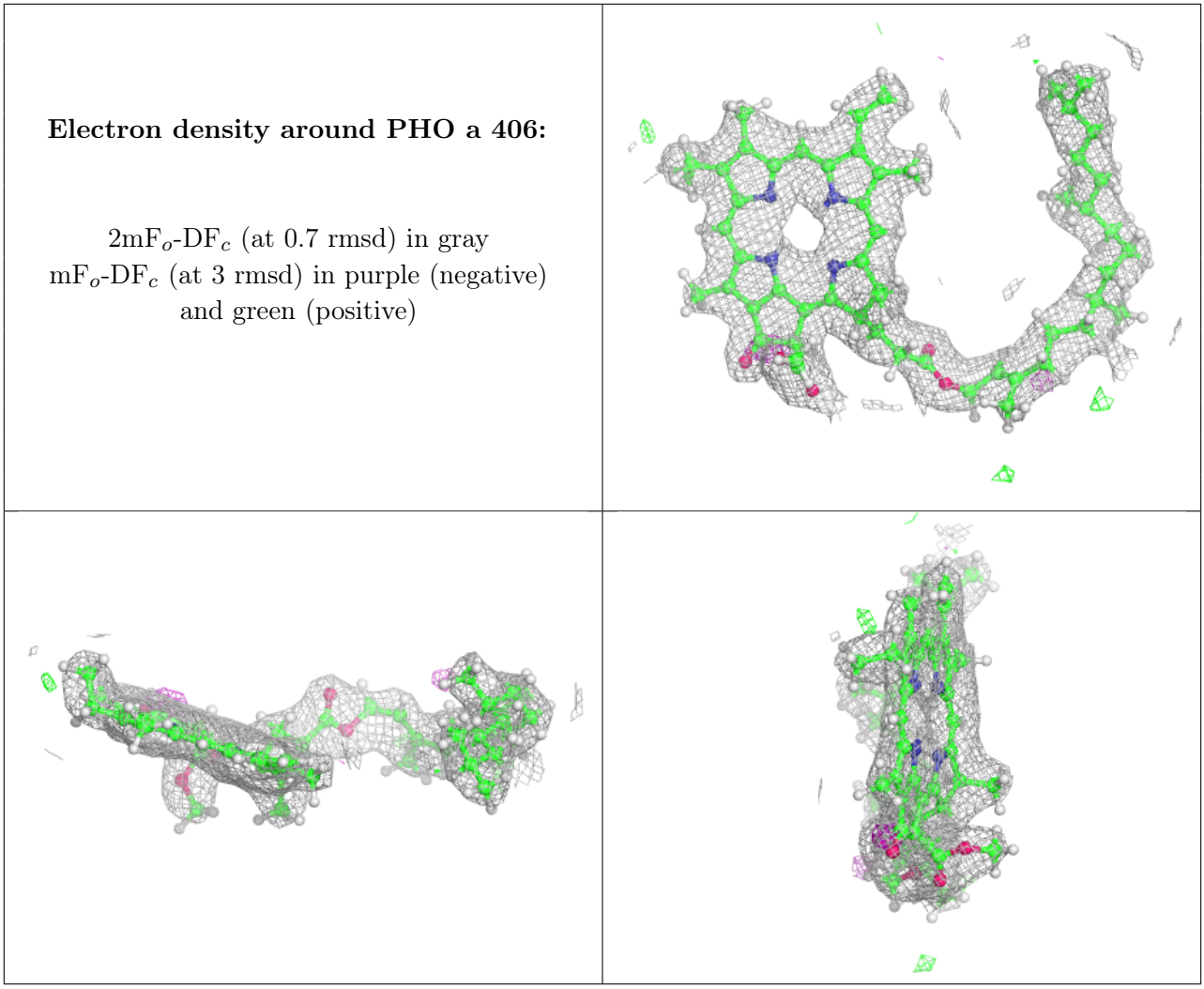
Electron density around CLA C 510:

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



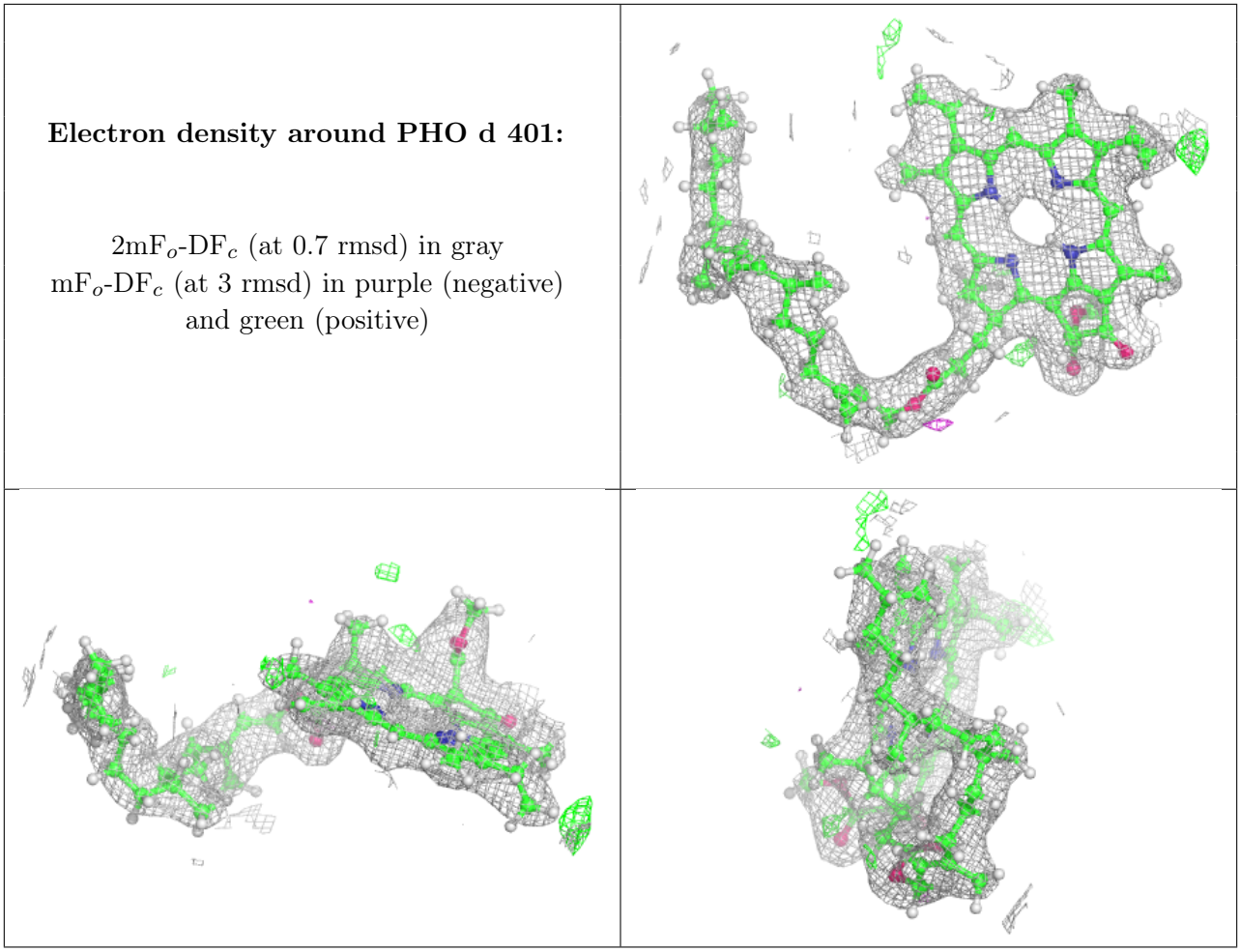
Electron density around PHO a 406:

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



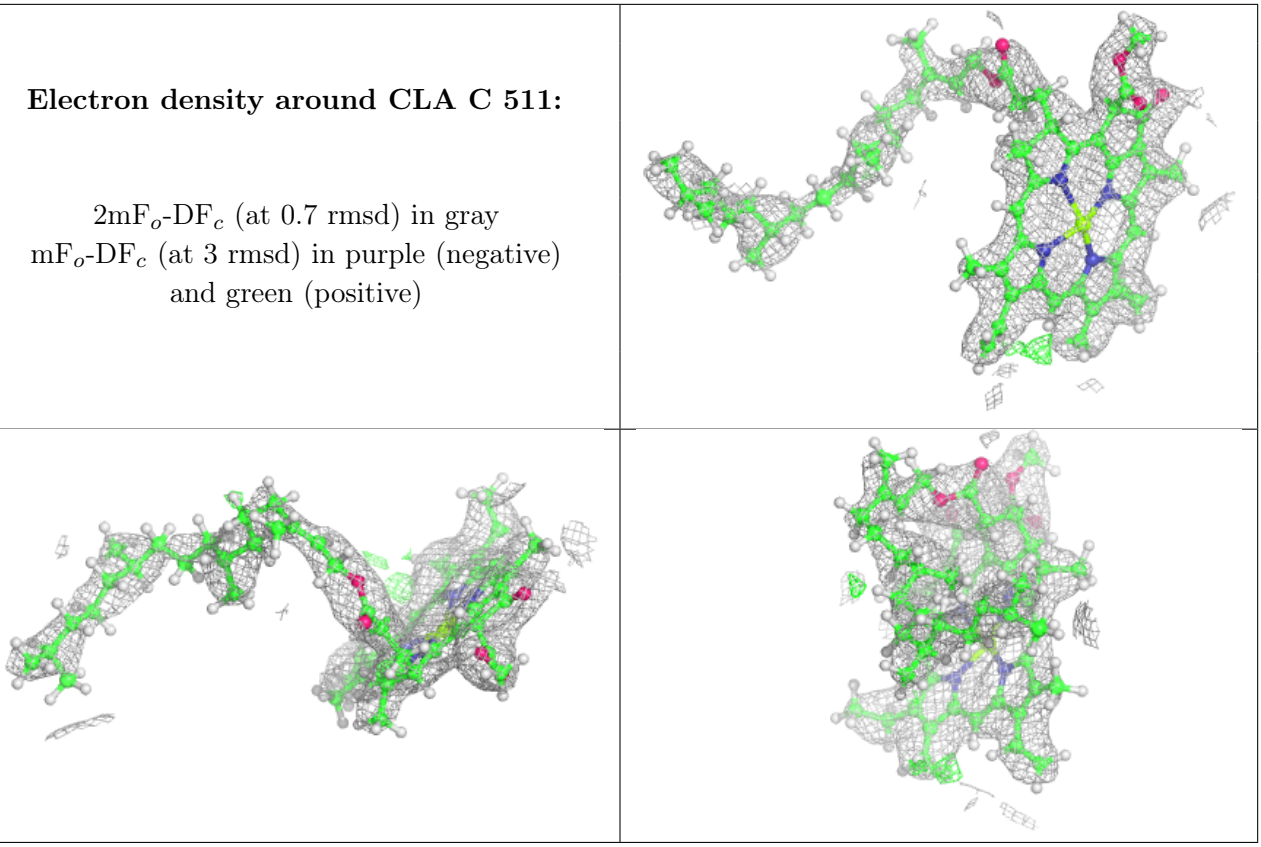
Electron density around PHO d 401:

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



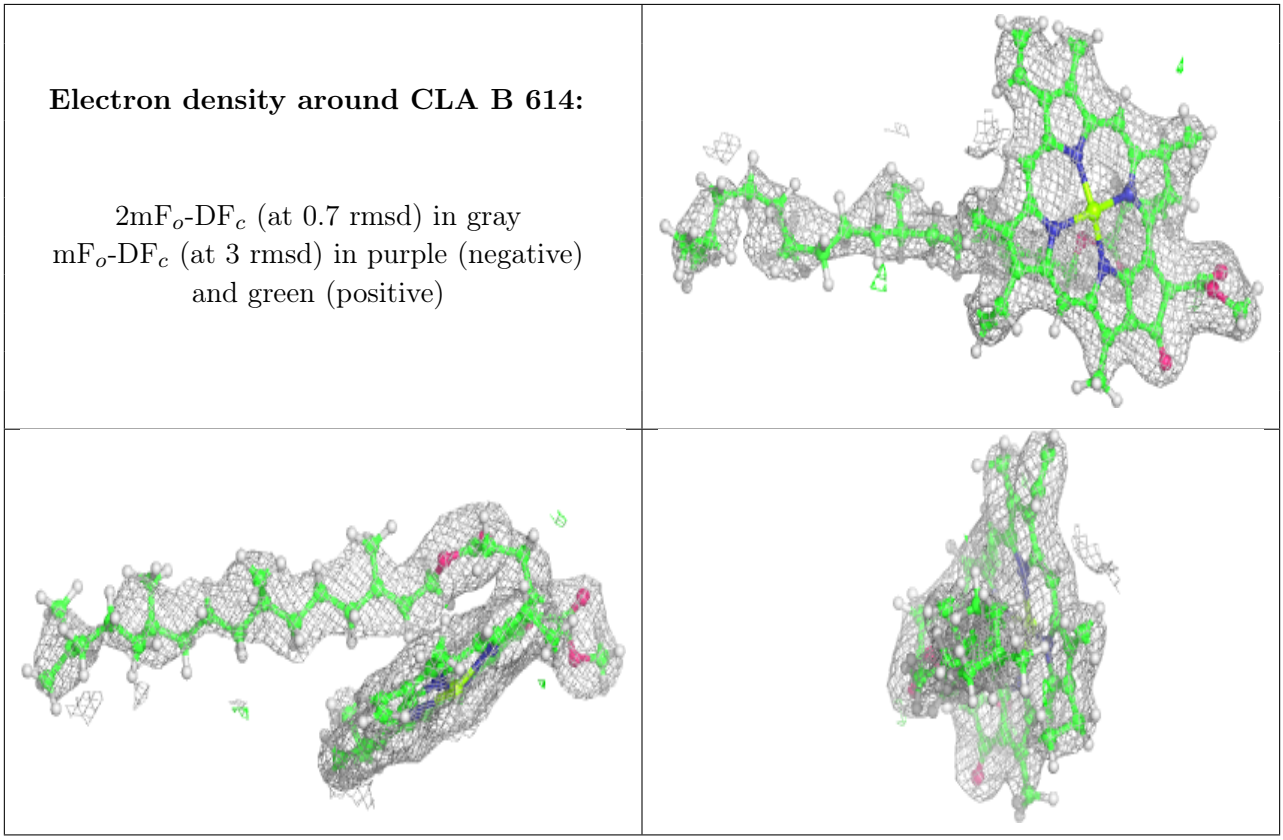
Electron density around CLA C 511:

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



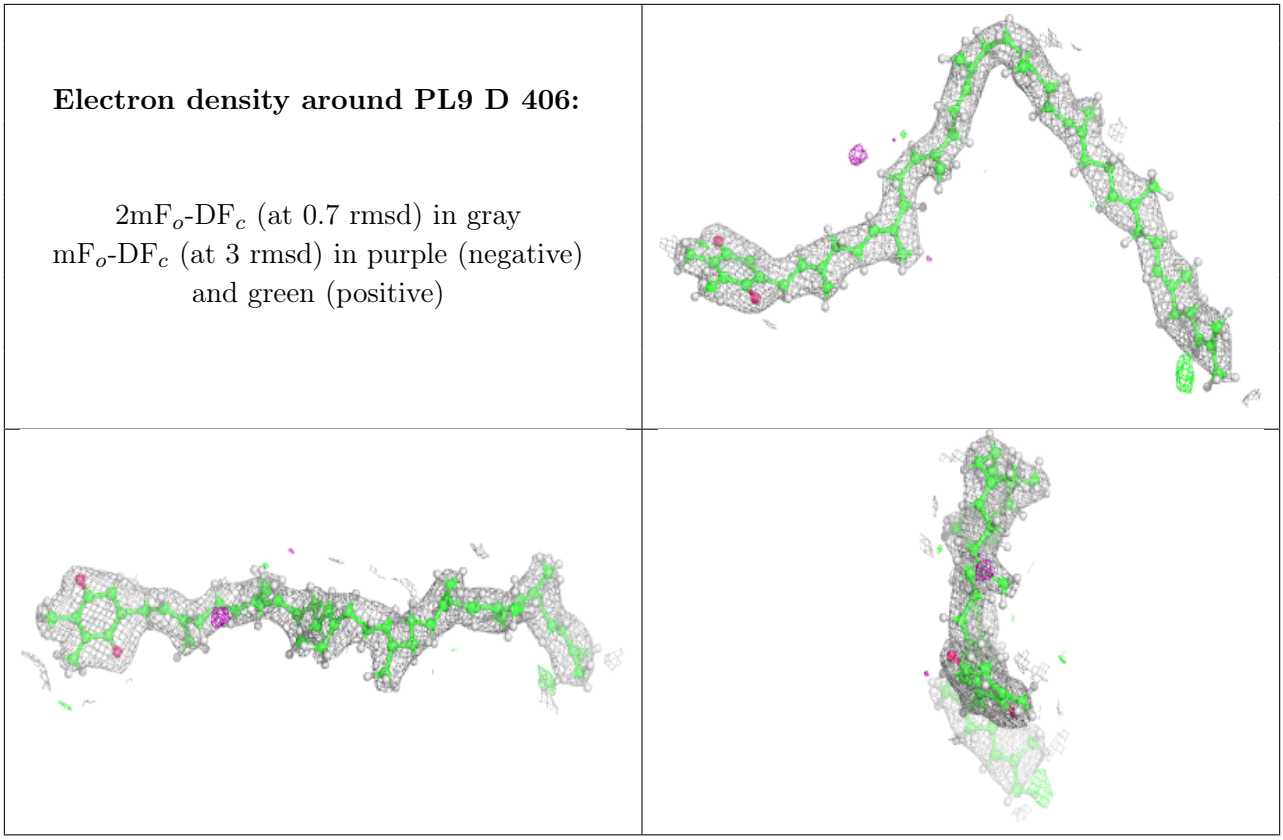
Electron density around CLA B 614:

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



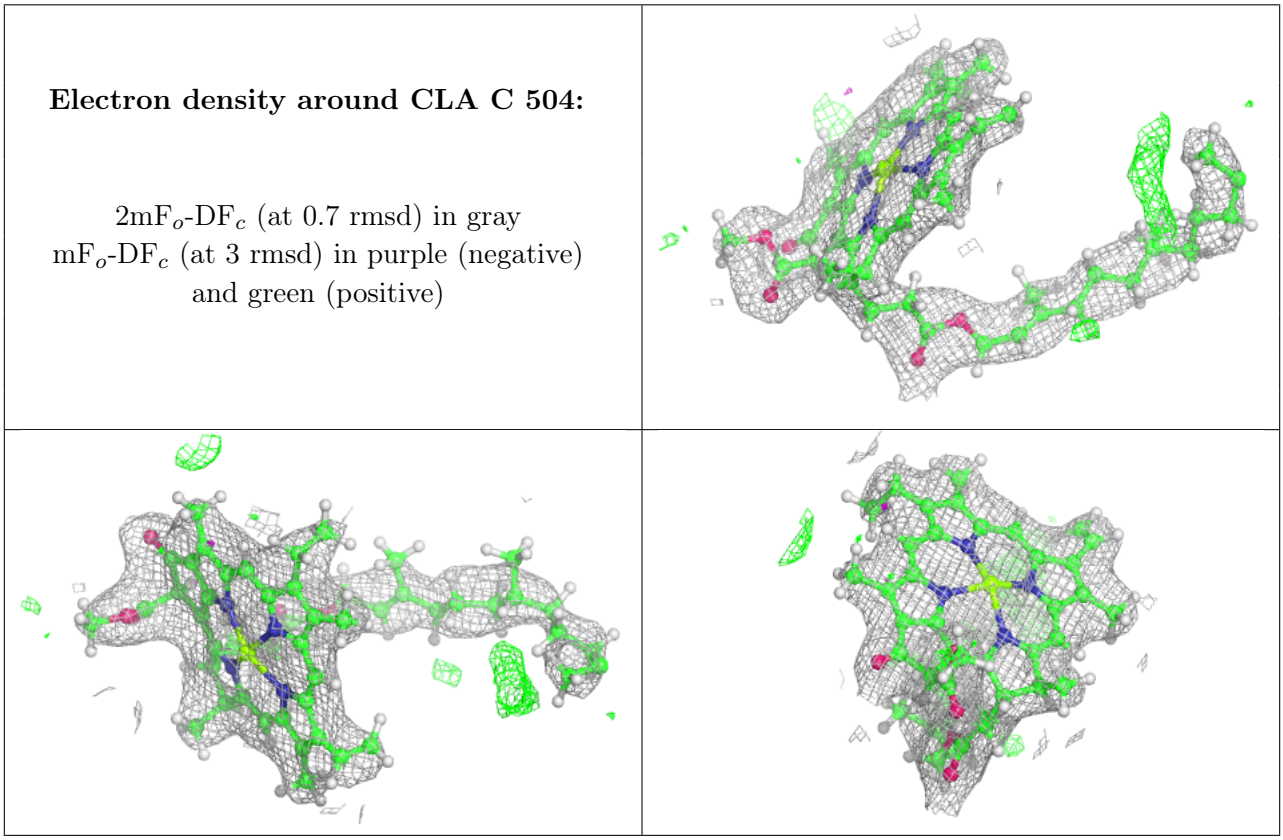
Electron density around PL9 D 406:

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



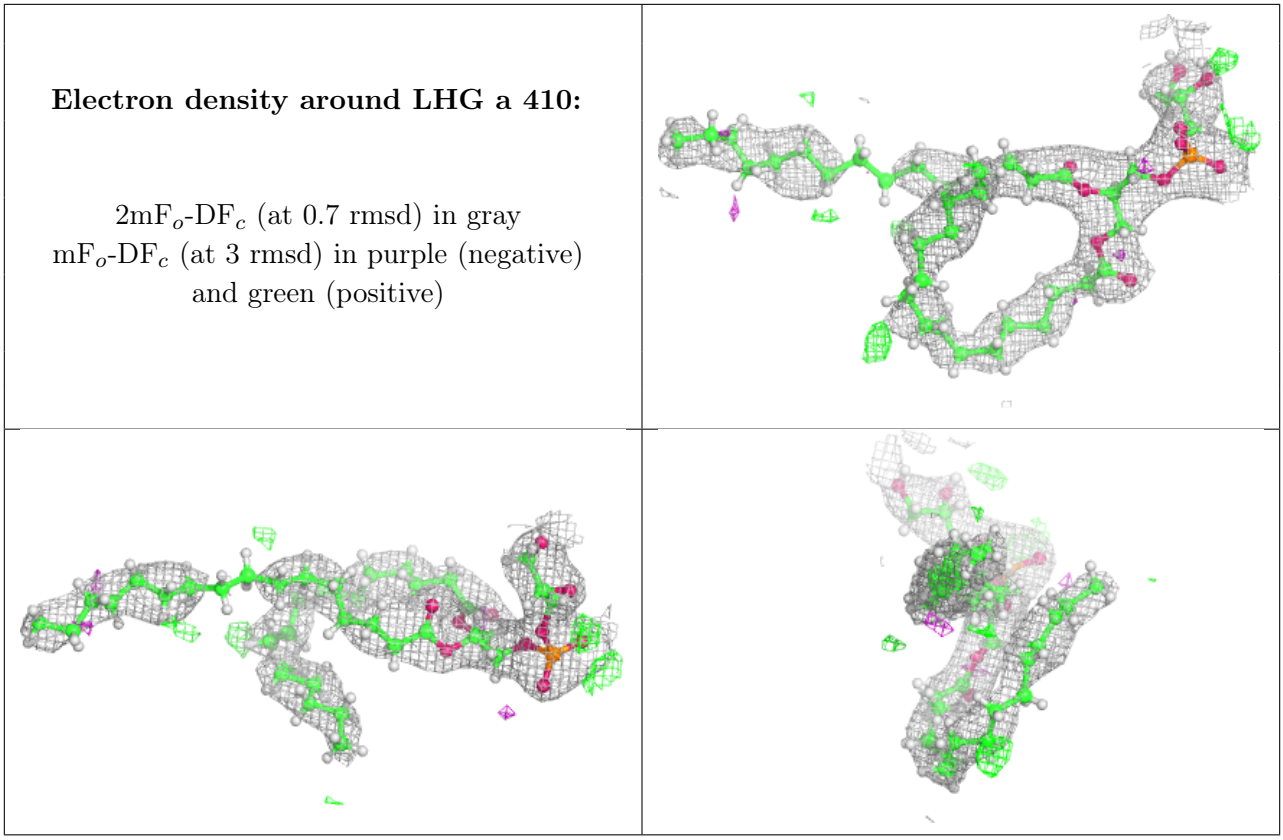
Electron density around CLA C 504:

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



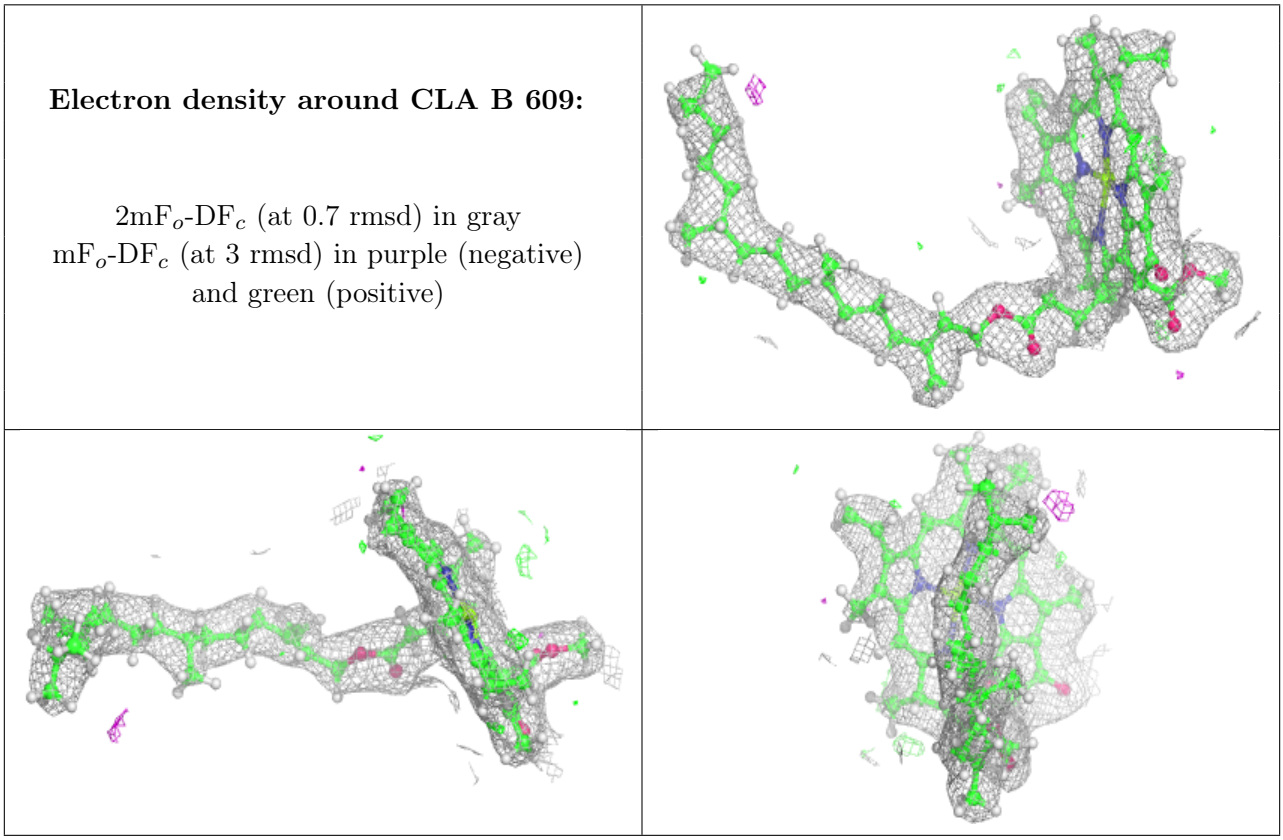
Electron density around LHG a 410:

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



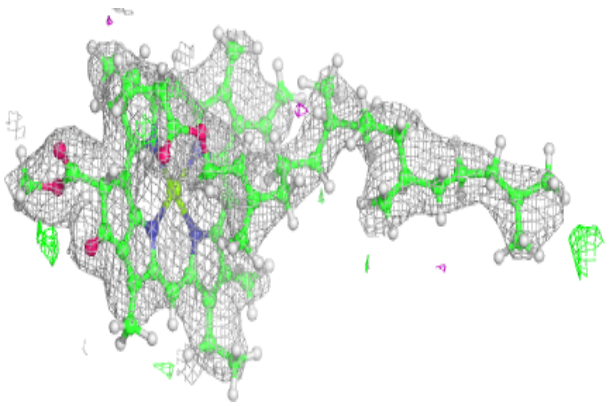
Electron density around CLA B 609:

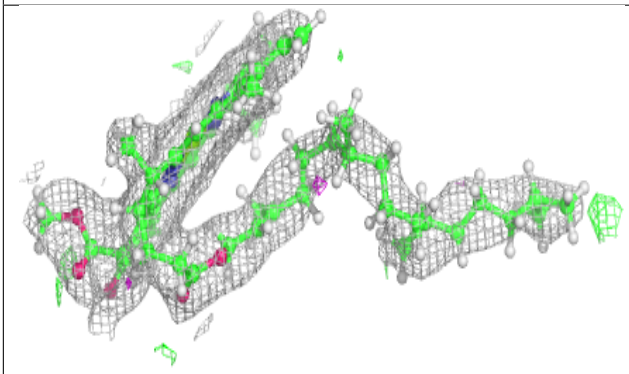
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

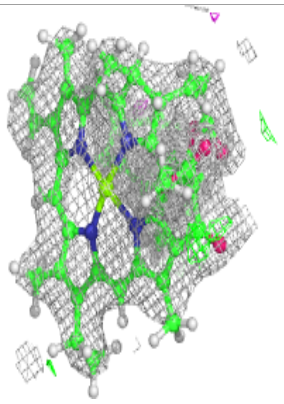


Electron density around CLA c 505:

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

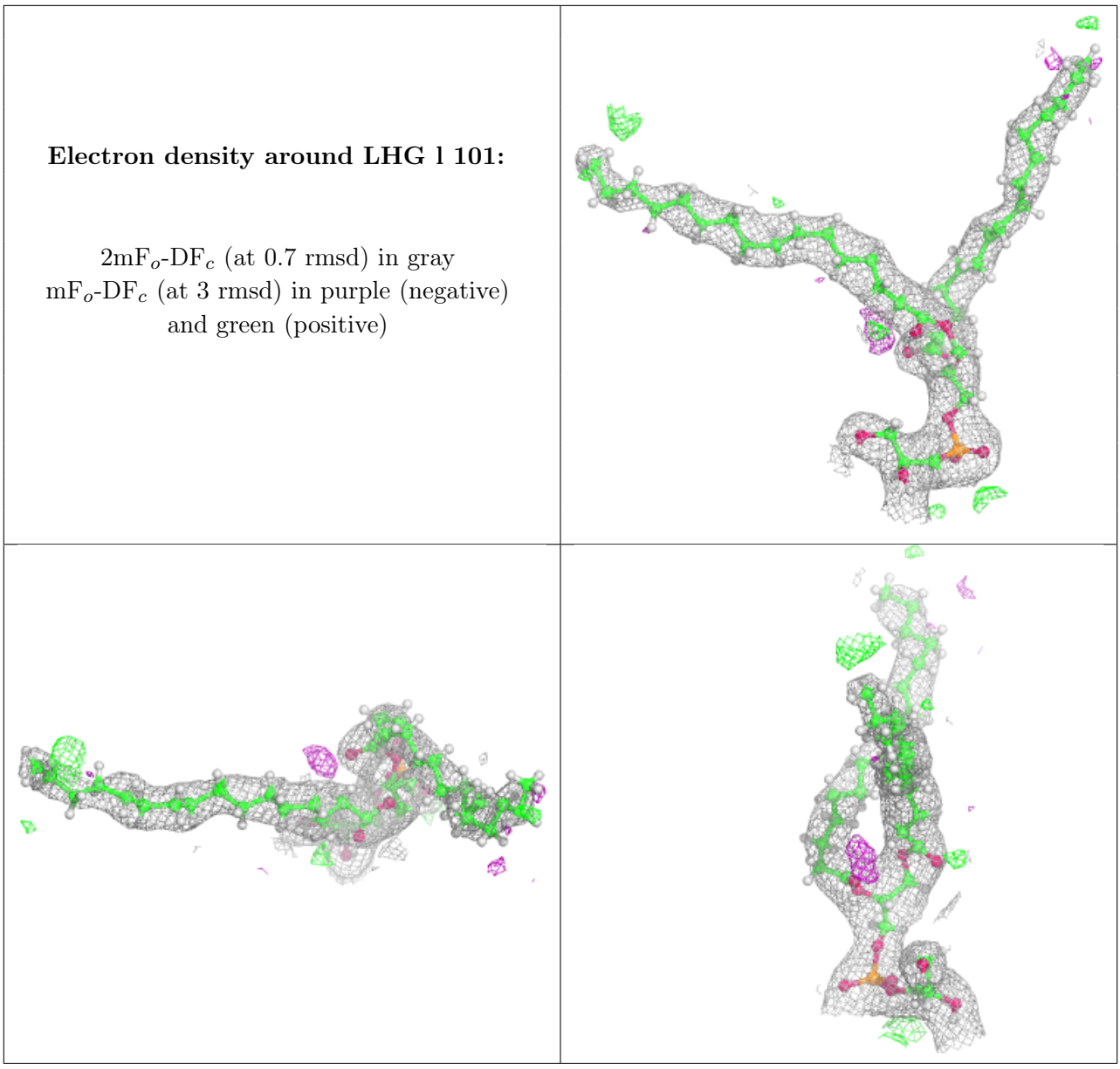






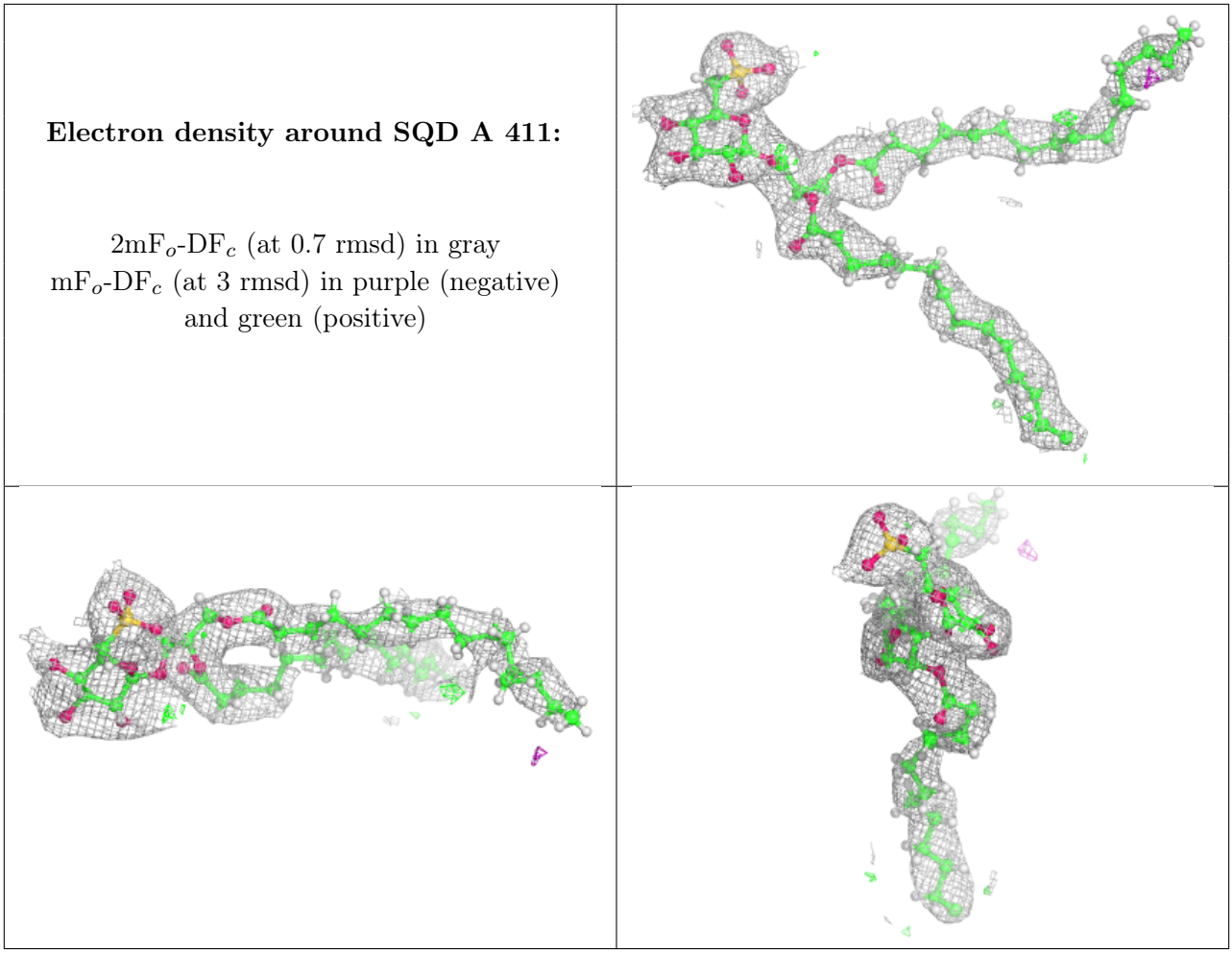
Electron density around LHG l 101:

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



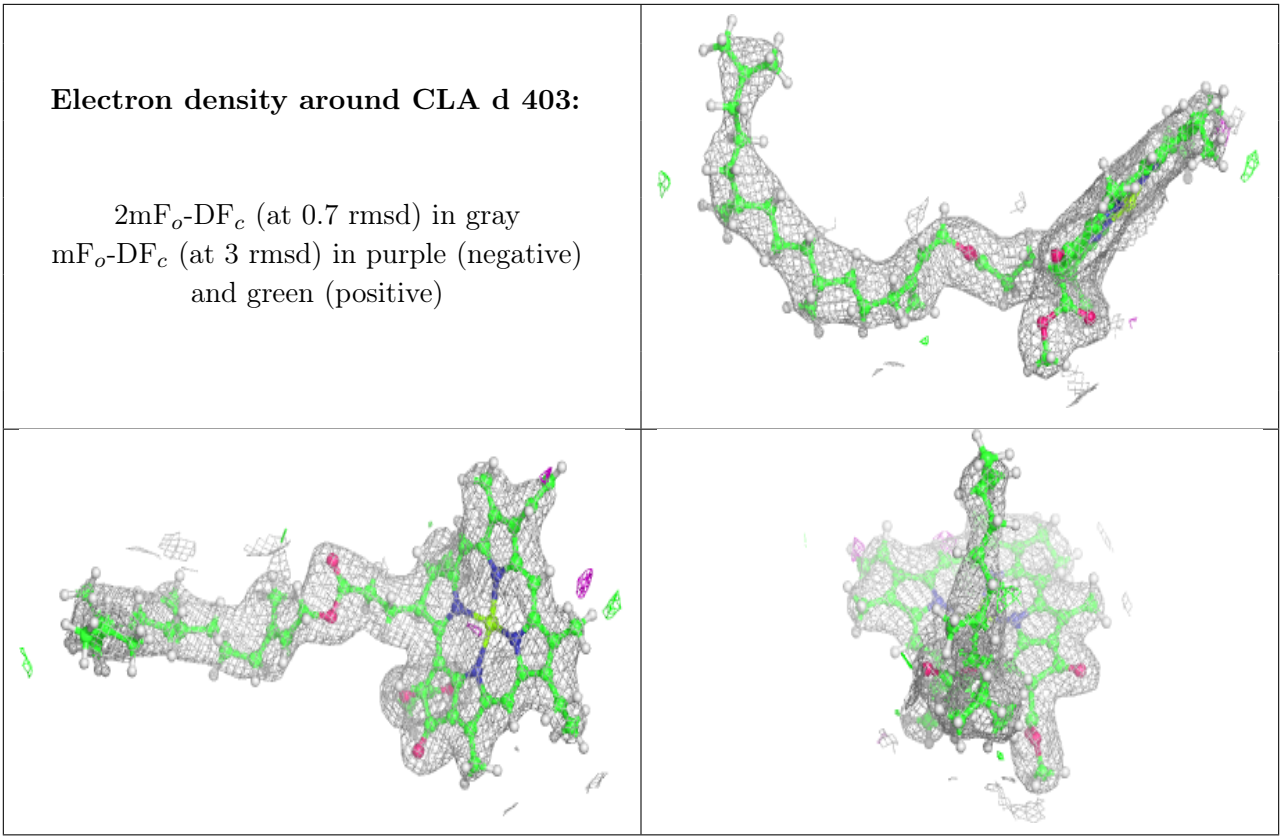
Electron density around SQD A 411:

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



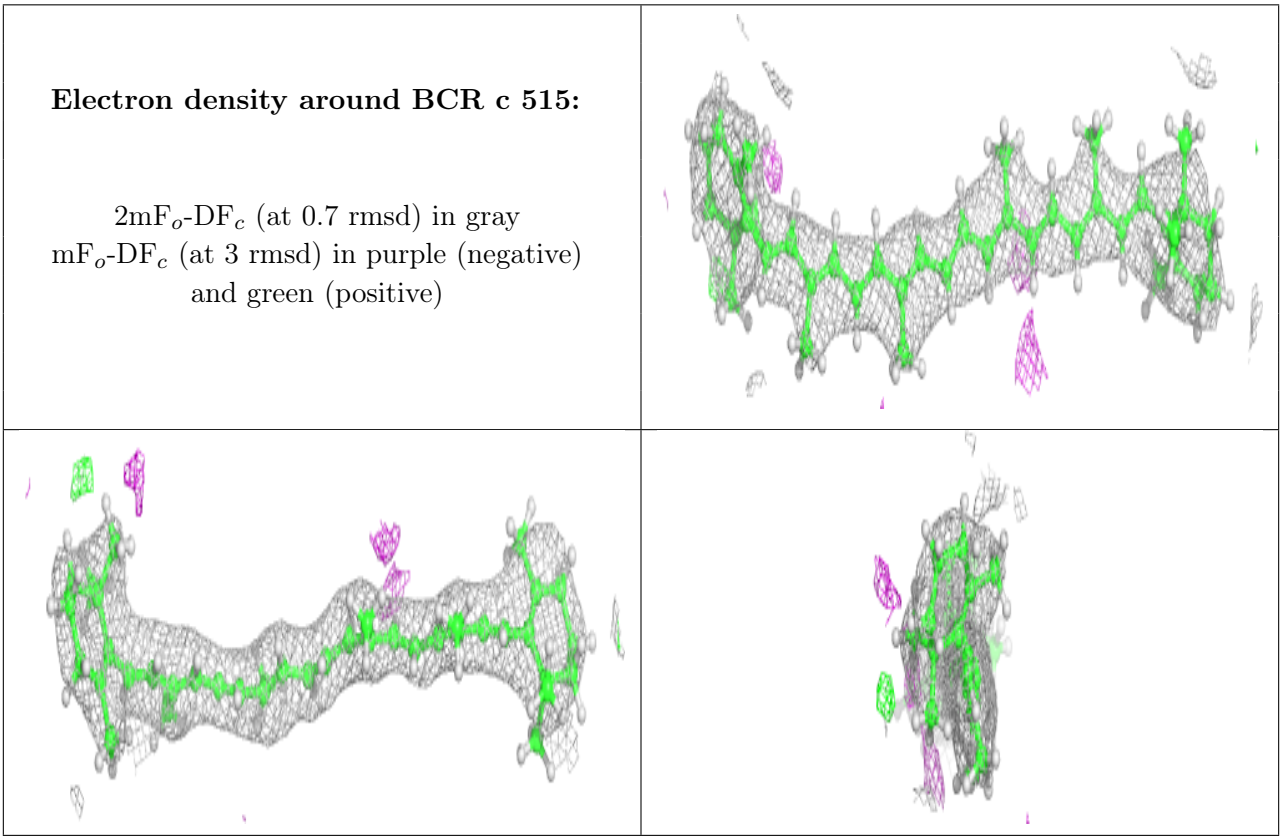
Electron density around CLA d 403:

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



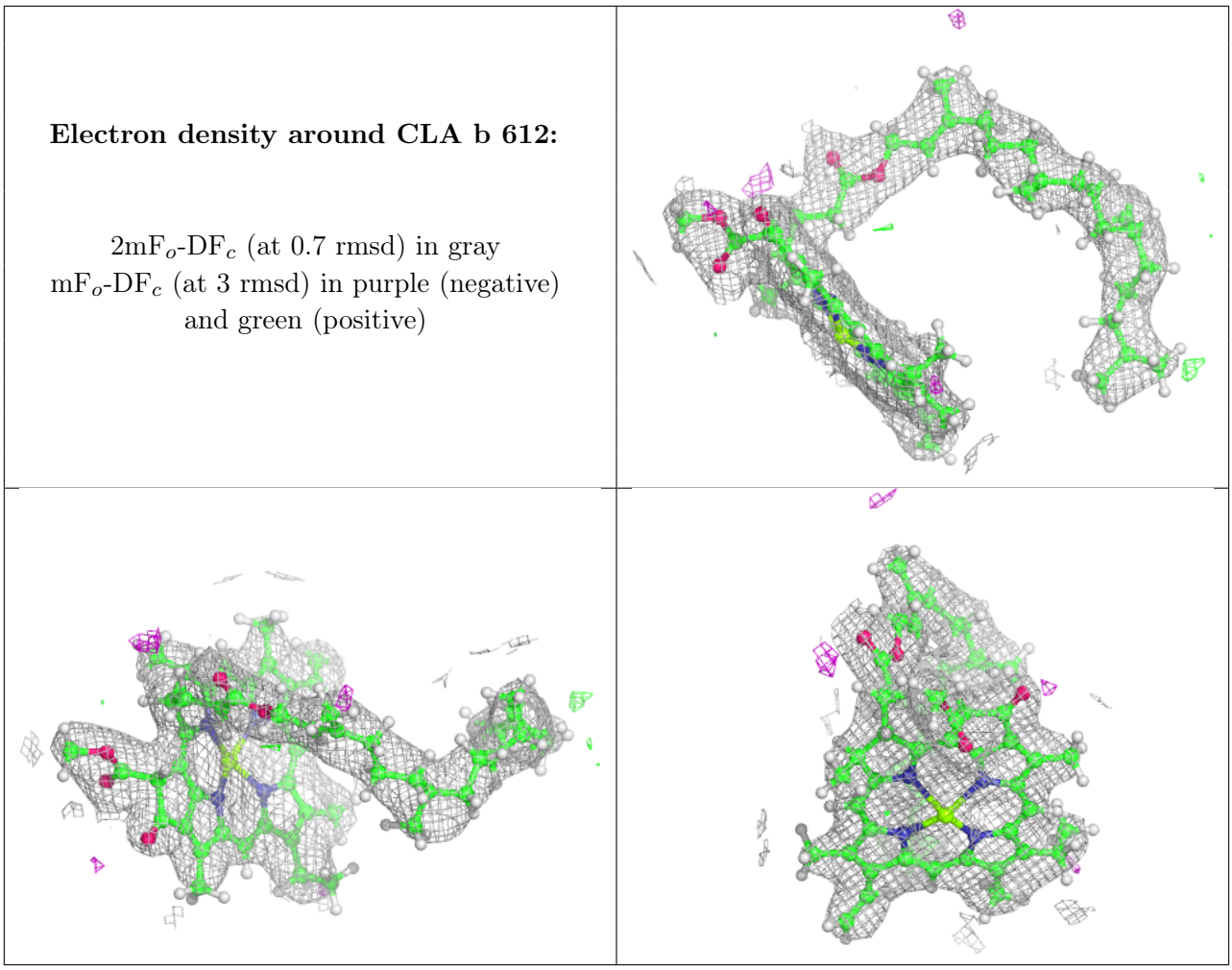
Electron density around BCR c 515:

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



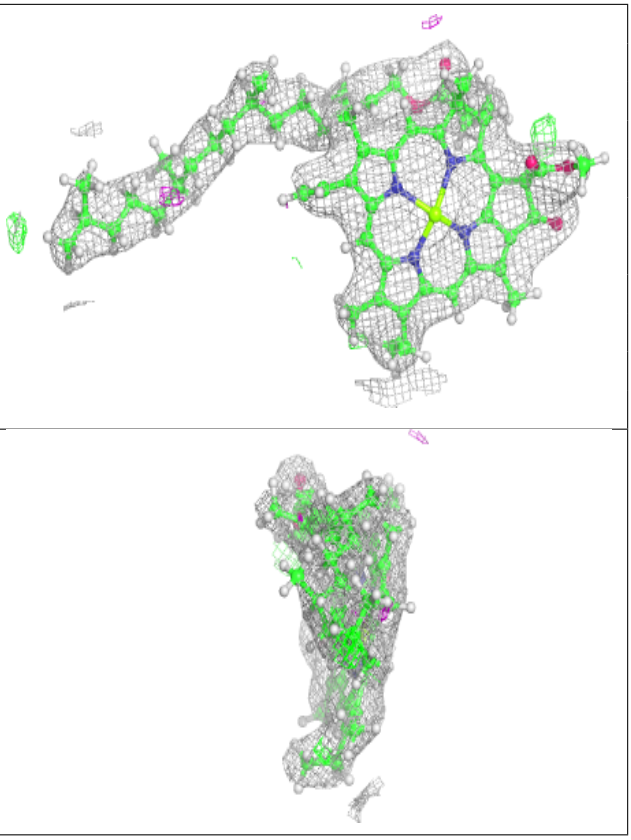
Electron density around CLA b 612:

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



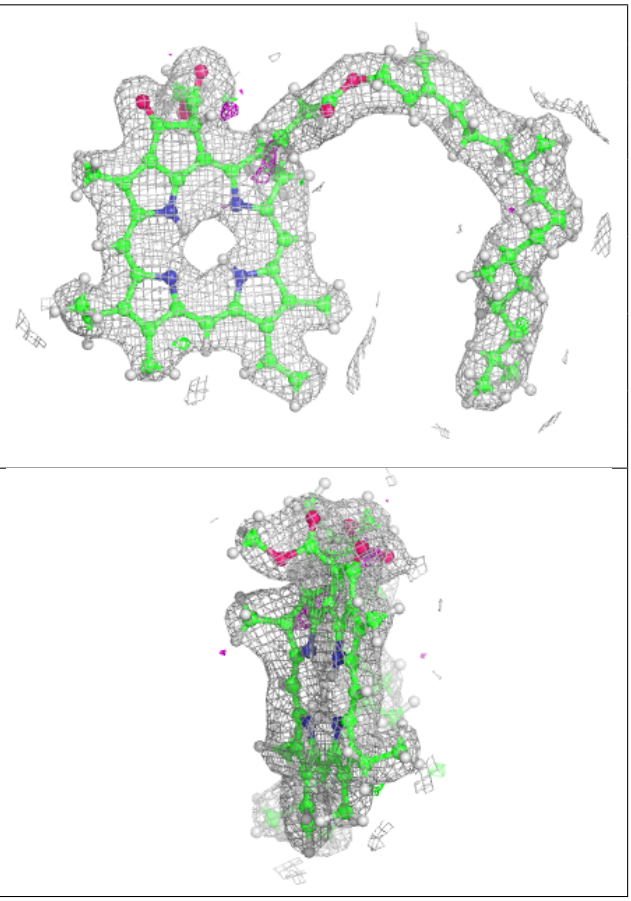
Electron density around CLA C 501:

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



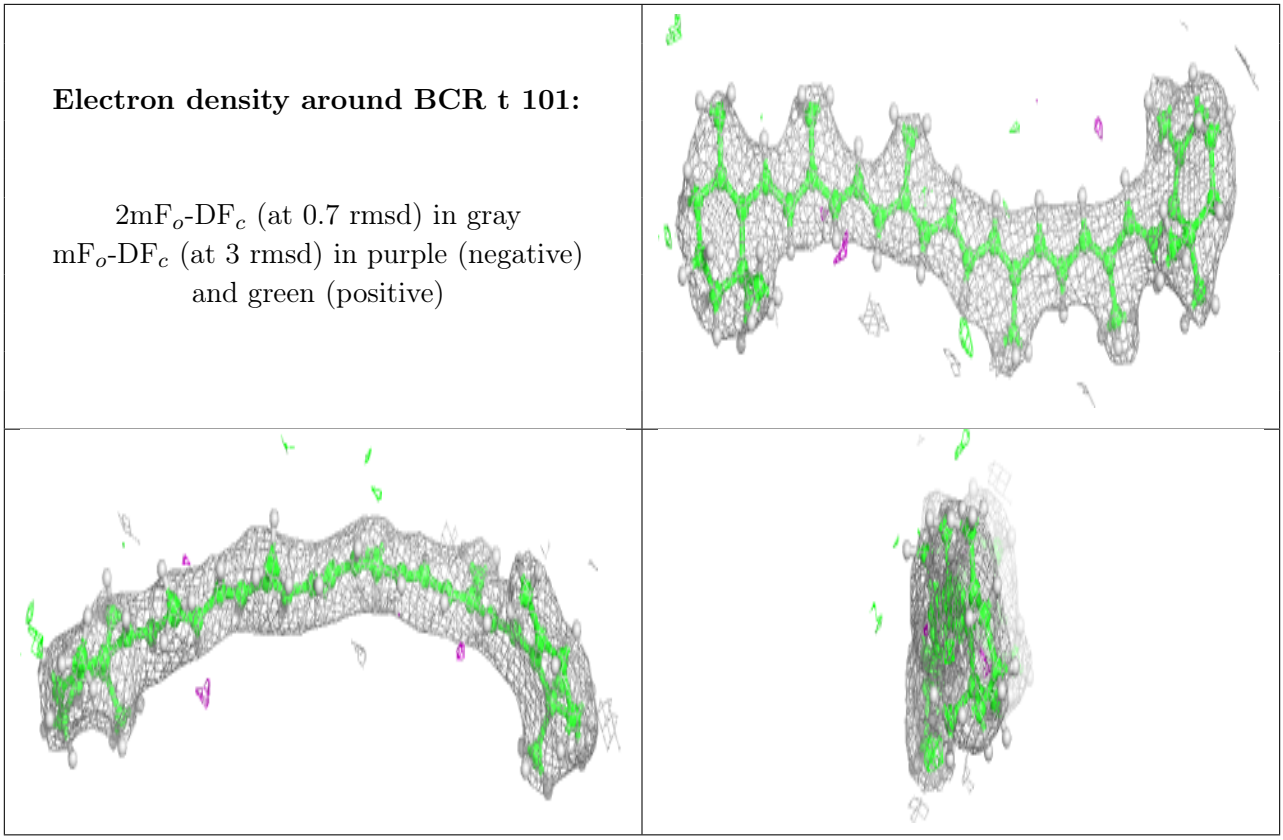
Electron density around PHO A 406:

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



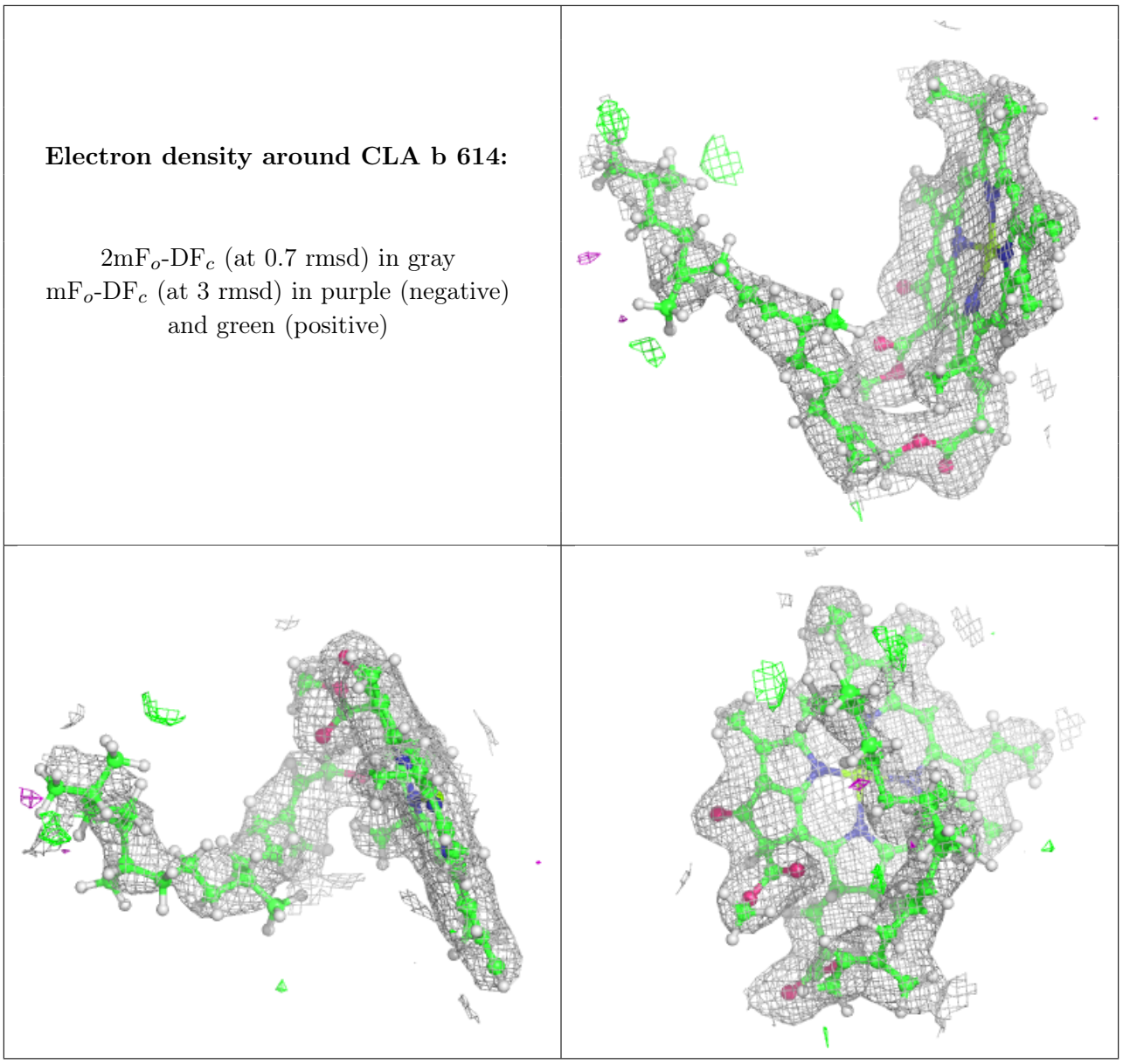
Electron density around BCR t 101:

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



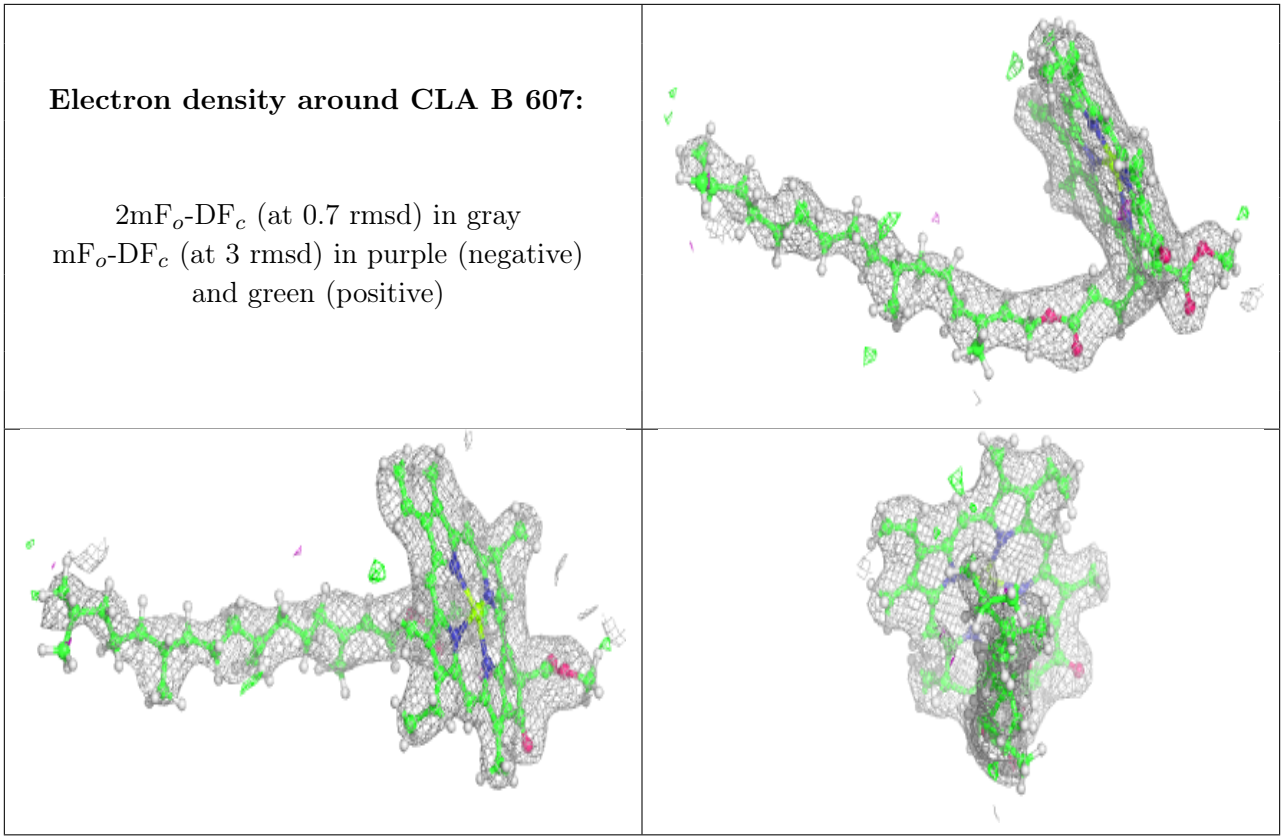
Electron density around CLA b 614:

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



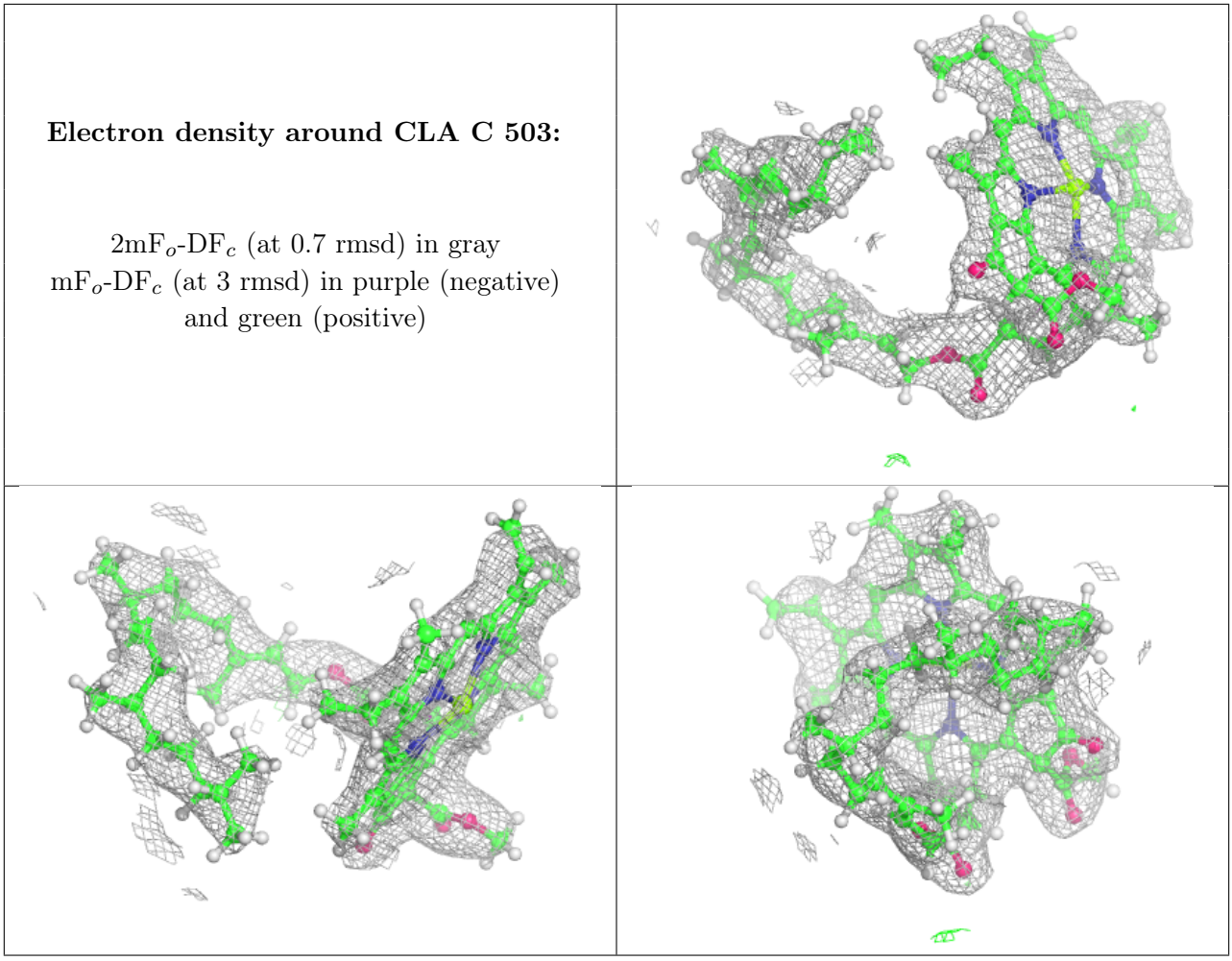
Electron density around CLA B 607:

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



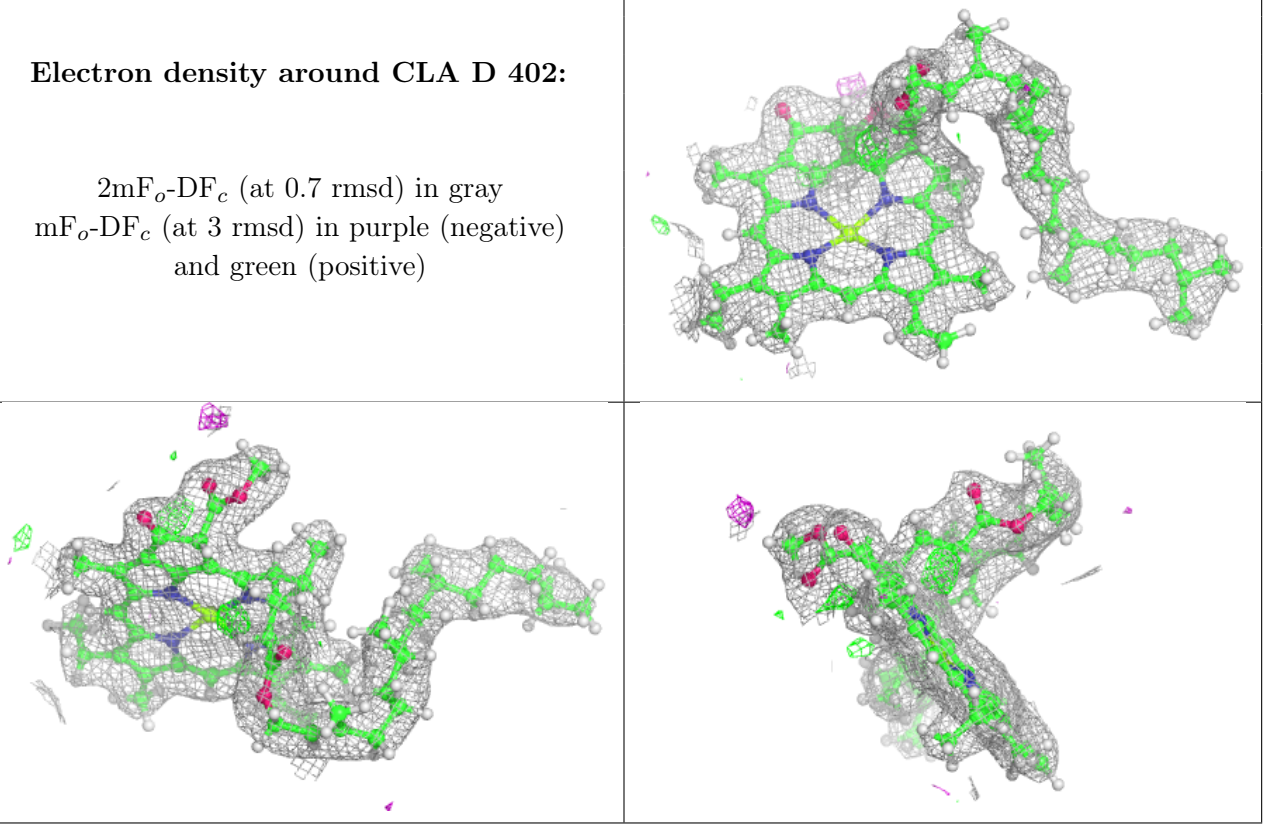
Electron density around CLA C 503:

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



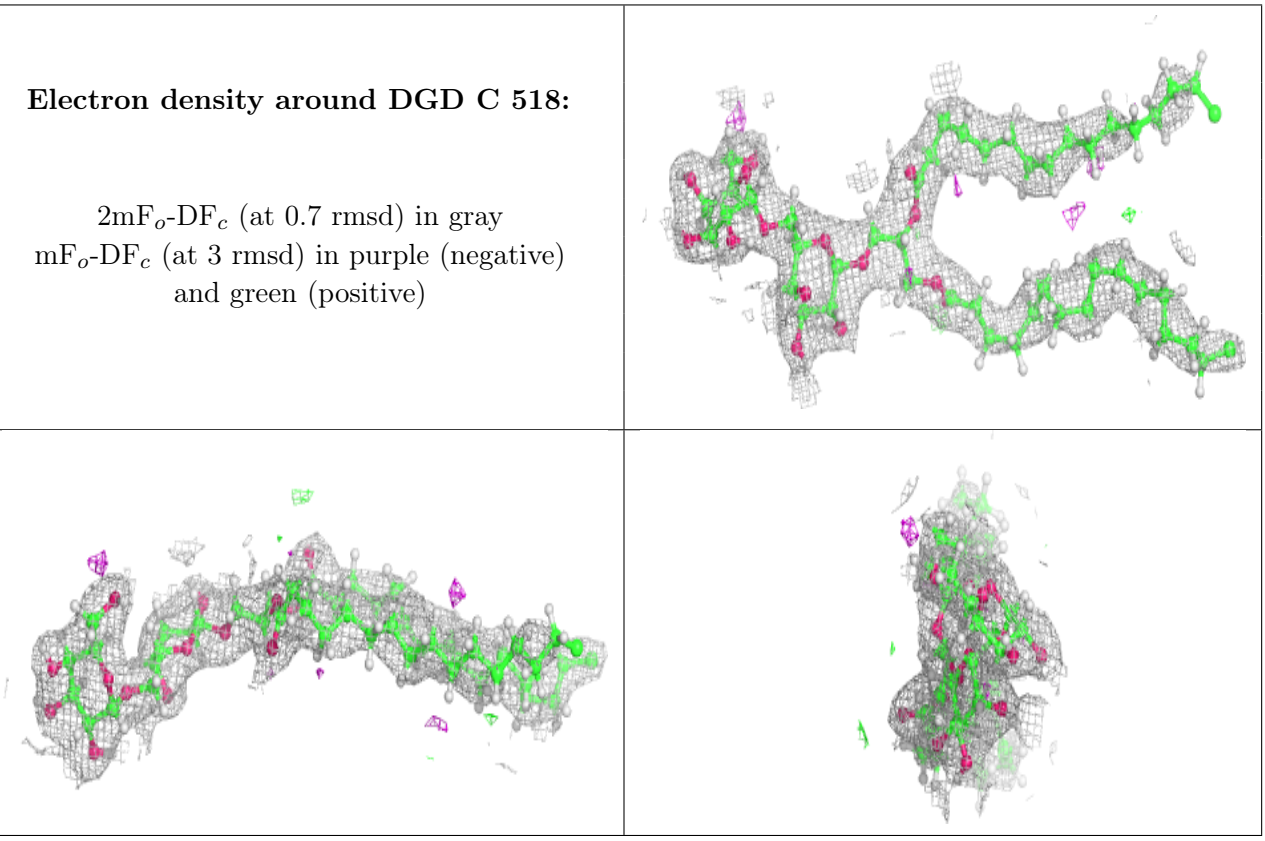
Electron density around CLA D 402:

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



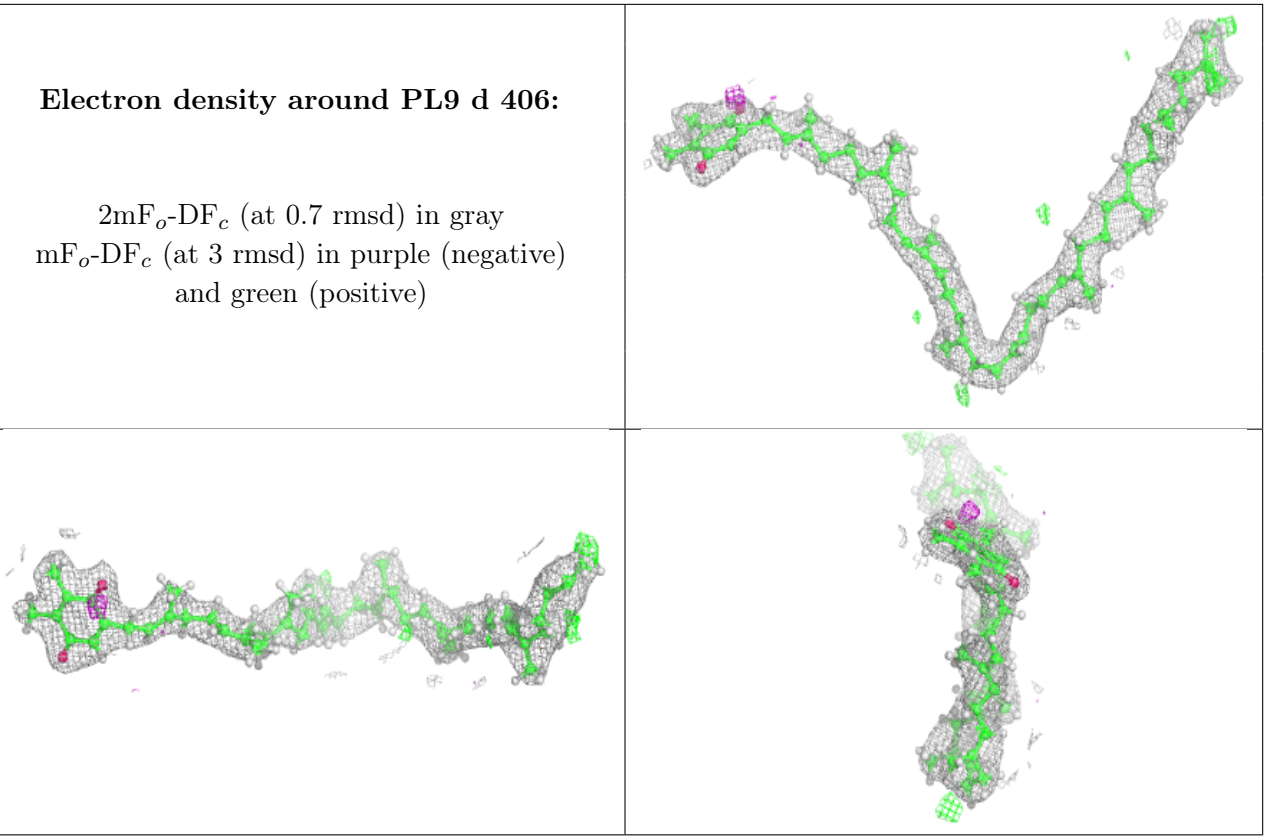
Electron density around DGD C 518:

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



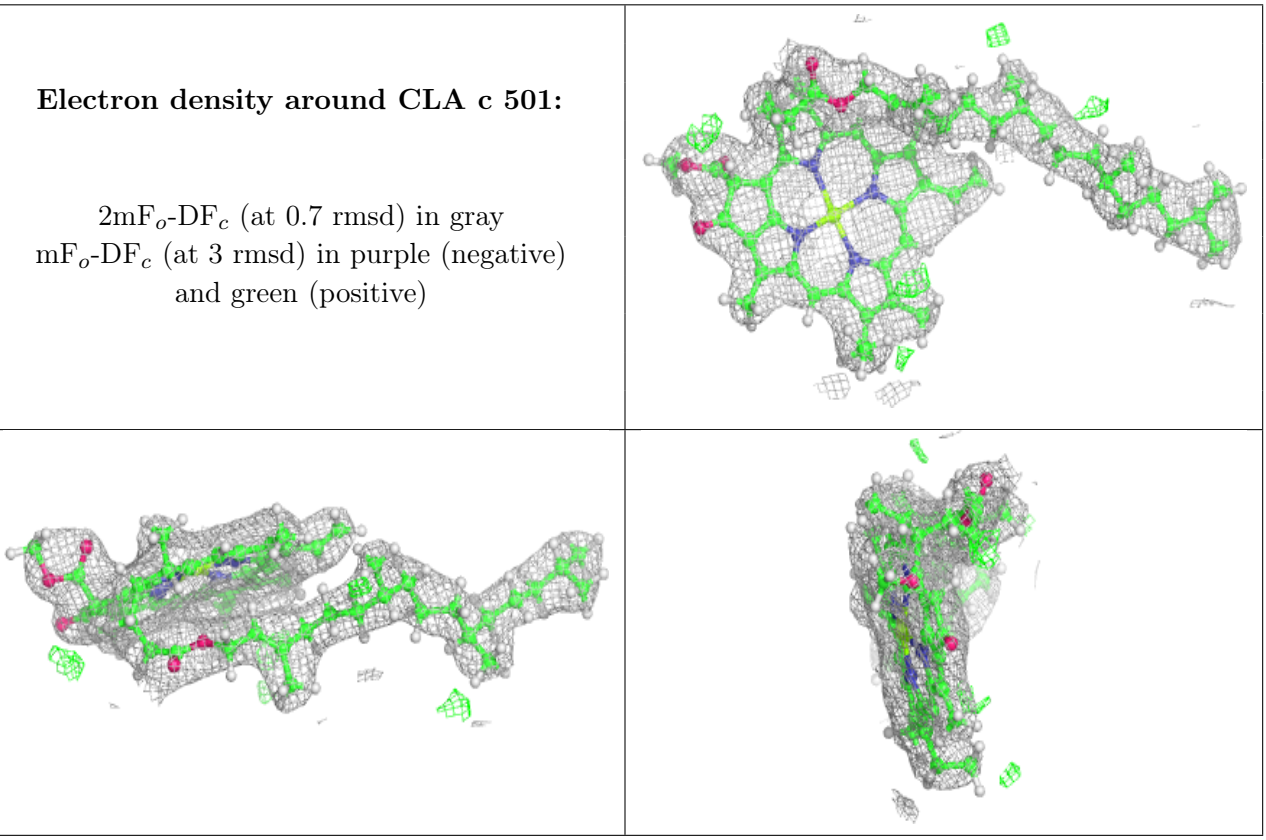
Electron density around PL9 d 406:

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



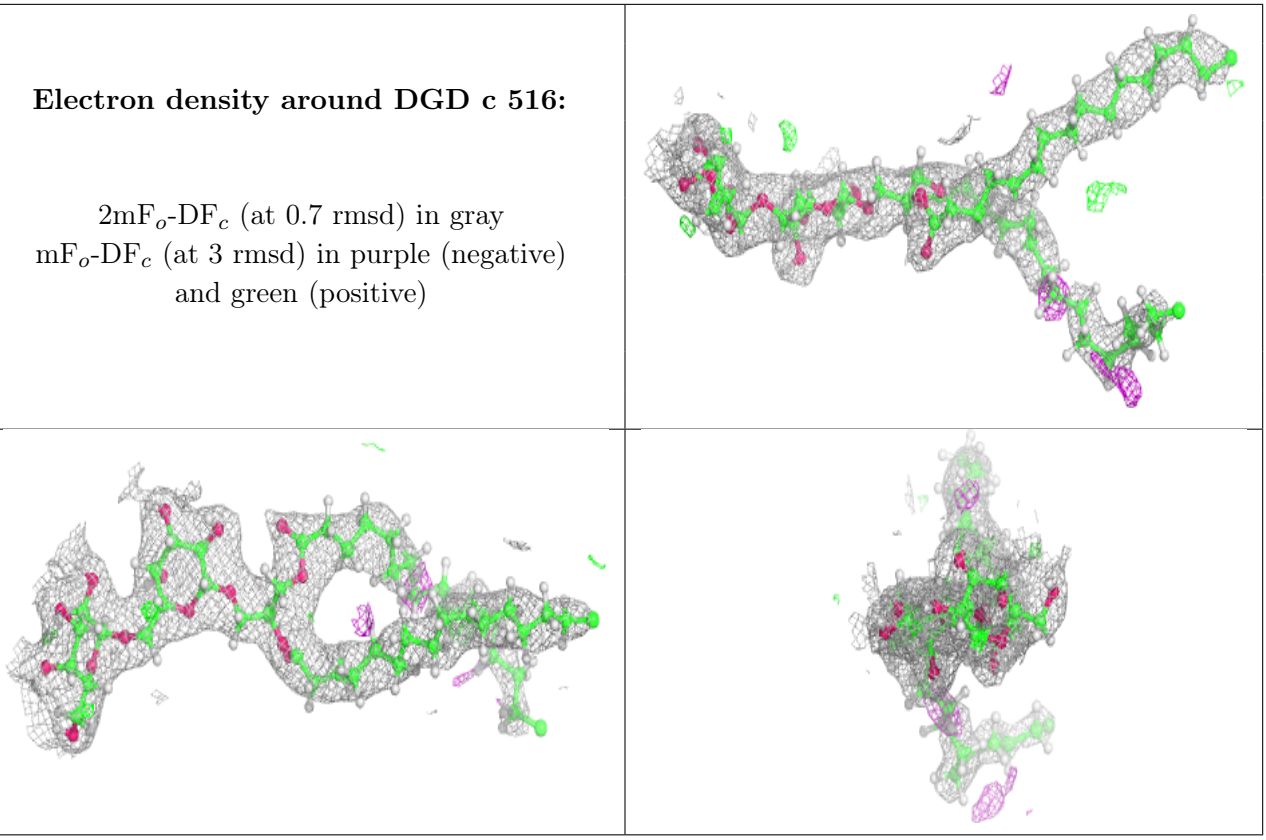
Electron density around CLA c 501:

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



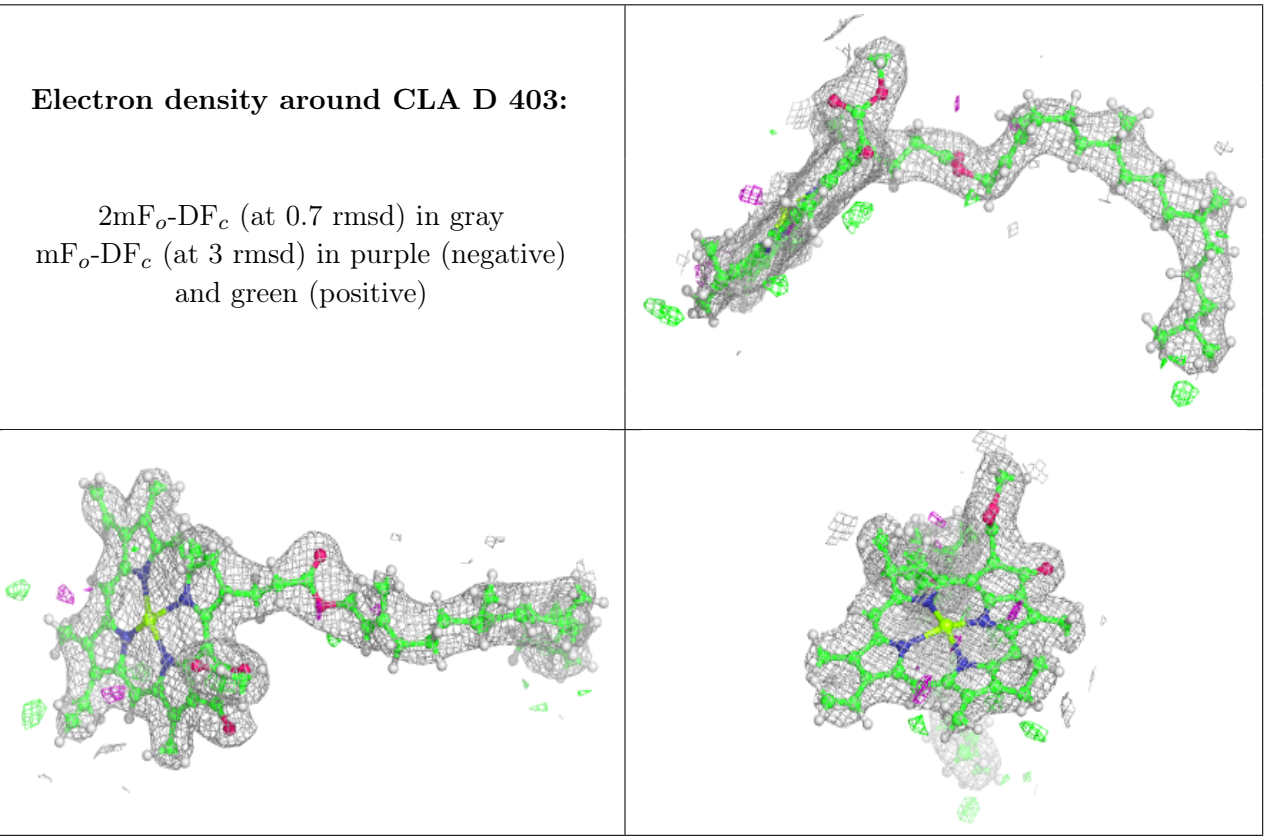
Electron density around DGD c 516:

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



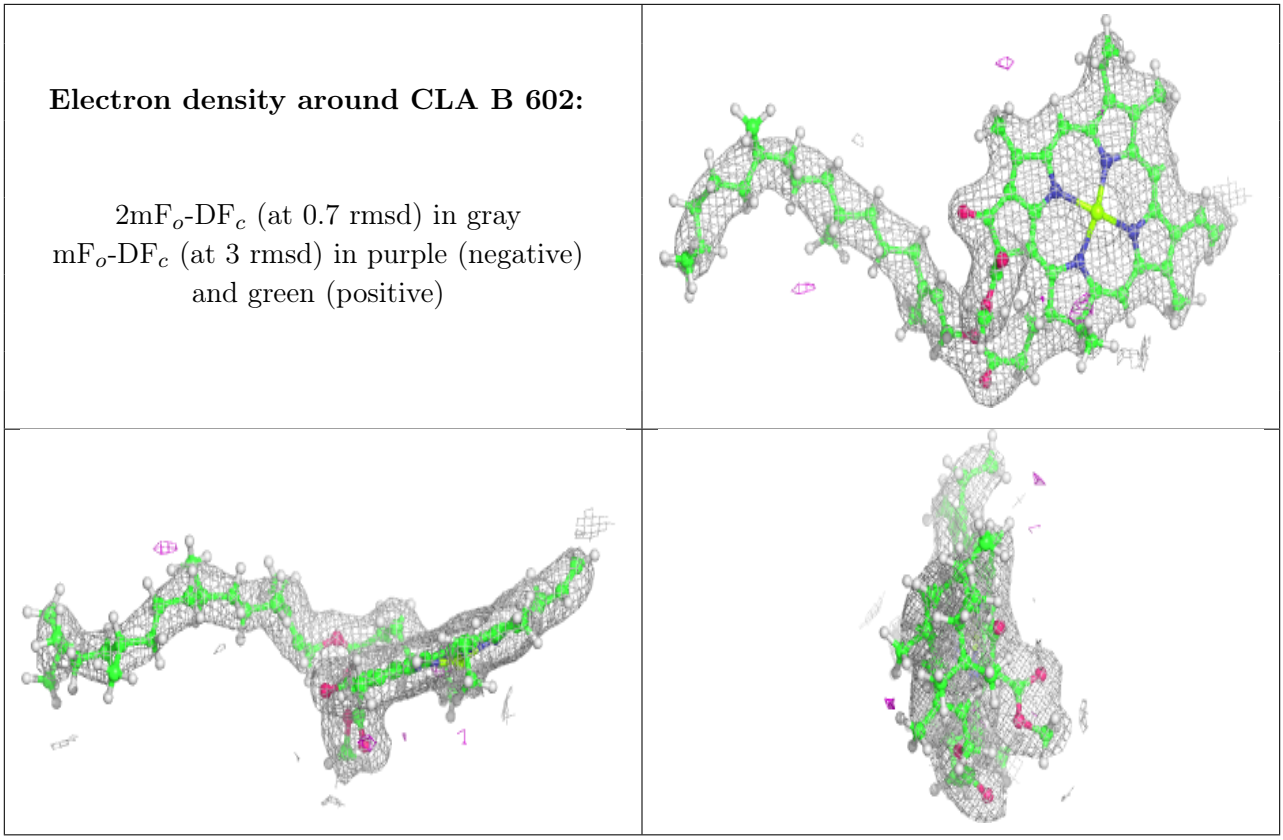
Electron density around CLA D 403:

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



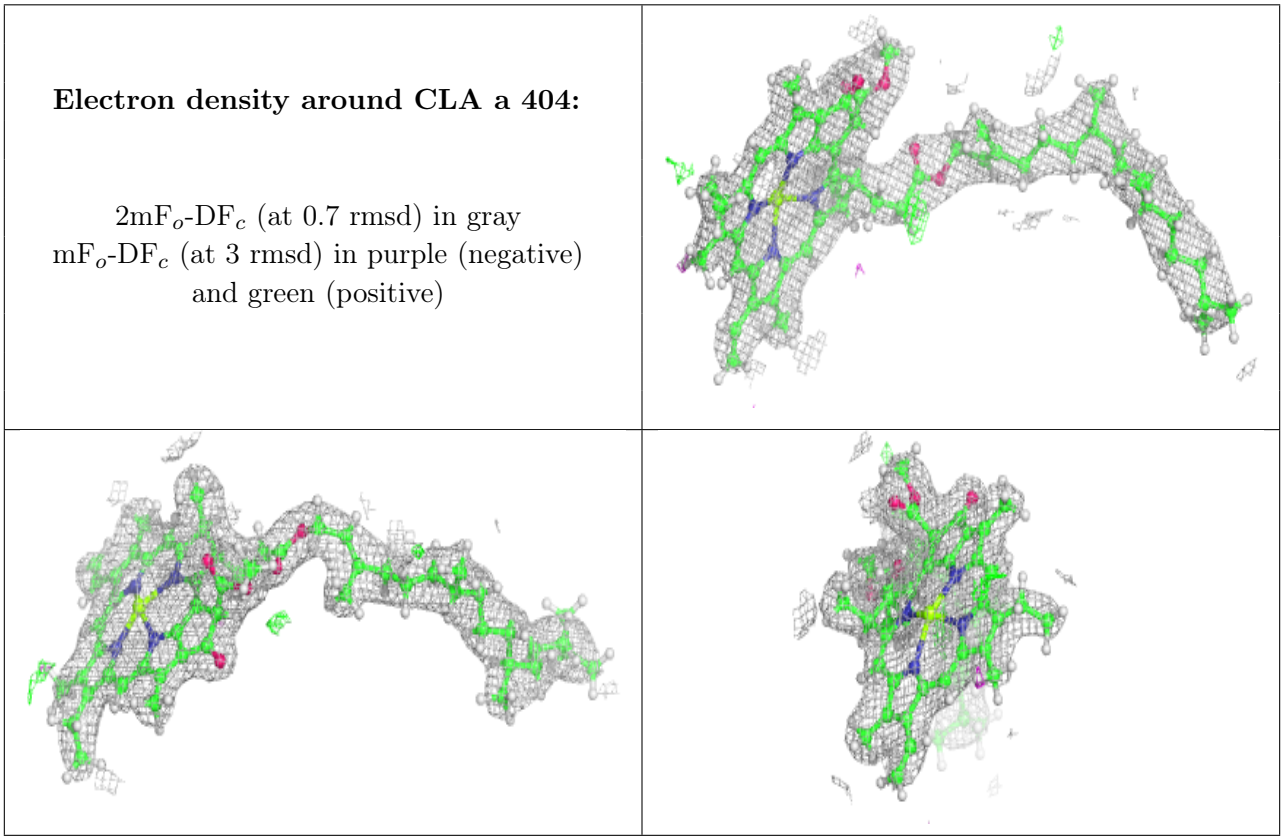
Electron density around CLA B 602:

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



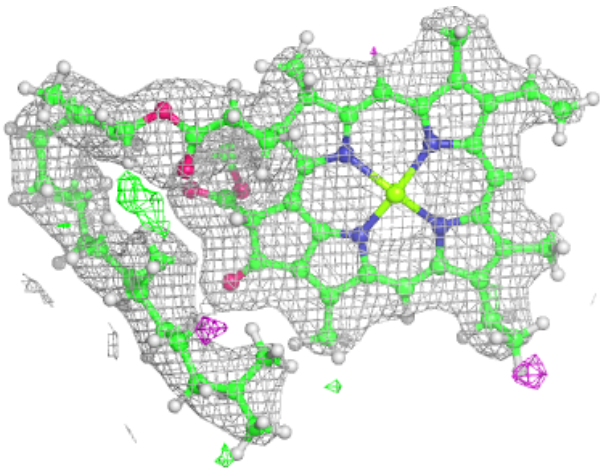
Electron density around CLA a 404:

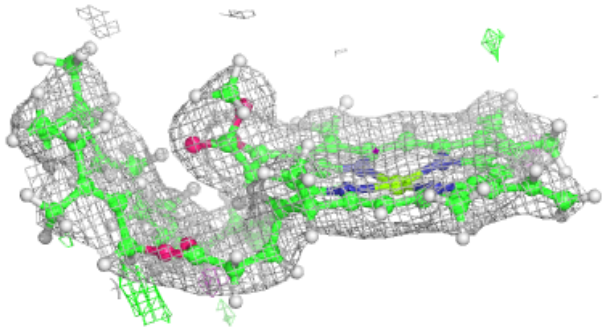
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

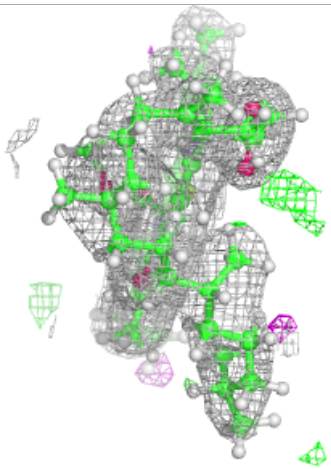


Electron density around CLA B 610:

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

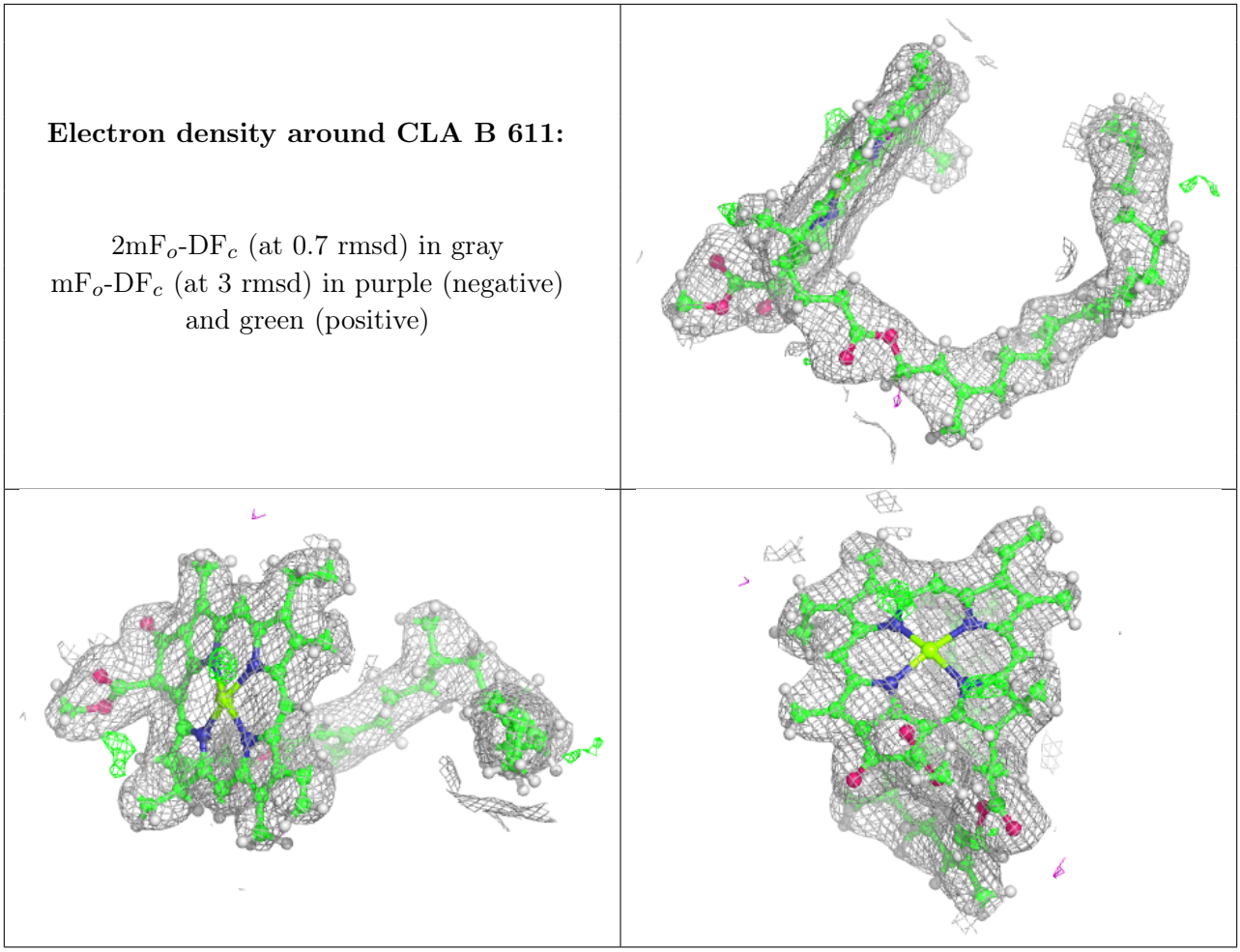






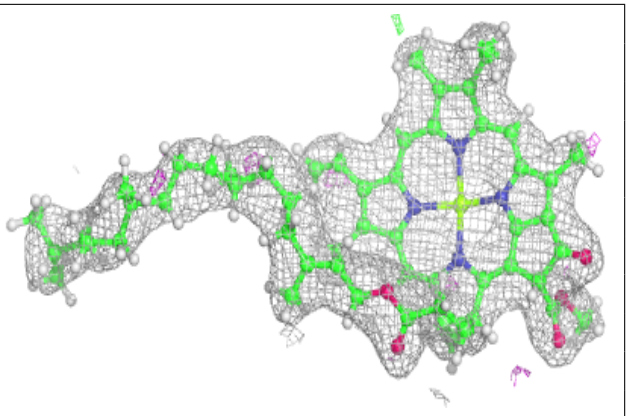
Electron density around CLA B 611:

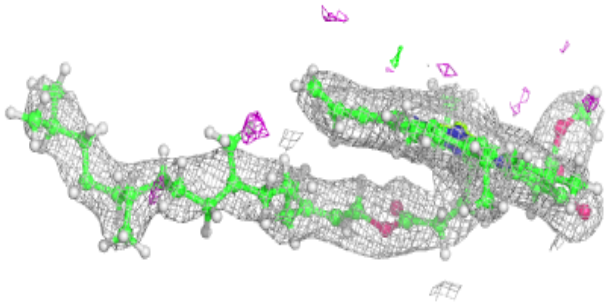
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 603:

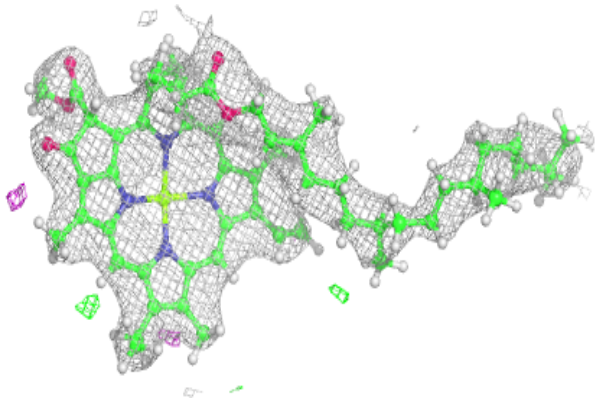
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

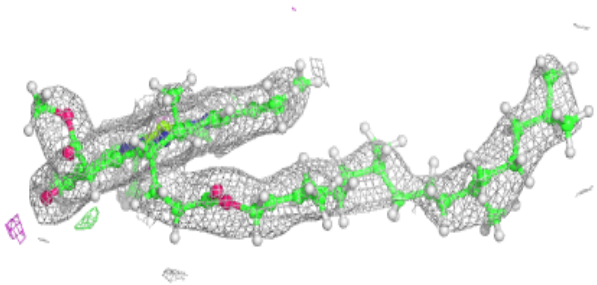


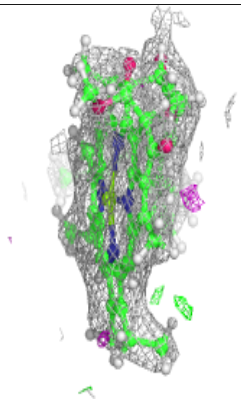


Electron density around CLA b 604:

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

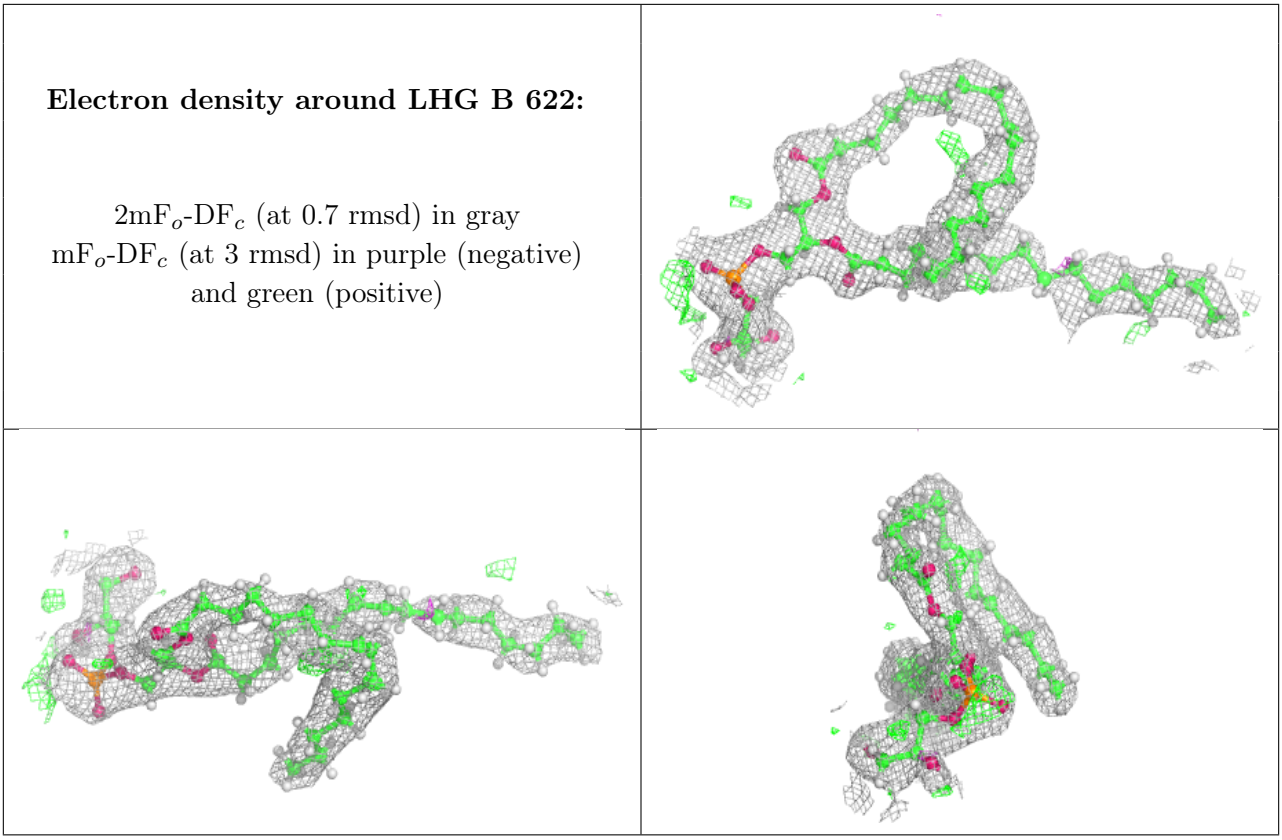






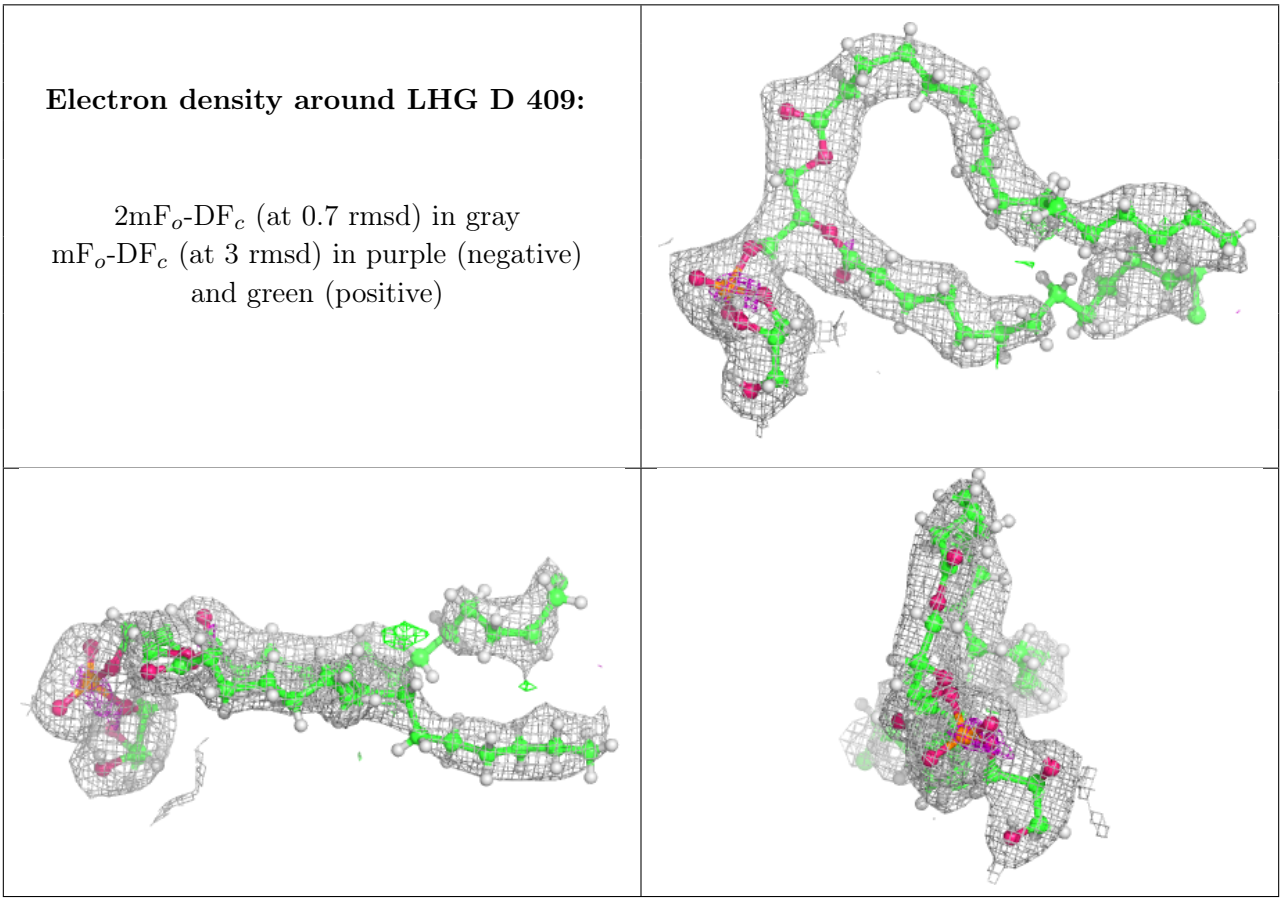
Electron density around LHG B 622:

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



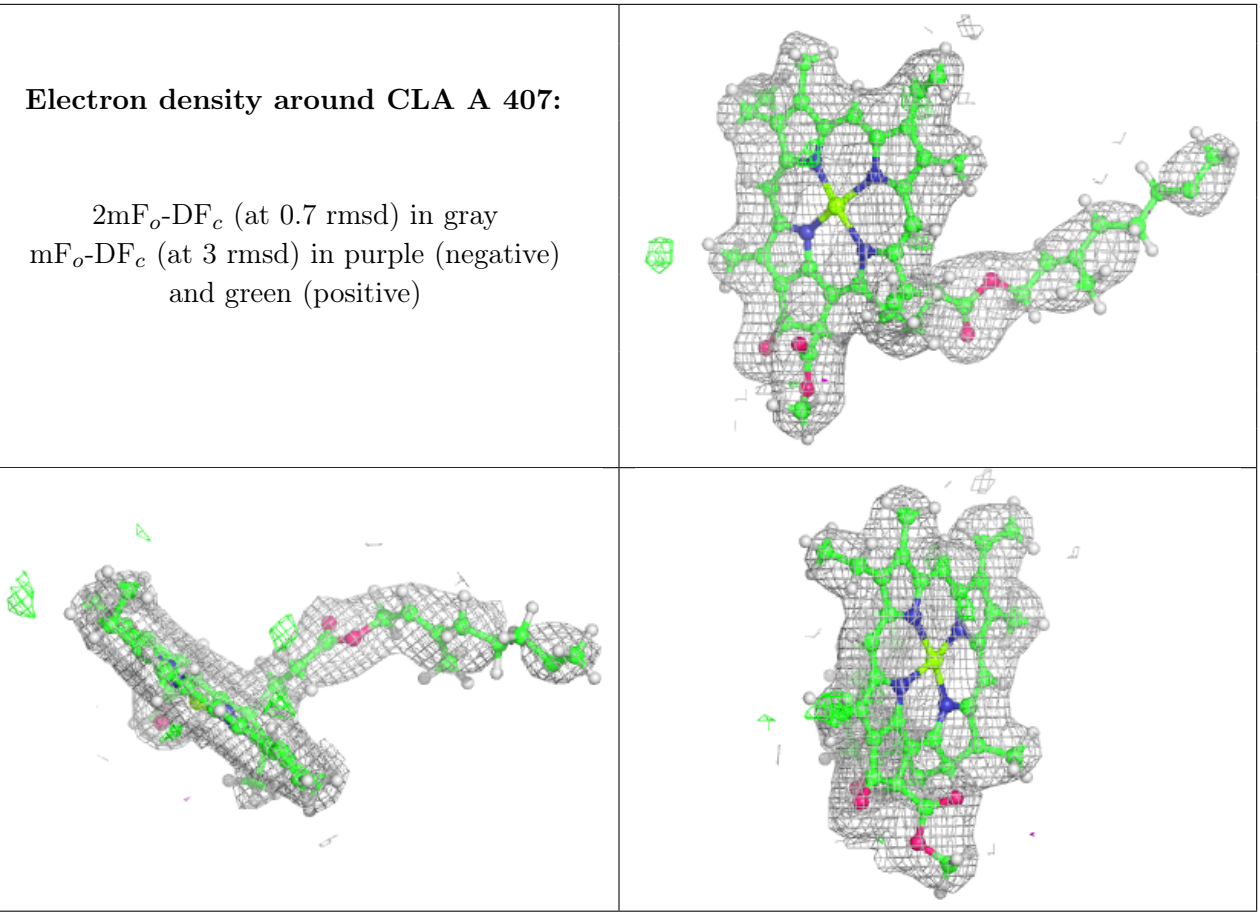
Electron density around LHG D 409:

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



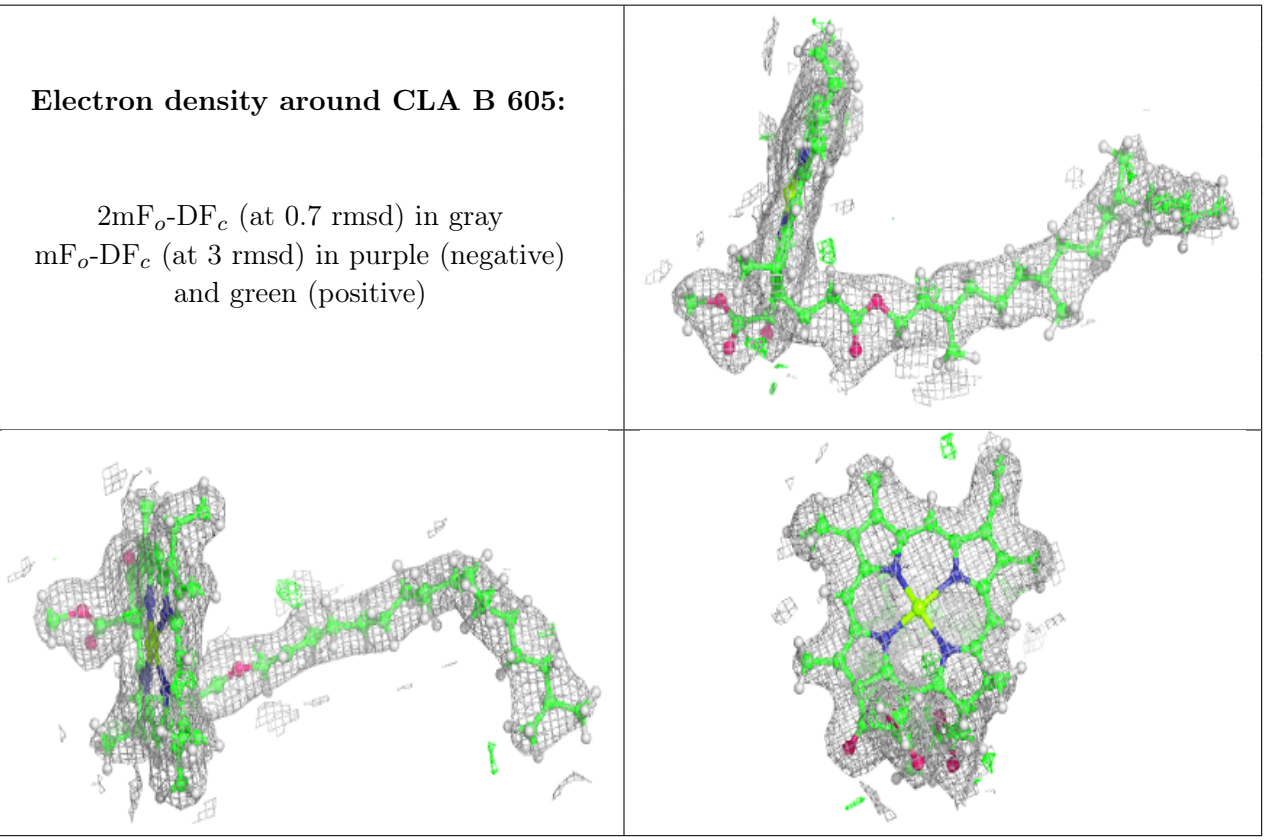
Electron density around CLA A 407:

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



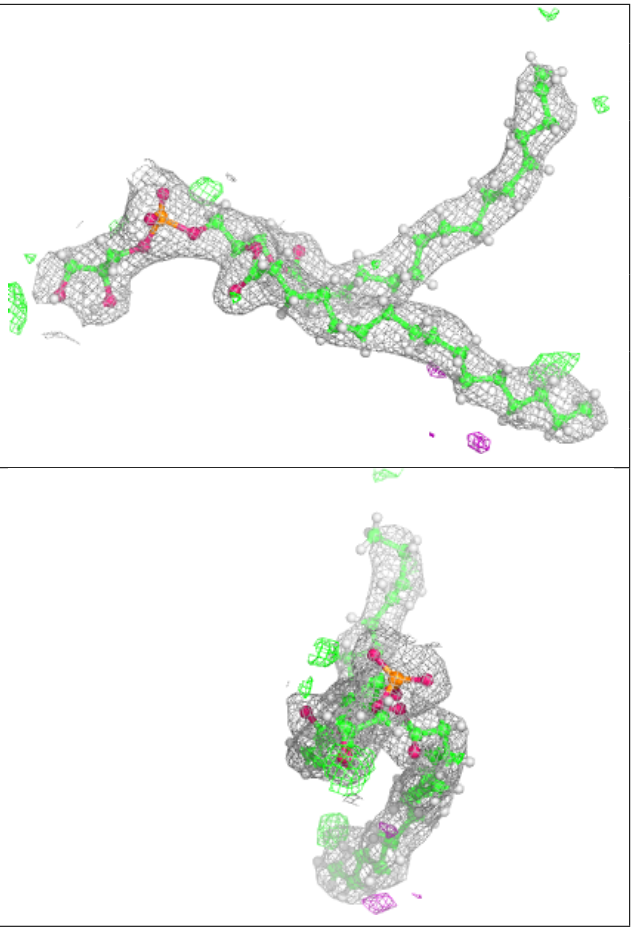
Electron density around CLA B 605:

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



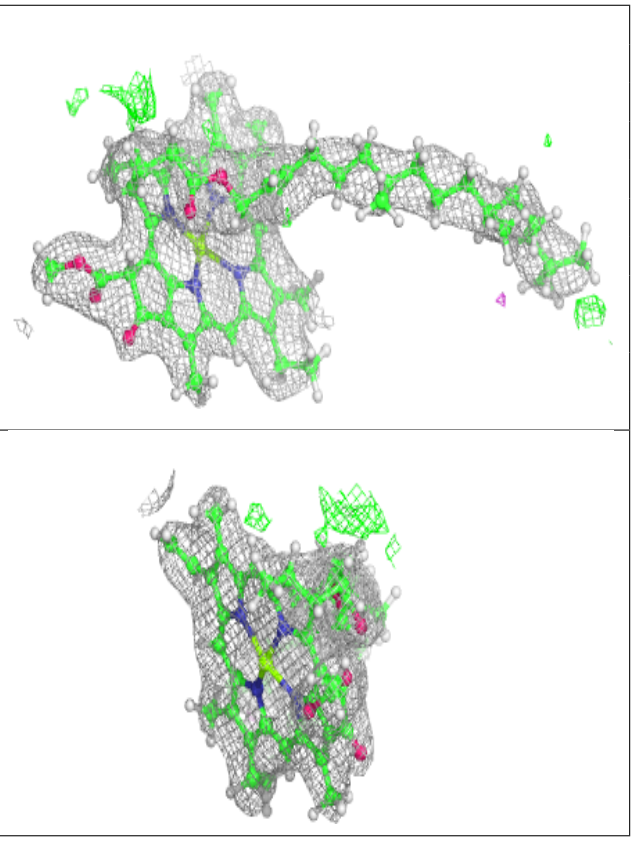
Electron density around LHG d 407:

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



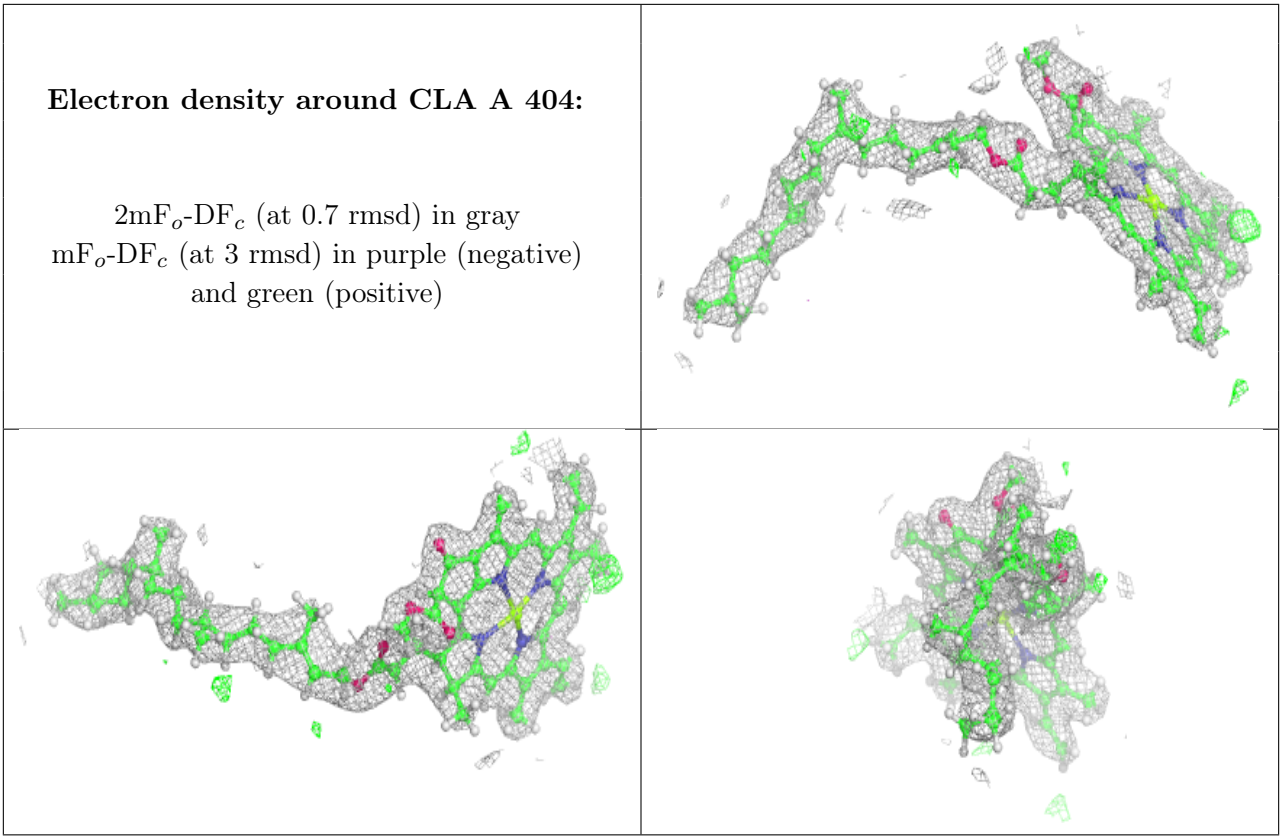
Electron density around CLA b 609:

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



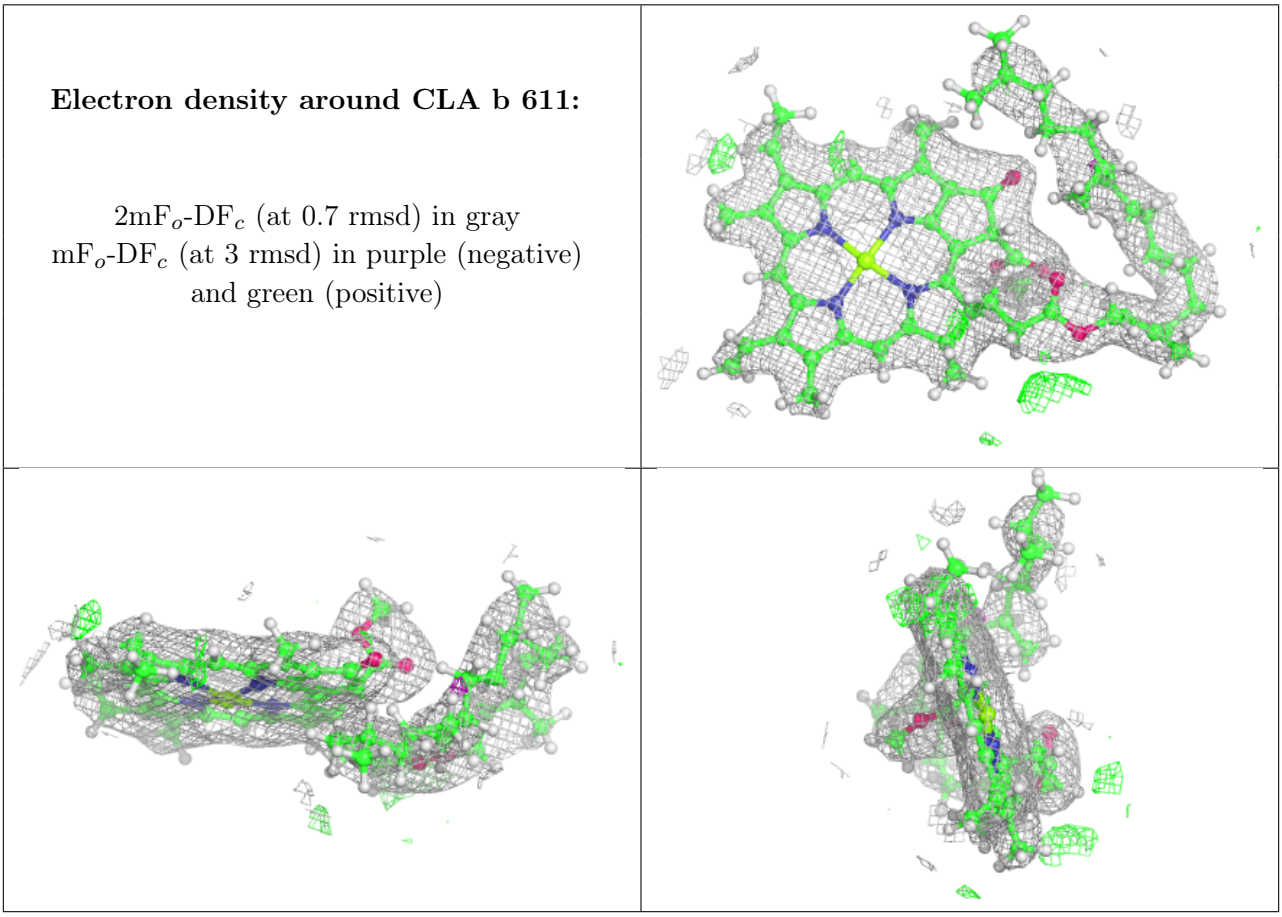
Electron density around CLA A 404:

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



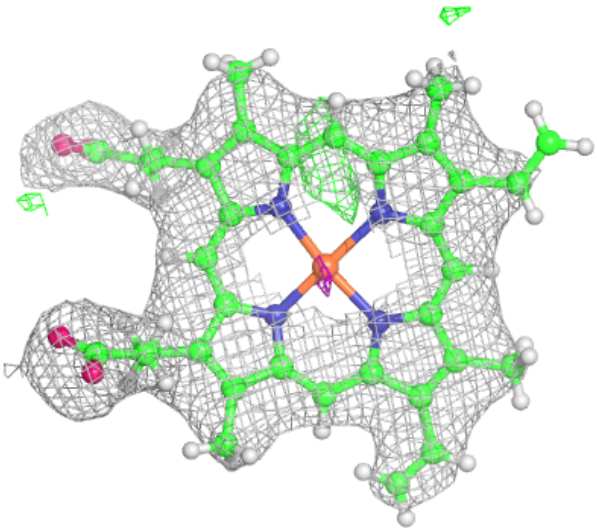
Electron density around CLA b 611:

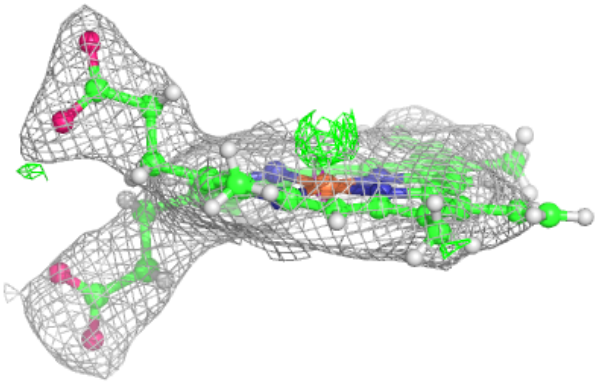
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

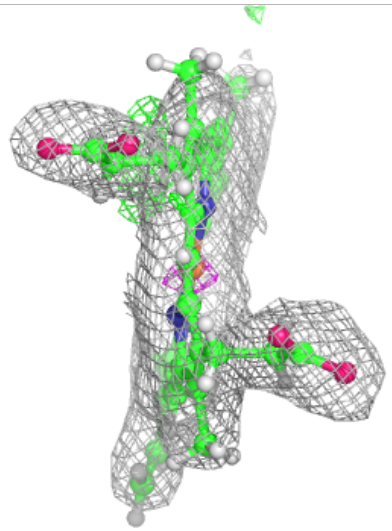


Electron density around HEM E 102:

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

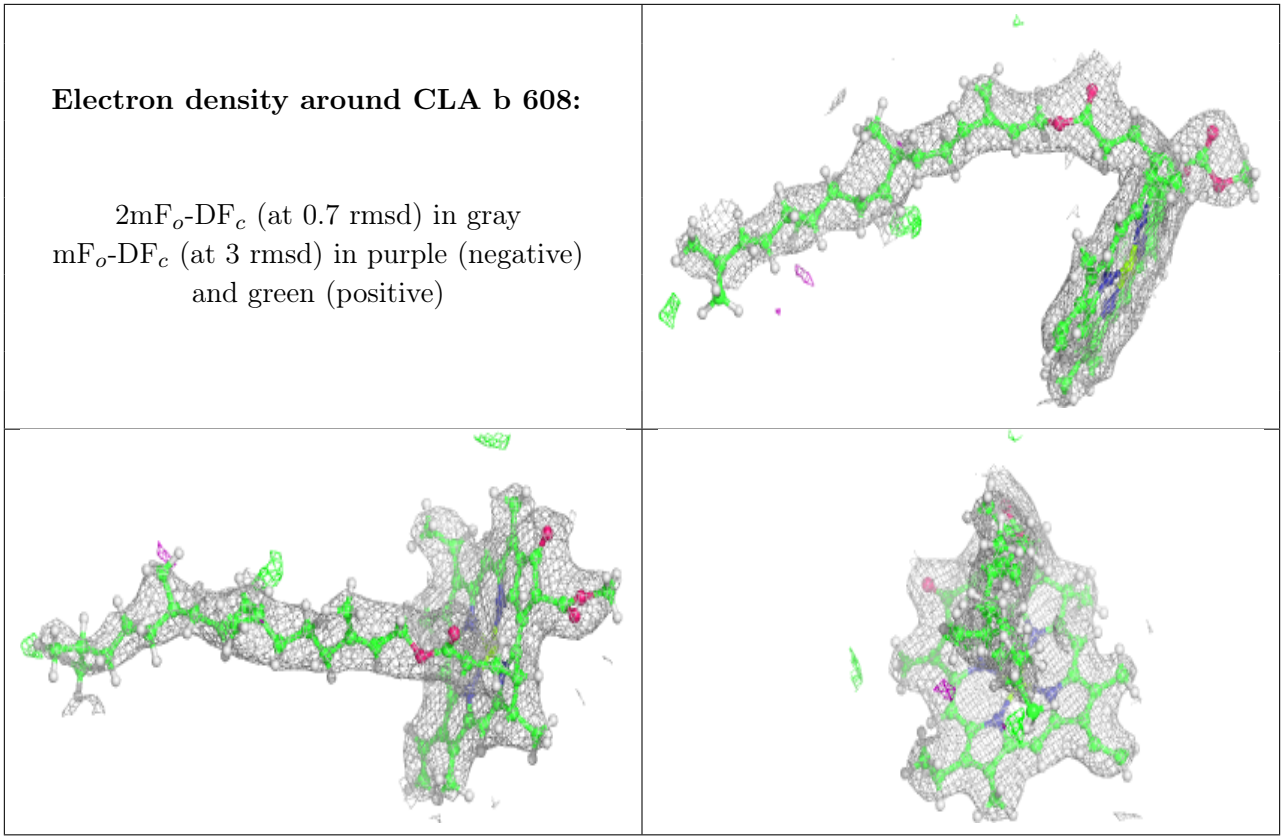






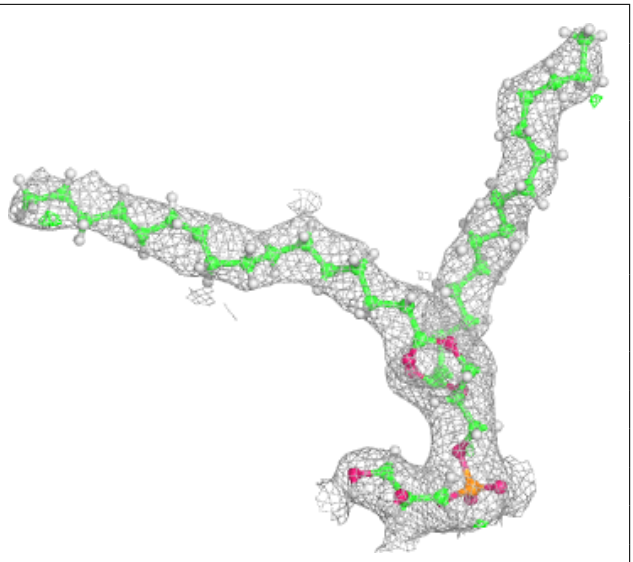
Electron density around CLA b 608:

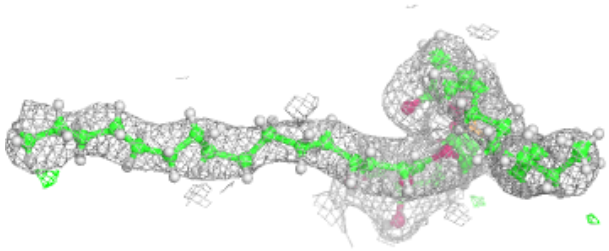
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

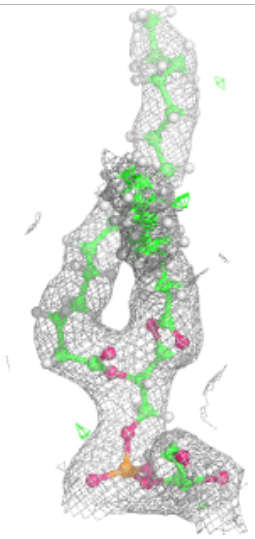


Electron density around LHG L 101:

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

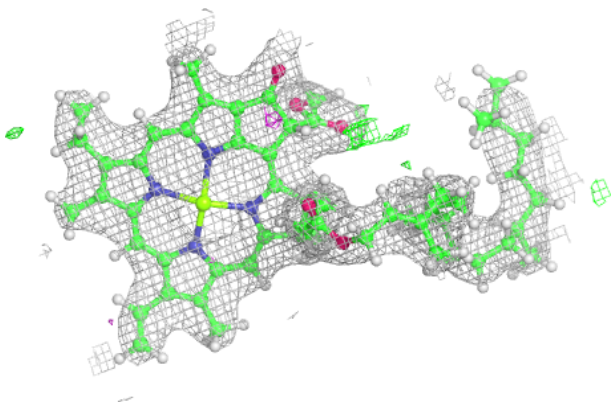


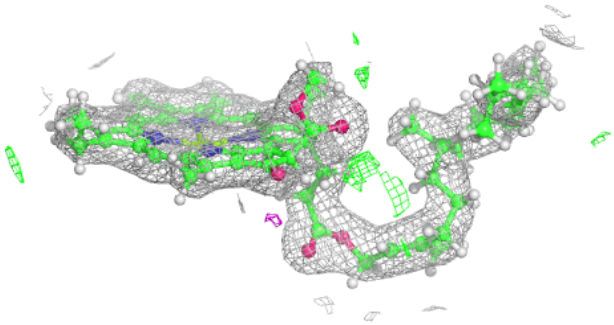


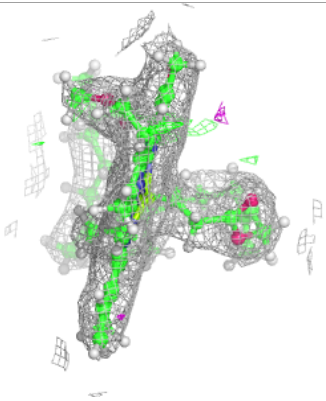


Electron density around CLA B 612:

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

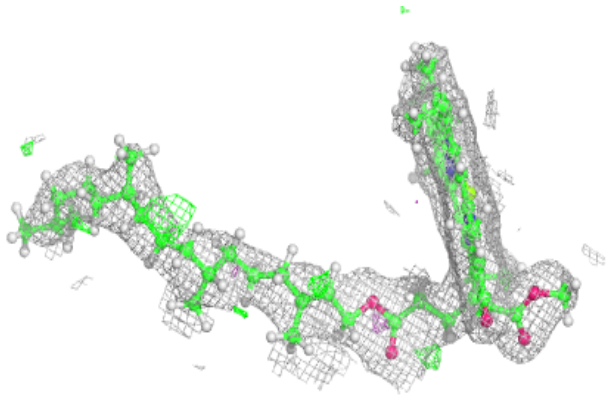


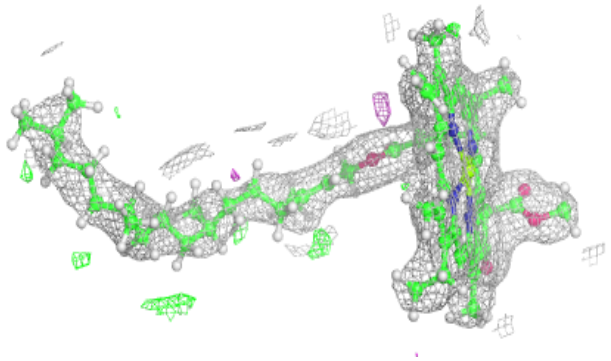


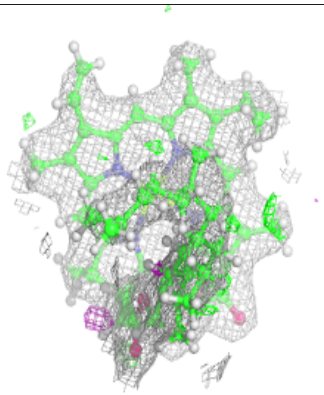


Electron density around CLA b 606:

