wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 03:44 AM EDT

PDB ID	:	4PJ0
Title	:	Structure of T.elongatus Photosystem II, rows of dimers crystal packing
Authors	:	Hellmich, J.; Bommer, M.; Burkhardt, A.; Ibrahim, M.; Kern, J.; Meents, A.; Mueh, F.; Dobbek, H.; Zouni, A.
Deposited on	:	2014-05-10
Resolution	:	2.44 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:

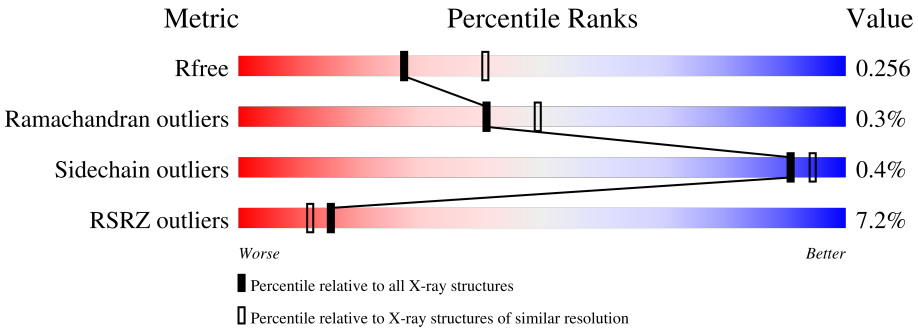
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.44 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	1564 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	344	3% 96%
1	a	344	% 97%
2	B	510	5% 98%
2	b	510	6% 98%
3	C	461	2% 97%
3	c	461	3% 97%

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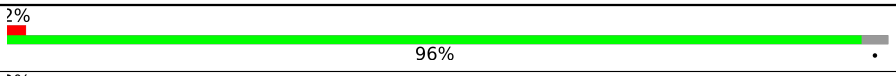
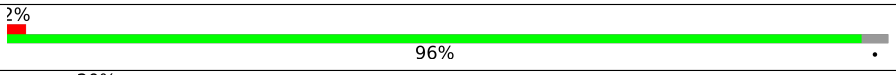
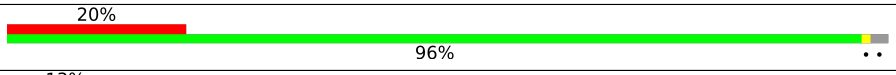
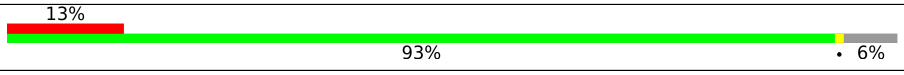
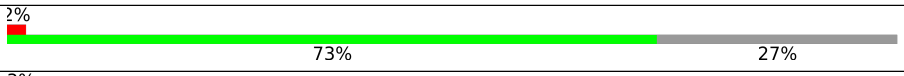
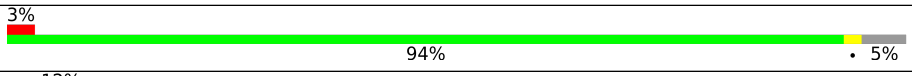
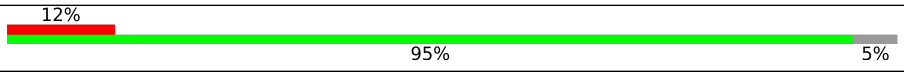
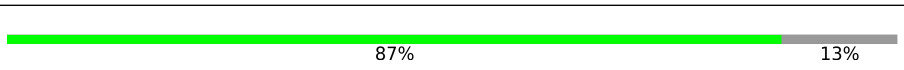
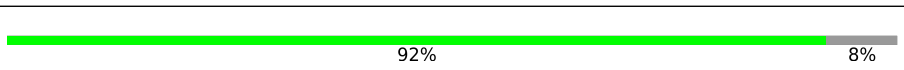
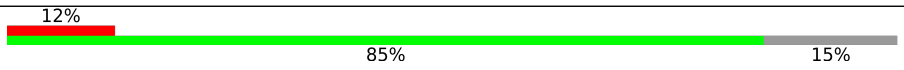
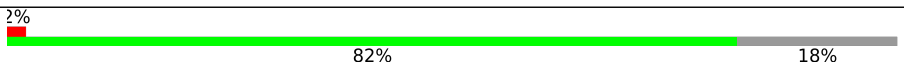
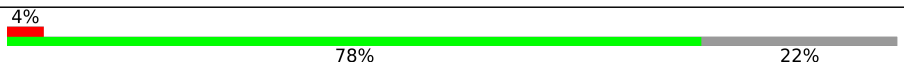
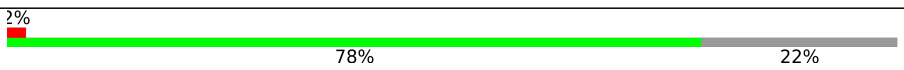
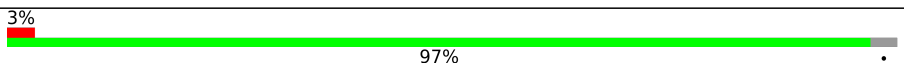
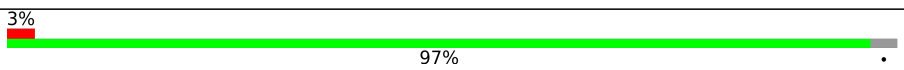
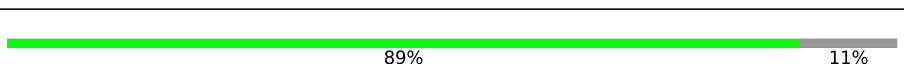
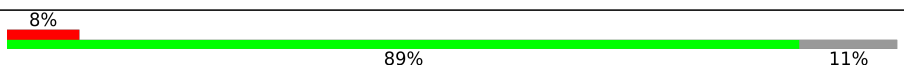
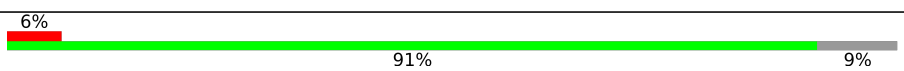
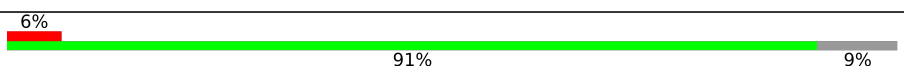
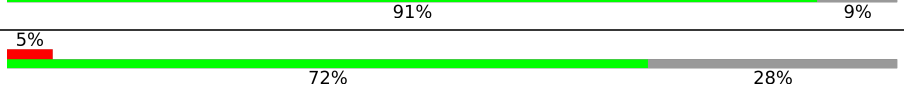
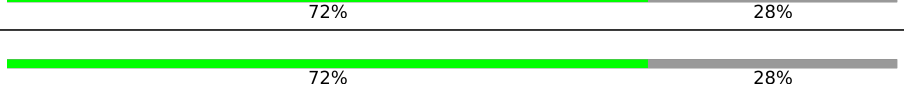
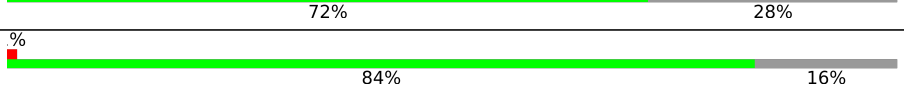
Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	

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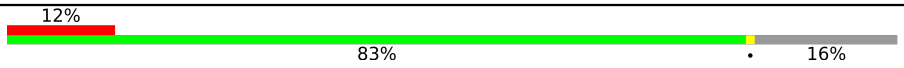
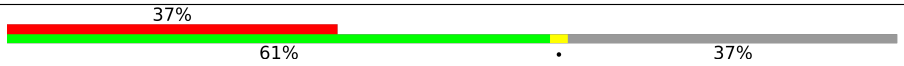
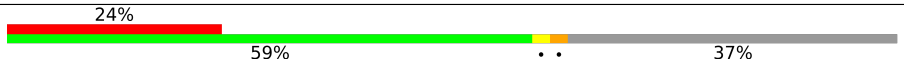
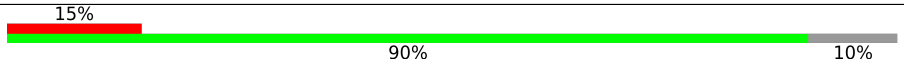
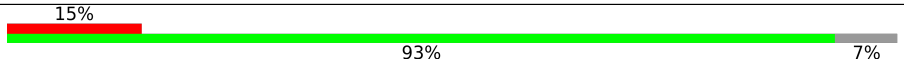
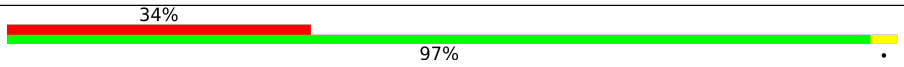
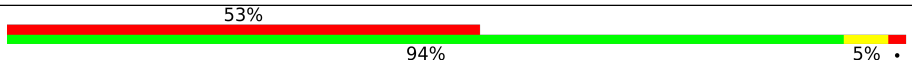
Mol	Chain	Length	Quality of chain
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 50236 atoms, of which 0 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total 661	C 431	N 107	O 123	0	0	0
5	e	79	Total 645	C 422	N 104	O 119	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total 269	C 184	N 44	O 40	S 1	0	0	0
6	f	33	Total 269	C 184	N 44	O 40	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total 498	C 333	N 80	O 83	S 2	0	0	0
7	h	63	Total 498	C 333	N 80	O 83	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	33	Total 266	C 183	N 39	O 43	S 1	0	0	0
8	i	35	Total 286	C 195	N 45	O 45	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total 249	C 170	N 38	O 40	S 1	0	0	0
9	j	33	Total 238	C 164	N 34	O 39	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total 284	C 198	N 41	O 45	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total 284	C 198	N 41	O 45	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total 296	C 197	N 47	O 52	0	0	0
11	l	36	Total 296	C 197	N 47	O 52	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total 249	C 167	N 36	O 45	S 1	0	0	0
12	m	32	Total 249	C 167	N 36	O 45	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total 1859	C 1162	N 314	O 379	S 4	0	0	0
13	o	243	Total 1865	C 1165	N 315	O 381	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total 249	C 176	N 35	O 36	S 2	0	0	0
14	t	29	Total 249	C 176	N 35	O 36	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total 765	C 486	N 128	O 151	0	0	0
15	u	96	Total 765	C 486	N 128	O 151	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

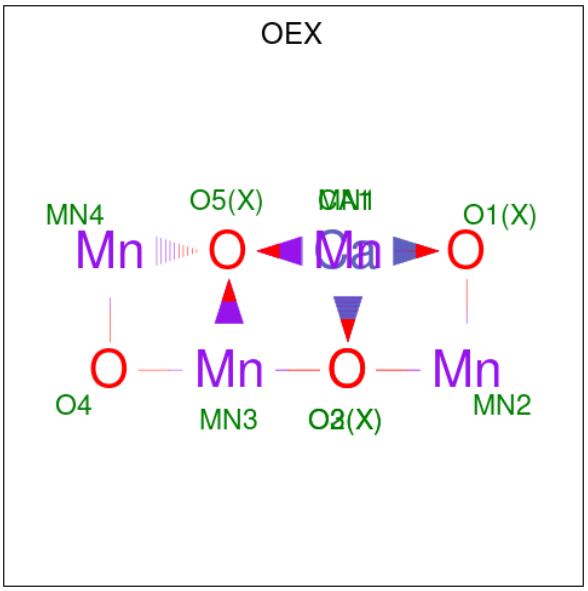
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	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	N	O	0	0	0
			273	186	47	40			
20	r	33	Total	C	N	O	0	0	0
			265	182	46	37			

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

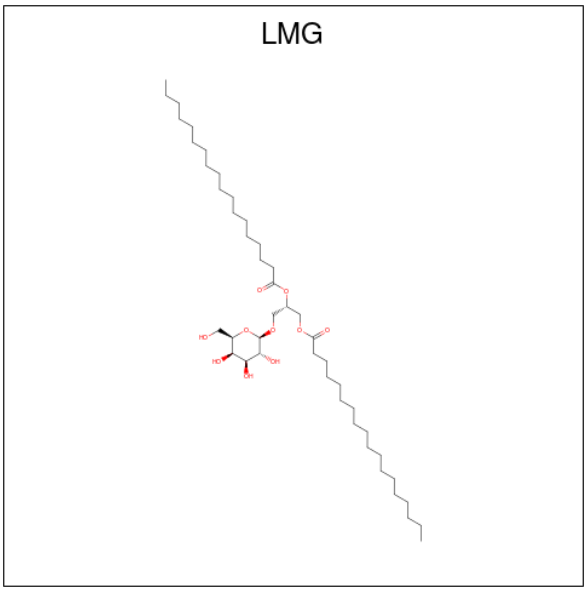


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 22 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

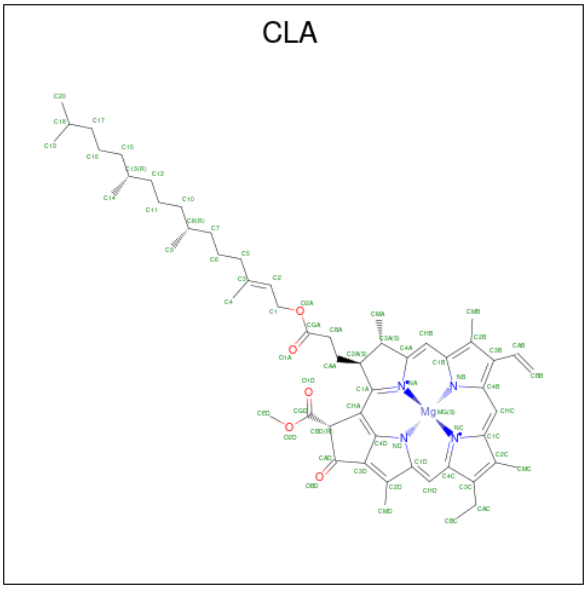


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 51 41 10	0	0
23	A	1	Total C O 51 41 10	0	0
23	B	1	Total C O 51 41 10	0	0
23	B	1	Total C O 51 41 10	0	0
23	C	1	Total C O 51 41 10	0	0
23	C	1	Total C O 51 41 10	0	0
23	D	1	Total C O 51 41 10	0	0
23	a	1	Total C O 51 41 10	0	0
23	a	1	Total C O 51 41 10	0	0
23	b	1	Total C O 51 41 10	0	0
23	b	1	Total C O 51 41 10	0	0
23	c	1	Total C O 51 41 10	0	0
23	c	1	Total C O 51 41 10	0	0
23	d	1	Total C O 51 41 10	0	0

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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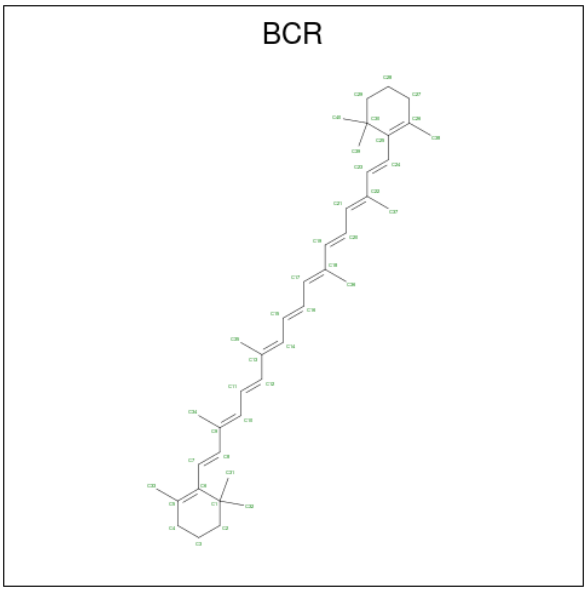
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- 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 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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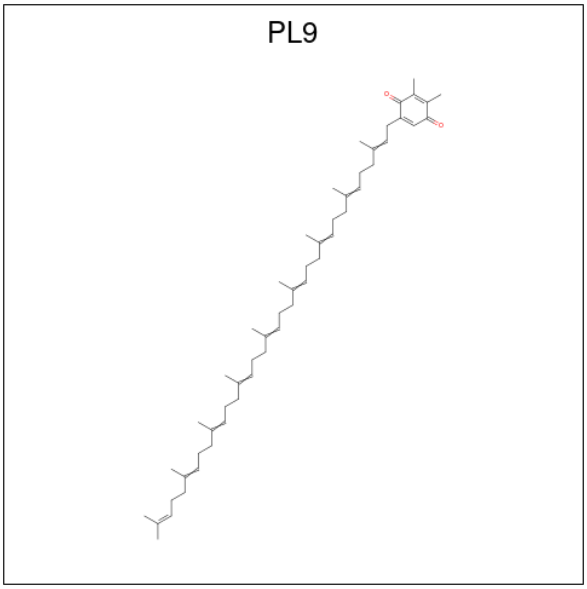
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

- 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 O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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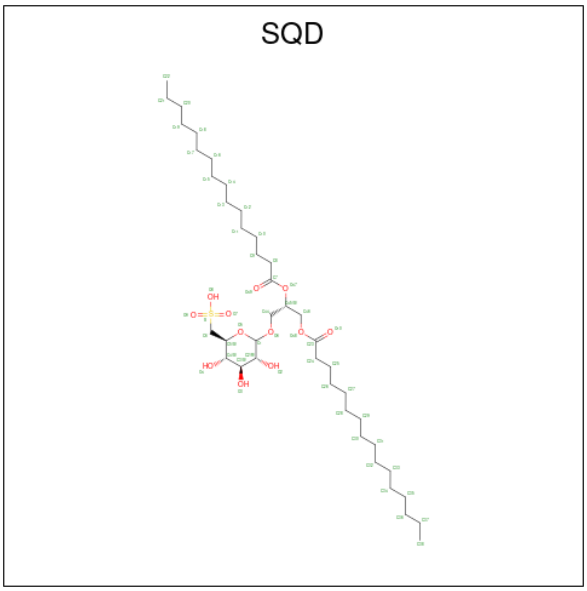
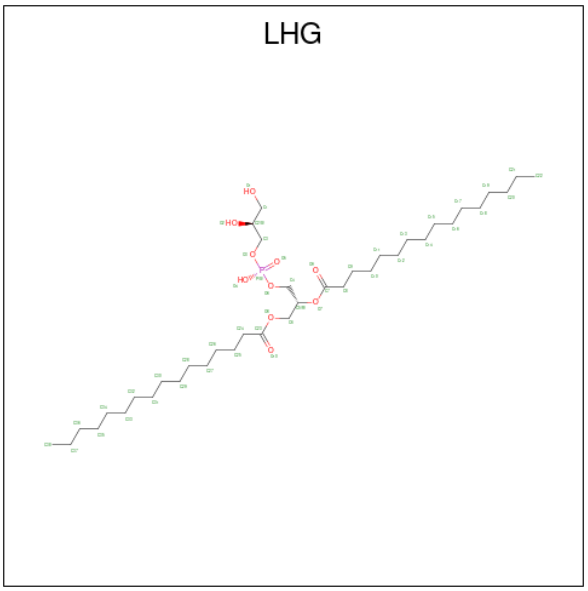
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

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



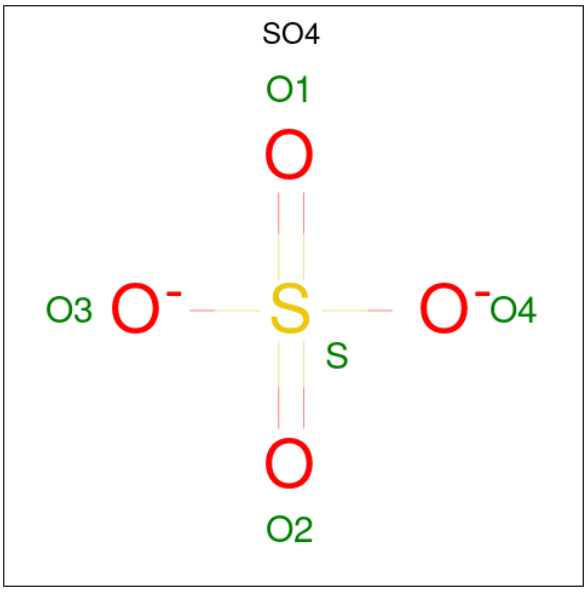
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 54 41 12 1	0	0
28	F	1	Total C O S 43 30 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	f	1	Total C O S 43 30 12 1	0	0

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



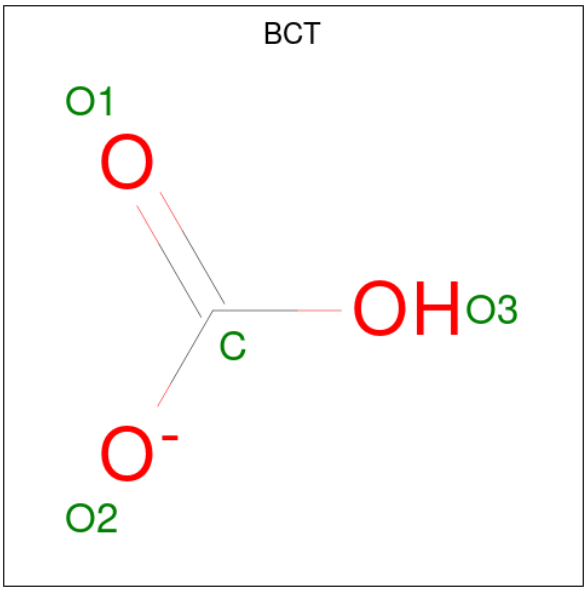
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			42	31	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total O S 5 4 1	0	0
30	O	1	Total O S 5 4 1	0	0
30	O	1	Total O S 5 4 1	0	0
30	U	1	Total O S 5 4 1	0	0
30	V	1	Total O S 5 4 1	0	0
30	a	1	Total O S 5 4 1	0	0
30	d	1	Total O S 5 4 1	0	0
30	o	1	Total O S 5 4 1	0	0
30	u	1	Total O S 5 4 1	0	0
30	u	1	Total O S 5 4 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 4 1 3	0	0
31	a	1	Total C O 4 1 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	6	Total C 68 68	0	0
32	C	1	Total C 15 15	0	0
32	D	1	Total C 15 15	0	0
32	I	1	Total C 14 14	0	0
32	J	1	Total C 11 11	0	0
32	M	2	Total C 26 26	0	0
32	T	2	Total C 27 27	0	0
32	X	1	Total C 10 10	0	0
32	b	5	Total C 60 60	0	0
32	c	1	Total C 15 15	0	0

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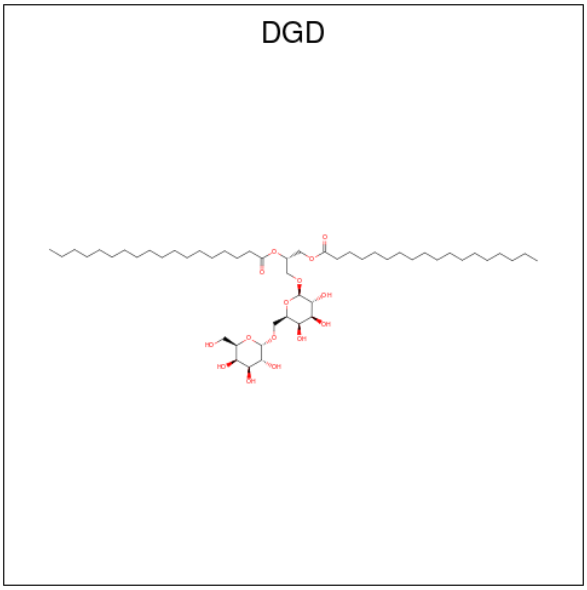
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	d	1	Total C 15 15	0	0
32	i	1	Total C 16 16	0	0
32	j	1	Total C 15 15	0	0
32	k	1	Total C 9 9	0	0
32	m	2	Total C 25 25	0	0
32	t	1	Total C 15 15	0	0
32	x	1	Total C 16 16	0	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0

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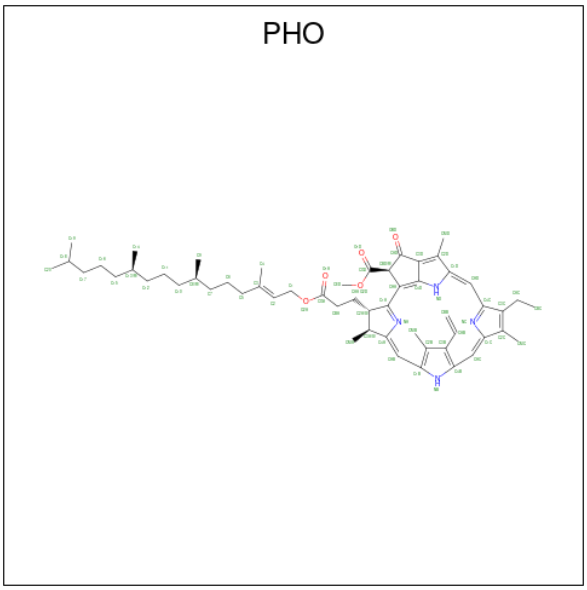
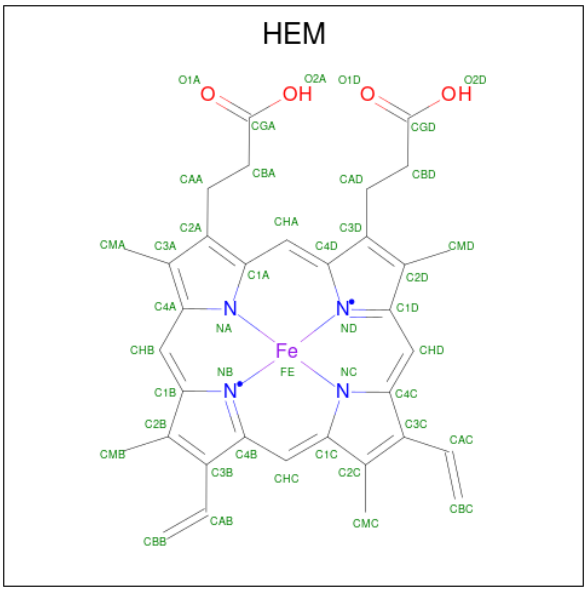
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	h	1	Total C O 62 47 15	0	0

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



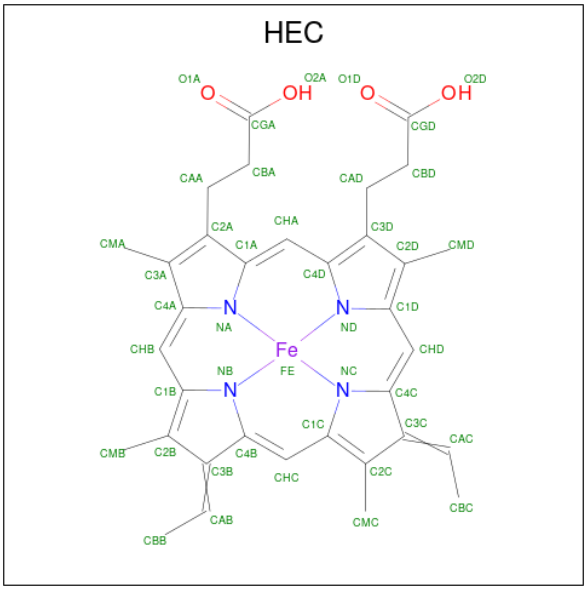
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	D	1	Total C N O 64 55 4 5	0	0
34	D	1	Total C N O 64 55 4 5	0	0
34	a	1	Total C N O 64 55 4 5	0	0
34	d	1	Total C N O 64 55 4 5	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
35	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
36	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	33	Total O 33 33	0	0
37	B	42	Total O 42 42	0	0
37	C	24	Total O 24 24	0	0
37	D	27	Total O 27 27	0	0
37	E	2	Total O 2 2	0	0
37	H	8	Total O 8 8	0	0
37	L	1	Total O 1 1	0	0
37	O	15	Total O 15 15	0	0
37	T	3	Total O 3 3	0	0
37	U	6	Total O 6 6	0	0
37	V	9	Total O 9 9	0	0
37	X	1	Total O 1 1	0	0
37	a	24	Total O 24 24	0	0
37	b	37	Total O 37 37	0	0
37	c	26	Total O 26 26	0	0
37	d	17	Total O 17 17	0	0
37	h	1	Total O 1 1	0	0
37	i	1	Total O 1 1	0	0
37	j	1	Total O 1 1	0	0
37	l	3	Total O 3 3	0	0
37	m	1	Total O 1 1	0	0

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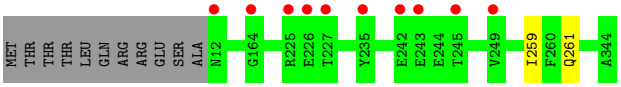
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	o	11	Total O 11 11	0	0
37	t	1	Total O 1 1	0	0
37	u	7	Total O 7 7	0	0
37	v	3	Total O 3 3	0	0

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.

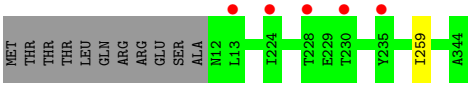
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



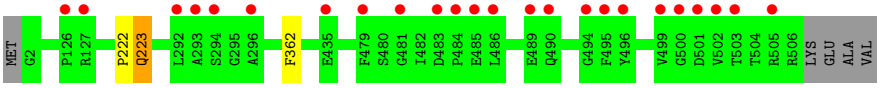
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



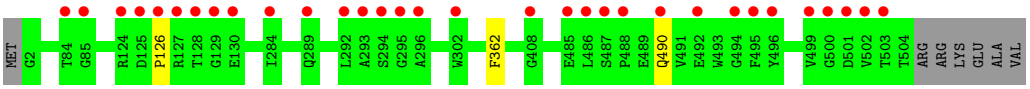
• Molecule 2: CP47 protein

Chain B:



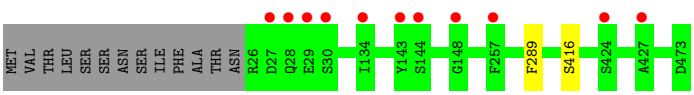
• Molecule 2: CP47 protein

Chain b:



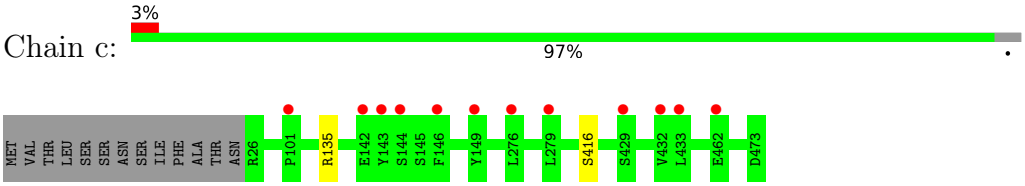
• Molecule 3: Photosystem II CP43 protein

Chain C:



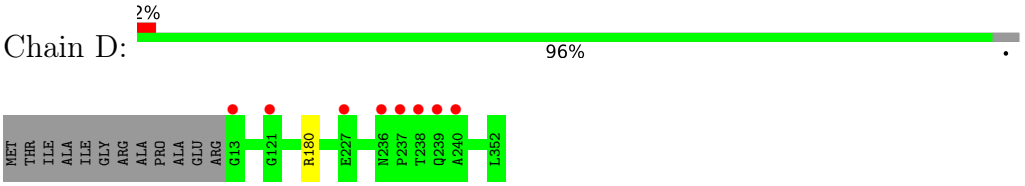
• Molecule 3: Photosystem II CP43 protein

Chain c:



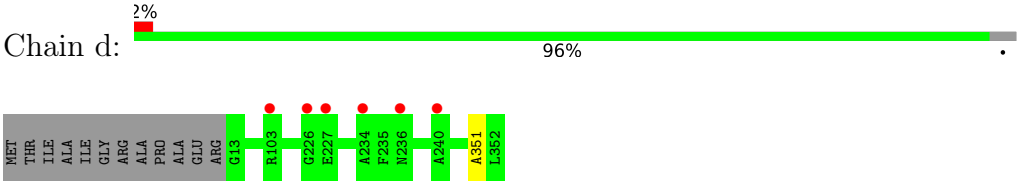
• Molecule 4: Photosystem II D2 protein

Chain D:



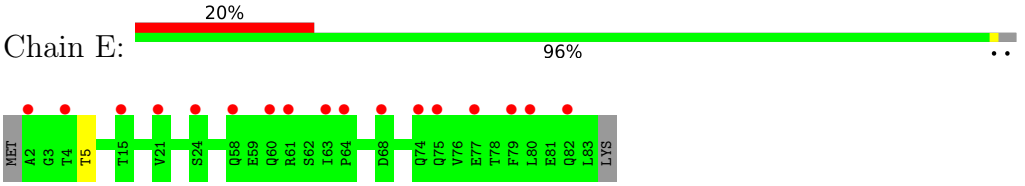
• Molecule 4: Photosystem II D2 protein

Chain d:



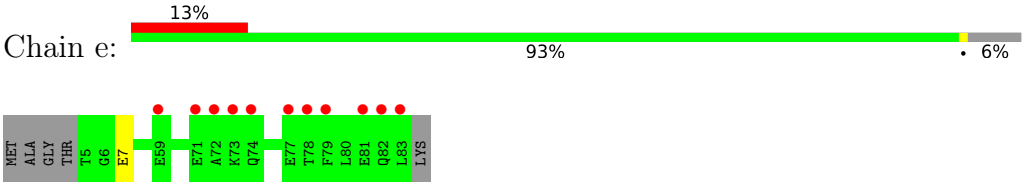
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



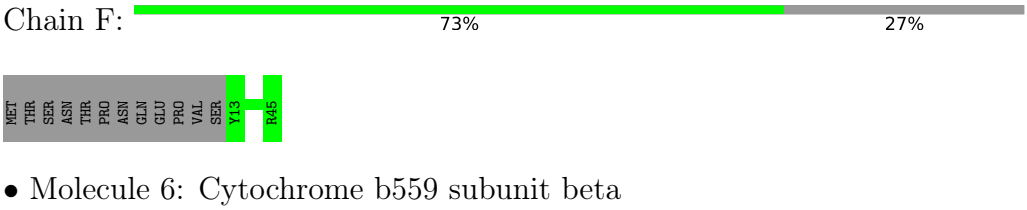
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



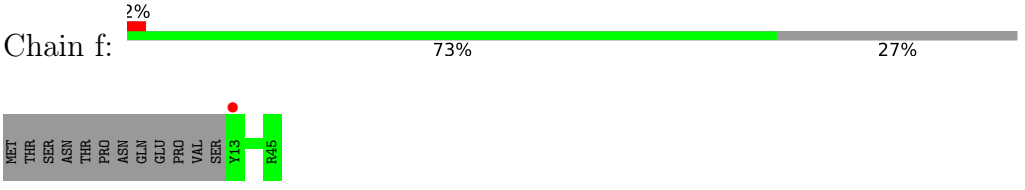
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



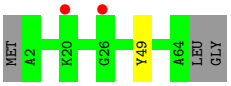
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



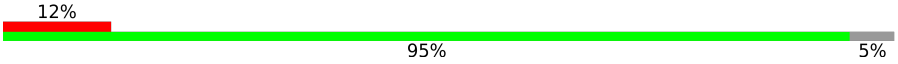
• Molecule 7: Photosystem II reaction center protein H

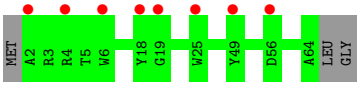
Chain H:



• Molecule 7: Photosystem II reaction center protein H

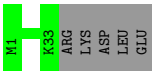
Chain h:





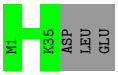
• Molecule 8: Photosystem II reaction center protein I

Chain I:



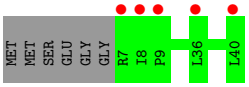
• Molecule 8: Photosystem II reaction center protein I

Chain i:



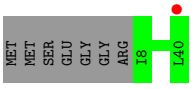
• Molecule 9: Photosystem II reaction center protein J

Chain J:



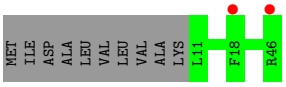
• Molecule 9: Photosystem II reaction center protein J

Chain j:



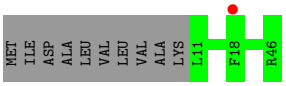
• Molecule 10: Photosystem II reaction center protein K

Chain K:



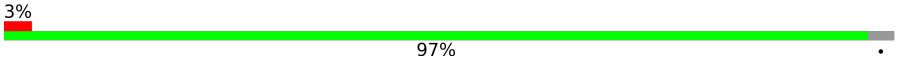
• Molecule 10: Photosystem II reaction center protein K

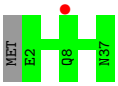
Chain k:



• Molecule 11: Photosystem II reaction center protein L

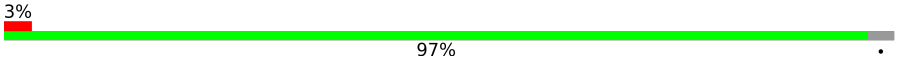
Chain L:





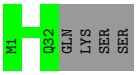
• Molecule 11: Photosystem II reaction center protein L

Chain l:



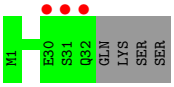
• Molecule 12: Photosystem II reaction center protein M

Chain M:



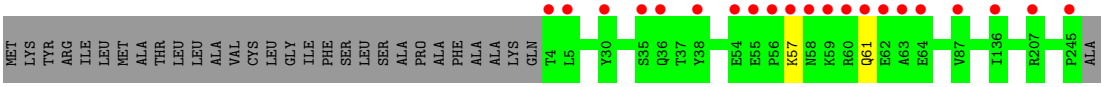
• Molecule 12: Photosystem II reaction center protein M

Chain m:



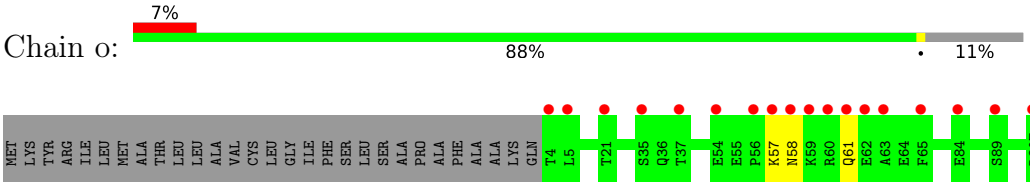
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



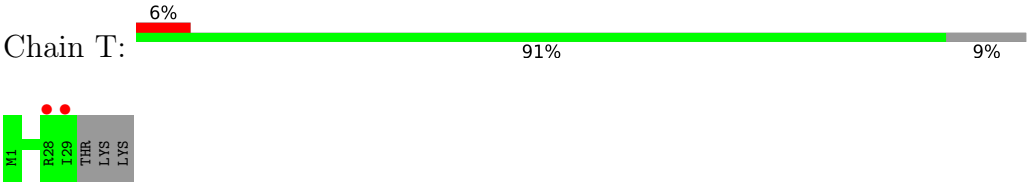
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



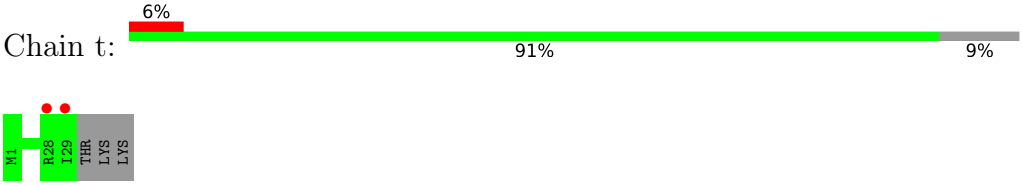
• Molecule 14: Photosystem II reaction center protein T

Chain T:



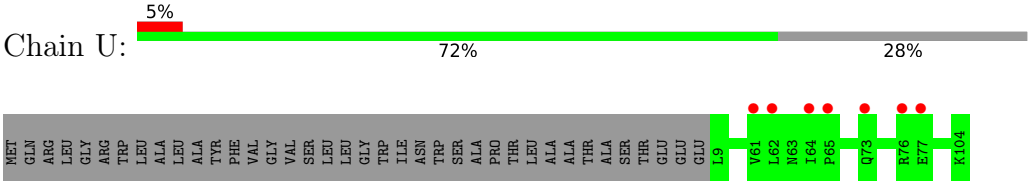
• Molecule 14: Photosystem II reaction center protein T

Chain t:



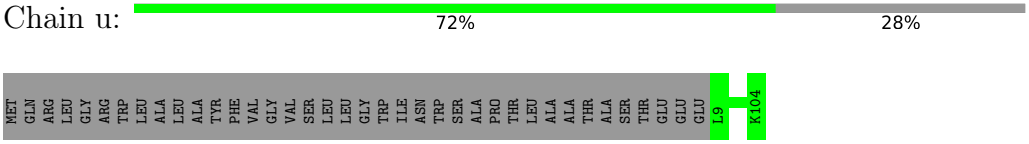
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



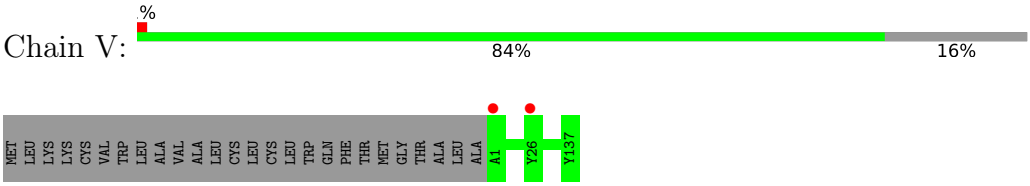
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



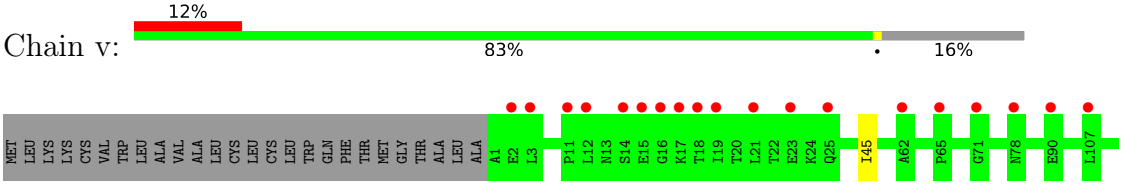
• Molecule 16: Cytochrome c-550

Chain V:



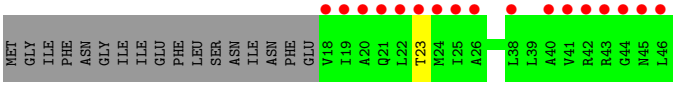
• Molecule 16: Cytochrome c-550

Chain v:



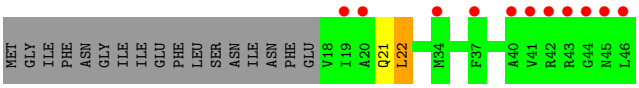
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



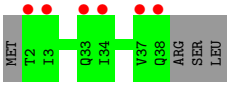
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



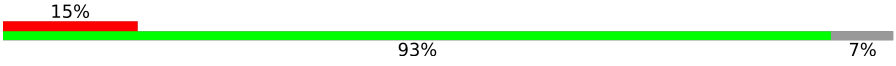
• Molecule 18: Photosystem II reaction center X protein

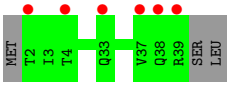
Chain X:



• Molecule 18: Photosystem II reaction center X protein

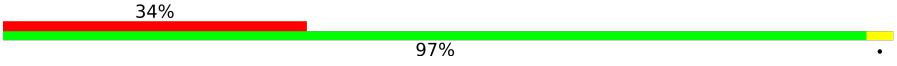
Chain x:

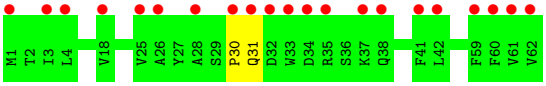




• Molecule 19: Photosystem II reaction center protein Z

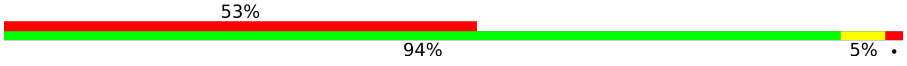
Chain Z:

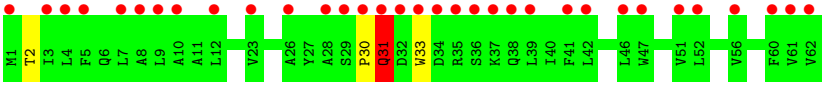




• Molecule 19: Photosystem II reaction center protein Z

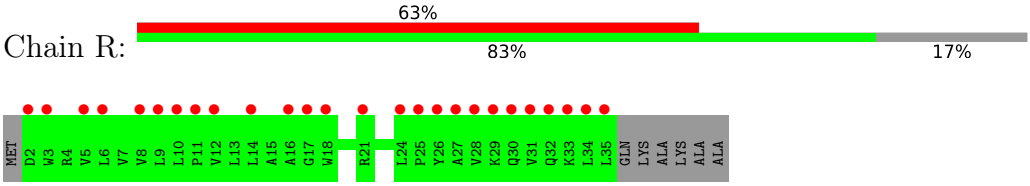
Chain z:





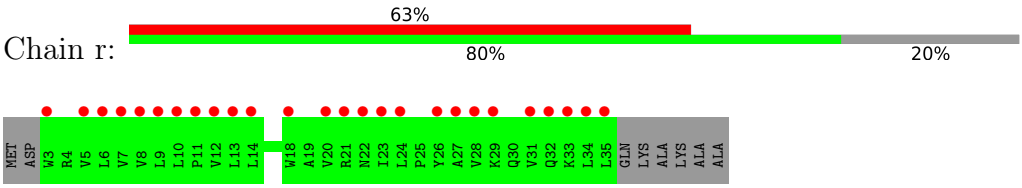
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.45Å 218.89Å 302.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.44 49.12 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.12-2.44) 98.4 (49.12-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.216 , 0.256 0.218 , 0.256	Depositor DCC
R_{free} test set	14111 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	50236	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, PHO, OEX, DGD, LHG, CL, PL9, HEM, SQD, LMG, BCR, SO4, HEC, FE, BCT, CLA

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	0.22	0/2702	0.39	0/3685
1	a	0.22	0/2702	0.37	0/3685
2	B	0.23	0/4120	0.38	1/5614 (0.0%)
2	b	0.22	0/4098	0.38	0/5586
3	C	0.21	0/3579	0.35	0/4872
3	c	0.21	0/3579	0.38	0/4872
4	D	0.22	0/2801	0.37	0/3818
4	d	0.22	0/2801	0.37	0/3818
5	E	0.21	0/680	0.39	0/929
5	e	0.21	0/664	0.38	0/907
6	F	0.22	0/278	0.38	0/379
6	f	0.22	0/278	0.39	0/379
7	H	0.22	0/511	0.37	0/697
7	h	0.22	0/511	0.38	0/697
8	I	0.23	0/273	0.37	0/370
8	i	0.23	0/293	0.39	0/395
9	J	0.20	0/255	0.33	0/346
9	j	0.21	0/244	0.36	0/332
10	K	0.30	0/294	0.55	0/405
10	k	0.23	0/294	0.40	0/405
11	L	0.22	0/303	0.34	0/412
11	l	0.22	0/303	0.35	0/412
12	M	0.22	0/252	0.40	0/344
12	m	0.22	0/252	0.39	0/344
13	O	0.21	0/1890	0.39	0/2564
13	o	0.22	0/1896	0.43	0/2571
14	T	0.24	0/258	0.37	0/349
14	t	0.24	0/258	0.37	0/349
15	U	0.20	0/776	0.36	0/1052
15	u	0.21	0/776	0.36	0/1052
16	V	0.20	0/1085	0.38	0/1473
16	v	0.20	0/1085	0.38	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.20	0/216	0.39	0/289
17	y	0.21	0/216	0.63	1/289 (0.3%)
18	X	0.21	0/273	0.34	0/370
18	x	0.21	0/284	0.35	0/384
19	Z	0.22	0/490	0.40	0/669
19	z	0.43	0/490	0.62	0/669
20	R	0.20	0/279	0.37	0/383
20	r	0.21	0/271	0.46	0/372
All	All	0.22	0/42610	0.39	2/58011 (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
2	B	0	1
19	z	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	y	22	LEU	CA-CB-CG	5.69	128.38	115.30
2	B	223	GLN	N-CA-C	-5.33	96.61	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	PRO	Peptide
19	z	31	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	41	49
1	a	331/344 (96%)	324 (98%)	6 (2%)	1 (0%)	41	49
2	B	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
2	b	501/510 (98%)	482 (96%)	18 (4%)	1 (0%)	47	57
3	C	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	47	57
3	c	446/461 (97%)	435 (98%)	9 (2%)	2 (0%)	34	41
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100	100
4	d	338/352 (96%)	323 (96%)	14 (4%)	1 (0%)	41	49
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	31/38 (82%)	31 (100%)	0	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/40 (80%)	32 (100%)	0	0	100	100
9	j	31/40 (78%)	31 (100%)	0	0	100	100
10	K	34/46 (74%)	31 (91%)	3 (9%)	0	100	100
10	k	34/46 (74%)	34 (100%)	0	0	100	100
11	L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	228 (95%)	11 (5%)	1 (0%)	34	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	241/272 (89%)	225 (93%)	13 (5%)	3 (1%)	13 13
14	T	27/32 (84%)	27 (100%)	0	0	100 100
14	t	27/32 (84%)	26 (96%)	1 (4%)	0	100 100
15	U	94/134 (70%)	89 (95%)	5 (5%)	0	100 100
15	u	94/134 (70%)	90 (96%)	4 (4%)	0	100 100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100 100
16	v	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22 26
17	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100 100
17	y	27/46 (59%)	24 (89%)	2 (7%)	1 (4%)	3 1
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100 100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9 7
19	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	4 1
20	R	32/41 (78%)	32 (100%)	0	0	100 100
20	r	31/41 (76%)	29 (94%)	2 (6%)	0	100 100
All	All	5199/5700 (91%)	5010 (96%)	173 (3%)	16 (0%)	41 49

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	30	PRO
13	o	57	LYS
3	c	416	SER
13	o	58	ASN

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	270/280 (96%)	269 (100%)	1 (0%)	91 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	403/407 (99%)	401 (100%)	2 (0%)	88	93
2	b	401/407 (98%)	399 (100%)	2 (0%)	88	93
3	C	350/362 (97%)	349 (100%)	1 (0%)	92	95
3	c	350/362 (97%)	350 (100%)	0	100	100
4	D	275/283 (97%)	274 (100%)	1 (0%)	91	94
4	d	275/283 (97%)	275 (100%)	0	100	100
5	E	71/73 (97%)	70 (99%)	1 (1%)	67	78
5	e	70/73 (96%)	69 (99%)	1 (1%)	67	78
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	52 (98%)	1 (2%)	57	69
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	30/35 (86%)	30 (100%)	0	100	100
8	i	32/35 (91%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	206/228 (90%)	205 (100%)	1 (0%)	88	93
13	o	206/228 (90%)	206 (100%)	0	100	100
14	T	26/29 (90%)	26 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	83 (100%)	0	100	100
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	22/37 (60%)	21 (96%)	1 (4%)	27 36
17	y	22/37 (60%)	21 (96%)	1 (4%)	27 36
18	X	30/34 (88%)	30 (100%)	0	100 100
18	x	31/34 (91%)	31 (100%)	0	100 100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57 69
19	z	52/52 (100%)	49 (94%)	3 (6%)	20 26
20	R	29/33 (88%)	29 (100%)	0	100 100
20	r	28/33 (85%)	28 (100%)	0	100 100
All	All	4318/4660 (93%)	4301 (100%)	17 (0%)	91 94

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	z	2	THR
19	z	33	TRP
13	O	61	GLN
17	Y	23	THR
19	Z	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	223	GLN
13	o	61	GLN
16	v	25	GLN
20	r	30	GLN
19	z	31	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 191 ligands modelled in this entry, 6 are monoatomic and 29 are unknown - leaving 156 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	$\#\|Z\| > 2$
25	CLA	b	609	-	65,73,73	2.18	10 (15%)	76,113,113	1.26	10 (13%)
29	LHG	D	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
28	SQD	F	101	-	42,43,54	1.31	4 (9%)	51,54,65	1.28	7 (13%)
35	HEM	e	101	6,5	41,50,50	1.41	4 (9%)	45,82,82	1.53	10 (22%)
25	CLA	C	510	-	65,73,73	2.12	9 (13%)	76,113,113	1.32	11 (14%)
26	BCR	B	617	-	41,41,41	0.69	0	56,56,56	1.96	17 (30%)
29	LHG	d	407	-	48,48,48	0.94	2 (4%)	51,54,54	0.99	2 (3%)
26	BCR	D	406	-	41,41,41	0.69	0	56,56,56	2.21	15 (26%)
25	CLA	c	509	-	65,73,73	2.12	9 (13%)	76,113,113	1.27	10 (13%)
25	CLA	c	505	-	65,73,73	2.17	9 (13%)	76,113,113	1.28	10 (13%)
25	CLA	A	606	-	65,73,73	2.11	9 (13%)	76,113,113	1.37	10 (13%)
26	BCR	B	618	-	41,41,41	0.69	0	56,56,56	1.86	11 (19%)
25	CLA	B	607	37	65,73,73	2.16	10 (15%)	76,113,113	1.30	12 (15%)
30	SO4	O	301	-	4,4,4	0.14	0	6,6,6	0.05	0
34	PHO	D	402	-	51,69,69	0.62	2 (3%)	47,99,99	0.72	1 (2%)
34	PHO	D	401	-	51,69,69	0.74	2 (3%)	47,99,99	0.61	0
21	OEX	A	601	3,37,1	0,15,15	-	-	-		
25	CLA	B	602	-	65,73,73	2.16	10 (15%)	76,113,113	1.35	12 (15%)
23	LMG	c	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.04	4 (6%)
31	BCT	A	616	22	2,3,3	0.71	0	2,3,3	0.27	0
25	CLA	a	606	-	65,73,73	2.12	9 (13%)	76,113,113	1.35	10 (13%)
26	BCR	k	102	-	41,41,41	0.72	0	56,56,56	1.84	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	615	-	65,73,73	2.16	10 (15%)	76,113,113	1.30	9 (11%)
26	BCR	C	522	-	41,41,41	0.66	0	56,56,56	2.07	15 (26%)
26	BCR	h	101	-	41,41,41	0.68	0	56,56,56	1.98	14 (25%)
25	CLA	C	504	-	65,73,73	2.12	9 (13%)	76,113,113	1.27	10 (13%)
23	LMG	a	603	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	6 (10%)
25	CLA	b	616	-	65,73,73	2.16	10 (15%)	76,113,113	1.33	10 (13%)
25	CLA	C	501	-	65,73,73	2.10	8 (12%)	76,113,113	1.27	11 (14%)
29	LHG	a	615	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
25	CLA	C	507	-	65,73,73	2.14	10 (15%)	76,113,113	1.26	10 (13%)
35	HEM	E	102	6,5	41,50,50	1.39	4 (9%)	45,82,82	1.51	9 (20%)
25	CLA	C	505	-	65,73,73	2.16	10 (15%)	76,113,113	1.28	10 (13%)
23	LMG	B	620	-	51,51,55	0.95	2 (3%)	59,59,63	0.97	3 (5%)
30	SO4	V	202	-	4,4,4	0.14	0	6,6,6	0.10	0
33	DGD	c	516	-	63,63,67	0.88	2 (3%)	77,77,81	0.92	3 (3%)
29	LHG	L	102	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	3 (5%)
25	CLA	C	503	-	65,73,73	2.13	10 (15%)	76,113,113	1.28	11 (14%)
25	CLA	B	610	-	65,73,73	2.16	9 (13%)	76,113,113	1.32	11 (14%)
26	BCR	C	515	-	41,41,41	0.71	0	56,56,56	1.83	14 (25%)
36	HEC	v	201	16	32,50,50	1.81	3 (9%)	24,82,82	1.48	4 (16%)
25	CLA	D	405	-	65,73,73	2.12	9 (13%)	76,113,113	1.29	11 (14%)
23	LMG	A	612	-	51,51,55	0.93	2 (3%)	59,59,63	1.01	3 (5%)
25	CLA	c	511	3	65,73,73	2.13	10 (15%)	76,113,113	1.24	10 (13%)
23	LMG	A	603	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
26	BCR	a	611	-	41,41,41	0.69	0	56,56,56	1.80	11 (19%)
25	CLA	A	608	-	65,73,73	2.15	10 (15%)	76,113,113	1.29	10 (13%)
25	CLA	b	611	-	65,73,73	2.15	10 (15%)	76,113,113	1.29	11 (14%)
25	CLA	c	503	-	65,73,73	2.16	10 (15%)	76,113,113	1.29	10 (13%)
25	CLA	C	502	-	65,73,73	2.15	10 (15%)	76,113,113	1.27	11 (14%)
23	LMG	B	624	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
23	LMG	a	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
26	BCR	z	101	-	41,41,41	0.70	0	56,56,56	1.86	10 (17%)
33	DGD	h	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	2 (2%)
25	CLA	b	606	-	65,73,73	2.19	10 (15%)	76,113,113	1.29	9 (11%)
25	CLA	D	404	-	65,73,73	2.19	10 (15%)	76,113,113	1.29	11 (14%)
34	PHO	a	609	-	51,69,69	0.72	2 (3%)	47,99,99	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	c	514	-	41,41,41	0.70	0	56,56,56	1.82	12 (21%)
25	CLA	c	501	-	65,73,73	2.13	10 (15%)	76,113,113	1.29	11 (14%)
27	PL9	d	405	-	55,55,55	0.61	1 (1%)	68,69,69	1.69	18 (26%)
26	BCR	K	101	-	41,41,41	0.73	0	56,56,56	1.79	14 (25%)
26	BCR	C	514	-	41,41,41	0.70	0	56,56,56	1.93	13 (23%)
30	SO4	o	301	-	4,4,4	0.14	0	6,6,6	0.05	0
25	CLA	B	611	-	65,73,73	2.13	9 (13%)	76,113,113	1.31	11 (14%)
26	BCR	d	404	-	41,41,41	0.72	0	56,56,56	2.04	14 (25%)
23	LMG	c	518	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
29	LHG	A	614	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	2 (3%)
30	SO4	u	202	-	4,4,4	0.14	0	6,6,6	0.05	0
33	DGD	c	515	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	4 (5%)
25	CLA	B	605	-	65,73,73	2.18	10 (15%)	76,113,113	1.32	10 (13%)
25	CLA	d	403	-	65,73,73	2.14	10 (15%)	76,113,113	1.24	10 (13%)
25	CLA	c	512	-	65,73,73	2.15	10 (15%)	76,113,113	1.24	10 (13%)
31	BCT	a	618	22	2,3,3	0.72	0	2,3,3	0.72	0
26	BCR	H	101	-	41,41,41	0.66	0	56,56,56	2.05	14 (25%)
26	BCR	c	521	-	41,41,41	0.66	0	56,56,56	2.06	12 (21%)
27	PL9	A	610	-	55,55,55	0.62	1 (1%)	68,69,69	1.75	20 (29%)
33	DGD	H	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.89	2 (2%)
29	LHG	E	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.08	3 (6%)
26	BCR	B	619	-	41,41,41	0.74	0	56,56,56	1.94	15 (26%)
25	CLA	b	607	37	65,73,73	2.14	9 (13%)	76,113,113	1.30	11 (14%)
25	CLA	C	509	-	65,73,73	2.11	10 (15%)	76,113,113	1.26	11 (14%)
28	SQD	L	101	-	53,54,54	1.20	4 (7%)	62,65,65	3.49	8 (12%)
25	CLA	C	513	-	65,73,73	2.16	9 (13%)	76,113,113	1.30	11 (14%)
29	LHG	a	616	-	41,41,48	1.00	2 (4%)	44,47,54	1.09	3 (6%)
25	CLA	B	604	-	65,73,73	2.14	10 (15%)	76,113,113	1.28	12 (15%)
23	LMG	d	408	-	51,51,55	0.95	2 (3%)	59,59,63	0.97	3 (5%)
25	CLA	B	612	-	65,73,73	2.13	8 (12%)	76,113,113	1.27	11 (14%)
25	CLA	C	506	-	65,73,73	2.15	10 (15%)	76,113,113	1.28	11 (14%)
25	CLA	a	607	37	65,73,73	2.16	9 (13%)	76,113,113	1.35	11 (14%)
33	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	3 (3%)
25	CLA	c	508	-	65,73,73	2.13	9 (13%)	76,113,113	1.31	11 (14%)
27	PL9	a	612	-	55,55,55	0.63	1 (1%)	68,69,69	1.67	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	614	-	65,73,73	2.16	9 (13%)	76,113,113	1.34	10 (13%)
27	PL9	D	407	-	55,55,55	0.61	1 (1%)	68,69,69	1.68	17 (25%)
33	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	4 (5%)
26	BCR	t	102	-	41,41,41	0.67	0	56,56,56	2.06	15 (26%)
30	SO4	u	201	-	4,4,4	0.14	0	6,6,6	0.05	0
36	HEC	V	201	16	32,50,50	1.82	3 (9%)	24,82,82	1.50	4 (16%)
25	CLA	B	609	-	65,73,73	2.18	10 (15%)	76,113,113	1.29	12 (15%)
25	CLA	C	511	3	65,73,73	2.13	10 (15%)	76,113,113	1.25	11 (14%)
25	CLA	c	513	-	65,73,73	2.16	9 (13%)	76,113,113	1.31	11 (14%)
25	CLA	A	607	-	65,73,73	2.15	9 (13%)	76,113,113	1.29	11 (14%)
23	LMG	b	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	4 (6%)
25	CLA	b	610	37	65,73,73	2.16	9 (13%)	76,113,113	1.30	11 (14%)
23	LMG	b	624	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
25	CLA	b	604	-	65,73,73	2.15	10 (15%)	76,113,113	1.27	11 (14%)
25	CLA	c	510	-	65,73,73	2.11	8 (12%)	76,113,113	1.31	11 (14%)
25	CLA	b	608	-	65,73,73	2.17	9 (13%)	76,113,113	1.30	11 (14%)
34	PHO	d	402	-	51,69,69	0.66	2 (3%)	47,99,99	0.69	1 (2%)
28	SQD	L	103	-	53,54,54	1.19	4 (7%)	62,65,65	1.16	4 (6%)
28	SQD	a	613	-	53,54,54	1.18	4 (7%)	62,65,65	1.21	8 (12%)
25	CLA	d	401	-	65,73,73	2.16	9 (13%)	76,113,113	1.30	11 (14%)
25	CLA	b	602	-	65,73,73	2.18	10 (15%)	76,113,113	1.37	11 (14%)
25	CLA	a	610	-	65,73,73	2.18	10 (15%)	76,113,113	1.30	11 (14%)
25	CLA	a	608	-	65,73,73	2.15	9 (13%)	76,113,113	1.30	12 (15%)
26	BCR	b	617	-	41,41,41	0.68	0	56,56,56	2.02	15 (26%)
29	LHG	A	613	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
30	SO4	d	410	-	4,4,4	0.13	0	6,6,6	0.05	0
25	CLA	C	508	-	65,73,73	2.13	9 (13%)	76,113,113	1.32	10 (13%)
26	BCR	A	609	-	41,41,41	0.69	0	56,56,56	1.85	12 (21%)
25	CLA	B	615	-	65,73,73	2.12	10 (15%)	76,113,113	1.30	9 (11%)
25	CLA	B	613	-	65,73,73	2.12	9 (13%)	76,113,113	1.28	11 (14%)
26	BCR	b	618	-	41,41,41	0.66	0	56,56,56	1.96	15 (26%)
25	CLA	c	504	-	65,73,73	2.13	9 (13%)	76,113,113	1.28	11 (14%)
25	CLA	b	605	-	65,73,73	2.18	10 (15%)	76,113,113	1.31	10 (13%)
23	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
30	SO4	O	302	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SO4	U	201	-	4,4,4	0.14	0	6,6,6	0.05	0
25	CLA	c	507	-	65,73,73	2.15	10 (15%)	76,113,113	1.26	10 (13%)
23	LMG	D	409	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
25	CLA	c	502	-	65,73,73	2.18	10 (15%)	76,113,113	1.27	11 (14%)
21	OEX	a	601	3,37,1	0,15,15	-	-	-		
25	CLA	B	603	-	65,73,73	2.15	9 (13%)	76,113,113	1.34	11 (14%)
25	CLA	b	601	-	65,73,73	2.16	10 (15%)	76,113,113	1.26	10 (13%)
30	SO4	a	617	-	4,4,4	0.14	0	6,6,6	0.05	0
25	CLA	B	606	-	65,73,73	2.17	10 (15%)	76,113,113	1.31	11 (14%)
23	LMG	C	521	-	51,51,55	0.97	3 (5%)	59,59,63	1.10	4 (6%)
26	BCR	b	619	-	41,41,41	0.72	0	56,56,56	1.93	13 (23%)
25	CLA	C	512	-	65,73,73	2.14	10 (15%)	76,113,113	1.25	10 (13%)
25	CLA	b	613	-	65,73,73	2.11	8 (12%)	76,113,113	1.26	11 (14%)
29	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
25	CLA	c	506	-	65,73,73	2.16	10 (15%)	76,113,113	1.30	11 (14%)
25	CLA	b	603	-	65,73,73	2.19	9 (13%)	76,113,113	1.29	11 (14%)
25	CLA	B	616	-	65,73,73	2.14	10 (15%)	76,113,113	1.39	11 (14%)
25	CLA	B	601	-	65,73,73	2.17	10 (15%)	76,113,113	1.27	10 (13%)
25	CLA	B	614	-	65,73,73	2.17	10 (15%)	76,113,113	1.33	11 (14%)
30	SO4	A	615	-	4,4,4	0.14	0	6,6,6	0.05	0
25	CLA	D	403	37	65,73,73	2.15	10 (15%)	76,113,113	1.35	11 (14%)
28	SQD	f	101	-	42,43,54	1.33	4 (9%)	51,54,65	1.31	7 (13%)
25	CLA	b	612	-	65,73,73	2.13	8 (12%)	76,113,113	1.30	11 (14%)
33	DGD	c	517	-	63,63,67	0.87	2 (3%)	77,77,81	0.89	3 (3%)
33	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.90	3 (3%)
29	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	3 (5%)
26	BCR	T	101	-	41,41,41	0.69	0	56,56,56	2.06	13 (23%)
25	CLA	B	608	-	65,73,73	2.13	9 (13%)	76,113,113	1.29	11 (14%)
28	SQD	A	611	-	53,54,54	1.17	4 (7%)	62,65,65	1.23	6 (9%)

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
25	CLA	b	609	-	1/1/15/20	2/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	D	408	-	-	6/53/53/53	-
28	SQD	F	101	-	-	6/38/58/69	0/1/1/1
35	HEM	e	101	6,5	-	6/12/54/54	-
25	CLA	C	510	-	1/1/15/20	4/37/115/115	-
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
29	LHG	d	407	-	-	14/53/53/53	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	3/37/115/115	-
25	CLA	c	505	-	1/1/15/20	1/37/115/115	-
25	CLA	A	606	-	1/1/15/20	1/37/115/115	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	CLA	B	607	37	1/1/15/20	6/37/115/115	-
34	PHO	D	402	-	-	2/37/103/103	0/5/6/6
34	PHO	D	401	-	-	6/37/103/103	0/5/6/6
25	CLA	B	602	-	1/1/15/20	9/37/115/115	-
23	LMG	c	520	-	-	13/46/66/70	0/1/1/1
25	CLA	a	606	-	1/1/15/20	1/37/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2
25	CLA	b	615	-	1/1/15/20	2/37/115/115	-
26	BCR	C	522	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	4/29/63/63	0/2/2/2
25	CLA	C	504	-	1/1/15/20	3/37/115/115	-
23	LMG	a	603	-	-	11/46/66/70	0/1/1/1
25	CLA	b	616	-	1/1/15/20	7/37/115/115	-
25	CLA	C	501	-	1/1/15/20	0/37/115/115	-
29	LHG	a	615	-	-	8/53/53/53	-
25	CLA	C	507	-	1/1/15/20	4/37/115/115	-
35	HEM	E	102	6,5	-	6/12/54/54	-
25	CLA	C	505	-	1/1/15/20	1/37/115/115	-
23	LMG	B	620	-	-	4/46/66/70	0/1/1/1
33	DGD	c	516	-	-	8/51/91/95	0/2/2/2
29	LHG	L	102	-	-	15/53/53/53	-
25	CLA	C	503	-	1/1/15/20	2/37/115/115	-
25	CLA	B	610	-	1/1/15/20	2/37/115/115	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
36	HEC	v	201	16	-	1/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	405	-	1/1/15/20	3/37/115/115	-
23	LMG	A	612	-	-	11/46/66/70	0/1/1/1
25	CLA	c	511	3	1/1/15/20	0/37/115/115	-
23	LMG	A	603	-	-	15/46/66/70	0/1/1/1
26	BCR	a	611	-	-	0/29/63/63	0/2/2/2
25	CLA	A	608	-	1/1/15/20	2/37/115/115	-
25	CLA	b	611	-	1/1/15/20	0/37/115/115	-
25	CLA	c	503	-	1/1/15/20	3/37/115/115	-
25	CLA	C	502	-	1/1/15/20	2/37/115/115	-
23	LMG	B	624	-	-	10/46/66/70	0/1/1/1
23	LMG	a	614	-	-	5/46/66/70	0/1/1/1
26	BCR	z	101	-	-	2/29/63/63	0/2/2/2
33	DGD	h	102	-	-	6/51/91/95	0/2/2/2
25	CLA	b	606	-	1/1/15/20	4/37/115/115	-
25	CLA	D	404	-	1/1/15/20	2/37/115/115	-
34	PHO	a	609	-	-	7/37/103/103	0/5/6/6
26	BCR	c	514	-	-	1/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/37/115/115	-
27	PL9	d	405	-	-	8/53/73/73	0/1/1/1
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	1/37/115/115	-
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
23	LMG	c	518	-	-	8/46/66/70	0/1/1/1
29	LHG	A	614	-	-	5/53/53/53	-
33	DGD	c	515	-	-	10/51/91/95	0/2/2/2
25	CLA	B	605	-	1/1/15/20	7/37/115/115	-
25	CLA	d	403	-	1/1/15/20	1/37/115/115	-
25	CLA	c	512	-	1/1/15/20	5/37/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	PL9	A	610	-	-	8/53/73/73	0/1/1/1
33	DGD	H	102	-	-	5/51/91/95	0/2/2/2
29	LHG	E	101	-	-	10/46/46/53	-
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	607	37	1/1/15/20	6/37/115/115	-
25	CLA	C	509	-	1/1/15/20	2/37/115/115	-
28	SQD	L	101	-	-	17/49/69/69	0/1/1/1
25	CLA	C	513	-	1/1/15/20	3/37/115/115	-
29	LHG	a	616	-	-	7/46/46/53	-
25	CLA	B	604	-	1/1/15/20	1/37/115/115	-
23	LMG	d	408	-	-	3/46/66/70	0/1/1/1
25	CLA	B	612	-	1/1/15/20	1/37/115/115	-
25	CLA	C	506	-	1/1/15/20	9/37/115/115	-
25	CLA	a	607	37	1/1/15/20	3/37/115/115	-
33	DGD	C	517	-	-	13/51/91/95	0/2/2/2
25	CLA	c	508	-	1/1/15/20	2/37/115/115	-
27	PL9	a	612	-	-	9/53/73/73	0/1/1/1
25	CLA	b	614	-	1/1/15/20	12/37/115/115	-
27	PL9	D	407	-	-	8/53/73/73	0/1/1/1
33	DGD	C	516	-	-	8/51/91/95	0/2/2/2
26	BCR	t	102	-	-	8/29/63/63	0/2/2/2
36	HEC	V	201	16	-	1/10/54/54	-
25	CLA	B	609	-	1/1/15/20	3/37/115/115	-
25	CLA	C	511	3	1/1/15/20	0/37/115/115	-
25	CLA	c	513	-	1/1/15/20	2/37/115/115	-
25	CLA	A	607	-	1/1/15/20	3/37/115/115	-
25	CLA	b	610	37	1/1/15/20	3/37/115/115	-
23	LMG	b	620	-	-	4/46/66/70	0/1/1/1
23	LMG	b	624	-	-	9/46/66/70	0/1/1/1
25	CLA	b	604	-	1/1/15/20	3/37/115/115	-
25	CLA	c	510	-	1/1/15/20	5/37/115/115	-
25	CLA	b	608	-	1/1/15/20	1/37/115/115	-
34	PHO	d	402	-	-	1/37/103/103	0/5/6/6
28	SQD	L	103	-	-	18/49/69/69	0/1/1/1
28	SQD	a	613	-	-	7/49/69/69	0/1/1/1
25	CLA	d	401	-	1/1/15/20	0/37/115/115	-
25	CLA	b	602	-	1/1/15/20	2/37/115/115	-
25	CLA	a	610	-	1/1/15/20	4/37/115/115	-
25	CLA	a	608	-	1/1/15/20	2/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
29	LHG	A	613	-	-	7/53/53/53	-
25	CLA	C	508	-	1/1/15/20	2/37/115/115	-
26	BCR	A	609	-	-	1/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	5/37/115/115	-
25	CLA	B	613	-	1/1/15/20	2/37/115/115	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	CLA	c	504	-	1/1/15/20	2/37/115/115	-
25	CLA	b	605	-	1/1/15/20	2/37/115/115	-
23	LMG	C	519	-	-	9/46/66/70	0/1/1/1
25	CLA	c	507	-	1/1/15/20	4/37/115/115	-
25	CLA	c	502	-	1/1/15/20	1/37/115/115	-
23	LMG	D	409	-	-	3/46/66/70	0/1/1/1
25	CLA	B	603	-	1/1/15/20	2/37/115/115	-
25	CLA	b	601	-	1/1/15/20	7/37/115/115	-
25	CLA	B	606	-	1/1/15/20	3/37/115/115	-
23	LMG	C	521	-	-	17/46/66/70	0/1/1/1
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	3/37/115/115	-
25	CLA	b	613	-	1/1/15/20	1/37/115/115	-
29	LHG	l	101	-	-	17/53/53/53	-
25	CLA	c	506	-	1/1/15/20	3/37/115/115	-
25	CLA	b	603	-	1/1/15/20	3/37/115/115	-
25	CLA	B	616	-	1/1/15/20	3/37/115/115	-
25	CLA	B	601	-	1/1/15/20	8/37/115/115	-
25	CLA	B	614	-	1/1/15/20	10/37/115/115	-
25	CLA	D	403	37	1/1/15/20	3/37/115/115	-
28	SQD	f	101	-	-	11/38/58/69	0/1/1/1
25	CLA	b	612	-	1/1/15/20	1/37/115/115	-
33	DGD	c	517	-	-	1/51/91/95	0/2/2/2
33	DGD	C	518	-	-	4/51/91/95	0/2/2/2
29	LHG	d	406	-	-	5/53/53/53	-
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	-	1/1/15/20	1/37/115/115	-
28	SQD	A	611	-	-	5/49/69/69	0/1/1/1

The worst 5 of 779 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	CLA	C4B-NB	12.18	1.46	1.35
25	B	609	CLA	C4B-NB	12.14	1.46	1.35
25	b	609	CLA	C4B-NB	12.12	1.46	1.35
25	c	503	CLA	C4B-NB	12.11	1.46	1.35
25	b	603	CLA	C4B-NB	12.05	1.46	1.35

The worst 5 of 1291 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	101	SQD	O9-S-C6	-17.82	85.76	106.94
28	L	101	SQD	O8-S-O9	-11.74	82.59	111.27
28	L	101	SQD	O7-S-C6	9.72	118.49	106.94
28	L	101	SQD	O9-S-O7	-9.24	81.97	113.95
28	L	101	SQD	O8-S-C6	7.84	118.24	105.74

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND

5 of 667 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C	521	LMG	O6-C1-O1-C7
25	A	607	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D

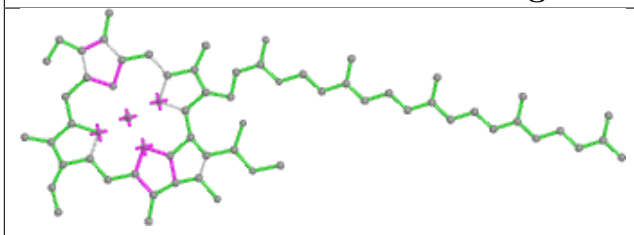
There are no ring outliers.

No monomer is involved in short contacts.

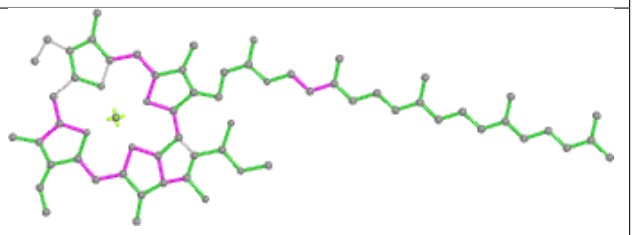
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

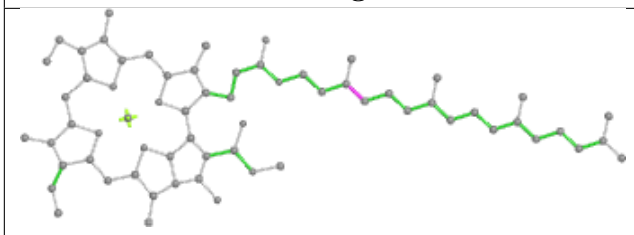
Ligand CLA b 609



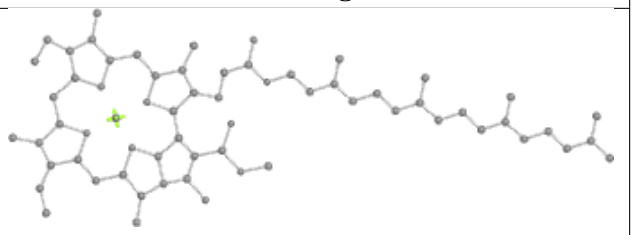
Bond lengths



Bond angles

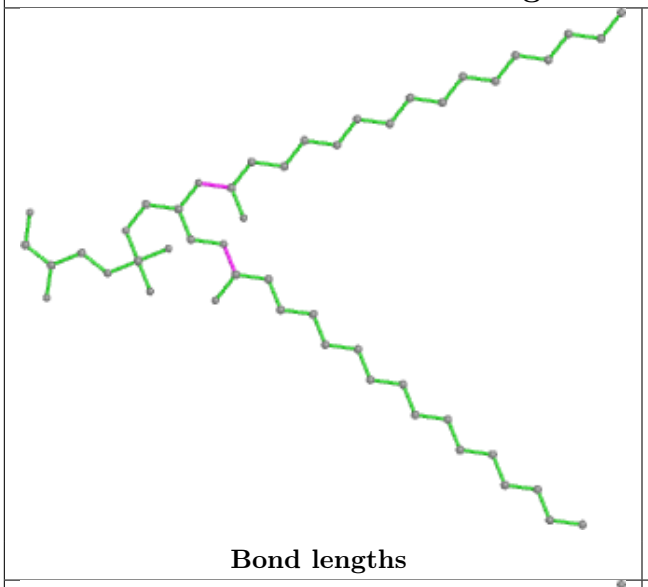


Torsions

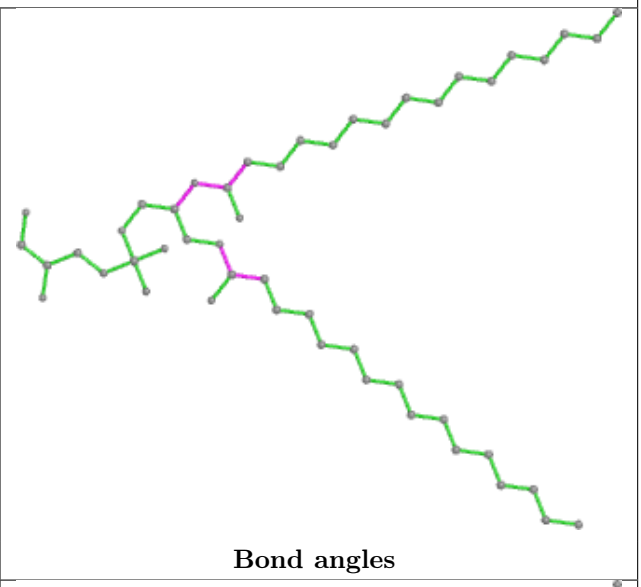


Rings

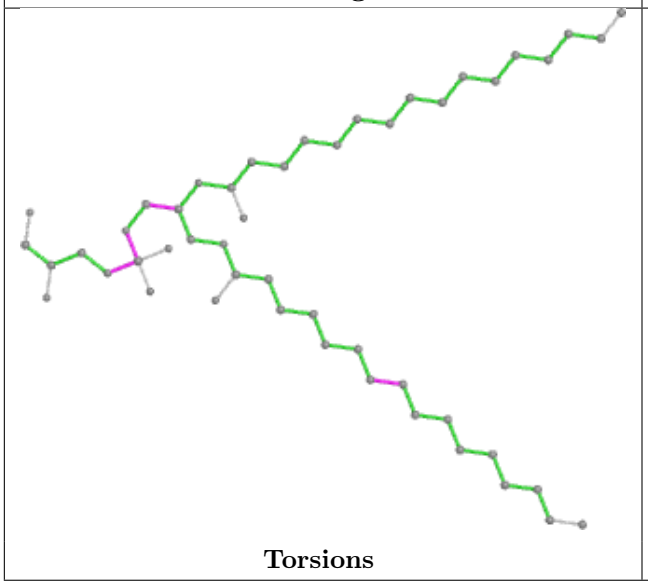
Ligand LHG D 408



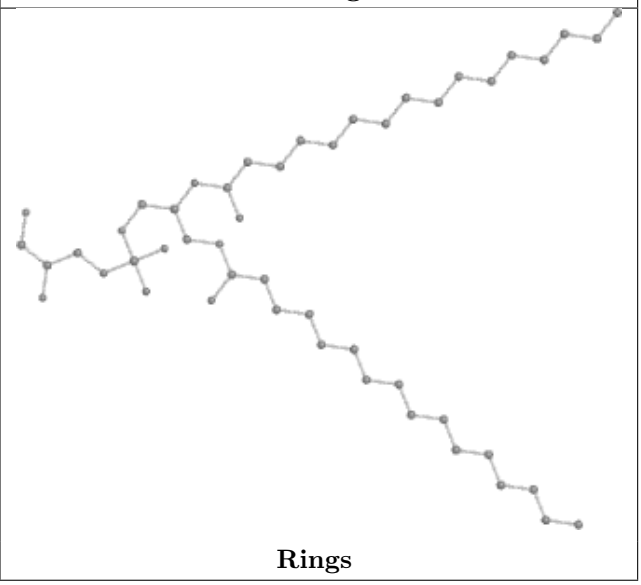
Bond lengths



Bond angles

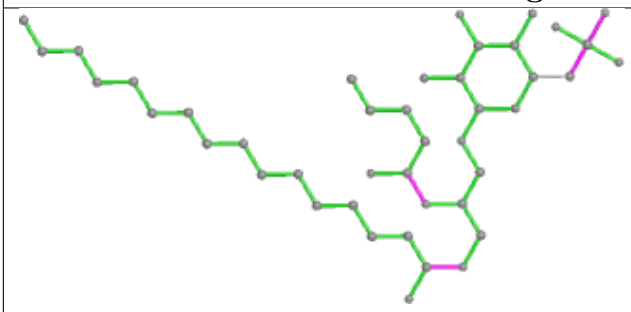


Torsions

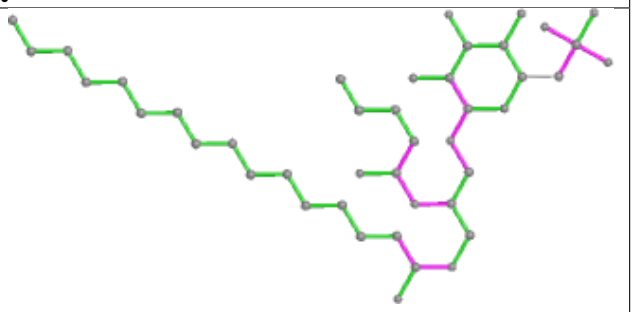


Rings

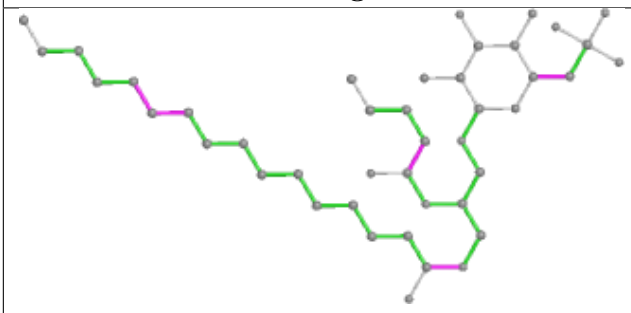
Ligand SQD F 101



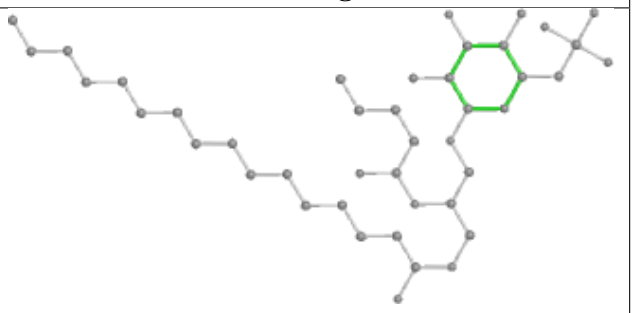
Bond lengths



Bond angles

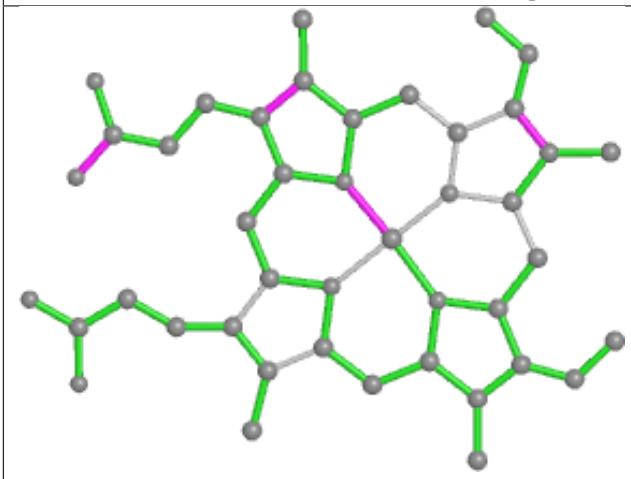


Torsions

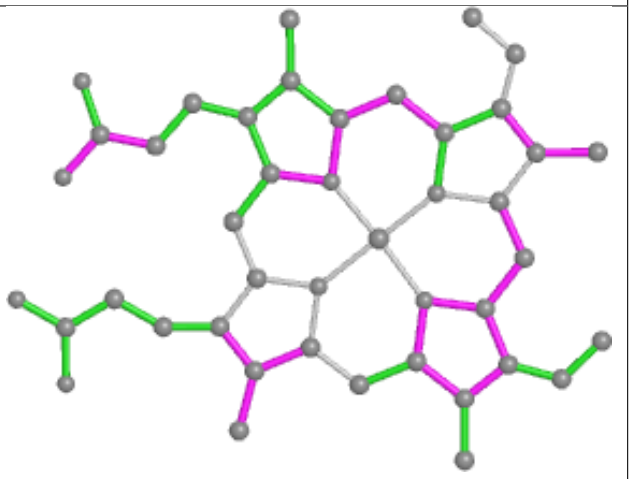


Rings

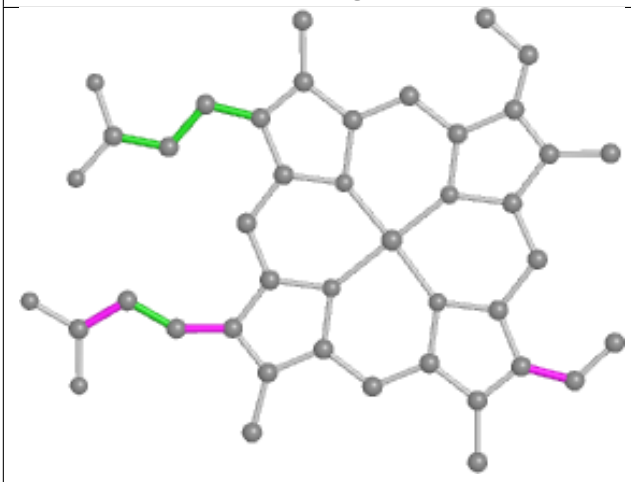
Ligand HEM e 101



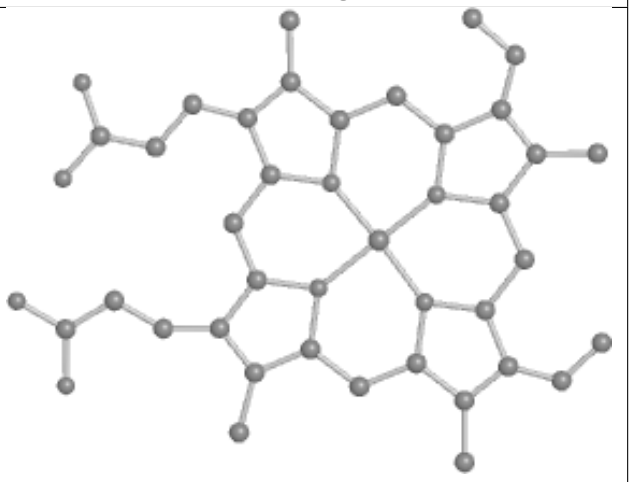
Bond lengths



Bond angles

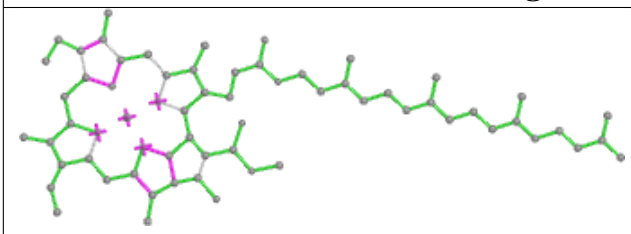


Torsions



Rings

Ligand CLA C 510



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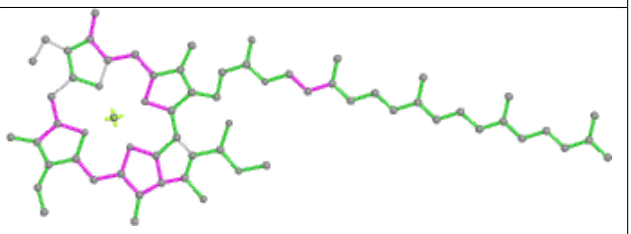
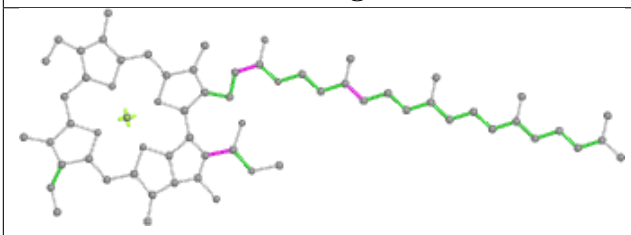
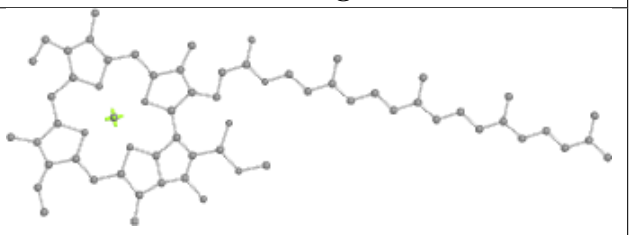


