wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2024 – 11:20 AM JST

PDB ID	:	4UB6
Title	:	Native structure of photosystem II (dataset-1) by a femtosecond X-ray laser
Authors	:	Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on	:	2014-08-12
Resolution	:	1.95 Å(reported)

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

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

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

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

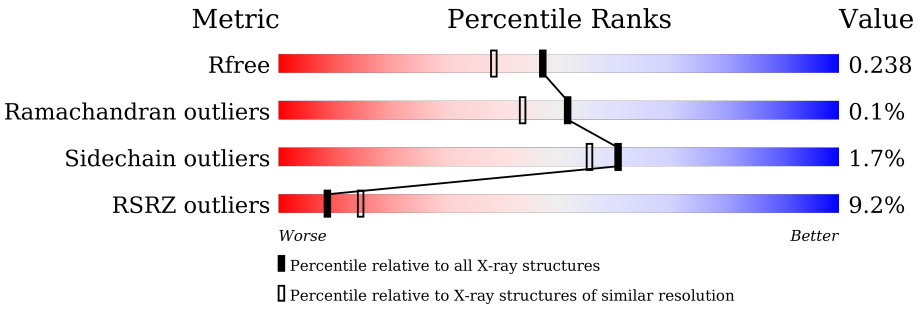
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	6% 97%
1	a	344	10% 96%
2	B	505	5% 98%
2	b	505	7% 98%
3	C	455	4% 98%
3	c	455	6% 99%
4	D	342	9% 99%

