wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 07:49 AM EST

PDB ID	:	6DHF
Title	:	RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.08 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	:	2.08 Å(reported)

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

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

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

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

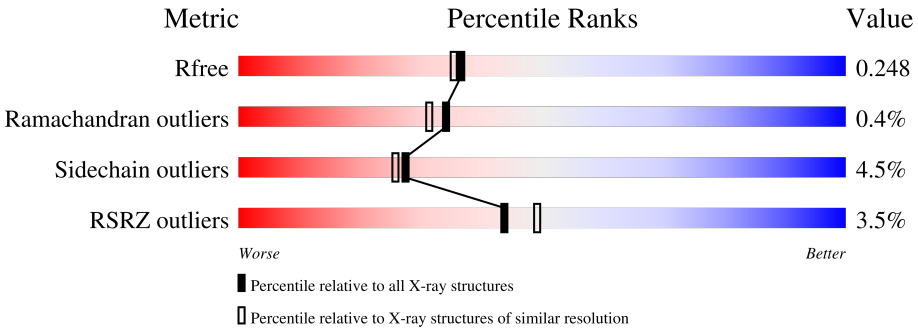
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

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 2.08 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	6189 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

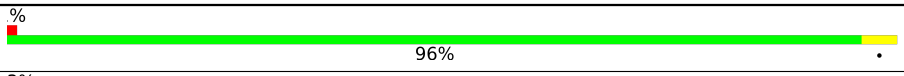
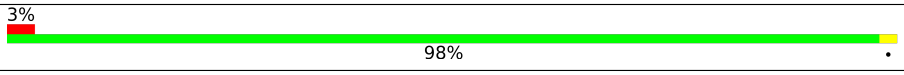
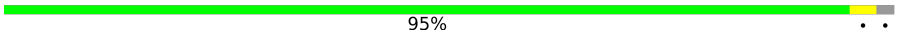
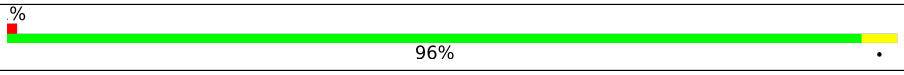
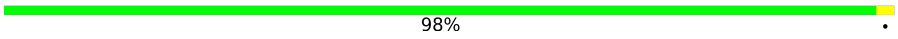
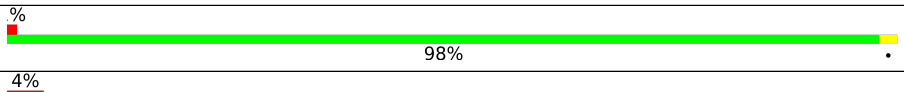
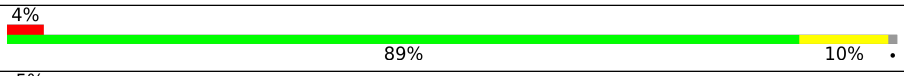
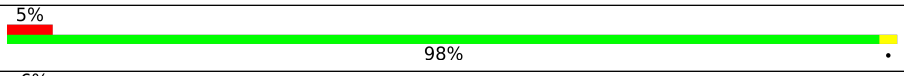
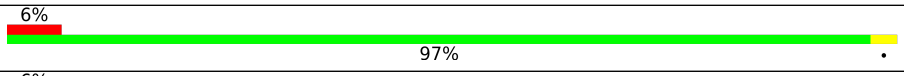
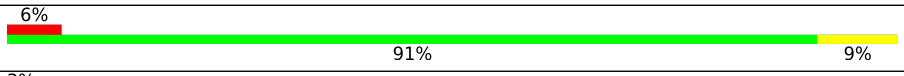
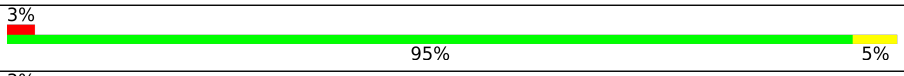
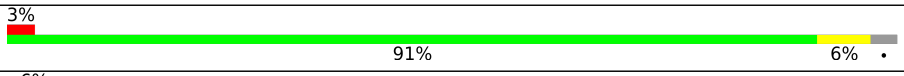
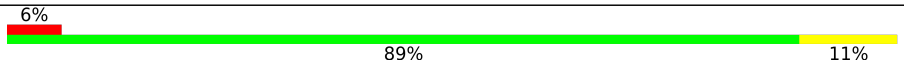
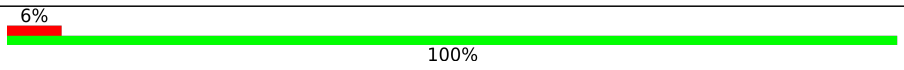
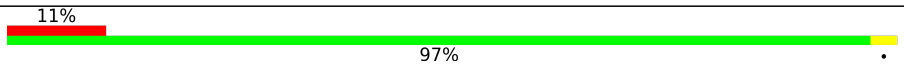
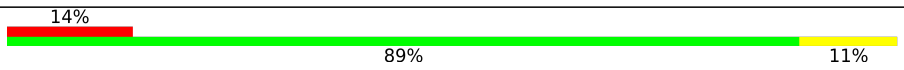
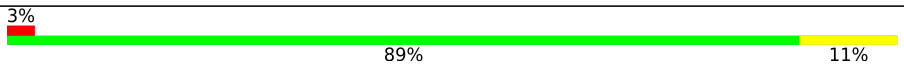
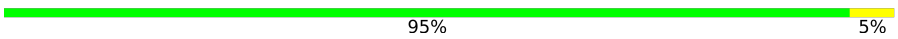
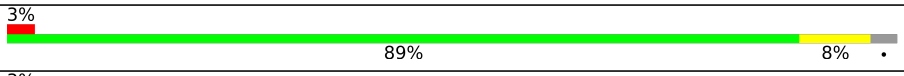
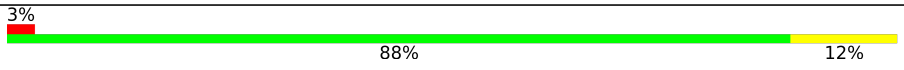
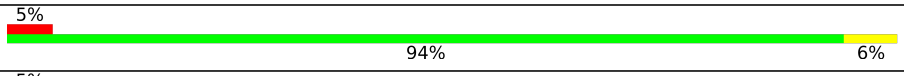
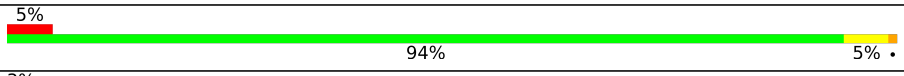
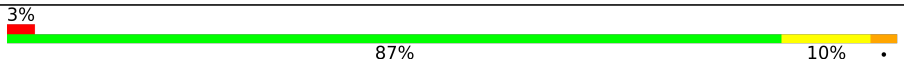
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	% 99% .
1	a	334	97% .

Continued on next page...

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

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	t	30	7% 97%
15	U	97	2% 96%
15	u	97	2% 97%
16	V	137	96%
16	v	137	% 96%
17	Y	30	37% 77% 10% 10%
17	y	30	27% 93% 7%
18	X	38	11% 97%
18	x	38	8% 95% 5%
19	Z	62	27% 89% 11%
19	z	62	24% 82% 18%
20	R	34	44% 85% 15%
20	r	34	62% 79% 12% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	h	101	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 103698 atoms, of which 51491 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	1	0
			6768	2249	3346	570	590	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6911	2290	3411	587	610	13			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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			

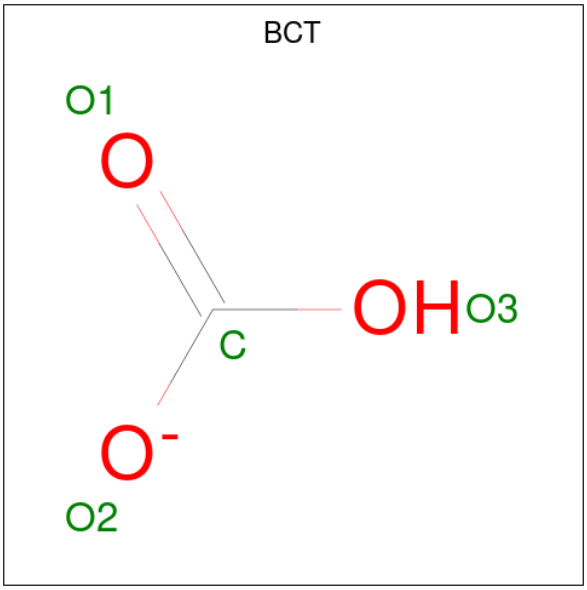
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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).

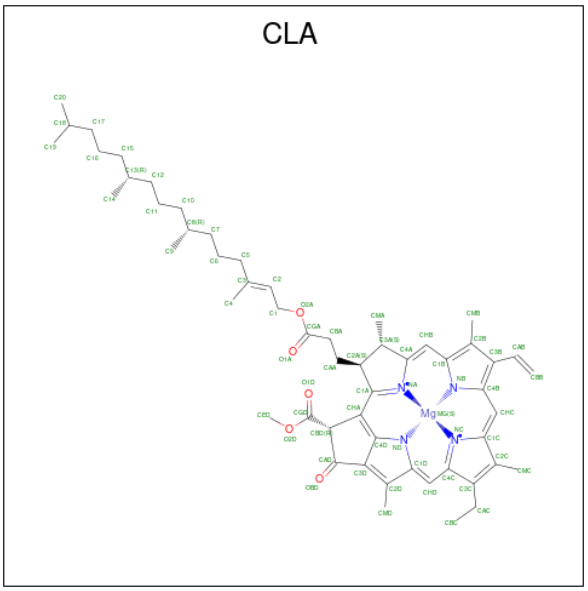
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	a	2	Total Cl 2 2	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

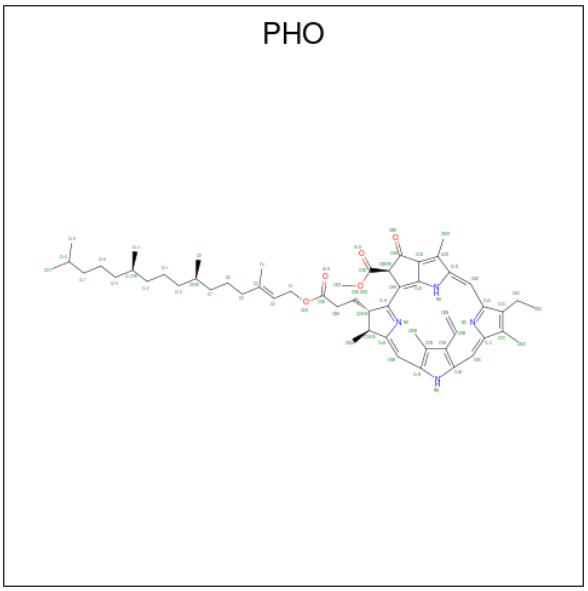
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

Continued from previous page...

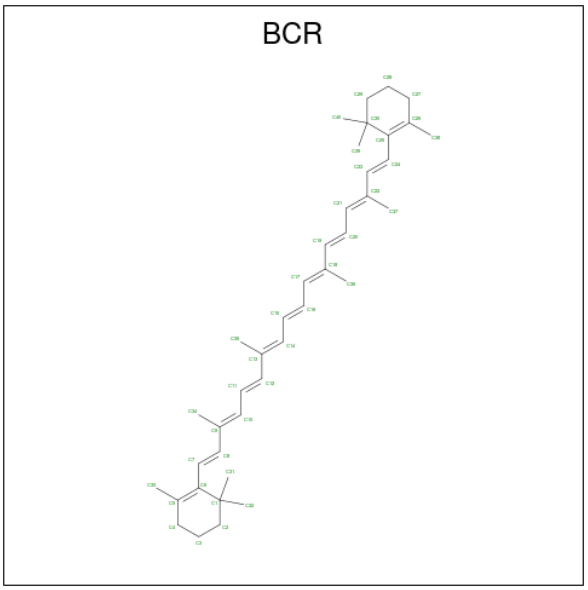
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
24	c	1	Total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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



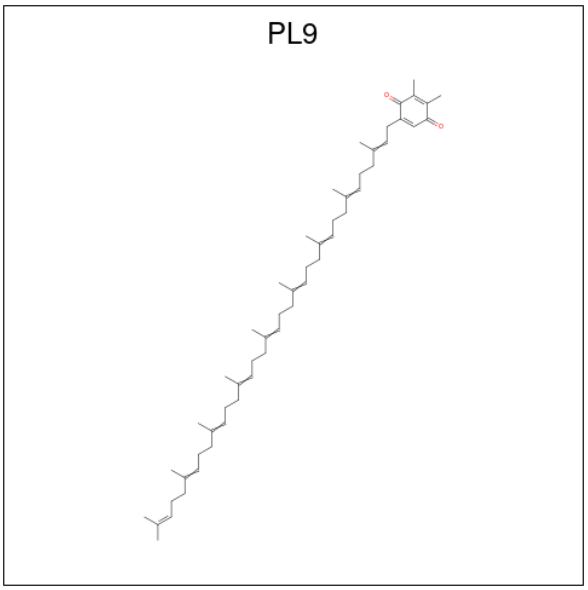
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



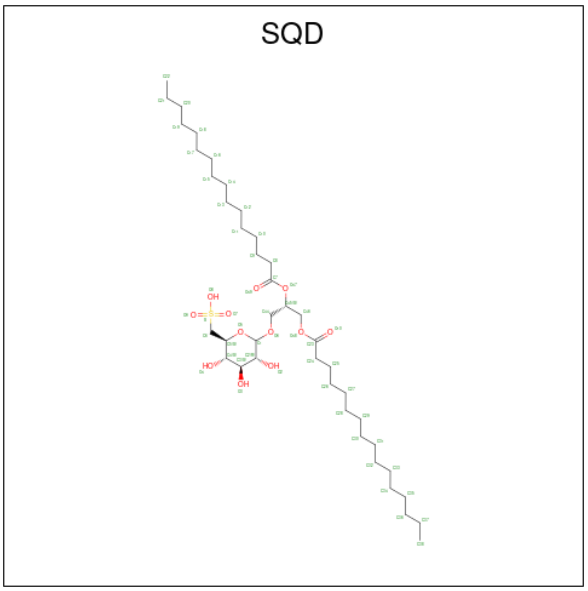
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C H 96 40 56	0	0
26	B	1	Total C H 96 40 56	0	0
26	B	1	Total C H 96 40 56	0	0
26	B	1	Total C H 96 40 56	0	0
26	C	1	Total C H 96 40 56	0	0
26	C	1	Total C H 96 40 56	0	0
26	D	1	Total C H 96 40 56	0	0
26	H	1	Total C H 96 40 56	0	0
26	K	1	Total C H 96 40 56	0	0
26	Y	1	Total C H 96 40 56	0	0
26	a	1	Total C H 96 40 56	0	0
26	b	1	Total C H 96 40 56	0	0
26	b	1	Total C H 96 40 56	0	0
26	b	1	Total C H 96 40 56	0	0
26	b	1	Total C H 96 40 56	0	0
26	c	1	Total C H 96 40 56	0	0
26	c	1	Total C H 96 40 56	0	0
26	c	1	Total C H 96 40 56	0	0
26	d	1	Total C H 96 40 56	0	0
26	h	1	Total C H 96 40 56	0	0
26	k	1	Total C H 96 40 56	0	0
26	t	1	Total C H 96 40 56	0	0

- Molecule 27 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: $C_{53}H_{80}O_2$).



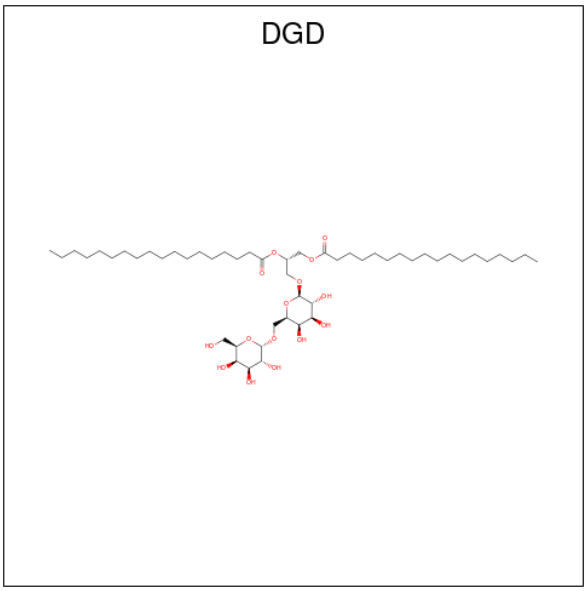
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



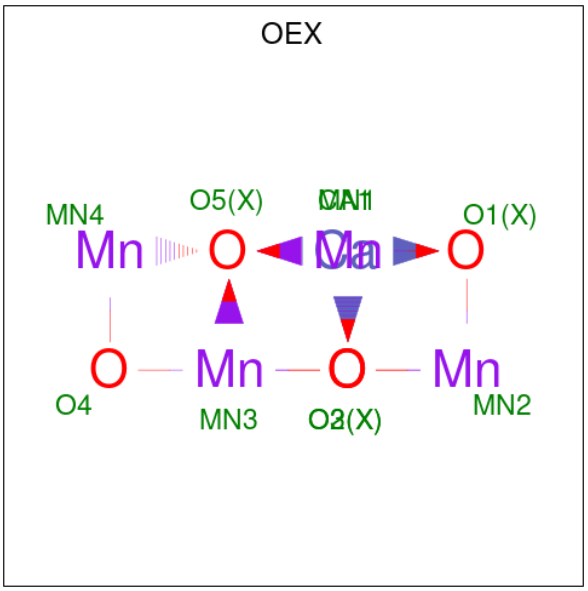
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H O S 122 39 70 12 1	0	0
28	A	1	Total C H O 104 35 65 4	0	0
28	B	1	Total C H O S 132 41 78 12 1	0	0
28	F	1	Total C H O S 81 25 45 10 1	0	0
28	a	1	Total C H O S 132 41 78 12 1	0	0
28	a	1	Total C H O 92 31 56 5	0	0
28	b	1	Total C H O S 114 36 65 12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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	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-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

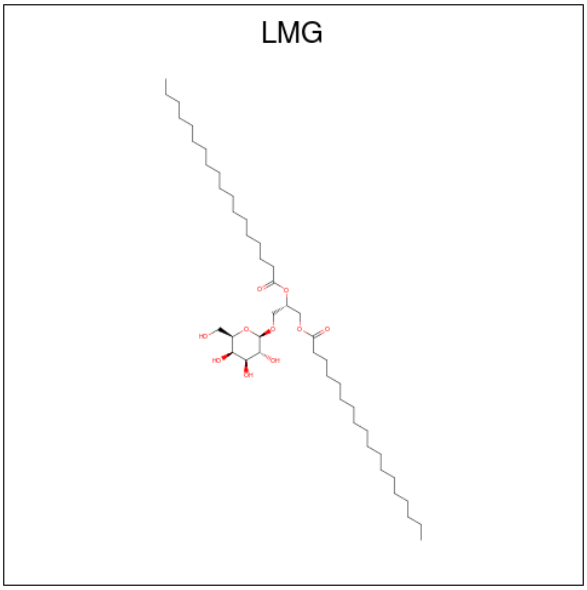
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	5	Total C H O 192 67 117 8	0	0
31	C	3	Total C H O 103 36 63 4	0	0
31	E	1	Total C H O 28 10 16 2	0	0
31	H	1	Total C H 53 18 35	0	0
31	I	1	Total C H 41 15 26	0	0
31	J	1	Total C H O 28 10 16 2	0	0
31	M	3	Total C H O 116 41 73 2	0	0
31	T	2	Total C H 91 31 60	0	0
31	X	1	Total C H O 55 18 35 2	0	0
31	a	1	Total C H O 28 10 16 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	4	Total	C	H	O	0	0
			176	60	110	6		
31	c	2	Total	C	H	O	0	0
			83	28	51	4		
31	d	1	Total	C	H	O	0	0
			43	15	26	2		
31	j	1	Total	C	H	O	0	0
			28	10	16	2		
31	m	1	Total	C	H	O	0	0
			28	10	16	2		
31	t	2	Total	C	H	O	0	0
			60	22	36	2		
31	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



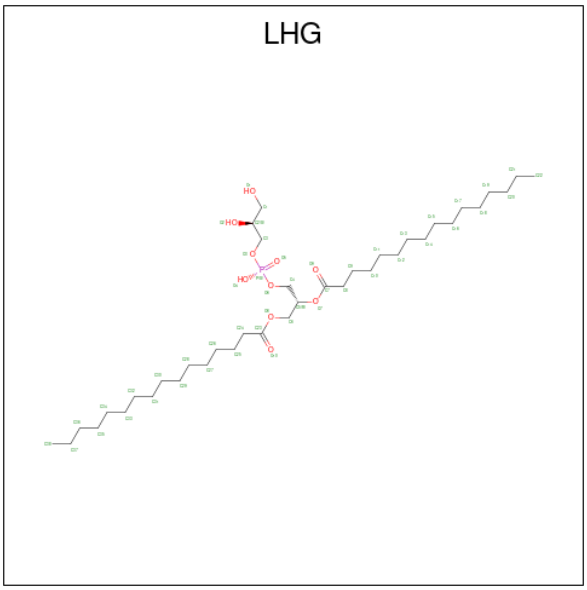
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			68	24	40	4		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			123	41	72	10		
32	D	1	Total	C	H	O	0	0
			78	27	45	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	K	1	Total	C	H	O		0	0
			114	38	66	10			
32	M	1	Total	C	H	O		0	0
			123	41	72	10			
32	b	1	Total	C	H	O		0	0
			123	41	72	10			
32	b	1	Total	C	H	O		0	0
			141	45	86	10			
32	c	1	Total	C	H	O		0	0
			81	27	44	10			
32	c	1	Total	C	H	O		0	0
			117	38	69	10			
32	c	1	Total	C	H	O		0	0
			117	39	68	10			
32	d	1	Total	C	H	O		0	0
			102	34	58	10			
32	h	1	Total	C	H	O		0	0
			57	21	34	2			

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



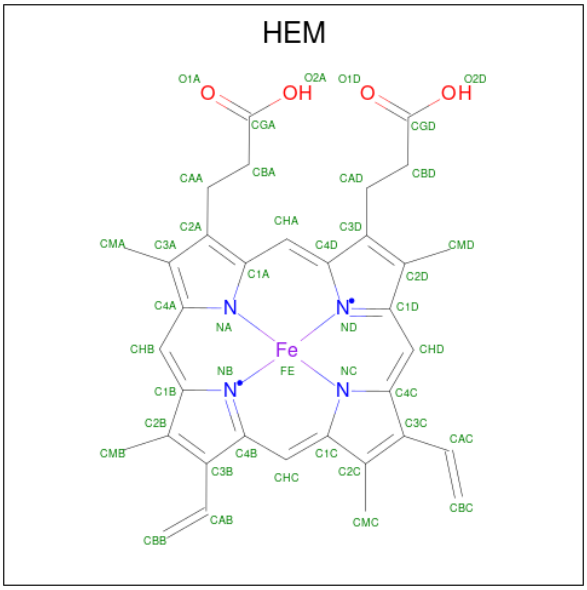
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

Continued on next page...

Continued from previous page...

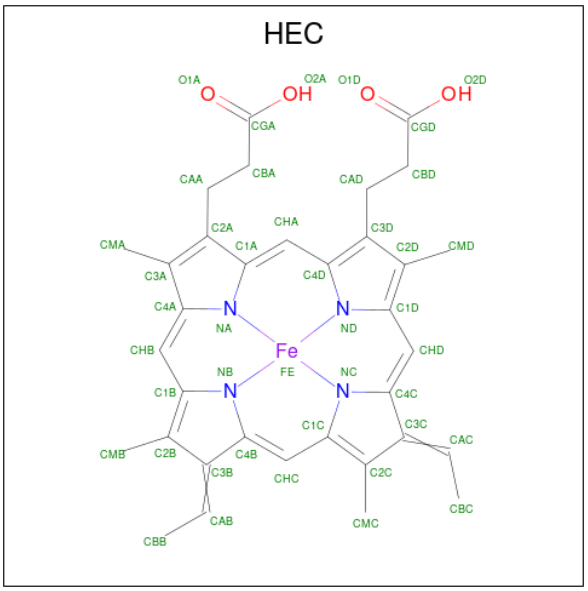
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	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	141	Total	O	0	0
			141	141		
36	B	218	Total	O	0	0
			218	218		
36	C	197	Total	O	0	0
			197	197		
36	D	138	Total	O	0	0
			138	138		
36	E	29	Total	O	0	0
			29	29		
36	F	14	Total	O	0	0
			14	14		
36	H	26	Total	O	0	0
			26	26		
36	I	16	Total	O	0	0
			16	16		
36	J	12	Total	O	0	0
			12	12		
36	K	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	L	9	Total O 9 9	0	0
36	M	5	Total O 5 5	0	0
36	O	125	Total O 125 125	0	0
36	T	11	Total O 11 11	0	0
36	U	52	Total O 52 52	0	0
36	V	68	Total O 68 68	0	0
36	Y	5	Total O 5 5	0	0
36	X	6	Total O 6 6	0	0
36	Z	3	Total O 3 3	0	0
36	R	4	Total O 4 4	0	0
36	a	121	Total O 121 121	0	0
36	b	187	Total O 187 187	0	0
36	c	156	Total O 156 156	0	0
36	d	123	Total O 123 123	0	0
36	e	22	Total O 22 22	0	0
36	f	2	Total O 2 2	0	0
36	h	19	Total O 19 19	0	0
36	i	10	Total O 10 10	0	0
36	j	10	Total O 10 10	0	0
36	k	5	Total O 5 5	0	0
36	l	9	Total O 9 9	0	0

Continued on next page...

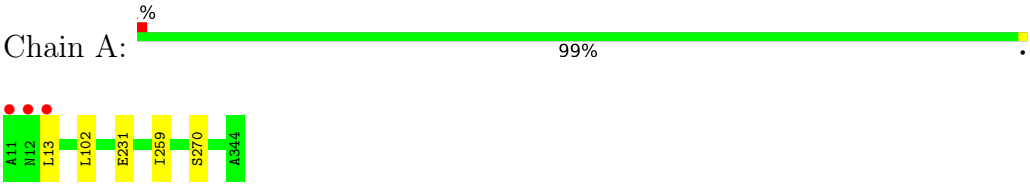
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	m	7	Total O 7 7	0	0
36	o	113	Total O 113 113	0	0
36	t	11	Total O 11 11	0	0
36	u	57	Total O 57 57	0	0
36	v	62	Total O 62 62	0	0
36	y	4	Total O 4 4	0	0
36	x	12	Total O 12 12	0	0
36	z	1	Total O 1 1	0	0
36	r	5	Total O 5 5	0	0

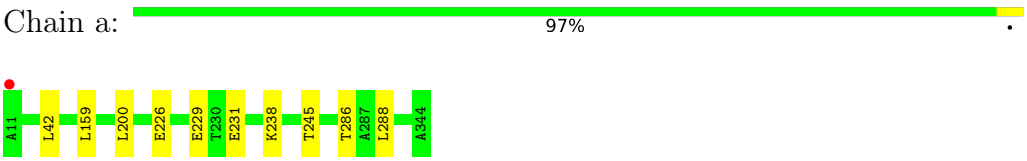
3 Residue-property plots (i)

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

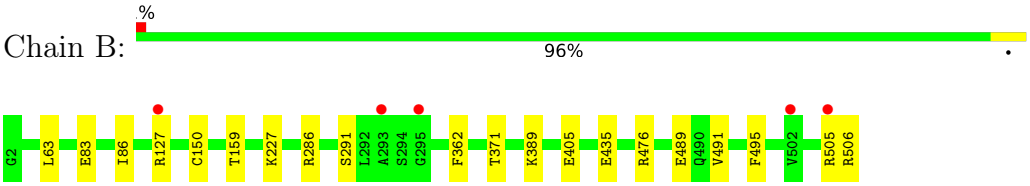
• Molecule 1: Photosystem II protein D1 1



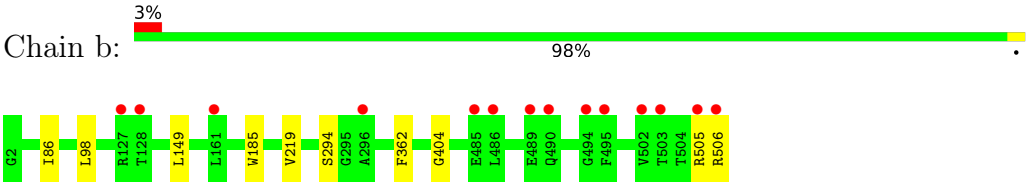
• Molecule 1: Photosystem II protein D1 1



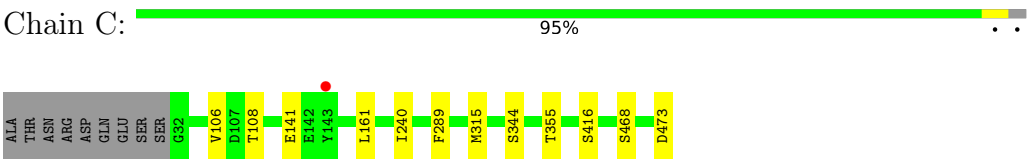
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

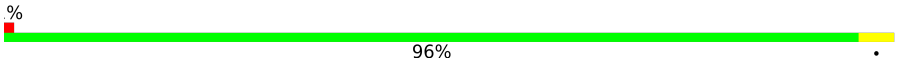


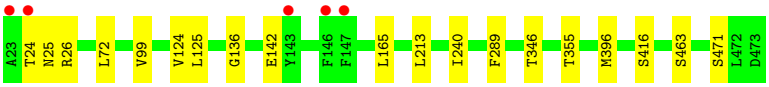
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

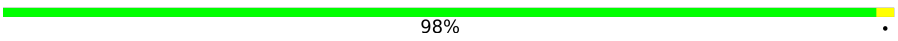
Chain c:

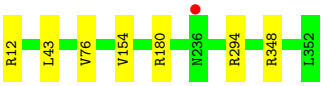




• Molecule 4: Photosystem II D2 protein

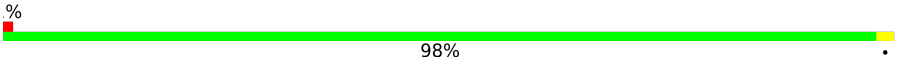
Chain D:

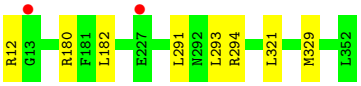




• Molecule 4: Photosystem II D2 protein

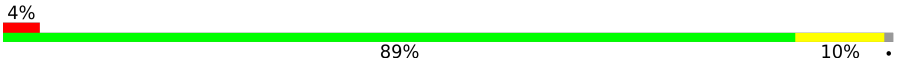
Chain d:

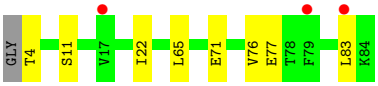




• Molecule 5: Cytochrome b559 subunit alpha

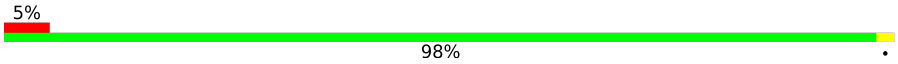
Chain E:

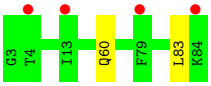




• Molecule 5: Cytochrome b559 subunit alpha

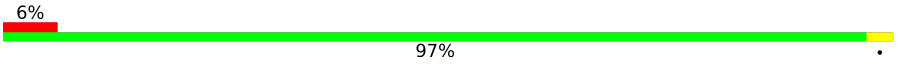
Chain e:

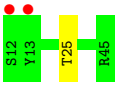




• Molecule 6: Cytochrome b559 subunit beta

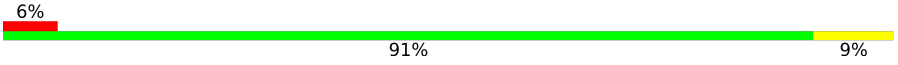
Chain F:





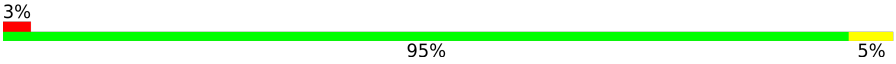
• Molecule 6: Cytochrome b559 subunit beta

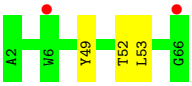
Chain f:



• Molecule 7: Photosystem II reaction center protein H

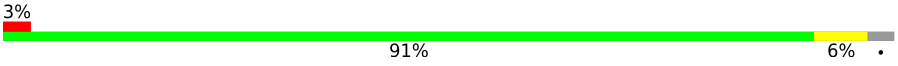
Chain H:

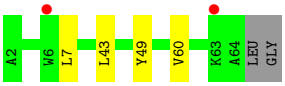




• Molecule 7: Photosystem II reaction center protein H

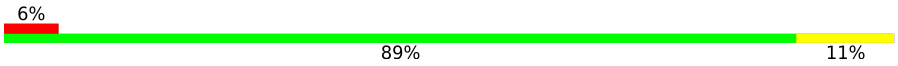
Chain h:

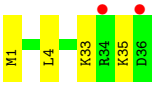




• Molecule 8: Photosystem II reaction center protein I

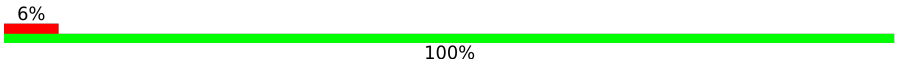
Chain I:





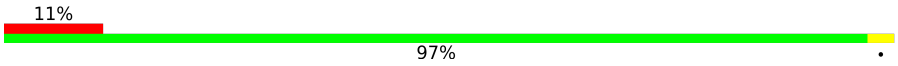
• Molecule 8: Photosystem II reaction center protein I

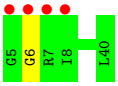
Chain i:



• Molecule 9: Photosystem II reaction center protein J

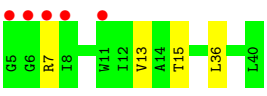
Chain J:





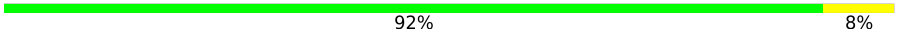
• Molecule 9: Photosystem II reaction center protein J

Chain j:



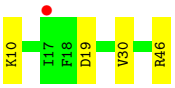
• Molecule 10: Photosystem II reaction center protein K

Chain K:



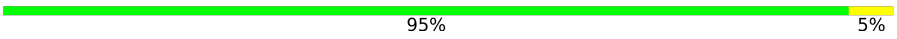
• Molecule 10: Photosystem II reaction center protein K

Chain k:



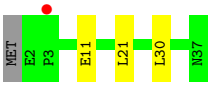
• Molecule 11: Photosystem II reaction center protein L

Chain L:



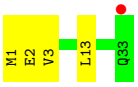
• Molecule 11: Photosystem II reaction center protein L

Chain l:



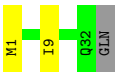
• Molecule 12: Photosystem II reaction center protein M

Chain M:



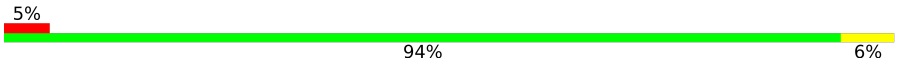
• Molecule 12: Photosystem II reaction center protein M

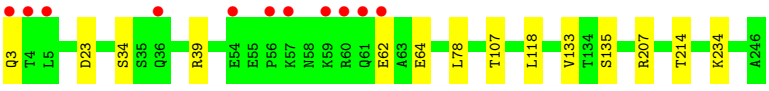
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

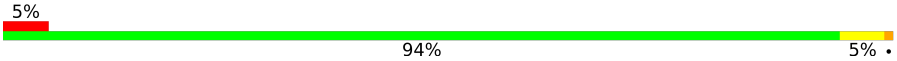
Chain O:

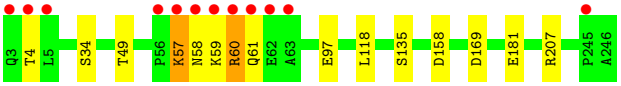




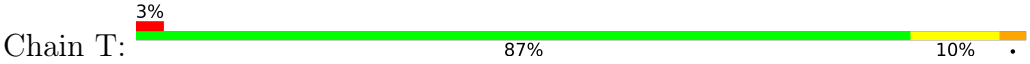
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

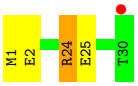
Chain o:



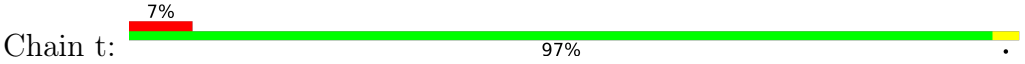


• Molecule 14: Photosystem II reaction center protein T

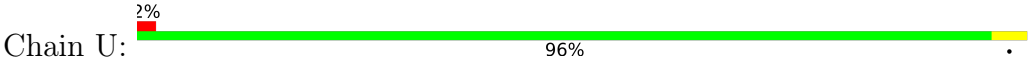


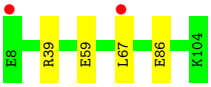


• Molecule 14: Photosystem II reaction center protein T

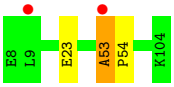


• Molecule 15: Photosystem II 12 kDa extrinsic protein

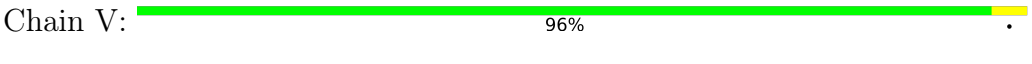


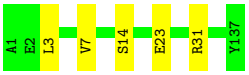


• Molecule 15: Photosystem II 12 kDa extrinsic protein

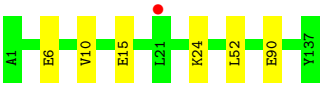


• Molecule 16: Cytochrome c-550



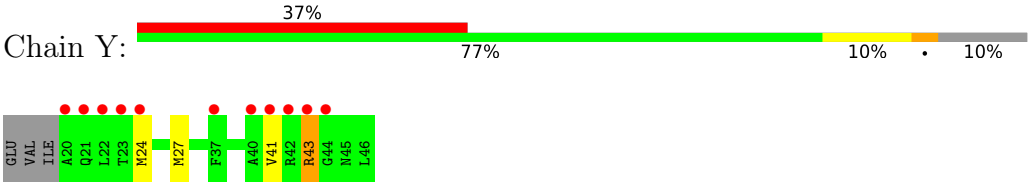


• Molecule 16: Cytochrome c-550



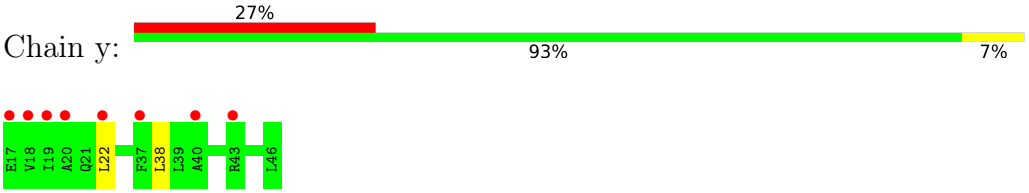
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



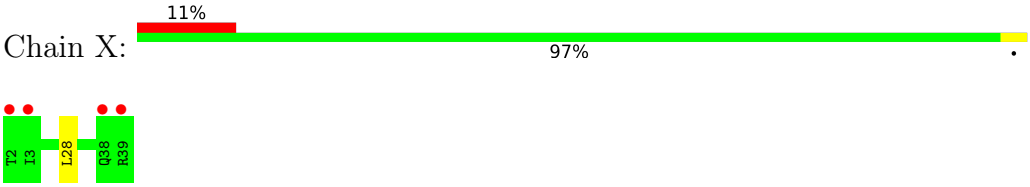
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



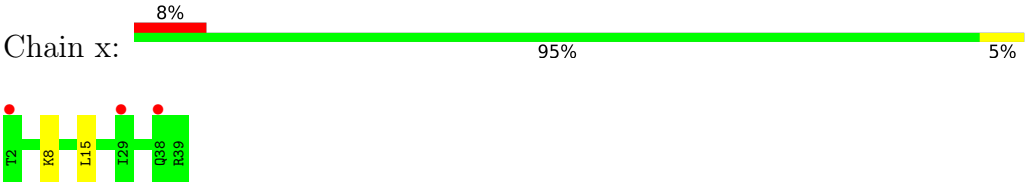
• Molecule 18: Photosystem II reaction center X protein

Chain X:



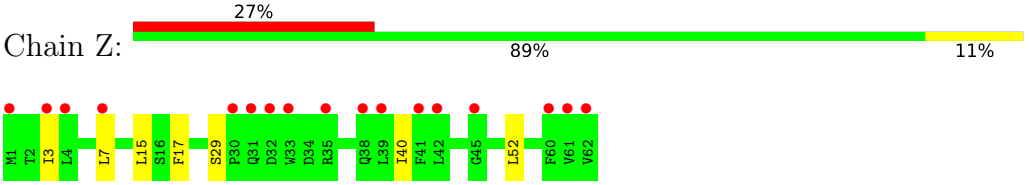
• Molecule 18: Photosystem II reaction center X protein

Chain x:



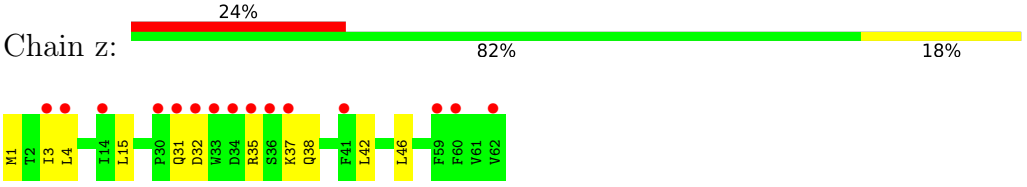
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



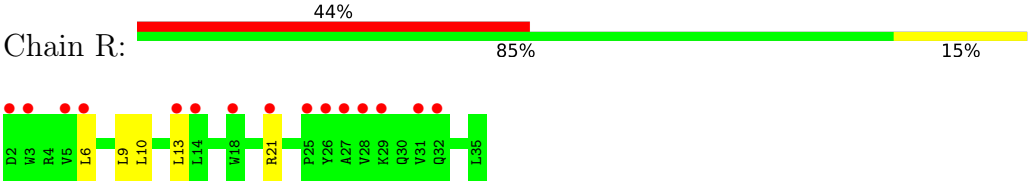
• Molecule 19: Photosystem II reaction center protein Z

Chain z:

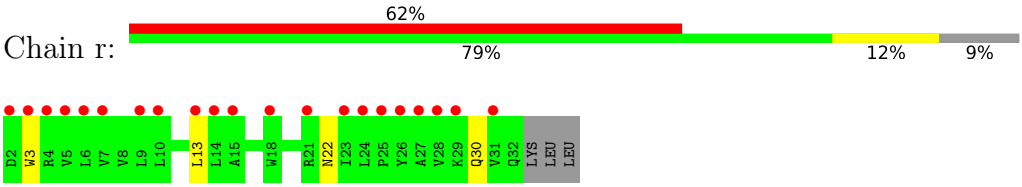


• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.82Å 220.89Å 307.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.43 – 2.08 30.43 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.43-2.08) 86.9 (30.43-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.56 (at 2.08Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.189 , 0.247 0.189 , 0.248	Depositor DCC
R_{free} test set	4194 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 72.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	103698	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: LMG, HEM, LHG, FME, PL9, UNL, CLA, SQD, BCR, FE2, BCT, DGD, CL, PHO, OEX, HEC

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	0.70	0/2707	0.72	0/3692
1	a	0.67	0/2704	0.71	0/3688
2	B	0.66	1/4160 (0.0%)	0.69	0/5668
2	b	0.64	1/4118 (0.0%)	0.67	0/5611
3	C	0.65	1/3538 (0.0%)	0.68	1/4818 (0.0%)
3	c	0.59	0/3619	0.67	0/4926
4	D	0.68	0/2812	0.71	2/3832 (0.1%)
4	d	0.62	0/2821	0.69	1/3844 (0.0%)
5	E	0.50	0/684	0.63	0/935
5	e	0.50	0/683	0.60	0/932
6	F	0.51	0/284	0.59	0/387
6	f	0.48	0/284	0.58	0/387
7	H	0.65	0/520	0.67	0/709
7	h	0.54	0/511	0.69	0/697
8	I	0.63	0/293	0.69	0/396
8	i	0.72	0/293	0.81	0/396
9	J	0.50	0/263	0.65	0/356
9	j	0.47	0/261	0.63	0/353
10	K	0.48	0/314	0.69	0/427
10	k	0.47	0/303	0.63	0/416
11	L	0.69	0/311	0.62	0/422
11	l	0.69	0/303	0.72	0/412
12	M	0.59	0/249	0.70	0/341
12	m	0.72	0/244	0.66	0/334
13	O	0.60	0/1914	0.73	0/2596
13	o	0.59	0/1905	0.74	2/2583 (0.1%)
14	T	0.68	0/257	0.89	2/349 (0.6%)
14	t	0.78	0/255	0.67	0/346
15	U	0.57	0/785	0.66	0/1064
15	u	0.64	0/785	0.72	0/1064
16	V	0.59	0/1085	0.68	0/1473
16	v	0.52	0/1085	0.66	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.39	0/197	0.61	0/264
17	y	0.33	0/219	0.53	0/294
18	X	0.52	0/284	0.66	0/384
18	x	0.38	0/284	0.55	0/384
19	Z	0.53	0/490	0.59	0/669
19	z	0.41	0/488	0.54	0/666
20	R	0.43	0/277	0.59	0/380
20	r	0.38	0/233	0.53	0/323
All	All	0.62	3/42822 (0.0%)	0.68	8/58291 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-7.37	1.17	1.34
2	B	150	CYS	CB-SG	-5.50	1.72	1.81
2	b	185	TRP	CB-CG	-5.06	1.41	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	24	ARG	NE-CZ-NH1	7.73	124.17	120.30
4	d	294	ARG	NE-CZ-NH1	6.17	123.38	120.30
3	C	473	ASP	CB-CG-OD1	5.50	123.25	118.30
13	o	169	ASP	CB-CG-OD1	5.48	123.23	118.30
4	D	294	ARG	NE-CZ-NH1	-5.44	117.58	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	53	ALA	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%)	325 (98%)	6 (2%)	1 (0%)	41 39
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100 100
2	B	508/505 (101%)	494 (97%)	14 (3%)	0	100 100
2	b	503/505 (100%)	491 (98%)	10 (2%)	2 (0%)	34 31
3	C	441/451 (98%)	428 (97%)	12 (3%)	1 (0%)	47 47
3	c	451/451 (100%)	433 (96%)	15 (3%)	3 (1%)	22 17
4	D	339/341 (99%)	328 (97%)	11 (3%)	0	100 100
4	d	340/341 (100%)	325 (96%)	15 (4%)	0	100 100
5	E	80/82 (98%)	76 (95%)	4 (5%)	0	100 100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100 100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
6	f	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
7	h	61/65 (94%)	55 (90%)	5 (8%)	1 (2%)	9 4
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%)	31 (91%)	2 (6%)	1 (3%)	4 1
9	j	34/36 (94%)	31 (91%)	3 (9%)	0	100 100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	4 1
10	k	35/37 (95%)	35 (100%)	0	0	100 100
11	L	35/37 (95%)	35 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

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%)	228 (94%)	13 (5%)	2 (1%)	19 14
13	o	242/244 (99%)	228 (94%)	11 (4%)	3 (1%)	13 7
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100 100
15	u	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	7 2
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100 100
16	v	135/137 (98%)	126 (93%)	9 (7%)	0	100 100
17	Y	25/30 (83%)	20 (80%)	3 (12%)	2 (8%)	1 0
17	y	28/30 (93%)	25 (89%)	3 (11%)	0	100 100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100 100
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9 4
20	R	32/34 (94%)	30 (94%)	2 (6%)	0	100 100
20	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3 1
All	All	5237/5326 (98%)	5019 (96%)	197 (4%)	21 (0%)	34 31

5 of 21 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/270 (100%)	266 (98%)	4 (2%)	65 69
1	a	269/270 (100%)	259 (96%)	10 (4%)	34 34
2	B	407/403 (101%)	388 (95%)	19 (5%)	26 24
2	b	402/403 (100%)	395 (98%)	7 (2%)	60 65
3	C	345/352 (98%)	336 (97%)	9 (3%)	46 49
3	c	354/352 (101%)	338 (96%)	16 (4%)	27 26
4	D	276/276 (100%)	271 (98%)	5 (2%)	59 63
4	d	277/276 (100%)	270 (98%)	7 (2%)	47 50
5	E	72/72 (100%)	63 (88%)	9 (12%)	4 2
5	e	71/72 (99%)	69 (97%)	2 (3%)	43 46
6	F	28/28 (100%)	27 (96%)	1 (4%)	35 35
6	f	28/28 (100%)	25 (89%)	3 (11%)	6 3
7	H	53/54 (98%)	50 (94%)	3 (6%)	20 17
7	h	53/54 (98%)	50 (94%)	3 (6%)	20 17
8	I	32/32 (100%)	29 (91%)	3 (9%)	8 5
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%)	19 (83%)	4 (17%)	2 1
10	K	31/30 (103%)	29 (94%)	2 (6%)	17 13
10	k	30/30 (100%)	26 (87%)	4 (13%)	4 2
11	L	35/35 (100%)	33 (94%)	2 (6%)	20 17
11	l	34/35 (97%)	31 (91%)	3 (9%)	10 6
12	M	28/29 (97%)	25 (89%)	3 (11%)	6 3
12	m	28/29 (97%)	27 (96%)	1 (4%)	35 35
13	O	208/207 (100%)	196 (94%)	12 (6%)	20 16
13	o	207/207 (100%)	195 (94%)	12 (6%)	20 16
14	T	26/26 (100%)	23 (88%)	3 (12%)	5 3
14	t	25/26 (96%)	25 (100%)	0	100 100
15	U	84/84 (100%)	80 (95%)	4 (5%)	25 23
15	u	84/84 (100%)	83 (99%)	1 (1%)	71 76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/117 (100%)	112 (96%)	5 (4%)	29	28
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	21
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	1
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	6
18	X	31/31 (100%)	30 (97%)	1 (3%)	39	40
18	x	31/31 (100%)	29 (94%)	2 (6%)	17	13
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	41 (80%)	10 (20%)	1	0
20	R	28/29 (97%)	23 (82%)	5 (18%)	2	1
20	r	19/29 (66%)	16 (84%)	3 (16%)	2	1
All	All	4323/4348 (99%)	4127 (96%)	196 (4%)	27	26

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	362	PHE
6	f	43	ILE
3	c	26	ARG
3	c	355	THR
9	j	15	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
19	z	38	GLN
13	o	58	ASN
2	b	282	GLN
17	Y	21	GLN
3	c	28	GLN

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	1.05	1 (12%)	7,9,11	1.58	2 (28%)
14	FME	t	1	14	8,9,10	1.41	1 (12%)	7,9,11	1.36	1 (14%)
8	FME	I	1	8	8,9,10	0.97	0	7,9,11	1.66	1 (14%)
8	FME	i	1	8	8,9,10	1.12	0	7,9,11	0.90	0
12	FME	m	1	12	8,9,10	1.18	1 (12%)	7,9,11	0.84	0
12	FME	M	1	12	8,9,10	1.25	1 (12%)	7,9,11	1.09	0

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-3.55	1.41	1.46
12	M	1	FME	CA-N	-2.84	1.42	1.46
12	m	1	FME	CA-N	-2.55	1.42	1.46
14	T	1	FME	CA-N	-2.27	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	C-CA-N	3.97	116.89	109.73
14	T	1	FME	CA-N-CN	-2.56	118.89	122.82
14	t	1	FME	C-CA-N	2.46	114.18	109.73
14	T	1	FME	O1-CN-N	-2.23	119.39	125.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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	$\#\|Z\| > 2$
32	LMG	c	522	-	48,48,55	1.19	6 (12%)	56,56,63	1.33	8 (14%)
29	DGD	c	517	-	63,63,67	1.23	9 (14%)	77,77,81	1.42	11 (14%)
24	CLA	C	514	-	65,73,73	1.44	7 (10%)	76,113,113	1.55	10 (13%)
24	CLA	C	504	-	65,73,73	1.64	12 (18%)	76,113,113	1.56	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	506	-	65,73,73	1.48	10 (15%)	76,113,113	1.29	11 (14%)
26	BCR	b	618	-	41,41,41	1.16	3 (7%)	56,56,56	1.41	12 (21%)
27	PL9	D	406	-	55,55,55	1.85	9 (16%)	68,69,69	1.47	15 (22%)
24	CLA	B	611	-	65,73,73	1.42	6 (9%)	76,113,113	1.56	13 (17%)
24	CLA	c	506	-	65,73,73	2.20	11 (16%)	76,113,113	1.39	12 (15%)
33	LHG	E	101	-	48,48,48	0.91	3 (6%)	51,54,54	1.12	2 (3%)
24	CLA	b	615	-	65,73,73	1.58	9 (13%)	76,113,113	1.68	10 (13%)
33	LHG	D	411	-	48,48,48	1.03	6 (12%)	51,54,54	1.42	8 (15%)
29	DGD	c	516	-	63,63,67	1.11	3 (4%)	77,77,81	1.40	9 (11%)
24	CLA	B	610	36	65,73,73	1.82	11 (16%)	76,113,113	1.58	13 (17%)
26	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	8 (14%)
24	CLA	B	603	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	14 (18%)
24	CLA	C	505	36	59,67,73	1.41	6 (10%)	68,105,113	1.54	12 (17%)
26	BCR	h	103	-	41,41,41	1.13	1 (2%)	56,56,56	1.47	13 (23%)
32	LMG	K	102	-	48,48,55	1.05	4 (8%)	56,56,63	1.33	5 (8%)
24	CLA	C	511	-	65,73,73	1.54	9 (13%)	76,113,113	1.39	7 (9%)
28	SQD	A	412	-	38,38,54	1.08	3 (7%)	40,40,65	1.32	3 (7%)
29	DGD	a	412	-	43,43,67	1.20	3 (6%)	45,45,81	1.33	8 (17%)
24	CLA	B	608	-	65,73,73	1.52	11 (16%)	76,113,113	1.27	9 (11%)
26	BCR	b	602	-	41,41,41	1.15	3 (7%)	56,56,56	1.32	5 (8%)
35	HEC	v	201	16	32,50,50	2.27	7 (21%)	24,82,82	1.40	5 (20%)
24	CLA	b	610	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	10 (13%)
24	CLA	c	503	-	65,73,73	1.66	7 (10%)	76,113,113	1.49	10 (13%)
24	CLA	c	505	-	65,73,73	1.52	8 (12%)	76,113,113	1.43	10 (13%)
24	CLA	c	512	-	65,73,73	1.49	8 (12%)	76,113,113	1.40	9 (11%)
24	CLA	D	403	-	65,73,73	1.49	13 (20%)	76,113,113	1.35	9 (11%)
25	PHO	A	407	-	51,69,69	1.08	5 (9%)	47,99,99	1.33	7 (14%)
24	CLA	c	507	36	65,73,73	1.46	11 (16%)	76,113,113	1.61	14 (18%)
27	PL9	A	410	-	55,55,55	1.39	4 (7%)	68,69,69	1.47	14 (20%)
28	SQD	A	411	-	51,52,54	1.02	4 (7%)	60,63,65	2.41	14 (23%)
24	CLA	D	402	36	65,73,73	1.66	9 (13%)	76,113,113	1.41	9 (11%)
24	CLA	c	508	-	64,72,73	1.60	9 (14%)	74,111,113	1.20	6 (8%)
24	CLA	C	509	-	65,73,73	1.67	8 (12%)	76,113,113	1.63	12 (15%)
26	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	7 (12%)
24	CLA	a	405	36	65,73,73	1.39	9 (13%)	76,113,113	1.34	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	DGD	c	518	-	63,63,67	1.09	4 (6%)	77,77,81	1.42	11 (14%)
28	SQD	f	101	-	40,41,54	1.14	5 (12%)	49,52,65	1.67	8 (16%)
34	HEM	e	102	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.43	7 (15%)
26	BCR	d	406	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
28	SQD	B	622	-	53,54,54	0.94	2 (3%)	62,65,65	1.85	13 (20%)
24	CLA	c	509	-	65,73,73	1.59	7 (10%)	76,113,113	1.56	12 (15%)
32	LMG	h	102	-	21,21,55	0.80	1 (4%)	20,20,63	1.01	1 (5%)
35	HEC	V	201	16	32,50,50	2.15	4 (12%)	24,82,82	1.29	2 (8%)
28	SQD	a	410	-	53,54,54	1.02	5 (9%)	62,65,65	2.02	13 (20%)
24	CLA	D	404	-	65,73,73	1.89	11 (16%)	76,113,113	1.02	5 (6%)
26	BCR	Y	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	4 (7%)
33	LHG	D	408	-	48,48,48	1.05	5 (10%)	51,54,54	1.25	5 (9%)
28	SQD	F	101	-	35,36,54	1.01	3 (8%)	42,45,65	1.85	12 (28%)
32	LMG	D	407	-	51,51,55	1.13	5 (9%)	59,59,63	1.24	4 (6%)
32	LMG	d	411	-	44,44,55	1.07	3 (6%)	52,52,63	1.35	5 (9%)
30	OEX	a	414	36,3,1	0,15,15	-	-	-		
24	CLA	c	501	-	65,73,73	1.63	10 (15%)	76,113,113	1.68	9 (11%)
24	CLA	A	408	-	54,62,73	1.76	11 (20%)	62,99,113	1.69	14 (22%)
25	PHO	d	402	-	51,69,69	1.11	6 (11%)	47,99,99	1.47	8 (17%)
24	CLA	B	604	-	65,73,73	1.64	8 (12%)	76,113,113	1.70	11 (14%)
33	LHG	d	408	-	48,48,48	0.71	0	51,54,54	1.22	5 (9%)
33	LHG	D	409	-	46,46,48	1.10	2 (4%)	49,52,54	1.40	7 (14%)
24	CLA	b	611	36	65,73,73	1.42	10 (15%)	76,113,113	1.47	14 (18%)
26	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.57	12 (21%)
24	CLA	b	605	-	65,73,73	1.55	9 (13%)	76,113,113	1.59	14 (18%)
28	SQD	a	411	-	35,35,54	1.10	2 (5%)	37,37,65	1.35	4 (10%)
24	CLA	a	407	-	65,73,73	1.71	11 (16%)	76,113,113	1.45	14 (18%)
24	CLA	c	511	3	65,73,73	1.98	8 (12%)	76,113,113	1.27	7 (9%)
24	CLA	A	406	36	65,73,73	1.44	12 (18%)	76,113,113	1.47	11 (14%)
24	CLA	B	609	-	65,73,73	1.61	10 (15%)	76,113,113	1.44	12 (15%)
32	LMG	c	519	-	37,37,55	1.10	3 (8%)	45,45,63	1.25	5 (11%)
24	CLA	c	502	-	65,73,73	1.48	8 (12%)	76,113,113	1.40	10 (13%)
24	CLA	b	604	-	65,73,73	1.53	11 (16%)	76,113,113	1.63	15 (19%)
26	BCR	b	619	-	41,41,41	1.26	2 (4%)	56,56,56	1.46	11 (19%)
24	CLA	b	617	-	60,68,73	1.73	12 (20%)	70,107,113	1.67	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	DGD	A	413	-	67,67,67	1.24	7 (10%)	81,81,81	1.49	10 (12%)
34	HEM	F	102	6,5	41,50,50	1.48	5 (12%)	45,82,82	1.28	4 (8%)
24	CLA	B	605	-	65,73,73	1.48	9 (13%)	76,113,113	1.57	13 (17%)
24	CLA	B	614	-	65,73,73	1.80	12 (18%)	76,113,113	1.24	6 (7%)
24	CLA	C	503	-	65,73,73	1.54	8 (12%)	76,113,113	1.62	11 (14%)
24	CLA	B	606	-	65,73,73	1.81	10 (15%)	76,113,113	1.46	10 (13%)
24	CLA	b	609	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	13 (17%)
32	LMG	B	621	-	26,26,55	0.80	1 (3%)	26,26,63	1.17	2 (7%)
26	BCR	c	521	-	41,41,41	0.95	2 (4%)	56,56,56	1.24	7 (12%)
30	OEX	A	414	36,3,1	0,15,15	-	-	-		
32	LMG	c	524	-	49,49,55	0.83	2 (4%)	57,57,63	1.36	4 (7%)
24	CLA	b	614	-	65,73,73	1.77	11 (16%)	76,113,113	1.47	12 (15%)
29	DGD	h	104	-	63,63,67	1.07	5 (7%)	77,77,81	1.39	8 (10%)
32	LMG	M	101	-	51,51,55	1.12	6 (11%)	59,59,63	1.58	14 (23%)
24	CLA	C	508	36	65,73,73	1.98	8 (12%)	76,113,113	1.45	7 (9%)
24	CLA	C	510	-	65,73,73	1.46	8 (12%)	76,113,113	1.30	7 (9%)
23	BCT	d	401	21	2,3,3	1.43	0	2,3,3	3.05	2 (100%)
26	BCR	a	408	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	8 (14%)
33	LHG	d	409	-	48,48,48	0.71	0	51,54,54	1.24	5 (9%)
24	CLA	A	405	-	65,73,73	1.50	10 (15%)	76,113,113	1.40	10 (13%)
33	LHG	d	410	-	38,38,48	0.78	2 (5%)	41,44,54	1.15	3 (7%)
27	PL9	d	407	-	55,55,55	1.40	5 (9%)	68,69,69	1.82	22 (32%)
24	CLA	b	608	36	65,73,73	1.37	7 (10%)	76,113,113	1.39	7 (9%)
26	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
29	DGD	C	518	-	63,63,67	1.06	4 (6%)	77,77,81	1.48	13 (16%)
27	PL9	a	409	-	55,55,55	1.11	4 (7%)	68,69,69	1.48	12 (17%)
26	BCR	t	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.39	8 (14%)
26	BCR	H	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
24	CLA	d	404	-	65,73,73	1.33	8 (12%)	76,113,113	1.42	9 (11%)
24	CLA	b	603	-	65,73,73	1.51	9 (13%)	76,113,113	1.67	12 (15%)
24	CLA	B	602	-	65,73,73	1.80	9 (13%)	76,113,113	1.39	12 (15%)
28	SQD	b	601	-	48,49,54	0.96	2 (4%)	57,60,65	2.00	13 (22%)
32	LMG	D	410	-	31,31,55	1.15	3 (9%)	33,33,63	1.08	0
24	CLA	b	606	-	65,73,73	1.53	8 (12%)	76,113,113	1.58	14 (18%)
24	CLA	b	616	-	65,73,73	1.78	11 (16%)	76,113,113	1.57	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	512	3	65,73,73	1.63	12 (18%)	76,113,113	1.58	8 (10%)
26	BCR	A	409	-	41,41,41	1.06	3 (7%)	56,56,56	1.30	7 (12%)
26	BCR	C	519	-	41,41,41	1.05	2 (4%)	56,56,56	1.38	9 (16%)
33	LHG	L	101	-	48,48,48	0.68	1 (2%)	51,54,54	1.17	3 (5%)
26	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.34	9 (16%)
24	CLA	B	601	36	65,73,73	1.98	9 (13%)	76,113,113	1.51	9 (11%)
24	CLA	c	510	-	65,73,73	1.63	7 (10%)	76,113,113	1.54	8 (10%)
24	CLA	B	616	-	60,68,73	1.79	12 (20%)	70,107,113	1.48	11 (15%)
24	CLA	b	613	-	65,73,73	1.56	7 (10%)	76,113,113	1.55	11 (14%)
26	BCR	c	515	-	41,41,41	1.35	4 (9%)	56,56,56	1.42	11 (19%)
25	PHO	a	406	-	51,69,69	1.15	5 (9%)	47,99,99	1.29	6 (12%)
29	DGD	C	517	-	63,63,67	1.15	6 (9%)	77,77,81	1.46	13 (16%)
33	LHG	l	101	-	48,48,48	0.84	1 (2%)	51,54,54	1.26	7 (13%)
29	DGD	C	516	-	63,63,67	1.19	6 (9%)	77,77,81	1.33	12 (15%)
32	LMG	C	501	-	48,48,55	0.90	1 (2%)	56,56,63	1.38	9 (16%)
24	CLA	h	101	36	65,73,73	1.80	11 (16%)	76,113,113	1.49	14 (18%)
24	CLA	b	612	-	65,73,73	1.71	11 (16%)	76,113,113	1.39	11 (14%)
25	PHO	D	401	-	51,69,69	1.13	5 (9%)	47,99,99	1.38	5 (10%)
24	CLA	C	502	-	65,73,73	1.90	11 (16%)	76,113,113	1.43	9 (11%)
26	BCR	D	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	3 (5%)
24	CLA	B	607	36	65,73,73	1.49	8 (12%)	76,113,113	1.48	11 (14%)
29	DGD	H	102	-	63,63,67	1.28	9 (14%)	77,77,81	1.45	9 (11%)
33	LHG	e	101	-	41,41,48	0.75	0	44,47,54	1.30	3 (6%)
32	LMG	b	623	-	55,55,55	0.95	5 (9%)	63,63,63	1.42	7 (11%)
24	CLA	B	612	-	65,73,73	1.31	6 (9%)	76,113,113	1.42	10 (13%)
24	CLA	c	513	-	65,73,73	1.57	9 (13%)	76,113,113	1.17	8 (10%)
24	CLA	c	504	36	60,68,73	1.59	10 (16%)	70,107,113	1.51	10 (14%)
24	CLA	B	613	-	65,73,73	1.73	12 (18%)	76,113,113	1.60	11 (14%)
24	CLA	C	507	-	65,73,73	1.72	9 (13%)	76,113,113	1.27	7 (9%)
24	CLA	d	403	36	65,73,73	1.57	9 (13%)	76,113,113	1.58	13 (17%)
26	BCR	B	617	-	41,41,41	1.20	3 (7%)	56,56,56	1.46	7 (12%)
32	LMG	b	621	-	51,51,55	0.82	0	59,59,63	1.52	10 (16%)
23	BCT	A	404	21	2,3,3	1.20	0	2,3,3	3.23	1 (50%)
26	BCR	B	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.51	12 (21%)
24	CLA	a	404	-	65,73,73	1.54	10 (15%)	76,113,113	1.59	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	607	-	65,73,73	2.03	9 (13%)	76,113,113	1.66	16 (21%)
24	CLA	d	405	-	65,73,73	1.83	9 (13%)	76,113,113	1.60	16 (21%)
24	CLA	C	513	-	65,73,73	1.48	10 (15%)	76,113,113	1.42	11 (14%)
26	BCR	C	515	-	41,41,41	1.41	4 (9%)	56,56,56	1.36	9 (16%)
24	CLA	B	615	-	65,73,73	1.63	11 (16%)	76,113,113	1.47	9 (11%)

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
32	LMG	c	522	-	-	24/43/63/70	0/1/1/1
29	DGD	c	517	-	-	15/51/91/95	0/2/2/2
24	CLA	C	514	-	1/1/20/20	10/37/115/115	-
24	CLA	C	504	-	1/1/20/20	5/37/115/115	-
24	CLA	C	506	-	1/1/20/20	11/37/115/115	-
26	BCR	b	618	-	-	6/29/63/63	0/2/2/2
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1
24	CLA	c	506	-	1/1/20/20	19/37/115/115	-
24	CLA	B	611	-	-	10/37/115/115	-
33	LHG	E	101	-	-	26/53/53/53	-
24	CLA	b	615	-	1/1/20/20	15/37/115/115	-
33	LHG	D	411	-	-	16/53/53/53	-
29	DGD	c	516	-	-	26/51/91/95	0/2/2/2
24	CLA	B	610	36	1/1/20/20	5/37/115/115	-
26	BCR	b	620	-	-	8/29/63/63	0/2/2/2
24	CLA	C	505	36	1/1/18/20	9/30/108/115	-
24	CLA	B	603	-	-	11/37/115/115	-
26	BCR	h	103	-	-	10/29/63/63	0/2/2/2
32	LMG	K	102	-	-	10/43/63/70	0/1/1/1
24	CLA	C	511	-	1/1/20/20	14/37/115/115	-
28	SQD	A	412	-	-	17/39/39/69	-
29	DGD	a	412	-	-	21/45/45/95	-
24	CLA	B	608	-	-	5/37/115/115	-
26	BCR	b	602	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEC	v	201	16	-	2/10/54/54	-
24	CLA	b	610	-	1/1/20/20	12/37/115/115	-
24	CLA	c	503	-	1/1/20/20	8/37/115/115	-
24	CLA	c	505	-	1/1/20/20	9/37/115/115	-
24	CLA	c	512	-	1/1/20/20	20/37/115/115	-
24	CLA	D	403	-	1/1/20/20	7/37/115/115	-
25	PHO	A	407	-	-	6/37/103/103	0/5/6/6
24	CLA	c	507	36	1/1/20/20	9/37/115/115	-
27	PL9	A	410	-	-	24/53/73/73	0/1/1/1
28	SQD	A	411	-	-	23/47/67/69	0/1/1/1
24	CLA	D	402	36	1/1/20/20	3/37/115/115	-
24	CLA	c	508	-	-	9/36/114/115	-
24	CLA	C	509	-	-	11/37/115/115	-
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
24	CLA	a	405	36	-	13/37/115/115	-
29	DGD	c	518	-	-	16/51/91/95	0/2/2/2
28	SQD	f	101	-	-	18/36/56/69	0/1/1/1
34	HEM	e	102	6,5	-	4/12/54/54	-
26	BCR	d	406	-	-	11/29/63/63	0/2/2/2
28	SQD	B	622	-	-	22/49/69/69	0/1/1/1
24	CLA	c	509	-	1/1/20/20	16/37/115/115	-
32	LMG	h	102	-	-	13/17/17/70	-
35	HEC	V	201	16	-	2/10/54/54	-
28	SQD	a	410	-	-	23/49/69/69	0/1/1/1
24	CLA	D	404	-	-	10/37/115/115	-
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	LHG	D	408	-	-	21/53/53/53	-
28	SQD	F	101	-	-	13/28/48/69	0/1/1/1
32	LMG	D	407	-	-	17/46/66/70	0/1/1/1
32	LMG	d	411	-	-	11/39/59/70	0/1/1/1
24	CLA	c	501	-	1/1/20/20	6/37/115/115	-
24	CLA	A	408	-	1/1/17/20	4/24/102/115	-
25	PHO	d	402	-	-	6/37/103/103	0/5/6/6
24	CLA	B	604	-	1/1/20/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	d	408	-	-	21/53/53/53	-
33	LHG	D	409	-	-	25/51/51/53	-
24	CLA	b	611	36	1/1/20/20	9/37/115/115	-
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/20/20	11/37/115/115	-
28	SQD	a	411	-	-	23/37/37/69	-
24	CLA	a	407	-	1/1/20/20	8/37/115/115	-
24	CLA	c	511	3	1/1/20/20	6/37/115/115	-
24	CLA	A	406	36	1/1/20/20	6/37/115/115	-
24	CLA	B	609	-	-	5/37/115/115	-
32	LMG	c	519	-	-	13/31/51/70	0/1/1/1
24	CLA	c	502	-	1/1/20/20	4/37/115/115	-
24	CLA	b	604	-	1/1/20/20	8/37/115/115	-
26	BCR	b	619	-	-	5/29/63/63	0/2/2/2
24	CLA	b	617	-	1/1/19/20	8/31/109/115	-
29	DGD	A	413	-	-	25/55/95/95	0/2/2/2
34	HEM	F	102	6,5	-	2/12/54/54	-
24	CLA	B	605	-	1/1/20/20	12/37/115/115	-
24	CLA	B	614	-	1/1/20/20	11/37/115/115	-
24	CLA	C	503	-	1/1/20/20	13/37/115/115	-
24	CLA	B	606	-	1/1/20/20	6/37/115/115	-
24	CLA	b	609	-	1/1/20/20	5/37/115/115	-
32	LMG	B	621	-	-	8/22/22/70	-
26	BCR	c	521	-	-	14/29/63/63	0/2/2/2
32	LMG	c	524	-	-	25/44/64/70	0/1/1/1
24	CLA	b	614	-	1/1/20/20	7/37/115/115	-
29	DGD	h	104	-	-	18/51/91/95	0/2/2/2
32	LMG	M	101	-	-	21/46/66/70	0/1/1/1
24	CLA	C	508	36	1/1/20/20	7/37/115/115	-
24	CLA	C	510	-	1/1/20/20	10/37/115/115	-
26	BCR	a	408	-	-	3/29/63/63	0/2/2/2
33	LHG	d	409	-	-	18/53/53/53	-
24	CLA	A	405	-	1/1/20/20	3/37/115/115	-
33	LHG	d	410	-	-	11/43/43/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	d	407	-	-	17/53/73/73	0/1/1/1
24	CLA	b	608	36	1/1/20/20	14/37/115/115	-
26	BCR	k	101	-	-	10/29/63/63	0/2/2/2
29	DGD	C	518	-	-	14/51/91/95	0/2/2/2
27	PL9	a	409	-	-	22/53/73/73	0/1/1/1
26	BCR	t	101	-	-	12/29/63/63	0/2/2/2
26	BCR	H	101	-	-	7/29/63/63	0/2/2/2
24	CLA	d	404	-	1/1/20/20	7/37/115/115	-
24	CLA	b	603	-	1/1/20/20	9/37/115/115	-
24	CLA	B	602	-	1/1/20/20	6/37/115/115	-
28	SQD	b	601	-	-	21/44/64/69	0/1/1/1
32	LMG	D	410	-	-	19/33/33/70	-
24	CLA	b	606	-	1/1/20/20	10/37/115/115	-
24	CLA	b	616	-	1/1/20/20	9/37/115/115	-
24	CLA	C	512	3	1/1/20/20	10/37/115/115	-
26	BCR	A	409	-	-	8/29/63/63	0/2/2/2
26	BCR	C	519	-	-	11/29/63/63	0/2/2/2
33	LHG	L	101	-	-	22/53/53/53	-
26	BCR	c	514	-	-	10/29/63/63	0/2/2/2
24	CLA	B	601	36	1/1/20/20	12/37/115/115	-
24	CLA	c	510	-	1/1/20/20	17/37/115/115	-
24	CLA	B	616	-	1/1/19/20	10/31/109/115	-
24	CLA	b	613	-	1/1/20/20	5/37/115/115	-
26	BCR	c	515	-	-	8/29/63/63	0/2/2/2
25	PHO	a	406	-	-	3/37/103/103	0/5/6/6
29	DGD	C	517	-	-	20/51/91/95	0/2/2/2
33	LHG	l	101	-	-	18/53/53/53	-
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
32	LMG	C	501	-	-	24/43/63/70	0/1/1/1
24	CLA	h	101	36	1/1/20/20	19/37/115/115	-
24	CLA	b	612	-	1/1/20/20	7/37/115/115	-
25	PHO	D	401	-	-	2/37/103/103	0/5/6/6
24	CLA	C	502	-	1/1/20/20	2/37/115/115	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607	36	1/1/20/20	12/37/115/115	-
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
33	LHG	e	101	-	-	29/46/46/53	-
32	LMG	b	623	-	-	18/50/70/70	0/1/1/1
24	CLA	B	612	-	1/1/20/20	14/37/115/115	-
24	CLA	c	513	-	1/1/20/20	11/37/115/115	-
24	CLA	c	504	36	1/1/19/20	8/31/109/115	-
24	CLA	B	613	-	1/1/20/20	11/37/115/115	-
24	CLA	d	403	36	1/1/20/20	3/37/115/115	-
24	CLA	C	507	-	-	13/37/115/115	-
26	BCR	B	617	-	-	5/29/63/63	0/2/2/2
32	LMG	b	621	-	-	21/46/66/70	0/1/1/1
26	BCR	B	619	-	-	7/29/63/63	0/2/2/2
24	CLA	a	404	-	1/1/20/20	6/37/115/115	-
24	CLA	b	607	-	1/1/20/20	11/37/115/115	-
24	CLA	d	405	-	1/1/20/20	4/37/115/115	-
24	CLA	C	513	-	1/1/20/20	12/37/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/20/20	11/37/115/115	-

The worst 5 of 917 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	MG-ND	-12.77	1.80	2.05
24	C	508	CLA	MG-NA	10.07	2.30	2.06
24	b	607	CLA	MG-NA	9.96	2.29	2.06
24	B	602	CLA	C4B-NB	9.47	1.43	1.35
24	c	511	CLA	C4B-NB	9.25	1.43	1.35

The worst 5 of 1337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	411	SQD	O6-C1-C2	9.52	123.17	108.30
28	A	411	SQD	O7-S-C6	9.51	118.24	106.94
28	a	410	SQD	O6-C1-C2	9.15	122.59	108.30
24	b	607	CLA	C4A-NA-C1A	8.45	110.51	106.71
24	a	404	CLA	C4A-NA-C1A	8.42	110.49	106.71

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND

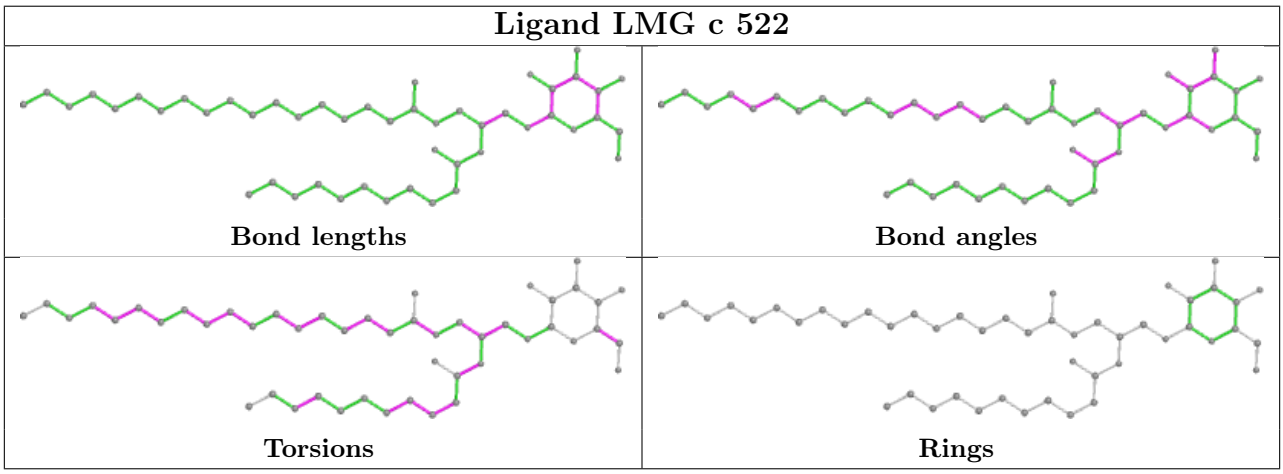
5 of 1710 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	408	CLA	C2-C3-C5-C6
24	A	408	CLA	C4-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	616	CLA	CBD-CGD-O2D-CED

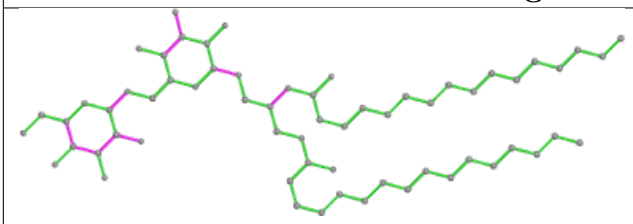
There are no ring outliers.

No monomer is involved in short contacts.

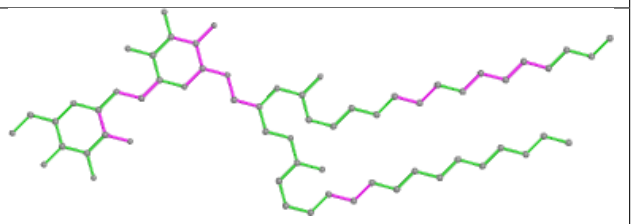
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