Bond angles

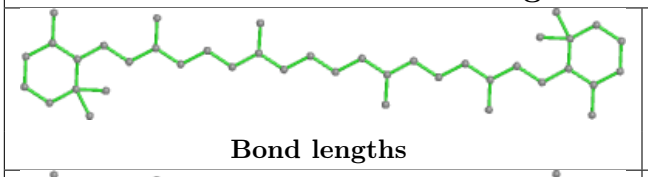


Torsions

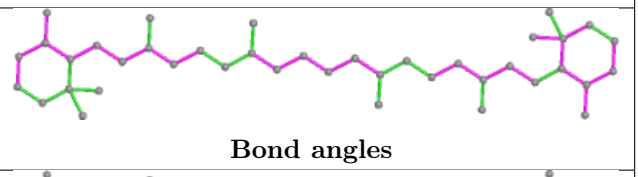


Rings

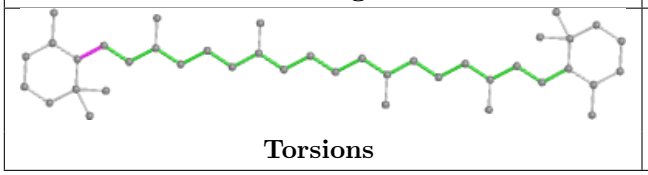
Ligand BCR B 617



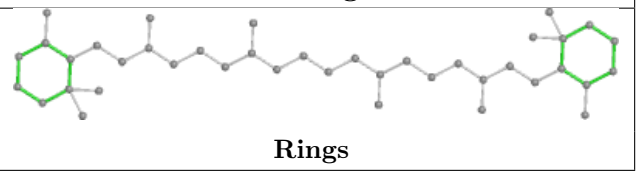
Bond lengths



Bond angles

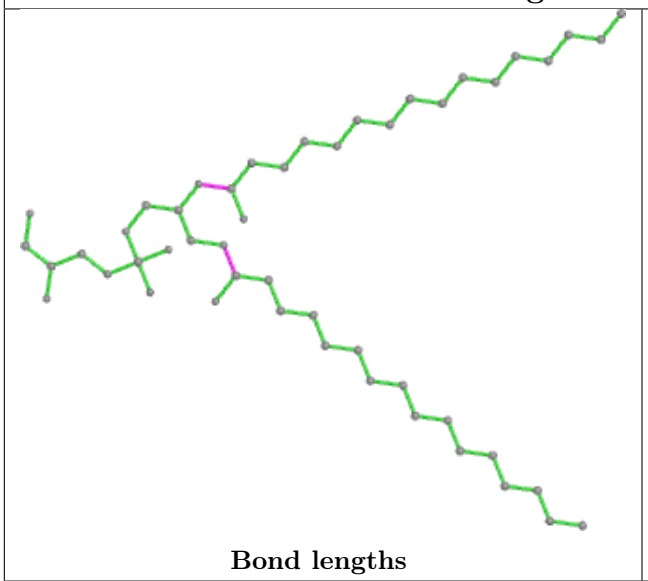


Torsions

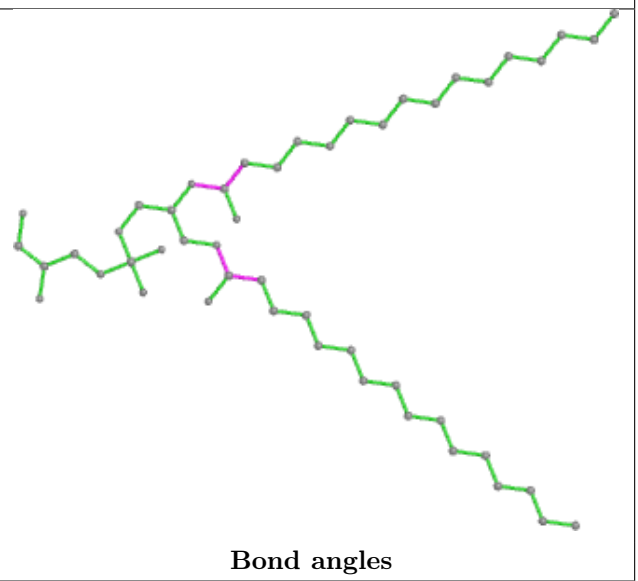


Rings

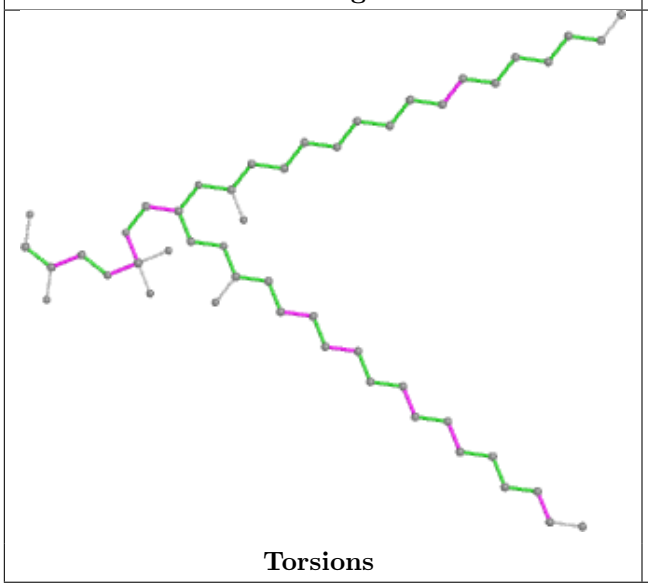
Ligand LHG d 407



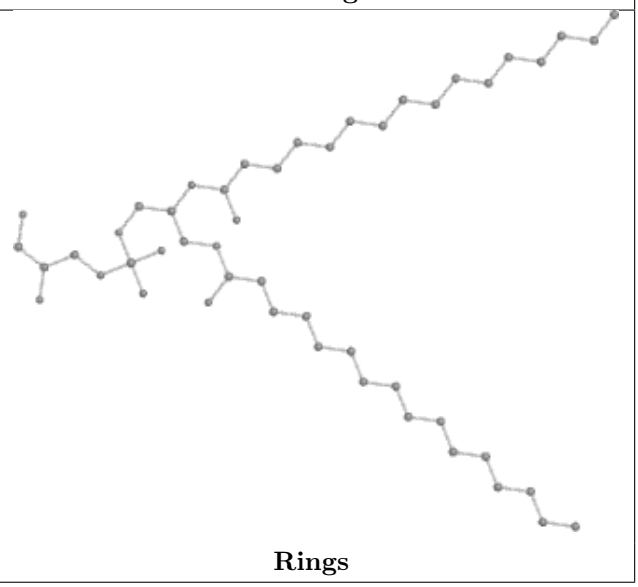
Bond lengths



Bond angles

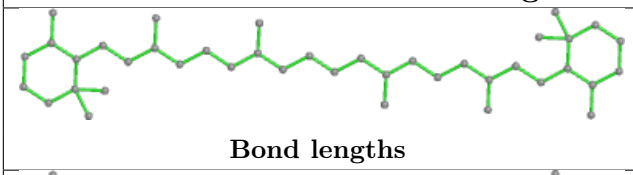


Torsions

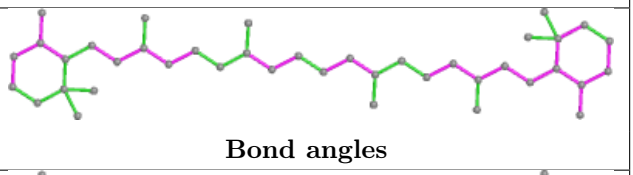


Rings

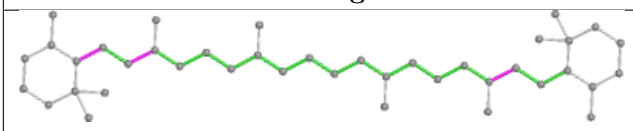
Ligand BCR D 406



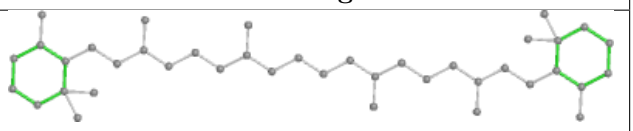
Bond lengths



Bond angles

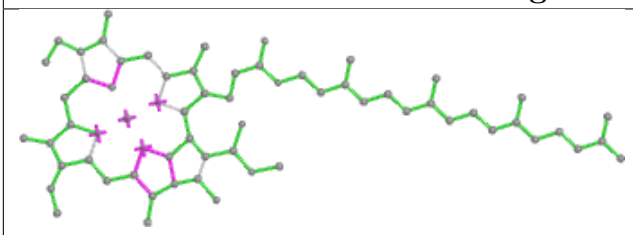


Torsions

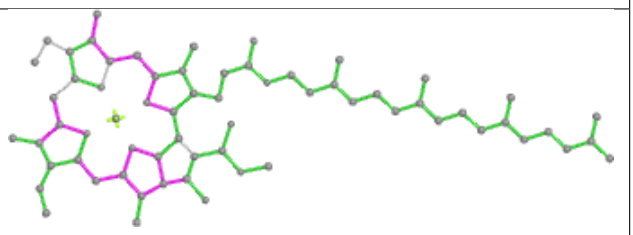


Rings

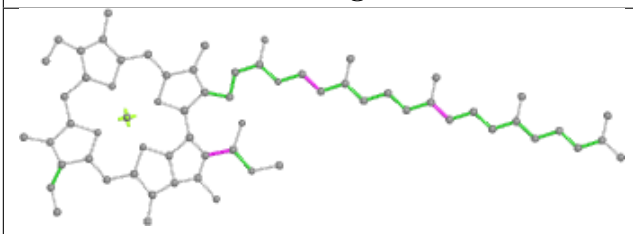
Ligand CLA c 509



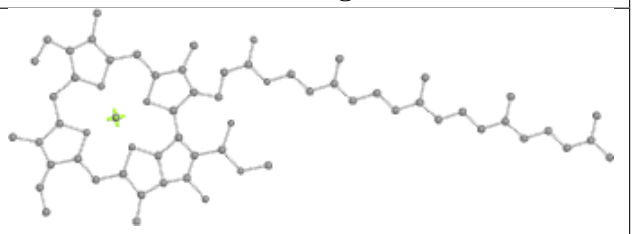
Bond lengths



Bond angles

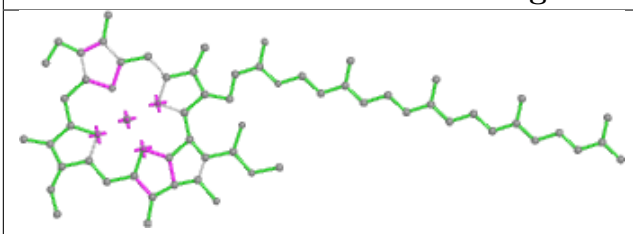


Torsions

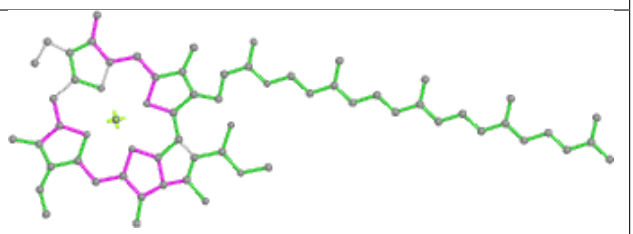


Rings

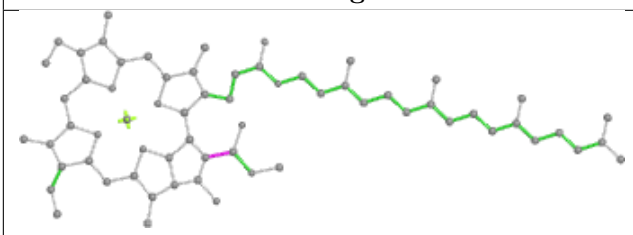
Ligand CLA c 505



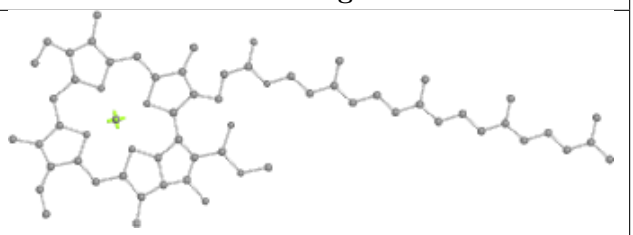
Bond lengths



Bond angles

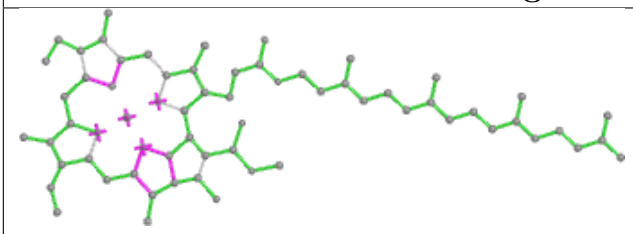


Torsions

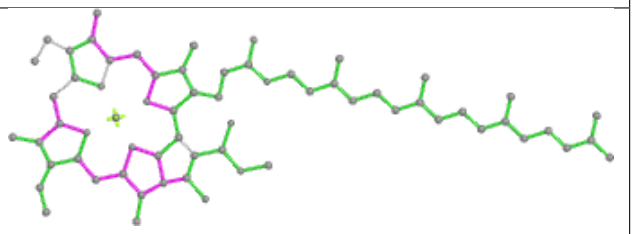


Rings

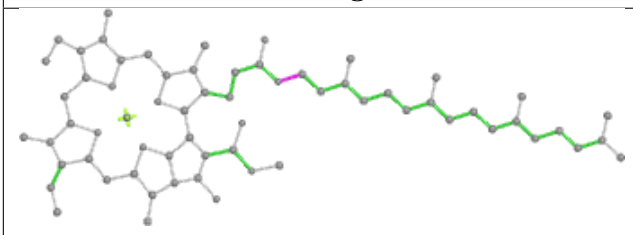
Ligand CLA A 606



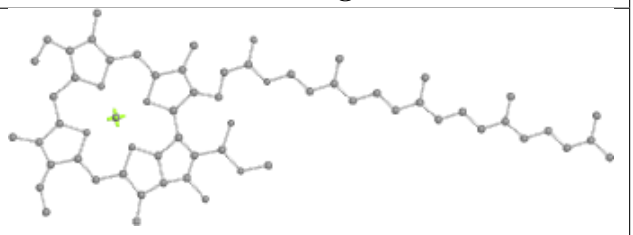
Bond lengths



Bond angles

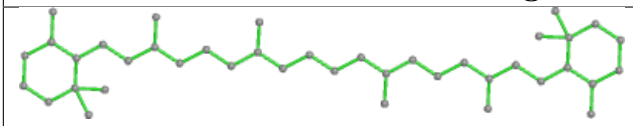


Torsions

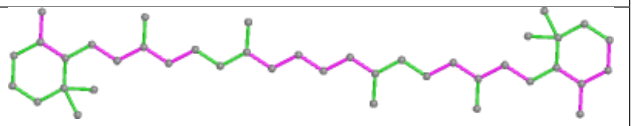


Rings

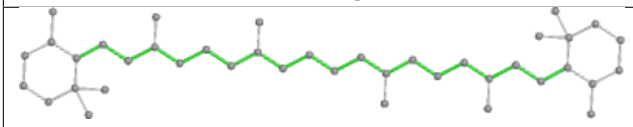
Ligand BCR B 618



Bond lengths



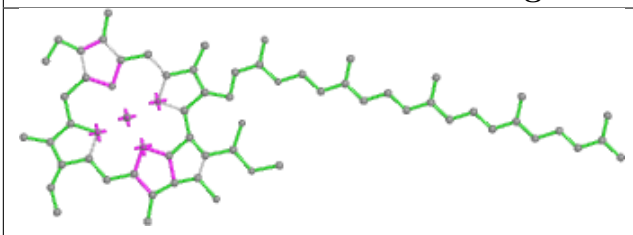
Bond angles



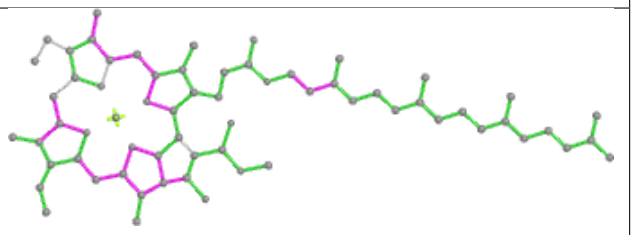
Torsions

Rings

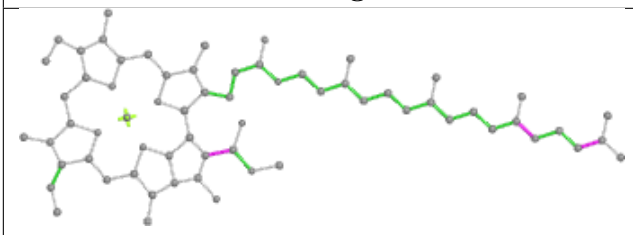
Ligand CLA B 607



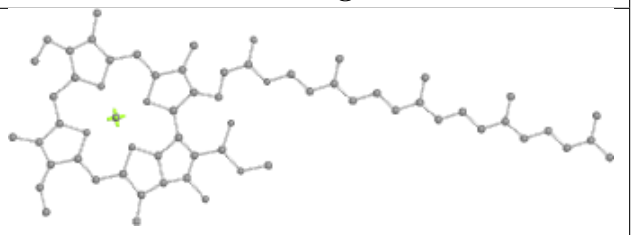
Bond lengths



Bond angles

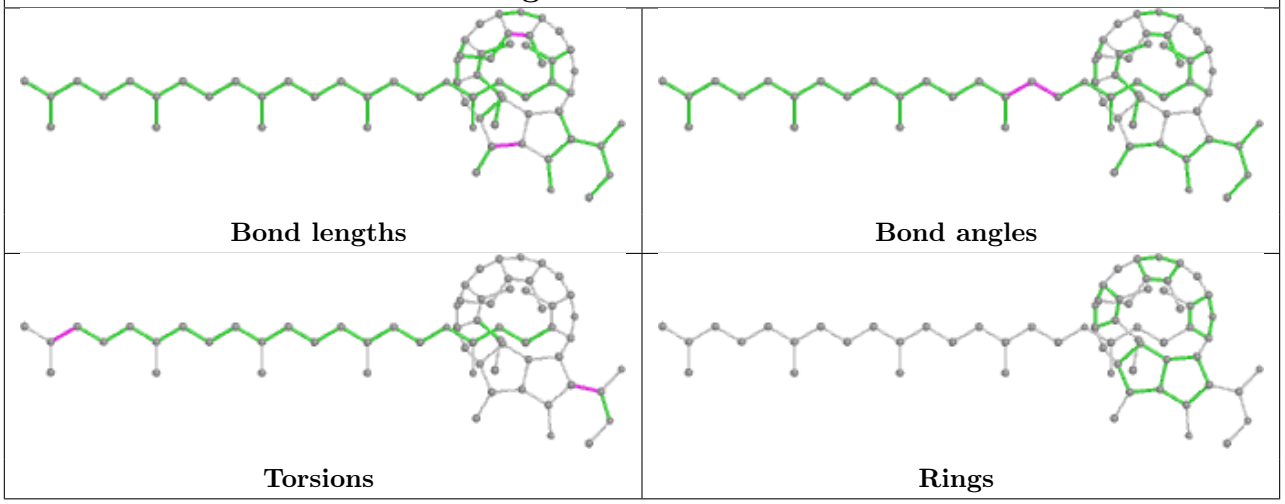


Torsions

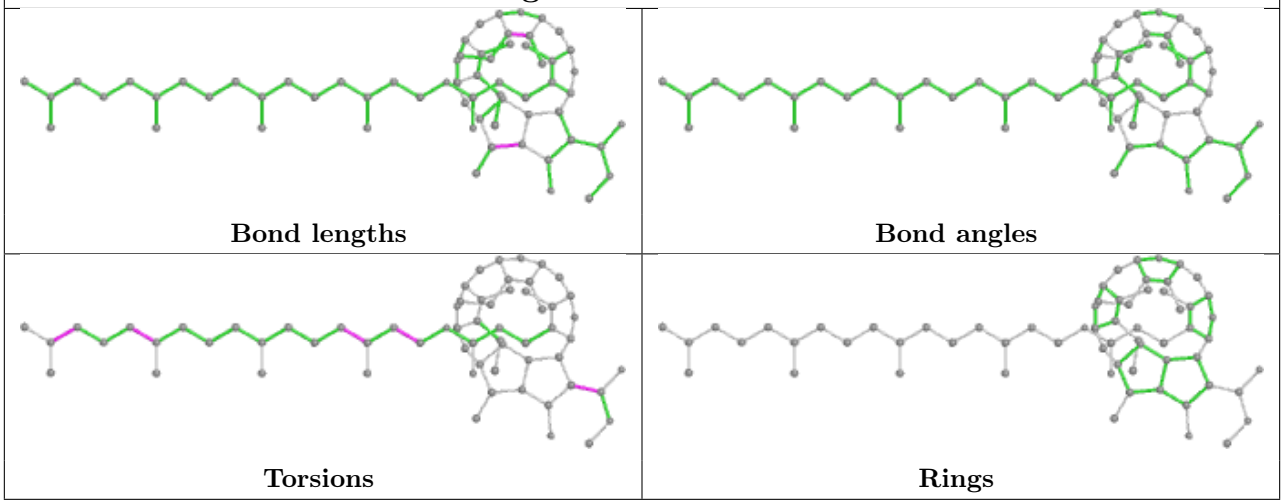


Rings

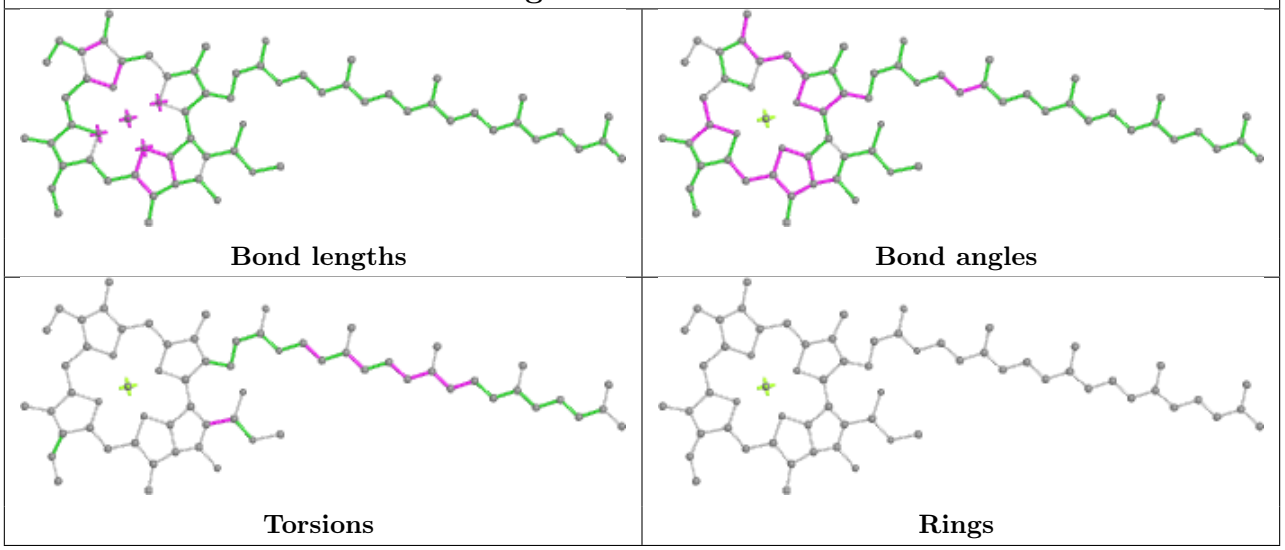
Ligand PHO D 402



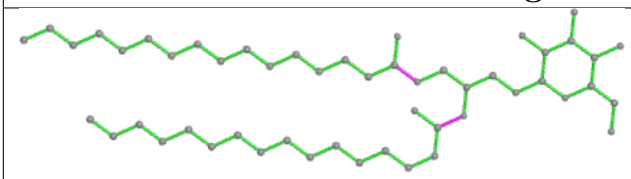
Ligand PHO D 401



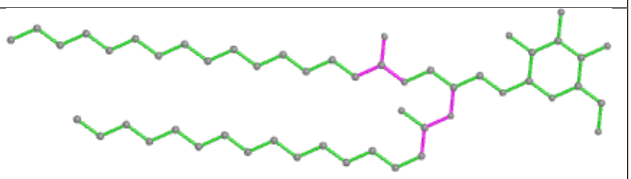
Ligand CLA B 602



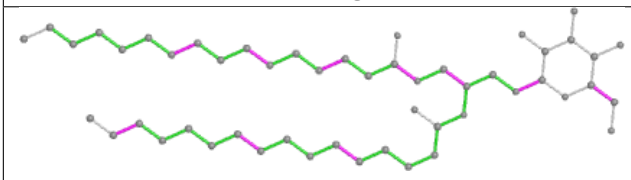
Ligand LMG c 520



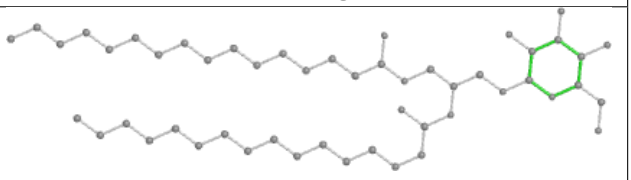
Bond lengths



Bond angles

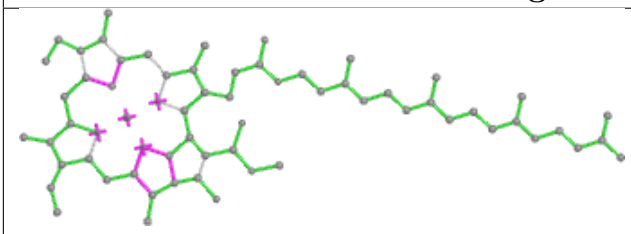


Torsions

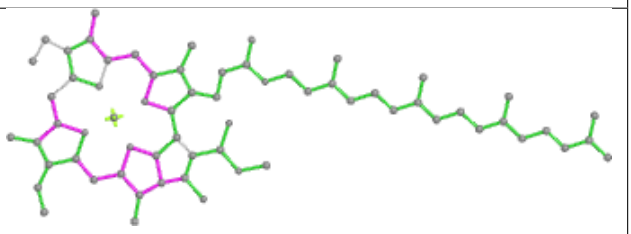


Rings

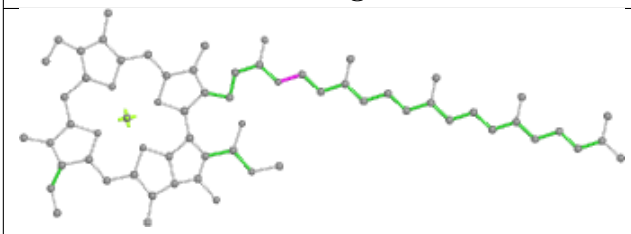
Ligand CLA a 606



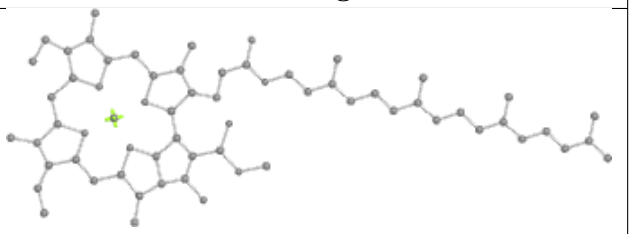
Bond lengths



Bond angles

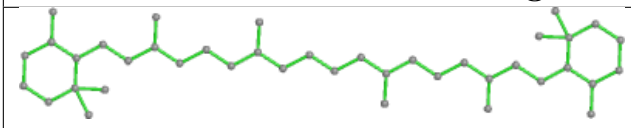


Torsions

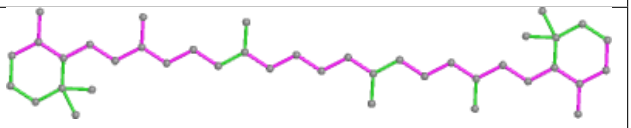


Rings

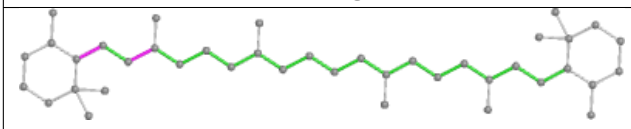
Ligand BCR k 102



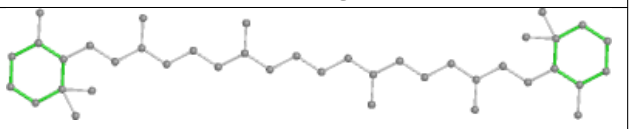
Bond lengths



Bond angles

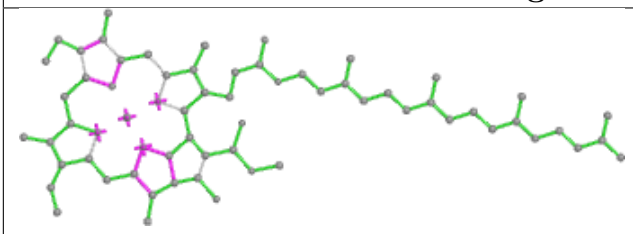


Torsions

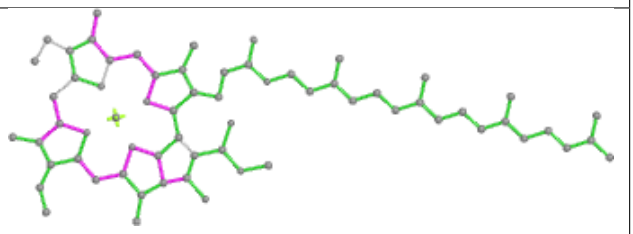


Rings

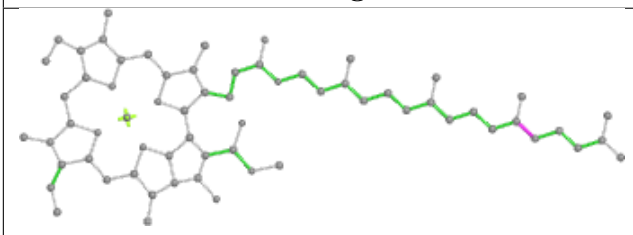
Ligand CLA b 615



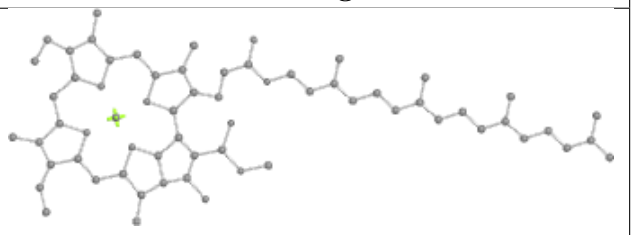
Bond lengths



Bond angles

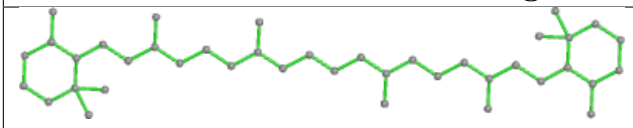


Torsions

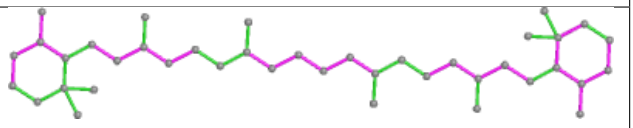


Rings

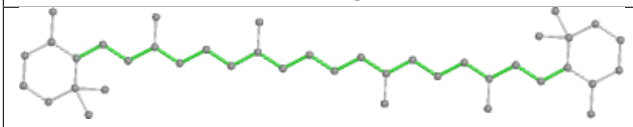
Ligand BCR C 522



Bond lengths



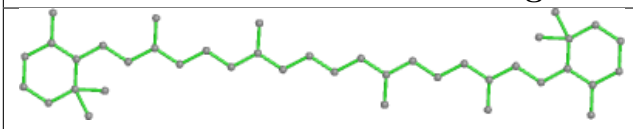
Bond angles



Torsions

Rings

Ligand BCR h 101



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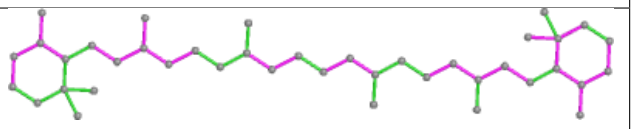
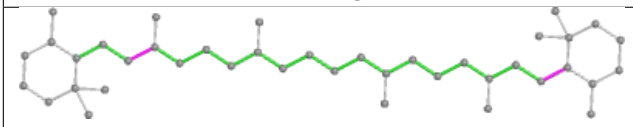


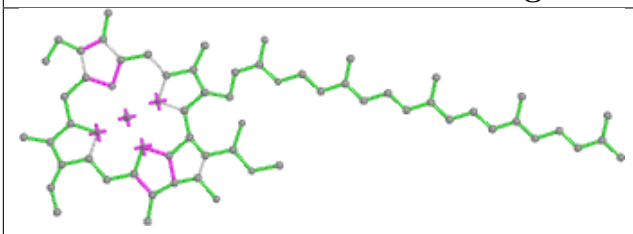
Bond angles



Torsions

Rings

Ligand CLA C 504



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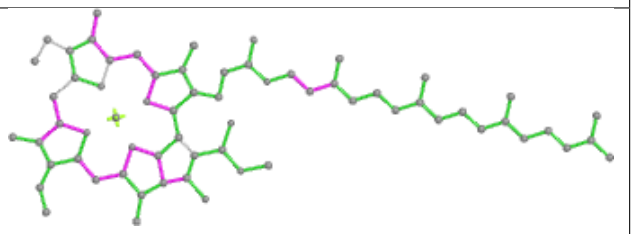
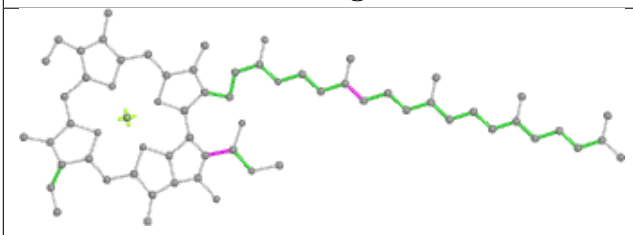
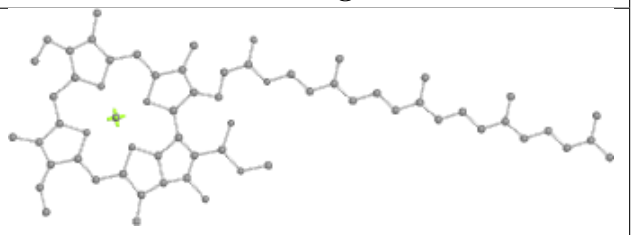


Bond angles

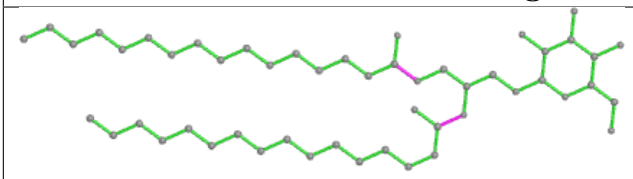


Torsions

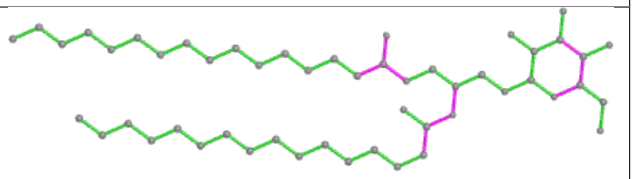


Rings

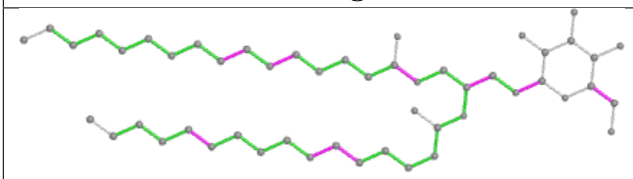
Ligand LMG a 603



Bond lengths



Bond angles



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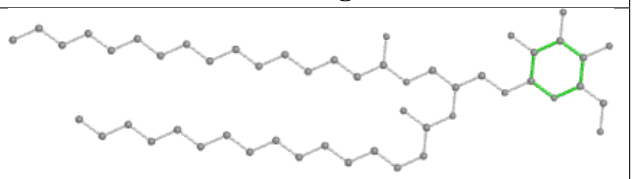
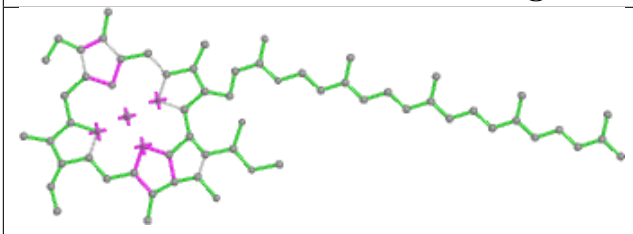


Rings

Ligand CLA b 616



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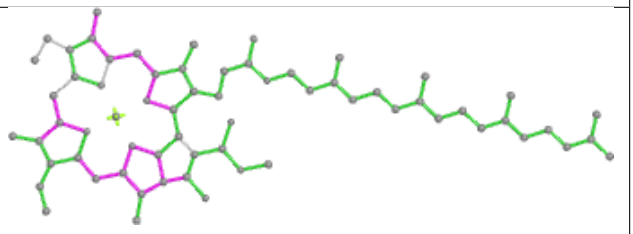
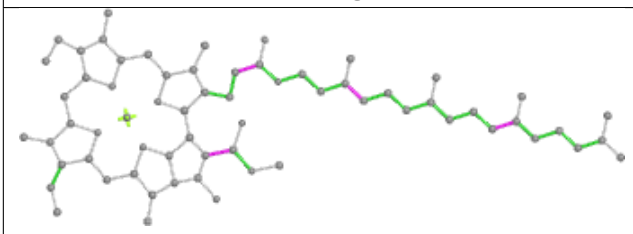
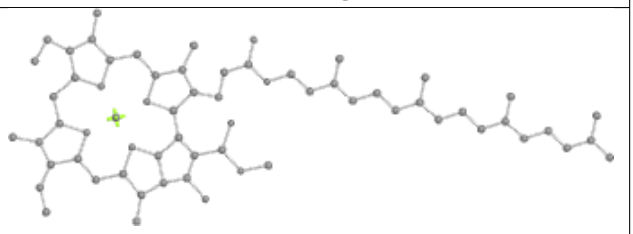


Bond angles

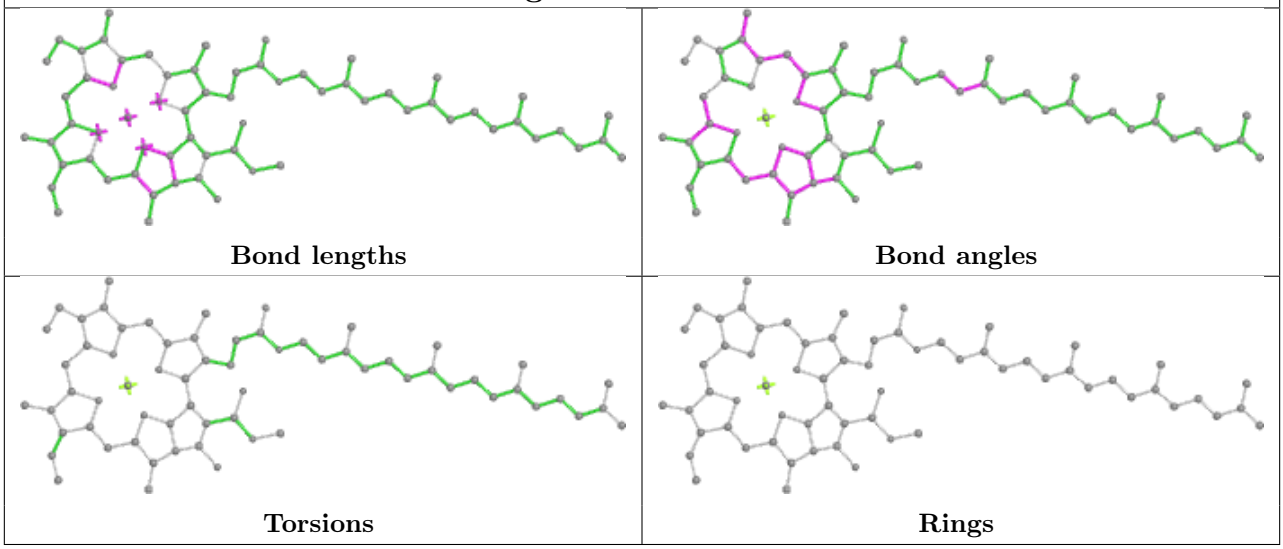


Torsions

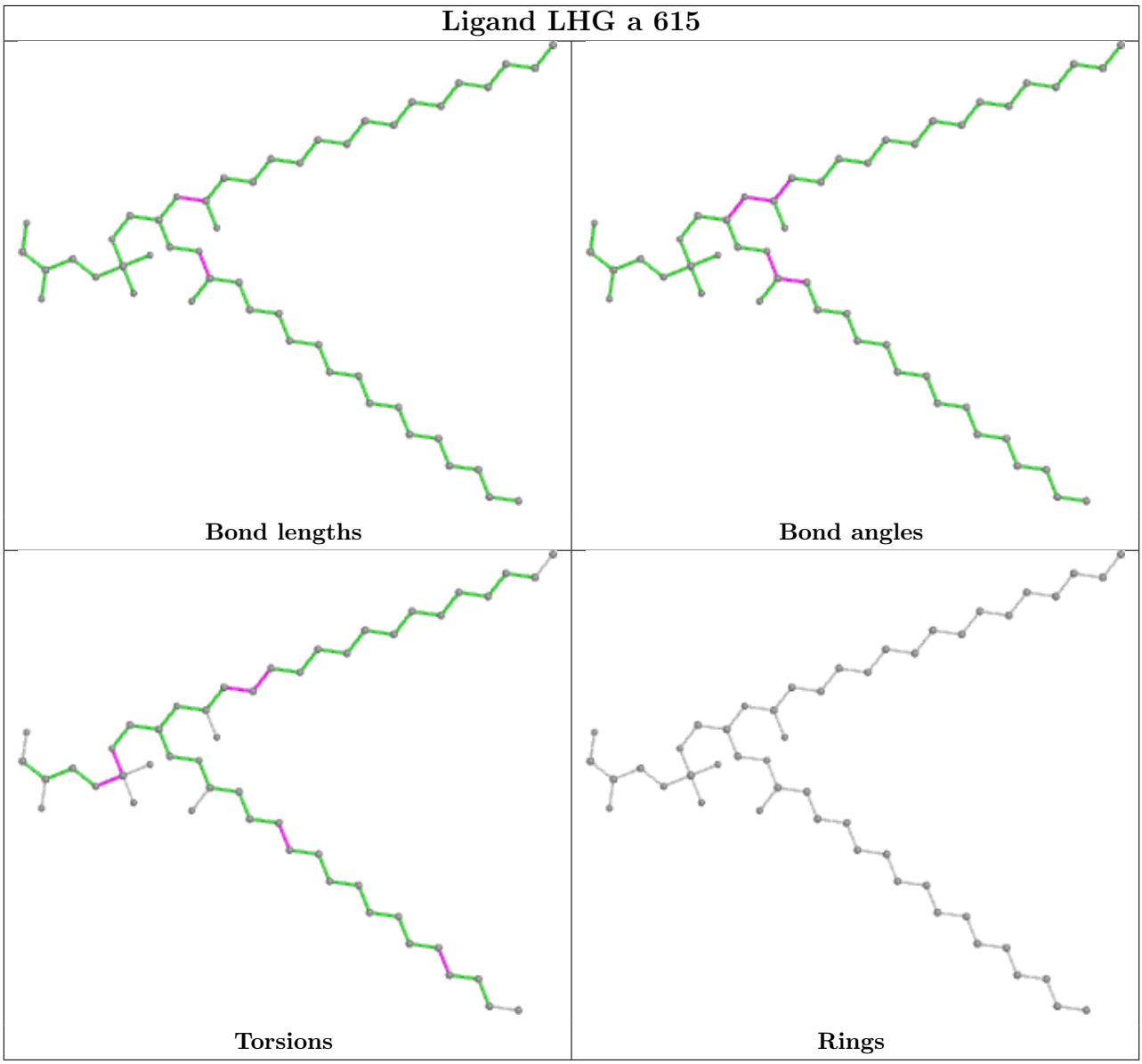


Rings

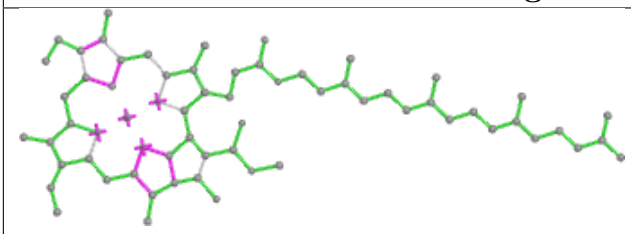
Ligand CLA C 501



Ligand LHG a 615



Ligand CLA C 507



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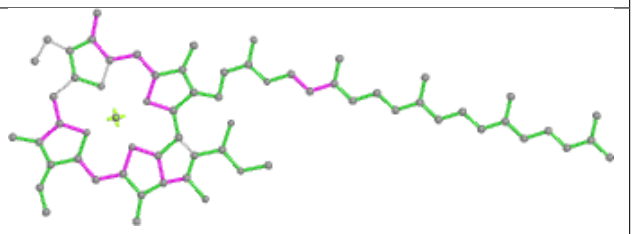
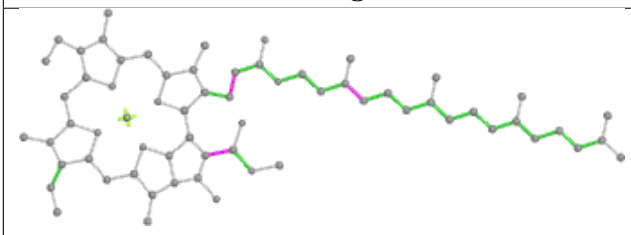


Bond angles



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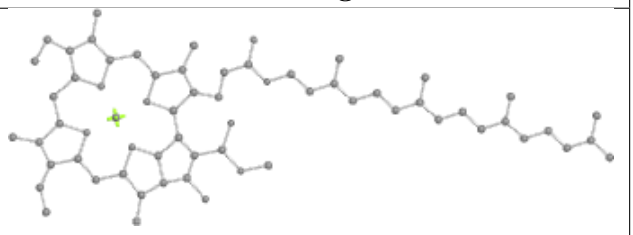
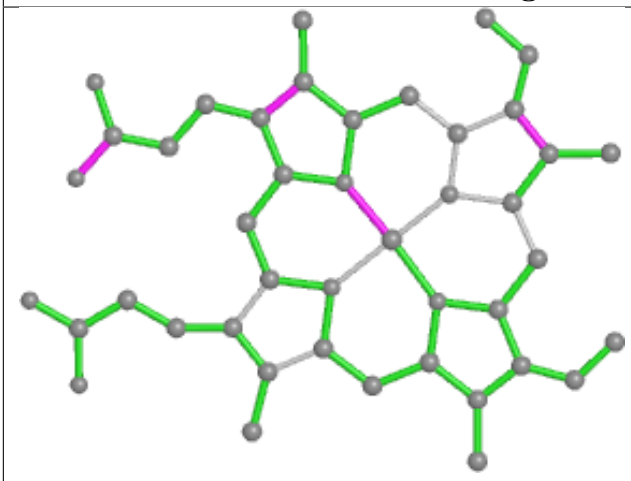
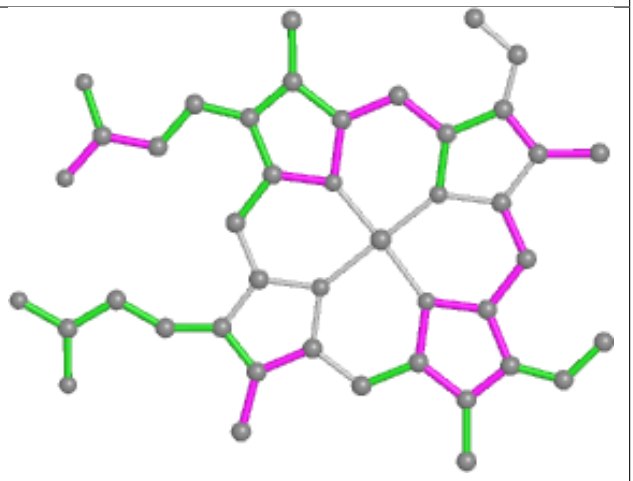


Rings

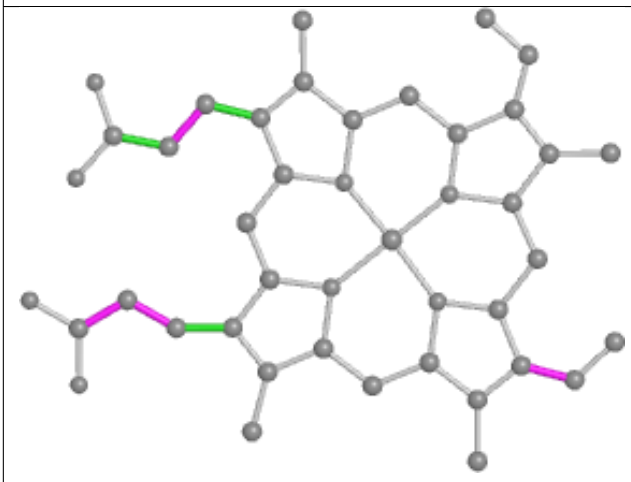
Ligand HEM E 102



Bond lengths



Bond angles



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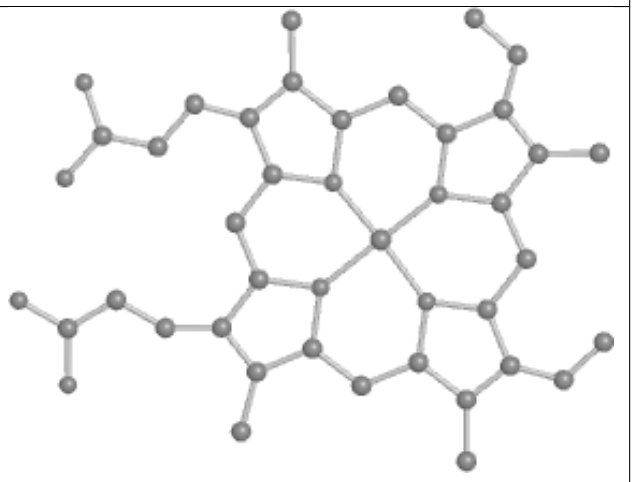
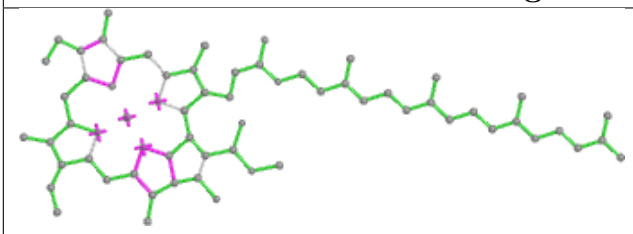
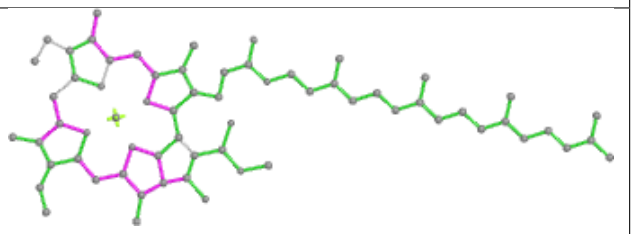


Rings

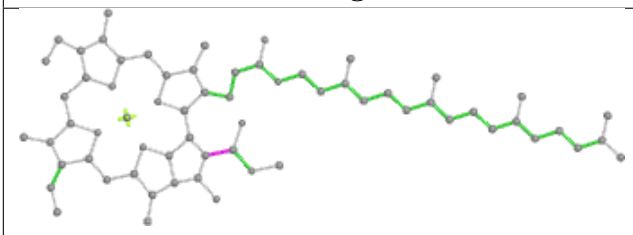
Ligand CLA C 505



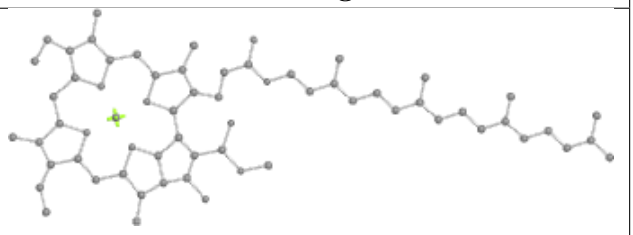
Bond lengths



Bond angles

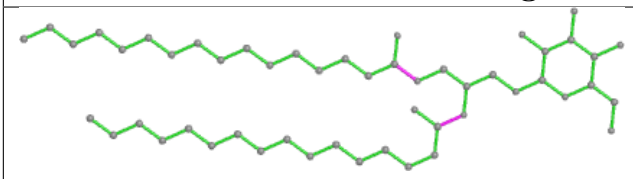


Torsions

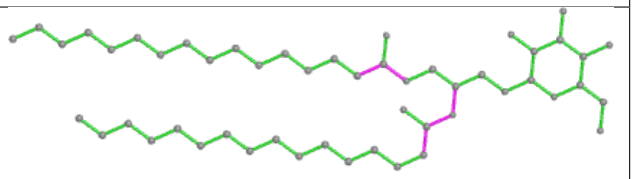


Rings

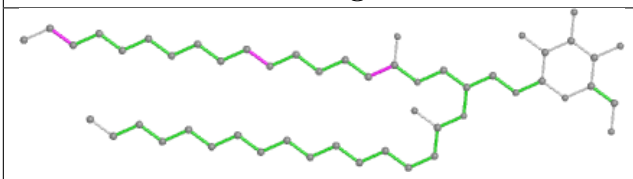
Ligand LMG B 620



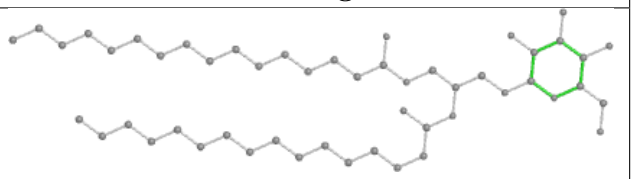
Bond lengths



Bond angles

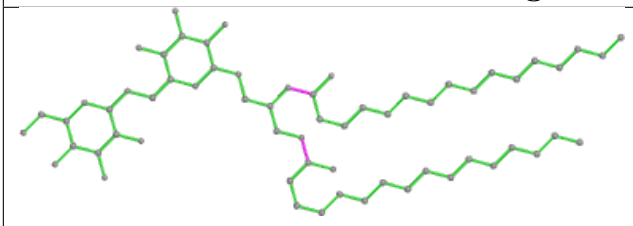


Torsions

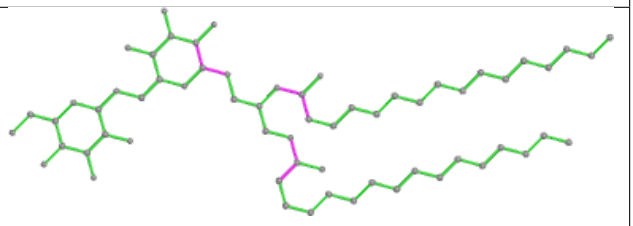


Rings

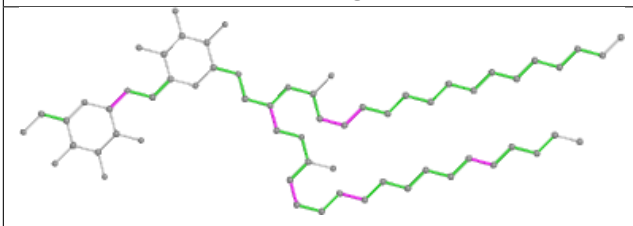
Ligand DGD c 516



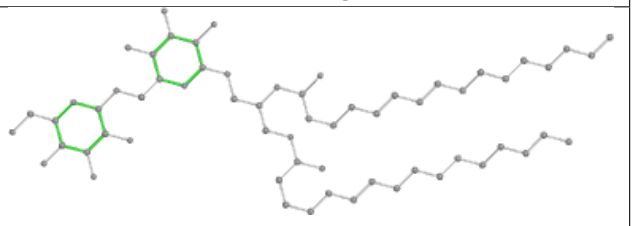
Bond lengths



Bond angles

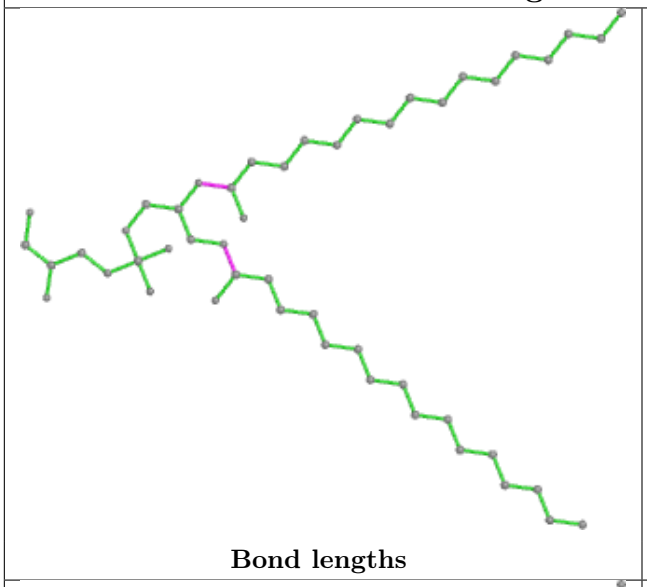


Torsions

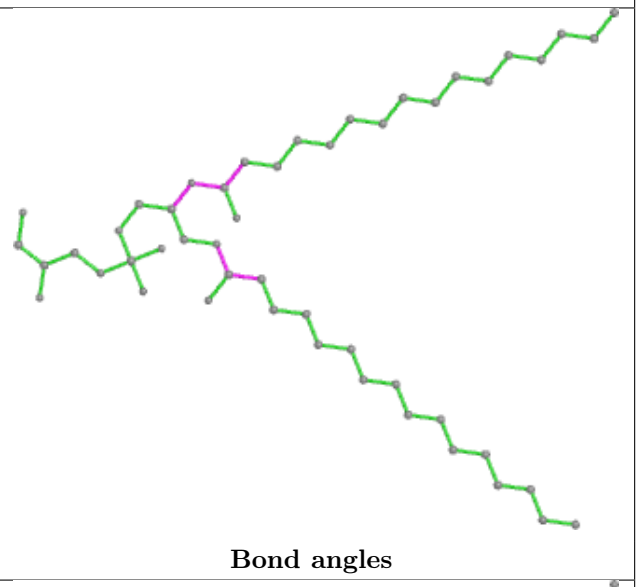


Rings

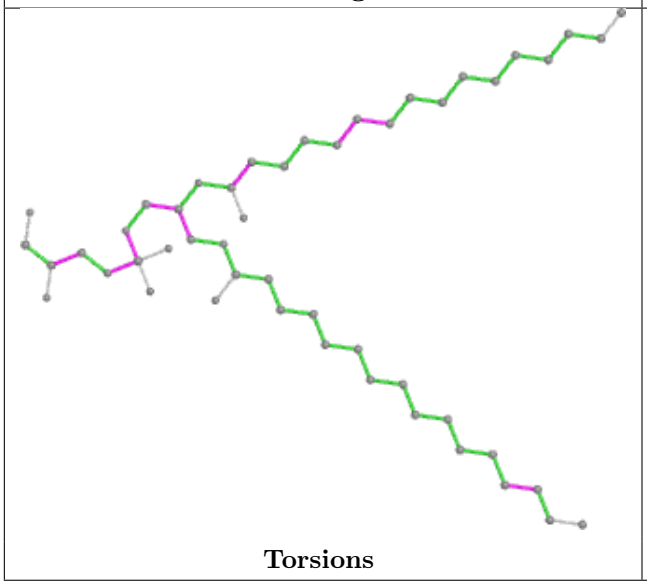
Ligand LHG L 102



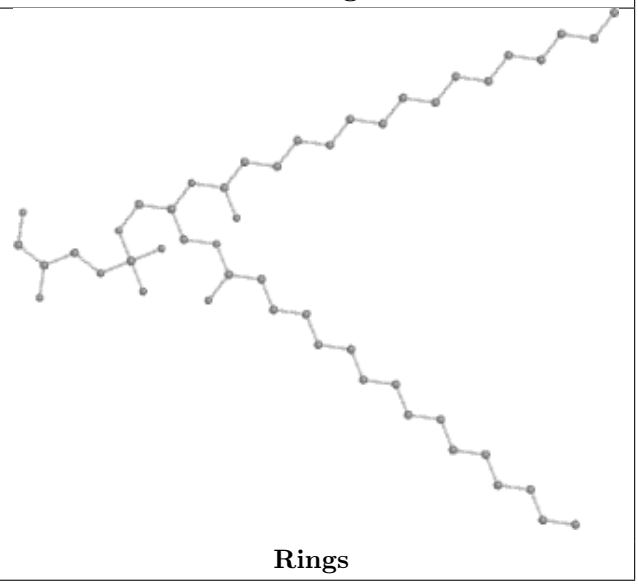
Bond lengths



Bond angles

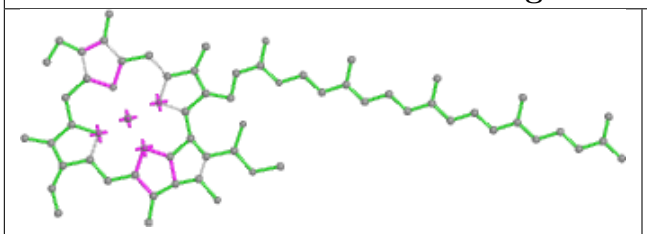


Torsions



Rings

Ligand CLA C 503



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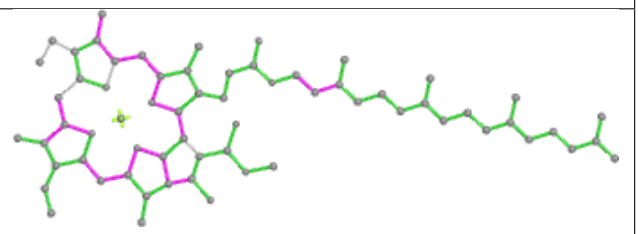
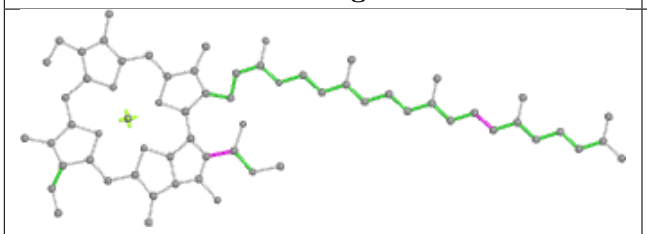
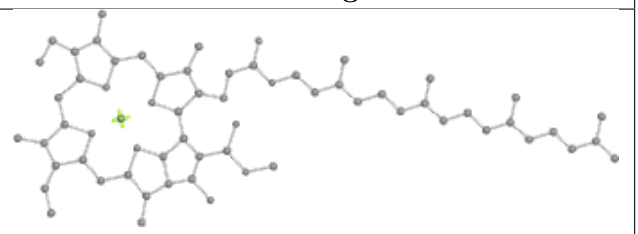


Bond angles

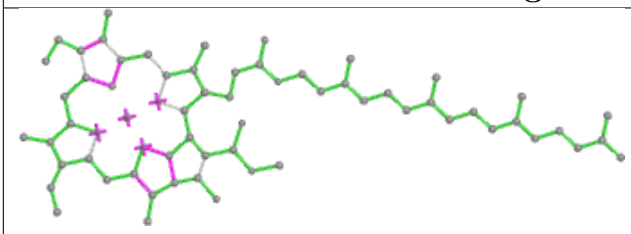


Torsions

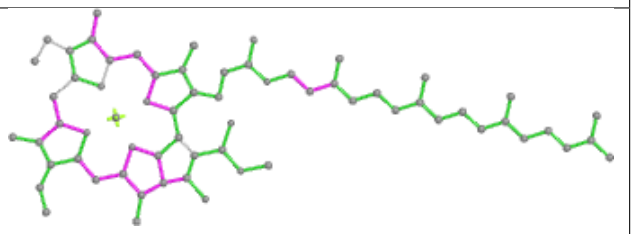


Rings

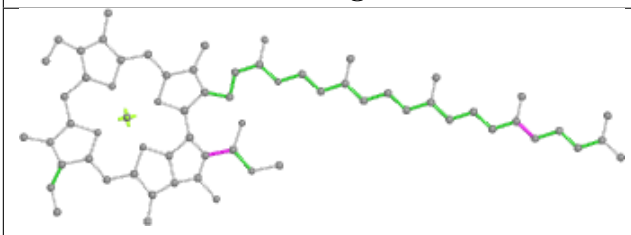
Ligand CLA B 610



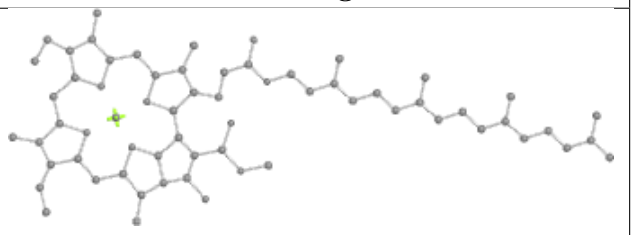
Bond lengths



Bond angles

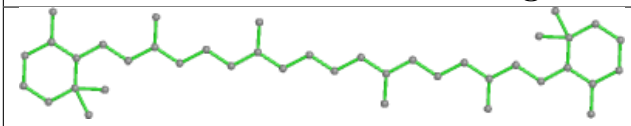


Torsions

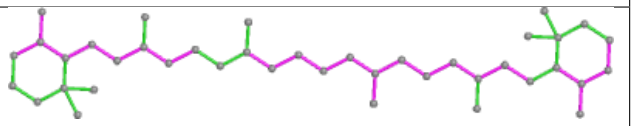


Rings

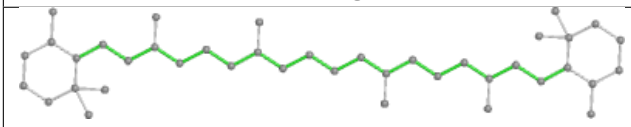
Ligand BCR C 515



Bond lengths



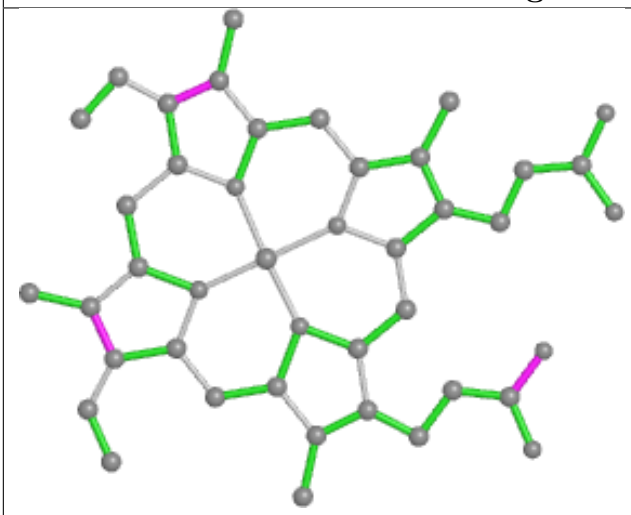
Bond angles



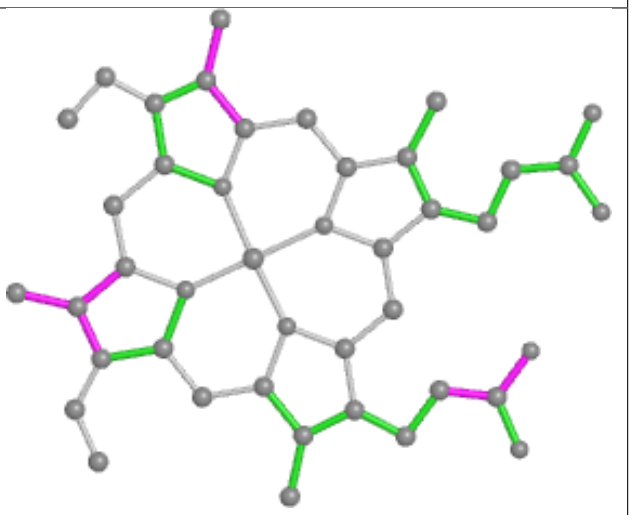
Torsions

Rings

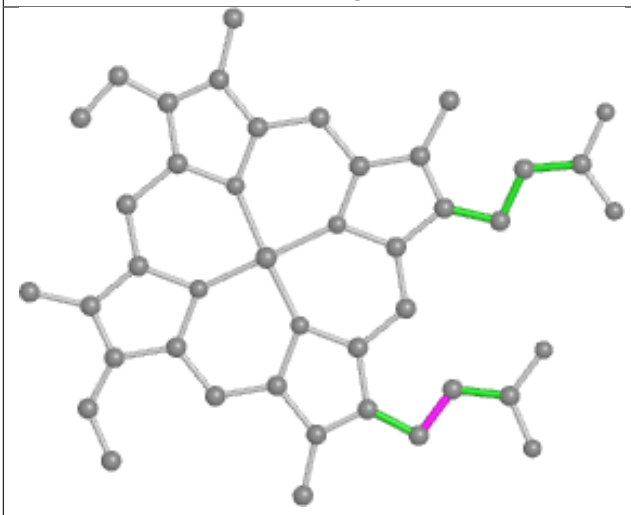
Ligand HEC v 201



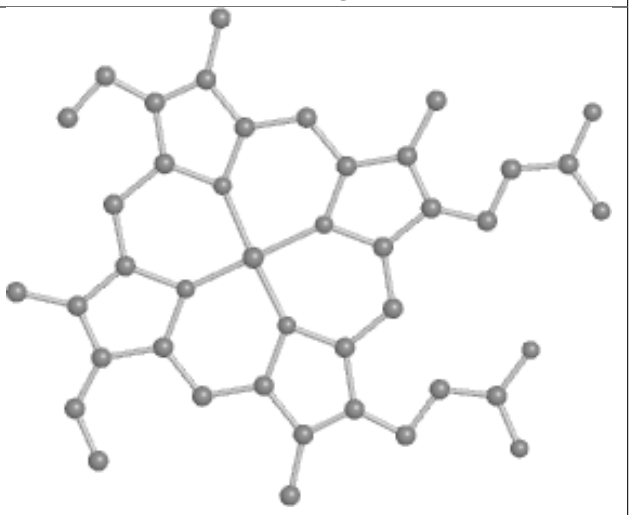
Bond lengths



Bond angles

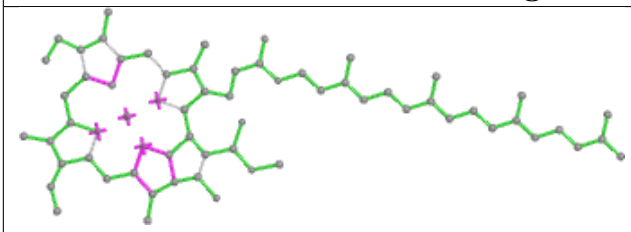


Torsions

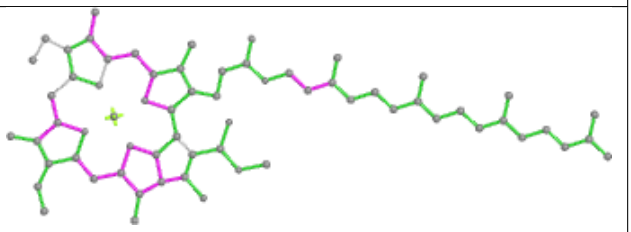


Rings

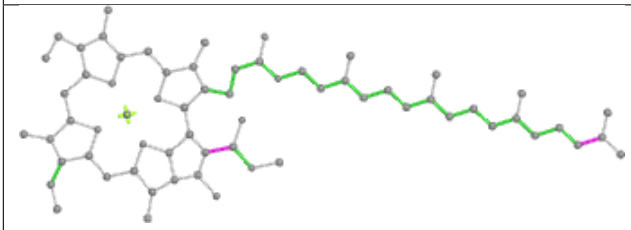
Ligand CLA D 405



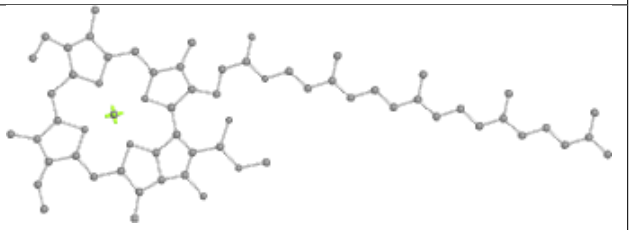
Bond lengths



Bond angles

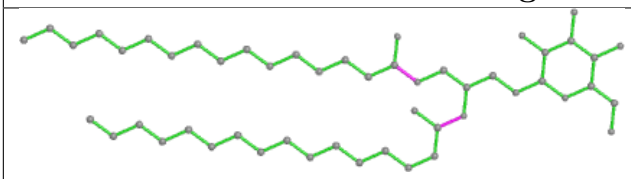


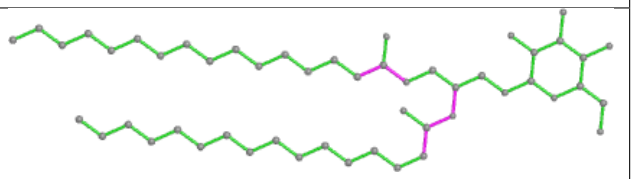
Torsions

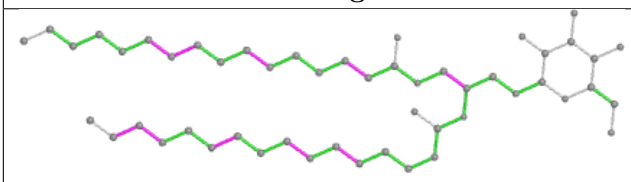


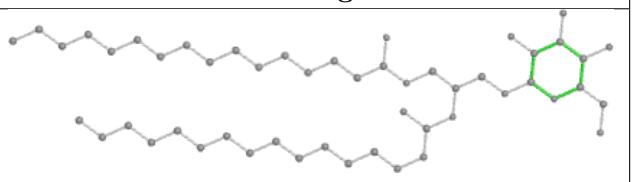
Rings

Ligand LMG A 612

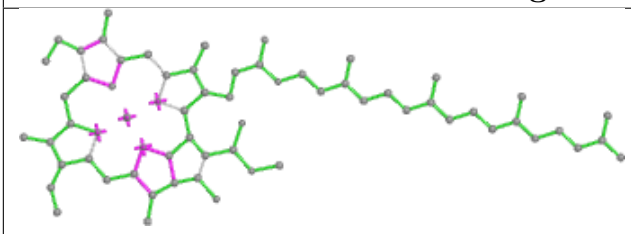

Bond lengths

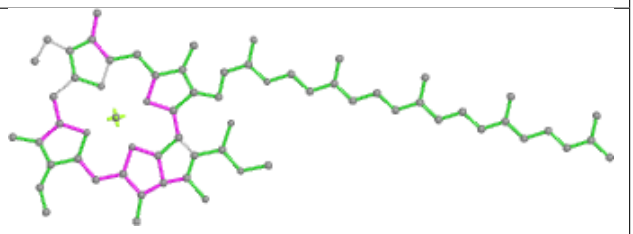

Bond angles

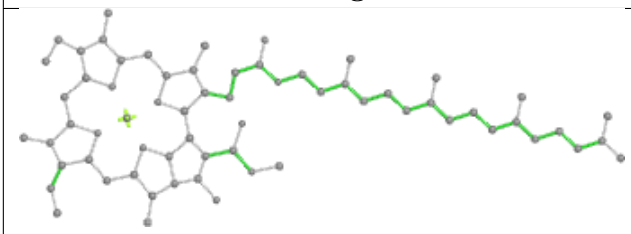

Torsions

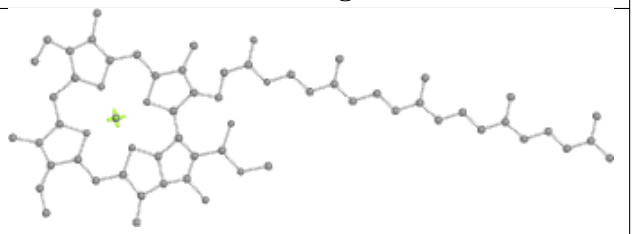

Rings

Ligand CLA c 511

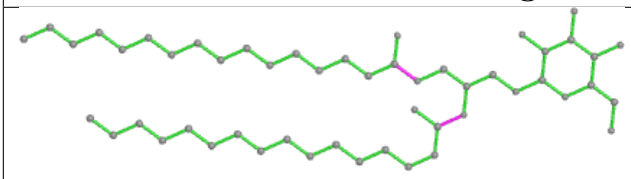

Bond lengths

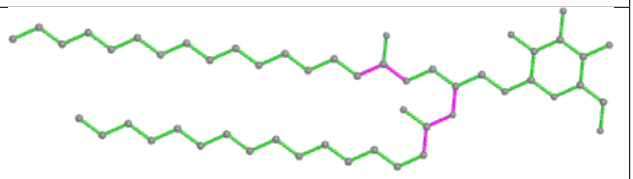

Bond angles

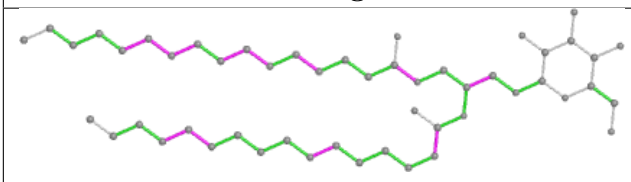

Torsions

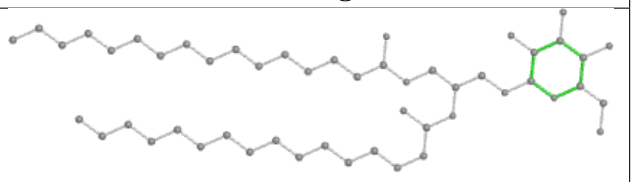

Rings

Ligand LMG A 603

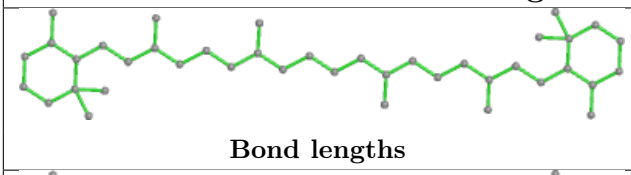

Bond lengths


Bond angles

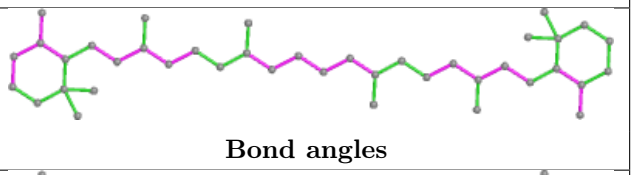

Torsions


Rings

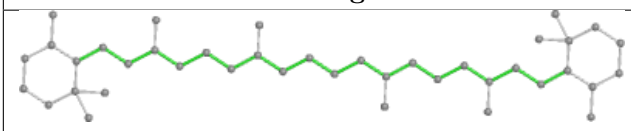
Ligand BCR a 611



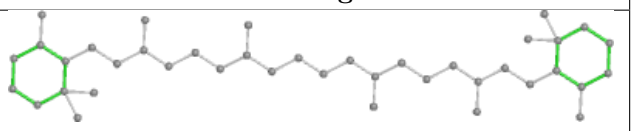
Bond lengths



Bond angles

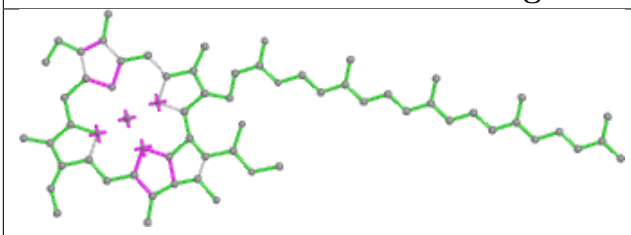


Torsions

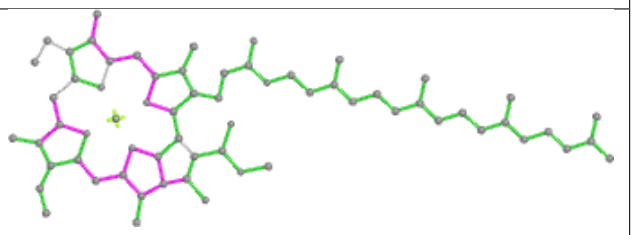


Rings

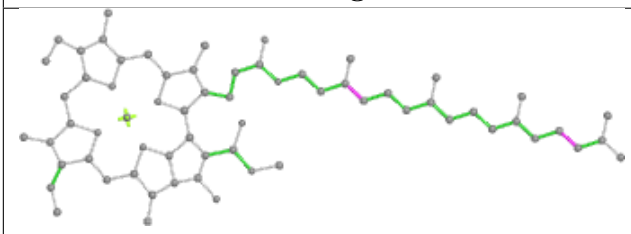
Ligand CLA A 608



Bond lengths



Bond angles



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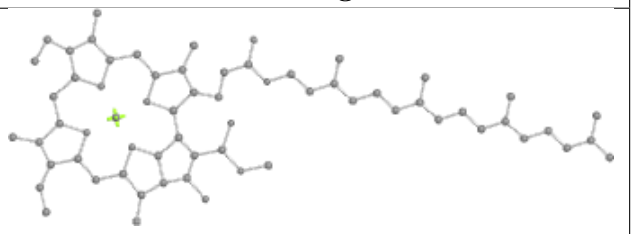
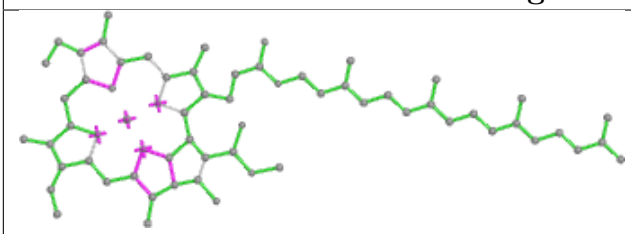
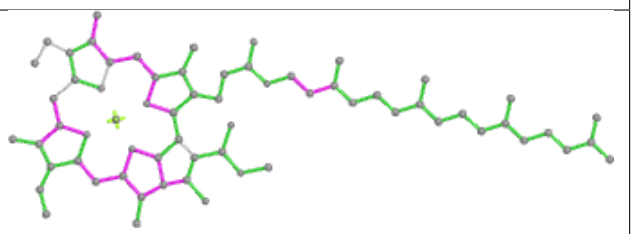


Rings

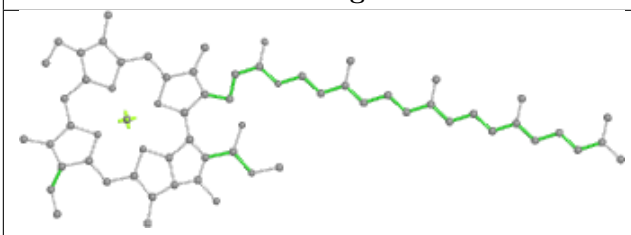
Ligand CLA b 611



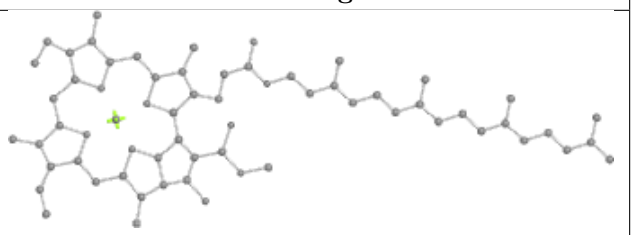
Bond lengths



Bond angles

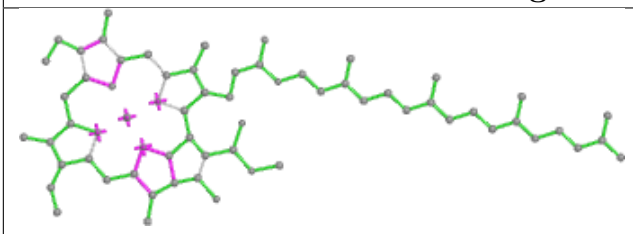


Torsions

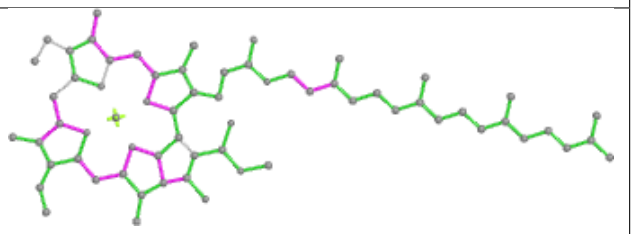


Rings

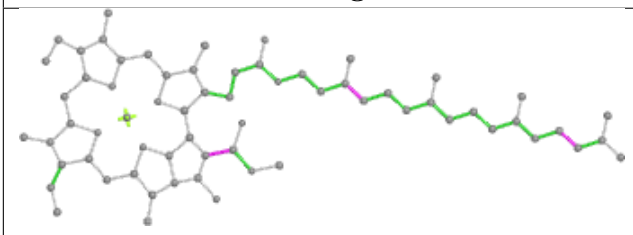
Ligand CLA c 503



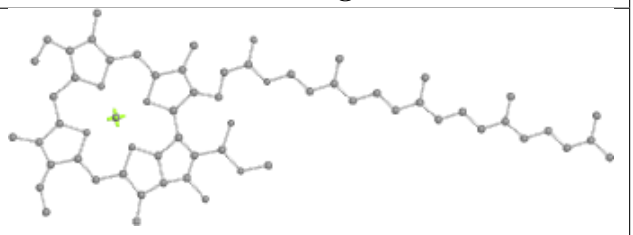
Bond lengths



Bond angles

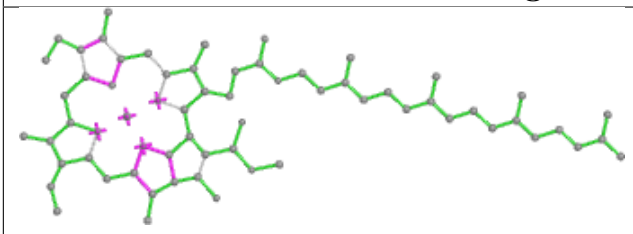


Torsions

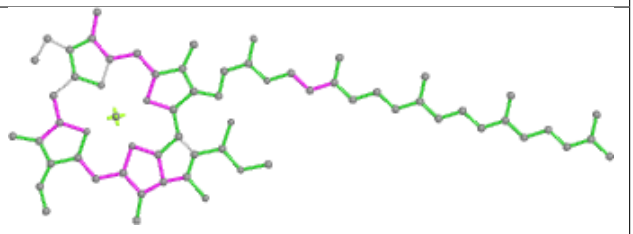


Rings

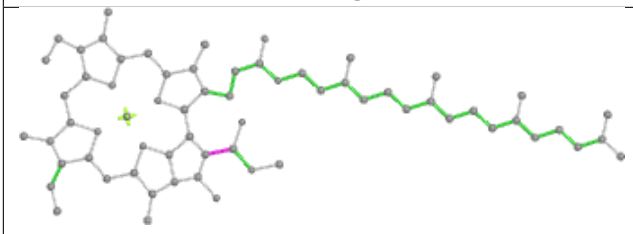
Ligand CLA C 502



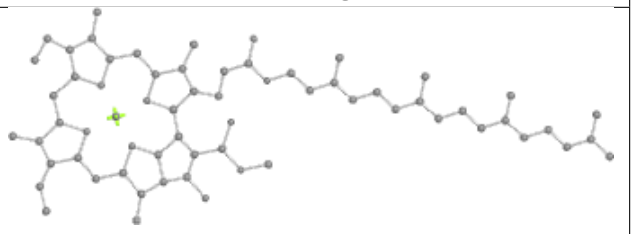
Bond lengths



Bond angles

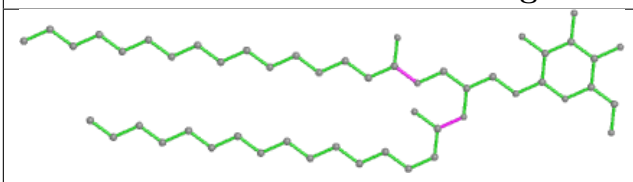


Torsions

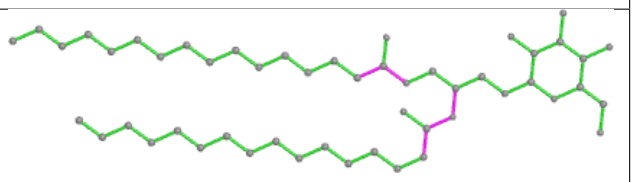


Rings

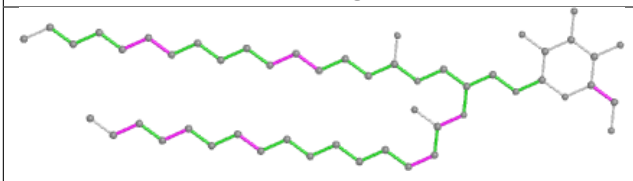
Ligand LMG B 624



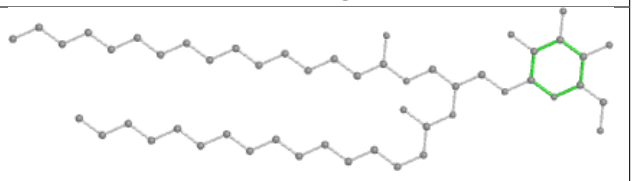
Bond lengths



Bond angles

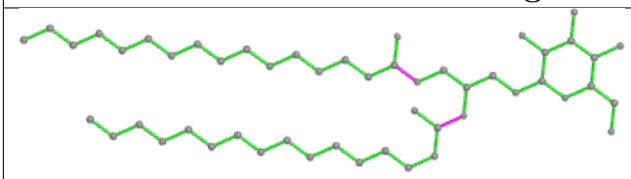


Torsions

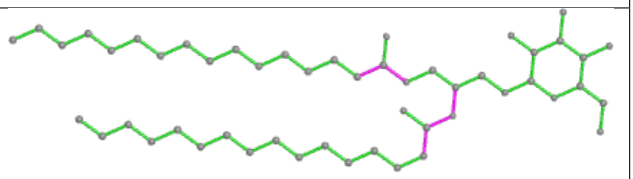


Rings

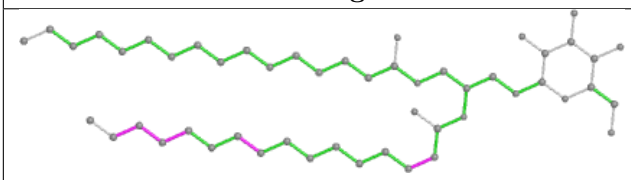
Ligand LMG a 614



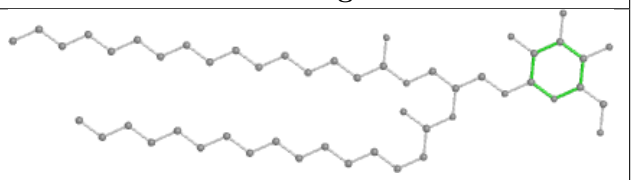
Bond lengths



Bond angles

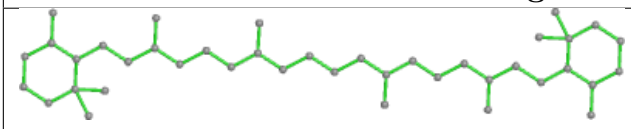


Torsions



Rings

Ligand BCR z 101



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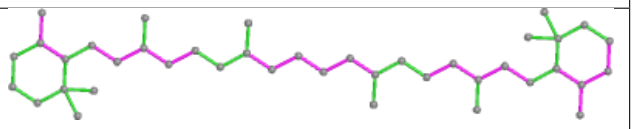
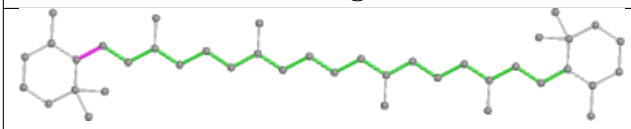


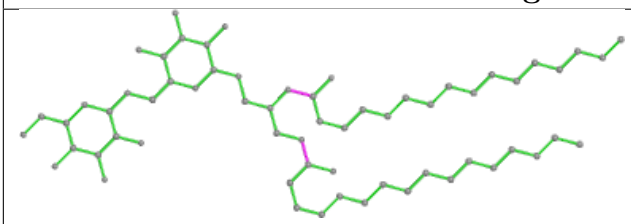
Bond angles



Torsions

Rings

Ligand DGD h 102



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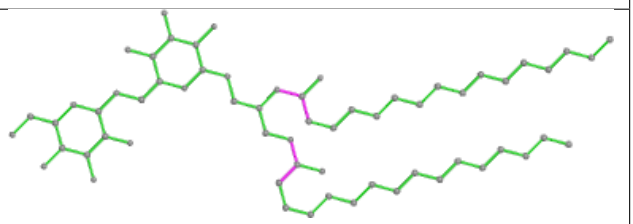
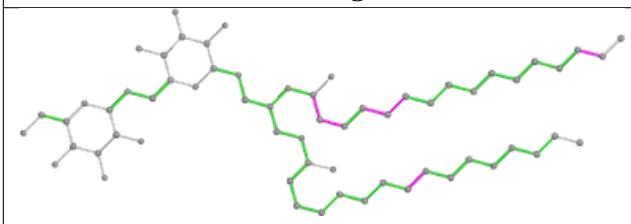
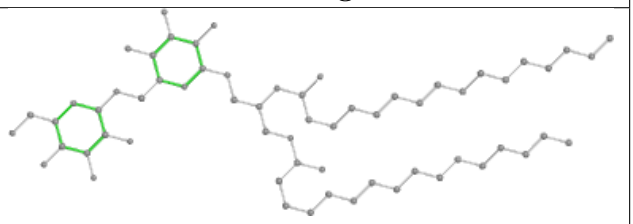


Bond angles

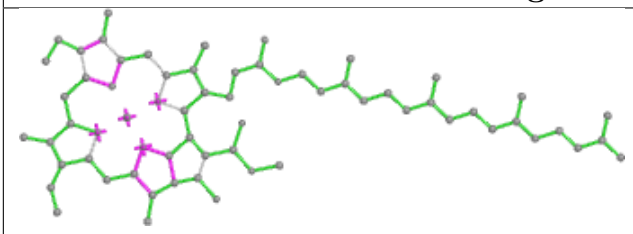


Torsions



Rings

Ligand CLA b 606



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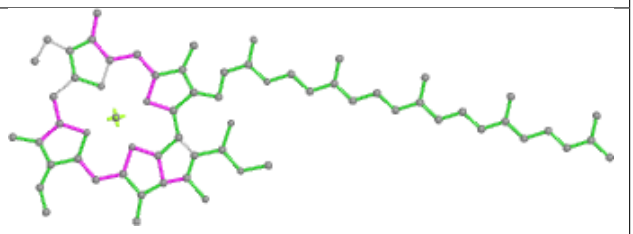
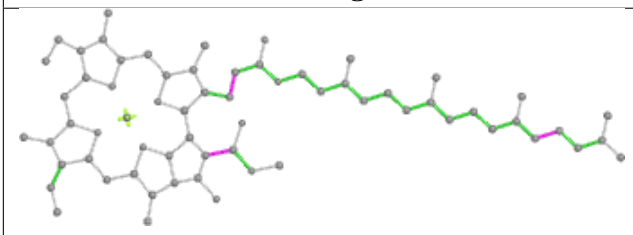
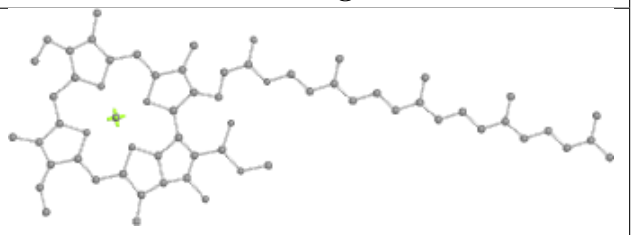


Bond angles

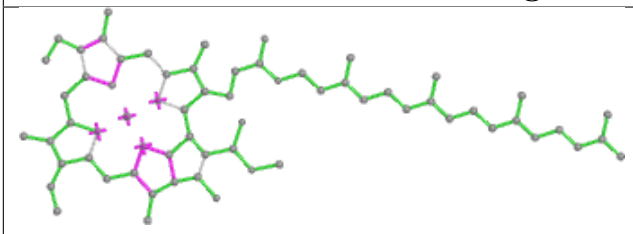


Torsions



Rings

Ligand CLA D 404



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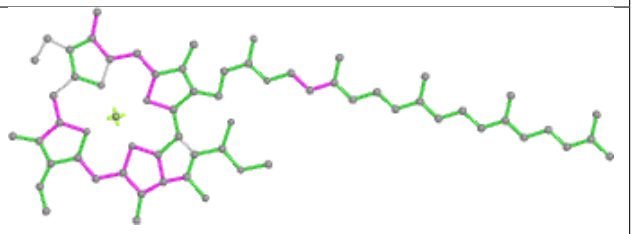
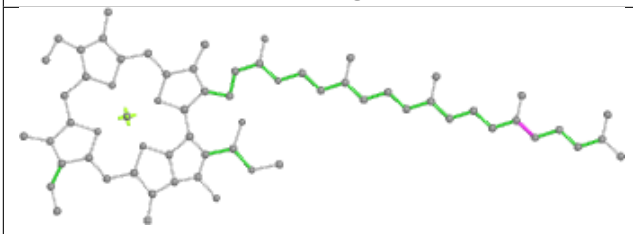
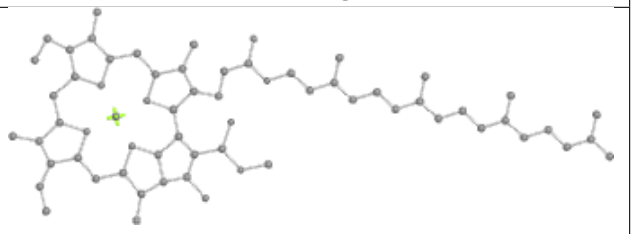


Bond angles

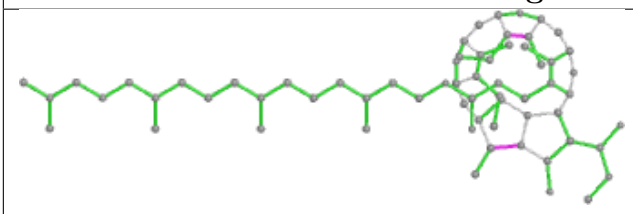


Torsions



Rings

Ligand PHO a 609



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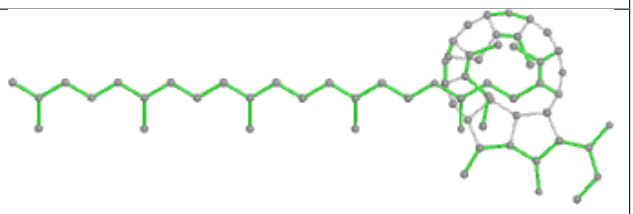
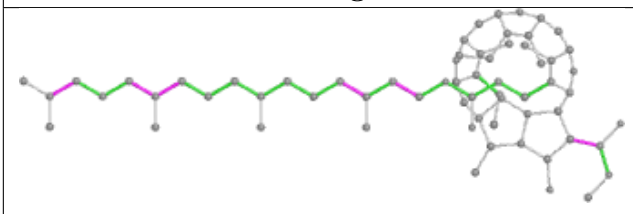
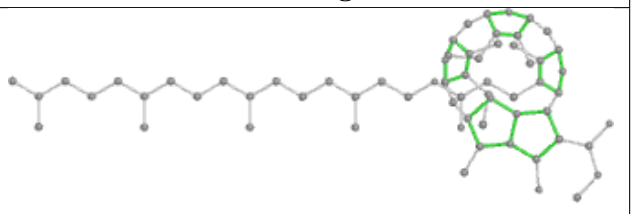