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

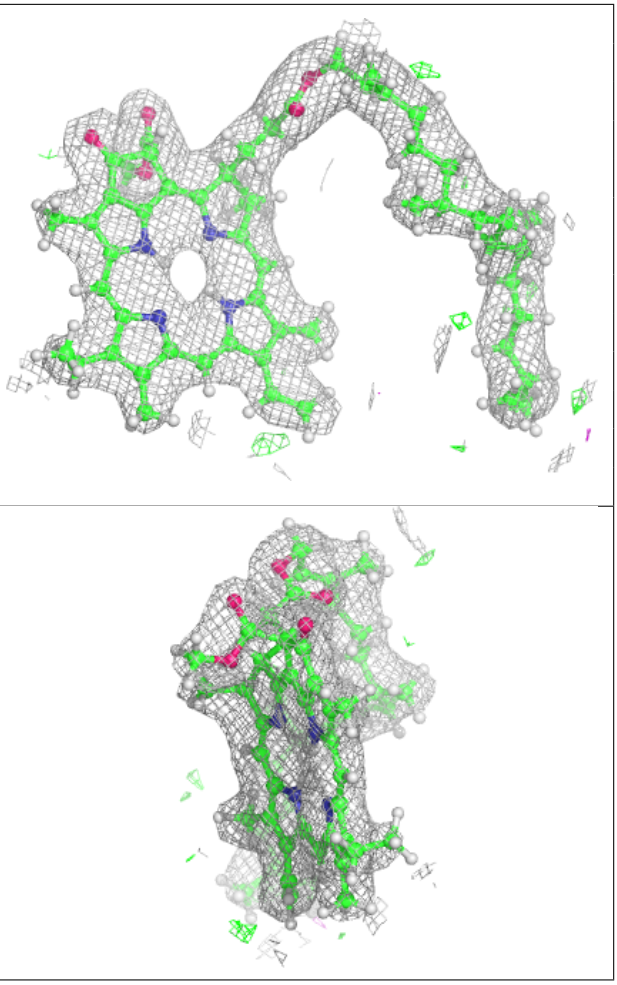






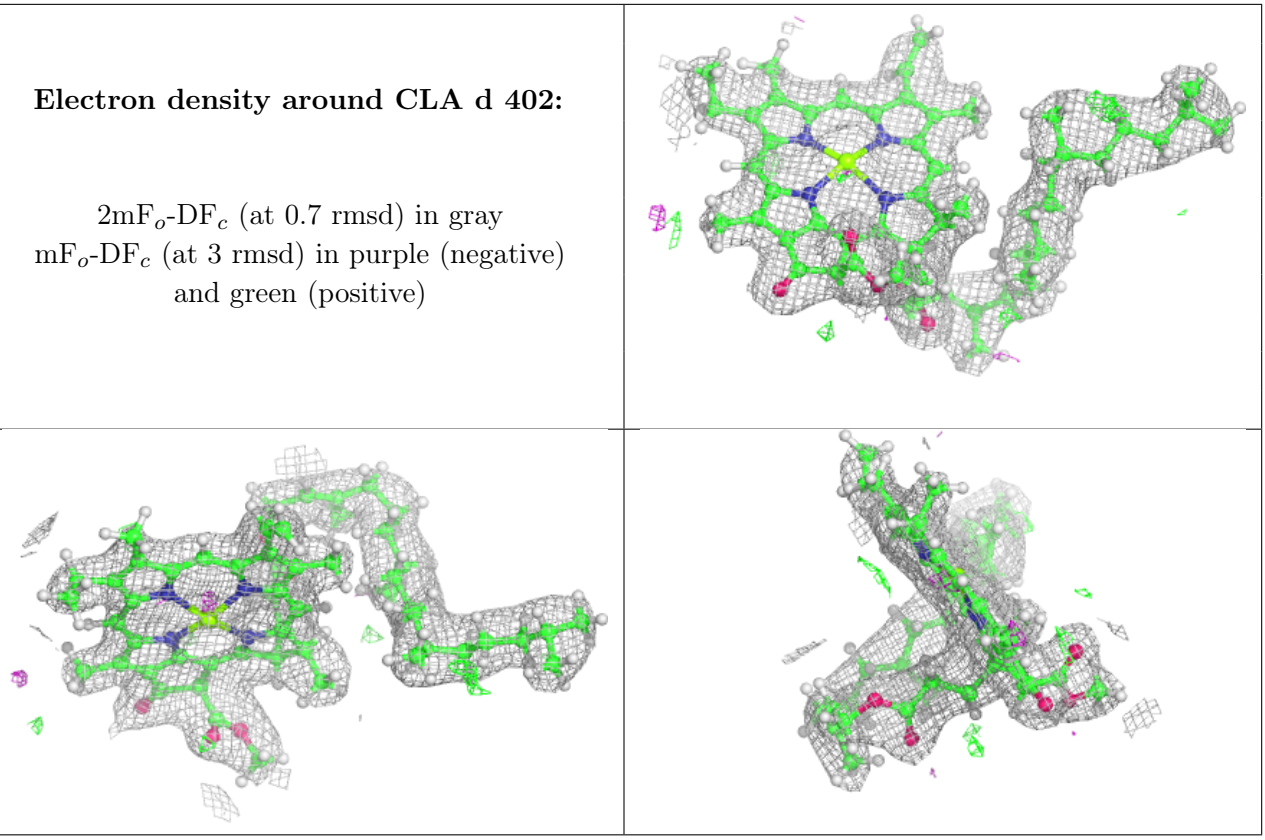
Electron density around PHO D 401:

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



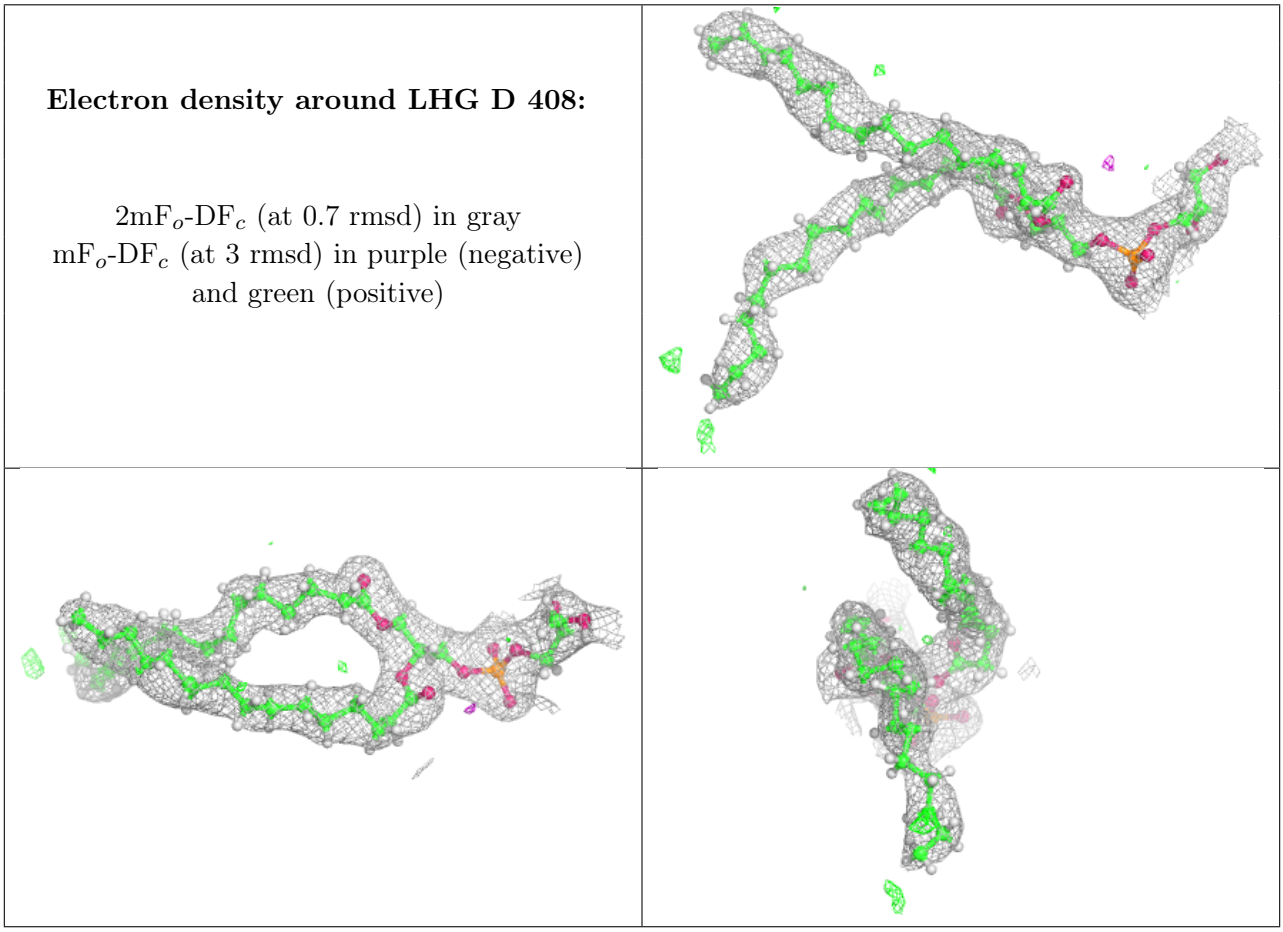
Electron density around CLA d 402:

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



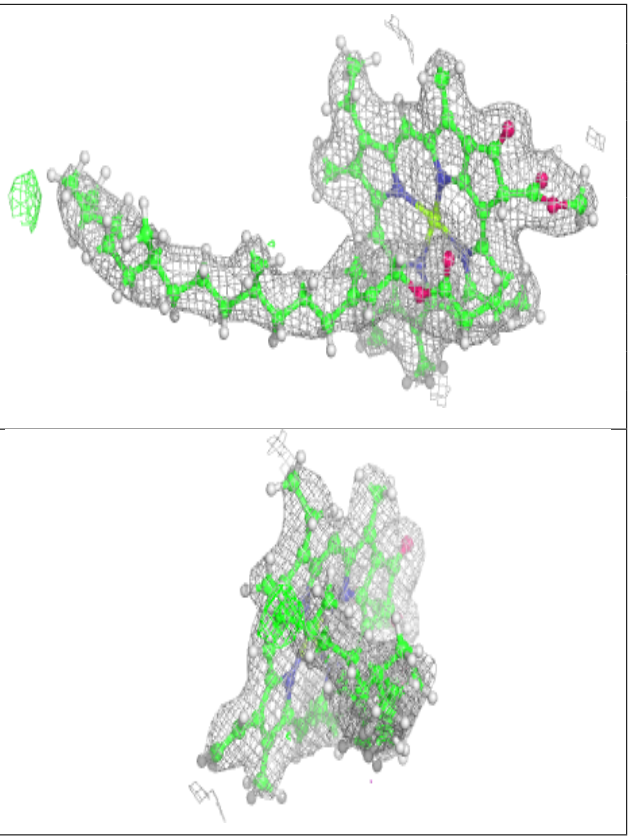
Electron density around LHG D 408:

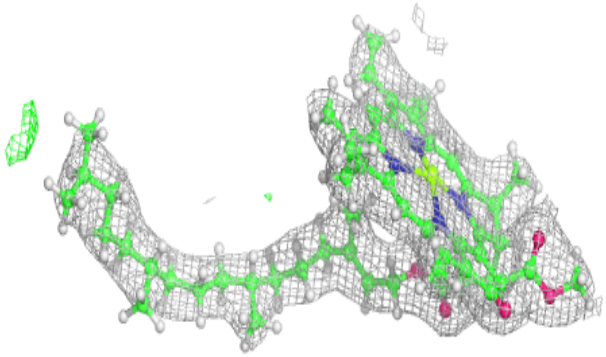
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 608:

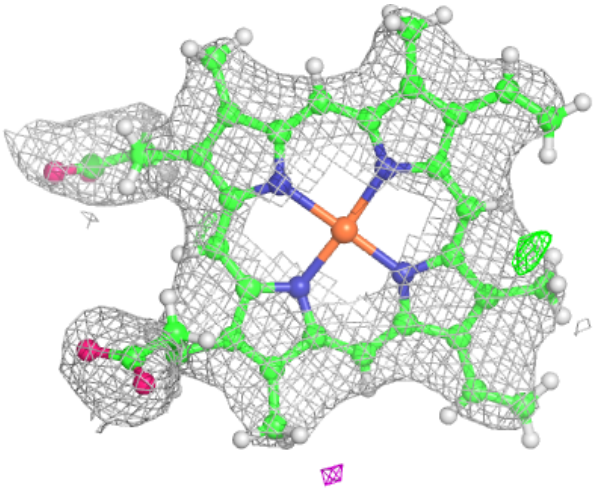
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

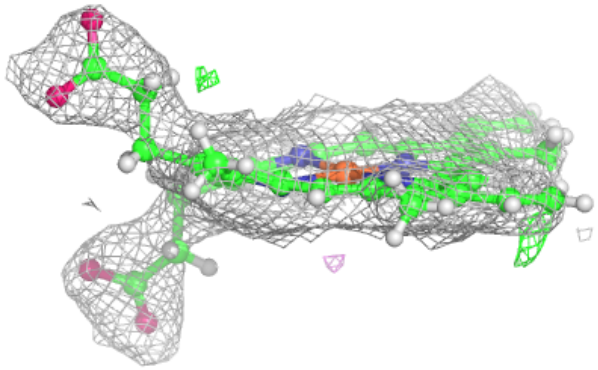


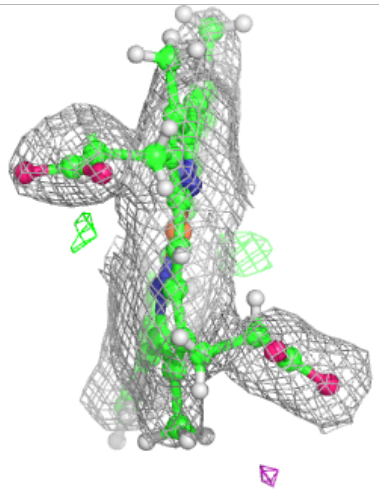


Electron density around HEM e 102:

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

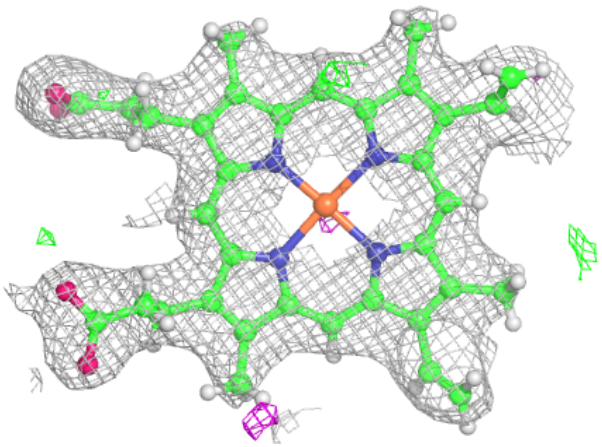


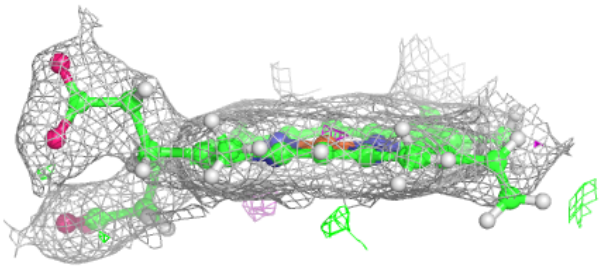




Electron density around HEC V 201:

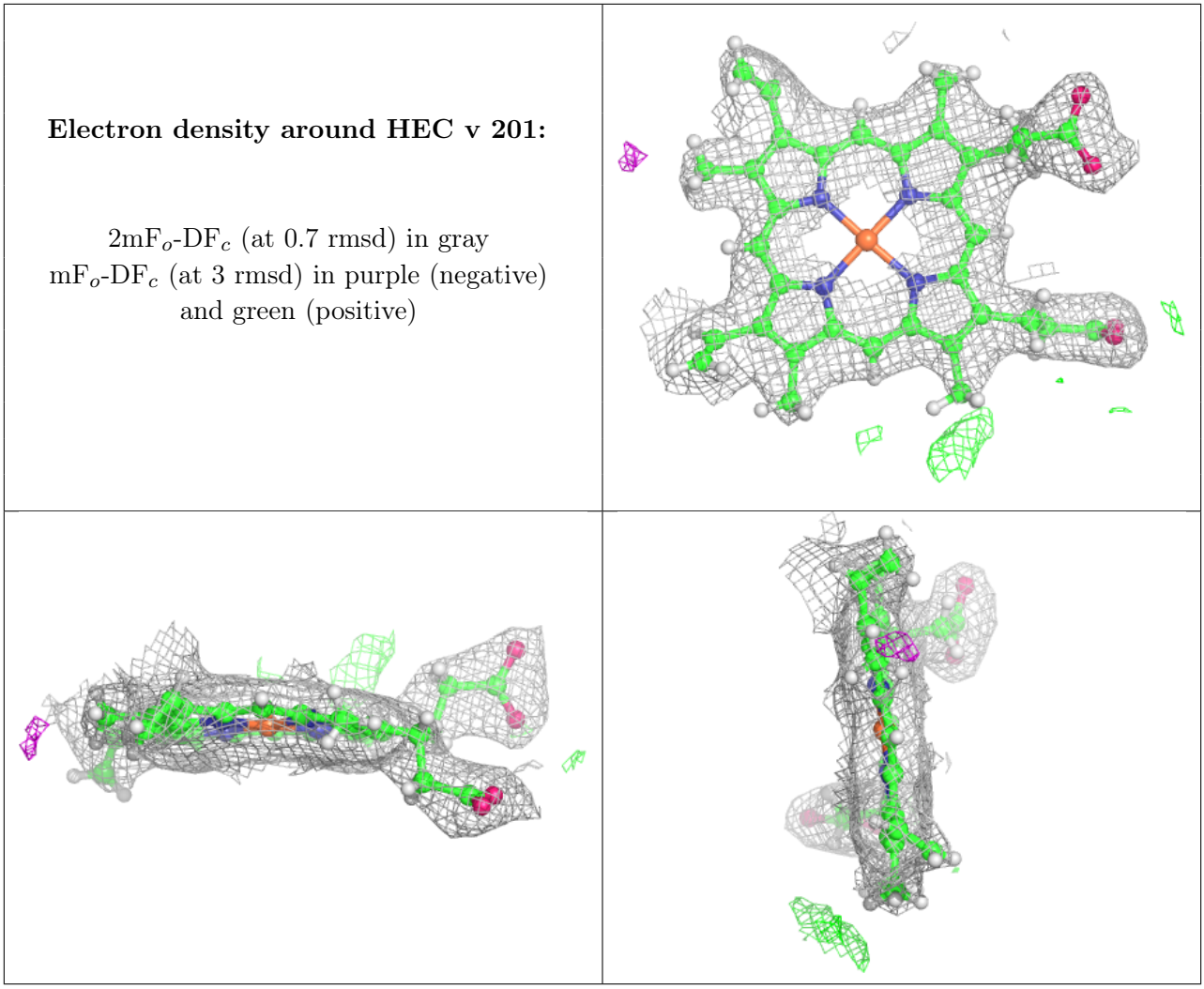
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC v 201:

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



6.5 Other polymers

There are no such residues in this entry.