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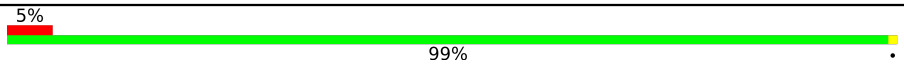
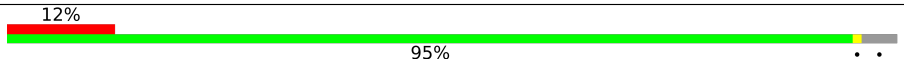
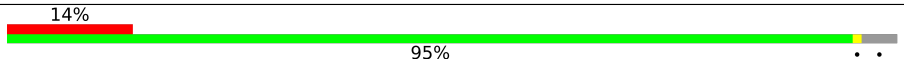
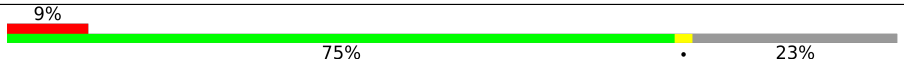
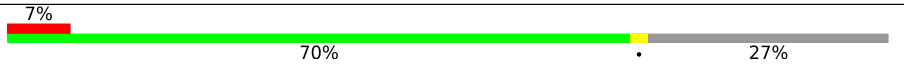
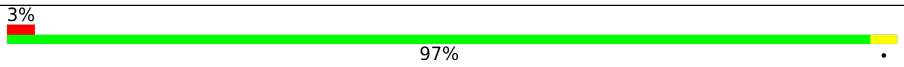
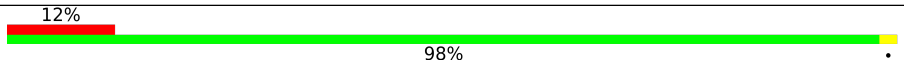
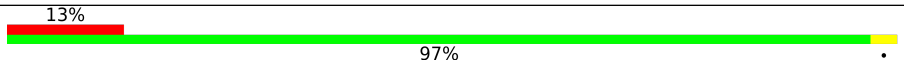
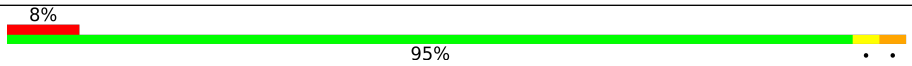
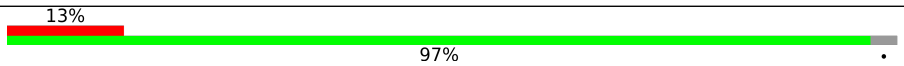
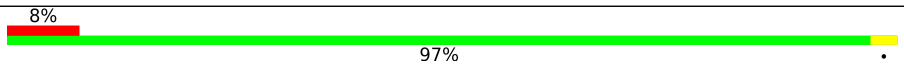
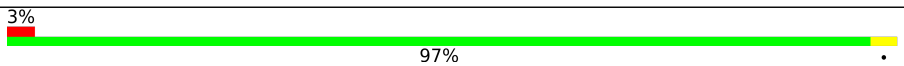
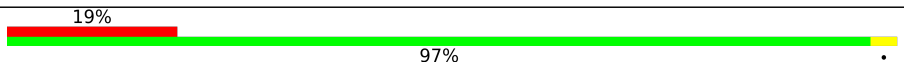
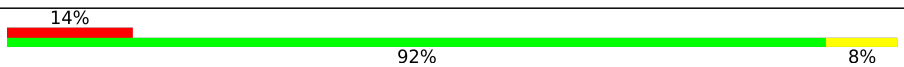
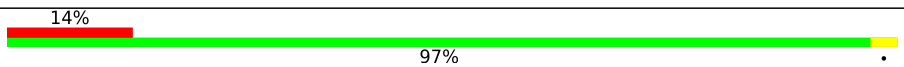
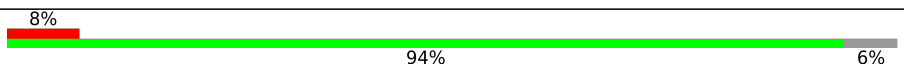
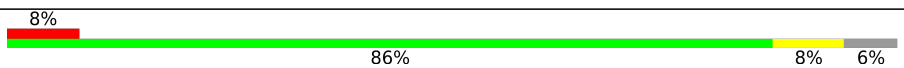
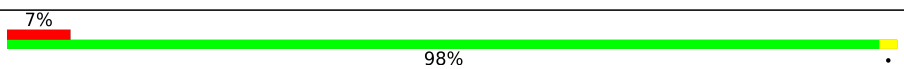
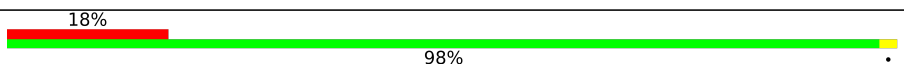
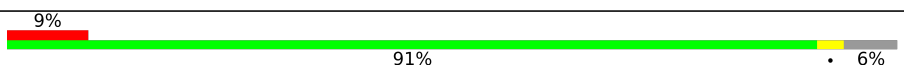
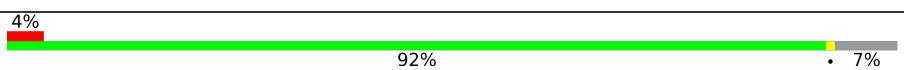
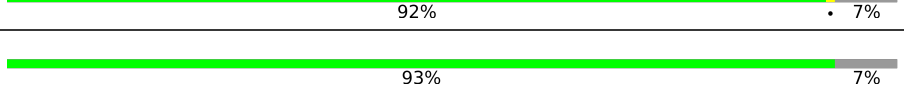
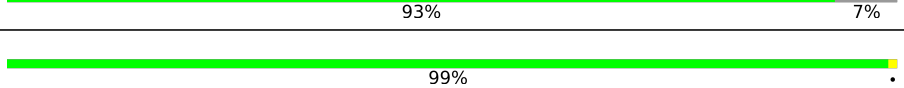
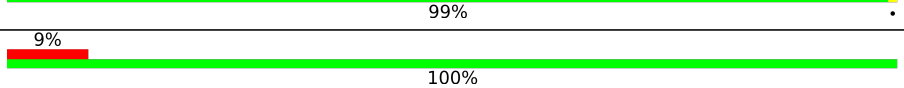
Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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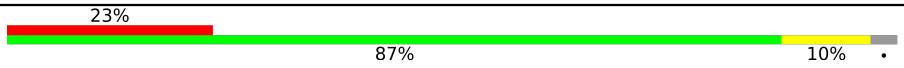
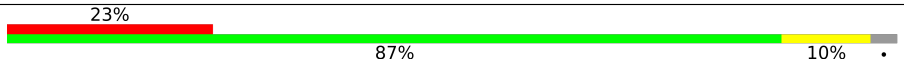
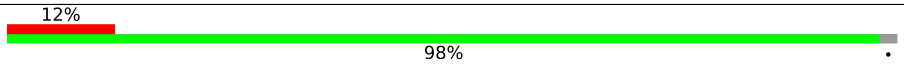
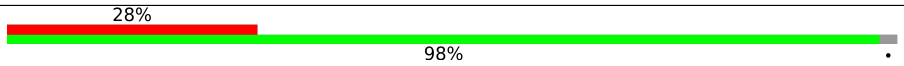
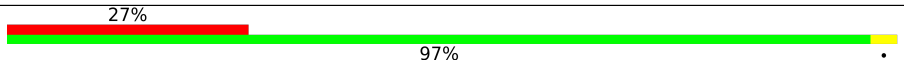
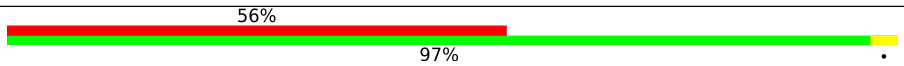
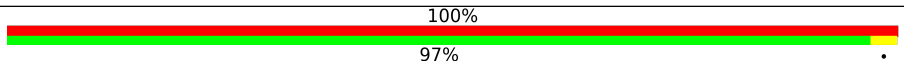
Mol	Chain	Length	Quality of chain
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
28	GOL	V	203	-	-	-	X
36	DGD	d	406	-	-	-	X