Bond angles

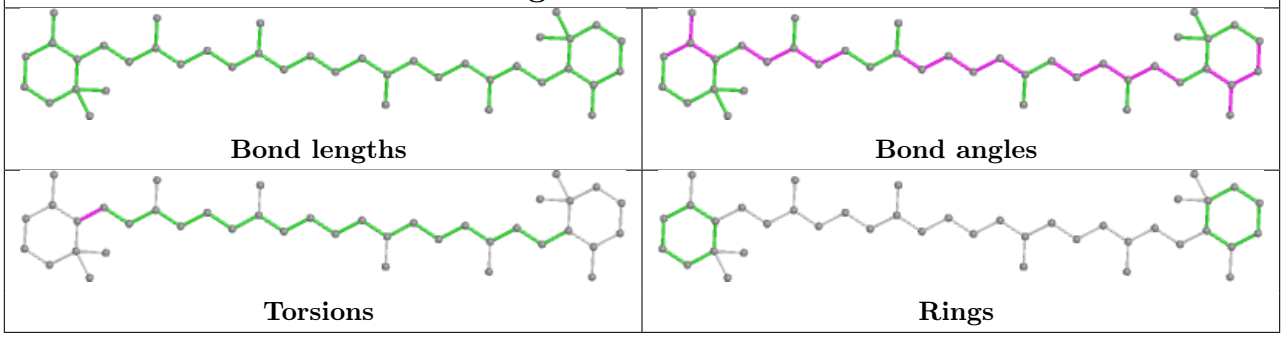


Torsions

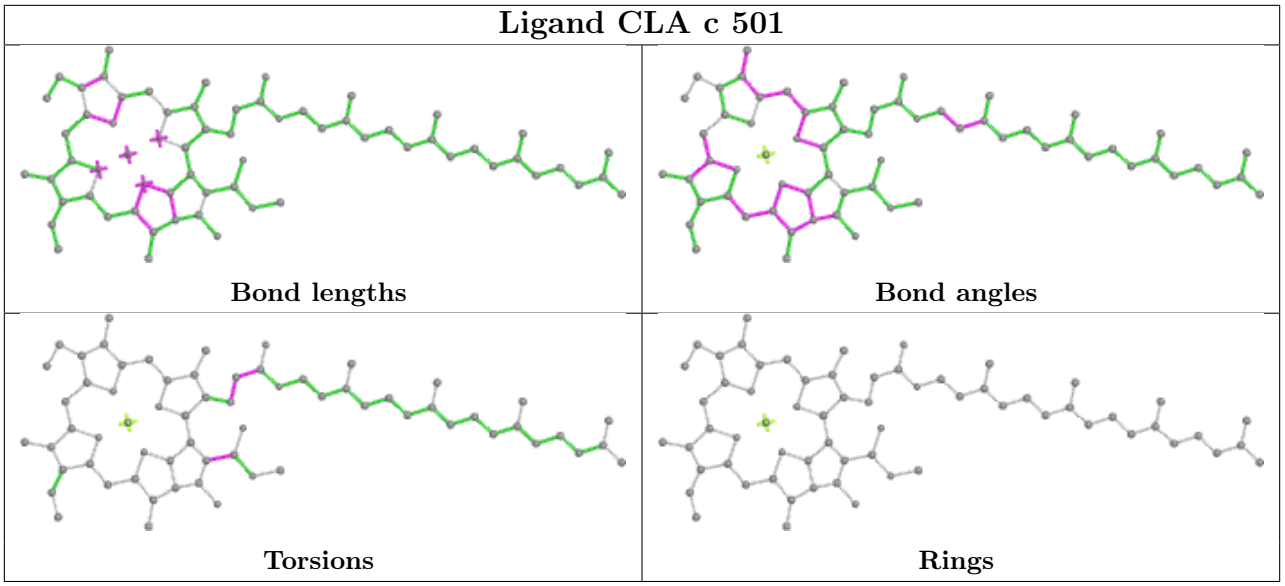


Rings

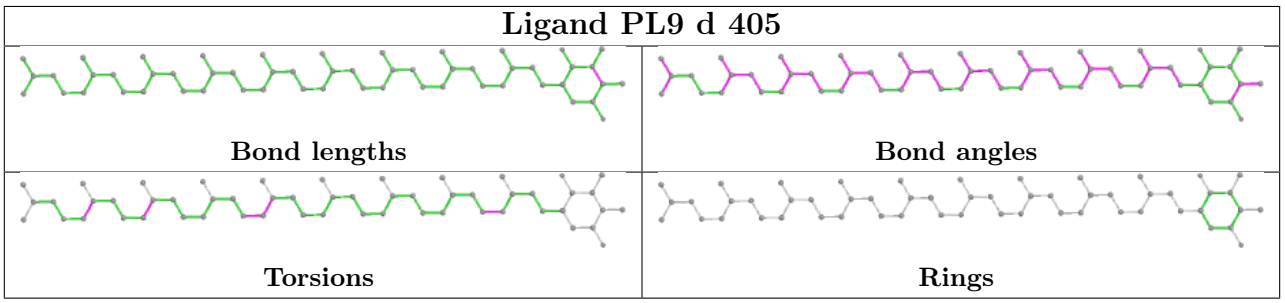
Ligand BCR c 514



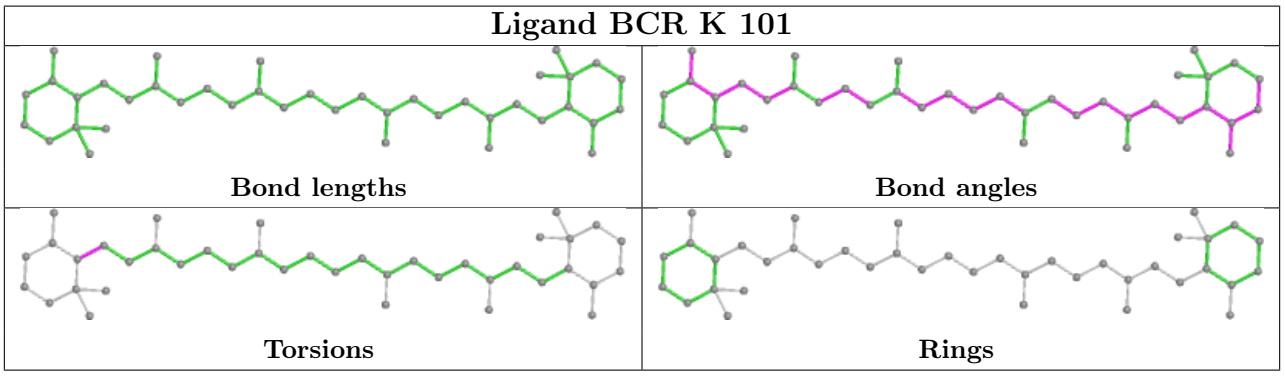
Ligand CLA c 501



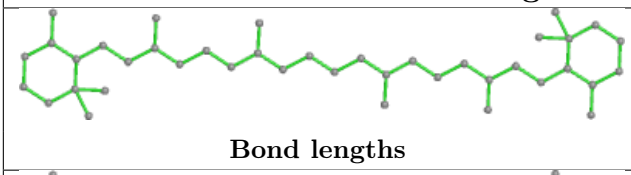
Ligand PL9 d 405



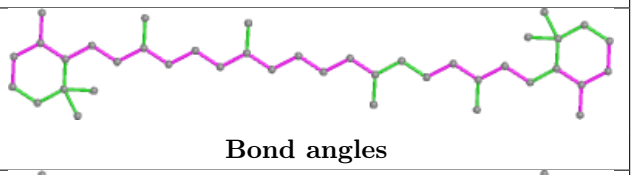
Ligand BCR K 101



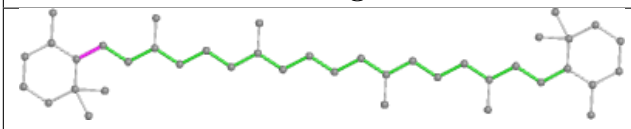
Ligand BCR C 514



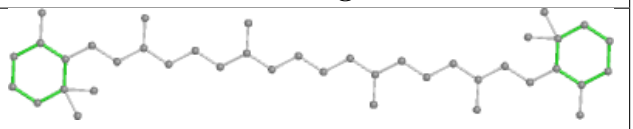
Bond lengths



Bond angles

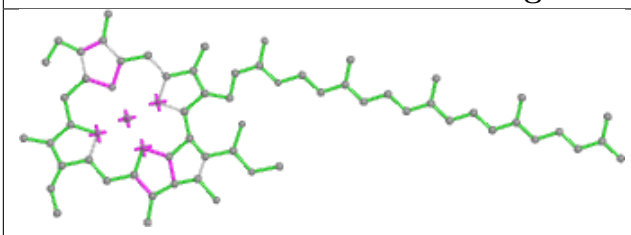


Torsions

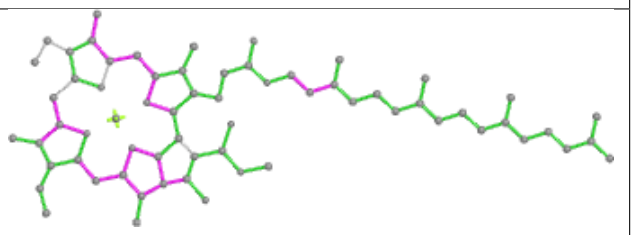


Rings

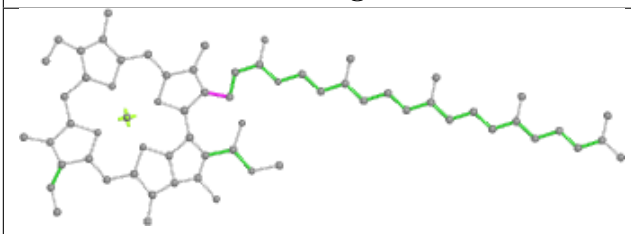
Ligand CLA B 611



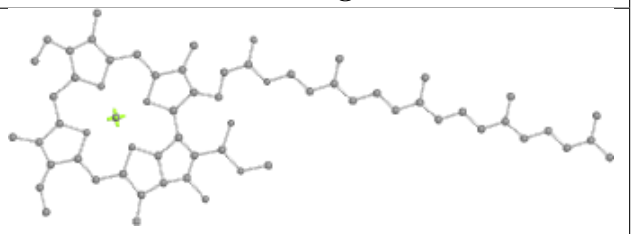
Bond lengths



Bond angles

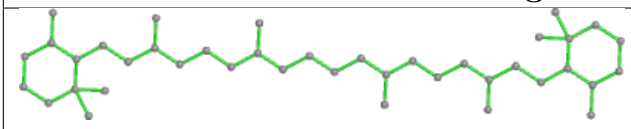


Torsions

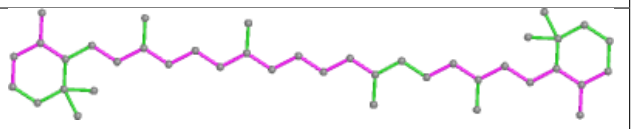


Rings

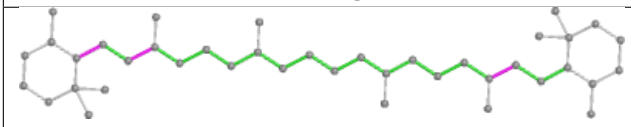
Ligand BCR d 404



Bond lengths



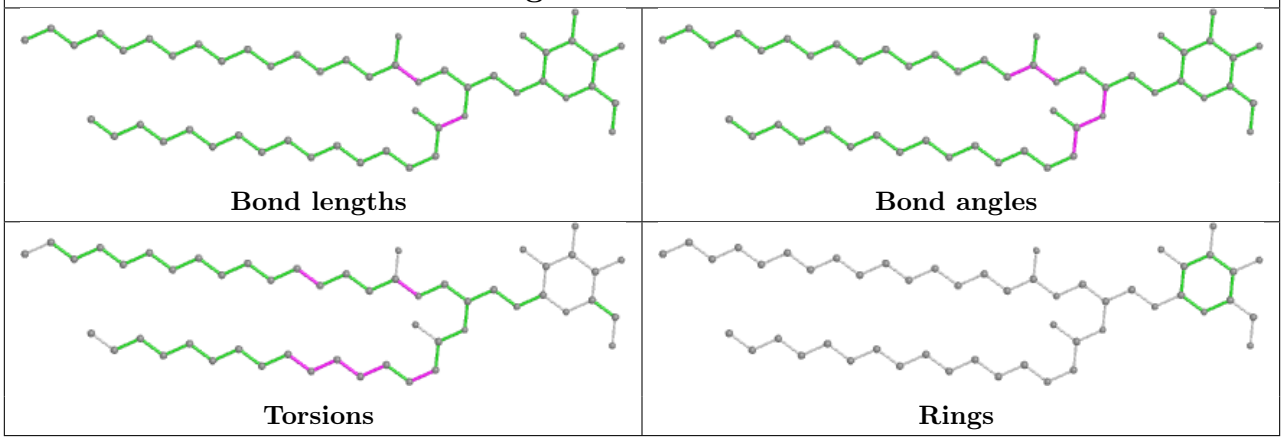
Bond angles



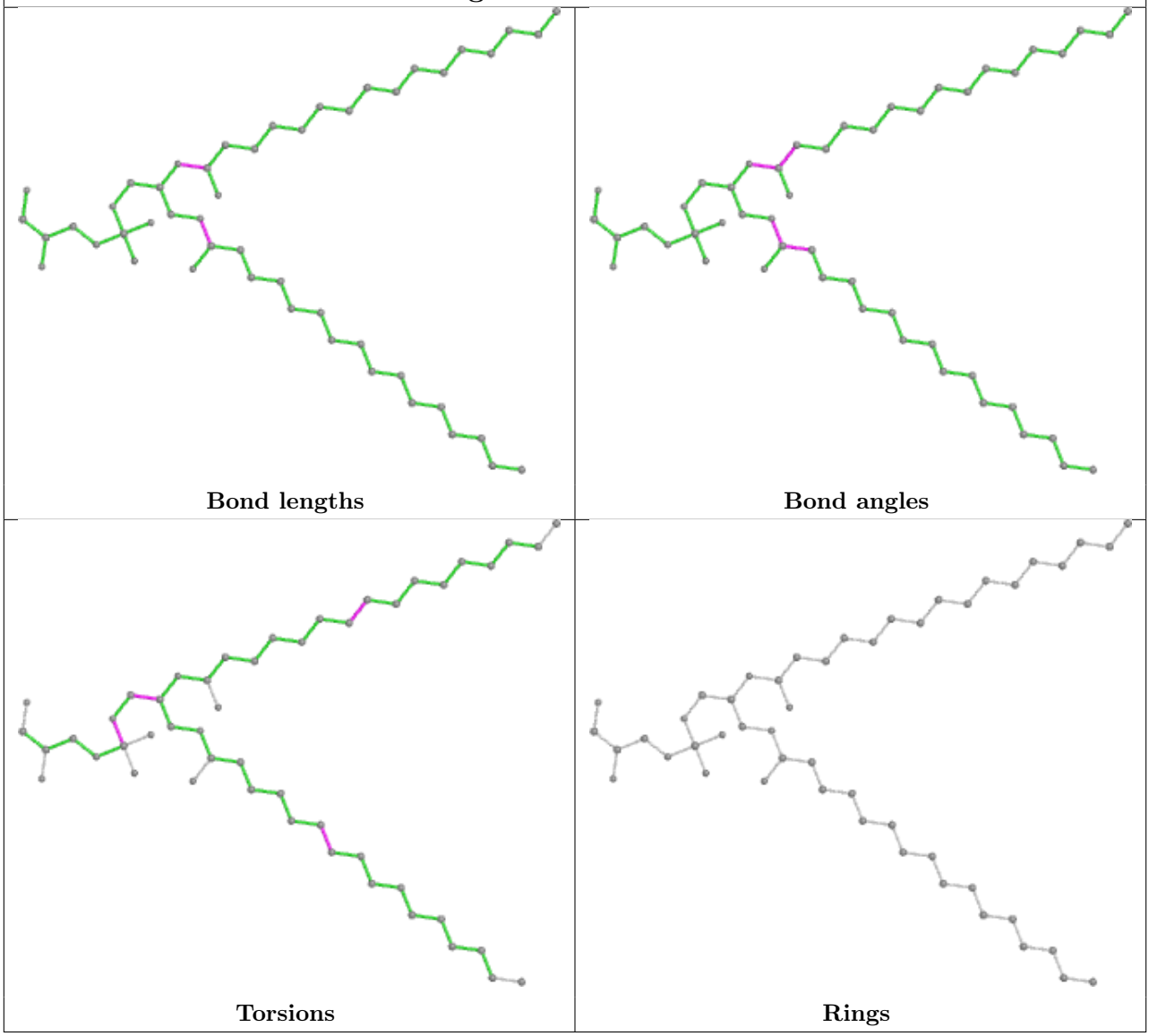
Torsions

Rings

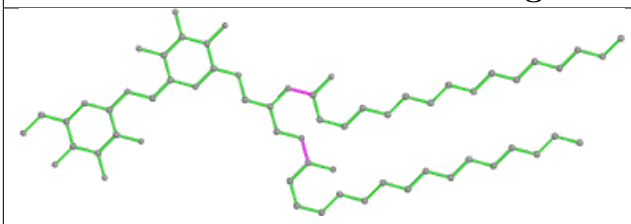
Ligand LMG c 518



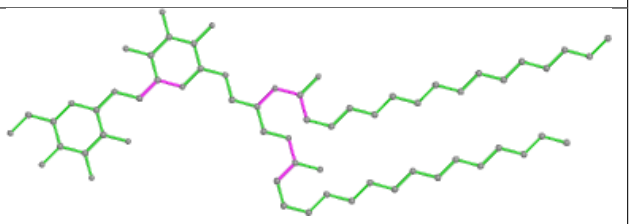
Ligand LHG A 614



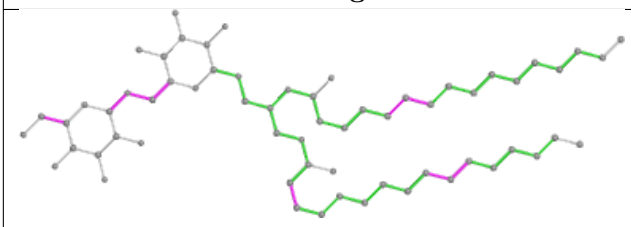
Ligand DGD c 515



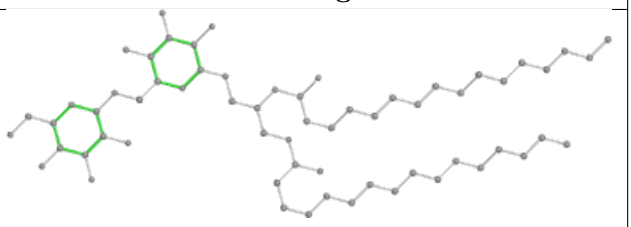
Bond lengths



Bond angles

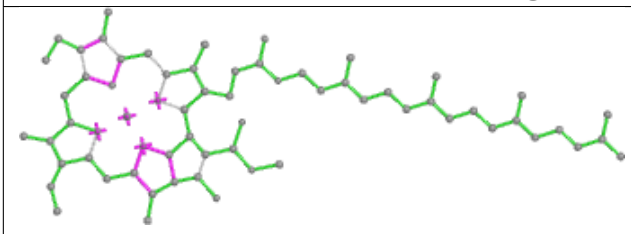


Torsions

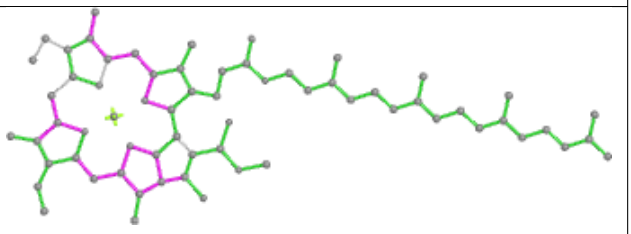


Rings

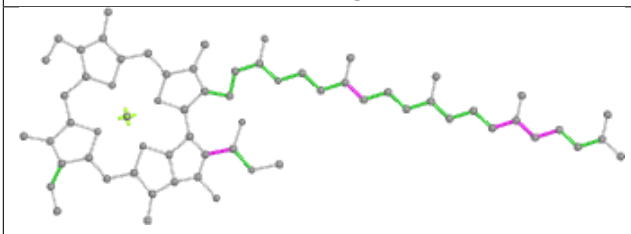
Ligand CLA B 605



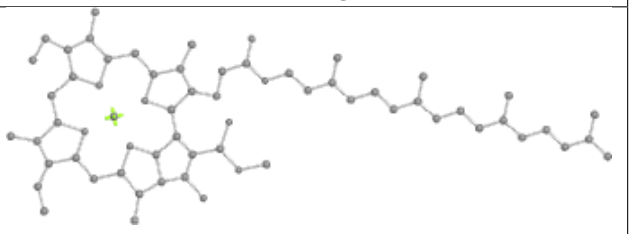
Bond lengths



Bond angles

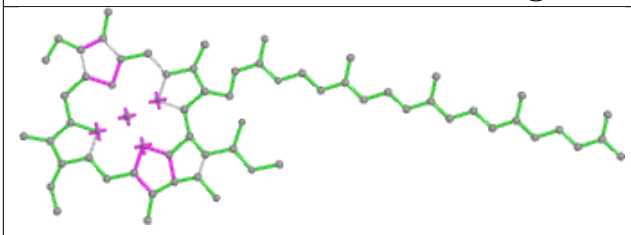


Torsions

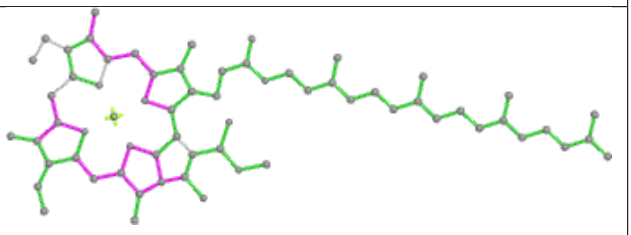


Rings

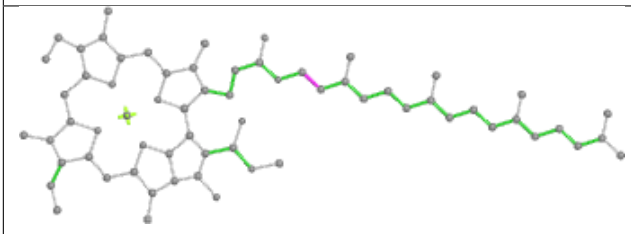
Ligand CLA d 403



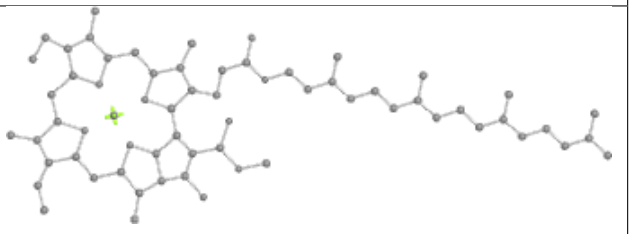
Bond lengths



Bond angles

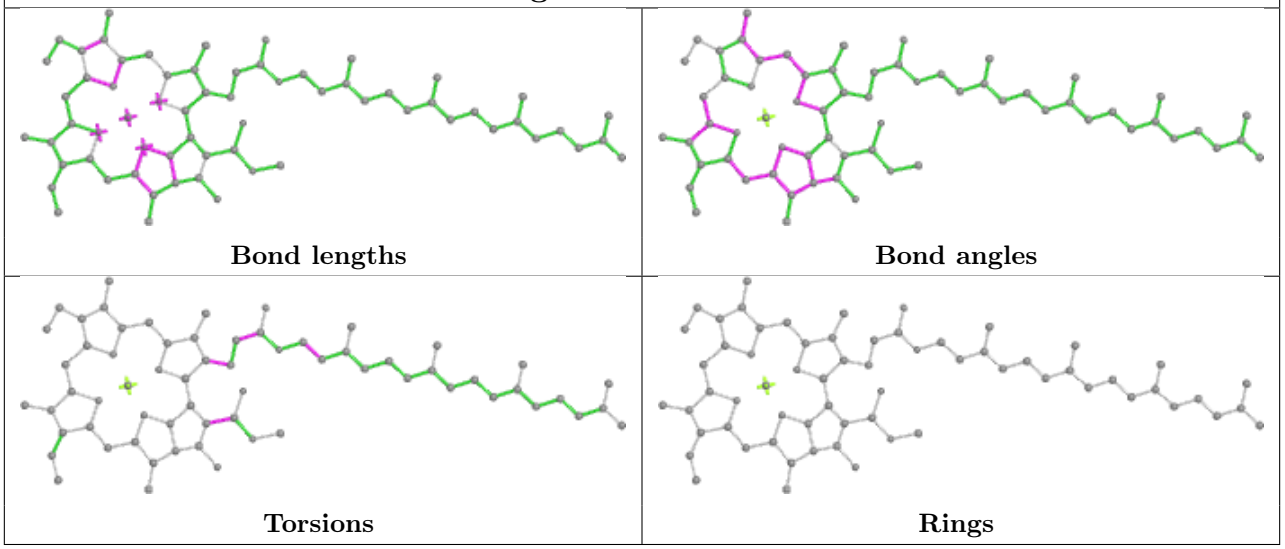


Torsions

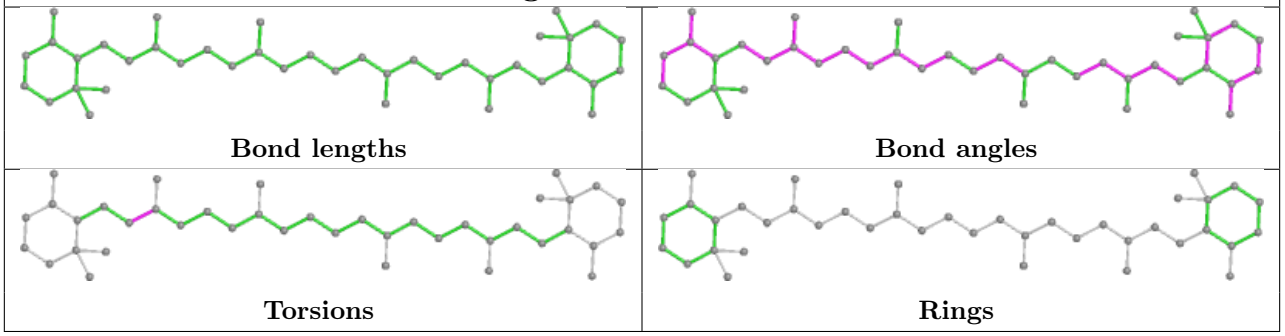


Rings

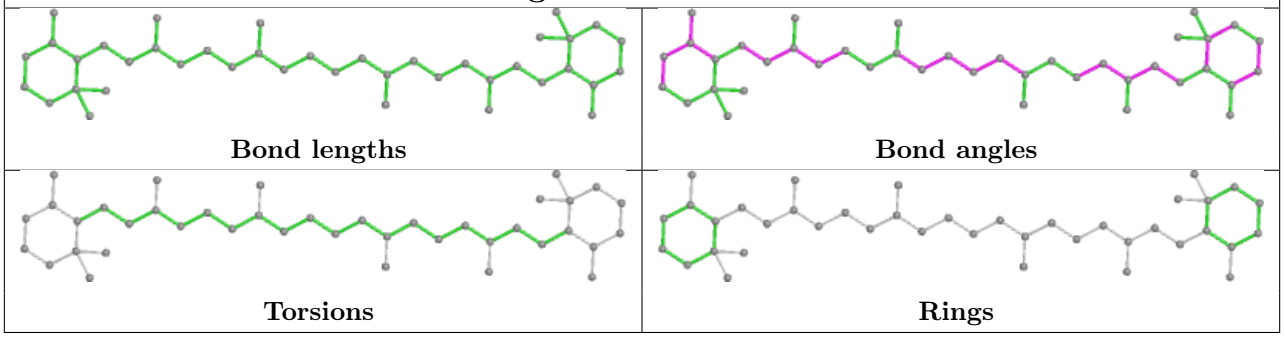
Ligand CLA c 512



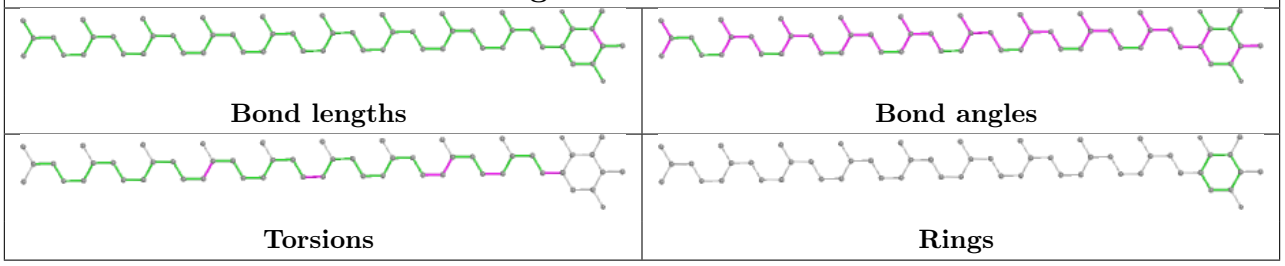
Ligand BCR H 101



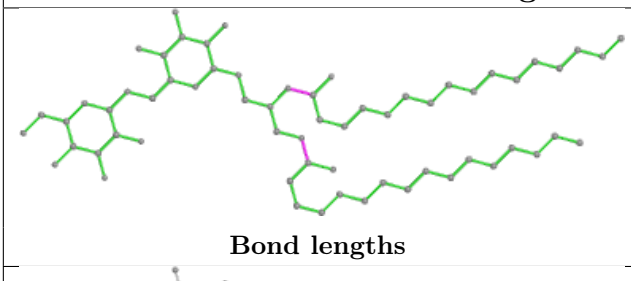
Ligand BCR c 521



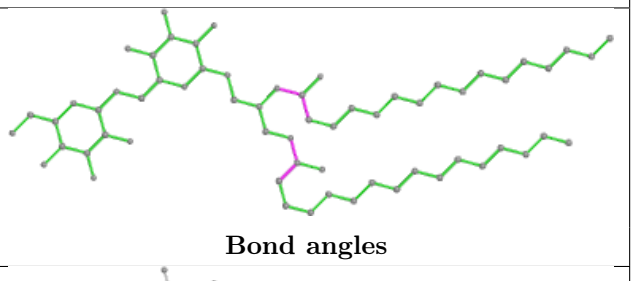
Ligand PL9 A 610



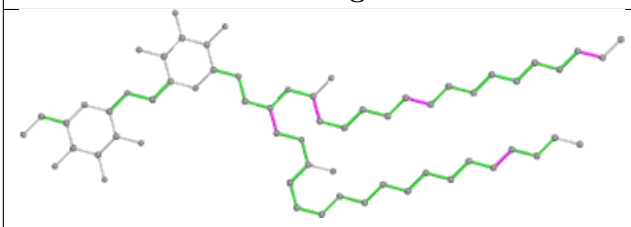
Ligand DGD H 102



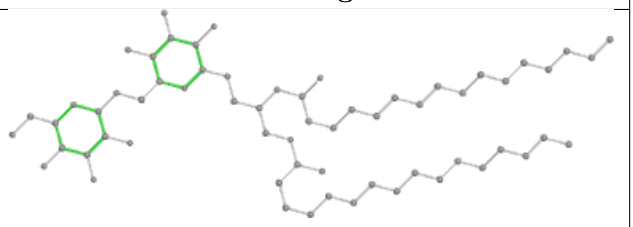
Bond lengths



Bond angles

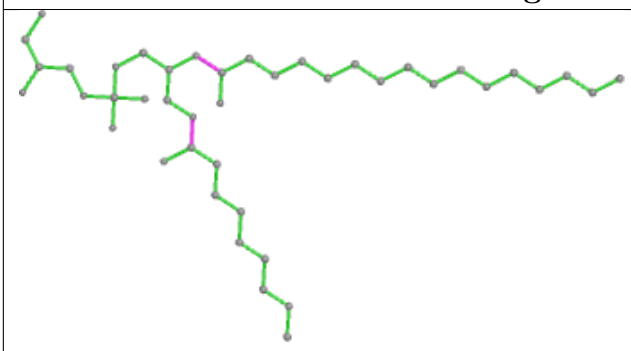


Torsions

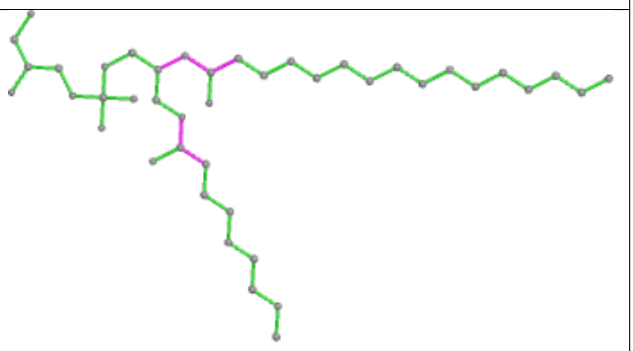


Rings

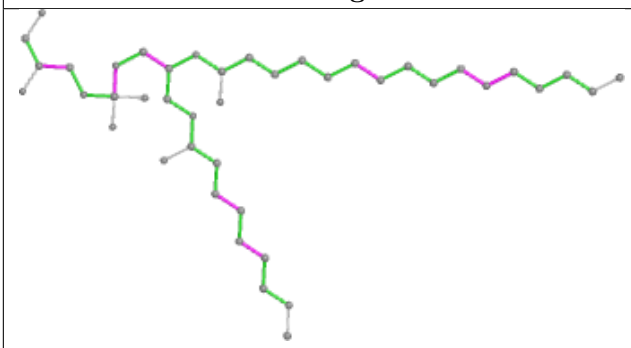
Ligand LHG E 101



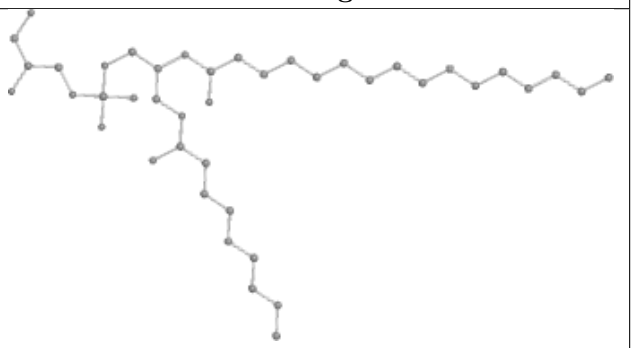
Bond lengths



Bond angles

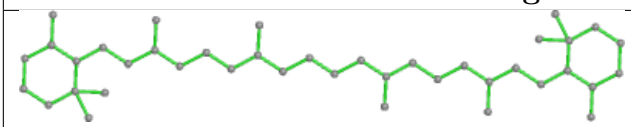


Torsions

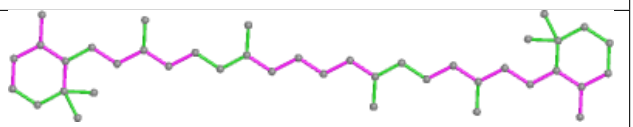


Rings

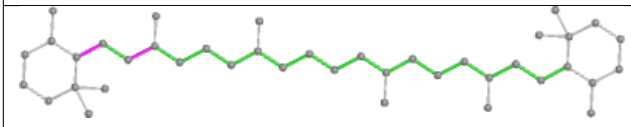
Ligand BCR B 619



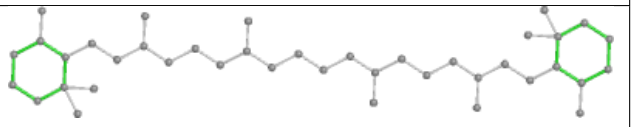
Bond lengths



Bond angles

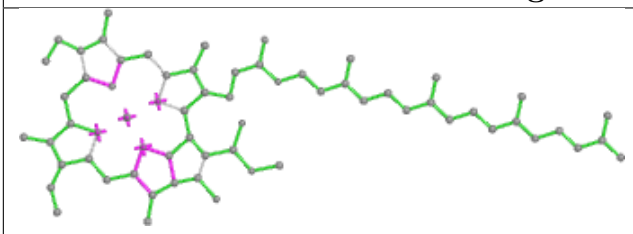


Torsions

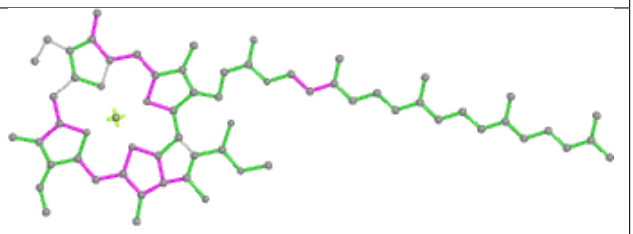


Rings

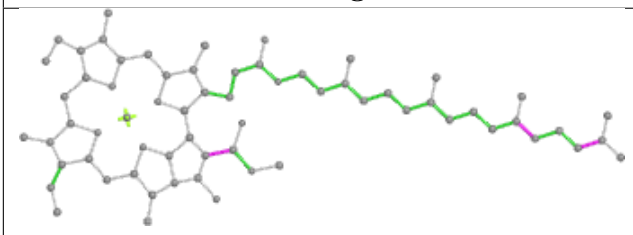
Ligand CLA b 607



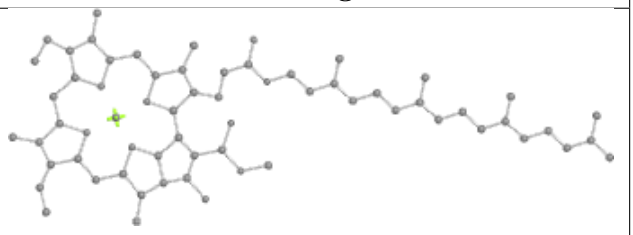
Bond lengths



Bond angles

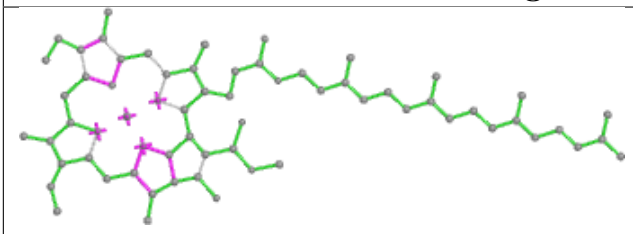


Torsions

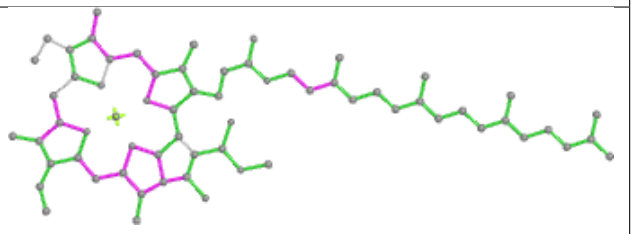


Rings

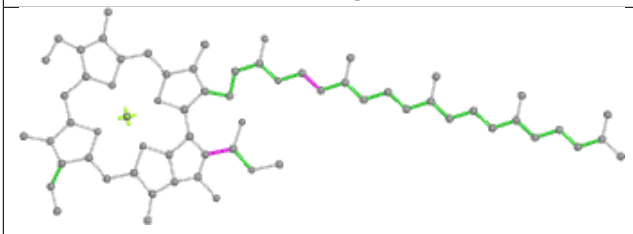
Ligand CLA C 509



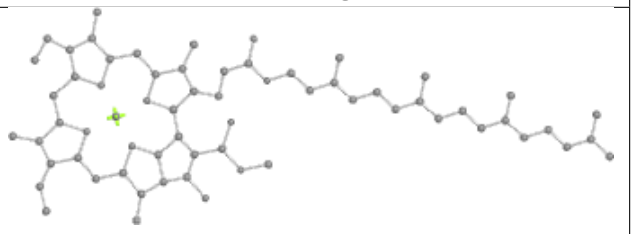
Bond lengths



Bond angles

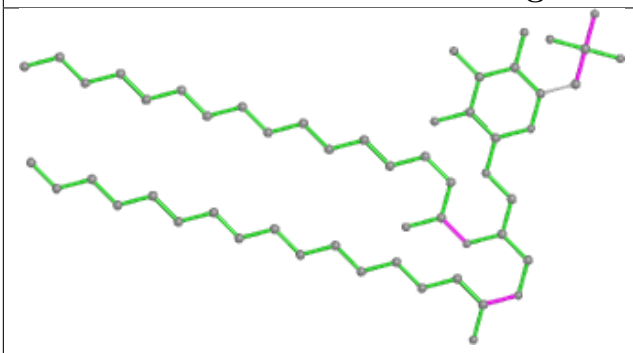


Torsions

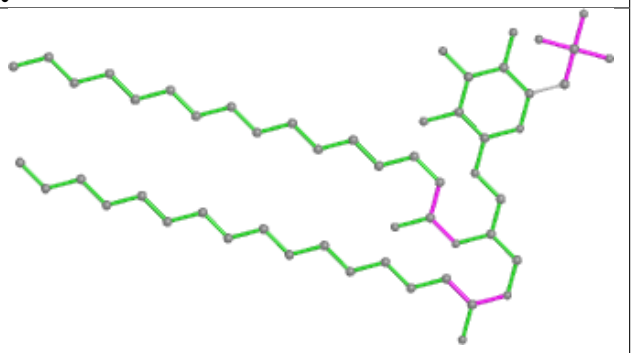


Rings

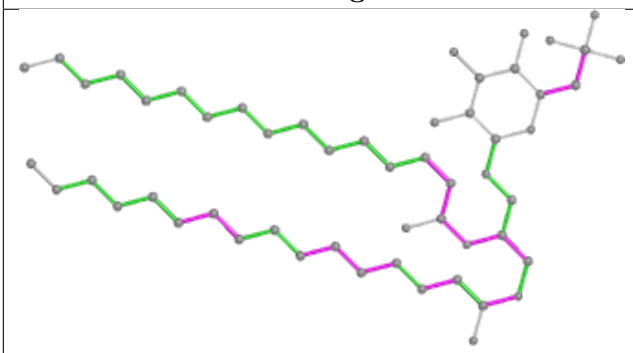
Ligand SQD L 101



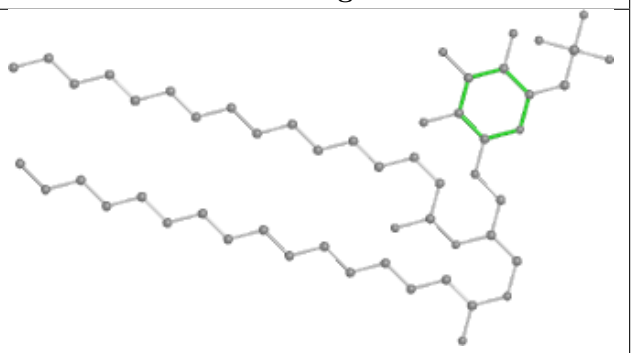
Bond lengths



Bond angles

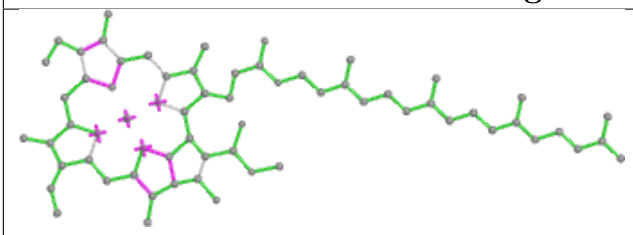


Torsions

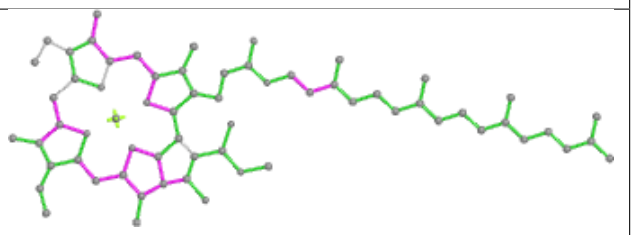


Rings

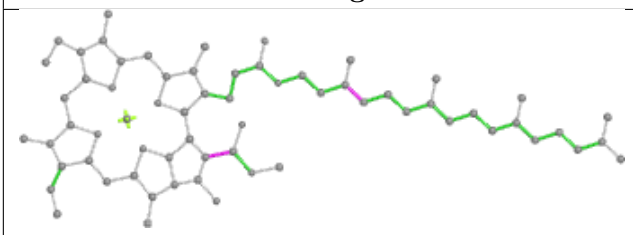
Ligand CLA C 513



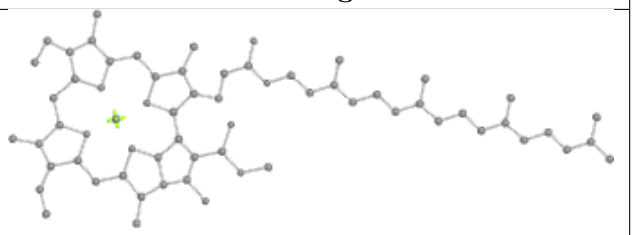
Bond lengths



Bond angles

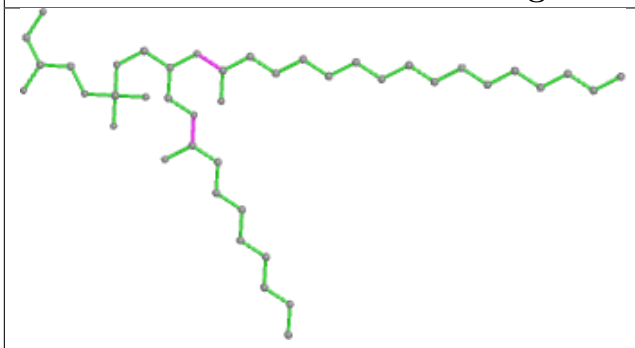


Torsions

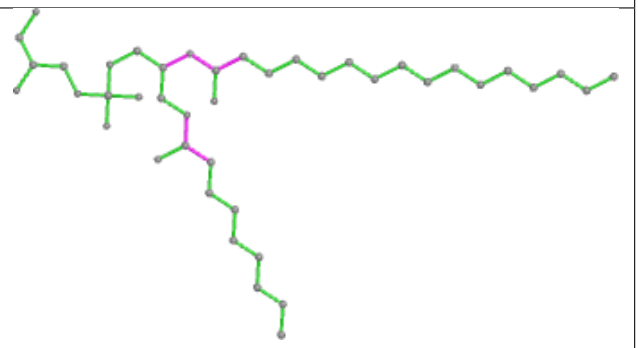


Rings

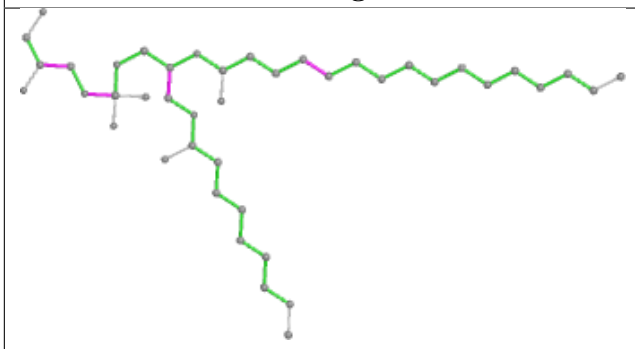
Ligand LHG a 616



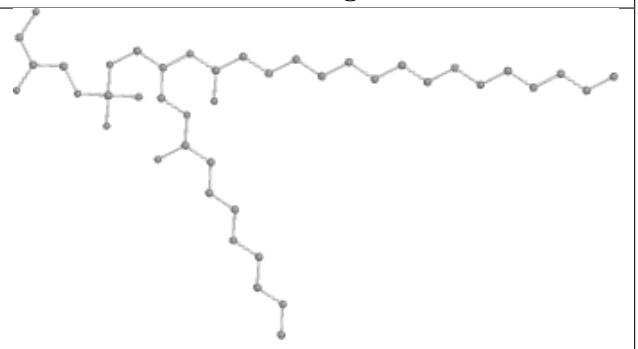
Bond lengths



Bond angles

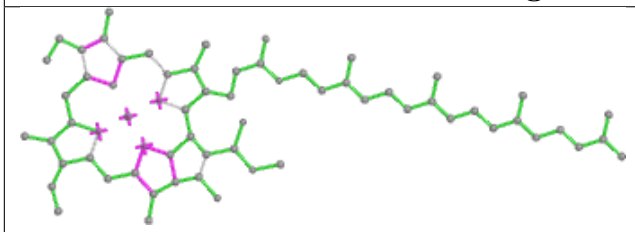


Torsions

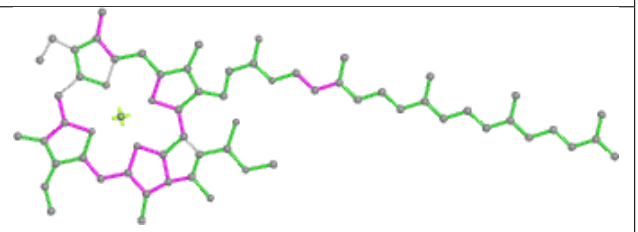


Rings

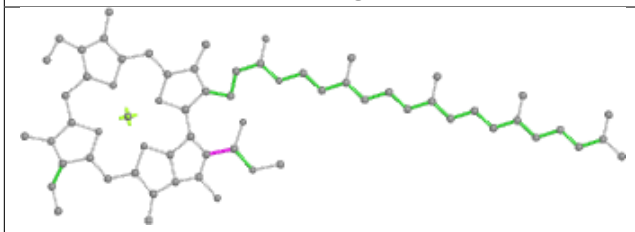
Ligand CLA B 604



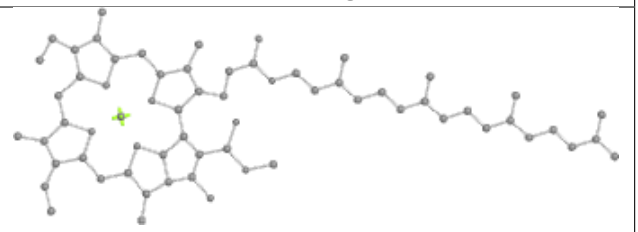
Bond lengths



Bond angles

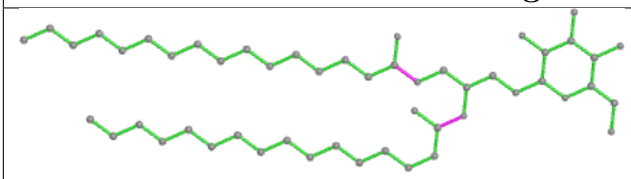


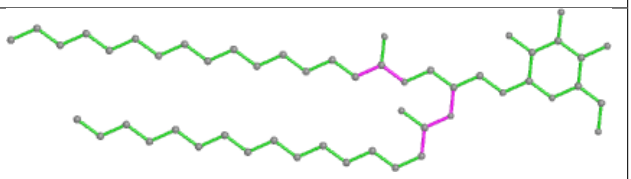
Torsions

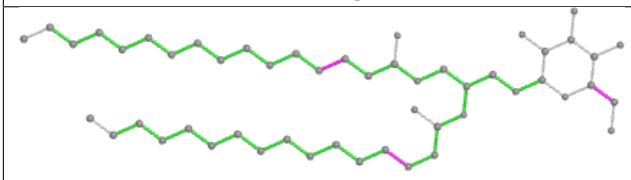


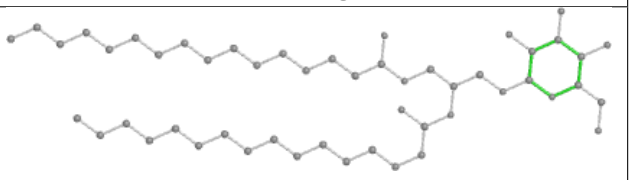
Rings

Ligand LMG d 408

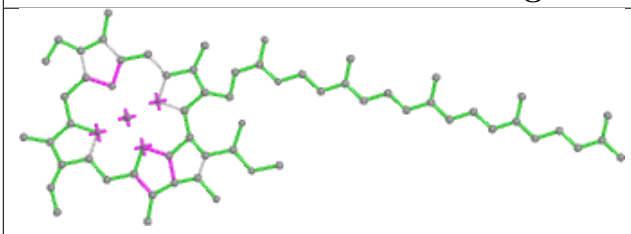

Bond lengths

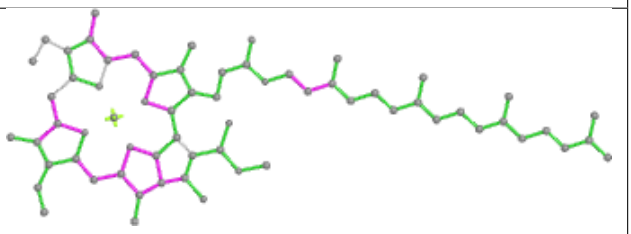

Bond angles

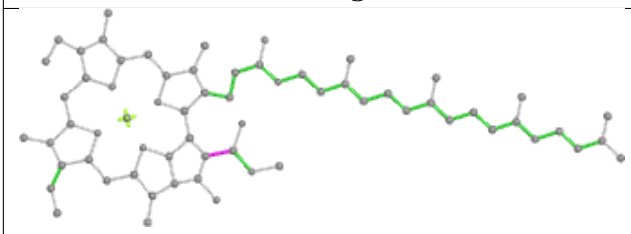

Torsions

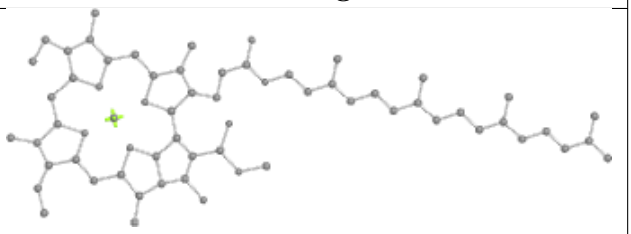

Rings

Ligand CLA B 612

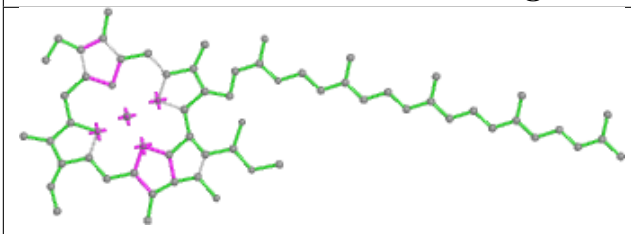

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA C 506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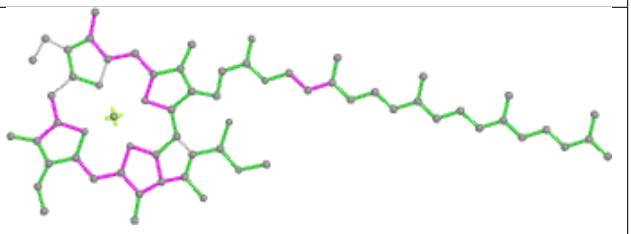
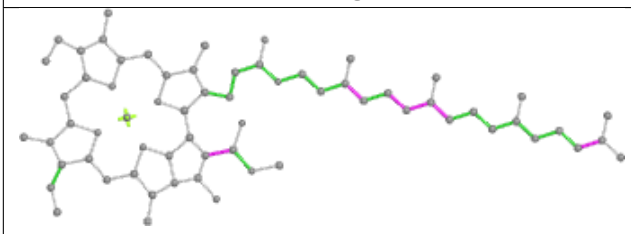

Bond angles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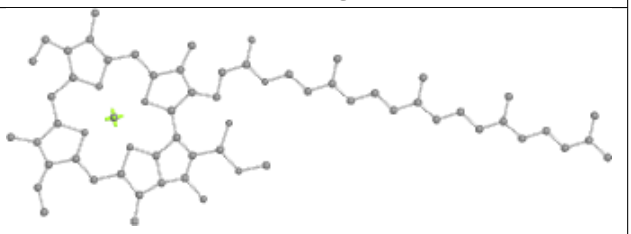
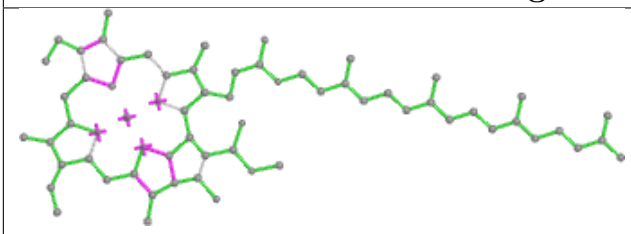
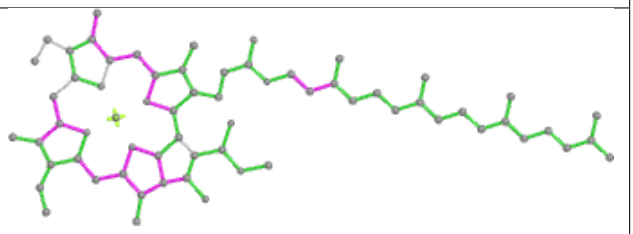

Rings

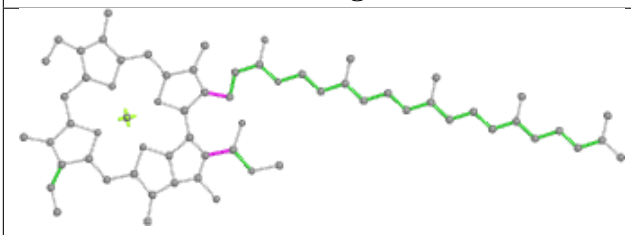
Ligand CLA a 607



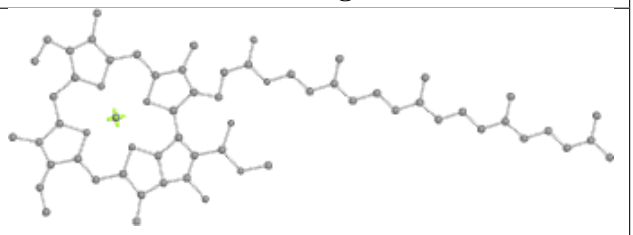
Bond lengths



Bond angles

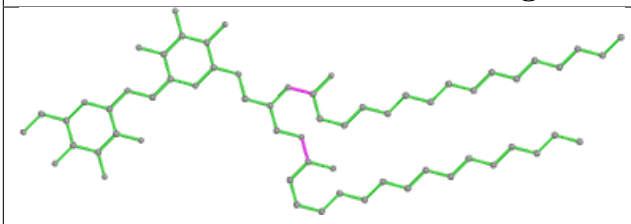


Torsions

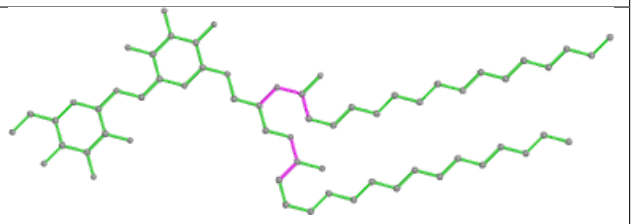


Rings

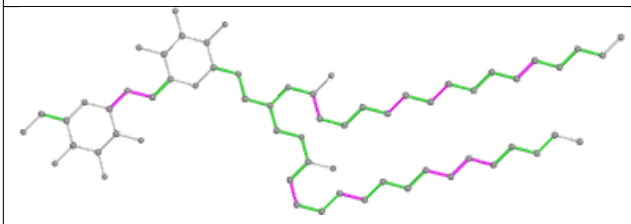
Ligand DGD C 517



Bond lengths



Bond angles



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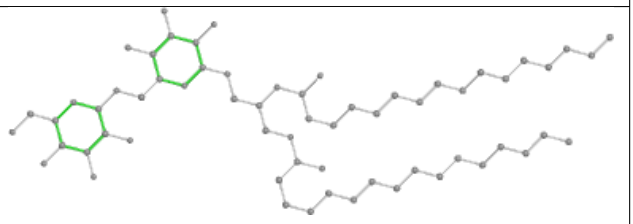
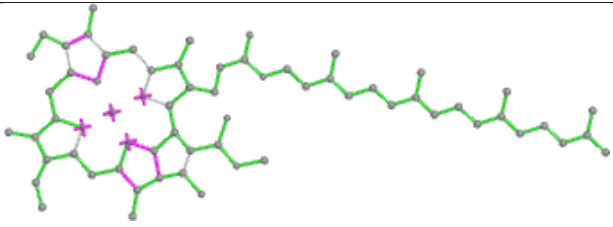
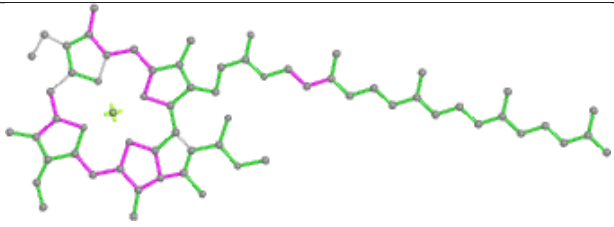


Rings

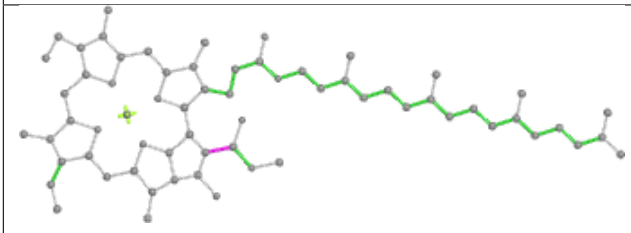
Ligand CLA c 508



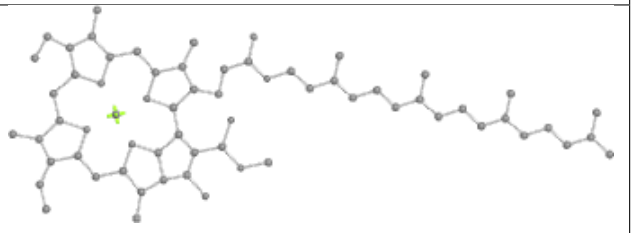
Bond lengths



Bond angles

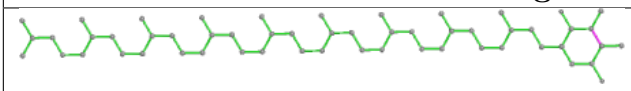


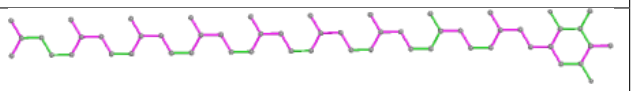
Torsions

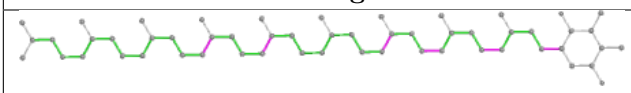


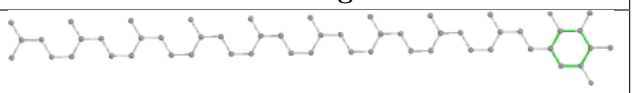
Rings

Ligand PL9 a 612

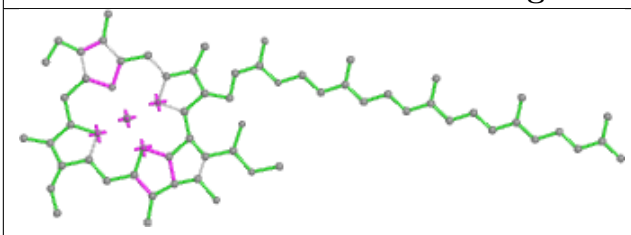

Bond lengths

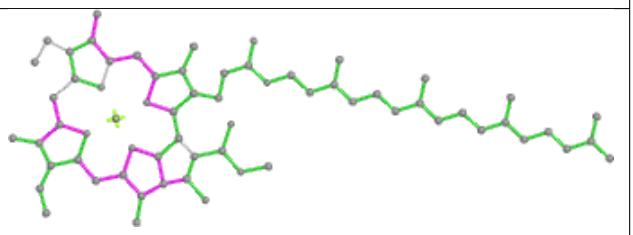

Bond angles

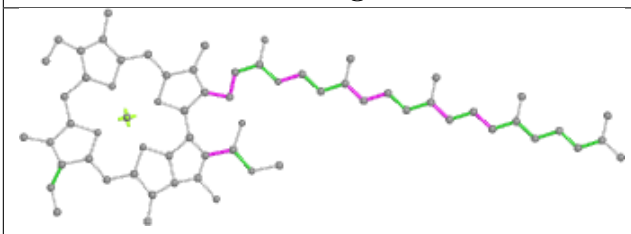

Torsions

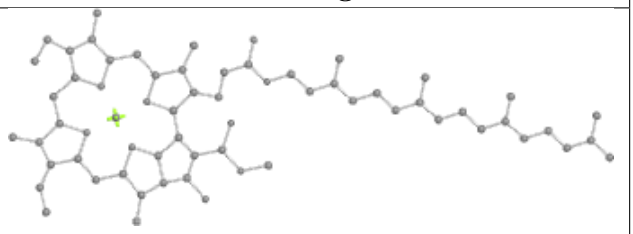

Rings

Ligand CLA b 614

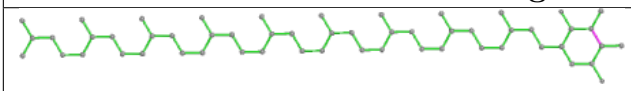

Bond lengths

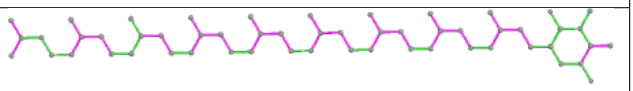

Bond angles

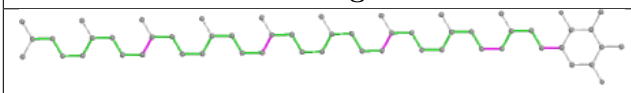

Torsions

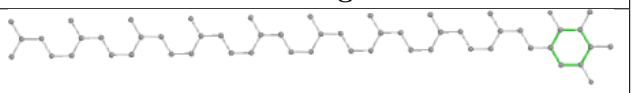

Rings

Ligand PL9 D 407

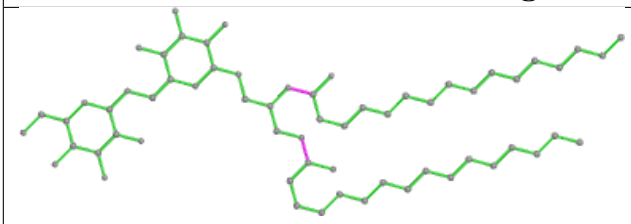

Bond lengths

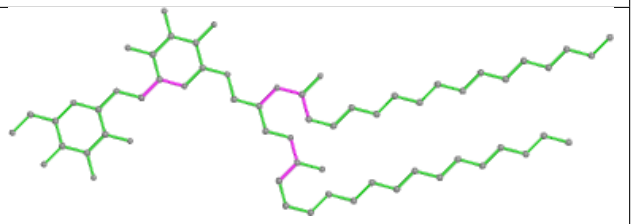

Bond angles

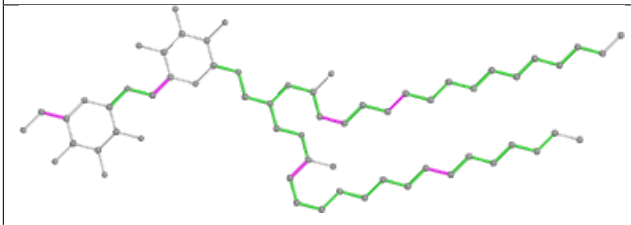

Torsions


Rings

Ligand DGD C 516


Bond lengths


Bond angles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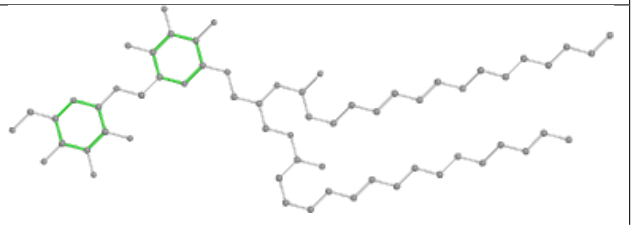
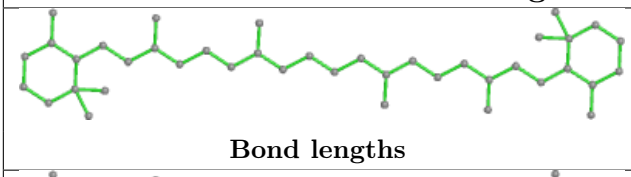
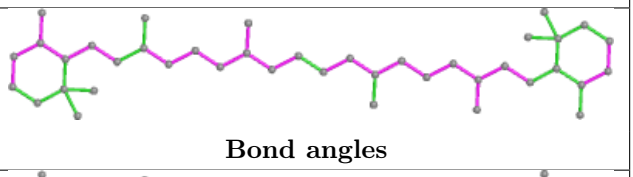

Rings

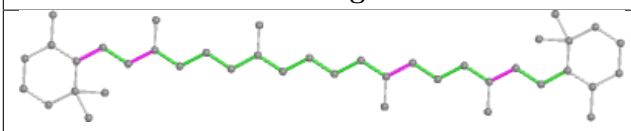
Ligand BCR t 102



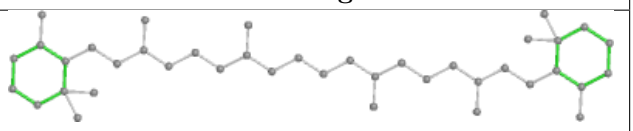
Bond lengths



Bond angles

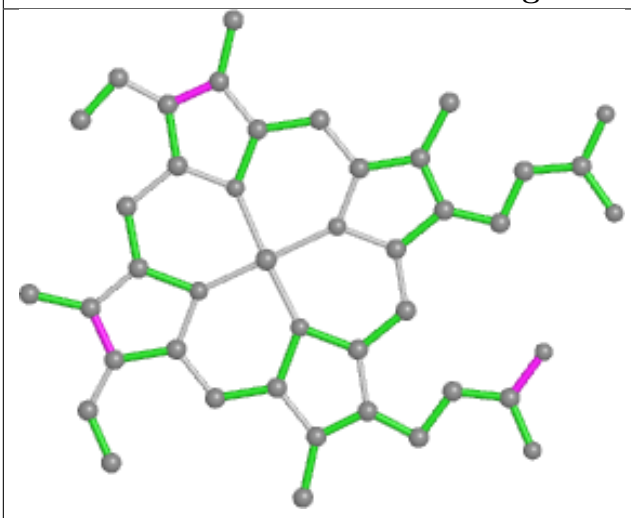


Torsions

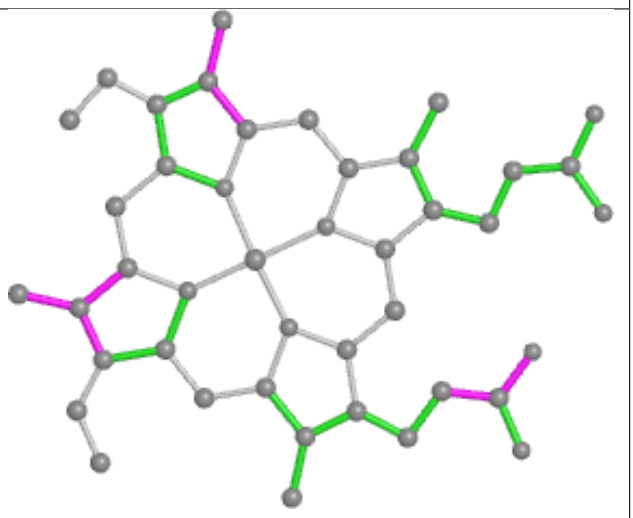


Rings

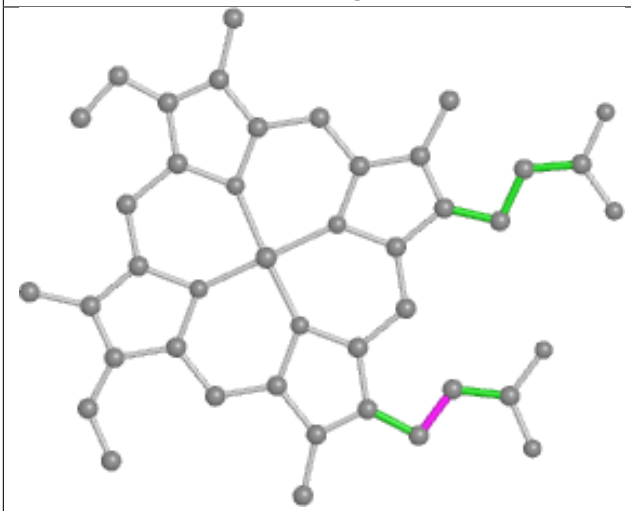
Ligand HEC V 201



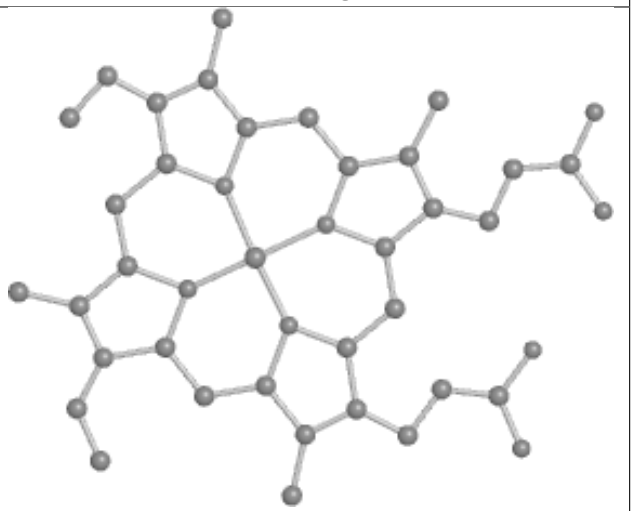
Bond lengths



Bond angles

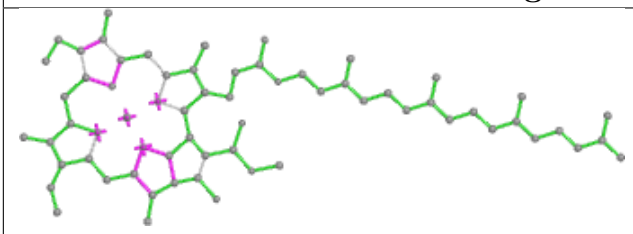


Torsions

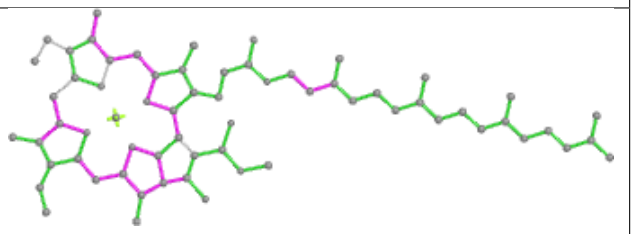


Rings

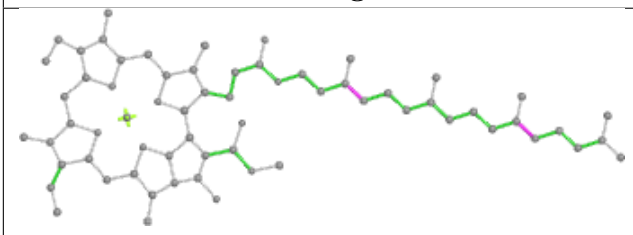
Ligand CLA B 609



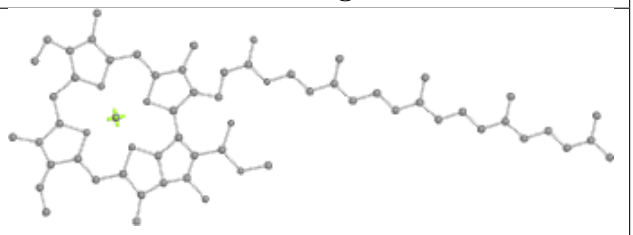
Bond lengths



Bond angles

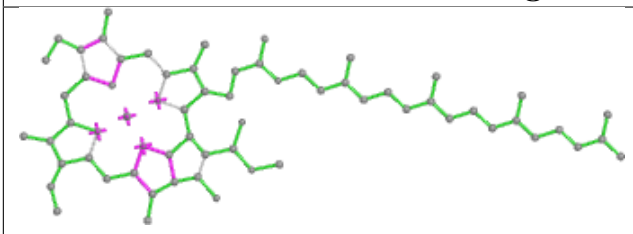


Torsions

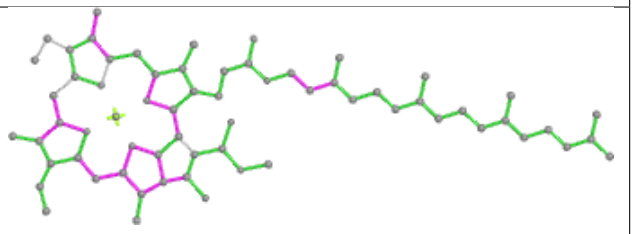


Rings

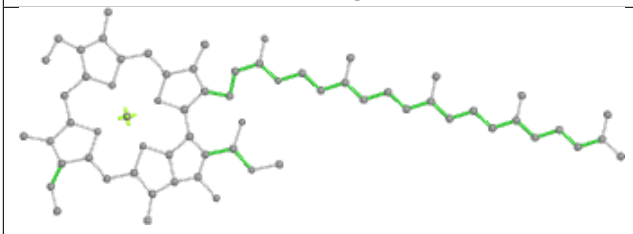
Ligand CLA C 511



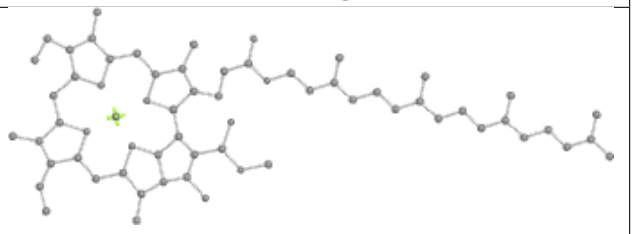
Bond lengths



Bond angles

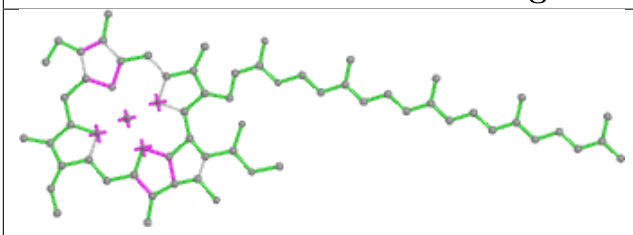


Torsions

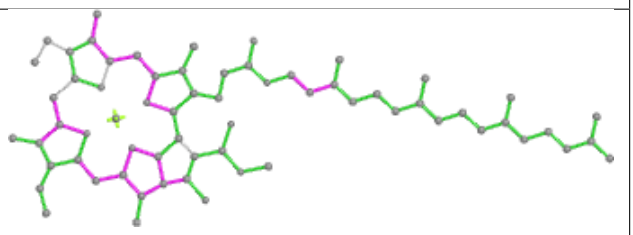


Rings

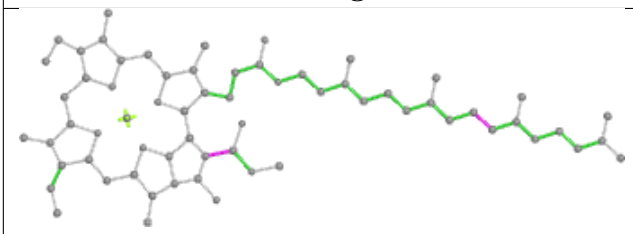
Ligand CLA c 513



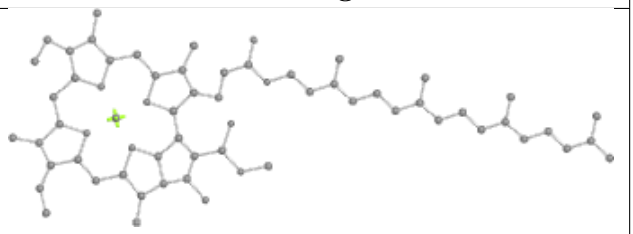
Bond lengths



Bond angles

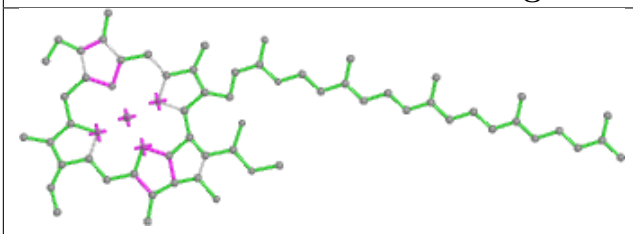


Torsions

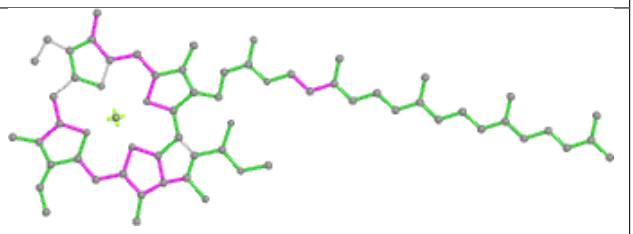


Rings

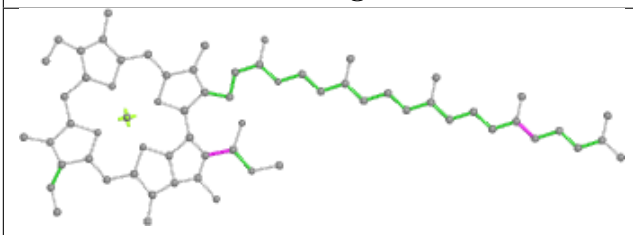
Ligand CLA A 607



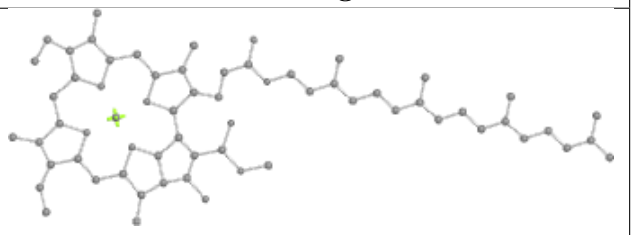
Bond lengths



Bond angles

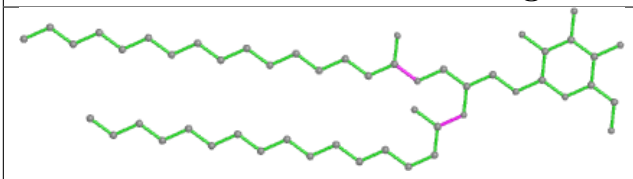


Torsions

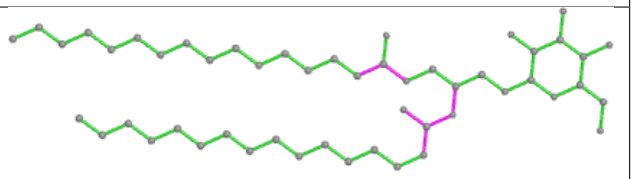


Rings

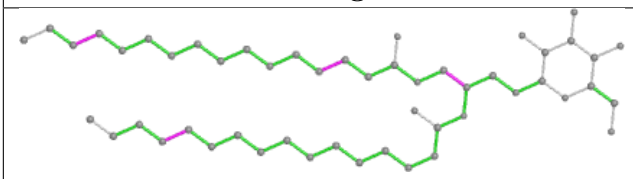
Ligand LMG b 620



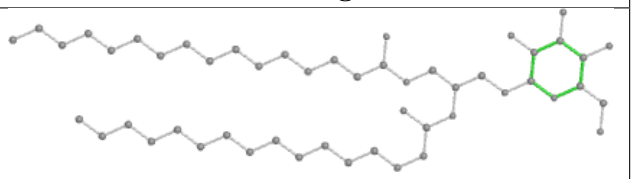
Bond lengths



Bond angles

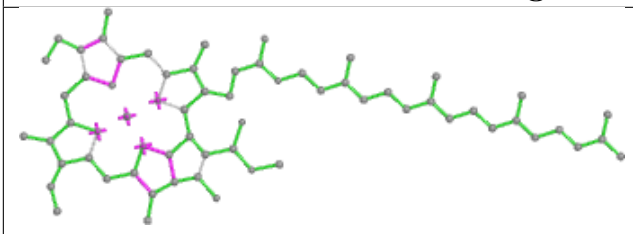


Torsions

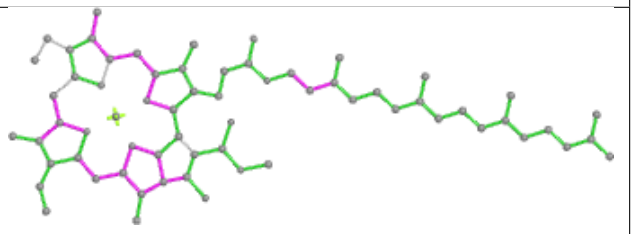


Rings

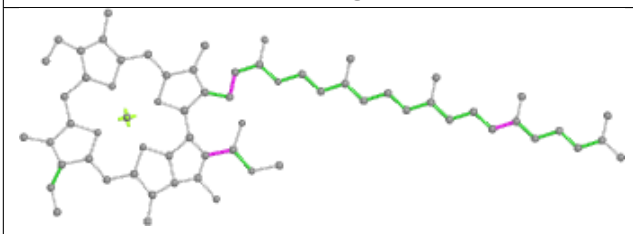
Ligand CLA b 610



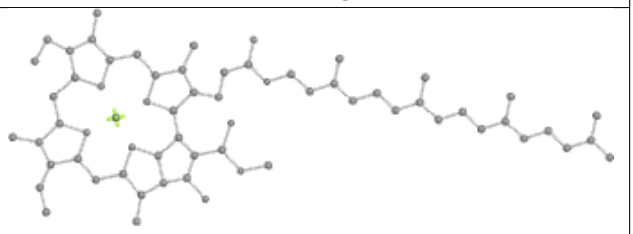
Bond lengths



Bond angles

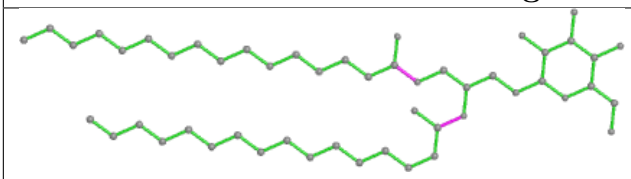


Torsions

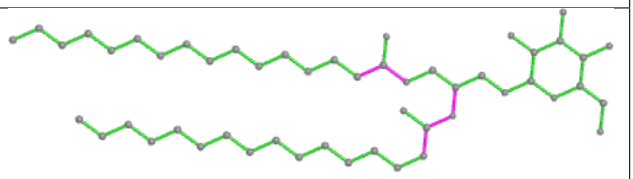


Rings

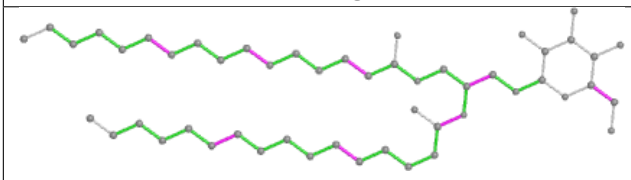
Ligand LMG b 624



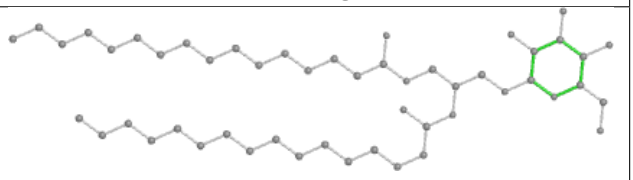
Bond lengths



Bond angles

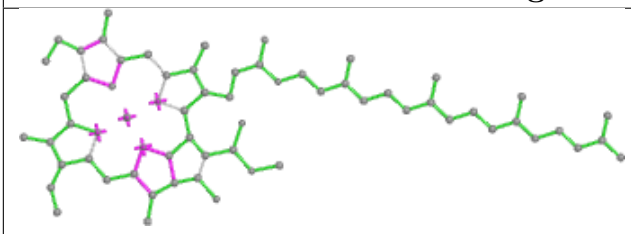


Torsions

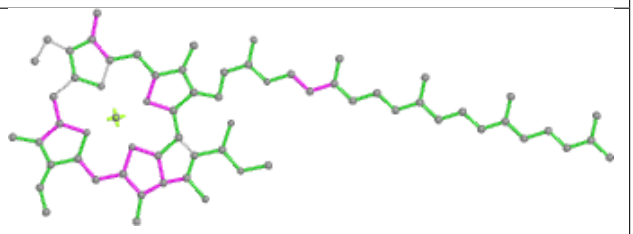


Rings

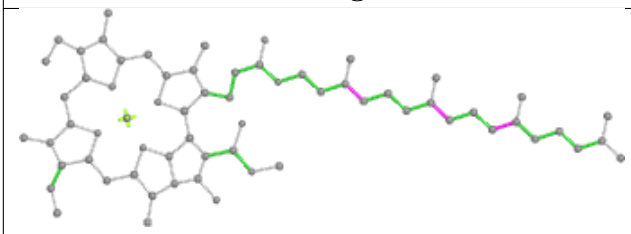
Ligand CLA b 604



Bond lengths



Bond angles



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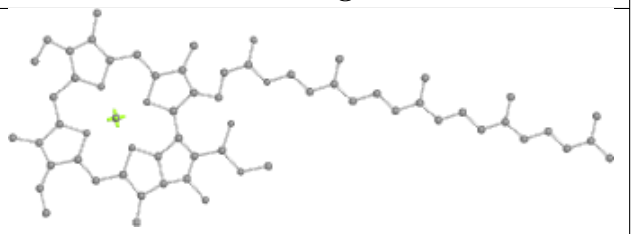
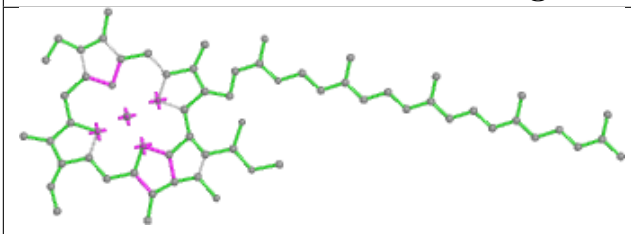


Rings

Ligand CLA c 510



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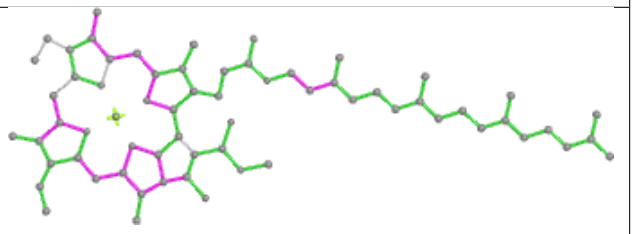
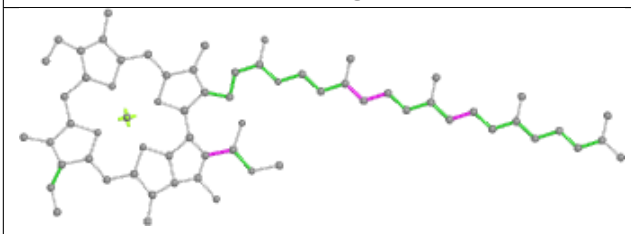
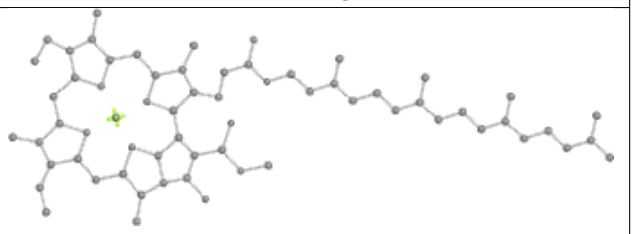