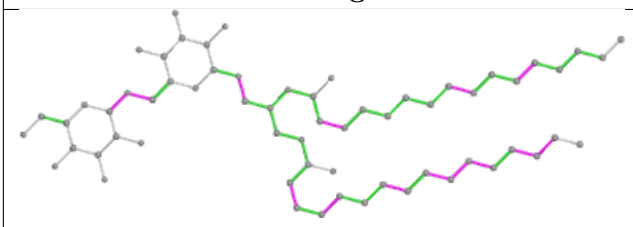
Ligand DGD c 517



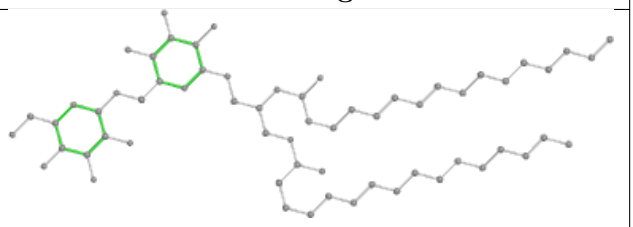
Bond lengths



Bond angles

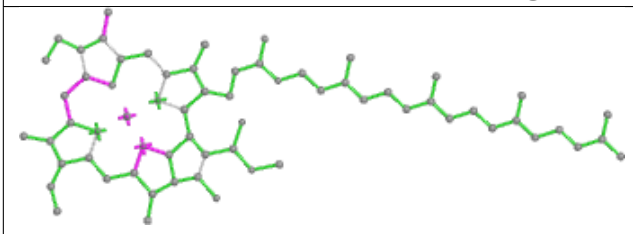


Torsions

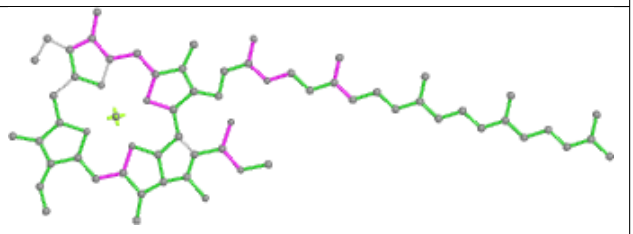


Rings

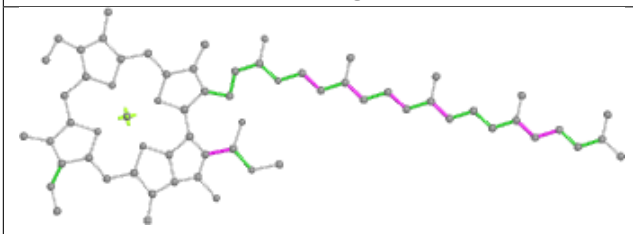
Ligand CLA C 514



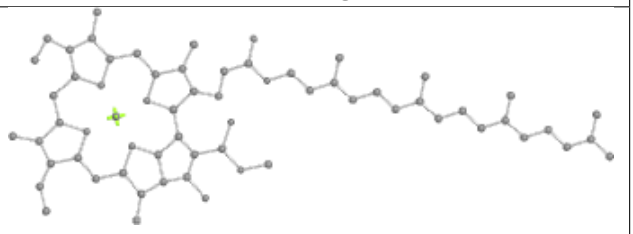
Bond lengths



Bond angles

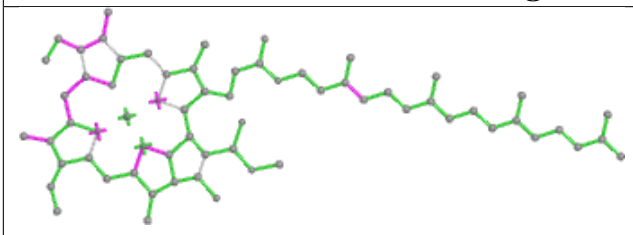


Torsions

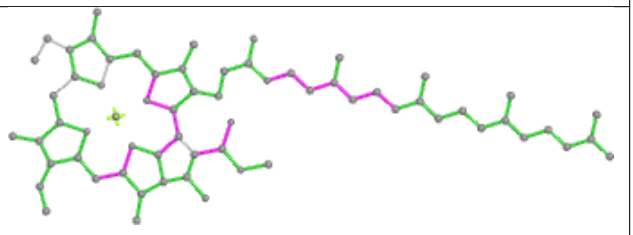


Rings

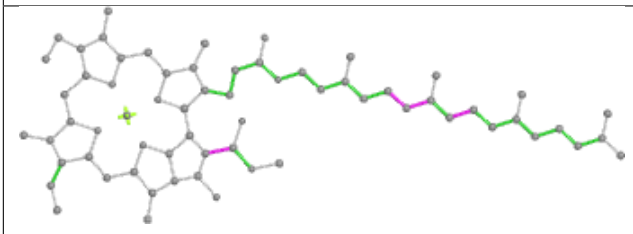
Ligand CLA C 504



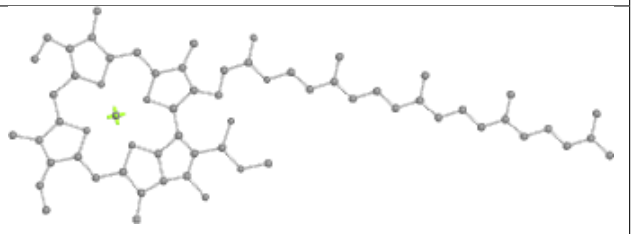
Bond lengths



Bond angles

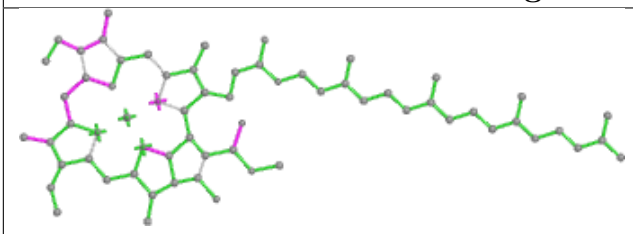


Torsions

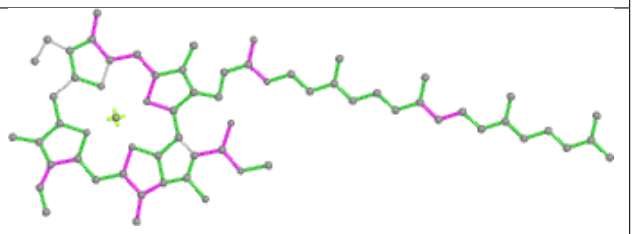


Rings

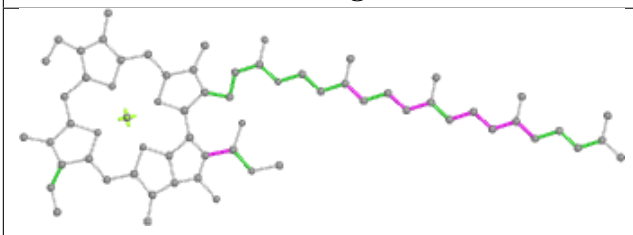
Ligand CLA C 506



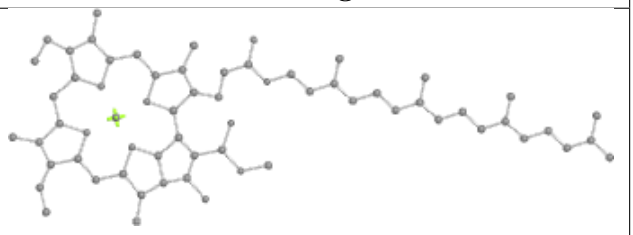
Bond lengths



Bond angles

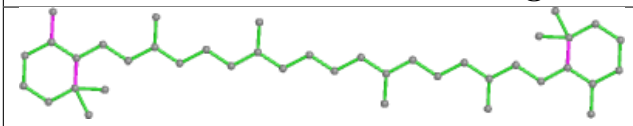


Torsions

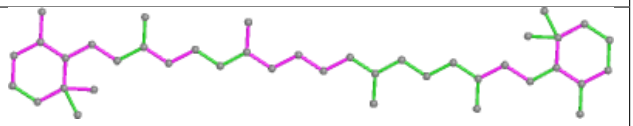


Rings

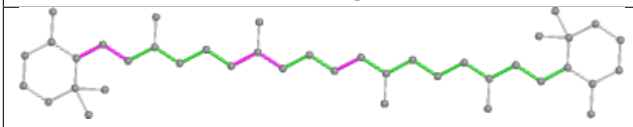
Ligand BCR b 618



Bond lengths



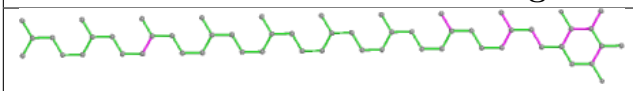
Bond angles



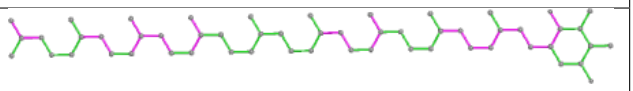
Torsions

Rings

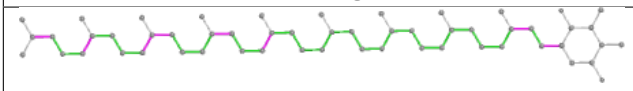
Ligand PL9 D 406



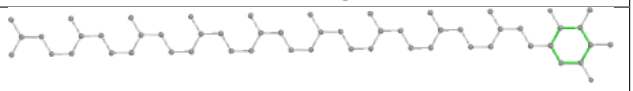
Bond lengths



Bond angles

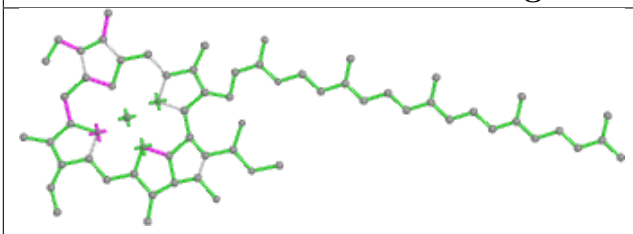


Torsions

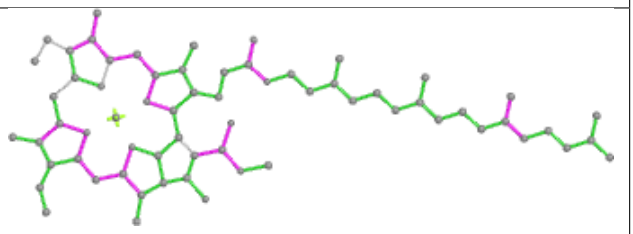


Rings

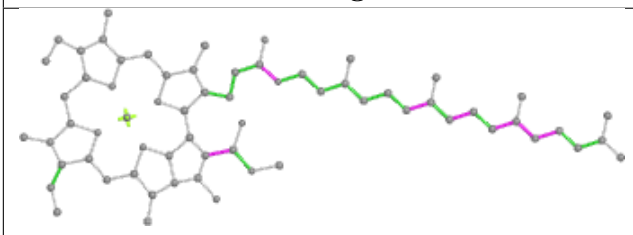
Ligand CLA B 611



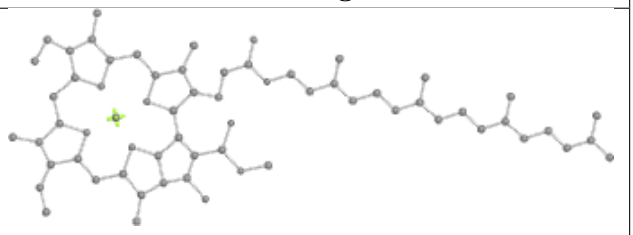
Bond lengths



Bond angles

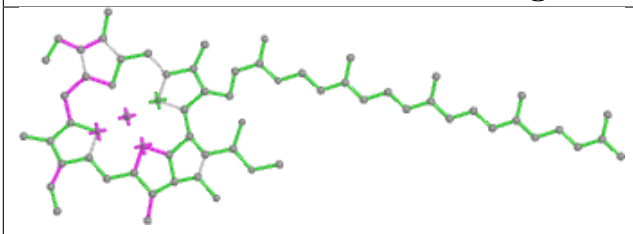


Torsions

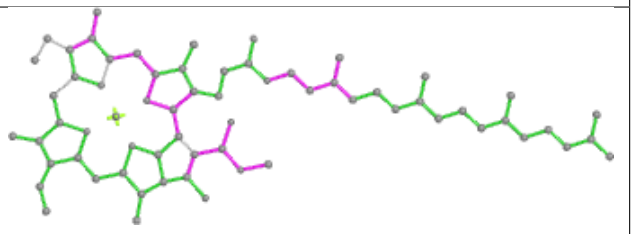


Rings

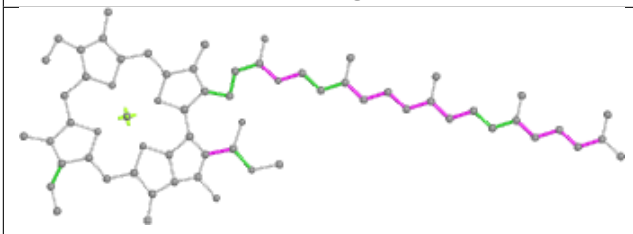
Ligand CLA c 506



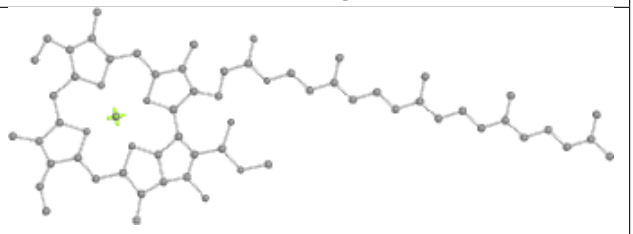
Bond lengths



Bond angles

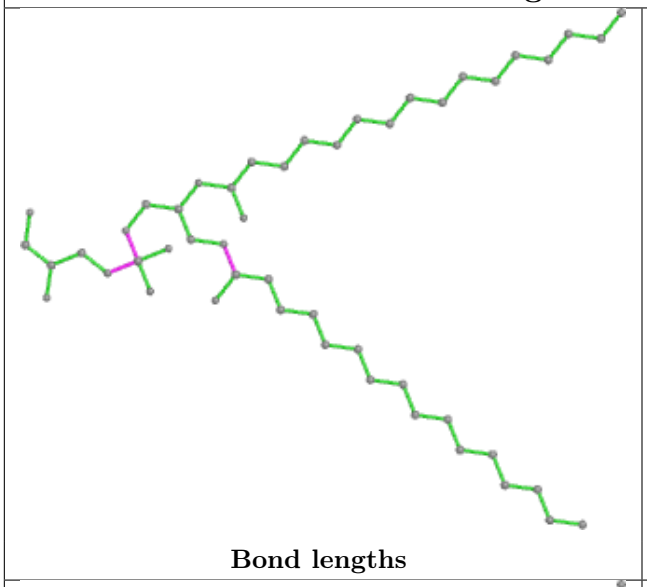


Torsions

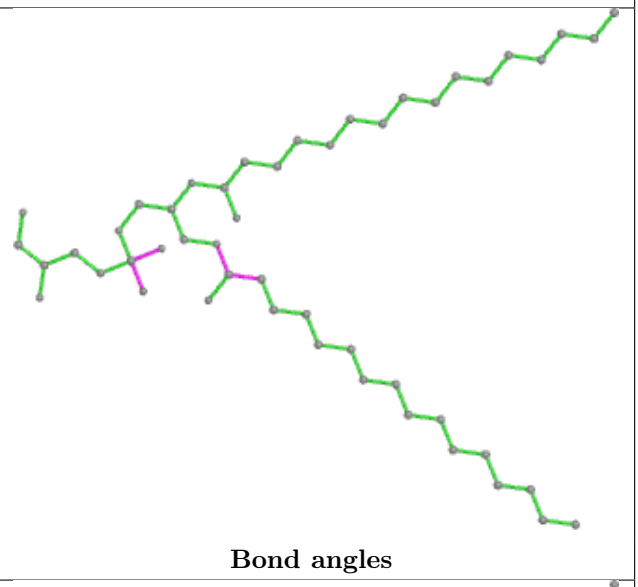


Rings

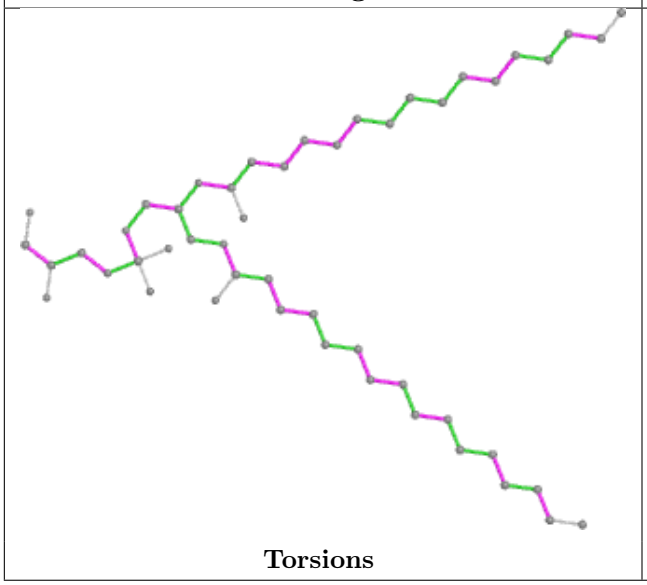
Ligand LHG E 101



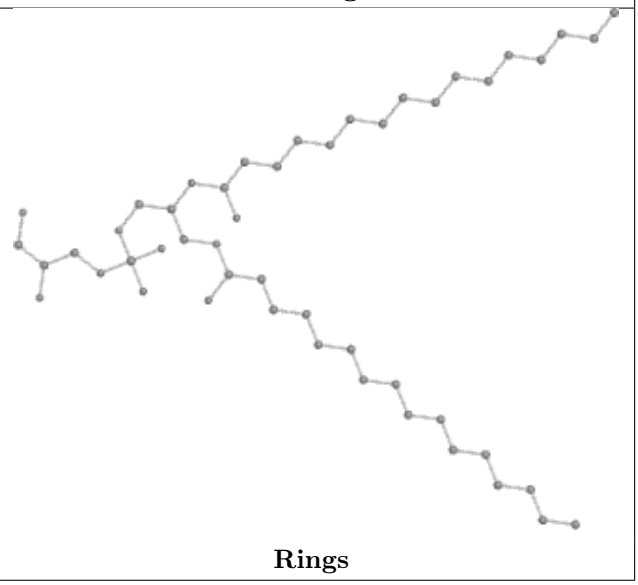
Bond lengths



Bond angles

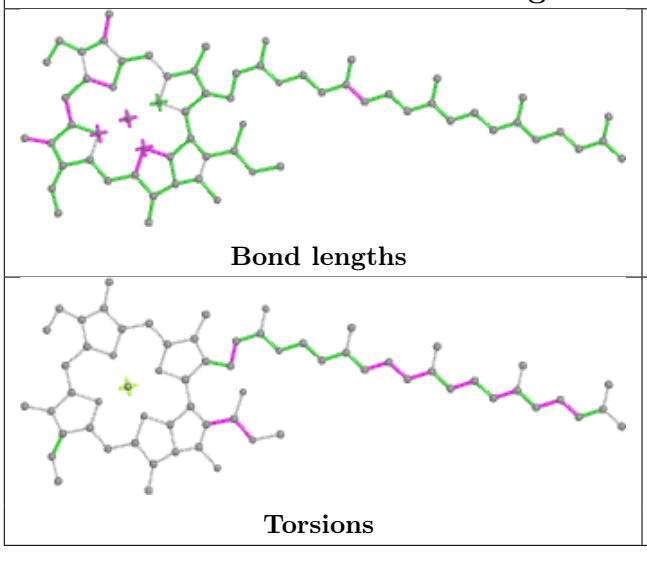


Torsions

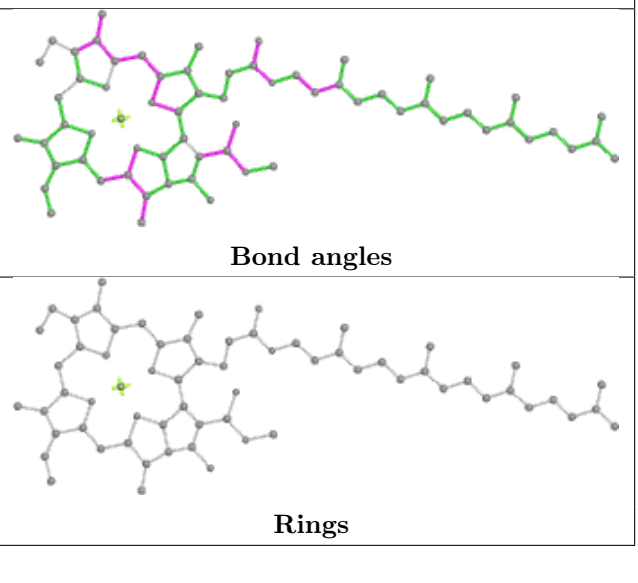


Rings

Ligand CLA b 615



Bond lengths

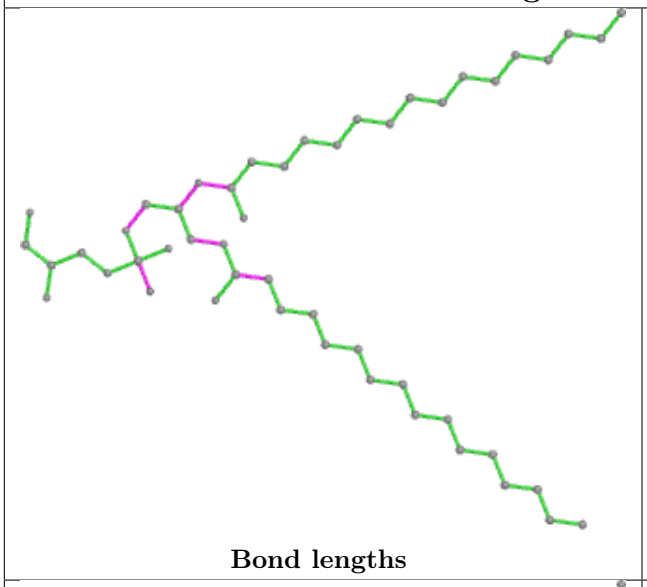


Bond angles

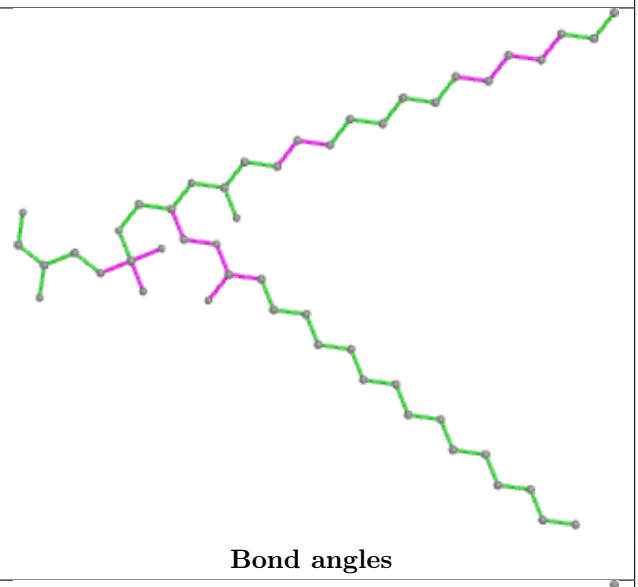
Torsions

Rings

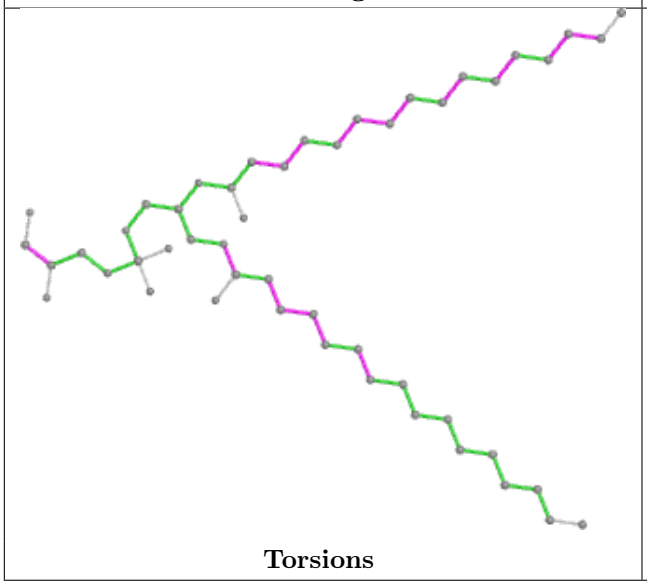
Ligand LHG D 411



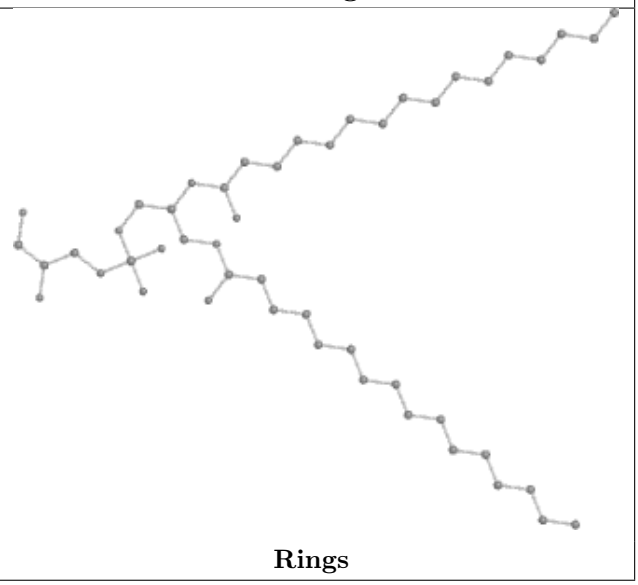
Bond lengths



Bond angles

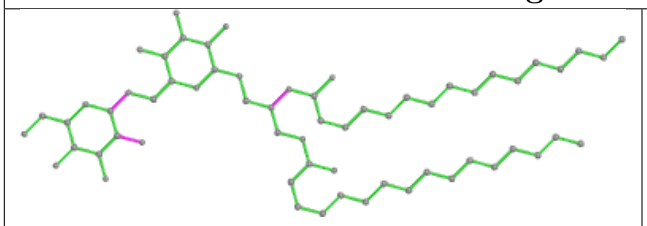


Torsions

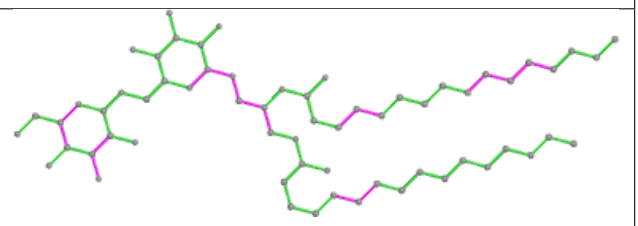


Rings

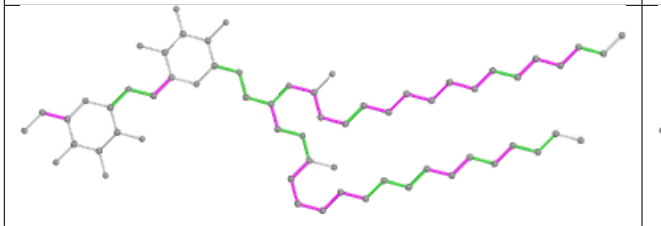
Ligand DGD c 516



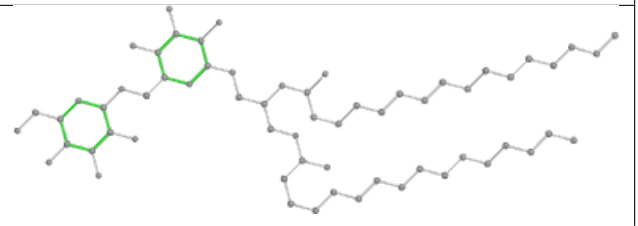
Bond lengths



Bond angles

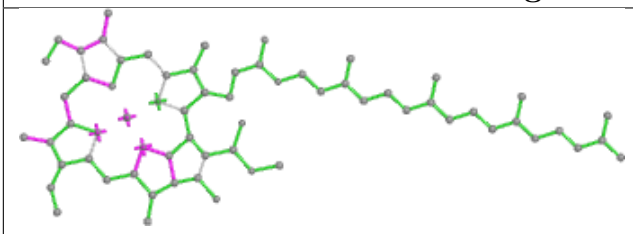


Torsions

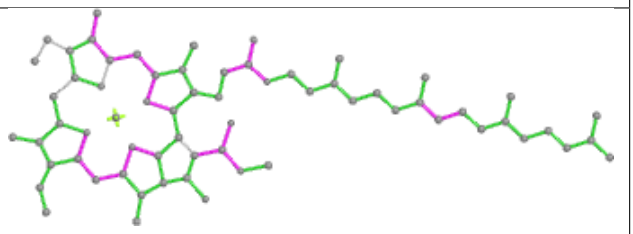


Rings

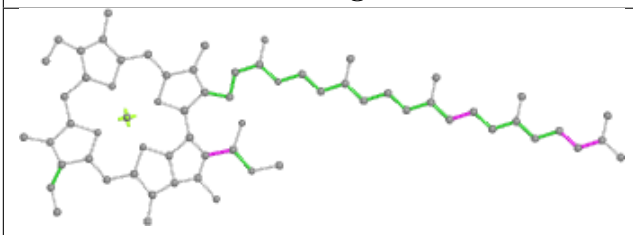
Ligand CLA B 610



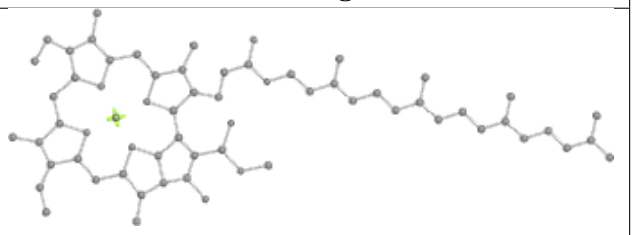
Bond lengths



Bond angles

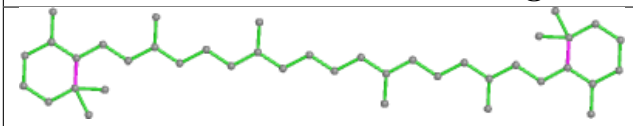


Torsions

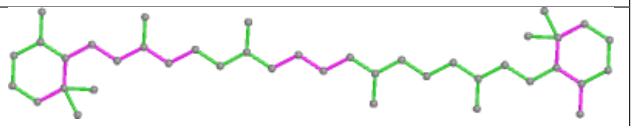


Rings

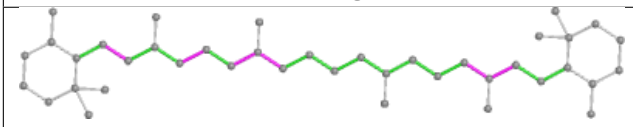
Ligand BCR b 620



Bond lengths



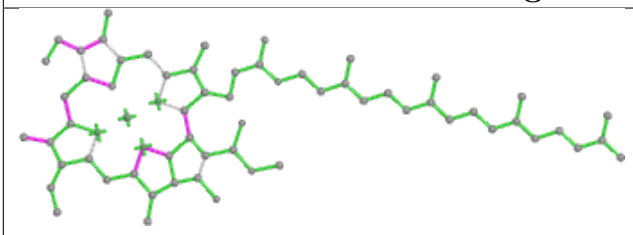
Bond angles



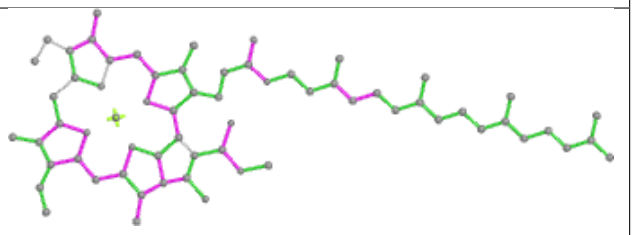
Torsions

Rings

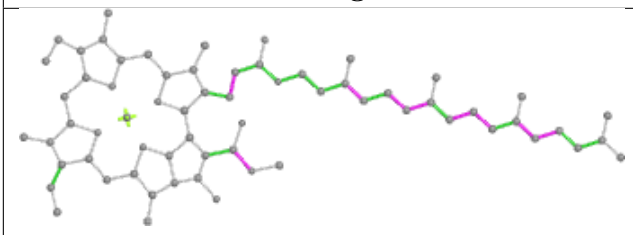
Ligand CLA B 603



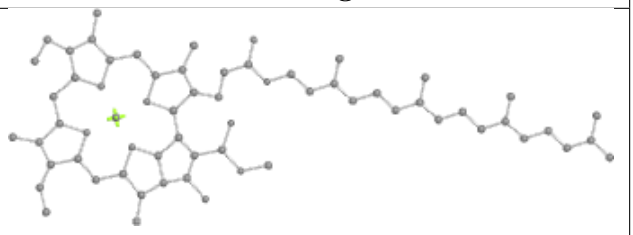
Bond lengths



Bond angles

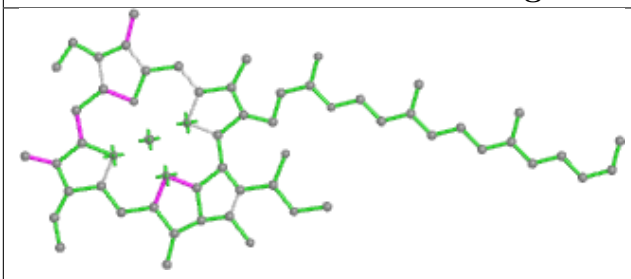


Torsions

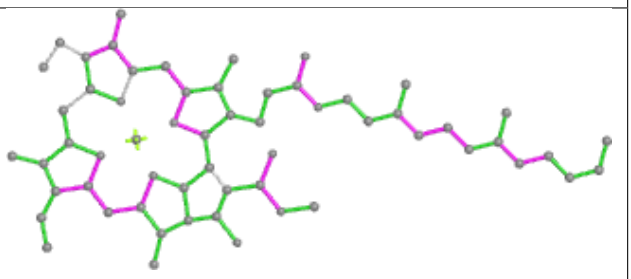


Rings

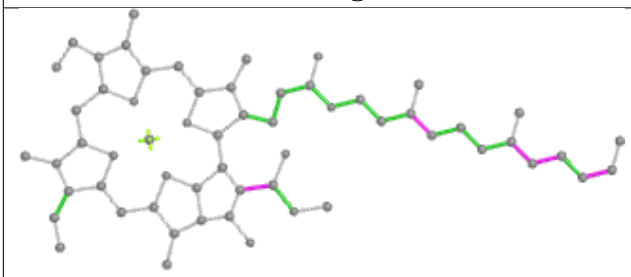
Ligand CLA C 505



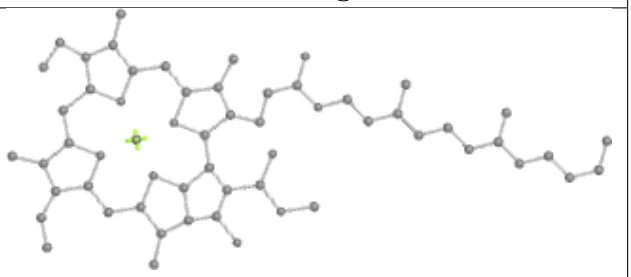
Bond lengths



Bond angles

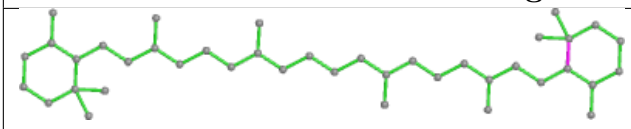


Torsions

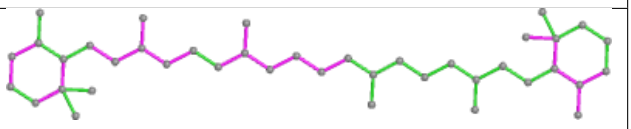


Rings

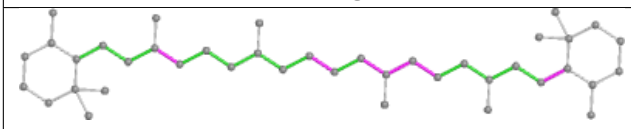
Ligand BCR h 103



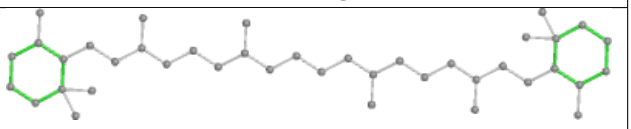
Bond lengths



Bond angles

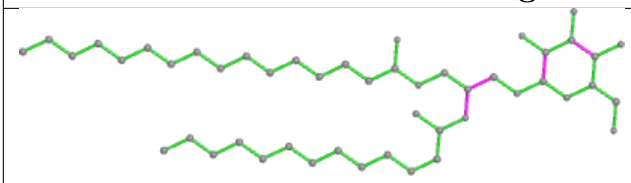


Torsions

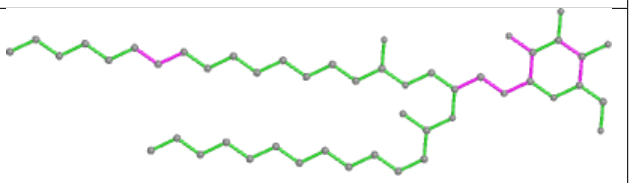


Rings

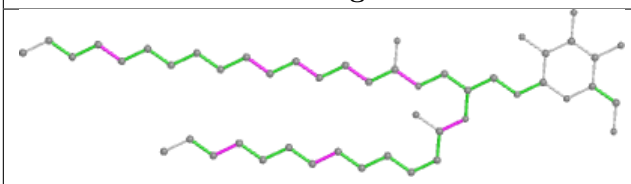
Ligand LMG K 102



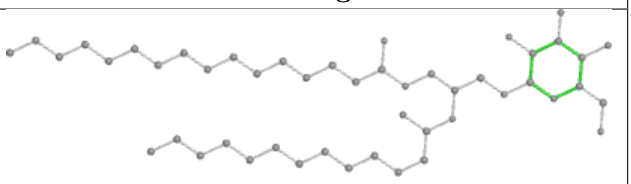
Bond lengths



Bond angles

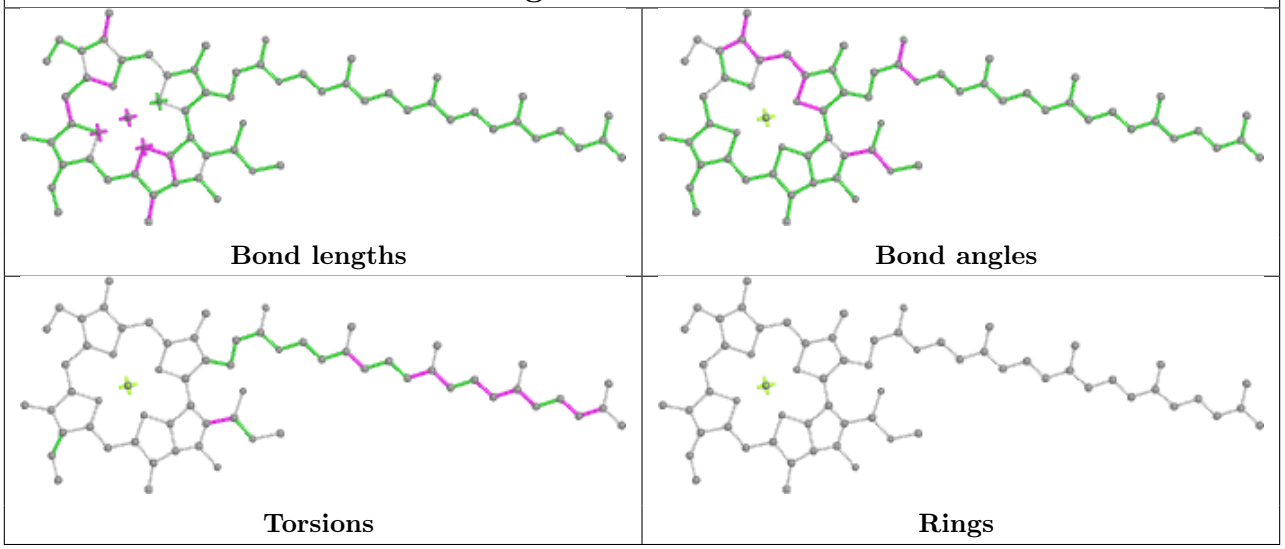


Torsions

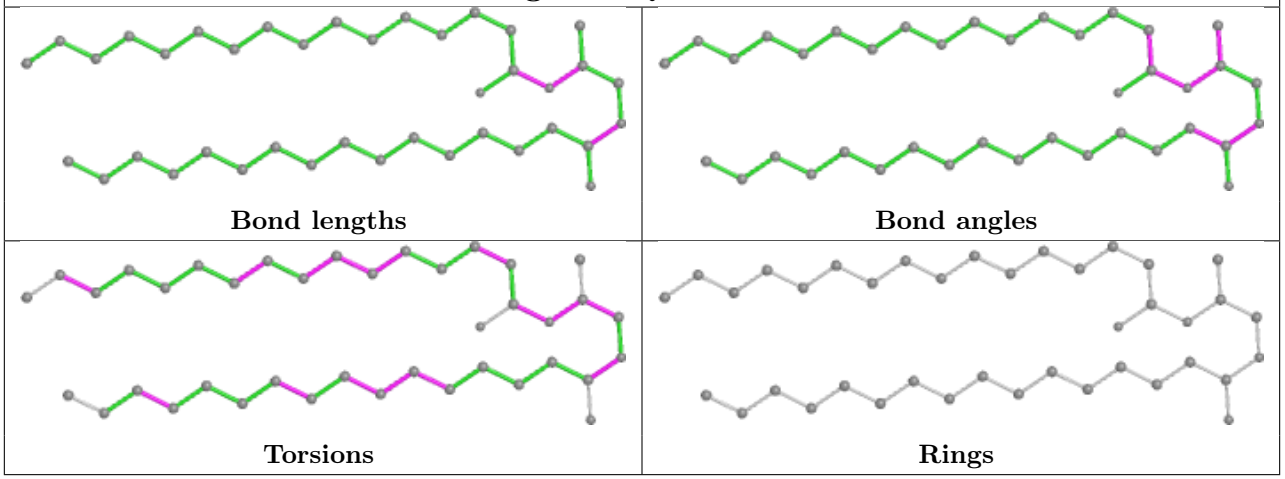


Rings

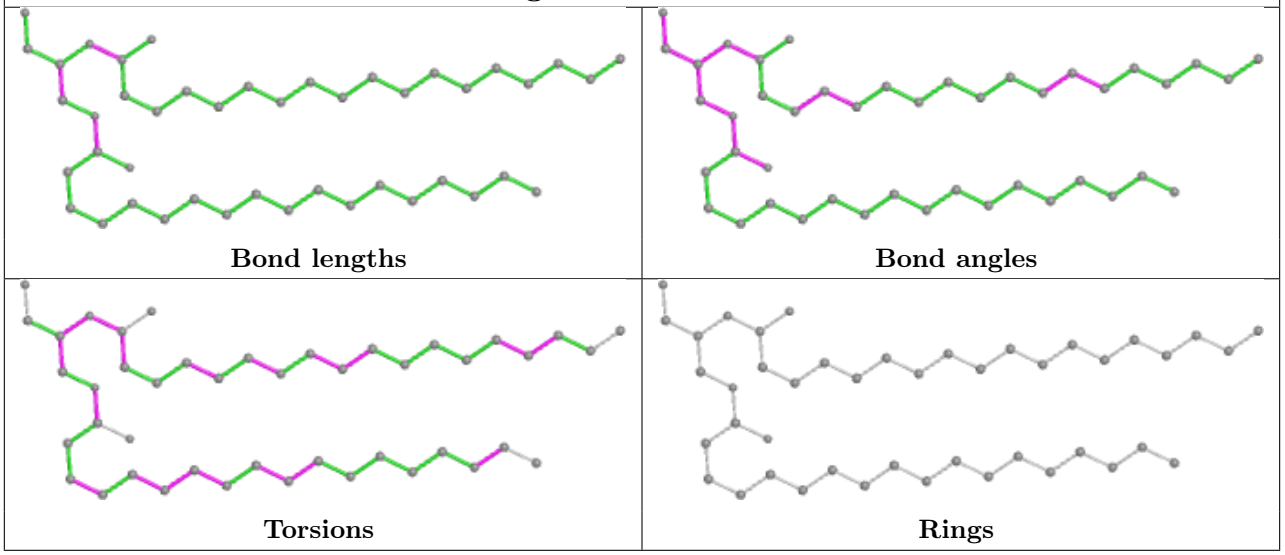
Ligand CLA C 511



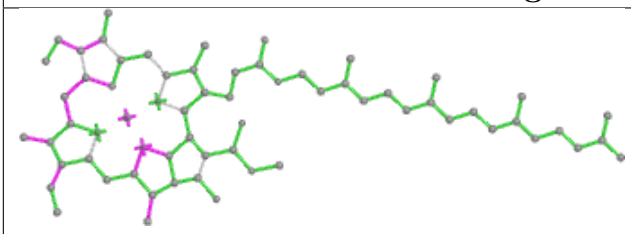
Ligand SQD A 412



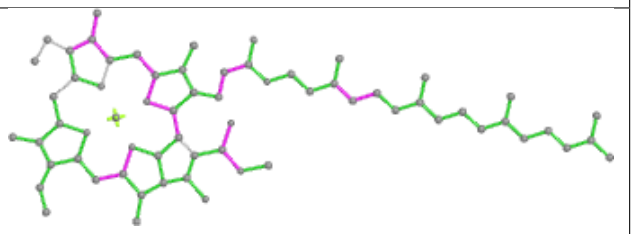
Ligand DGD a 412



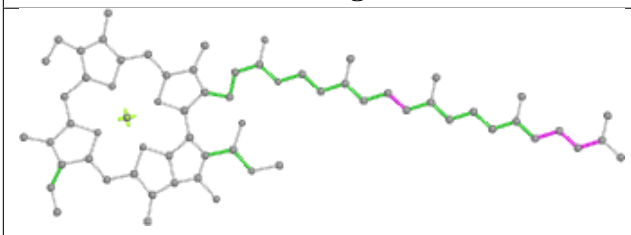
Ligand CLA B 608



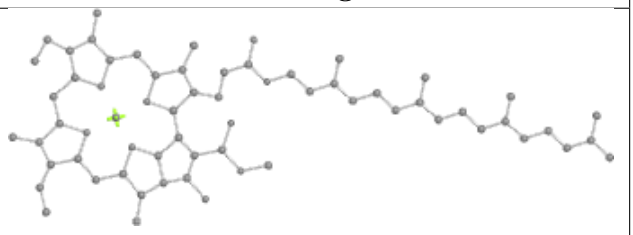
Bond lengths



Bond angles

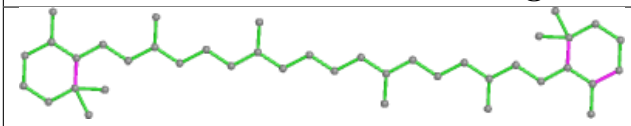


Torsions

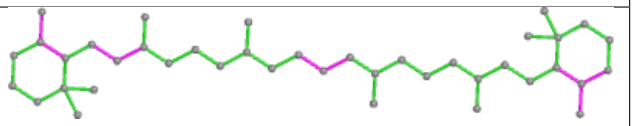


Rings

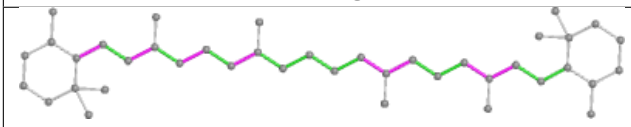
Ligand BCR b 602



Bond lengths



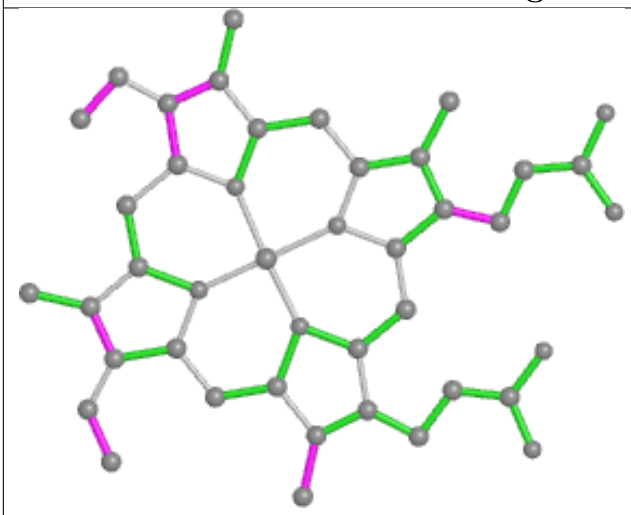
Bond angles



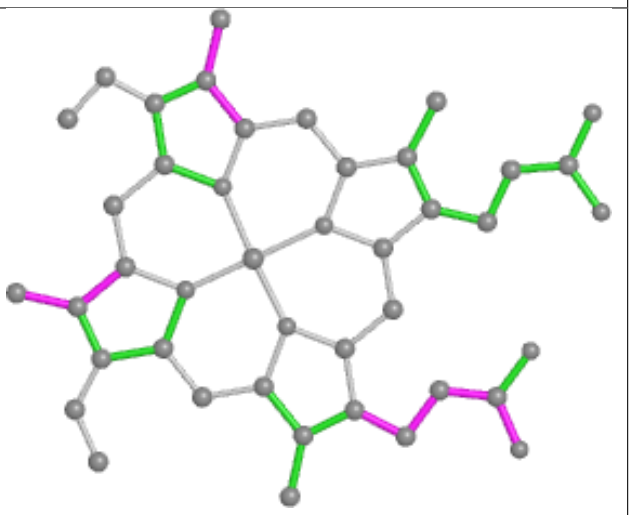
Torsions

Rings

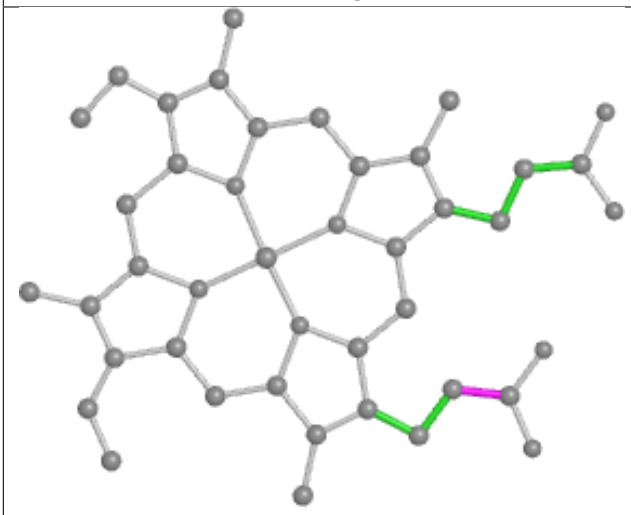
Ligand HEC v 201



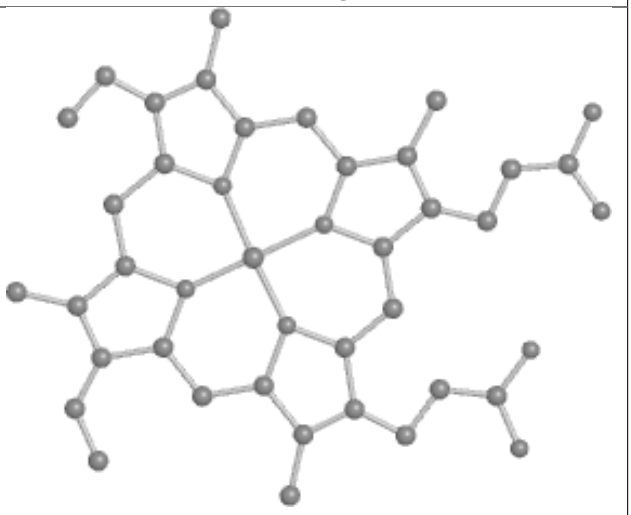
Bond lengths



Bond angles

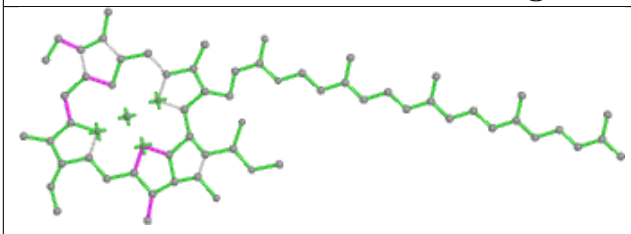


Torsions

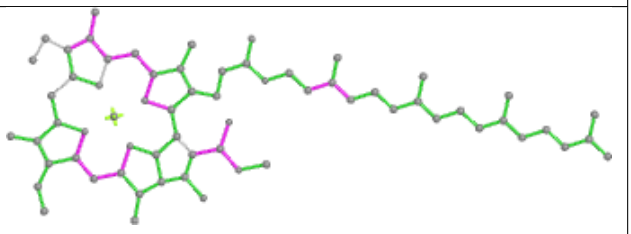


Rings

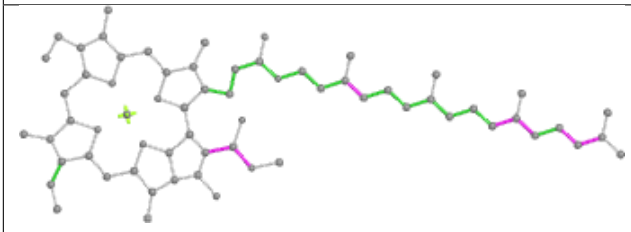
Ligand CLA b 610



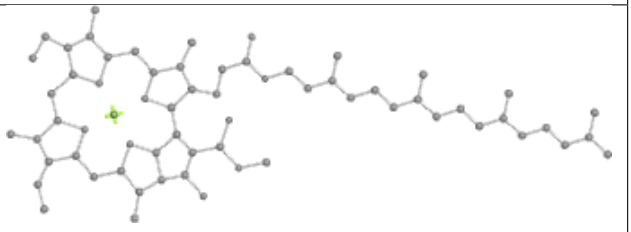
Bond lengths



Bond angles

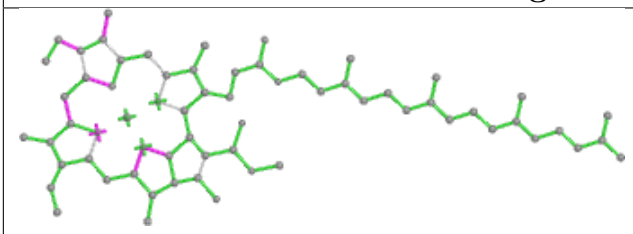


Torsions

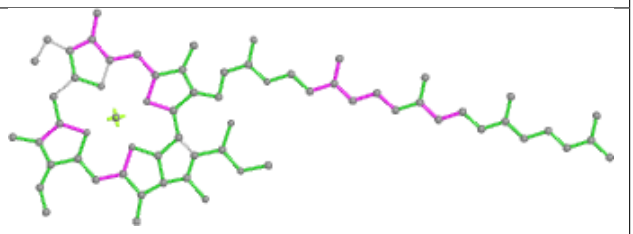


Rings

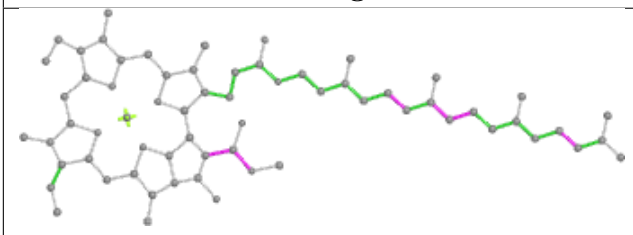
Ligand CLA c 503



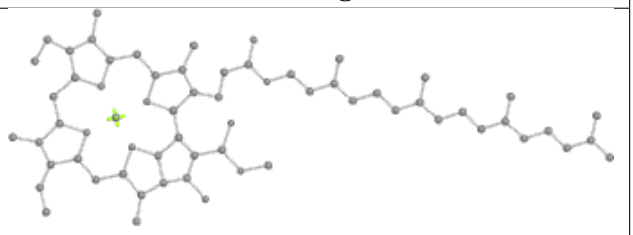
Bond lengths



Bond angles

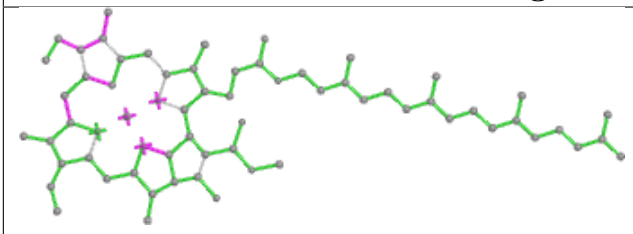


Torsions

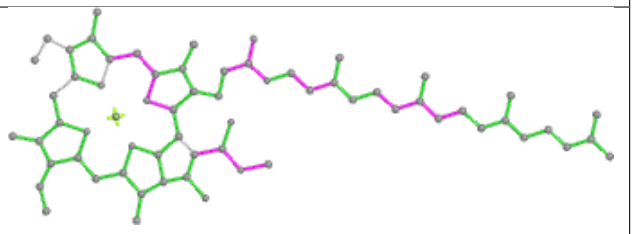


Rings

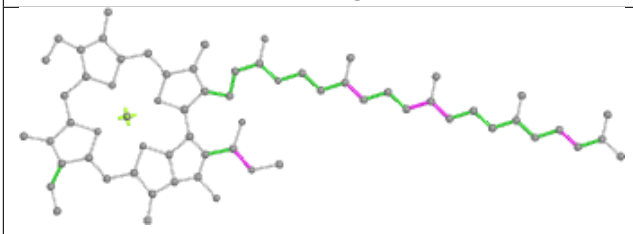
Ligand CLA c 505



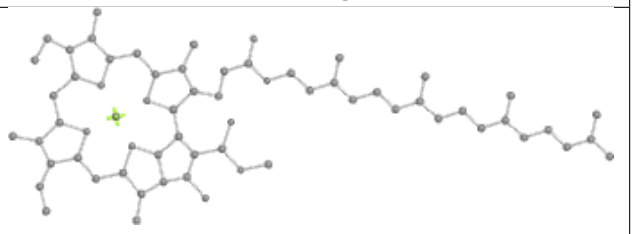
Bond lengths



Bond angles

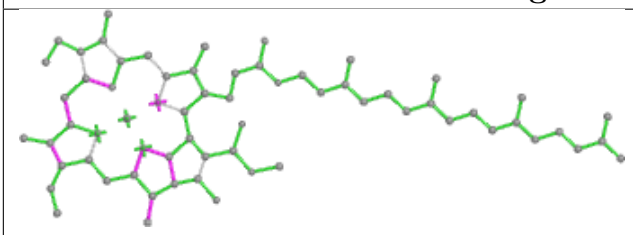


Torsions

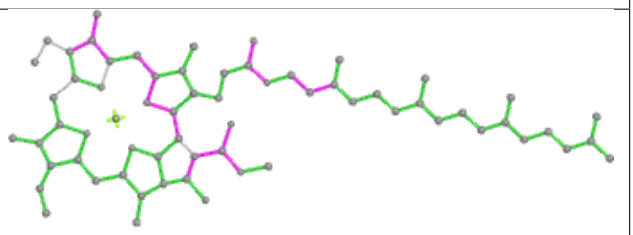


Rings

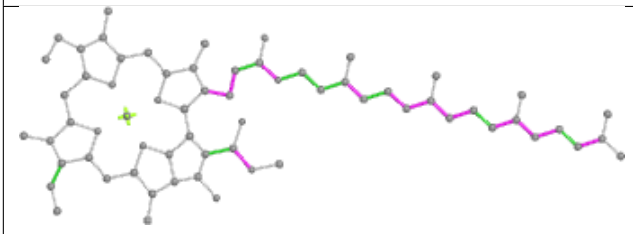
Ligand CLA c 512



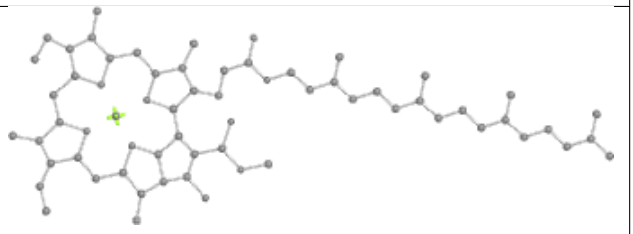
Bond lengths



Bond angles

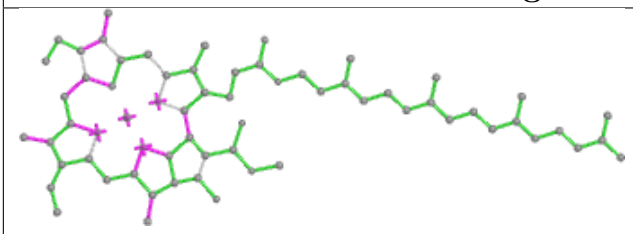


Torsions

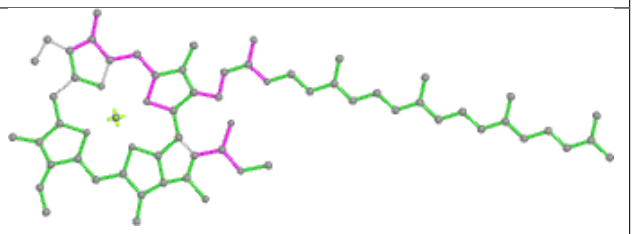


Rings

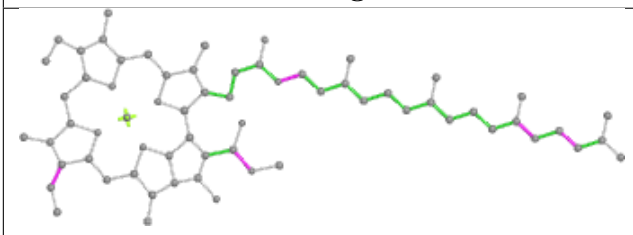
Ligand CLA D 403



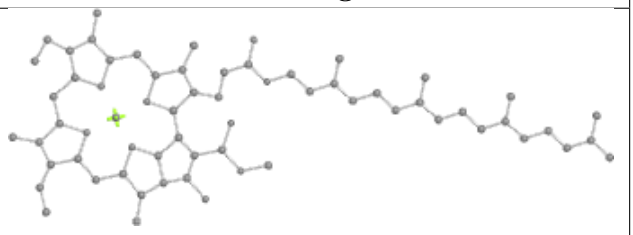
Bond lengths



Bond angles

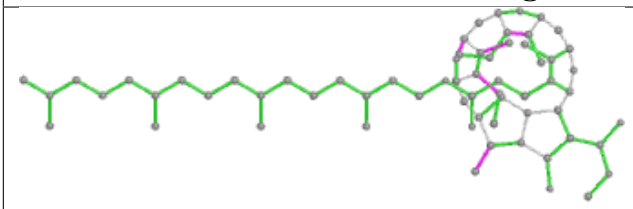


Torsions

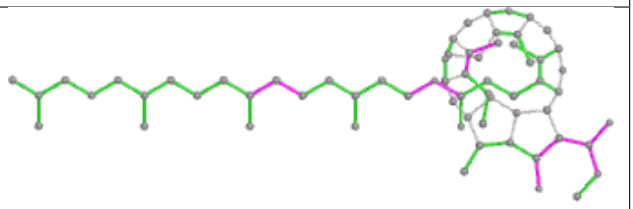


Rings

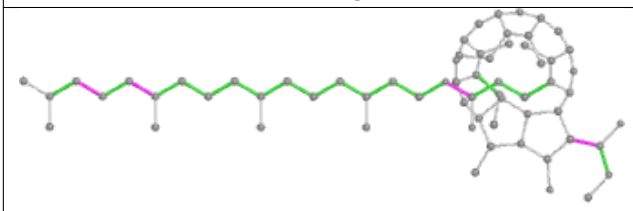
Ligand PHO A 407



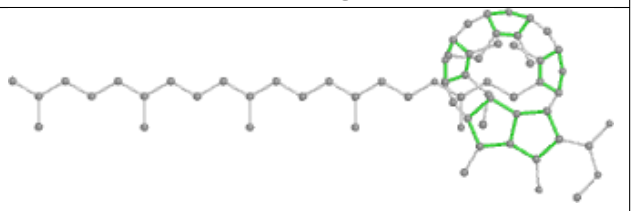
Bond lengths



Bond angles

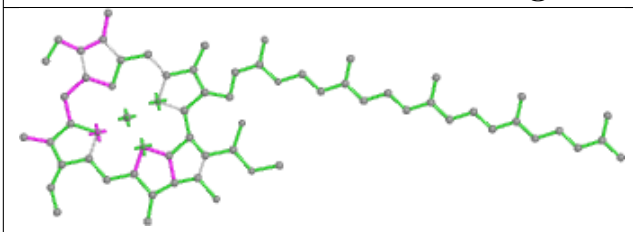


Torsions

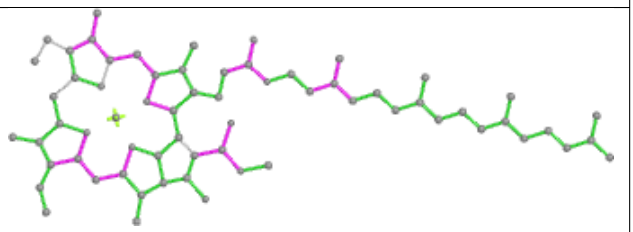


Rings

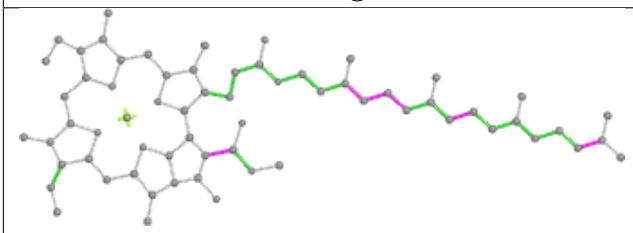
Ligand CLA c 507



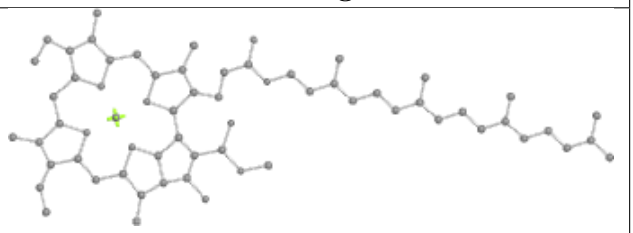
Bond lengths



Bond angles

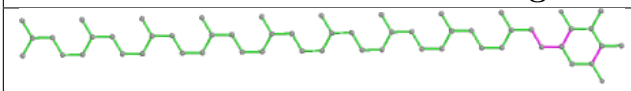


Torsions

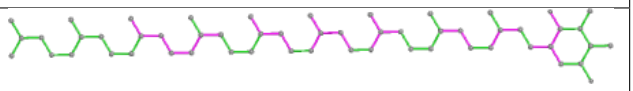


Rings

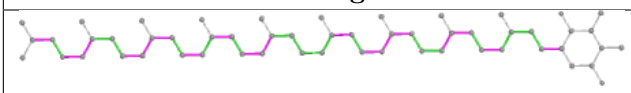
Ligand PL9 A 410



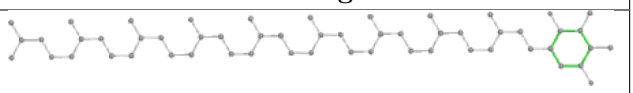
Bond lengths



Bond angles

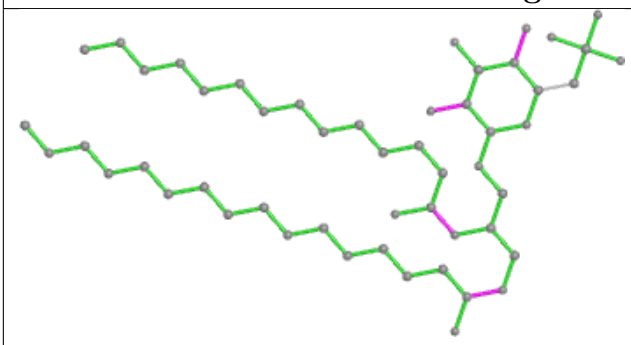


Torsions

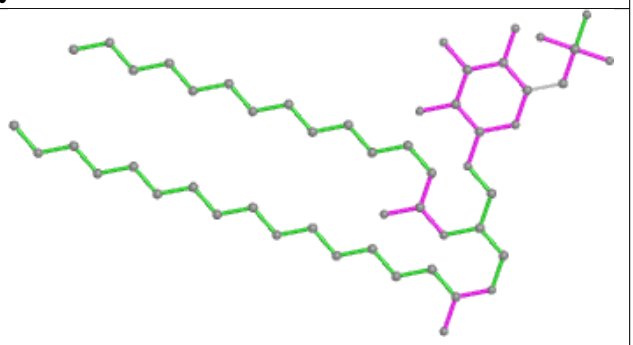


Rings

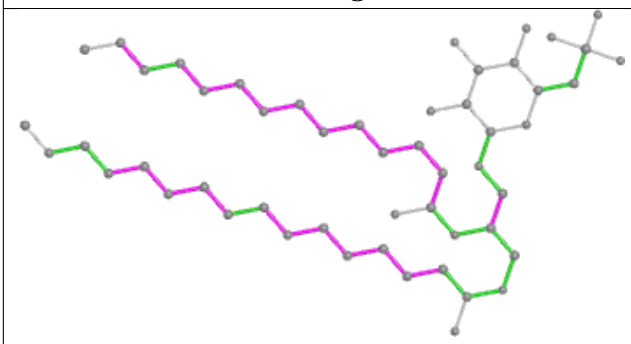
Ligand SQD A 411



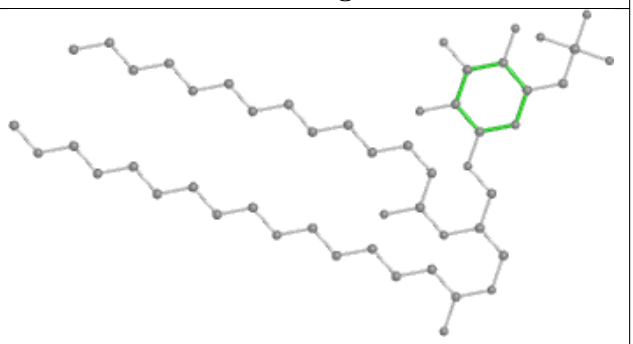
Bond lengths



Bond angles

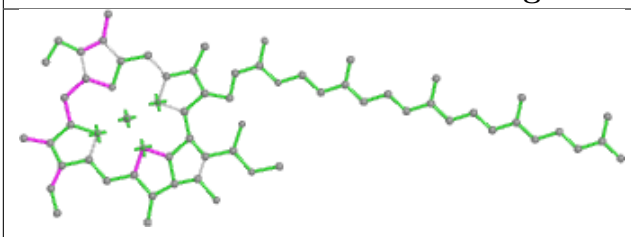


Torsions

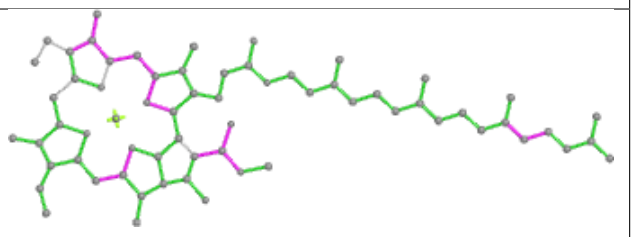


Rings

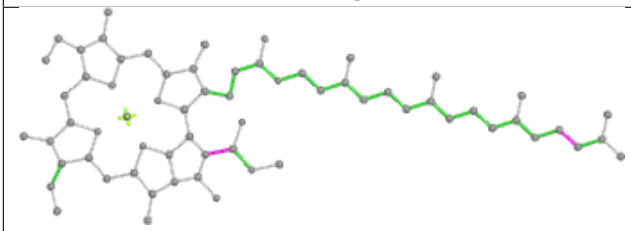
Ligand CLA D 402



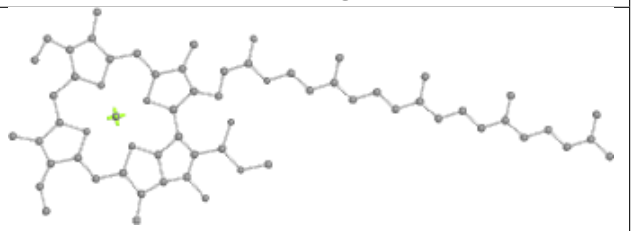
Bond lengths



Bond angles

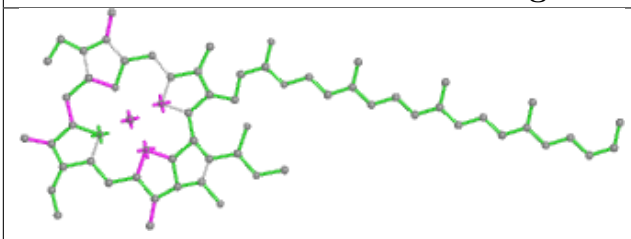


Torsions

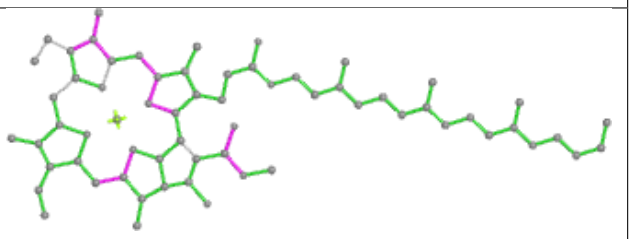


Rings

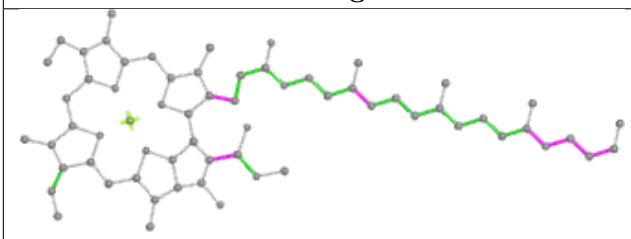
Ligand CLA c 508



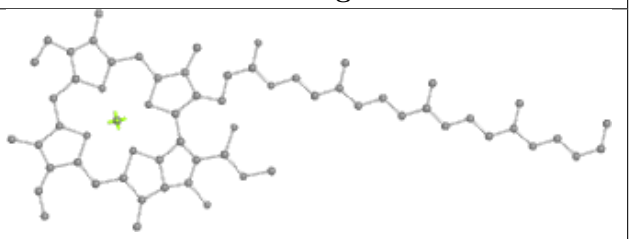
Bond lengths



Bond angles

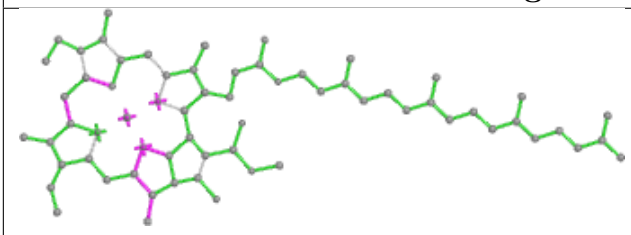


Torsions

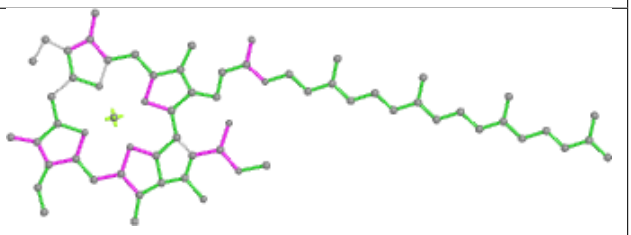


Rings

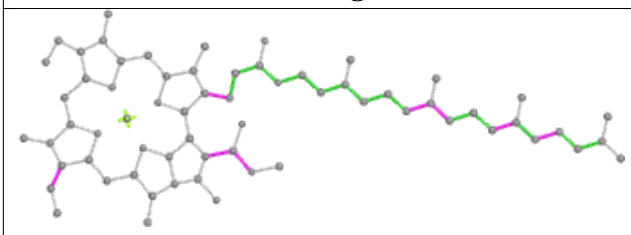
Ligand CLA C 509



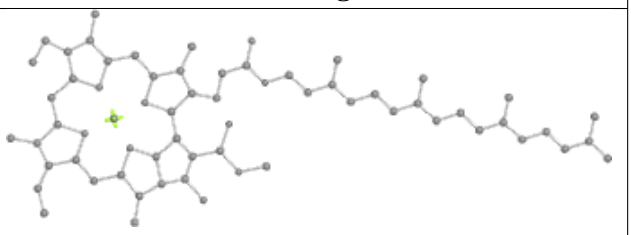
Bond lengths



Bond angles

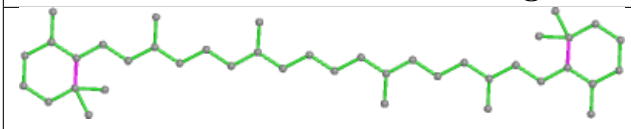


Torsions

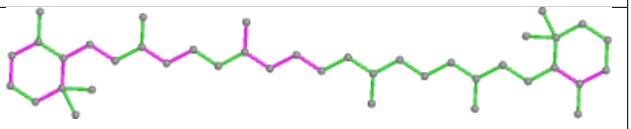


Rings

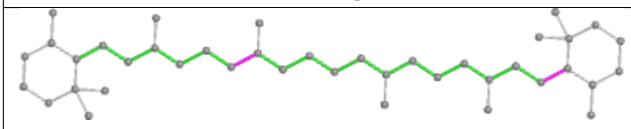
Ligand BCR B 618



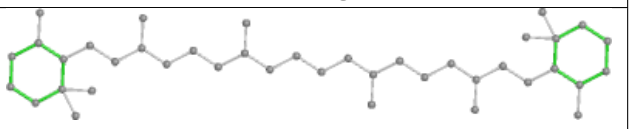
Bond lengths



Bond angles

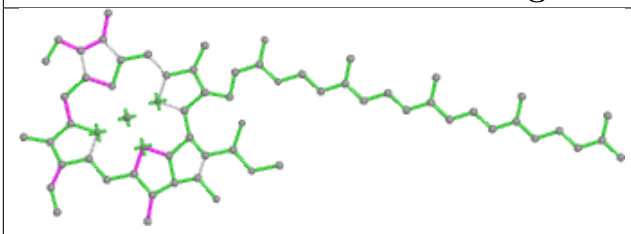


Torsions

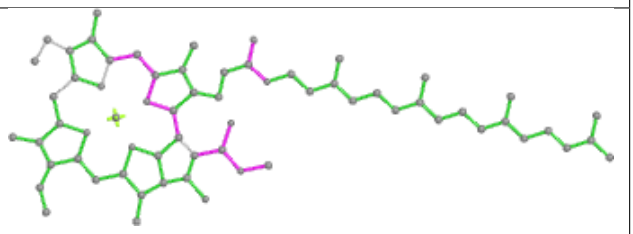


Rings

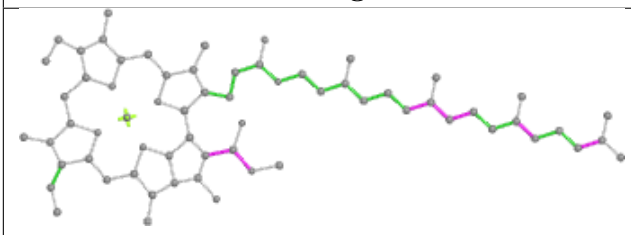
Ligand CLA a 405



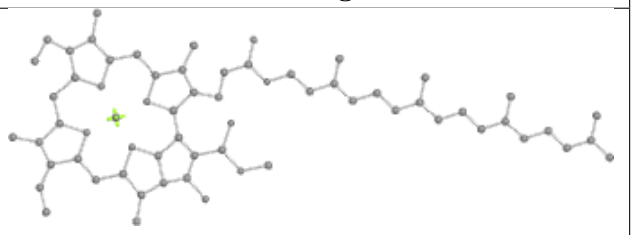
Bond lengths



Bond angles

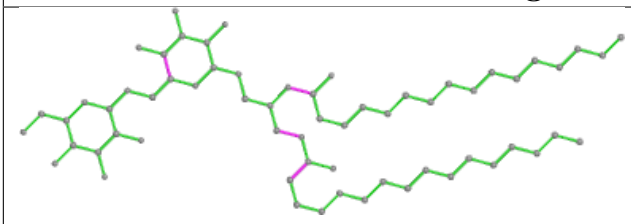


Torsions

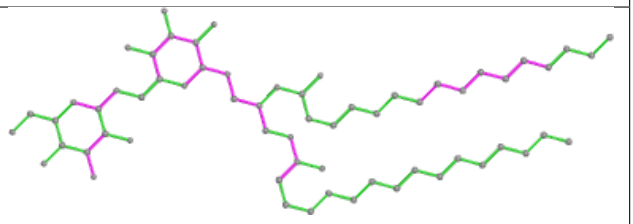


Rings

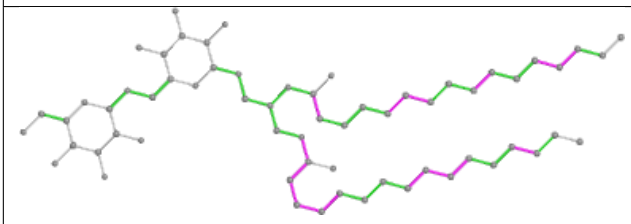
Ligand DGD c 518



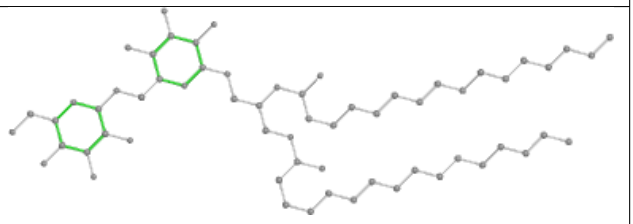
Bond lengths



Bond angles

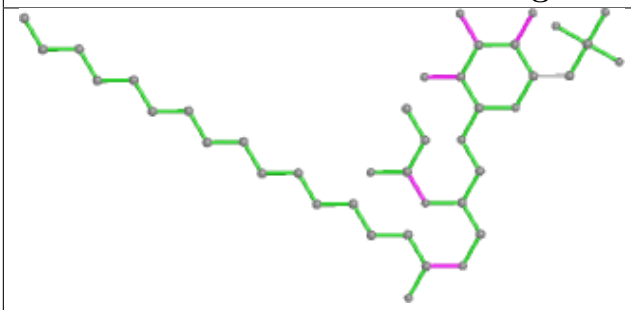


Torsions

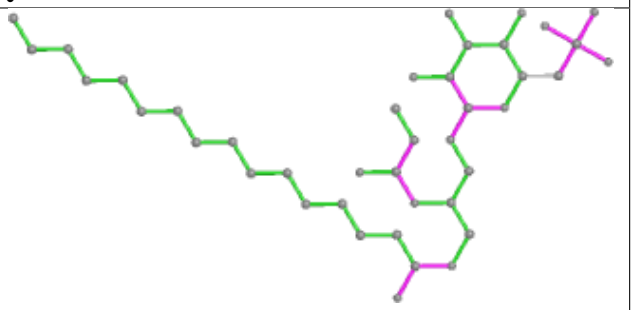


Rings

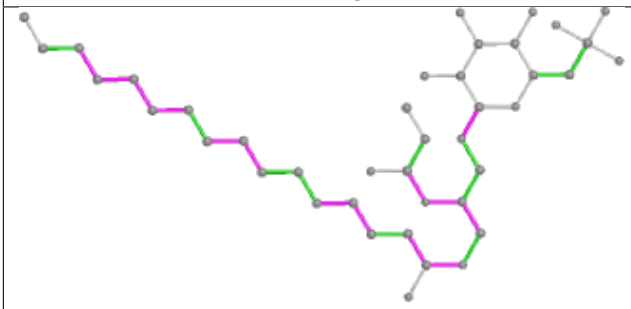
Ligand SQD f 101



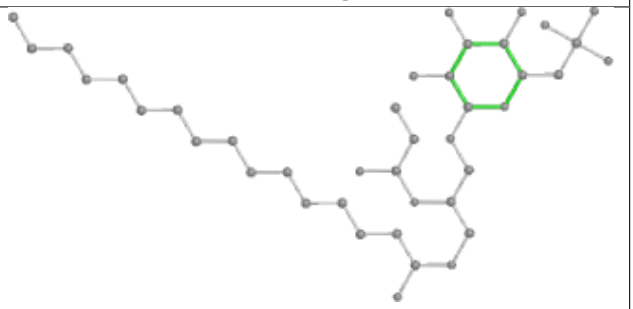
Bond lengths



Bond angles

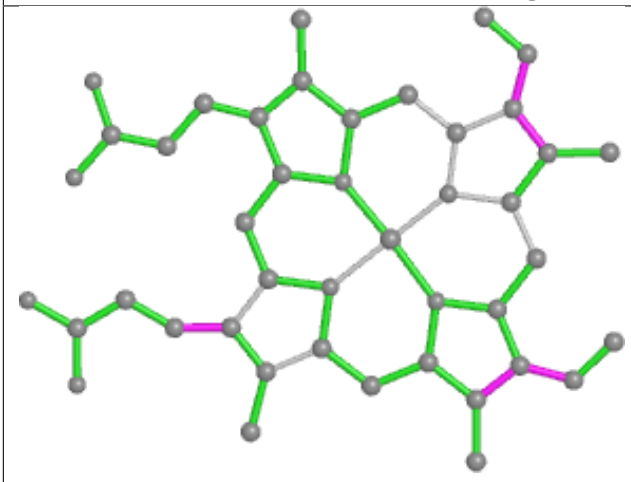


Torsions

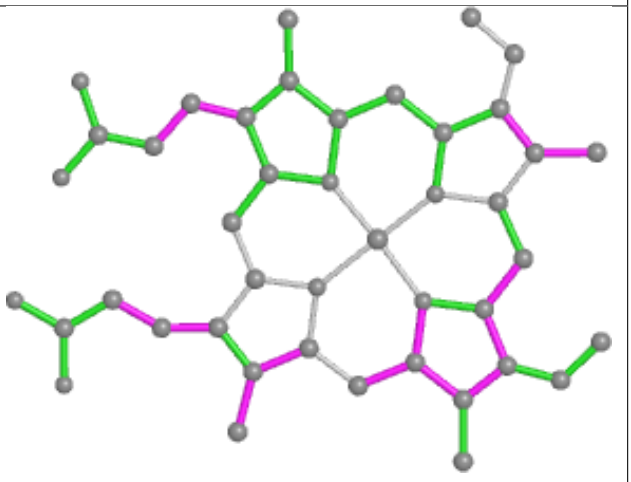


Rings

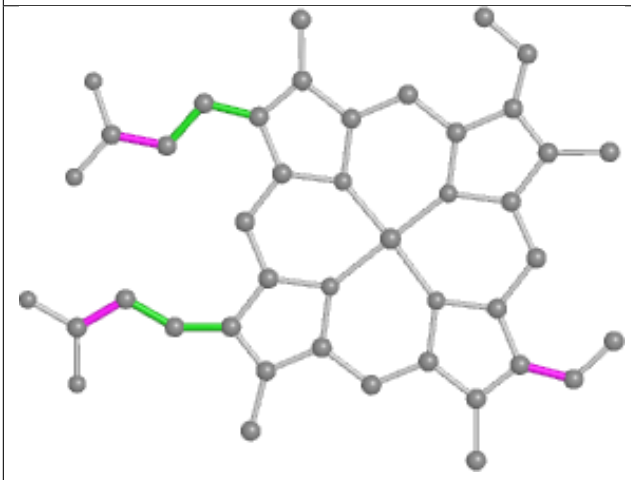
Ligand HEM e 102



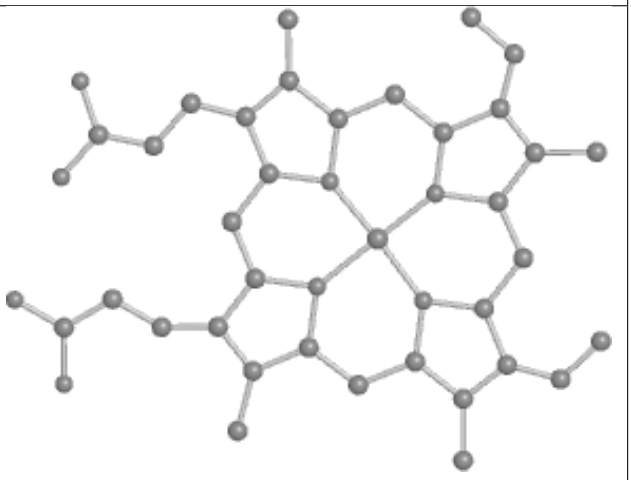
Bond lengths



Bond angles

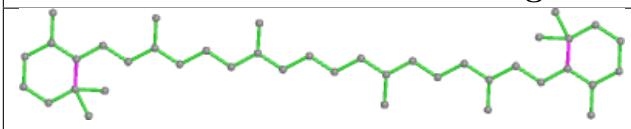


Torsions

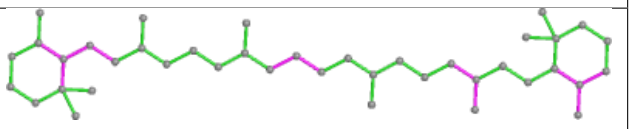


Rings

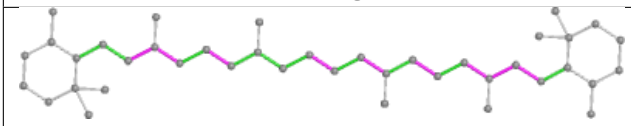
Ligand BCR d 406



Bond lengths



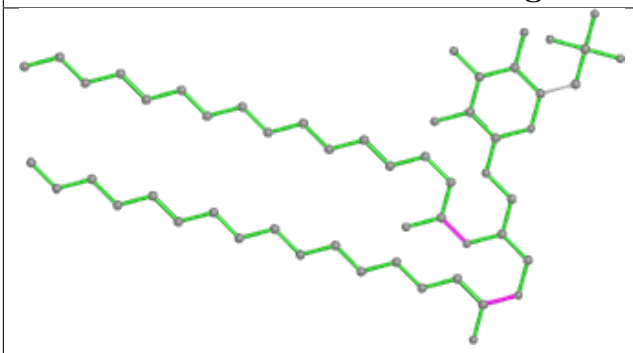
Bond angles



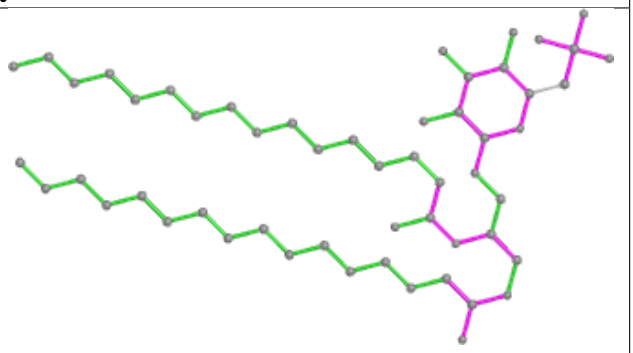
Torsions

Rings

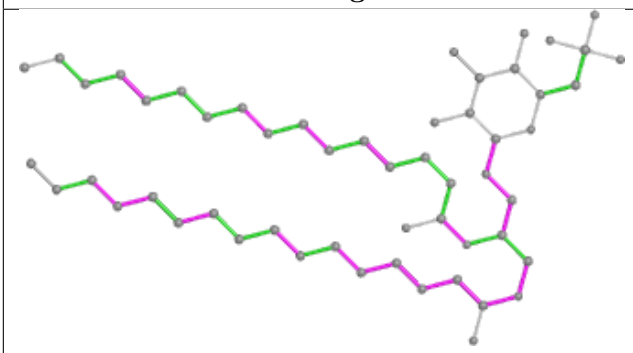
Ligand SQD B 622



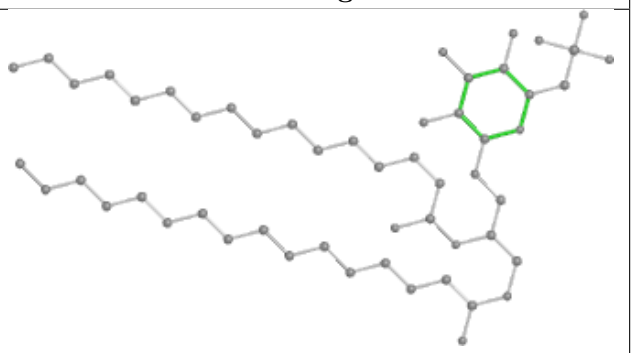
Bond lengths



Bond angles

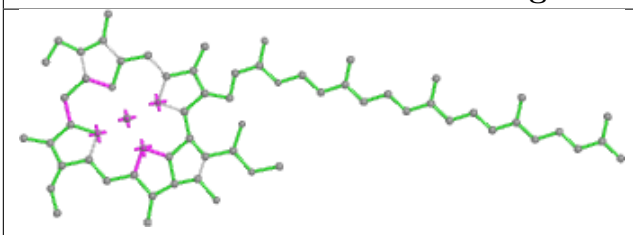


Torsions

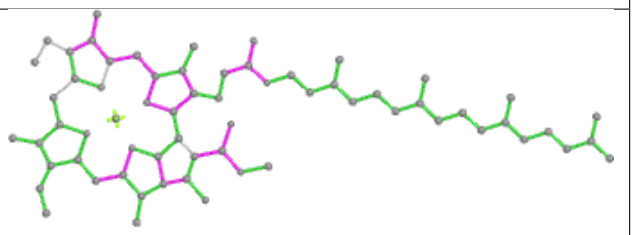


Rings

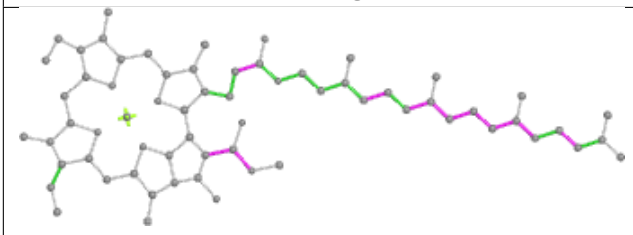
Ligand CLA c 509



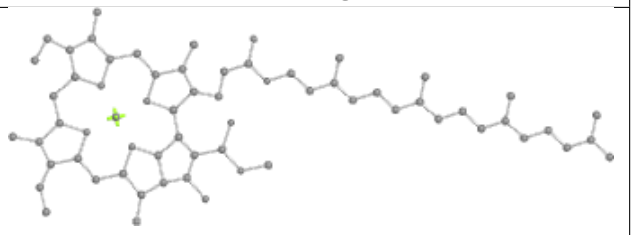
Bond lengths



Bond angles

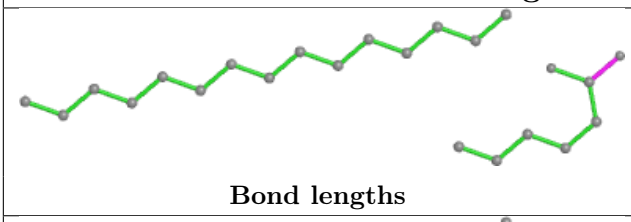


Torsions

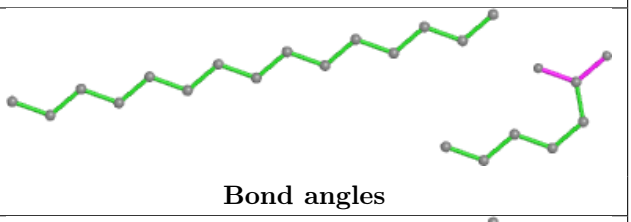


Rings

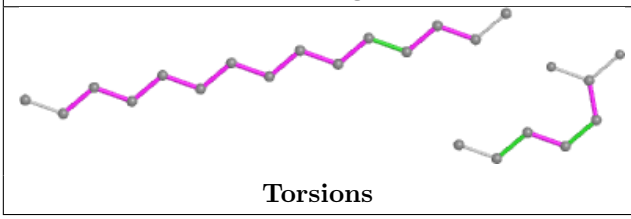
Ligand LMG h 102



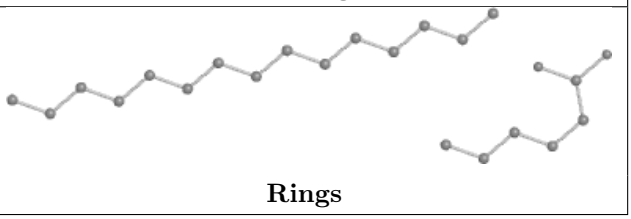
Bond lengths



Bond angles

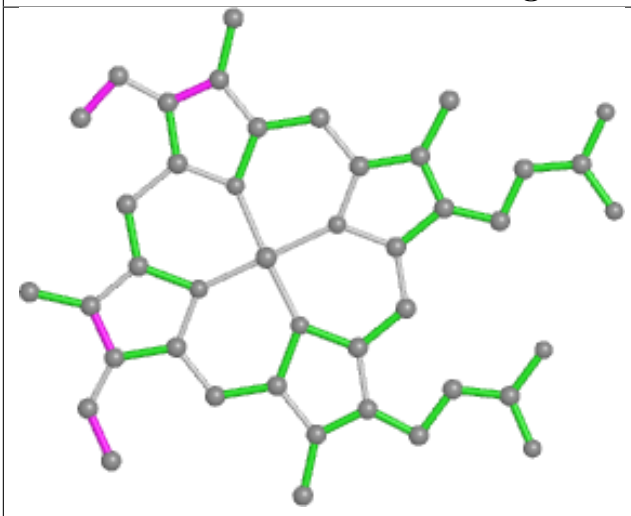


Torsions

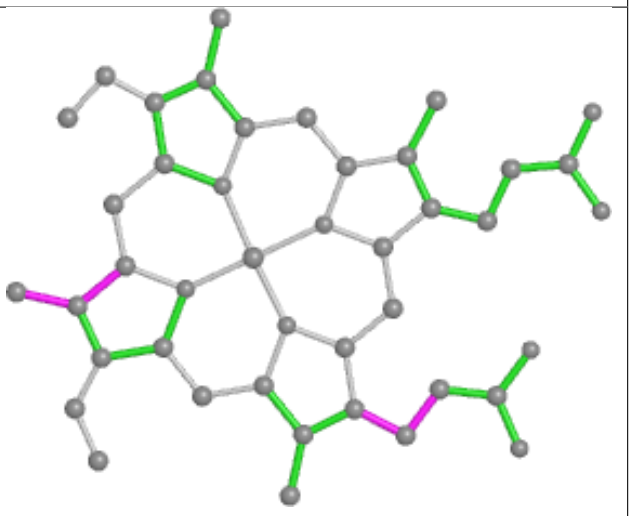


Rings

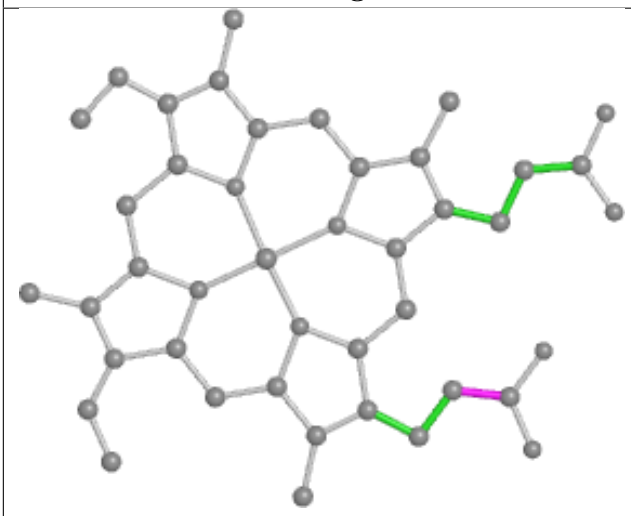
Ligand HEC V 201



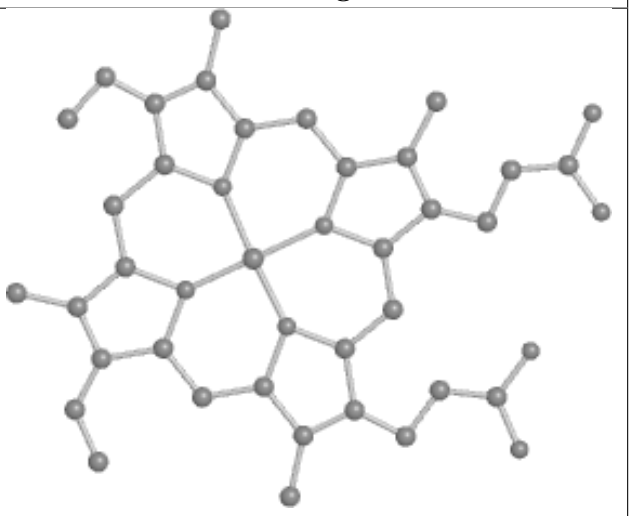
Bond lengths



Bond angles

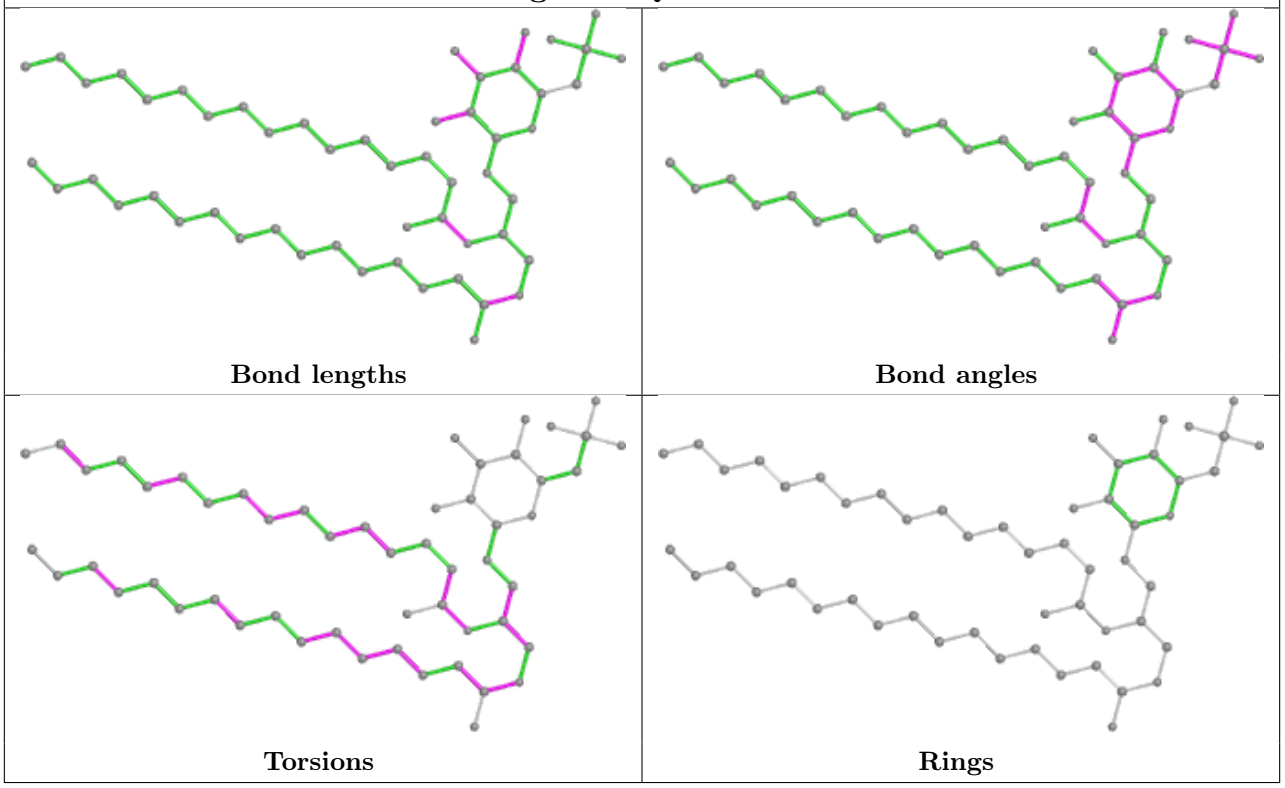


Torsions

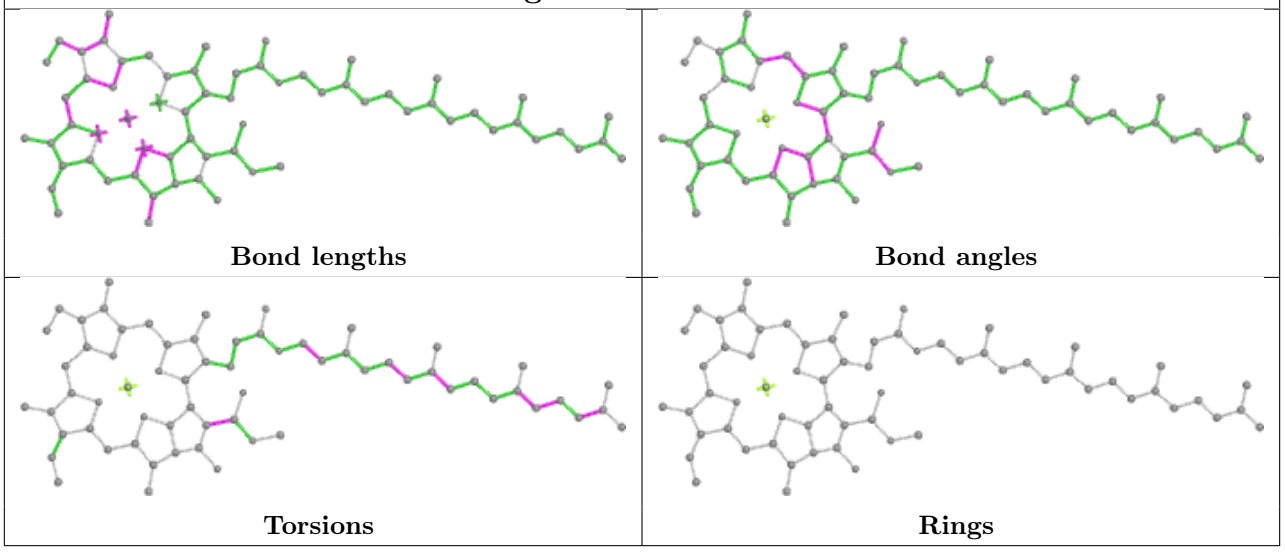


Rings

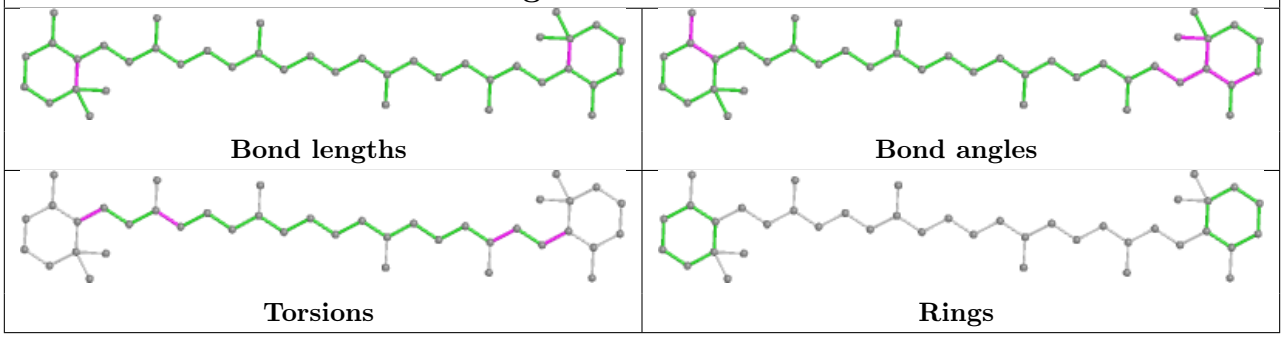
Ligand SQD a 410



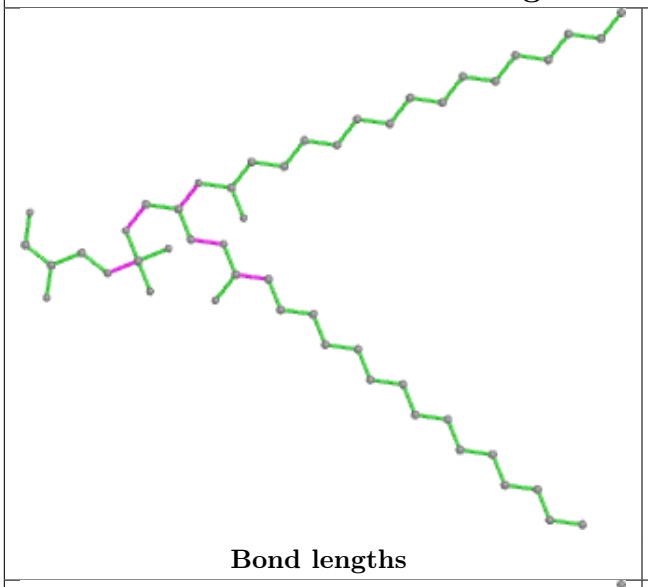
Ligand CLA D 404



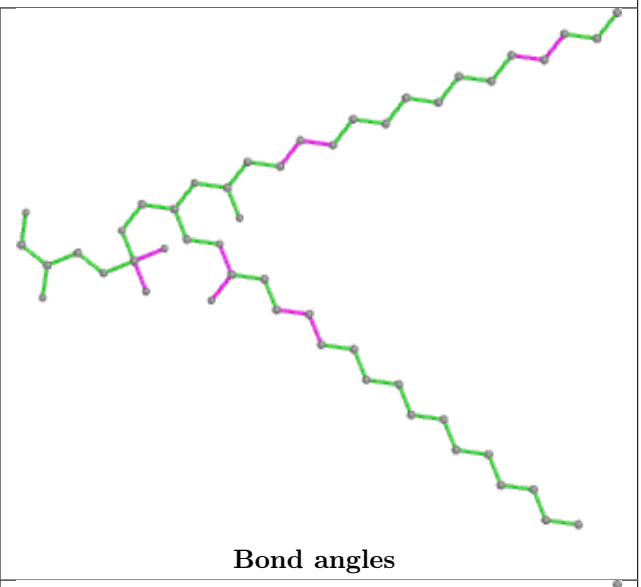
Ligand BCR Y 101



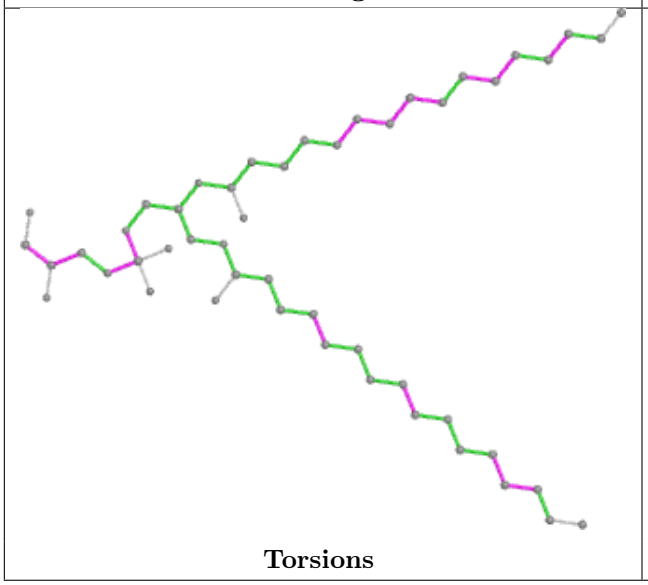
Ligand LHG D 408



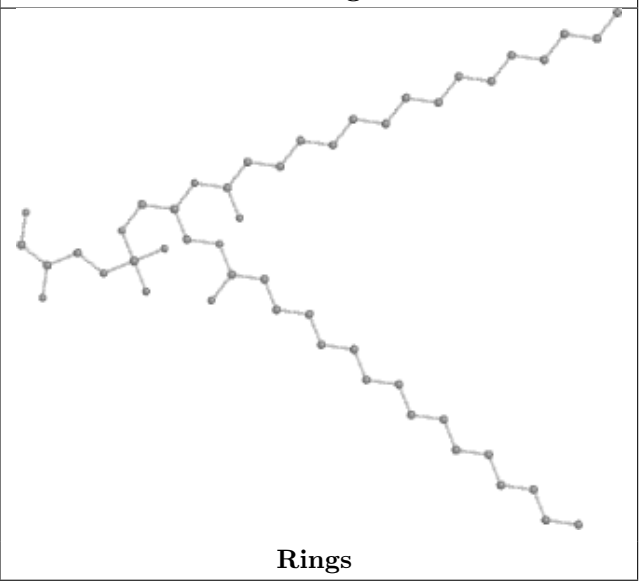
Bond lengths



Bond angles

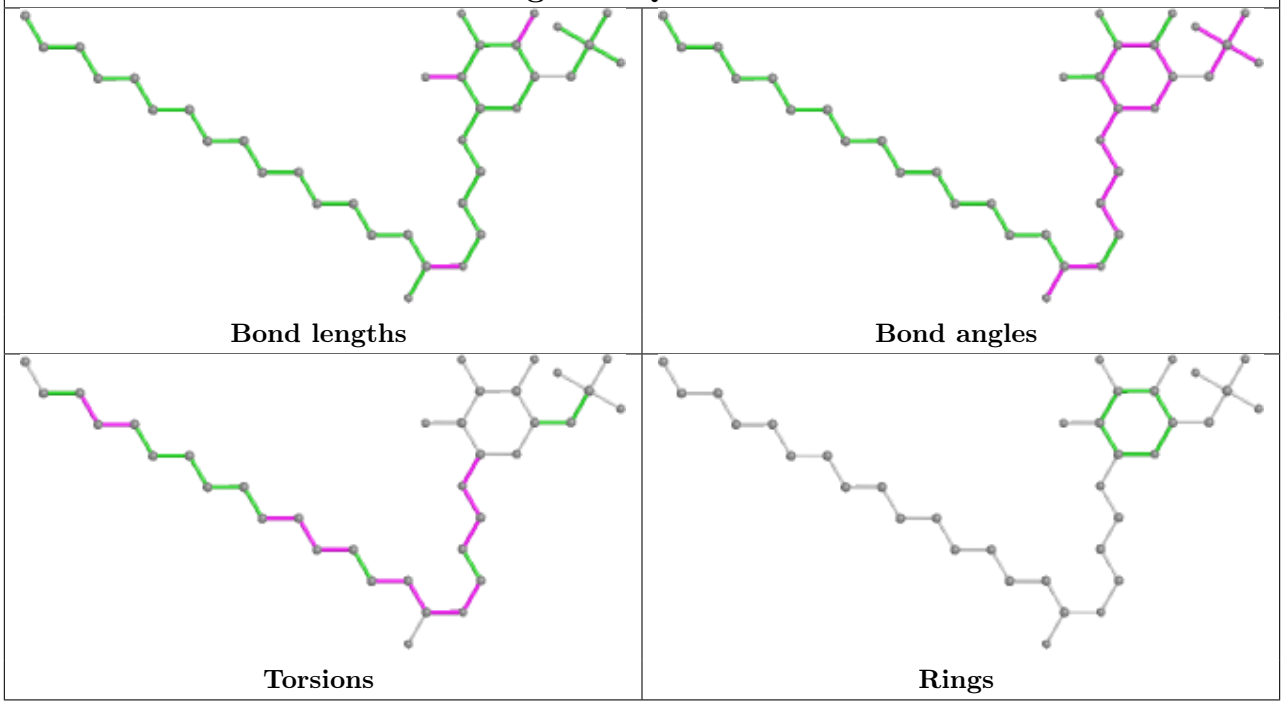


Torsions

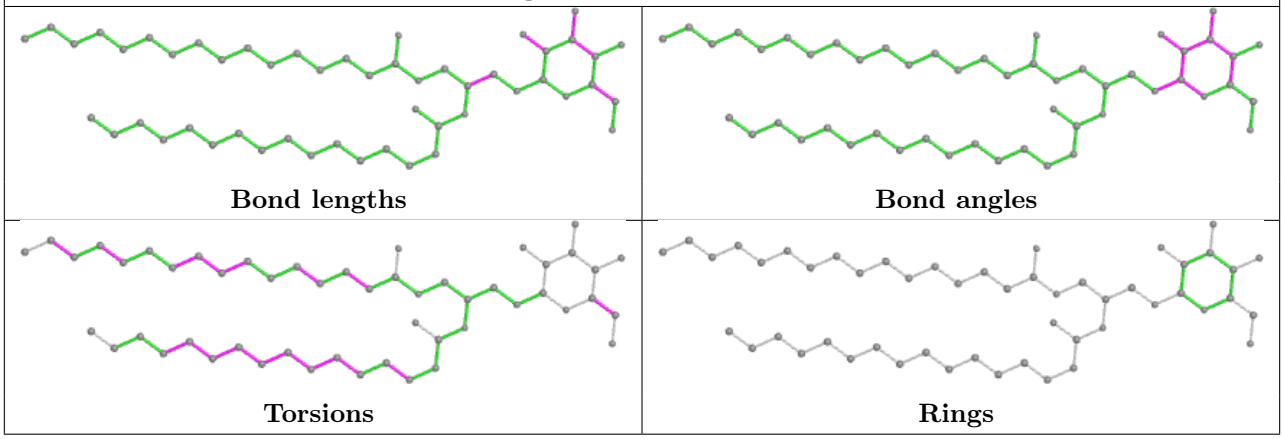


Rings

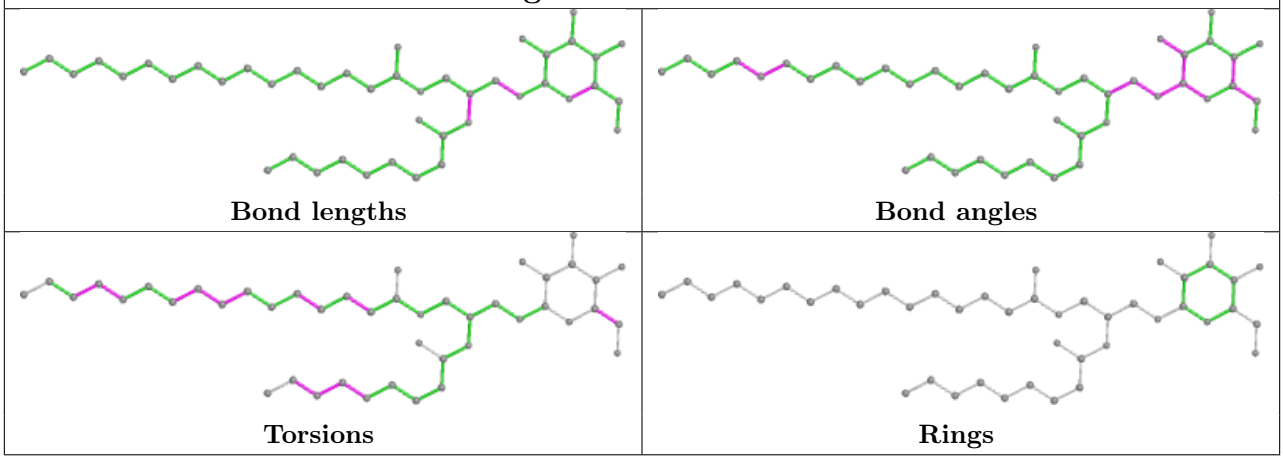
Ligand SQD F 101



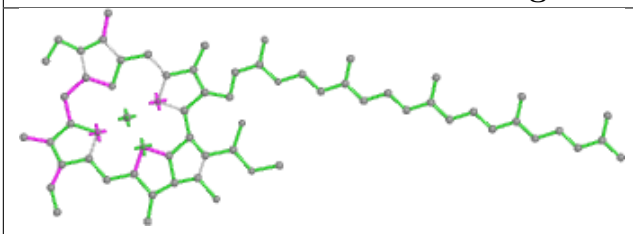
Ligand LMG D 407



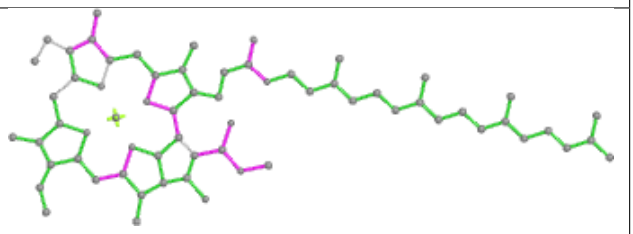
Ligand LMG d 411



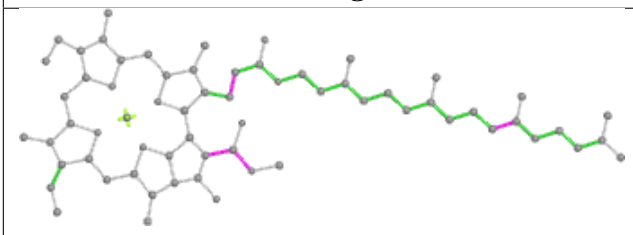
Ligand CLA c 501



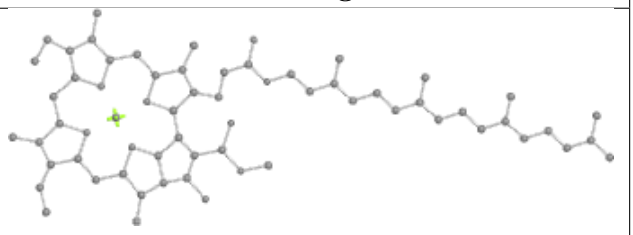
Bond lengths



Bond angles

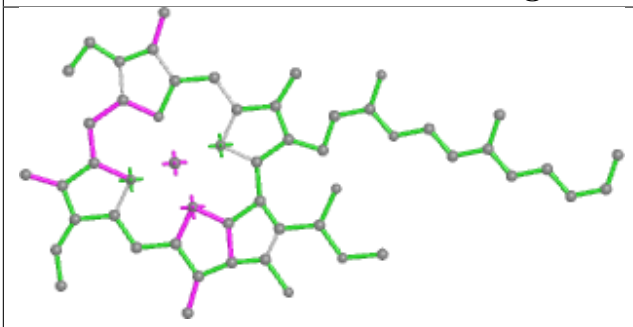


Torsions

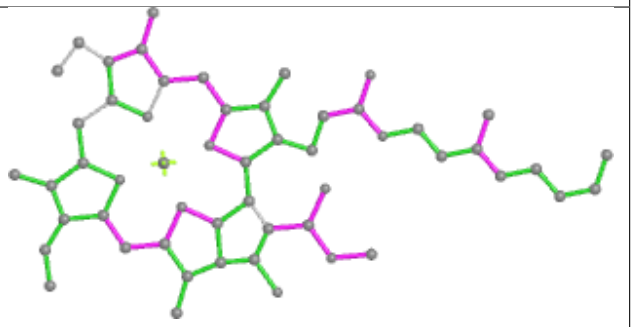


Rings

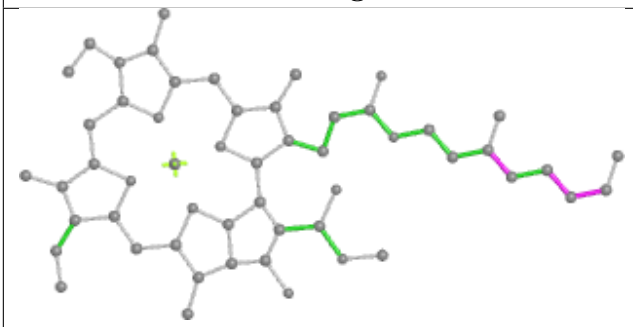
Ligand CLA A 408



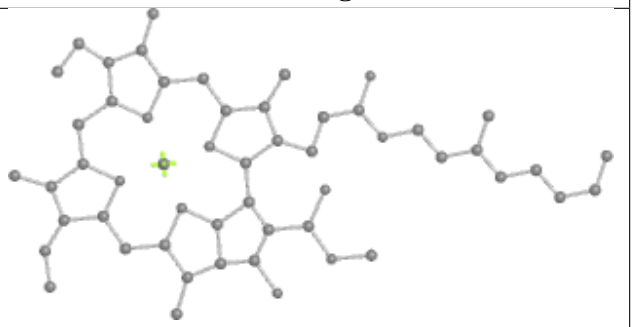
Bond lengths



Bond angles

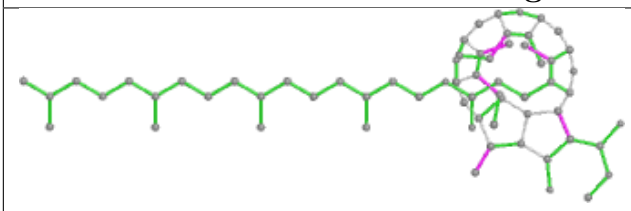


Torsions

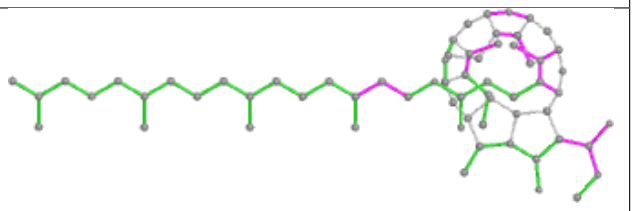


Rings

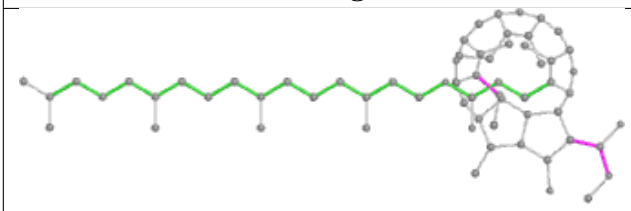
Ligand PHO d 402



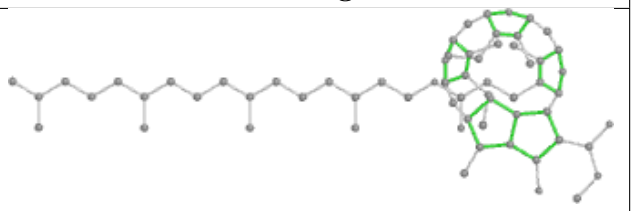
Bond lengths



Bond angles

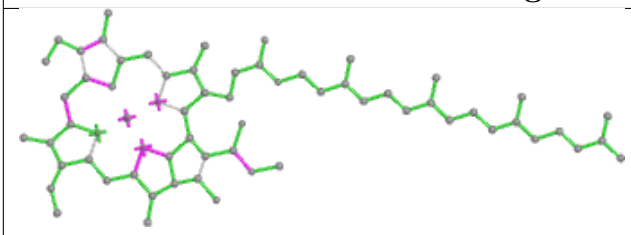


Torsions

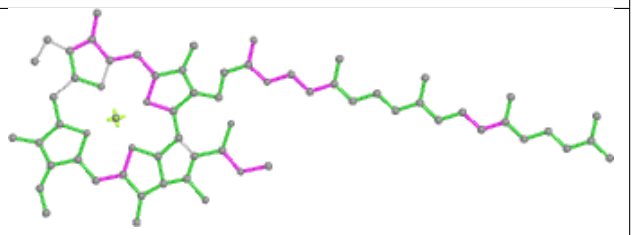


Rings

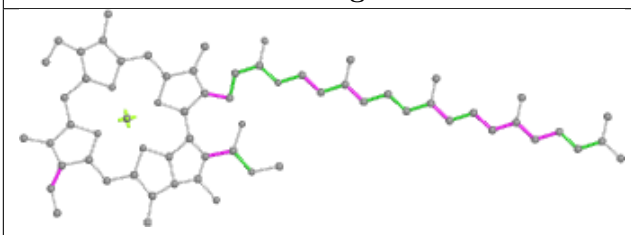
Ligand CLA B 604



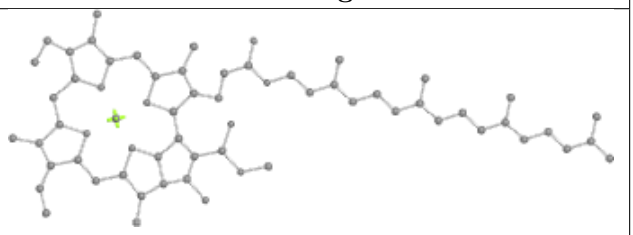
Bond lengths



Bond angles

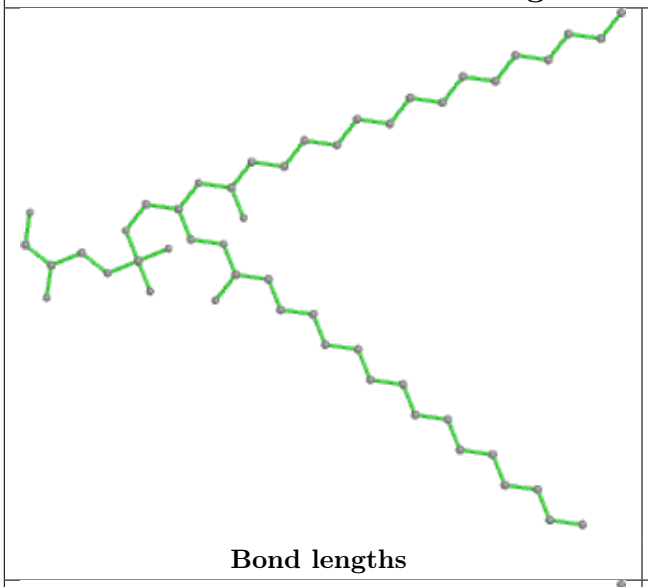


Torsions

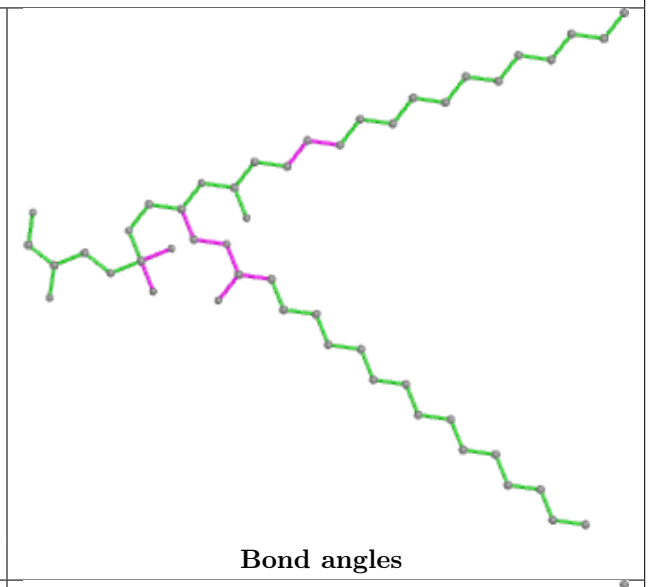


Rings

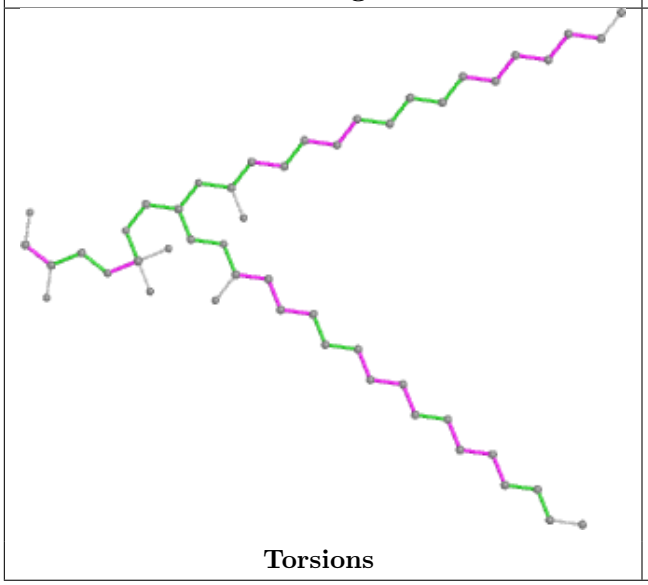
Ligand LHG d 408



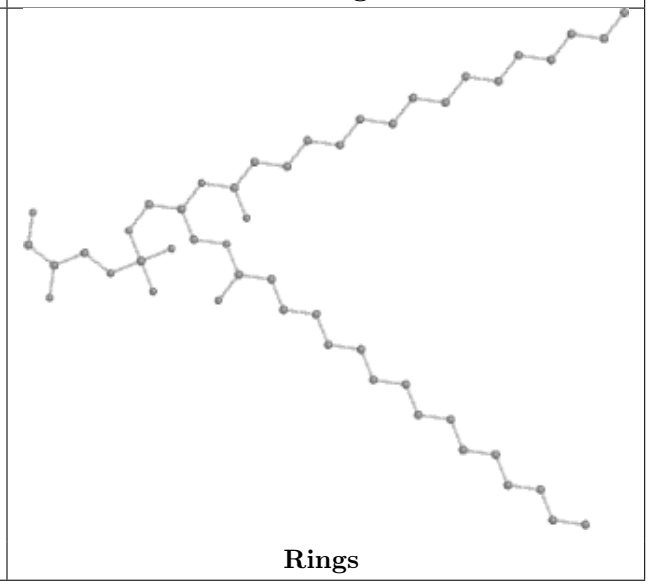
Bond lengths



Bond angles

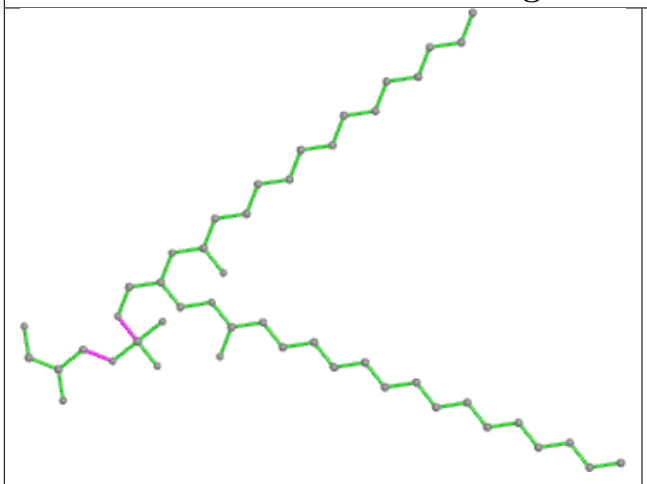


Torsions

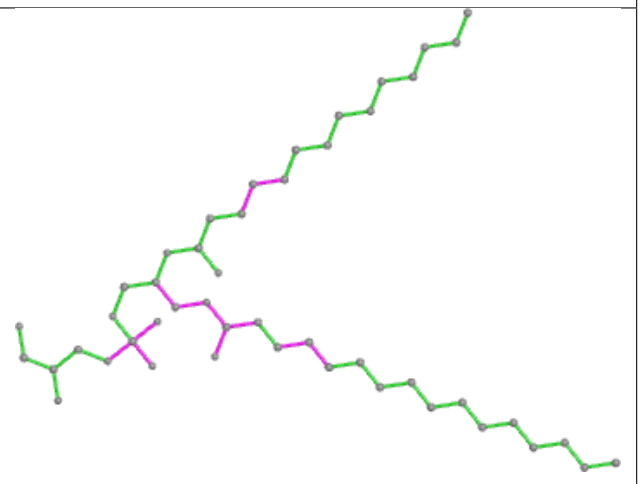


Rings

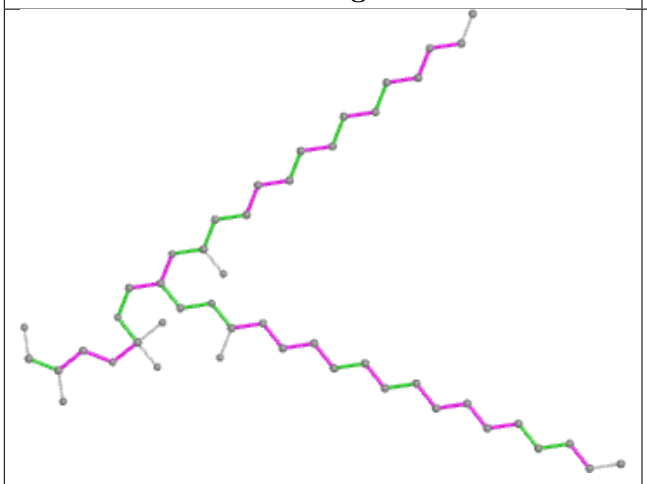
Ligand LHG D 409



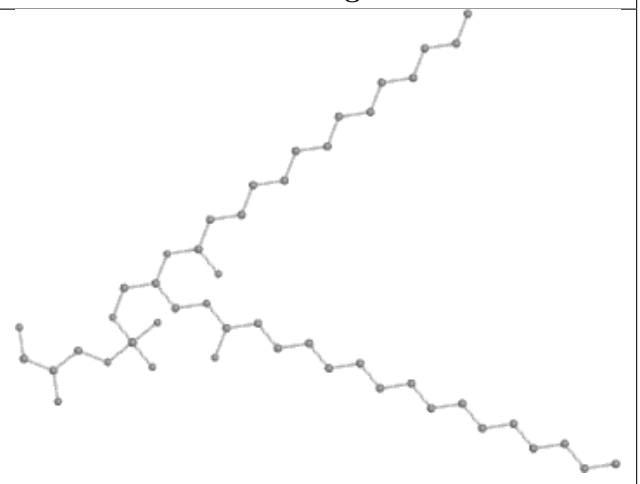
Bond lengths



Bond angles

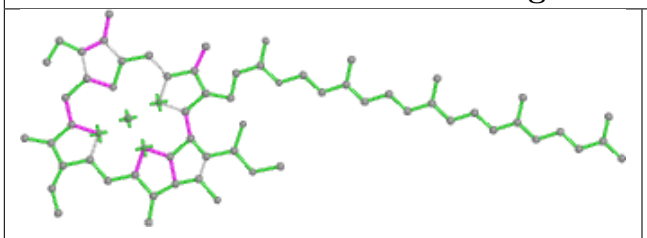


Torsions

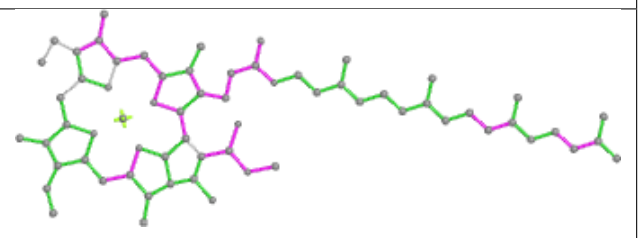


Rings

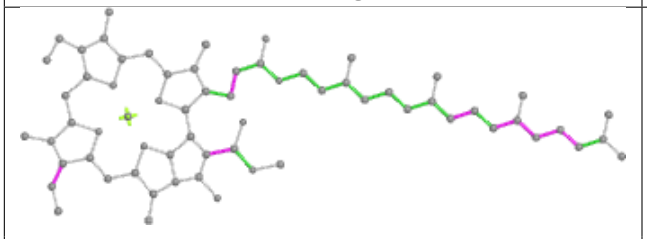
Ligand CLA b 611



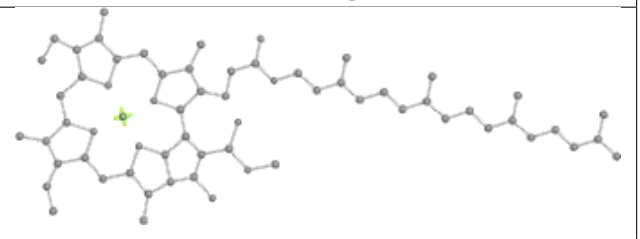
Bond lengths



Bond angles

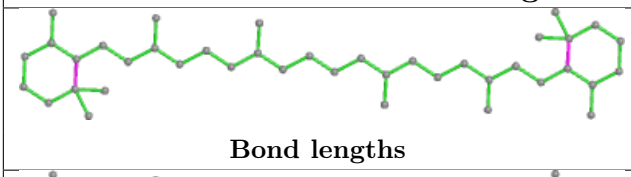


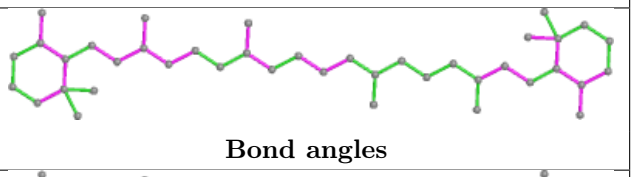
Torsions

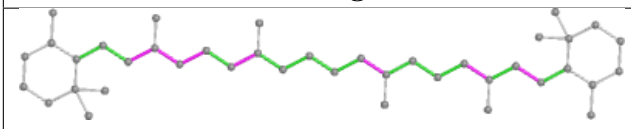


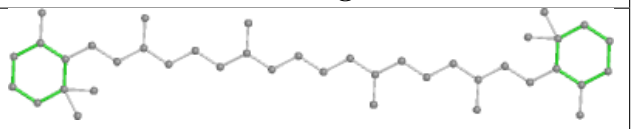
Rings

Ligand BCR K 101

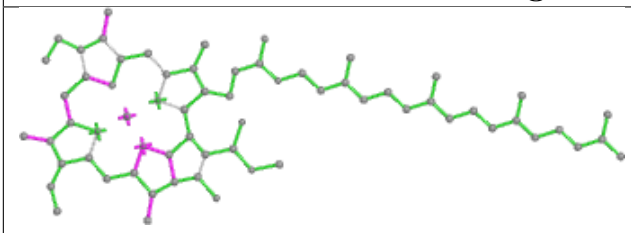

Bond lengths

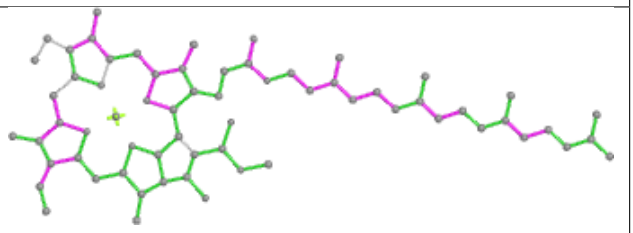

Bond angles

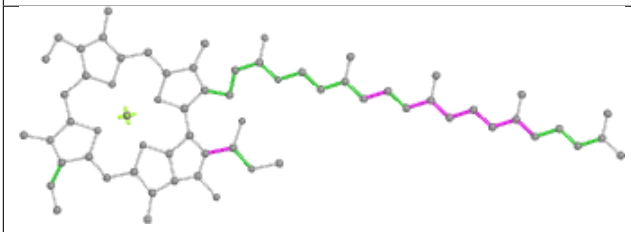

Torsions

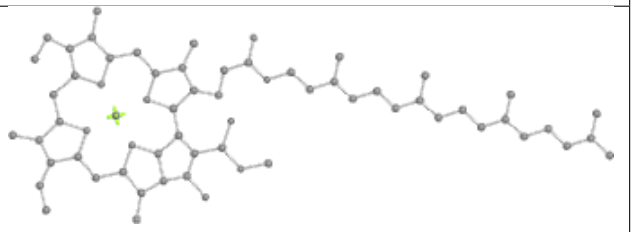

Rings

Ligand CLA b 605

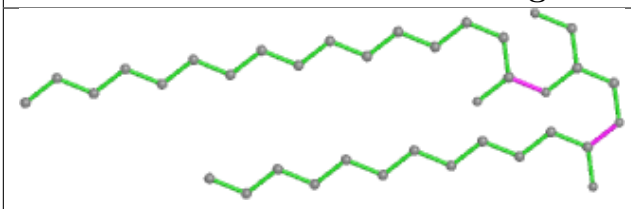

Bond lengths

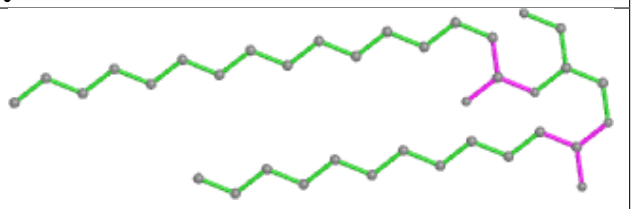

Bond angles

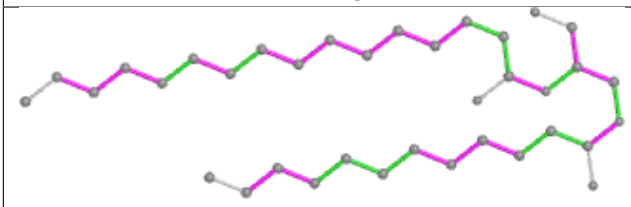

Torsions

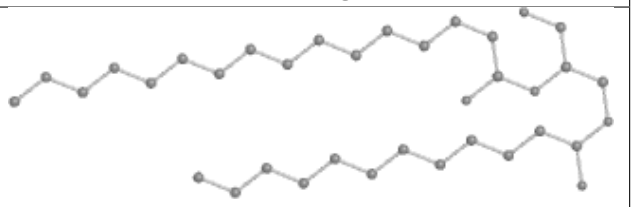

Rings

Ligand SQD a 411

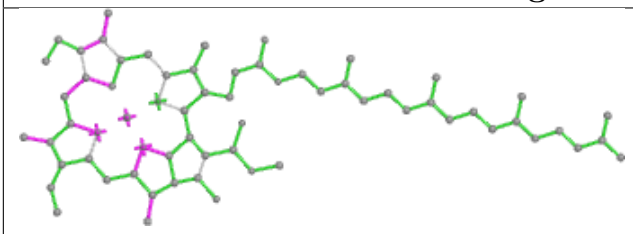

Bond lengths


Bond angles

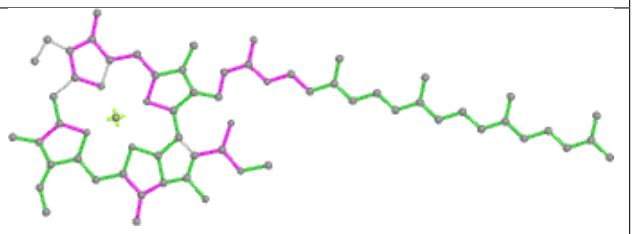

Torsions


Rings

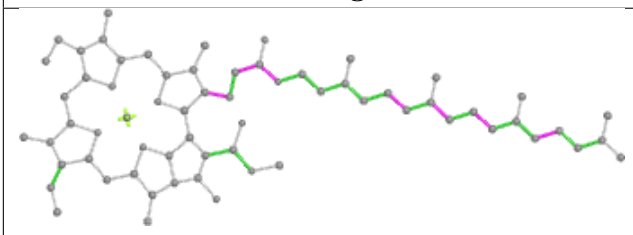
Ligand CLA a 407



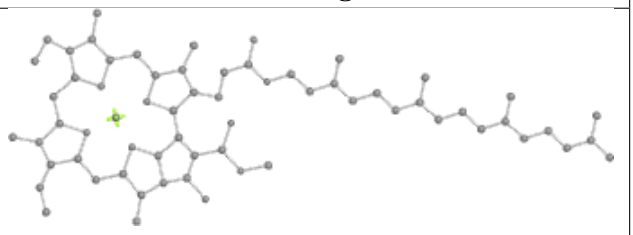
Bond lengths



Bond angles

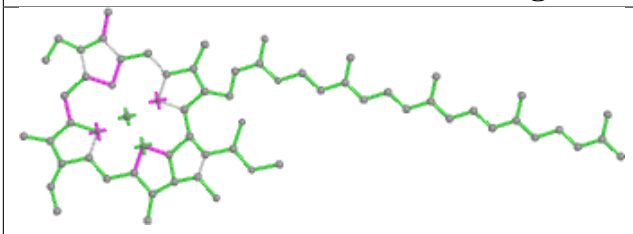


Torsions

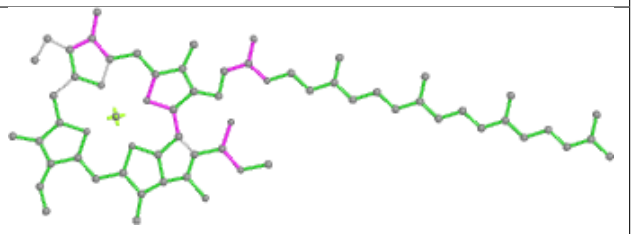


Rings

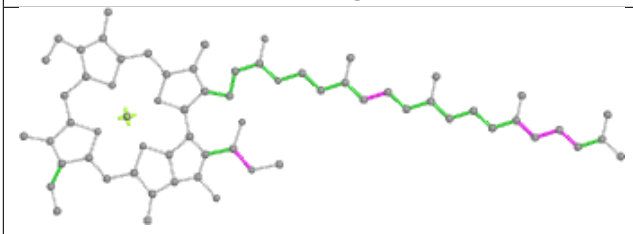
Ligand CLA c 511



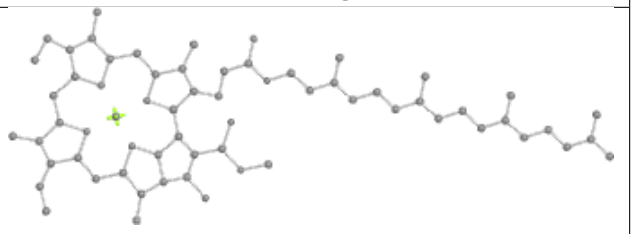
Bond lengths



Bond angles

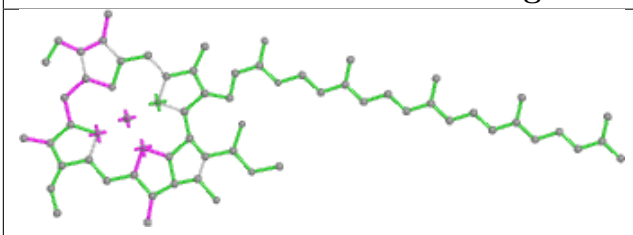


Torsions

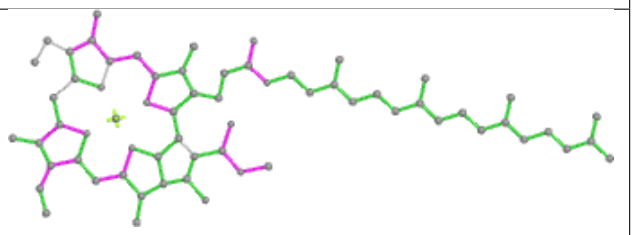


Rings

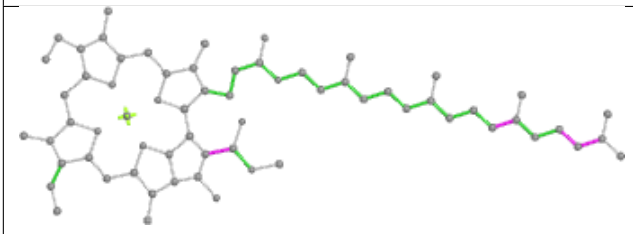
Ligand CLA A 406