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 54195 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	11	0
			4027	2643	668	703	13			
2	b	504	Total	C	N	O	S	0	12	0
			4033	2650	668	702	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 668	C 436	N 107	O 125	0	2	0
5	e	81	Total 670	C 439	N 107	O 124	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	32	Total 257	C 175	N 43	O 38	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	65	Total 519	C 346	N 85	O 86	S 2	0	1	0
7	h	65	Total 511	C 341	N 82	O 86	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	38	Total 314	C 211	N 48	O 54	S 1	0	0	0
8	i	38	Total 314	C 211	N 48	O 54	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	38	Total 272	C 182	N 42	O 47	S 1	0	0	0
9	j	39	Total 280	C 187	N 43	O 48	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 204	N 43	O 46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total 293	C 204	N 43	O 46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 309	C 207	N 48	O 53	S 1	0	1	0
11	l	37	Total 309	C 207	N 48	O 53	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 274	C 184	N 40	O 49	S 1	0	1	0
12	m	34	Total 269	C 179	N 40	O 49	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	243	Total 1903	C 1191	N 315	O 392	S 5	0	8	0
13	o	243	Total 1891	C 1183	N 315	O 388	S 5	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total 264	C 185	N 36	O 41	S 2	0	1	0
14	t	30	Total 264	C 185	N 36	O 41	S 2	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total 774	C 491	N 129	O 154	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	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 protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

- 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			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		

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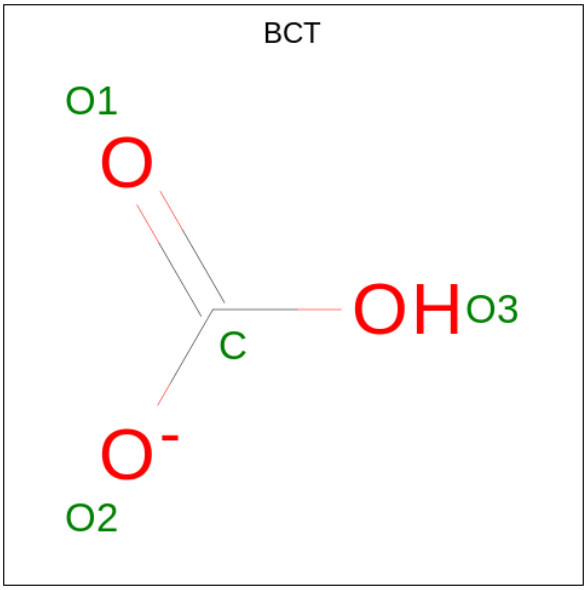
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