Bond angles

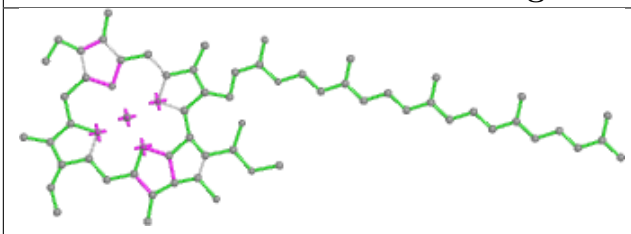


Torsions

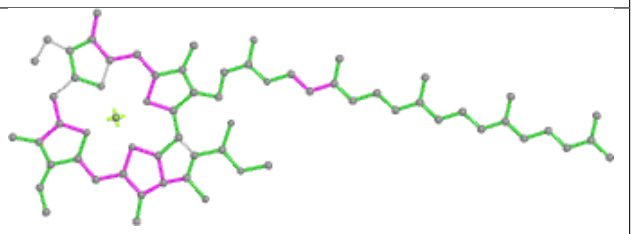


Rings

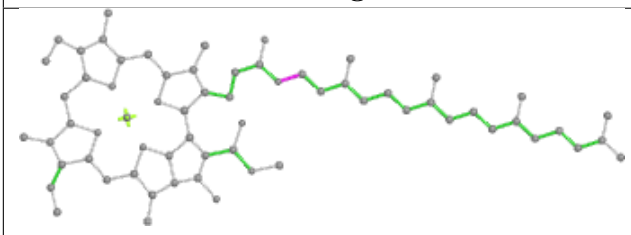
Ligand CLA b 608



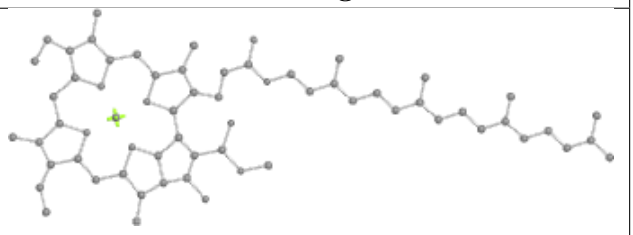
Bond lengths



Bond angles

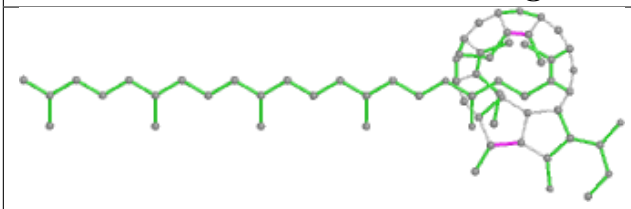


Torsions

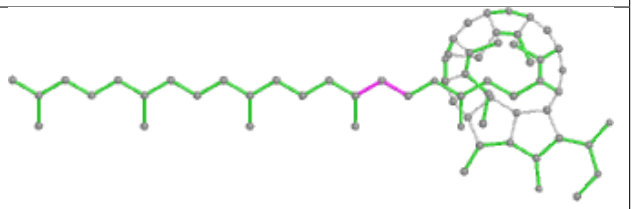


Rings

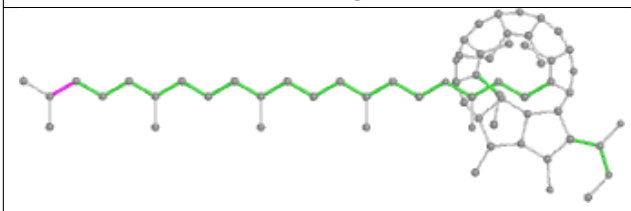
Ligand PHO d 402



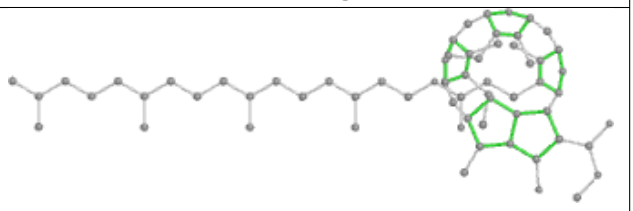
Bond lengths



Bond angles

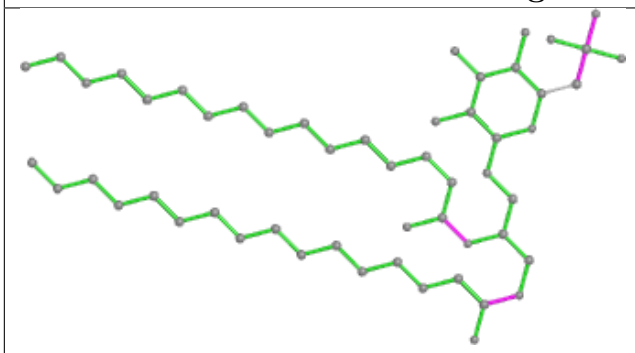


Torsions

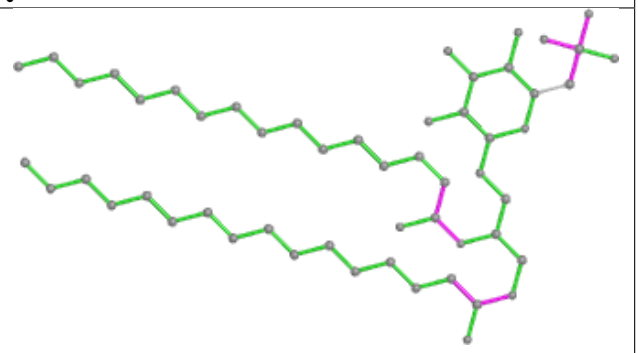


Rings

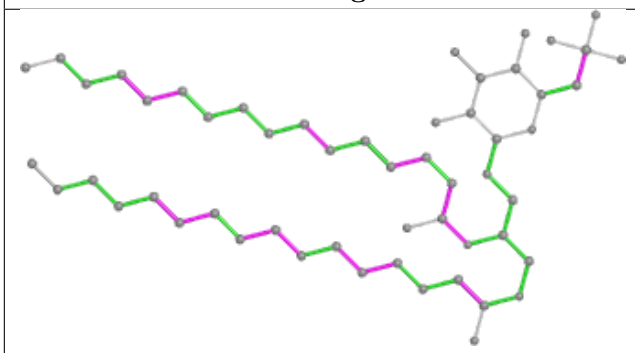
Ligand SQD L 103



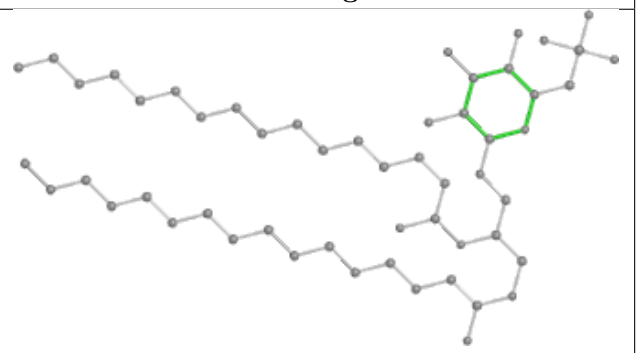
Bond lengths



Bond angles

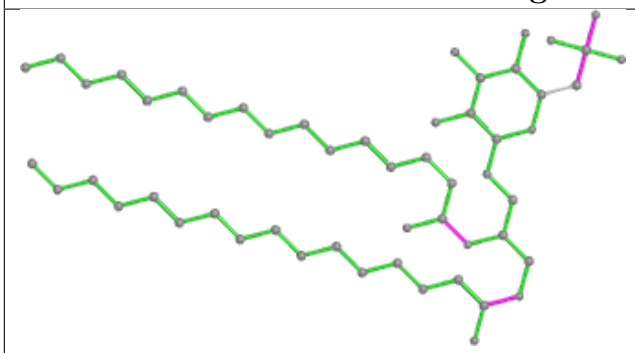


Torsions

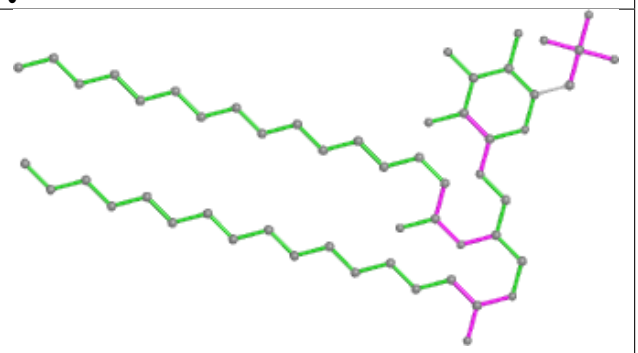


Rings

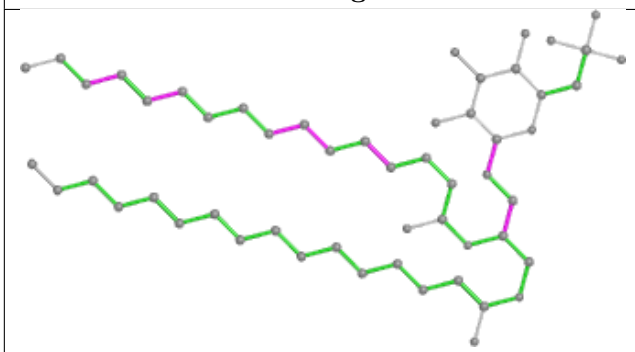
Ligand SQD a 613



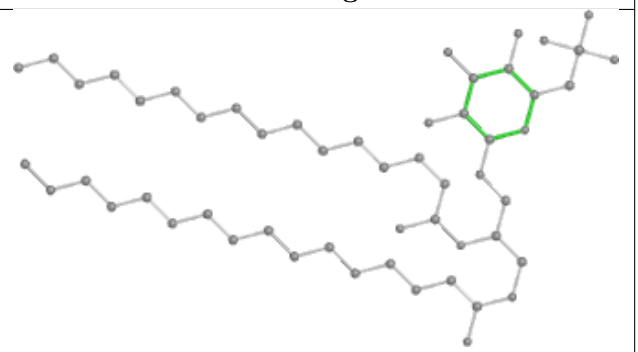
Bond lengths



Bond angles

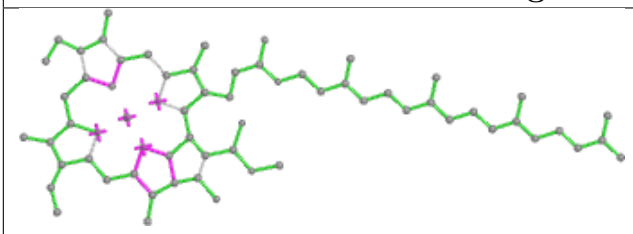


Torsions

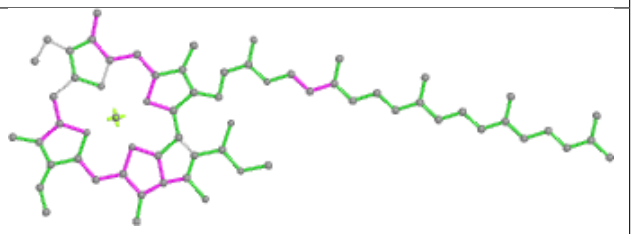


Rings

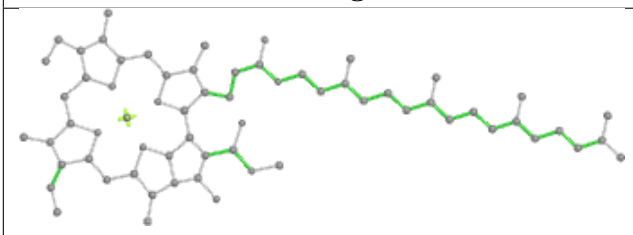
Ligand CLA d 401



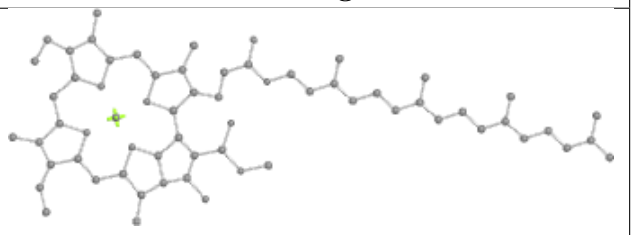
Bond lengths



Bond angles

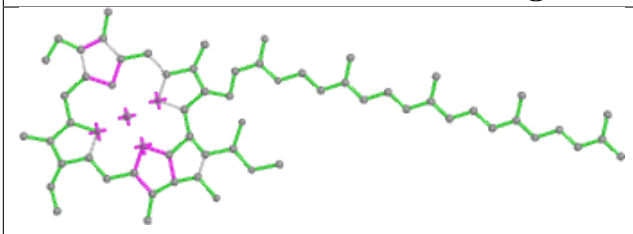


Torsions

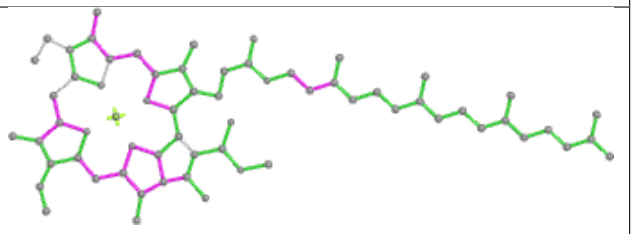


Rings

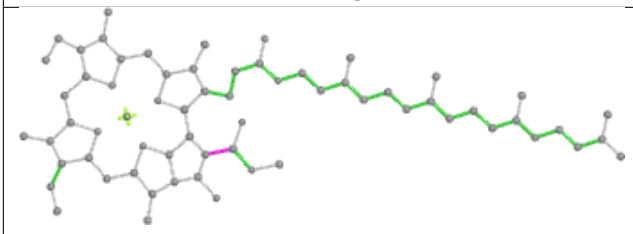
Ligand CLA b 602



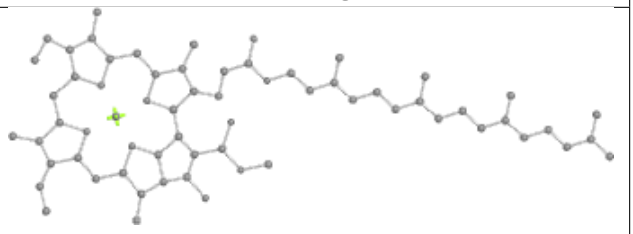
Bond lengths



Bond angles

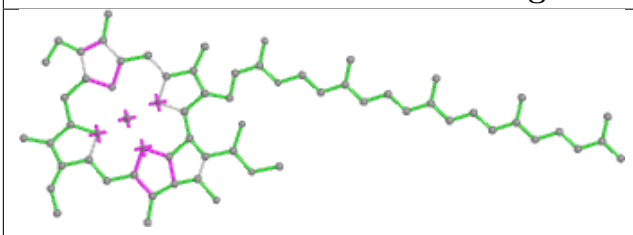


Torsions

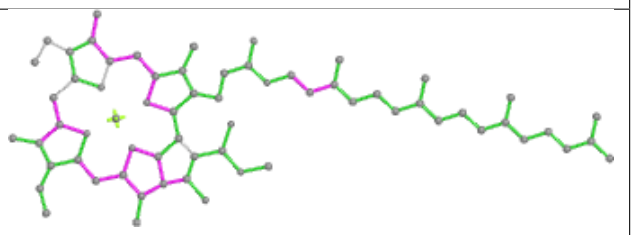


Rings

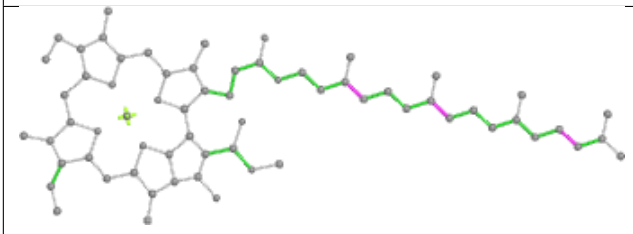
Ligand CLA a 610



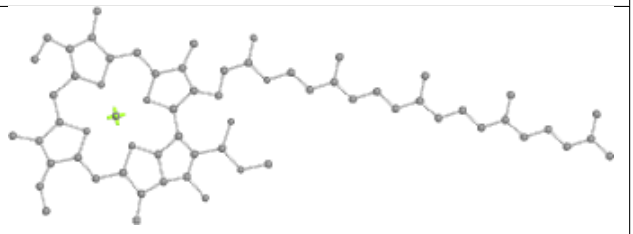
Bond lengths



Bond angles

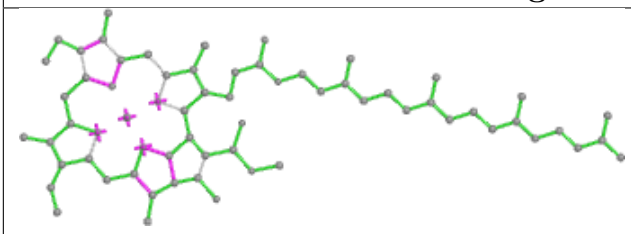


Torsions

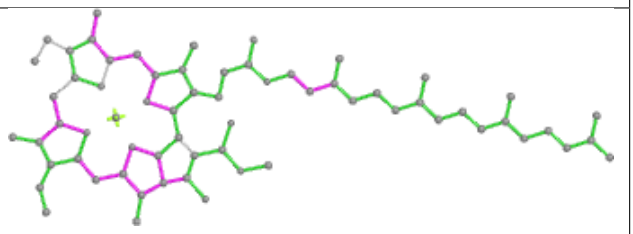


Rings

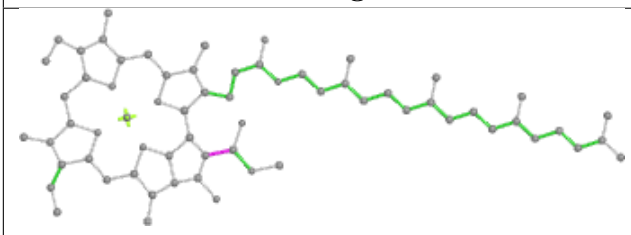
Ligand CLA a 608



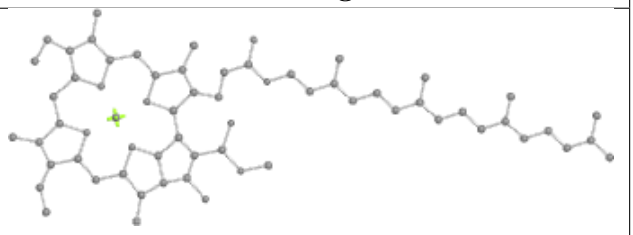
Bond lengths



Bond angles

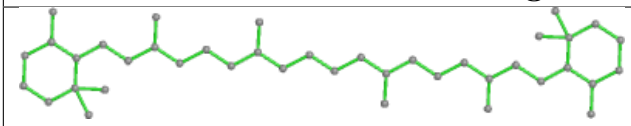


Torsions

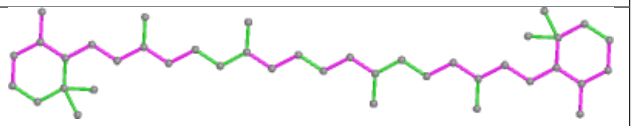


Rings

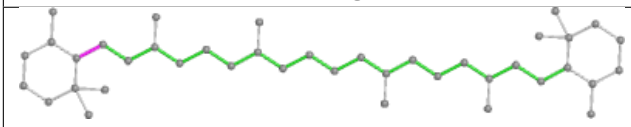
Ligand BCR b 617



Bond lengths



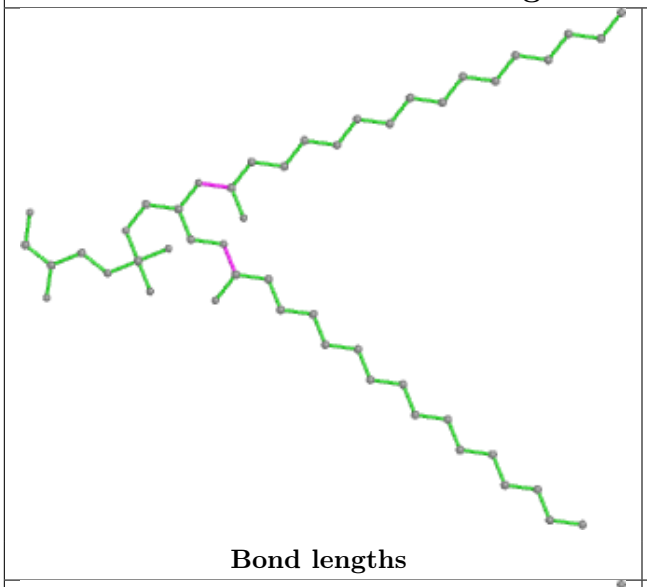
Bond angles



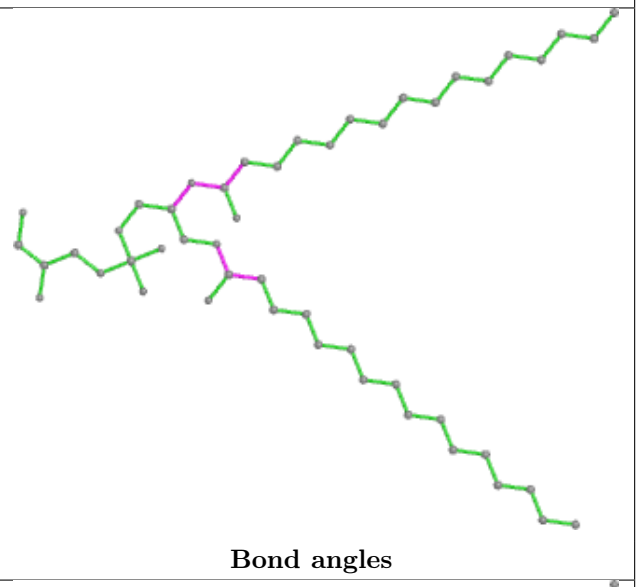
Torsions

Rings

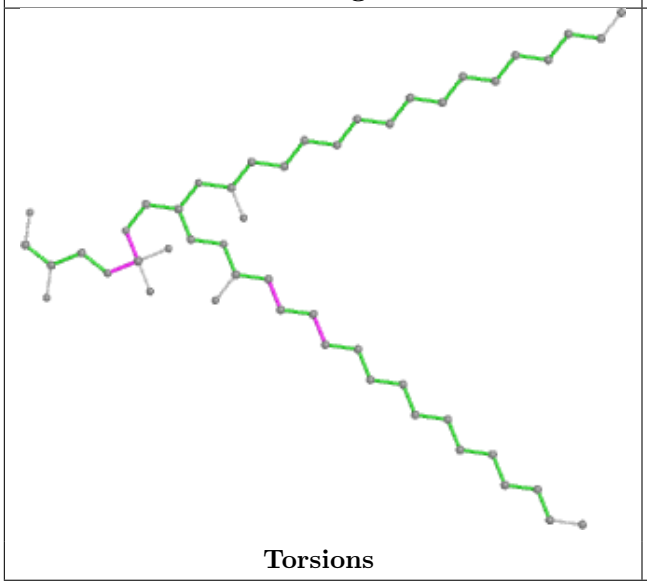
Ligand LHG A 613



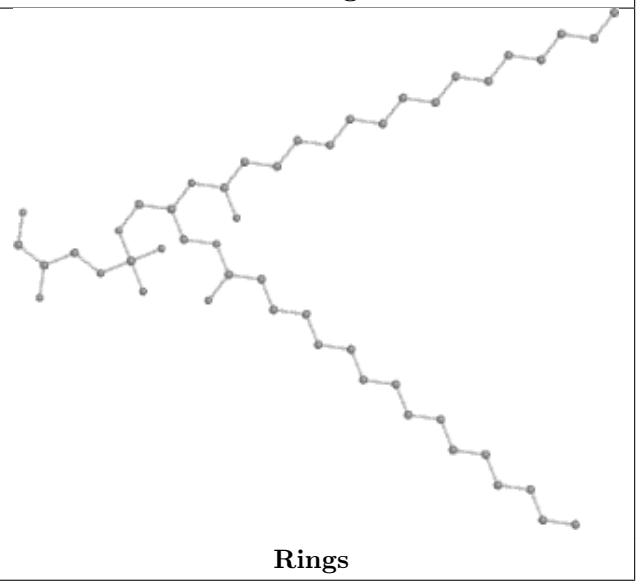
Bond lengths



Bond angles

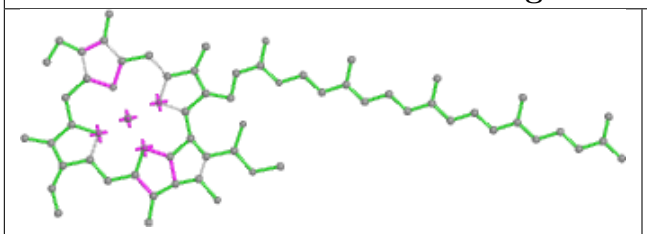


Torsions

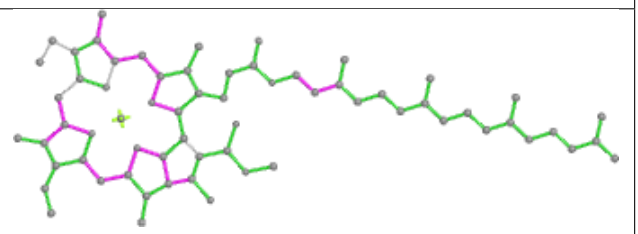


Rings

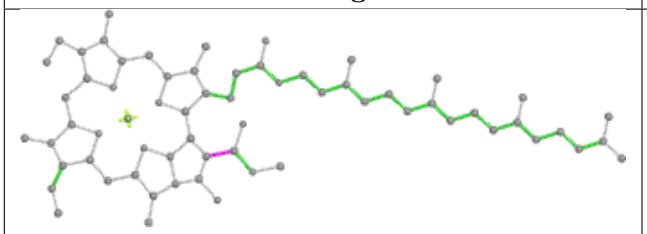
Ligand CLA C 508



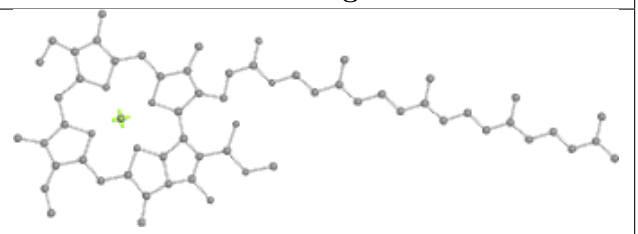
Bond lengths



Bond angles

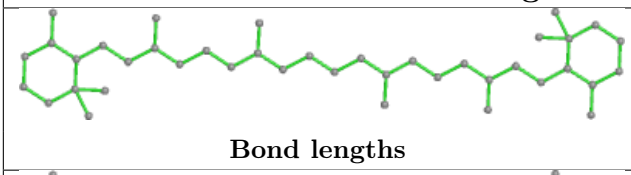


Torsions

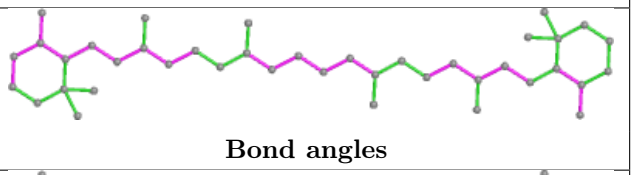


Rings

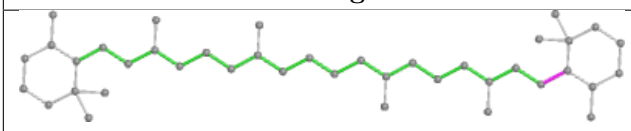
Ligand BCR A 609



Bond lengths



Bond angles



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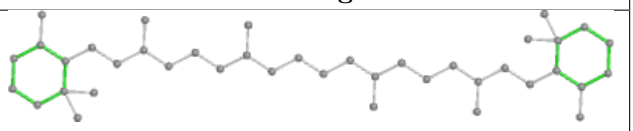
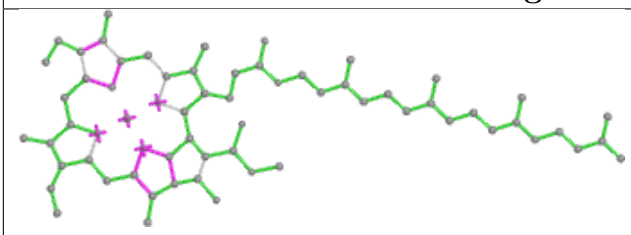
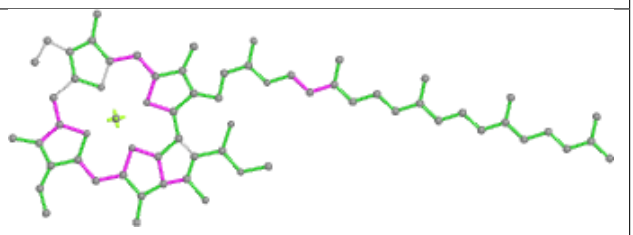


Rings

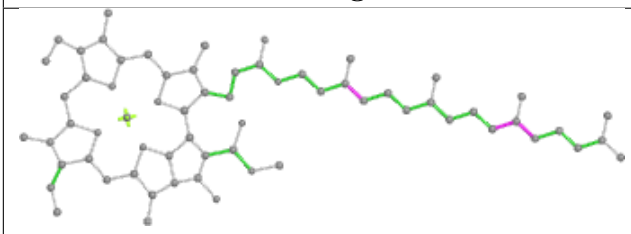
Ligand CLA B 615



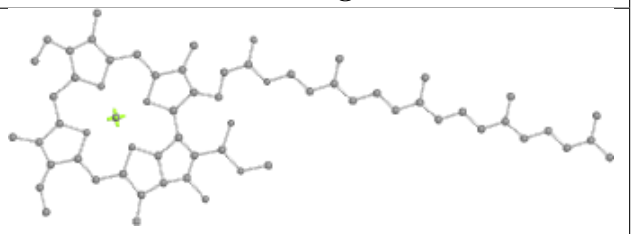
Bond lengths



Bond angles

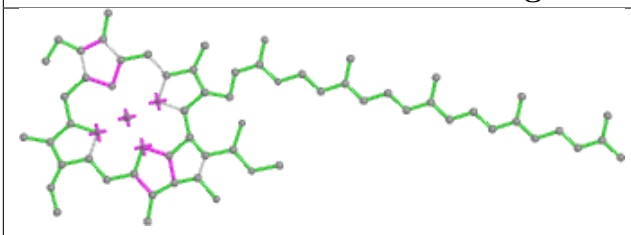


Torsions

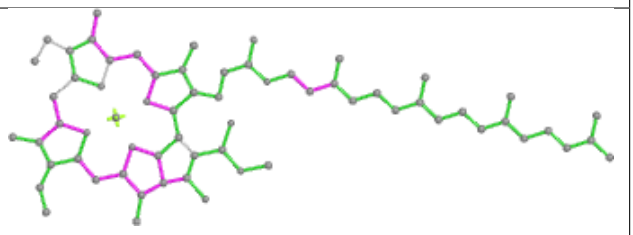


Rings

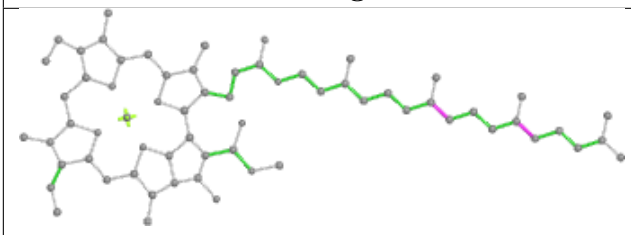
Ligand CLA B 613



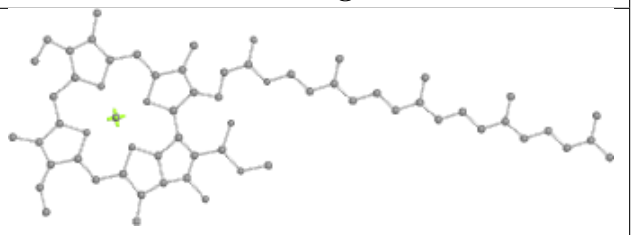
Bond lengths



Bond angles

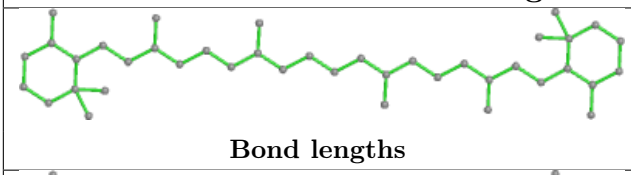


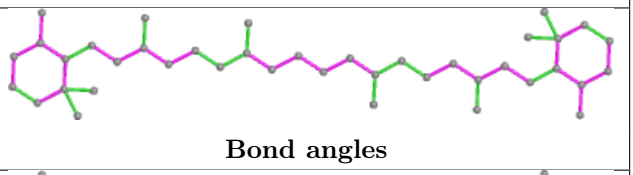
Torsions

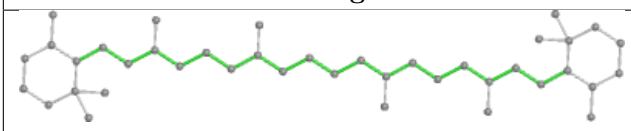


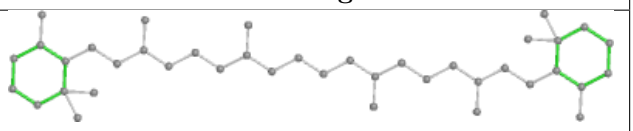
Rings

Ligand BCR b 618

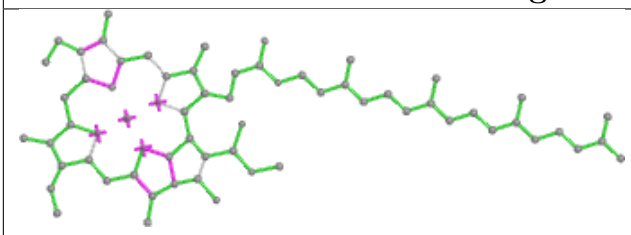

Bond lengths

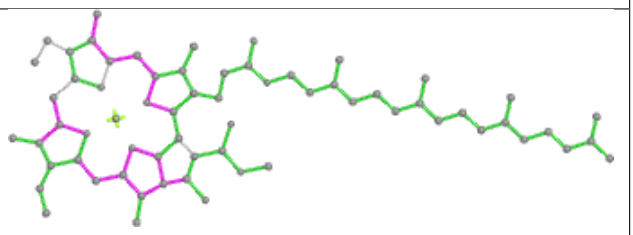

Bond angles

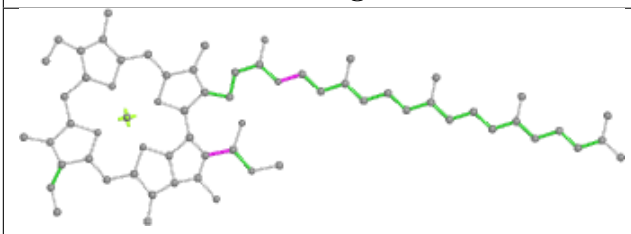

Torsions

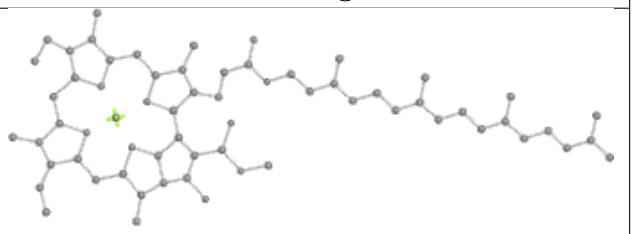

Rings

Ligand CLA c 504

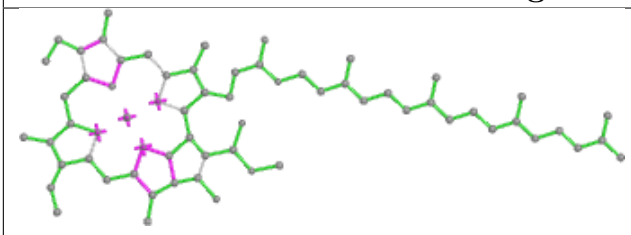

Bond lengths

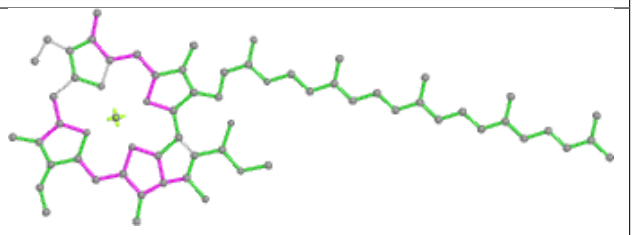

Bond angles

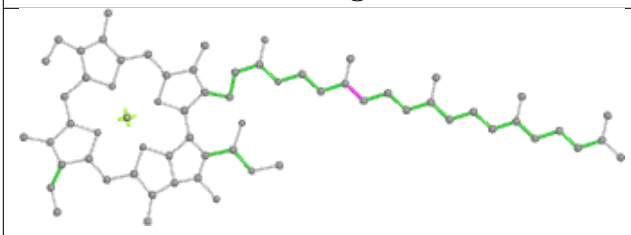

Torsions

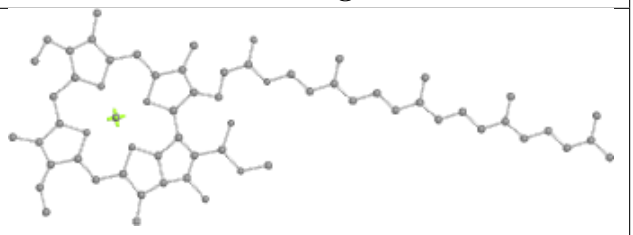

Rings

Ligand CLA b 605

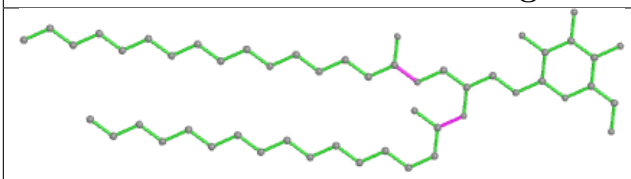

Bond lengths

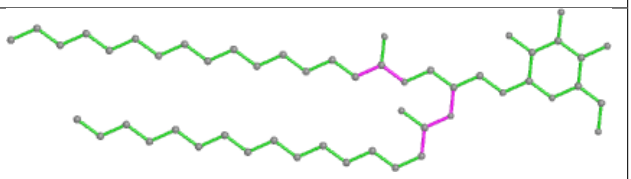

Bond angles

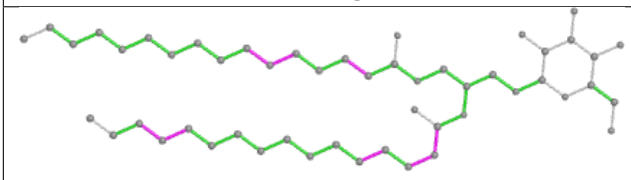

Torsions


Rings

Ligand LMG C 519


Bond lengths


Bond angles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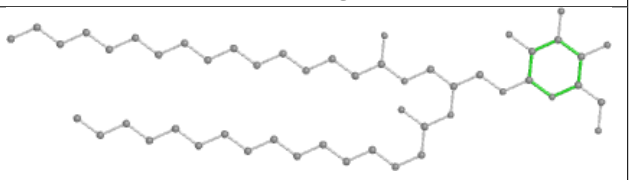
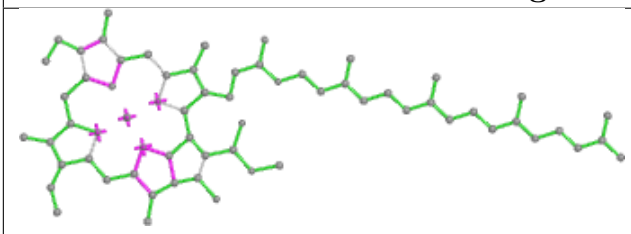
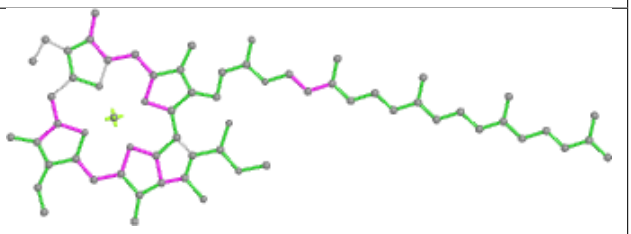
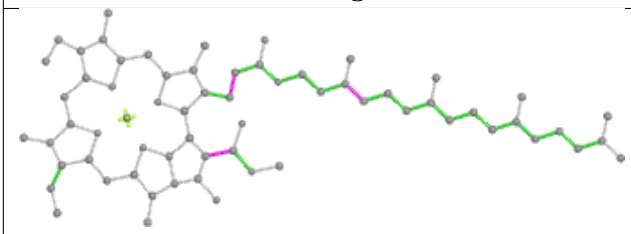
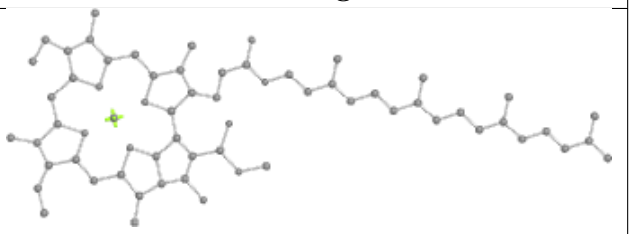

Rings

Ligand CLA c 507

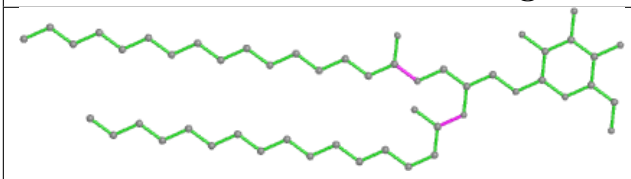

Bond lengths

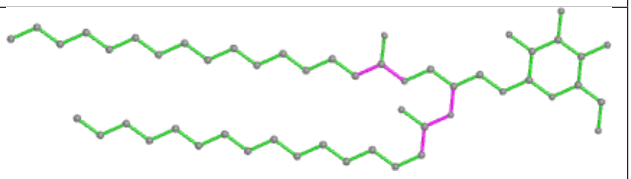

Bond angles

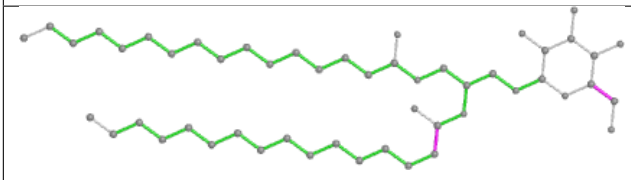

Torsions


Rings

Ligand LMG D 409


Bond lengths


Bond angles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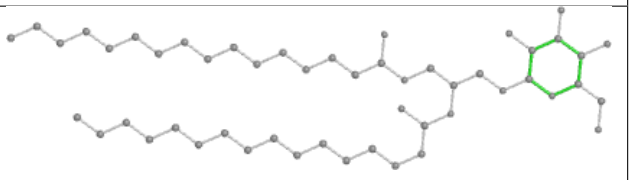
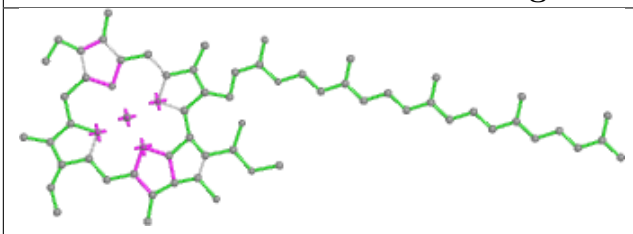
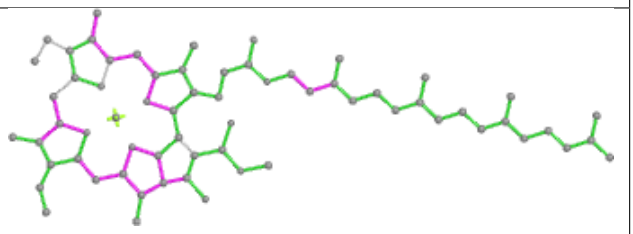

Rings

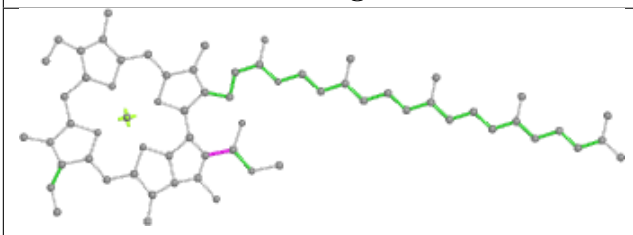
Ligand CLA c 502



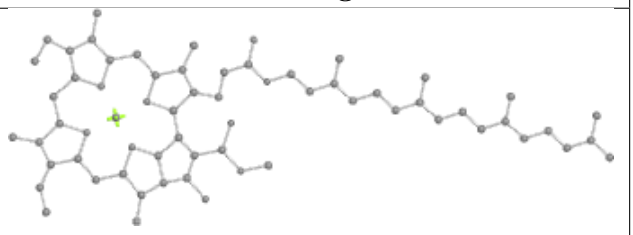
Bond lengths



Bond angles

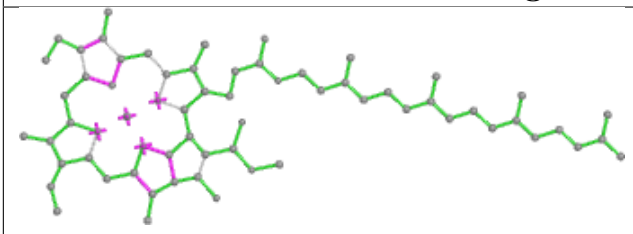


Torsions

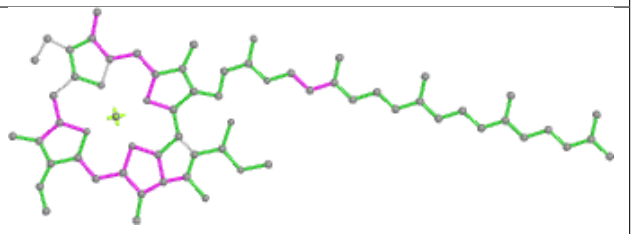


Rings

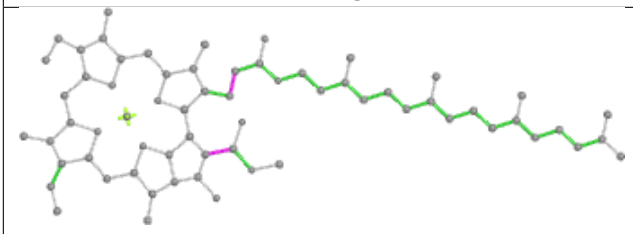
Ligand CLA B 603



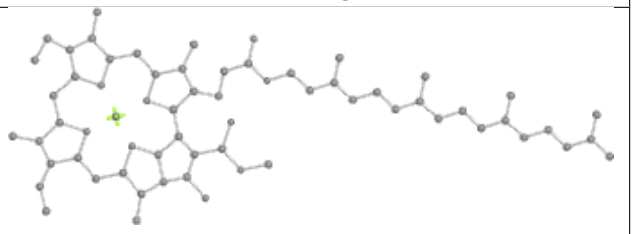
Bond lengths



Bond angles

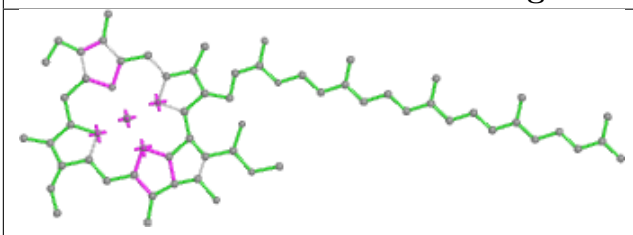


Torsions

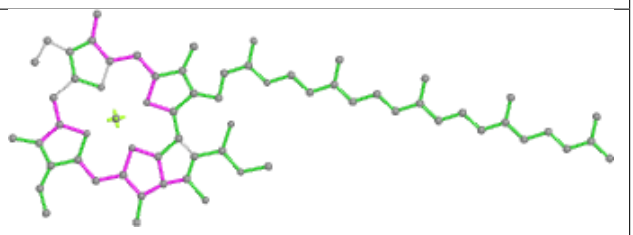


Rings

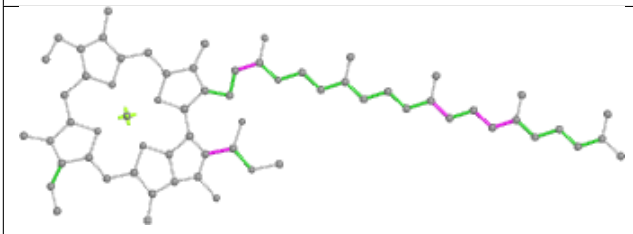
Ligand CLA b 601



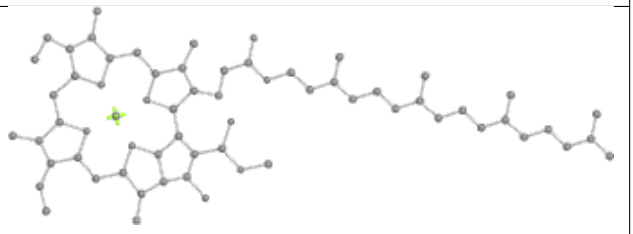
Bond lengths



Bond angles

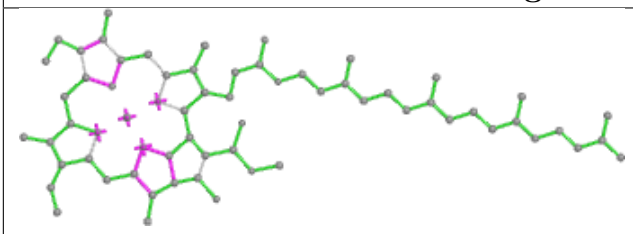


Torsions

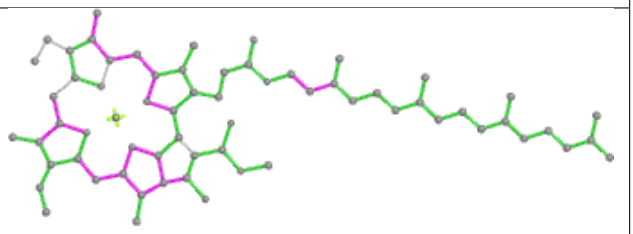


Rings

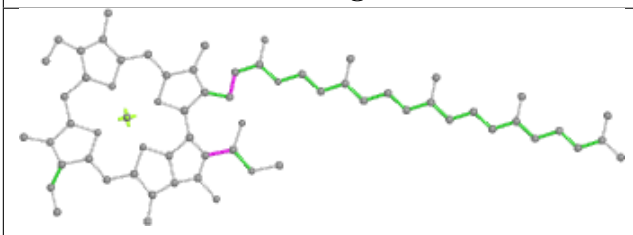
Ligand CLA B 606



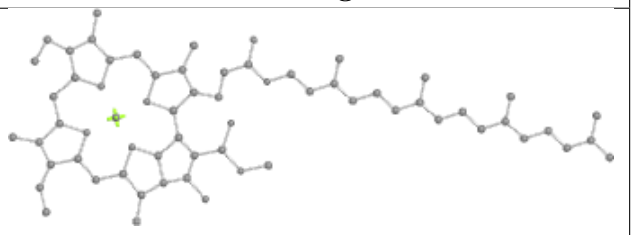
Bond lengths



Bond angles

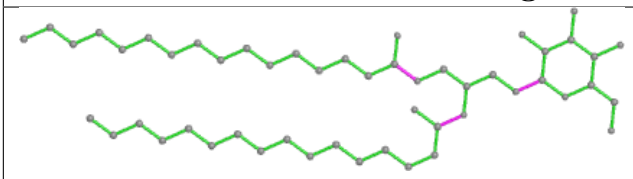


Torsions

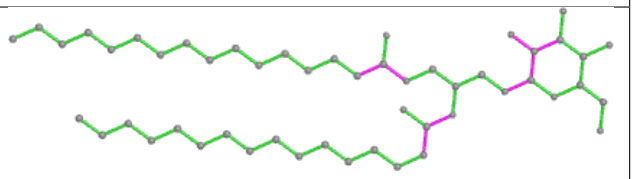


Rings

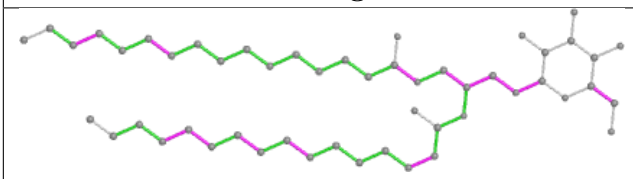
Ligand LMG C 521



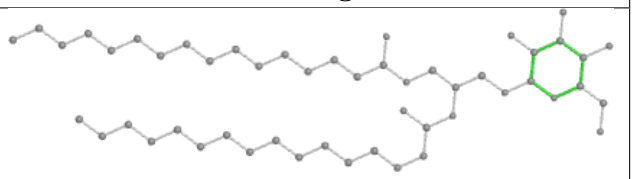
Bond lengths



Bond angles

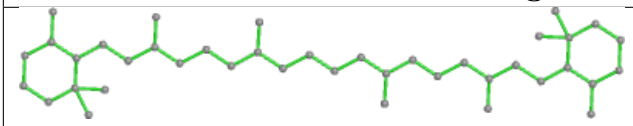


Torsions

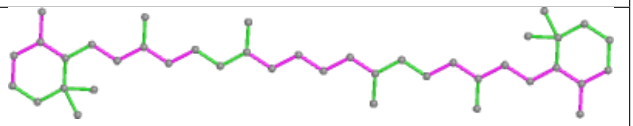


Rings

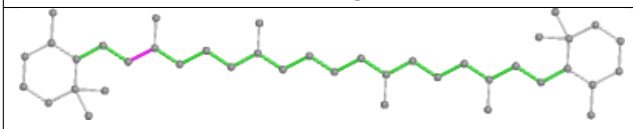
Ligand BCR b 619



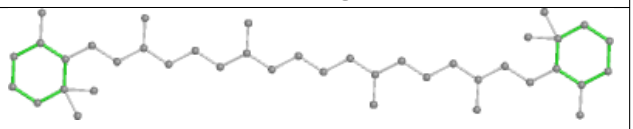
Bond lengths



Bond angles

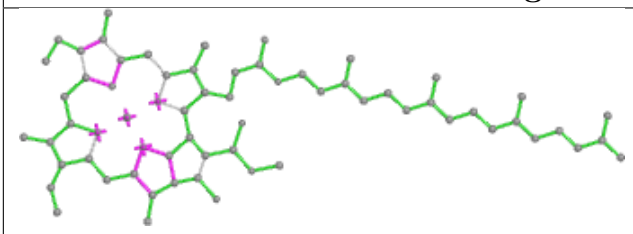


Torsions

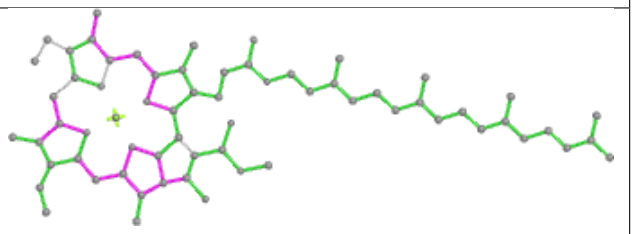


Rings

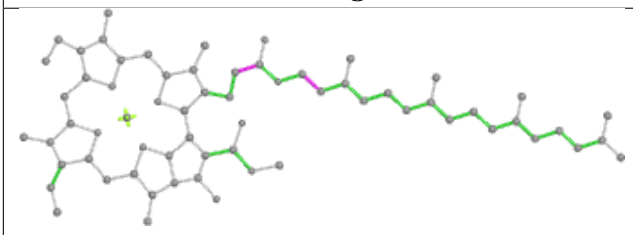
Ligand CLA C 512



Bond lengths



Bond angles



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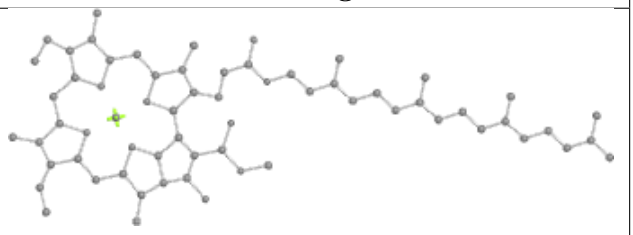
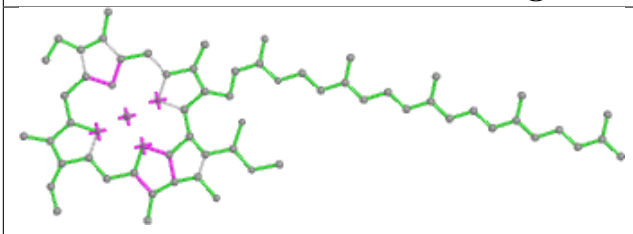
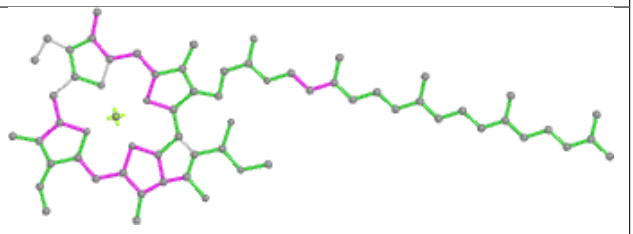


Rings

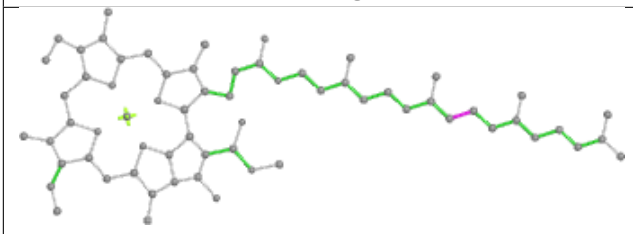
Ligand CLA b 613



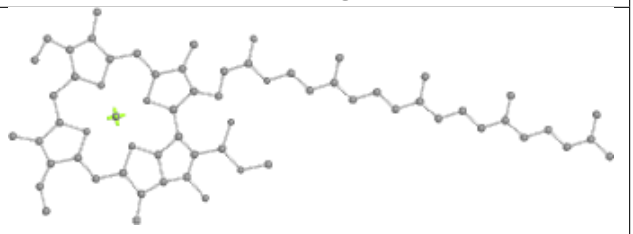
Bond lengths



Bond angles

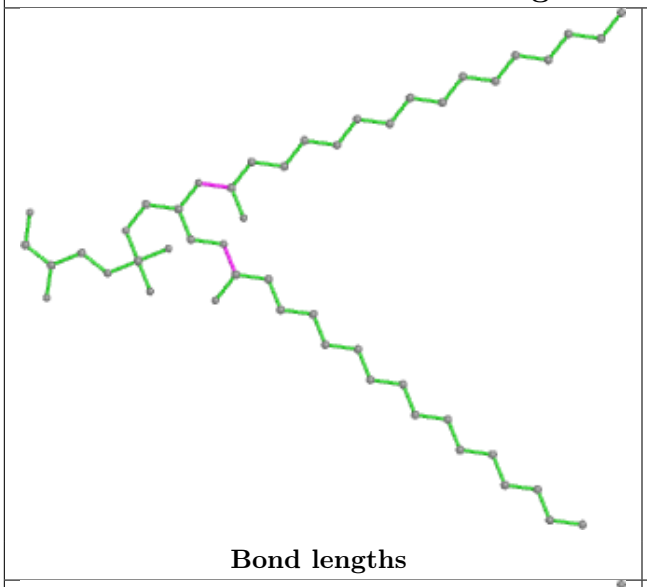


Torsions

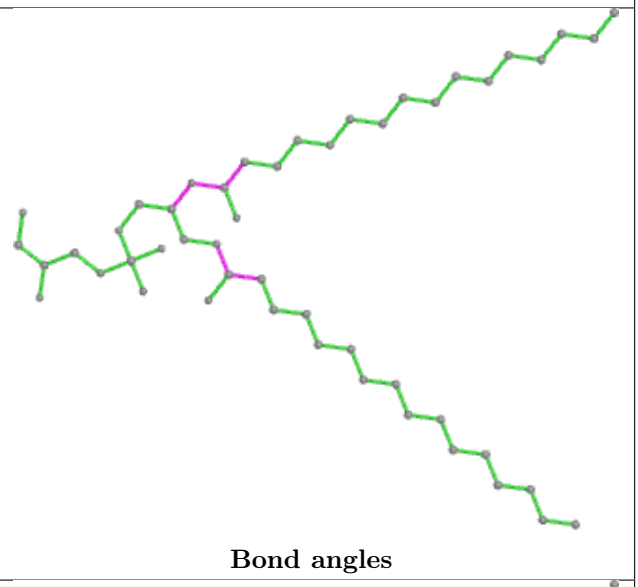


Rings

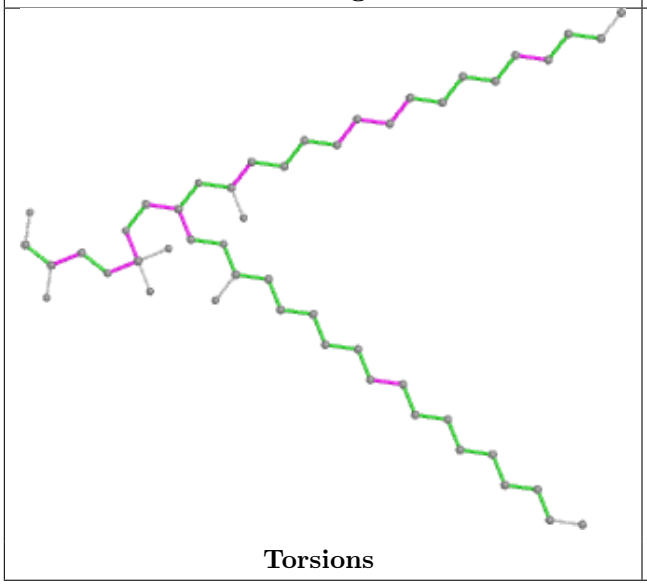
Ligand LHG l 101



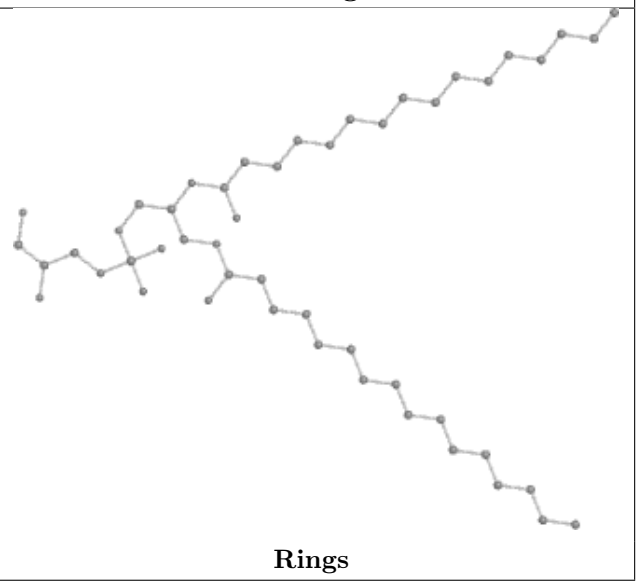
Bond lengths



Bond angles

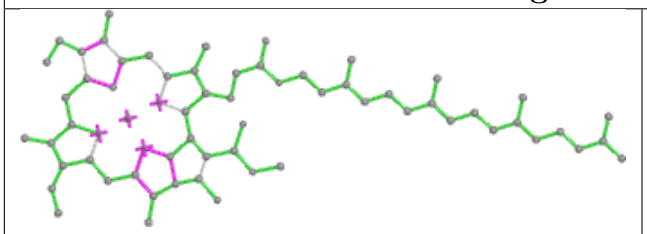


Torsions

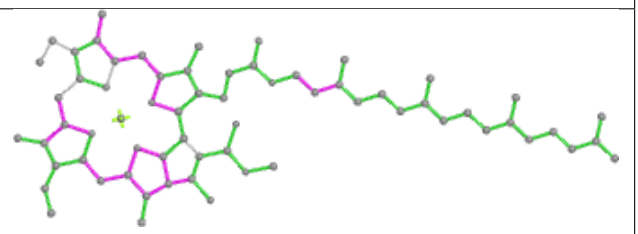


Rings

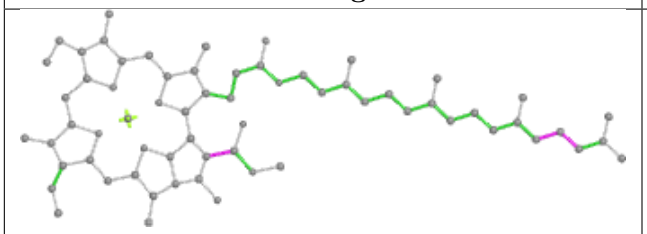
Ligand CLA c 506



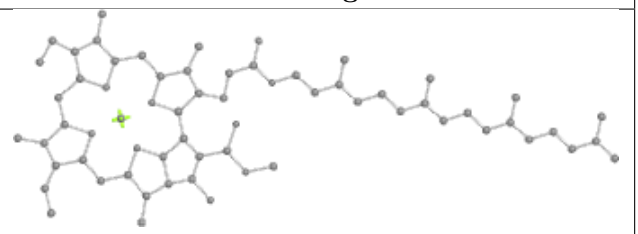
Bond lengths



Bond angles

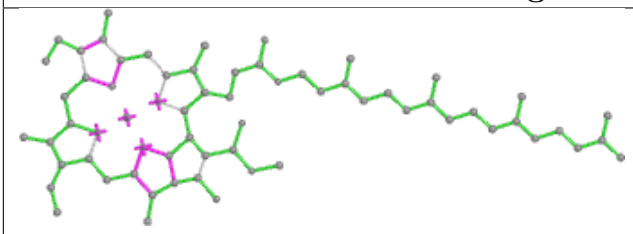


Torsions

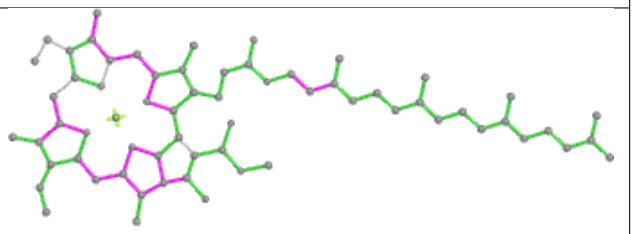


Rings

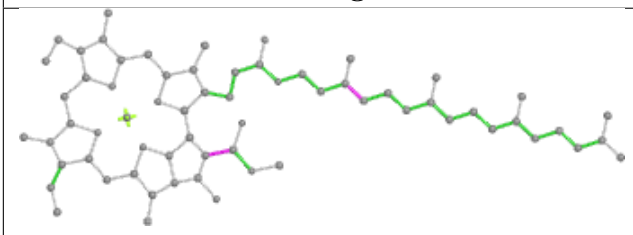
Ligand CLA b 603



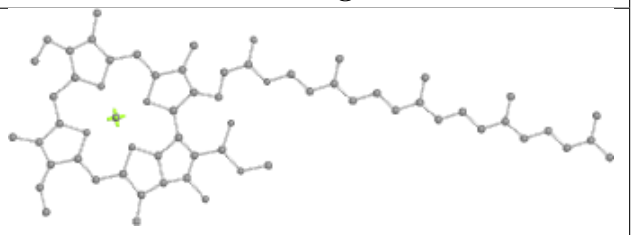
Bond lengths



Bond angles

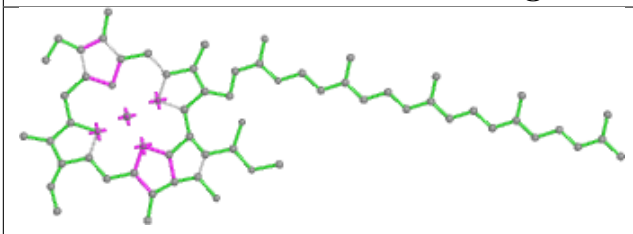


Torsions

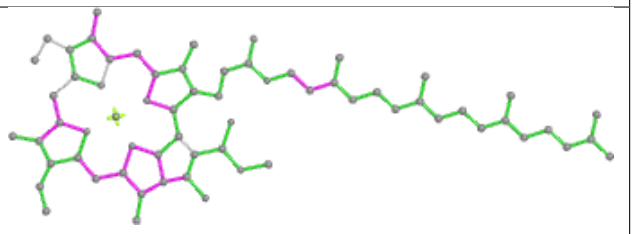


Rings

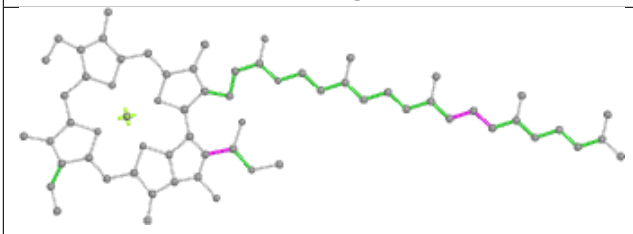
Ligand CLA B 616



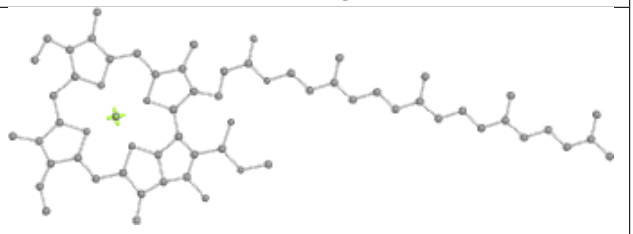
Bond lengths



Bond angles

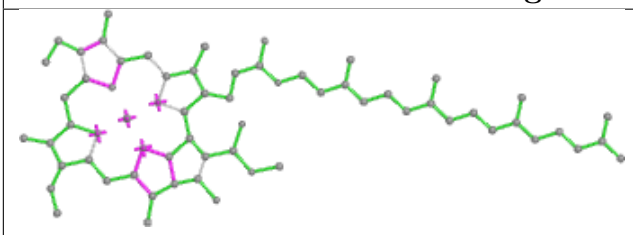


Torsions

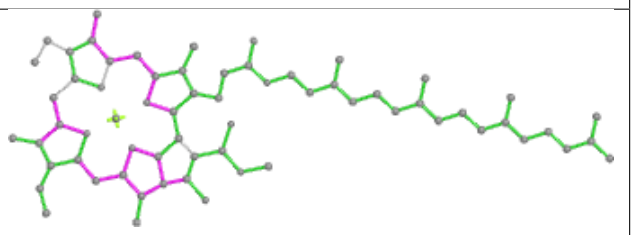


Rings

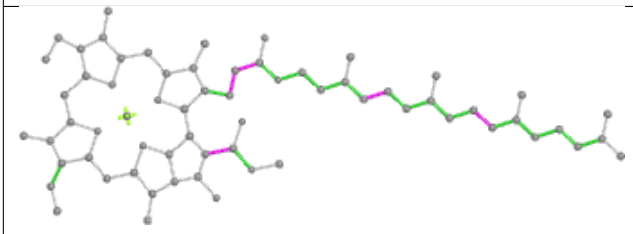
Ligand CLA B 601



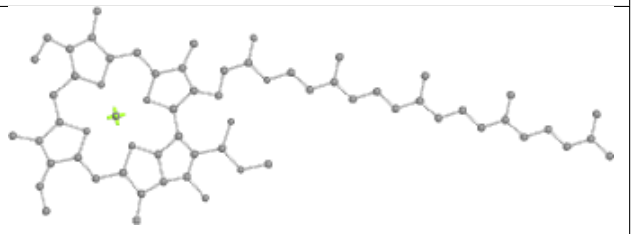
Bond lengths



Bond angles

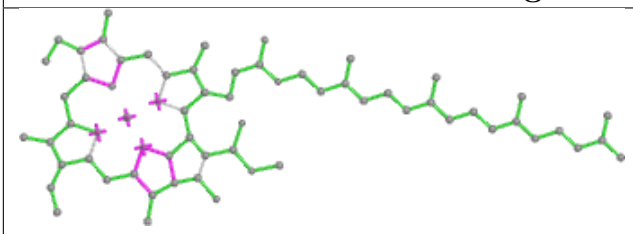


Torsions

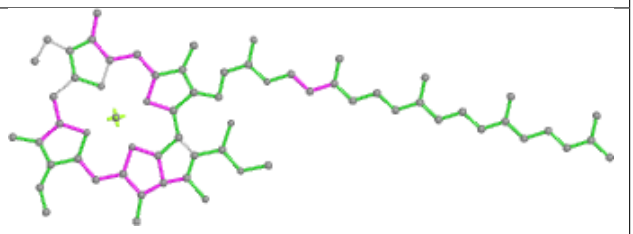


Rings

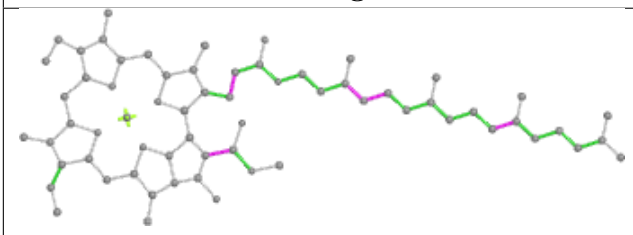
Ligand CLA B 614



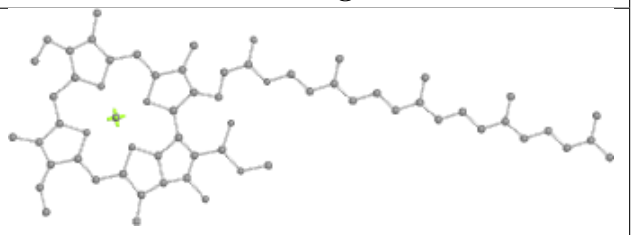
Bond lengths



Bond angles

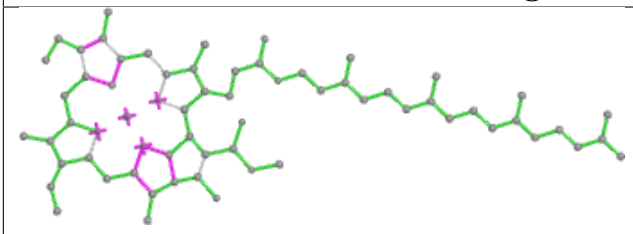


Torsions

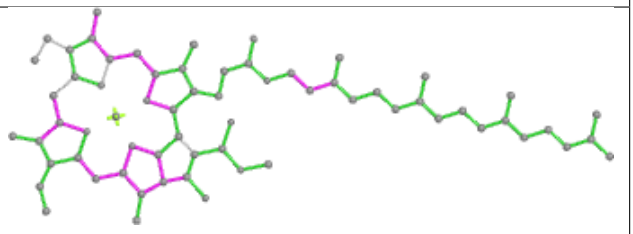


Rings

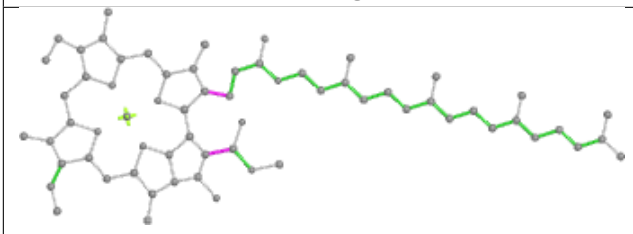
Ligand CLA D 403



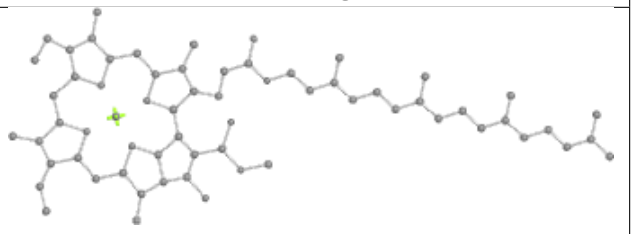
Bond lengths



Bond angles

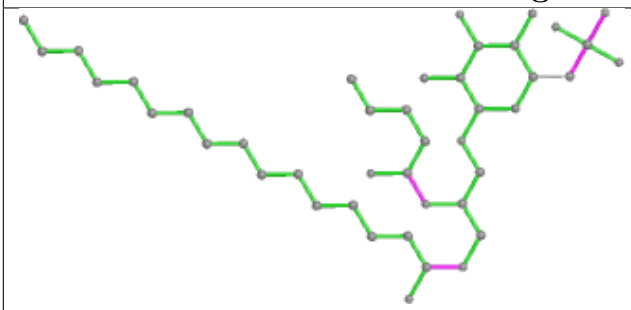


Torsions

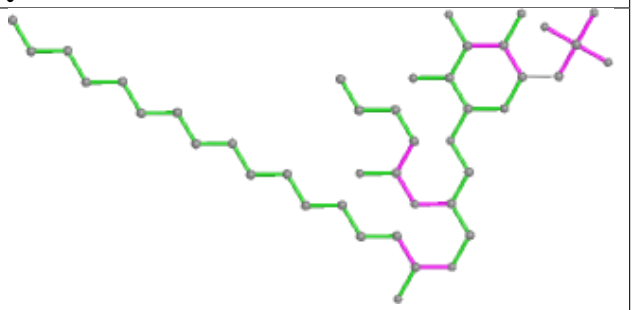


Rings

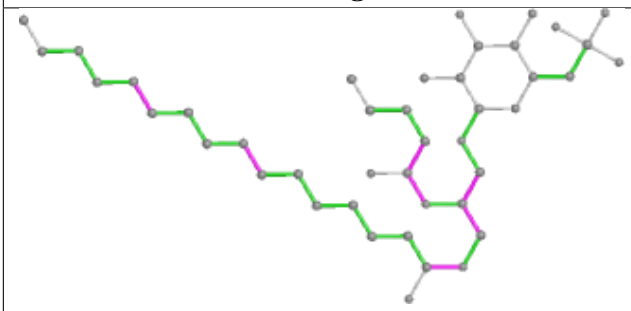
Ligand SQD f 101



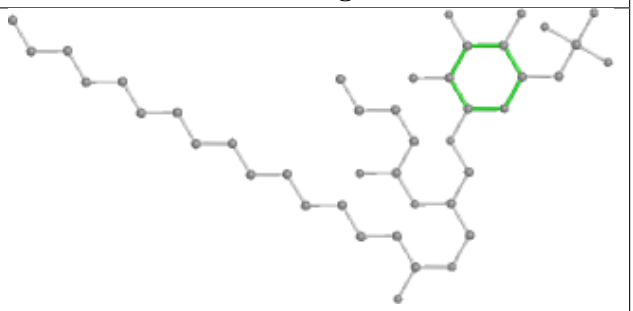
Bond lengths



Bond angles

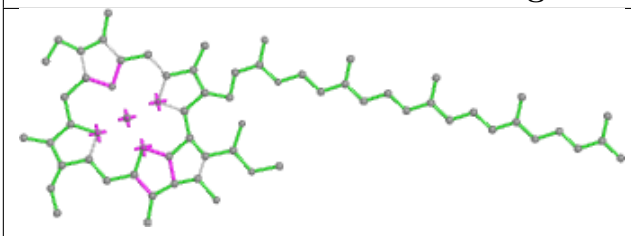


Torsions

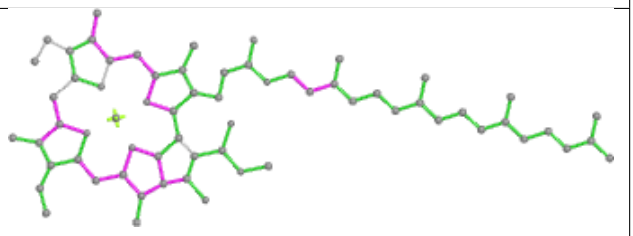


Rings

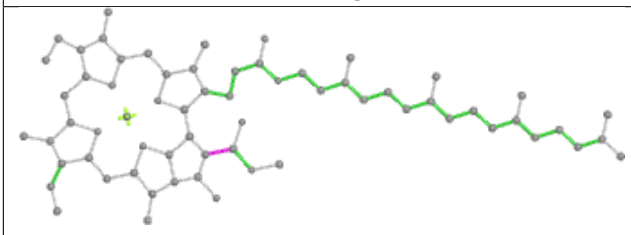
Ligand CLA b 612



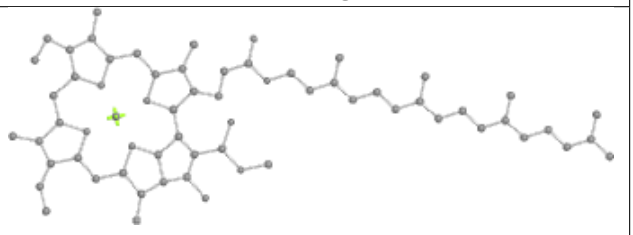
Bond lengths



Bond angles

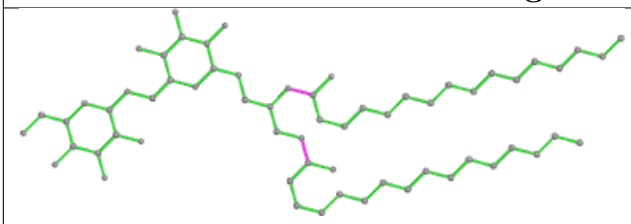


Torsions

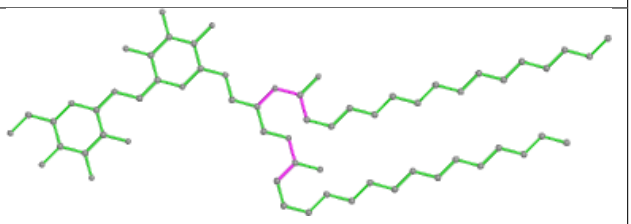


Rings

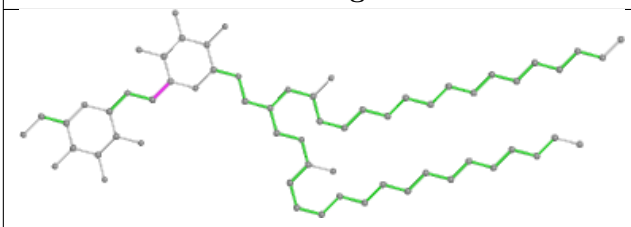
Ligand DGD c 517



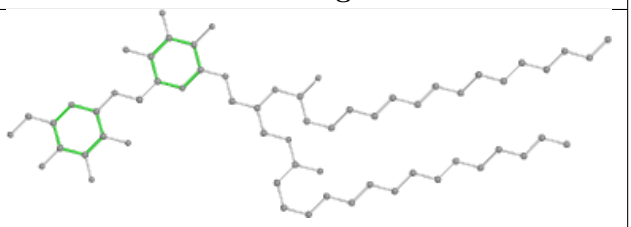
Bond lengths



Bond angles

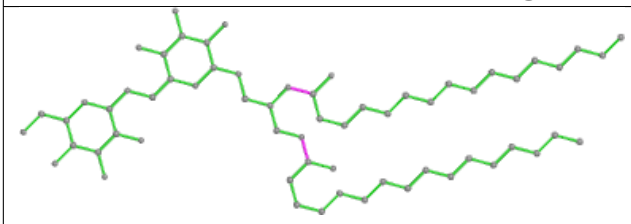


Torsions

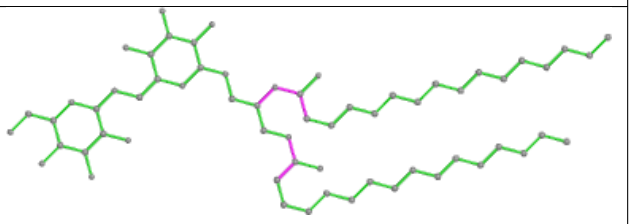


Rings

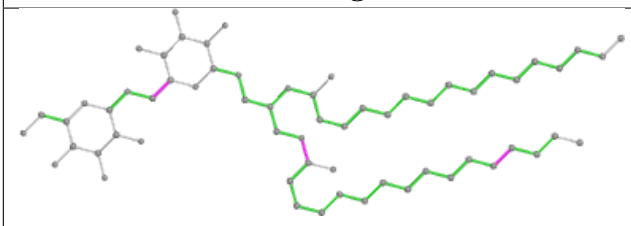
Ligand DGD C 518



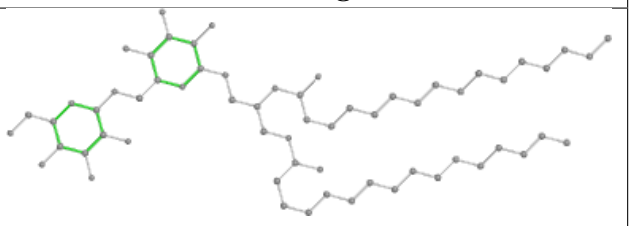
Bond lengths



Bond angles

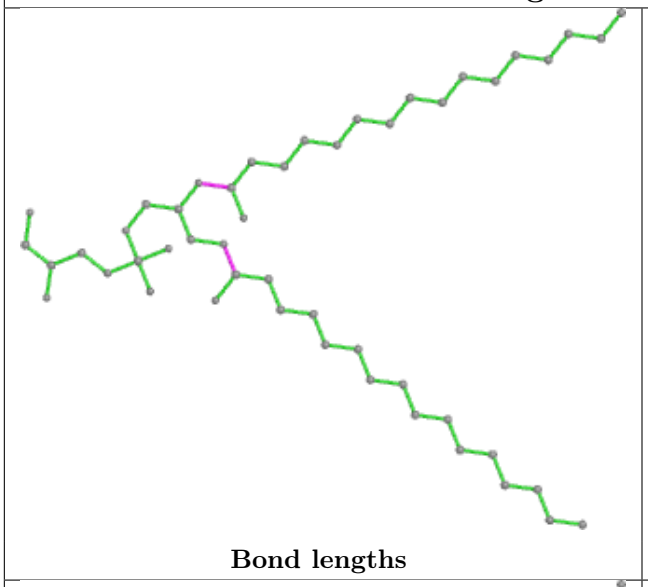


Torsions

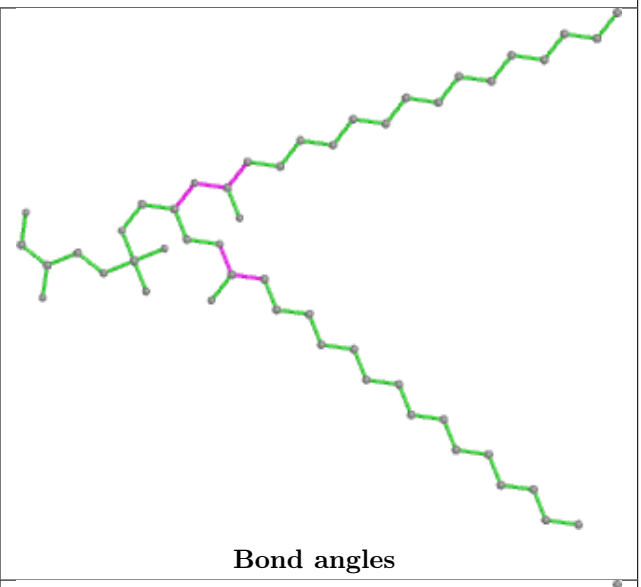


Rings

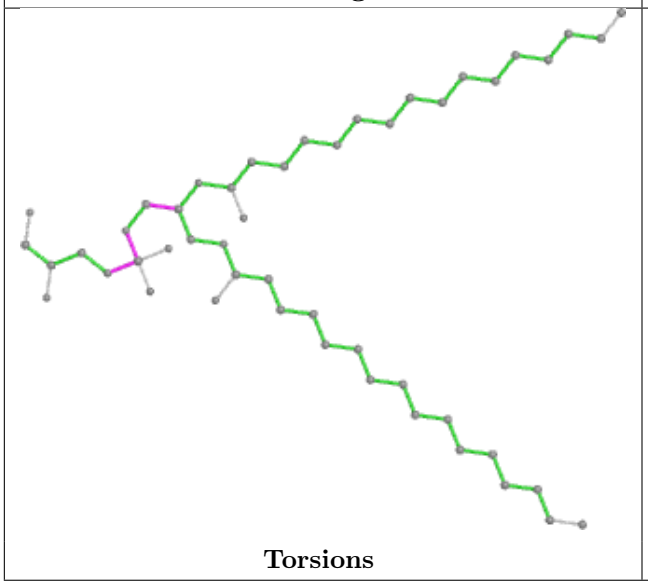
Ligand LHG d 406



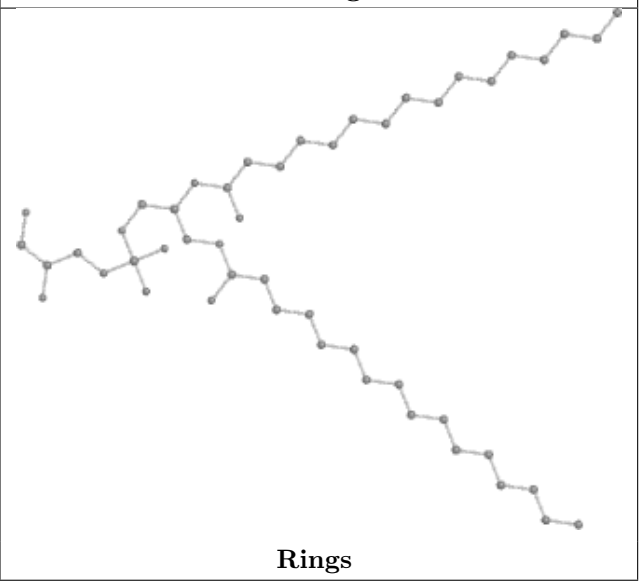
Bond lengths



Bond angles

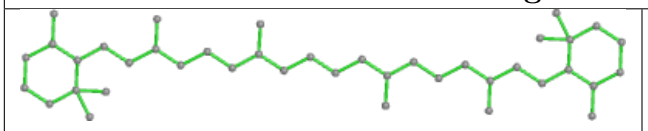


Torsions

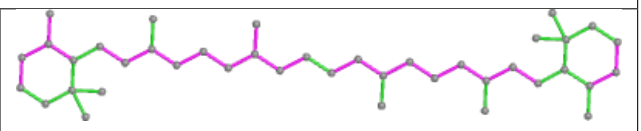


Rings

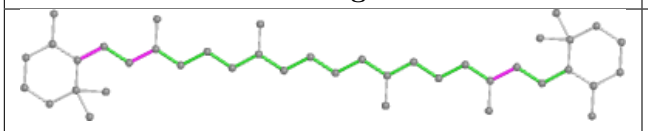
Ligand BCR T 101



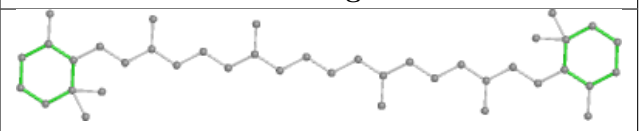
Bond lengths



Bond angles

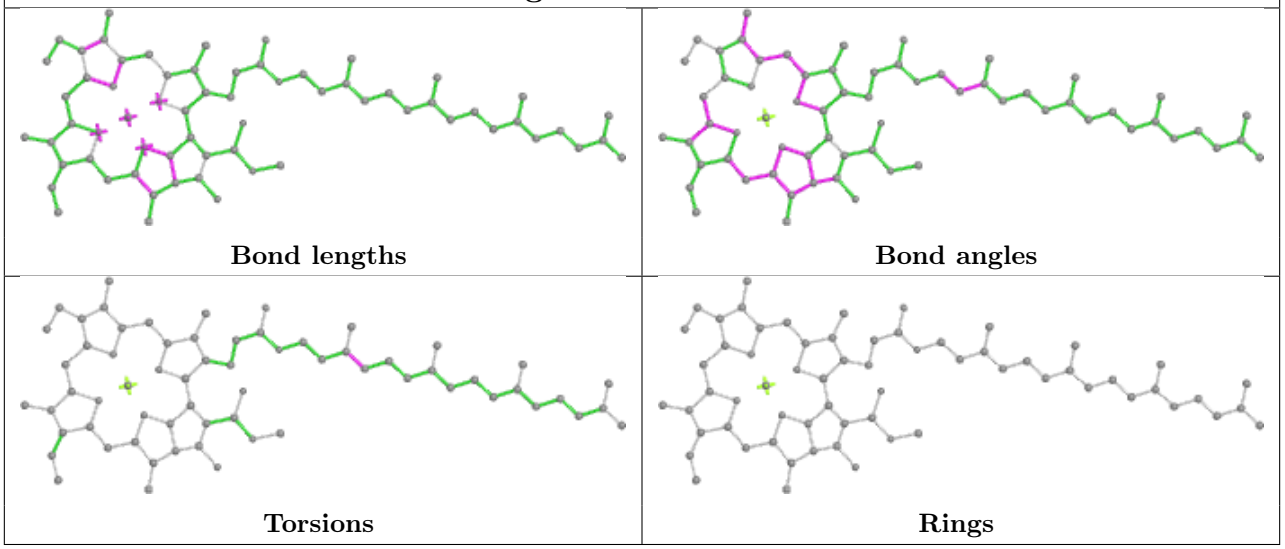


Torsions

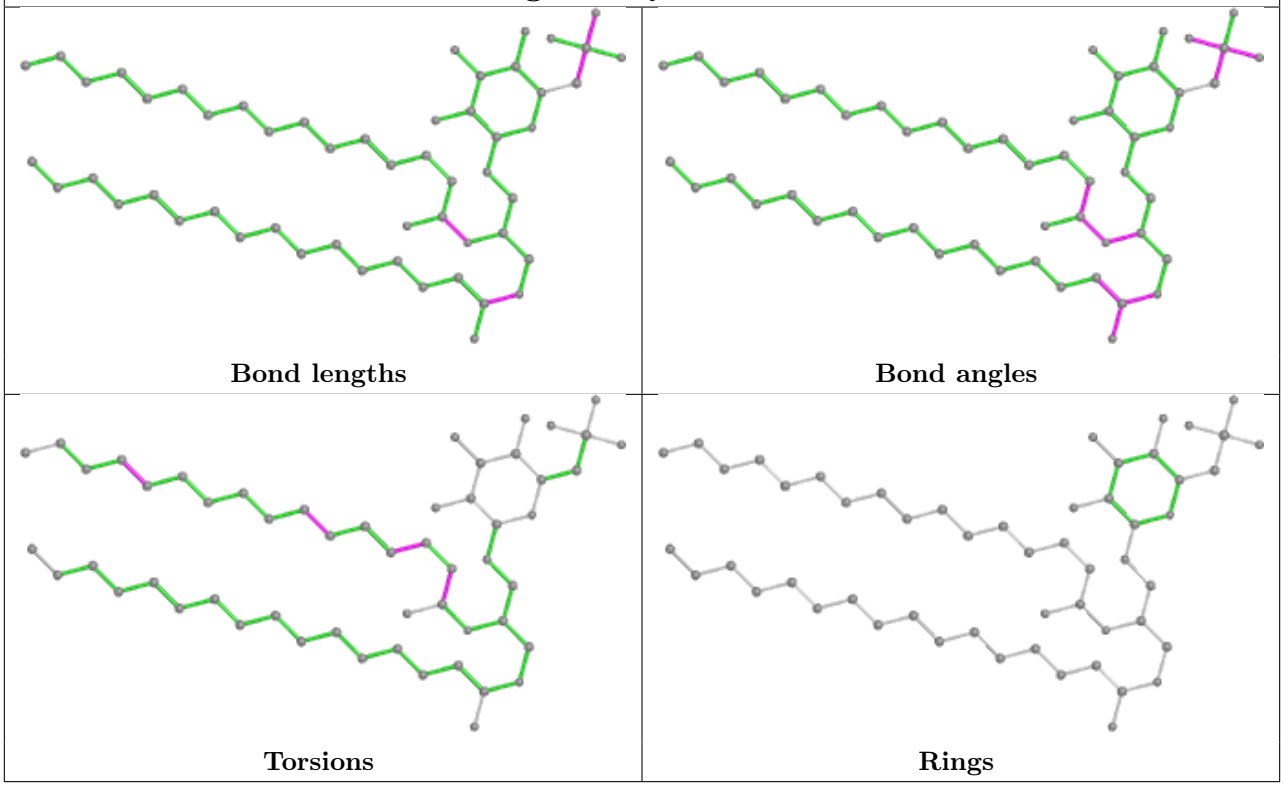


Rings

Ligand CLA B 608



Ligand SQD A 611



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	333/344 (96%)	0.12	10 (3%) 50 46	24, 32, 54, 72	0
1	a	333/344 (96%)	0.00	5 (1%) 73 71	24, 34, 62, 76	0
2	B	505/510 (99%)	0.04	24 (4%) 30 28	24, 35, 61, 84	0
2	b	503/510 (98%)	0.14	32 (6%) 19 16	26, 38, 67, 87	0
3	C	448/461 (97%)	0.09	11 (2%) 57 53	24, 40, 59, 77	0
3	c	448/461 (97%)	0.03	12 (2%) 54 50	29, 42, 60, 80	0
4	D	340/352 (96%)	-0.01	8 (2%) 59 54	25, 34, 52, 70	0
4	d	340/352 (96%)	-0.13	6 (1%) 68 64	26, 37, 59, 74	0
5	E	82/84 (97%)	1.03	17 (20%) 1 0	39, 57, 71, 75	0
5	e	79/84 (94%)	0.57	11 (13%) 2 1	43, 58, 71, 81	0
6	F	33/45 (73%)	-0.18	0 100 100	42, 49, 63, 71	0
6	f	33/45 (73%)	-0.08	1 (3%) 50 46	46, 52, 73, 82	0
7	H	63/66 (95%)	0.12	2 (3%) 47 44	34, 41, 48, 60	0
7	h	63/66 (95%)	0.48	8 (12%) 3 2	39, 48, 59, 69	0
8	I	33/38 (86%)	-0.33	0 100 100	30, 36, 44, 55	0
8	i	35/38 (92%)	-0.24	0 100 100	31, 39, 56, 66	0
9	J	34/40 (85%)	0.16	5 (14%) 2 1	40, 53, 64, 78	0
9	j	33/40 (82%)	0.15	1 (3%) 50 46	43, 52, 61, 65	0
10	K	36/46 (78%)	0.42	2 (5%) 24 20	52, 61, 75, 77	0
10	k	36/46 (78%)	0.17	1 (2%) 53 49	48, 60, 76, 78	0
11	L	36/37 (97%)	-0.26	1 (2%) 53 49	26, 33, 53, 59	0
11	l	36/37 (97%)	-0.09	1 (2%) 53 49	28, 35, 50, 62	0
12	M	32/36 (88%)	-0.11	0 100 100	30, 36, 56, 58	0
12	m	32/36 (88%)	0.11	3 (9%) 8 5	30, 38, 57, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	242/272 (88%)	0.44	21 (8%) 10 7	30, 44, 70, 104	0
13	o	243/272 (89%)	0.30	20 (8%) 11 8	28, 45, 72, 108	0
14	T	29/32 (90%)	0.19	2 (6%) 16 13	26, 35, 56, 62	0
14	t	29/32 (90%)	0.16	2 (6%) 16 13	31, 36, 55, 67	0
15	U	96/134 (71%)	0.38	7 (7%) 15 11	34, 43, 64, 72	0
15	u	96/134 (71%)	0.01	0 100 100	35, 45, 58, 65	0
16	V	137/163 (84%)	0.13	2 (1%) 73 71	33, 44, 56, 64	0
16	v	137/163 (84%)	0.72	20 (14%) 2 1	37, 50, 67, 82	0
17	Y	29/46 (63%)	2.59	17 (58%) 0 0	63, 76, 95, 96	0
17	y	29/46 (63%)	1.58	11 (37%) 0 0	61, 71, 90, 91	0
18	X	37/41 (90%)	0.26	6 (16%) 1 1	42, 50, 65, 79	0
18	x	38/41 (92%)	0.55	6 (15%) 2 1	41, 52, 74, 84	0
19	Z	62/62 (100%)	1.75	21 (33%) 0 0	57, 73, 104, 111	0
19	z	62/62 (100%)	2.31	33 (53%) 0 0	62, 74, 100, 107	0
20	R	34/41 (82%)	3.15	26 (76%) 0 0	61, 74, 88, 92	0
20	r	33/41 (80%)	2.94	26 (78%) 0 0	64, 73, 86, 91	0
All	All	5279/5700 (92%)	0.24	381 (7%) 15 12	24, 41, 72, 111	0

The worst 5 of 381 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	61	GLN	9.1
13	O	56	PRO	8.8
13	O	63	ALA	8.2
19	Z	33	TRP	7.5
17	Y	22	LEU	7.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
28	SQD	L	103	54/54	0.72	0.28	34,53,92,102	0
30	SO4	u	202	5/5	0.75	0.23	64,73,90,96	0
23	LMG	C	519	51/55	0.77	0.26	48,64,79,84	0
27	PL9	a	612	55/55	0.77	0.29	48,64,76,81	0
28	SQD	L	101	54/54	0.81	0.23	34,54,89,94	0
27	PL9	A	610	55/55	0.81	0.26	34,52,63,70	0
26	BCR	K	101	40/40	0.81	0.22	51,61,70,73	0
23	LMG	a	603	51/55	0.82	0.21	37,52,70,80	0
23	LMG	B	620	51/55	0.82	0.25	27,50,57,64	0
26	BCR	c	521	40/40	0.82	0.23	43,53,62,66	0
23	LMG	A	612	51/55	0.82	0.25	38,52,61,63	0
32	UNL	D	410	15/-	0.82	0.21	36,44,67,68	0
32	UNL	b	625	16/-	0.82	0.18	37,43,48,49	0
23	LMG	A	603	51/55	0.83	0.20	36,49,64,72	0
23	LMG	a	614	51/55	0.83	0.23	34,50,68,75	0
29	LHG	E	101	42/49	0.83	0.23	44,67,78,83	0
23	LMG	b	624	51/55	0.84	0.27	43,59,69,72	0
32	UNL	J	101	11/-	0.84	0.25	48,58,64,67	0
32	UNL	B	626	9/-	0.84	0.27	35,40,44,47	0
32	UNL	i	101	16/-	0.84	0.23	33,42,48,48	0
28	SQD	F	101	43/54	0.85	0.25	46,63,76,85	0
32	UNL	M	101	10/-	0.85	0.22	45,49,60,62	0
23	LMG	C	521	51/55	0.85	0.27	38,51,63,67	0
29	LHG	a	616	42/49	0.85	0.23	53,71,80,87	0
32	UNL	x	101	16/-	0.85	0.18	31,42,52,54	0
32	UNL	B	623	13/-	0.86	0.19	36,40,48,51	0
23	LMG	c	518	51/55	0.86	0.23	38,58,76,80	0
26	BCR	d	404	40/40	0.86	0.22	38,50,62,67	0
26	BCR	k	102	40/40	0.86	0.19	48,59,65,65	0
26	BCR	z	101	40/40	0.86	0.25	49,59,63,67	0
32	UNL	T	102	15/-	0.86	0.24	36,46,51,51	0
32	UNL	T	103	12/-	0.86	0.22	35,42,49,49	0
32	UNL	b	621	10/-	0.86	0.20	32,41,44,46	0
32	UNL	b	622	12/-	0.86	0.23	37,47,51,51	0
25	CLA	C	512	65/65	0.86	0.23	45,56,66,71	0
32	UNL	d	409	15/-	0.86	0.25	39,45,52,53	0
23	LMG	b	620	51/55	0.86	0.23	31,44,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	j	101	15/-	0.86	0.20	43,53,57,59	0
32	UNL	m	101	10/-	0.86	0.21	44,53,58,59	0
32	UNL	B	622	8/-	0.86	0.33	38,42,45,46	0
28	SQD	f	101	43/54	0.87	0.33	55,77,85,88	0
25	CLA	b	601	65/65	0.87	0.24	39,59,77,84	0
26	BCR	h	101	40/40	0.87	0.18	34,44,52,53	0
26	BCR	C	514	40/40	0.87	0.23	50,58,65,66	0
32	UNL	m	102	15/-	0.87	0.19	34,43,51,52	0
32	UNL	t	101	15/-	0.87	0.21	31,49,57,57	0
28	SQD	a	613	54/54	0.87	0.21	37,65,73,77	0
26	BCR	t	102	40/40	0.88	0.22	28,39,45,49	0
23	LMG	B	624	51/55	0.88	0.22	41,50,60,66	0
26	BCR	D	406	40/40	0.88	0.21	28,45,64,66	0
32	UNL	b	623	13/-	0.88	0.17	37,44,53,54	0
26	BCR	H	101	40/40	0.88	0.17	32,37,53,54	0
32	UNL	c	519	15/-	0.88	0.18	40,46,51,53	0
27	PL9	d	405	55/55	0.88	0.20	29,37,50,55	0
25	CLA	C	513	65/65	0.88	0.20	51,62,77,82	0
32	UNL	B	627	12/-	0.88	0.24	33,39,45,50	0
23	LMG	c	520	51/55	0.88	0.30	41,54,74,79	0
25	CLA	c	502	65/65	0.88	0.24	31,41,49,55	0
25	CLA	c	513	65/65	0.88	0.24	45,60,76,79	0
26	BCR	B	619	40/40	0.88	0.17	33,39,46,50	0
33	DGD	C	517	62/66	0.88	0.21	36,50,69,82	0
33	DGD	c	516	62/66	0.88	0.23	32,46,78,87	0
28	SQD	A	611	54/54	0.89	0.20	32,57,74,79	0
25	CLA	B	601	65/65	0.89	0.16	36,49,72,80	0
25	CLA	c	503	65/65	0.89	0.20	33,43,50,57	0
32	UNL	b	626	9/-	0.89	0.26	32,45,53,56	0
32	UNL	B	625	16/-	0.89	0.15	37,42,49,50	0
26	BCR	T	101	40/40	0.89	0.21	30,41,48,50	0
33	DGD	C	518	62/66	0.89	0.20	30,46,63,70	0
30	SO4	V	202	5/5	0.89	0.55	71,72,81,81	0
25	CLA	B	609	65/65	0.90	0.15	28,36,43,52	0
25	CLA	C	502	65/65	0.90	0.20	35,43,48,50	0
25	CLA	c	511	65/65	0.90	0.15	39,54,62,66	0
25	CLA	C	511	65/65	0.90	0.18	42,58,67,70	0
30	SO4	O	301	5/5	0.90	0.31	51,67,76,82	0
26	BCR	A	609	40/40	0.90	0.17	24,34,39,40	0
32	UNL	I	101	14/-	0.90	0.15	32,41,48,49	0
25	CLA	b	616	65/65	0.90	0.20	28,42,62,69	0
33	DGD	H	102	62/66	0.90	0.23	27,36,47,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	BCT	a	618	4/4	0.90	0.13	36,38,43,44	0
33	DGD	h	102	62/66	0.90	0.19	35,44,51,56	0
30	SO4	a	617	5/5	0.91	0.20	52,57,70,79	0
25	CLA	C	510	65/65	0.91	0.22	36,46,58,68	0
22	FE	a	602	1/1	0.91	0.08	37,37,37,37	0
32	UNL	B	621	10/-	0.91	0.19	34,41,45,46	0
25	CLA	B	616	65/65	0.91	0.18	26,36,78,87	0
26	BCR	a	611	40/40	0.91	0.15	26,35,41,44	0
26	BCR	b	617	40/40	0.91	0.21	31,41,48,51	0
25	CLA	c	512	65/65	0.91	0.19	44,57,65,68	0
25	CLA	B	606	65/65	0.91	0.17	25,33,57,62	0
32	UNL	C	520	15/-	0.91	0.14	31,42,47,47	0
25	CLA	D	405	65/65	0.91	0.19	24,35,63,68	0
29	LHG	A	614	49/49	0.91	0.20	29,48,70,78	0
25	CLA	C	503	65/65	0.91	0.17	32,44,49,50	0
29	LHG	a	615	49/49	0.91	0.19	32,42,53,62	0
25	CLA	b	604	65/65	0.91	0.23	23,34,50,58	0
26	BCR	C	522	40/40	0.91	0.19	45,55,63,64	0
25	CLA	C	508	65/65	0.91	0.21	36,43,79,88	0
29	LHG	l	101	49/49	0.92	0.17	28,39,50,53	0
27	PL9	D	407	55/55	0.92	0.19	21,37,44,47	0
25	CLA	c	505	65/65	0.92	0.16	32,40,48,51	0
25	CLA	c	508	65/65	0.92	0.21	35,44,73,77	0
25	CLA	a	608	65/65	0.92	0.18	28,36,75,85	0
23	LMG	d	408	51/55	0.92	0.17	35,49,72,80	0
25	CLA	C	504	65/65	0.92	0.20	35,49,67,75	0
25	CLA	d	403	65/65	0.92	0.17	28,39,77,85	0
25	CLA	b	606	65/65	0.92	0.15	24,35,55,62	0
26	BCR	B	617	40/40	0.92	0.17	32,38,44,47	0
29	LHG	A	613	49/49	0.92	0.18	21,37,47,56	0
25	CLA	b	614	65/65	0.92	0.16	25,38,57,65	0
25	CLA	C	507	65/65	0.92	0.16	26,41,51,57	0
29	LHG	L	102	49/49	0.92	0.17	27,39,46,50	0
25	CLA	B	614	65/65	0.92	0.17	27,36,57,61	0
25	CLA	C	509	65/65	0.92	0.17	35,43,55,60	0
29	LHG	d	406	49/49	0.92	0.16	25,41,48,53	0
32	UNL	M	102	16/-	0.92	0.15	28,43,53,56	0
29	LHG	d	407	49/49	0.92	0.22	38,50,68,76	0
26	BCR	b	619	40/40	0.93	0.16	35,44,50,54	0
26	BCR	c	514	40/40	0.93	0.16	26,42,50,53	0
25	CLA	c	510	65/65	0.93	0.25	41,46,53,57	0
23	LMG	D	409	51/55	0.93	0.17	31,48,74,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	B	604	65/65	0.93	0.20	20,32,50,65	0
25	CLA	b	613	65/65	0.93	0.23	21,29,52,58	0
30	SO4	A	615	5/5	0.93	0.29	49,50,62,64	0
25	CLA	C	505	65/65	0.93	0.17	29,39,49,57	0
25	CLA	b	615	65/65	0.93	0.14	31,39,49,52	0
25	CLA	C	506	65/65	0.93	0.13	32,41,67,71	0
26	BCR	B	618	40/40	0.93	0.18	23,35,48,50	0
25	CLA	c	501	65/65	0.93	0.18	27,39,45,54	0
25	CLA	B	615	65/65	0.93	0.15	28,36,47,55	0
32	UNL	k	101	9/-	0.93	0.27	44,52,56,56	0
26	BCR	C	515	40/40	0.93	0.16	30,40,50,54	0
25	CLA	a	607	65/65	0.93	0.16	22,30,37,45	0
25	CLA	c	504	65/65	0.93	0.23	35,42,61,74	0
24	CL	a	604	1/1	0.93	0.22	40,40,40,40	0
25	CLA	c	506	65/65	0.93	0.17	35,44,66,73	0
25	CLA	c	507	65/65	0.93	0.17	31,41,50,52	0
25	CLA	B	608	65/65	0.93	0.19	21,32,41,47	0
25	CLA	c	509	65/65	0.93	0.20	32,45,56,61	0
33	DGD	c	517	62/66	0.93	0.17	33,45,66,77	0
26	BCR	b	618	40/40	0.93	0.21	27,36,41,48	0
34	PHO	d	402	64/64	0.93	0.17	29,40,48,54	0
35	HEM	E	102	43/43	0.93	0.17	42,53,68,74	0
25	CLA	B	605	65/65	0.94	0.17	21,30,37,42	0
25	CLA	B	612	65/65	0.94	0.18	25,31,40,44	0
25	CLA	B	602	65/65	0.94	0.16	21,34,47,50	0
25	CLA	b	608	65/65	0.94	0.20	28,40,49,56	0
25	CLA	b	609	65/65	0.94	0.15	28,41,55,60	0
30	SO4	O	302	5/5	0.94	0.31	65,66,78,80	0
30	SO4	U	201	5/5	0.94	0.14	47,60,63,71	5
33	DGD	c	515	62/66	0.94	0.18	26,37,70,73	0
25	CLA	b	611	65/65	0.94	0.17	23,36,45,48	0
25	CLA	b	612	65/65	0.94	0.21	24,34,43,48	0
30	SO4	o	301	5/5	0.94	0.29	62,68,71,91	0
34	PHO	D	402	64/64	0.94	0.20	24,33,41,49	0
34	PHO	a	609	64/64	0.94	0.15	24,30,39,42	0
25	CLA	A	607	65/65	0.94	0.19	23,36,71,74	0
25	CLA	a	610	65/65	0.94	0.16	23,30,65,76	0
35	HEM	e	101	43/43	0.94	0.16	49,57,69,72	0
25	CLA	b	610	65/65	0.95	0.17	23,35,45,48	0
25	CLA	a	606	65/65	0.95	0.15	19,30,40,48	0
25	CLA	C	501	65/65	0.95	0.15	21,34,46,51	0
25	CLA	B	611	65/65	0.95	0.17	19,27,39,42	0