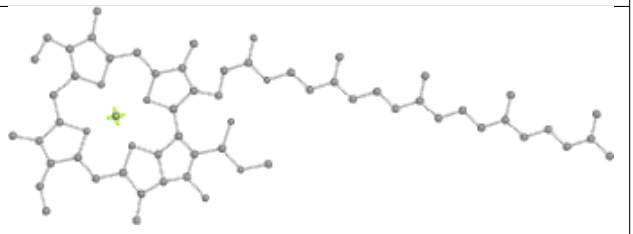
Bond lengths



Bond angles

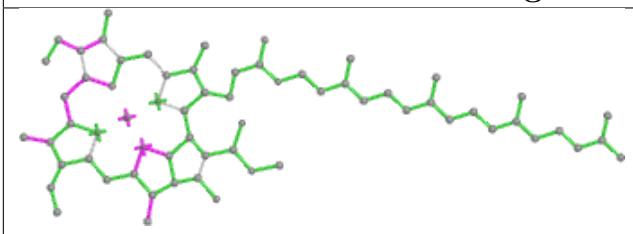


Torsions

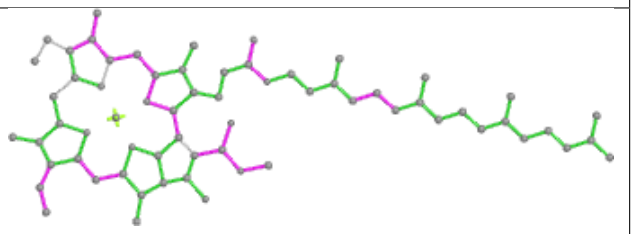


Rings

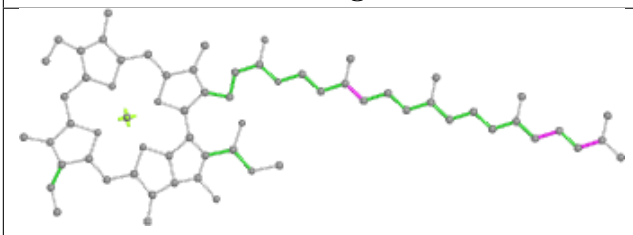
Ligand CLA B 609



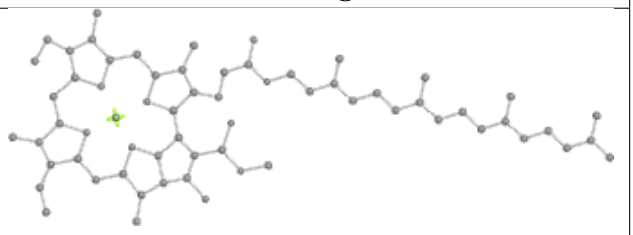
Bond lengths



Bond angles

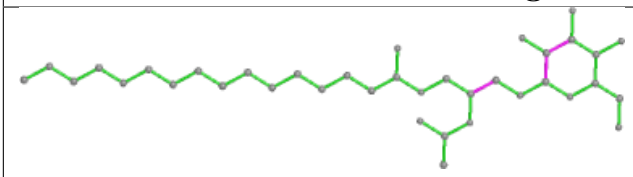


Torsions

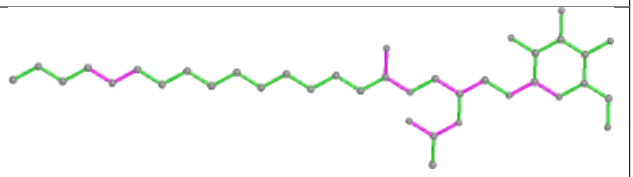


Rings

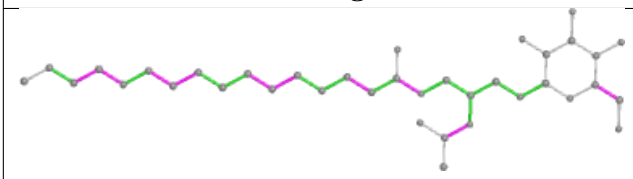
Ligand LMG c 519



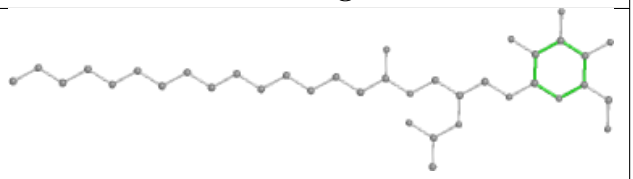
Bond lengths



Bond angles

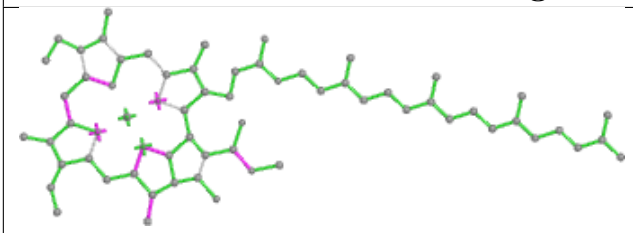


Torsions

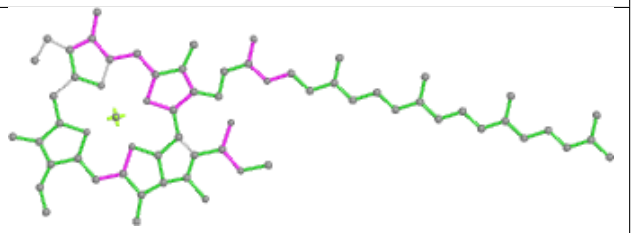


Rings

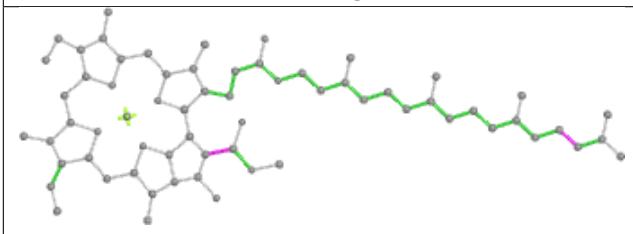
Ligand CLA c 502



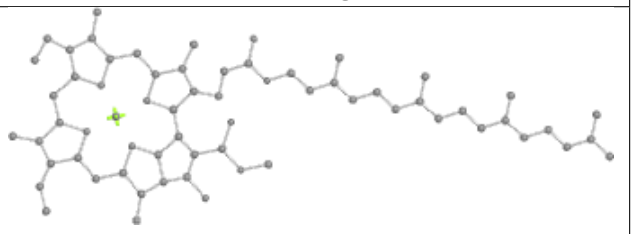
Bond lengths



Bond angles

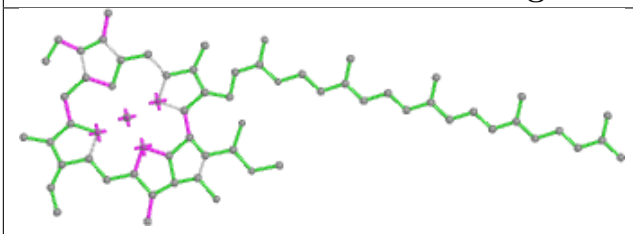


Torsions

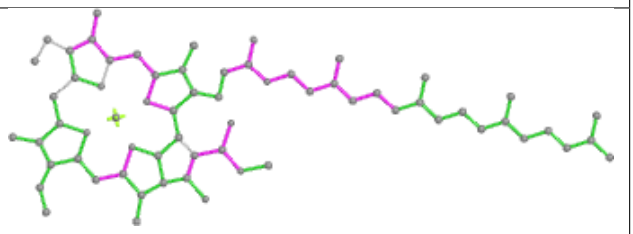


Rings

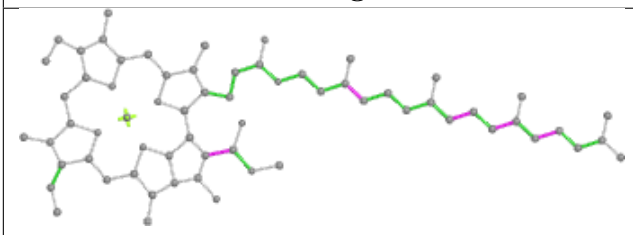
Ligand CLA b 604



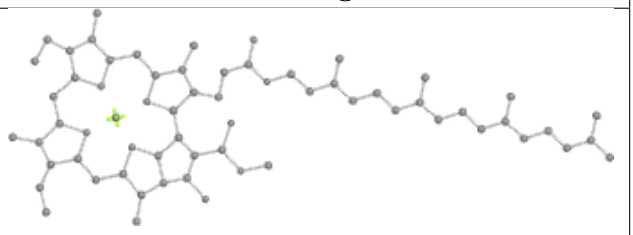
Bond lengths



Bond angles

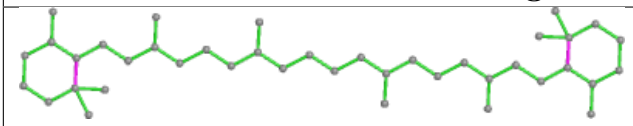


Torsions

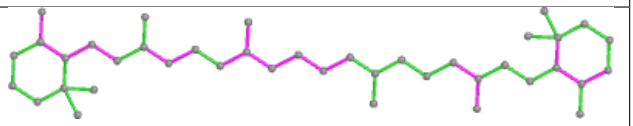


Rings

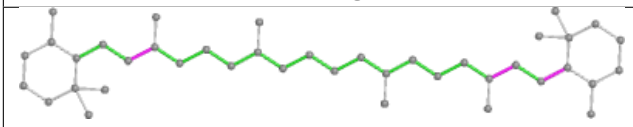
Ligand BCR b 619



Bond lengths



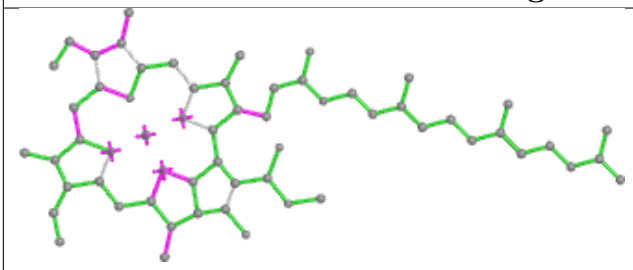
Bond angles



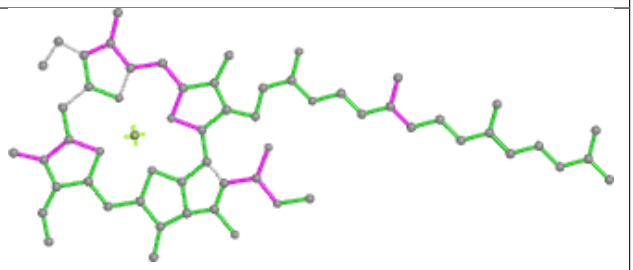
Torsions

Rings

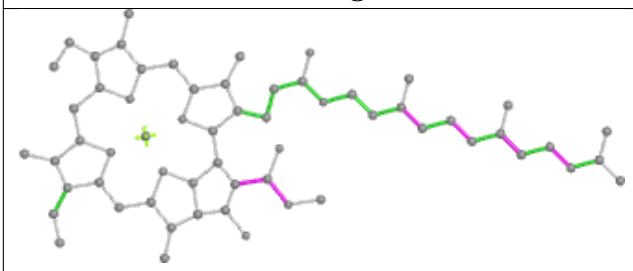
Ligand CLA b 617



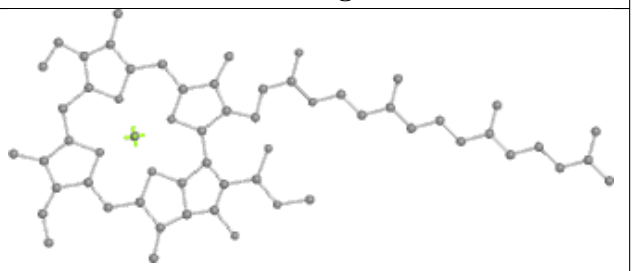
Bond lengths



Bond angles

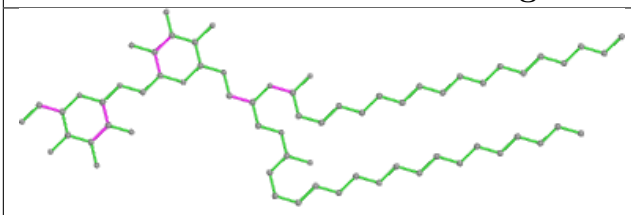


Torsions

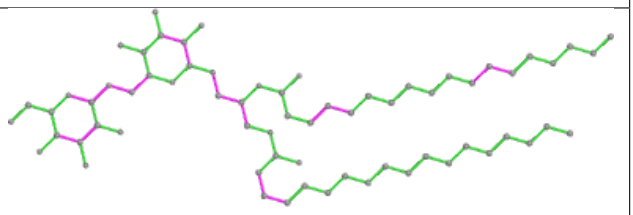


Rings

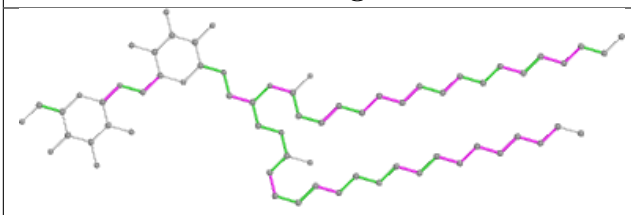
Ligand DGD A 413



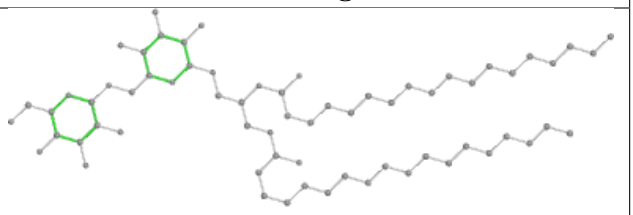
Bond lengths



Bond angles

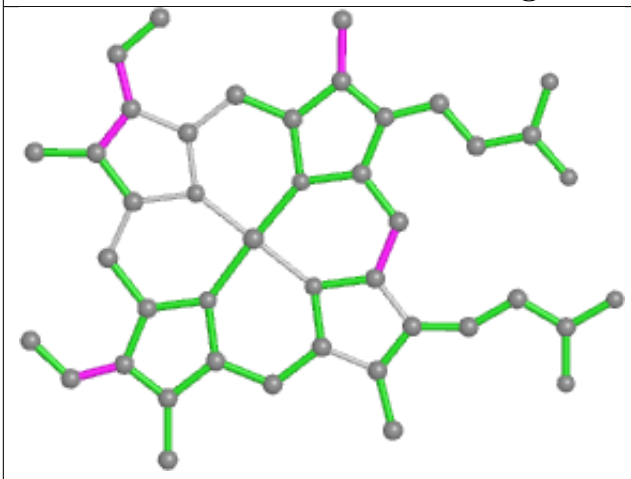


Torsions

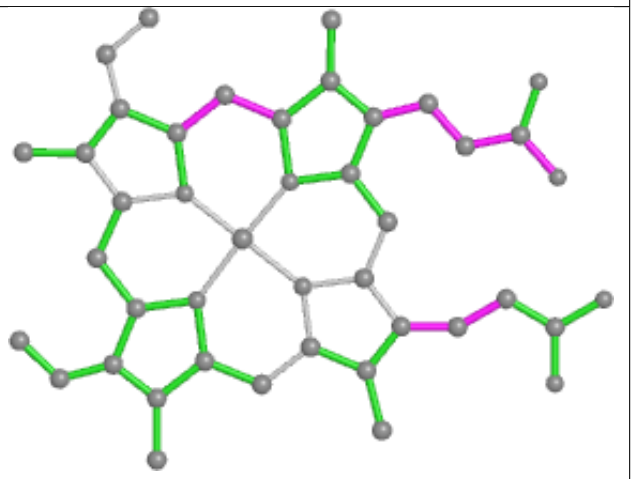


Rings

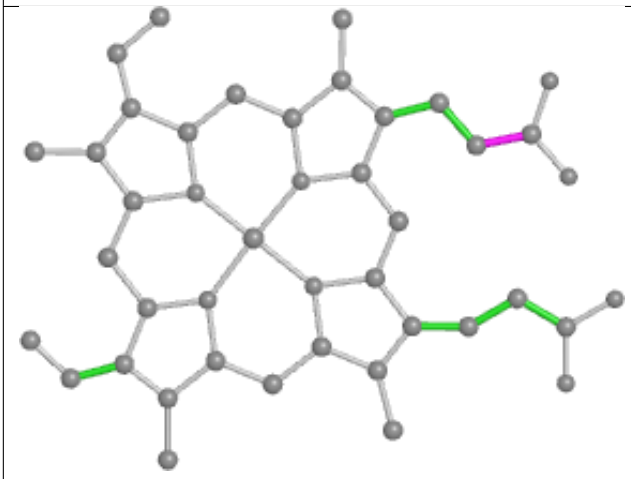
Ligand HEM F 102



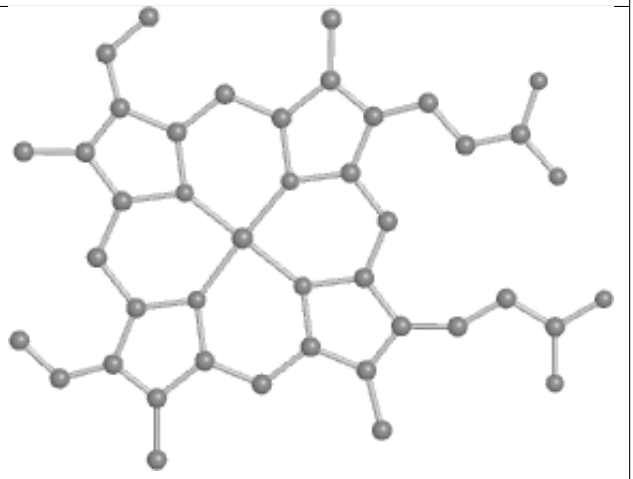
Bond lengths



Bond angles

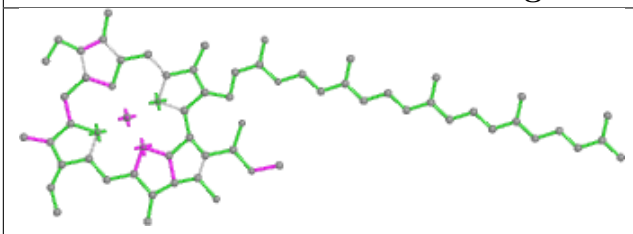


Torsions

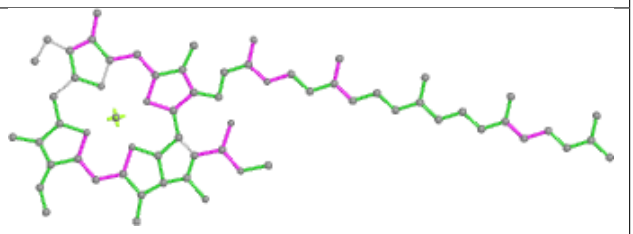


Rings

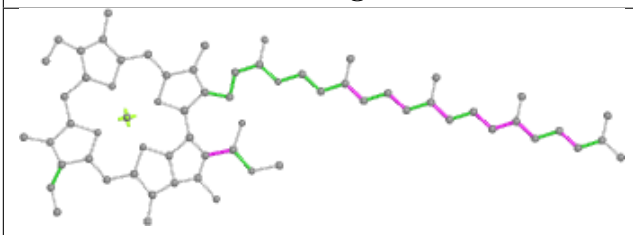
Ligand CLA B 605



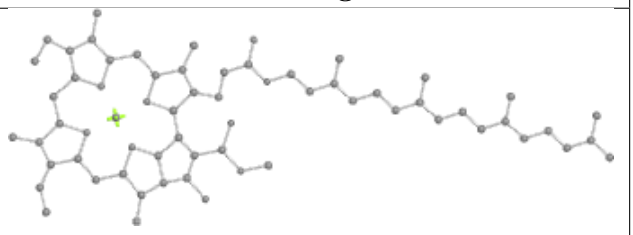
Bond lengths



Bond angles

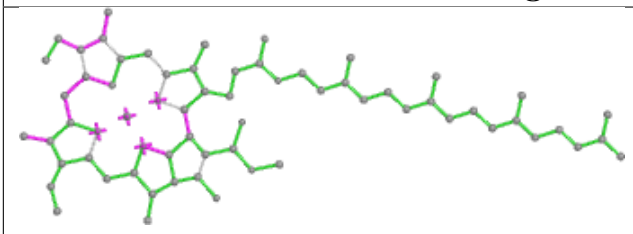


Torsions

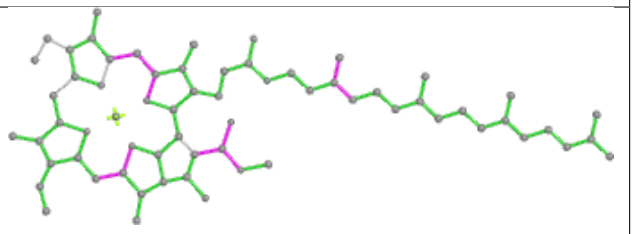


Rings

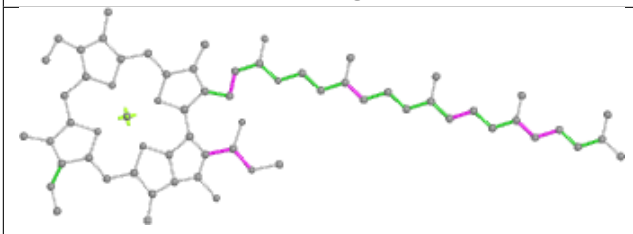
Ligand CLA B 614



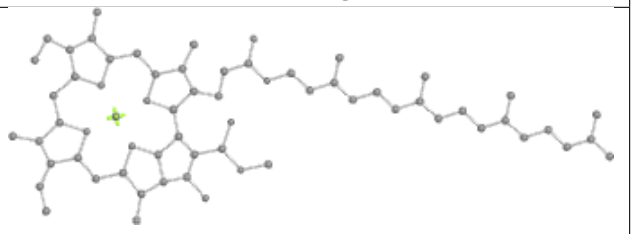
Bond lengths



Bond angles

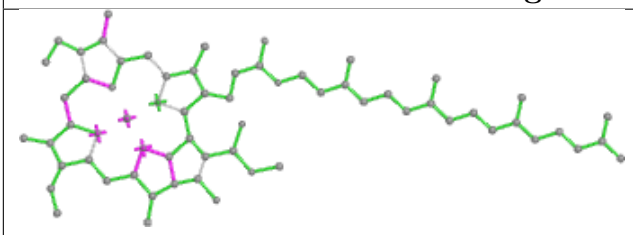


Torsions

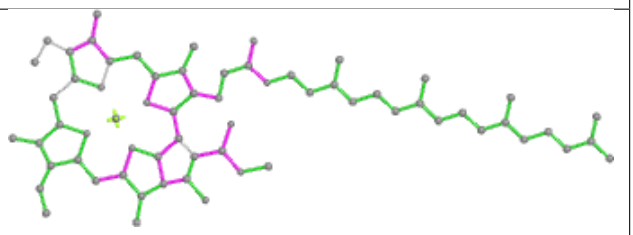


Rings

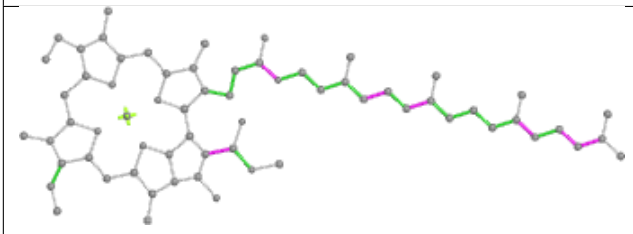
Ligand CLA C 503



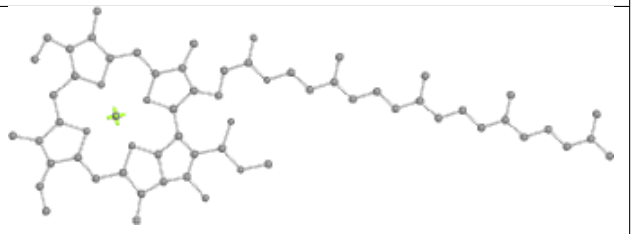
Bond lengths



Bond angles

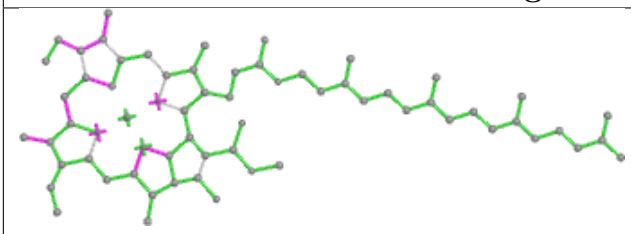


Torsions

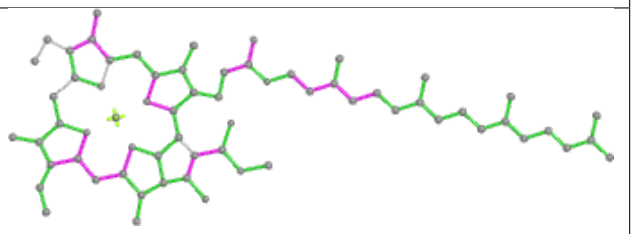


Rings

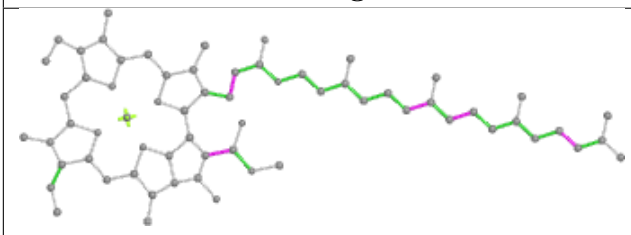
Ligand CLA B 606



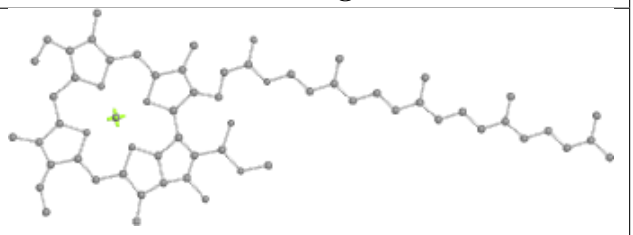
Bond lengths



Bond angles

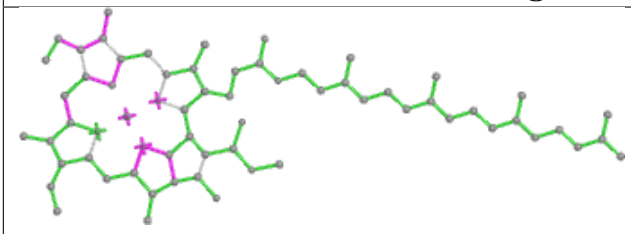


Torsions

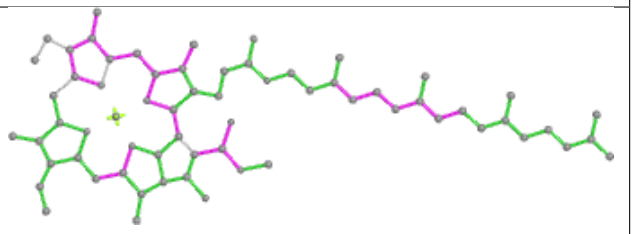


Rings

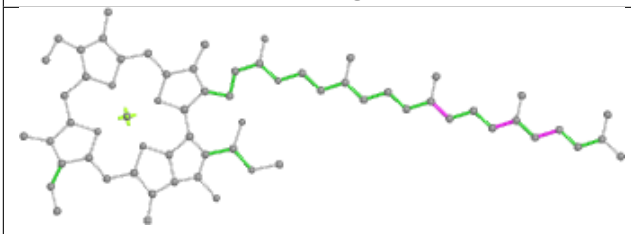
Ligand CLA b 609



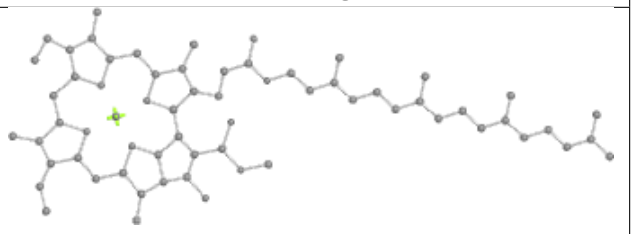
Bond lengths



Bond angles

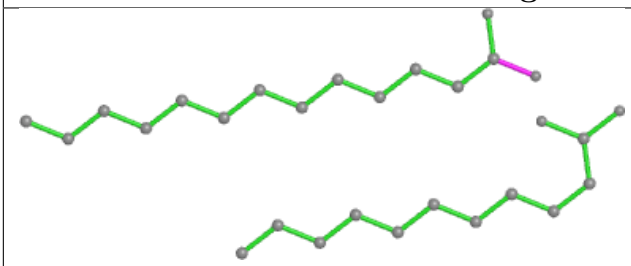


Torsions

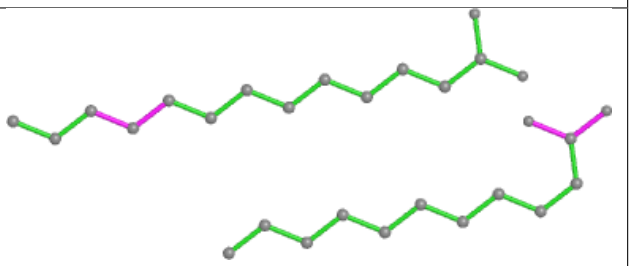


Rings

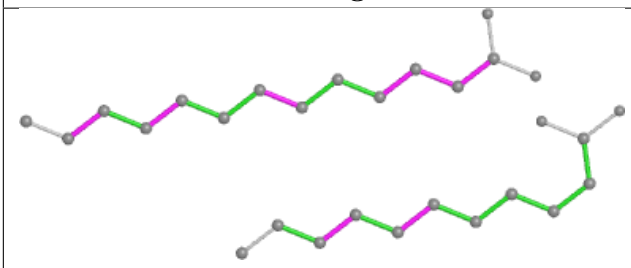
Ligand LMG B 621



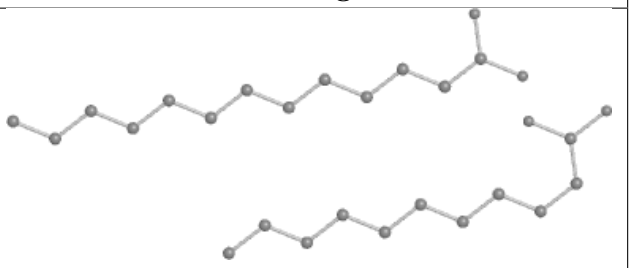
Bond lengths



Bond angles

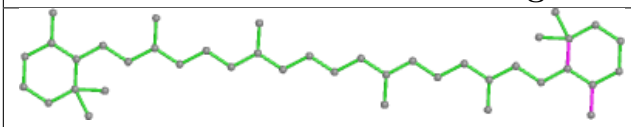


Torsions

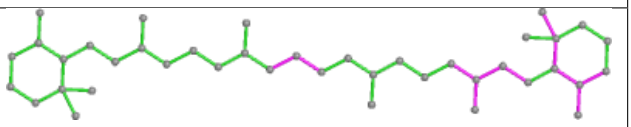


Rings

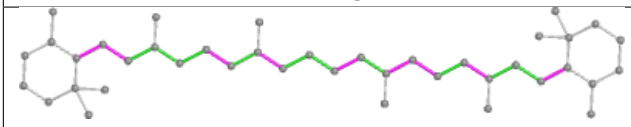
Ligand BCR c 521



Bond lengths



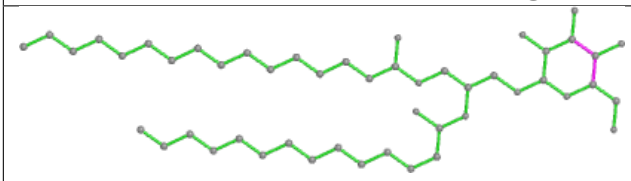
Bond angles



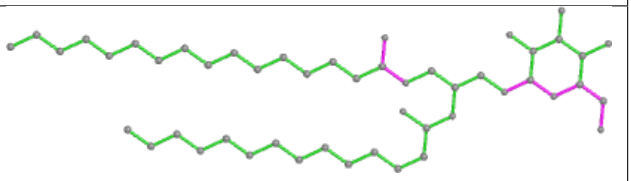
Torsions

Rings

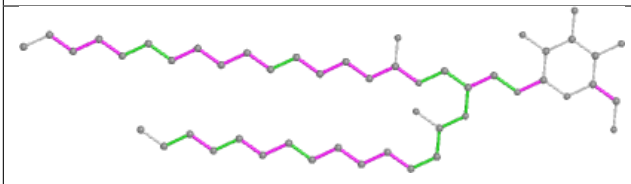
Ligand LMG c 524



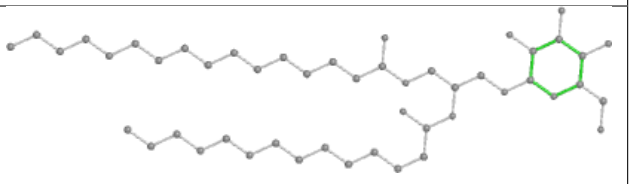
Bond lengths



Bond angles

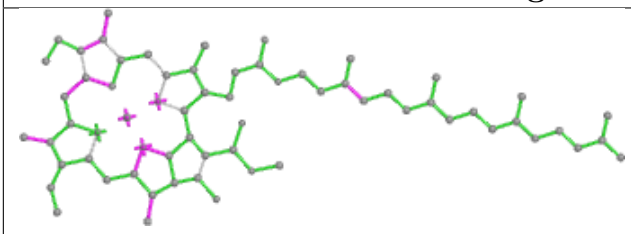


Torsions

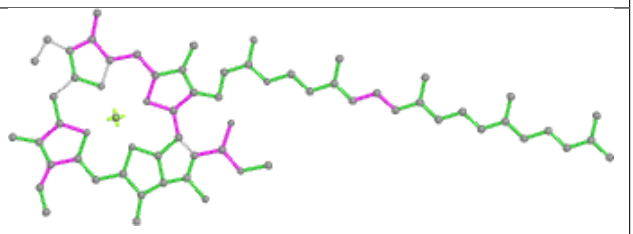


Rings

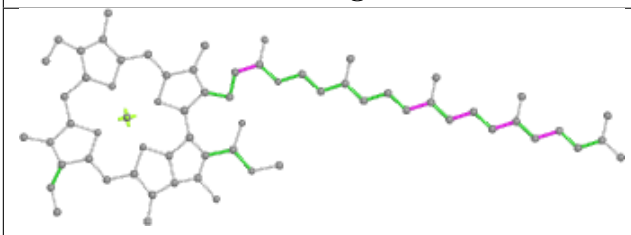
Ligand CLA b 614



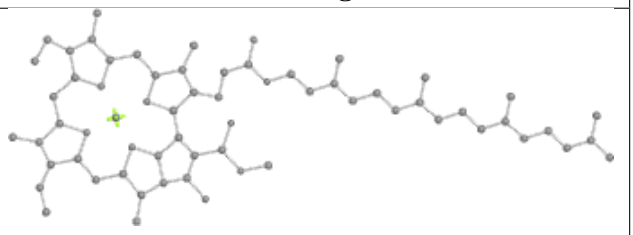
Bond lengths



Bond angles

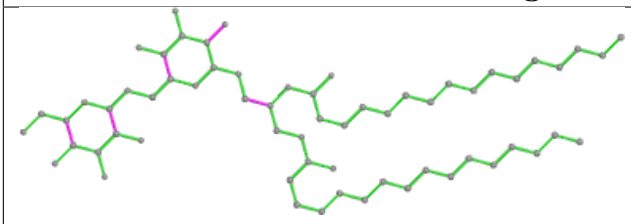


Torsions

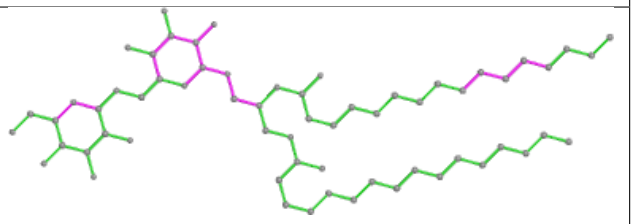


Rings

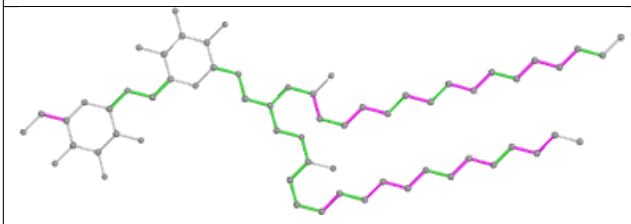
Ligand DGD h 104



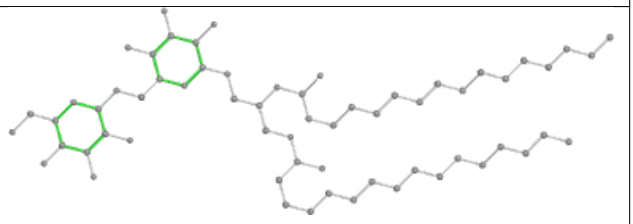
Bond lengths



Bond angles

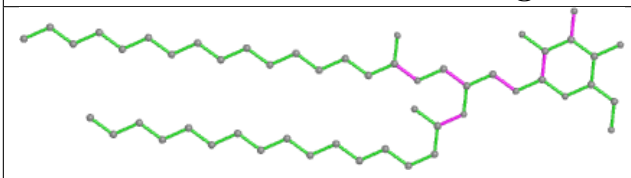


Torsions

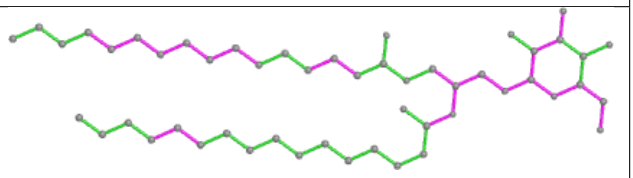


Rings

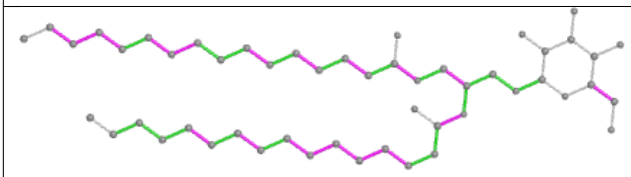
Ligand LMG M 101



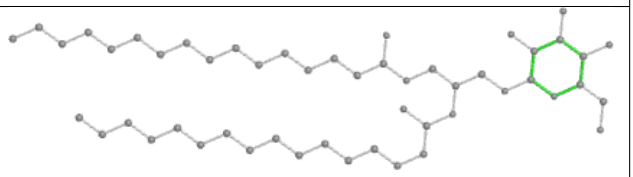
Bond lengths



Bond angles

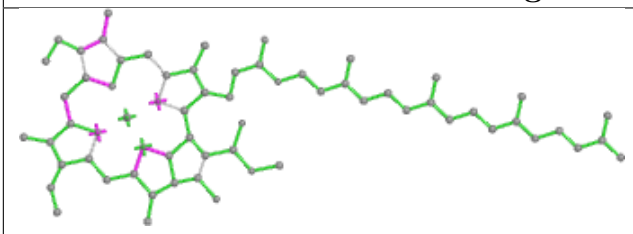


Torsions

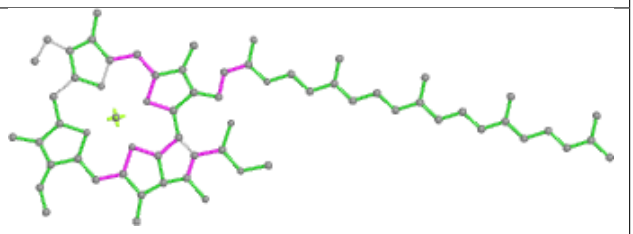


Rings

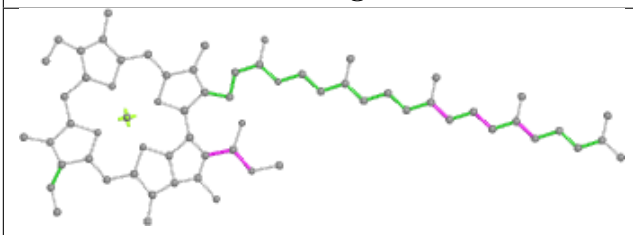
Ligand CLA C 508



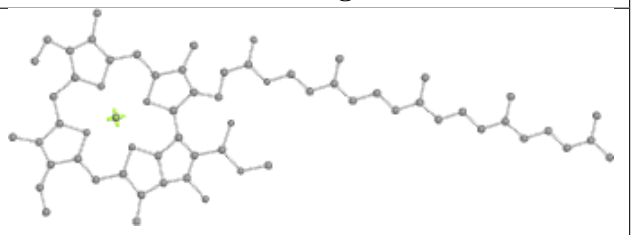
Bond lengths



Bond angles

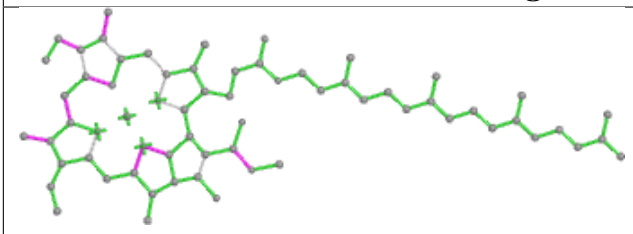


Torsions

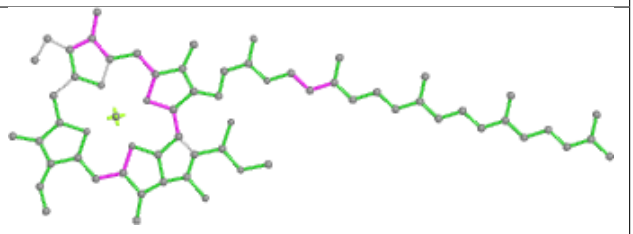


Rings

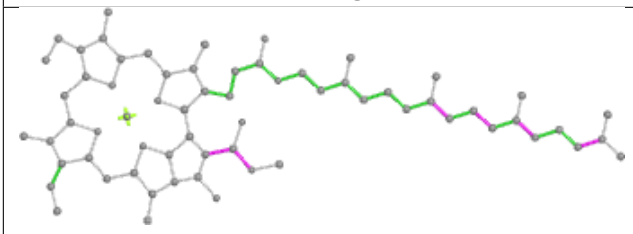
Ligand CLA C 510



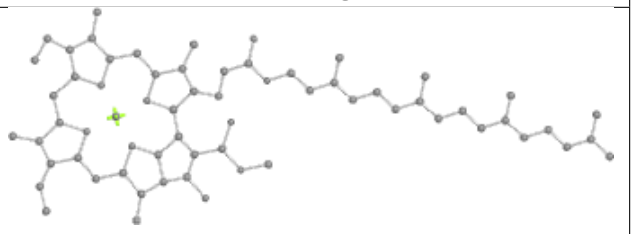
Bond lengths



Bond angles

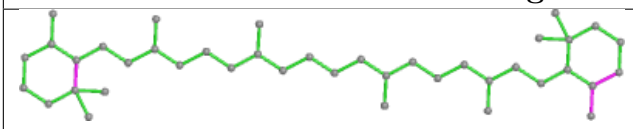


Torsions

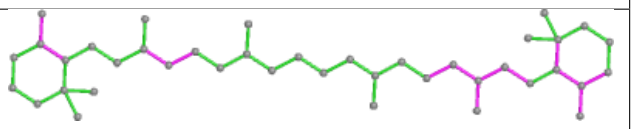


Rings

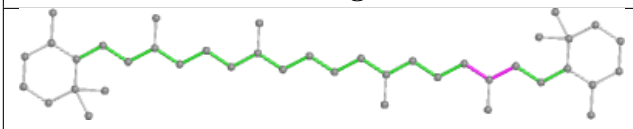
Ligand BCR a 408



Bond lengths



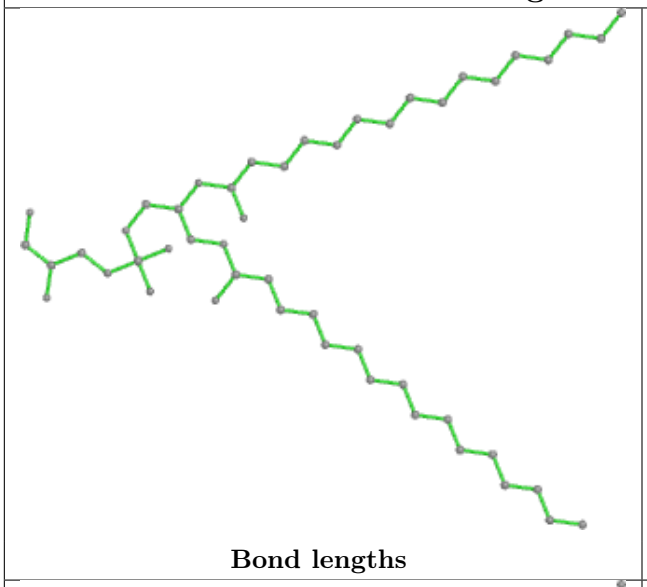
Bond angles



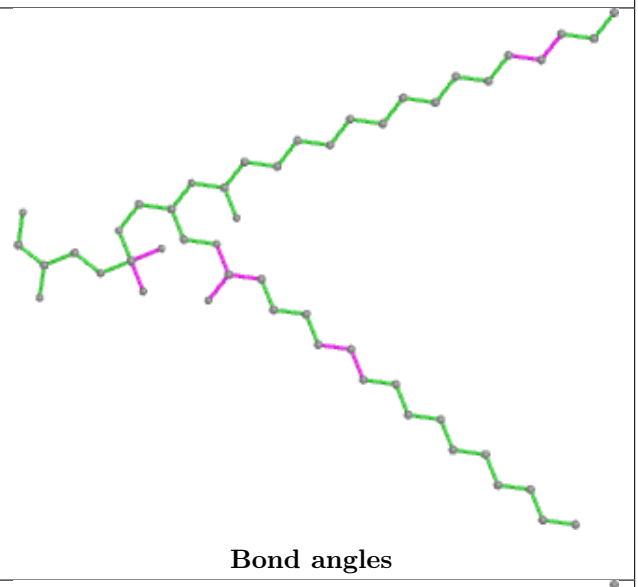
Torsions

Rings

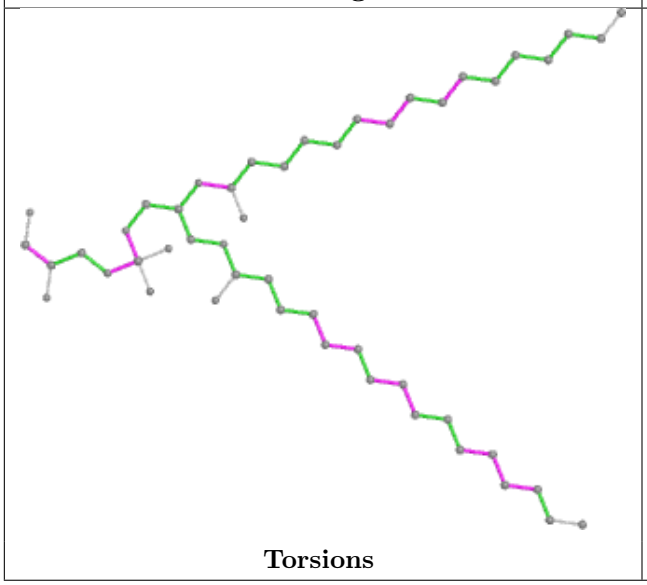
Ligand LHG d 409



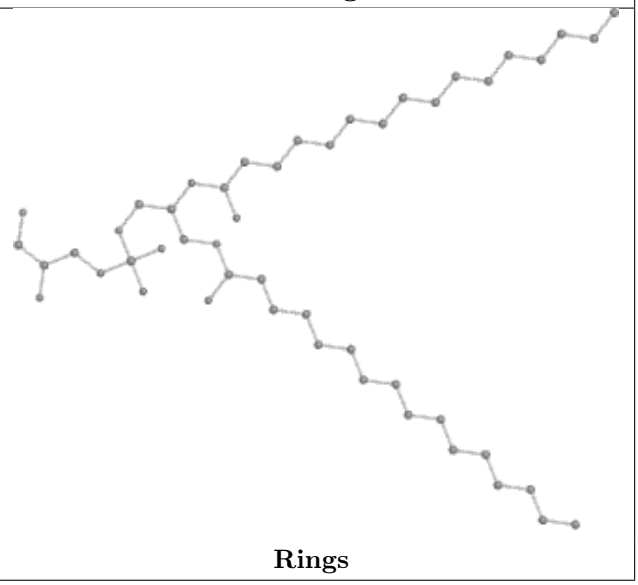
Bond lengths



Bond angles

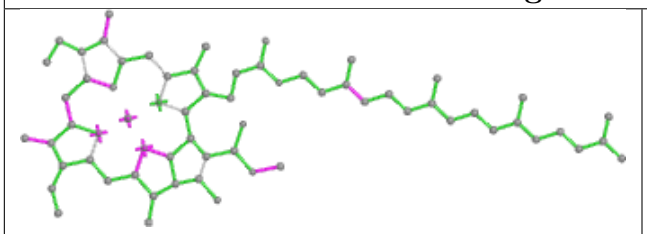


Torsions

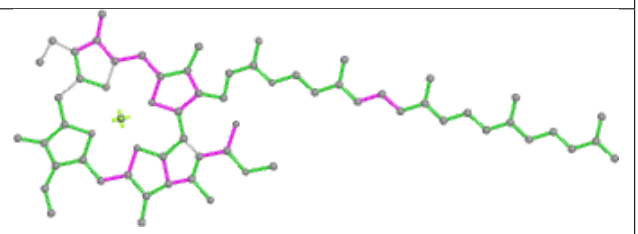


Rings

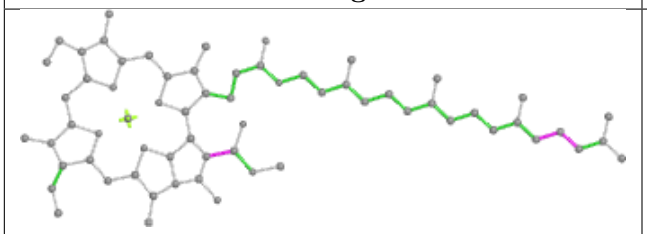
Ligand CLA A 405



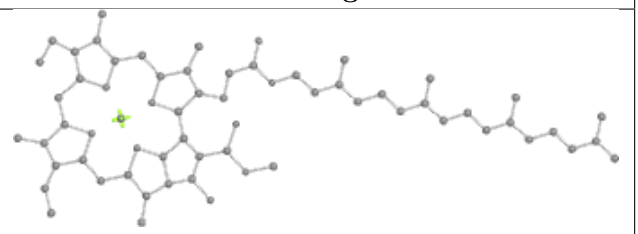
Bond lengths



Bond angles

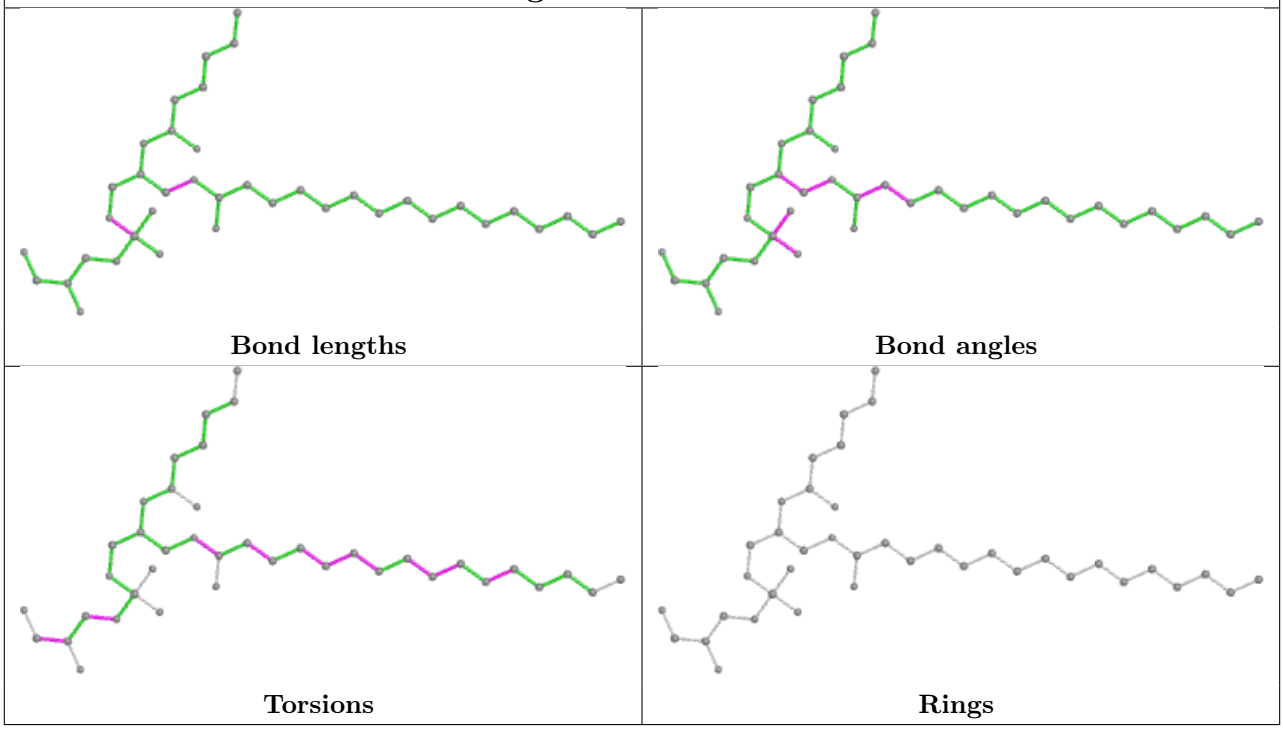


Torsions

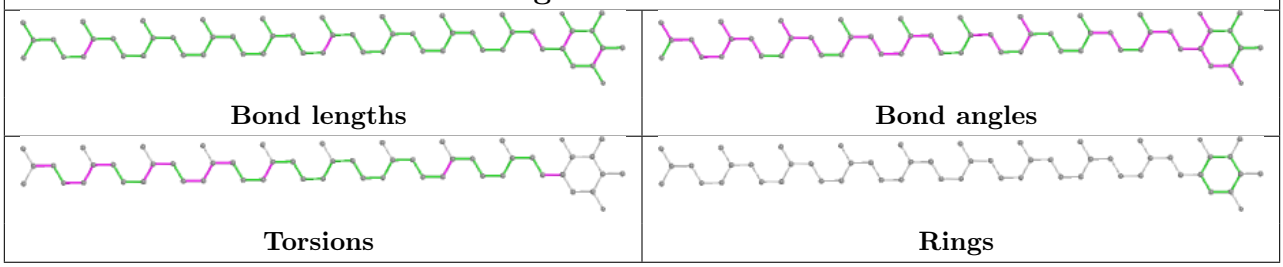


Rings

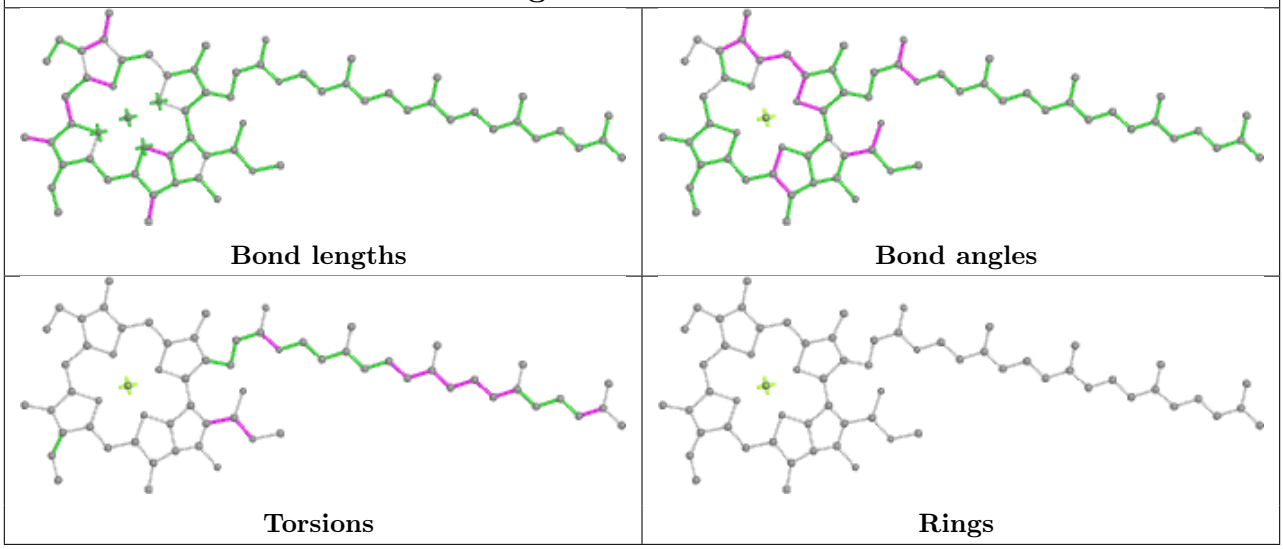
Ligand LHG d 410



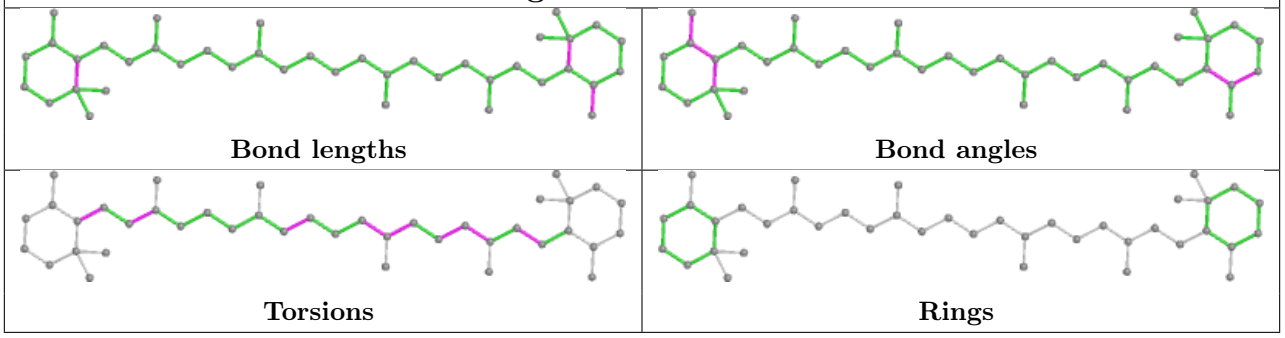
Ligand PL9 d 407



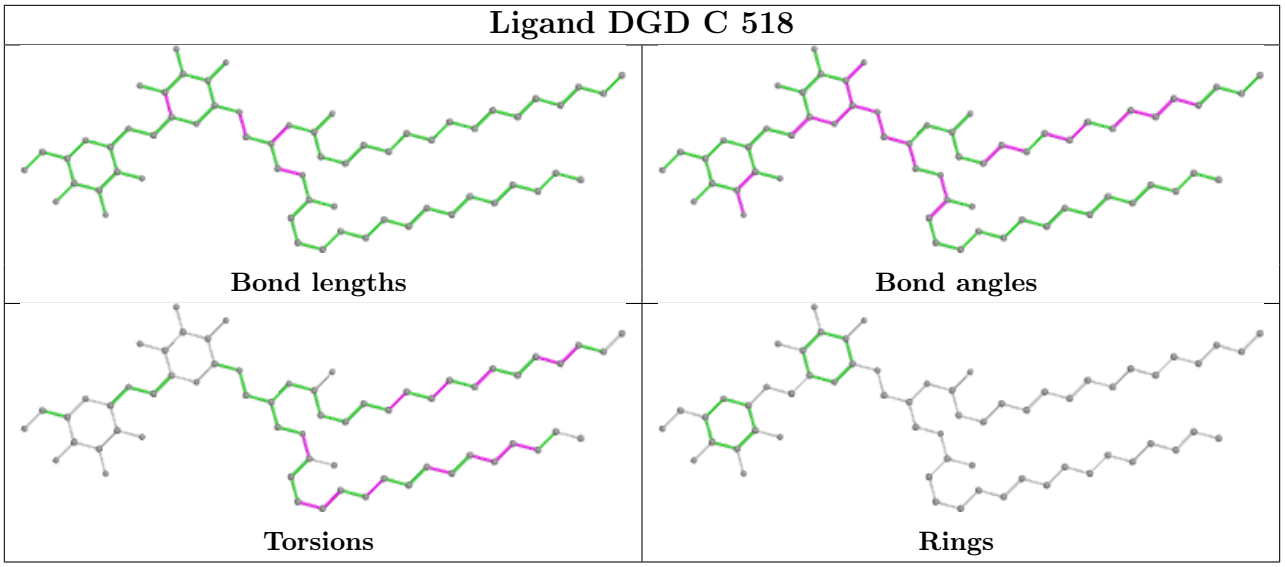
Ligand CLA b 608



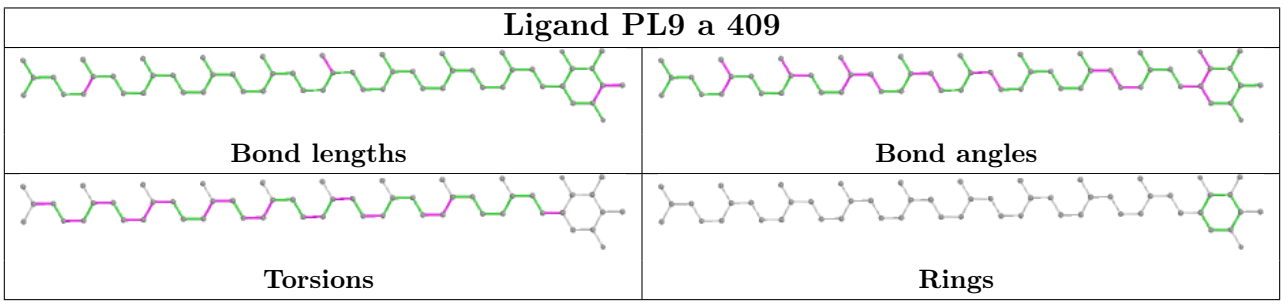
Ligand BCR k 101



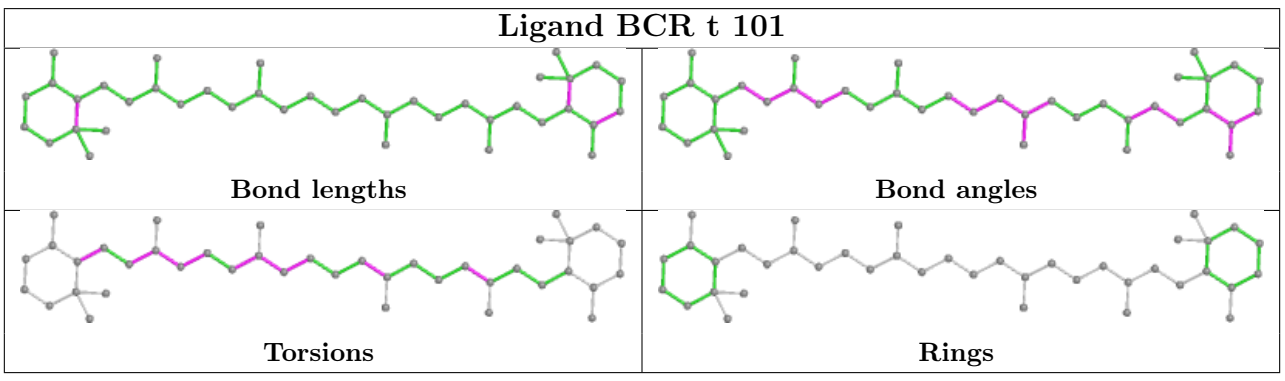
Ligand DGD C 518



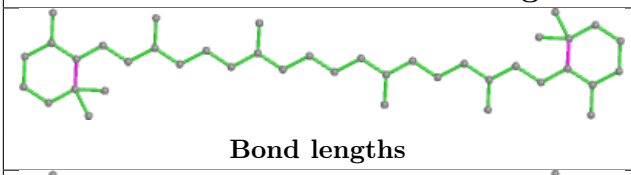
Ligand PL9 a 409



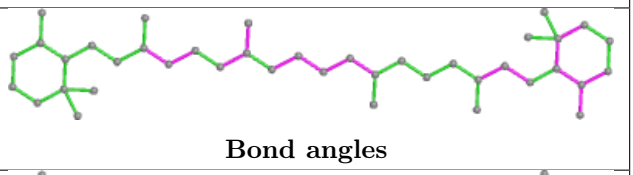
Ligand BCR t 101



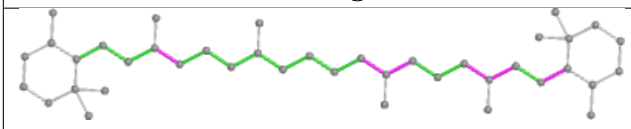
Ligand BCR H 101



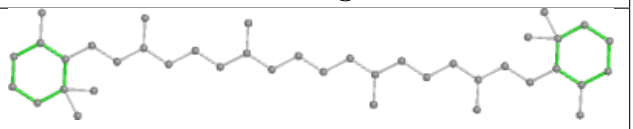
Bond lengths



Bond angles

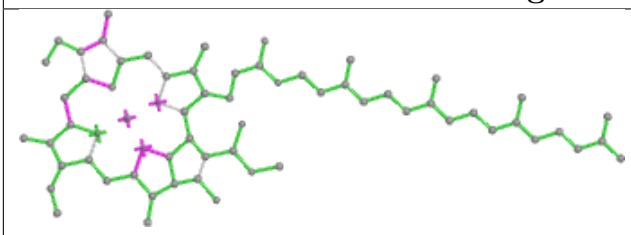


Torsions

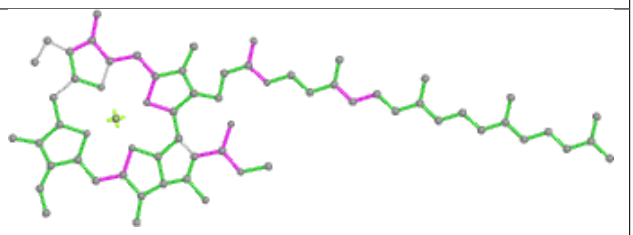


Rings

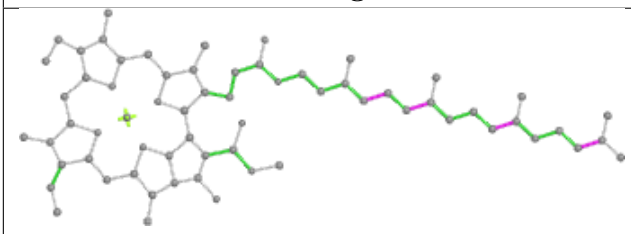
Ligand CLA d 404



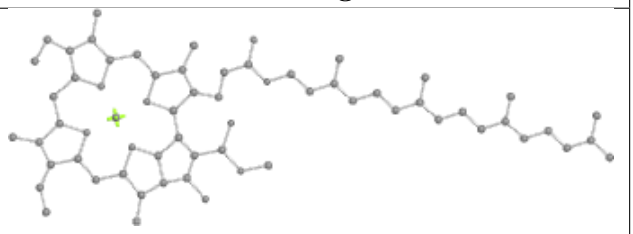
Bond lengths



Bond angles

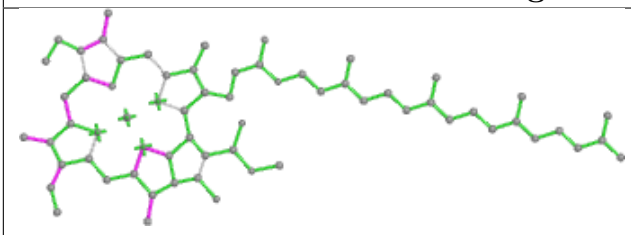


Torsions

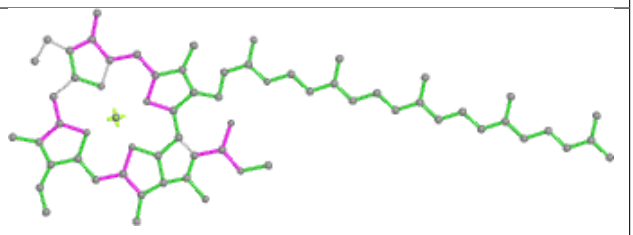


Rings

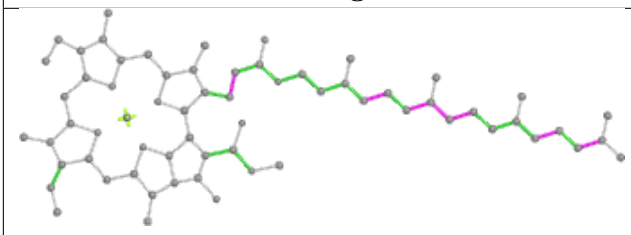
Ligand CLA b 603



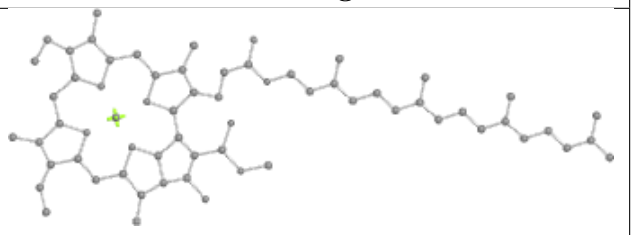
Bond lengths



Bond angles

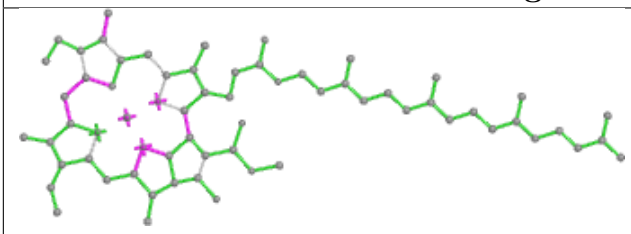


Torsions

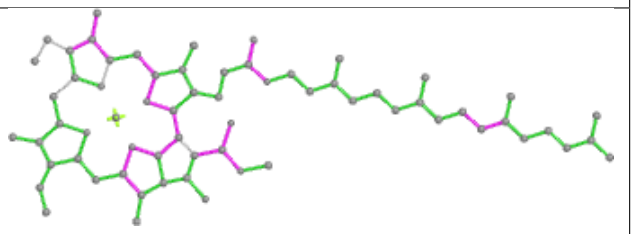


Rings

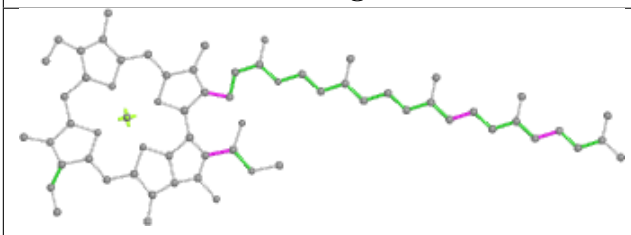
Ligand CLA B 602



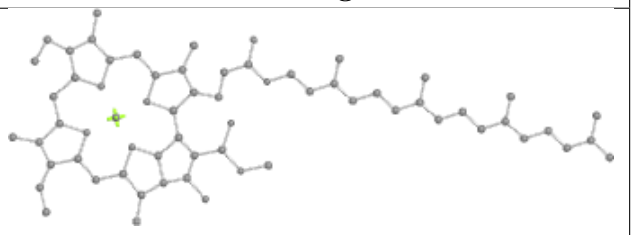
Bond lengths



Bond angles

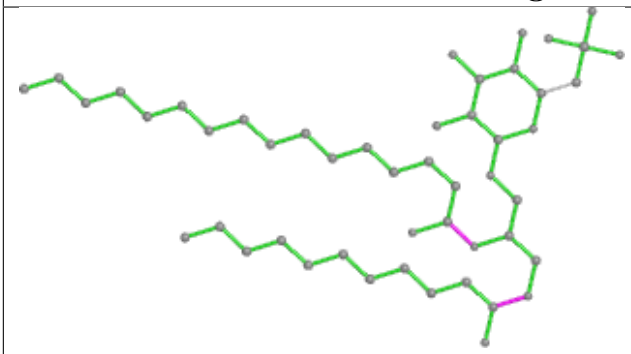


Torsions

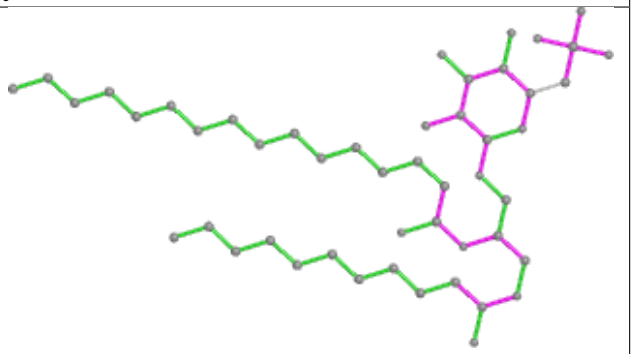


Rings

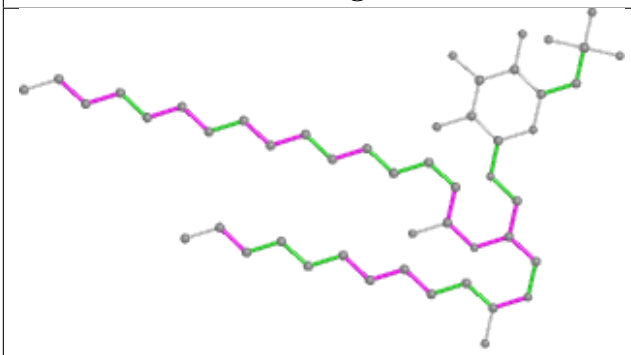
Ligand SQD b 601



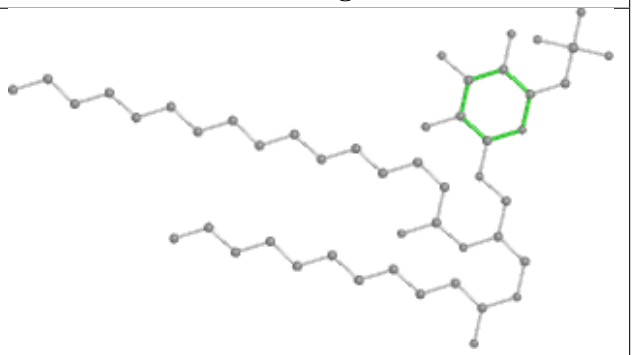
Bond lengths



Bond angles

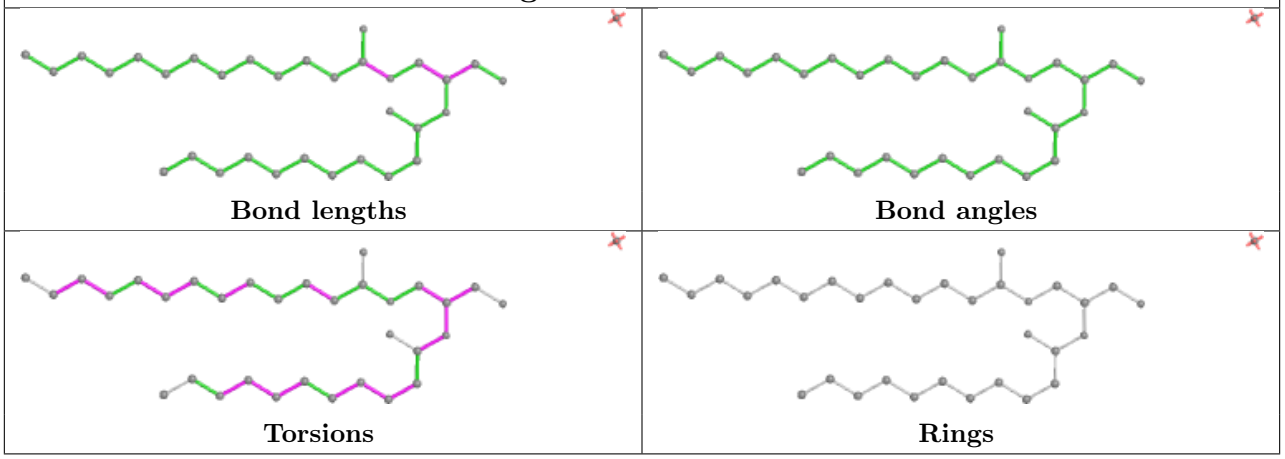


Torsions

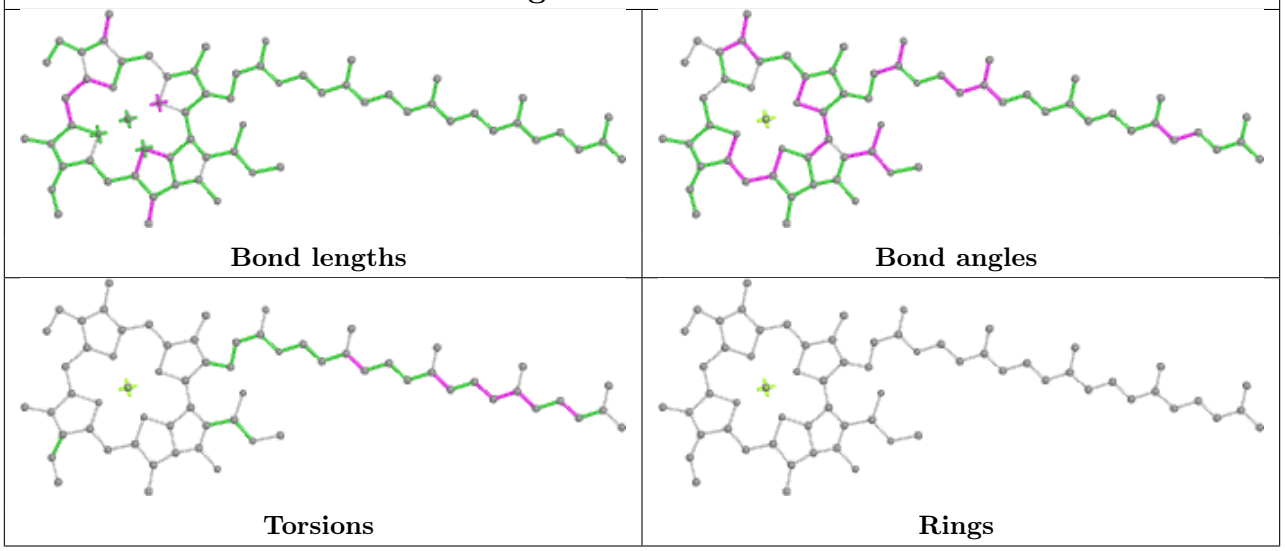


Rings

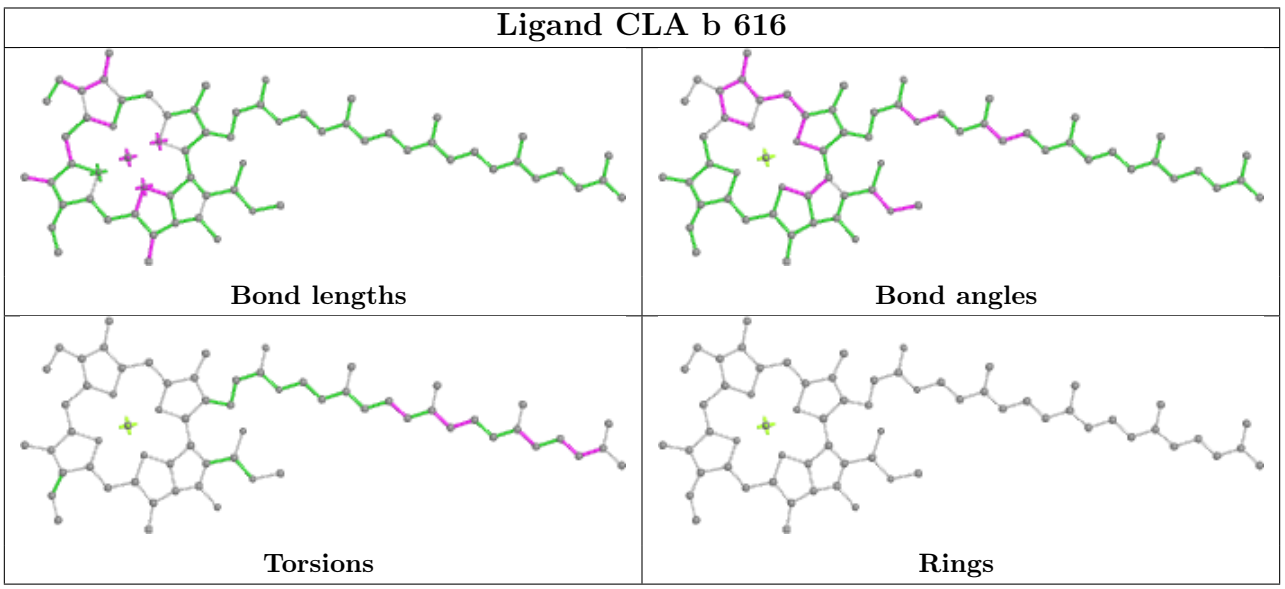
Ligand LMG D 410



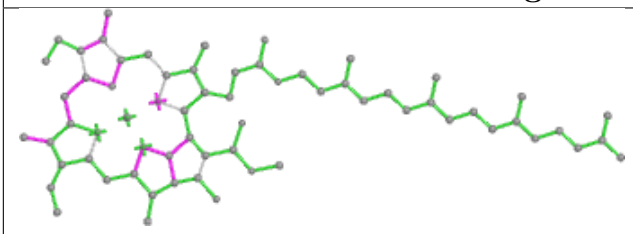
Ligand CLA b 606



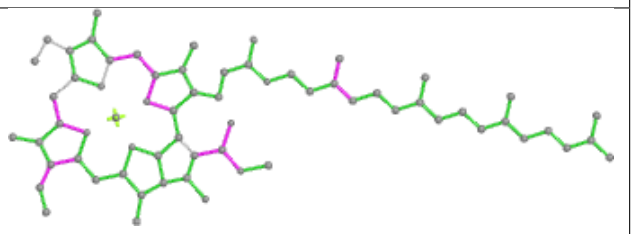
Ligand CLA b 616



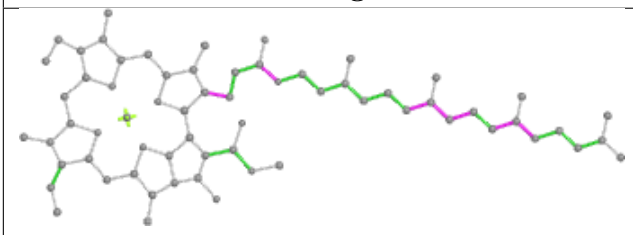
Ligand CLA C 512



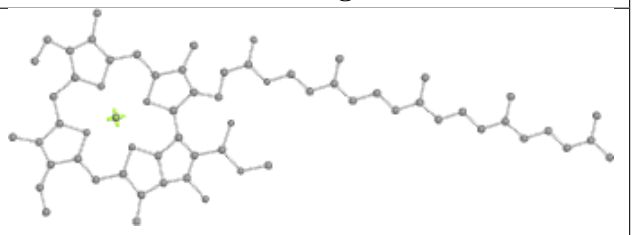
Bond lengths



Bond angles

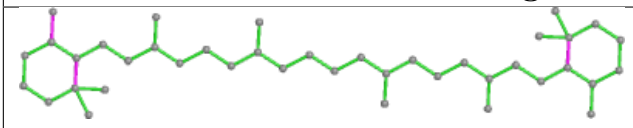


Torsions

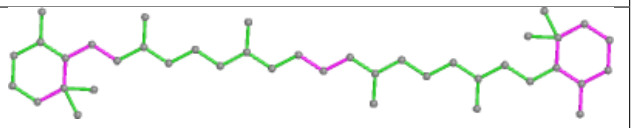


Rings

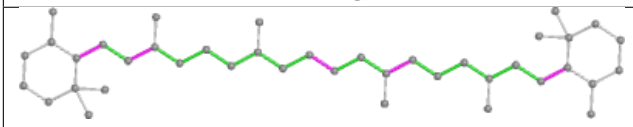
Ligand BCR A 409



Bond lengths



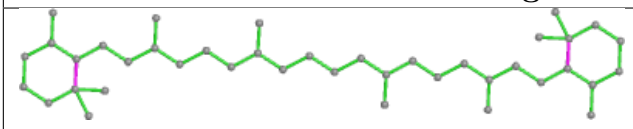
Bond angles



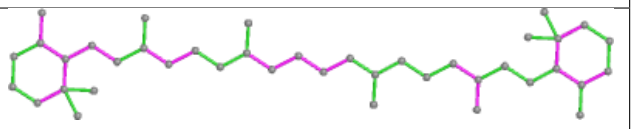
Torsions

Rings

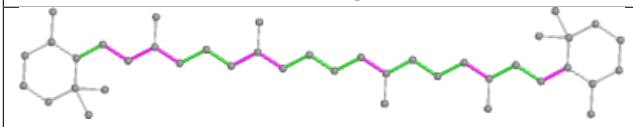
Ligand BCR C 519



Bond lengths



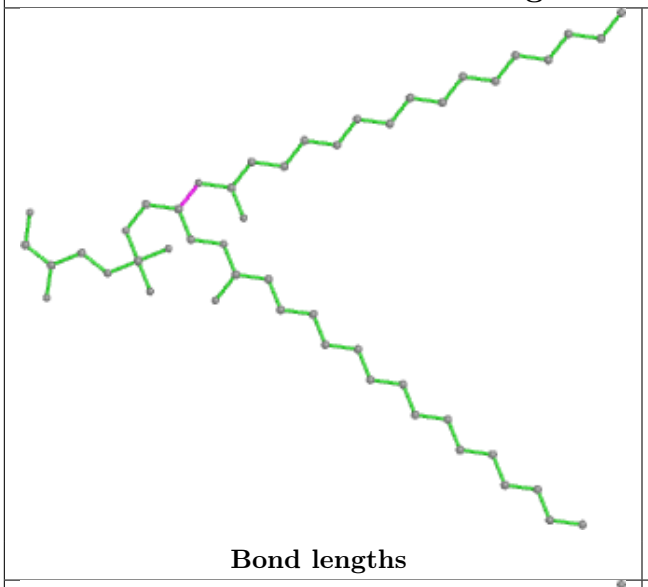
Bond angles



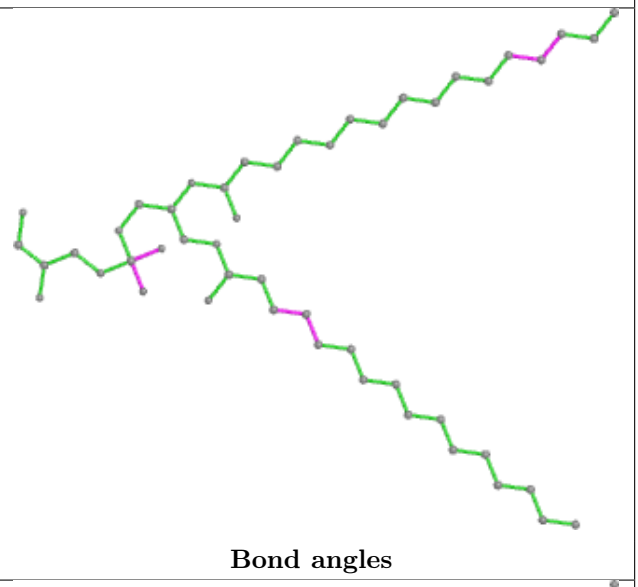
Torsions

Rings

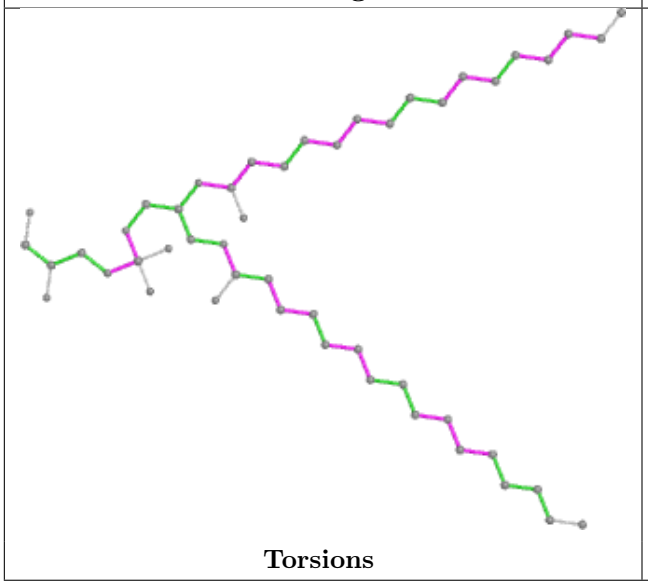
Ligand LHG L 101



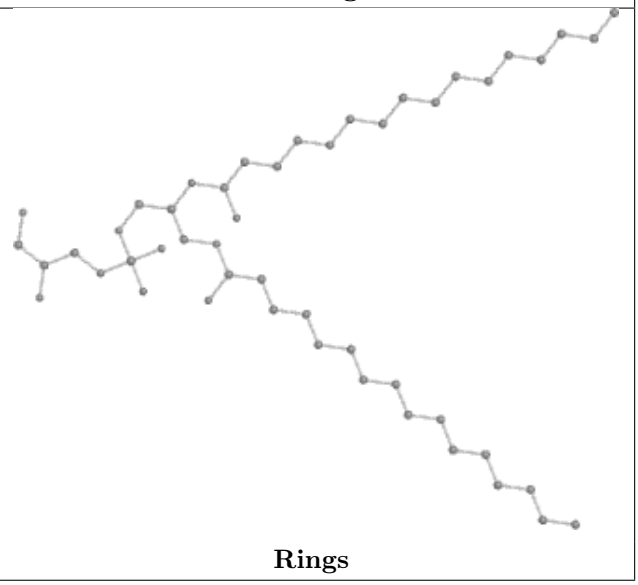
Bond lengths



Bond angles

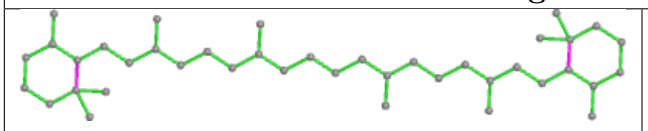


Torsions

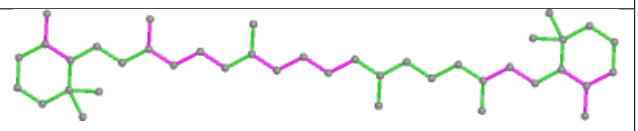


Rings

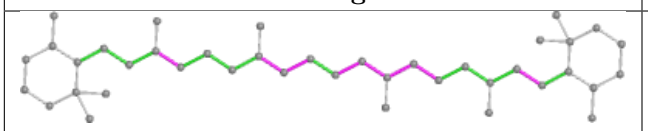
Ligand BCR c 514



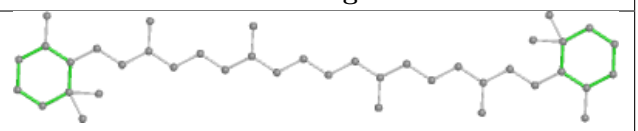
Bond lengths



Bond angles

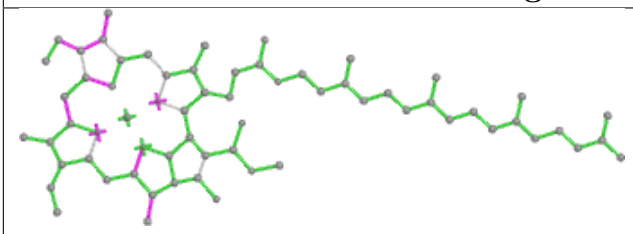


Torsions

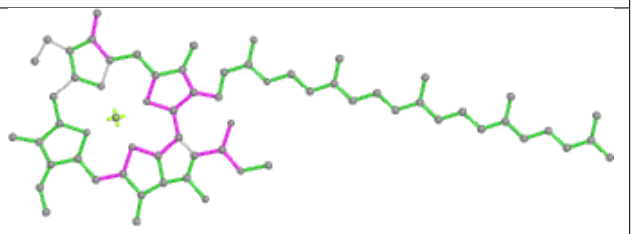


Rings

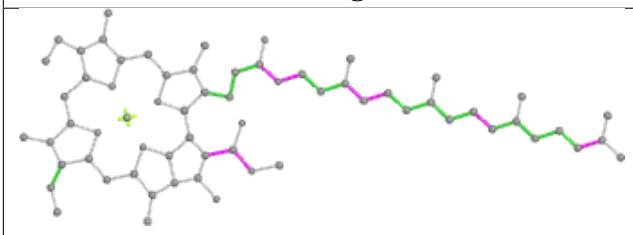
Ligand CLA B 601



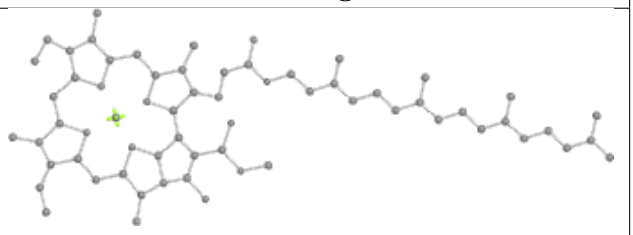
Bond lengths



Bond angles

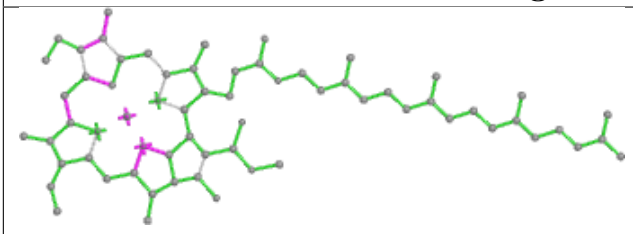


Torsions

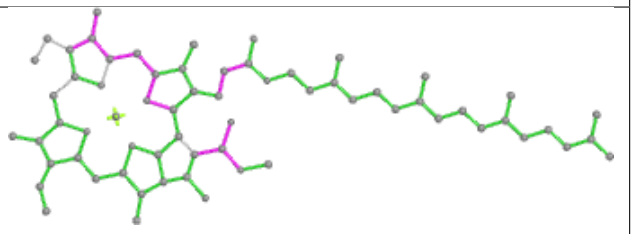


Rings

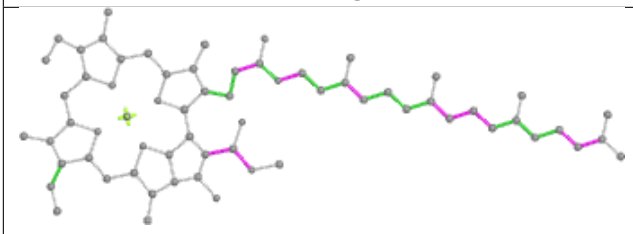
Ligand CLA c 510



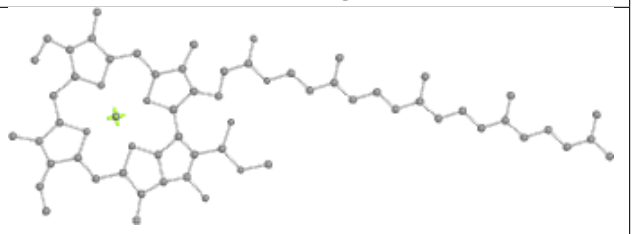
Bond lengths



Bond angles

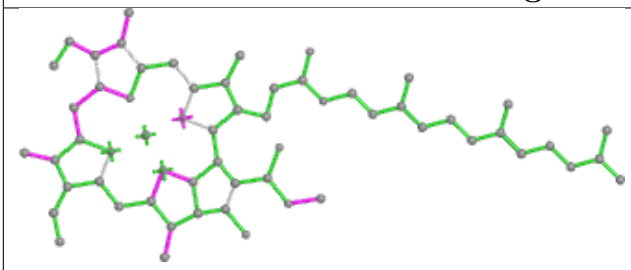


Torsions

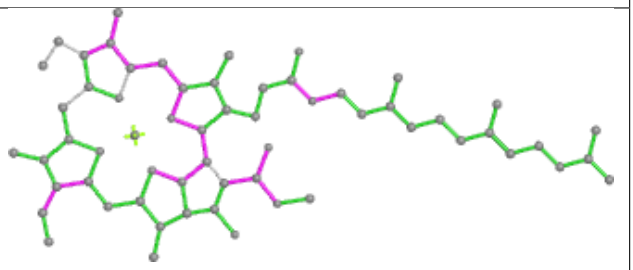


Rings

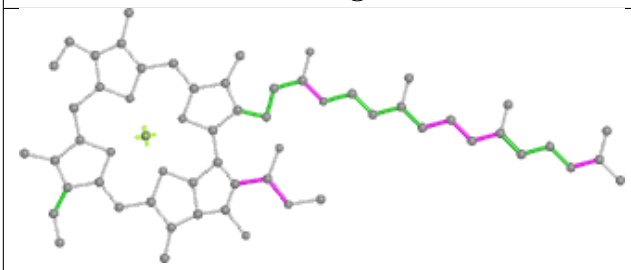
Ligand CLA B 616



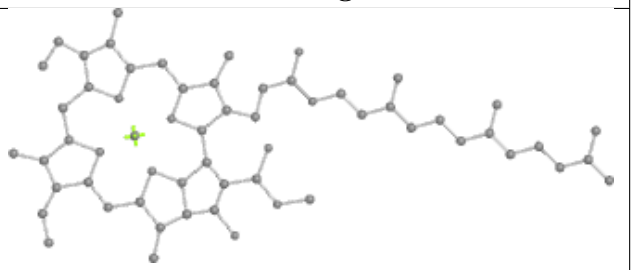
Bond lengths



Bond angles

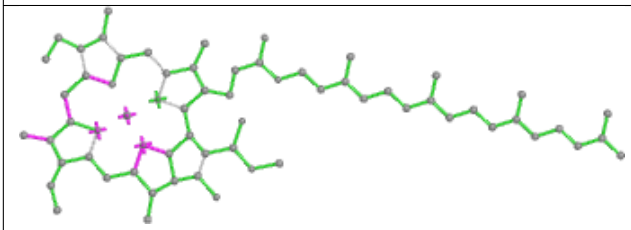


Torsions

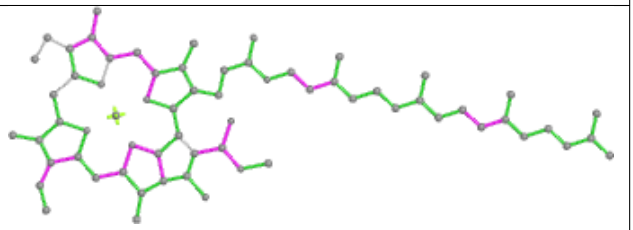


Rings

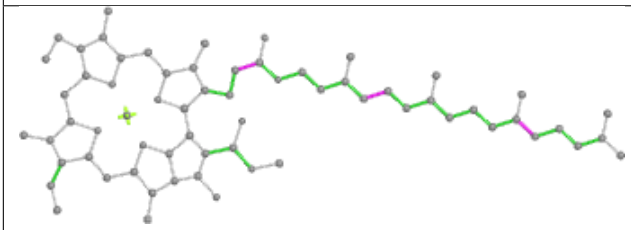
Ligand CLA b 613



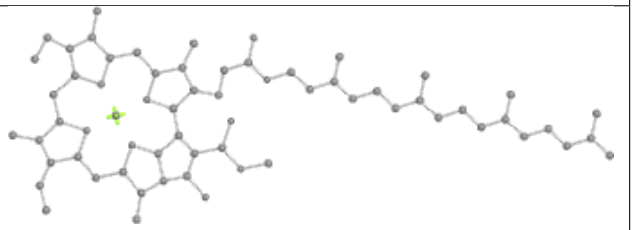
Bond lengths



Bond angles

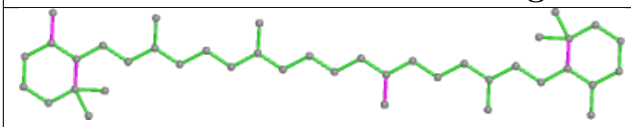


Torsions

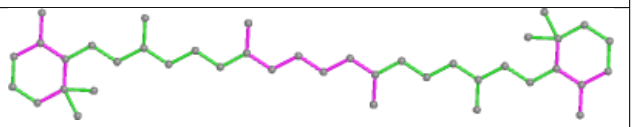


Rings

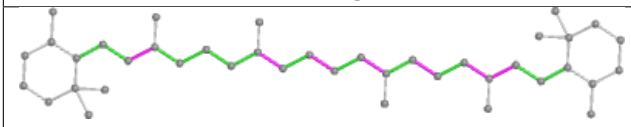
Ligand BCR c 515



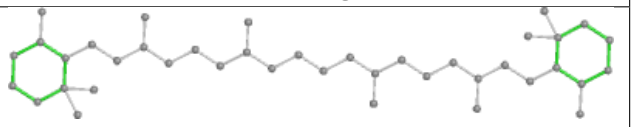
Bond lengths



Bond angles

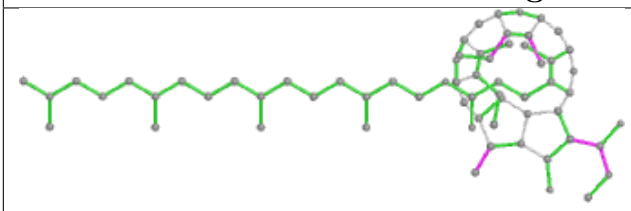


Torsions

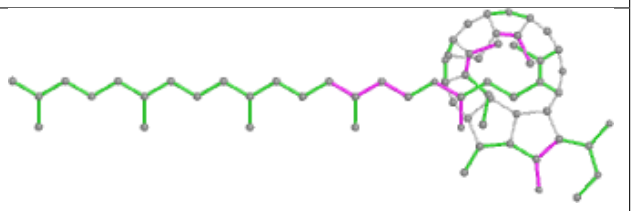


Rings

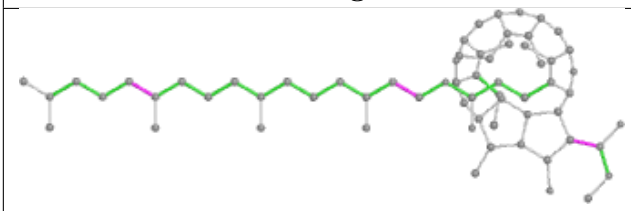
Ligand PHO a 406



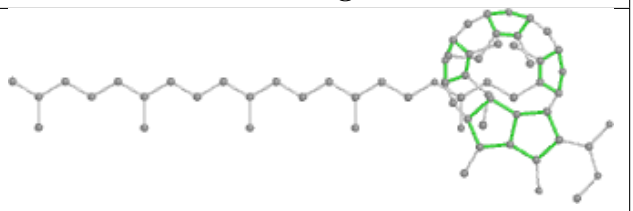
Bond lengths



Bond angles

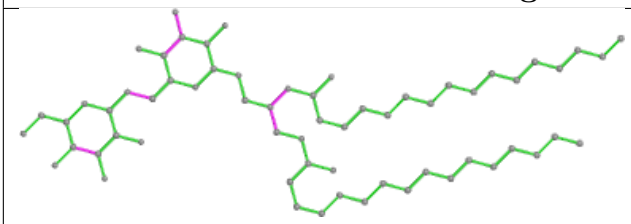


Torsions

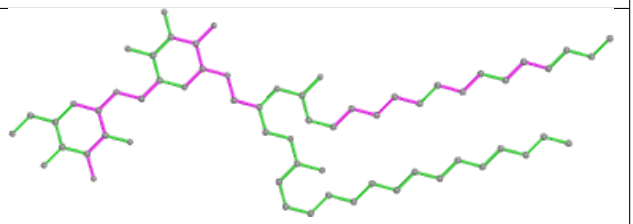


Rings

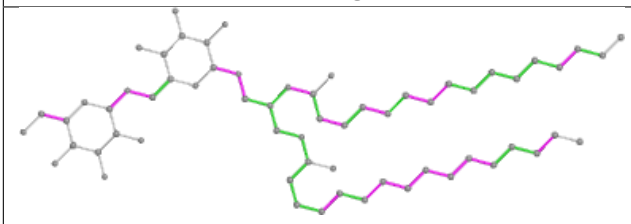
Ligand DGD C 517



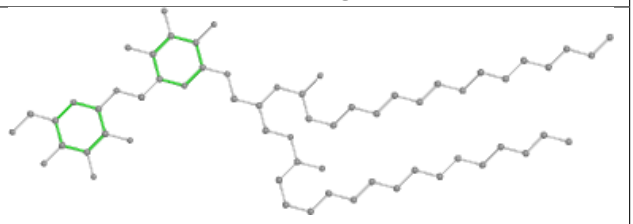
Bond lengths



Bond angles

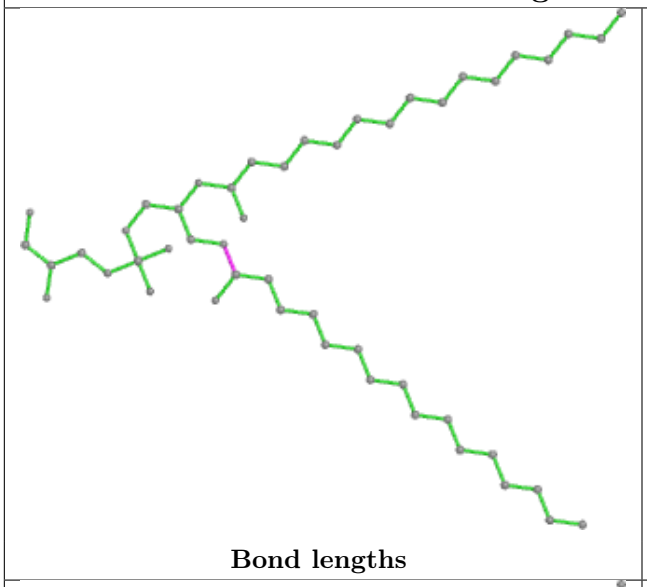


Torsions

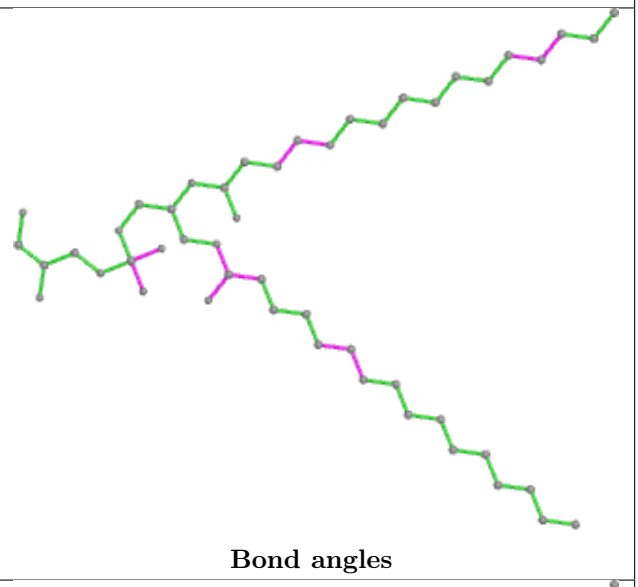


Rings

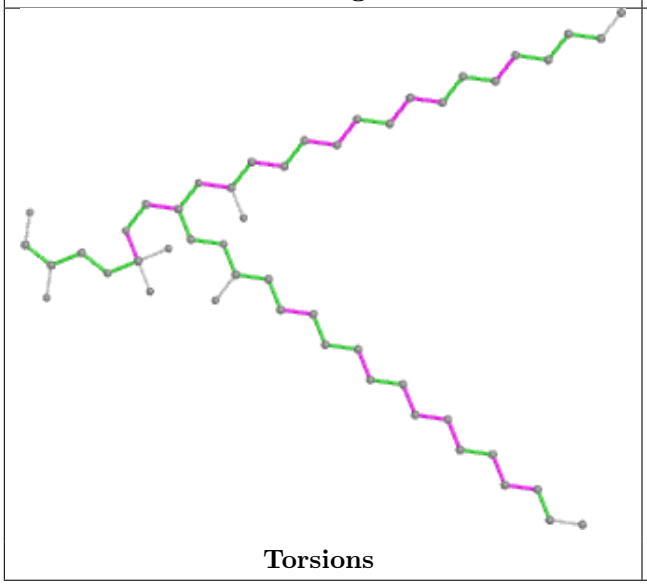
Ligand LHG l 101



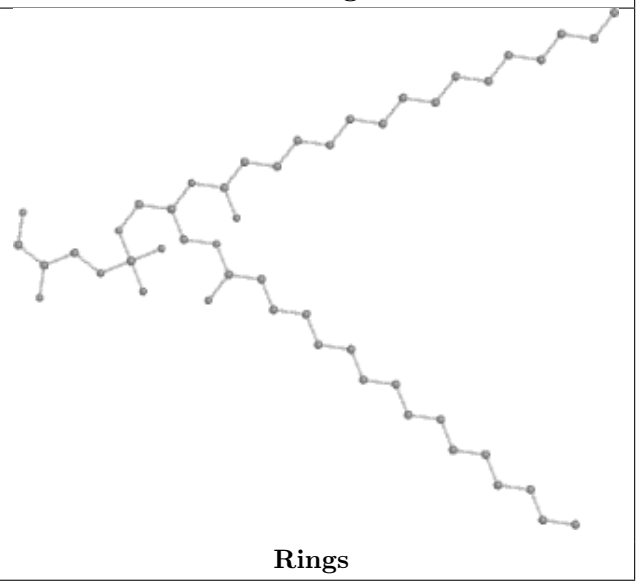
Bond lengths



Bond angles

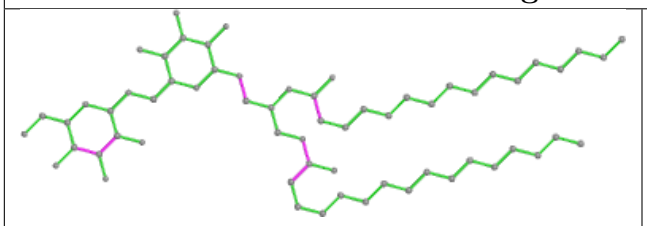


Torsions

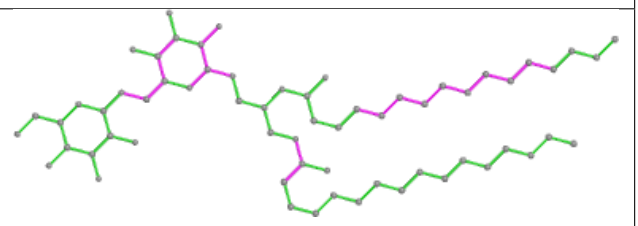


Rings

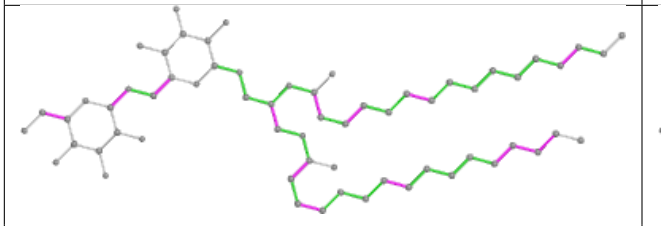
Ligand DGD C 516



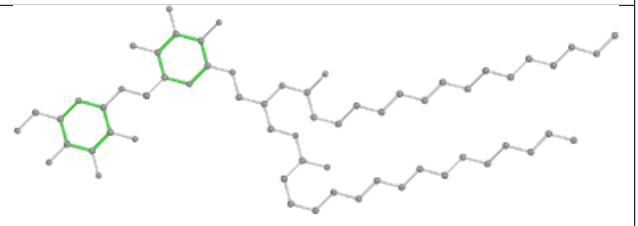
Bond lengths



Bond angles

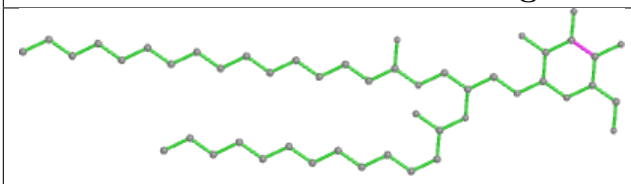


Torsions

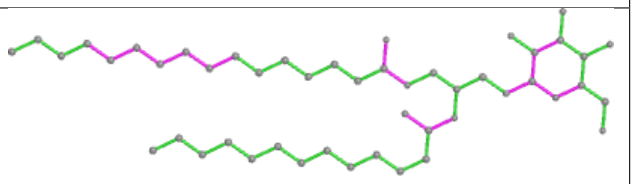


Rings

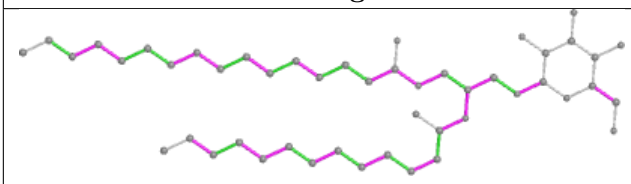
Ligand LMG C 501



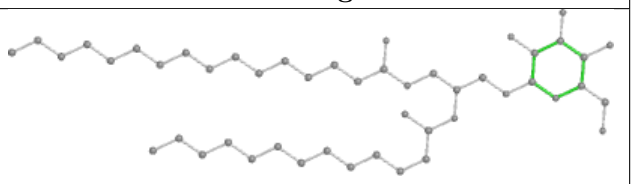
Bond lengths



Bond angles

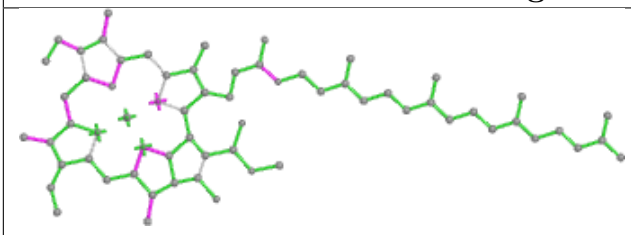


Torsions

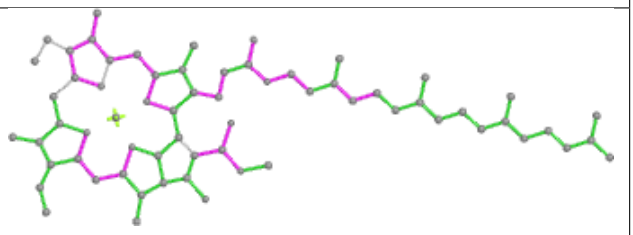


Rings

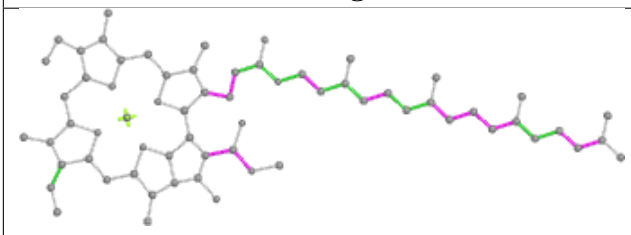
Ligand CLA h 101



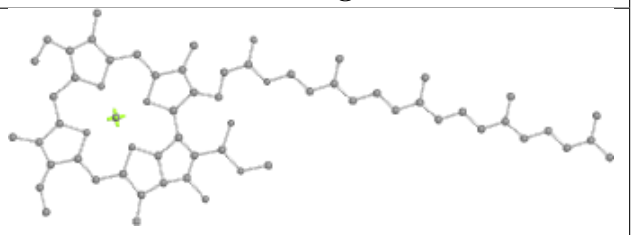
Bond lengths



Bond angles

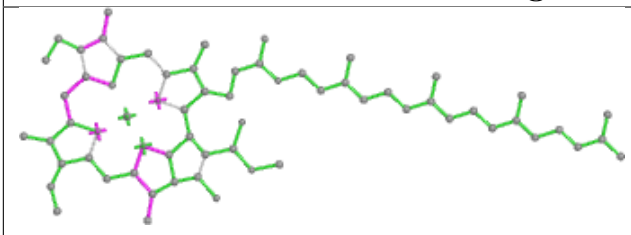


Torsions

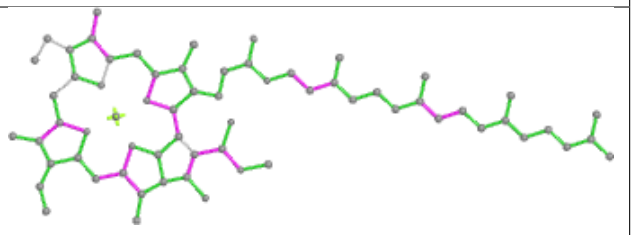


Rings

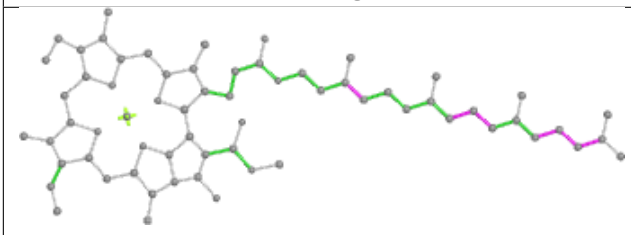
Ligand CLA b 612



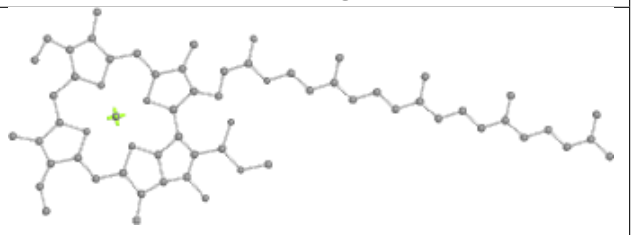
Bond lengths



Bond angles

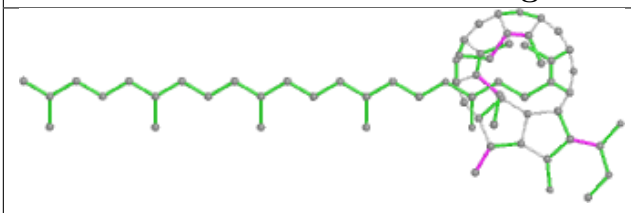


Torsions

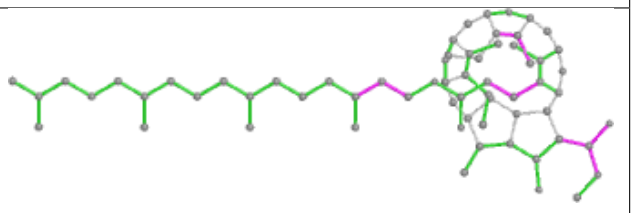


Rings

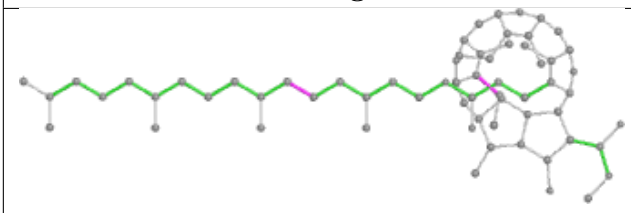
Ligand PHO D 401



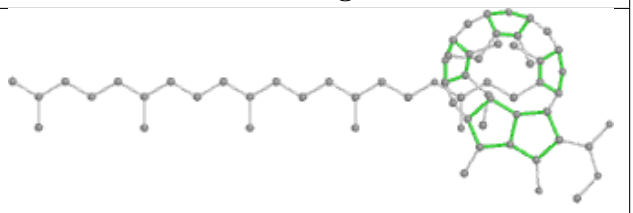
Bond lengths



Bond angles

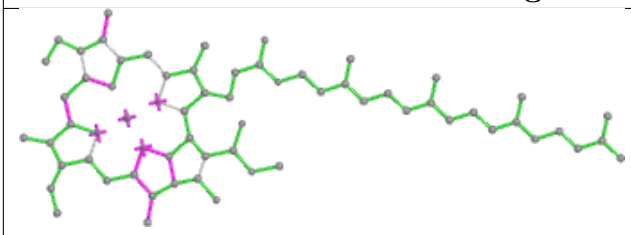


Torsions

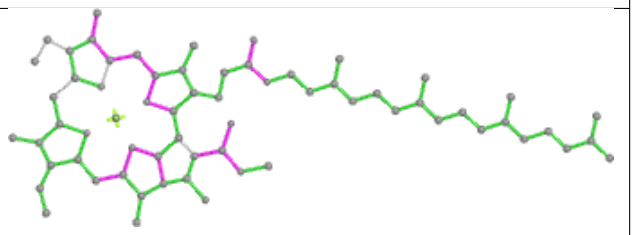


Rings

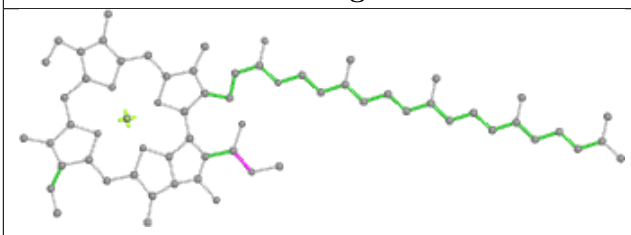
Ligand CLA C 502



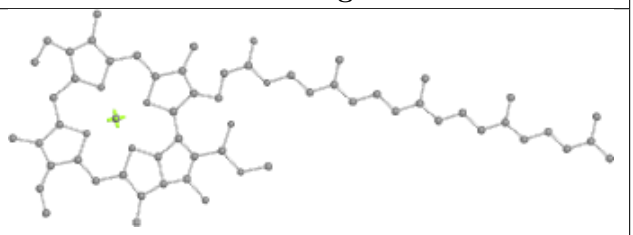
Bond lengths



Bond angles

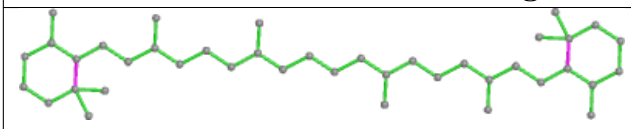


Torsions

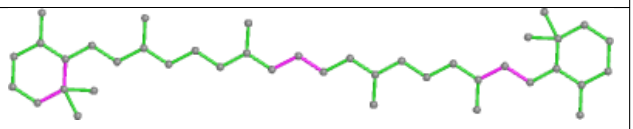


Rings

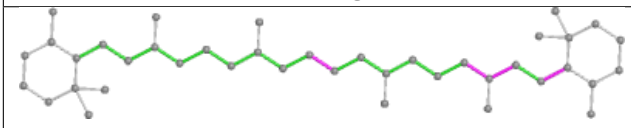
Ligand BCR D 405



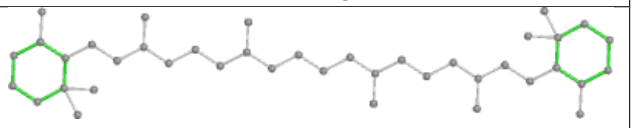
Bond lengths



Bond angles

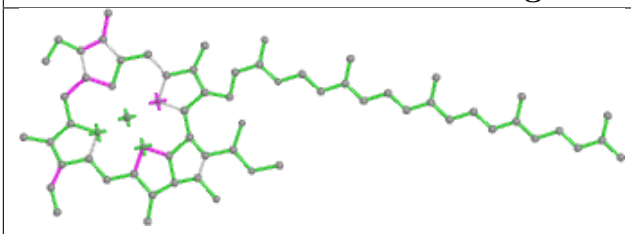


Torsions

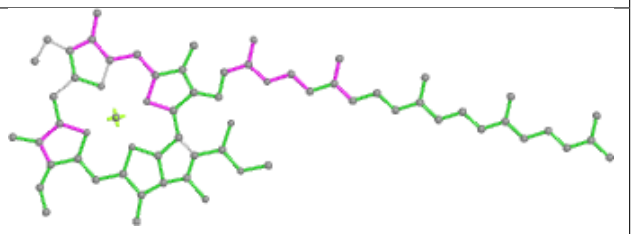


Rings

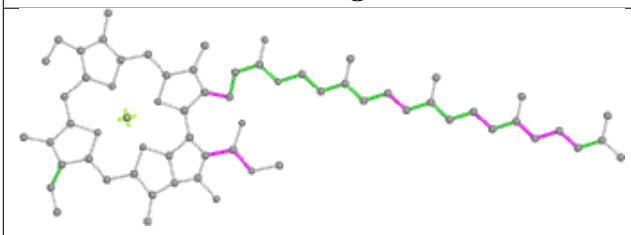
Ligand CLA B 607



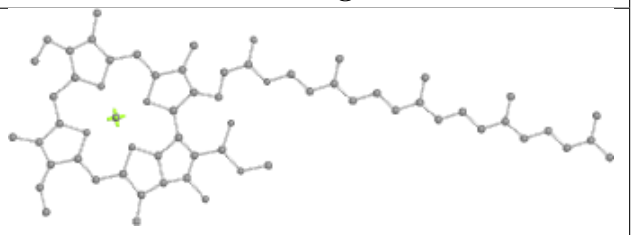
Bond lengths



Bond angles

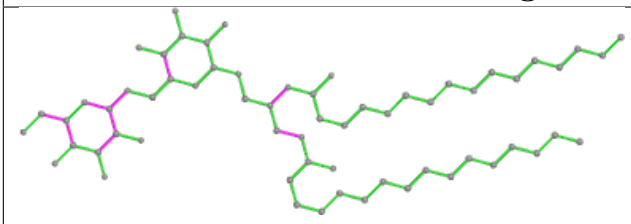


Torsions

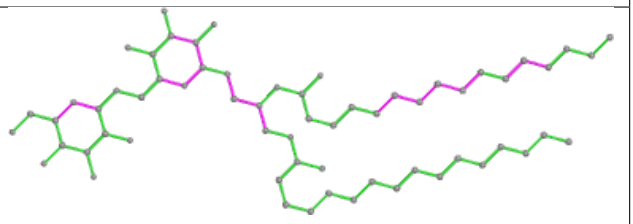


Rings

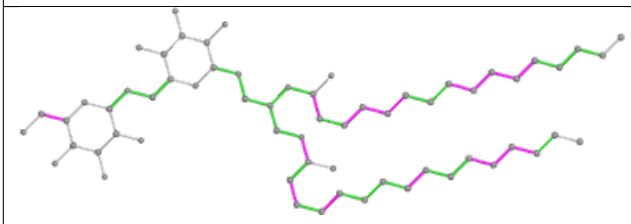
Ligand DGD H 102



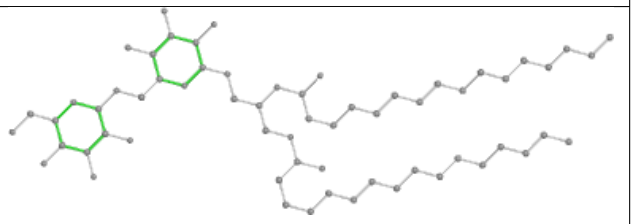
Bond lengths



Bond angles

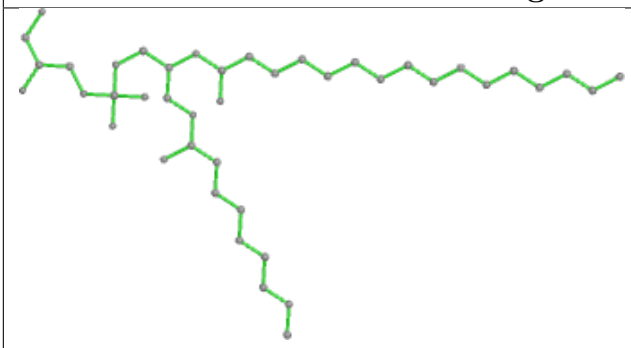


Torsions

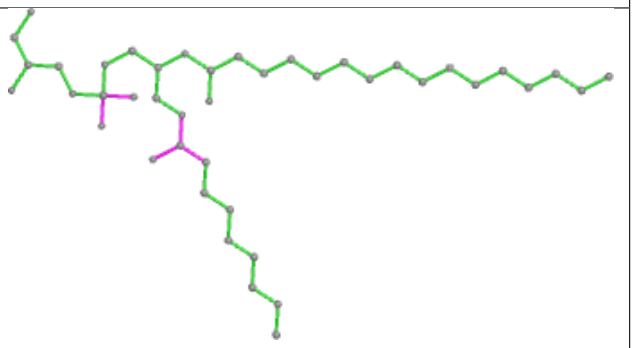


Rings

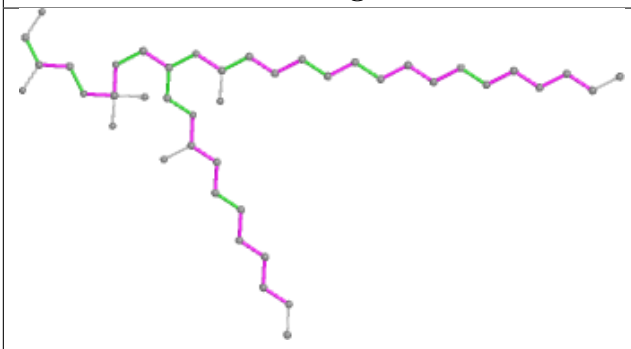
Ligand LHG e 101



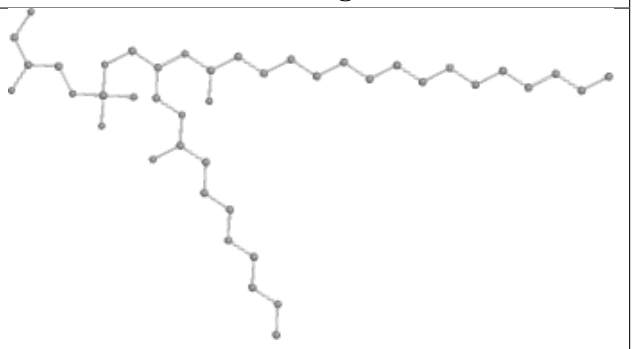
Bond lengths



Bond angles

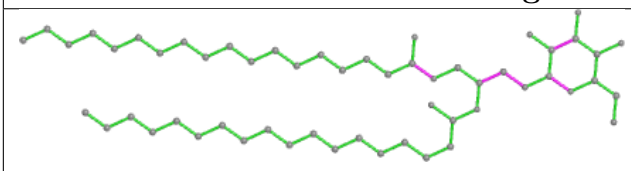


Torsions

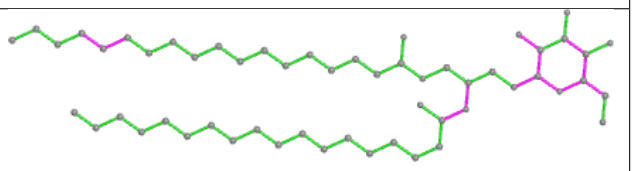


Rings

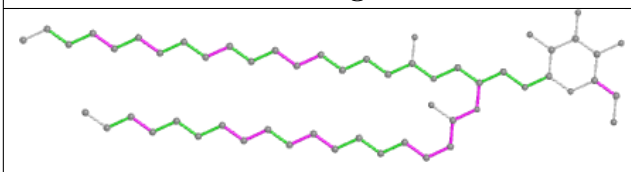
Ligand LMG b 623



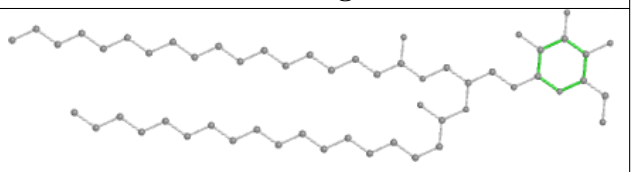
Bond lengths



Bond angles

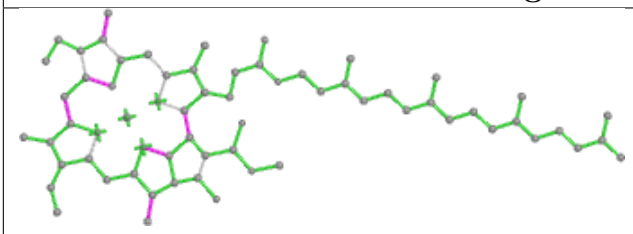


Torsions

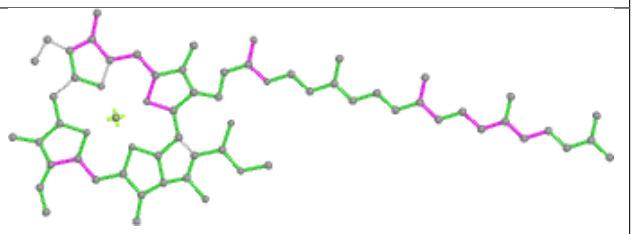


Rings

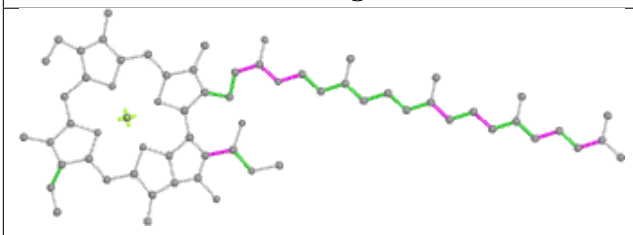
Ligand CLA B 612



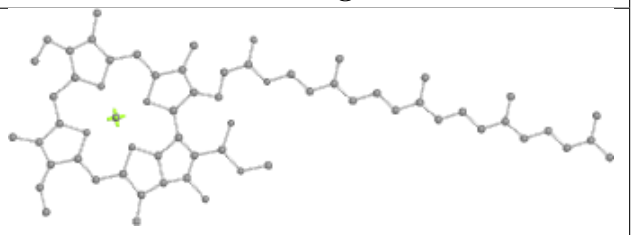
Bond lengths



Bond angles

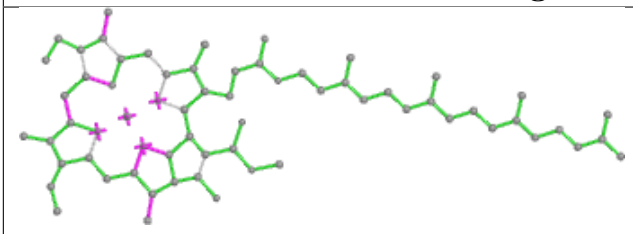


Torsions

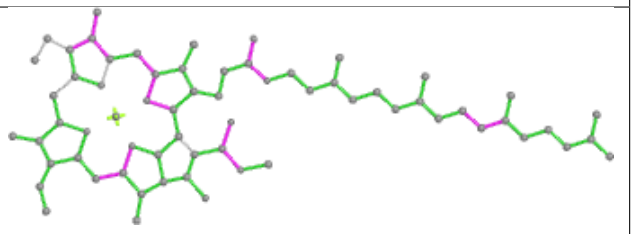


Rings

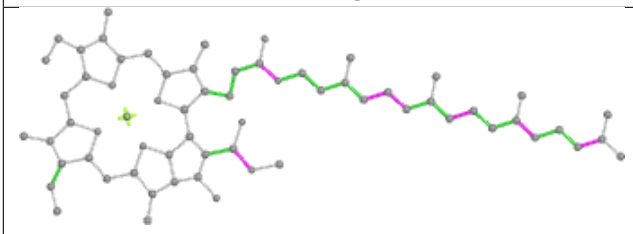
Ligand CLA c 513



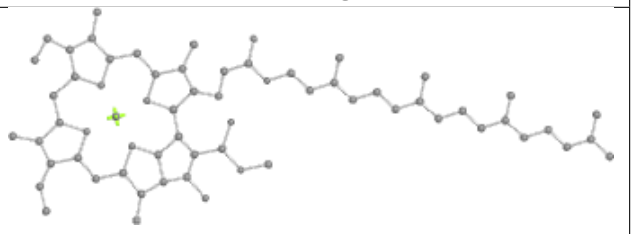
Bond lengths



Bond angles

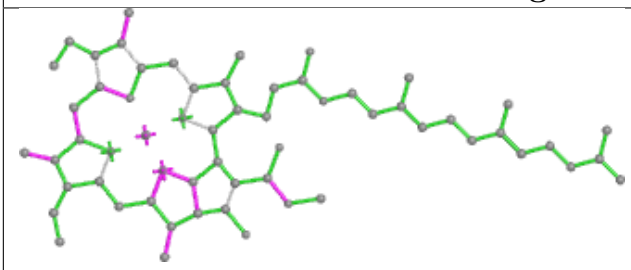


Torsions

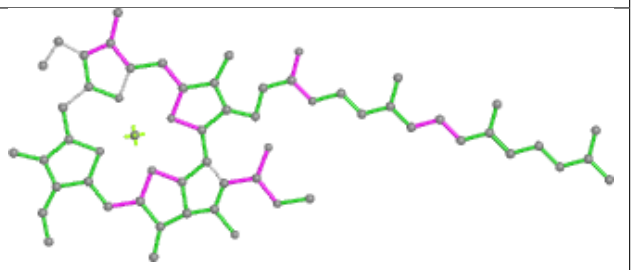