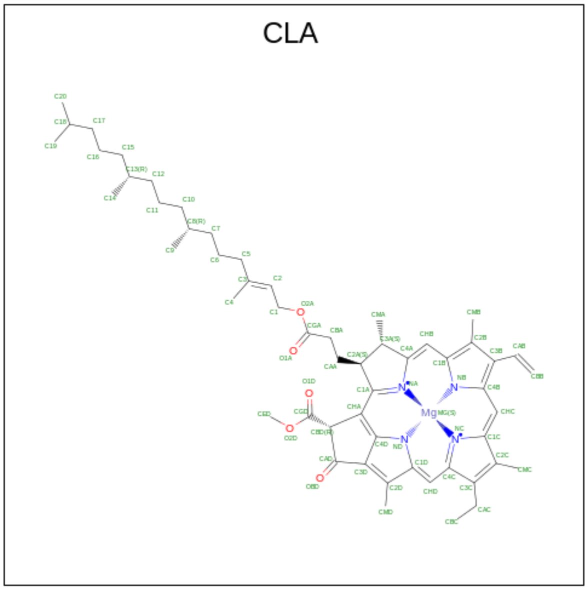
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	U	1	Total Cl 1 1	0	0
22	a	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0

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



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

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



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

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

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

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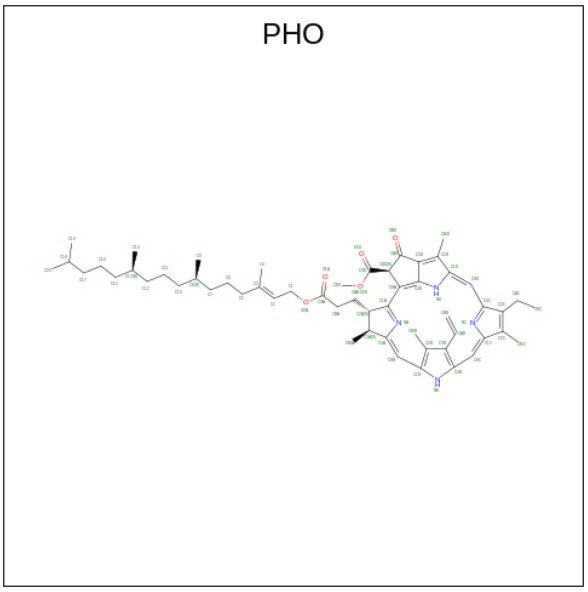
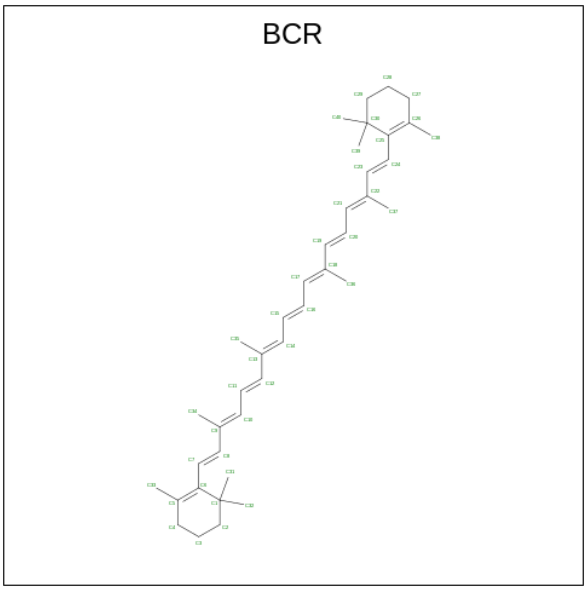
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

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



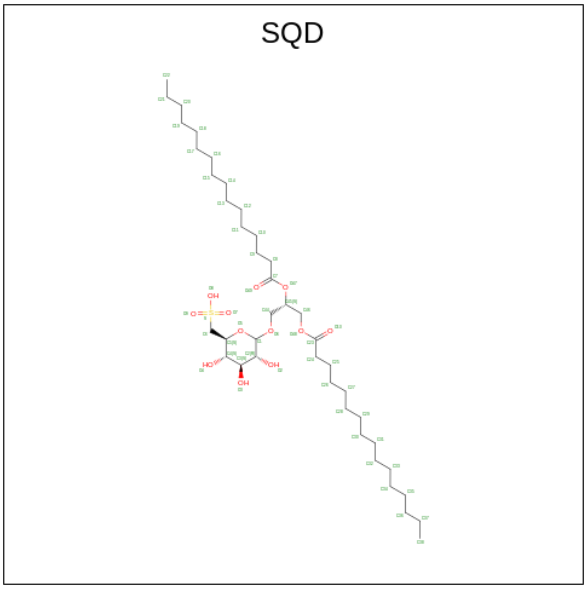
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