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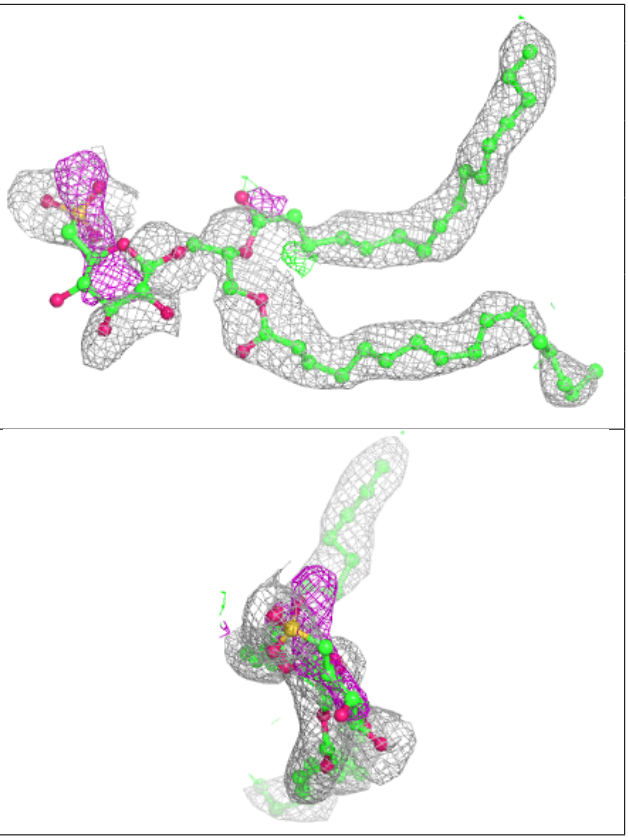
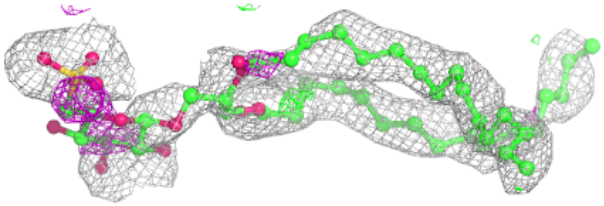
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	B	603	65/65	0.95	0.16	21,31,48,53	0
25	CLA	B	613	65/65	0.95	0.18	21,30,50,60	0
25	CLA	d	401	65/65	0.95	0.15	20,30,45,53	0
33	DGD	C	516	62/66	0.95	0.18	25,35,67,72	0
25	CLA	b	602	65/65	0.95	0.15	29,41,55,60	0
25	CLA	b	603	65/65	0.95	0.18	24,36,50,60	0
25	CLA	A	606	65/65	0.95	0.16	19,29,35,47	0
30	SO4	d	410	5/5	0.95	0.18	73,73,83,84	0
32	UNL	X	101	10/-	0.95	0.22	36,38,40,40	0
25	CLA	b	605	65/65	0.95	0.18	24,33,42,47	0
30	SO4	u	201	5/5	0.95	0.19	63,66,73,73	0
25	CLA	A	608	65/65	0.95	0.17	14,27,68,74	0
29	LHG	D	408	49/49	0.95	0.15	20,36,45,51	0
25	CLA	b	607	65/65	0.95	0.21	22,29,42,44	0
25	CLA	D	403	65/65	0.95	0.14	23,30,39,49	0
25	CLA	B	610	65/65	0.95	0.16	20,29,37,40	0
36	HEC	v	201	43/43	0.95	0.15	29,39,47,55	0
25	CLA	D	404	65/65	0.96	0.15	18,28,40,43	0
34	PHO	D	401	64/64	0.96	0.16	24,30,36,39	0
25	CLA	B	607	65/65	0.96	0.16	19,28,53,54	0
24	CL	A	604	1/1	0.96	0.15	35,35,35,35	0
22	FE	A	602	1/1	0.97	0.06	34,34,34,34	0
21	OEX	a	601	10/10	0.97	0.11	33,37,46,51	0
31	BCT	A	616	4/4	0.97	0.11	28,33,33,38	0
36	HEC	V	201	43/43	0.97	0.15	31,38,46,48	0
24	CL	a	605	1/1	0.97	0.17	38,38,38,38	1
21	OEX	A	601	10/10	0.98	0.13	34,40,52,57	0
24	CL	A	605	1/1	0.99	0.18	26,26,26,26	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 SQD L 103:

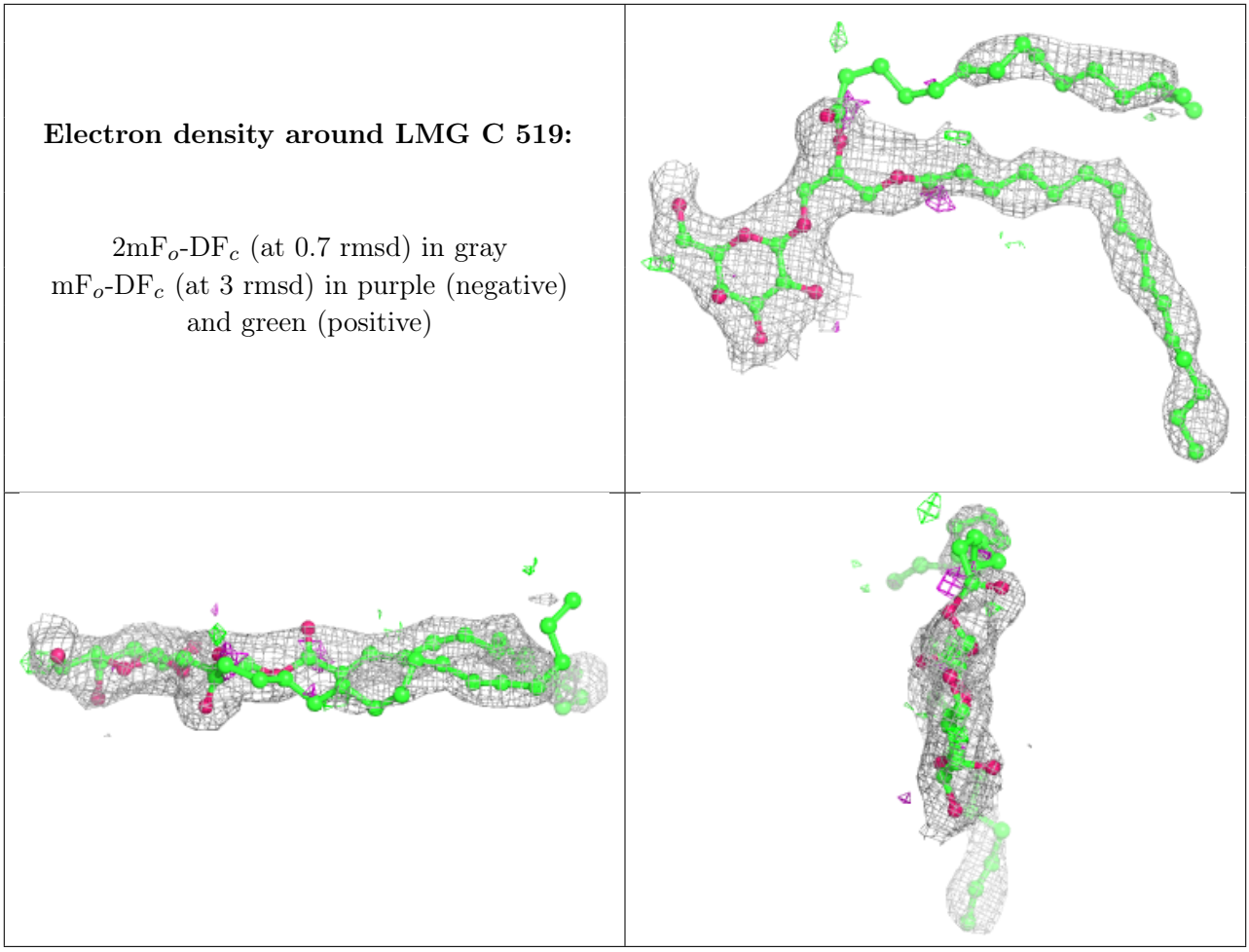
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





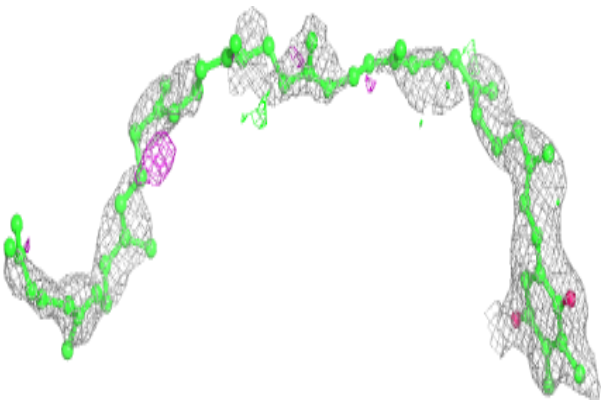
Electron density around LMG C 519:

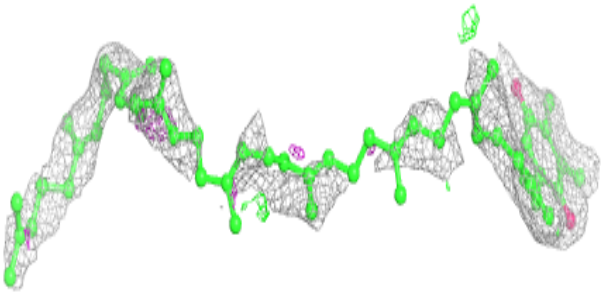
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

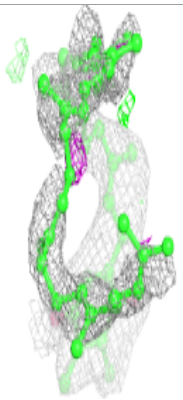


Electron density around PL9 a 612:

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

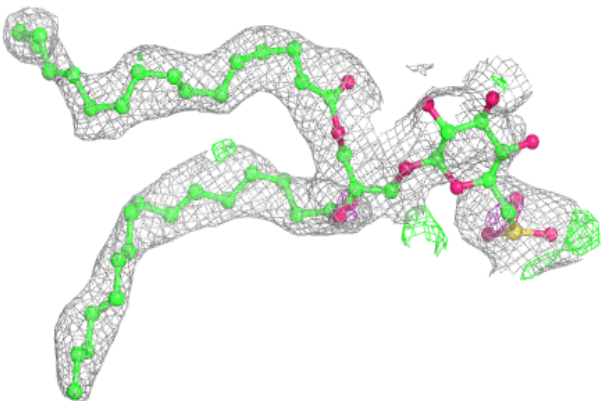


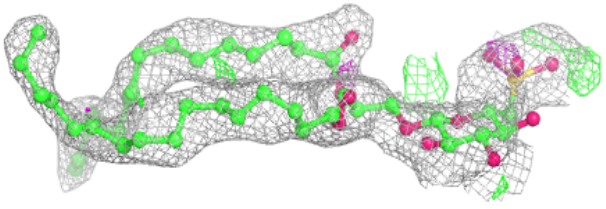


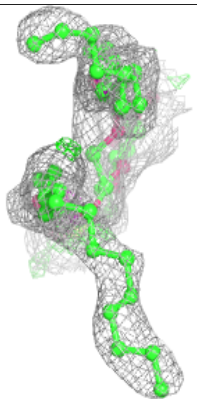


Electron density around SQD L 101:

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

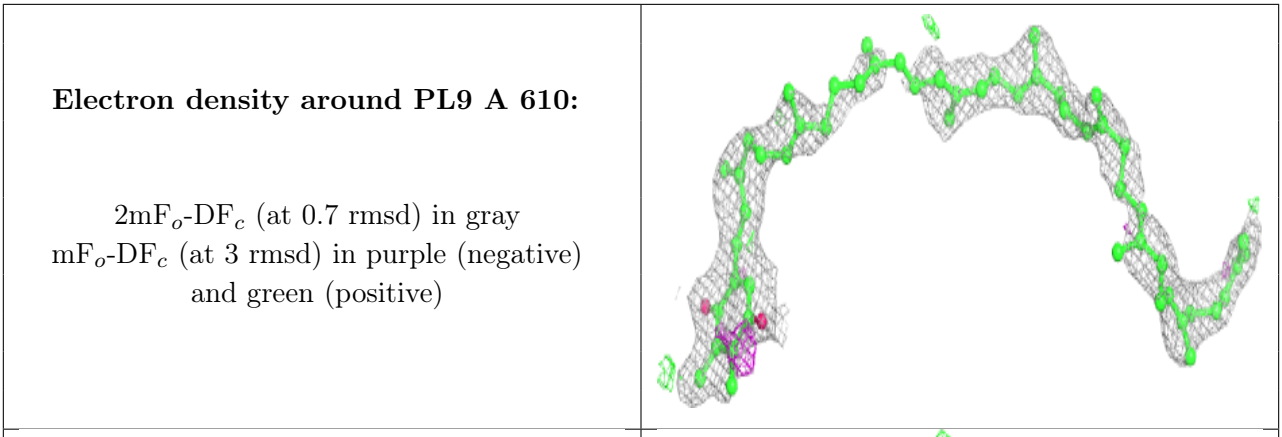






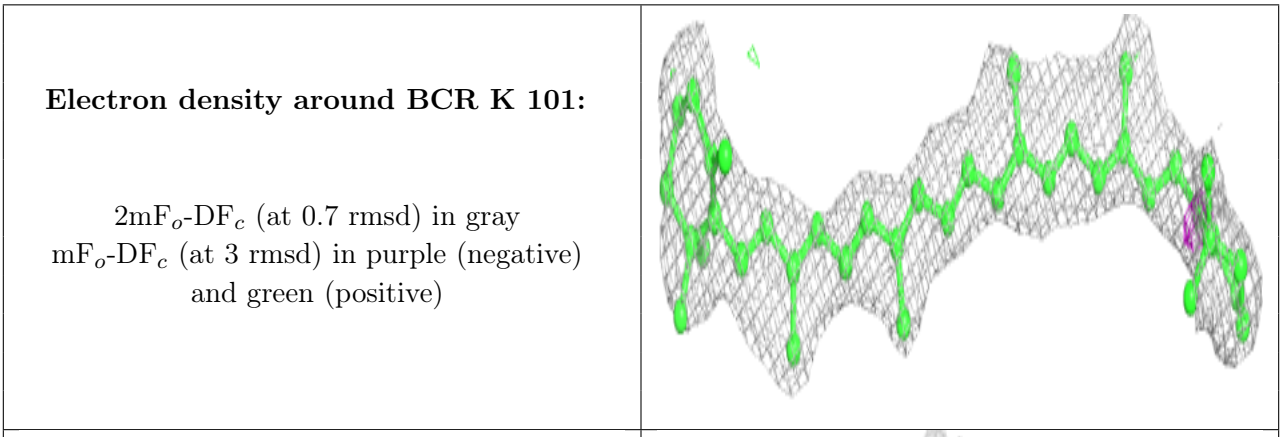
Electron density around PL9 A 610:

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



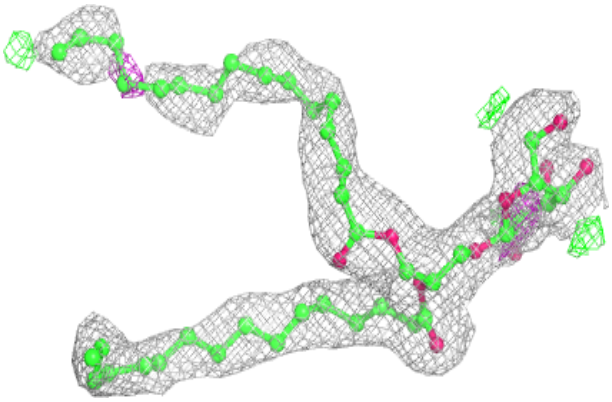
Electron density around BCR K 101:

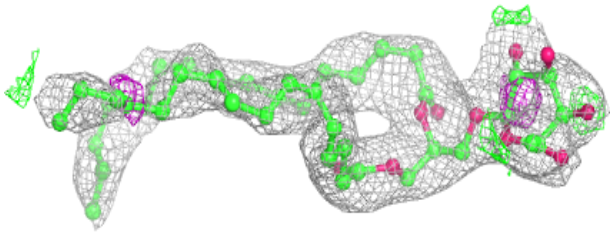
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

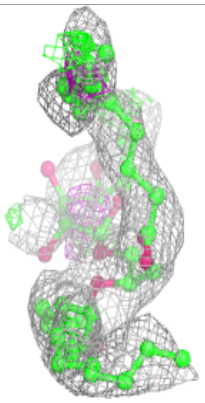


Electron density around LMG a 603:

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

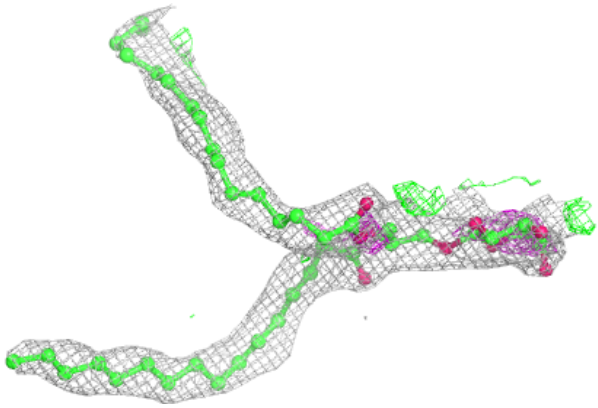


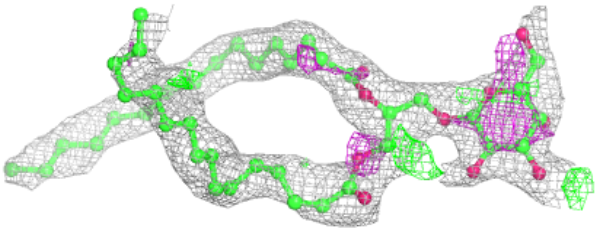


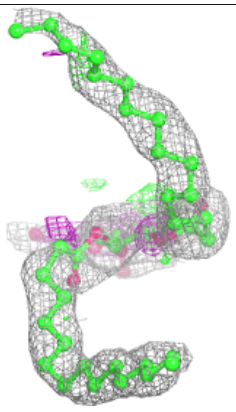


Electron density around LMG B 620:

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

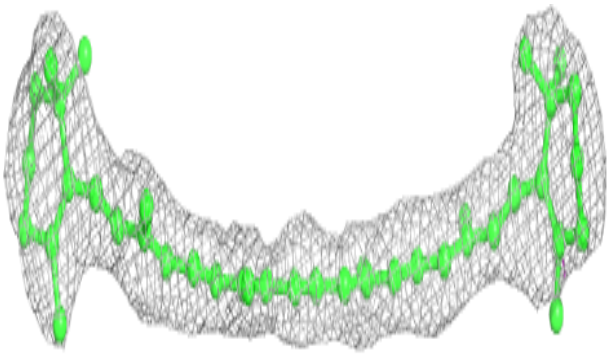


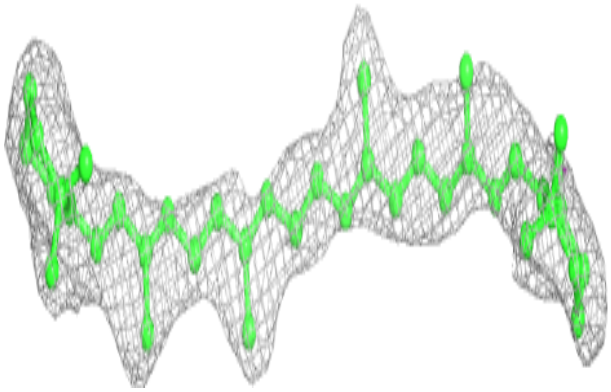


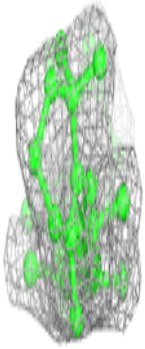


Electron density around BCR c 521:

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

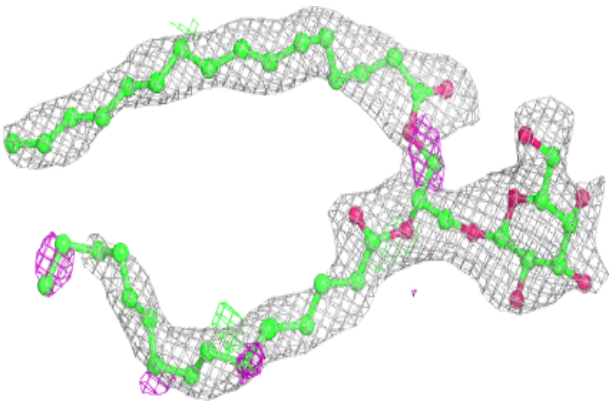


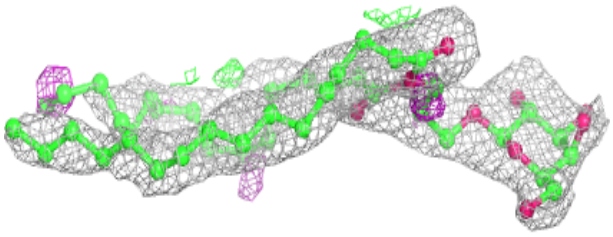


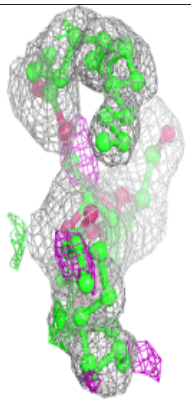


Electron density around LMG A 612:

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

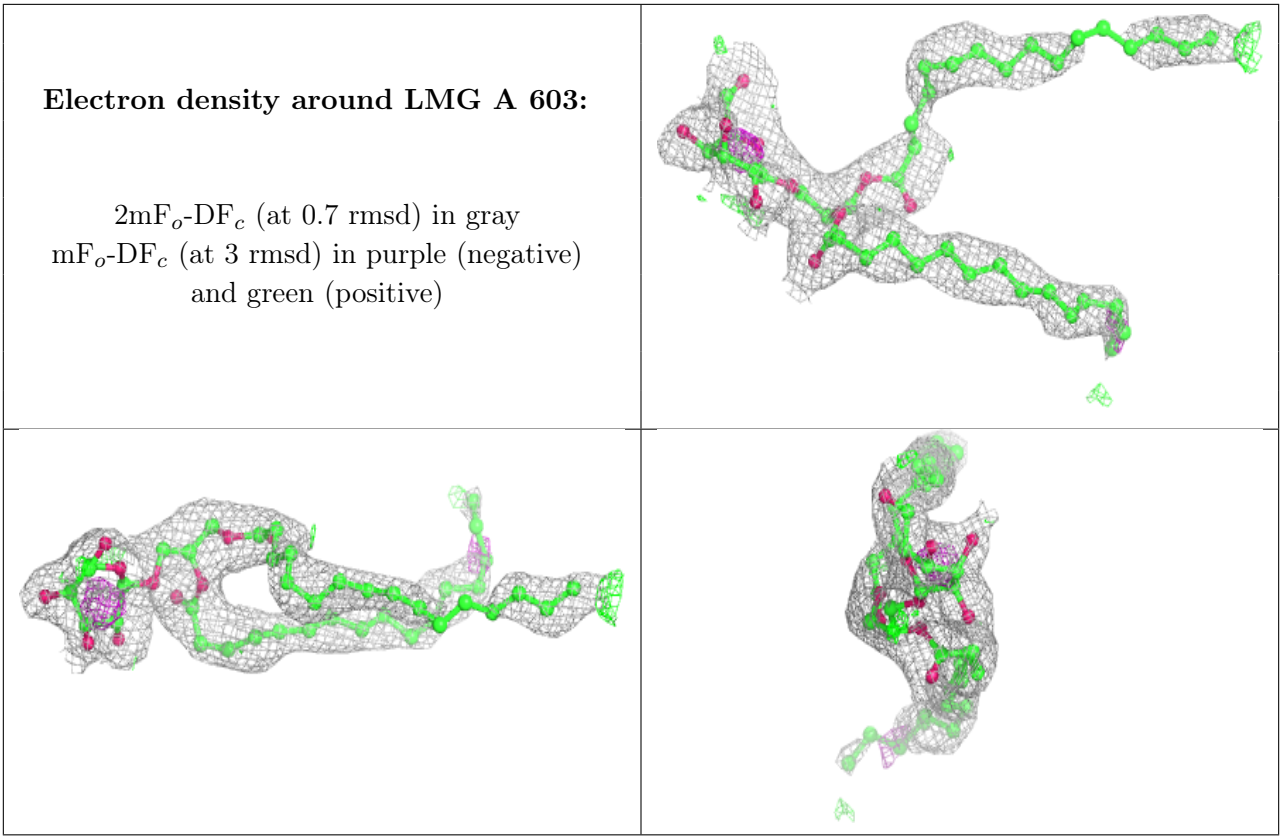






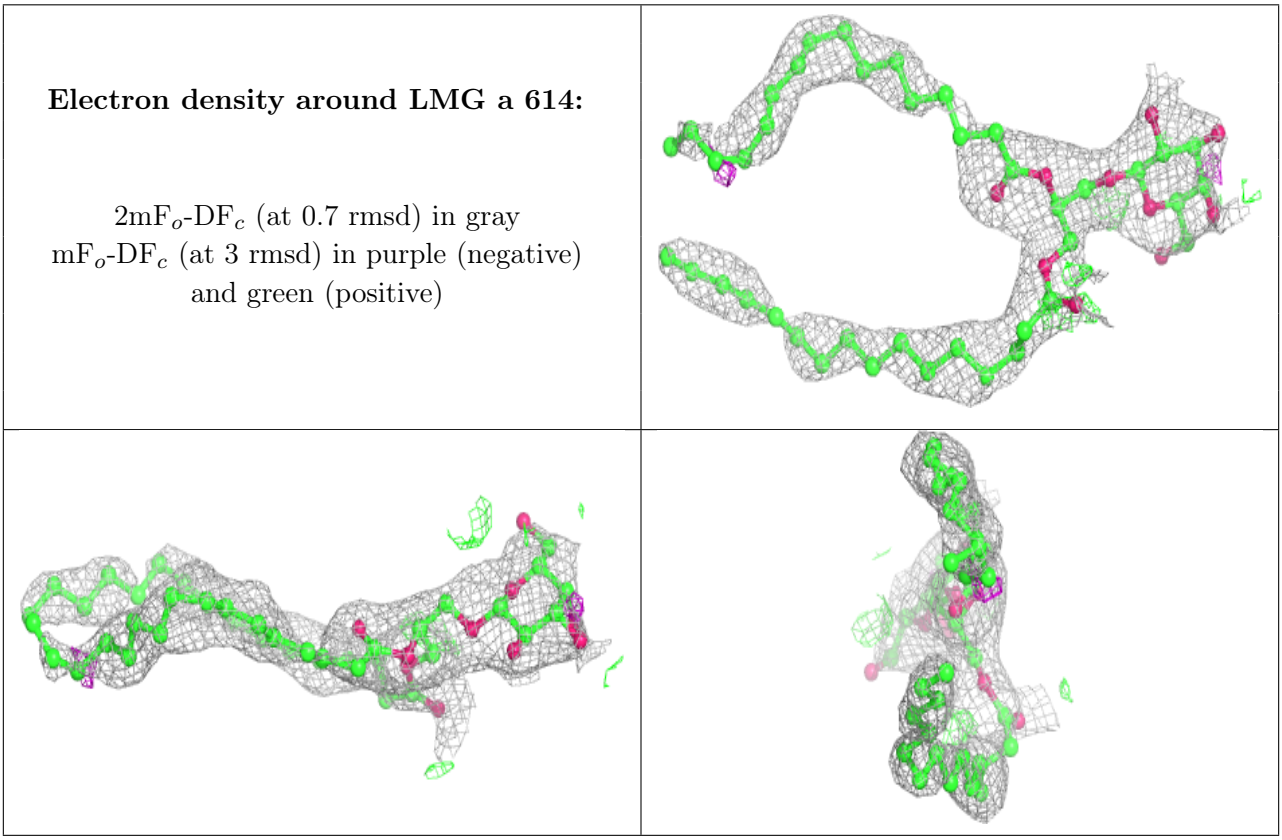
Electron density around LMG A 603:

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



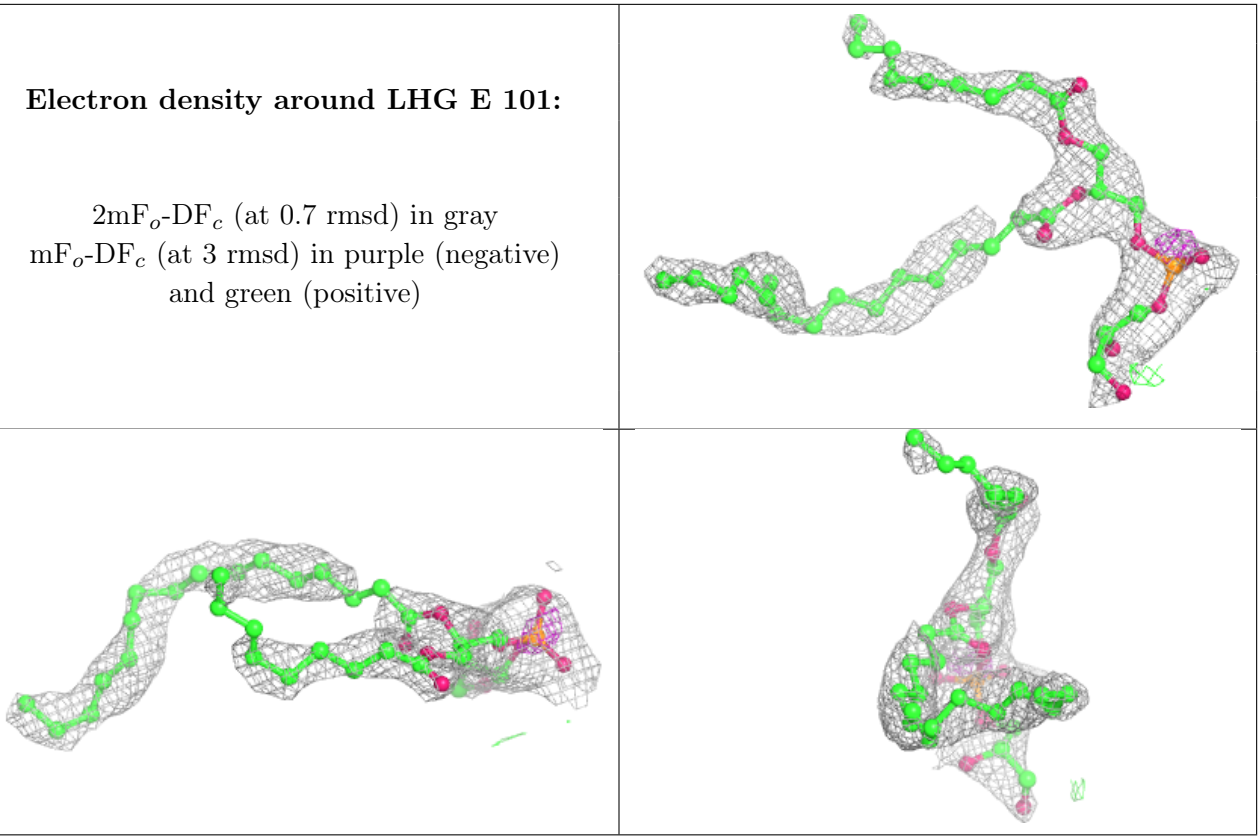
Electron density around LMG a 614:

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



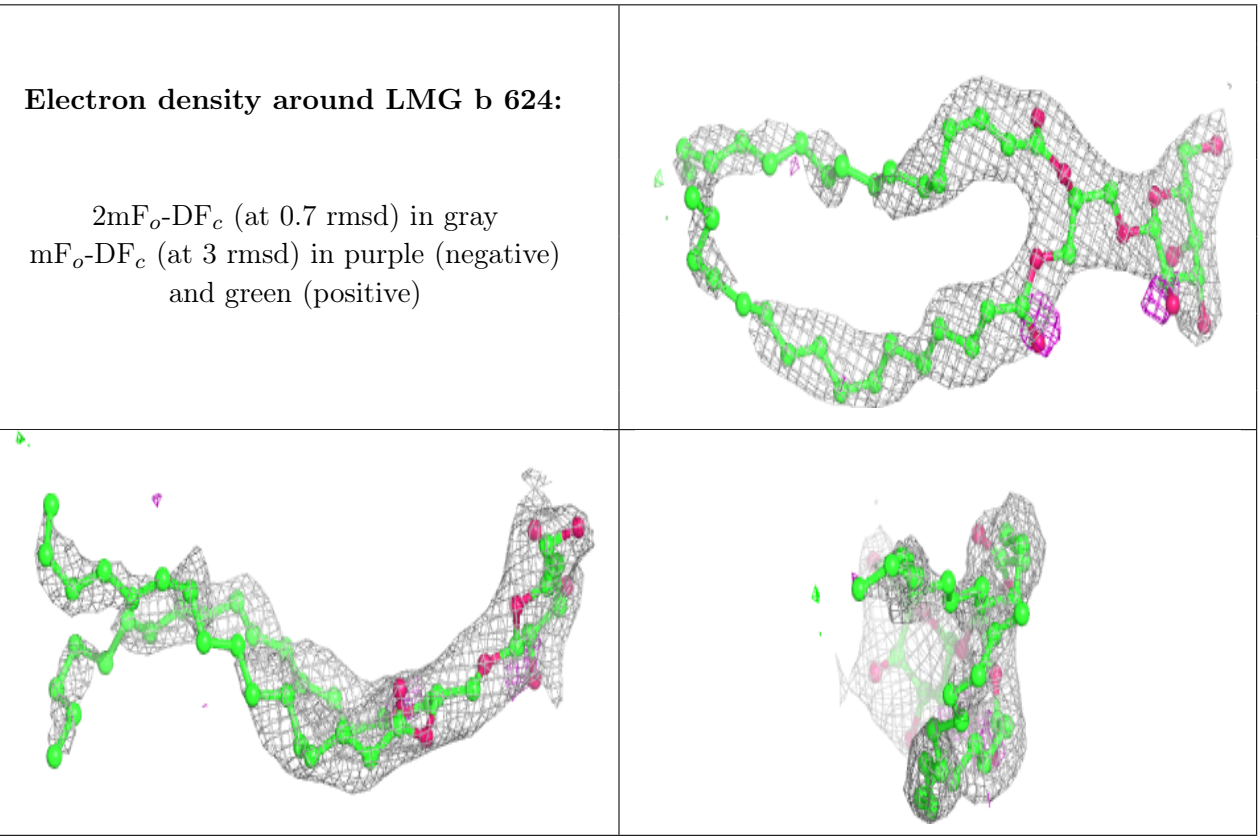
Electron density around LHG E 101:

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



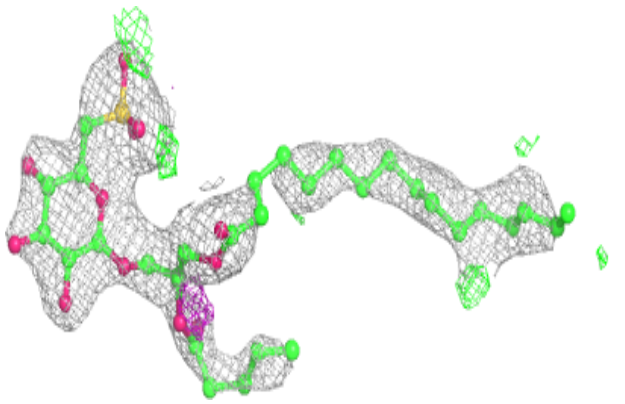
Electron density around LMG b 624:

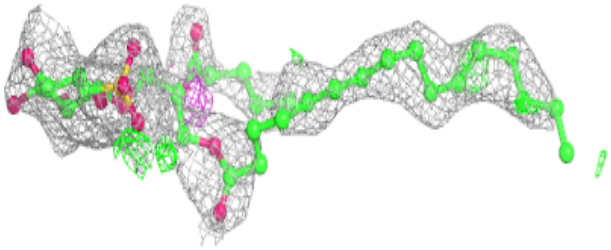
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

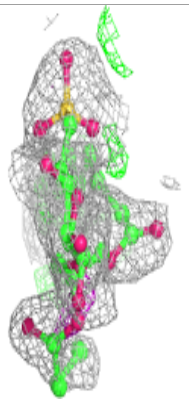


Electron density around SQD F 101:

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

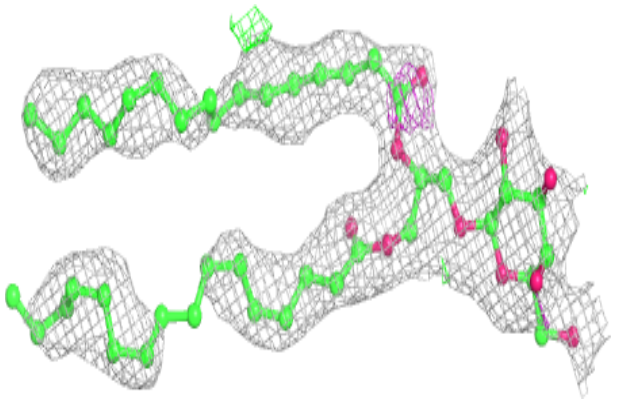


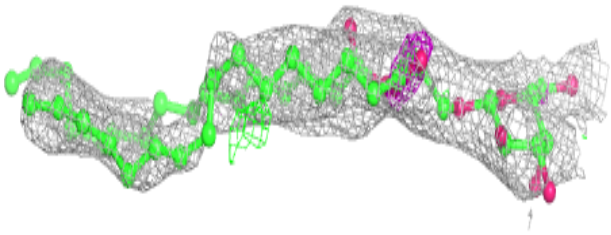


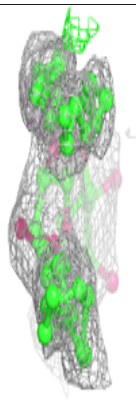


Electron density around LMG C 521:

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

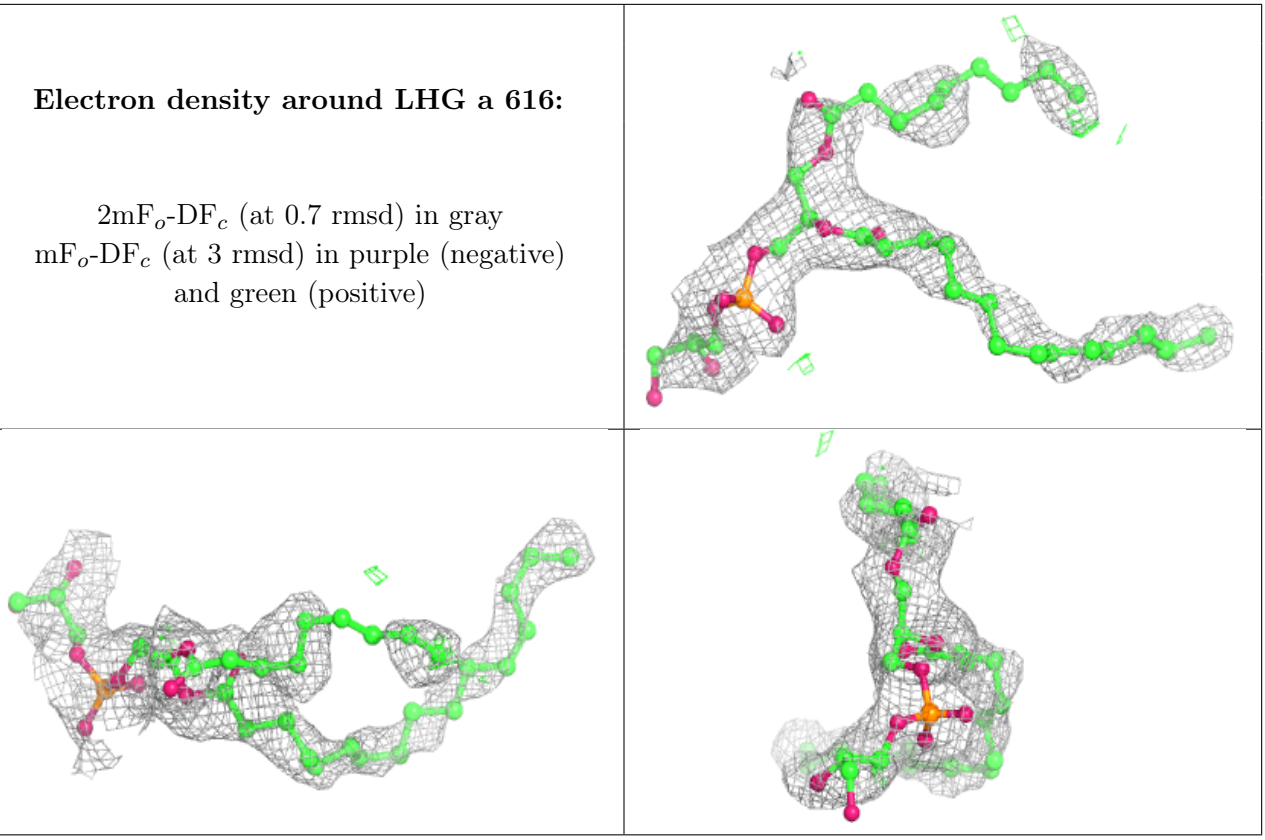






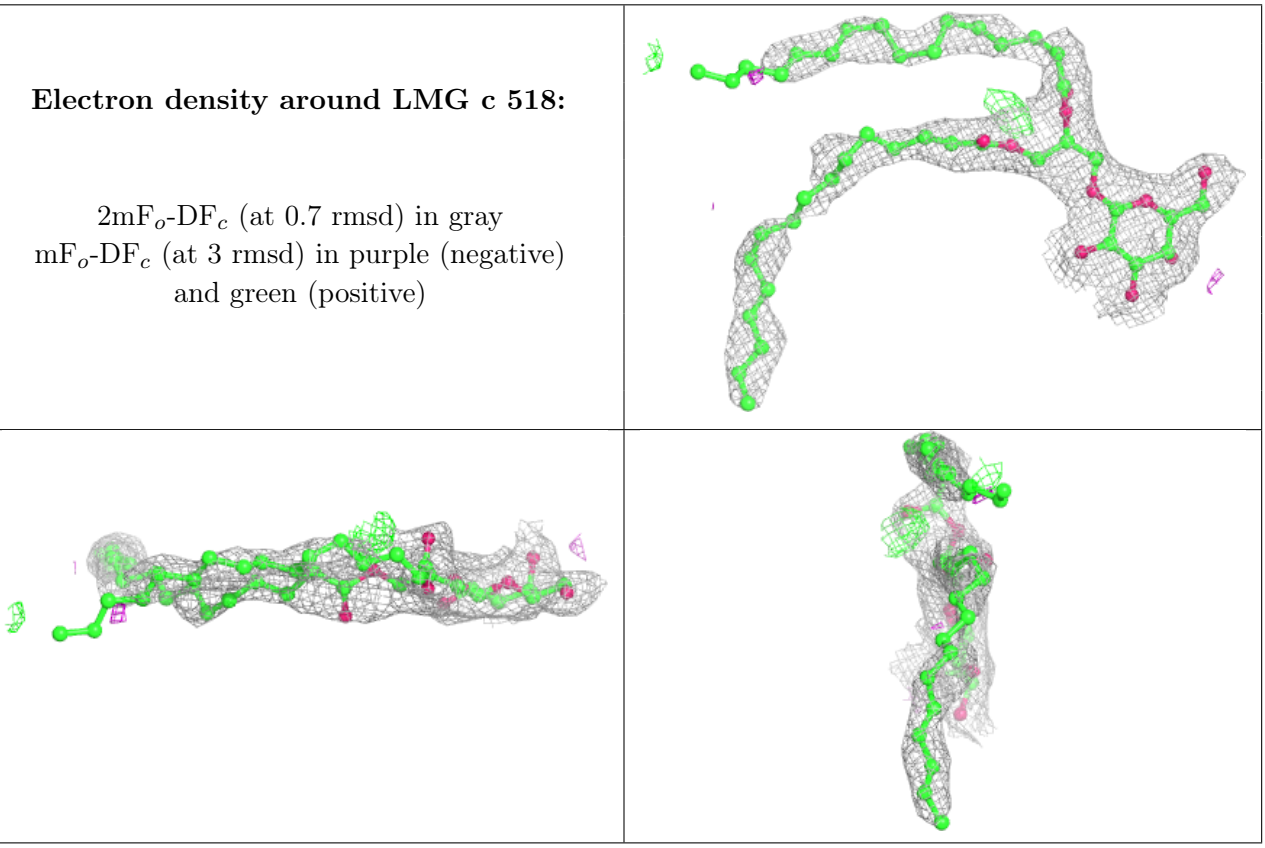
Electron density around LHG a 616:

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



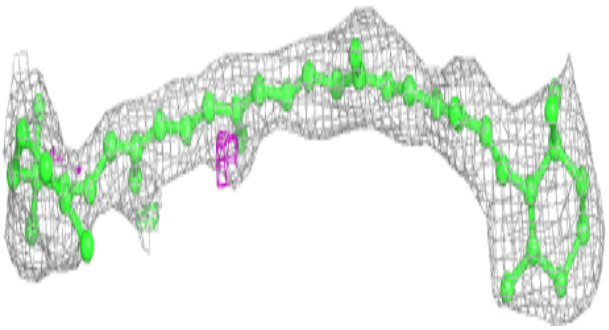
Electron density around LMG c 518:

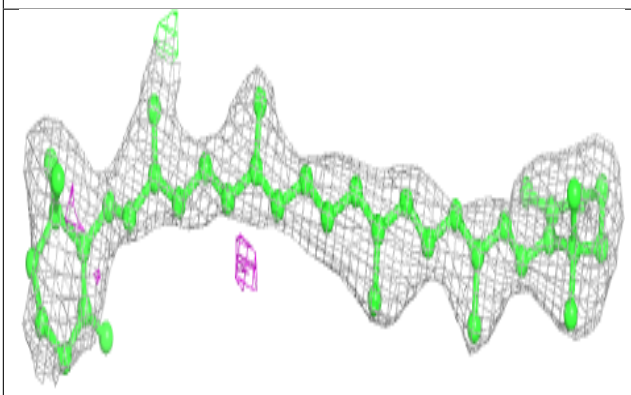
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

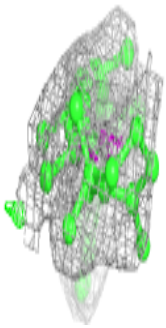


Electron density around BCR d 404:

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

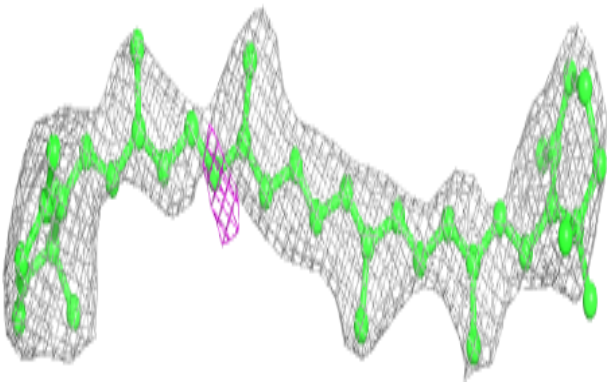


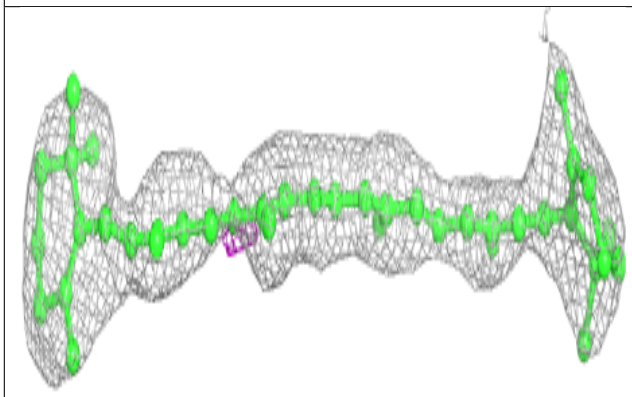


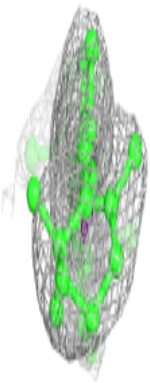


Electron density around BCR k 102:

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

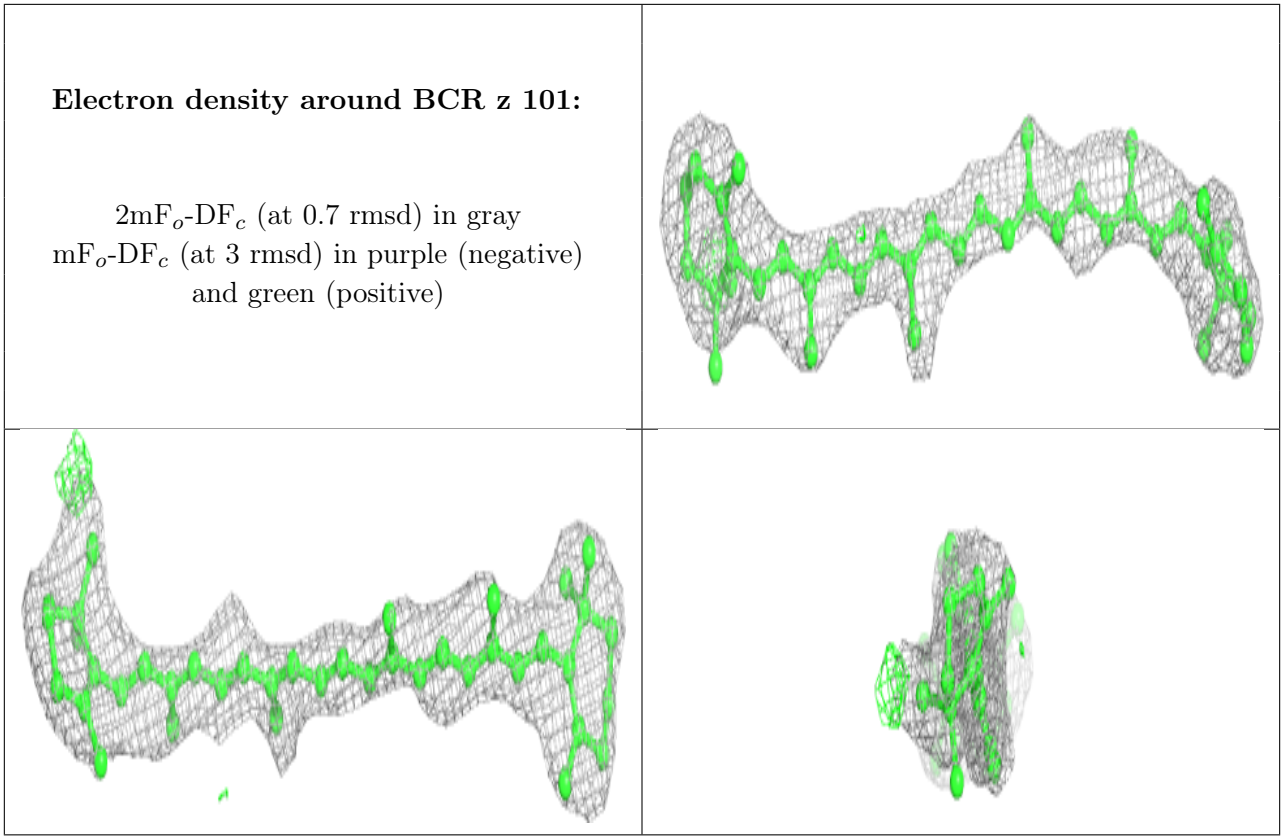






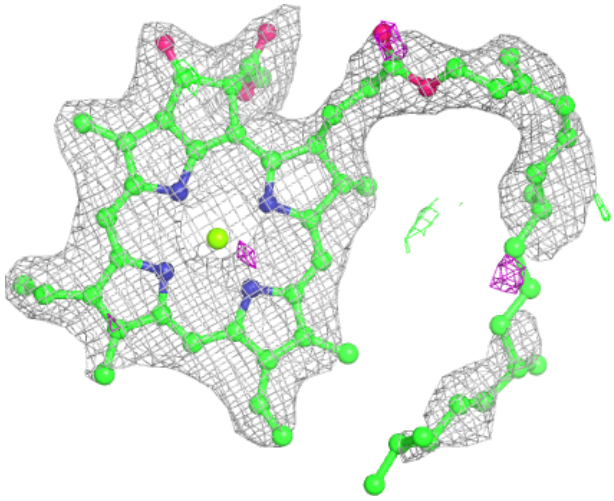
Electron density around BCR z 101:

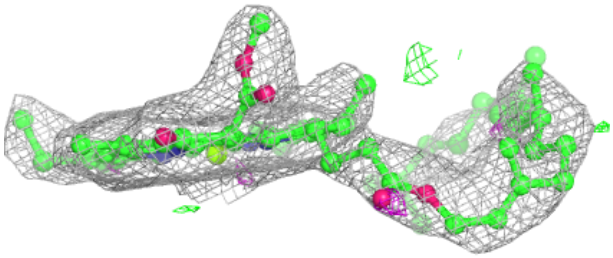
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

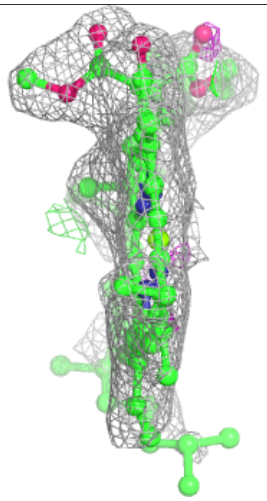


Electron density around CLA C 512:

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

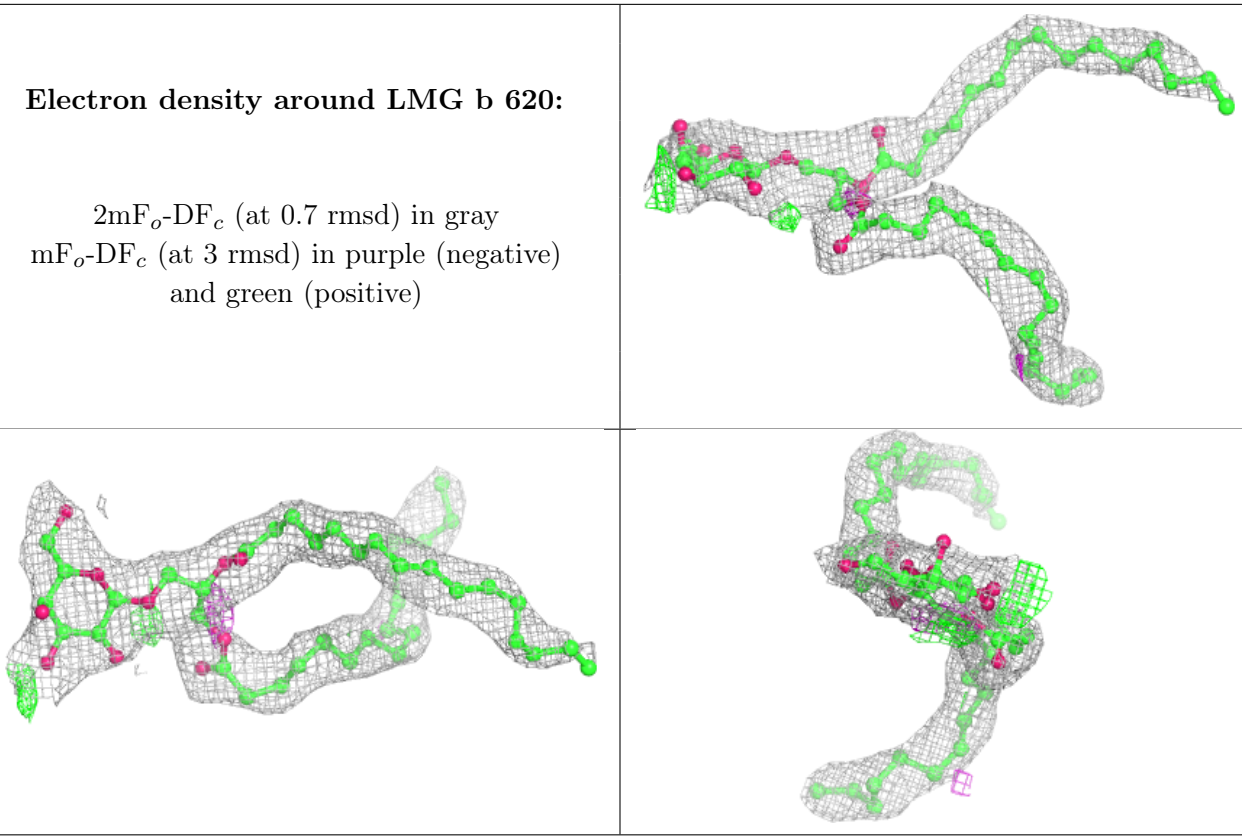






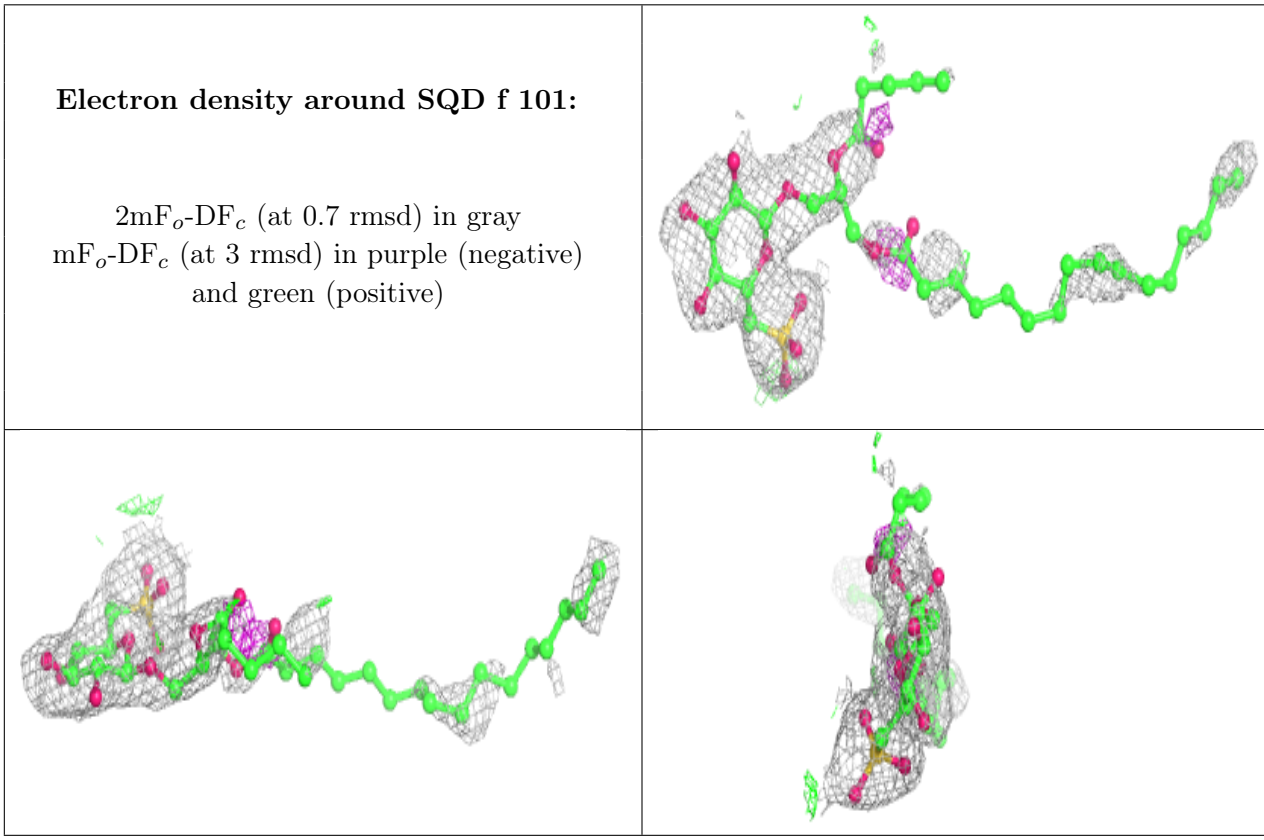
Electron density around LMG b 620:

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



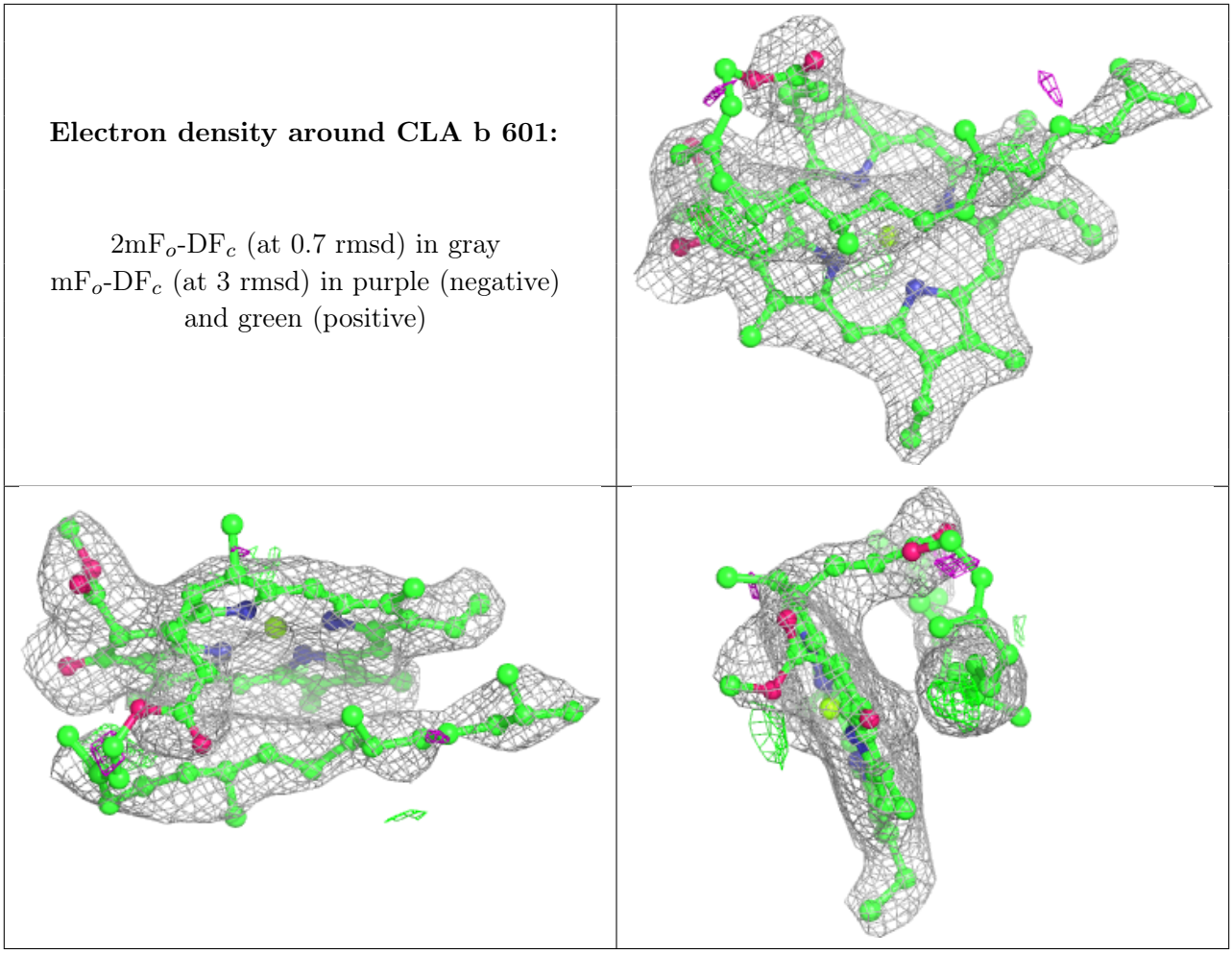
Electron density around SQD f 101:

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



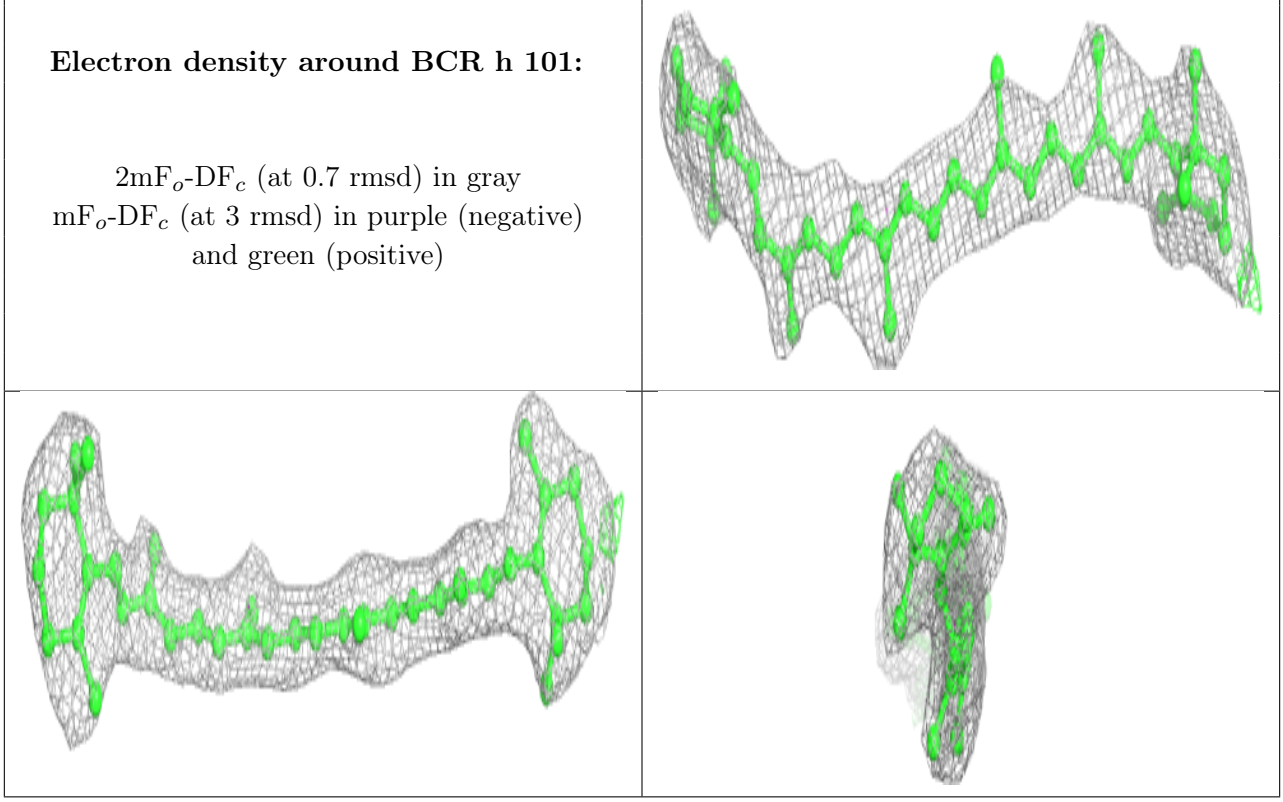
Electron density around CLA b 601:

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



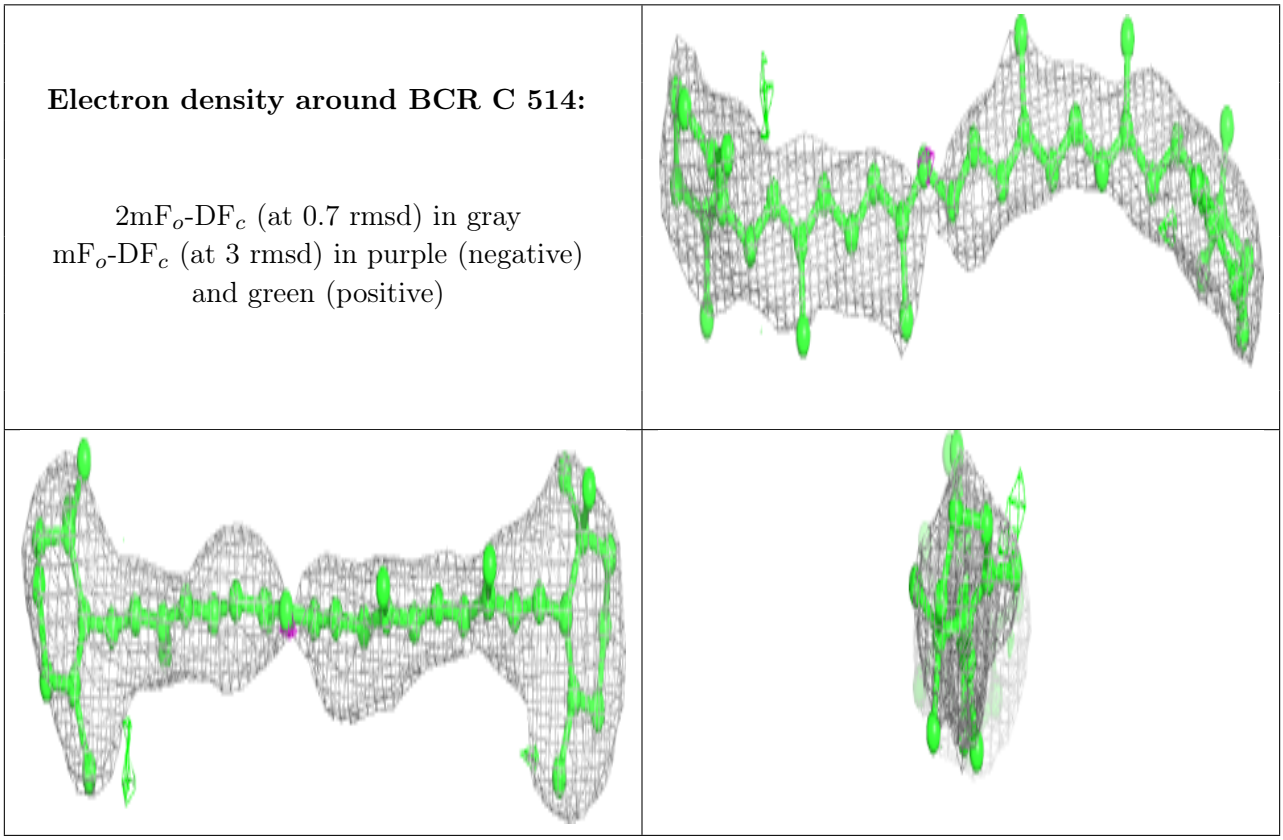
Electron density around BCR h 101:

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



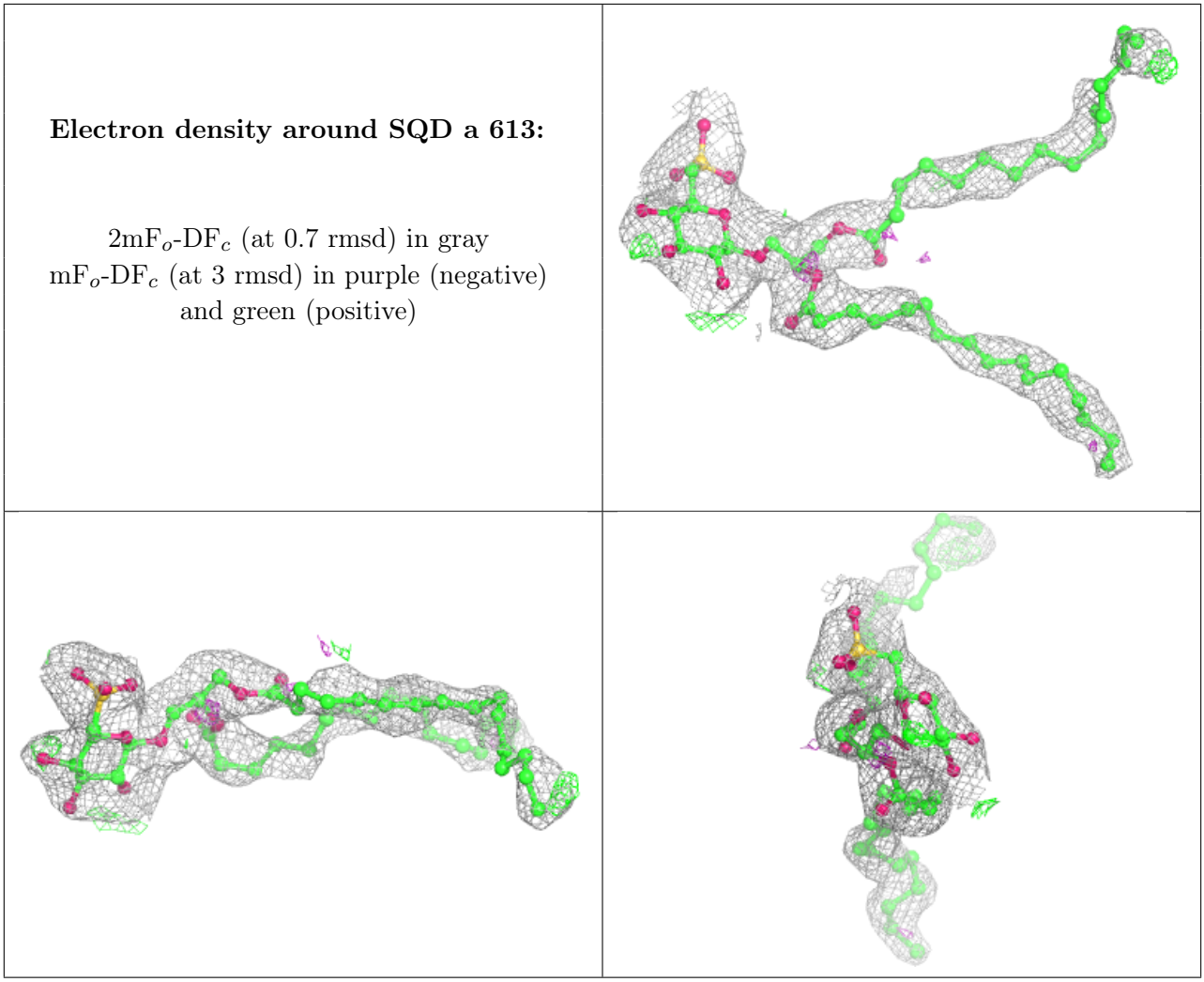
Electron density around BCR C 514:

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



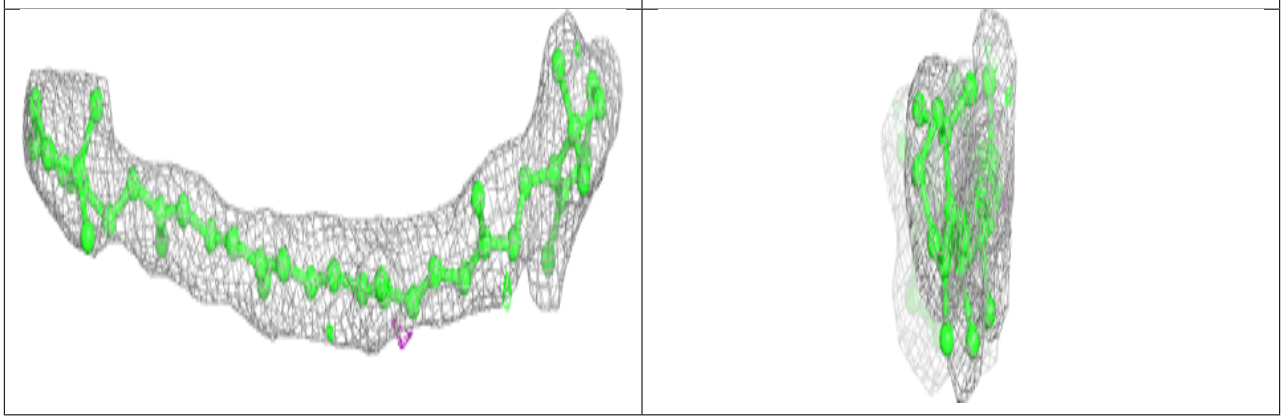
Electron density around SQD a 613:

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



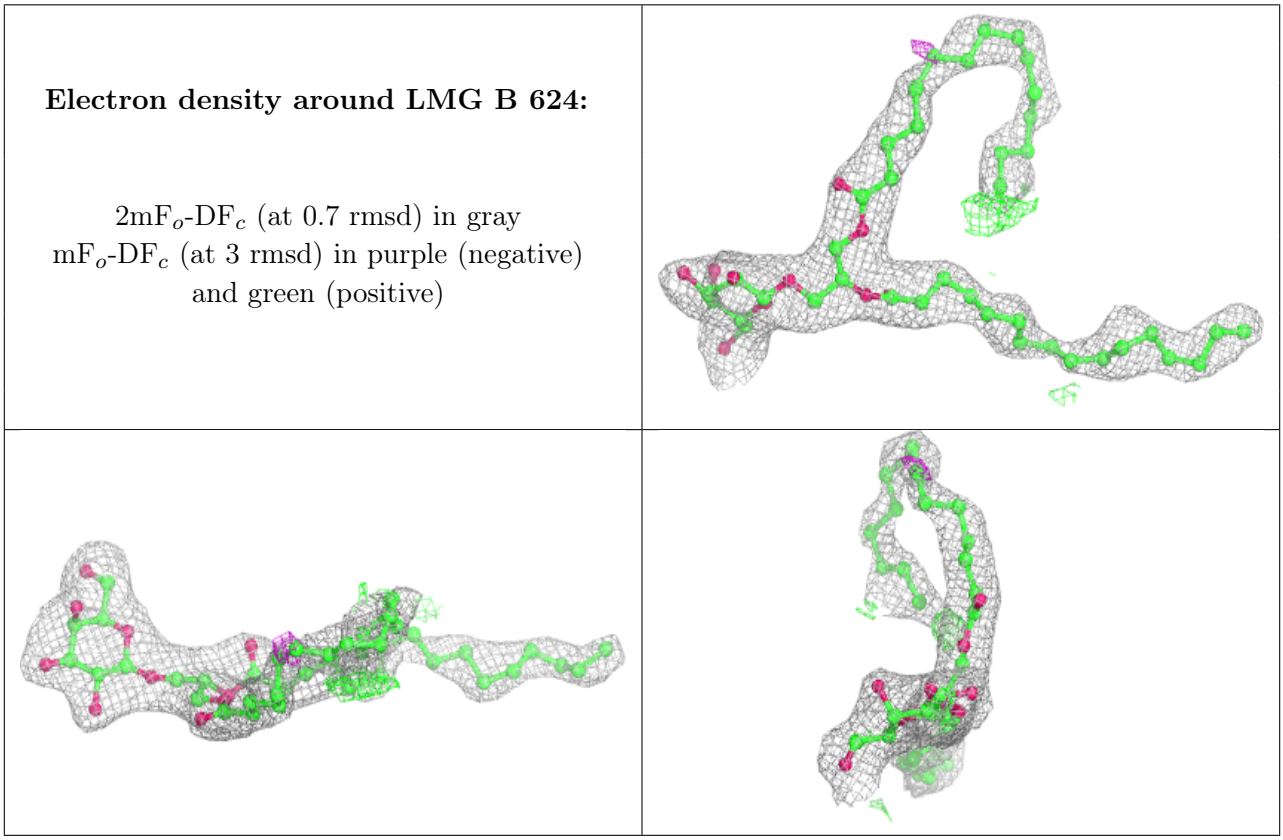
Electron density around BCR t 102:

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



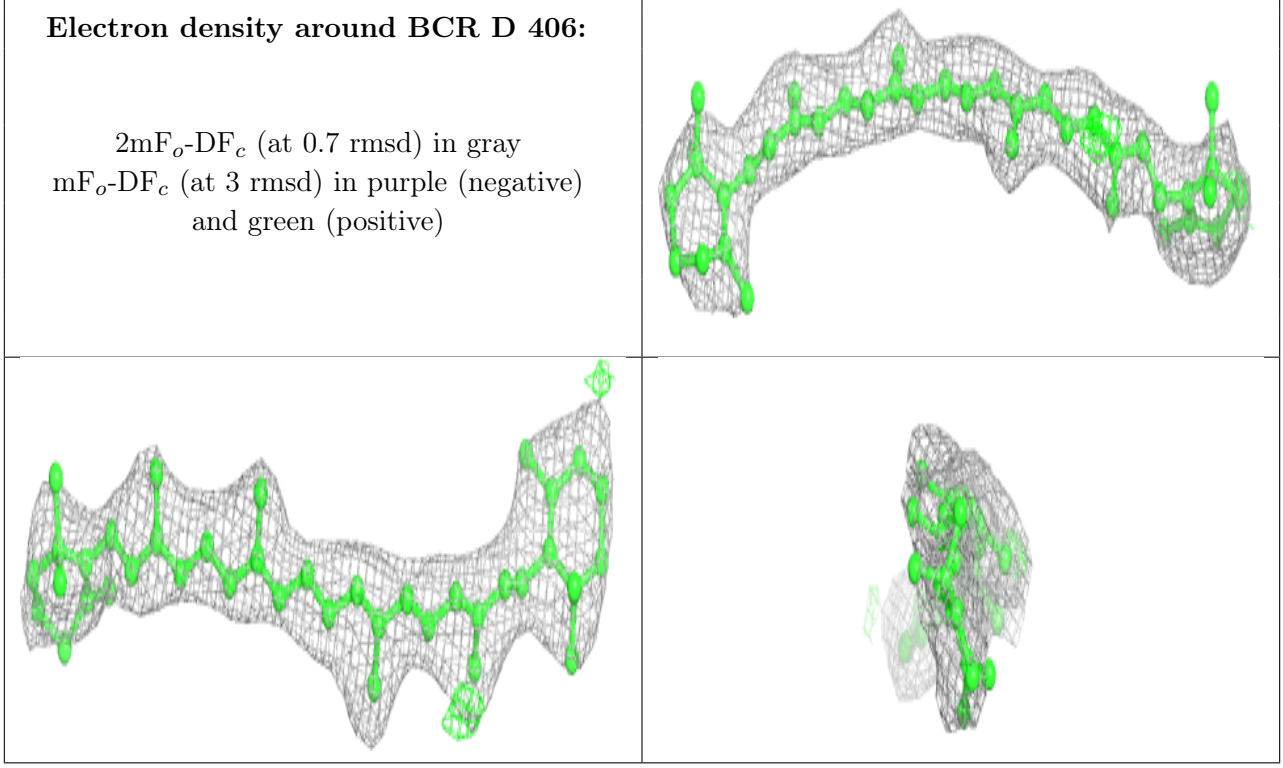
Electron density around LMG B 624:

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



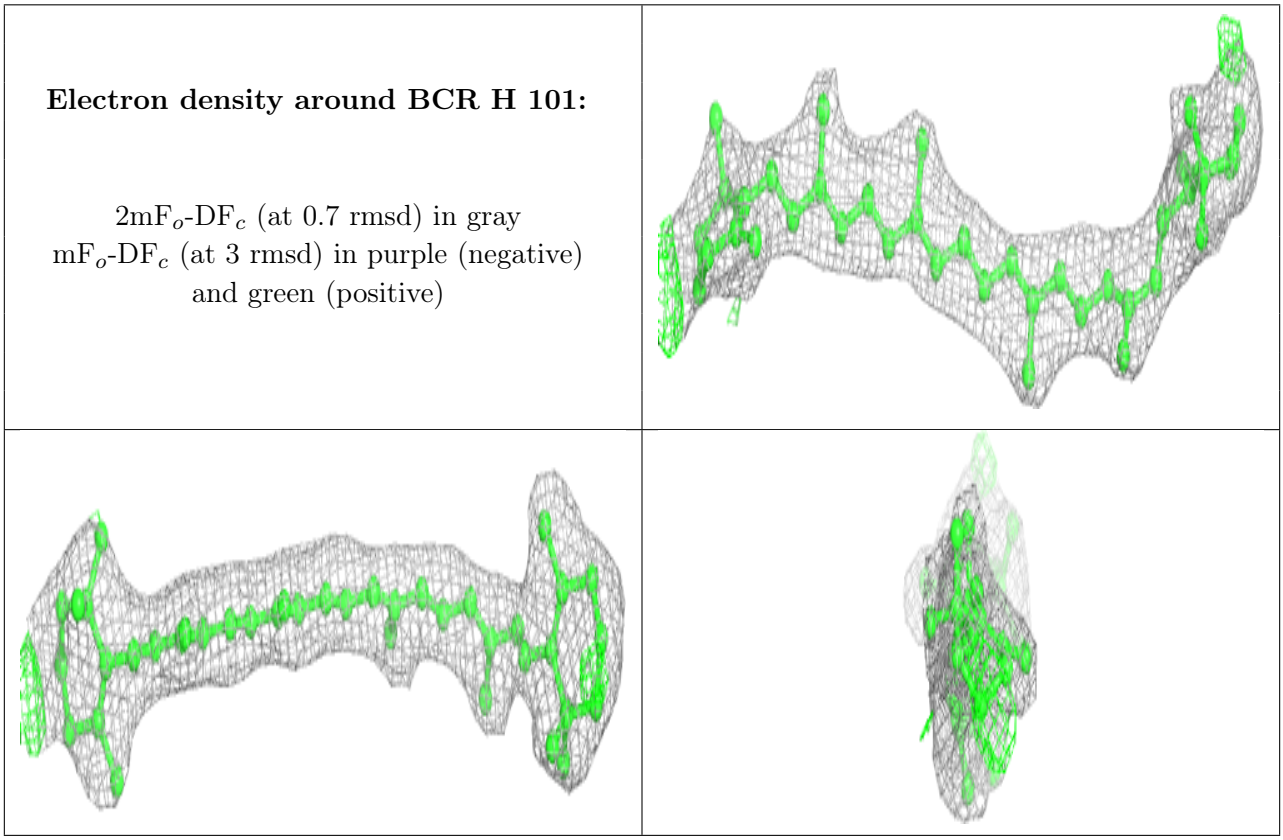
Electron density around BCR D 406:

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



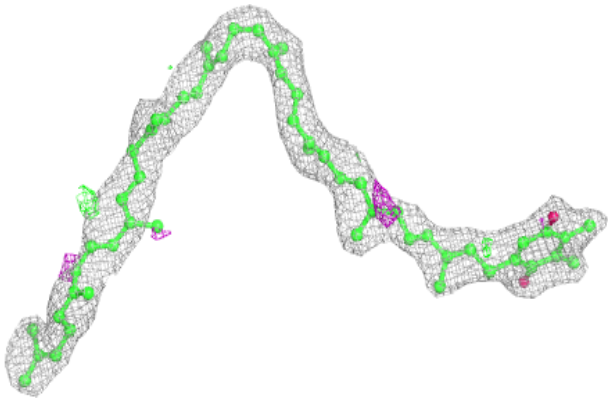
Electron density around BCR H 101:

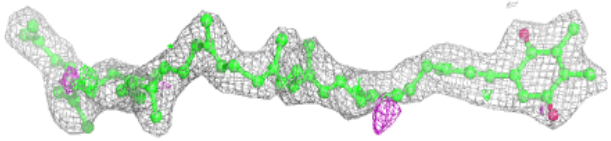
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

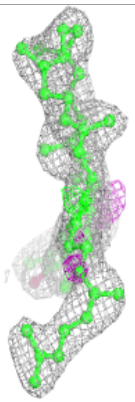


Electron density around PL9 d 405:

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

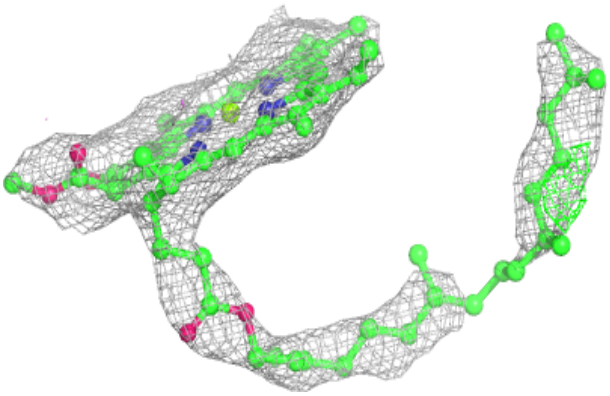


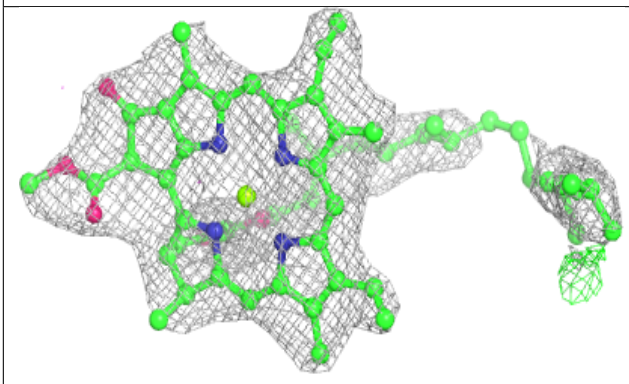


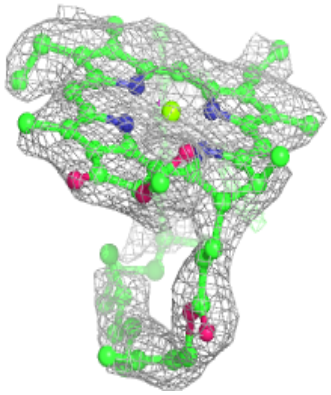


Electron density around CLA C 513:

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

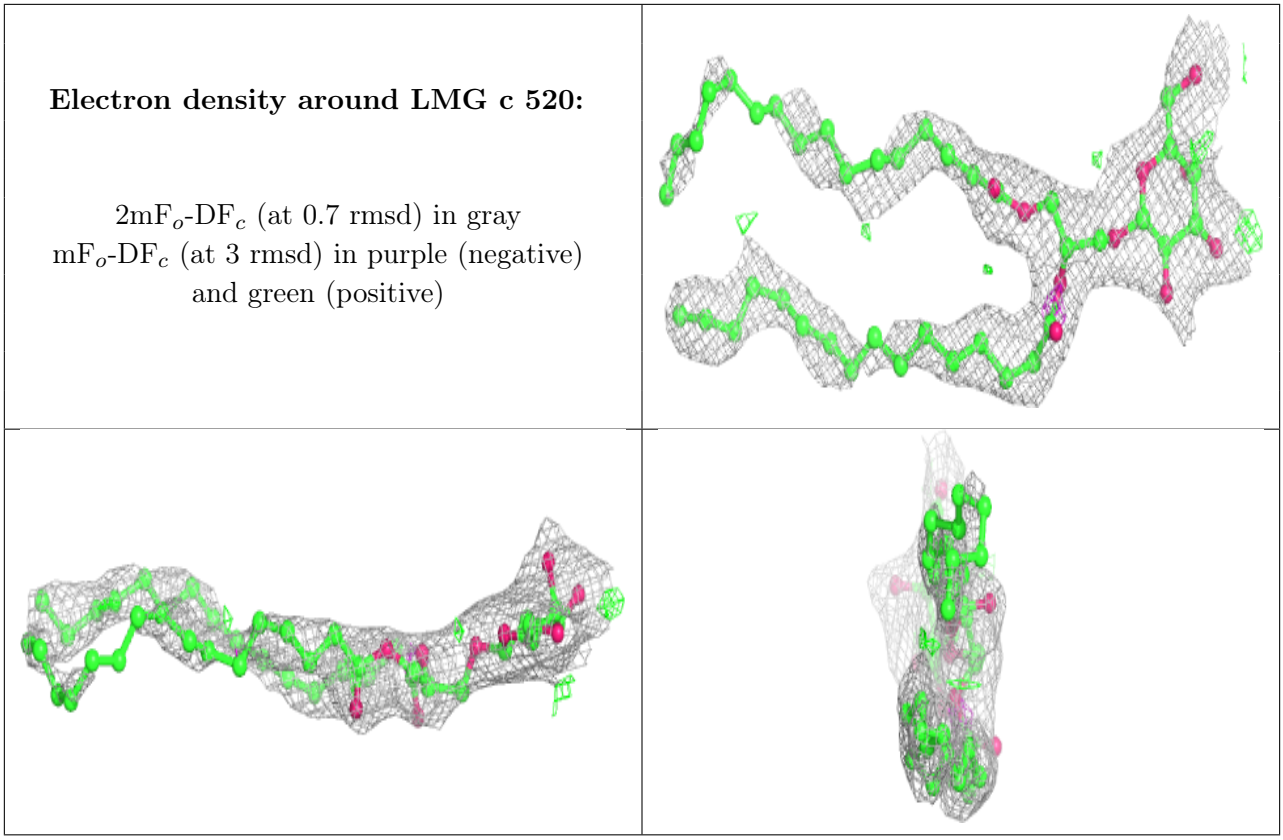






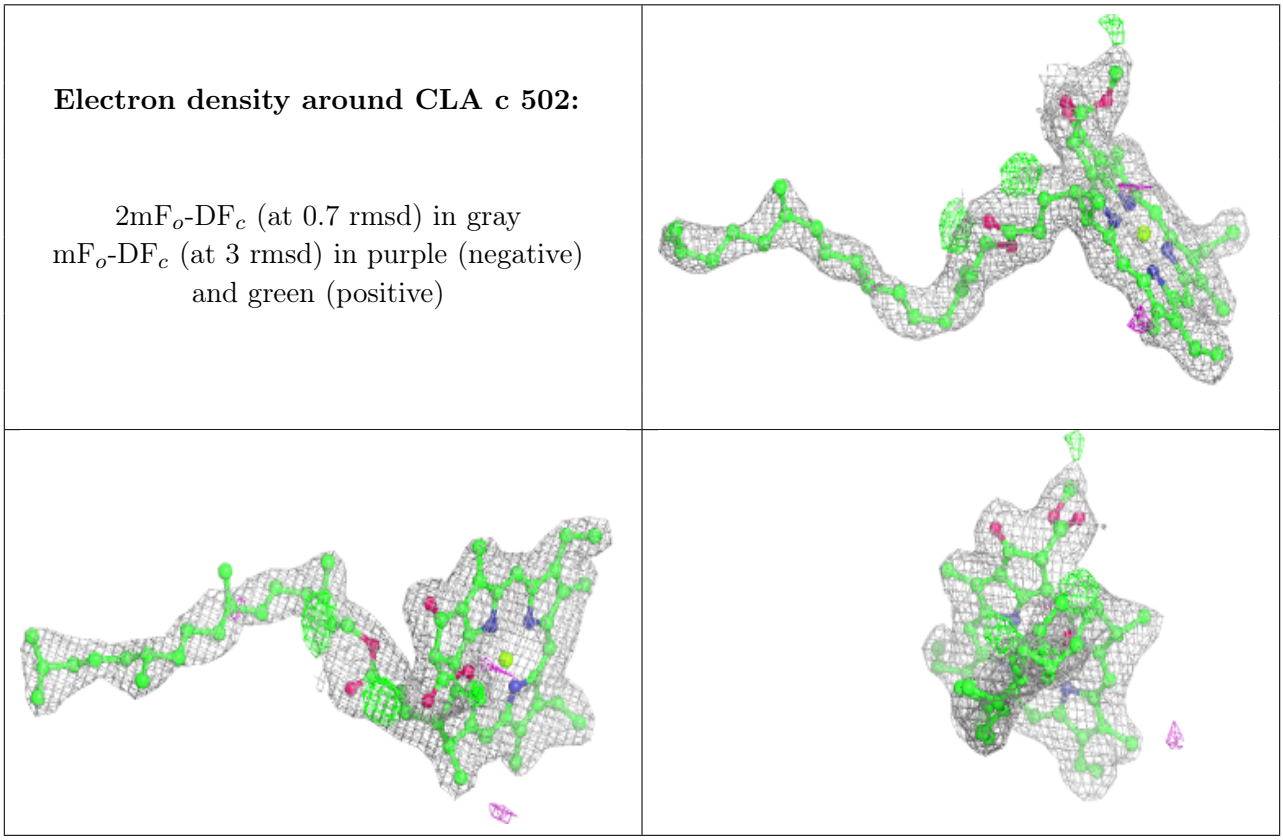
Electron density around LMG c 520:

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



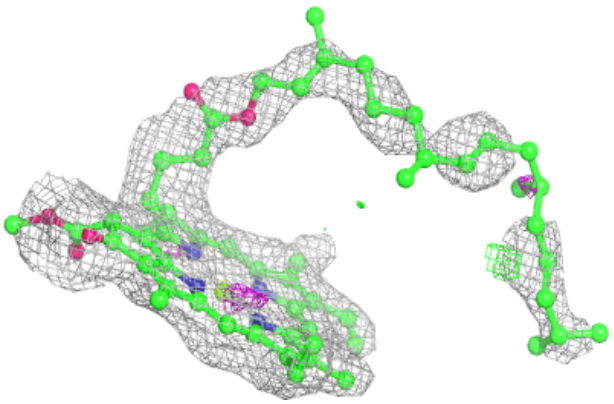
Electron density around CLA c 502:

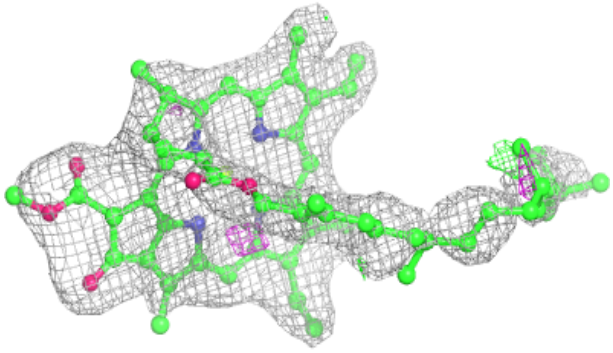
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

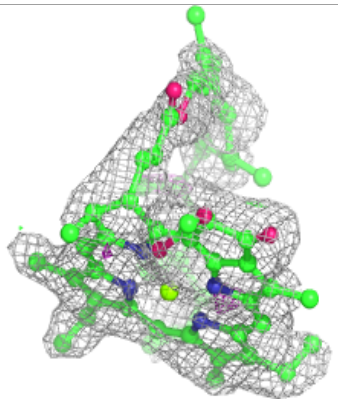


Electron density around CLA c 513:

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

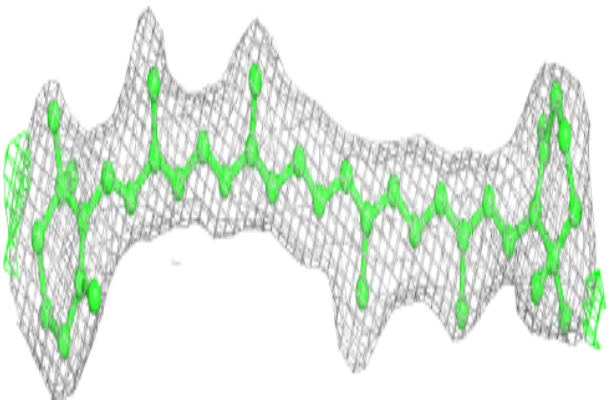


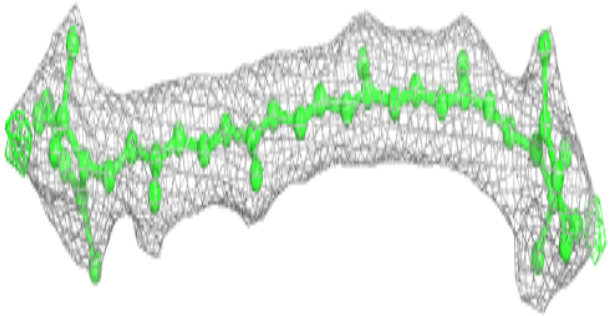


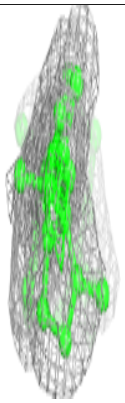


Electron density around BCR B 619:

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

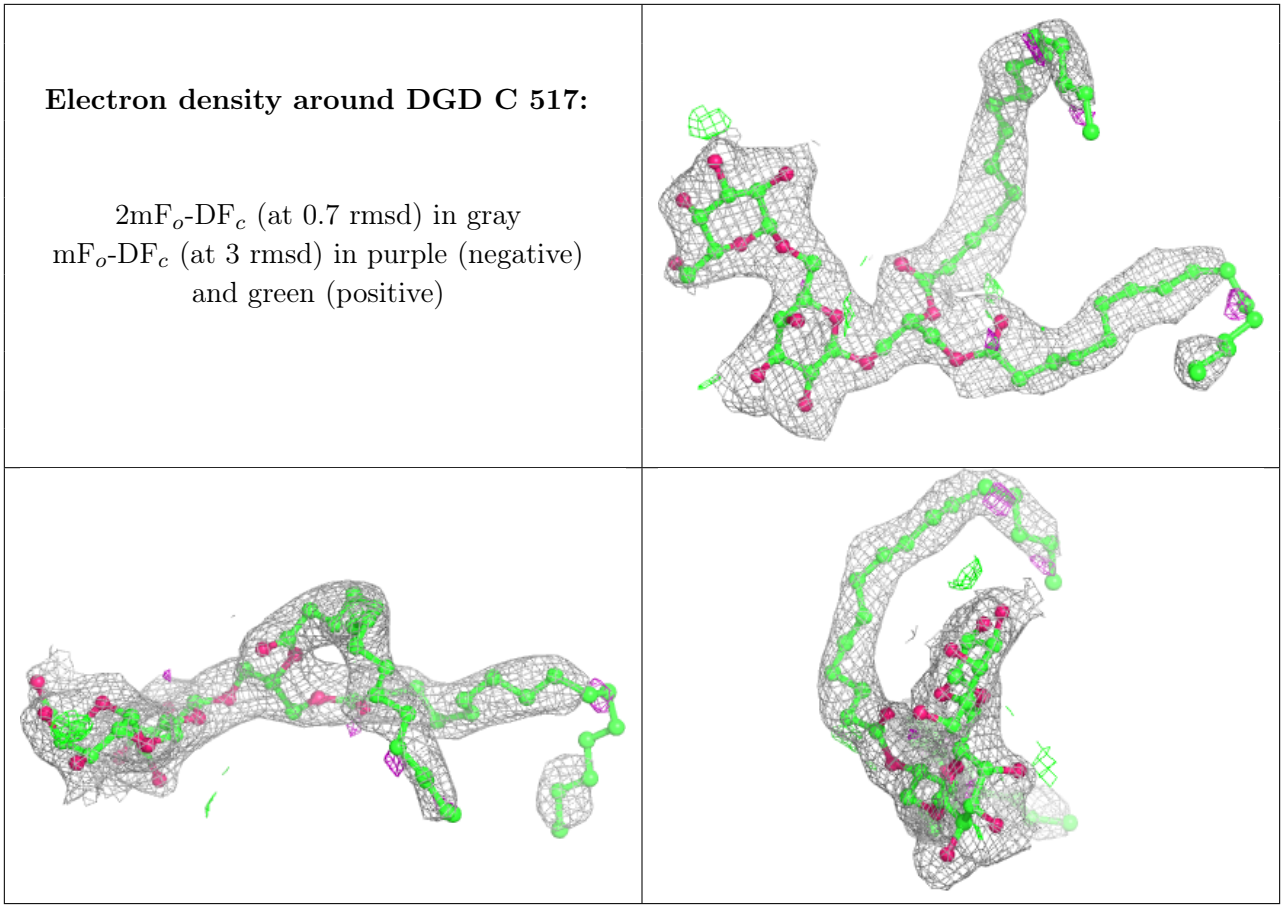






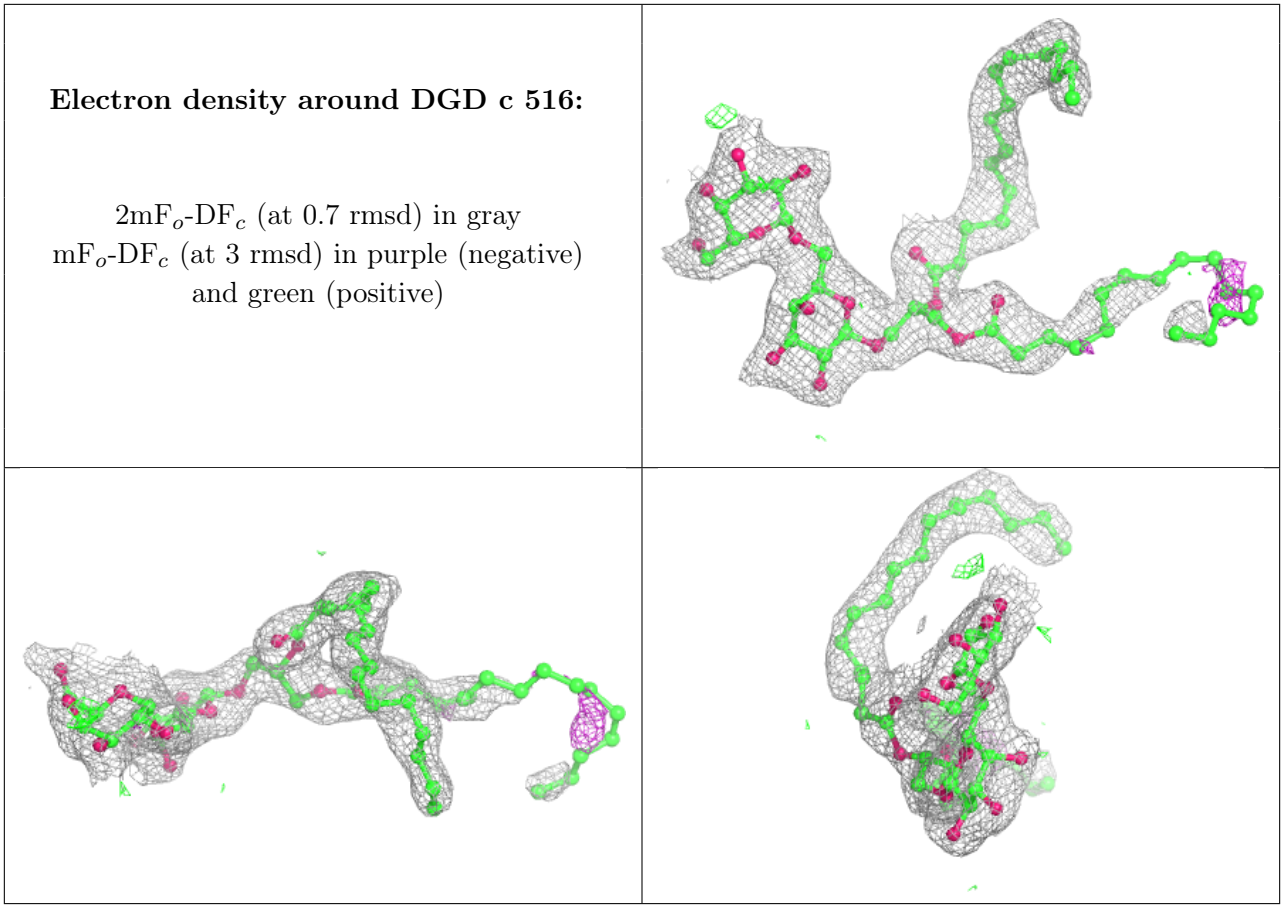
Electron density around DGD C 517:

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



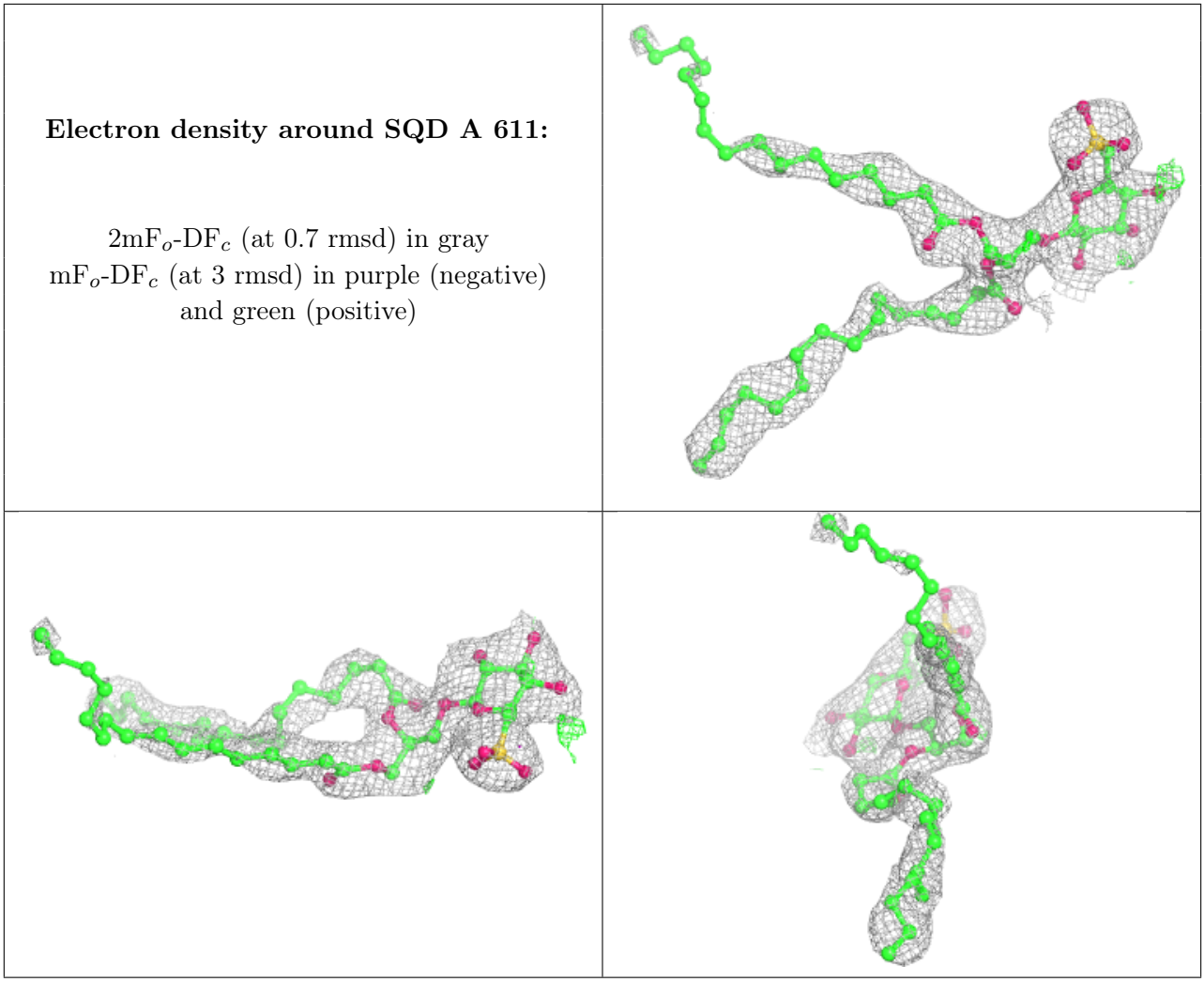
Electron density around DGD c 516:

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



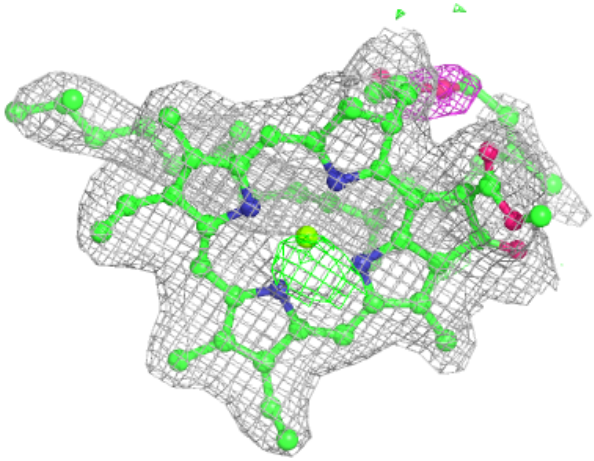
Electron density around SQD A 611:

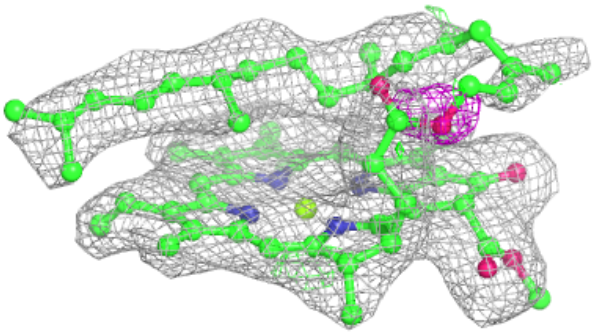
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

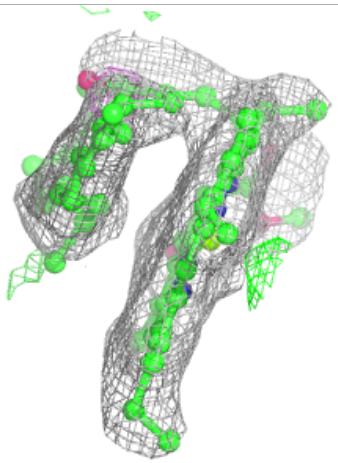


Electron density around CLA B 601:

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

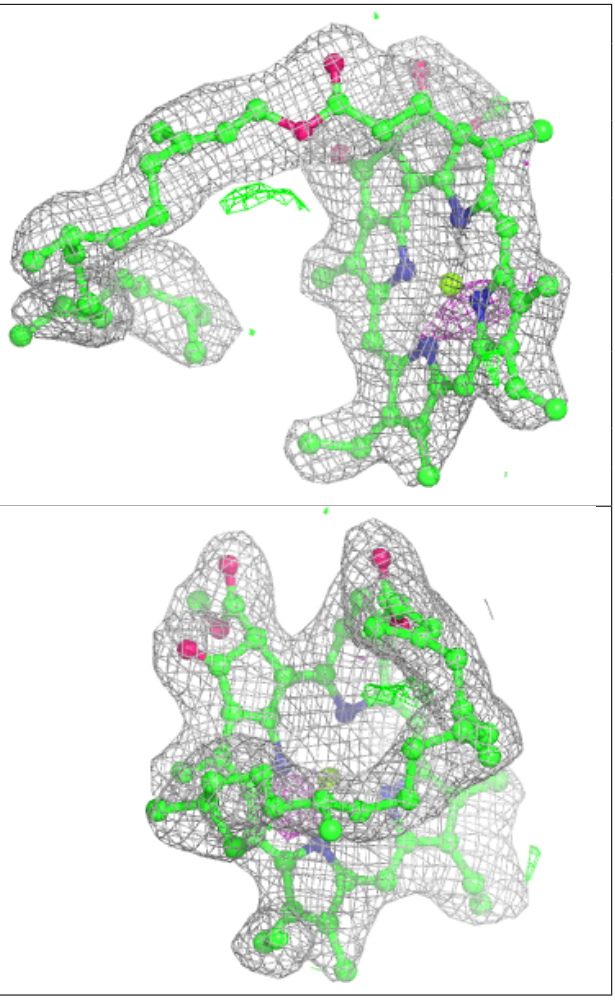






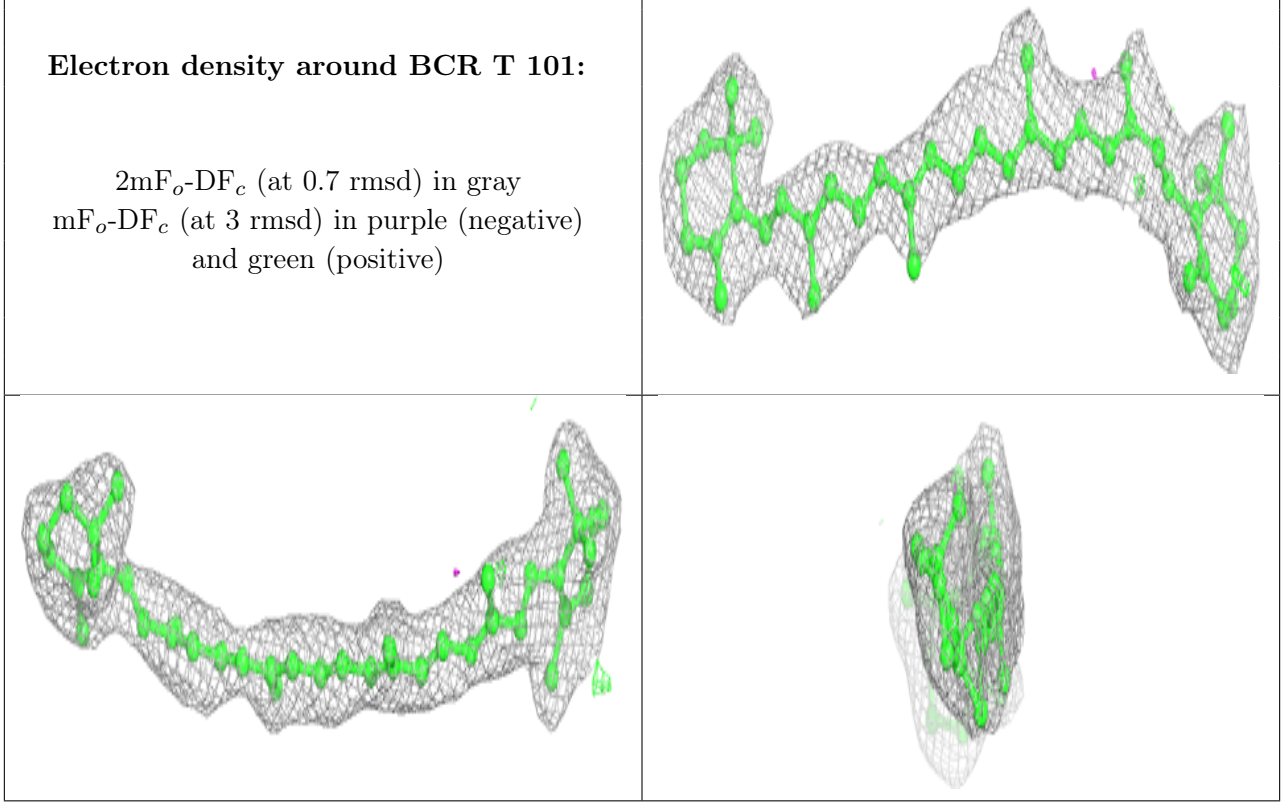
Electron density around CLA c 503:

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



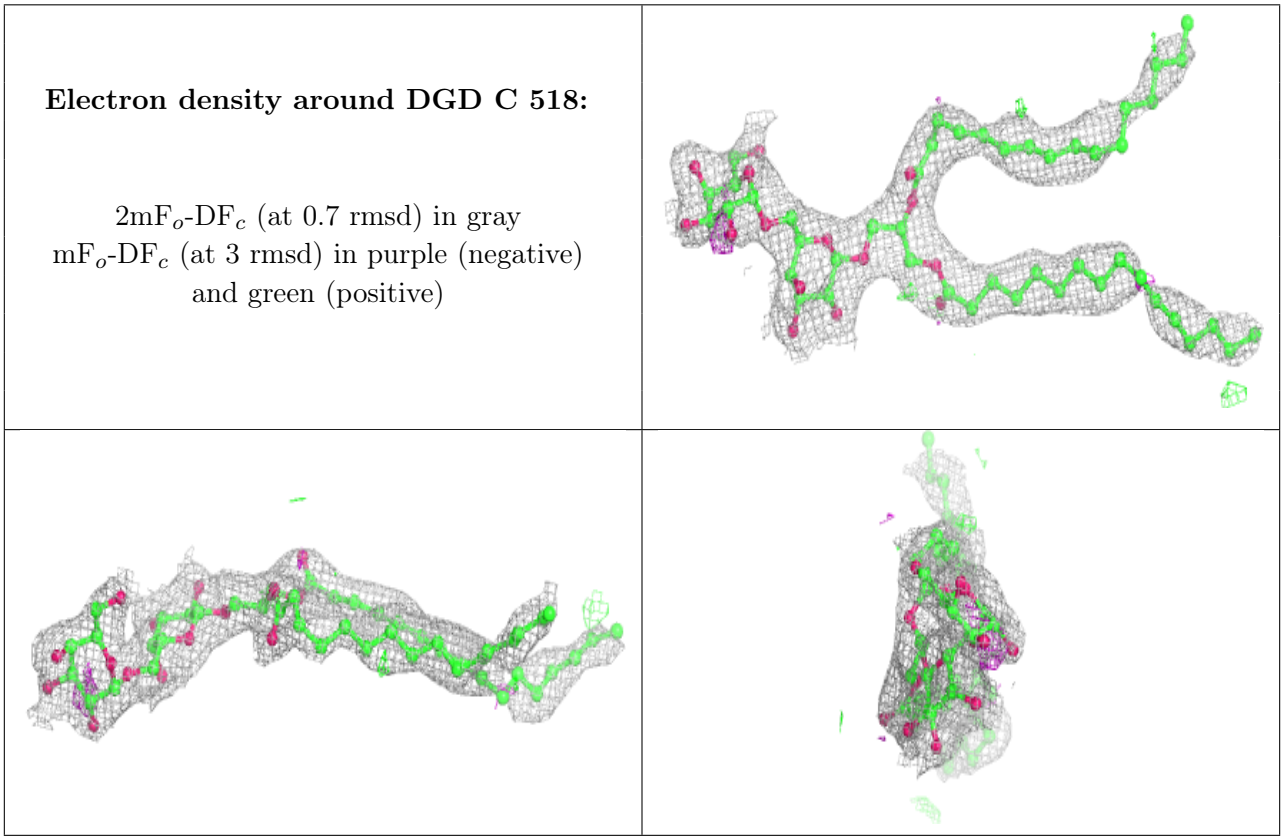
Electron density around BCR T 101:

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



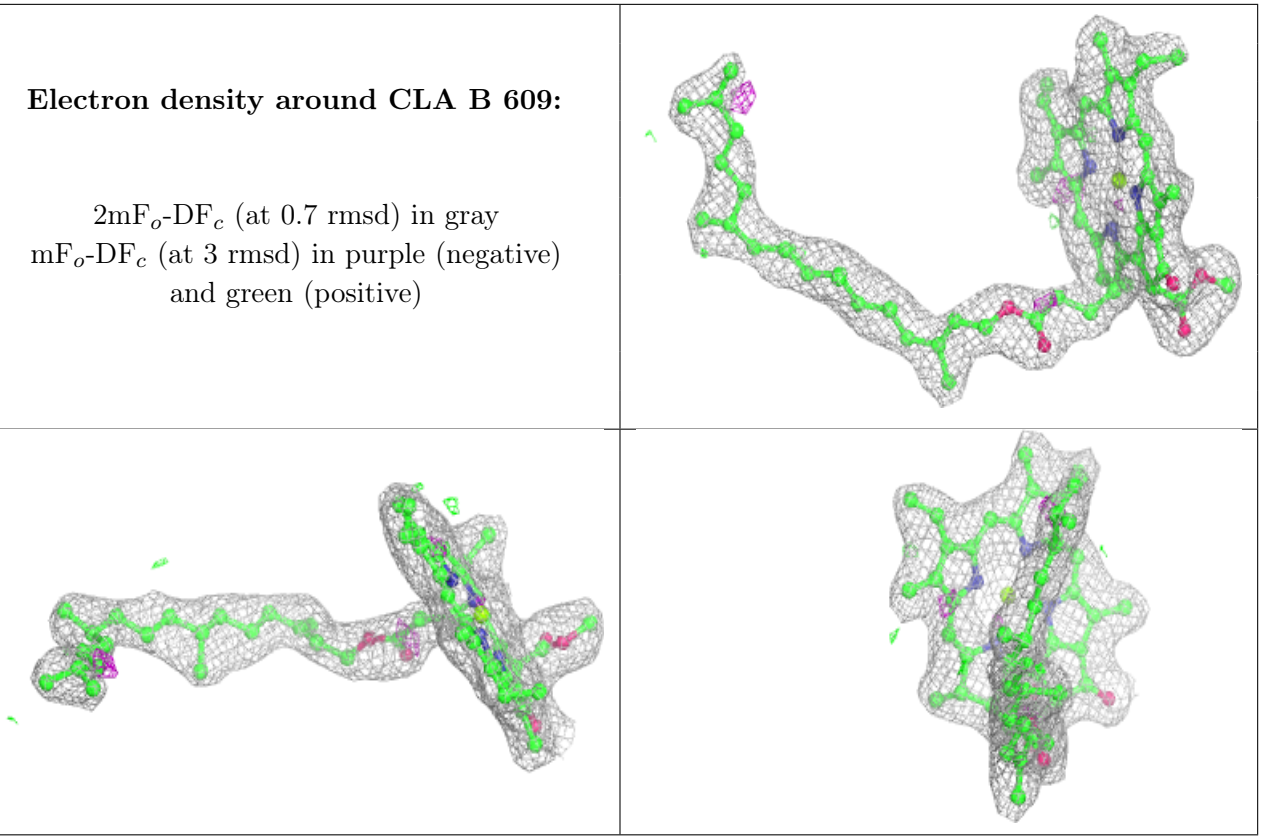
Electron density around DGD C 518:

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



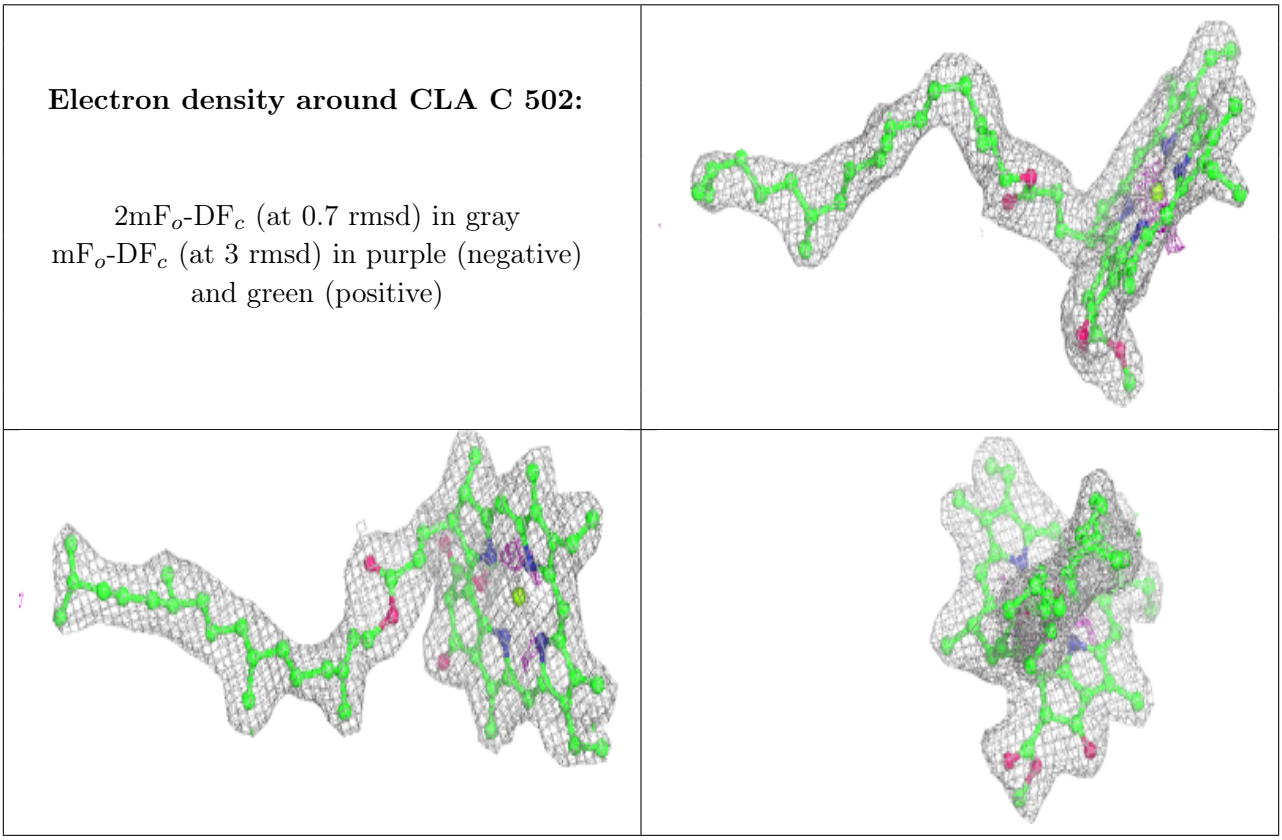
Electron density around CLA B 609:

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



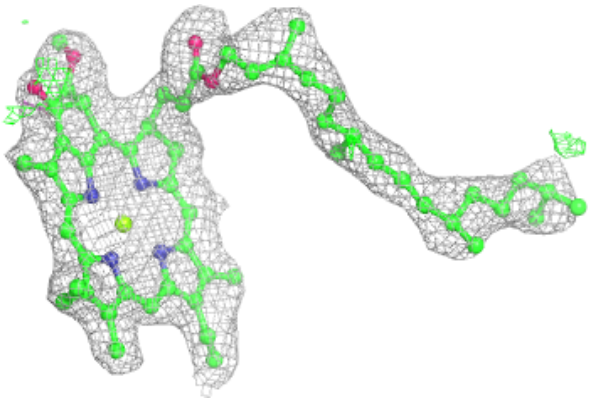
Electron density around CLA C 502:

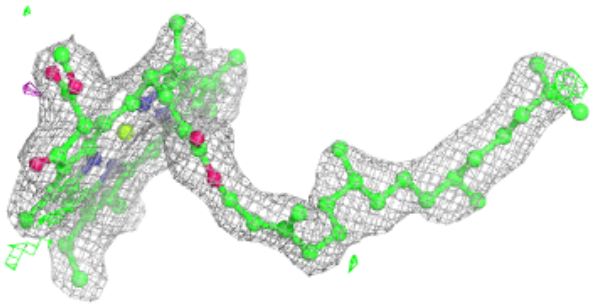
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

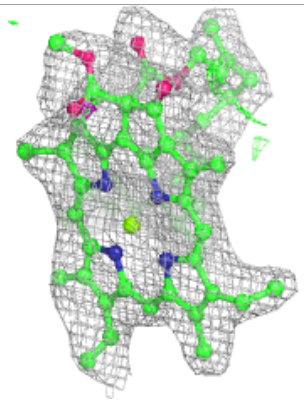


Electron density around CLA c 511:

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

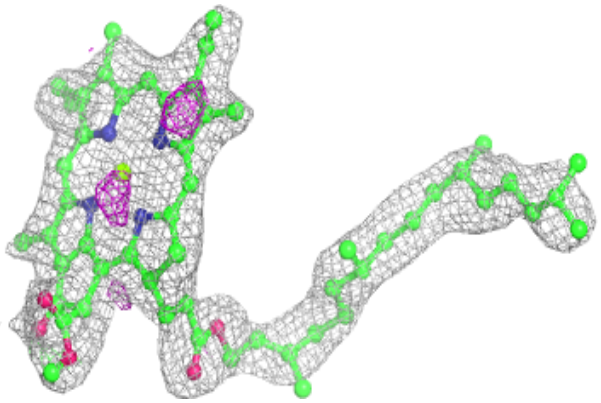


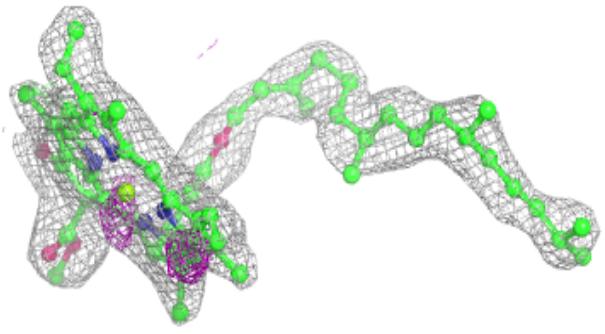


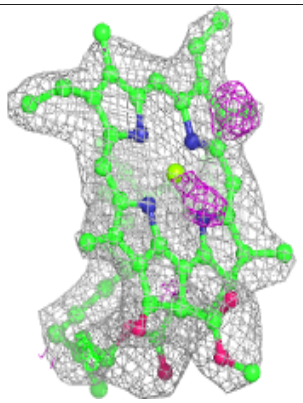


Electron density around CLA C 511:

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

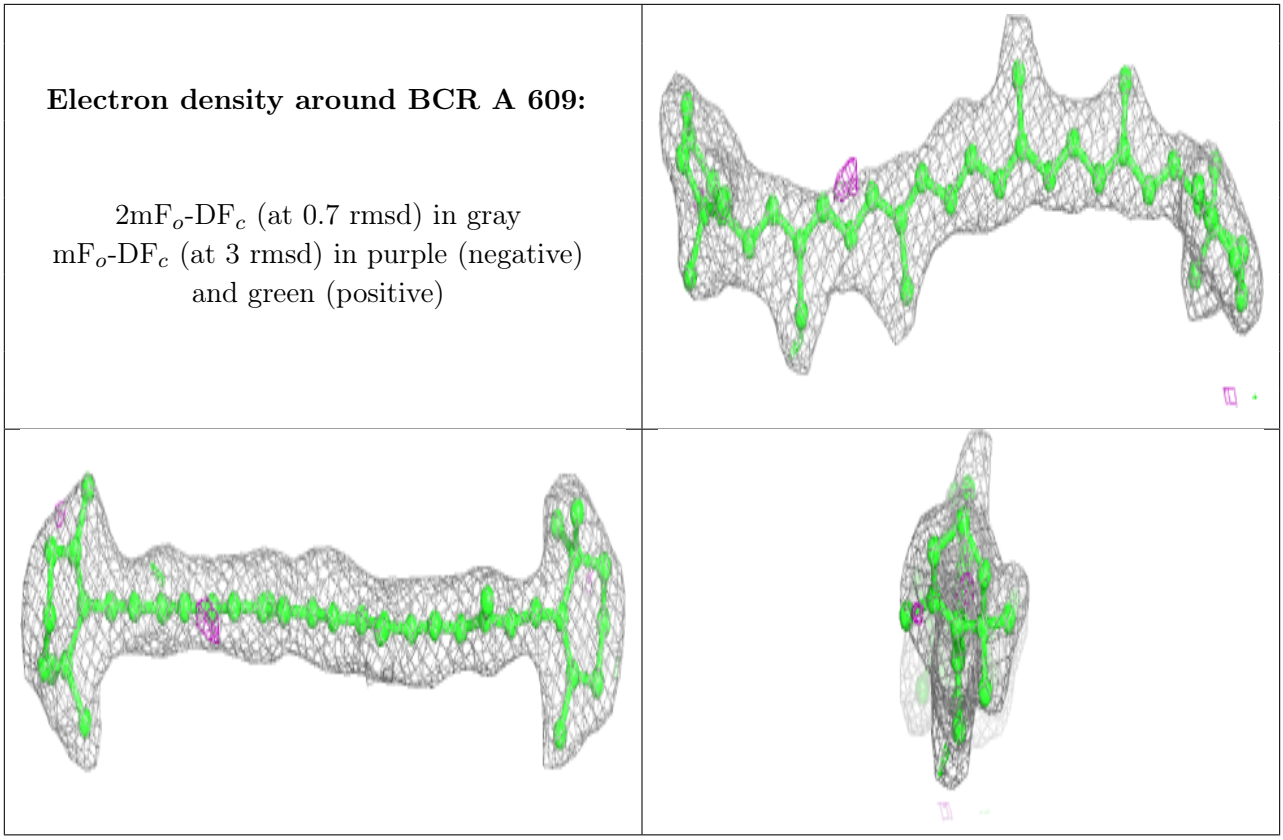






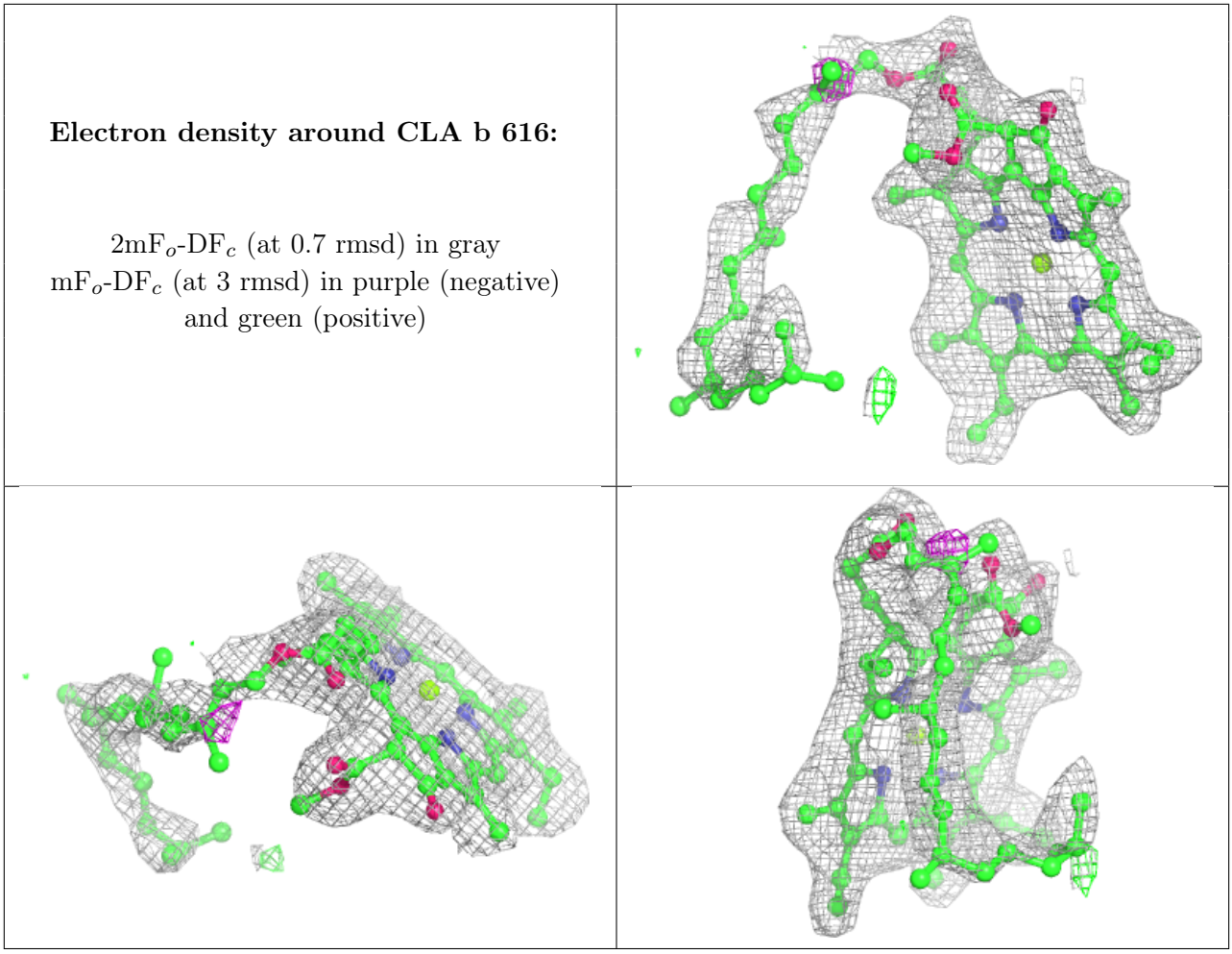
Electron density around BCR A 609:

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



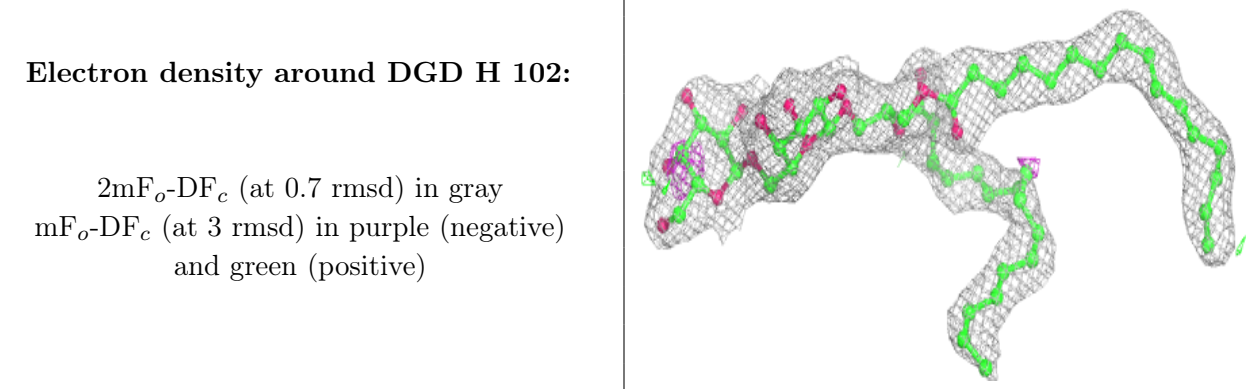
Electron density around CLA b 616:

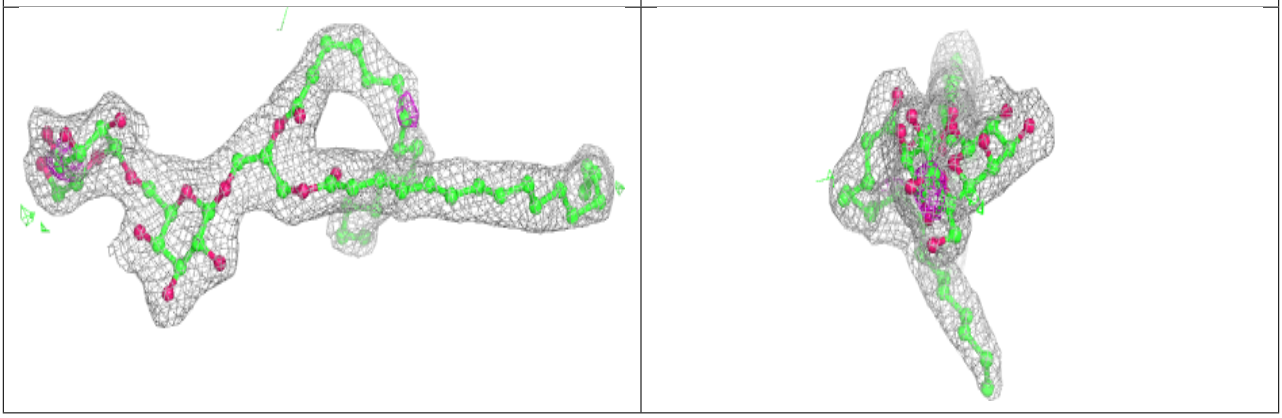
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD H 102:

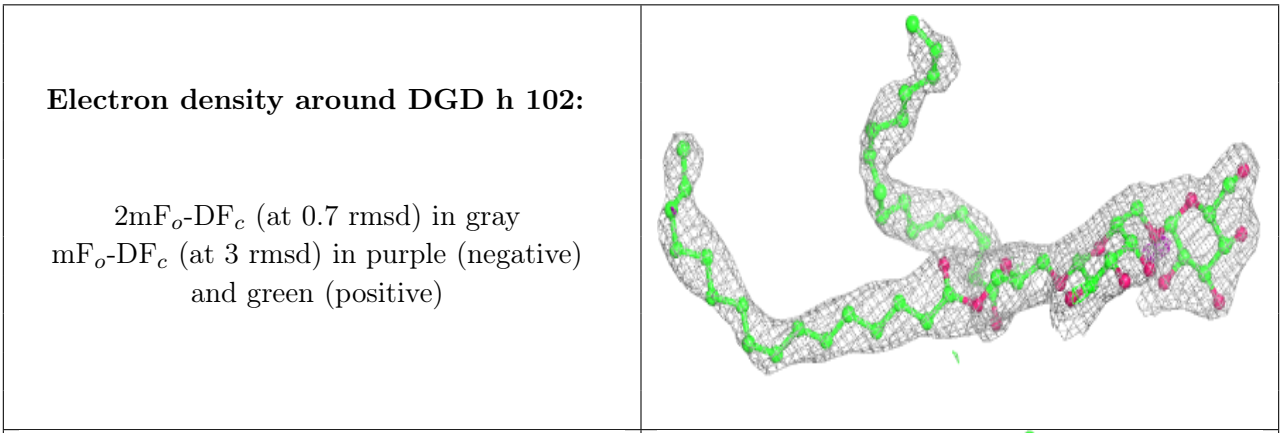
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

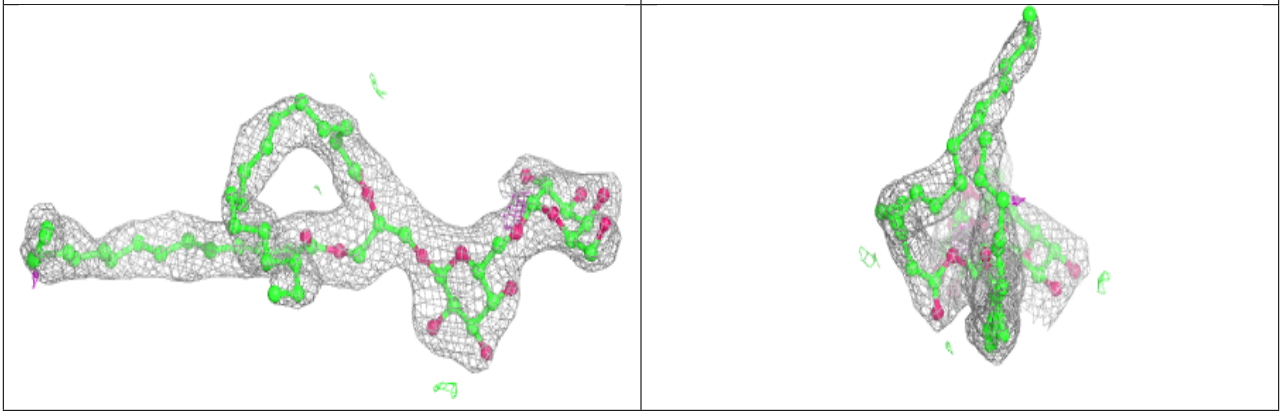




Electron density around DGD h 102:

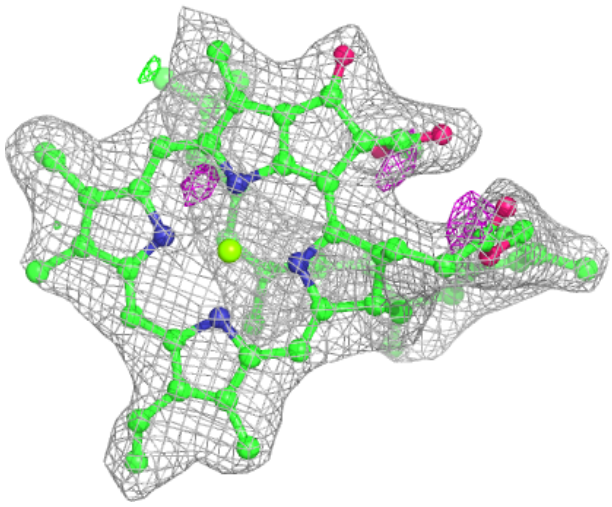
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

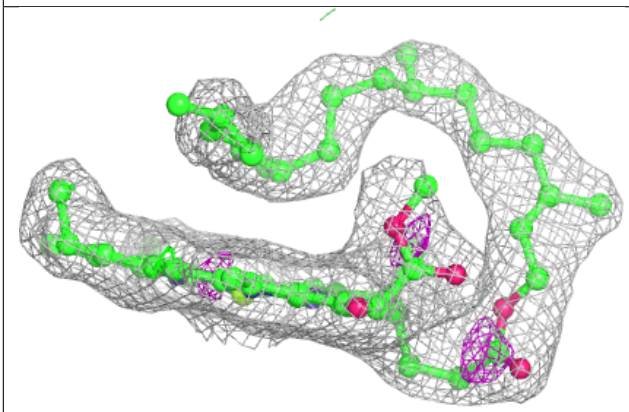


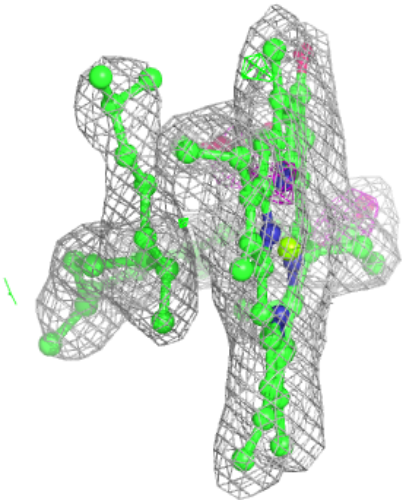


Electron density around CLA C 510:

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

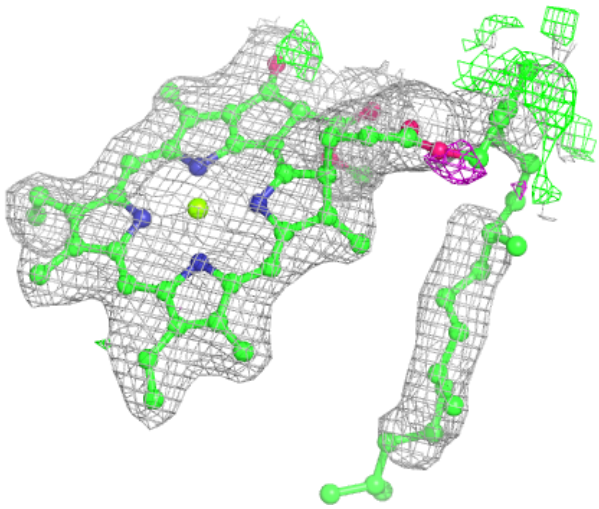


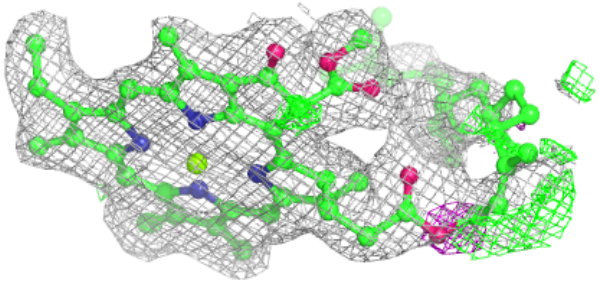


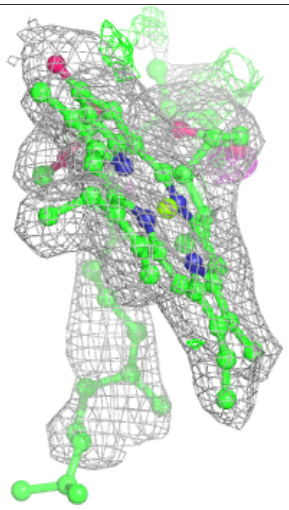


Electron density around CLA B 616:

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

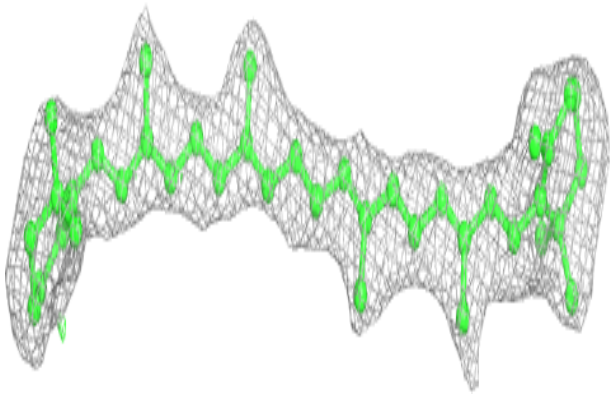


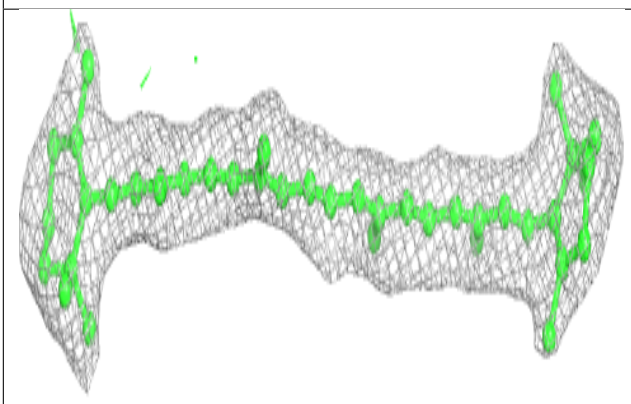


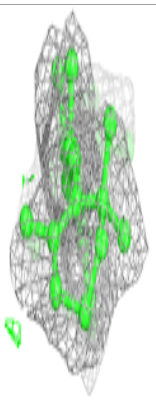


Electron density around BCR a 611:

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

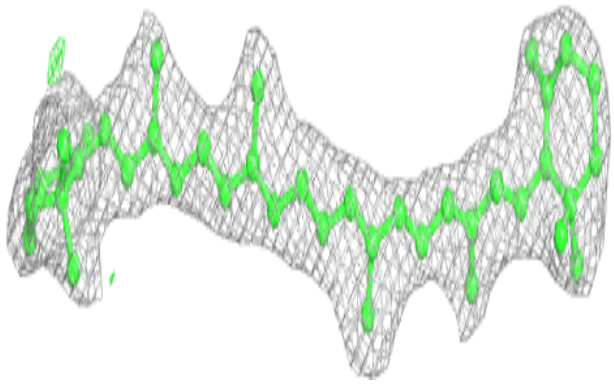


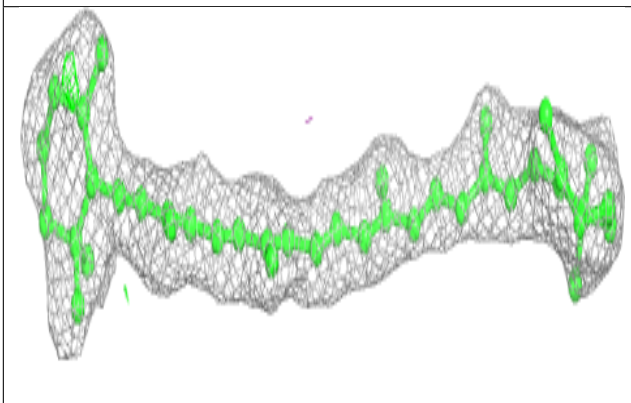


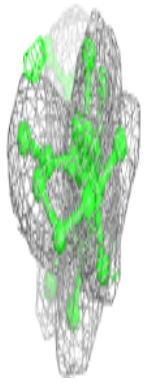


Electron density around BCR b 617:

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

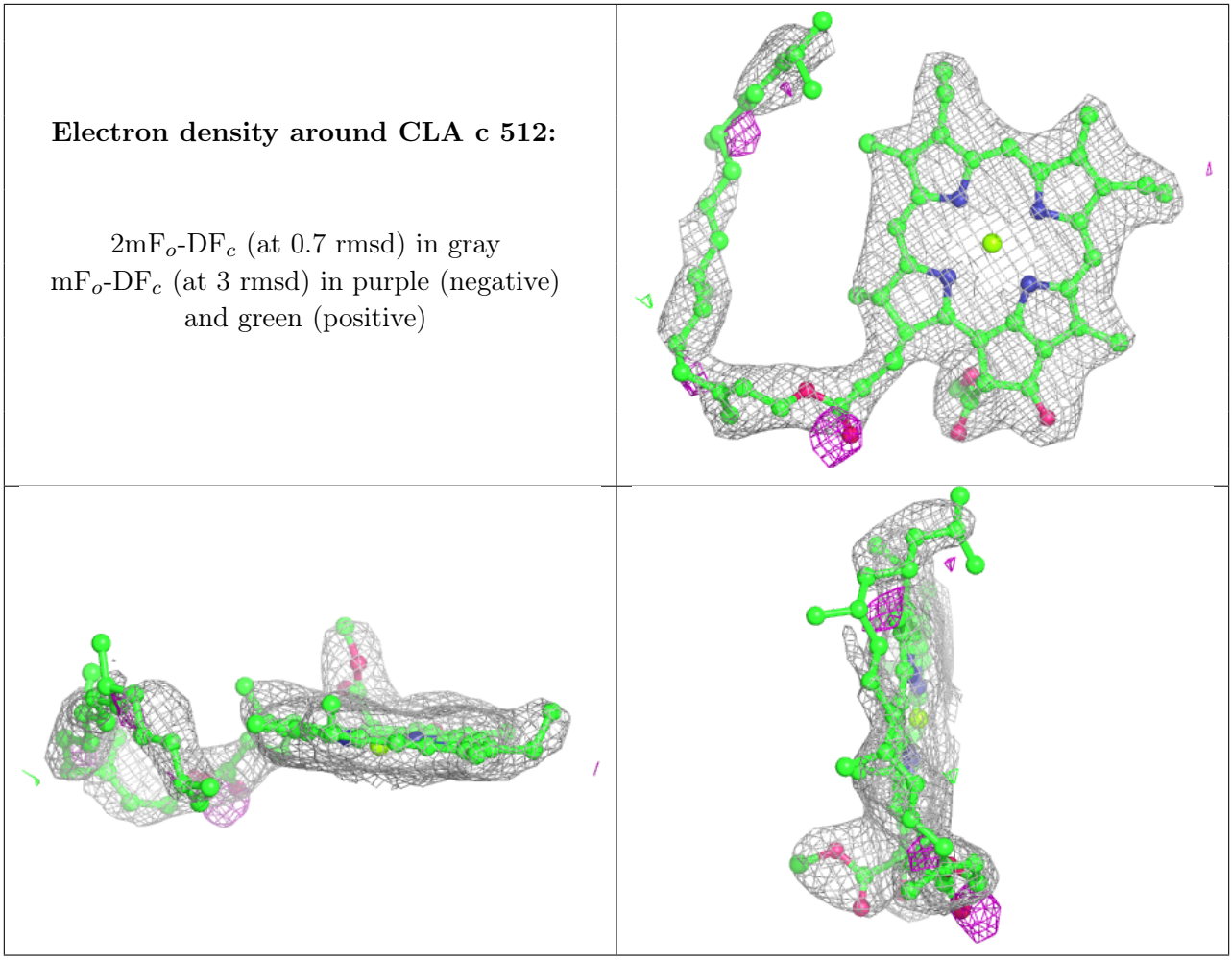






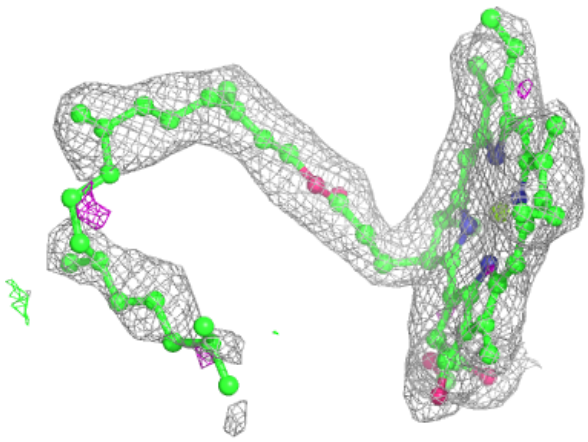
Electron density around CLA c 512:

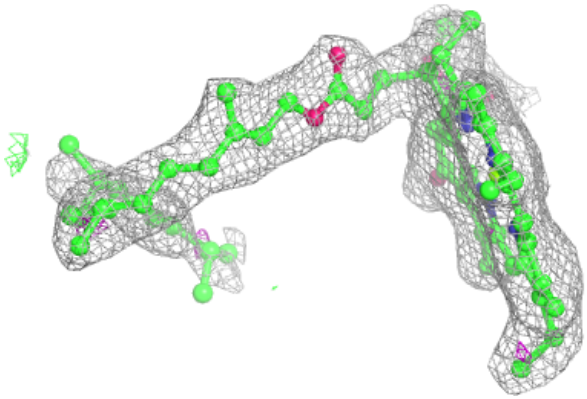
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

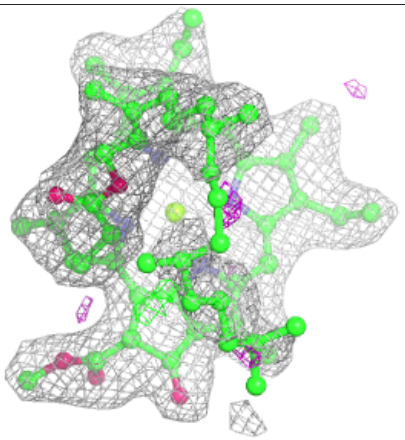


Electron density around CLA B 606:

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

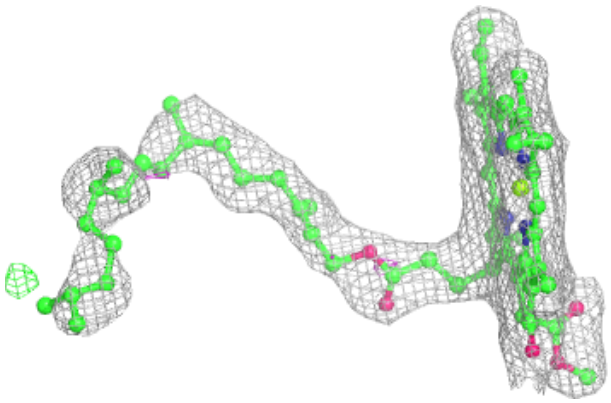


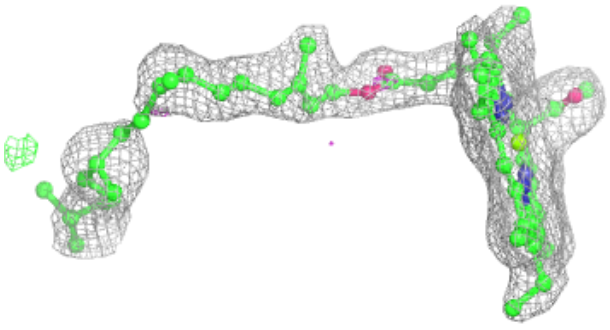


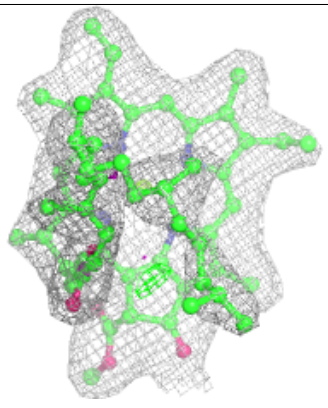


Electron density around CLA D 405:

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

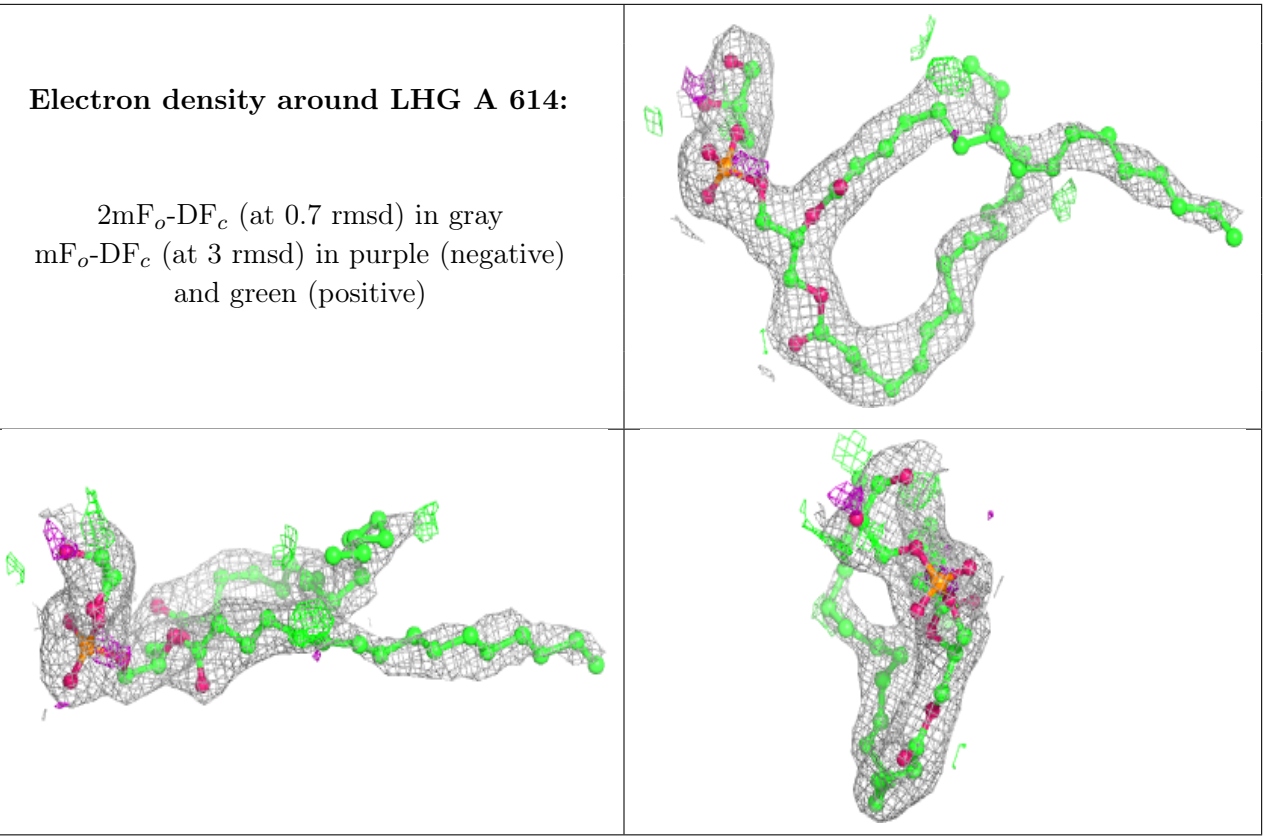






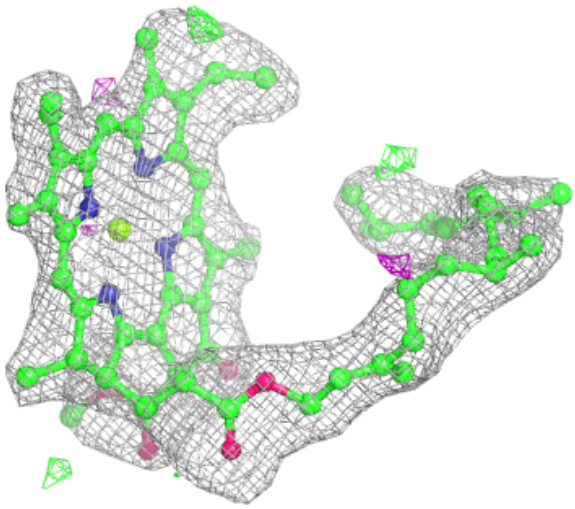
Electron density around LHG A 614:

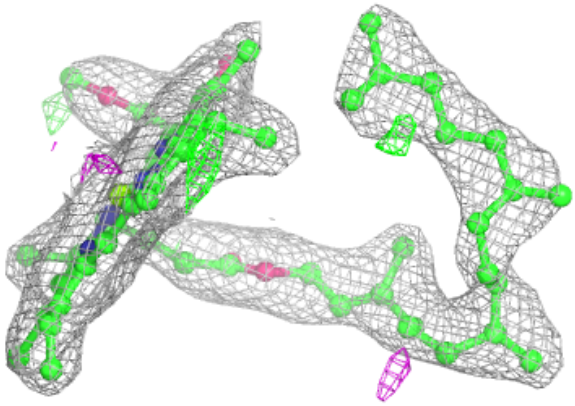
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

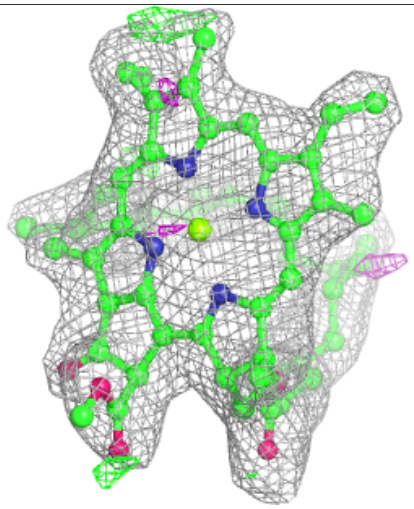


Electron density around CLA C 503:

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

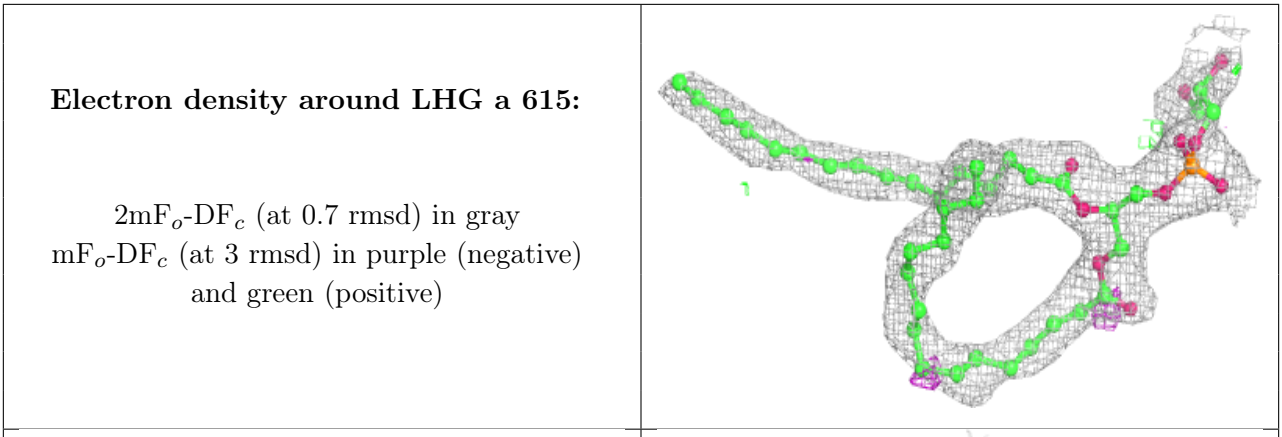






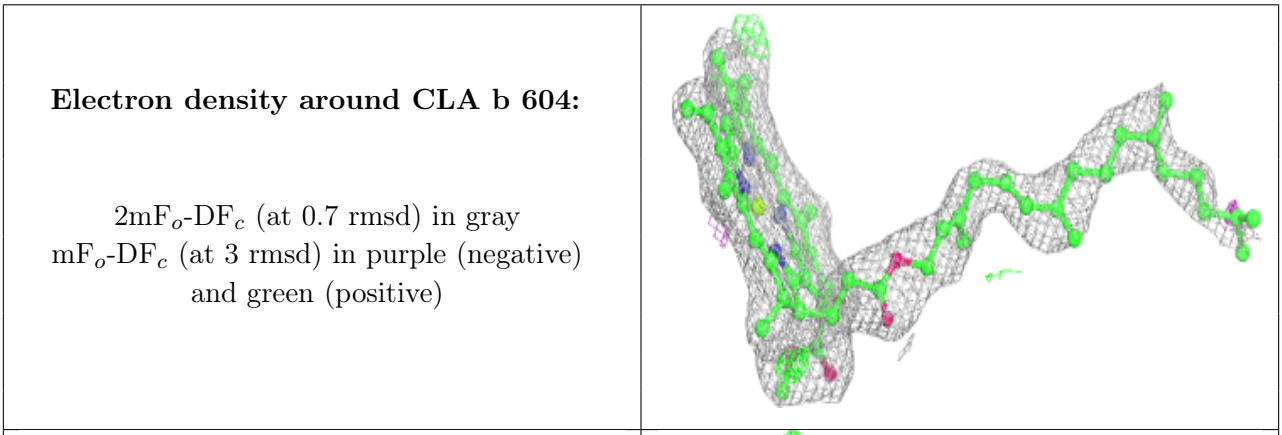
Electron density around LHG a 615:

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



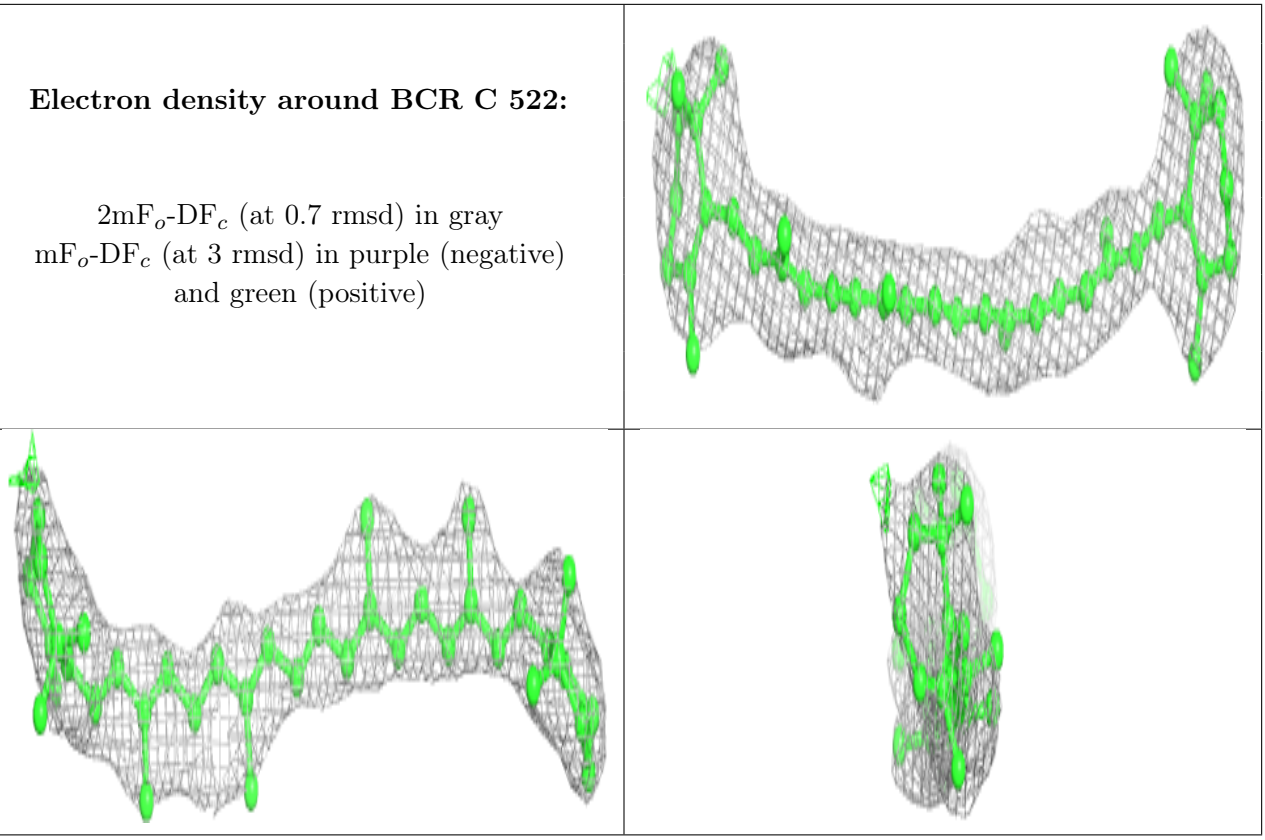
Electron density around CLA b 604:

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



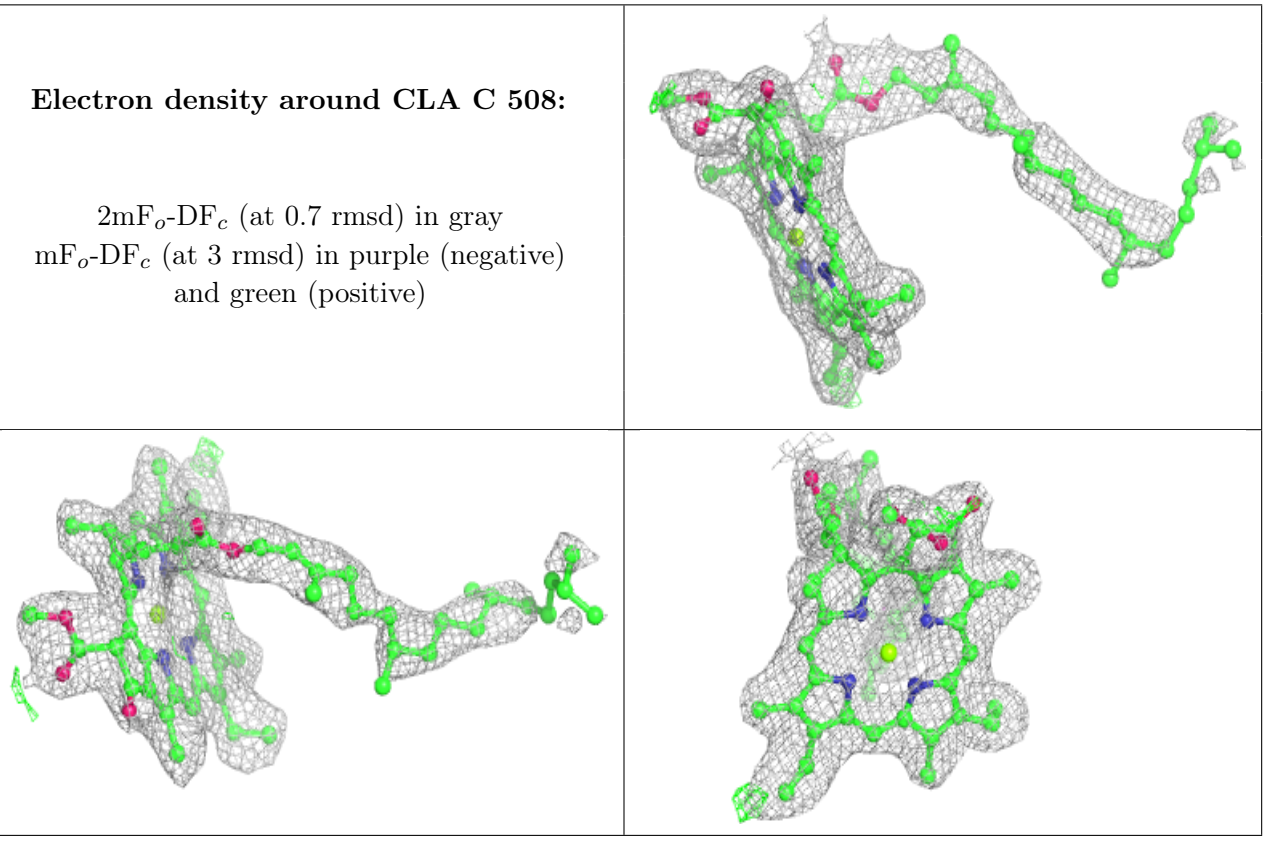
Electron density around BCR C 522:

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



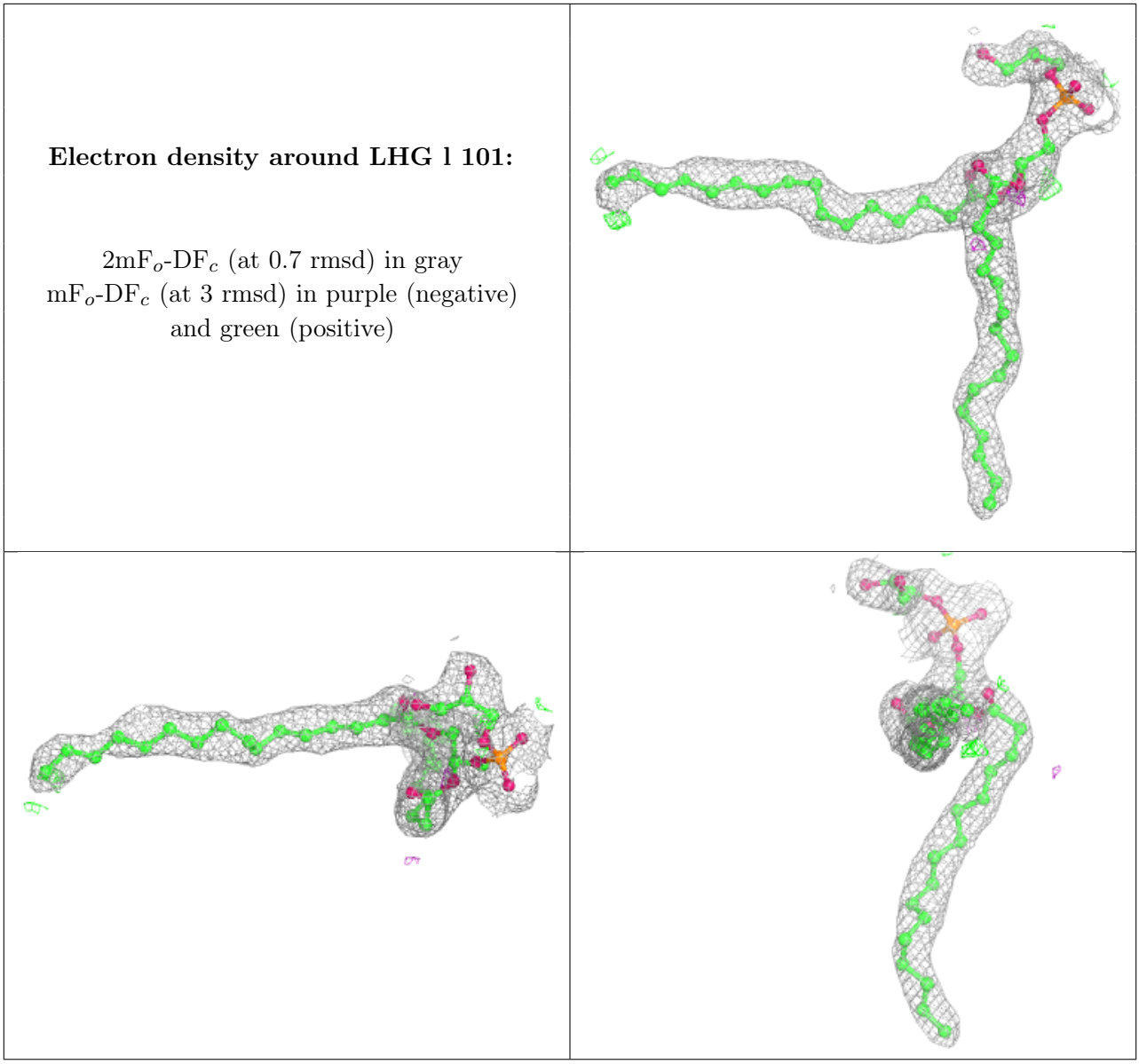
Electron density around CLA C 508:

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



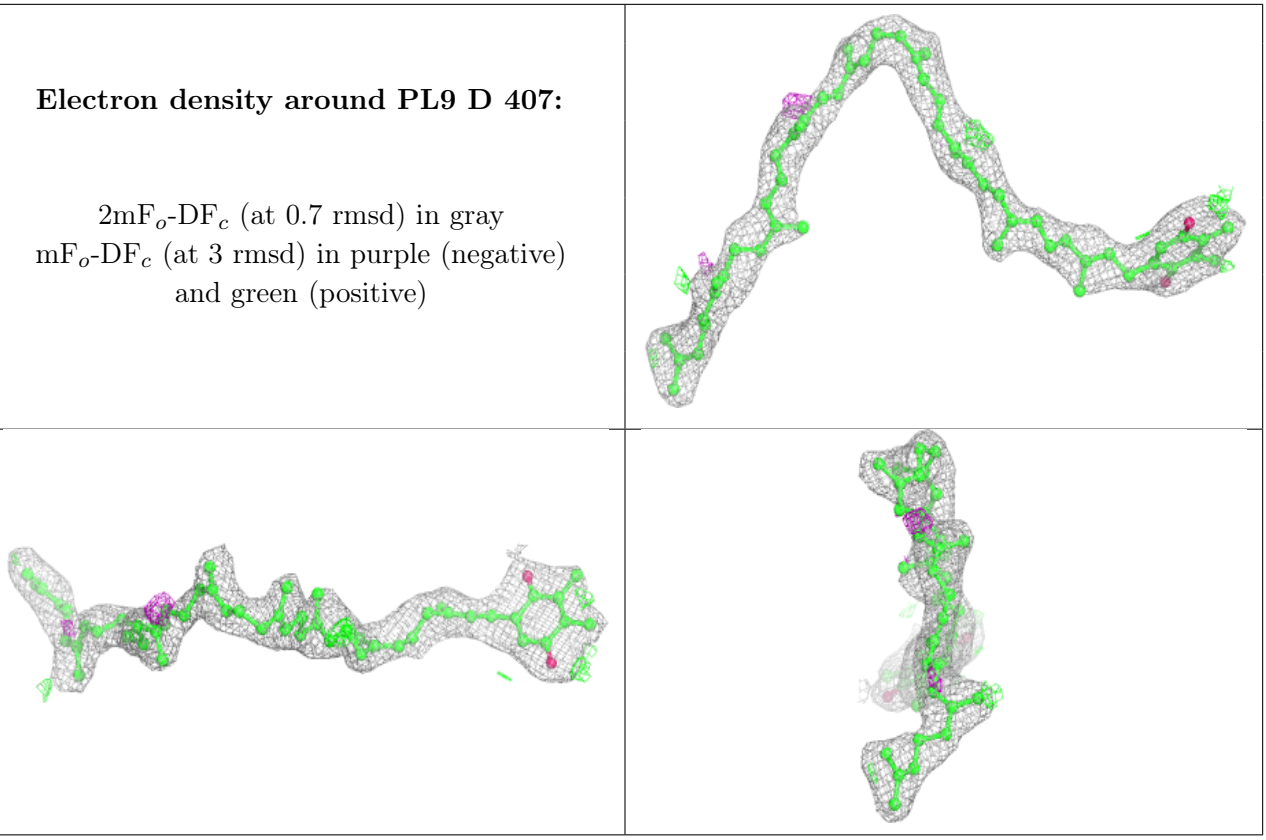
Electron density around LHG l 101:

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



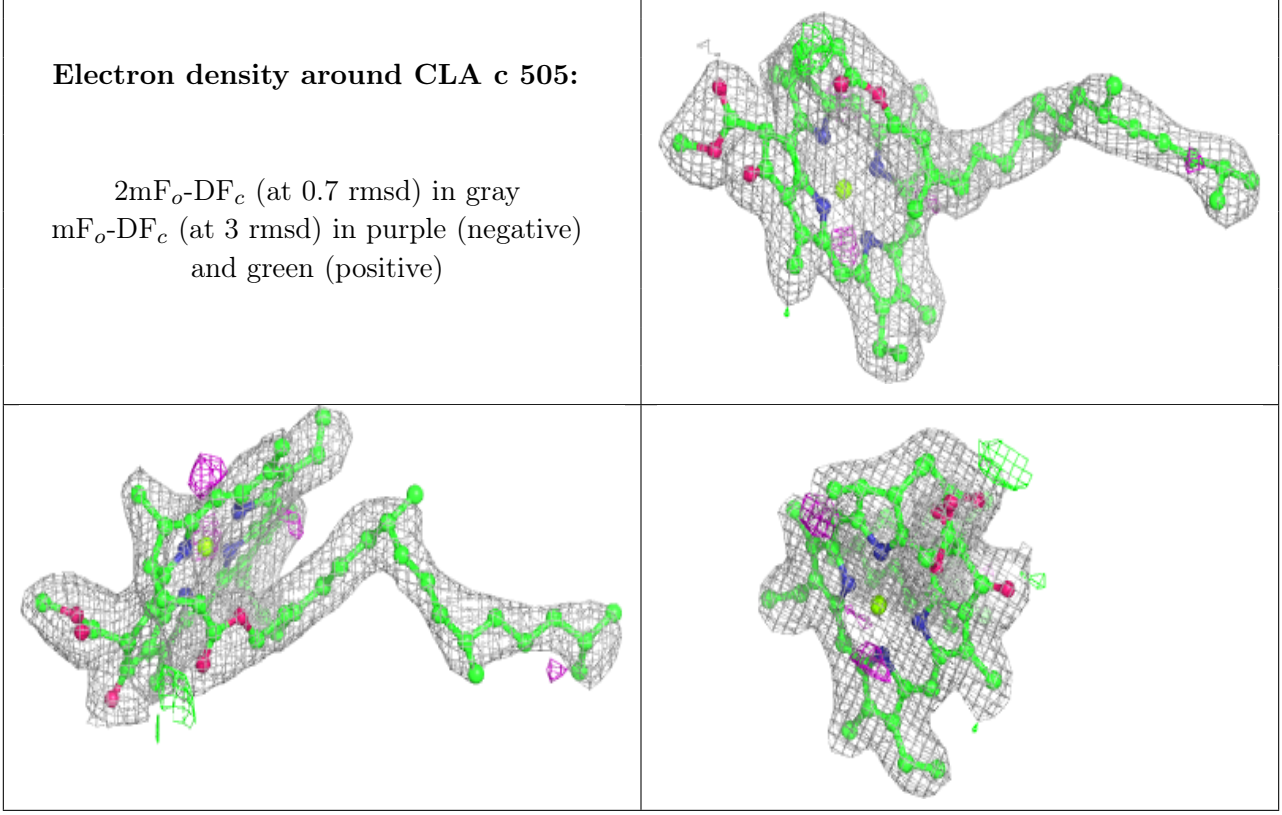
Electron density around PL9 D 407:

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



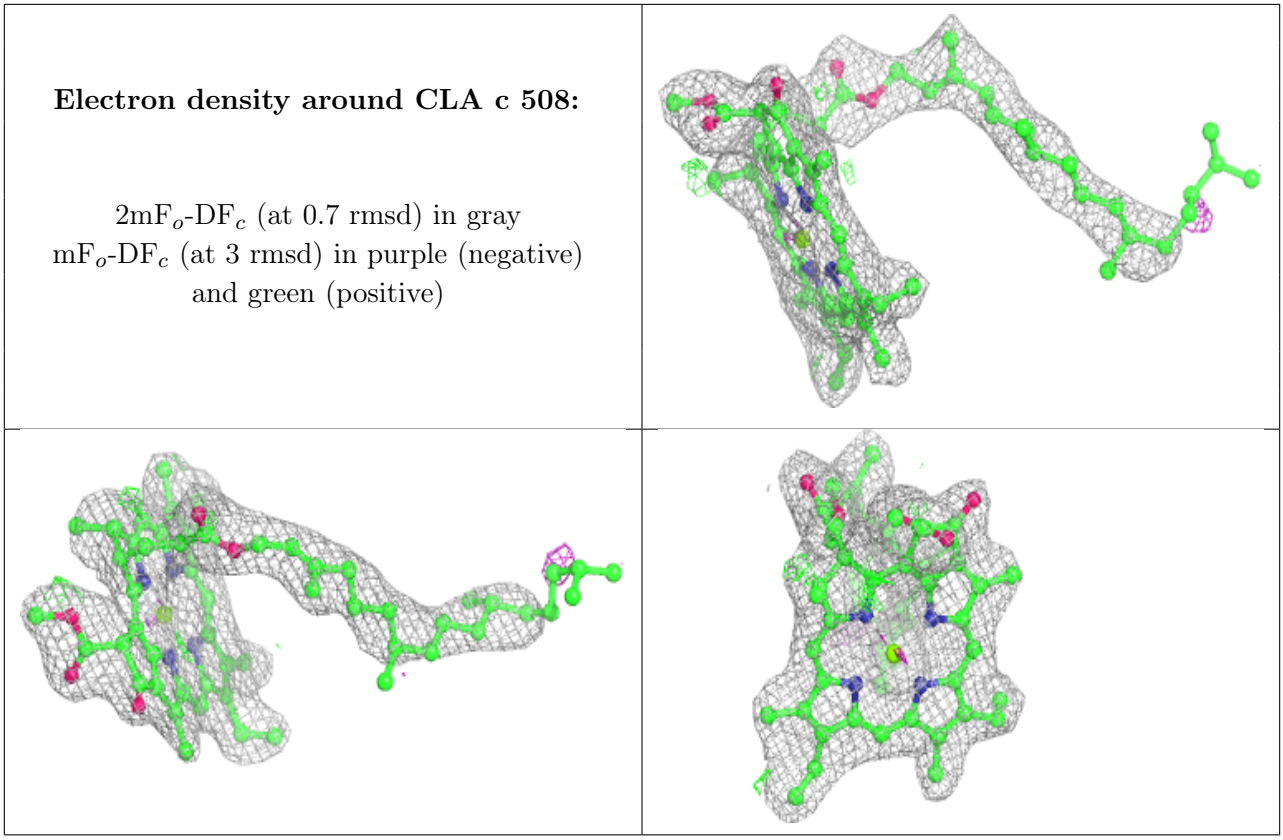
Electron density around CLA c 505:

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



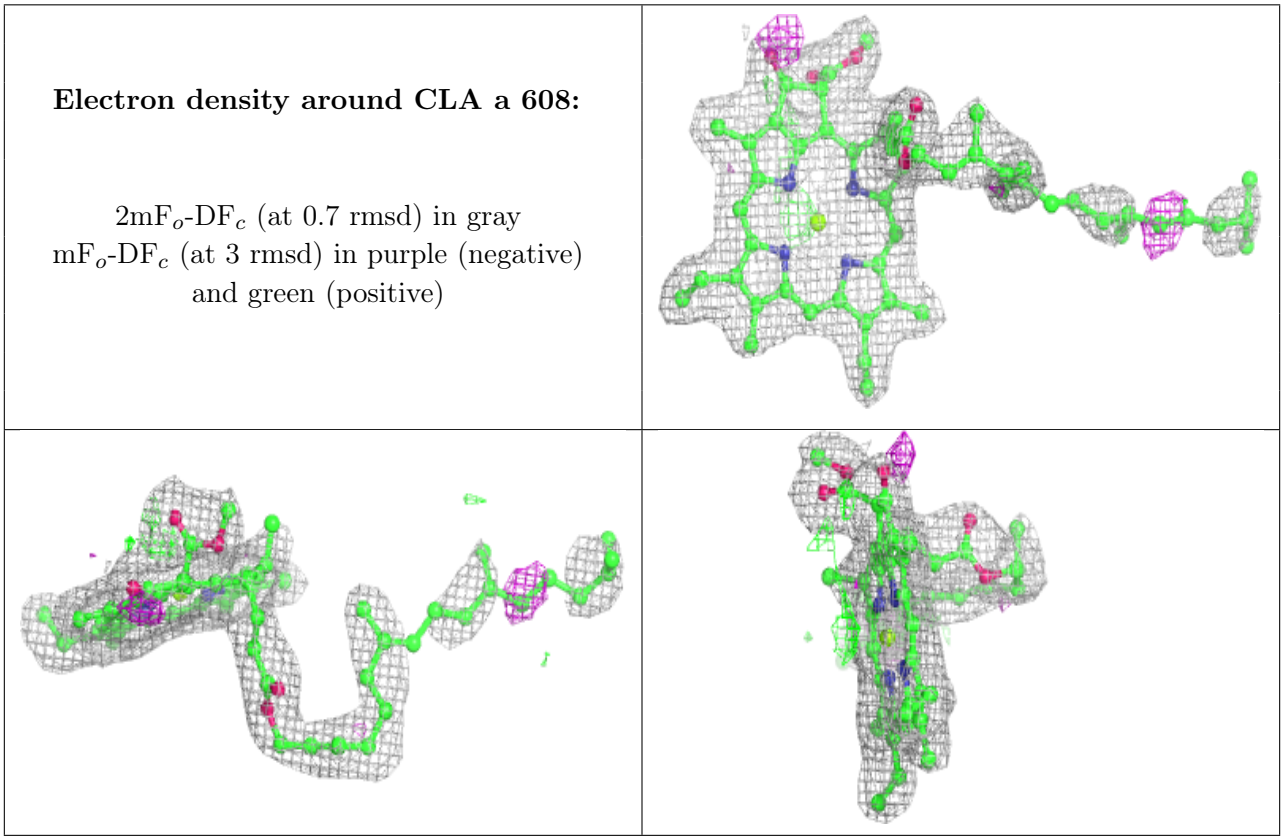
Electron density around CLA c 508:

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



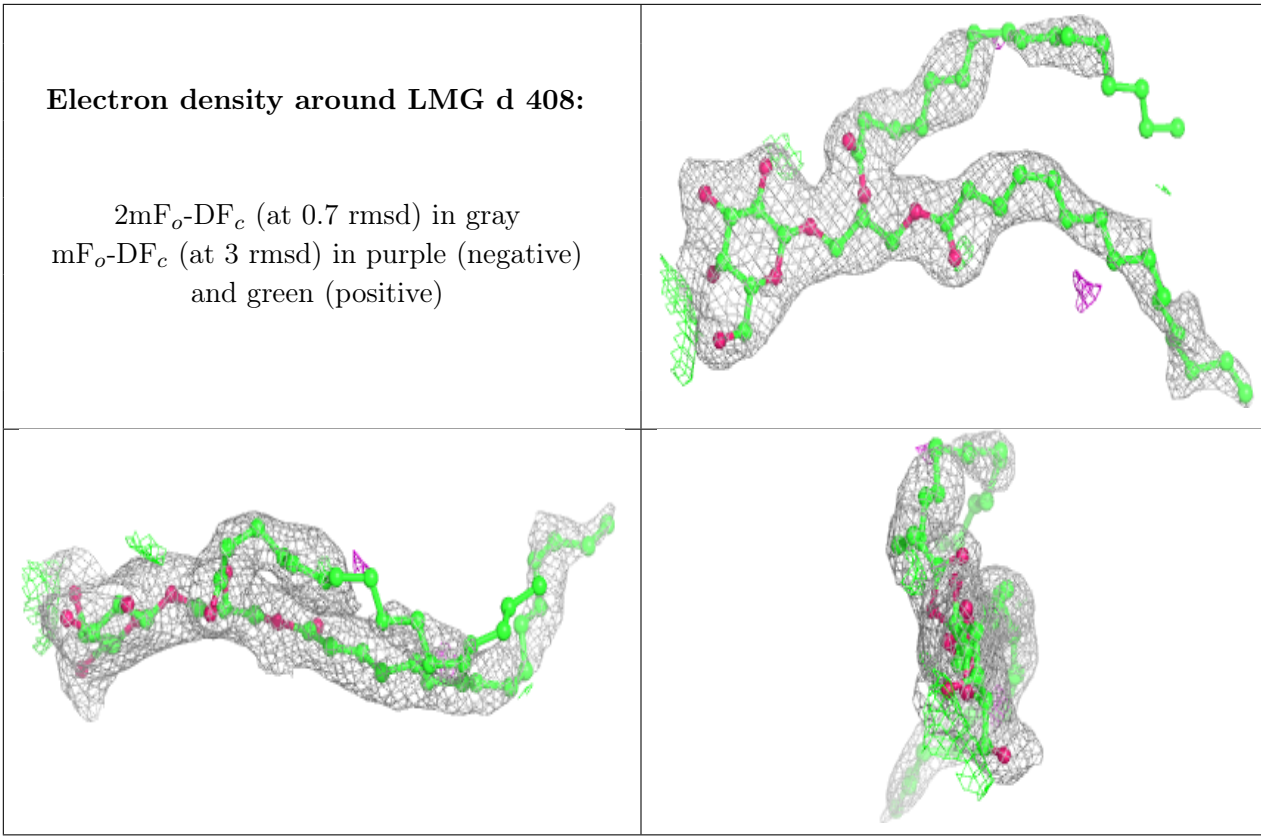
Electron density around CLA a 608:

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



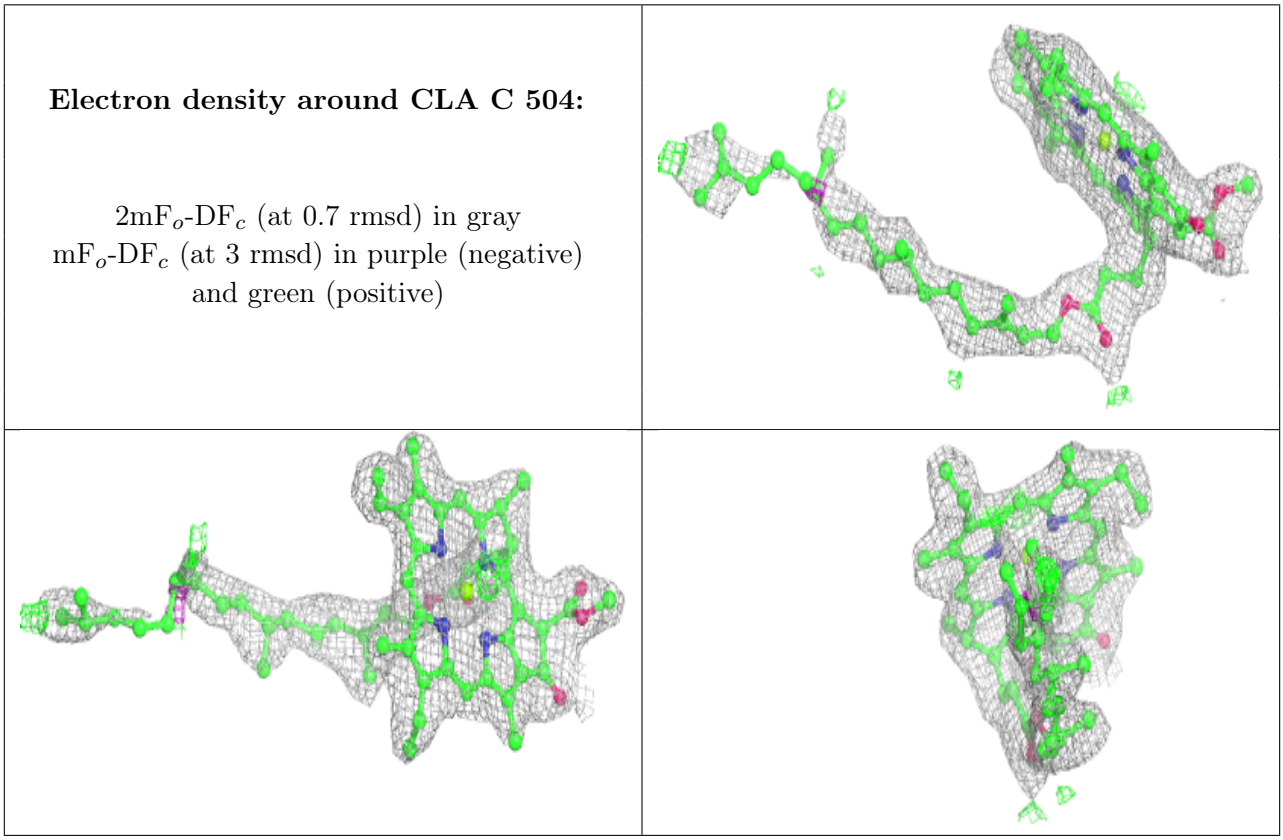
Electron density around LMG d 408:

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



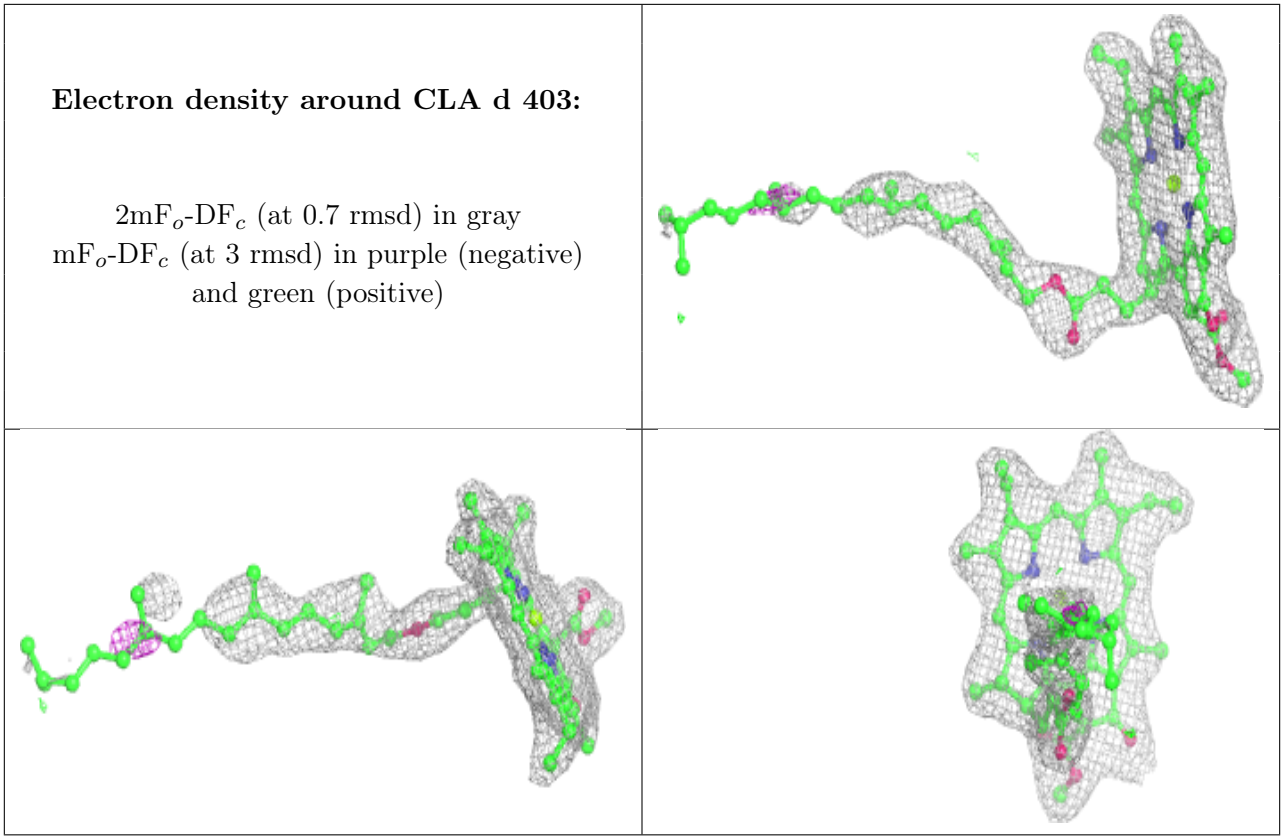
Electron density around CLA C 504:

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



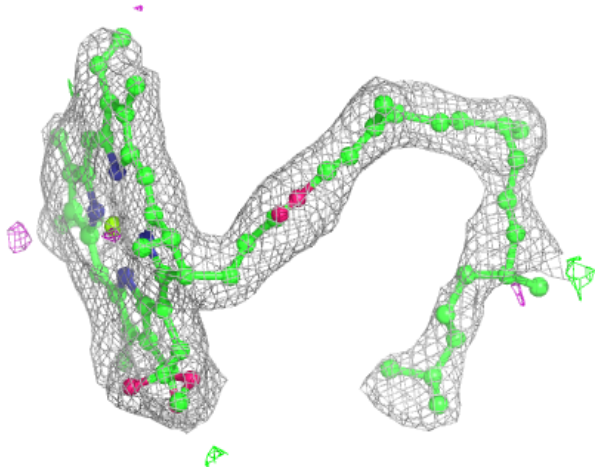
Electron density around CLA d 403:

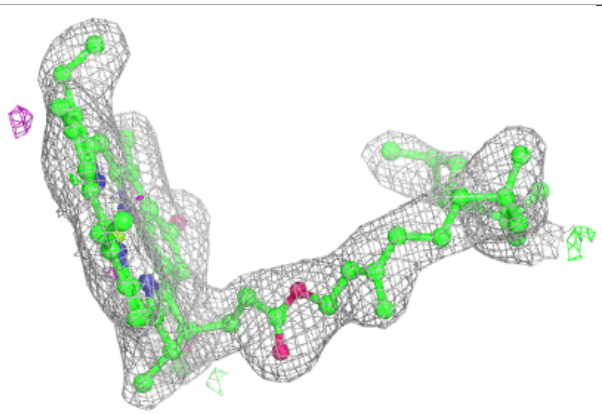
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

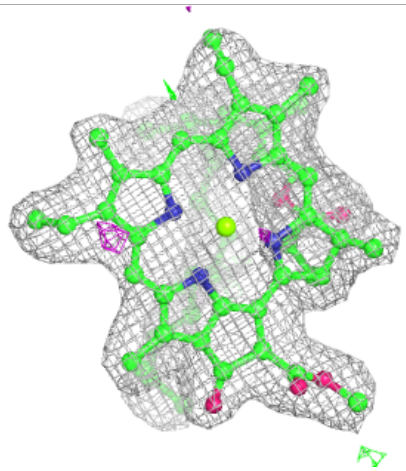


Electron density around CLA b 606:

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

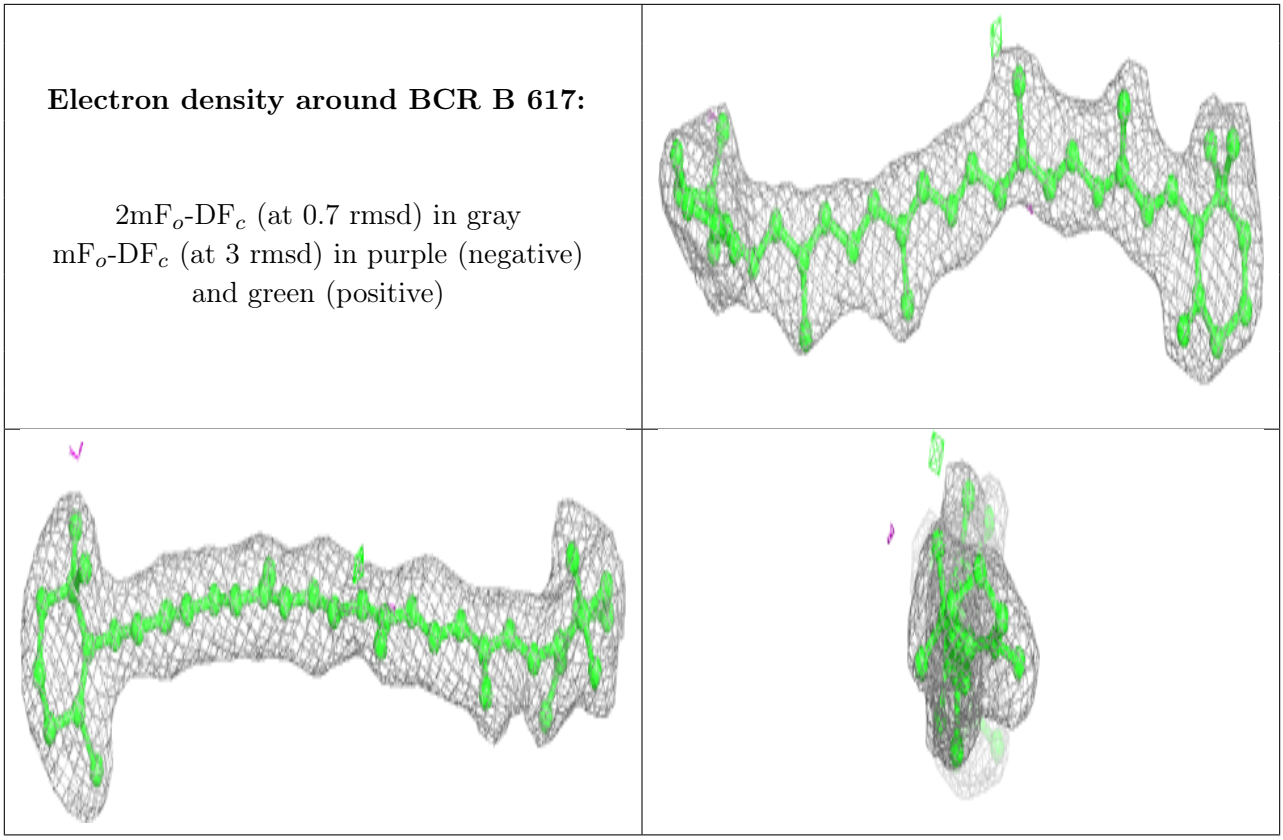






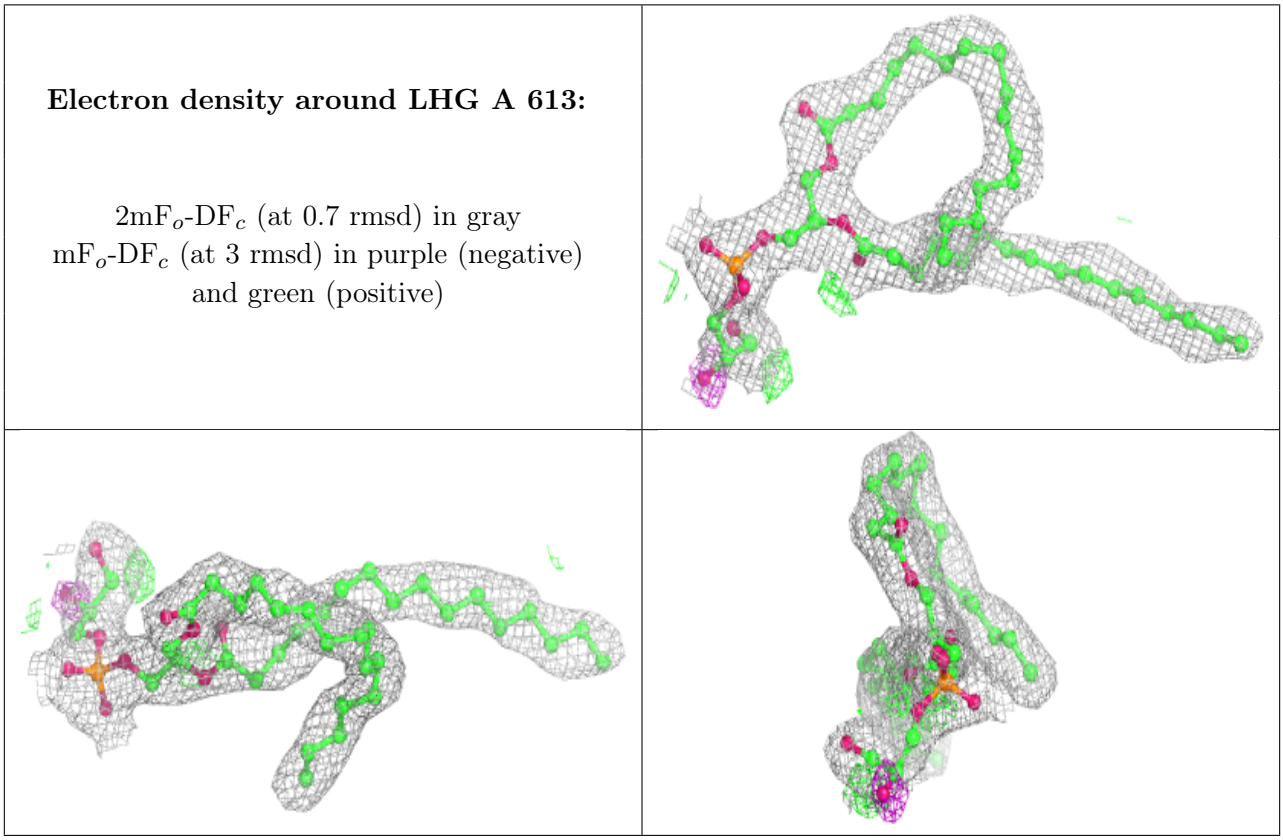
Electron density around BCR B 617:

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



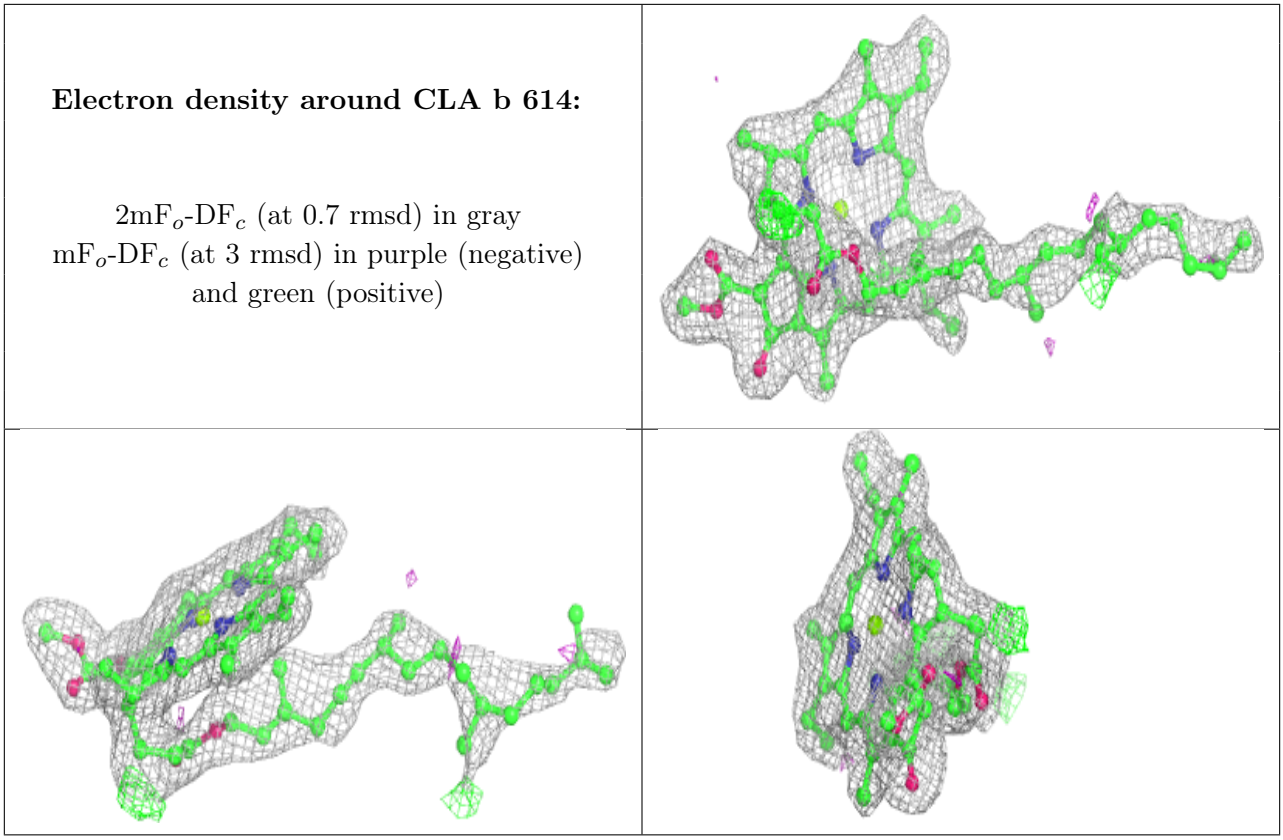
Electron density around LHG A 613:

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



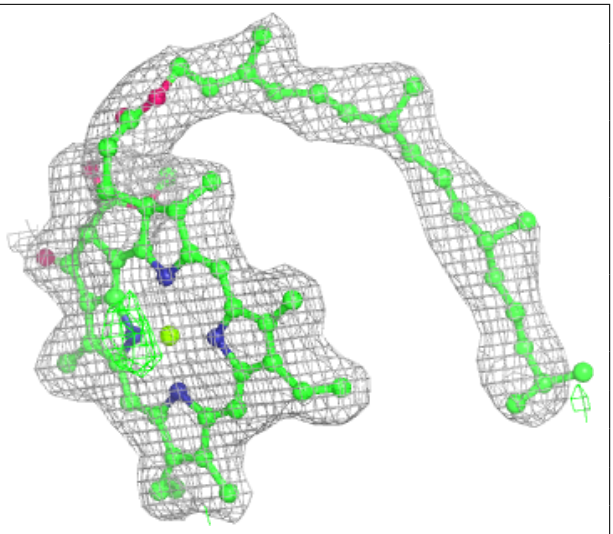
Electron density around CLA b 614:

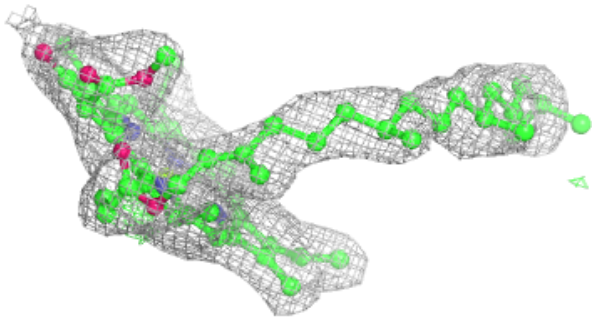
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

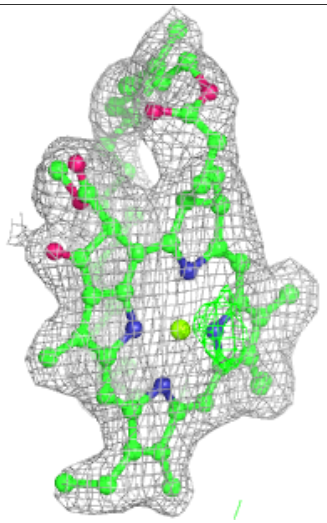


Electron density around CLA C 507:

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

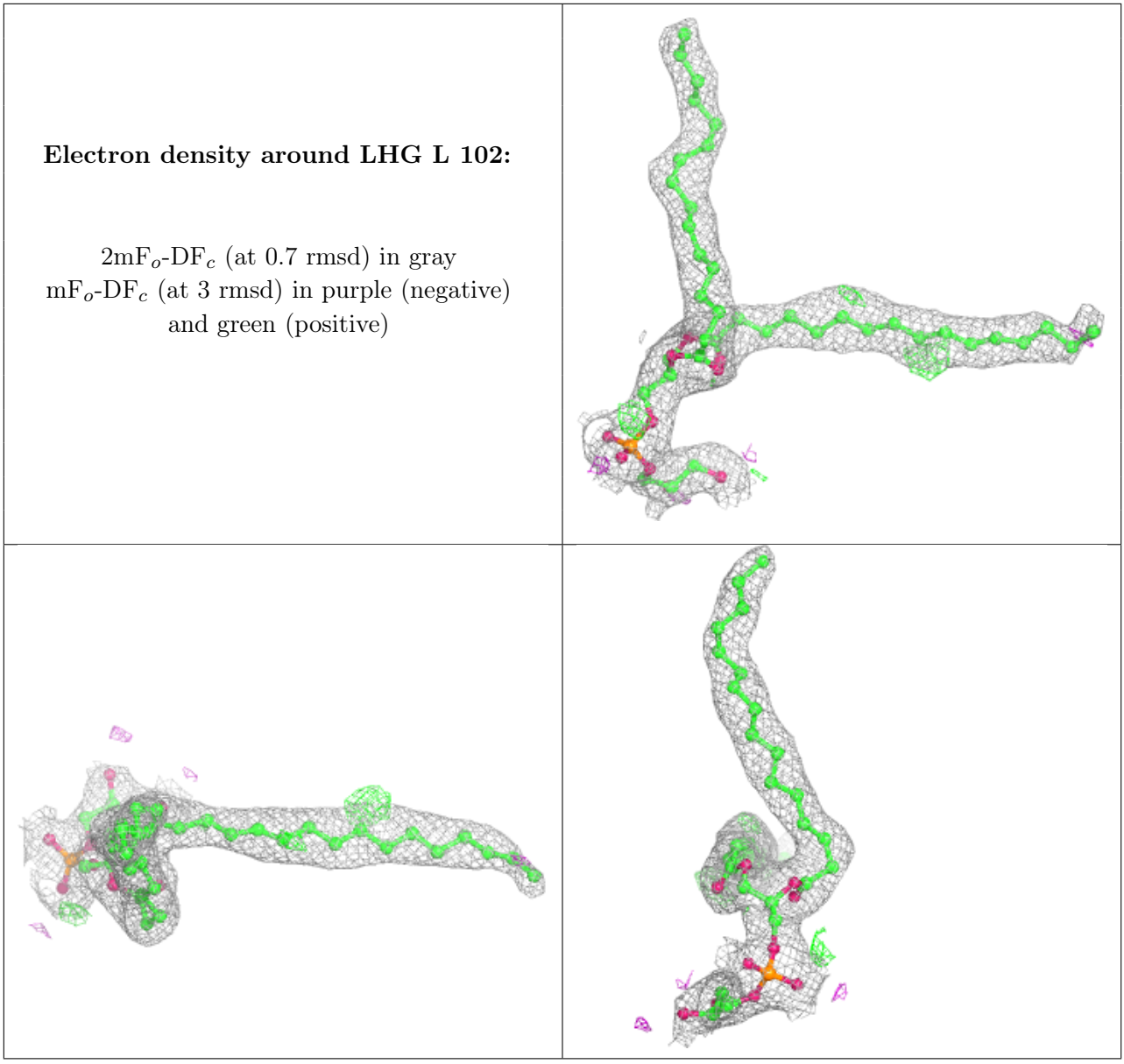






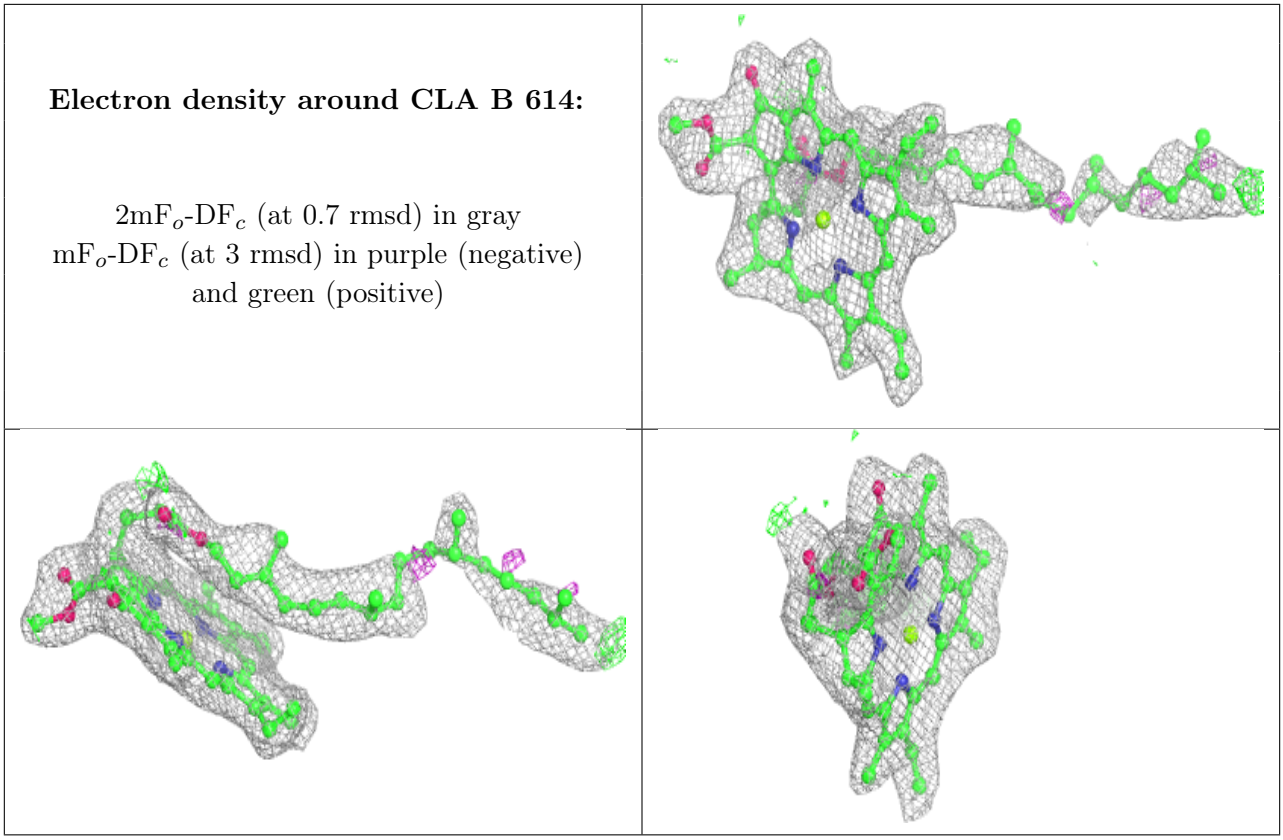
Electron density around LHG L 102:

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



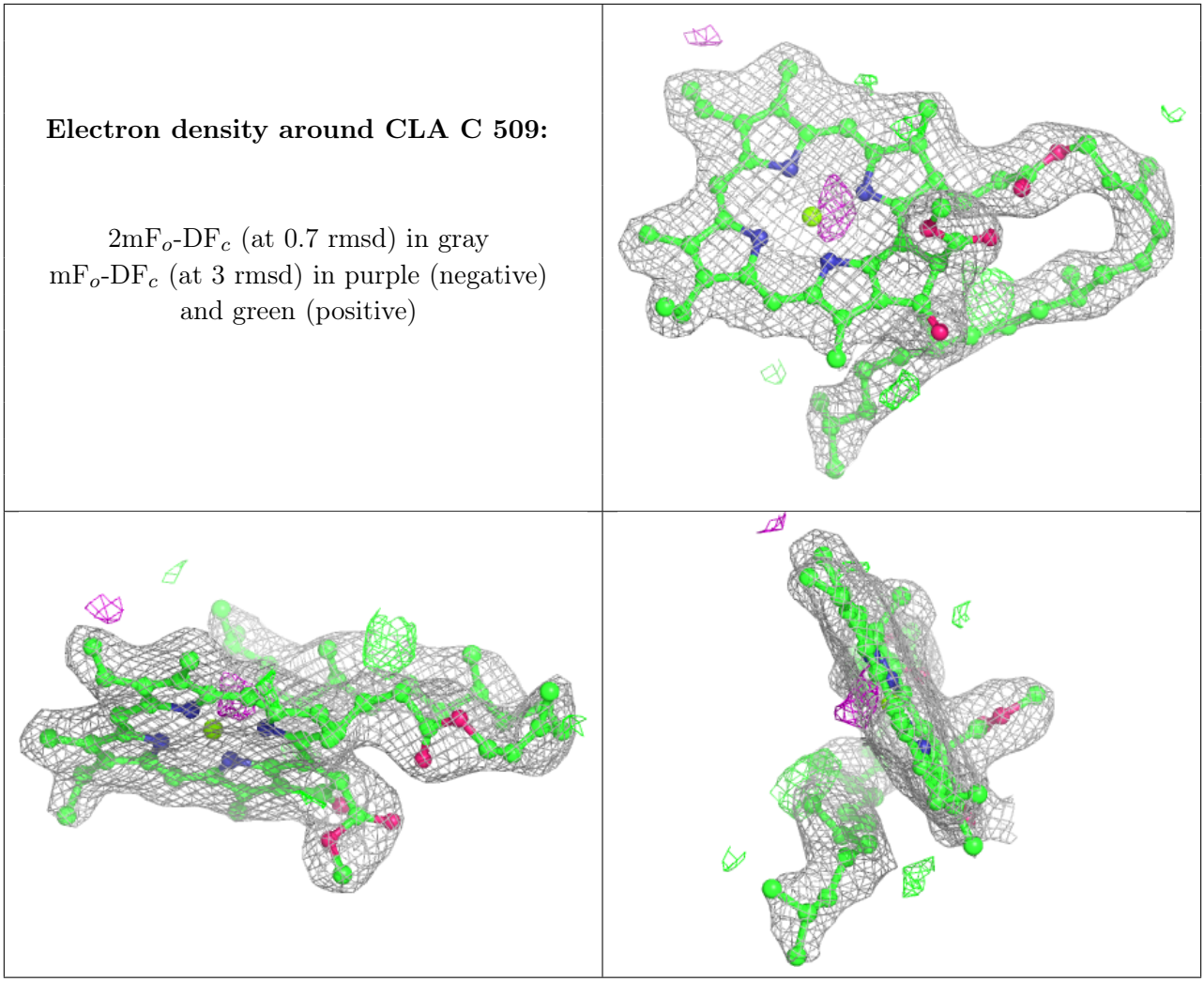
Electron density around CLA B 614:

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



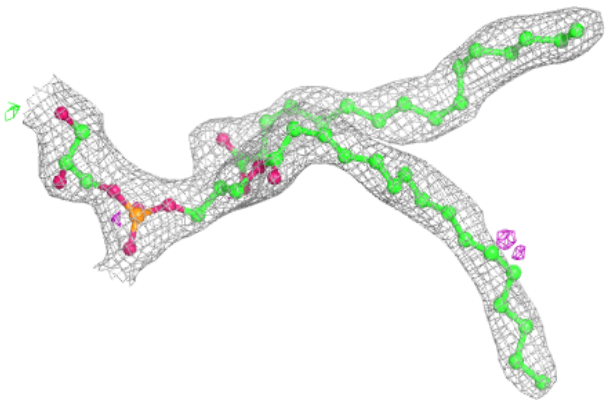
Electron density around CLA C 509:

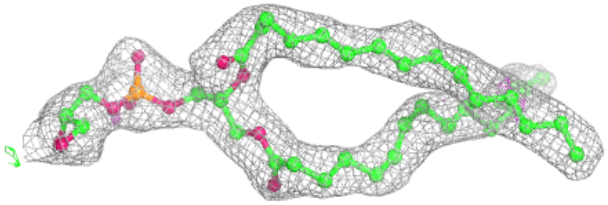
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

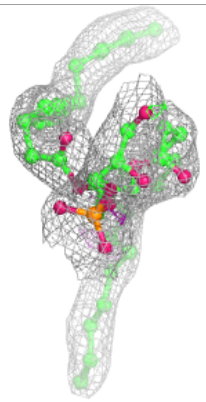


Electron density around LHG d 406:

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

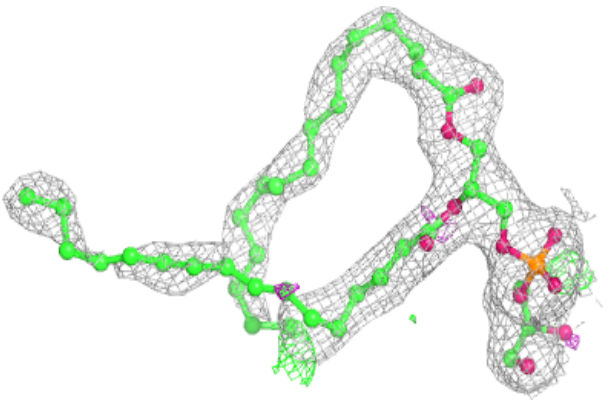


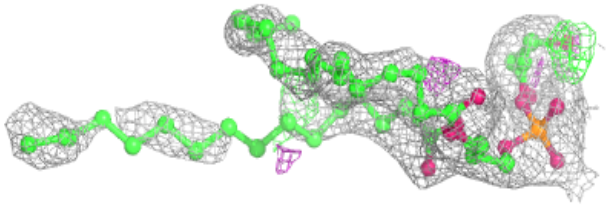


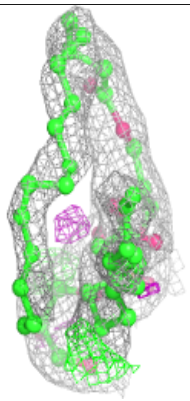


Electron density around LHG d 407:

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

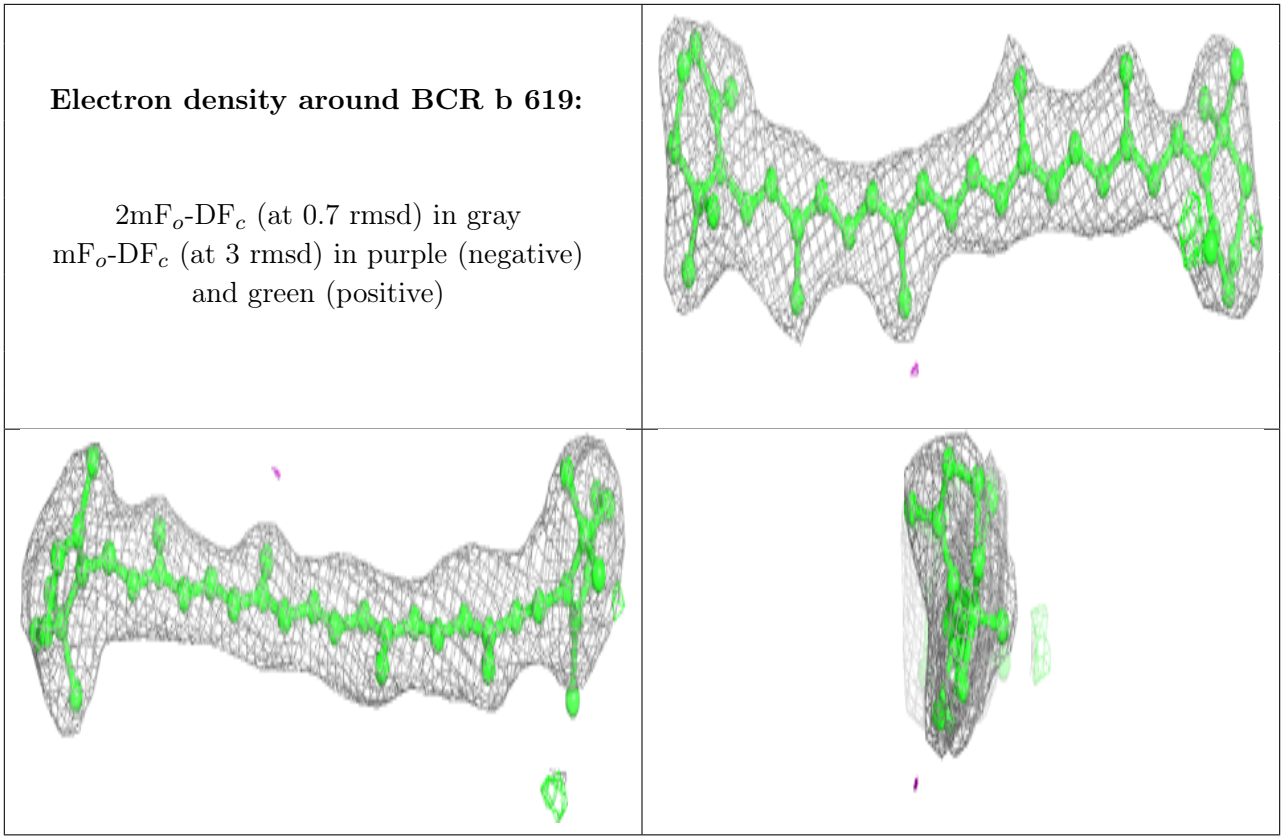






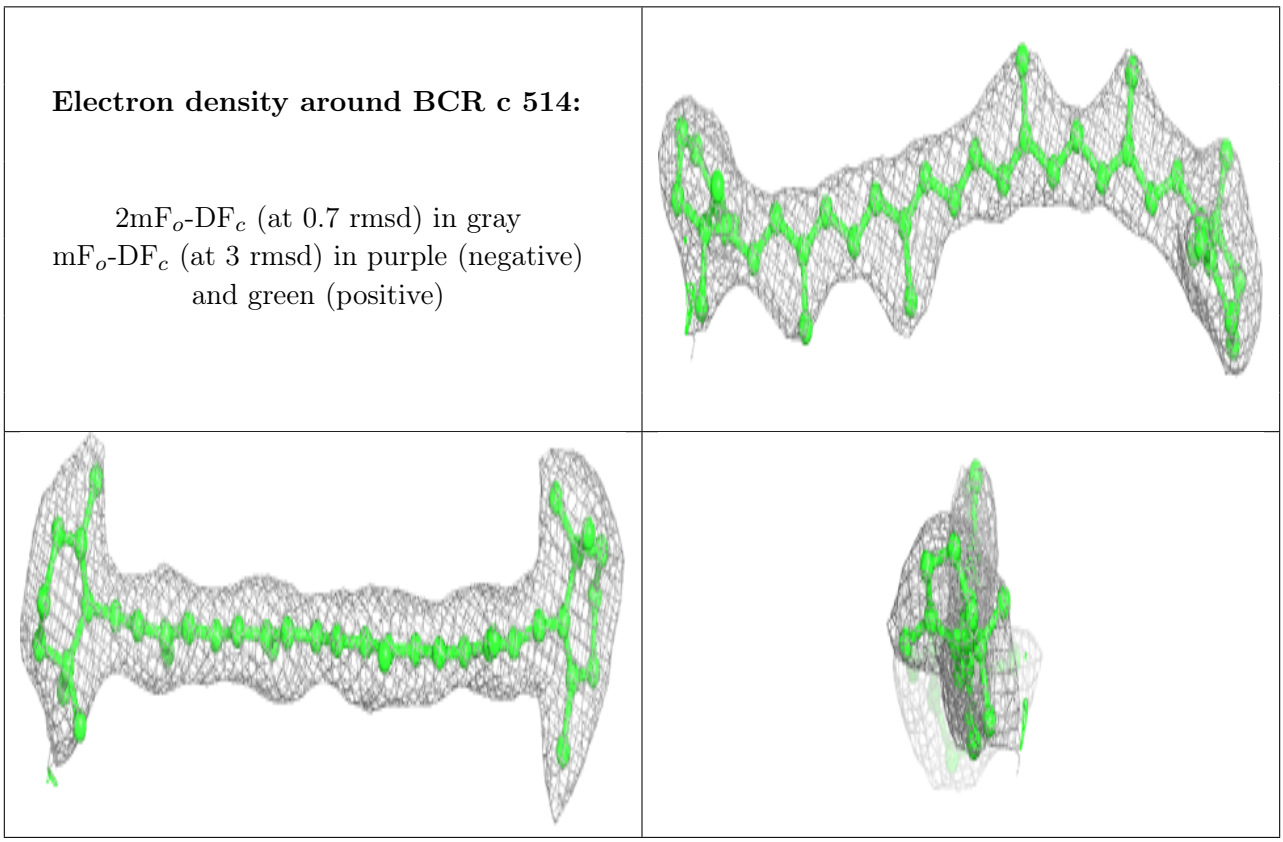
Electron density around BCR b 619:

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



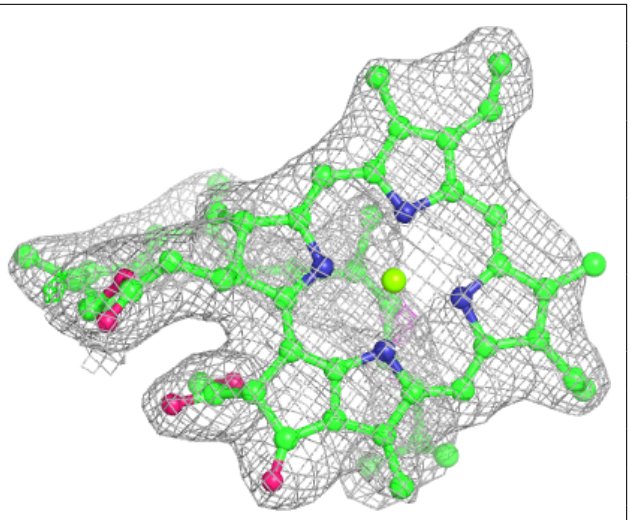
Electron density around BCR c 514:

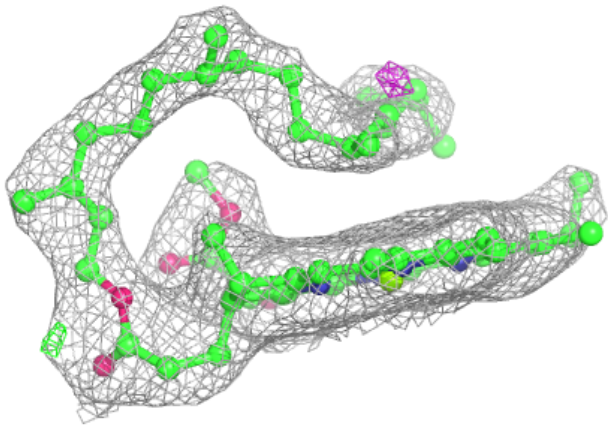
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

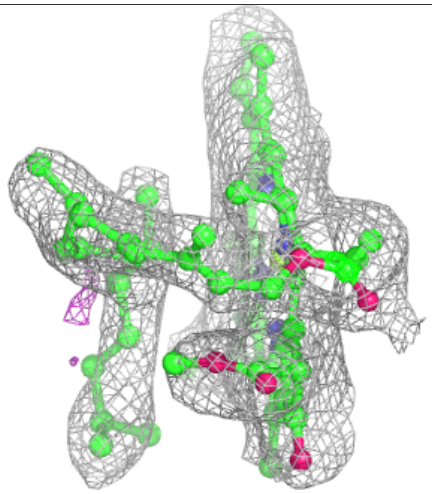


Electron density around CLA c 510:

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

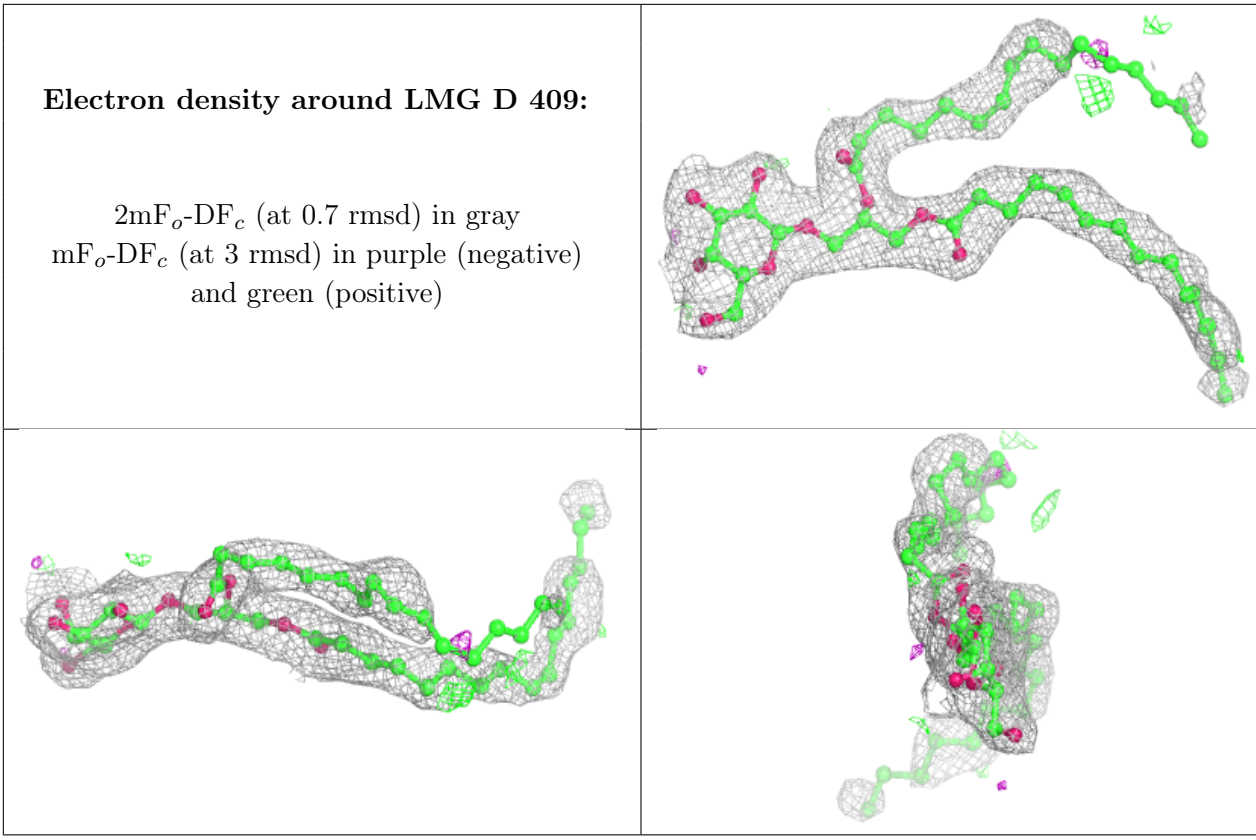






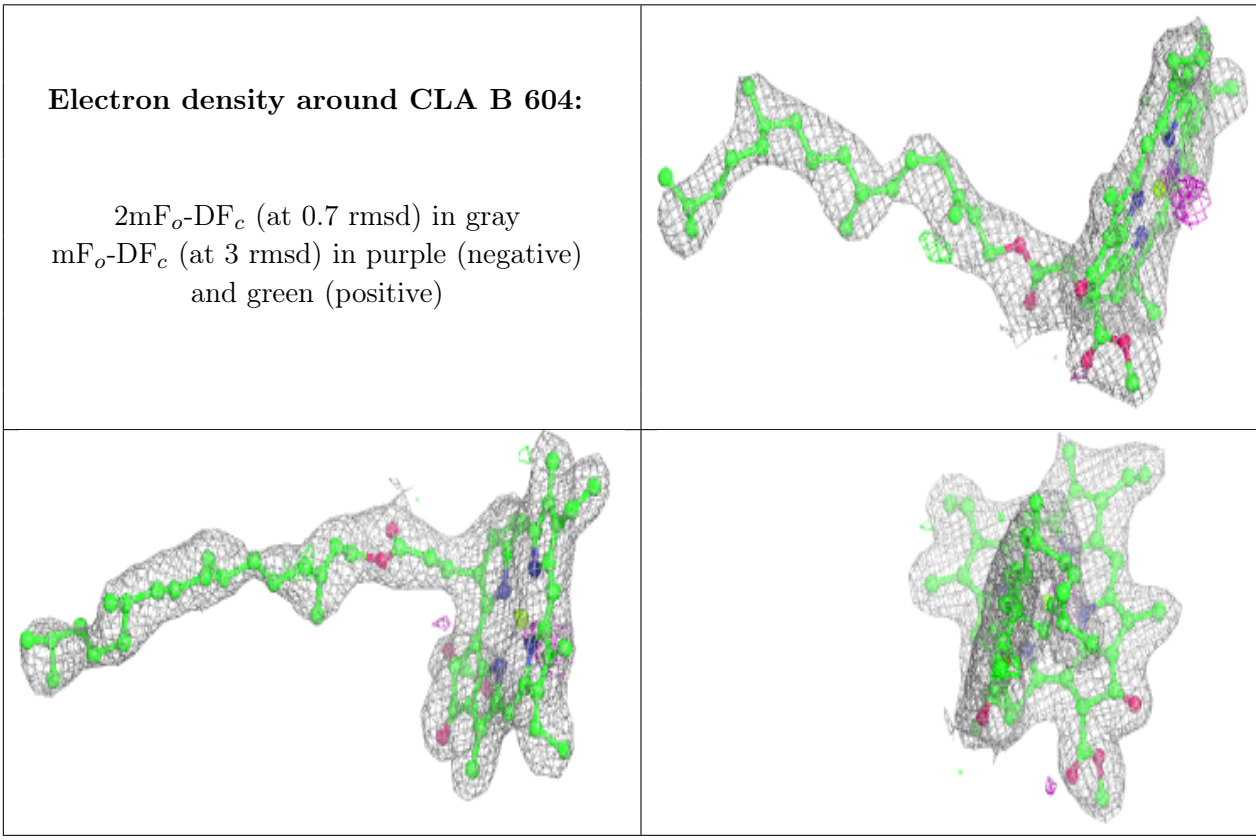
Electron density around LMG D 409:

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



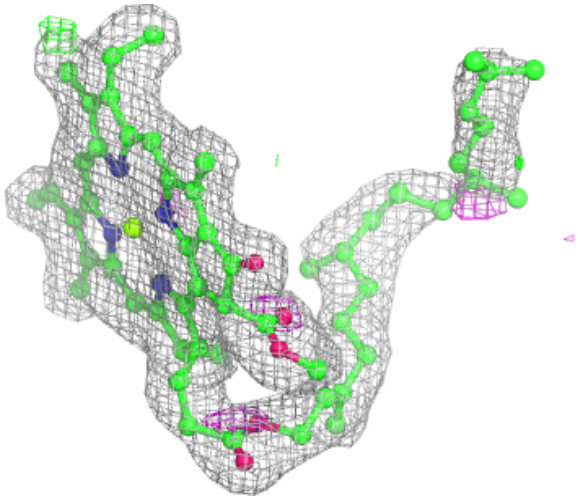
Electron density around CLA B 604:

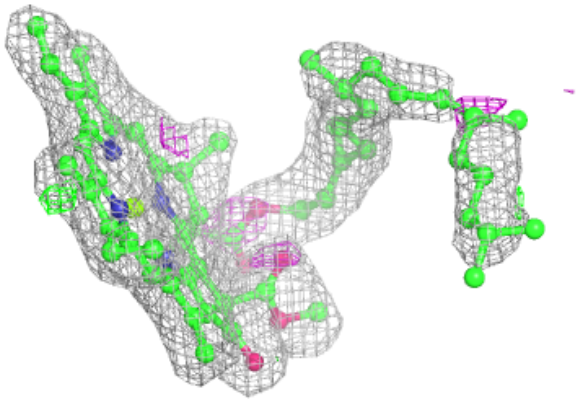
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

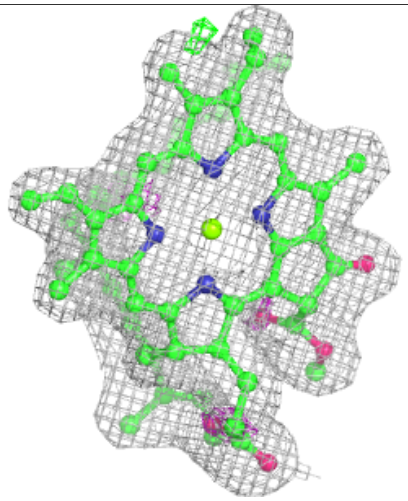


Electron density around CLA b 613:

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

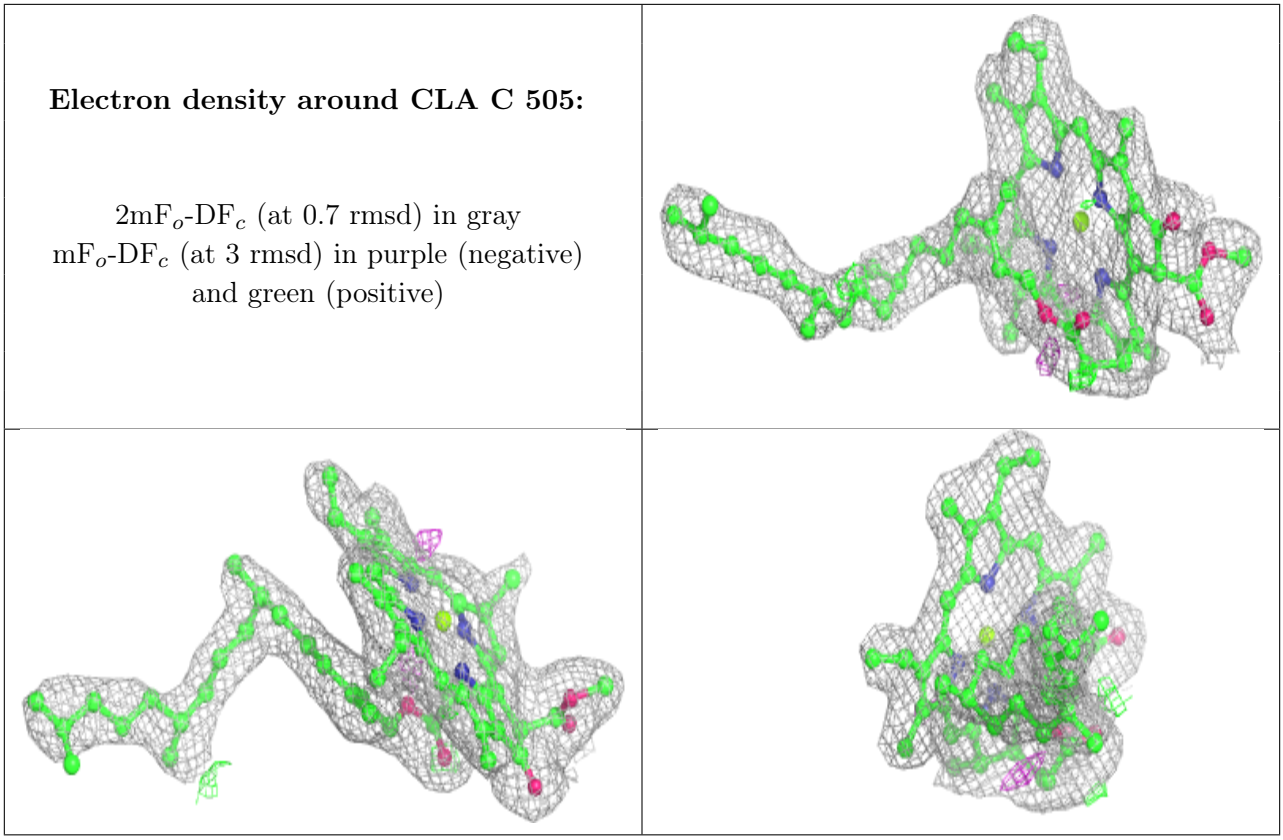






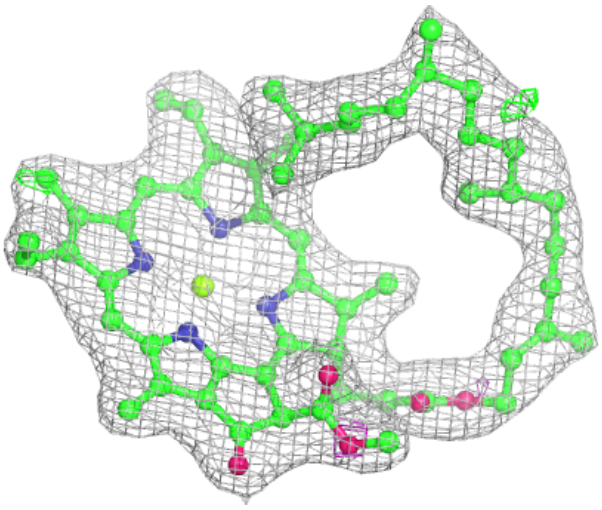
Electron density around CLA C 505:

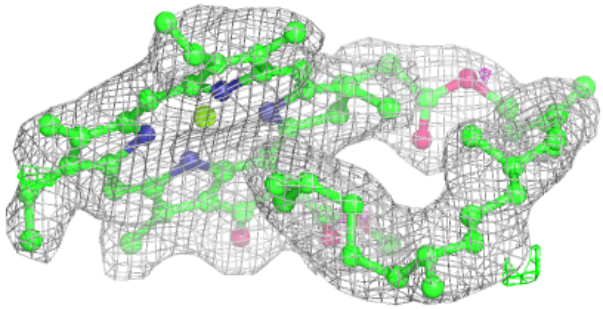
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

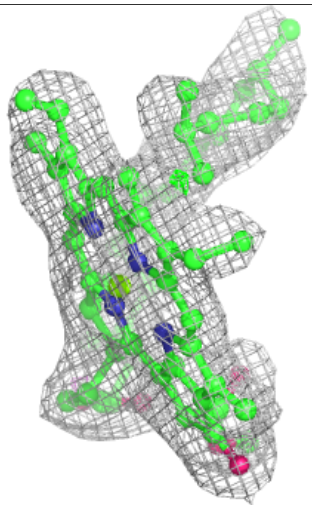


Electron density around CLA b 615:

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

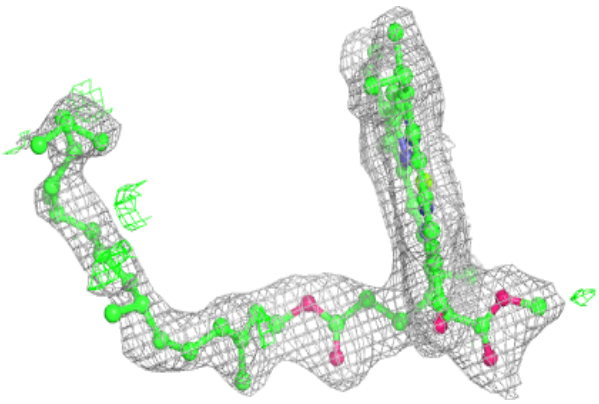


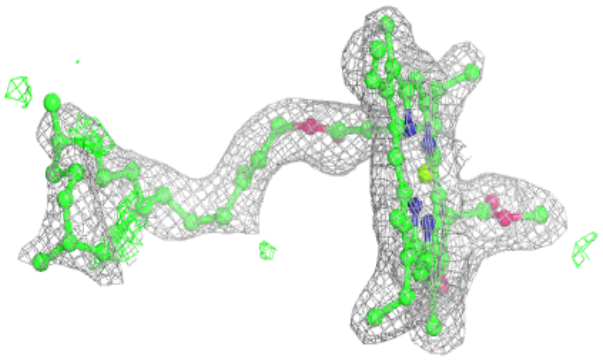


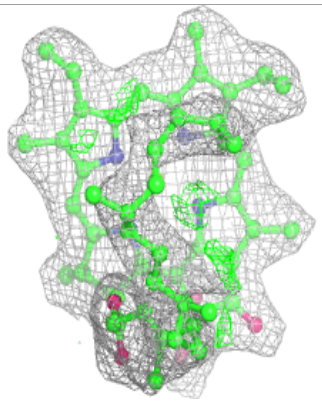


Electron density around CLA C 506:

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

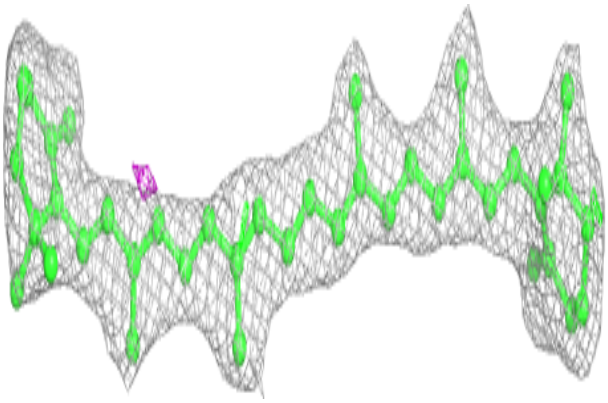


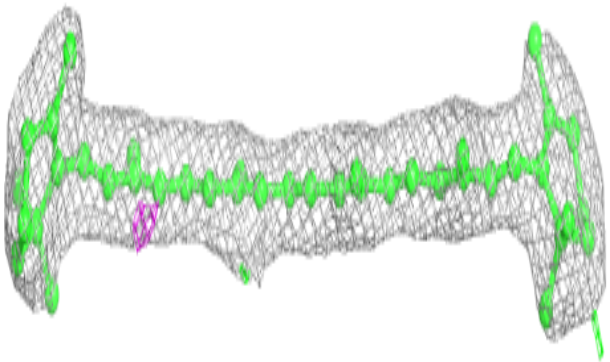


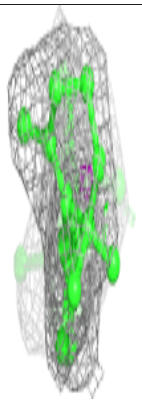


Electron density around BCR B 618:

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

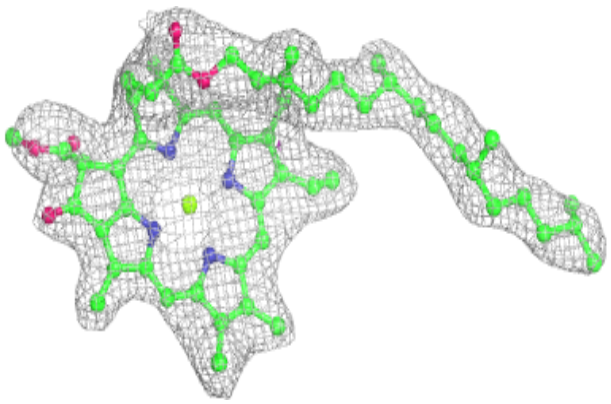


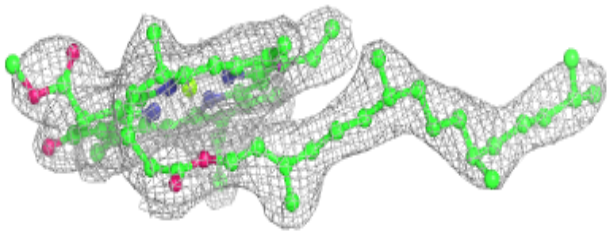


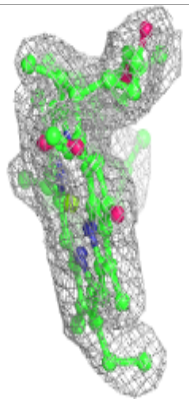


Electron density around CLA c 501:

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

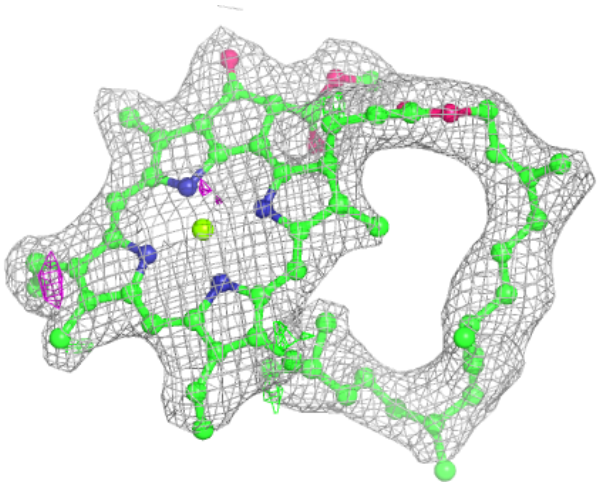


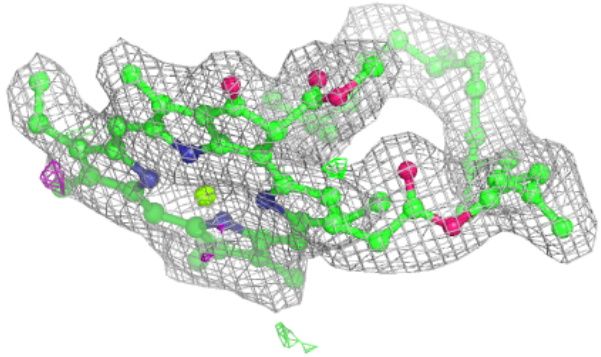


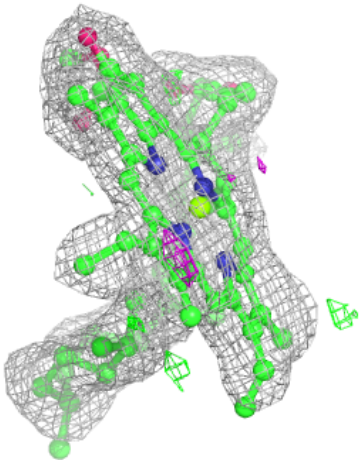


Electron density around CLA B 615:

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

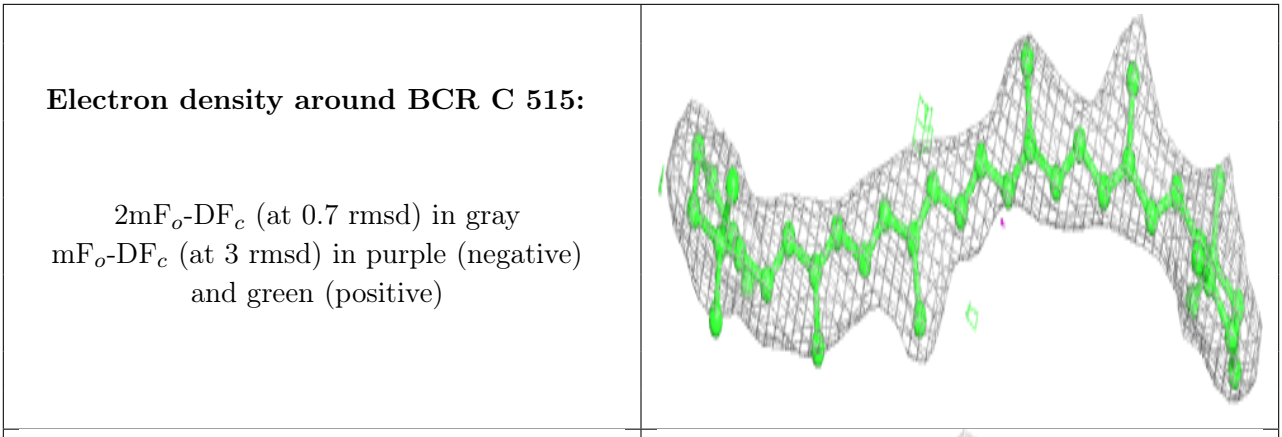






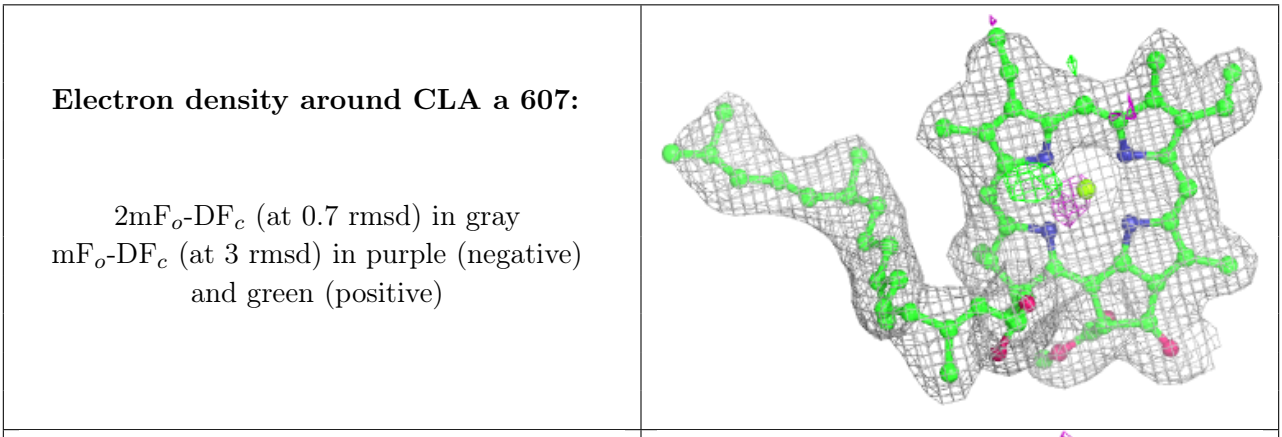
Electron density around BCR C 515:

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



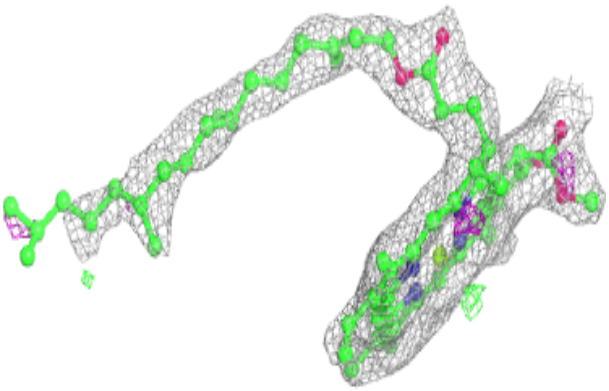
Electron density around CLA a 607:

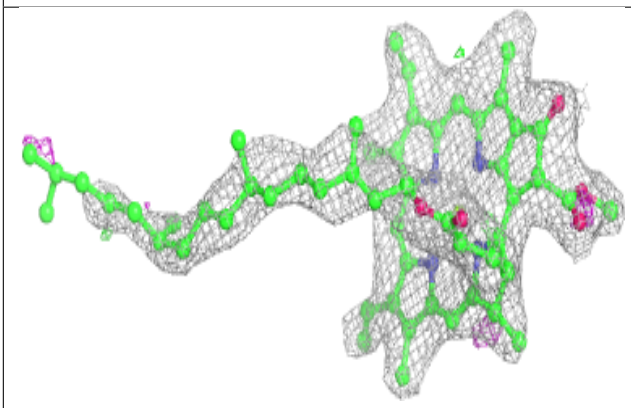
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

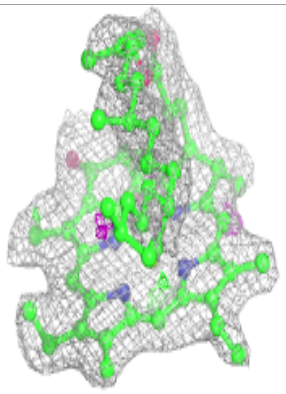


Electron density around CLA c 504:

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

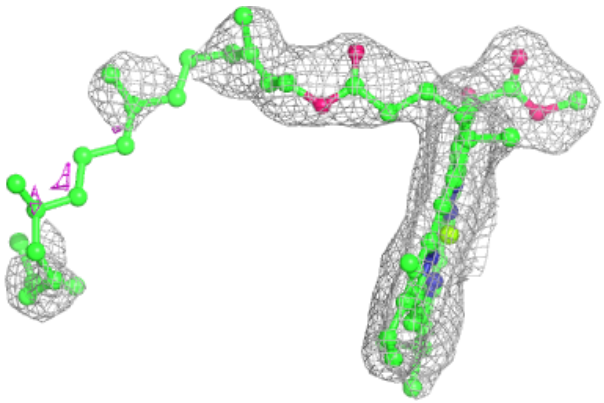


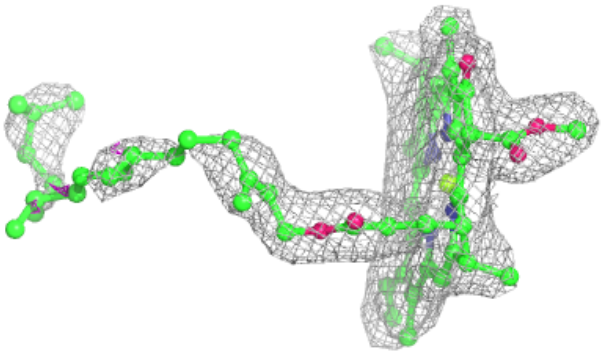


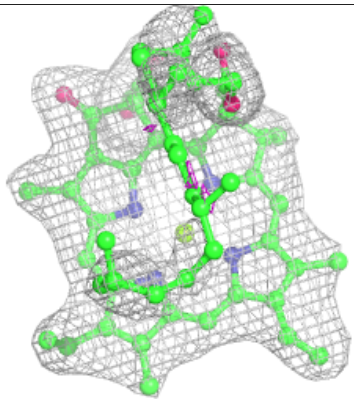


Electron density around CLA c 506:

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

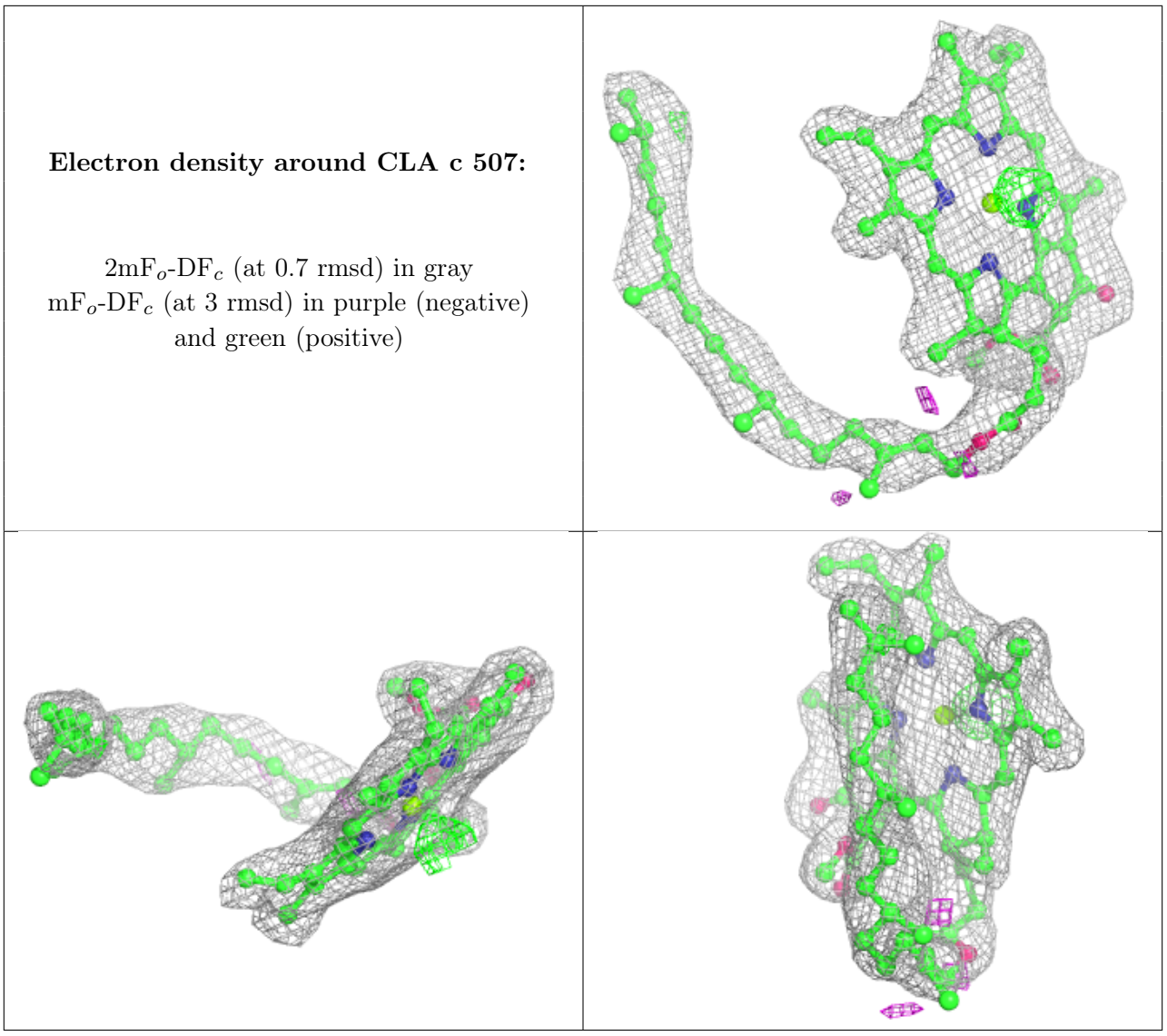






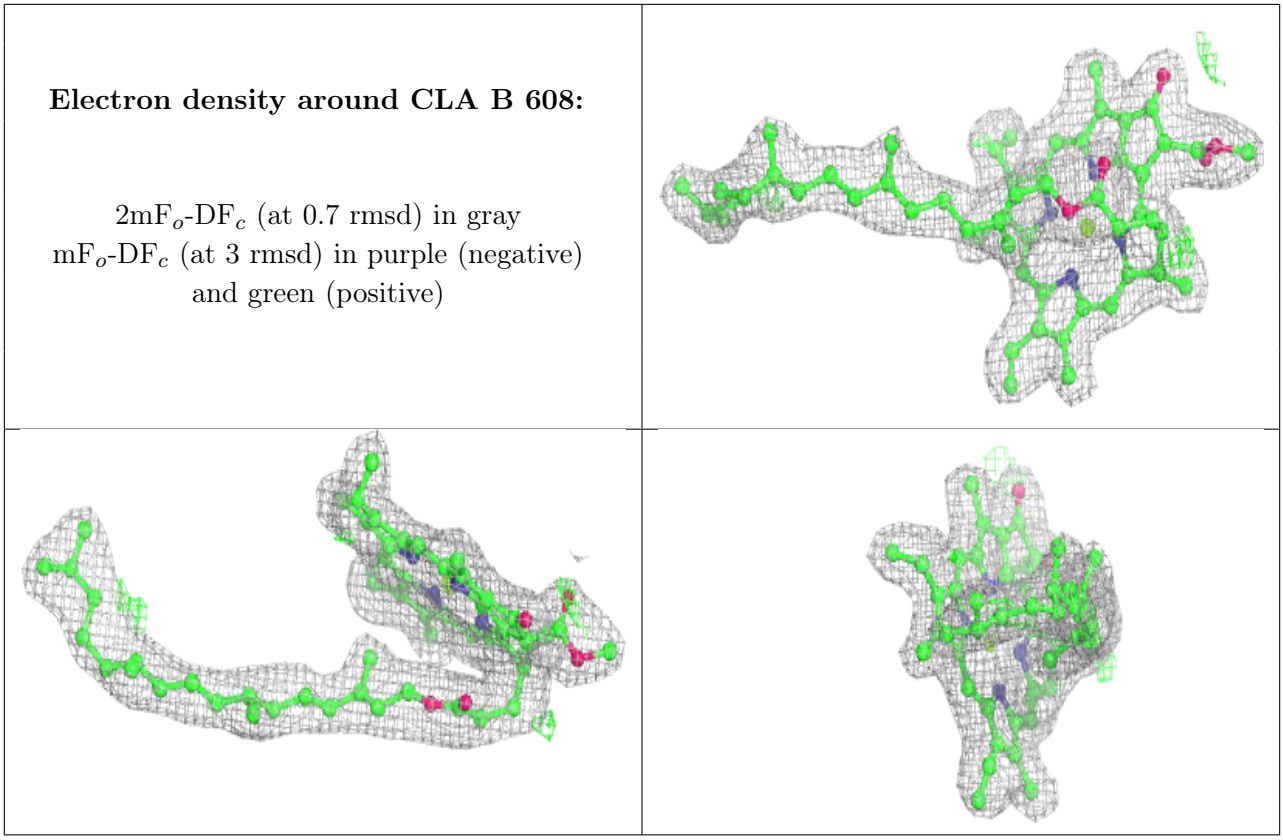
Electron density around CLA c 507:

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



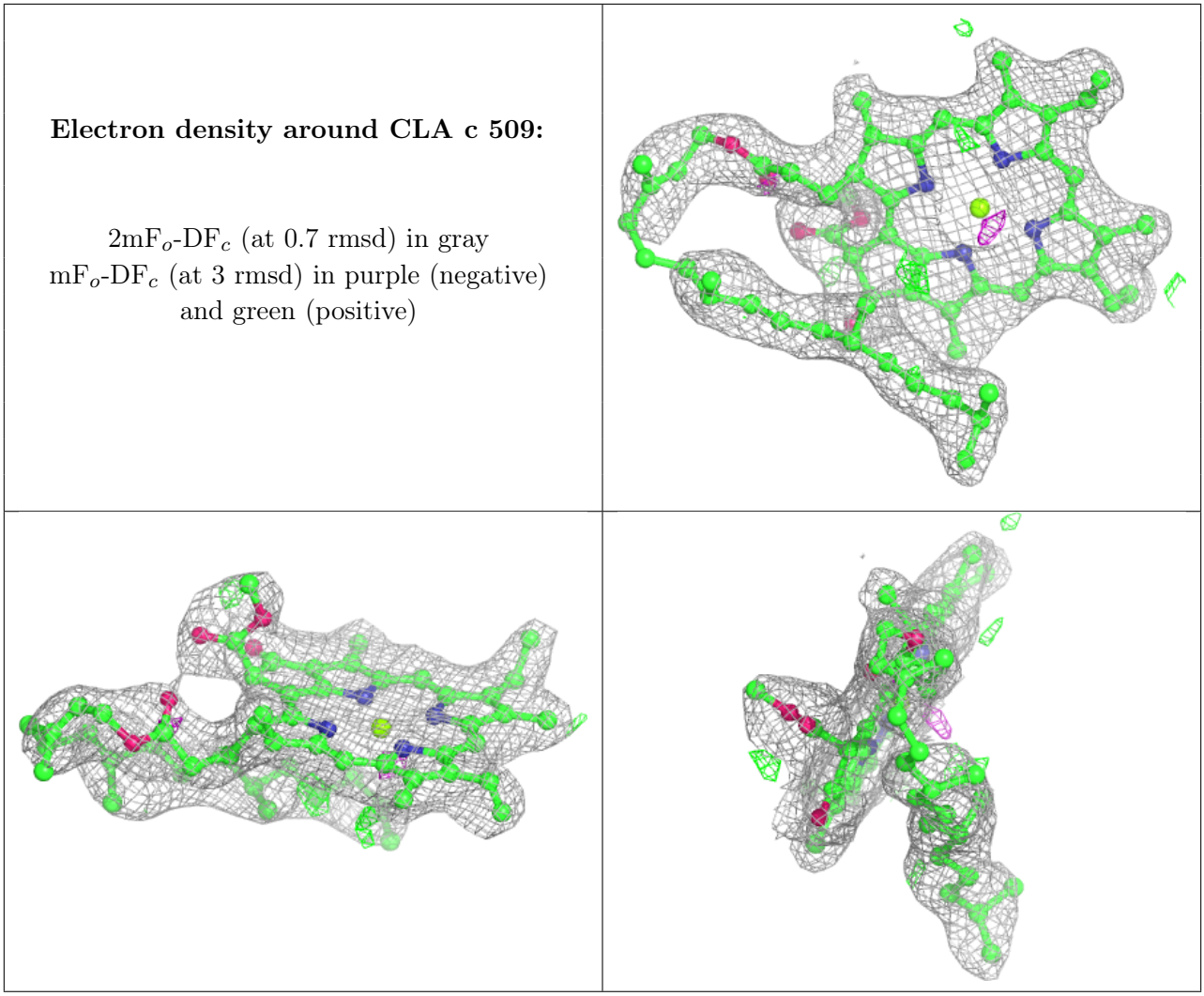
Electron density around CLA B 608:

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



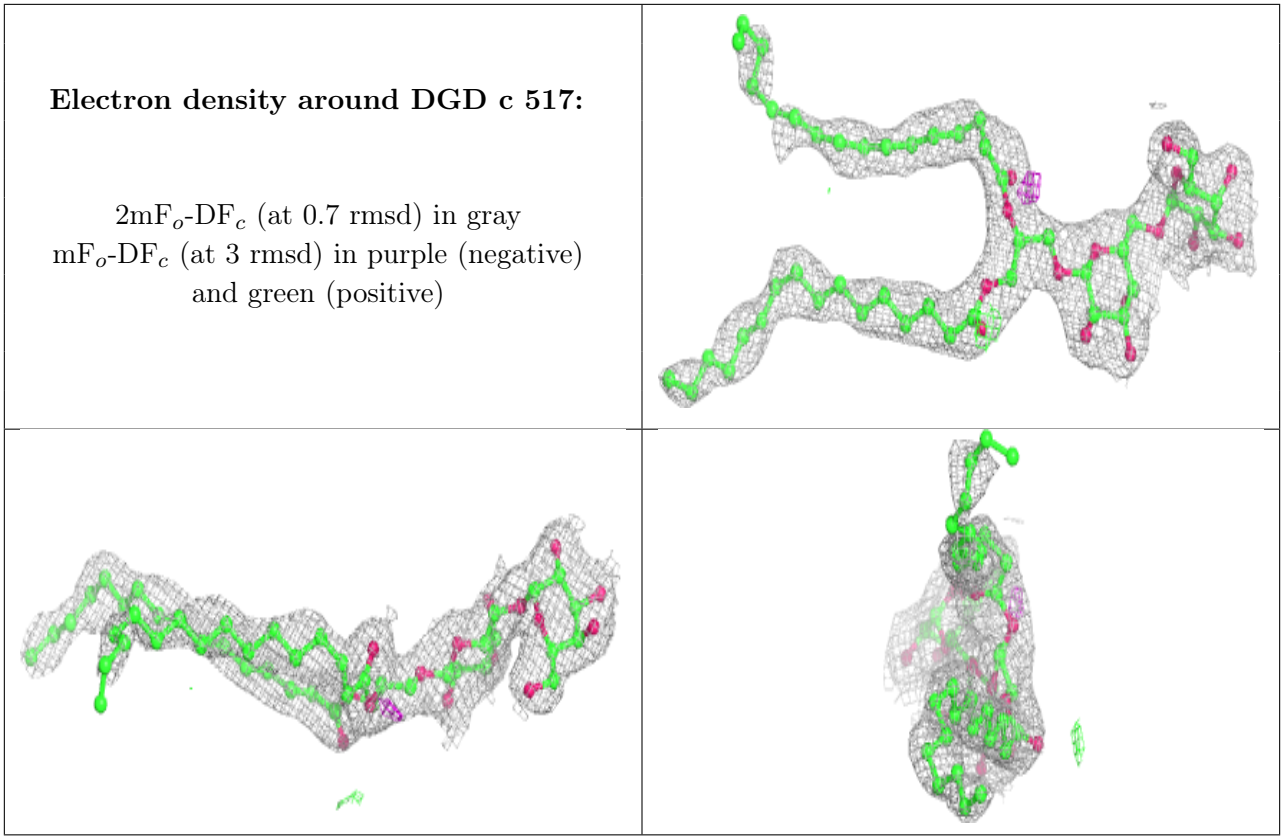
Electron density around CLA c 509:

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



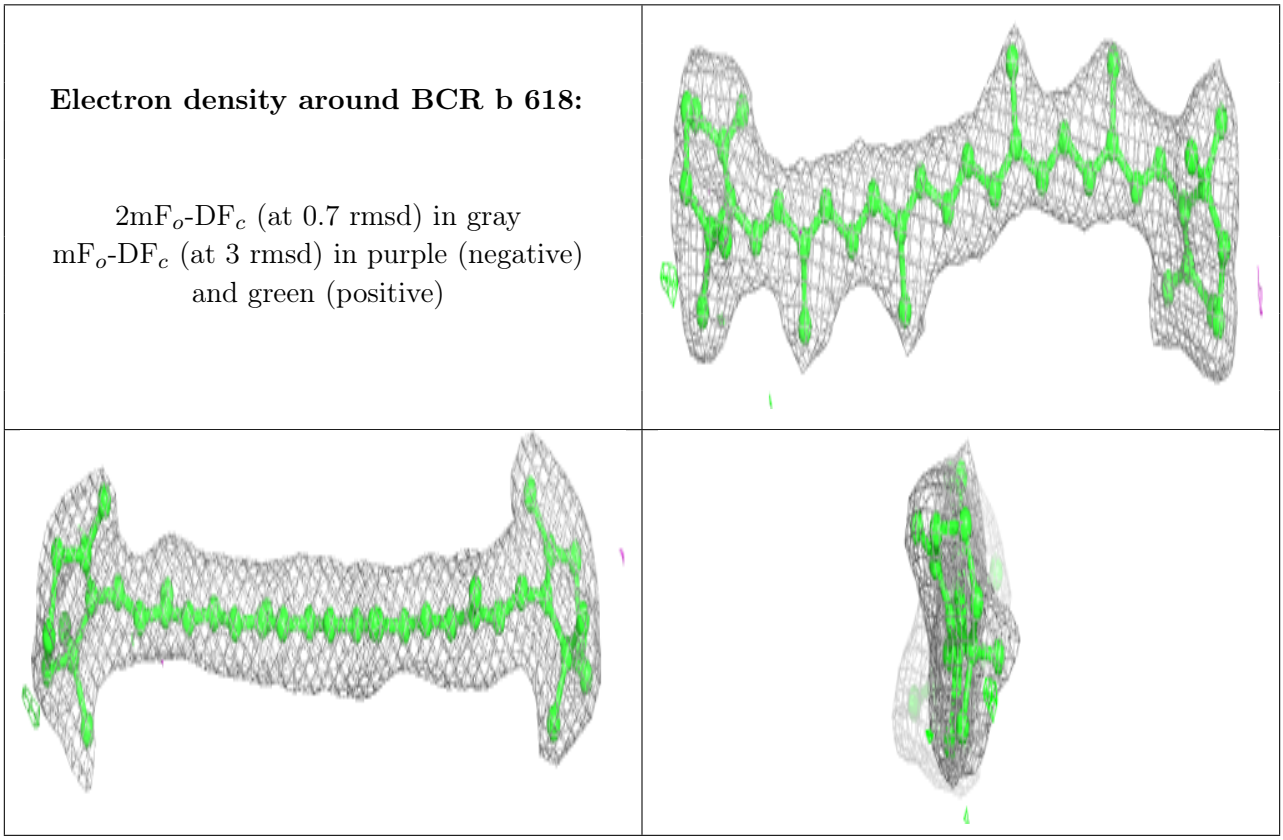
Electron density around DGD c 517:

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



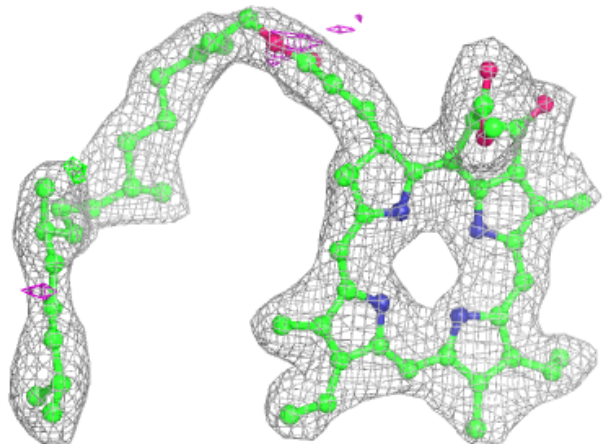
Electron density around BCR b 618:

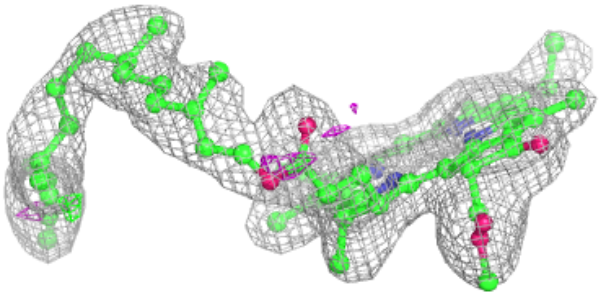
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO d 402:

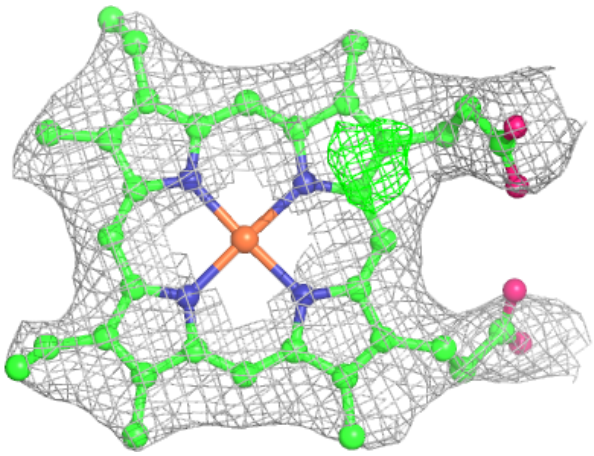
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

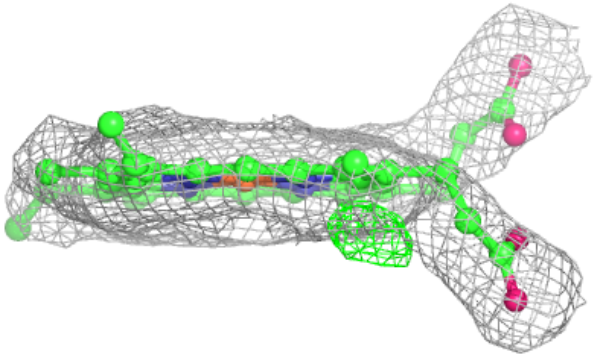


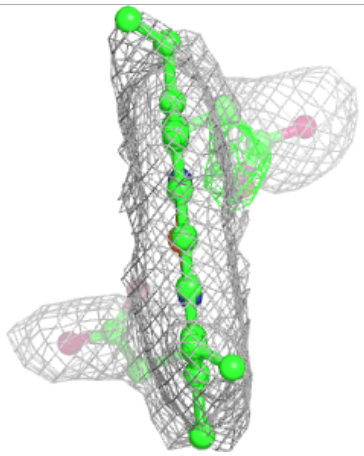


Electron density around HEM E 102:

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

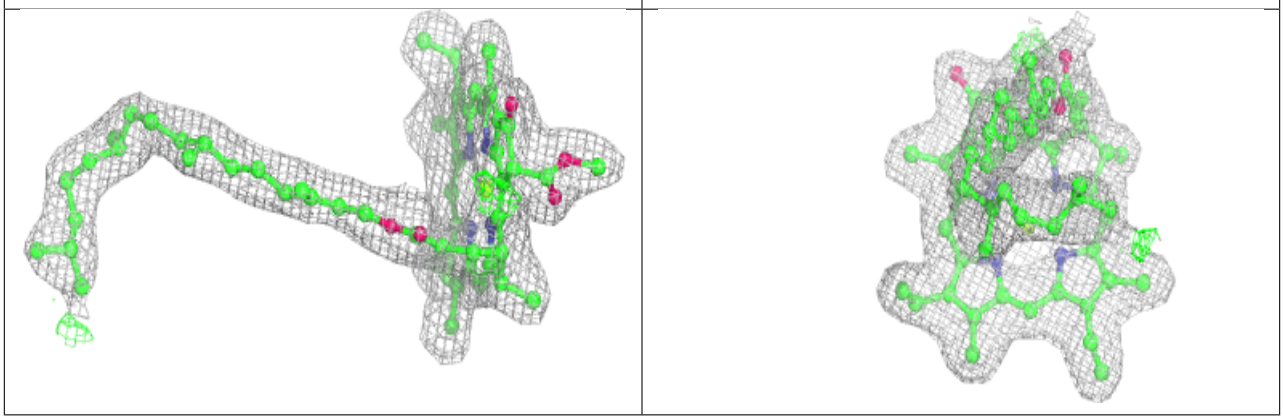






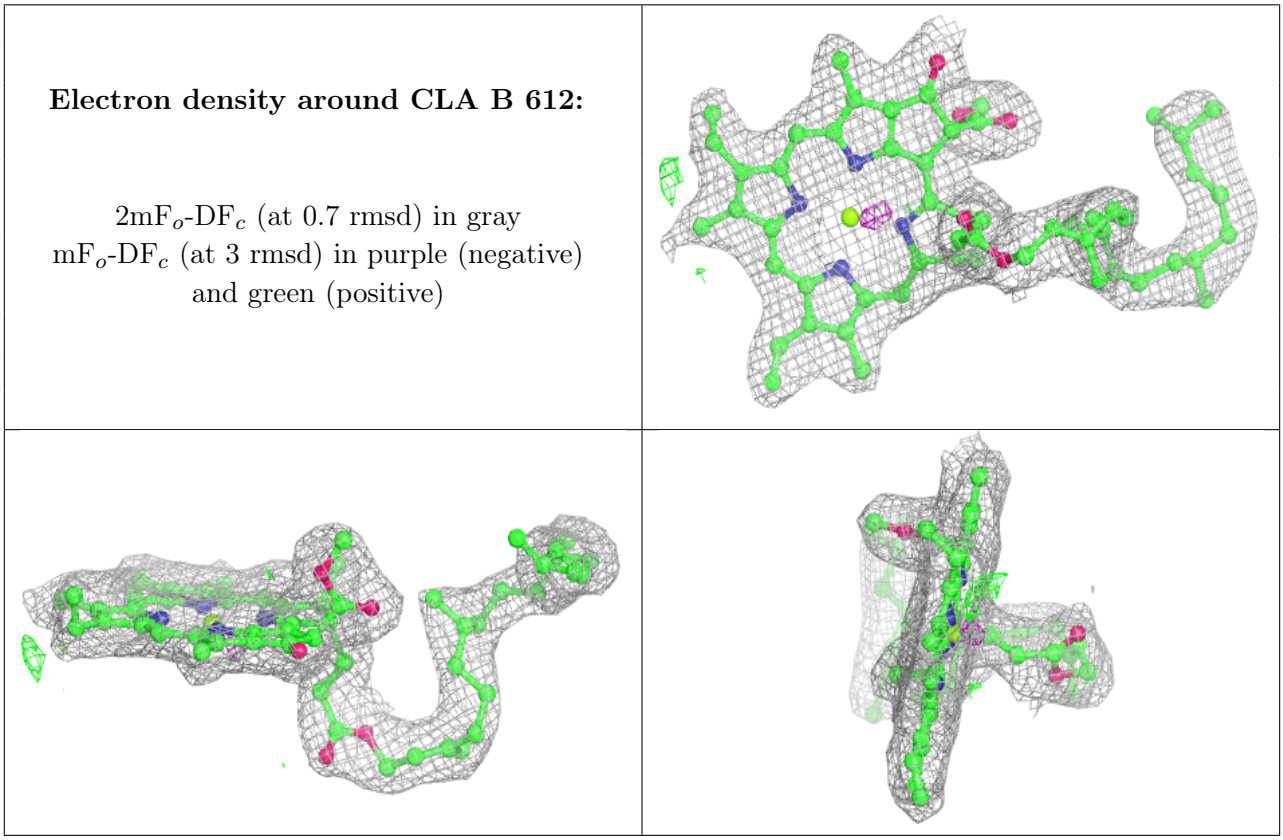
Electron density around CLA B 605:

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



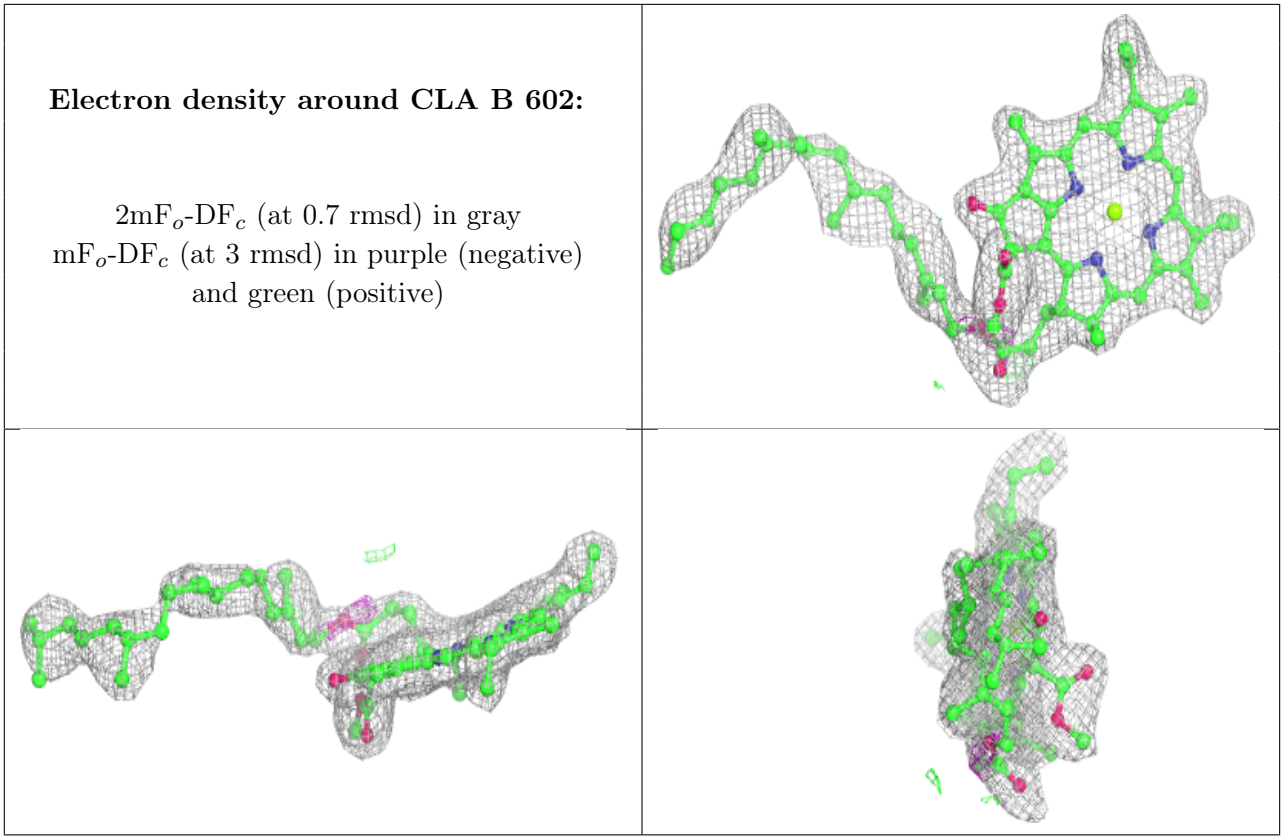
Electron density around CLA B 612:

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



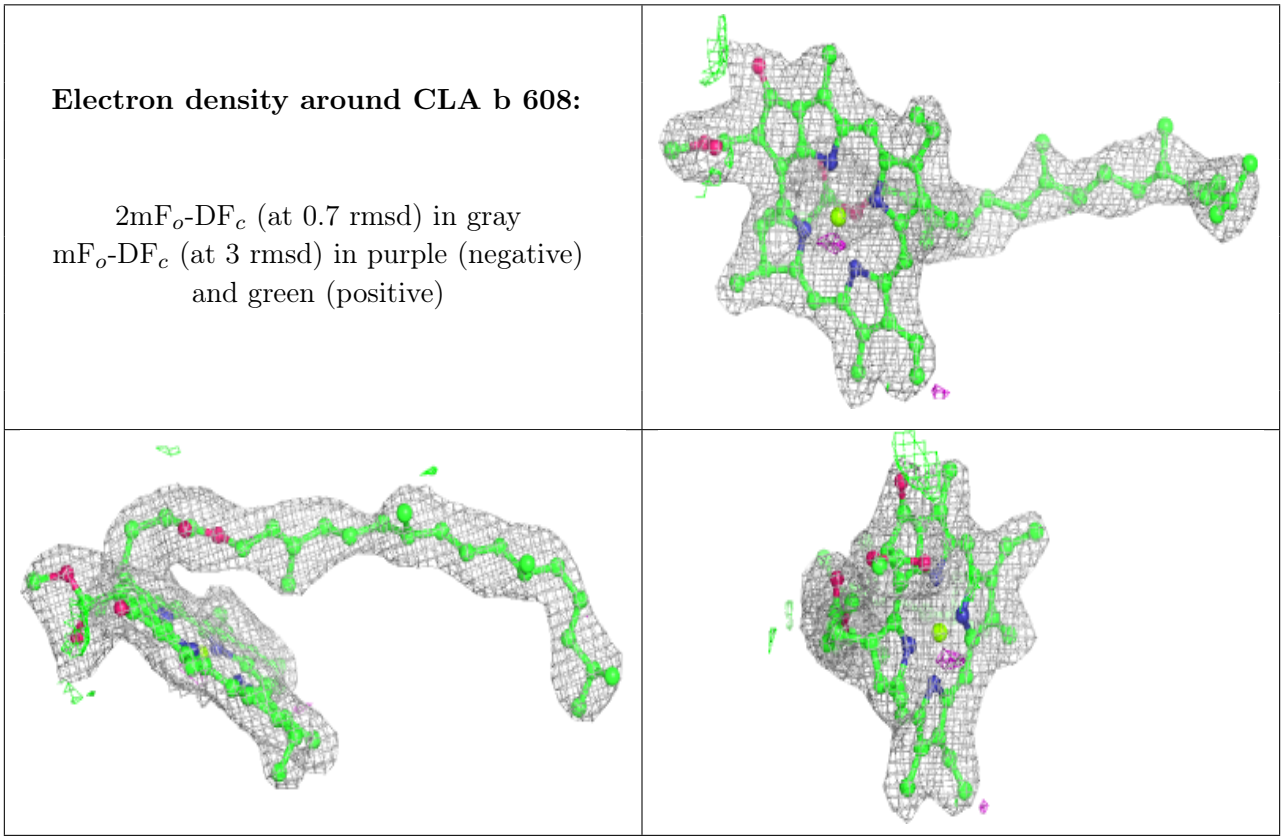
Electron density around CLA B 602:

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



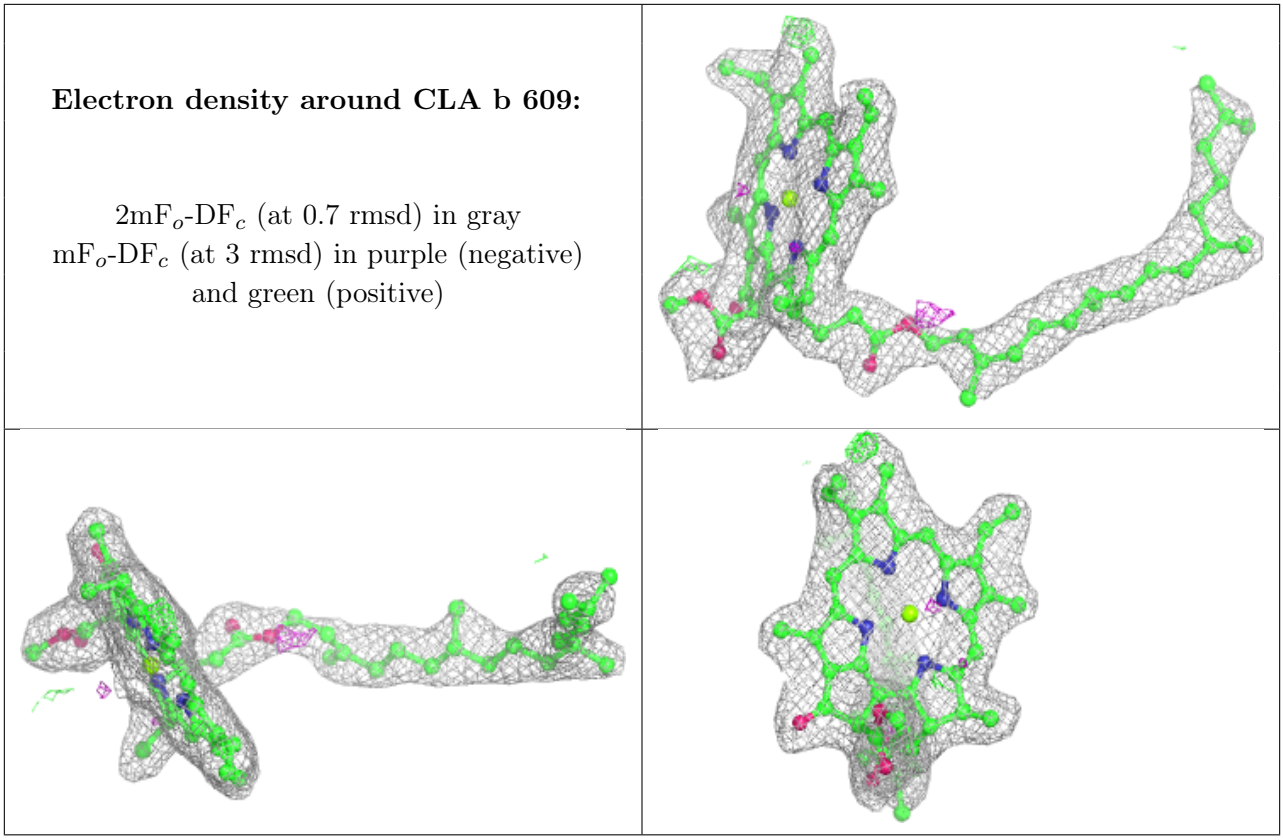
Electron density around CLA b 608:

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



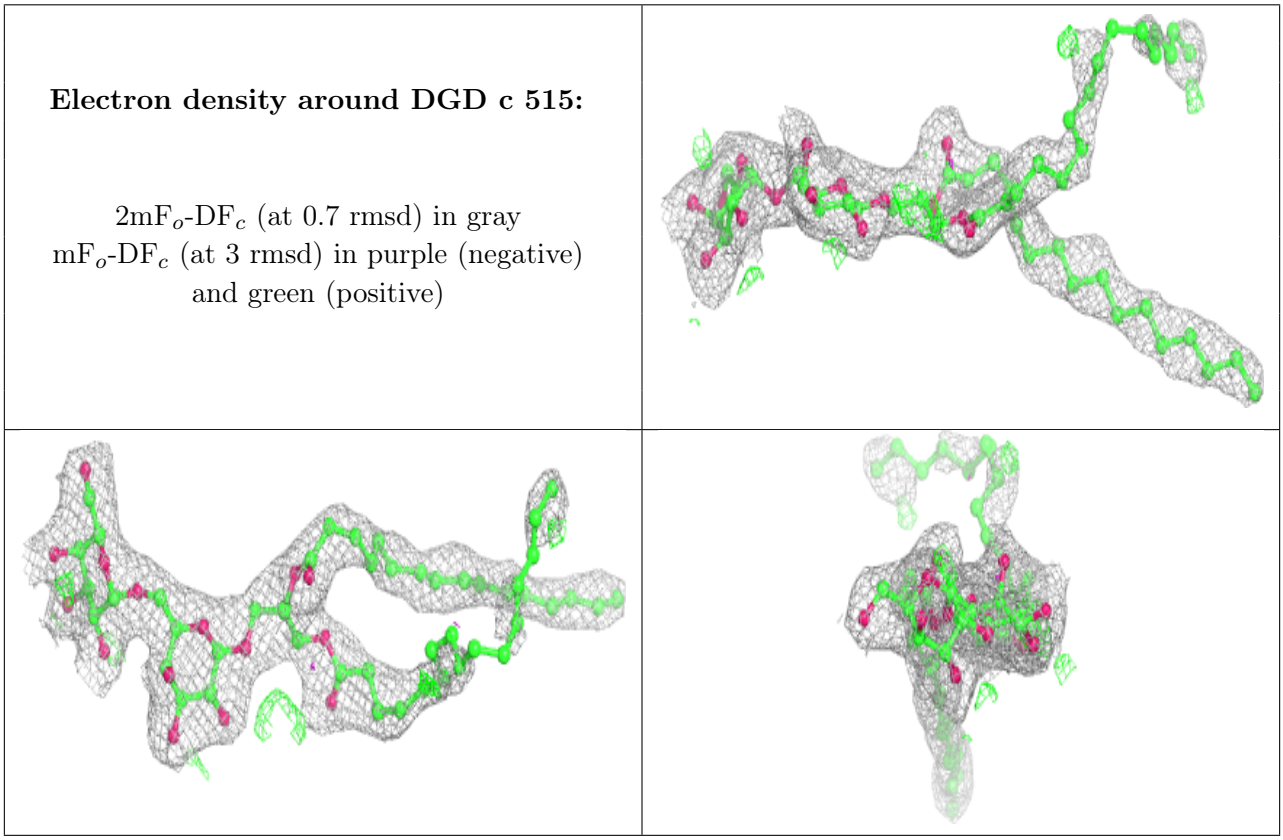
Electron density around CLA b 609:

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



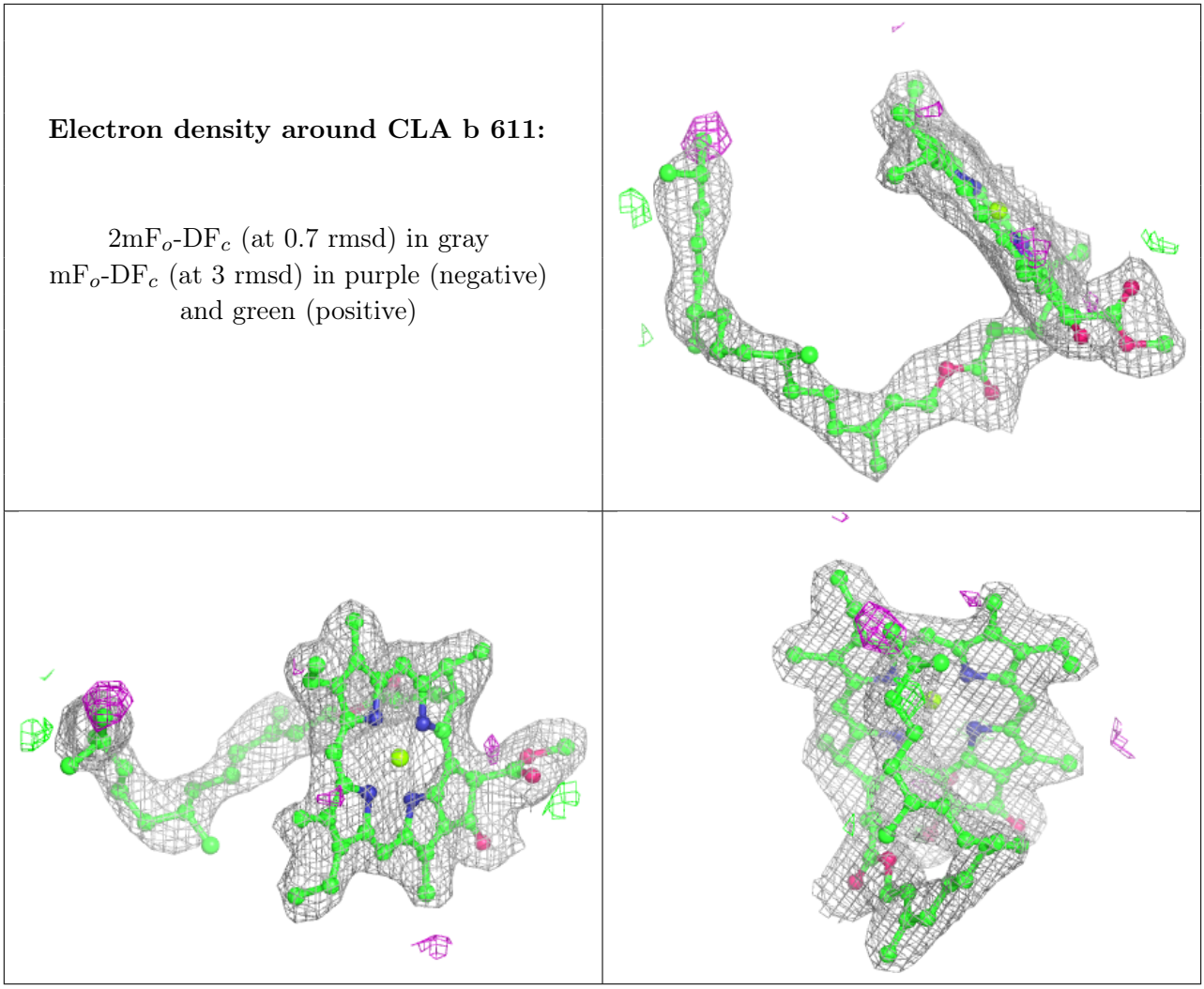
Electron density around DGD c 515:

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



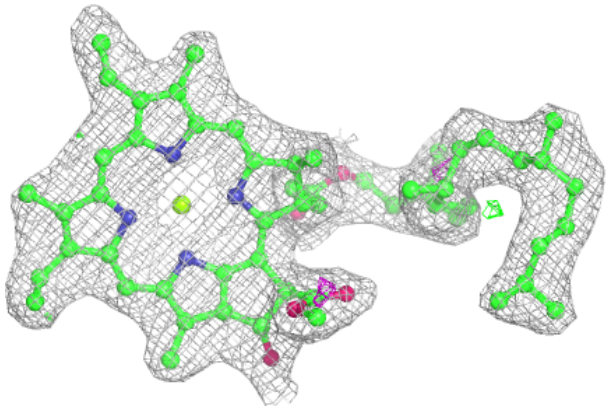
Electron density around CLA b 611:

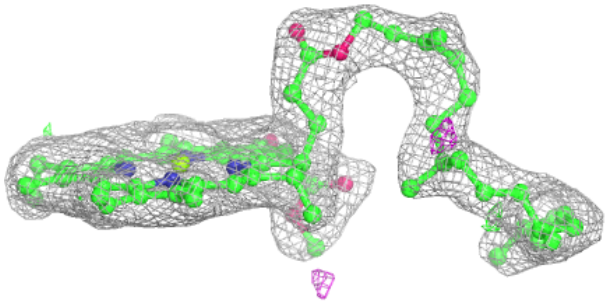
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

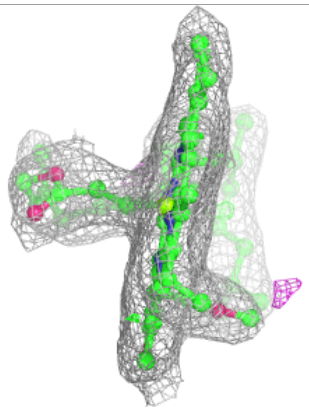


Electron density around CLA b 612:

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

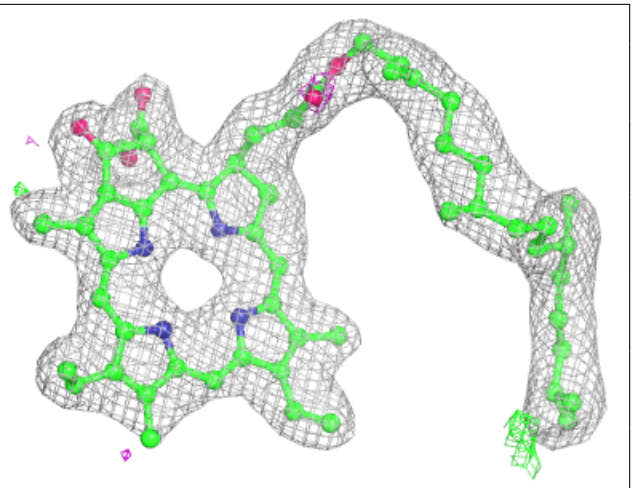


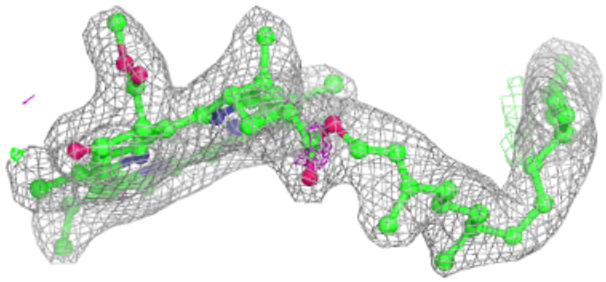


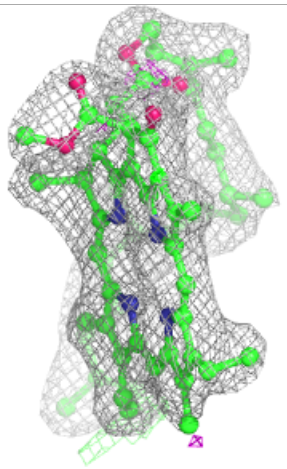


Electron density around PHO D 402:

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

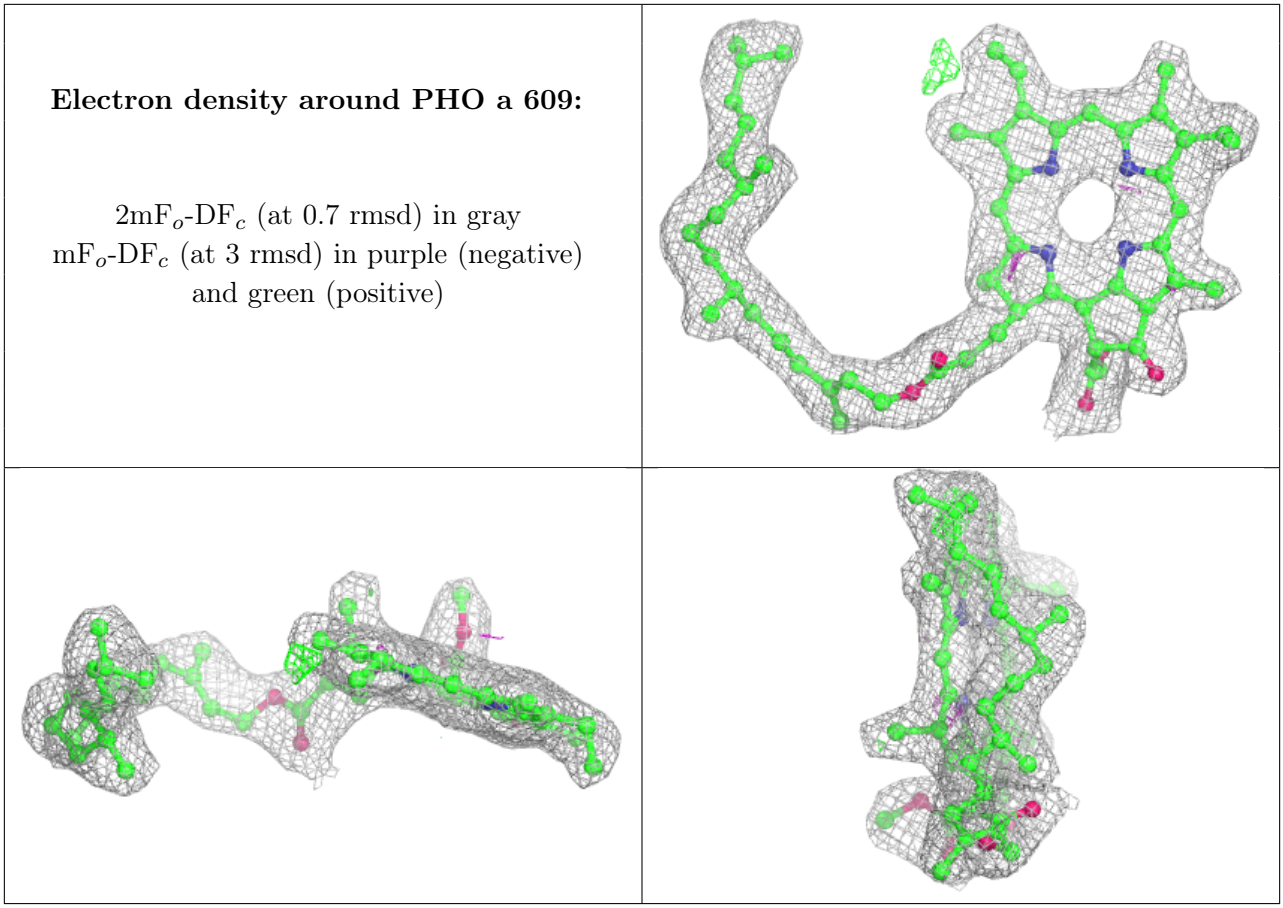






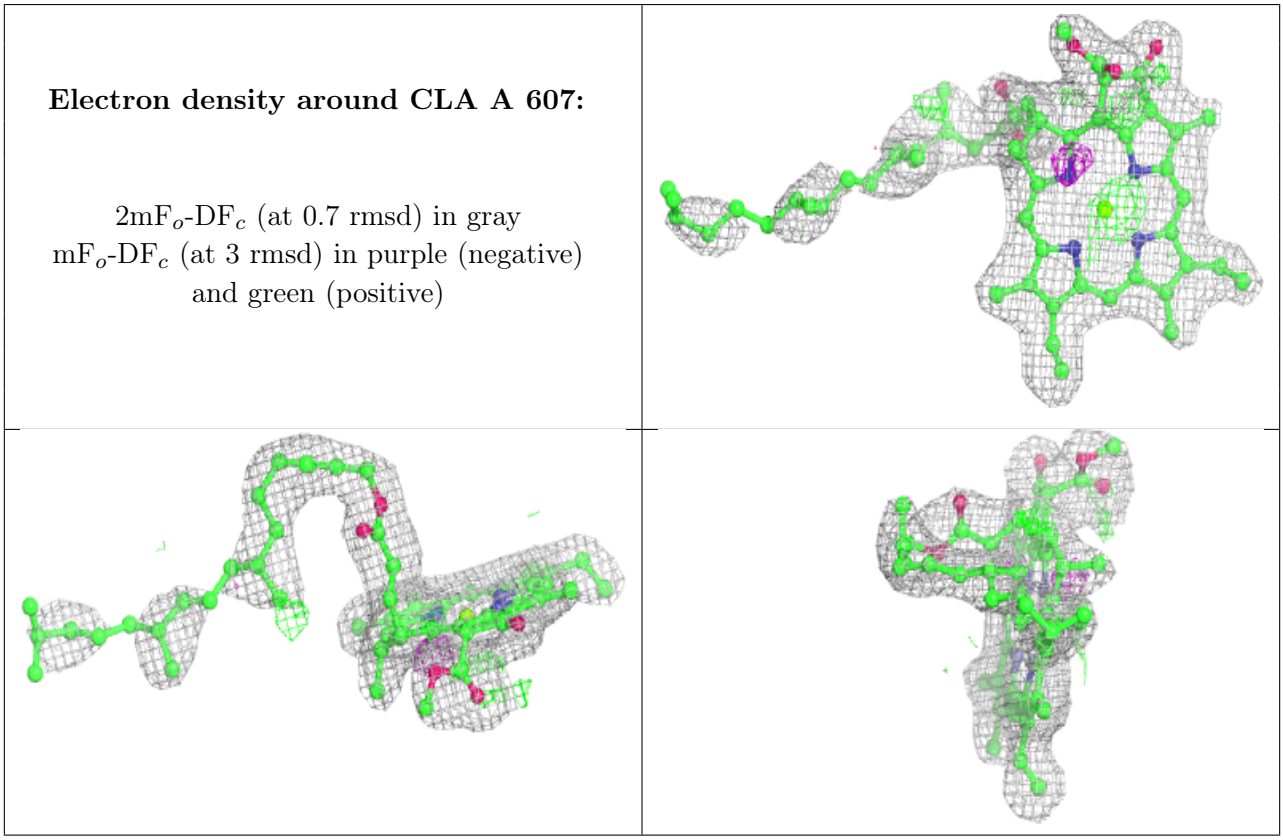
Electron density around PHO a 609:

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



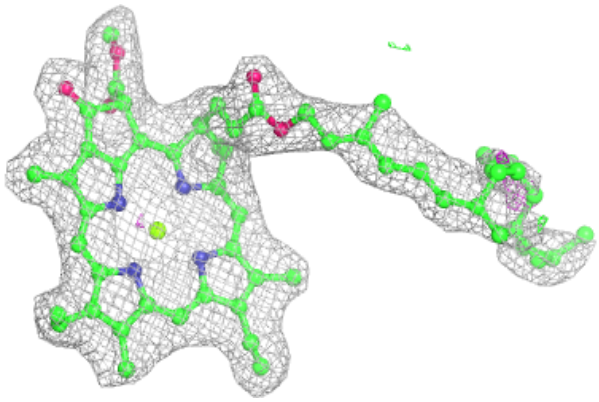
Electron density around CLA A 607:

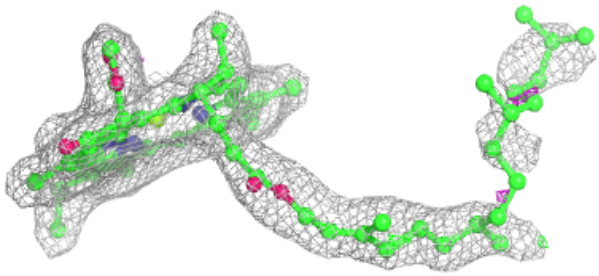
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

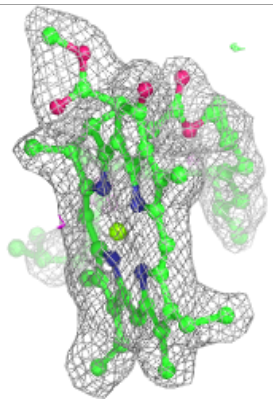


Electron density around CLA a 610:

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

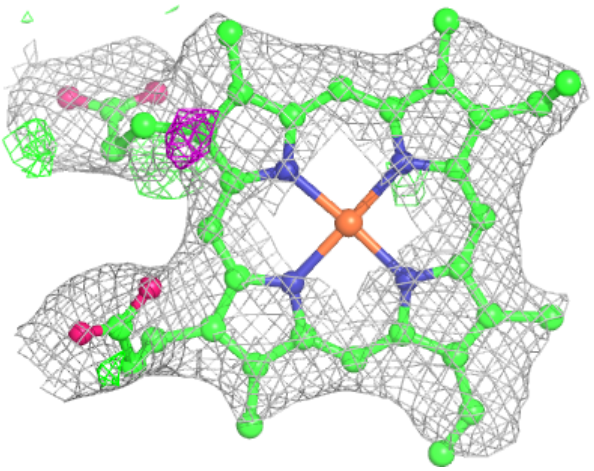


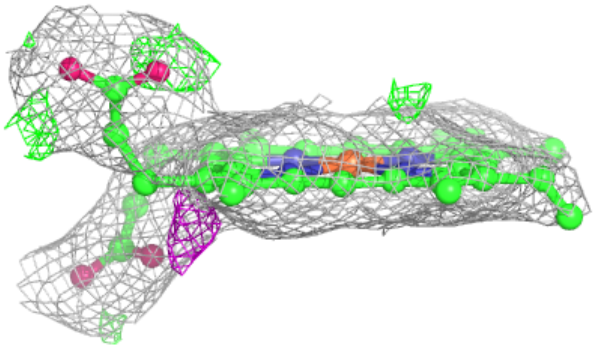


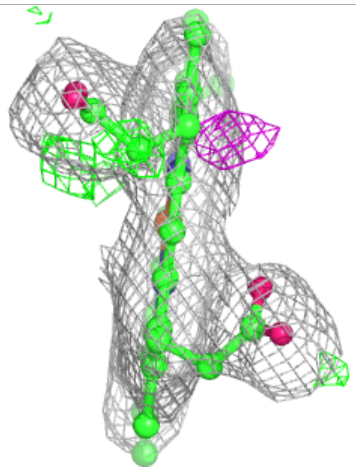


Electron density around HEM e 101:

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

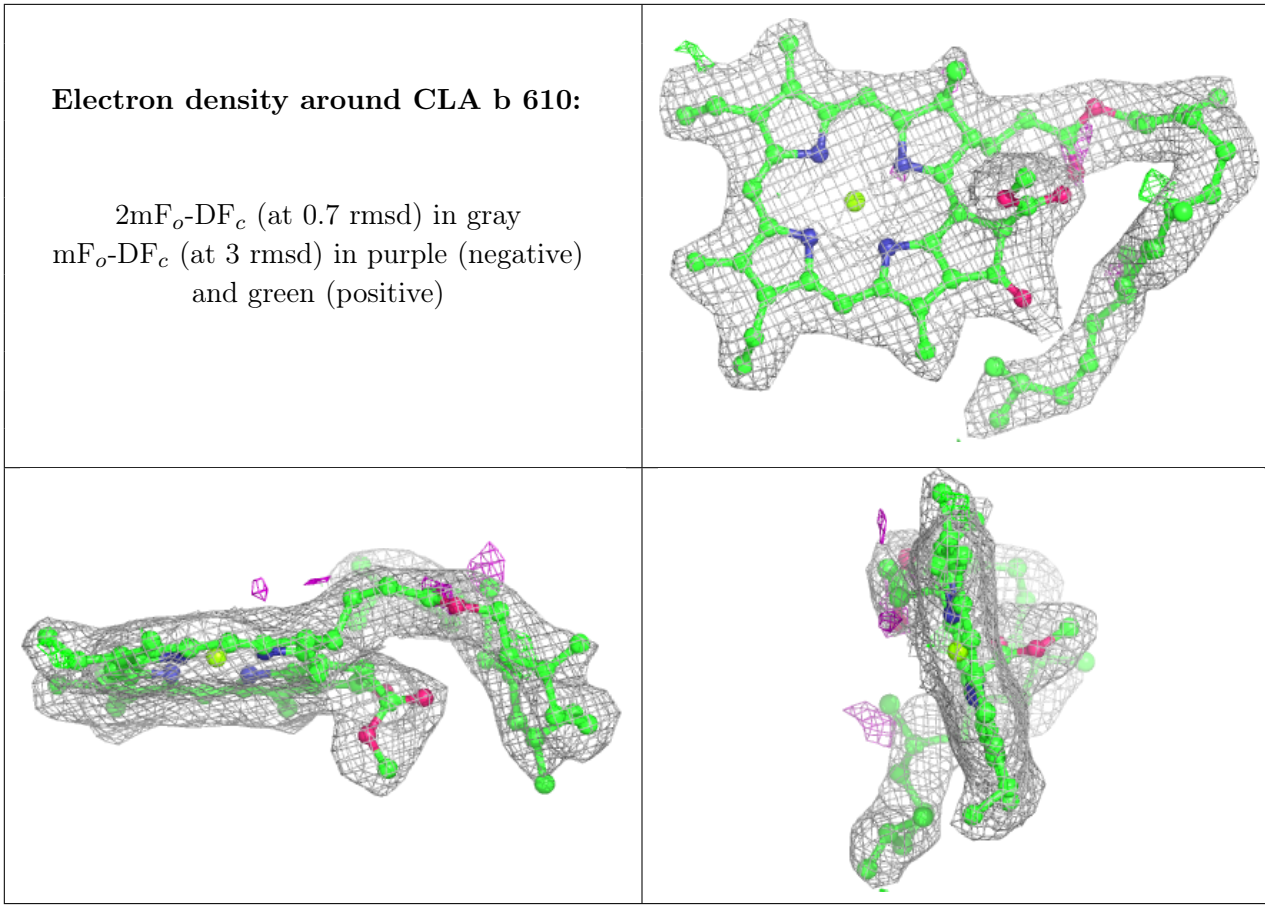






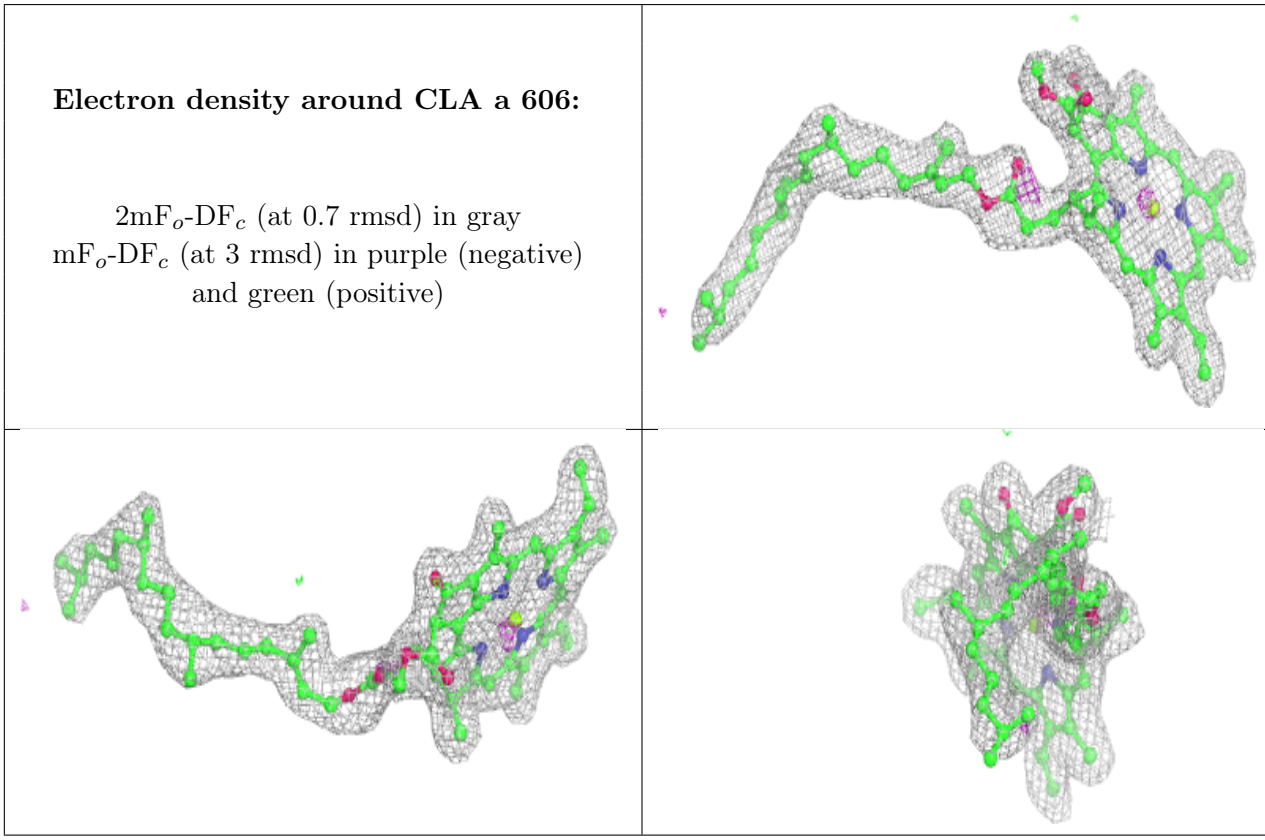
Electron density around CLA b 610:

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



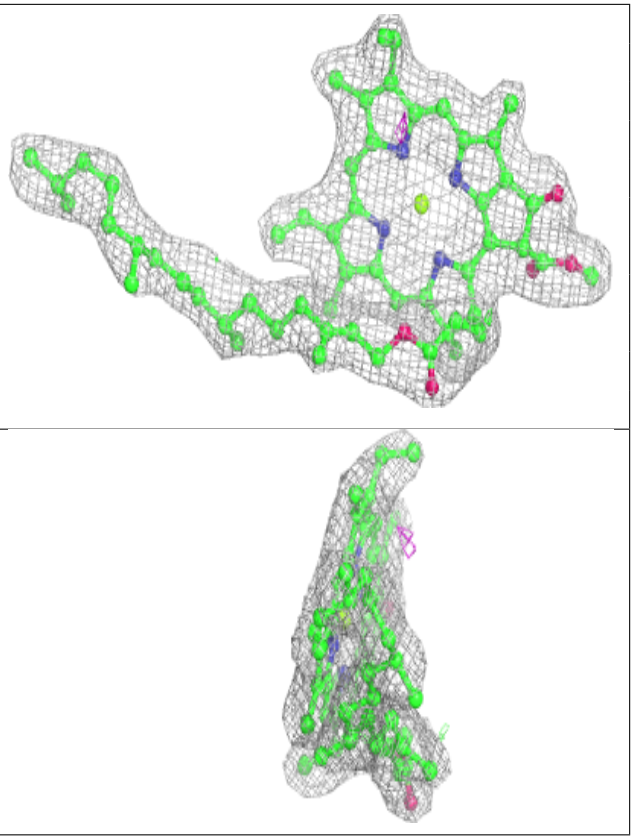
Electron density around CLA a 606:

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



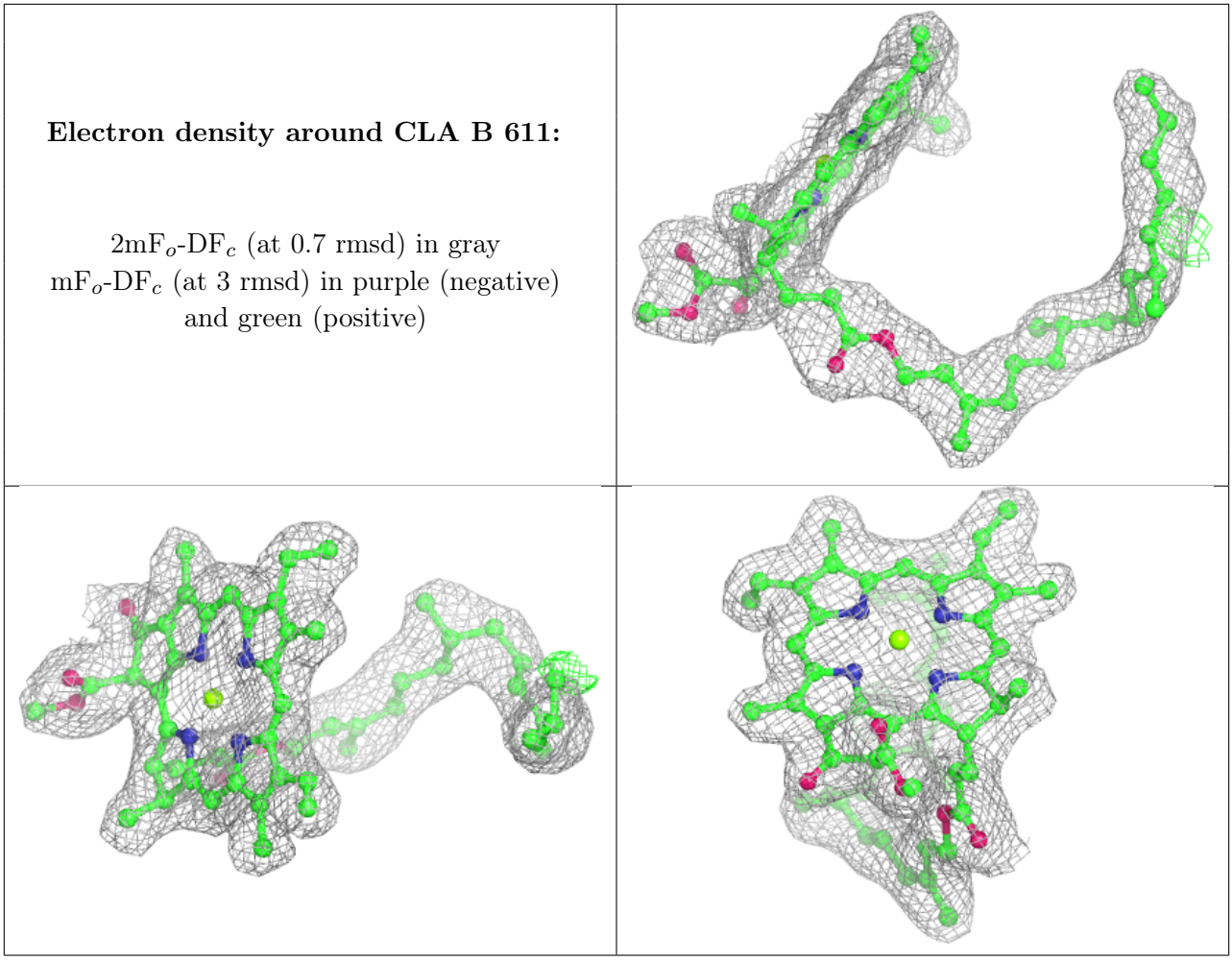
Electron density around CLA C 501:

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



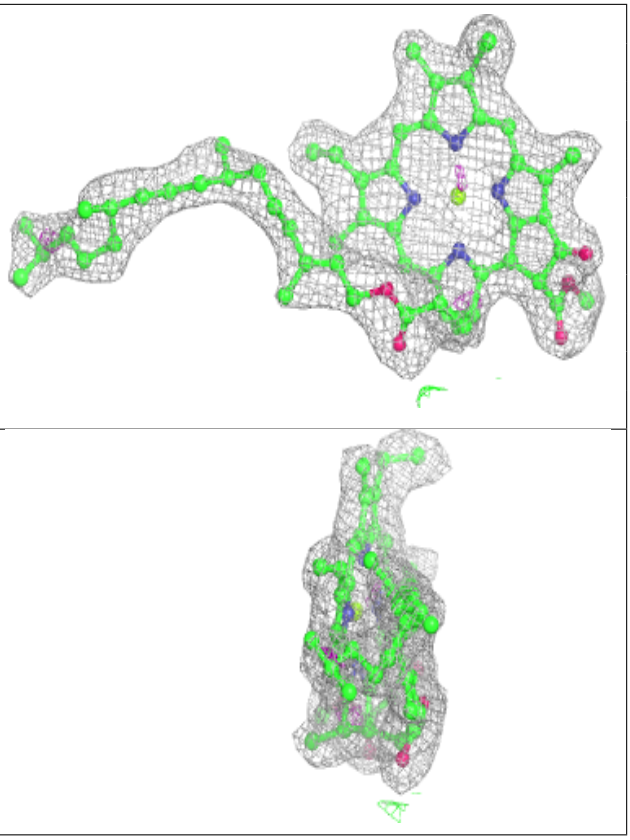
Electron density around CLA B 611:

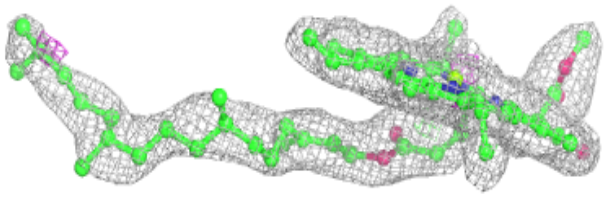
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 603:

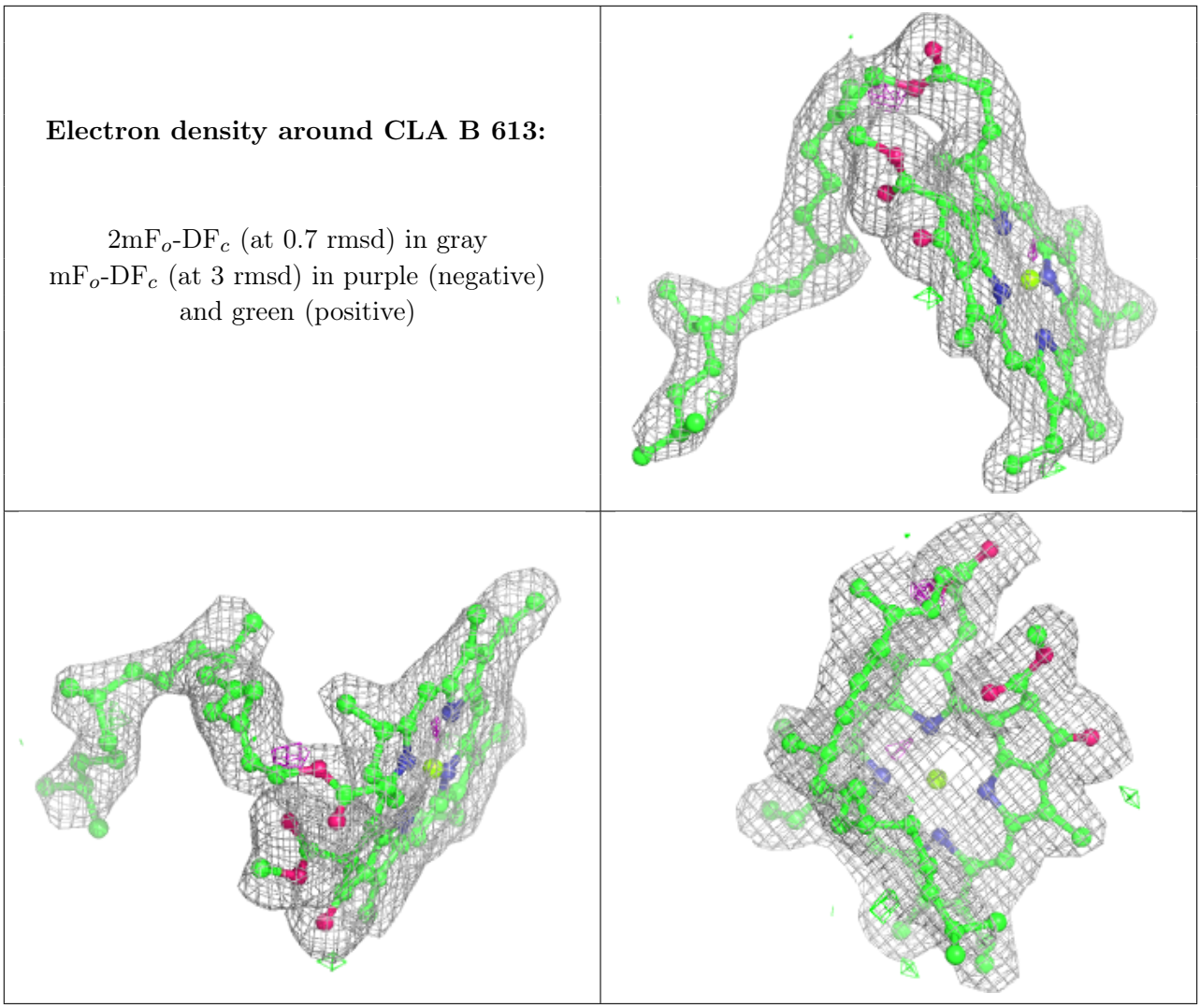
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





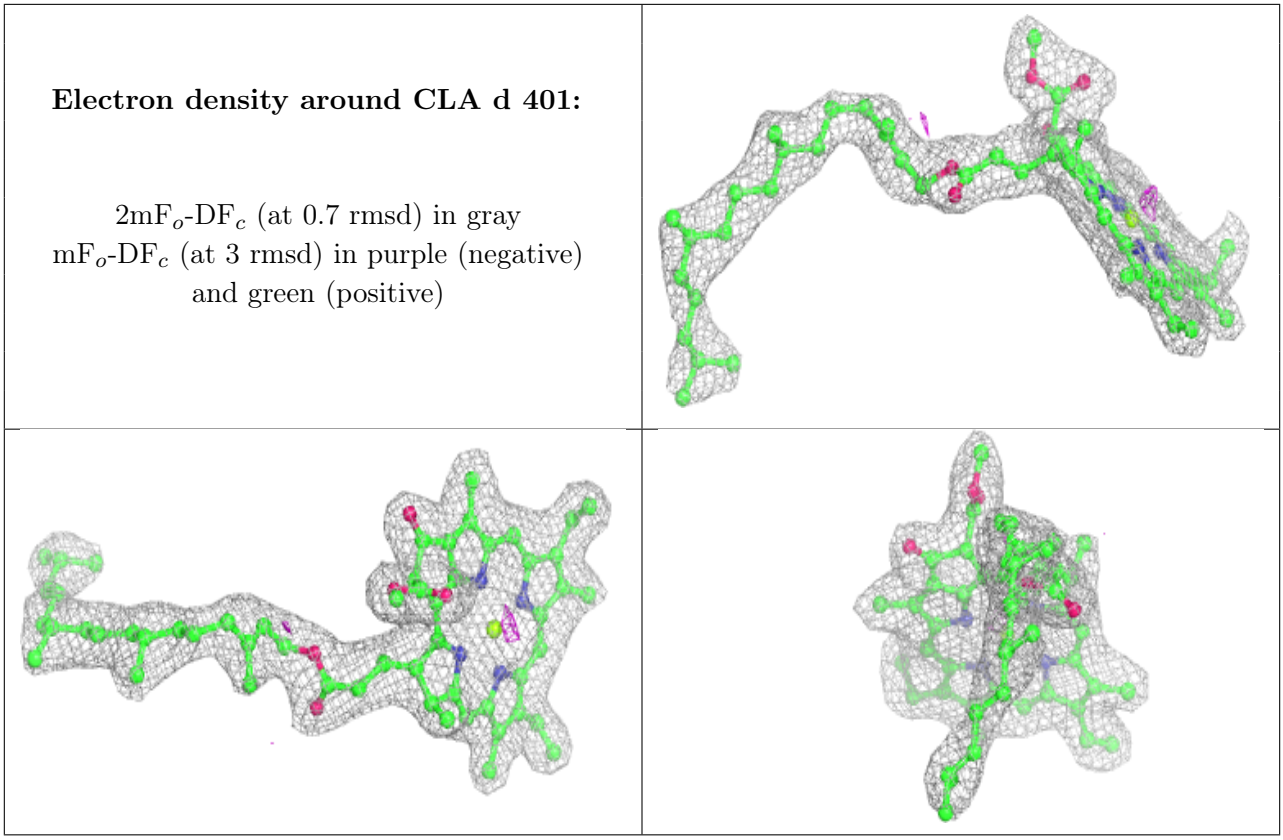
Electron density around CLA B 613:

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



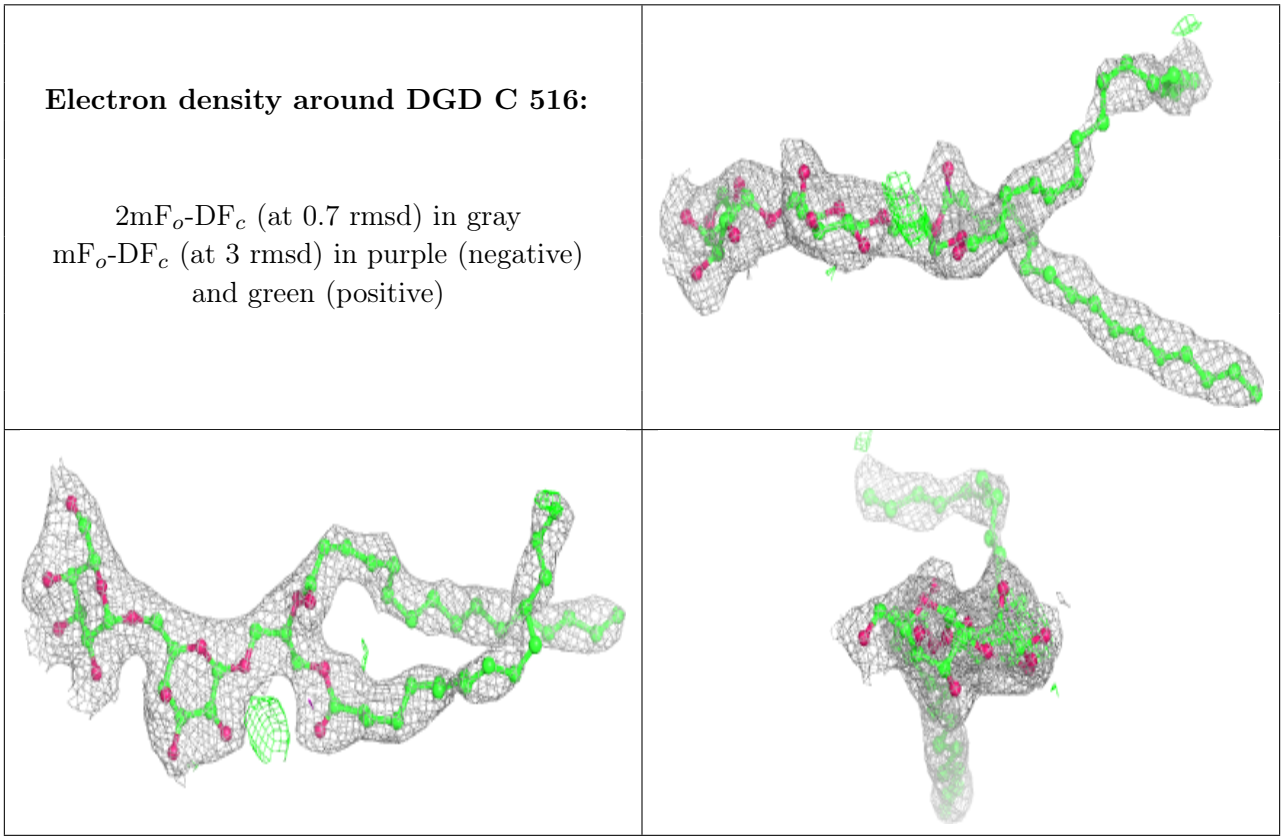
Electron density around CLA d 401:

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



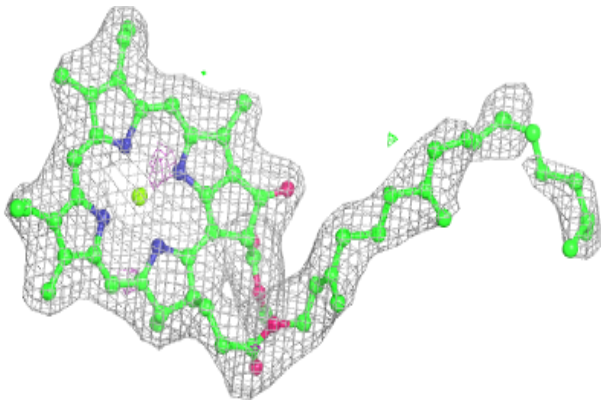
Electron density around DGD C 516:

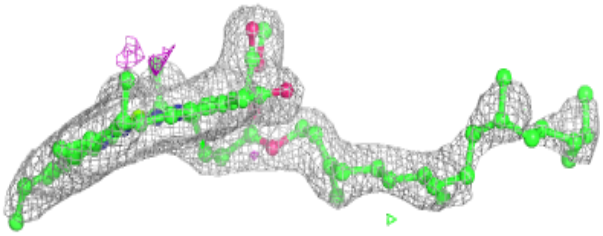
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

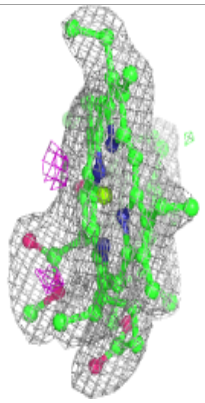


Electron density around CLA b 602:

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

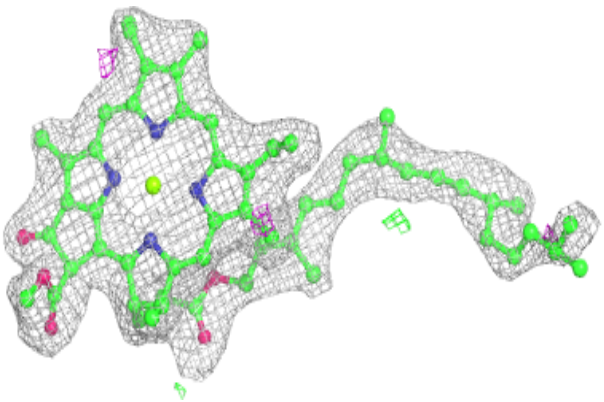


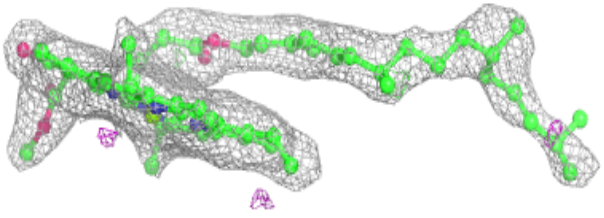


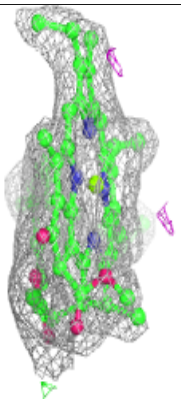


Electron density around CLA b 603:

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

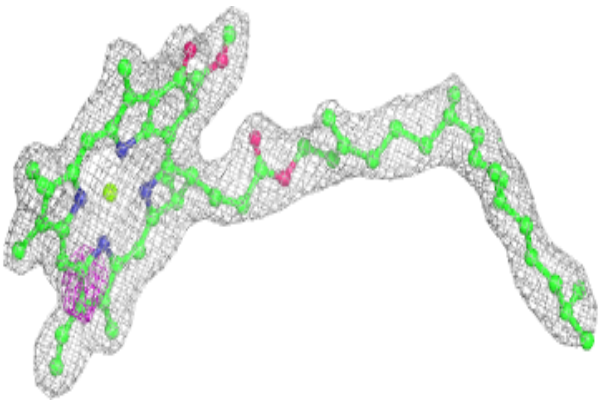


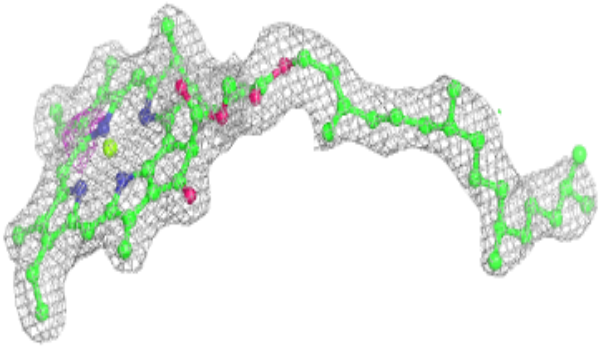


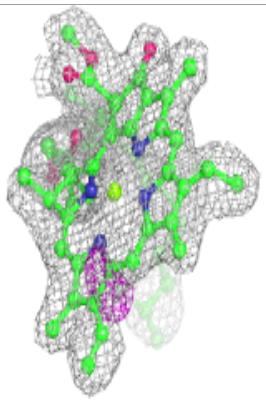


Electron density around CLA A 606:

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

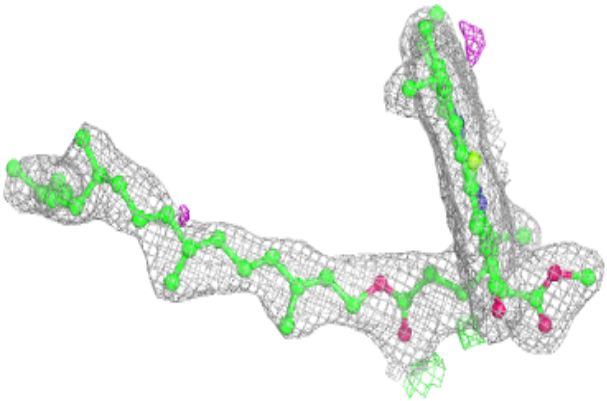


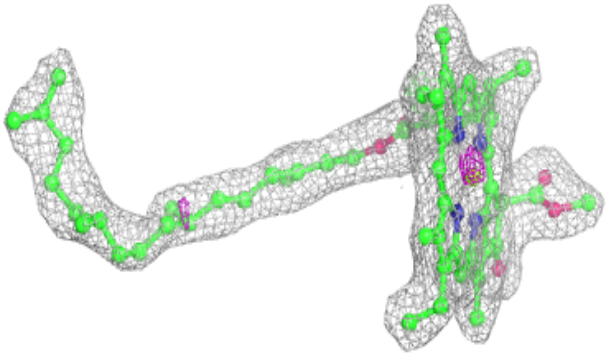


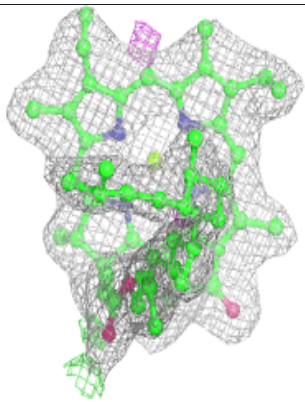


Electron density around CLA b 605:

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

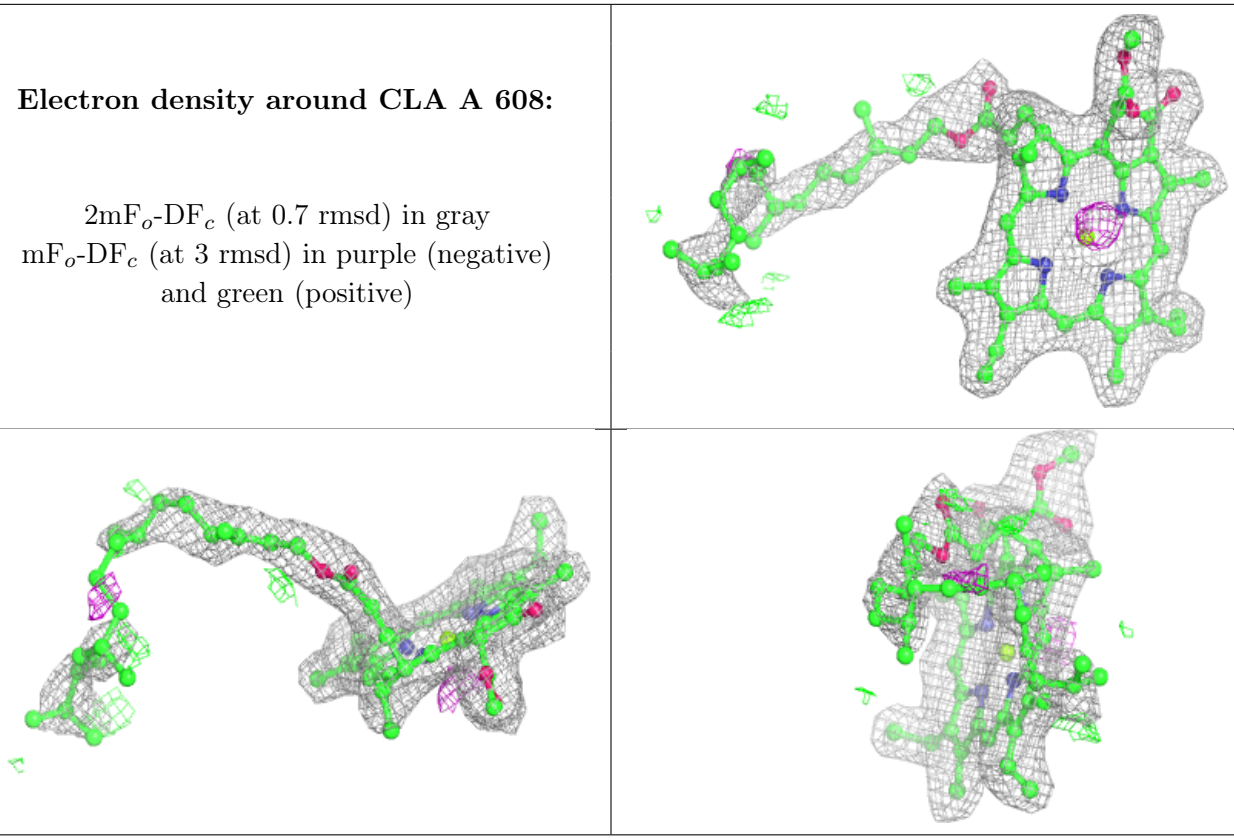






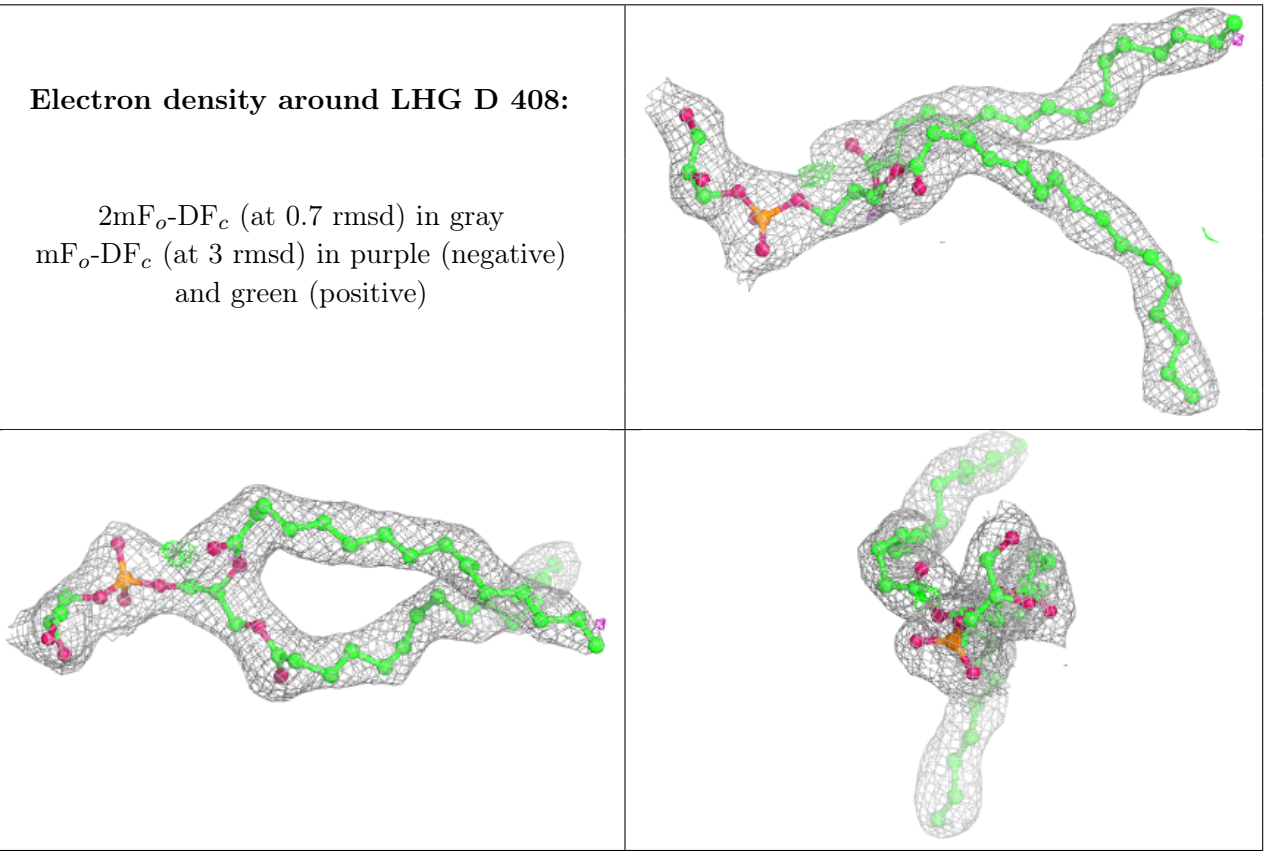
Electron density around CLA A 608:

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



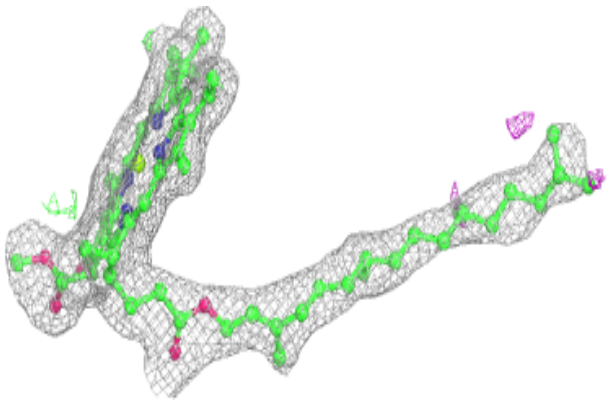
Electron density around LHG D 408:

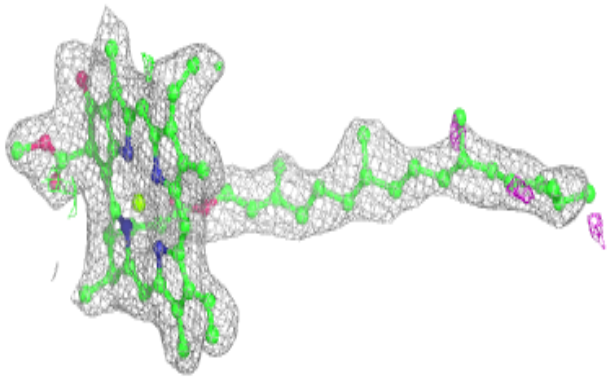
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

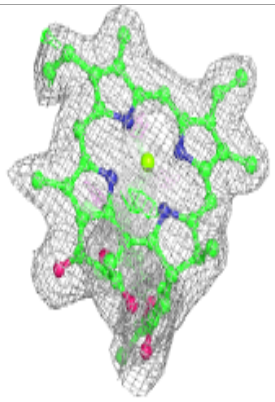


Electron density around CLA b 607:

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

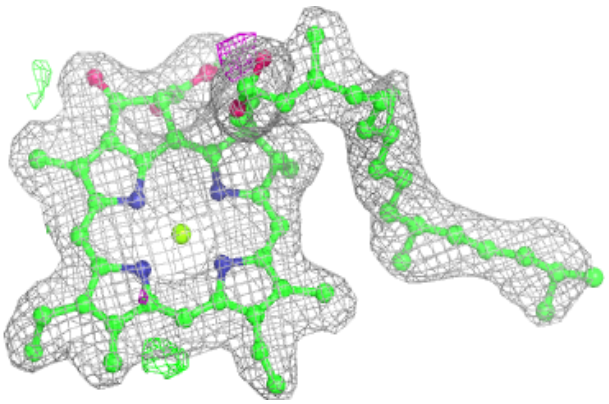


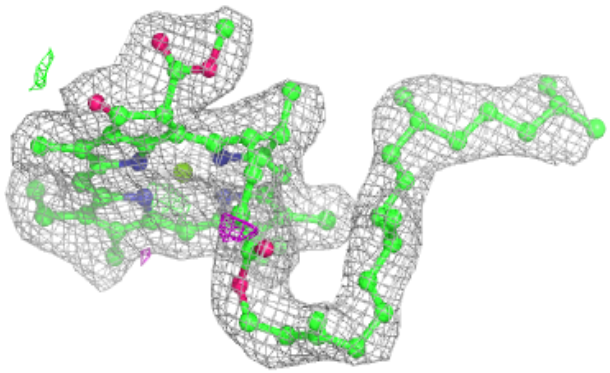


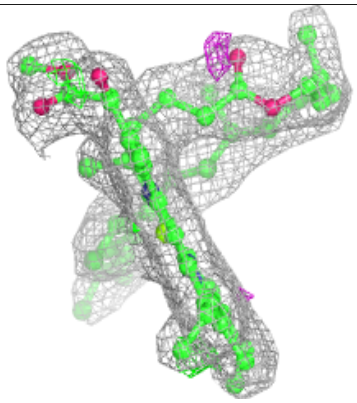


Electron density around CLA D 403:

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

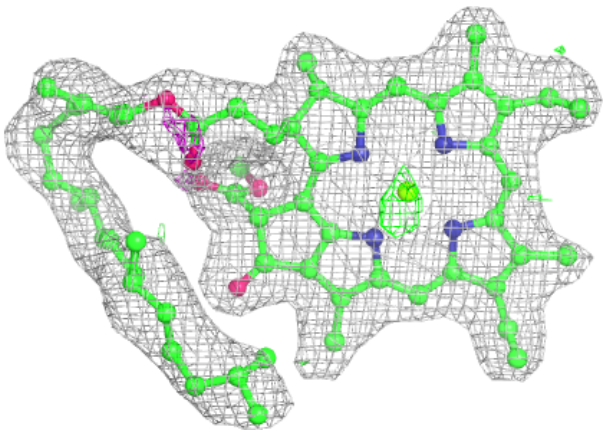


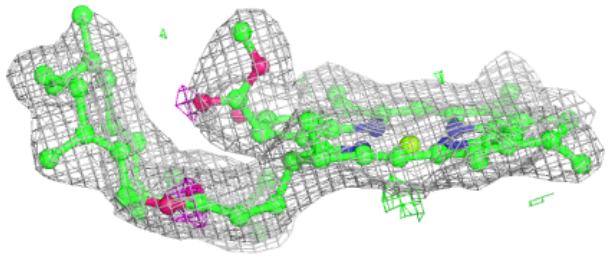


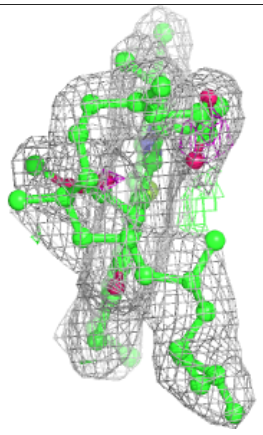


Electron density around CLA B 610:

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

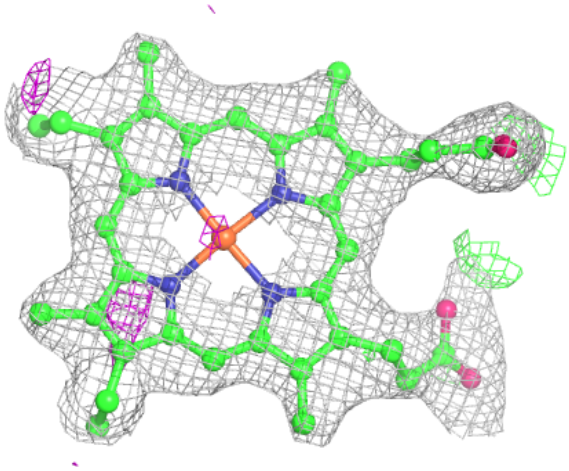


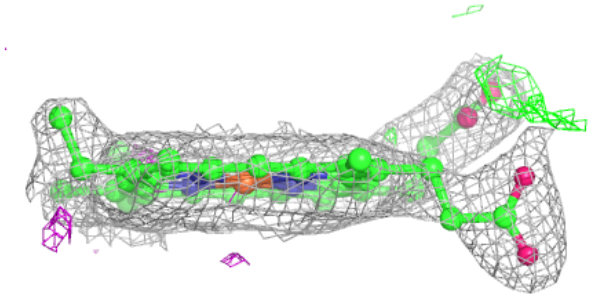


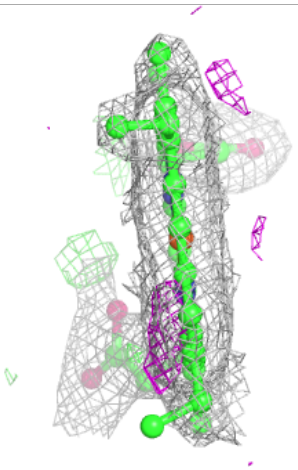


Electron density around HEC v 201:

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

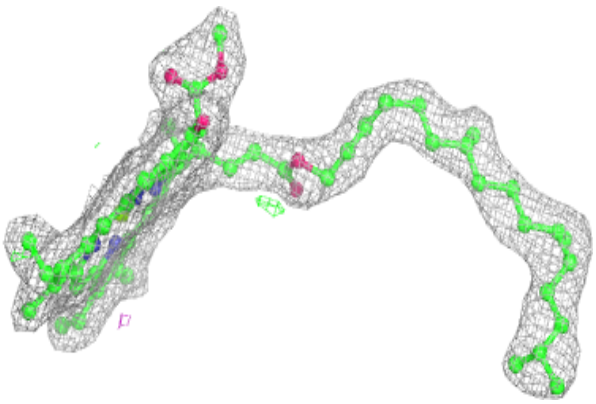


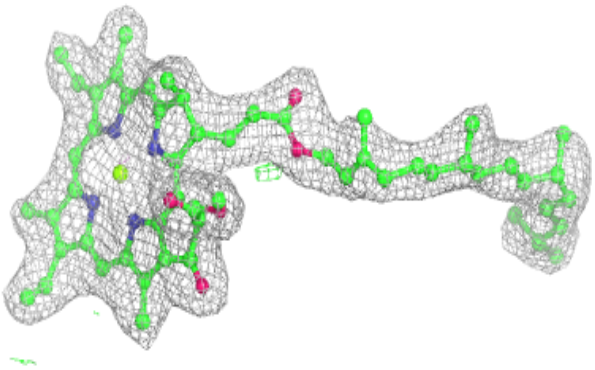


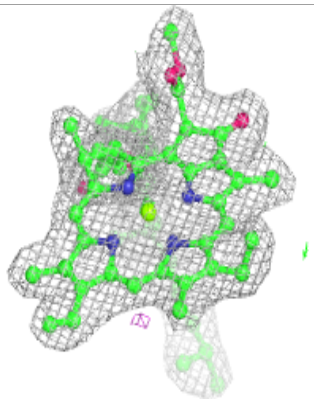


Electron density around CLA D 404:

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

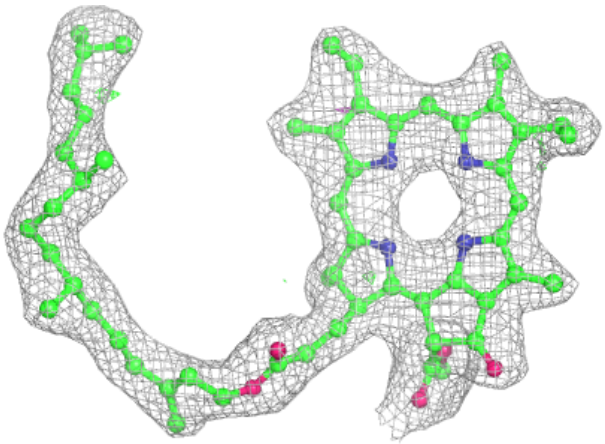


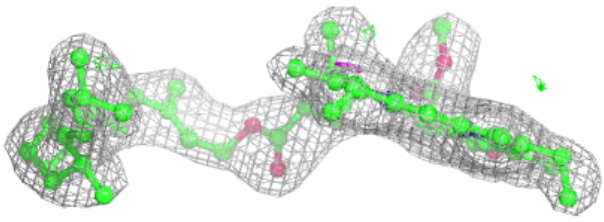


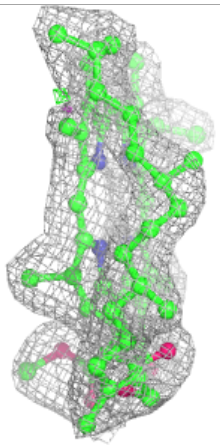


Electron density around PHO D 401:

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

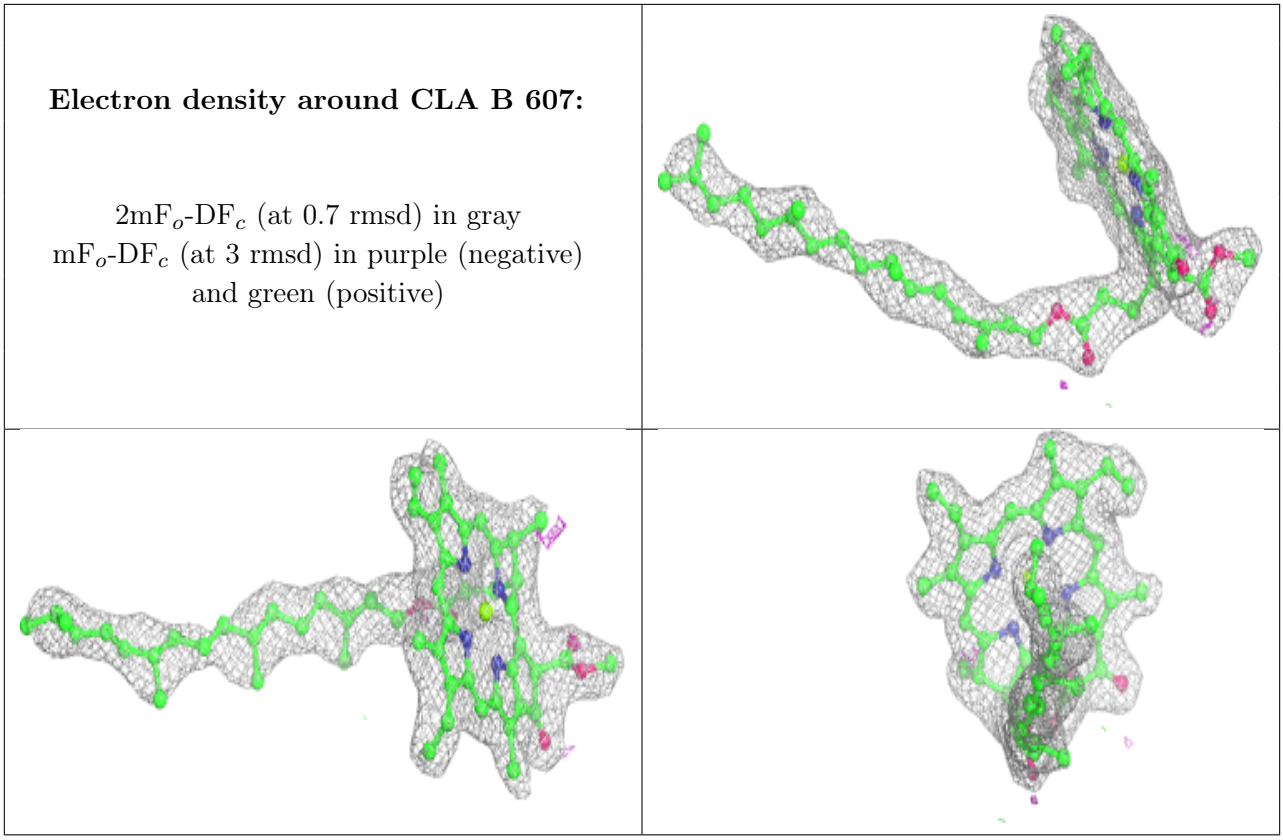






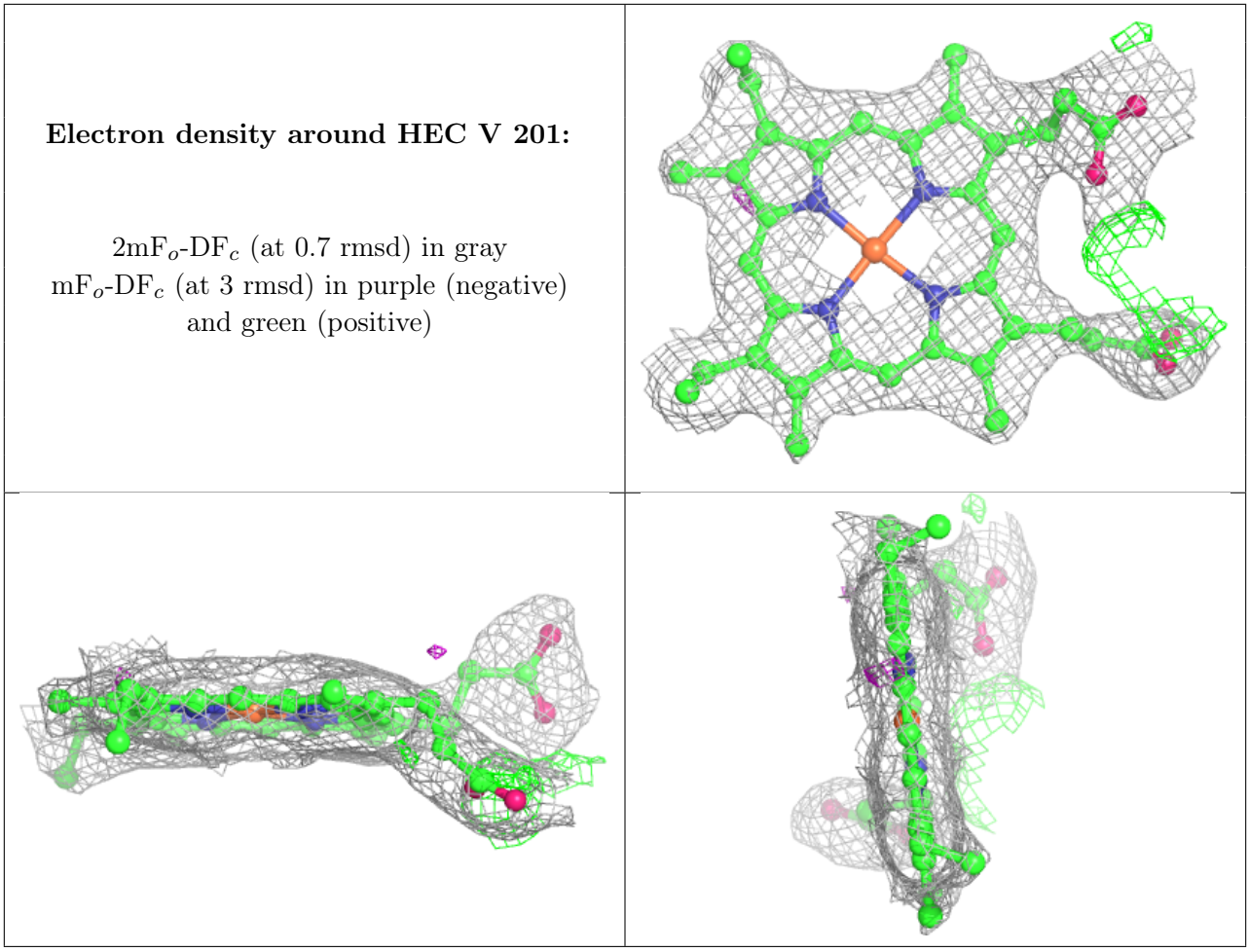
Electron density around CLA B 607:

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



Electron density around 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.