Rings

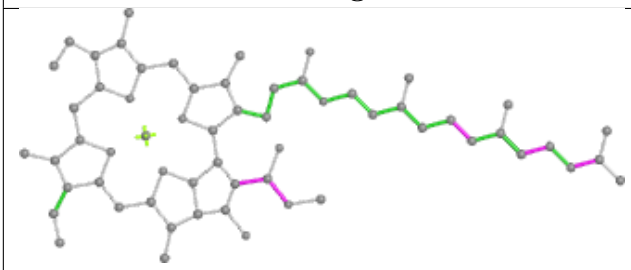
Ligand CLA c 504



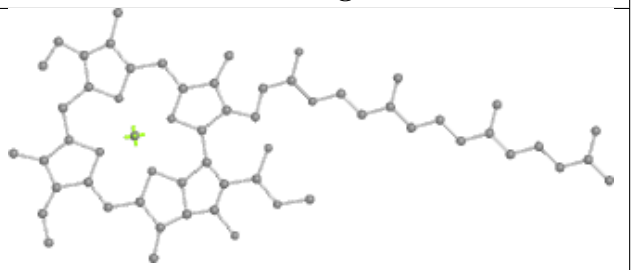
Bond lengths



Bond angles

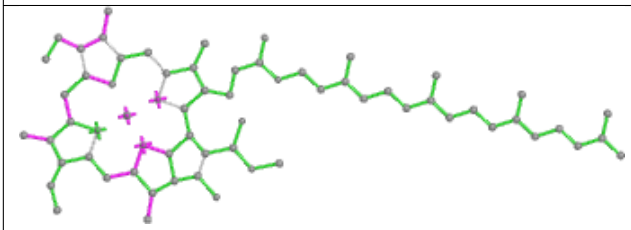


Torsions

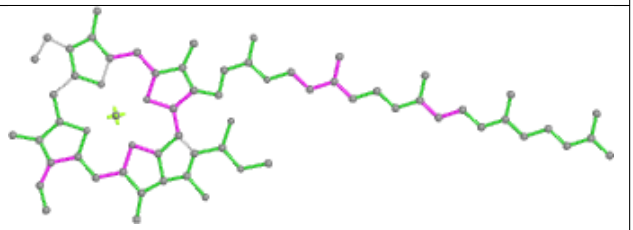


Rings

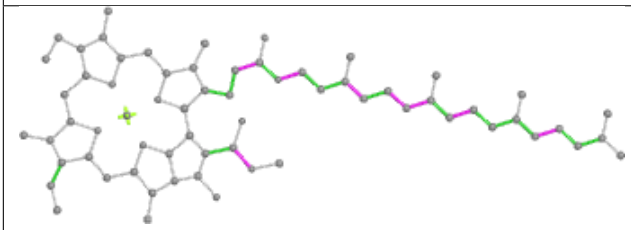
Ligand CLA B 613



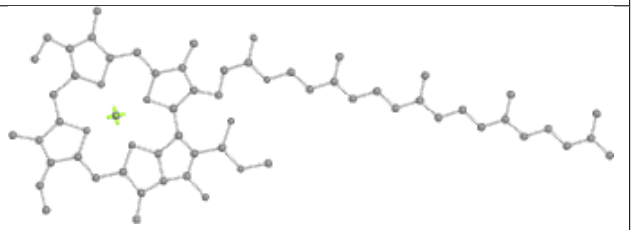
Bond lengths



Bond angles

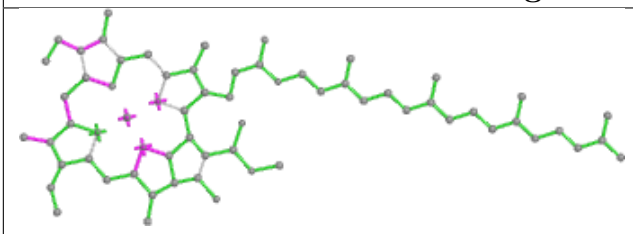


Torsions

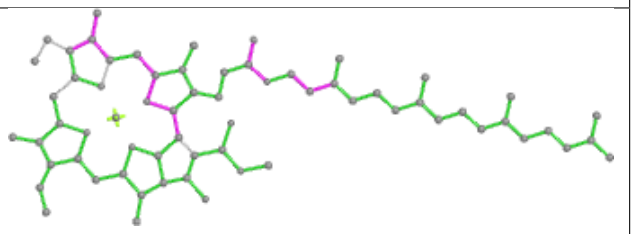


Rings

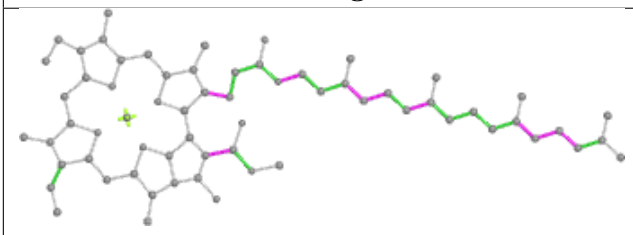
Ligand CLA C 507



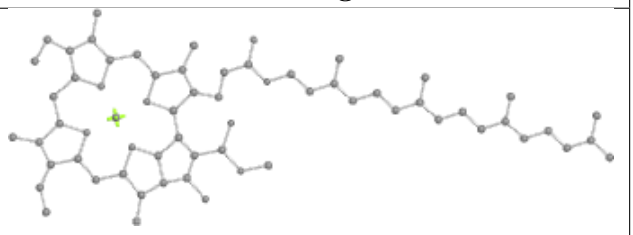
Bond lengths



Bond angles

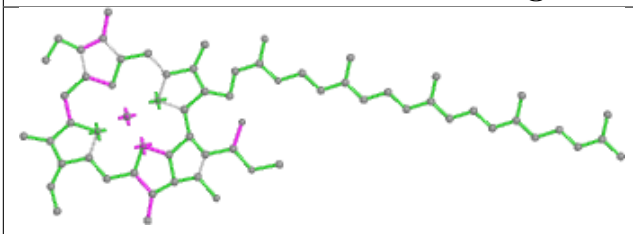


Torsions

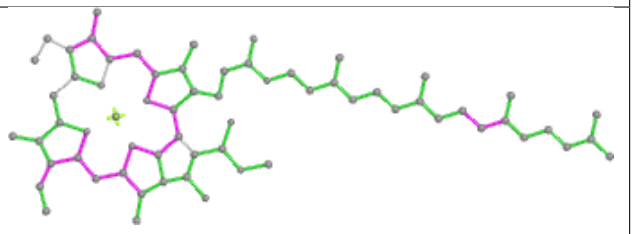


Rings

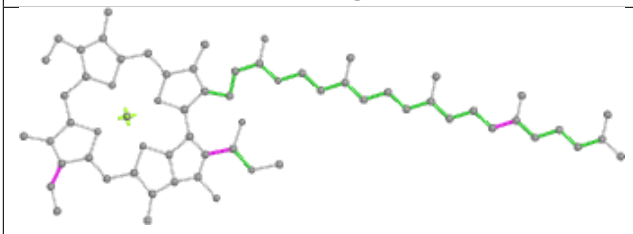
Ligand CLA d 403



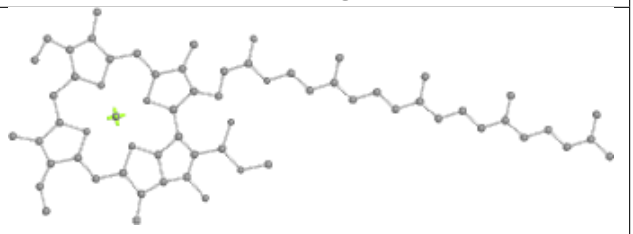
Bond lengths



Bond angles

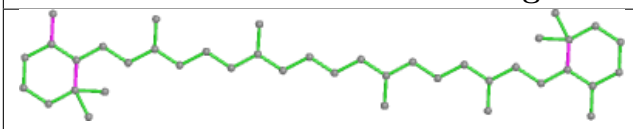


Torsions

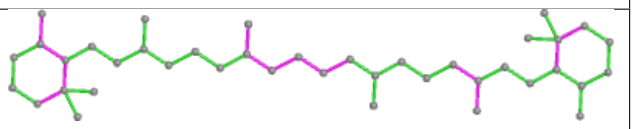


Rings

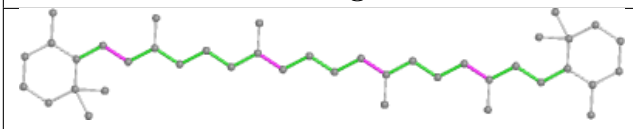
Ligand BCR B 617



Bond lengths



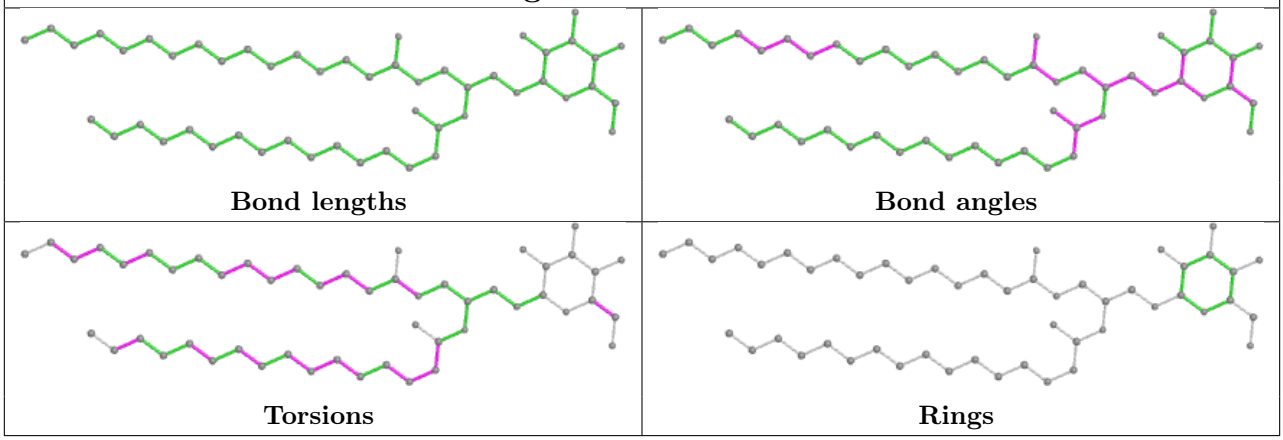
Bond angles



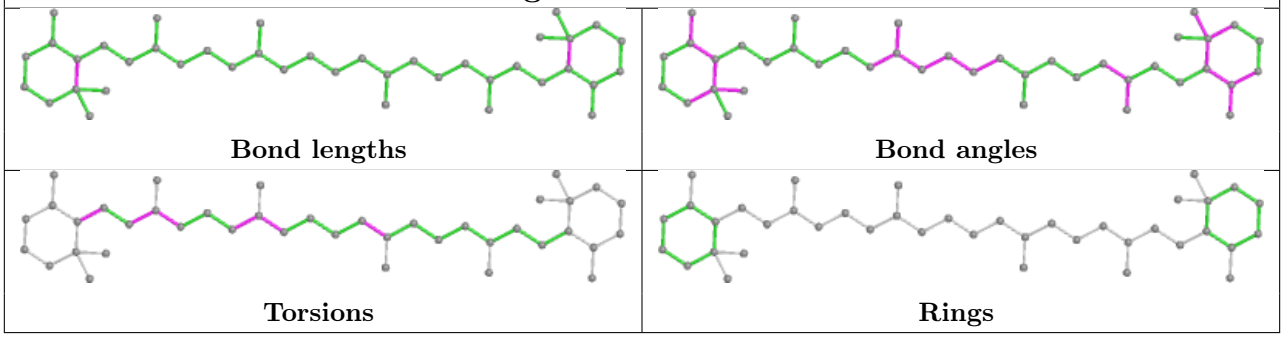
Torsions

Rings

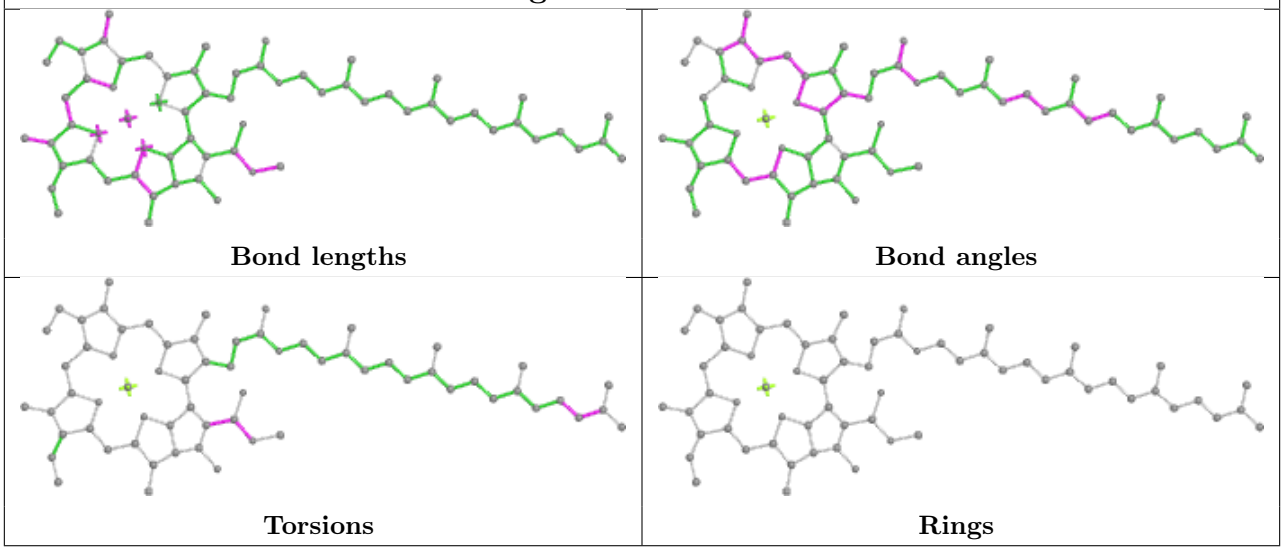
Ligand LMG b 621



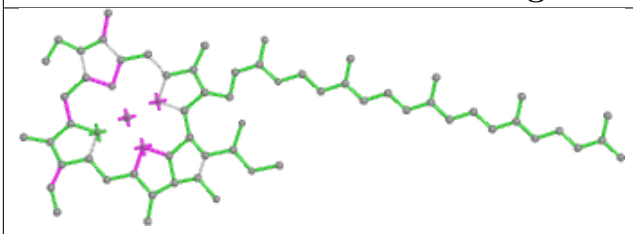
Ligand BCR B 619



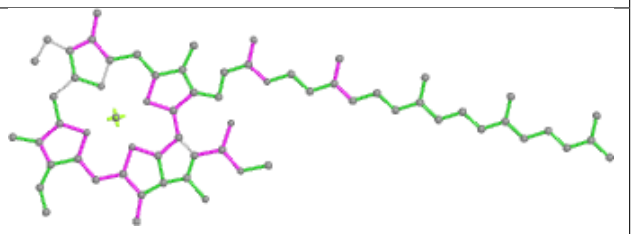
Ligand CLA a 404



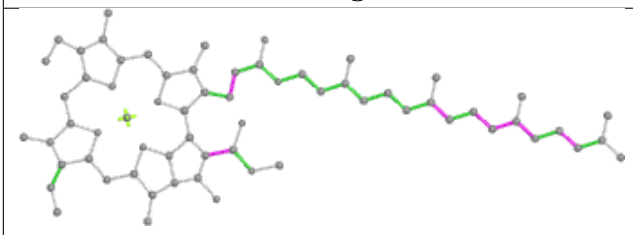
Ligand CLA b 607



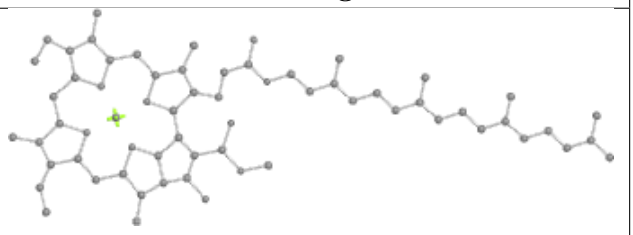
Bond lengths



Bond angles

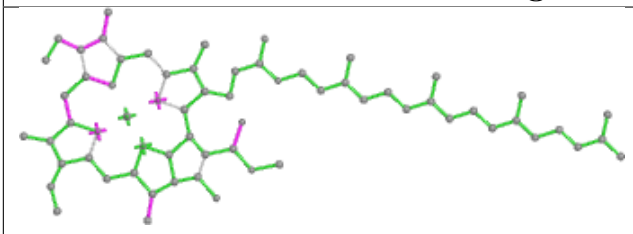


Torsions

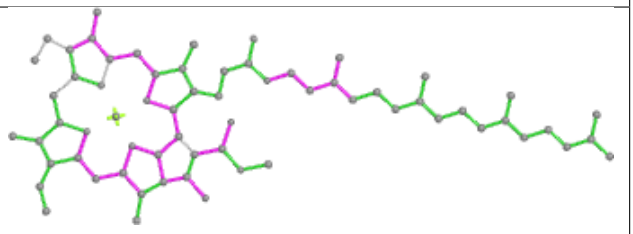


Rings

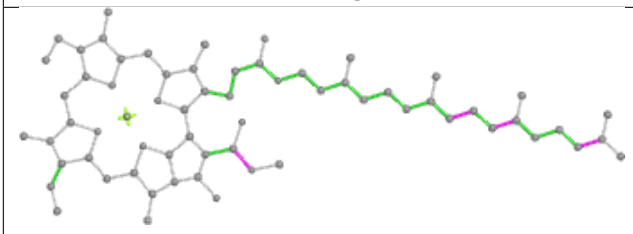
Ligand CLA d 405



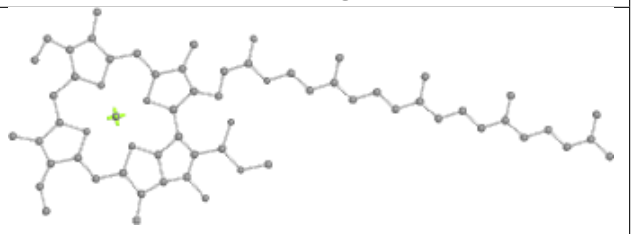
Bond lengths



Bond angles

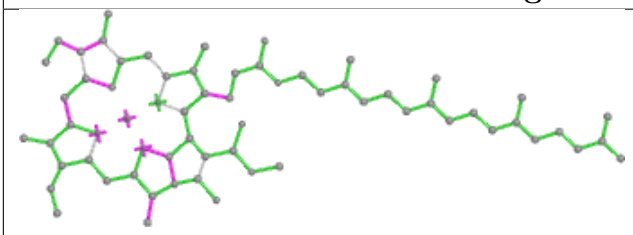


Torsions

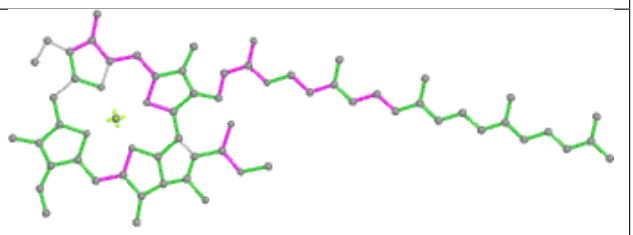


Rings

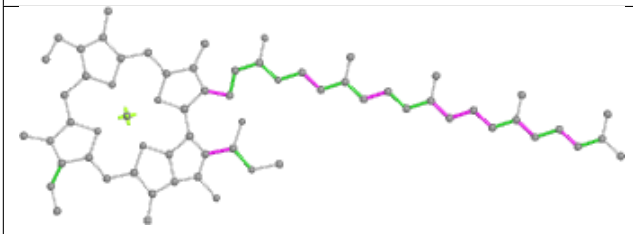
Ligand CLA C 513



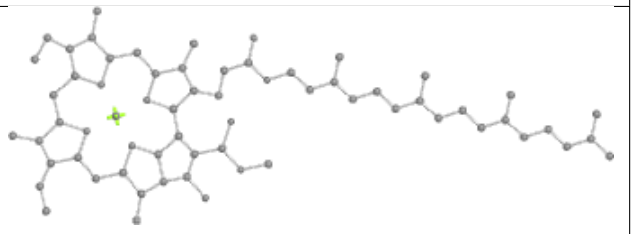
Bond lengths



Bond angles

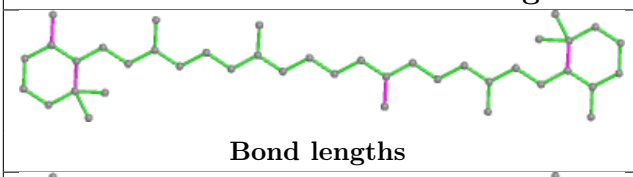


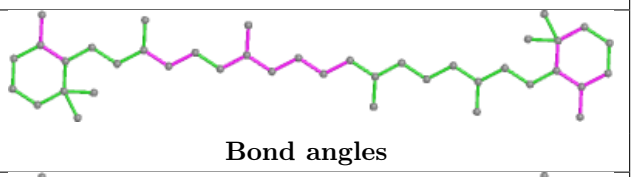
Torsions

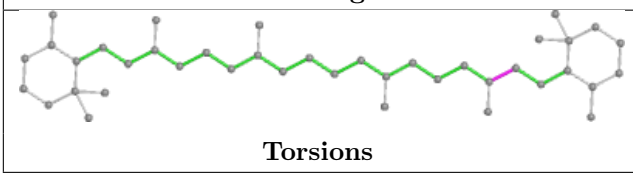


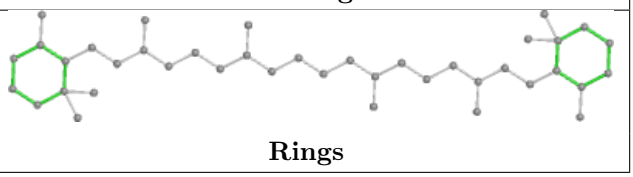
Rings

Ligand BCR C 515

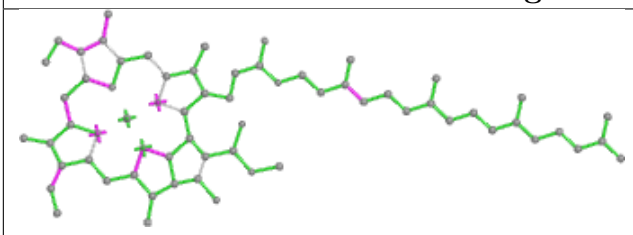


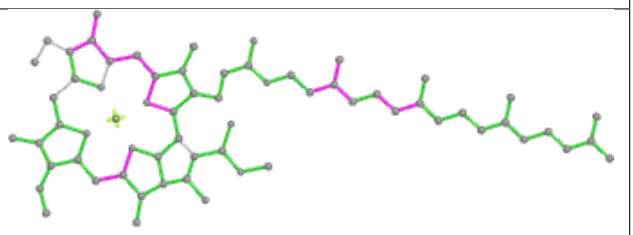


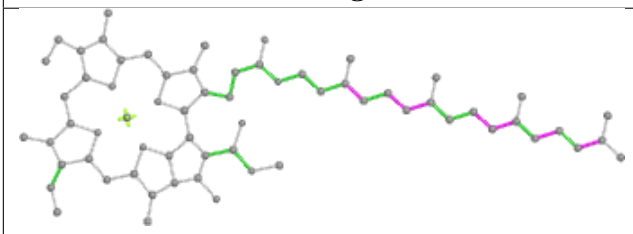


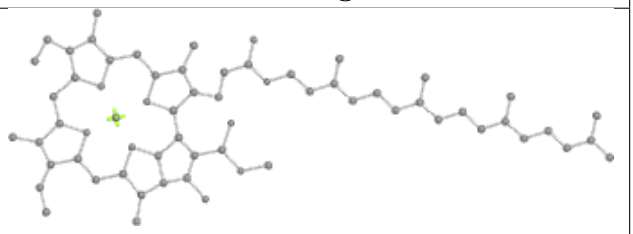


Ligand CLA B 615









5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

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%)	-0.42	3 (0%) 84 86	20, 28, 47, 75	0
1	a	334/334 (100%)	-0.42	1 (0%) 94 94	22, 30, 59, 81	0
2	B	505/505 (100%)	-0.36	5 (0%) 82 84	21, 32, 62, 87	0
2	b	505/505 (100%)	-0.25	14 (2%) 53 58	23, 35, 71, 104	0
3	C	442/451 (98%)	-0.29	1 (0%) 95 95	23, 35, 54, 79	0
3	c	451/451 (100%)	-0.27	5 (1%) 80 83	25, 39, 60, 106	0
4	D	341/341 (100%)	-0.31	1 (0%) 94 94	20, 30, 47, 75	0
4	d	341/341 (100%)	-0.30	2 (0%) 89 91	20, 33, 59, 84	0
5	E	81/82 (98%)	0.09	3 (3%) 41 46	30, 50, 69, 81	0
5	e	82/82 (100%)	0.30	4 (4%) 29 34	39, 59, 79, 87	0
6	F	34/34 (100%)	-0.29	2 (5%) 22 26	35, 41, 64, 84	0
6	f	34/34 (100%)	-0.13	2 (5%) 22 26	40, 48, 74, 93	0
7	H	65/65 (100%)	-0.03	2 (3%) 49 54	33, 40, 57, 72	0
7	h	63/65 (96%)	0.09	2 (3%) 47 53	40, 49, 59, 66	0
8	I	35/36 (97%)	-0.22	2 (5%) 23 28	30, 36, 65, 72	0
8	i	35/36 (97%)	-0.20	2 (5%) 23 28	30, 39, 69, 76	0
9	J	36/36 (100%)	0.24	4 (11%) 5 6	34, 48, 76, 94	0
9	j	36/36 (100%)	0.32	5 (13%) 2 3	40, 53, 82, 85	0
10	K	37/37 (100%)	-0.05	0 100 100	42, 51, 67, 70	0
10	k	37/37 (100%)	0.11	1 (2%) 54 59	45, 57, 74, 85	0
11	L	37/37 (100%)	-0.36	0 100 100	22, 29, 62, 69	0
11	l	36/37 (97%)	-0.24	1 (2%) 53 58	25, 29, 68, 75	0
12	M	32/33 (96%)	-0.20	1 (3%) 49 54	26, 31, 61, 74	0
12	m	31/33 (93%)	-0.19	0 100 100	26, 32, 48, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.05	11 (4%) 33 37	25, 41, 82, 133	0
13	o	244/244 (100%)	-0.11	12 (4%) 29 34	22, 39, 76, 127	0
14	T	29/30 (96%)	-0.59	1 (3%) 45 50	24, 31, 59, 68	0
14	t	29/30 (96%)	-0.36	2 (6%) 16 20	25, 31, 76, 94	0
15	U	97/97 (100%)	-0.24	2 (2%) 63 67	30, 41, 68, 90	0
15	u	97/97 (100%)	-0.41	2 (2%) 63 67	30, 40, 57, 83	0
16	V	137/137 (100%)	-0.47	0 100 100	25, 40, 55, 85	0
16	v	137/137 (100%)	-0.21	1 (0%) 87 89	32, 46, 65, 81	0
17	Y	27/30 (90%)	1.86	11 (40%) 0 0	53, 75, 110, 122	0
17	y	30/30 (100%)	1.03	8 (26%) 0 0	59, 71, 98, 102	0
18	X	38/38 (100%)	0.28	4 (10%) 6 7	37, 49, 76, 84	0
18	x	38/38 (100%)	0.60	3 (7%) 12 15	48, 60, 84, 103	0
19	Z	62/62 (100%)	0.87	17 (27%) 0 0	50, 65, 108, 122	0
19	z	62/62 (100%)	1.09	15 (24%) 0 0	56, 73, 115, 119	0
20	R	34/34 (100%)	1.89	15 (44%) 0 0	59, 70, 86, 92	0
20	r	31/34 (91%)	2.56	21 (67%) 0 0	69, 85, 97, 104	0
All	All	5300/5326 (99%)	-0.17	188 (3%) 44 49	20, 37, 73, 133	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	8.8
13	o	3	GLN	8.6
13	O	3	GLN	7.6
13	o	58	ASN	7.6
18	X	2	THR	7.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.95	0.14	33,47,76,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.95	0.10	30,49,70,70	0
14	FME	t	1	10/11	0.95	0.09	26,38,64,65	0
8	FME	i	1	10/11	0.96	0.16	38,52,64,68	0
8	FME	I	1	10/11	0.96	0.13	33,53,72,72	0
12	FME	m	1	10/11	0.98	0.12	29,50,66,80	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	UNL	H	103	53/-	0.76	0.22	51,73,94,97	0
31	UNL	a	413	28/-	0.77	0.31	31,63,70,81	0
32	LMG	c	522	48/55	0.77	0.24	42,80,114,117	0
33	LHG	E	101	49/49	0.79	0.22	48,83,108,119	0
32	LMG	h	102	23/55	0.80	0.24	41,77,102,105	0
28	SQD	a	411	36/54	0.80	0.17	38,65,87,97	0
31	UNL	c	523	28/-	0.81	0.17	49,72,88,89	0
29	DGD	a	412	44/66	0.81	0.15	32,57,76,84	0
31	UNL	E	102	28/-	0.81	0.29	53,74,84,86	0
31	UNL	b	624	40/-	0.81	0.18	52,69,88,88	0
27	PL9	A	410	55/55	0.82	0.20	31,58,79,91	0
31	UNL	B	626	47/-	0.82	0.35	48,66,91,94	0
31	UNL	b	625	55/-	0.82	0.17	40,60,80,81	0
31	UNL	b	626	26/-	0.82	0.21	39,52,61,63	0
29	DGD	A	413	66/66	0.83	0.18	36,68,84,102	0
31	UNL	B	625	28/-	0.83	0.38	52,73,90,103	0
32	LMG	D	410	33/55	0.83	0.16	35,54,89,98	0
24	CLA	h	101	65/65	0.84	0.16	45,67,92,104	0
31	UNL	t	103	26/-	0.84	0.20	38,64,77,81	0
31	UNL	c	520	55/-	0.84	0.18	34,61,83,90	0
32	LMG	b	623	55/55	0.85	0.27	44,76,98,109	0
28	SQD	b	601	49/54	0.85	0.14	39,58,97,111	0
31	UNL	b	622	55/-	0.86	0.21	39,60,84,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	Y	101	40/40	0.86	0.13	37,54,73,75	0
24	CLA	c	512	65/65	0.86	0.14	42,60,99,125	0
27	PL9	a	409	55/55	0.86	0.21	36,66,86,99	0
31	UNL	X	101	55/-	0.86	0.16	33,54,76,78	0
24	CLA	C	514	65/65	0.86	0.18	45,65,91,105	0
24	CLA	C	513	65/65	0.87	0.15	33,56,93,103	0
31	UNL	M	104	53/-	0.87	0.16	36,48,88,90	0
31	UNL	C	522	47/-	0.87	0.13	44,56,66,67	0
24	CLA	B	616	60/65	0.87	0.16	23,42,93,98	0
31	UNL	J	101	28/-	0.88	0.15	50,63,71,81	0
31	UNL	M	103	26/-	0.88	0.18	39,51,59,64	0
32	LMG	K	102	48/55	0.88	0.16	48,71,92,101	0
26	BCR	h	103	40/40	0.88	0.13	31,54,78,88	0
32	LMG	c	519	37/55	0.88	0.16	41,70,83,88	0
31	UNL	T	101	47/-	0.88	0.18	38,49,65,71	0
28	SQD	f	101	41/54	0.88	0.22	55,90,116,124	0
24	CLA	c	513	65/65	0.88	0.21	40,74,109,115	0
33	LHG	e	101	42/49	0.88	0.28	58,87,114,129	0
31	UNL	m	101	28/-	0.89	0.14	38,53,74,82	0
26	BCR	H	101	40/40	0.89	0.11	30,47,67,71	0
31	UNL	x	101	55/-	0.89	0.19	39,58,75,78	0
31	UNL	B	623	28/-	0.89	0.11	35,51,67,77	0
31	UNL	I	101	41/-	0.89	0.14	40,51,76,78	0
26	BCR	k	101	40/40	0.89	0.12	41,64,77,79	0
28	SQD	A	412	39/54	0.89	0.19	41,68,96,103	0
31	UNL	C	520	28/-	0.89	0.10	33,46,50,62	0
28	SQD	B	622	54/54	0.89	0.13	33,60,88,102	0
31	UNL	T	102	44/-	0.89	0.19	41,57,76,77	0
31	UNL	d	412	43/-	0.89	0.20	43,58,70,77	0
31	UNL	C	521	28/-	0.90	0.11	44,54,60,67	0
24	CLA	B	601	65/65	0.90	0.14	32,65,102,107	0
32	LMG	c	524	49/55	0.90	0.13	37,54,88,107	0
24	CLA	D	404	65/65	0.90	0.15	21,42,123,126	0
24	CLA	a	407	65/65	0.90	0.15	17,36,89,116	0
24	CLA	b	617	60/65	0.90	0.14	24,44,89,98	0
32	LMG	C	501	48/55	0.91	0.15	34,57,72,109	0
32	LMG	D	407	51/55	0.91	0.17	24,58,93,98	0
26	BCR	C	515	40/40	0.91	0.13	28,39,49,64	0
31	UNL	B	620	43/-	0.91	0.11	35,49,60,70	0
32	LMG	b	621	51/55	0.91	0.12	32,51,76,91	0
28	SQD	F	101	36/54	0.91	0.15	41,74,93,99	0
26	BCR	D	405	40/40	0.91	0.12	29,46,90,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	UNL	j	101	28/-	0.91	0.12	44,56,67,68	0
24	CLA	B	615	65/65	0.91	0.12	20,38,64,87	0
31	UNL	t	102	34/-	0.91	0.13	38,51,64,77	0
26	BCR	K	101	40/40	0.91	0.12	33,56,69,76	0
24	CLA	b	616	65/65	0.91	0.13	26,41,60,72	0
24	CLA	C	507	65/65	0.92	0.12	25,42,99,113	0
24	CLA	c	507	65/65	0.92	0.15	28,45,64,65	0
24	CLA	d	405	65/65	0.92	0.13	25,49,107,114	0
32	LMG	M	101	51/55	0.92	0.11	25,47,71,81	0
29	DGD	H	102	62/66	0.92	0.12	27,48,63,78	0
26	BCR	c	521	40/40	0.92	0.15	40,56,70,75	0
26	BCR	b	619	40/40	0.93	0.09	27,41,54,56	0
32	LMG	B	621	28/55	0.93	0.12	33,50,62,66	0
26	BCR	b	620	40/40	0.93	0.10	29,50,62,66	0
28	SQD	a	410	54/54	0.93	0.13	41,68,93,95	0
24	CLA	c	508	64/65	0.93	0.12	29,48,80,108	0
26	BCR	d	406	40/40	0.93	0.12	32,56,100,106	0
24	CLA	C	508	65/65	0.93	0.13	23,40,61,67	0
24	CLA	c	502	65/65	0.93	0.13	27,42,63,71	0
29	DGD	C	516	62/66	0.93	0.12	21,40,79,95	0
29	DGD	C	517	62/66	0.93	0.11	32,56,96,109	0
24	CLA	c	504	60/65	0.93	0.12	26,46,87,91	0
31	UNL	M	102	37/-	0.93	0.11	33,47,65,67	0
32	LMG	d	411	44/55	0.93	0.13	31,55,91,97	0
24	CLA	C	506	65/65	0.93	0.17	23,39,65,76	0
29	DGD	h	104	62/66	0.93	0.11	30,51,68,76	0
26	BCR	b	618	40/40	0.93	0.11	25,43,56,61	0
24	CLA	c	511	65/65	0.94	0.14	43,56,76,80	0
24	CLA	A	406	65/65	0.94	0.12	21,37,99,112	0
24	CLA	a	405	65/65	0.94	0.13	22,40,97,115	0
24	CLA	C	503	65/65	0.94	0.11	27,42,60,69	0
24	CLA	b	605	65/65	0.94	0.13	18,33,82,98	0
26	BCR	A	409	40/40	0.94	0.09	21,34,44,48	0
26	BCR	B	618	40/40	0.94	0.07	22,39,51,56	0
26	BCR	B	619	40/40	0.94	0.09	21,40,62,72	0
24	CLA	b	607	65/65	0.94	0.10	22,41,77,84	0
26	BCR	C	519	40/40	0.94	0.16	29,56,68,74	0
24	CLA	b	610	65/65	0.94	0.11	26,46,64,79	0
29	DGD	c	517	62/66	0.94	0.11	31,55,92,107	0
29	DGD	c	518	62/66	0.94	0.11	26,53,78,88	0
24	CLA	b	613	65/65	0.94	0.17	20,35,45,61	0
24	CLA	b	615	65/65	0.94	0.15	24,42,81,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	602	65/65	0.94	0.12	22,36,63,74	0
31	UNL	B	624	46/-	0.94	0.10	39,54,66,72	0
26	BCR	b	602	40/40	0.94	0.10	23,41,66,72	0
24	CLA	B	604	65/65	0.94	0.12	18,33,77,84	0
24	CLA	B	606	65/65	0.94	0.10	24,38,76,83	0
24	CLA	c	503	65/65	0.94	0.14	24,44,55,60	0
26	BCR	c	514	40/40	0.94	0.16	35,60,72,74	0
24	CLA	C	512	65/65	0.94	0.11	34,53,69,75	0
24	CLA	c	505	65/65	0.94	0.14	24,42,66,70	0
24	CLA	c	506	65/65	0.94	0.14	25,53,110,118	0
24	CLA	B	614	65/65	0.94	0.14	16,37,88,97	0
24	CLA	A	408	54/65	0.94	0.13	16,32,62,73	0
24	CLA	c	509	65/65	0.94	0.17	29,48,64,68	0
28	SQD	A	411	52/54	0.94	0.13	33,59,89,94	0
24	CLA	c	510	65/65	0.94	0.13	32,49,73,84	0
29	DGD	C	518	62/66	0.95	0.10	26,48,79,89	0
24	CLA	b	609	65/65	0.95	0.12	25,42,58,69	0
24	CLA	C	511	65/65	0.95	0.12	28,47,67,72	0
24	CLA	A	405	65/65	0.95	0.11	15,28,41,49	0
24	CLA	b	614	65/65	0.95	0.13	15,33,74,88	0
26	BCR	c	515	40/40	0.95	0.11	25,45,64,78	0
24	CLA	d	403	65/65	0.95	0.10	16,30,44,47	0
24	CLA	C	504	65/65	0.95	0.11	22,42,54,57	0
24	CLA	C	505	59/65	0.95	0.12	26,46,75,87	0
25	PHO	a	406	64/64	0.95	0.11	22,32,41,45	0
26	BCR	t	101	40/40	0.95	0.09	25,40,56,60	0
25	PHO	d	402	64/64	0.95	0.11	25,39,53,62	0
27	PL9	D	406	55/55	0.95	0.11	18,34,46,50	0
24	CLA	D	402	65/65	0.95	0.11	17,28,50,57	0
27	PL9	d	407	55/55	0.95	0.10	19,35,43,50	0
26	BCR	B	617	40/40	0.95	0.10	24,42,54,55	0
24	CLA	c	501	65/65	0.95	0.13	28,39,53,55	0
24	CLA	D	403	65/65	0.95	0.11	16,29,61,74	0
24	CLA	B	609	65/65	0.95	0.10	22,40,57,64	0
24	CLA	a	404	65/65	0.95	0.10	16,29,44,59	0
24	CLA	B	613	65/65	0.95	0.12	17,30,65,73	0
24	CLA	C	502	65/65	0.95	0.11	22,36,50,60	0
24	CLA	b	603	65/65	0.95	0.14	24,44,69,80	0
24	CLA	C	509	65/65	0.95	0.12	24,42,96,114	0
33	LHG	D	411	49/49	0.95	0.11	26,44,69,81	0
26	BCR	a	408	40/40	0.95	0.09	17,32,48,53	0
33	LHG	d	408	49/49	0.95	0.11	31,51,85,94	0

Continued on next page...

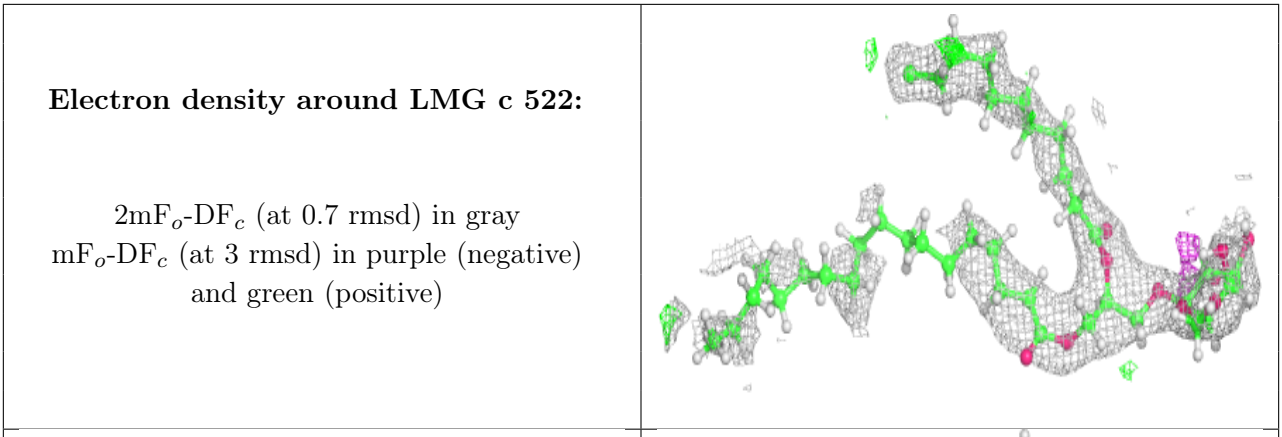
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LHG	d	410	39/49	0.95	0.10	32,48,71,76	0
24	CLA	C	510	65/65	0.95	0.14	22,46,61,72	0
24	CLA	B	610	65/65	0.96	0.15	18,32,43,48	0
24	CLA	d	404	65/65	0.96	0.11	19,33,63,70	0
24	CLA	B	612	65/65	0.96	0.15	17,32,49,59	0
24	CLA	b	606	65/65	0.96	0.12	20,35,50,52	0
25	PHO	A	407	64/64	0.96	0.10	16,28,39,44	0
25	PHO	D	401	64/64	0.96	0.09	21,33,48,50	0
24	CLA	B	603	65/65	0.96	0.13	17,34,66,68	0
24	CLA	b	608	65/65	0.96	0.11	16,36,69,79	0
33	LHG	D	408	49/49	0.96	0.12	19,42,59,63	0
33	LHG	D	409	47/49	0.96	0.10	20,45,83,99	0
24	CLA	B	607	65/65	0.96	0.10	15,34,62,70	0
24	CLA	B	605	65/65	0.96	0.14	15,30,44,61	0
24	CLA	b	611	65/65	0.96	0.14	19,38,53,61	0
33	LHG	d	409	49/49	0.96	0.12	22,39,62,67	0
24	CLA	b	612	65/65	0.96	0.10	19,32,48,58	0
29	DGD	c	516	62/66	0.96	0.11	22,41,77,90	0
33	LHG	l	101	49/49	0.96	0.10	28,46,61,67	0
34	HEM	F	102	43/43	0.96	0.12	35,49,65,69	0
24	CLA	b	604	65/65	0.97	0.11	21,35,67,77	0
24	CLA	B	608	65/65	0.97	0.10	17,34,59,63	0
24	CLA	B	611	65/65	0.97	0.12	18,32,46,54	0
33	LHG	L	101	49/49	0.97	0.11	25,41,56,66	0
23	BCT	d	401	4/4	0.97	0.20	29,29,38,46	0
34	HEM	e	102	43/43	0.97	0.11	43,55,79,79	0
35	HEC	v	201	43/43	0.97	0.13	27,36,47,54	0
35	HEC	V	201	43/43	0.98	0.11	22,33,42,48	0
21	FE2	a	401	1/1	0.99	0.06	33,33,33,33	0
22	CL	A	402	1/1	0.99	0.07	25,25,25,25	0
22	CL	a	402	1/1	0.99	0.06	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.03	25,25,25,25	0
30	OEX	A	414	10/10	0.99	0.11	19,29,33,33	0
30	OEX	a	414	10/10	0.99	0.11	23,29,33,34	1
23	BCT	A	404	4/4	0.99	0.13	28,28,30,36	0
21	FE2	A	401	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	1.00	0.06	29,29,29,29	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.

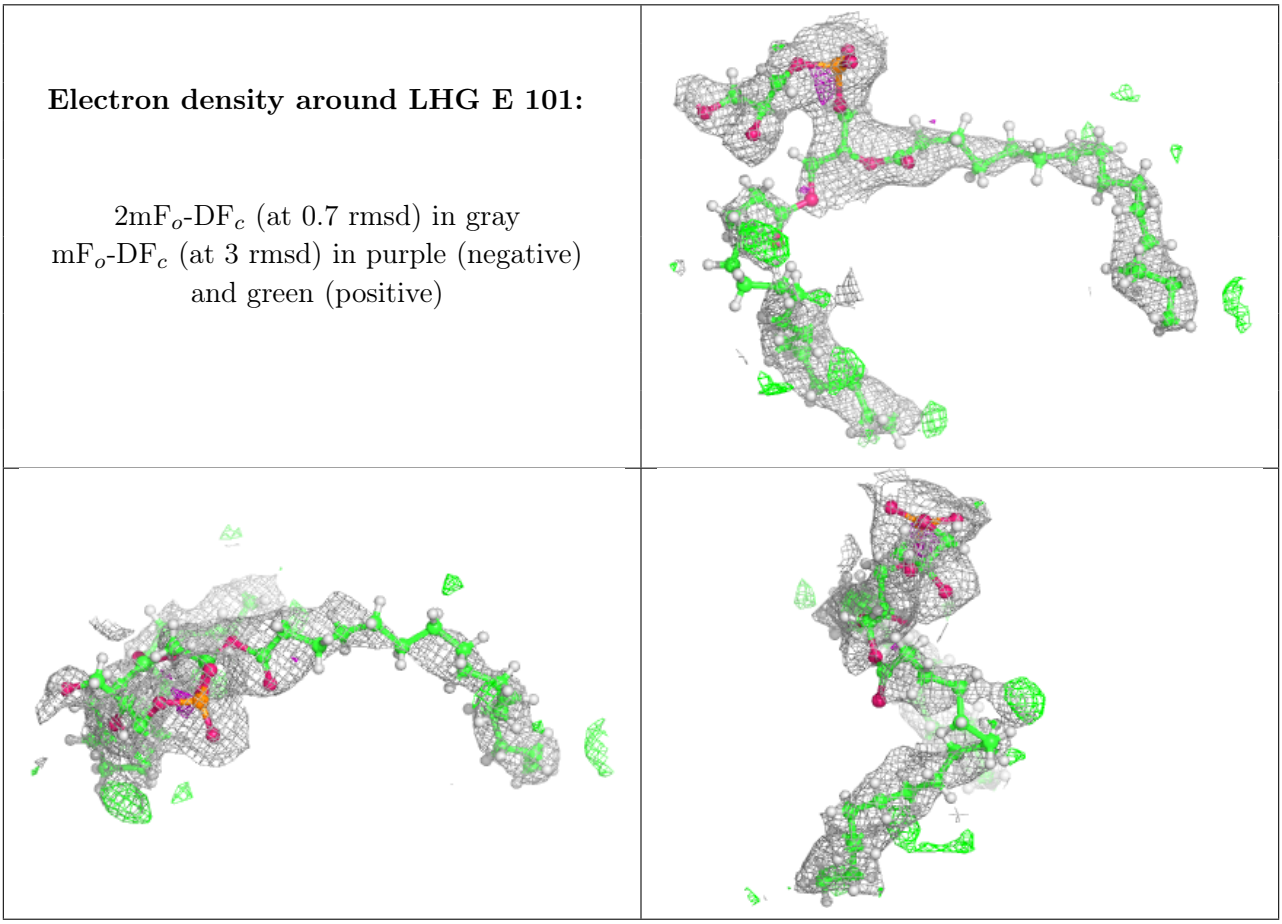
Electron density around LMG c 522:

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



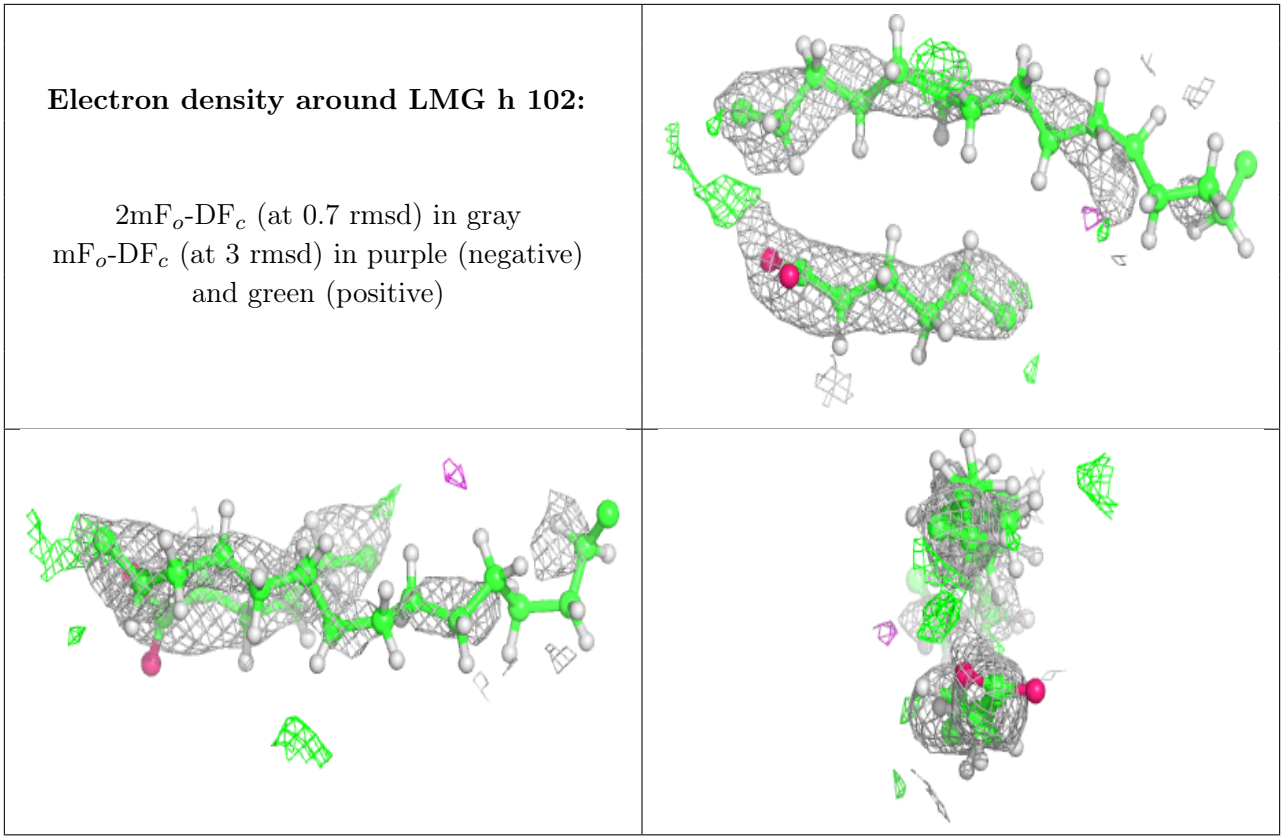
Electron density around LHG E 101:

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



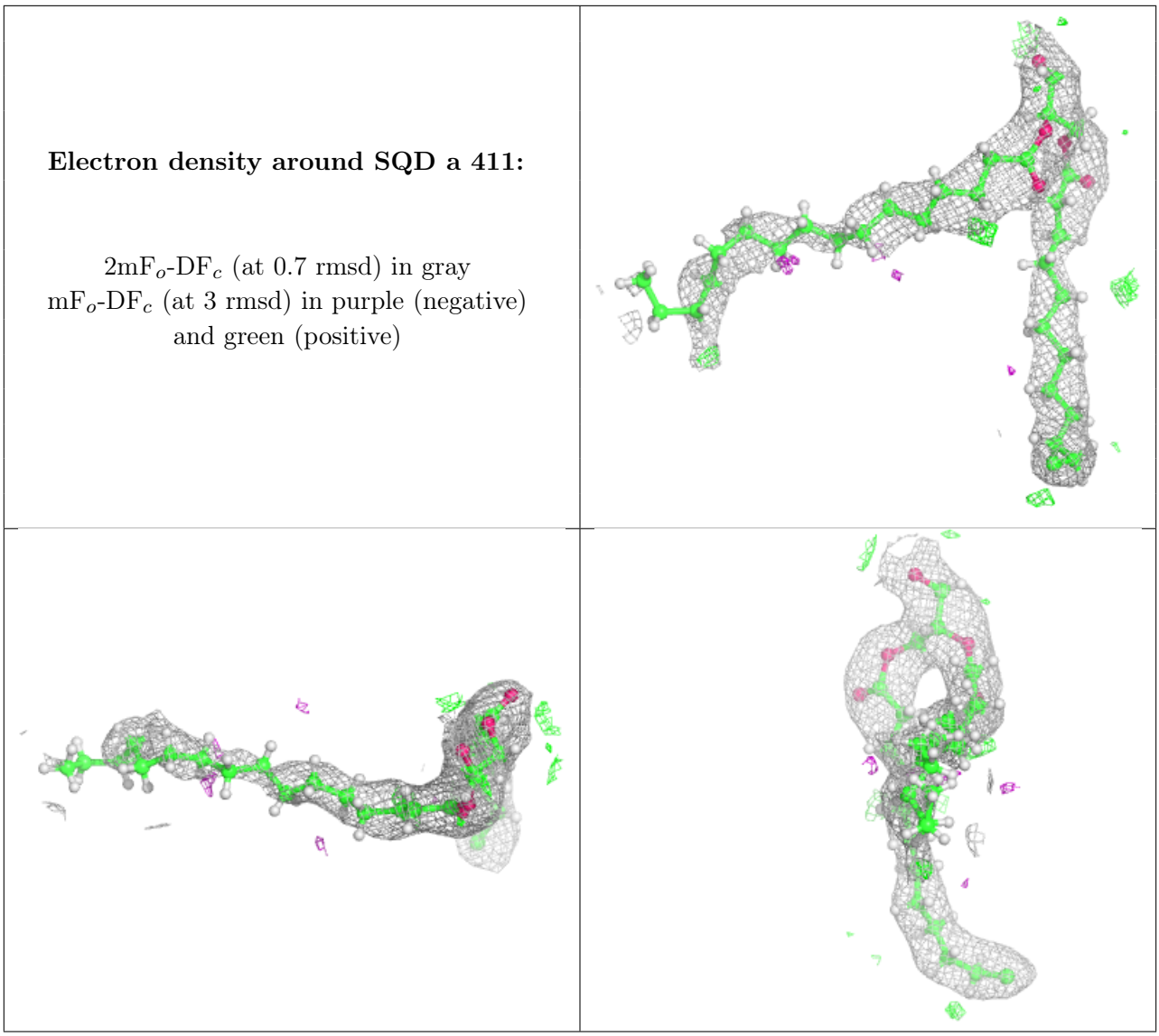
Electron density around LMG h 102:

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



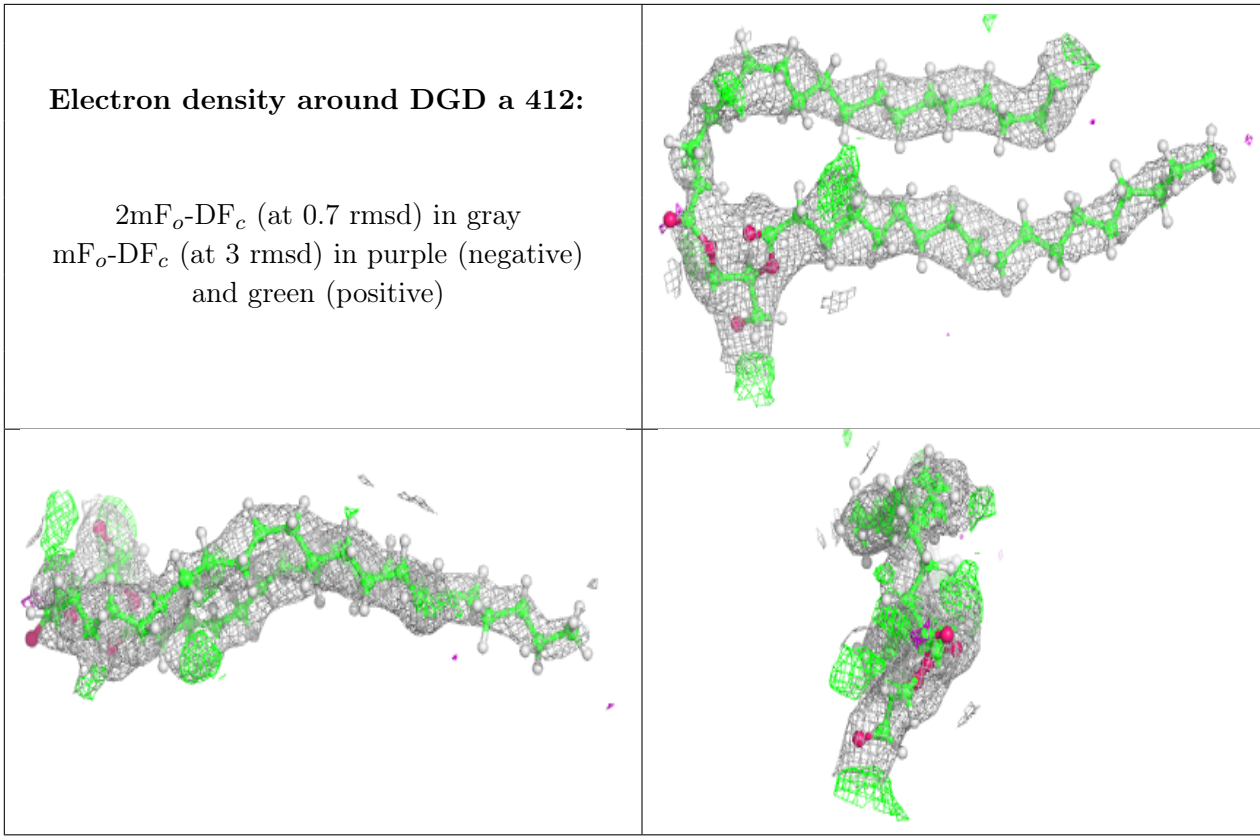
Electron density around SQD a 411:

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



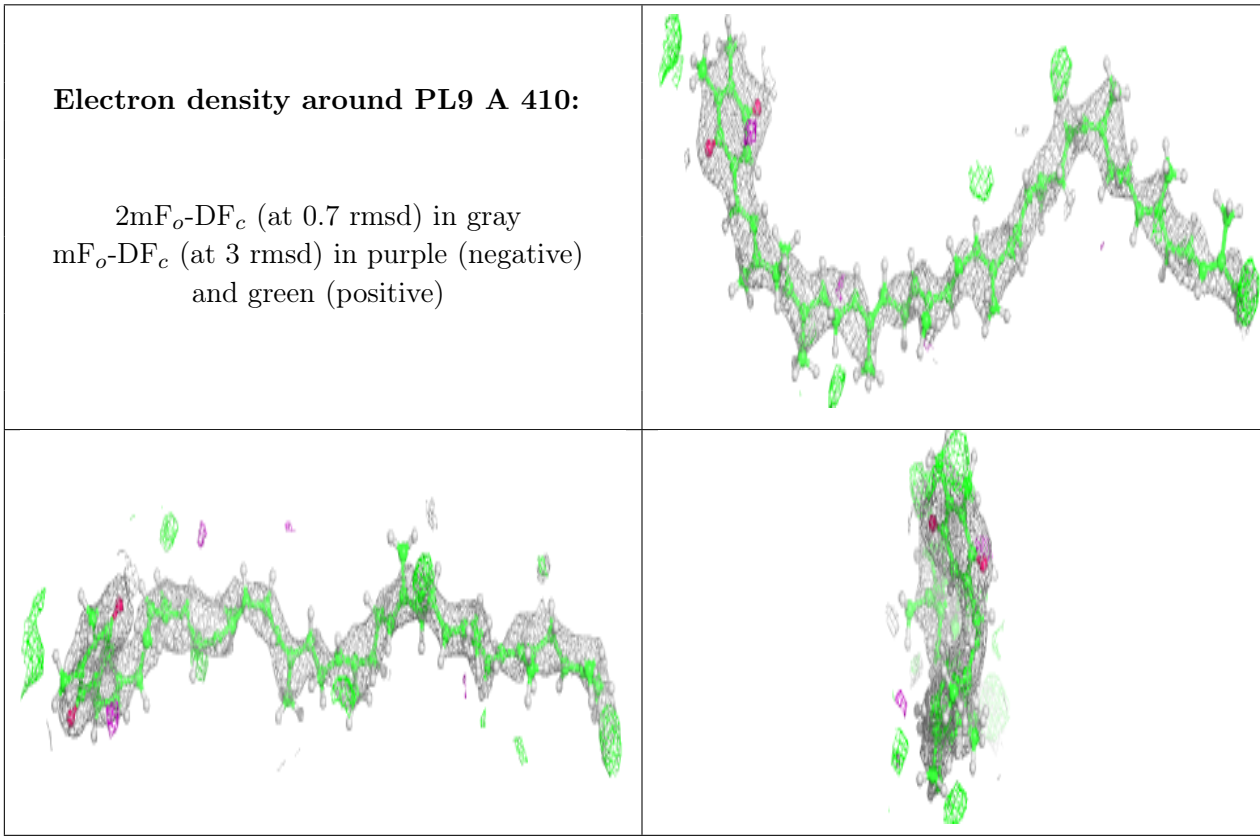
Electron density around DGD a 412:

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



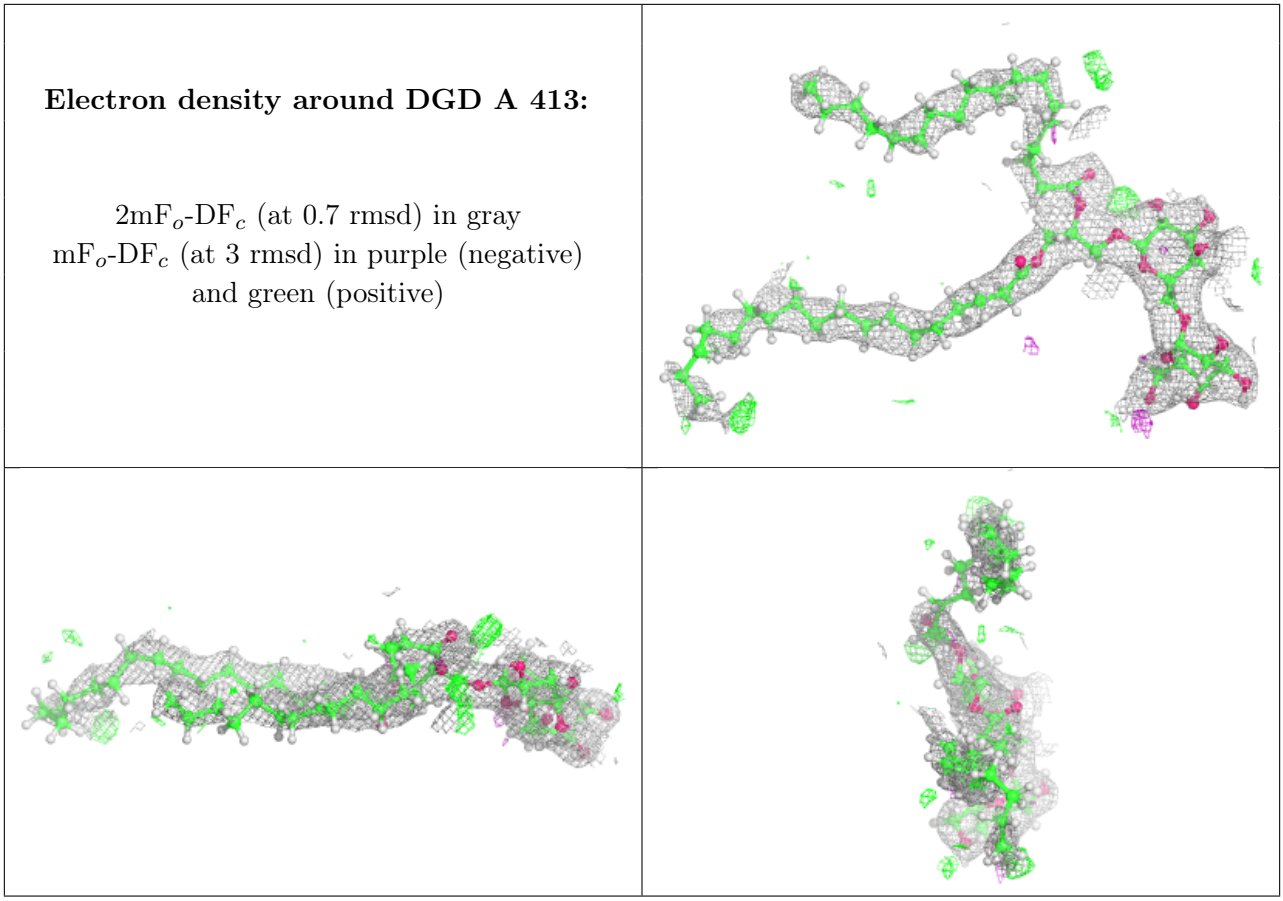
Electron density around PL9 A 410:

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



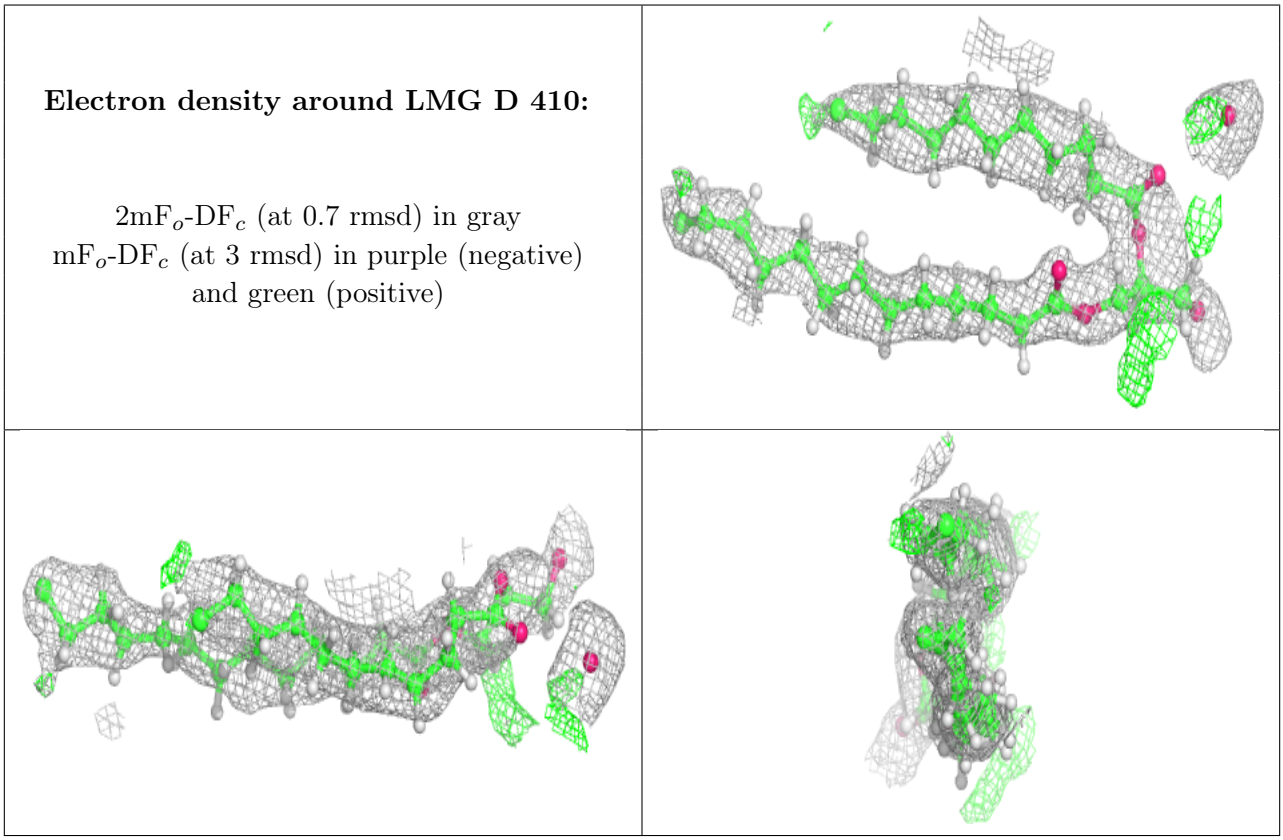
Electron density around DGD A 413:

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



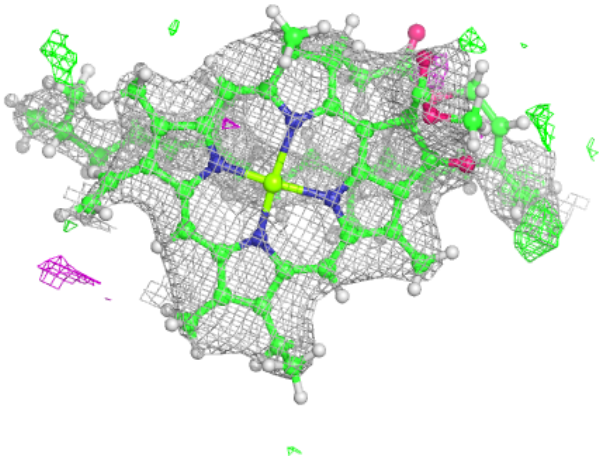
Electron density around LMG D 410:

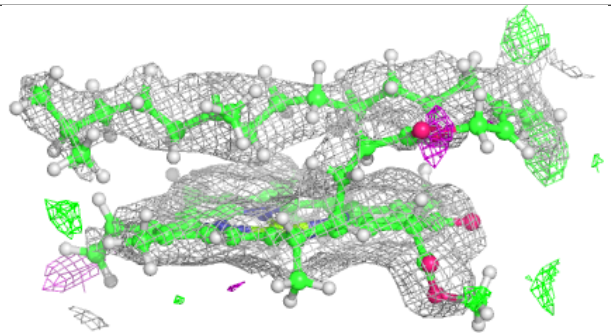
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA h 101:

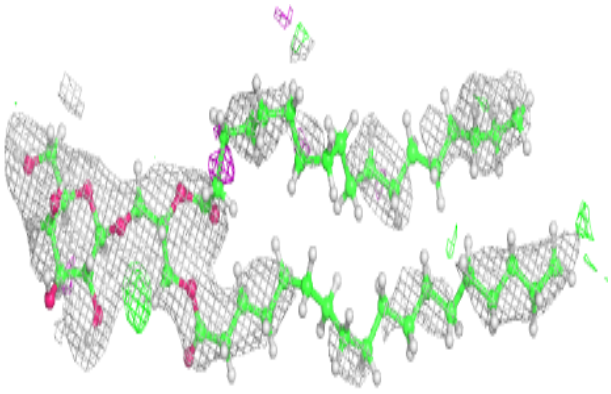
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

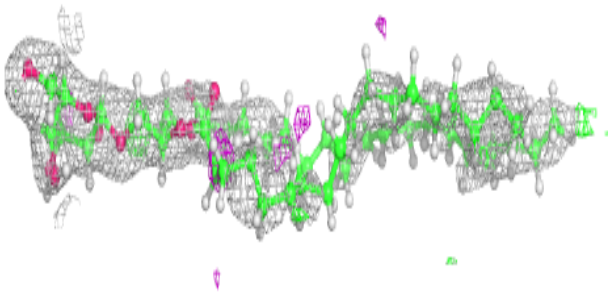


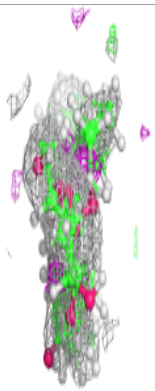


Electron density around LMG b 623:

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

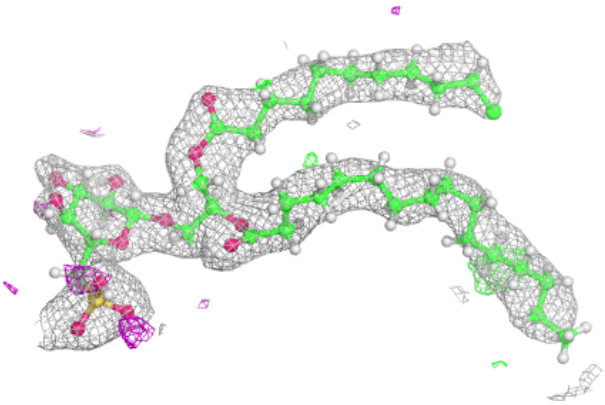


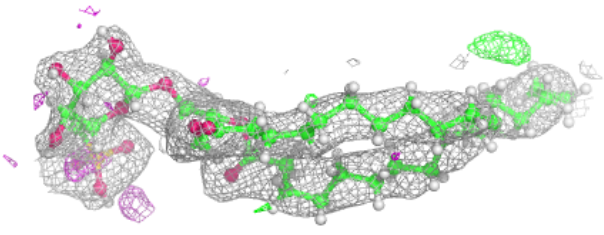


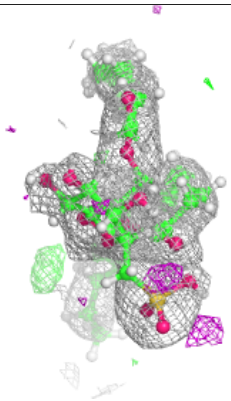


Electron density around SQD b 601:

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

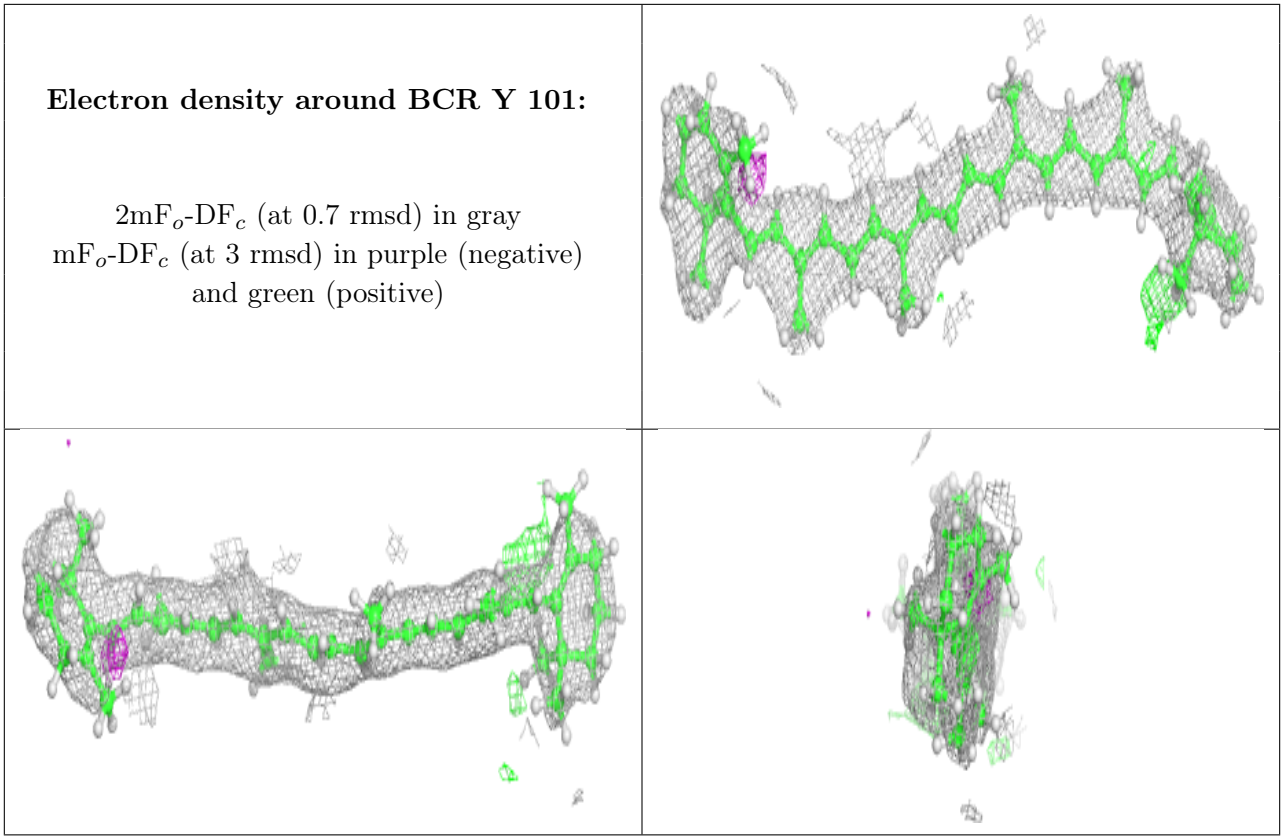






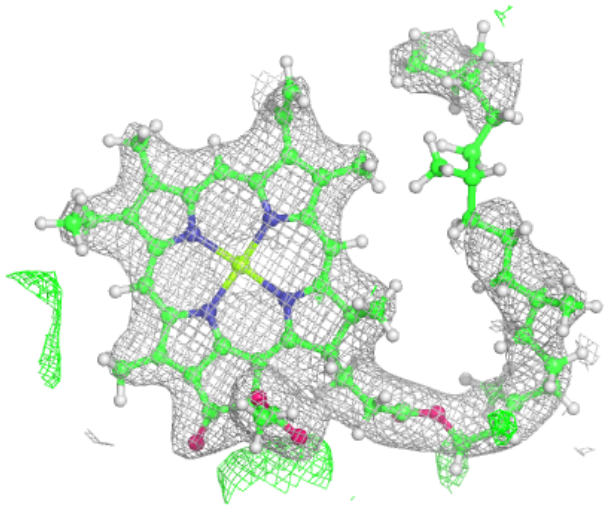
Electron density around BCR Y 101:

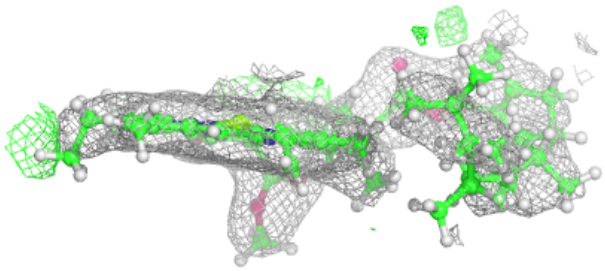
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

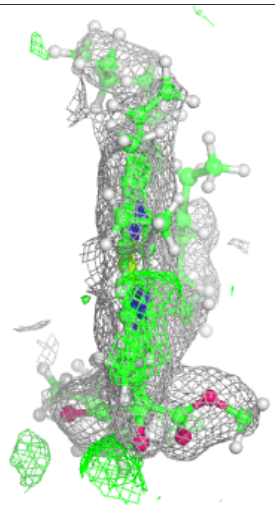


Electron density around CLA c 512:

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

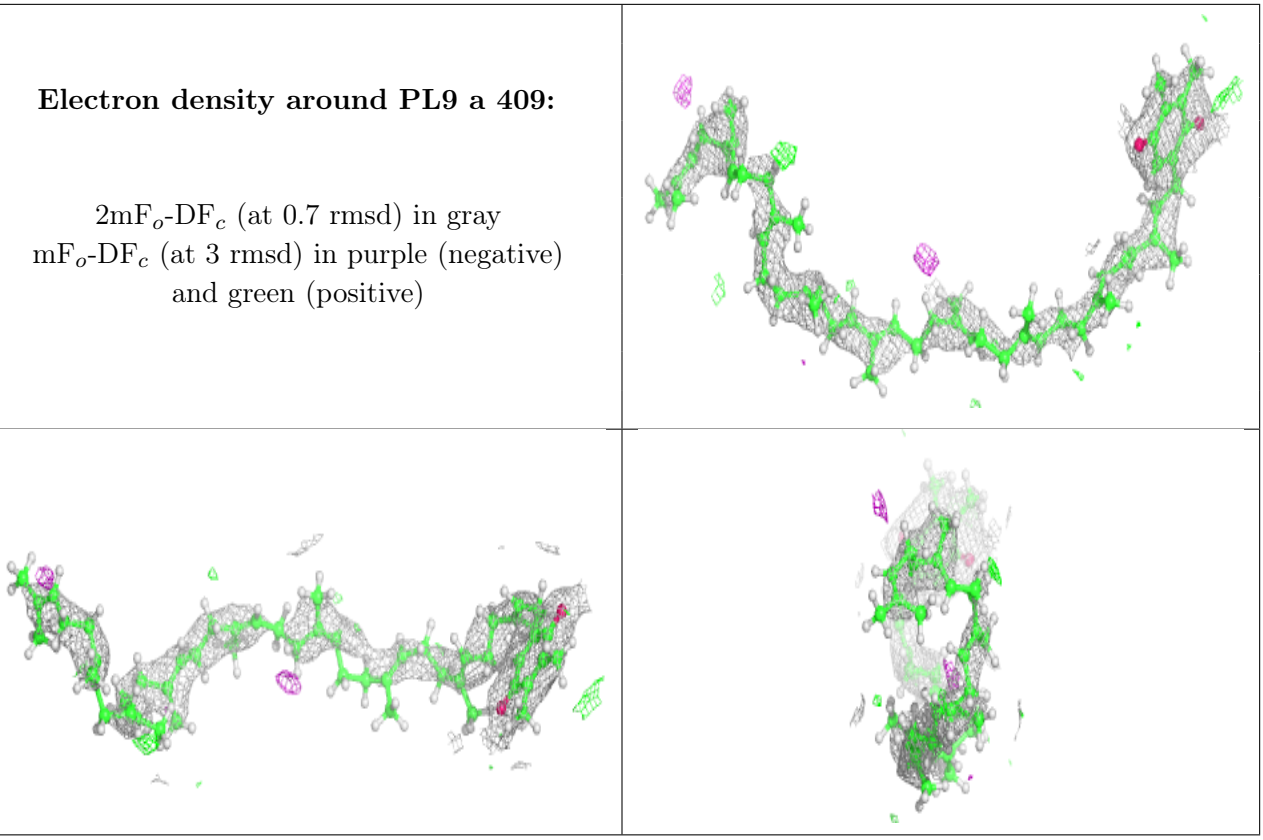






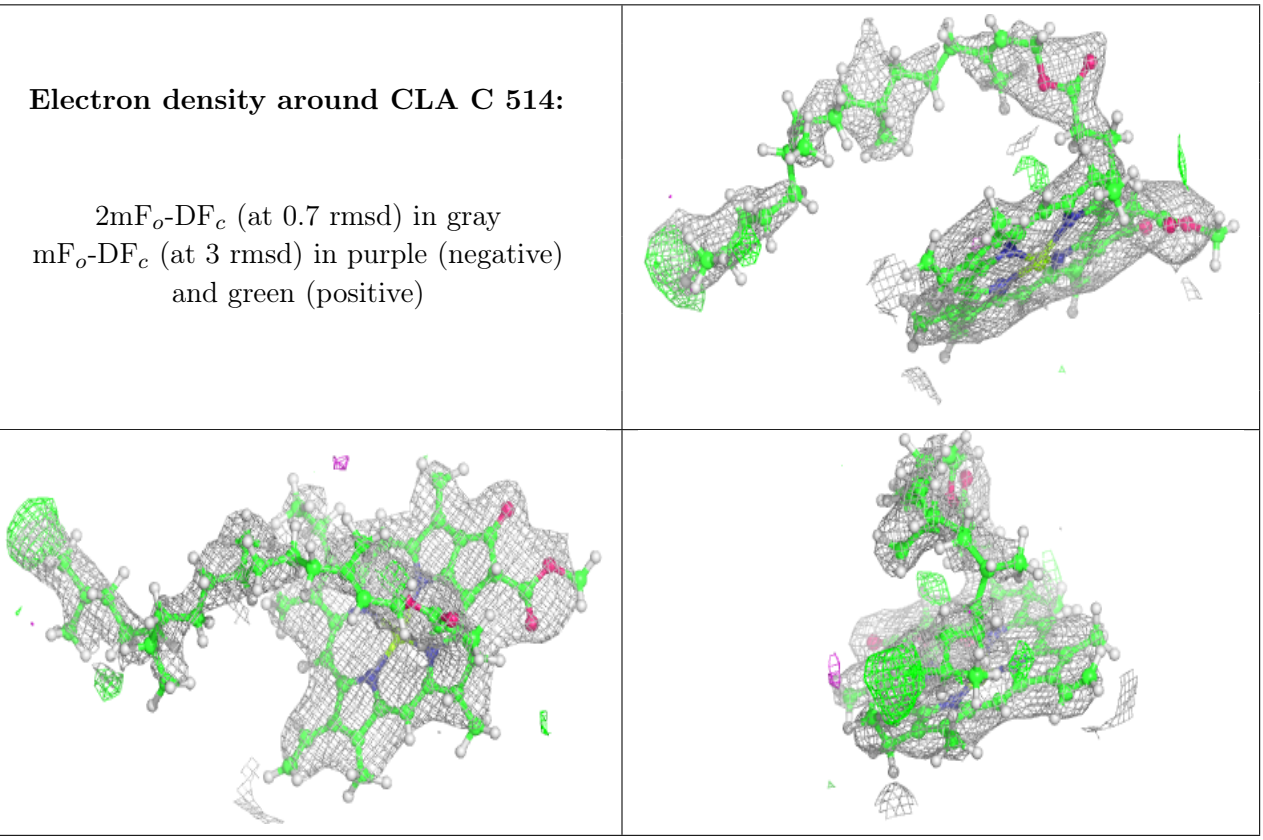
Electron density around PL9 a 409:

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



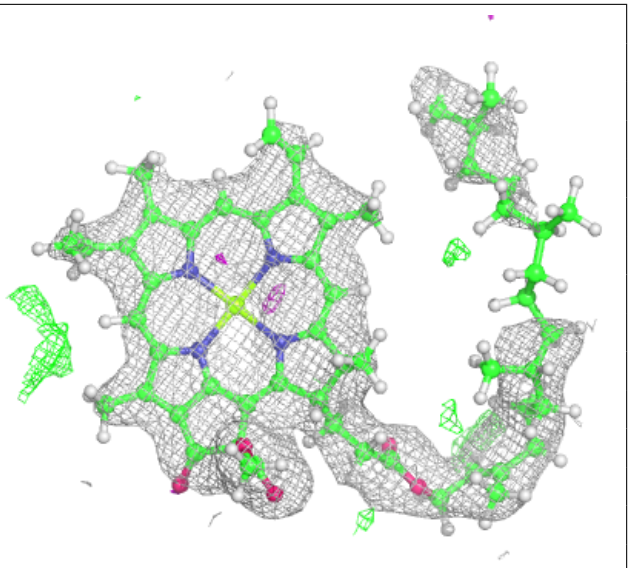
Electron density around CLA C 514:

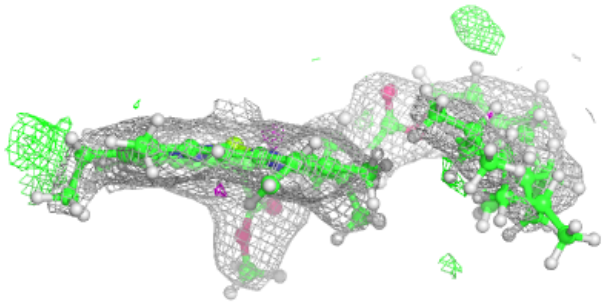
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

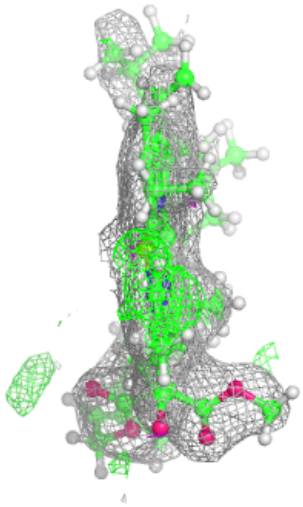


Electron density around CLA C 513:

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

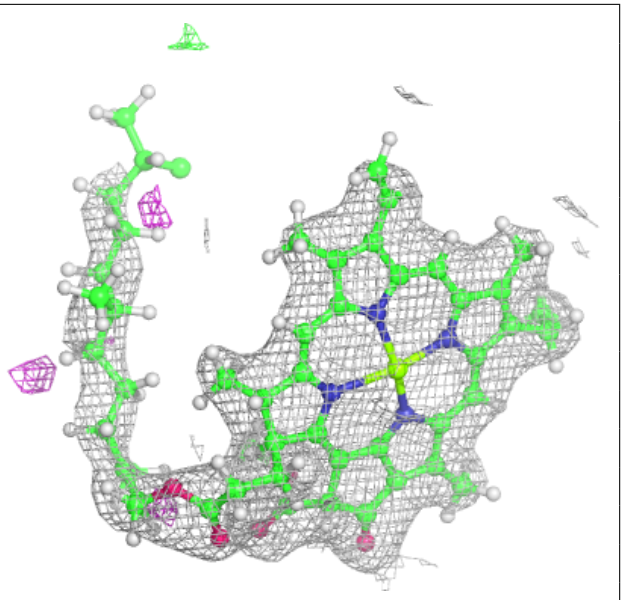


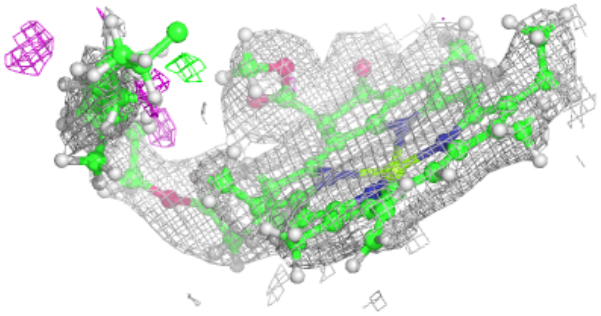


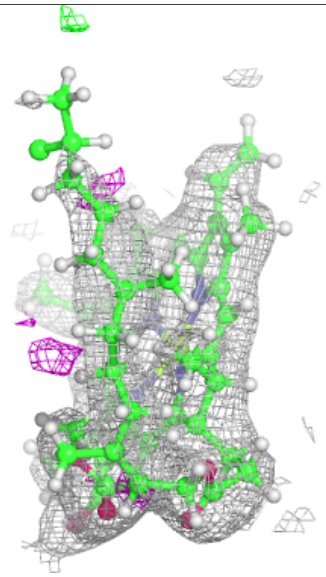


Electron density around CLA B 616:

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

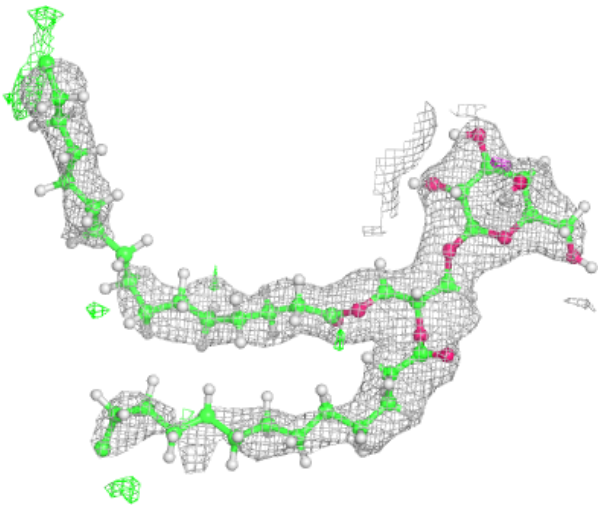


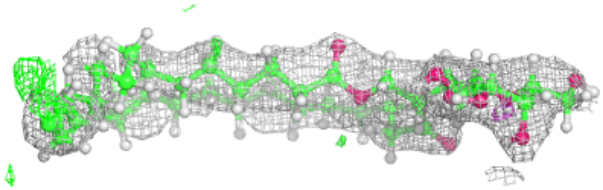


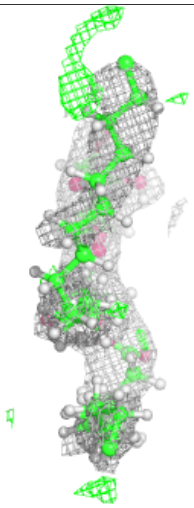


Electron density around LMG K 102:

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

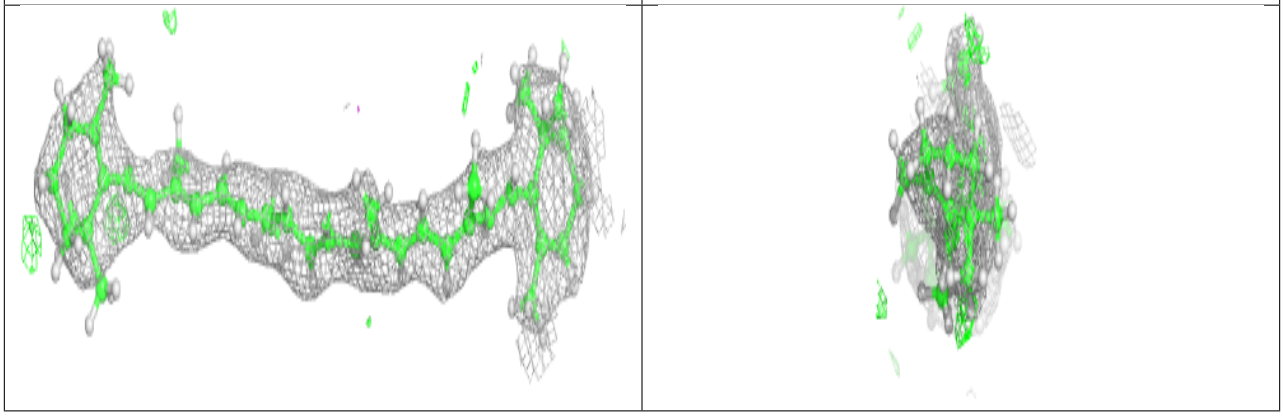






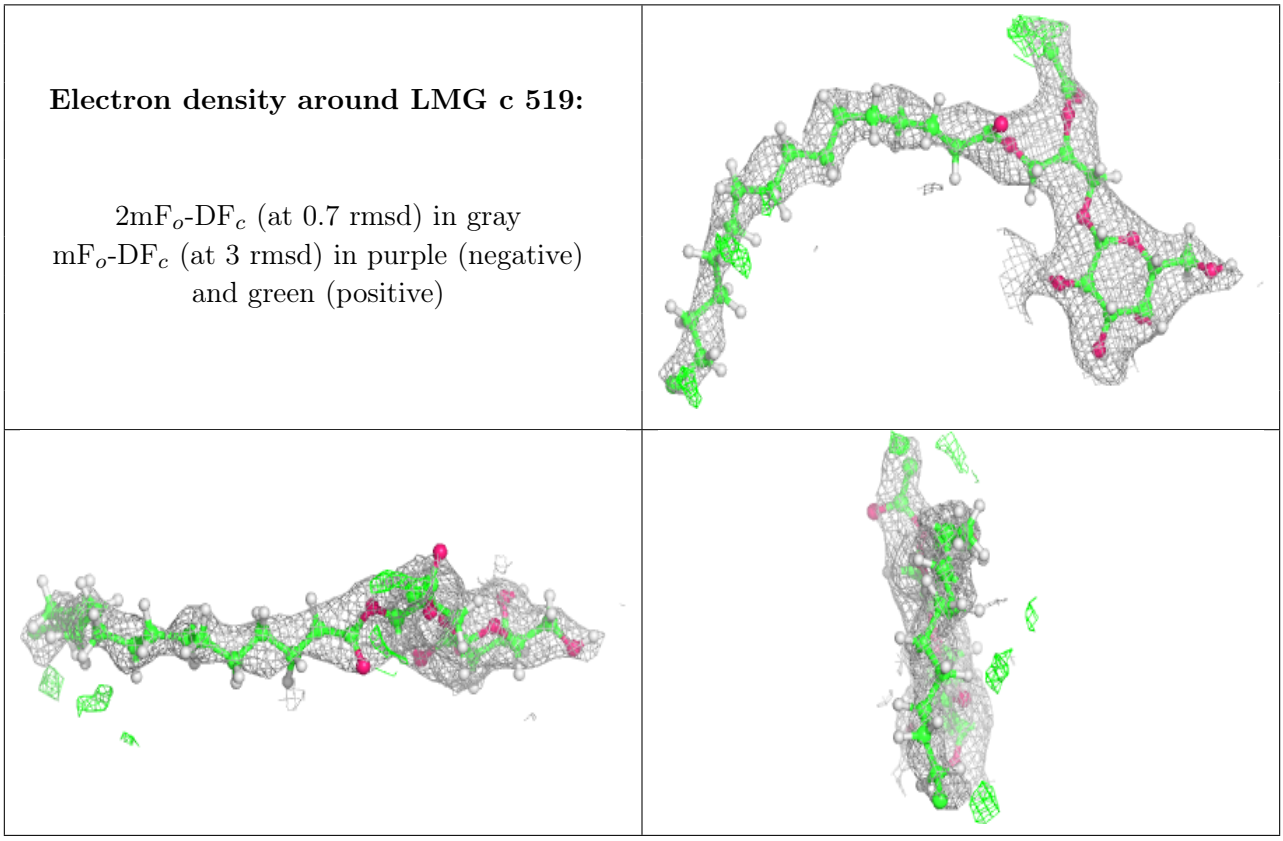
Electron density around BCR h 103:

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



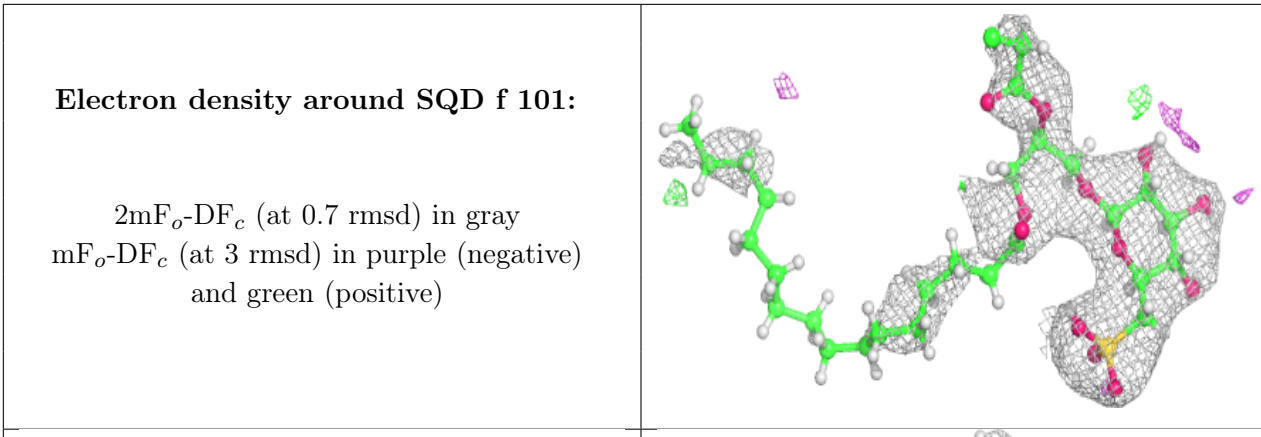
Electron density around LMG c 519:

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



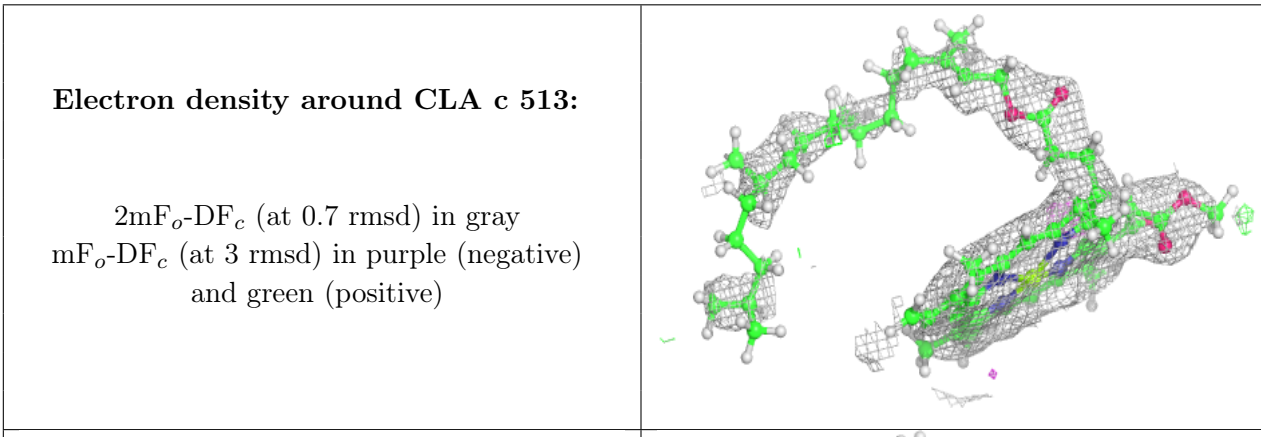
Electron density around SQD f 101:

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



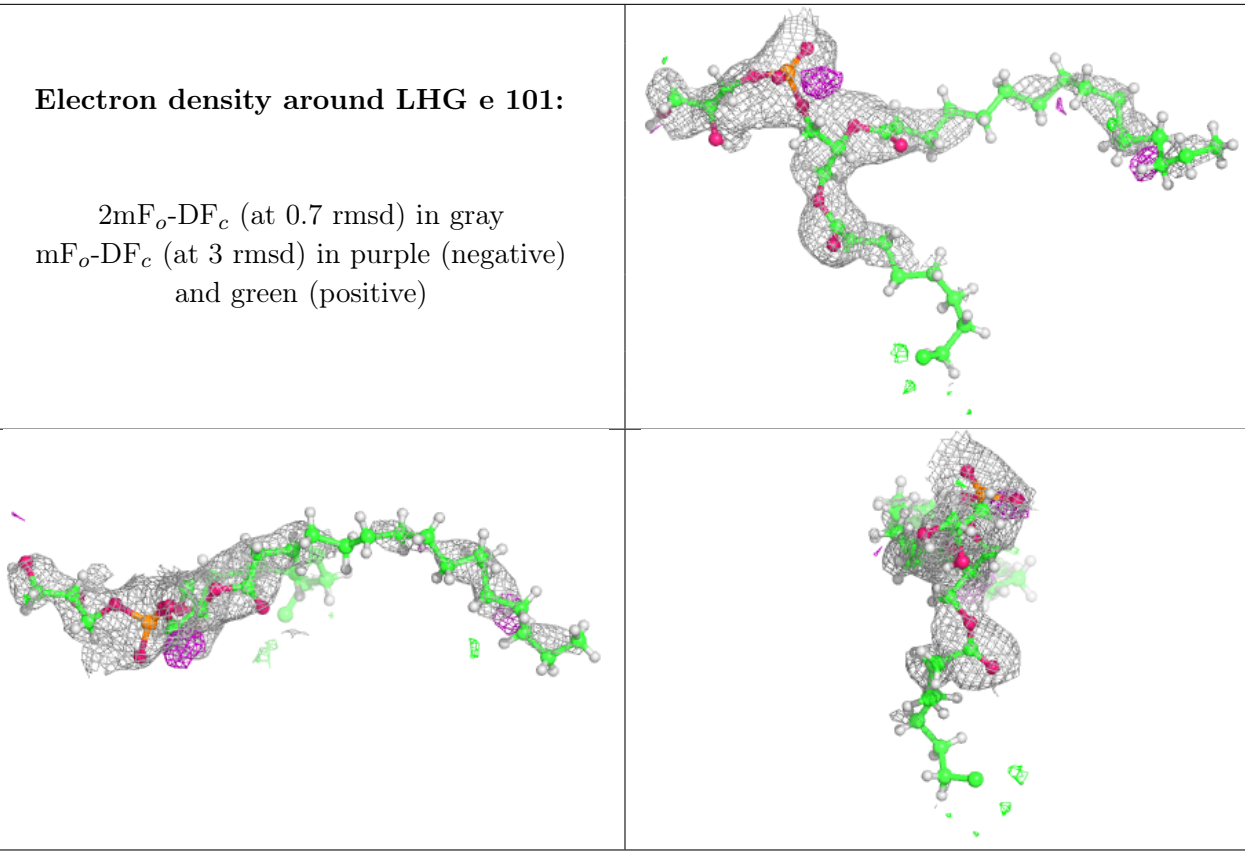
Electron density around CLA c 513:

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



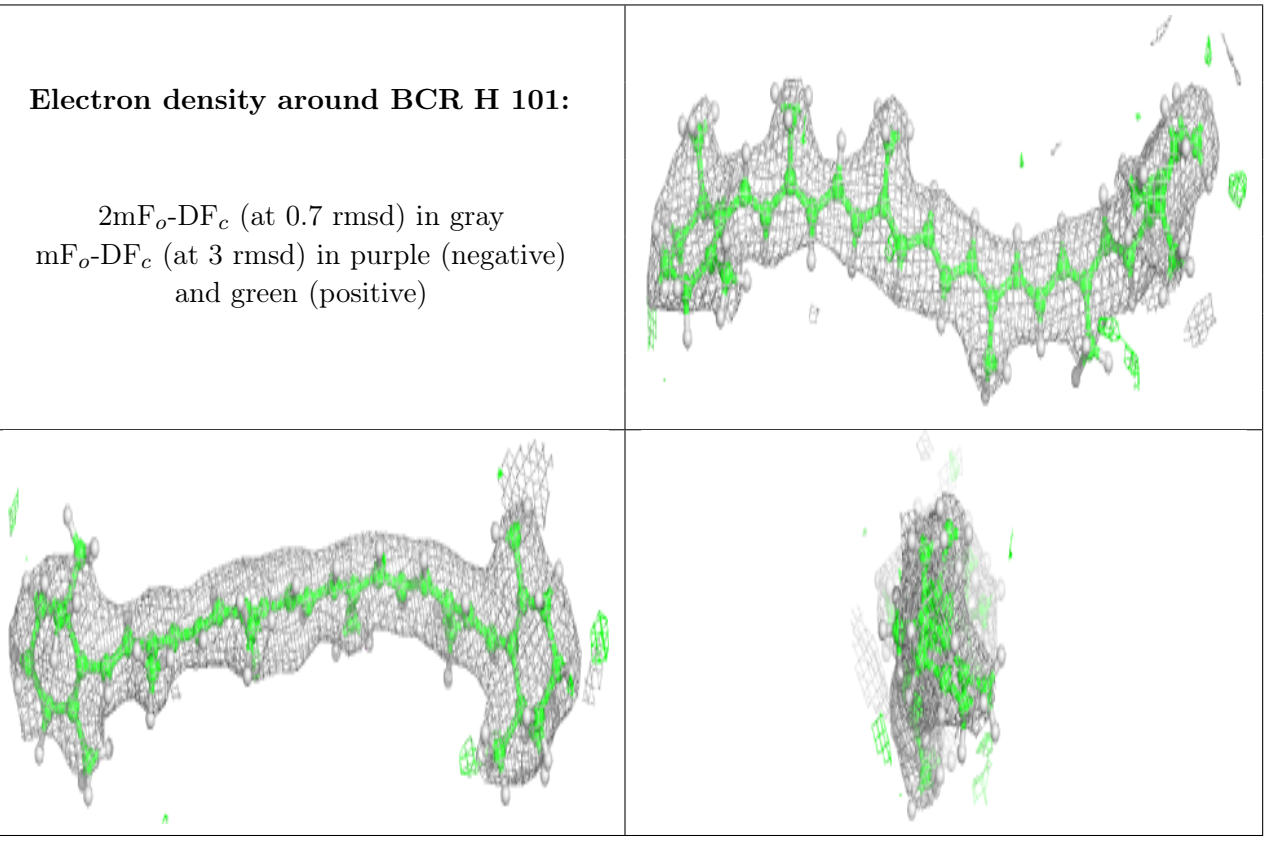
Electron density around LHG e 101:

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



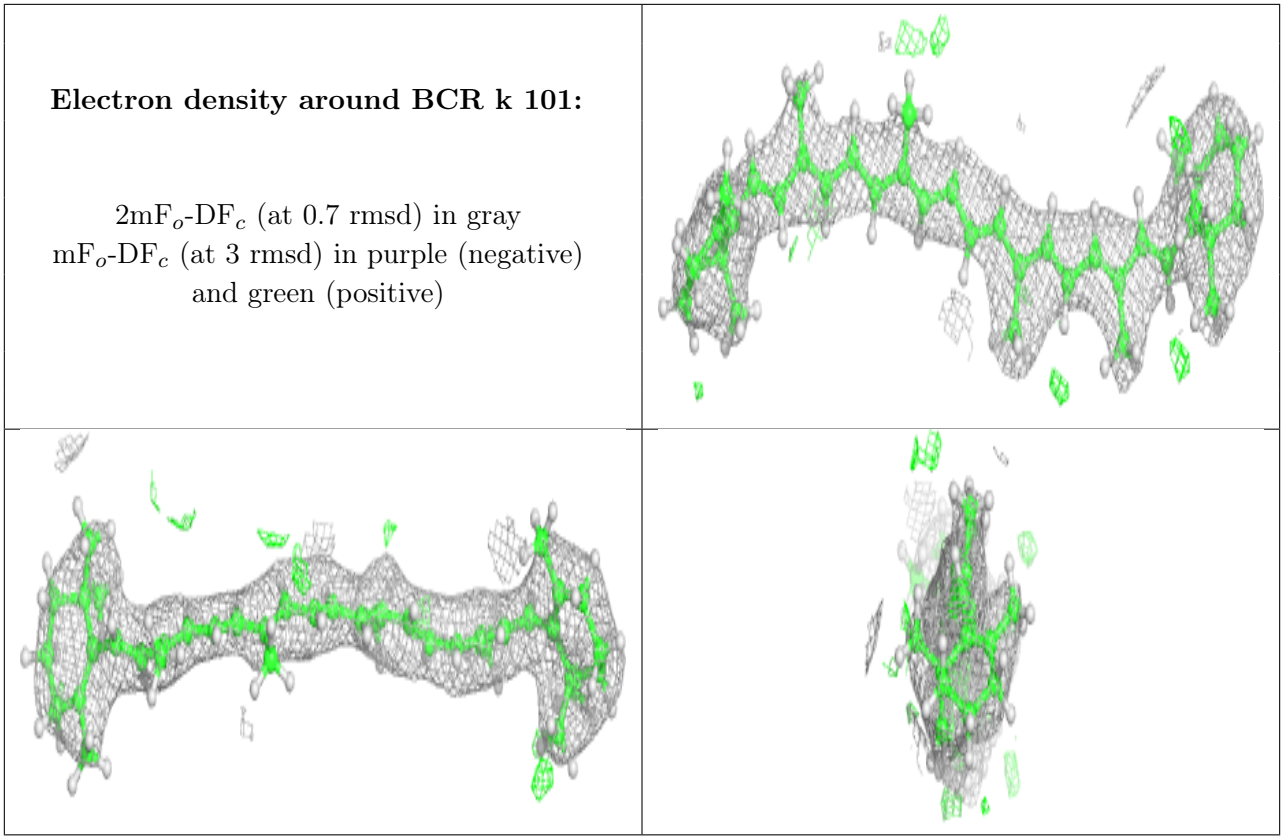
Electron density around BCR H 101:

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



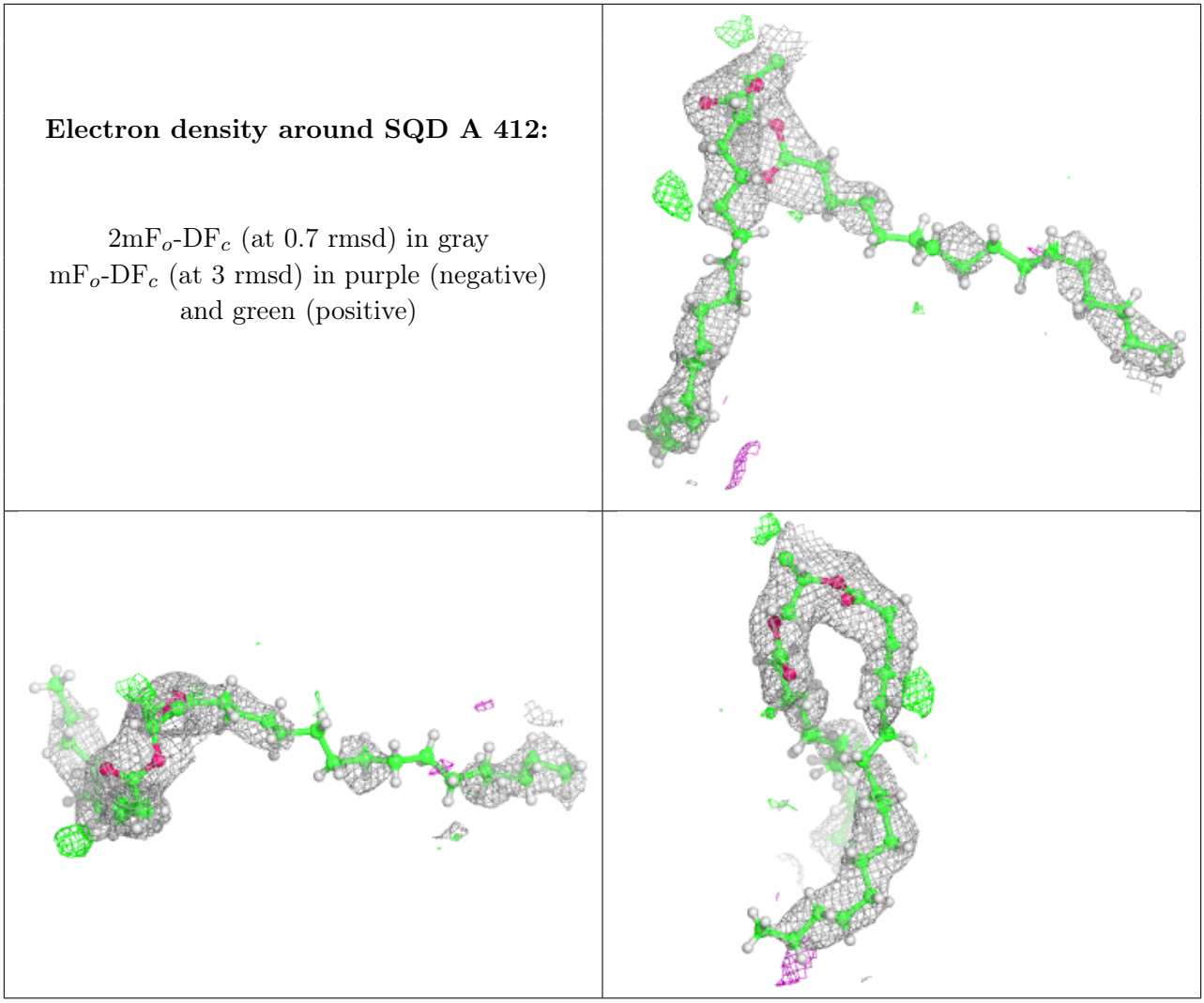
Electron density around BCR k 101:

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



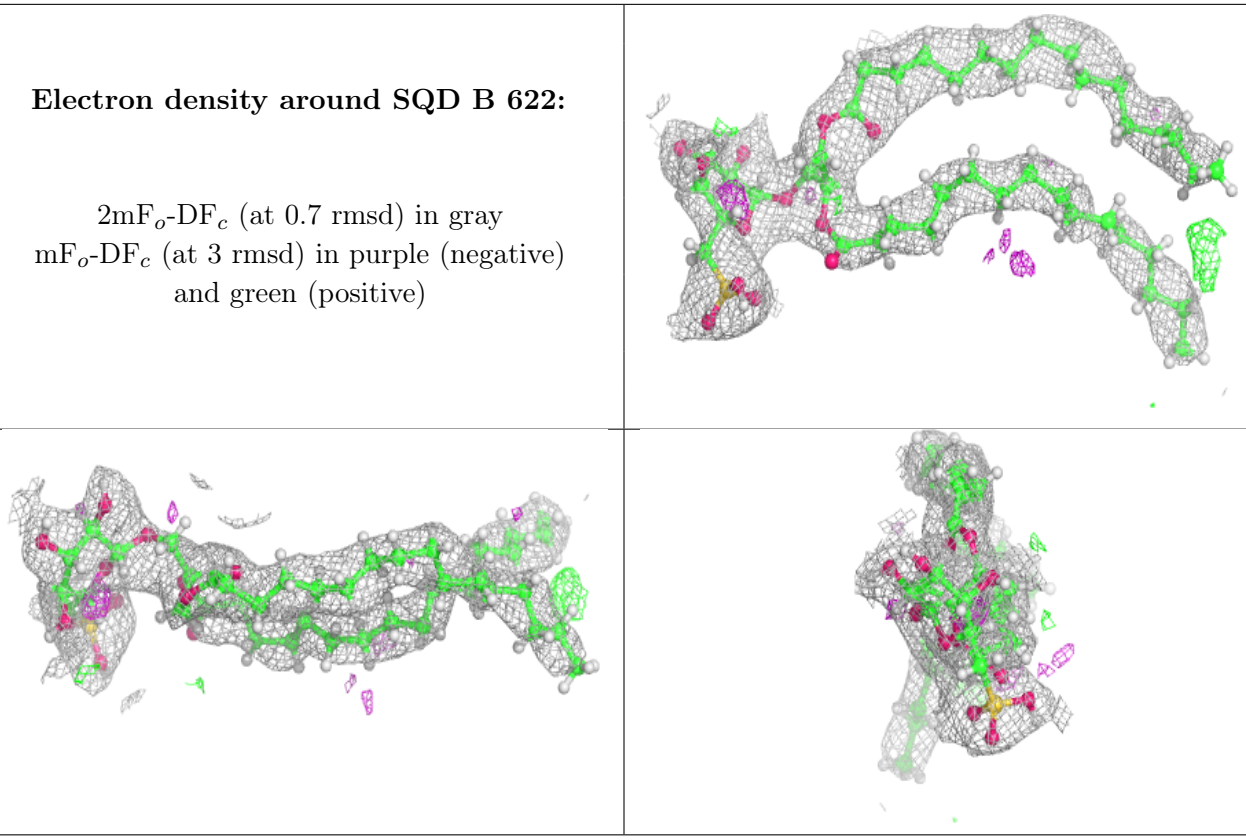
Electron density around SQD A 412:

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



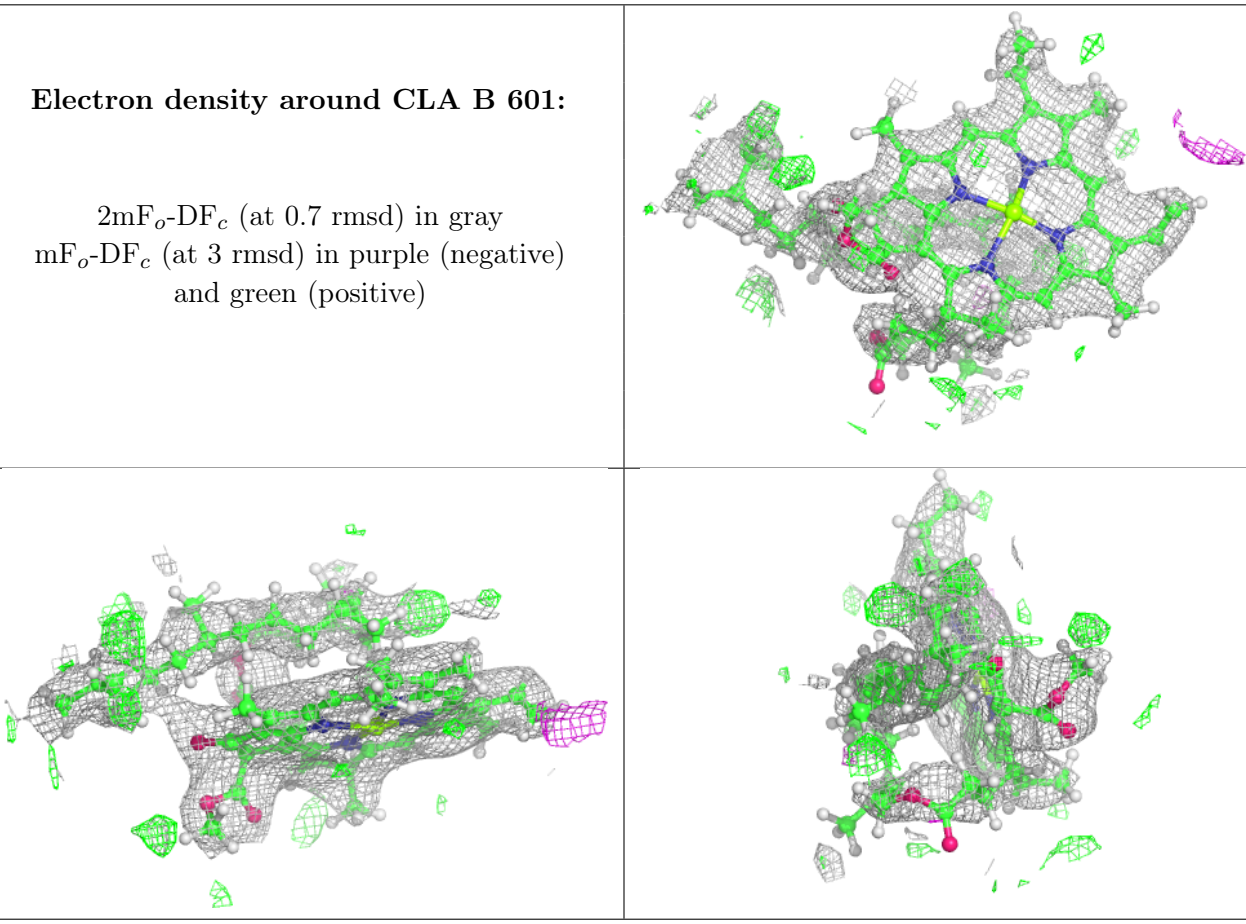
Electron density around SQD B 622:

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



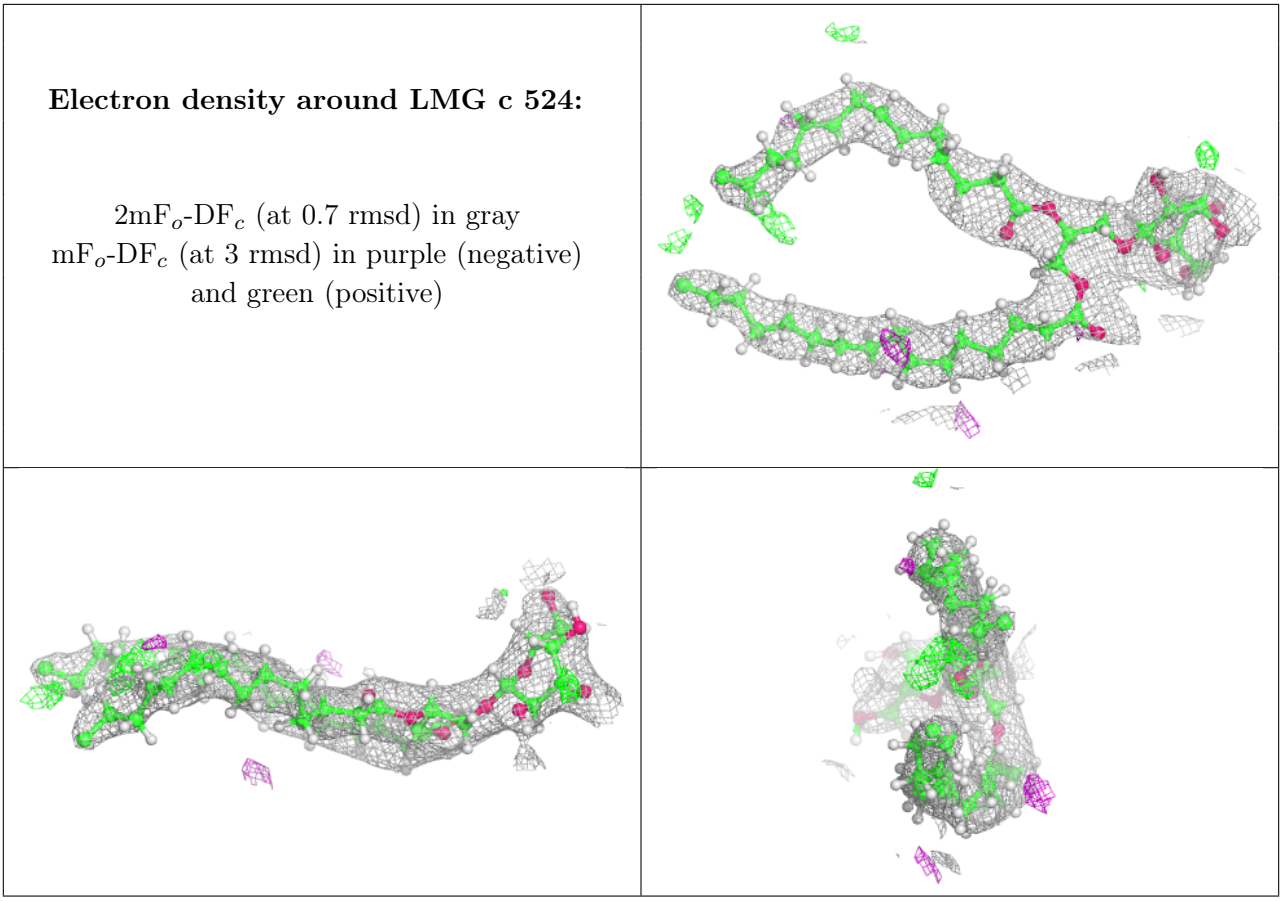
Electron density around CLA B 601:

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



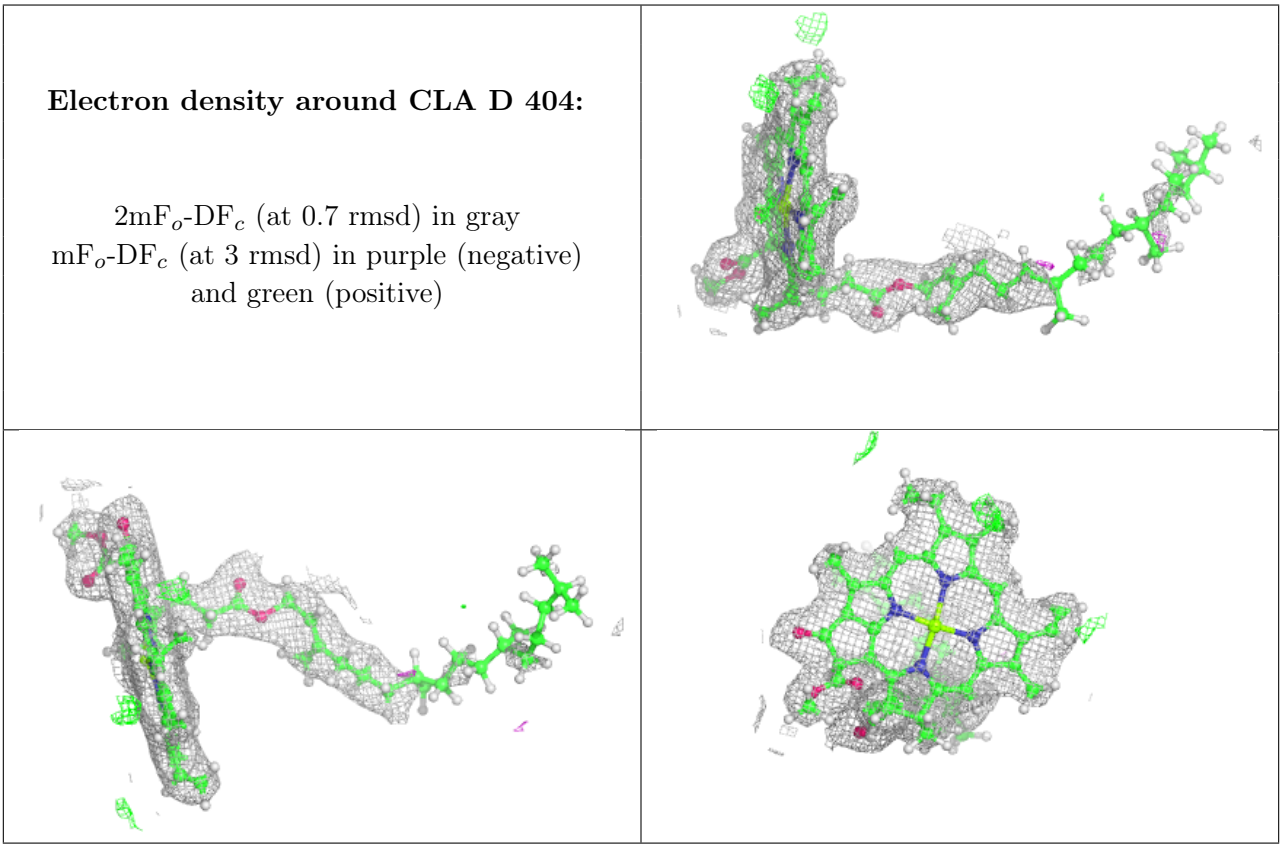
Electron density around LMG c 524:

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



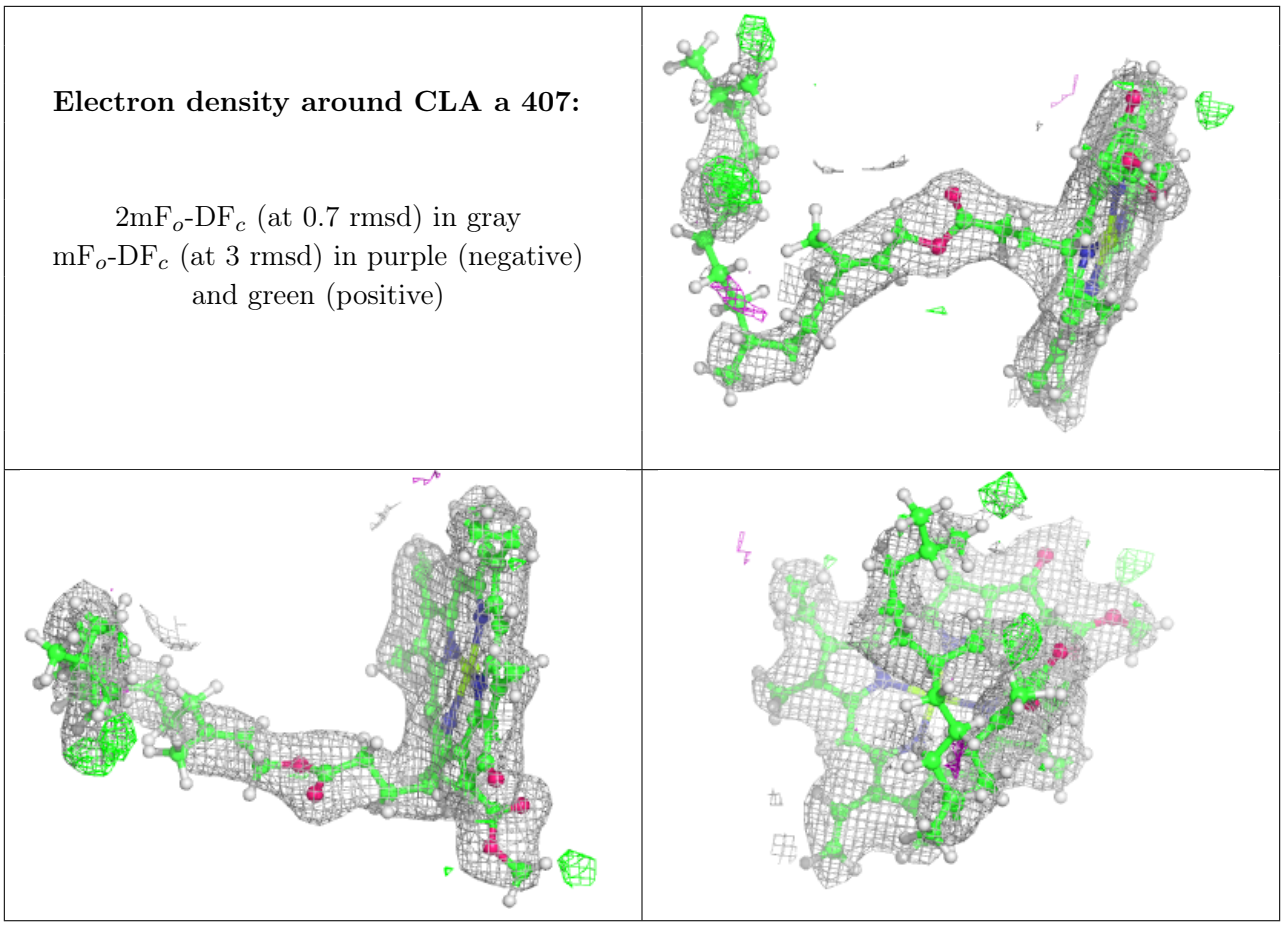
Electron density around CLA D 404:

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



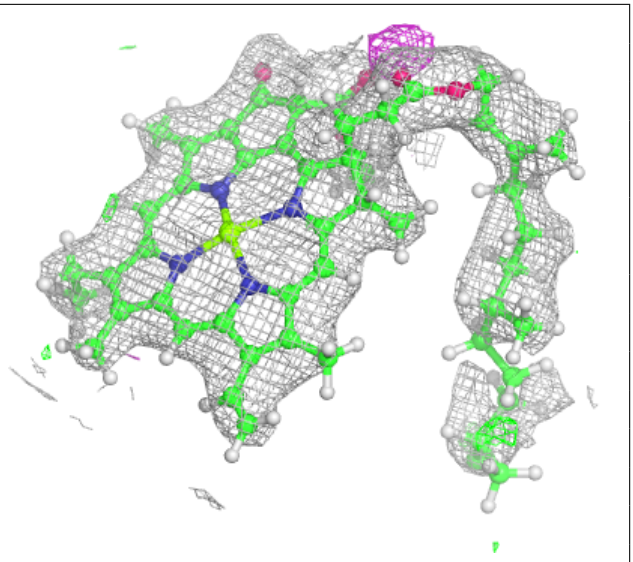
Electron density around CLA a 407:

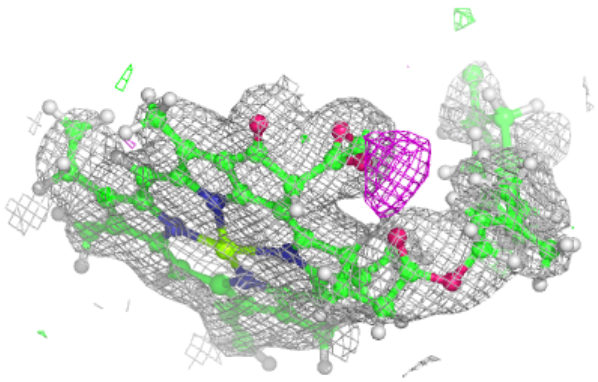
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

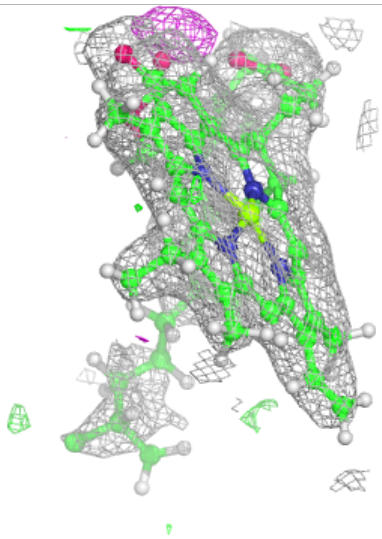


Electron density around CLA b 617:

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

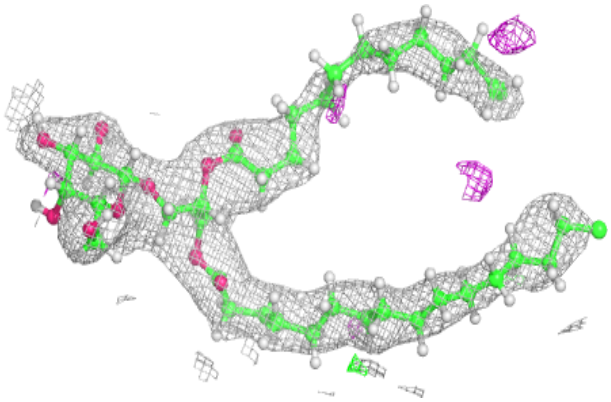


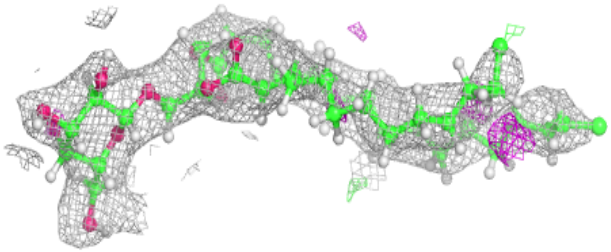


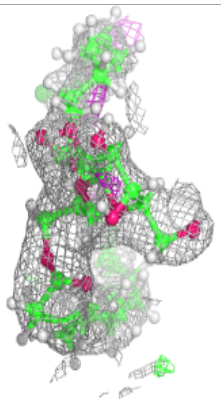


Electron density around LMG C 501:

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

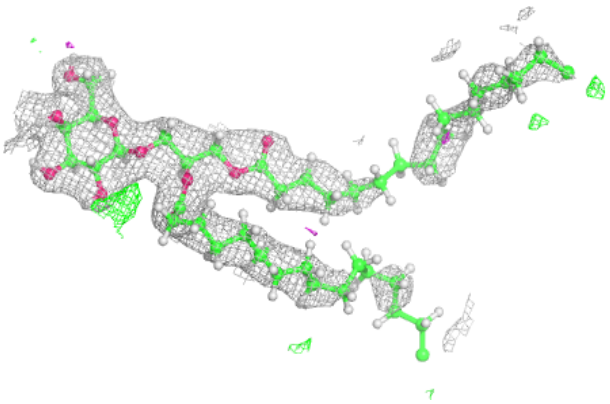


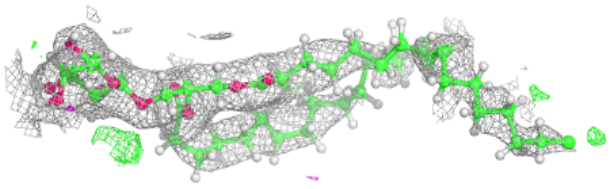


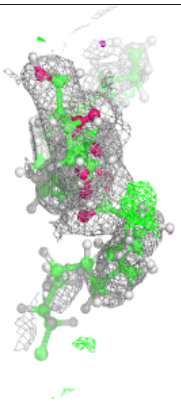


Electron density around LMG D 407:

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

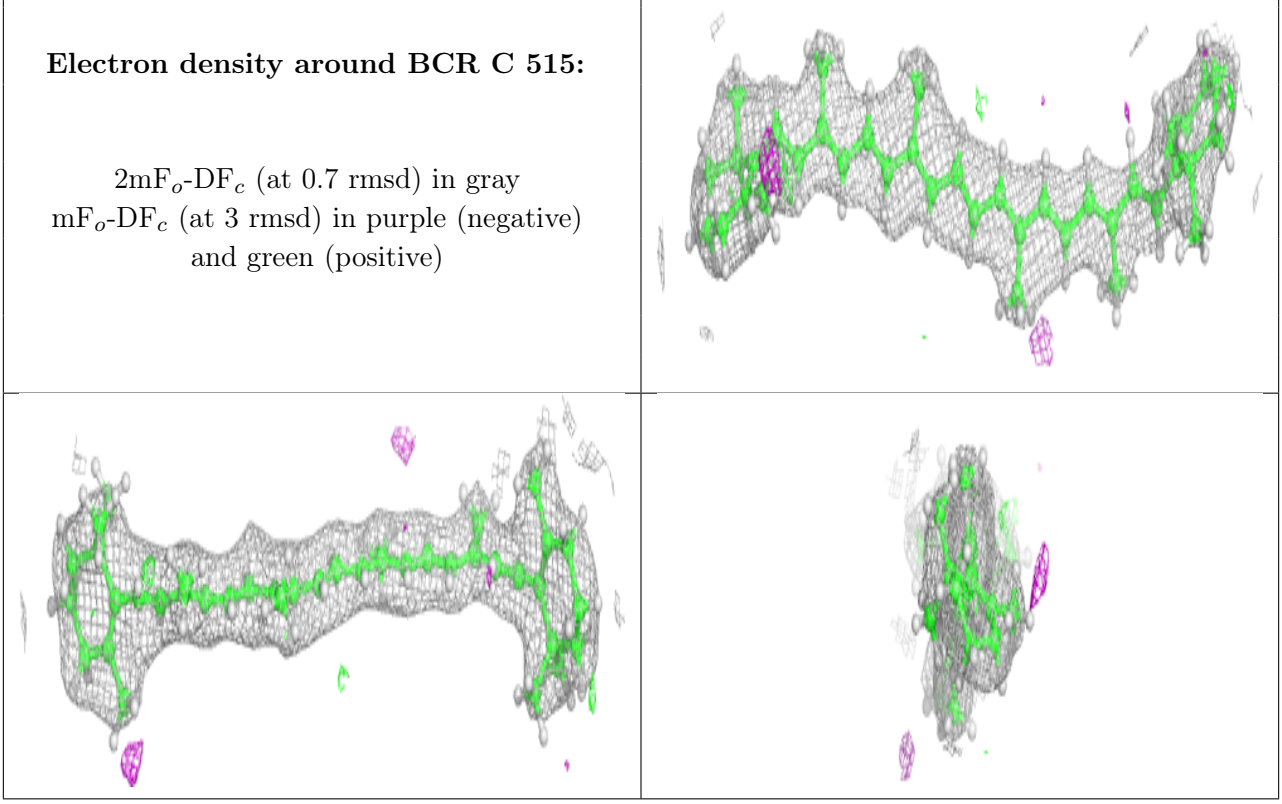






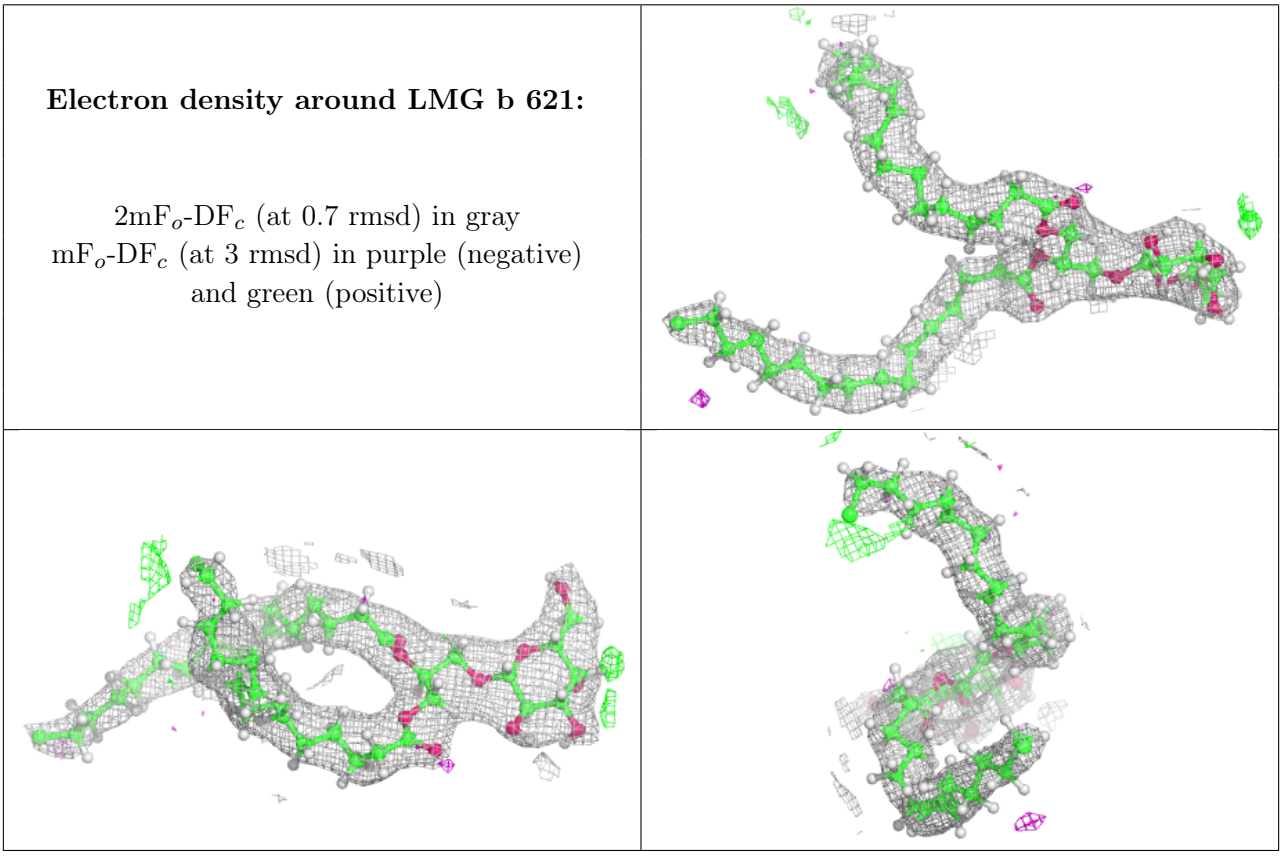
Electron density around BCR C 515:

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



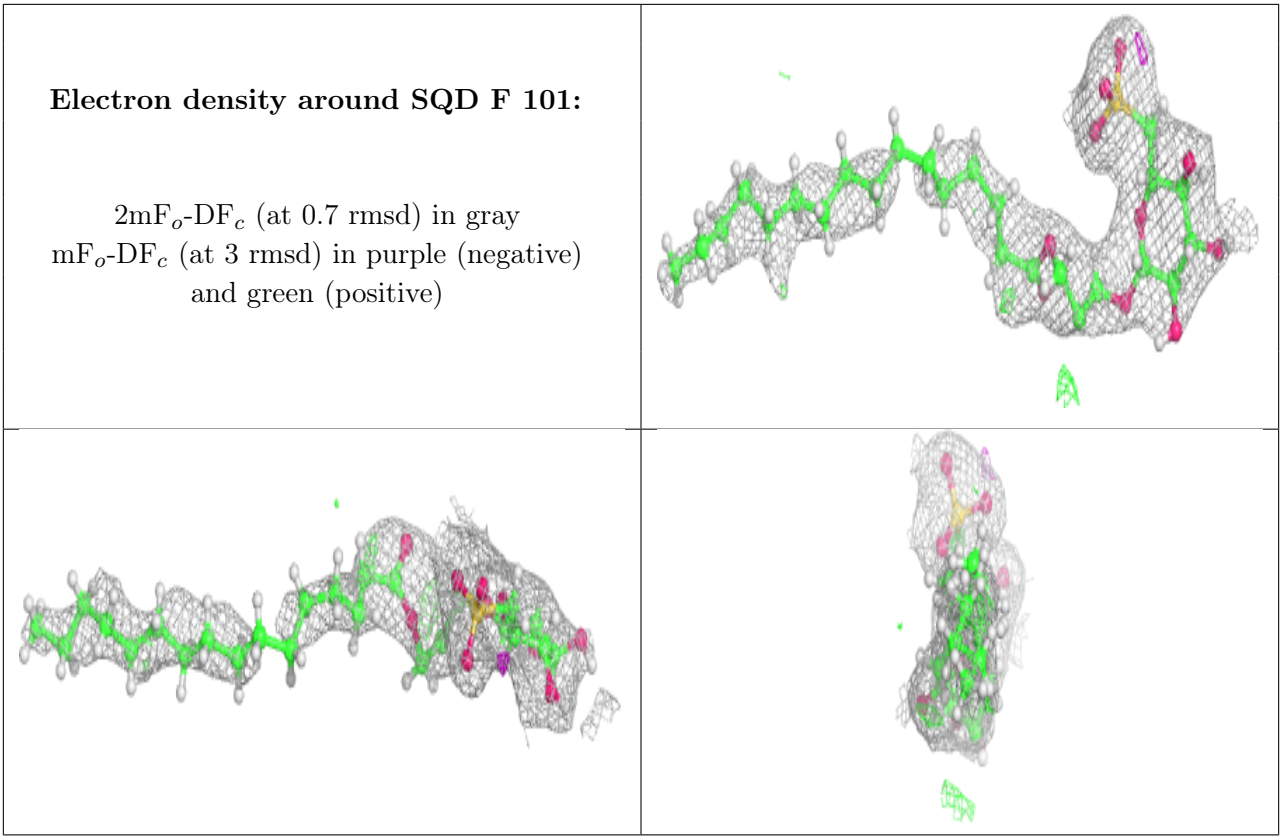
Electron density around LMG b 621:

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



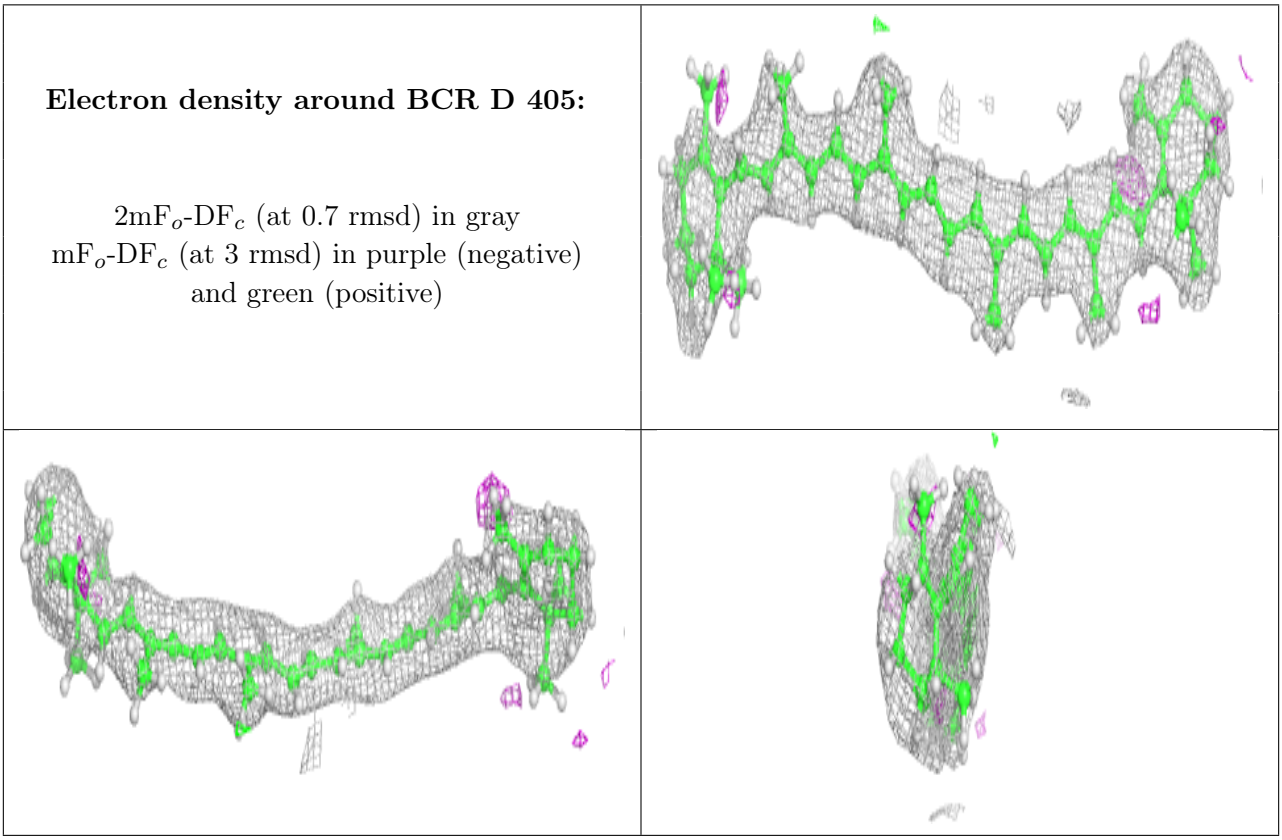
Electron density around SQD F 101:

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



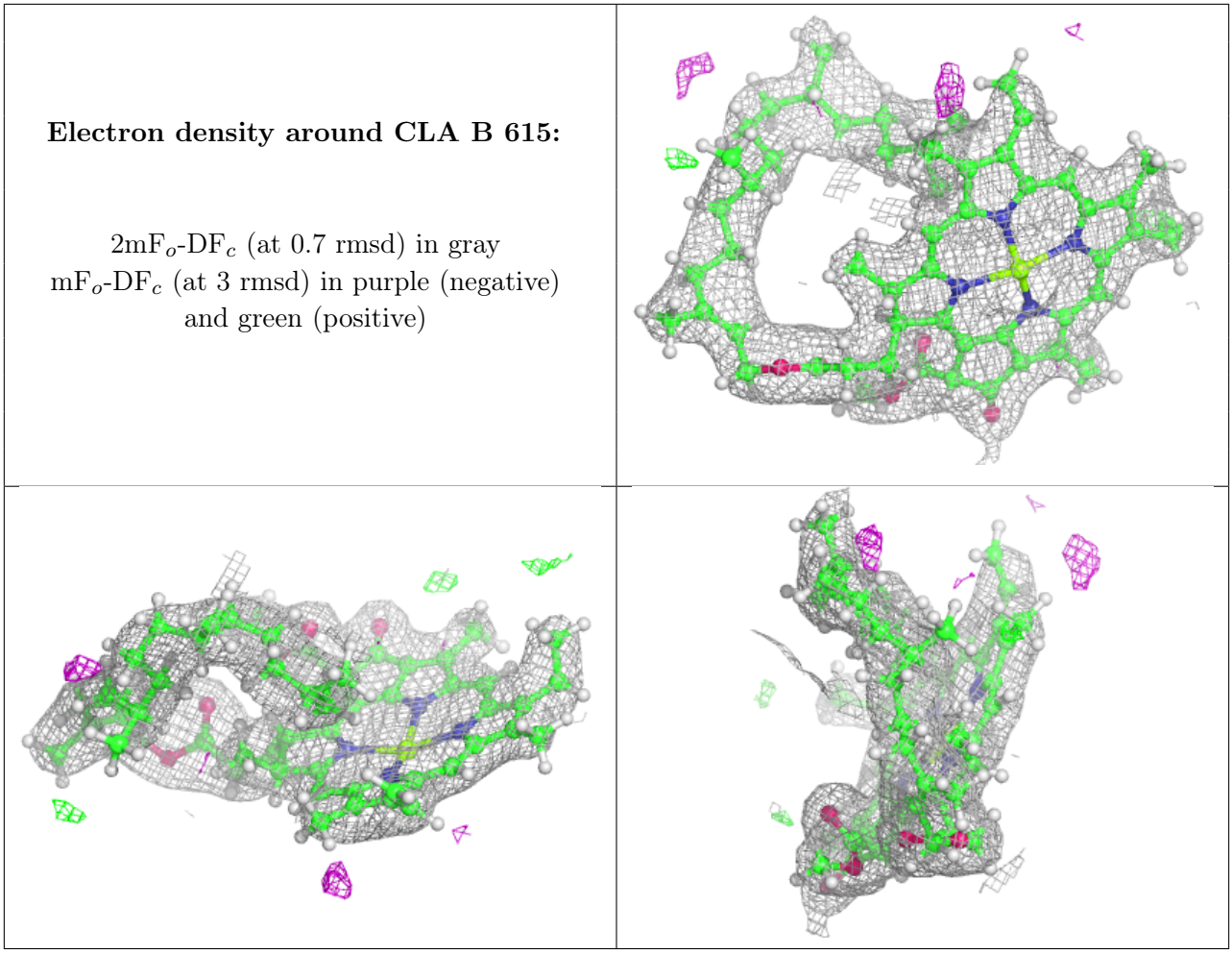
Electron density around BCR D 405:

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



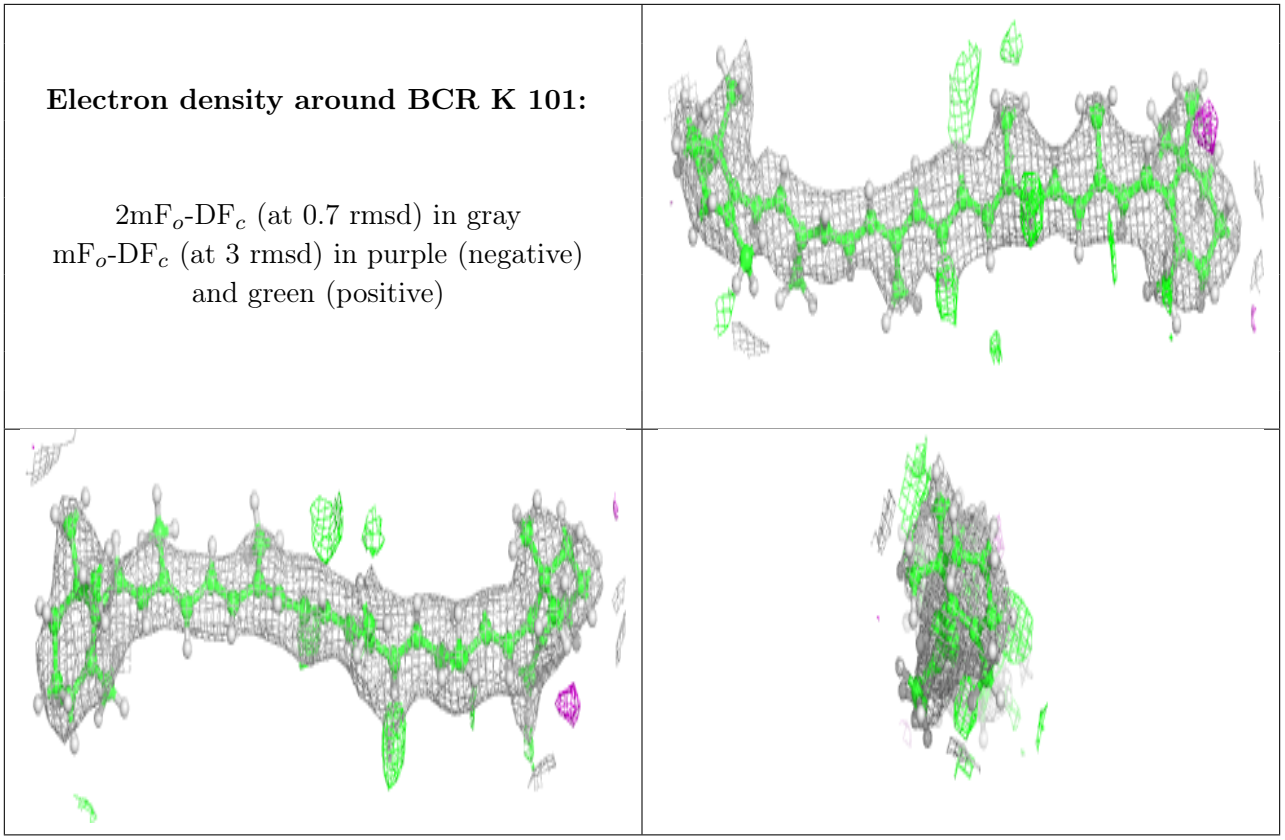
Electron density around CLA B 615:

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



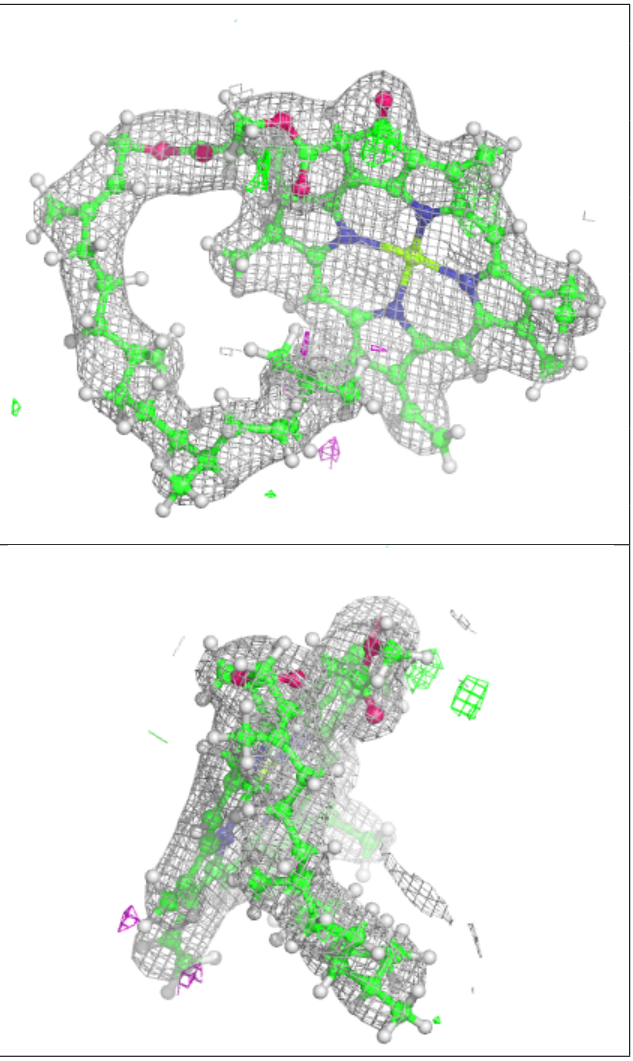
Electron density around BCR K 101:

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



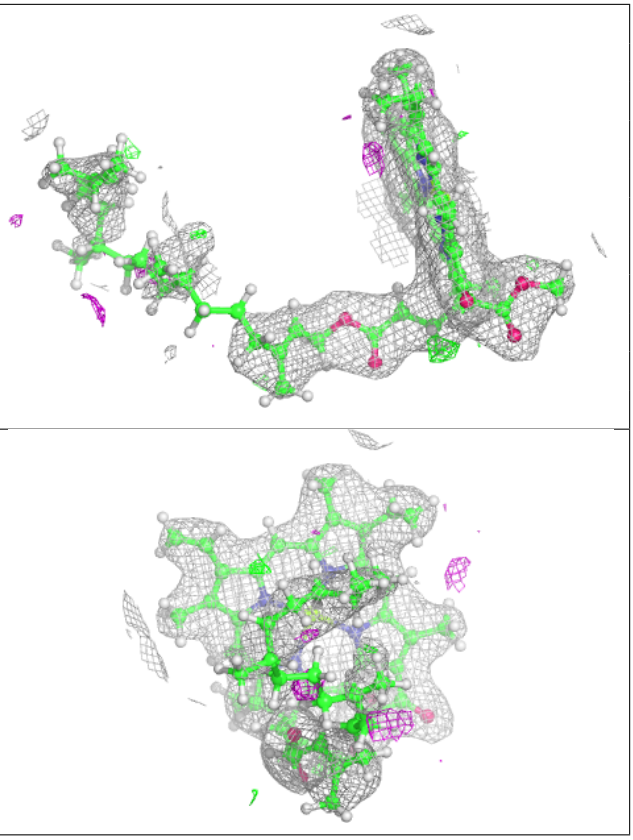
Electron density around CLA b 616:

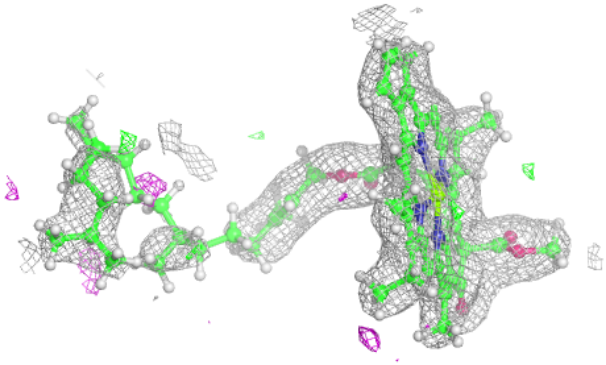
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 507:

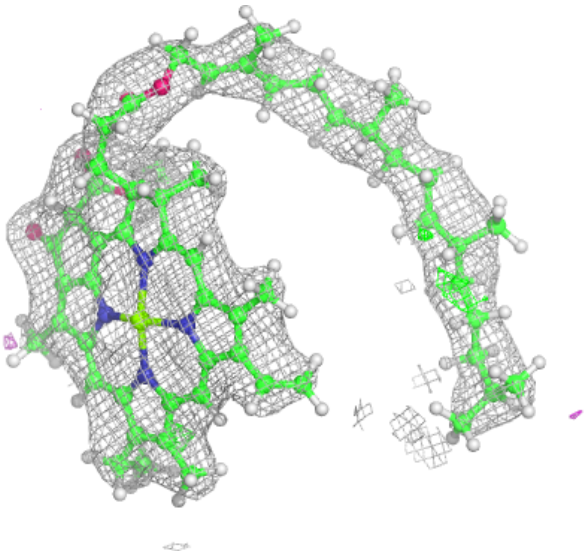
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

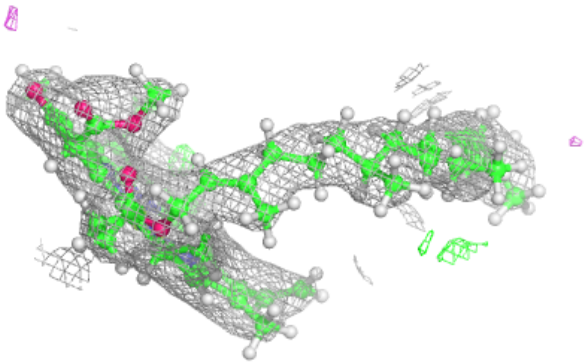


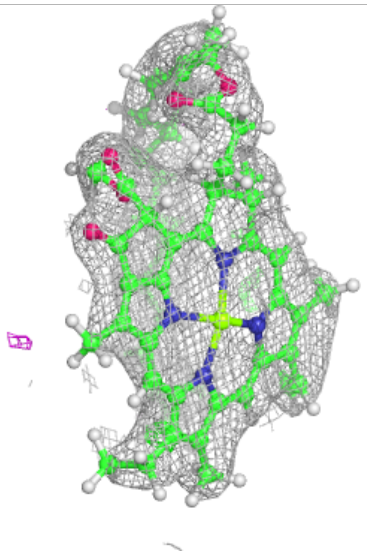


Electron density around CLA c 507:

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

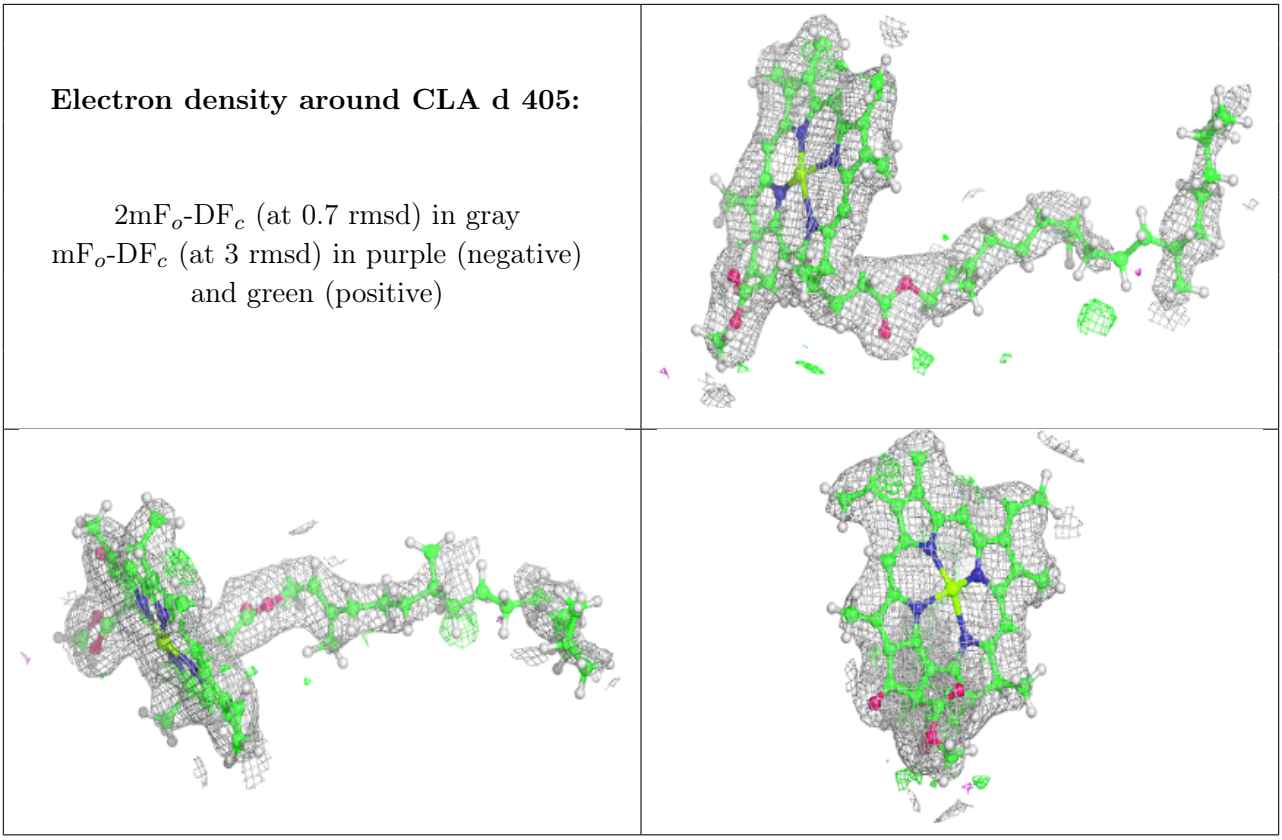






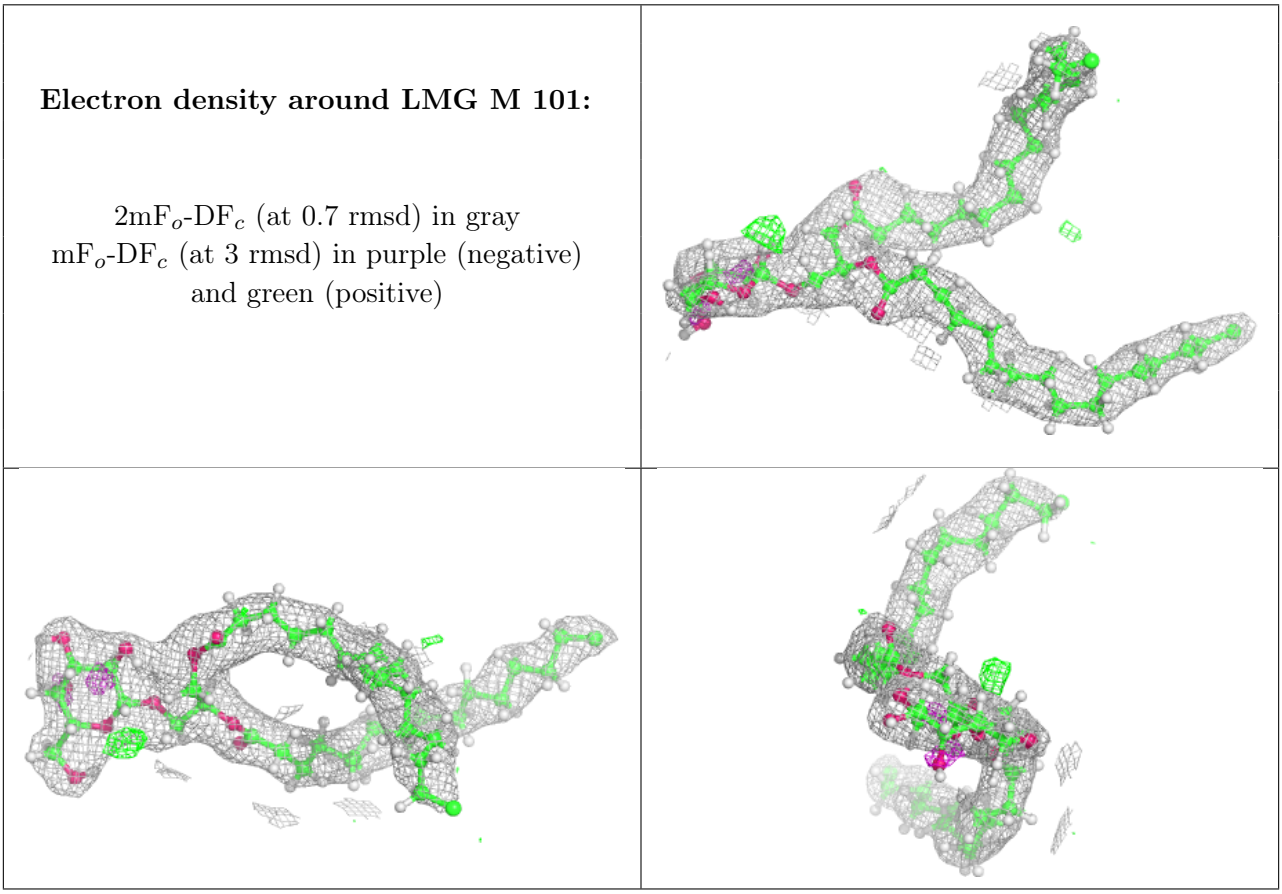
Electron density around CLA d 405:

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



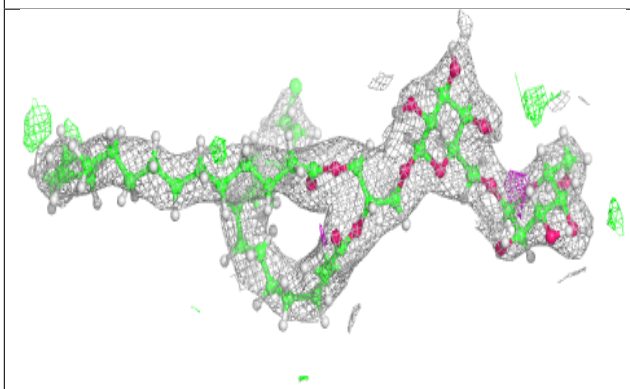
Electron density around LMG M 101:

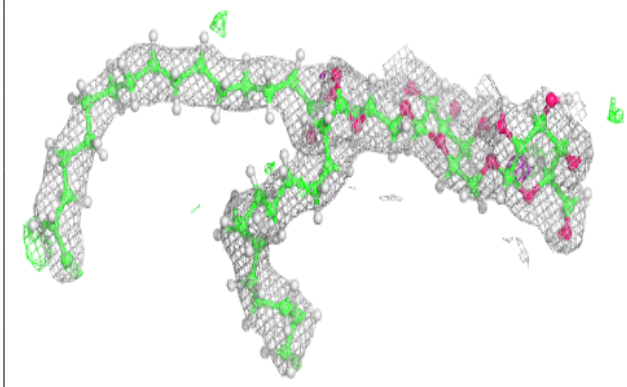
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

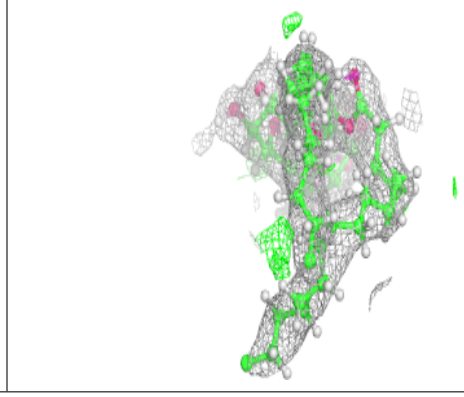


Electron density around DGD H 102:

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

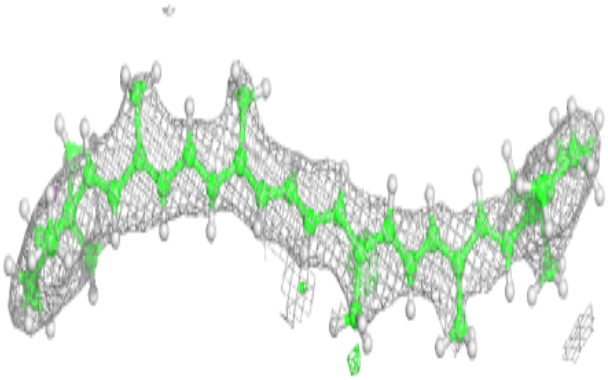


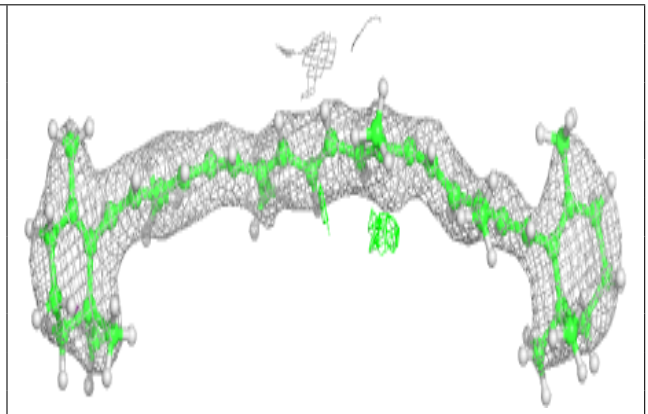


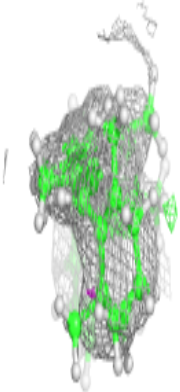


Electron density around BCR c 521:

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

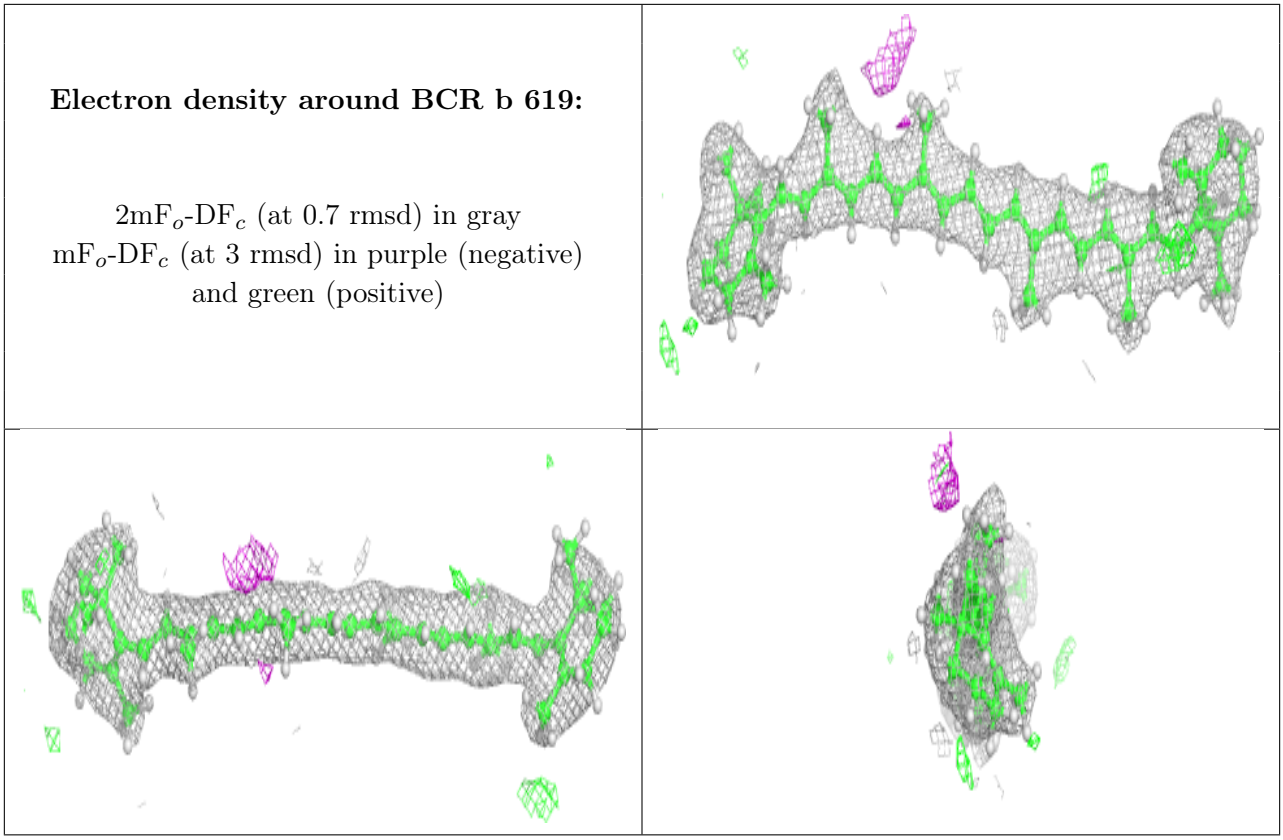






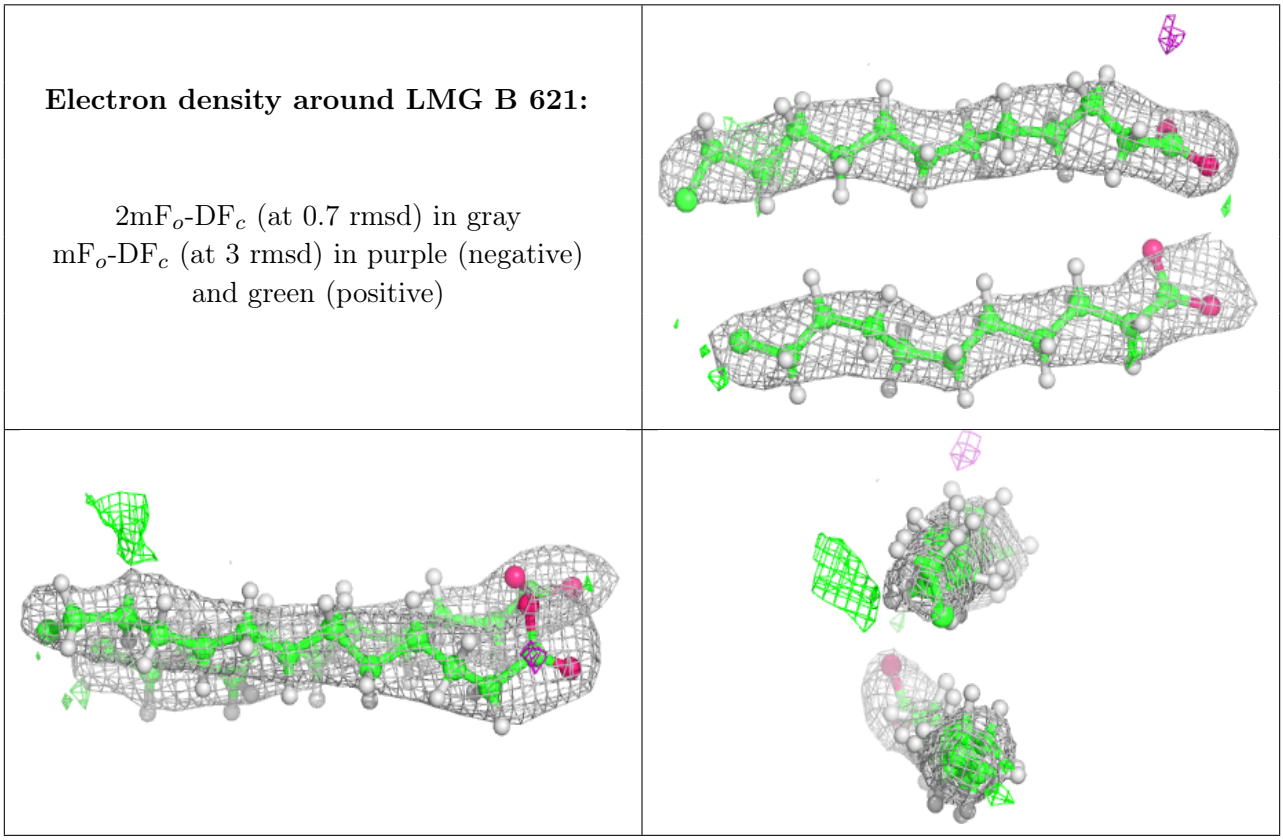
Electron density around BCR b 619:

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



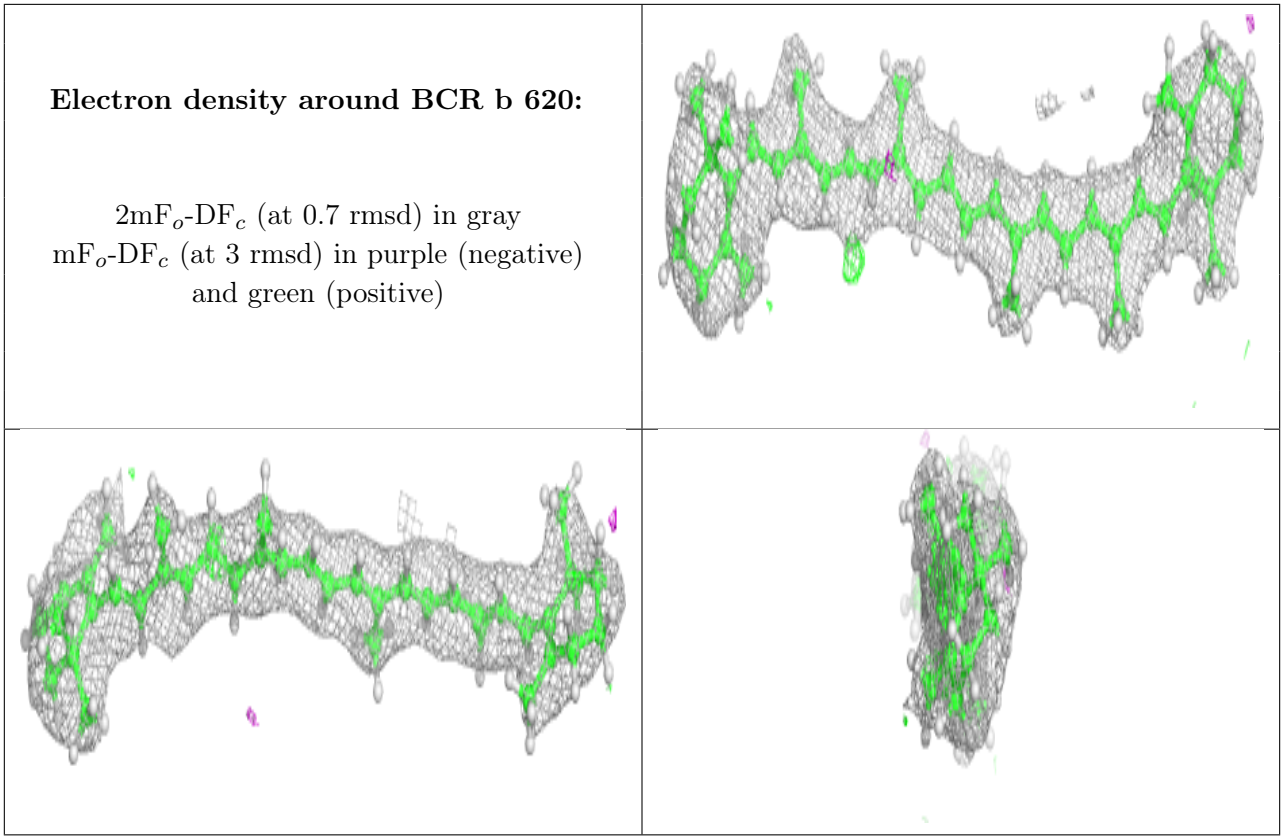
Electron density around LMG B 621:

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



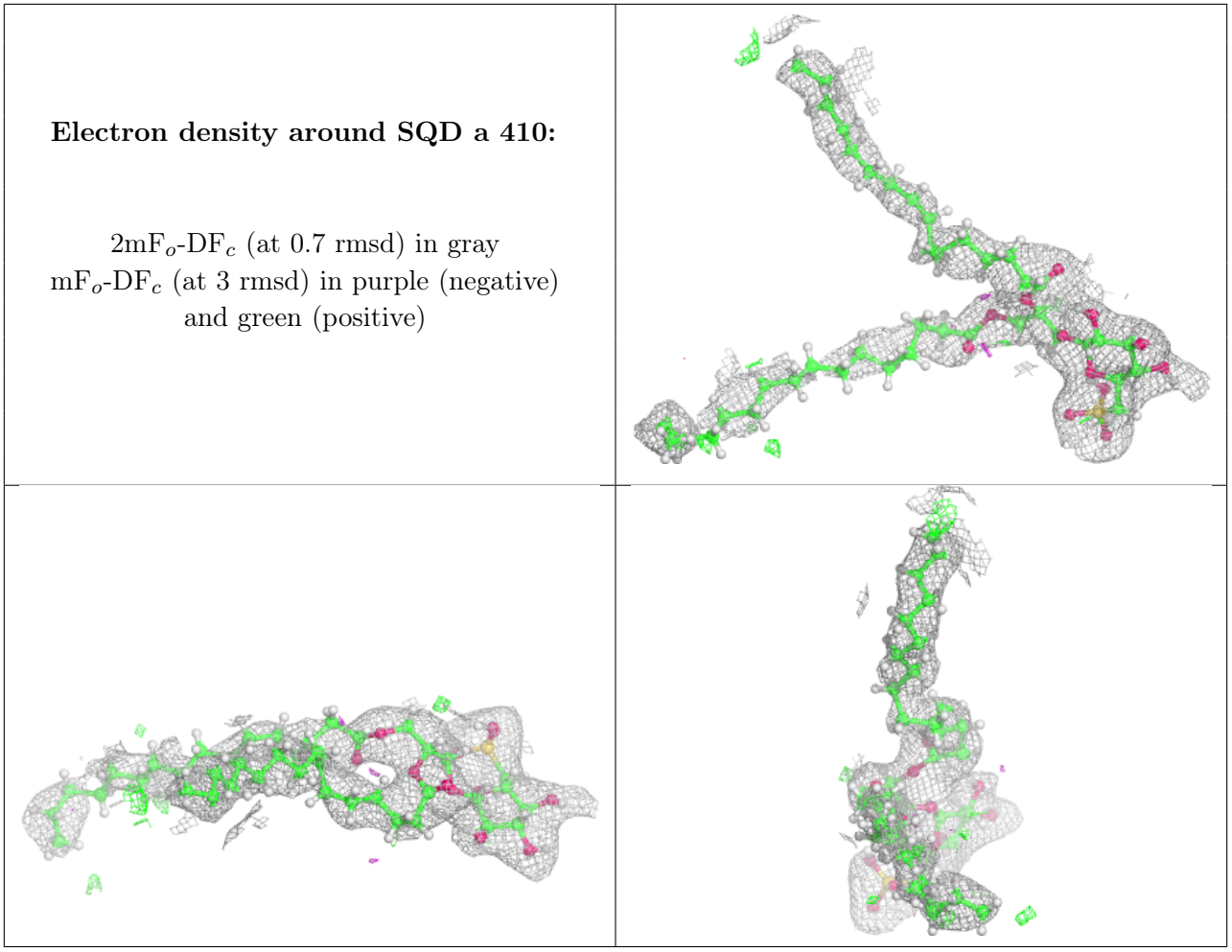
Electron density around BCR b 620:

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



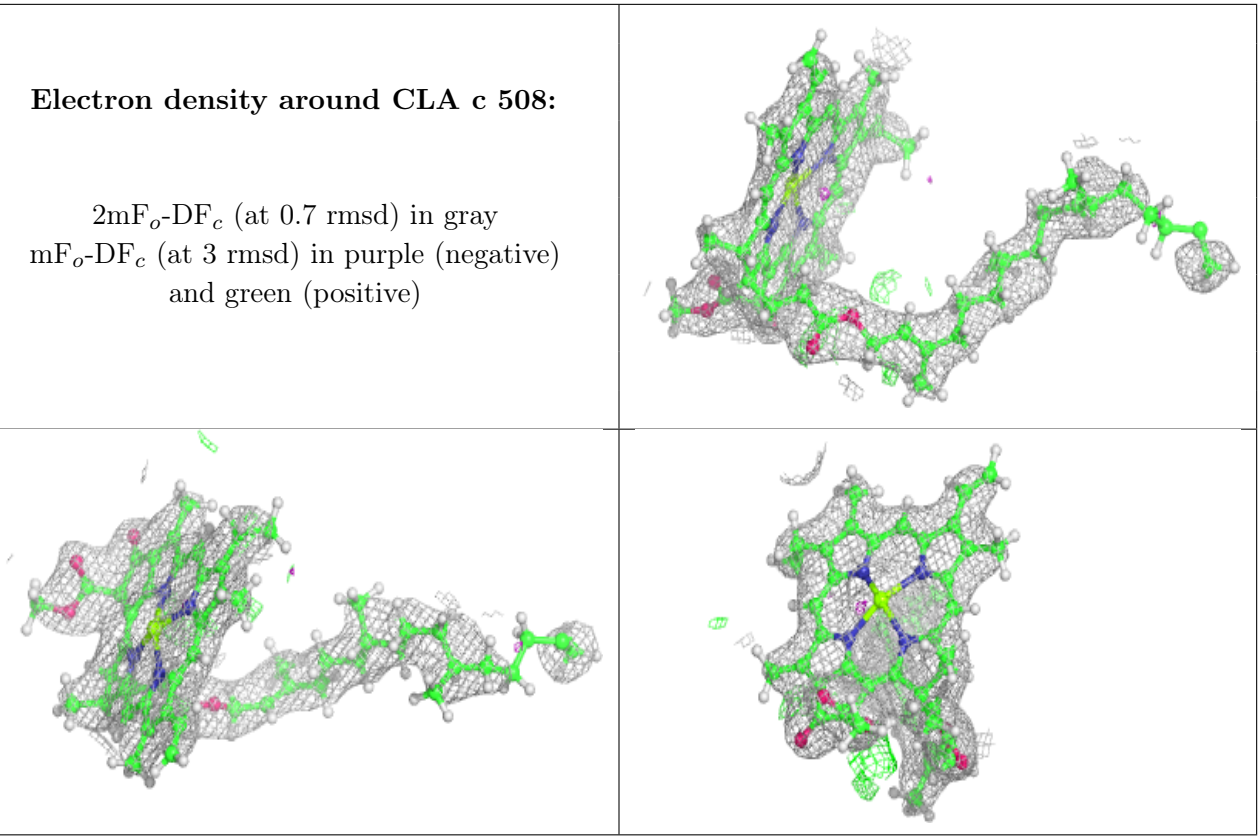
Electron density around SQD a 410:

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



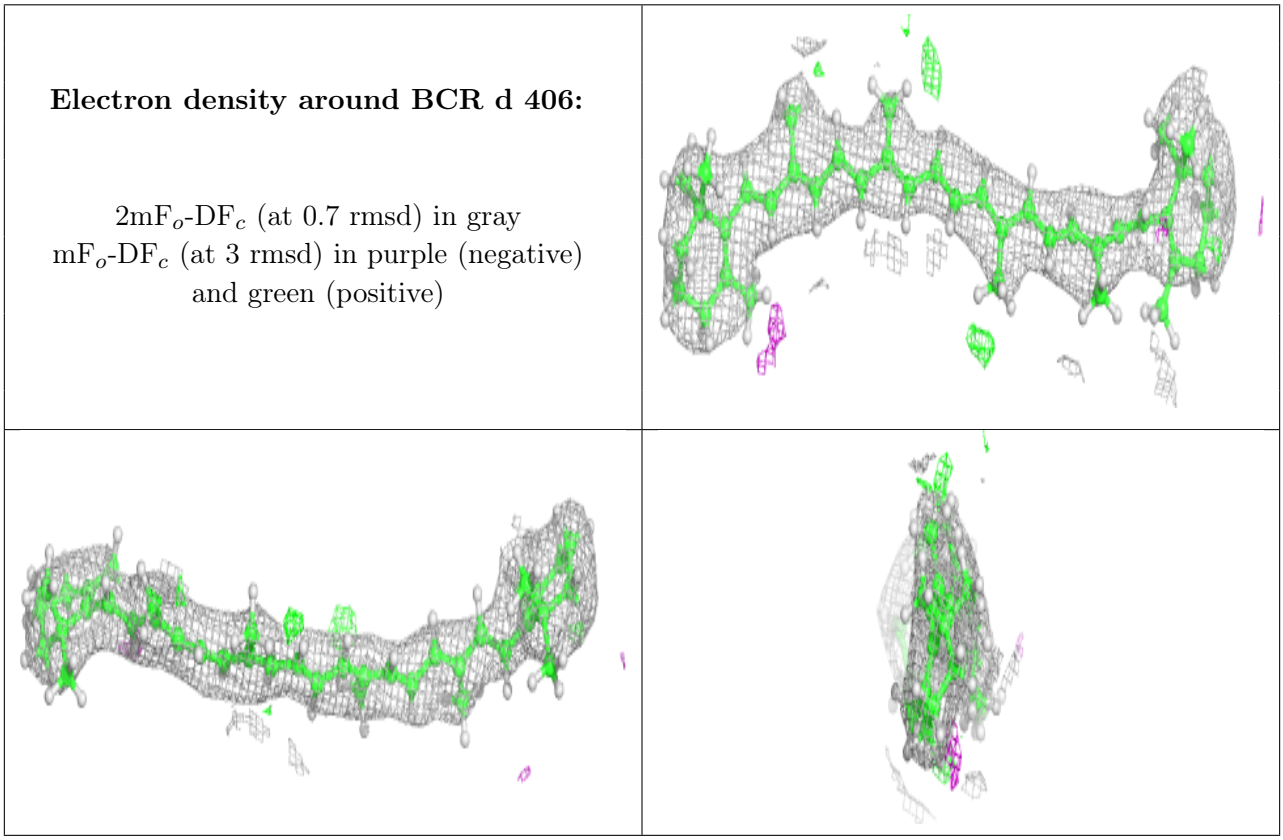
Electron density around CLA c 508:

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



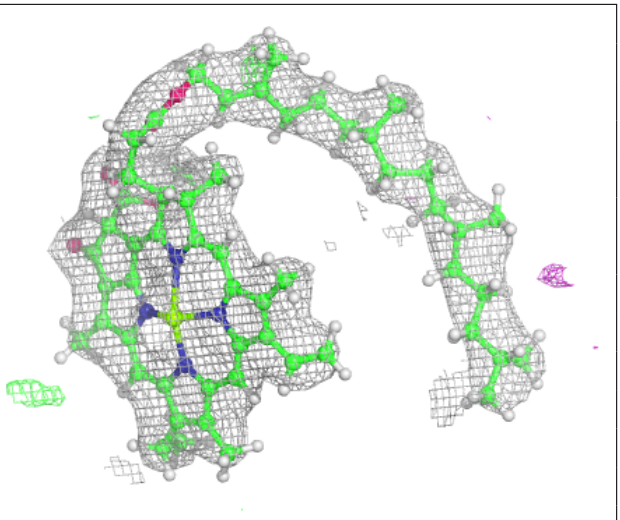
Electron density around BCR d 406:

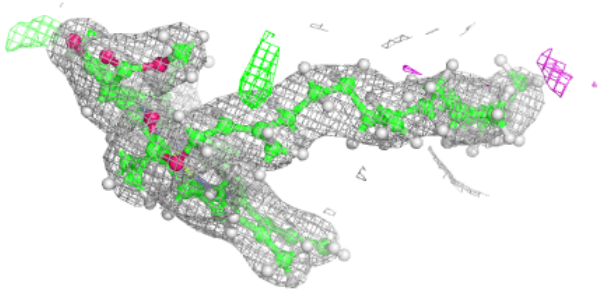
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

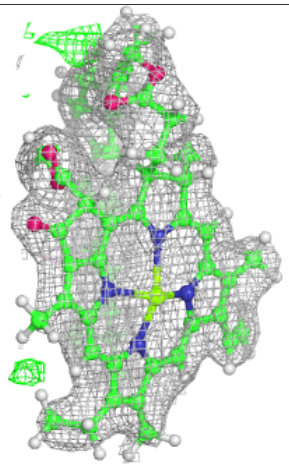


Electron density around CLA C 508:

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

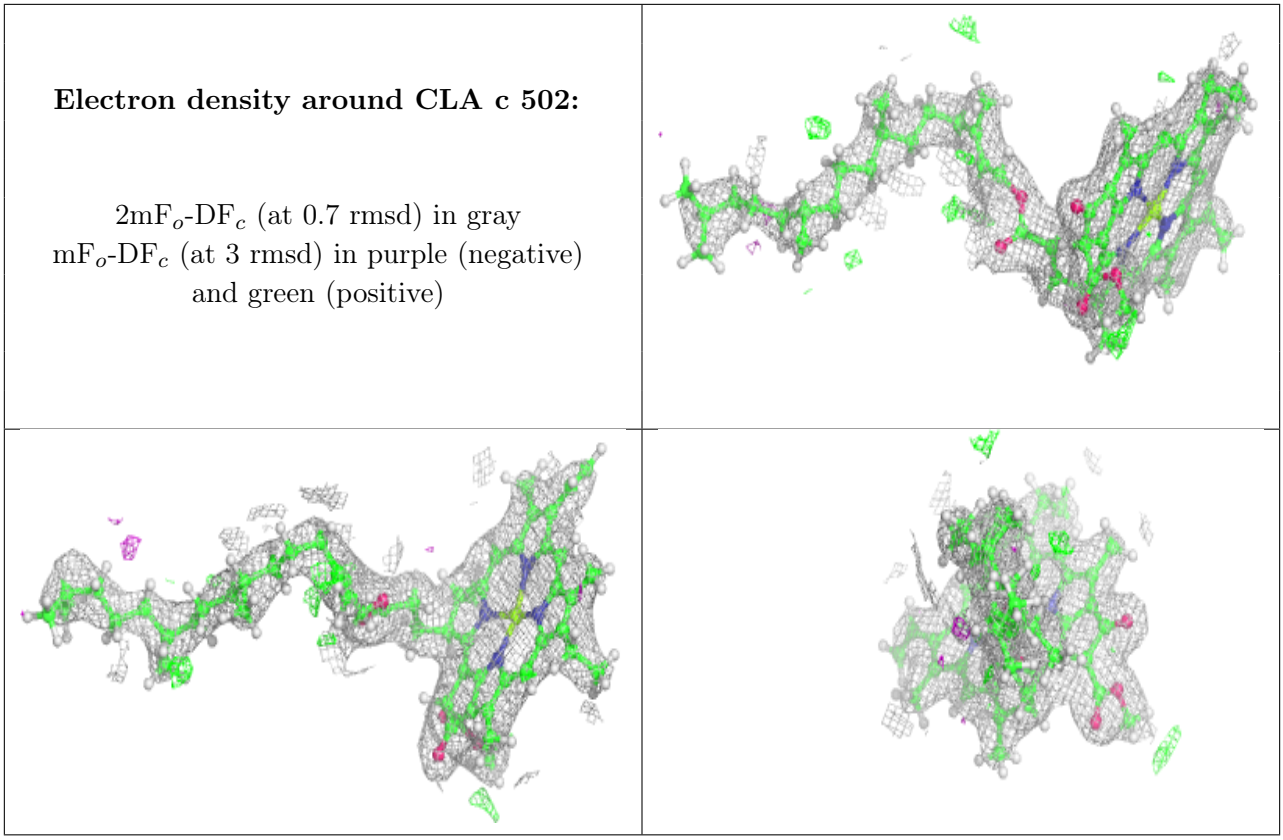






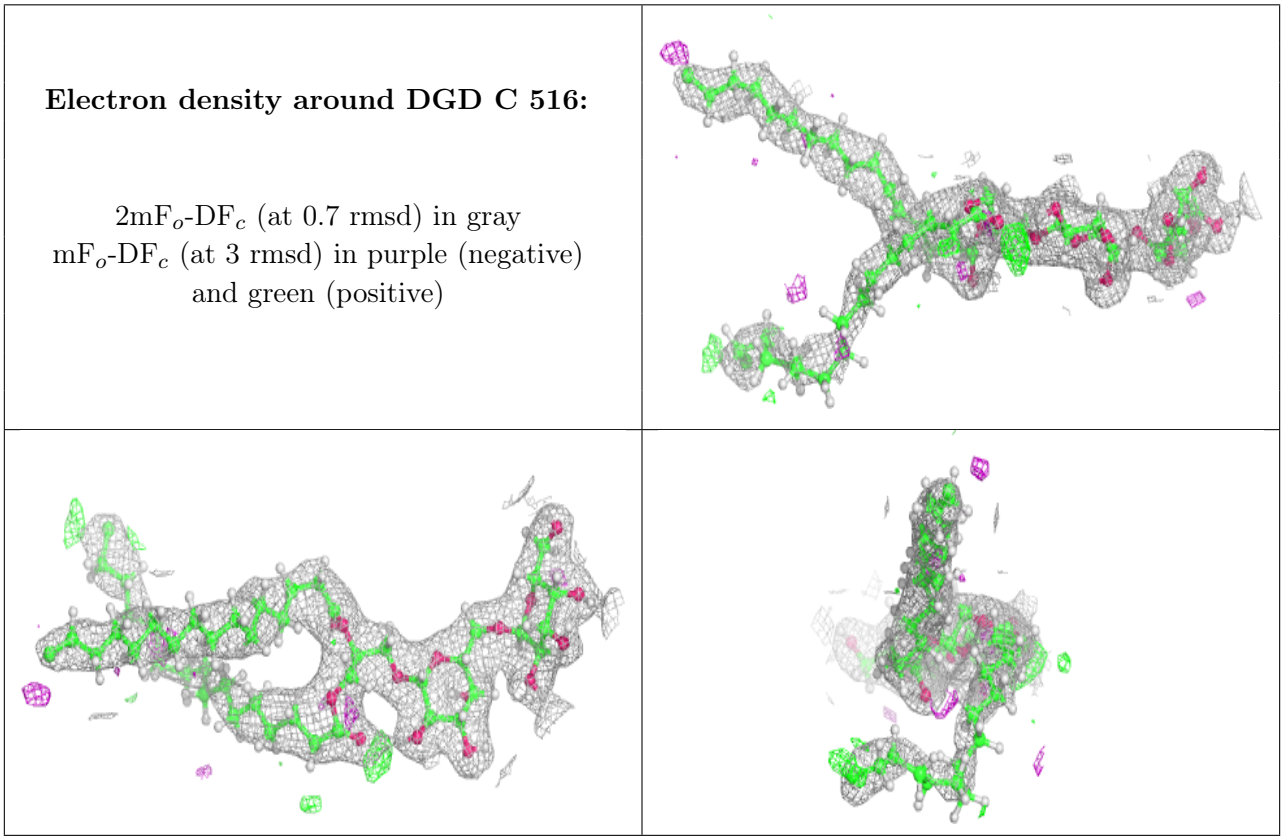
Electron density around CLA c 502:

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



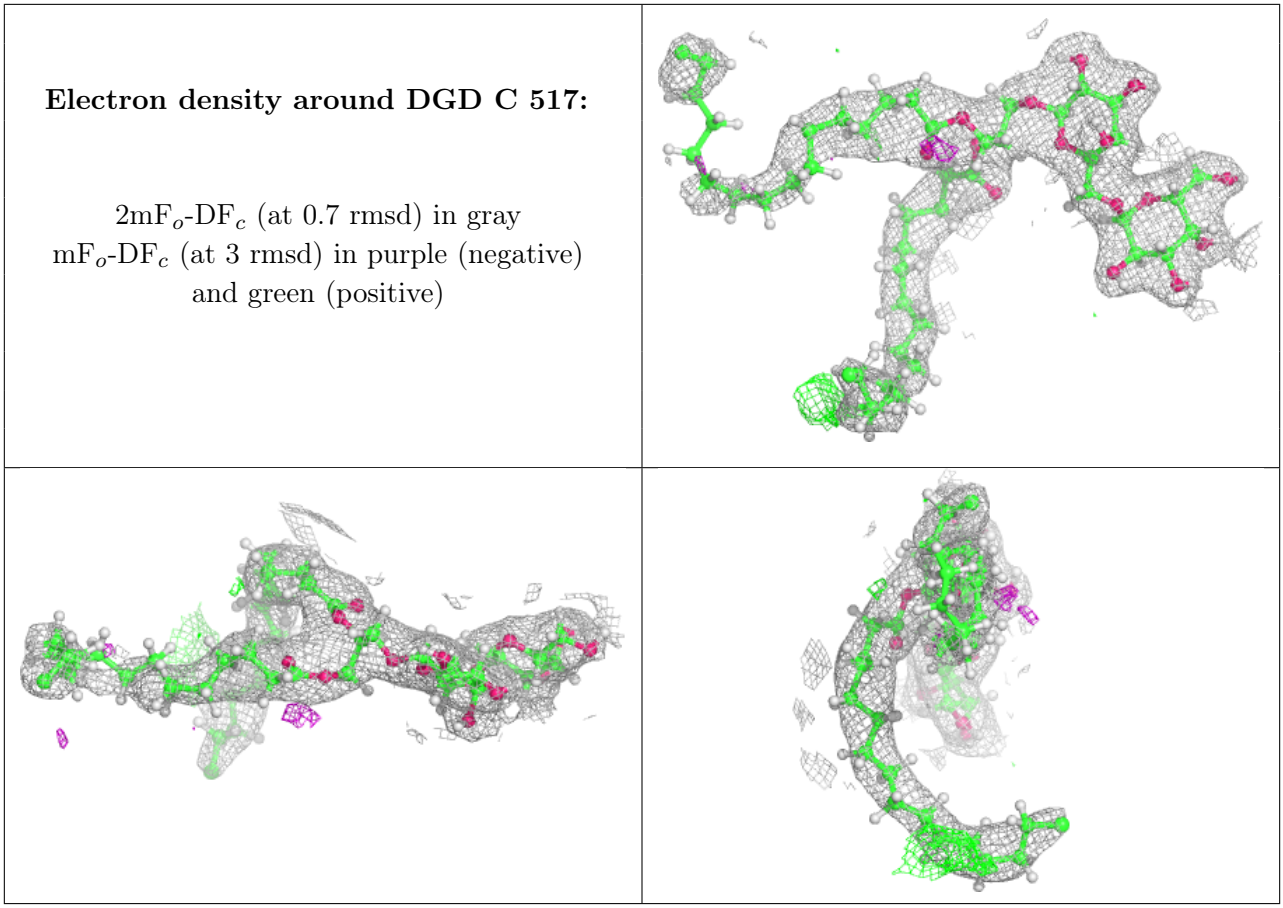
Electron density around DGD C 516:

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



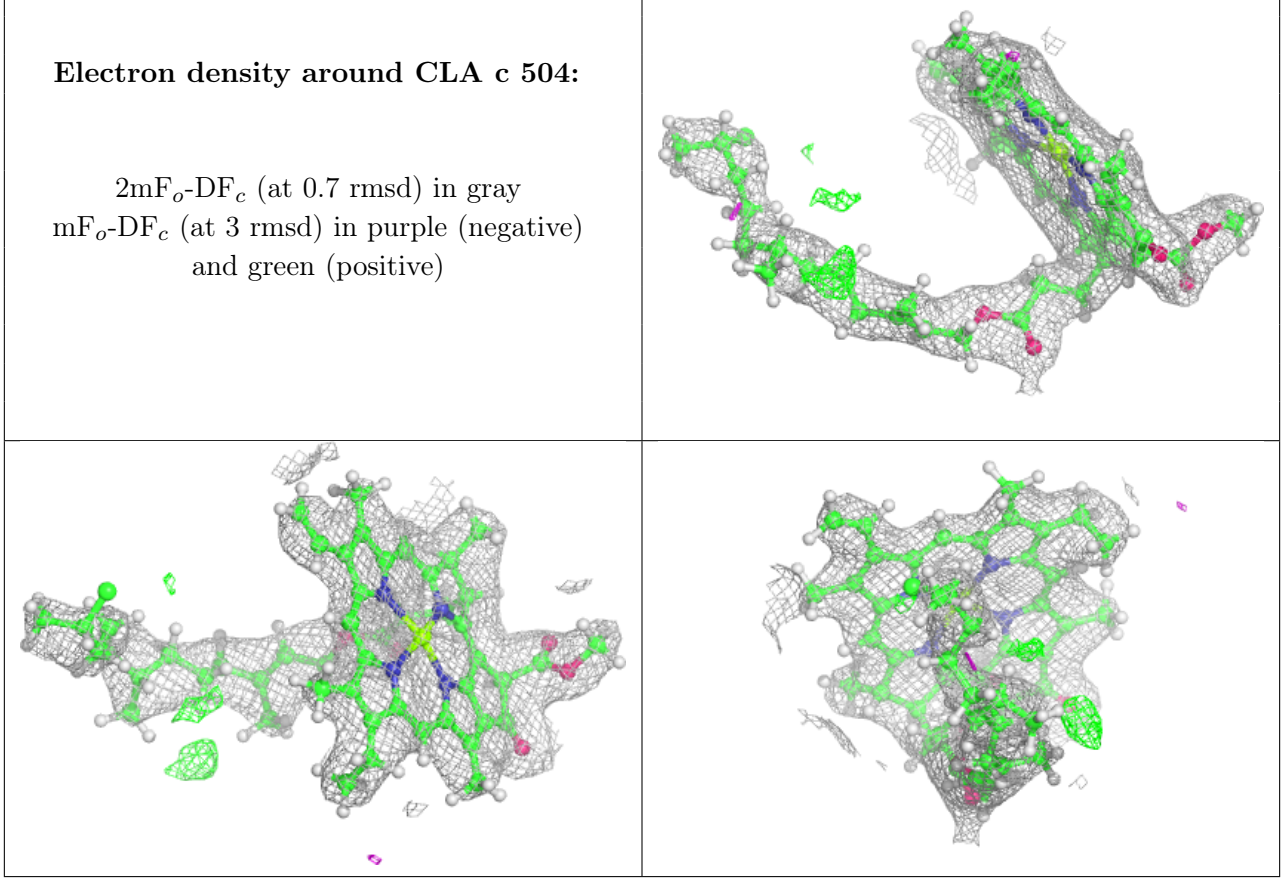
Electron density around DGD C 517:

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



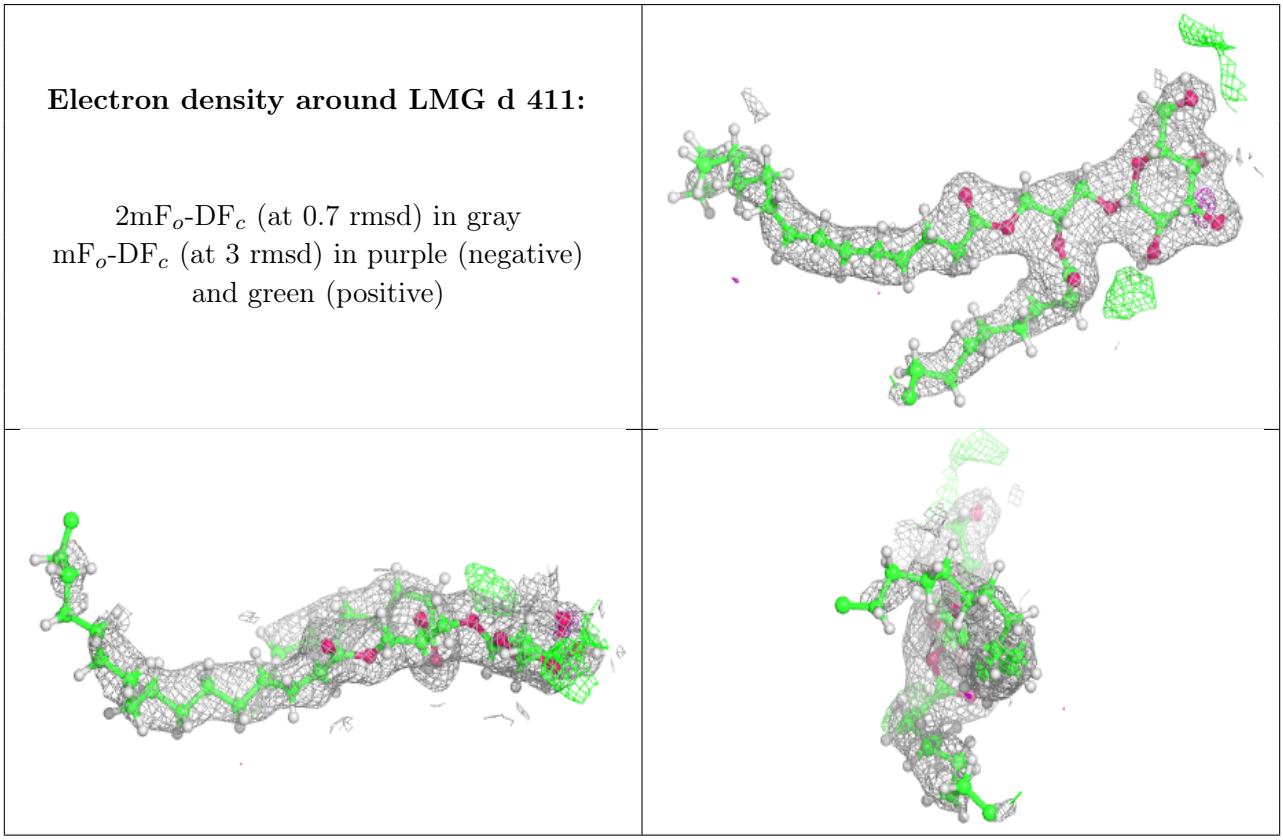
Electron density around CLA c 504:

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



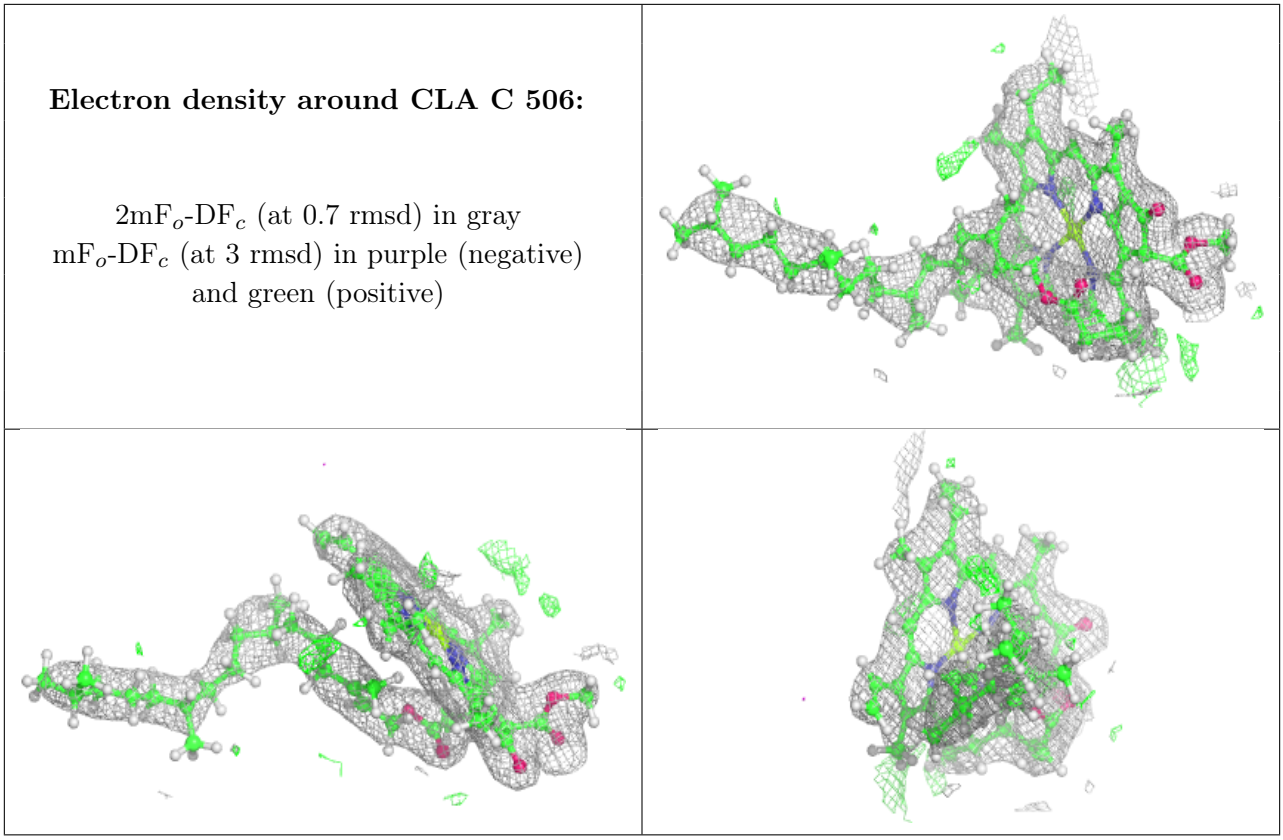
Electron density around LMG d 411:

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



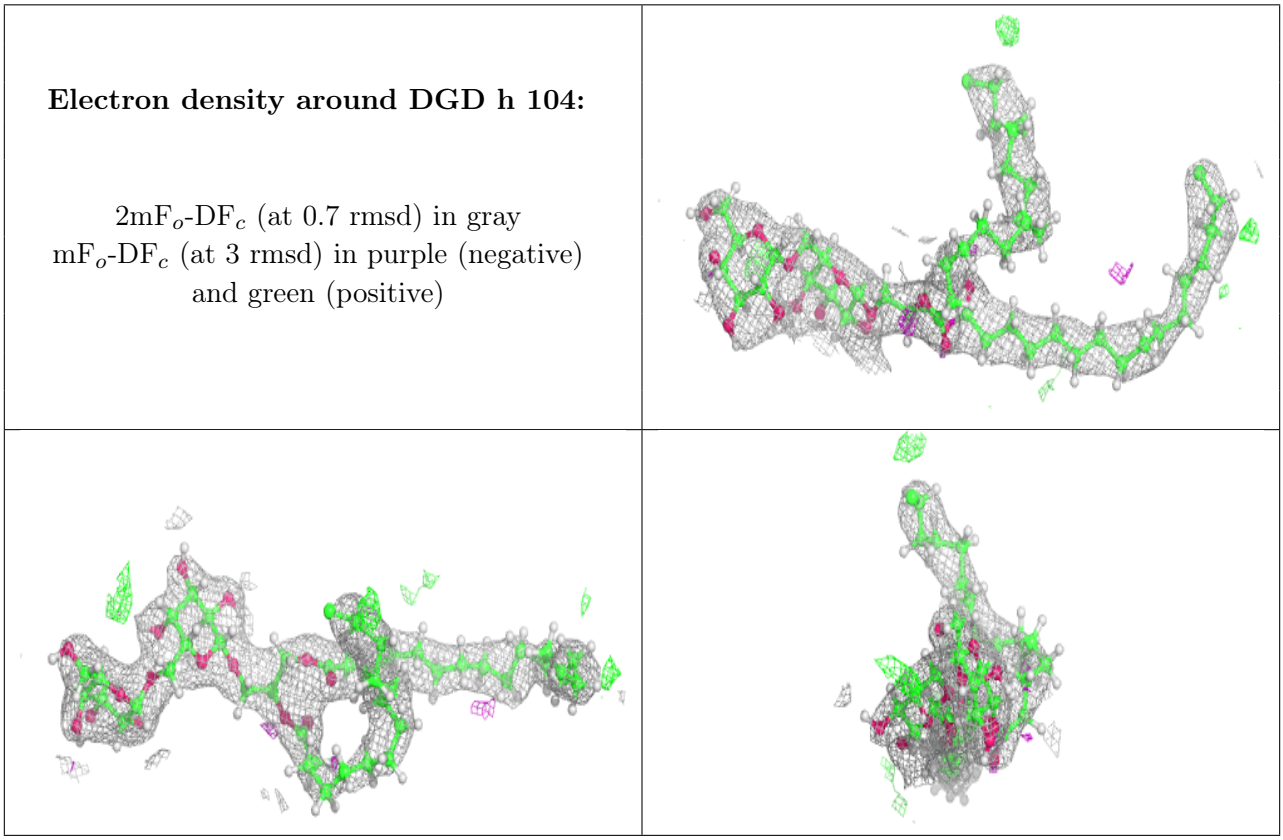
Electron density around CLA C 506:

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



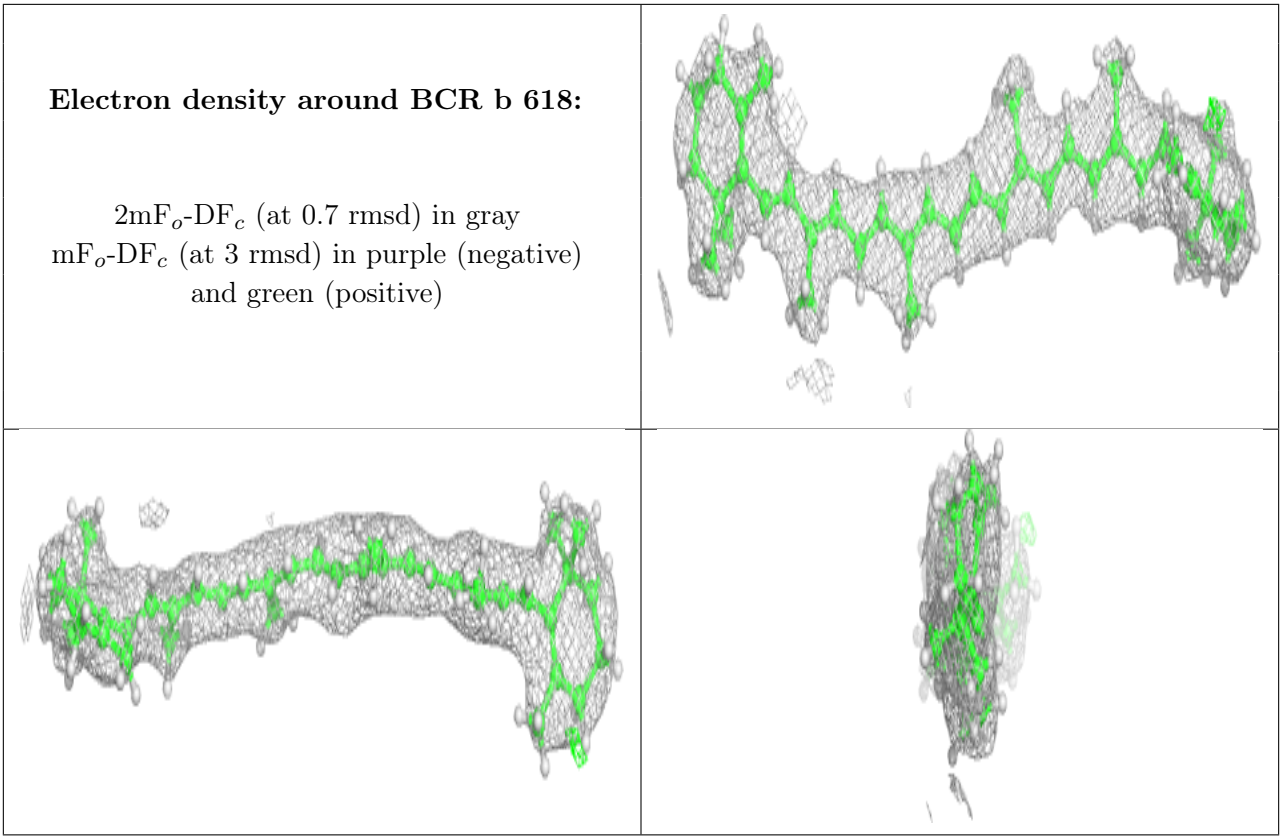
Electron density around DGD h 104:

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



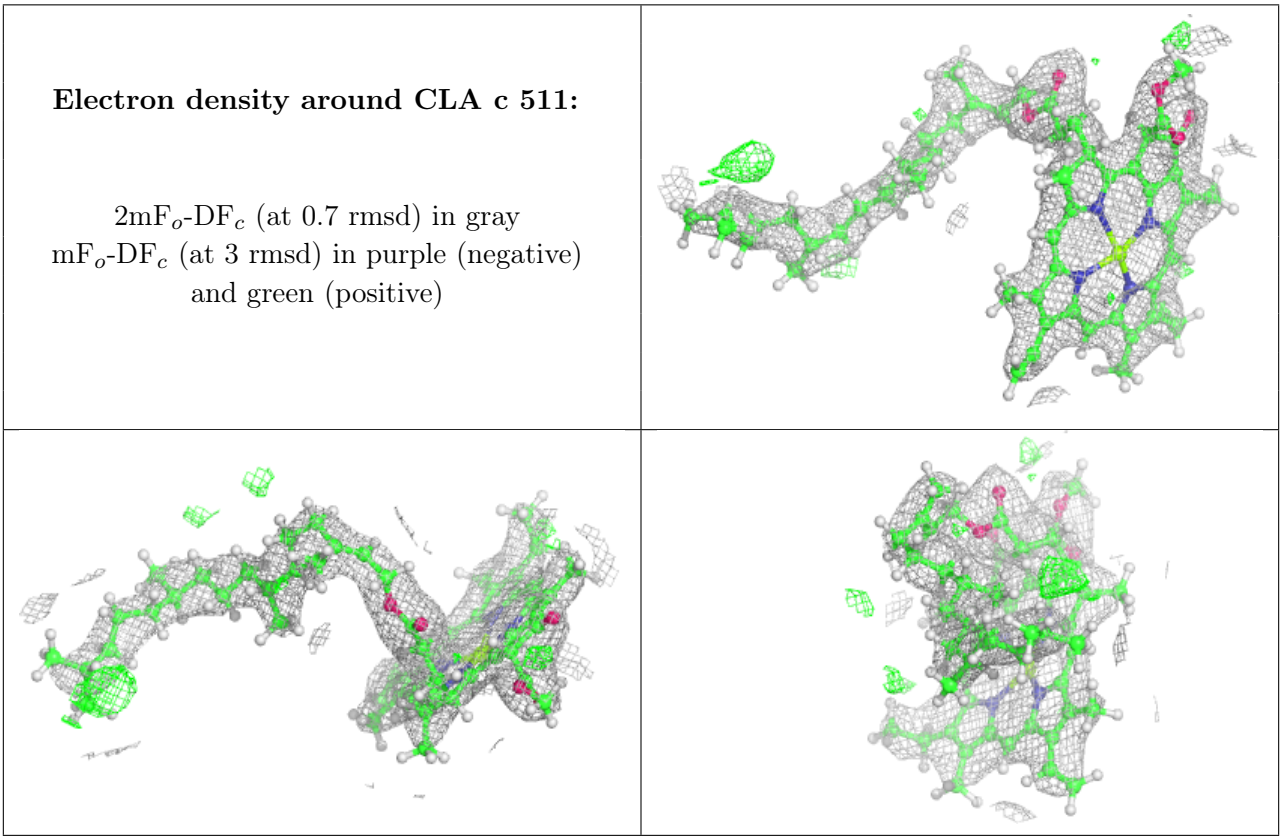
Electron density around BCR b 618:

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



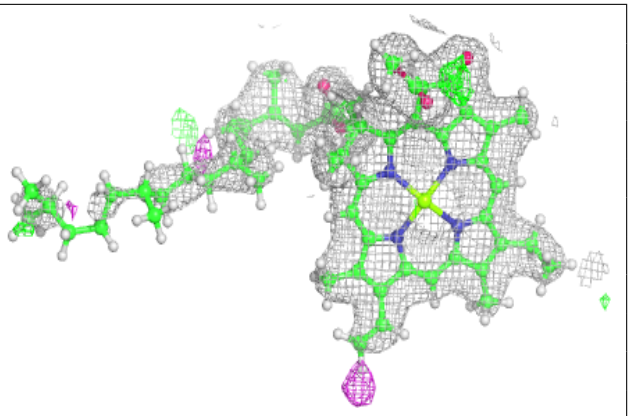
Electron density around CLA c 511:

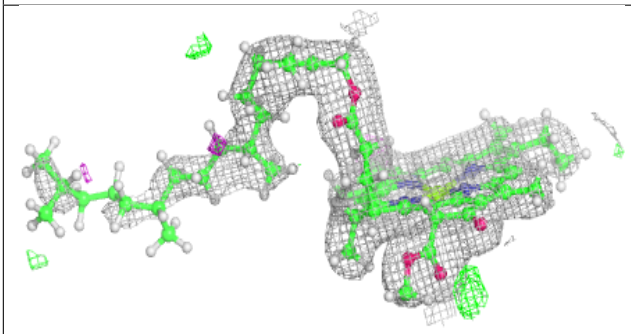
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

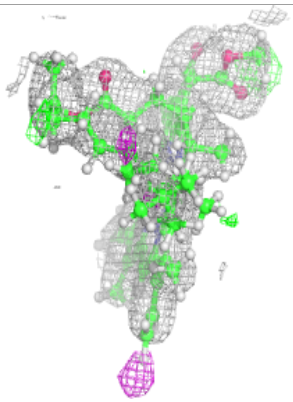


Electron density around CLA A 406:

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

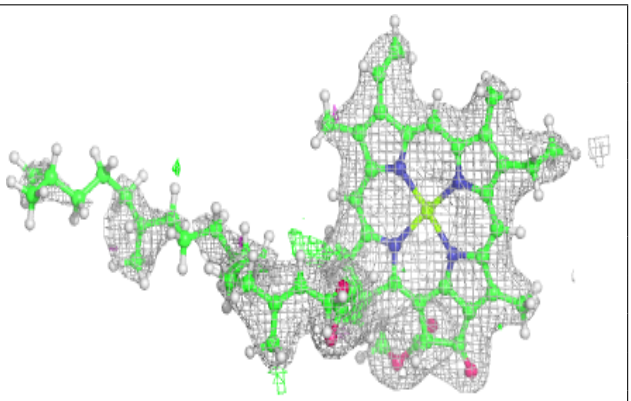


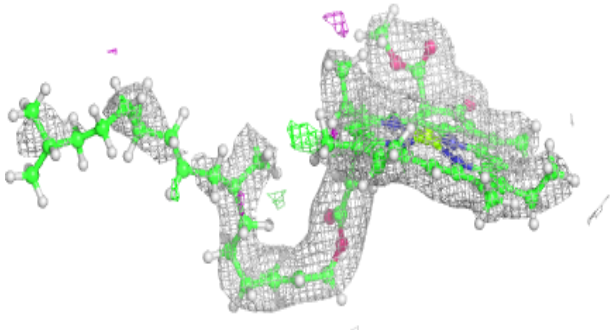


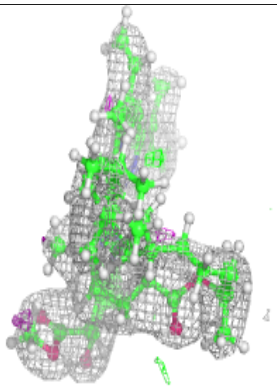


Electron density around CLA a 405:

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

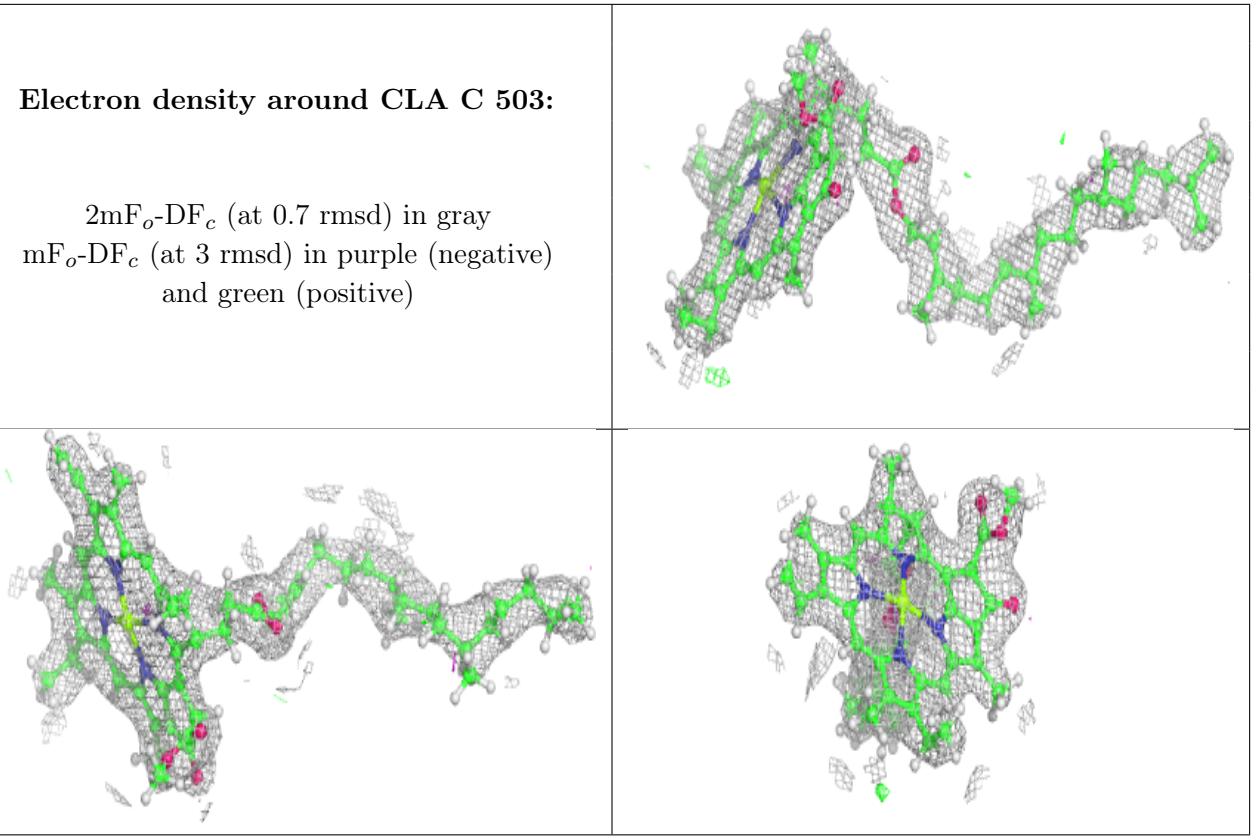






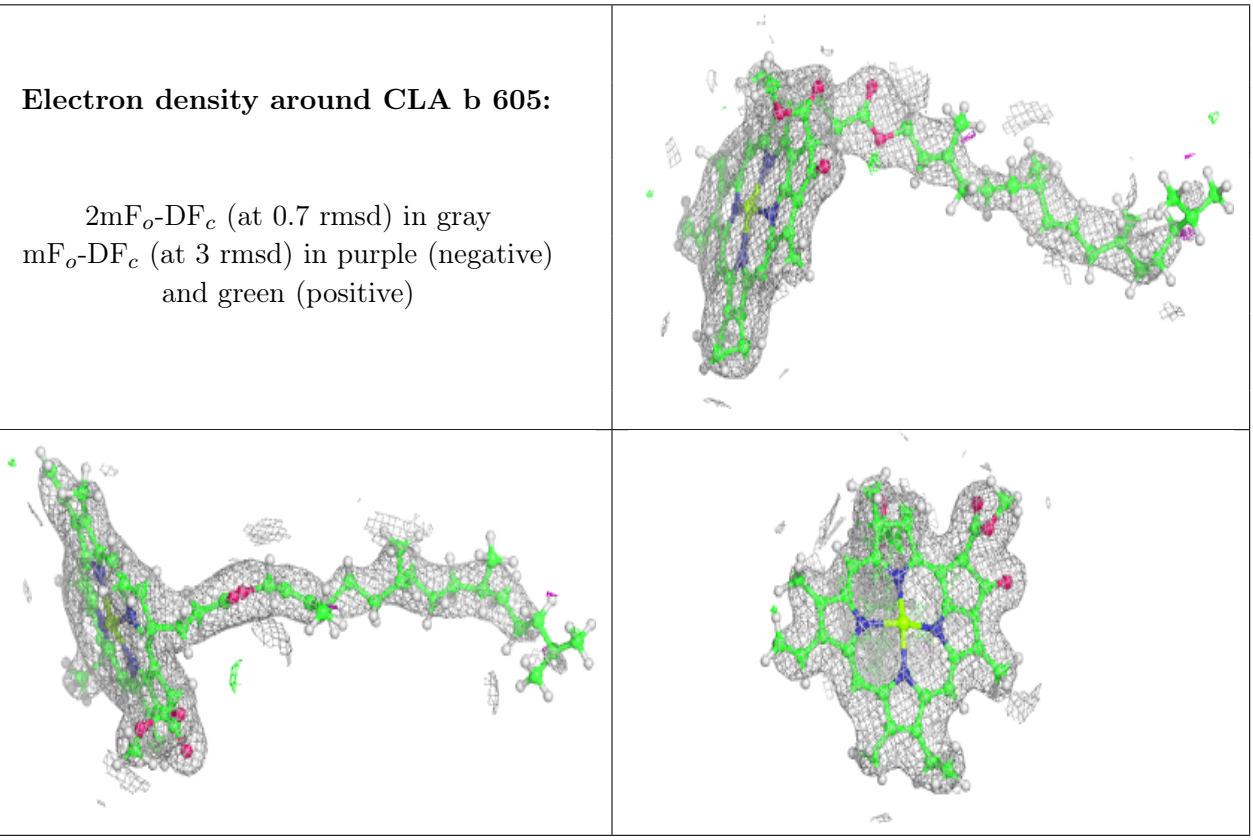
Electron density around CLA C 503:

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



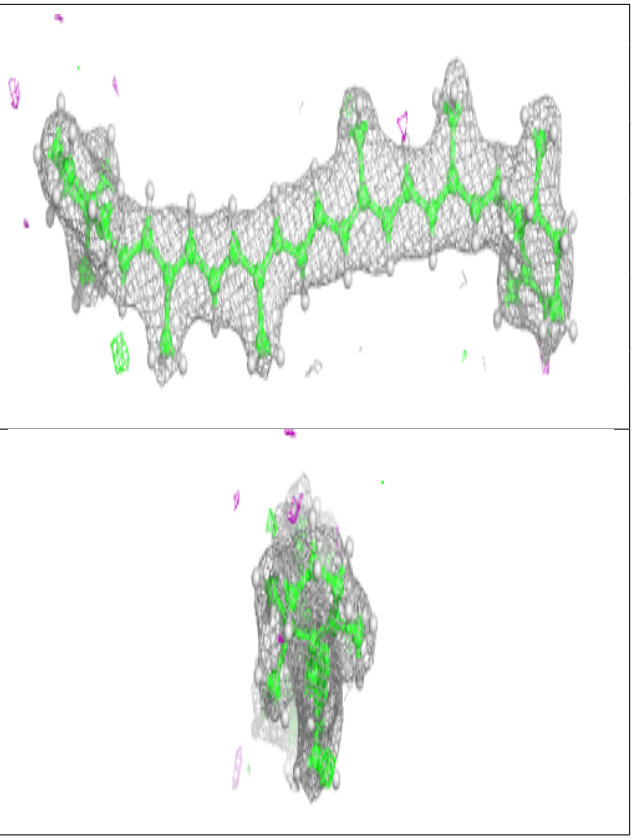
Electron density around CLA b 605:

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



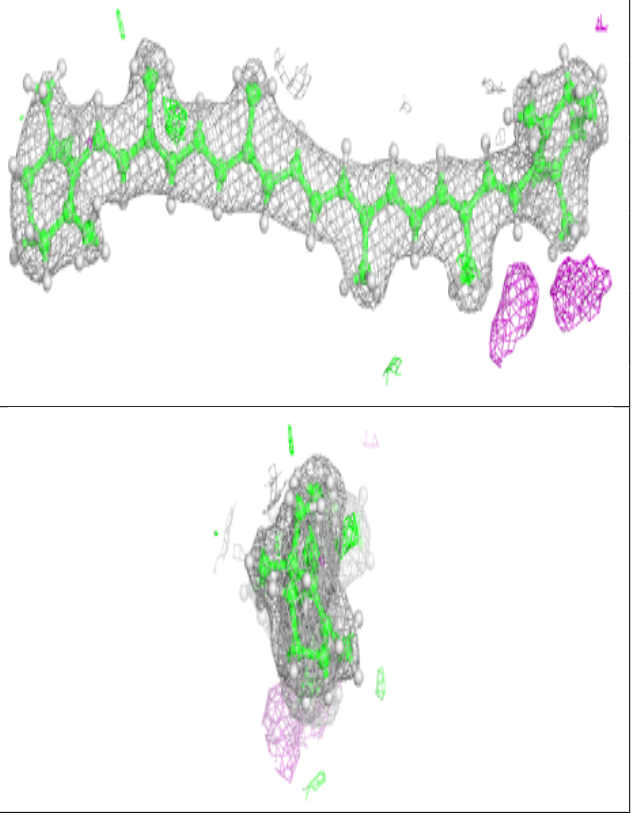
Electron density around BCR A 409:

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



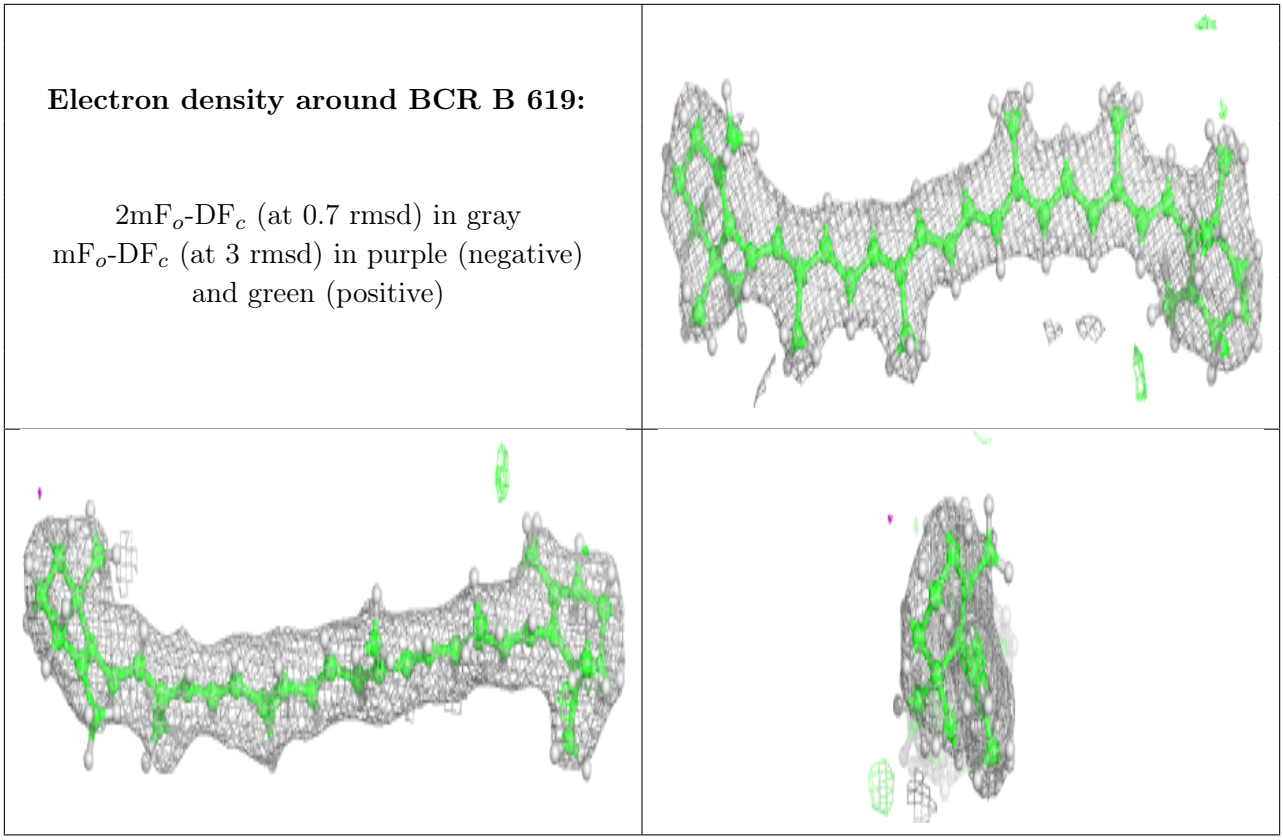
Electron density around BCR B 618:

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



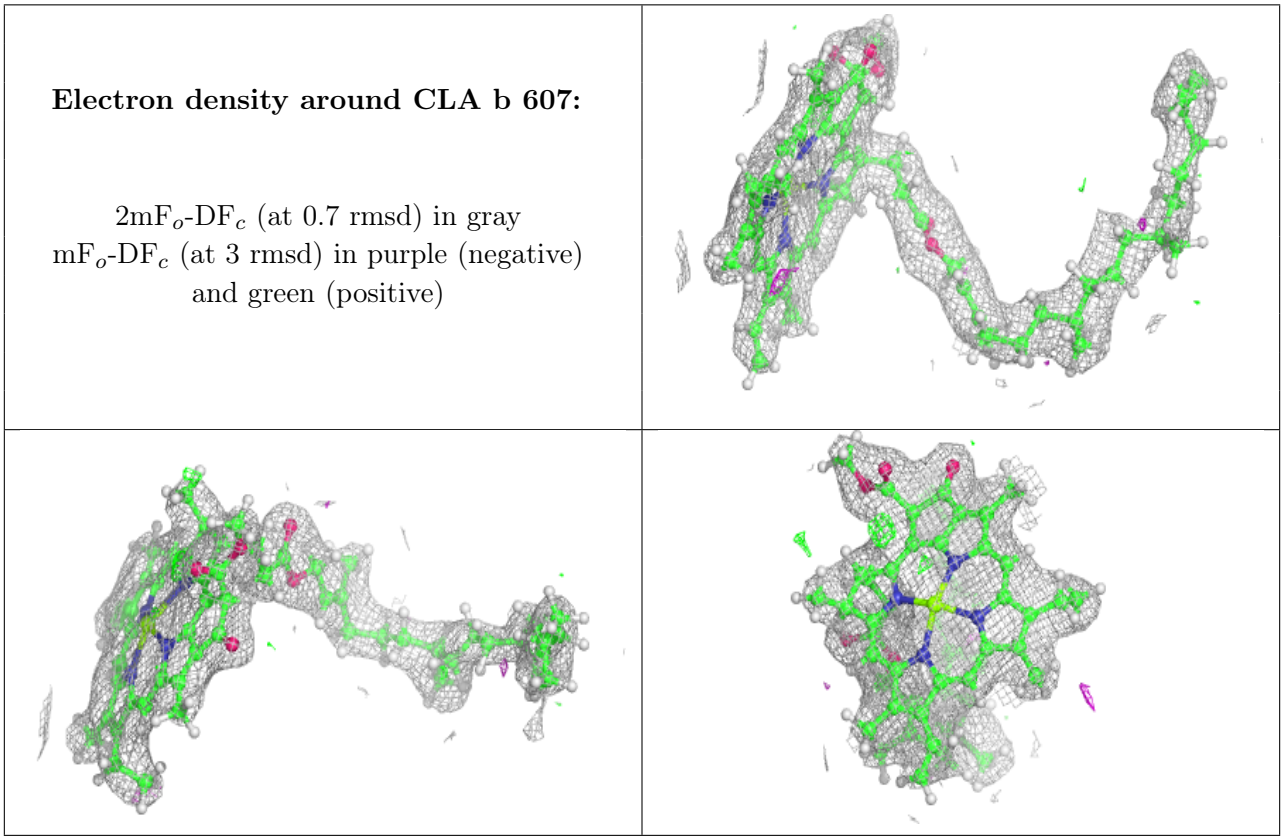
Electron density around BCR B 619:

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



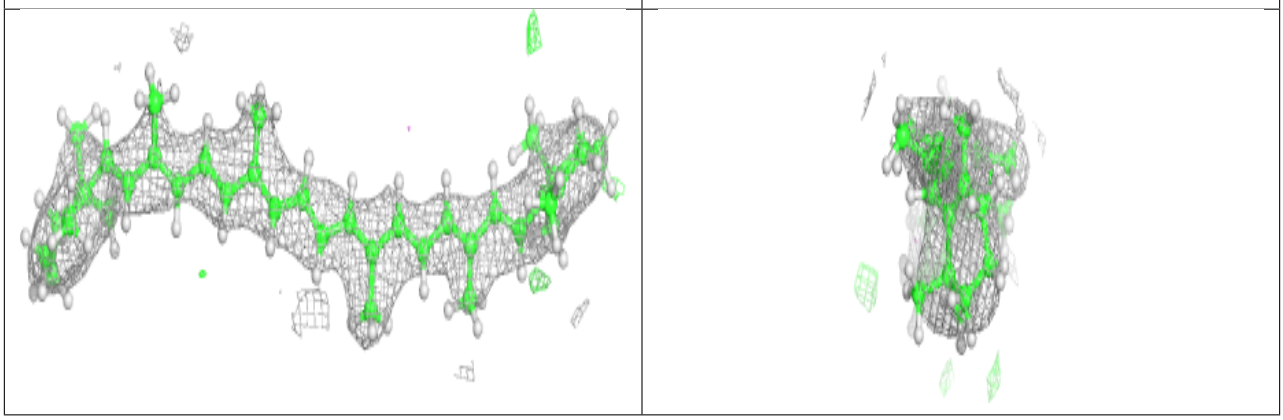
Electron density around CLA b 607:

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



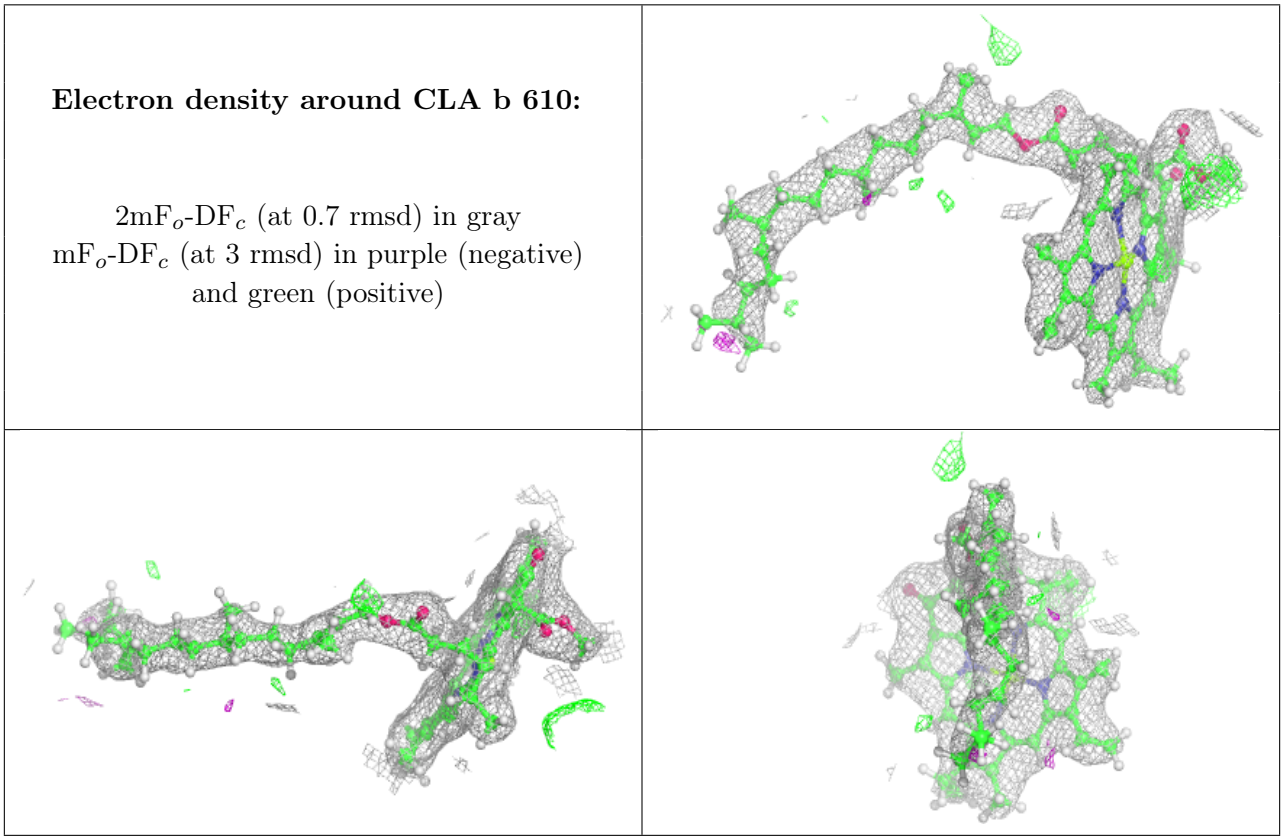
Electron density around BCR C 519:

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



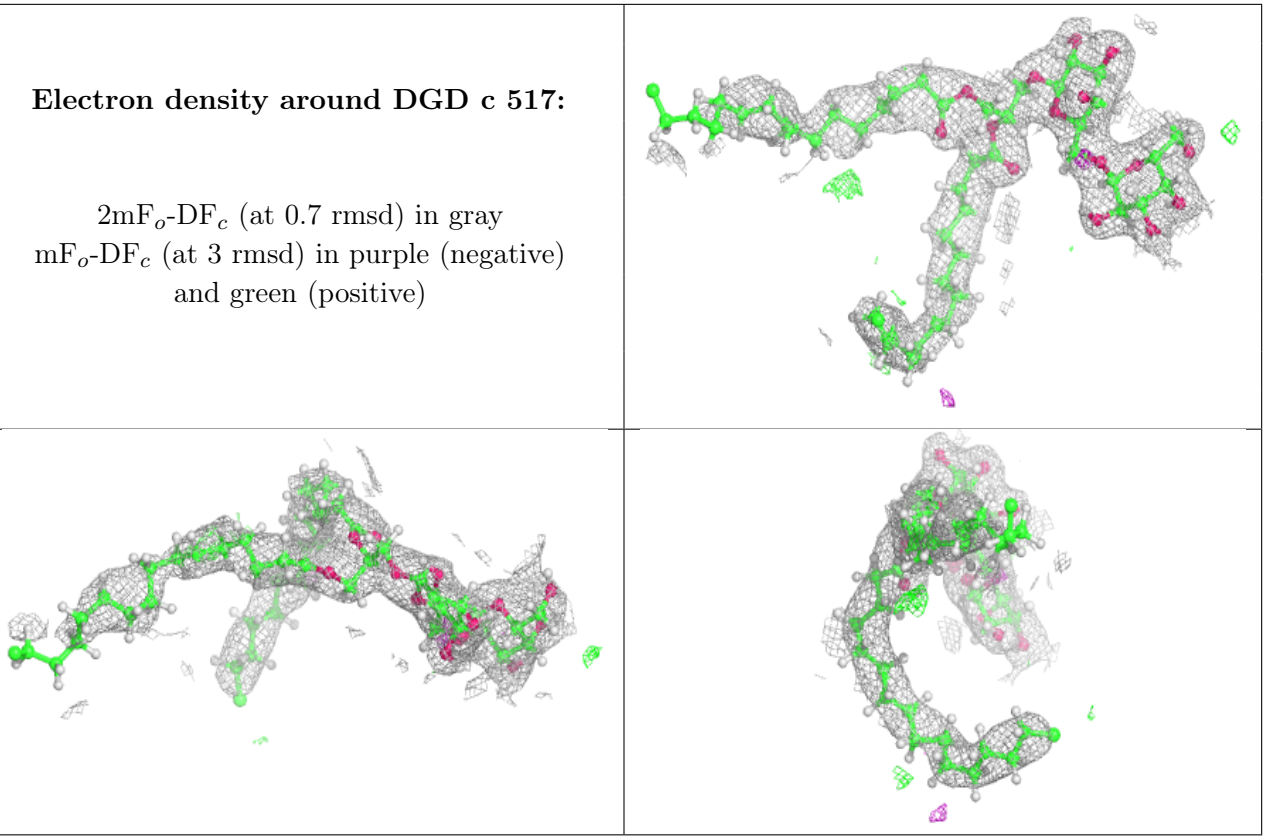
Electron density around CLA b 610:

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



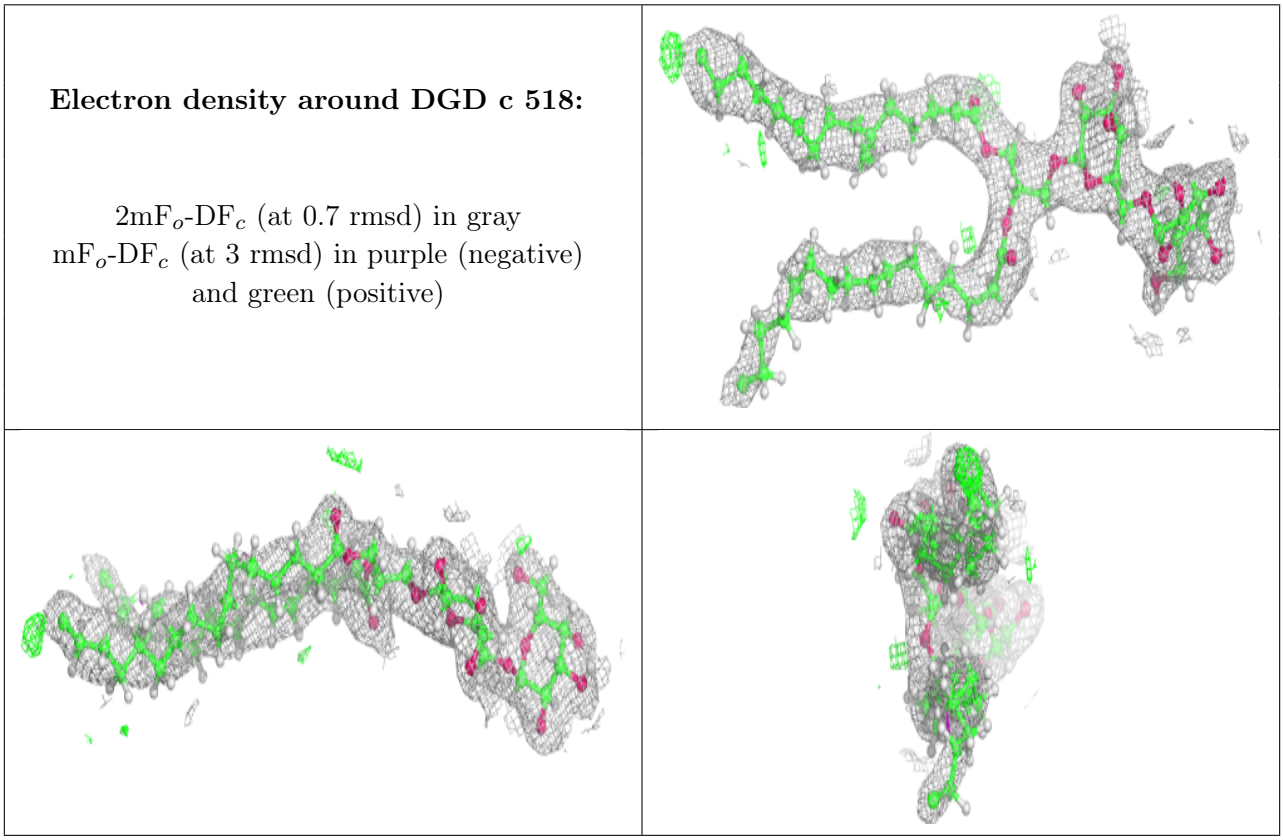
Electron density around DGD c 517:

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



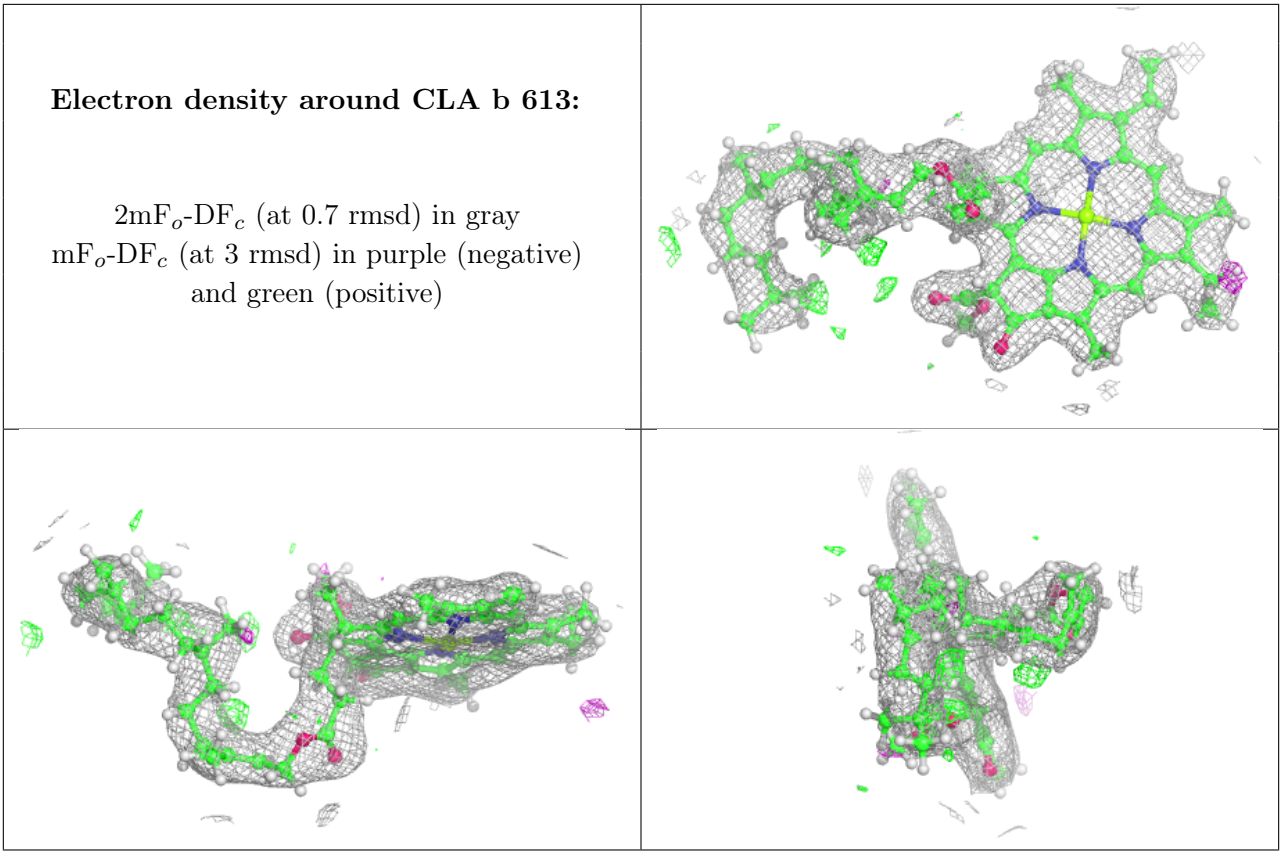
Electron density around DGD c 518:

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



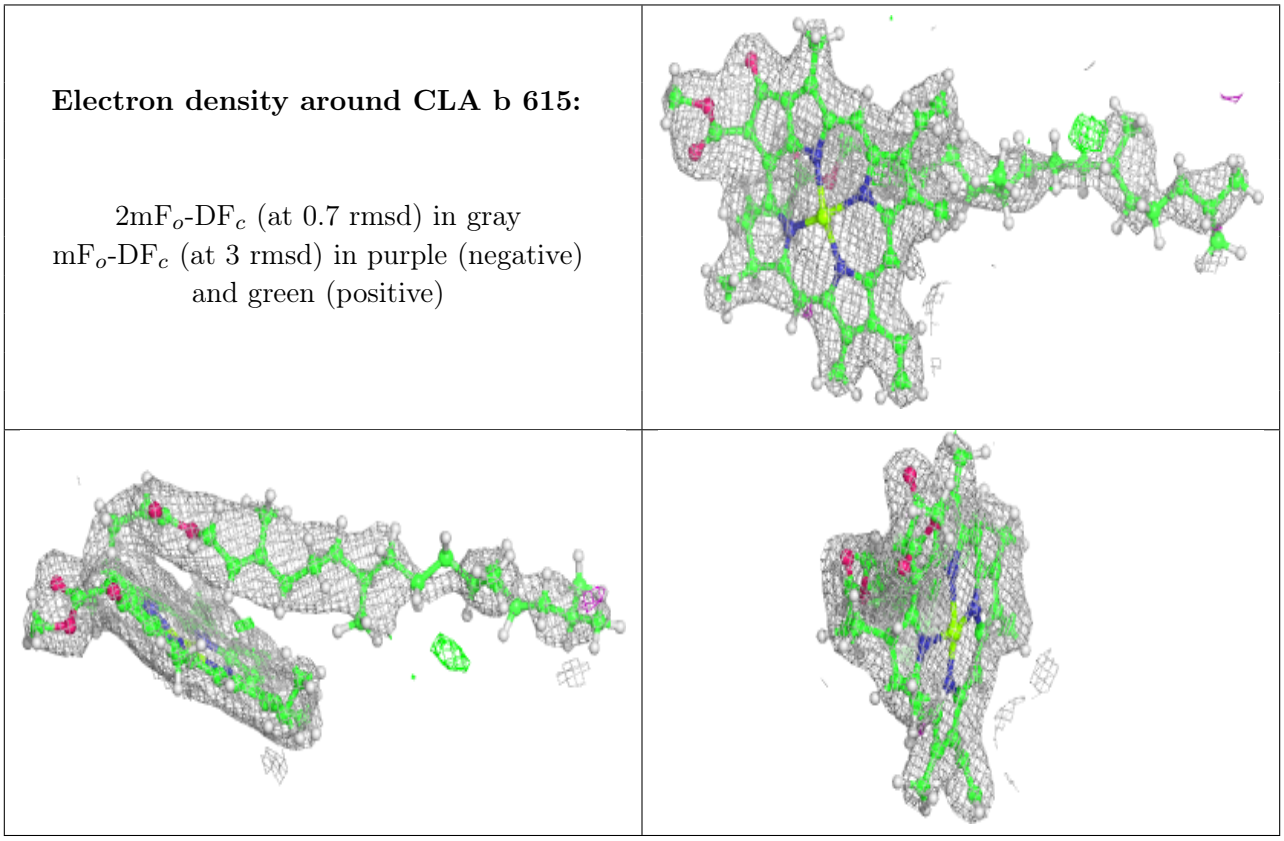
Electron density around CLA b 613:

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



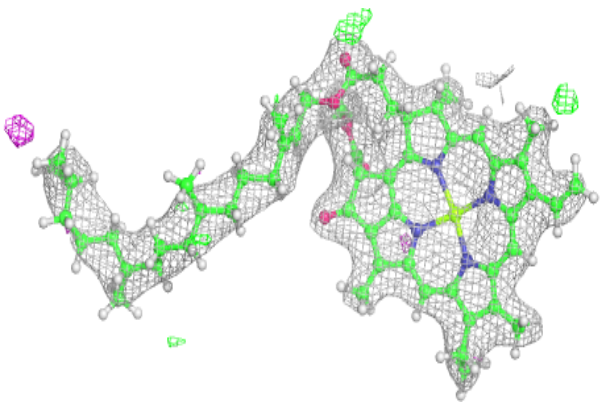
Electron density around CLA b 615:

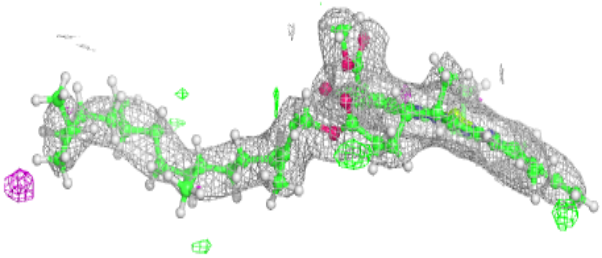
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

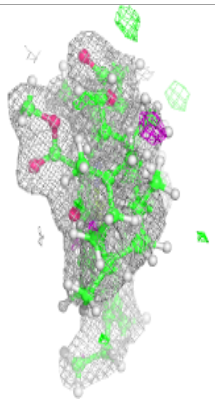


Electron density around CLA B 602:

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

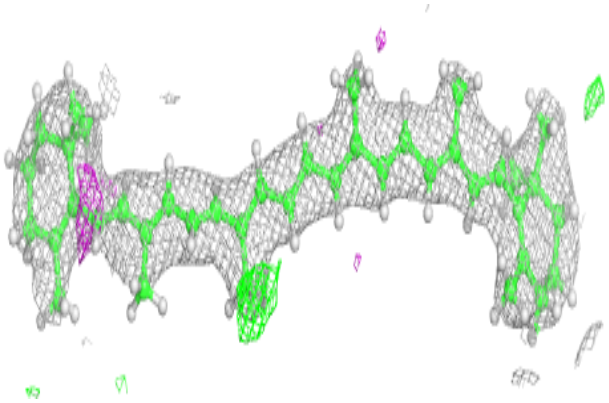


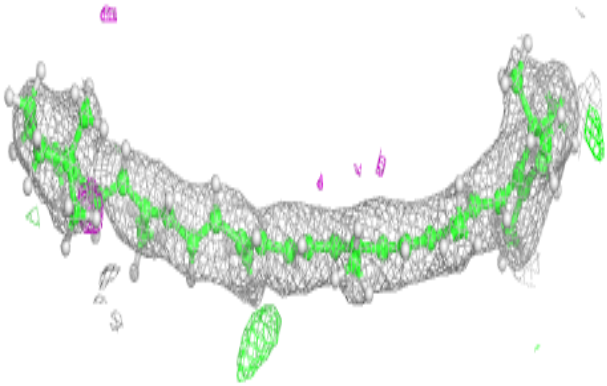


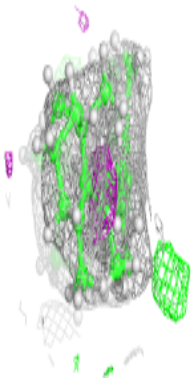


Electron density around BCR b 602:

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

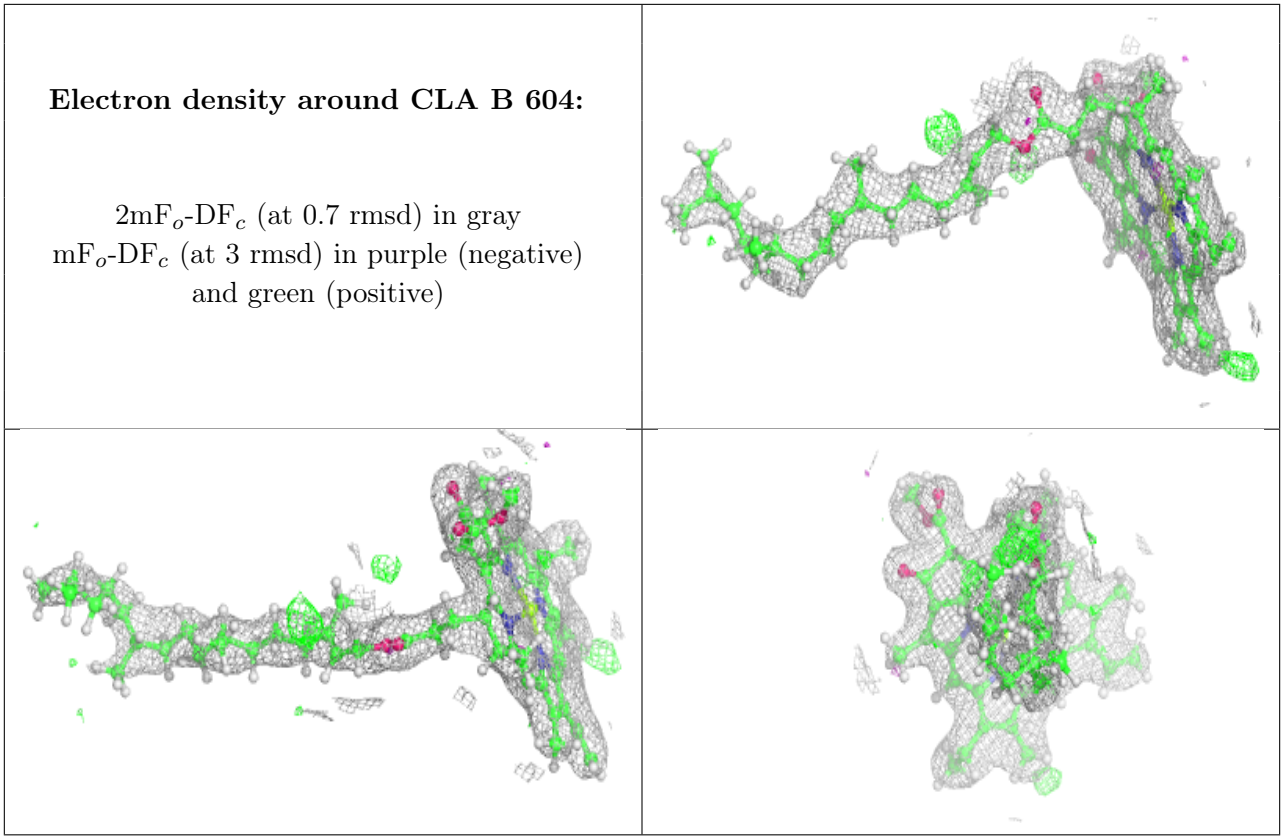






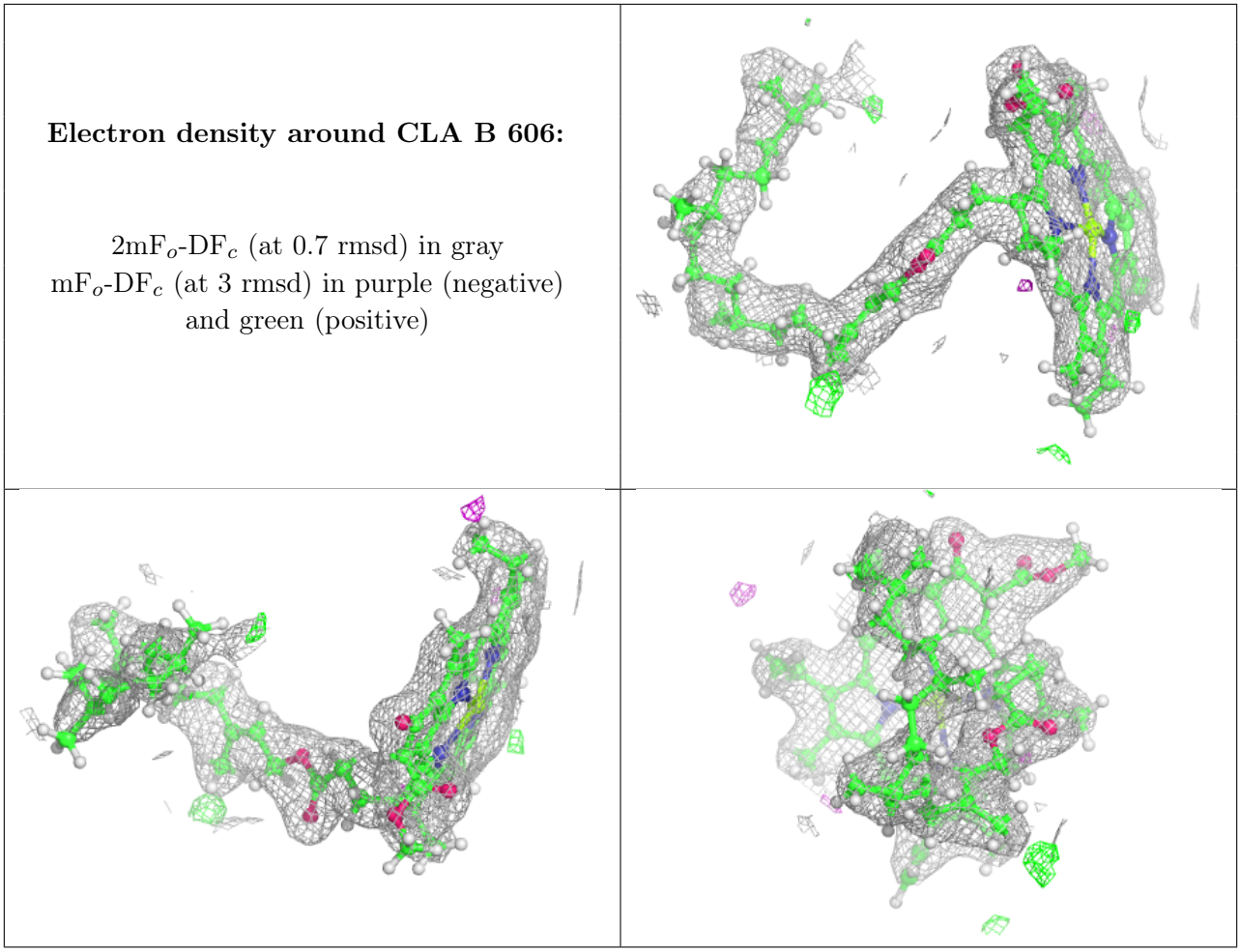
Electron density around CLA B 604:

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



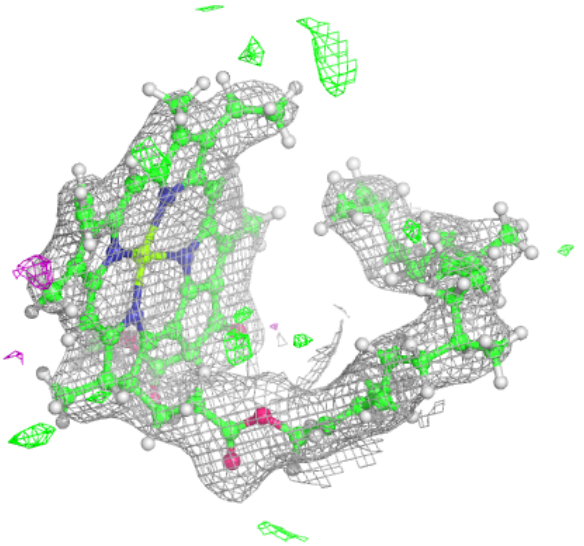
Electron density around CLA B 606:

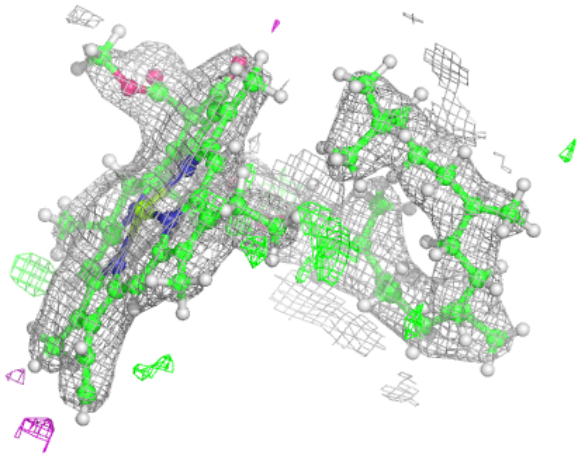
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

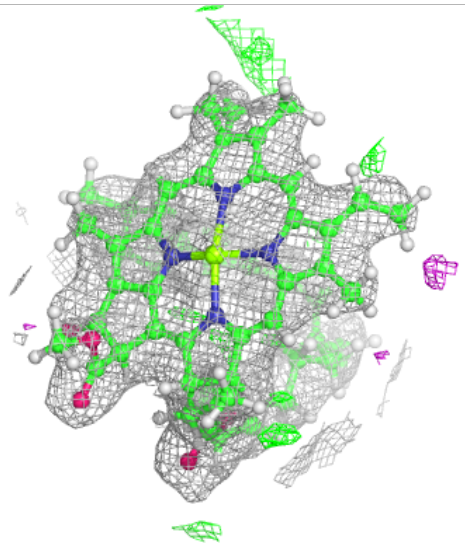


Electron density around CLA c 503:

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

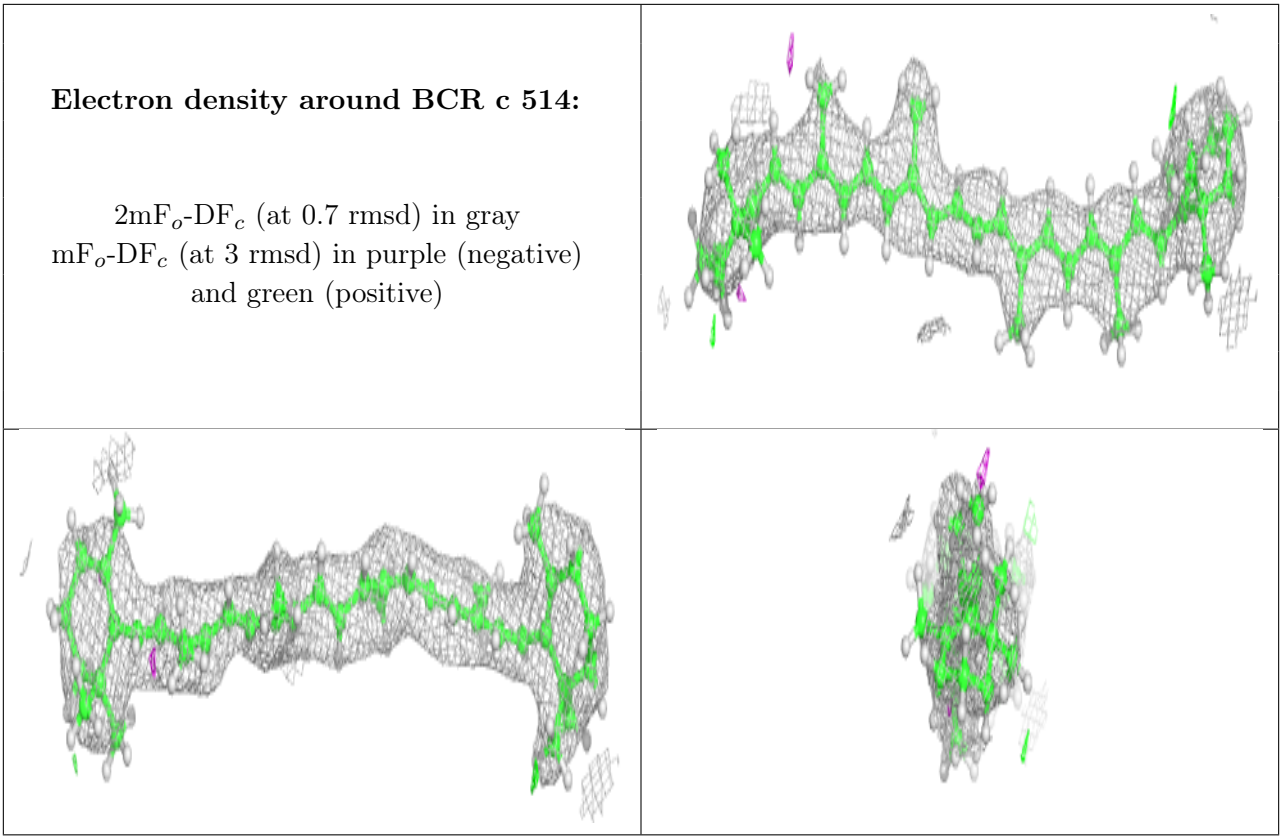






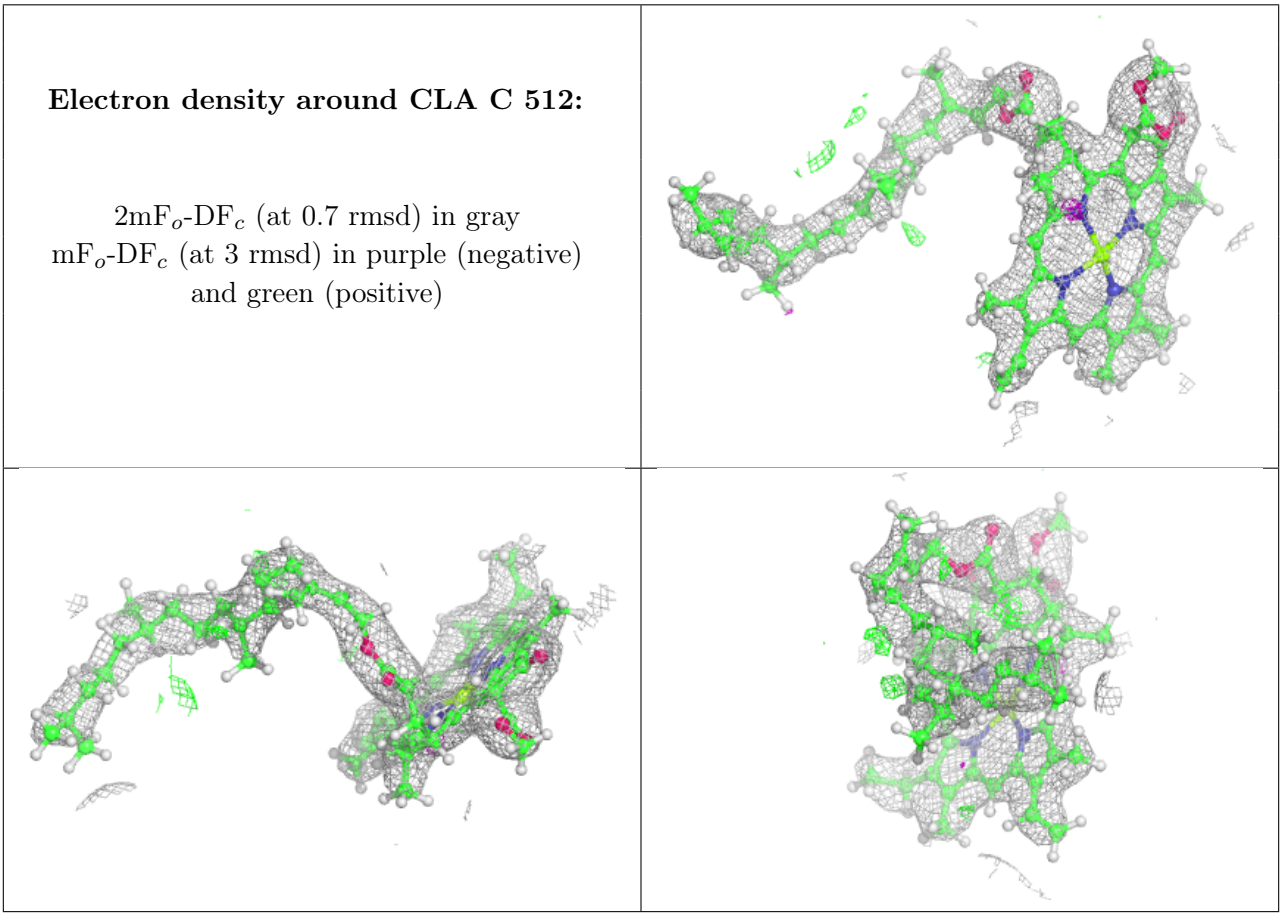
Electron density around BCR c 514:

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



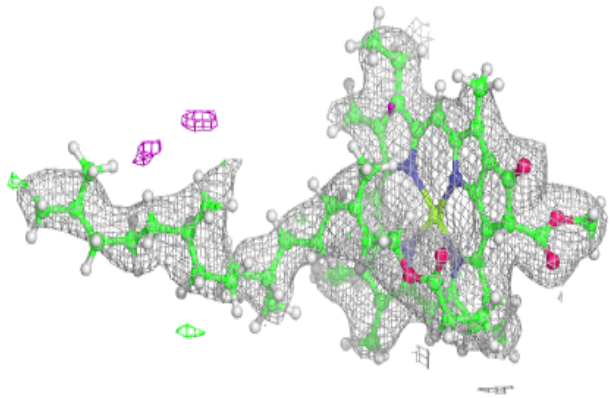
Electron density around CLA C 512:

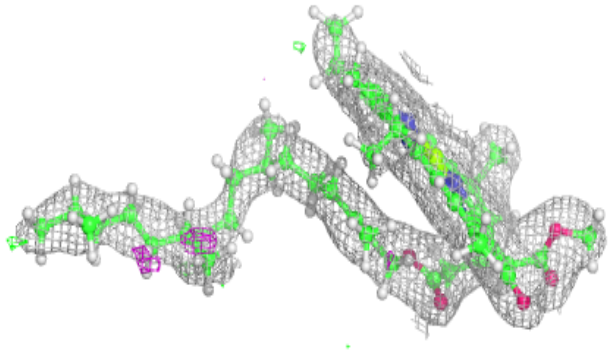
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

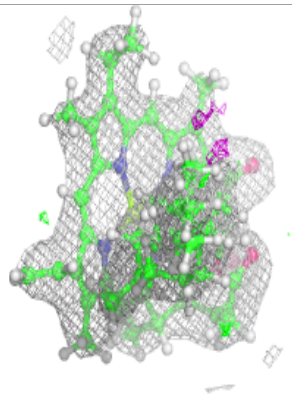


Electron density around CLA c 505:

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

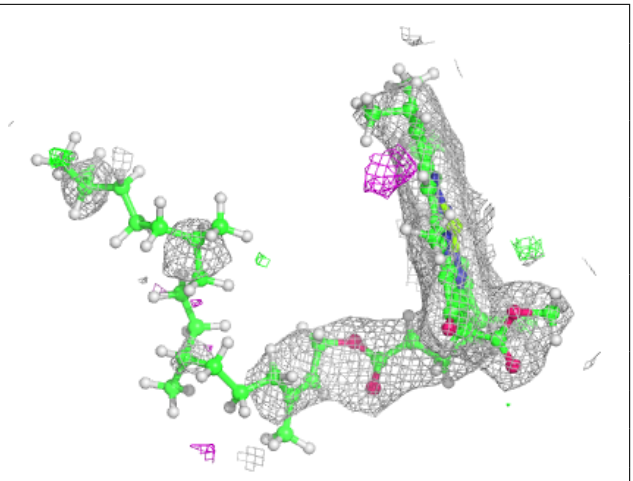


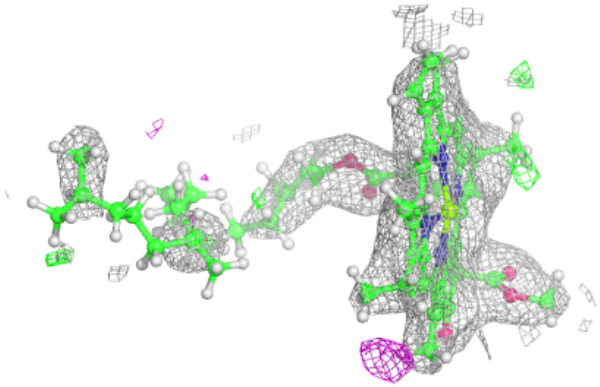


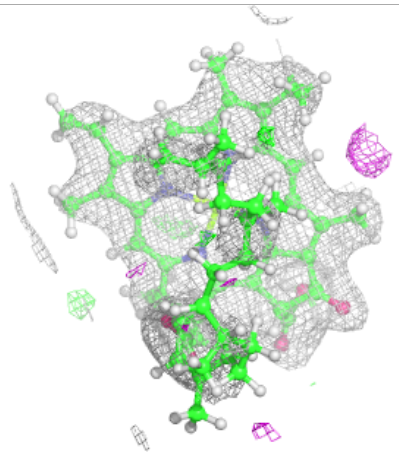


Electron density around CLA c 506:

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

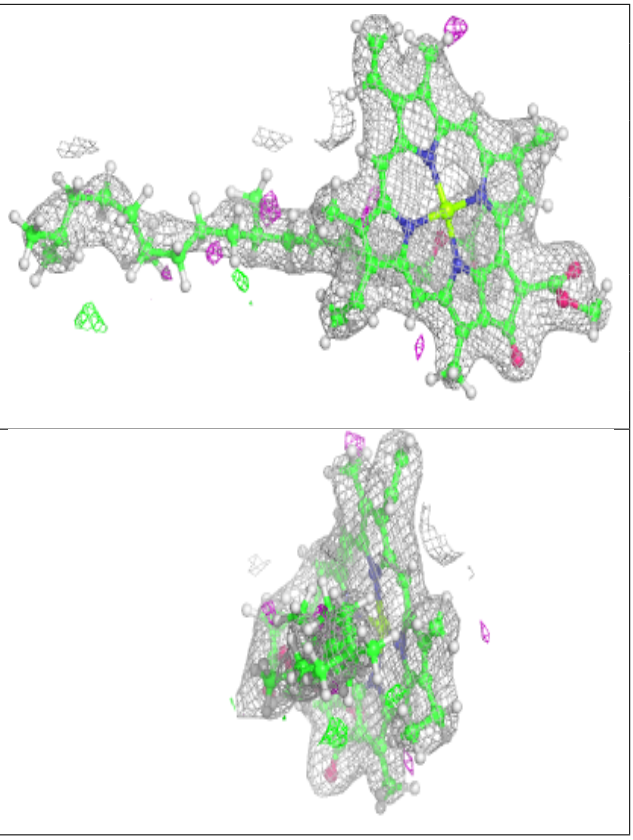






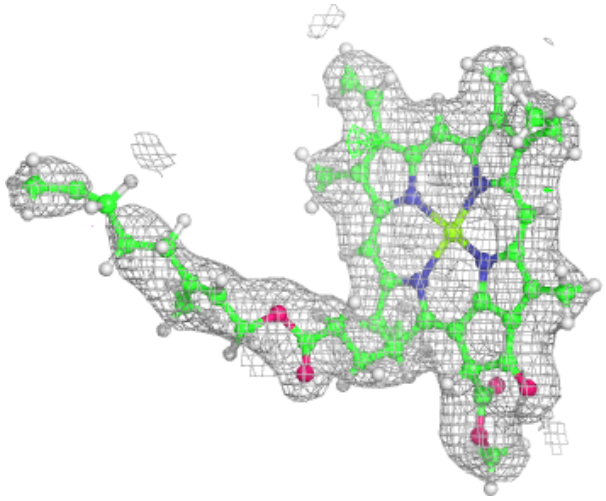
Electron density around CLA B 614:

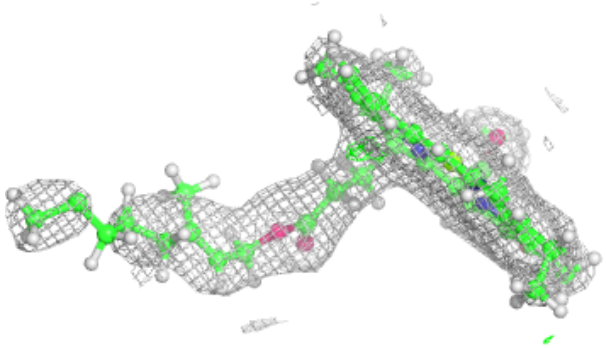
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

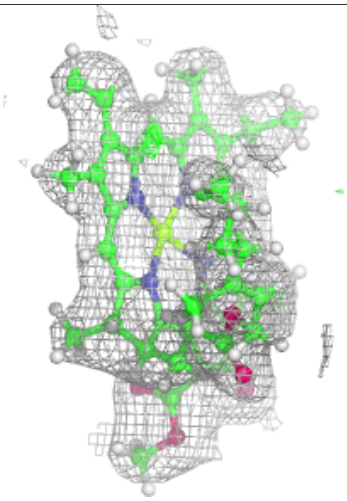


Electron density around CLA A 408:

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

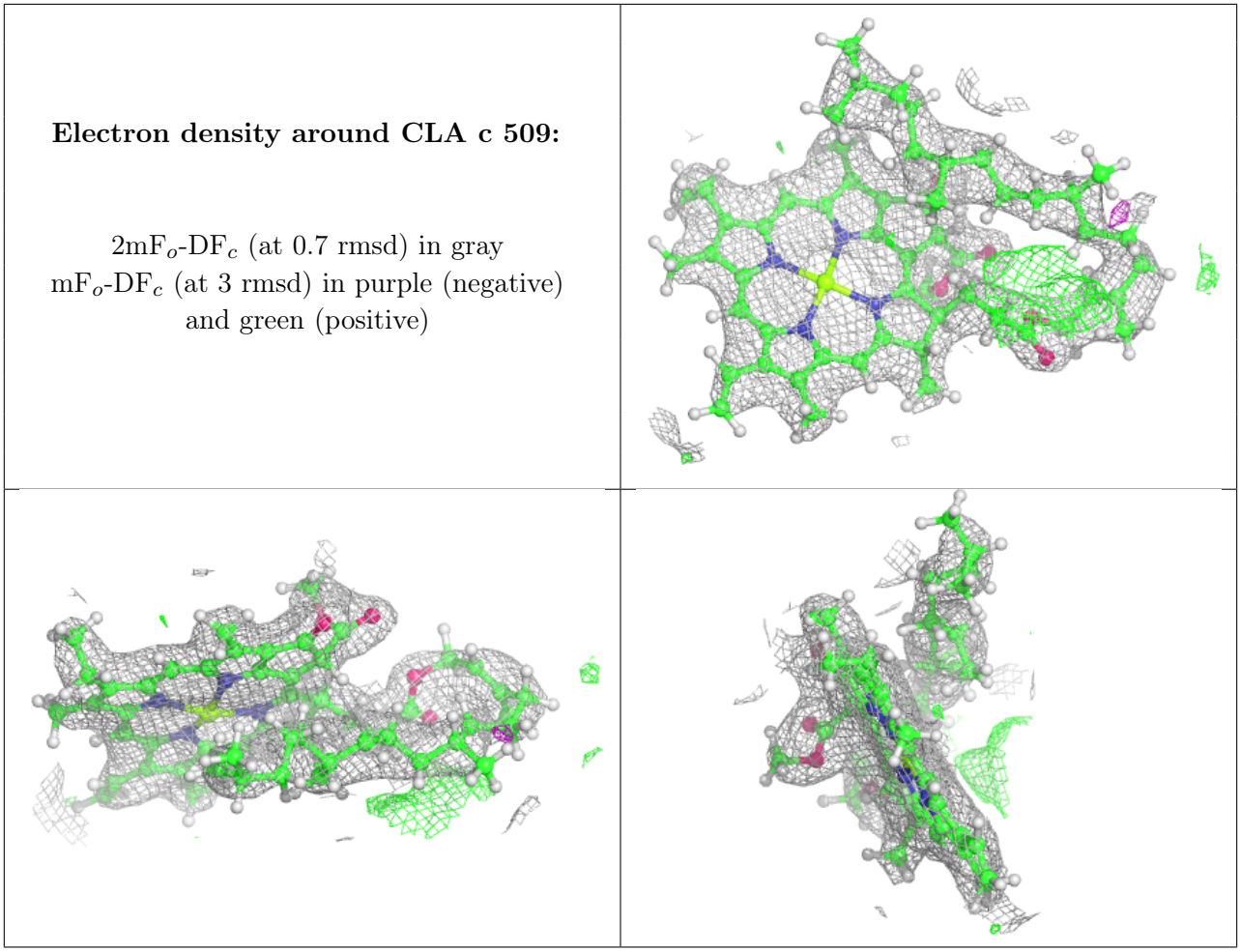






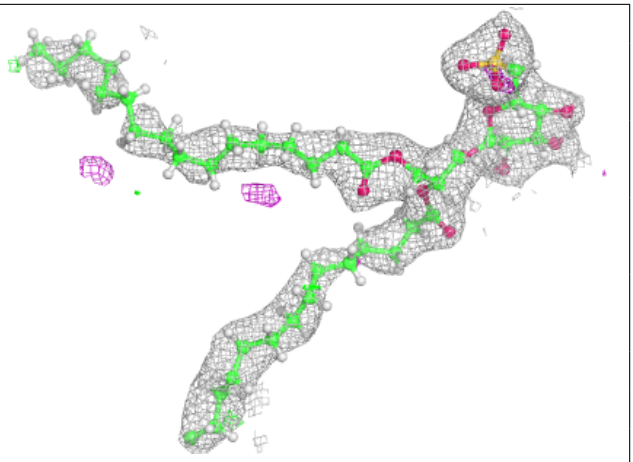
Electron density around CLA c 509:

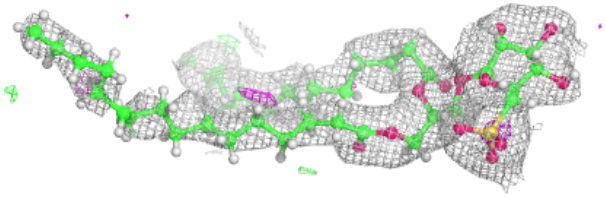
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

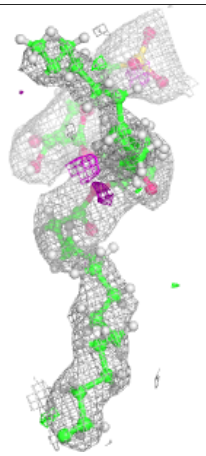


Electron density around SQD A 411:

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

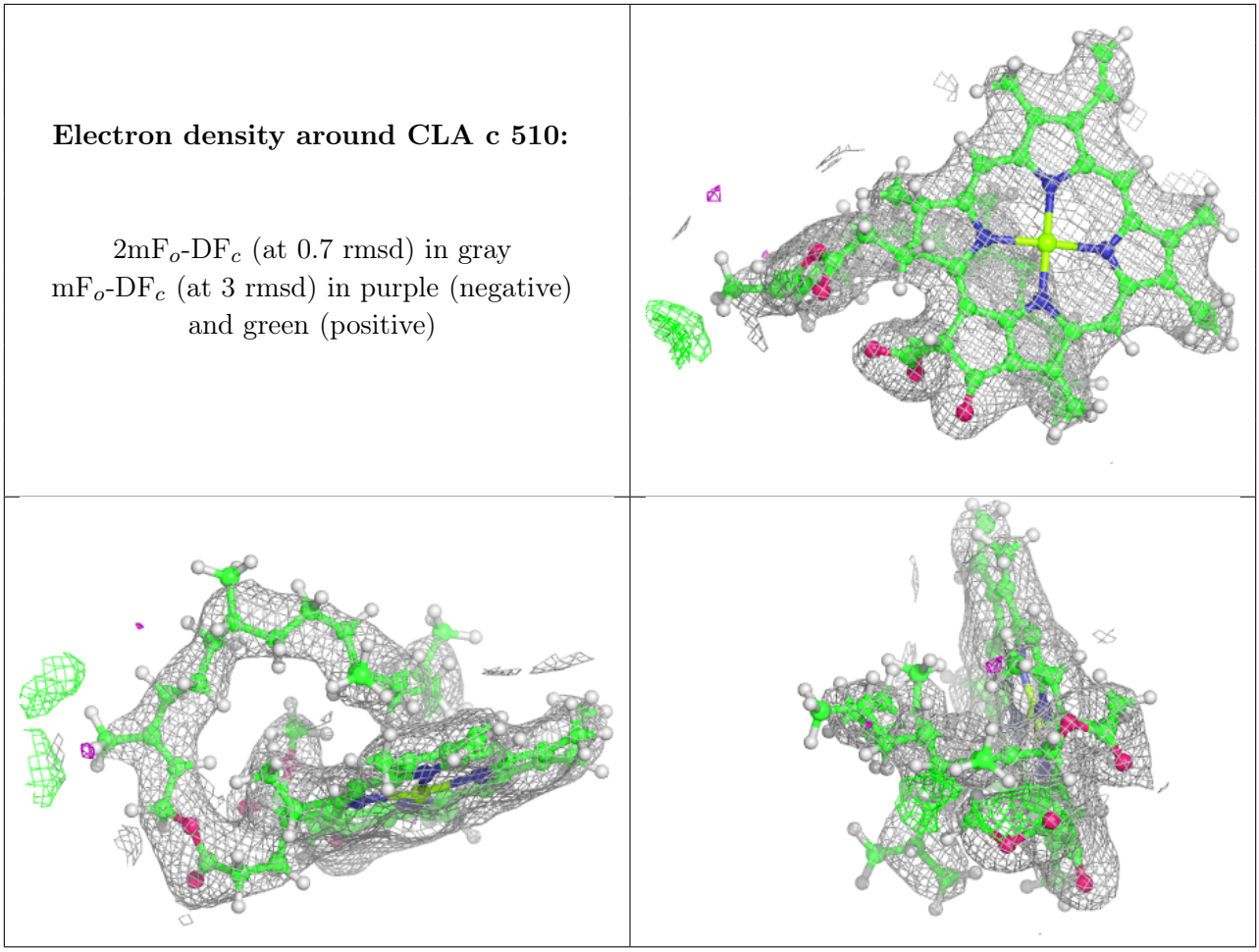






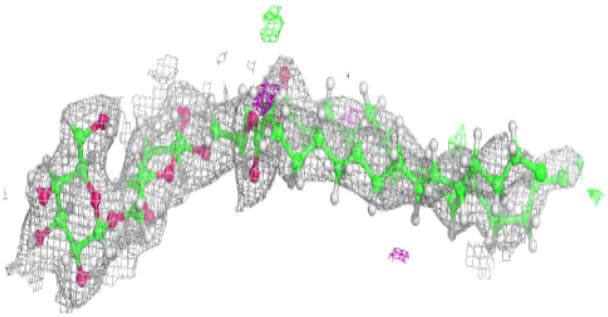
Electron density around CLA c 510:

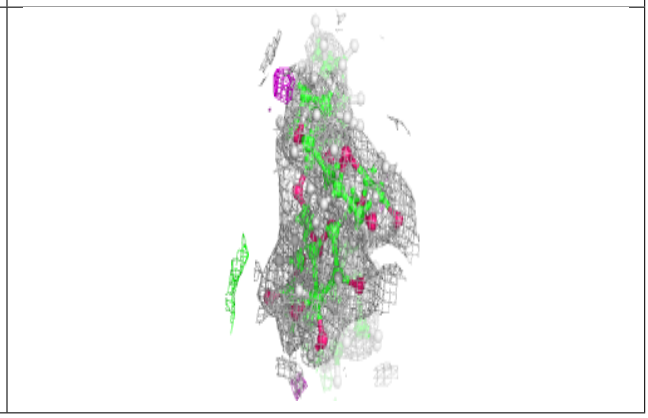
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD C 518:

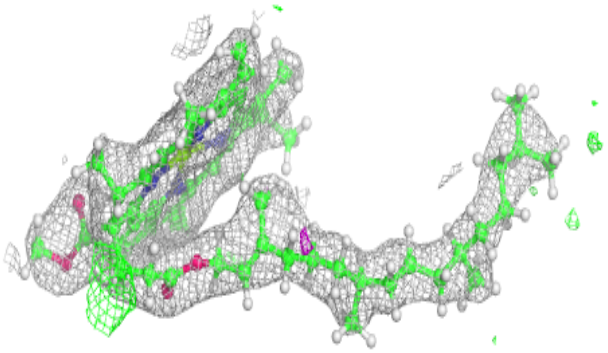
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

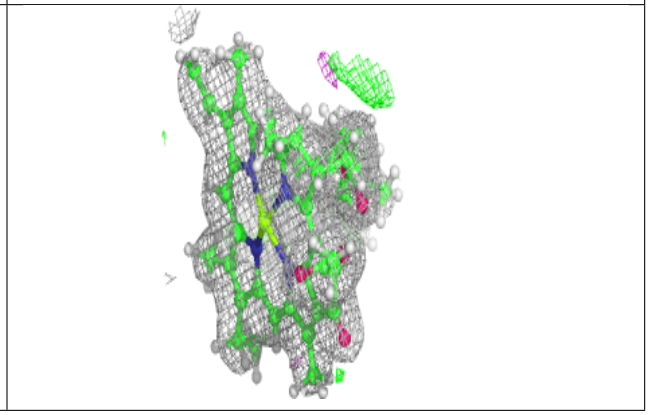




Electron density around CLA b 609:

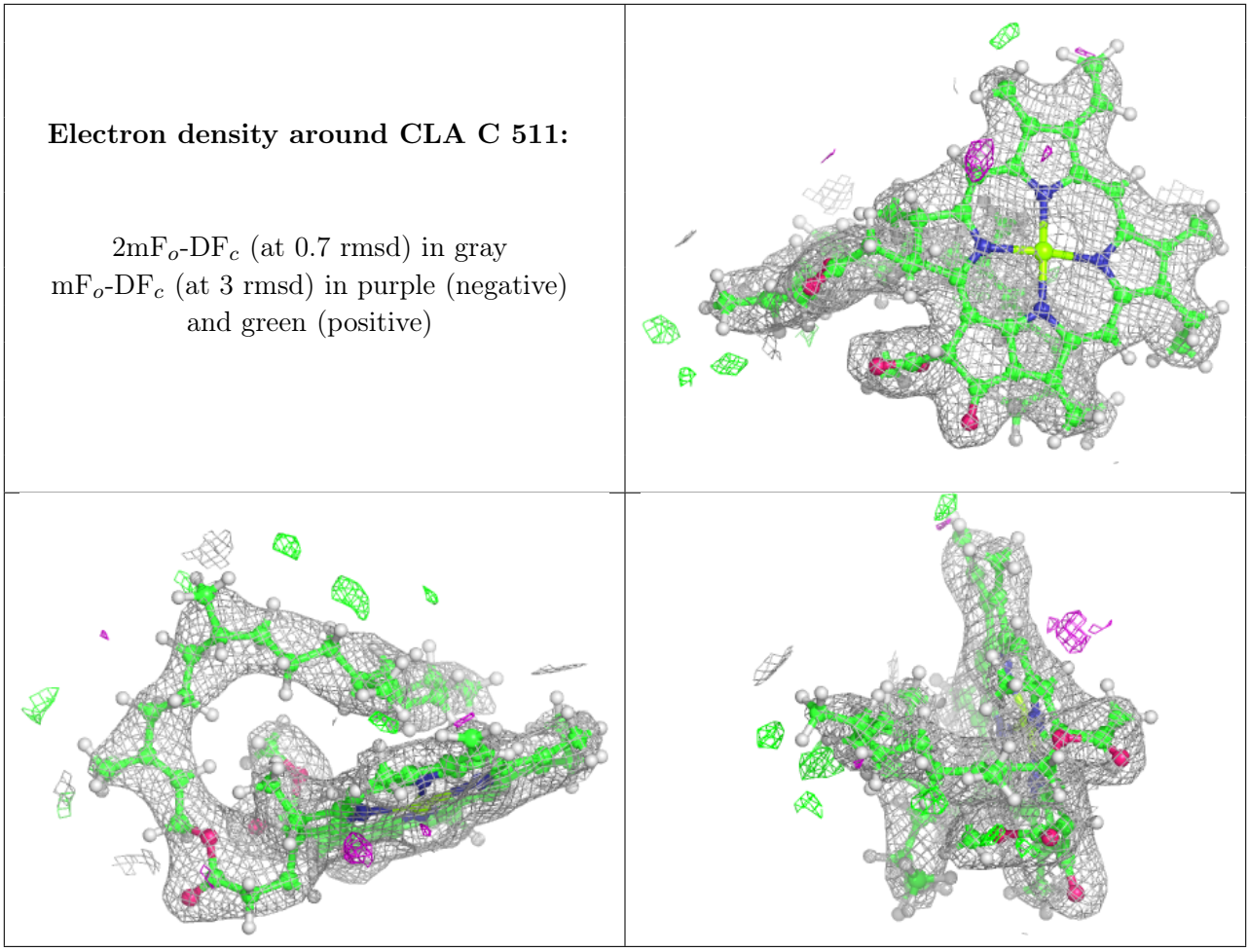
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





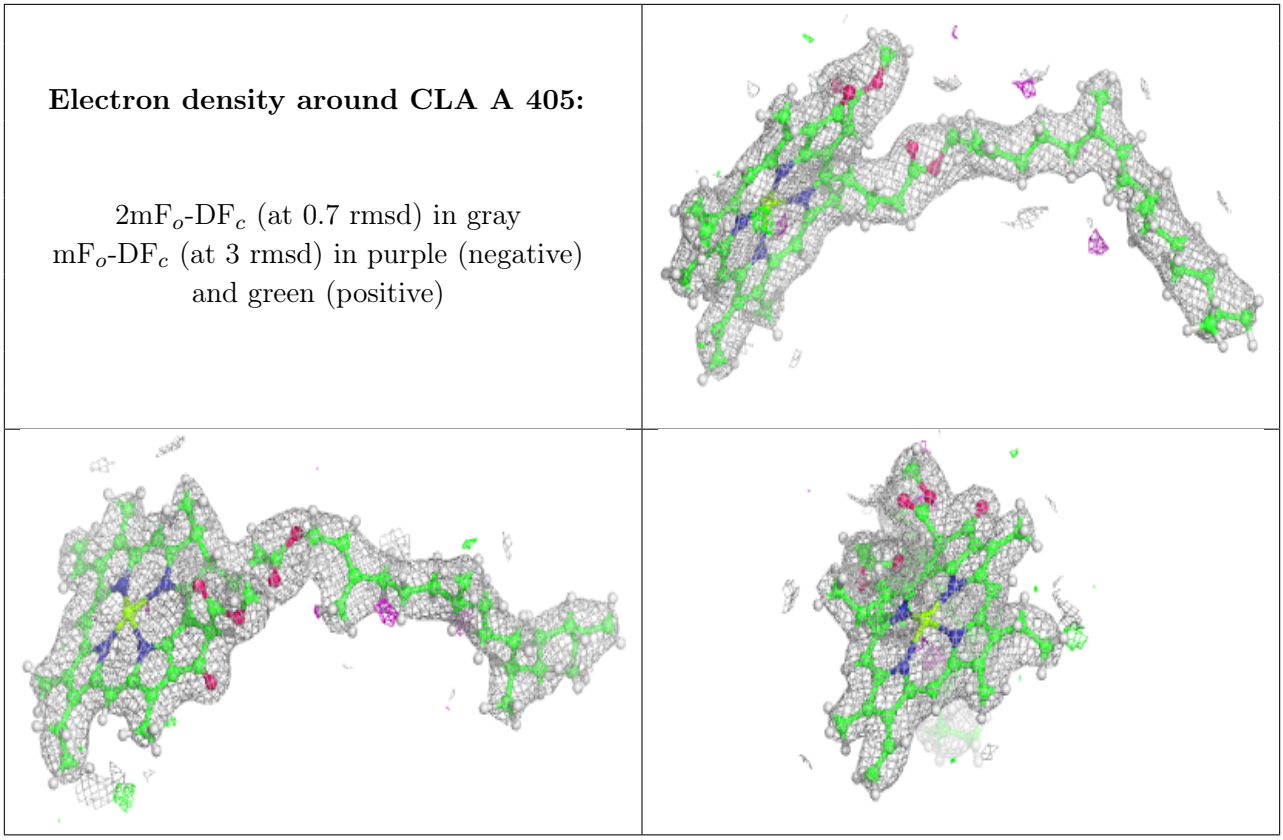
Electron density around CLA C 511:

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



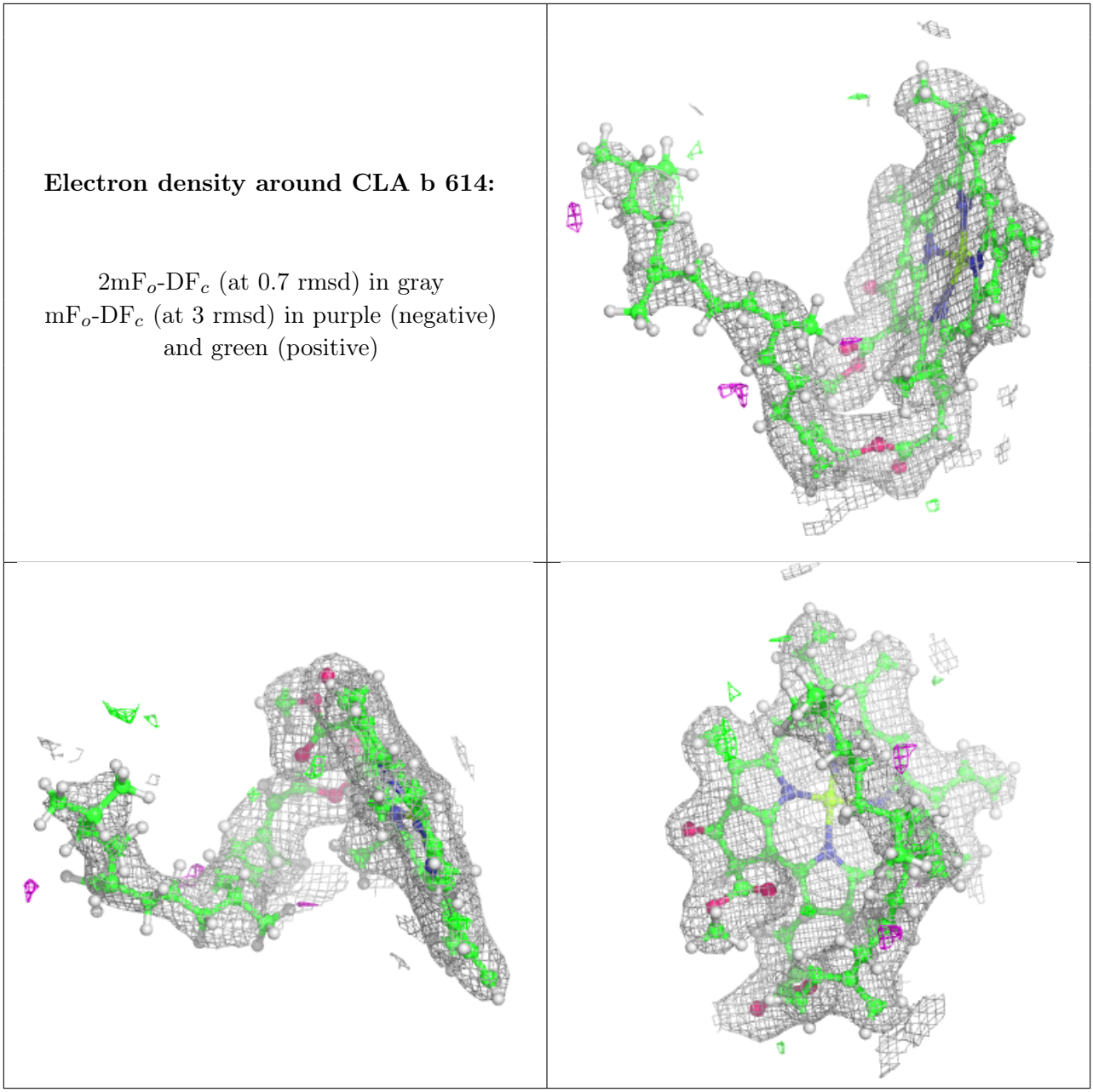
Electron density around CLA A 405:

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



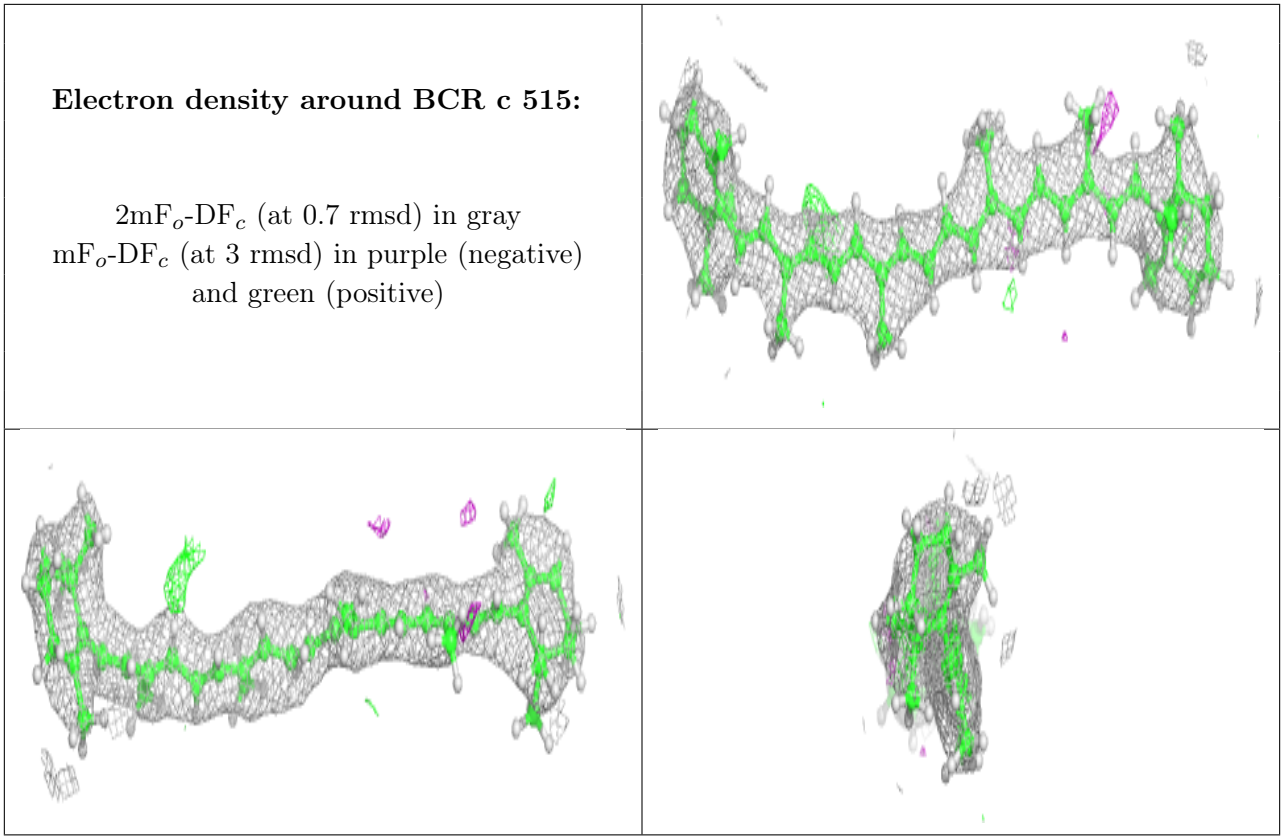
Electron density around CLA b 614:

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



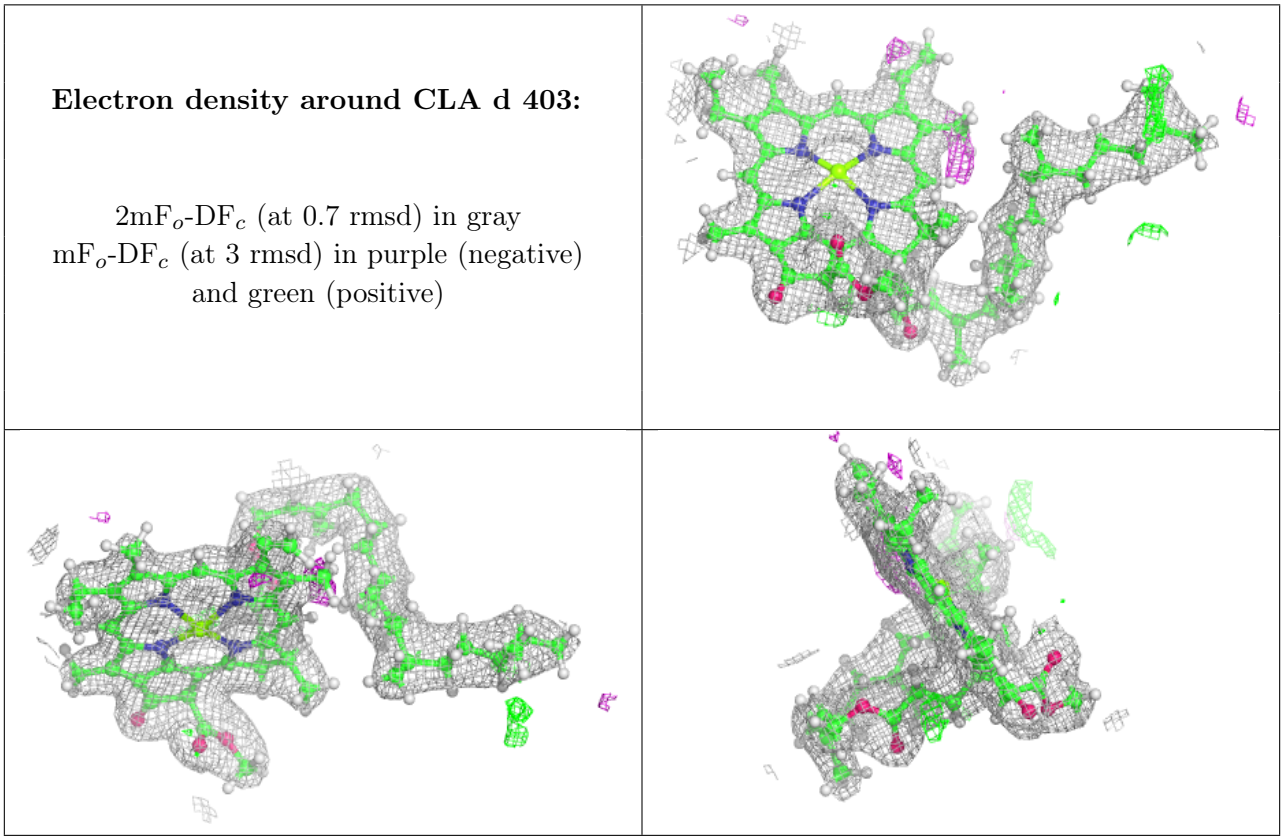
Electron density around BCR c 515:

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



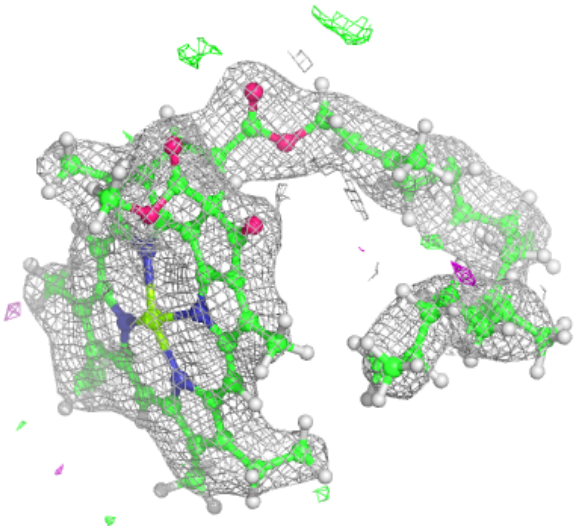
Electron density around CLA d 403:

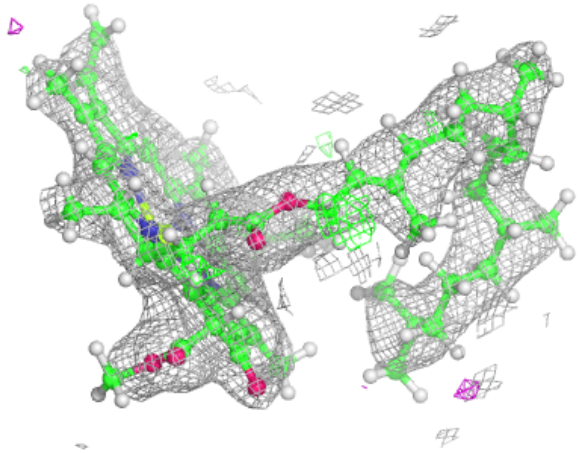
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

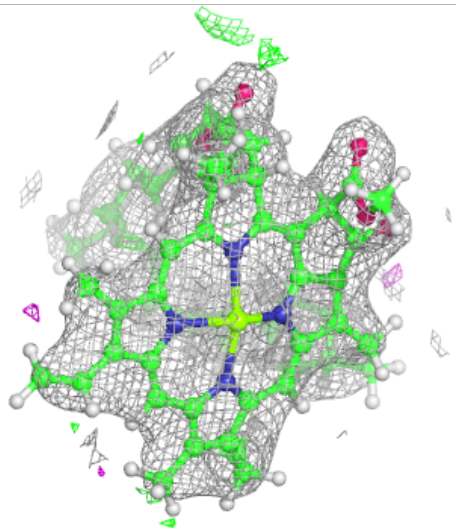


Electron density around CLA C 504:

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

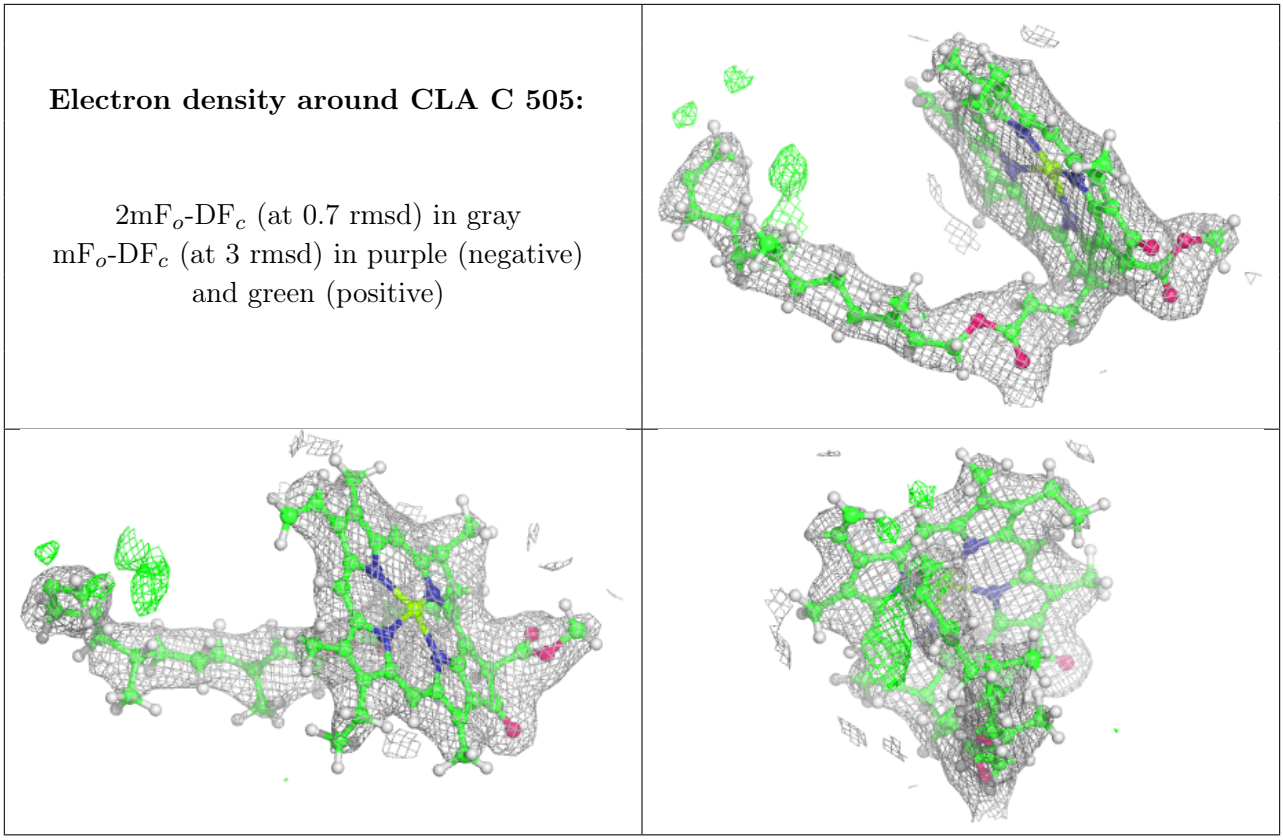






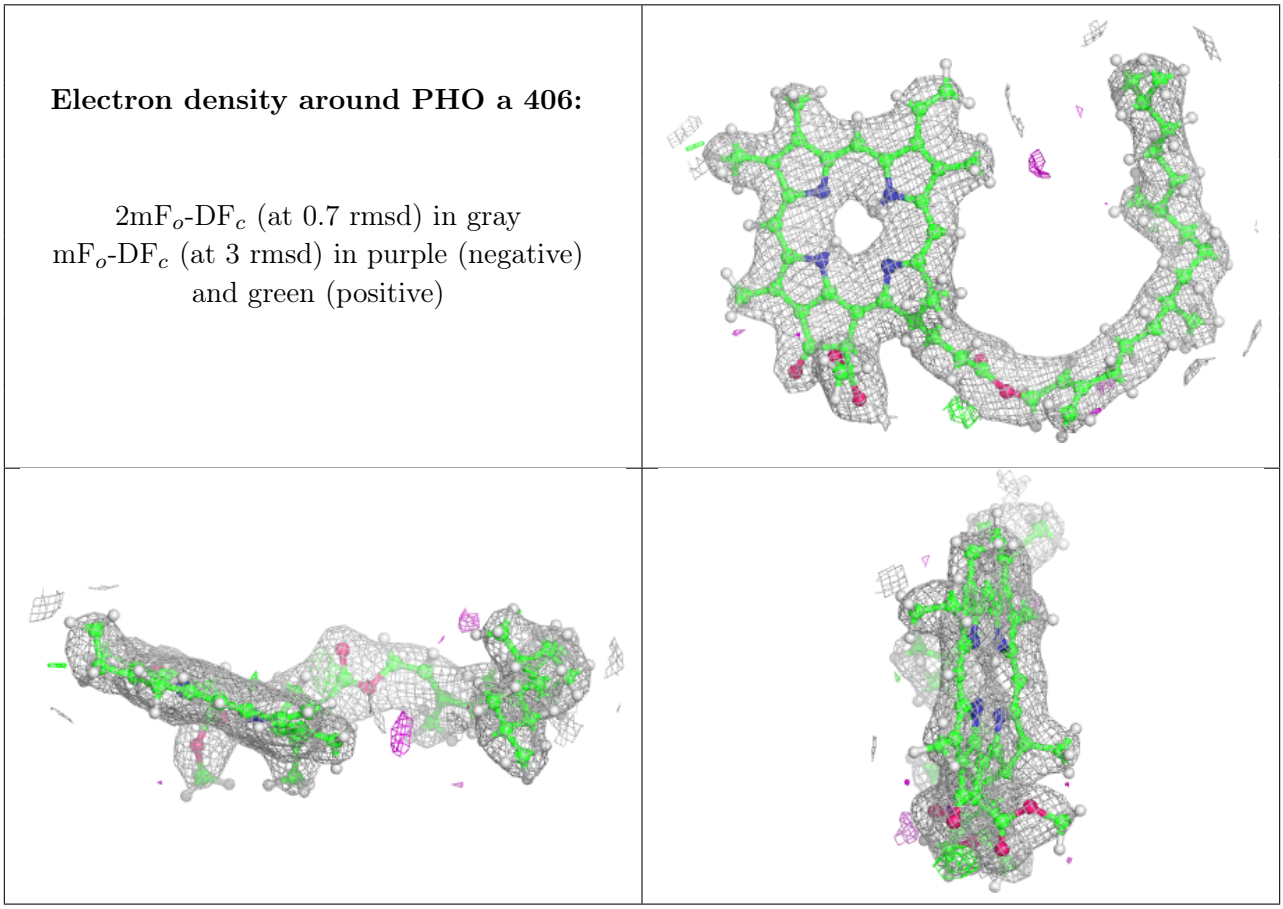
Electron density around CLA C 505:

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



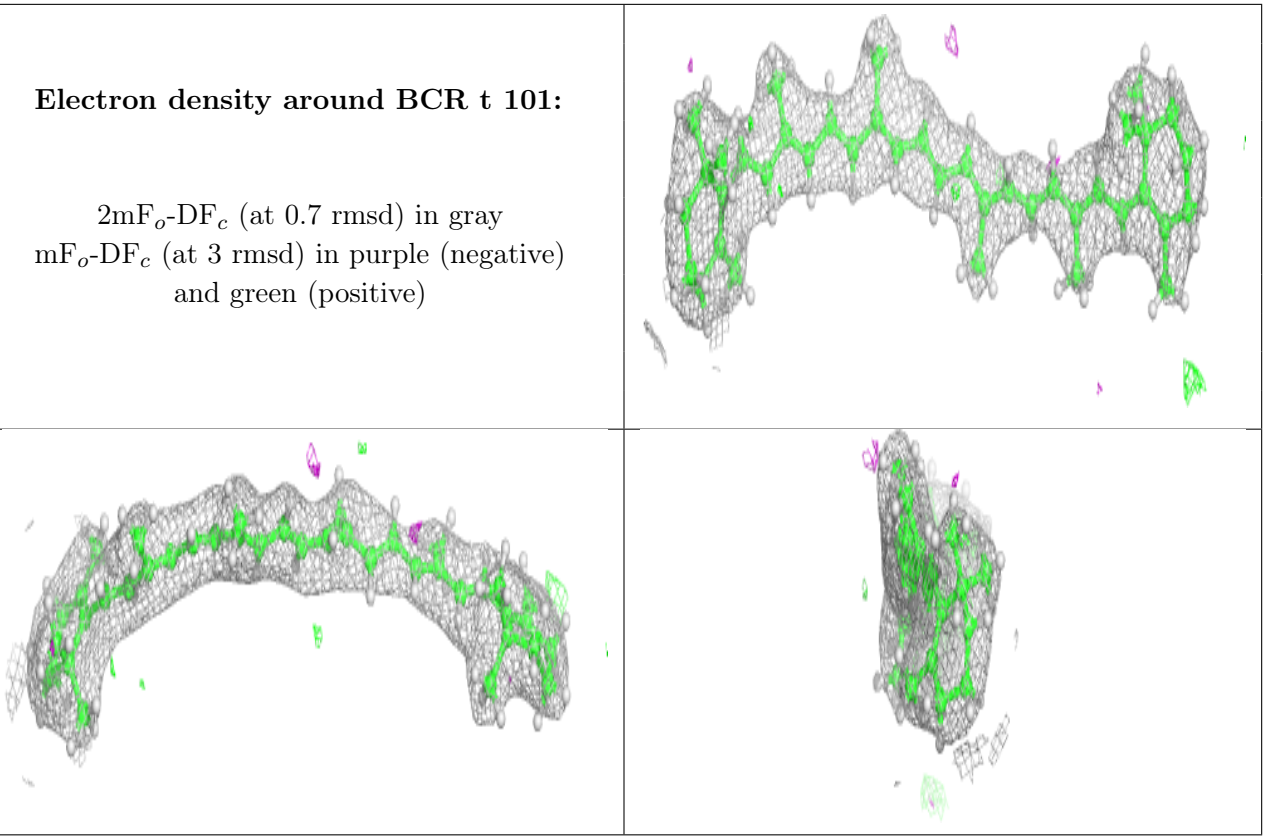
Electron density around PHO a 406:

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



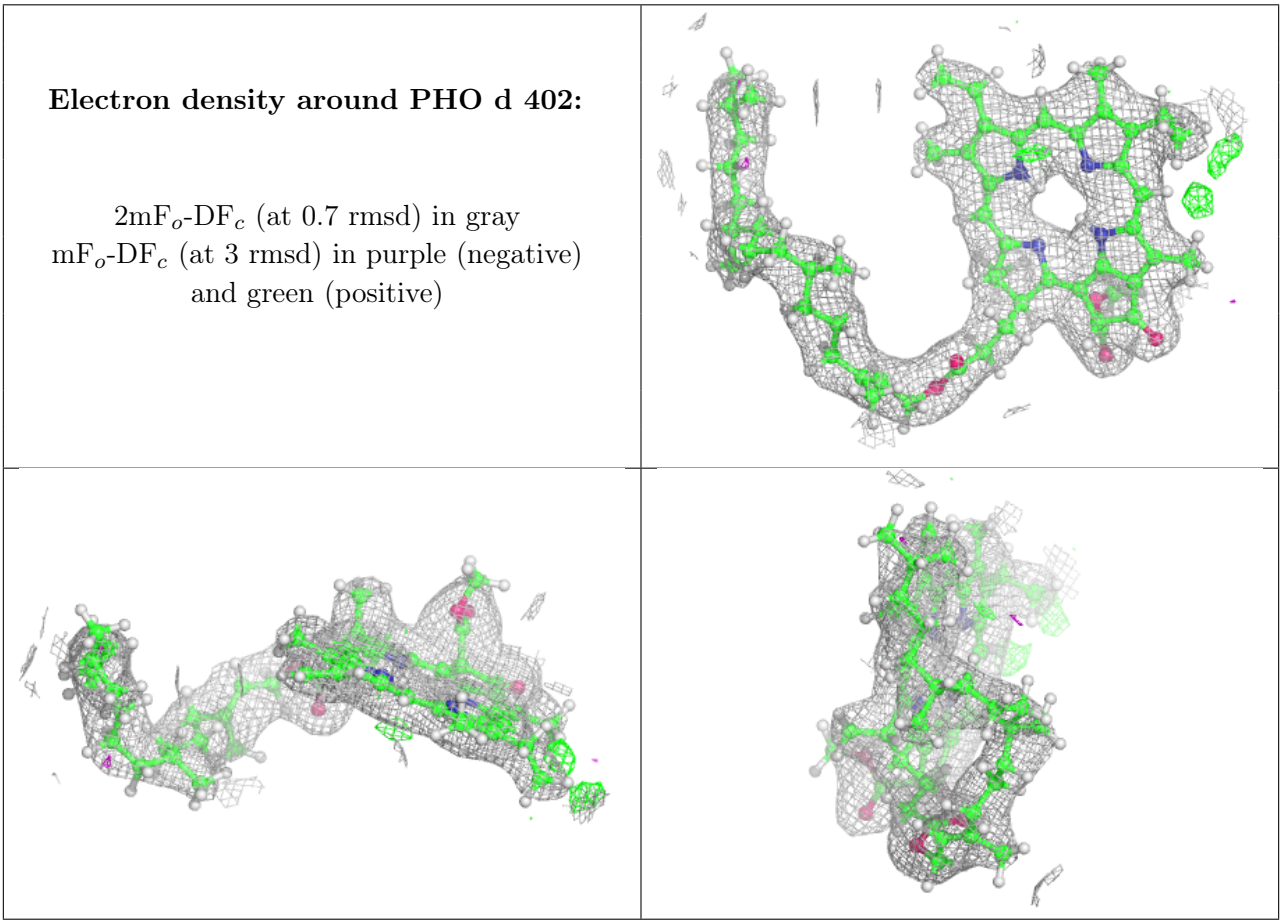
Electron density around BCR t 101:

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



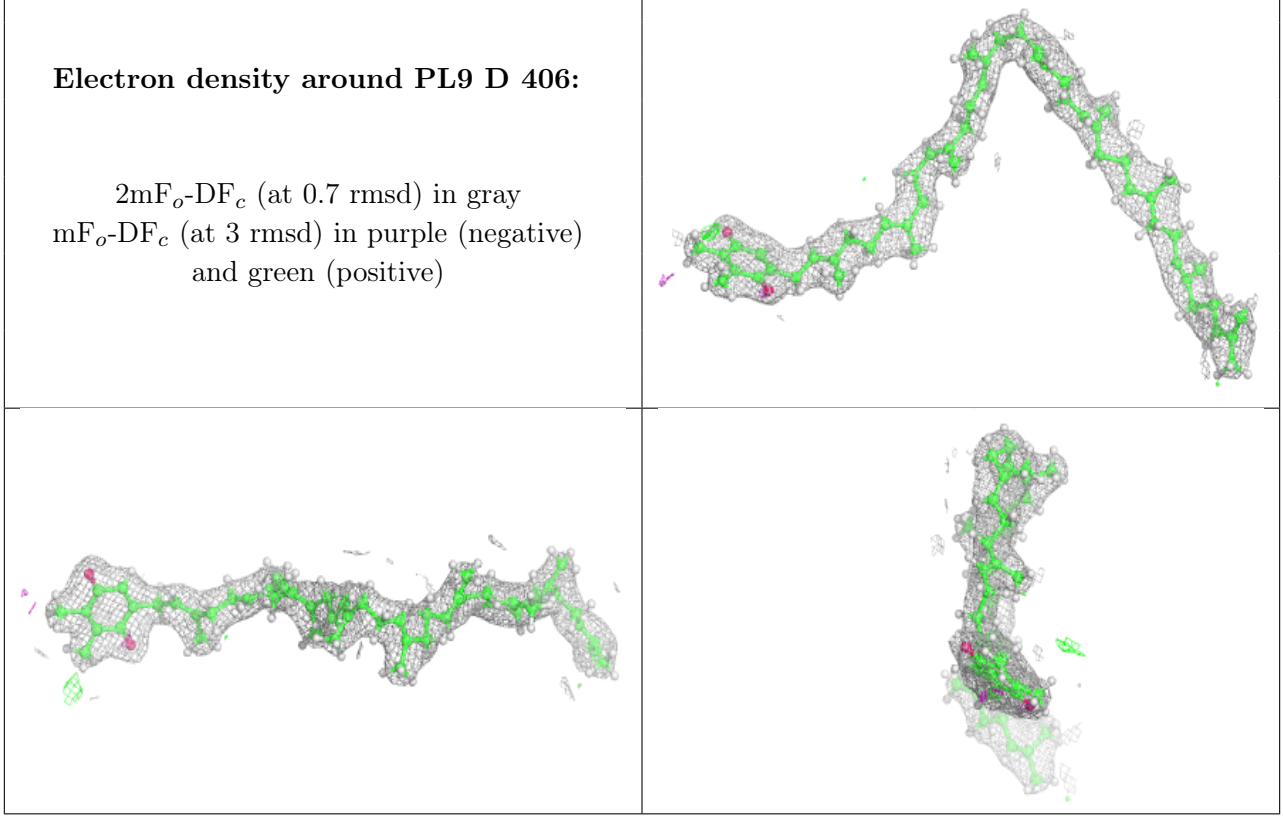
Electron density around PHO d 402:

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



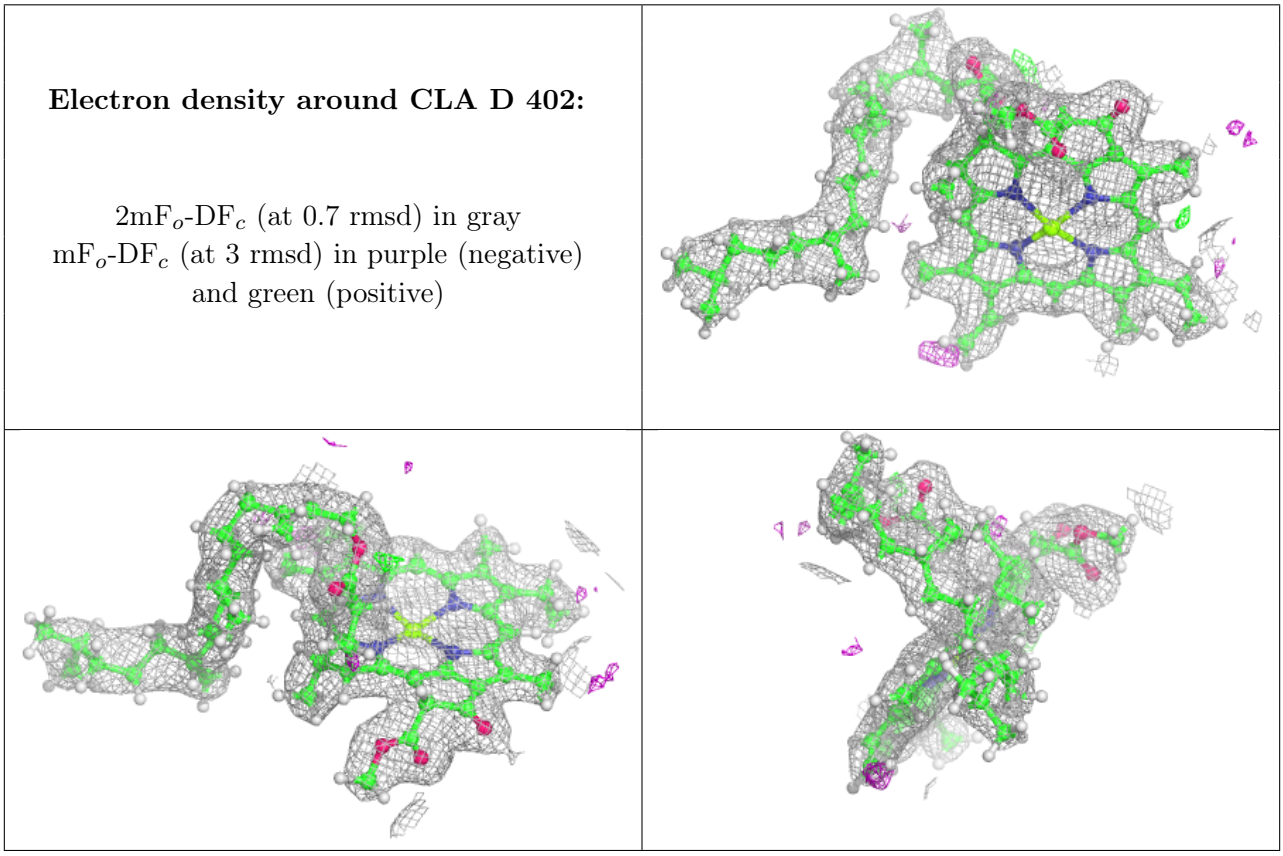
Electron density around PL9 D 406:

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



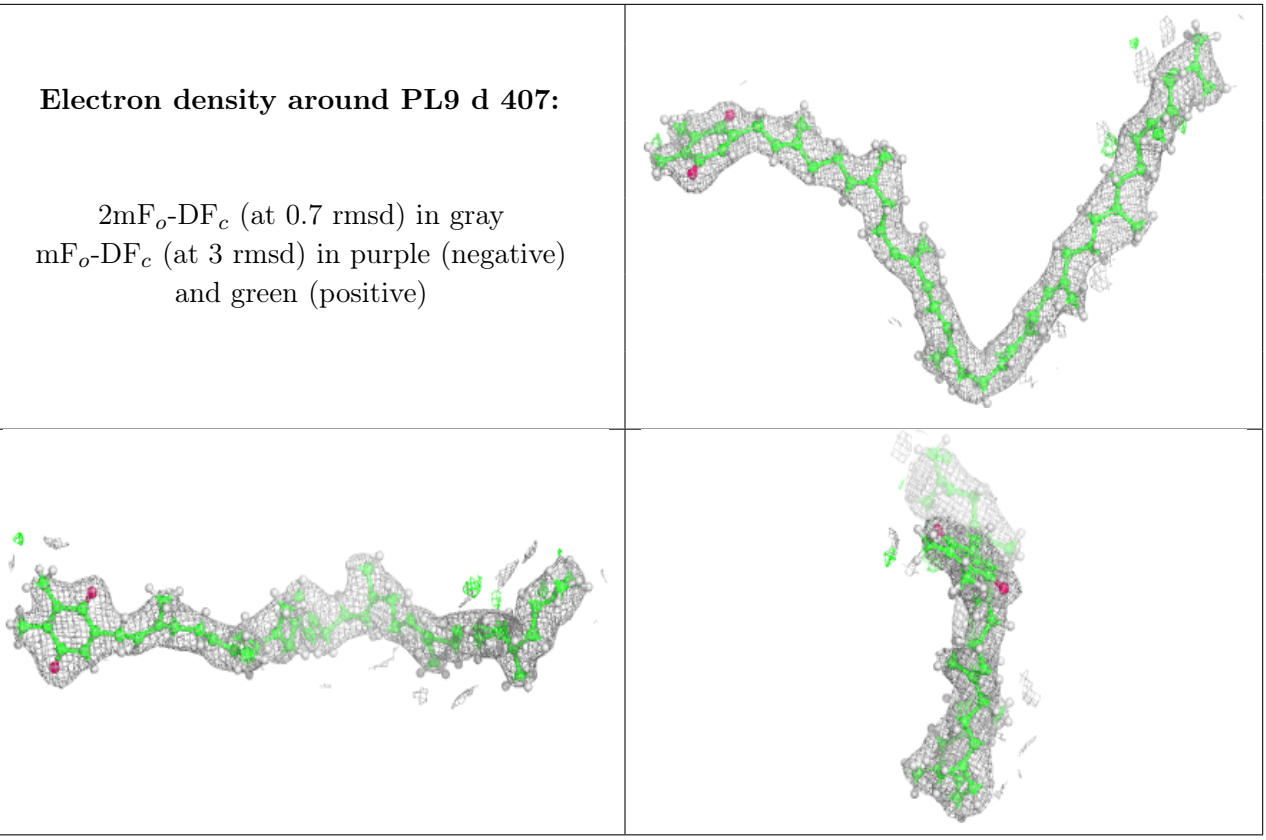
Electron density around CLA D 402:

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



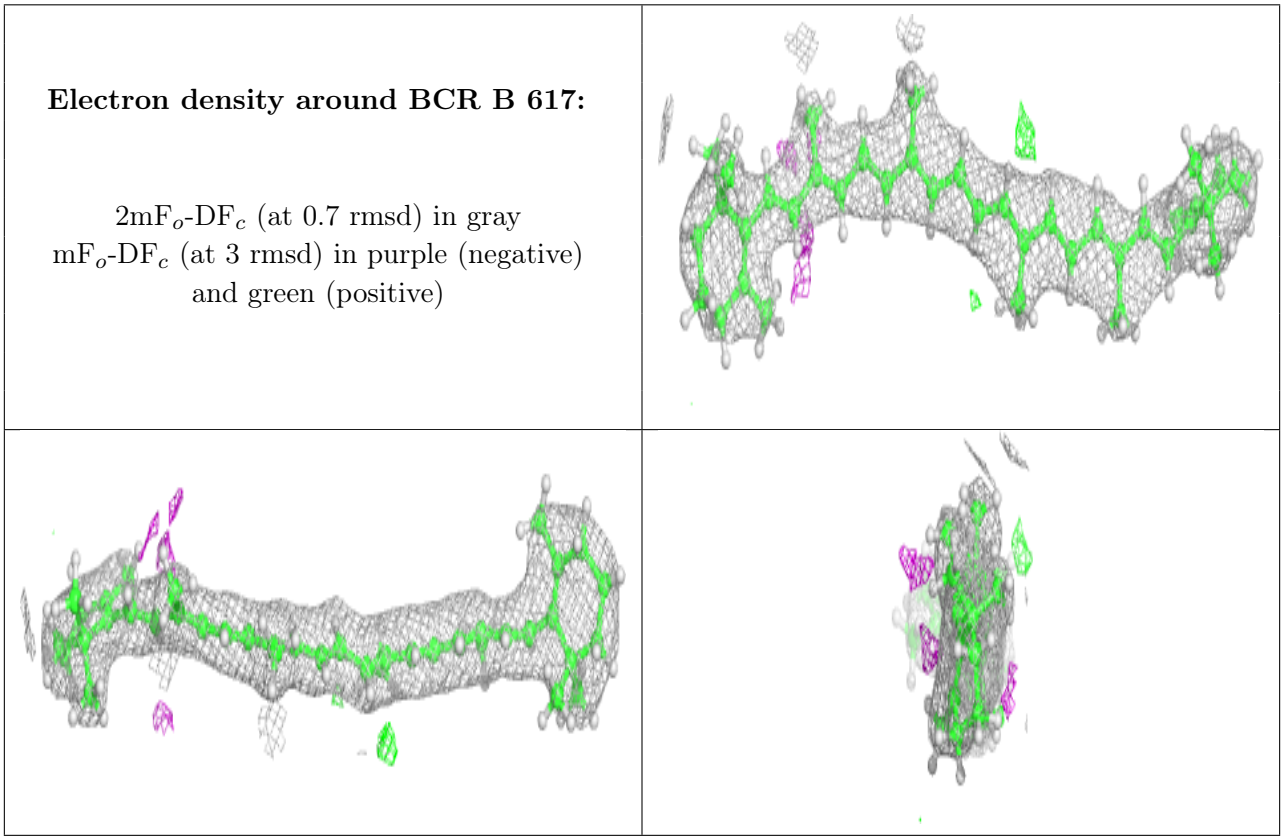
Electron density around PL9 d 407:

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



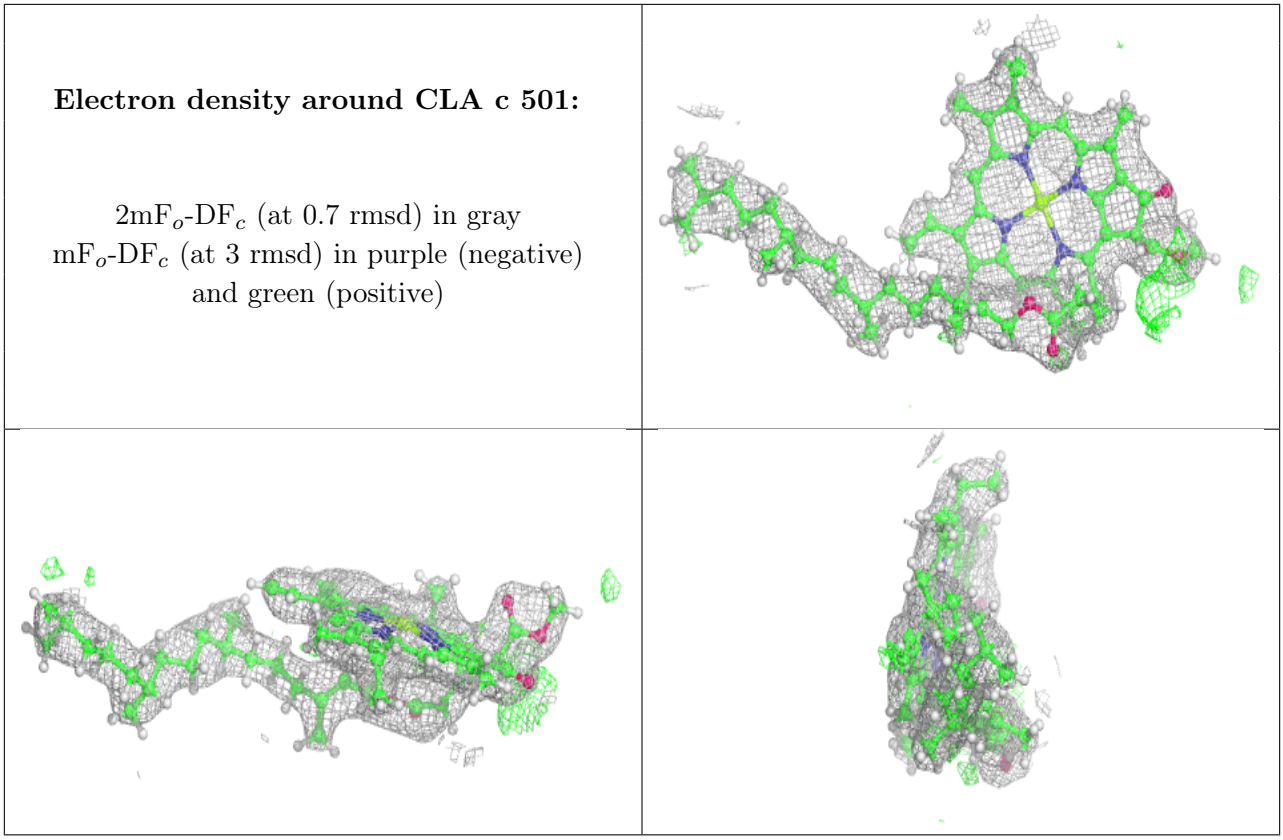
Electron density around BCR B 617:

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



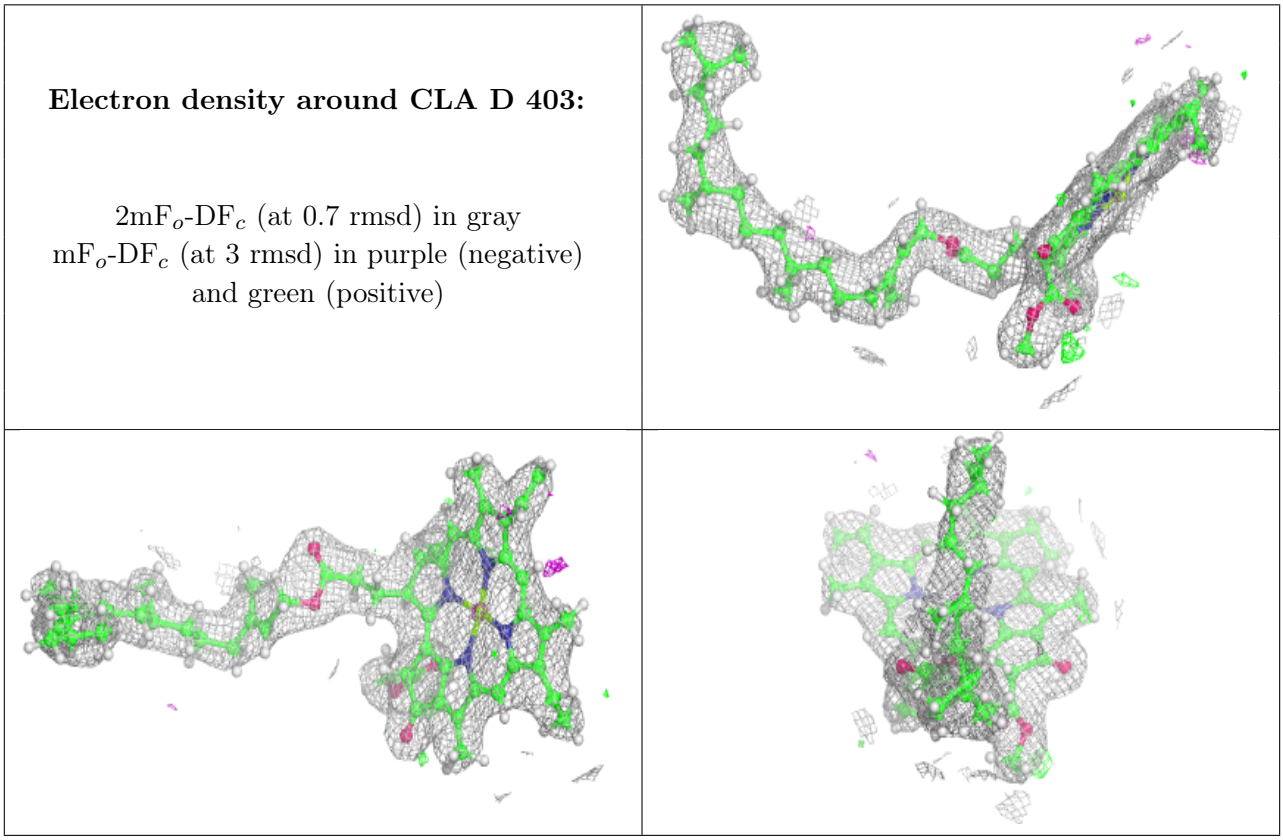
Electron density around CLA c 501:

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



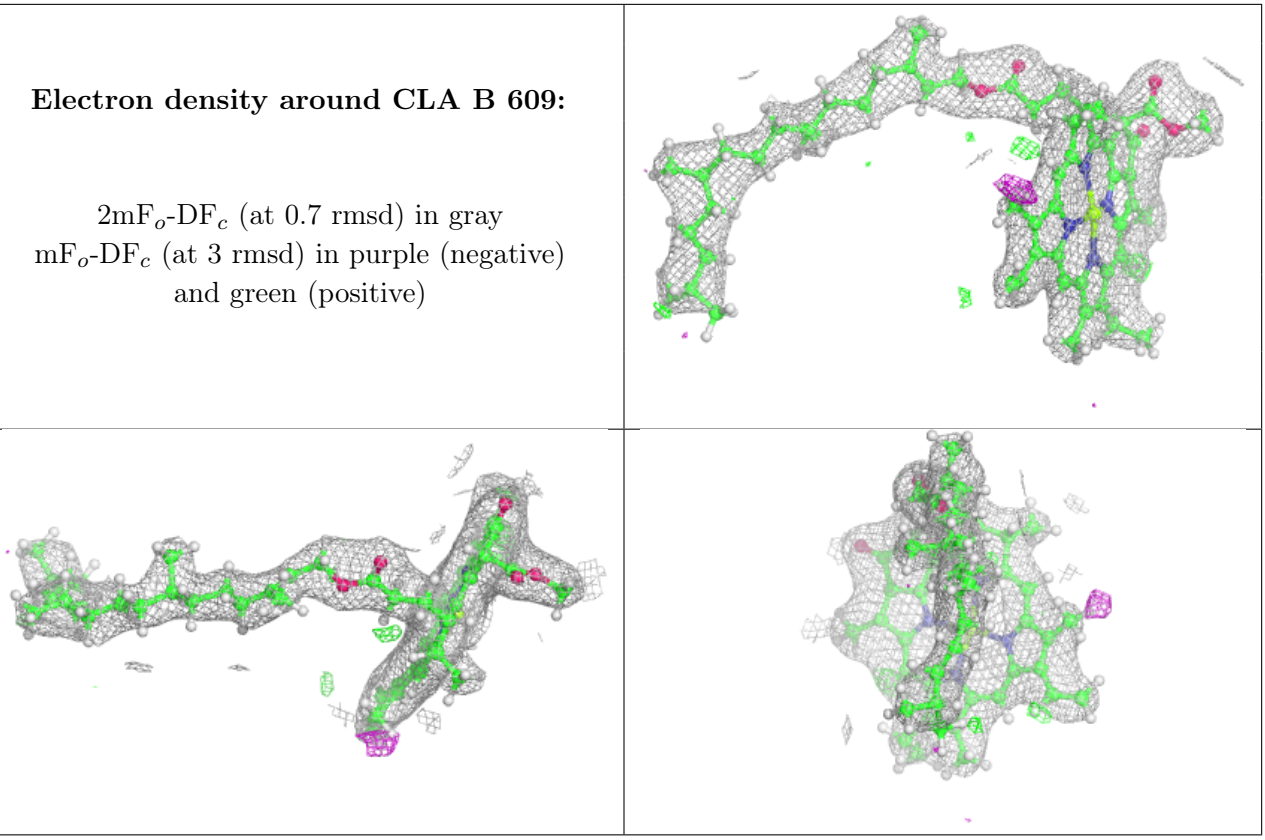
Electron density around CLA D 403:

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



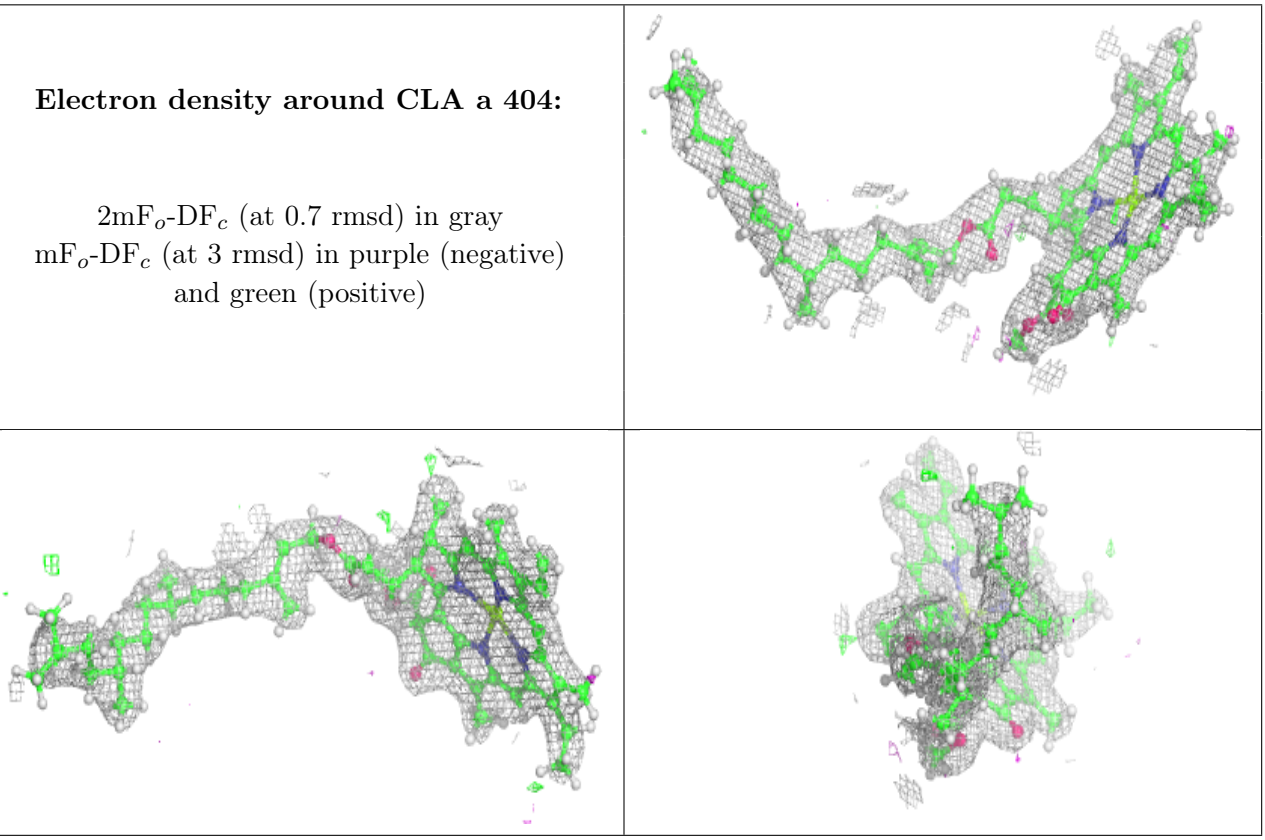
Electron density around CLA B 609:

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



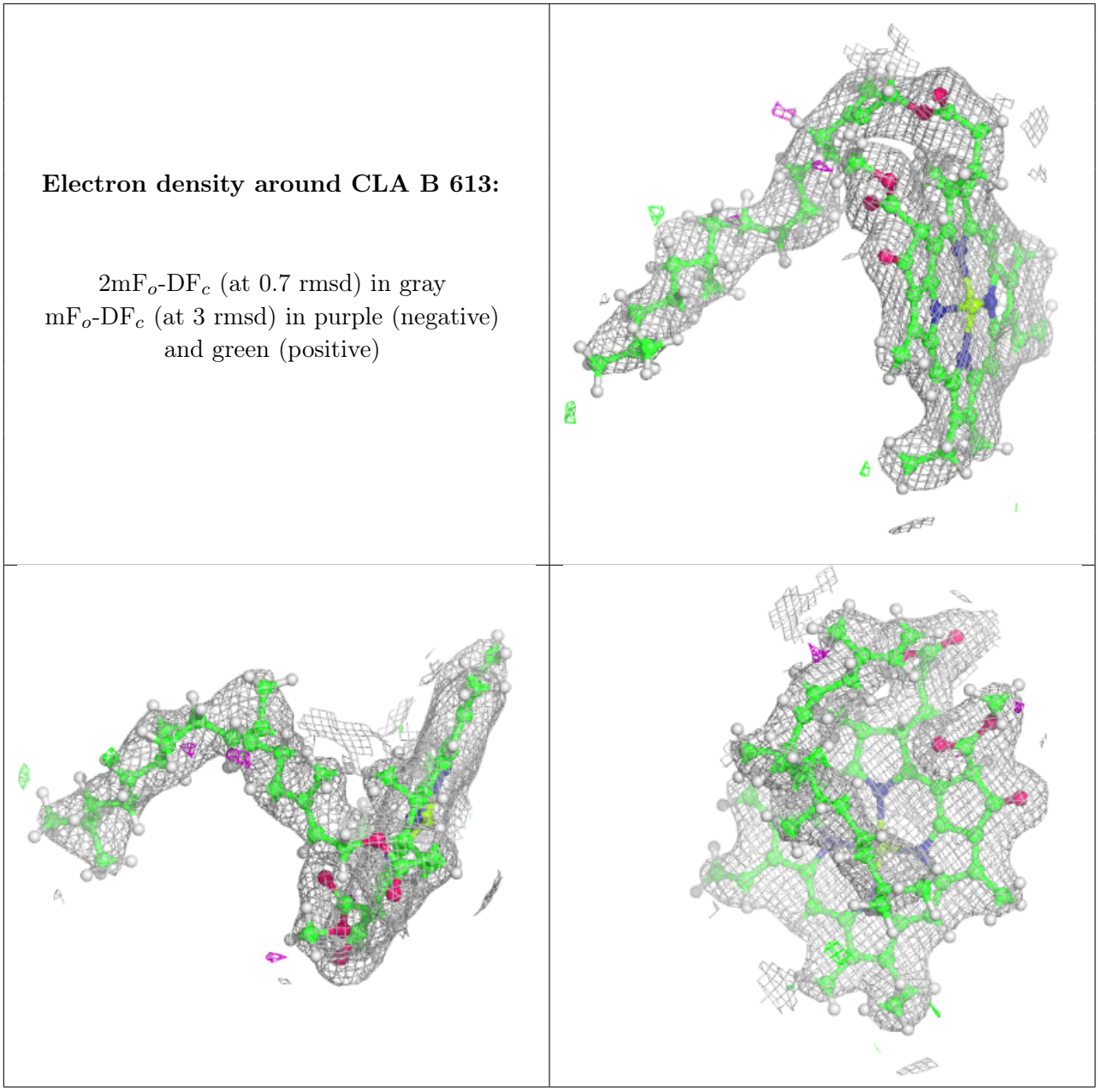
Electron density around CLA a 404:

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



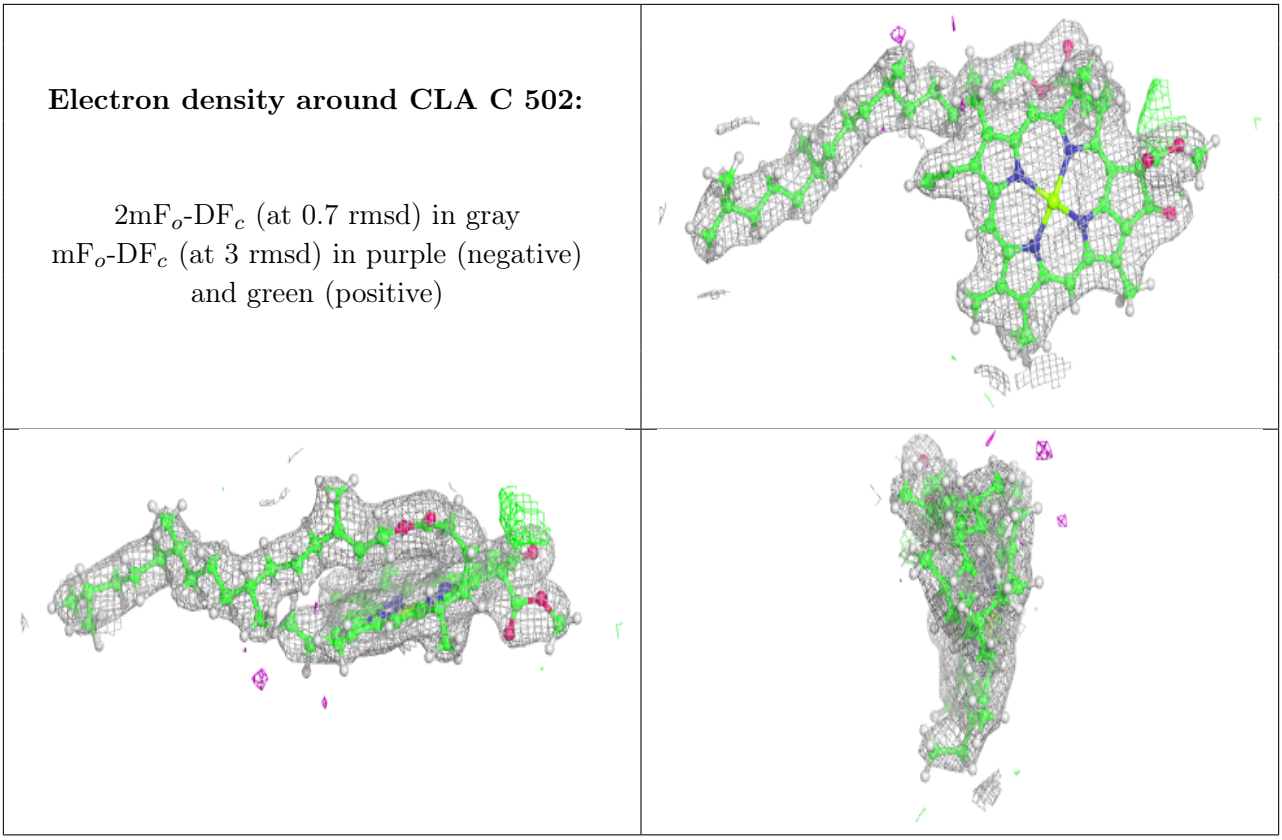
Electron density around CLA B 613:

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



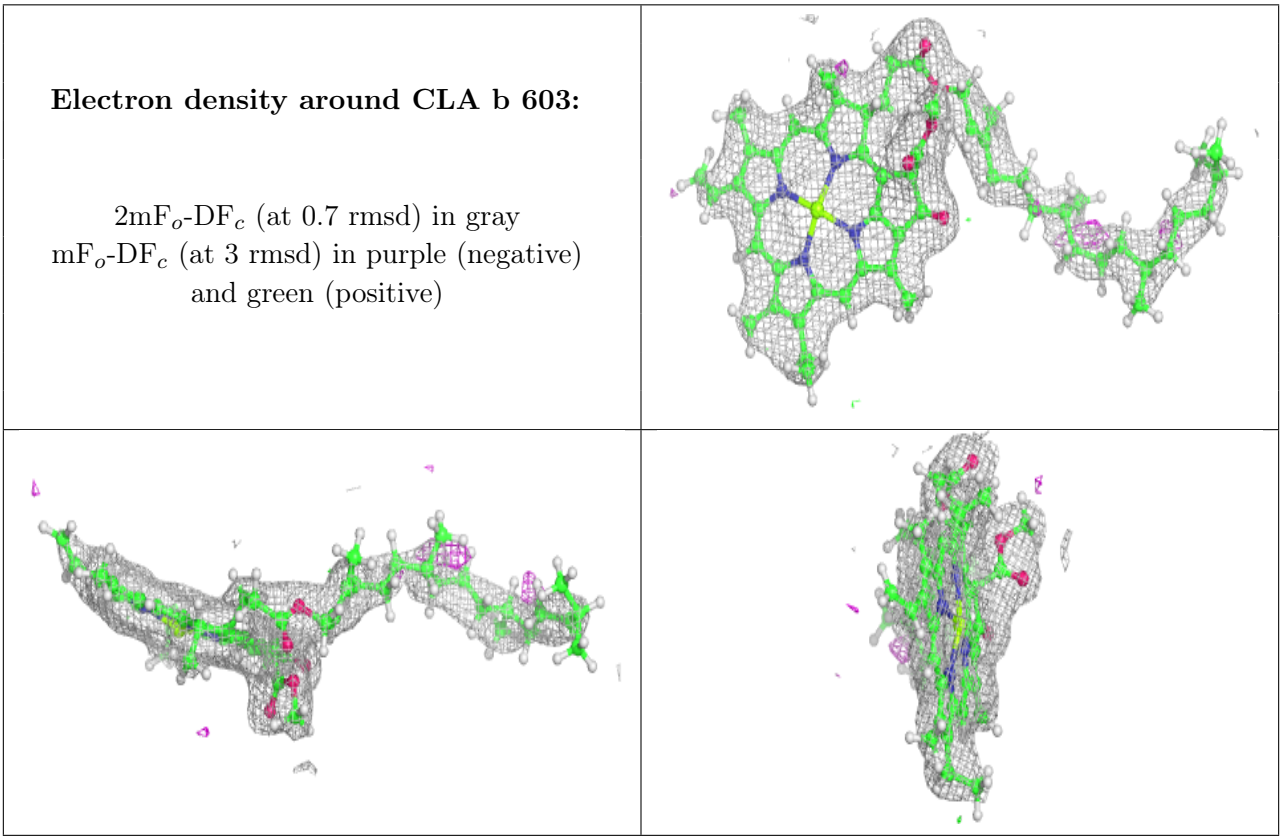
Electron density around CLA C 502:

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



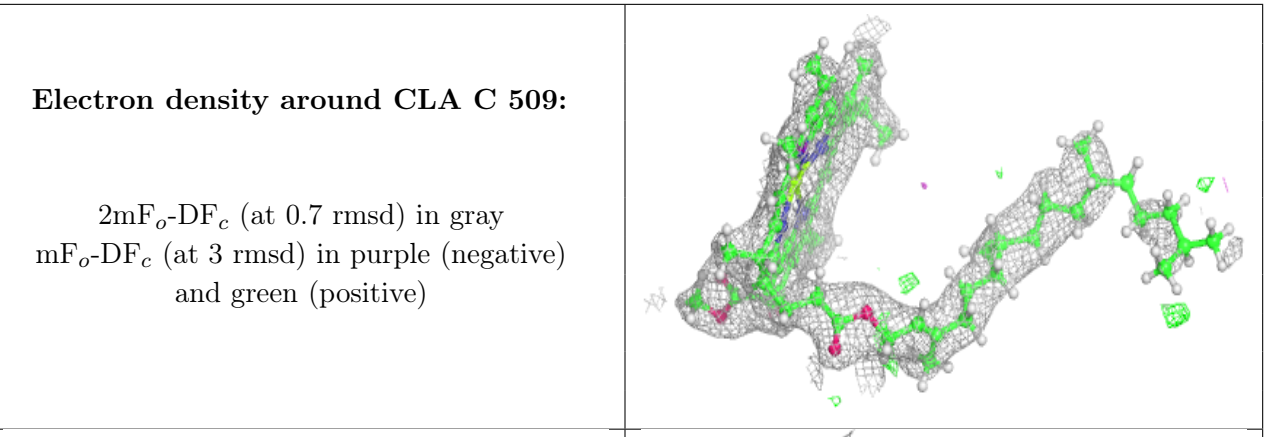
Electron density around CLA b 603:

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



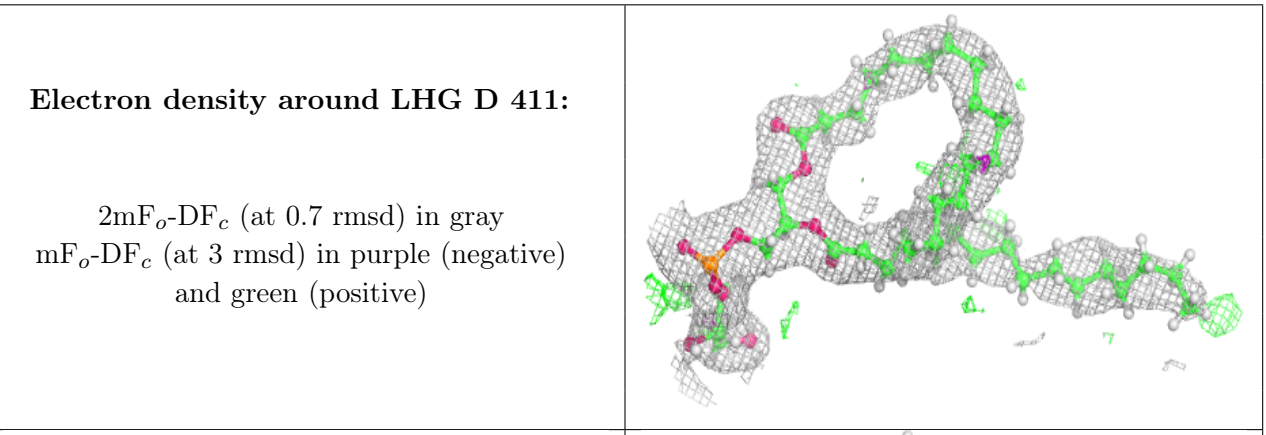
Electron density around CLA C 509:

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



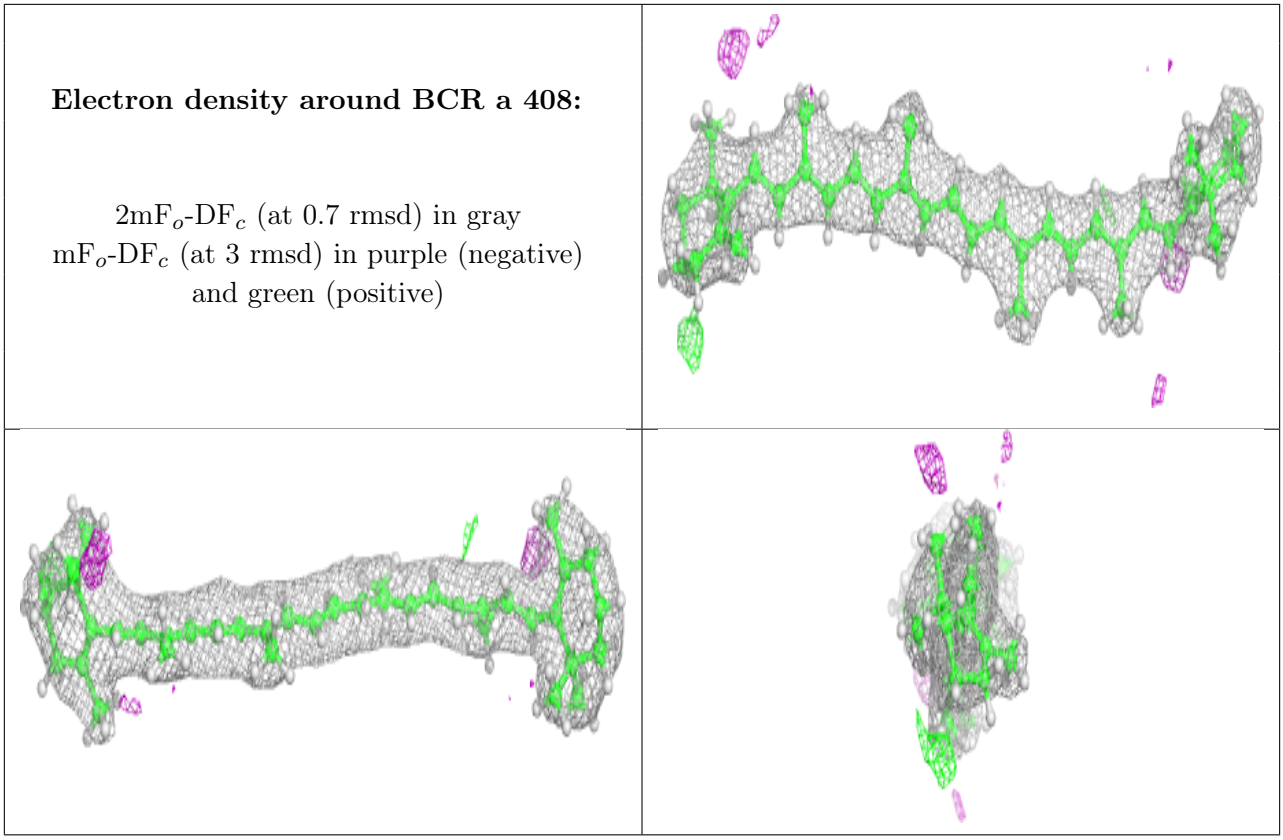
Electron density around LHG D 411:

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



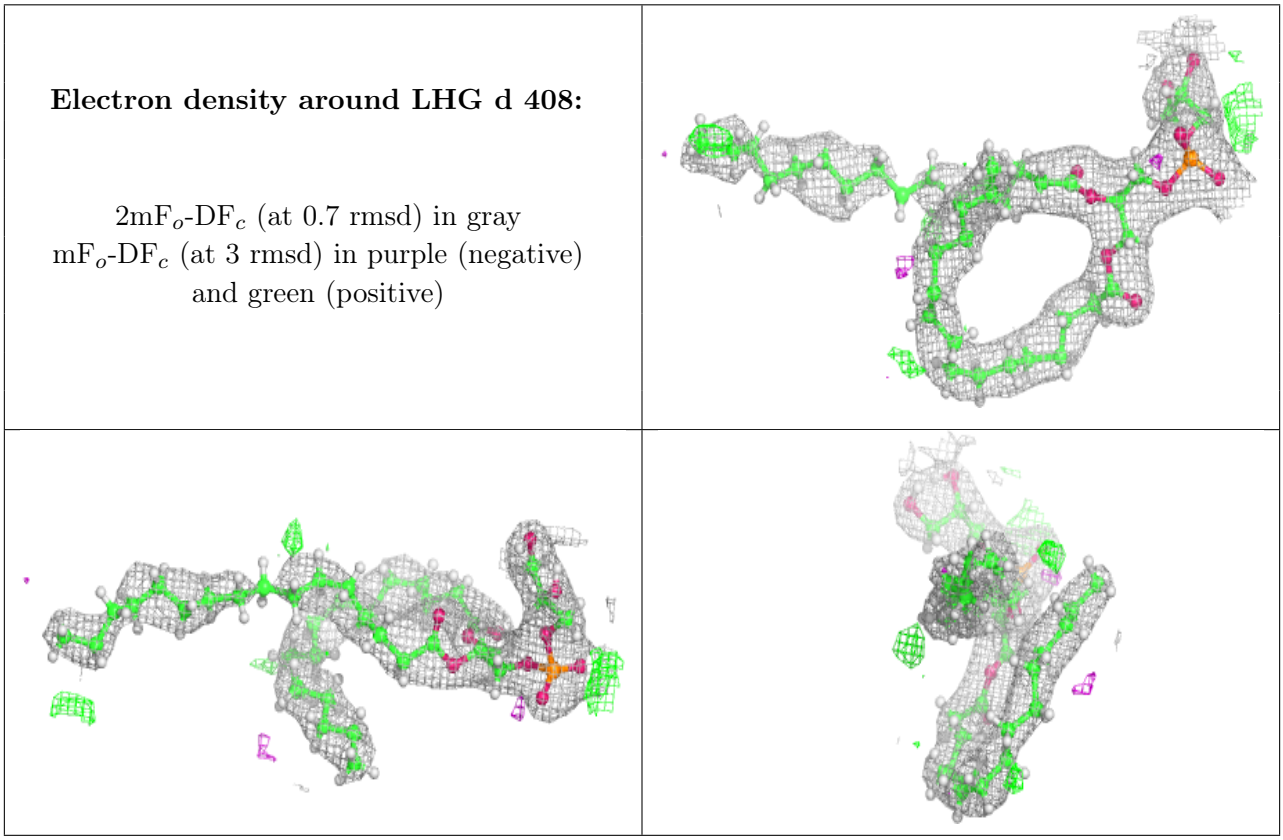
Electron density around BCR a 408:

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



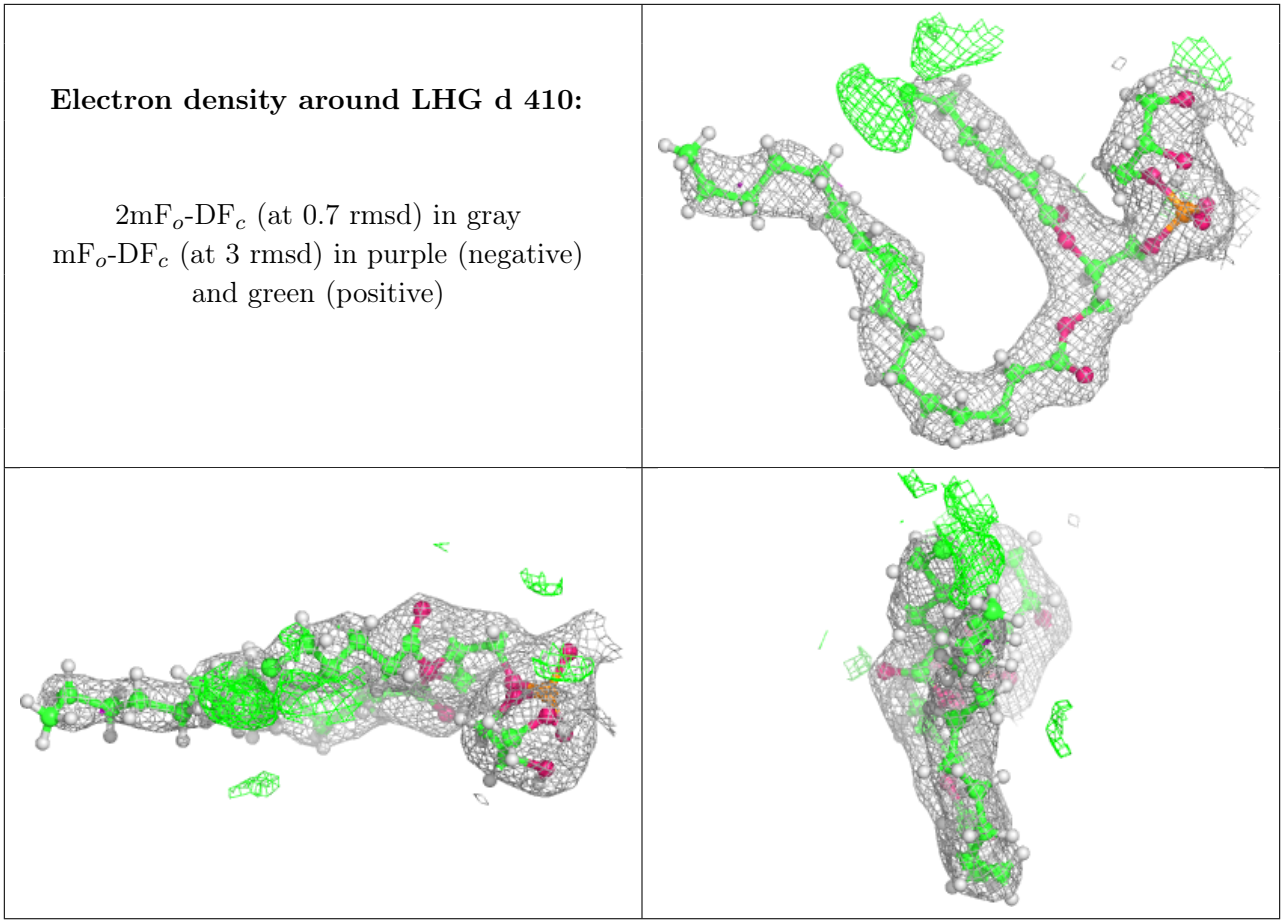
Electron density around LHG d 408:

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



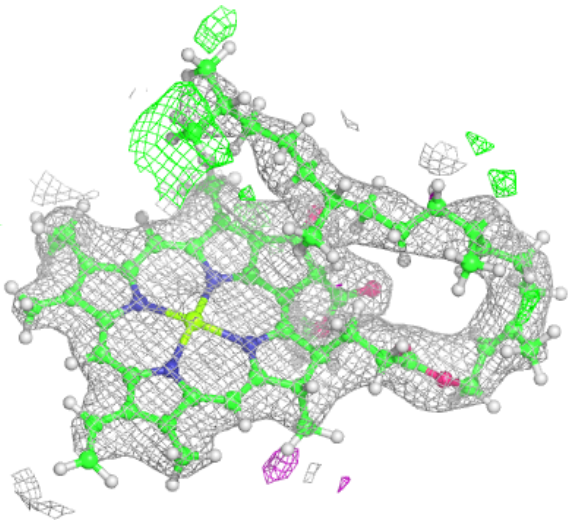
Electron density around LHG d 410:

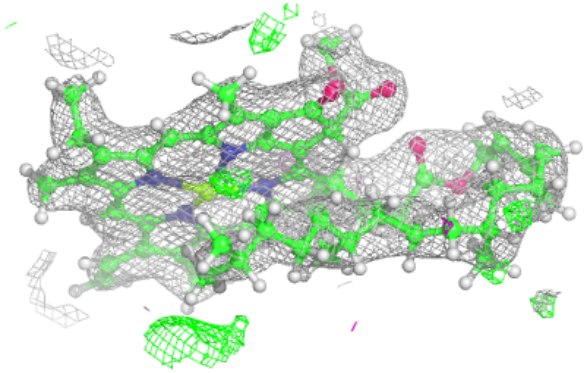
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

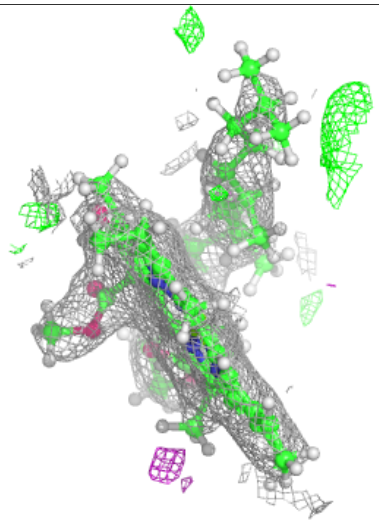


Electron density around CLA C 510:

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

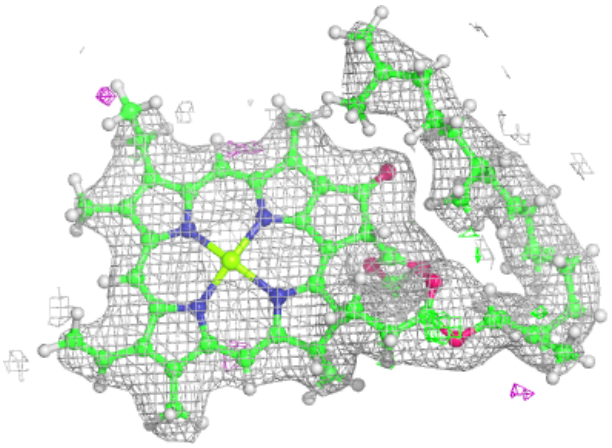


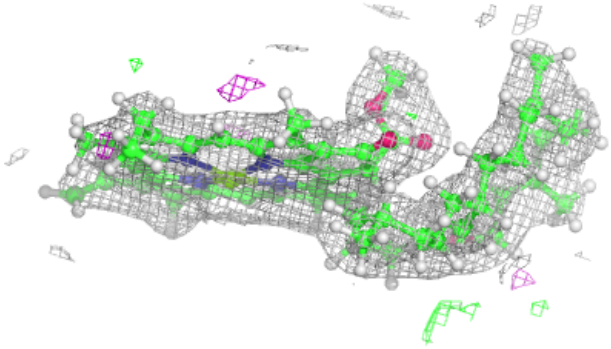


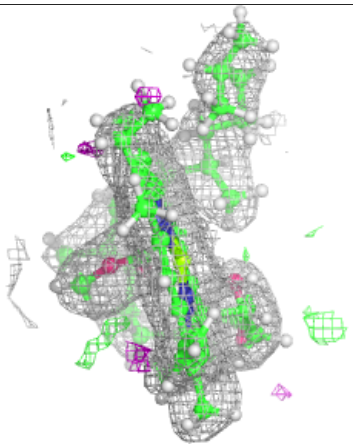


Electron density around CLA B 610:

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

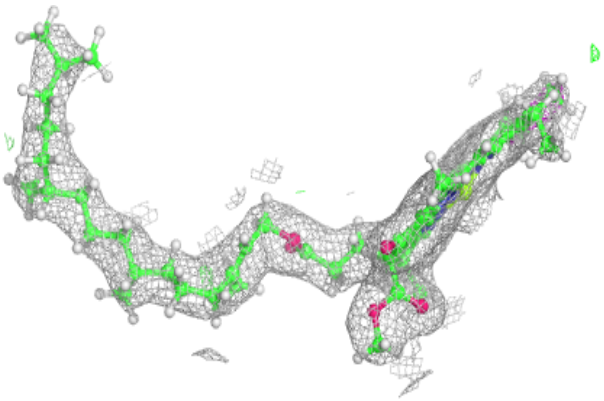


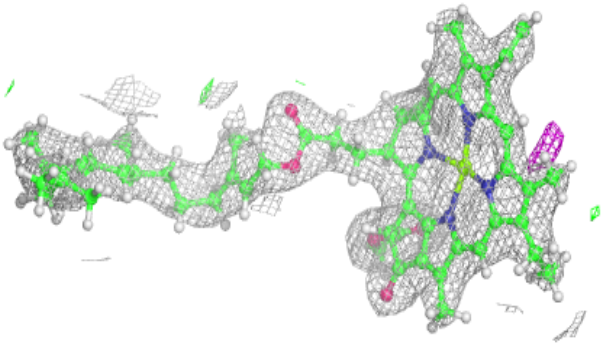


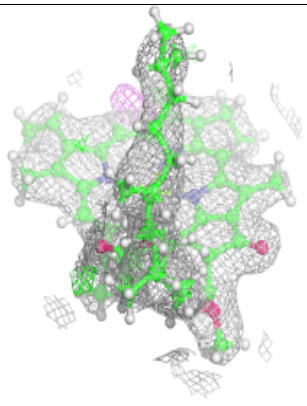


Electron density around CLA d 404:

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

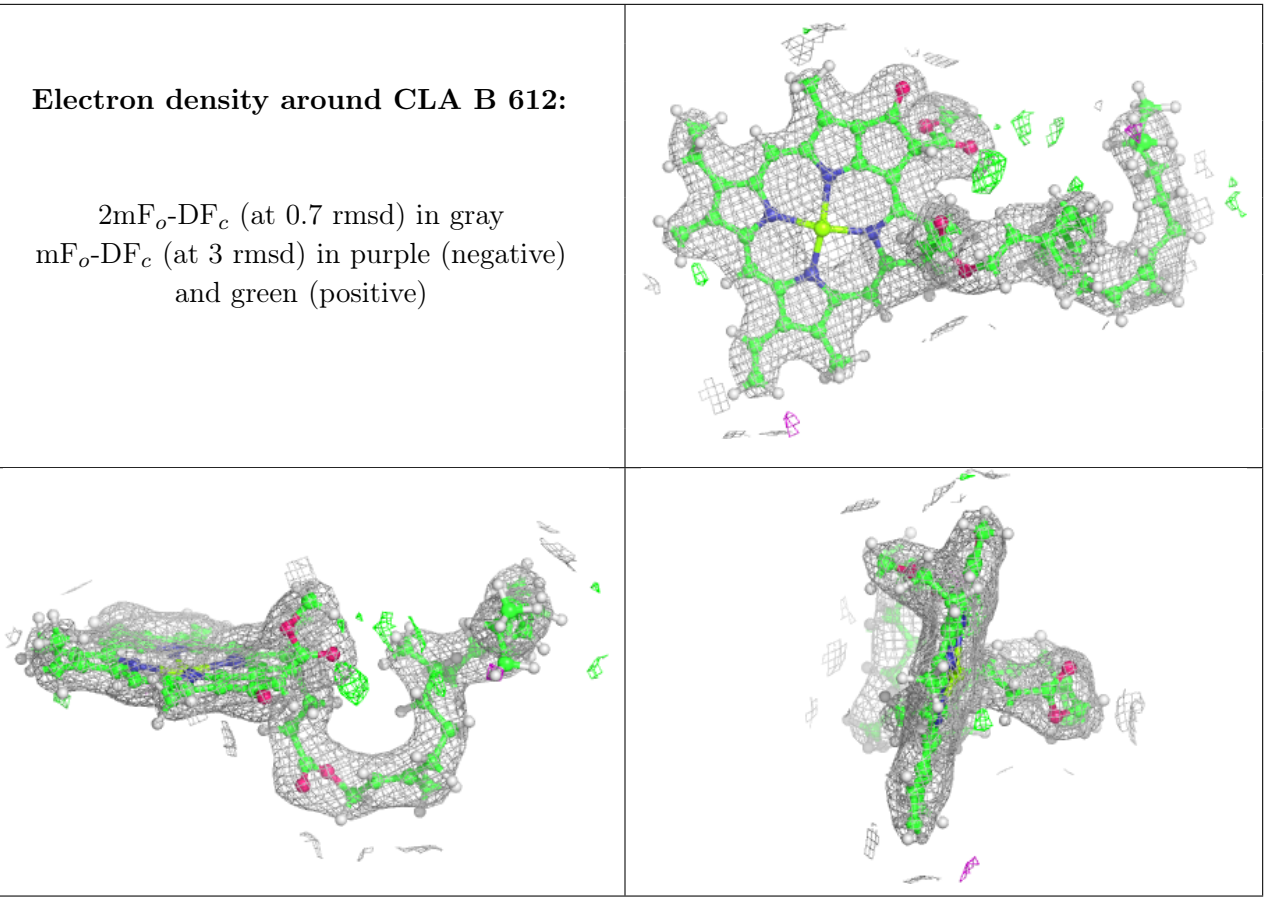






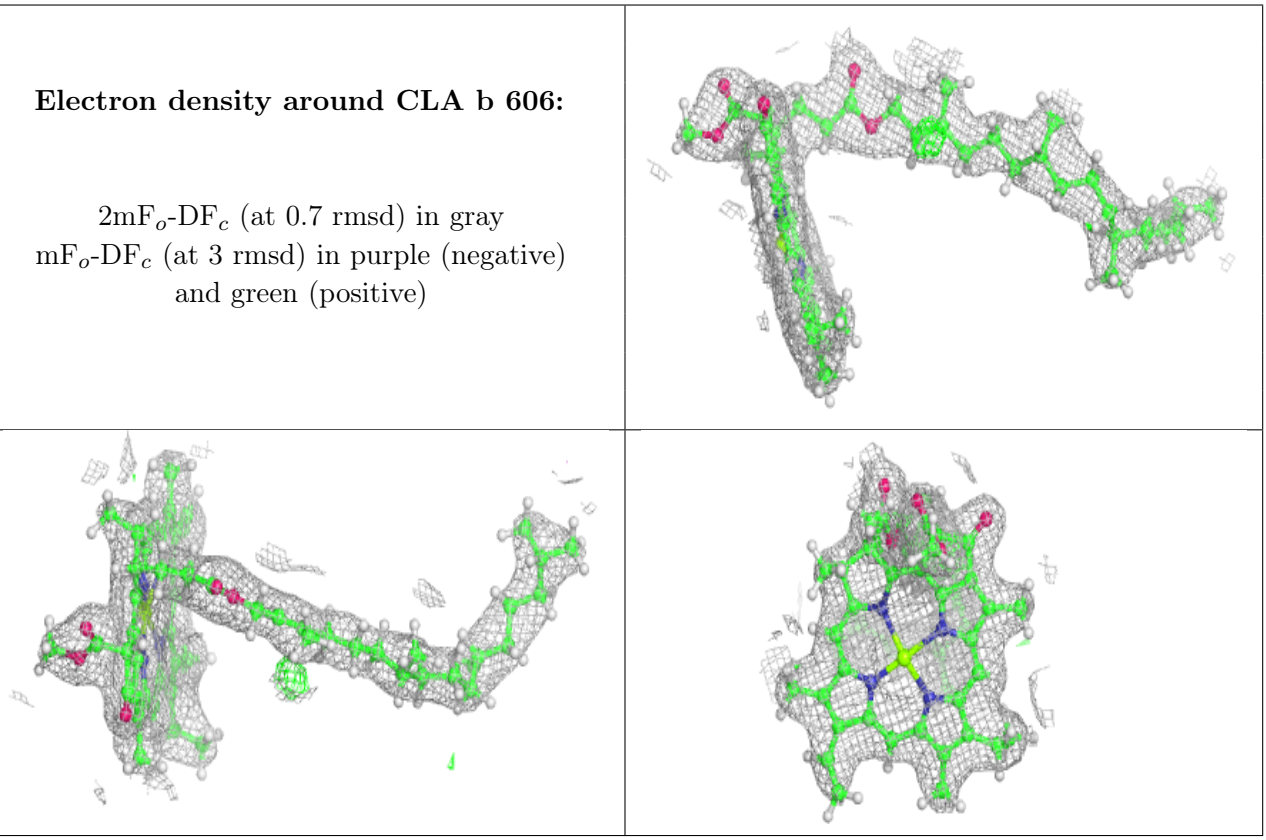
Electron density around CLA B 612:

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



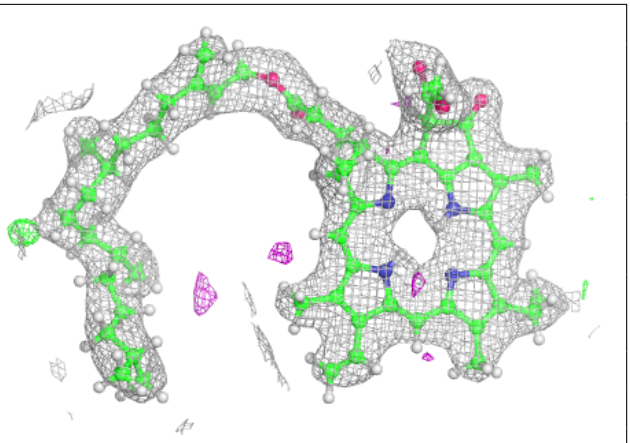
Electron density around CLA b 606:

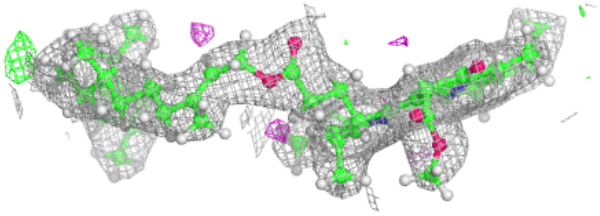
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

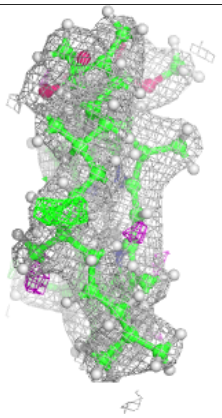


Electron density around PHO A 407:

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

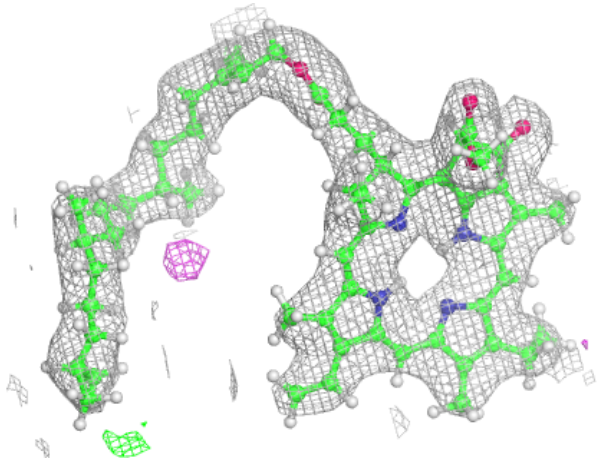


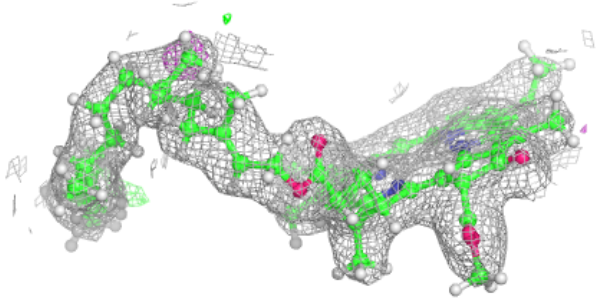


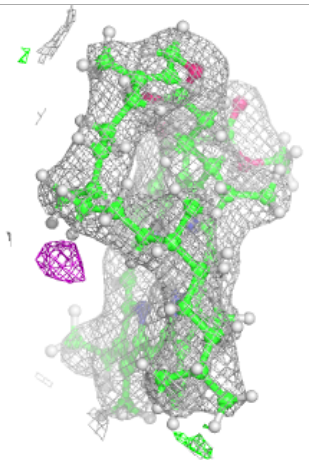


Electron density around PHO D 401:

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

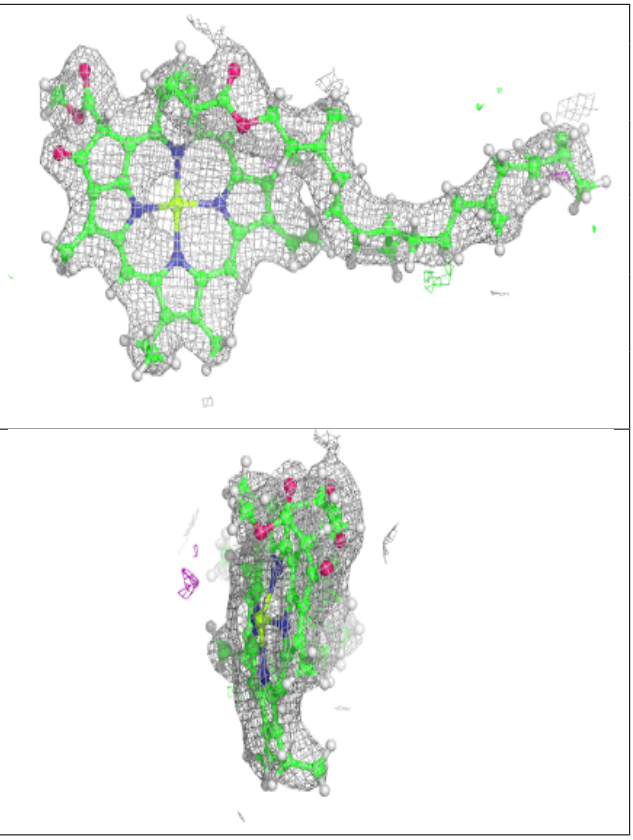






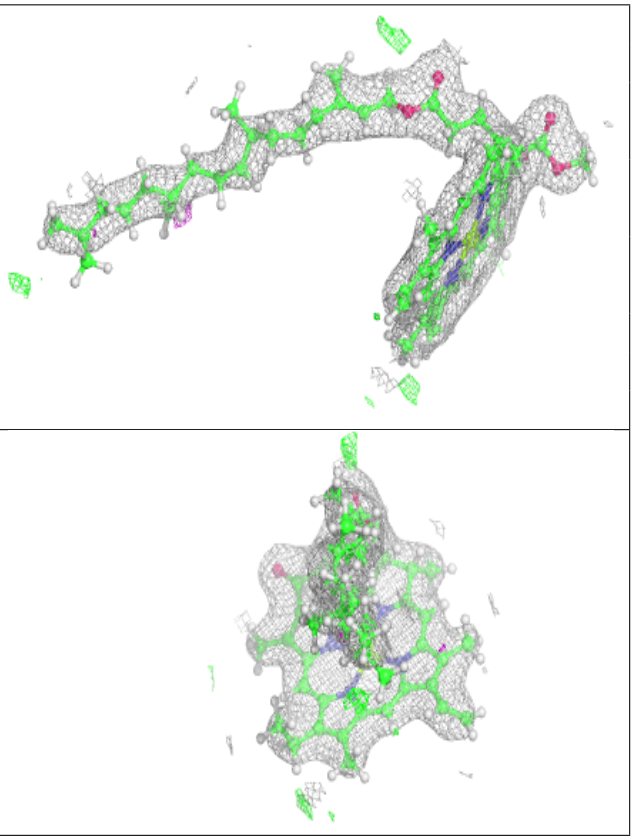
Electron density around CLA B 603:

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



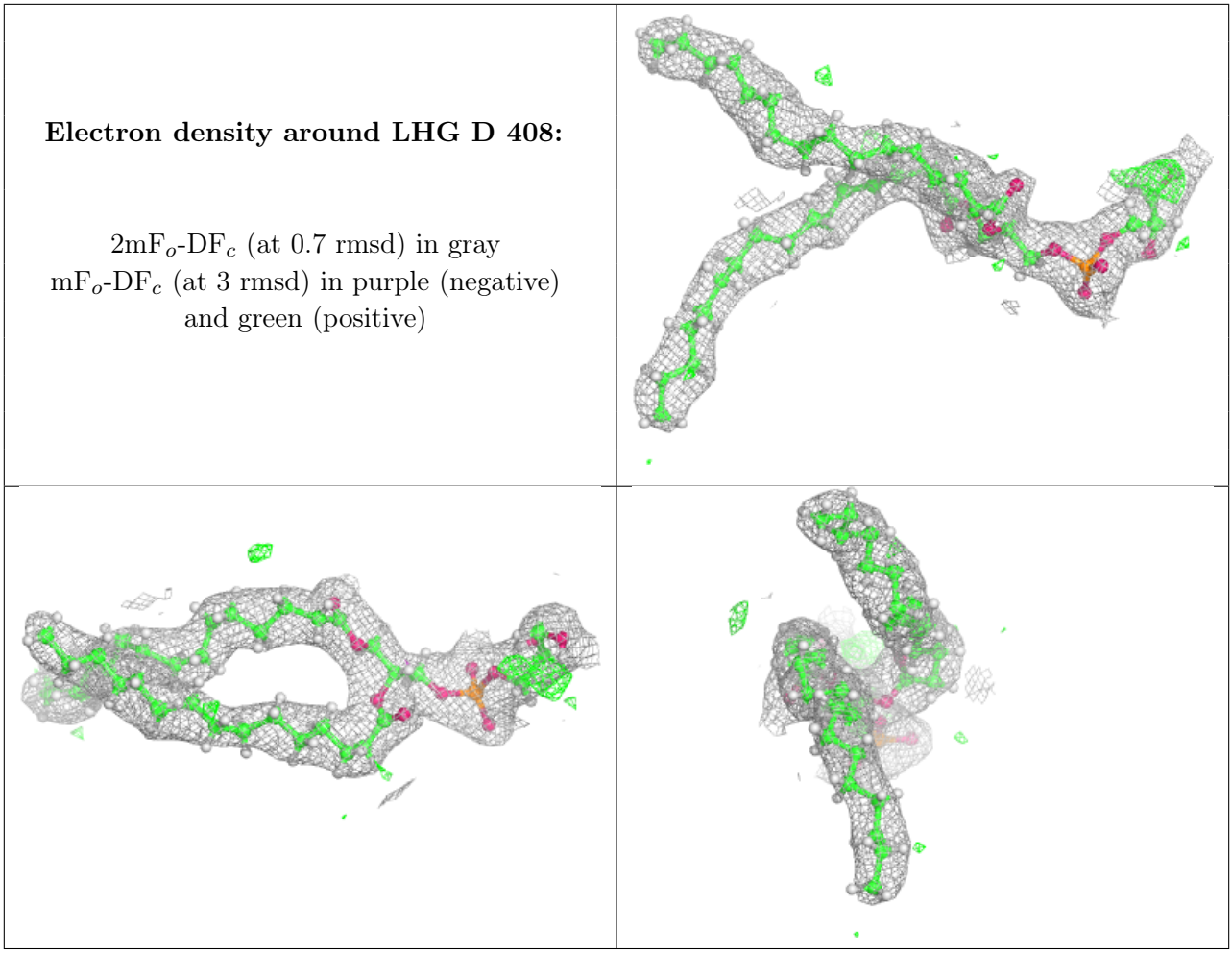
Electron density around CLA b 608:

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



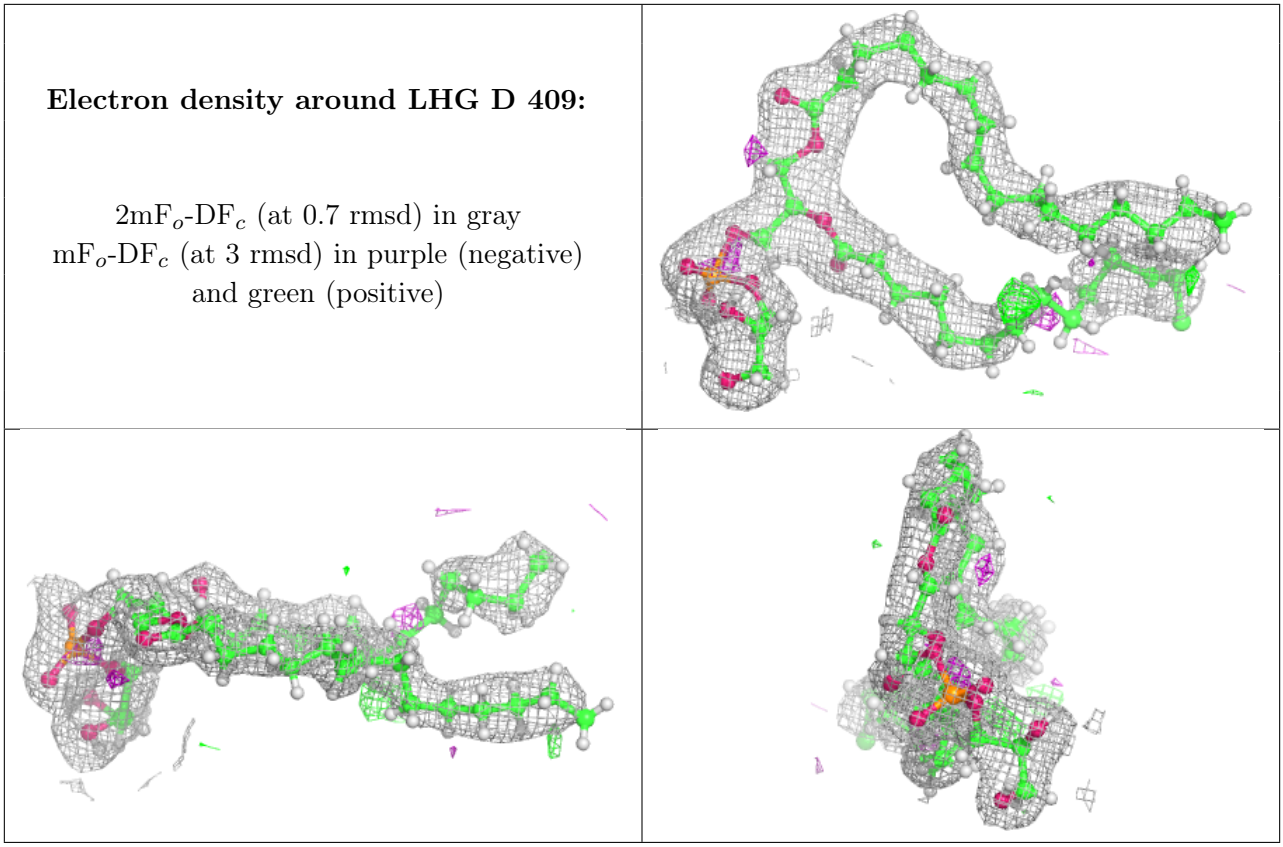
Electron density around LHG D 408:

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



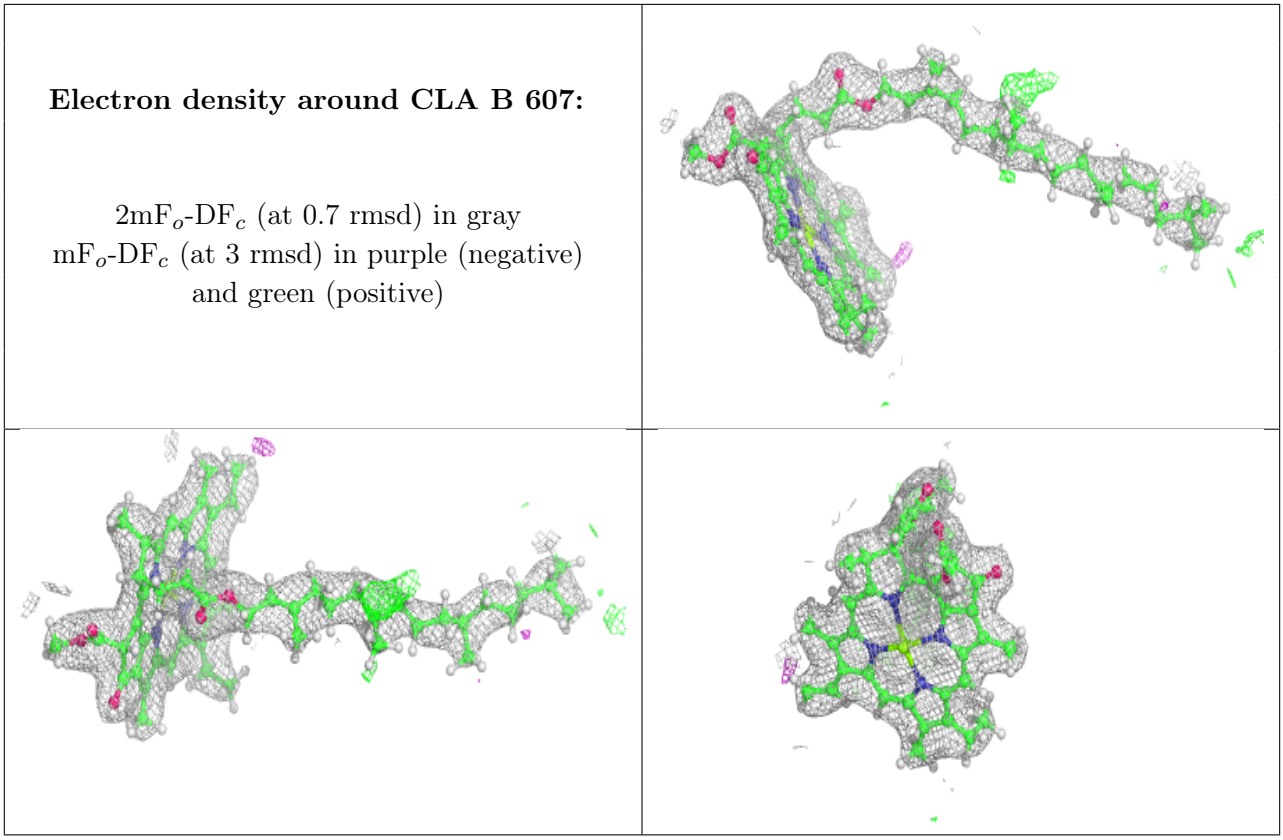
Electron density around LHG D 409:

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



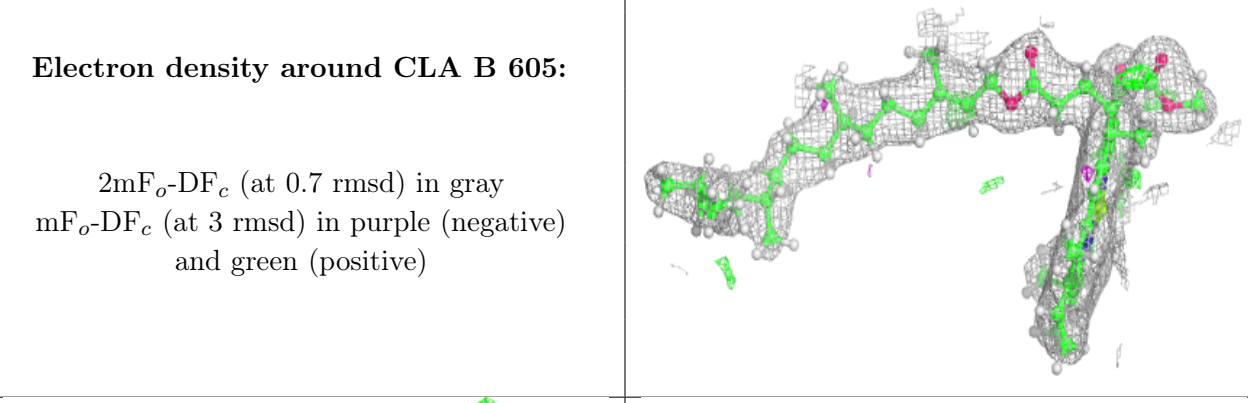
Electron density around CLA B 607:

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



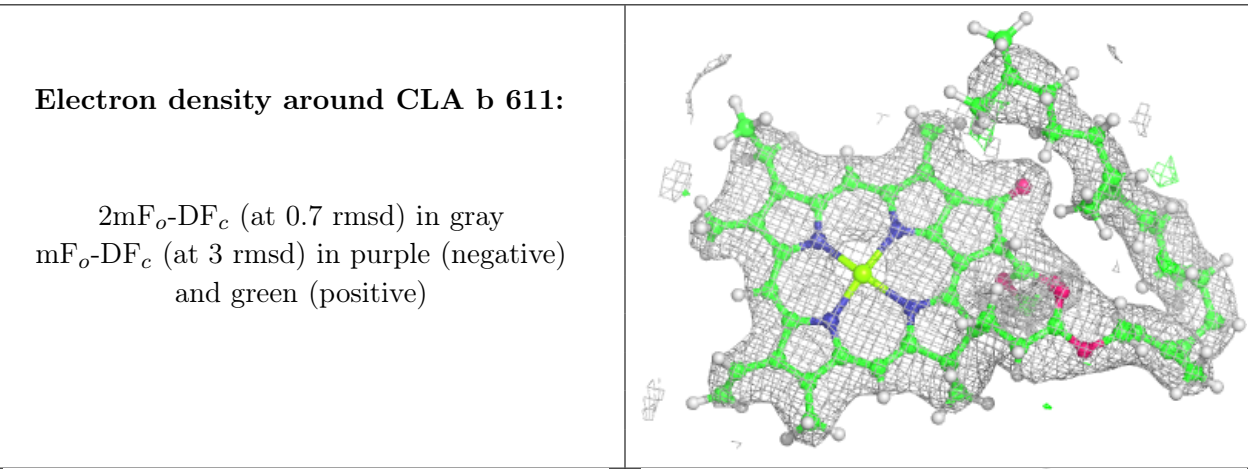
Electron density around CLA B 605:

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



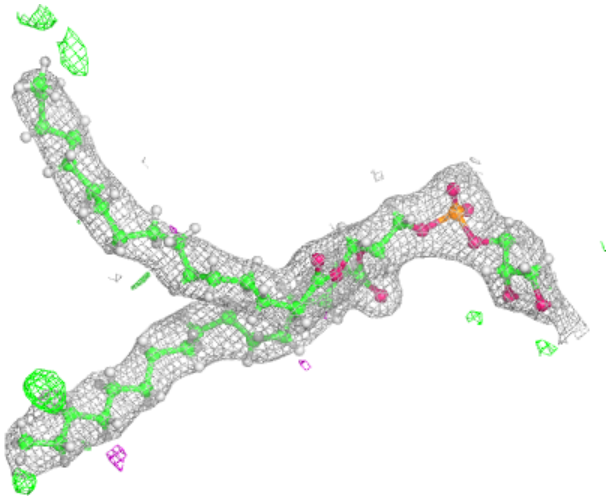
Electron density around CLA b 611:

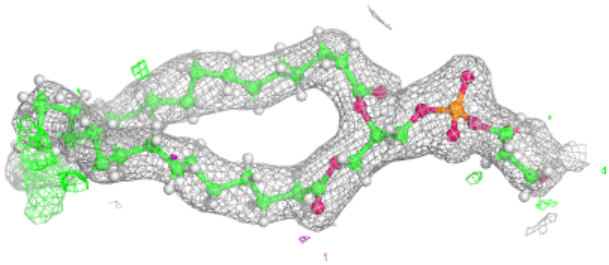
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

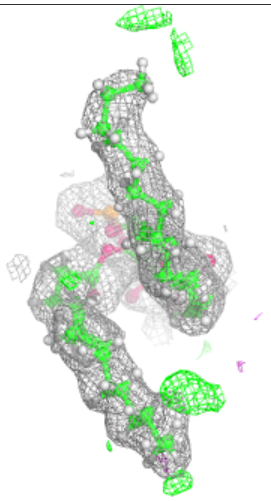


Electron density around LHG d 409:

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

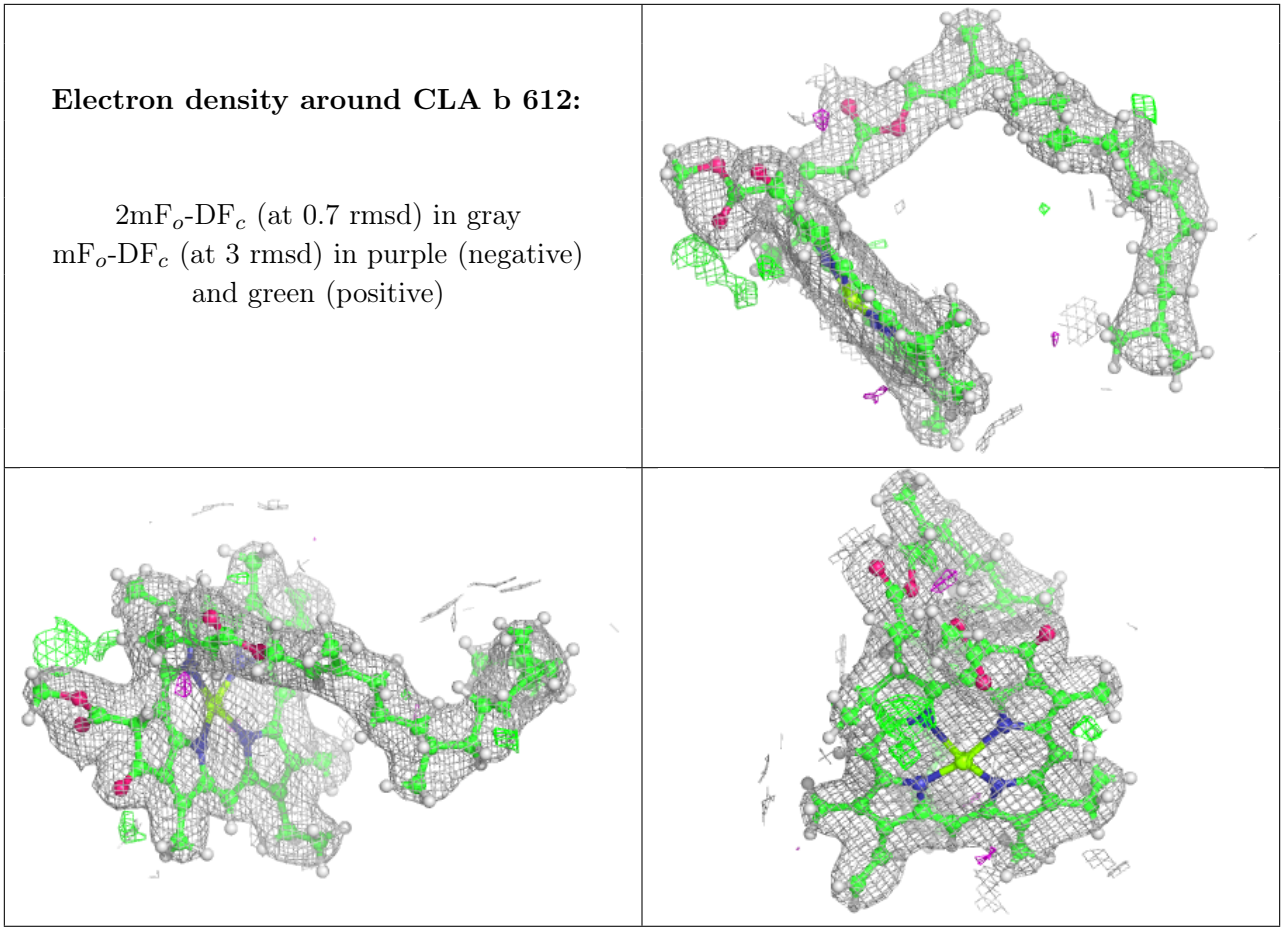






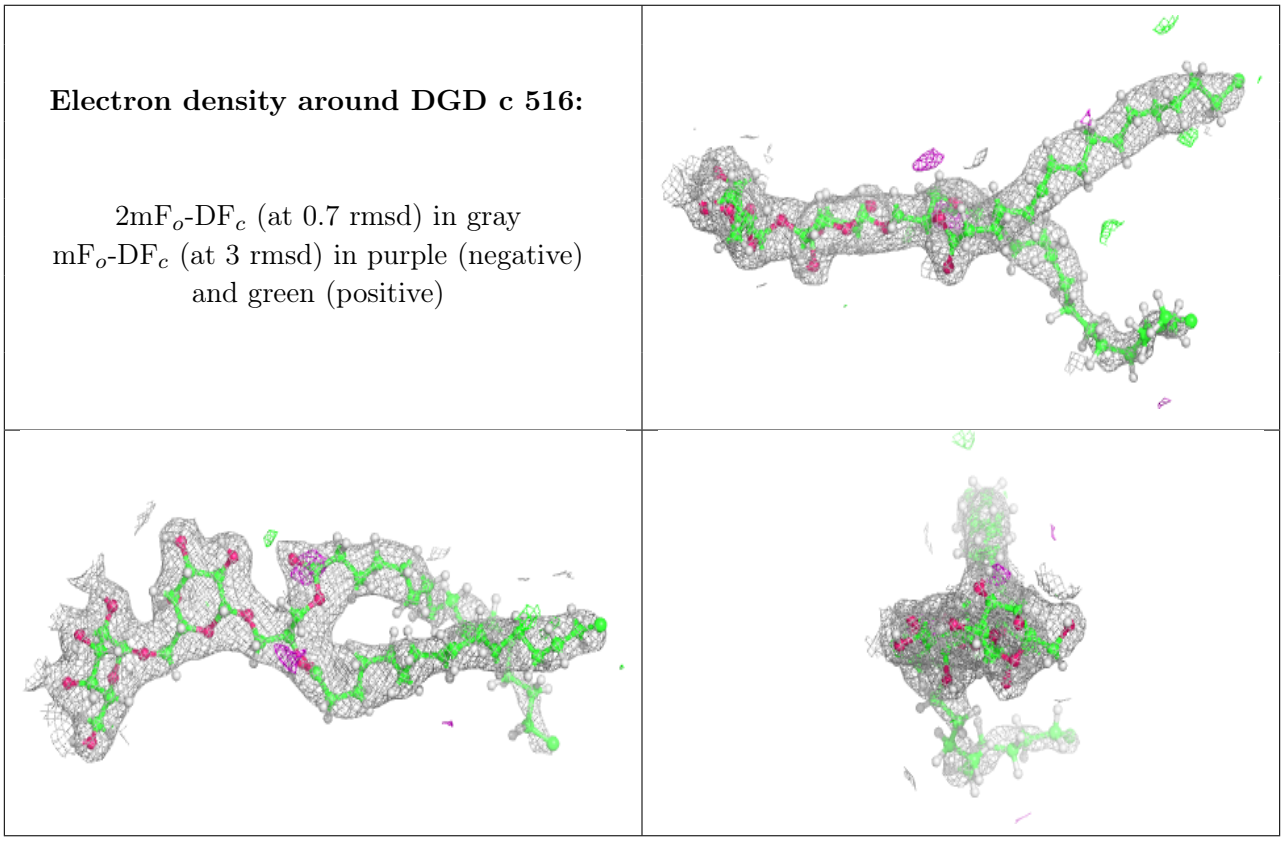
Electron density around CLA b 612:

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



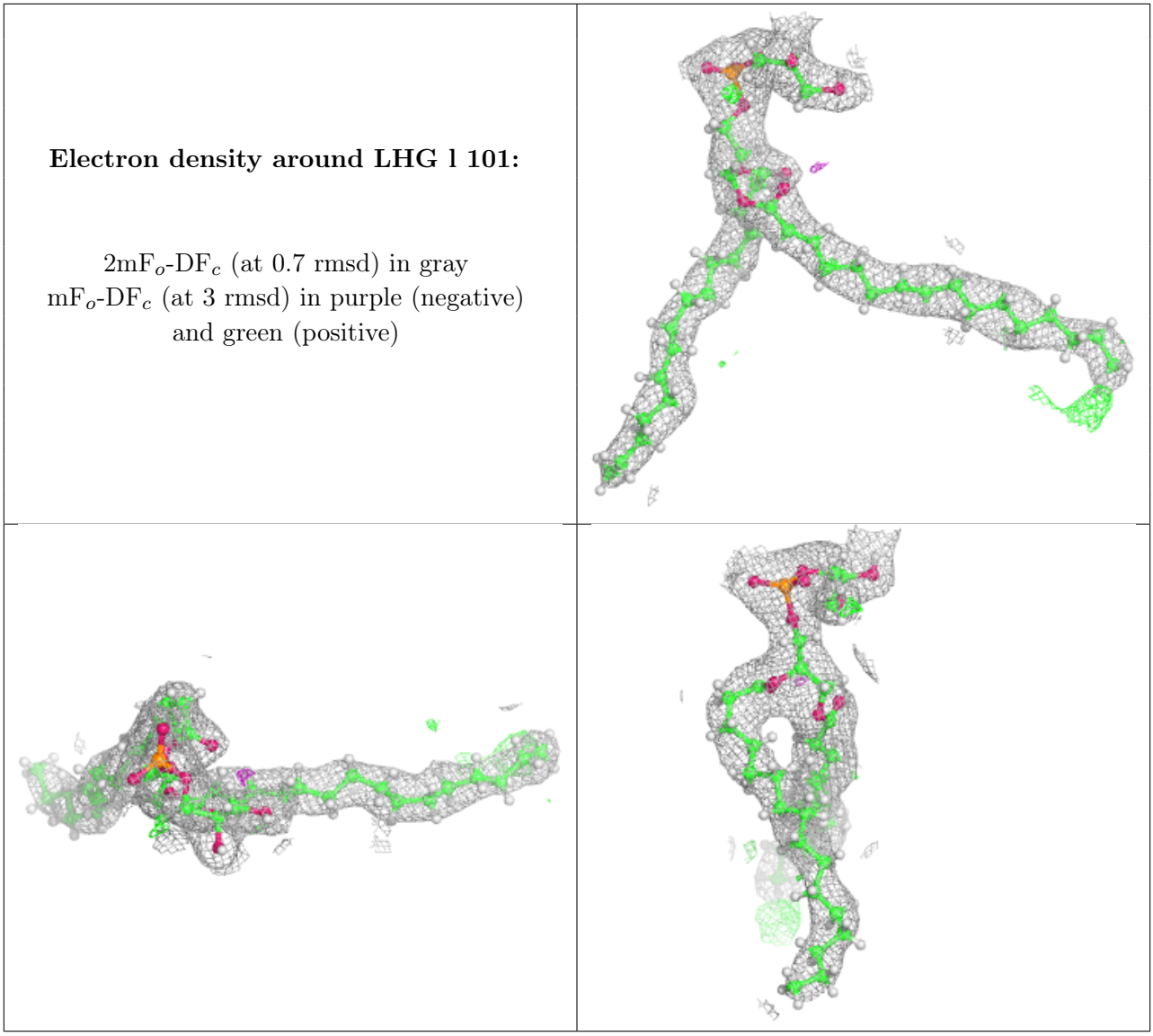
Electron density around DGD c 516:

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



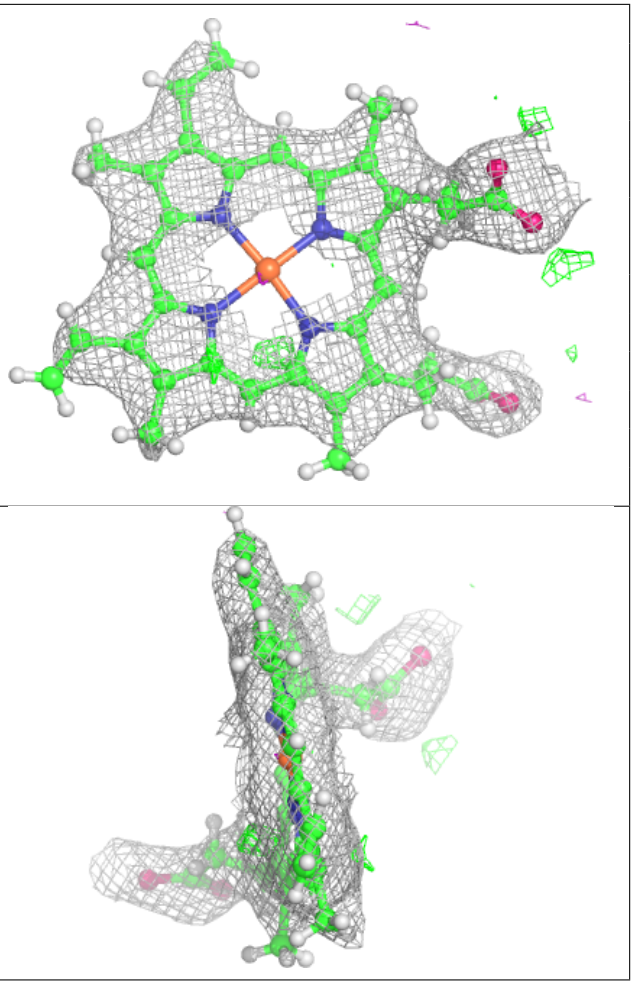
Electron density around LHG l 101:

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



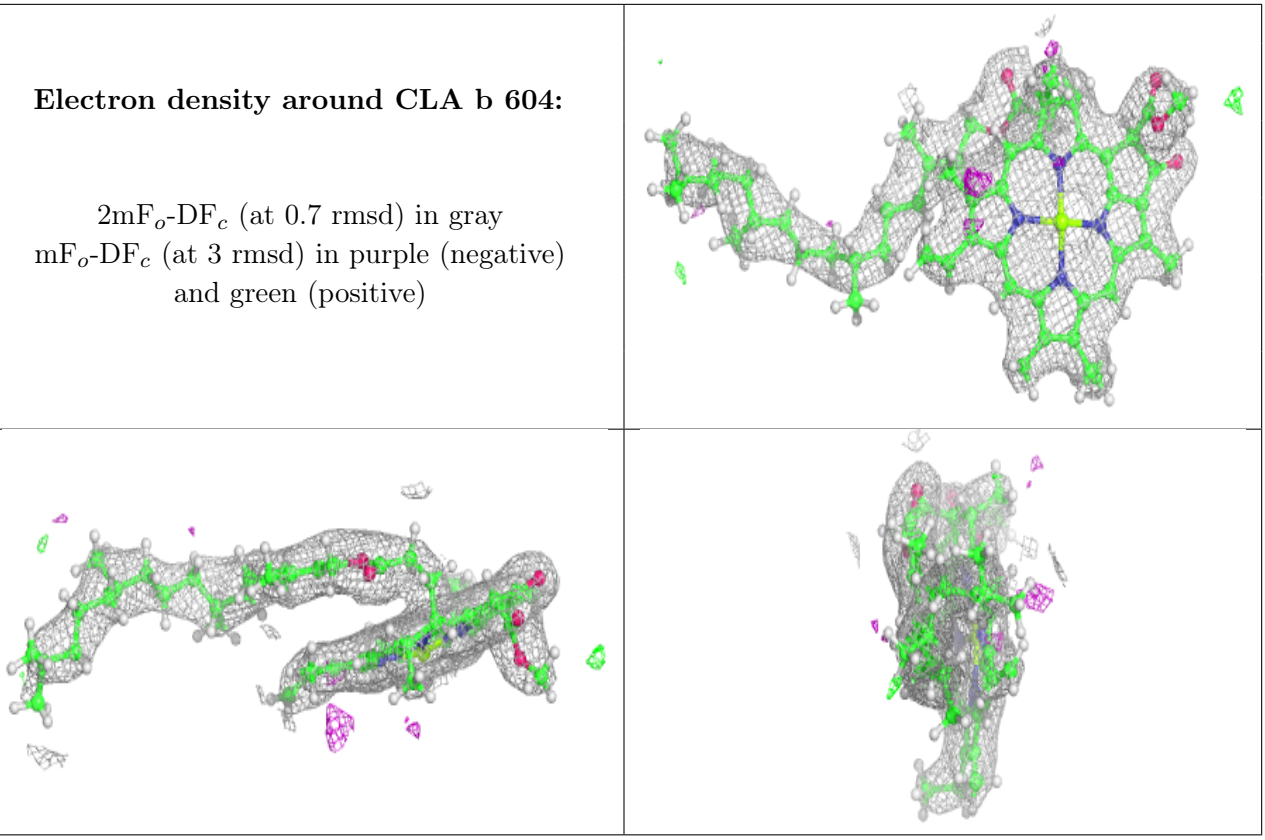
Electron density around HEM F 102:

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



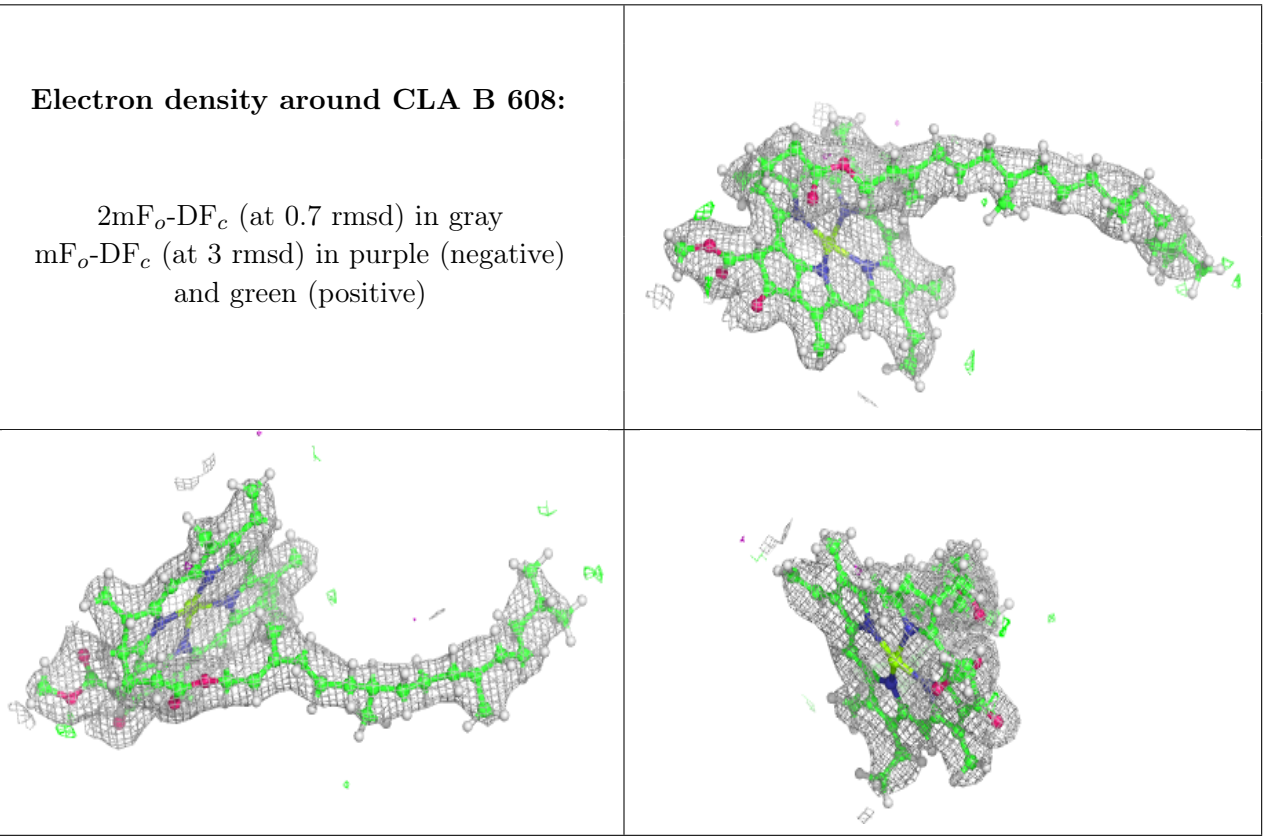
Electron density around CLA b 604:

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



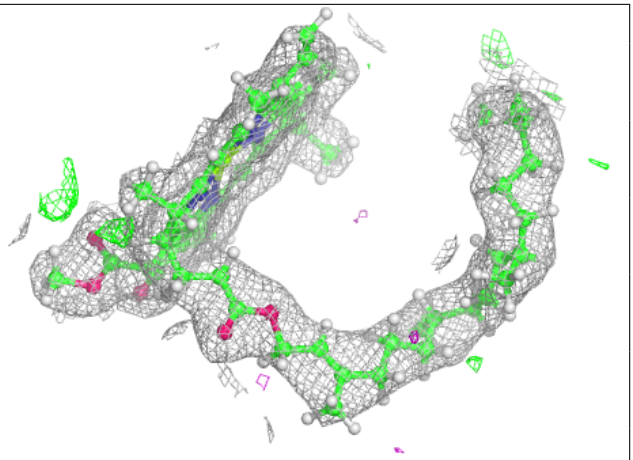
Electron density around CLA B 608:

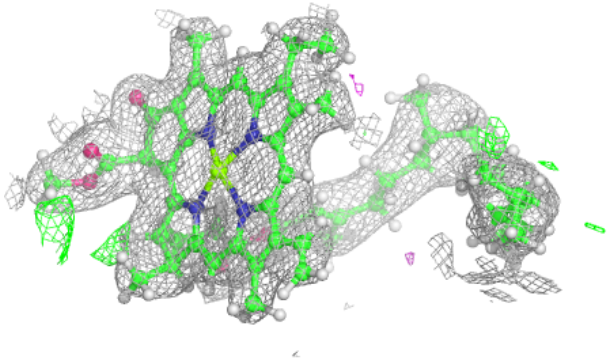
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

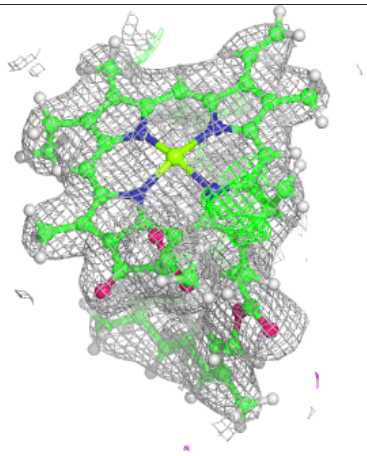


Electron density around CLA B 611:

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

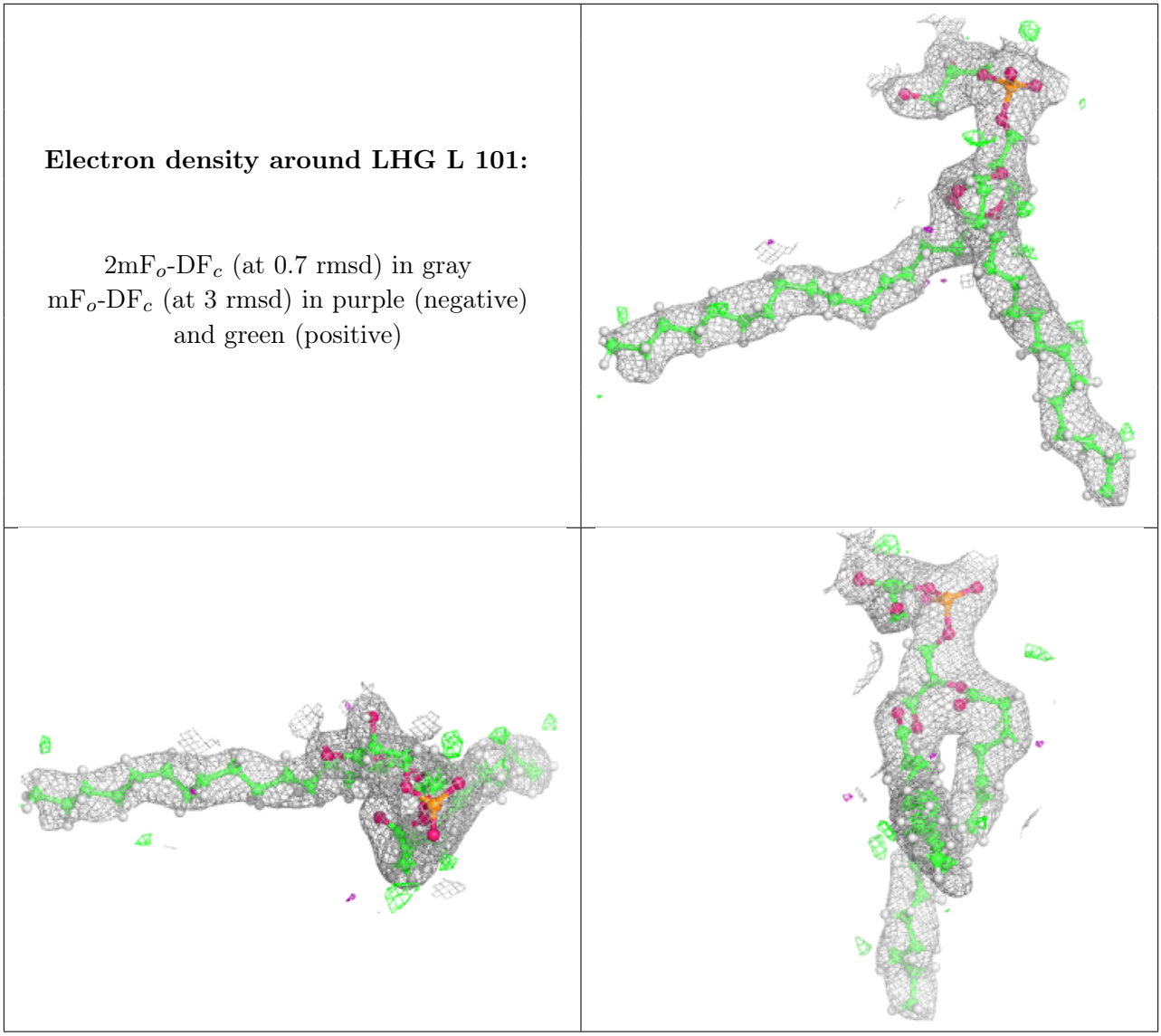






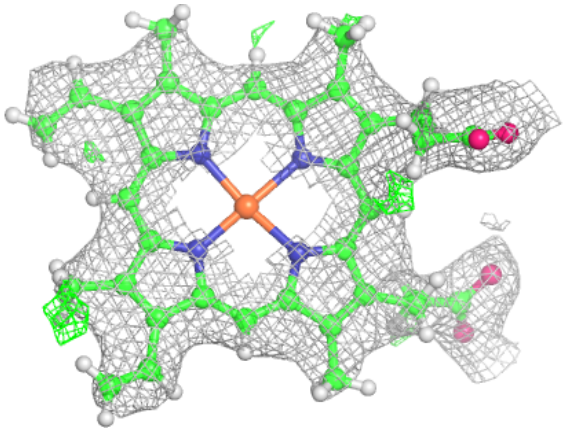
Electron density around LHG L 101:

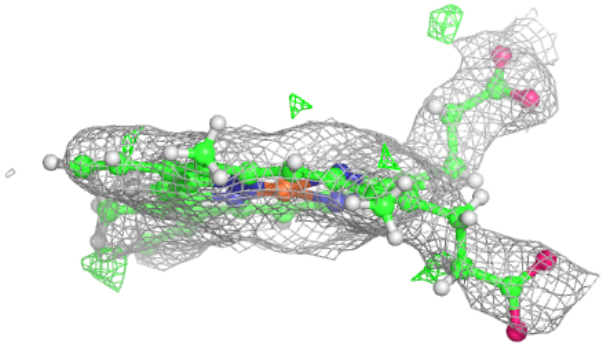
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

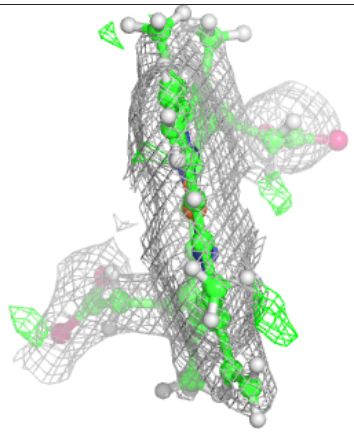


Electron density around HEM e 102:

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

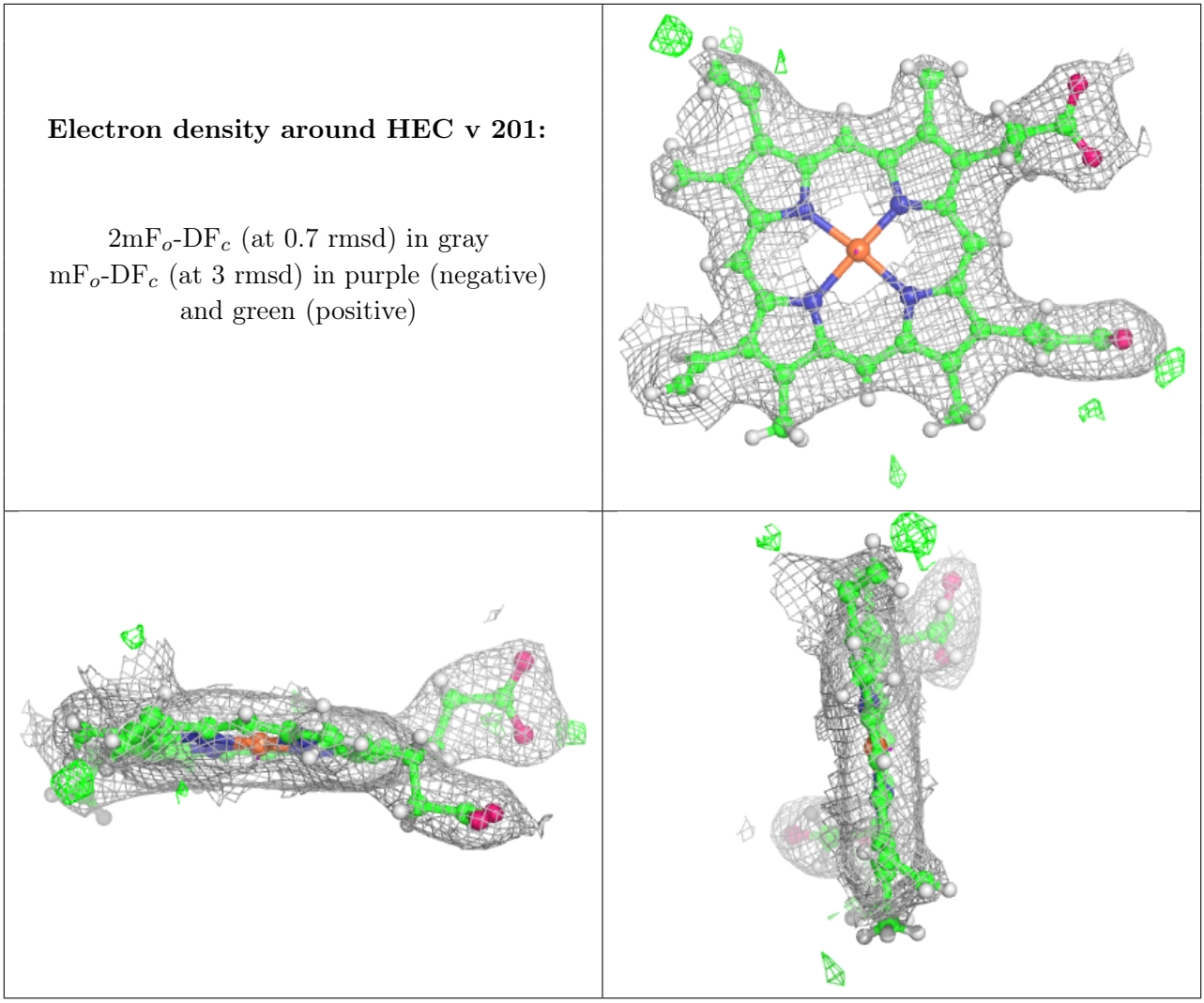






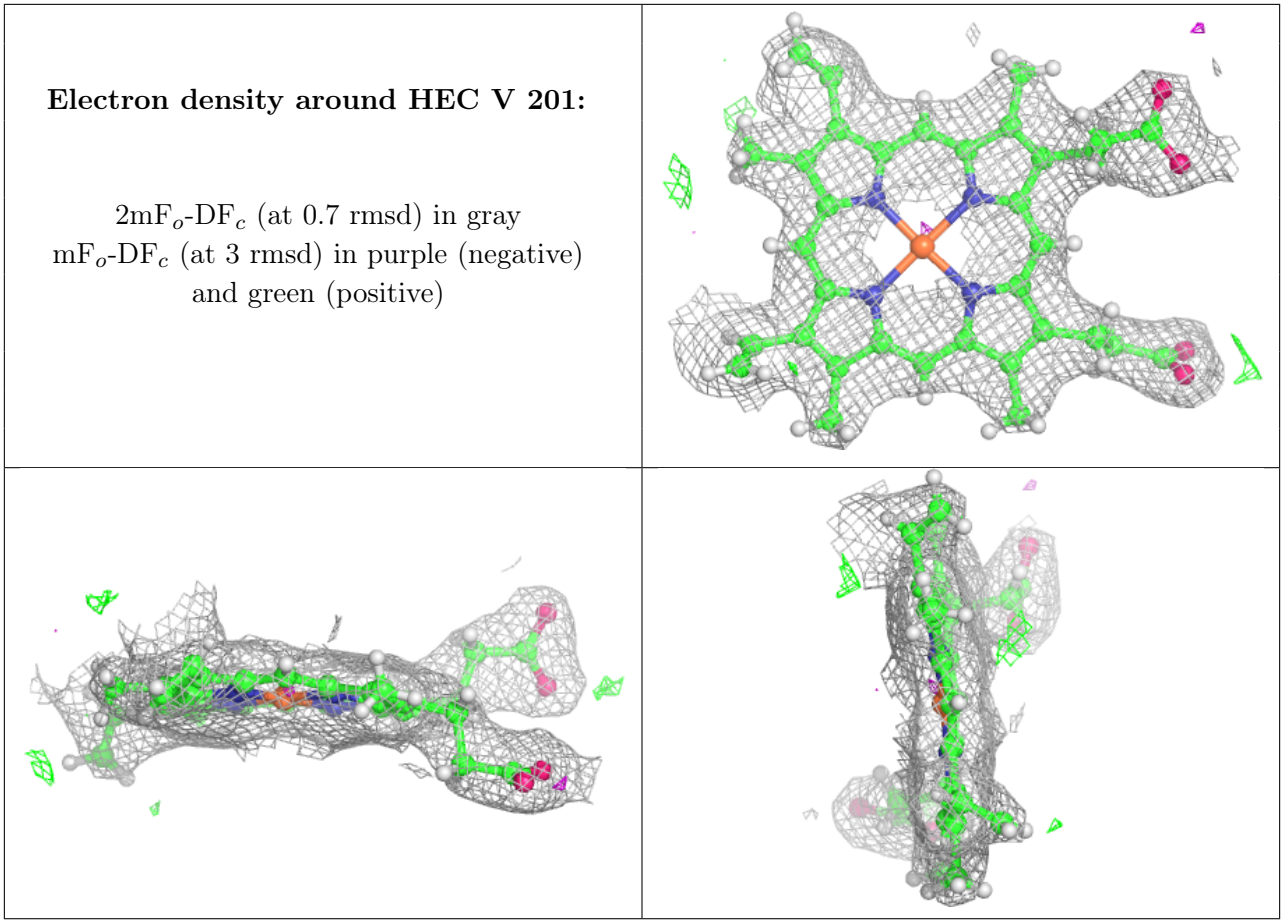
Electron density around HEC v 201:

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



Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.