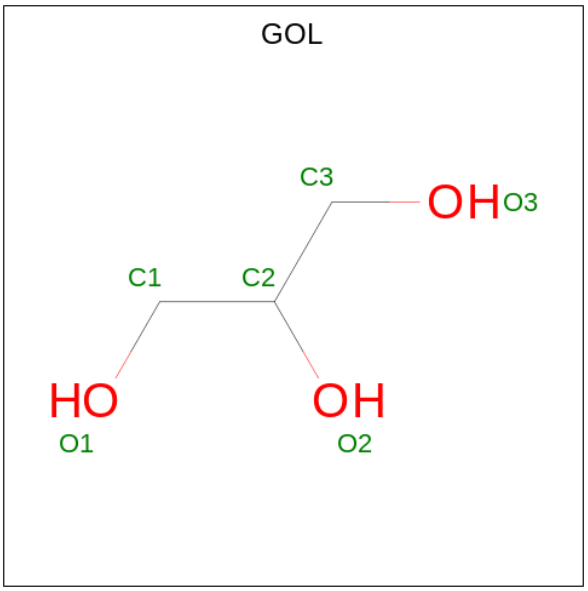
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total 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
26	b	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	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 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
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	f	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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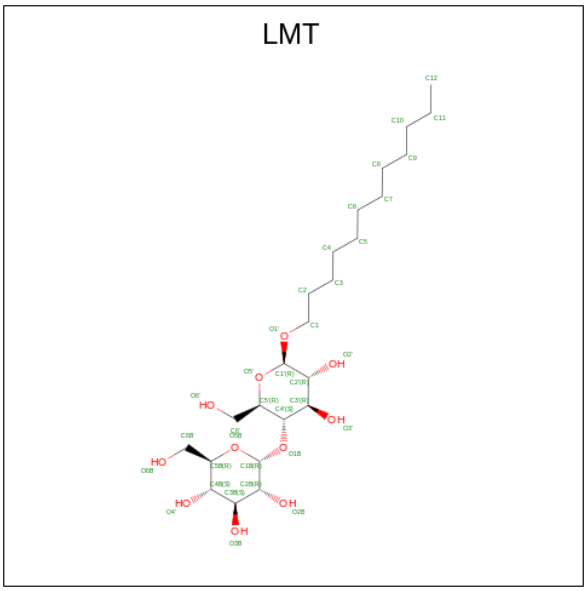
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 25 19 6	0	0
29	C	1	Total C O 35 24 11	0	0
29	E	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	b	1	Total C O 25 19 6	0	0
29	b	1	Total C O 25 19 6	0	0

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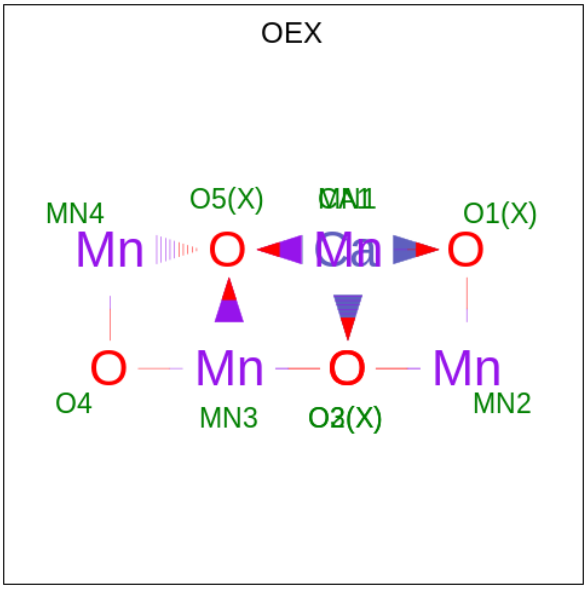
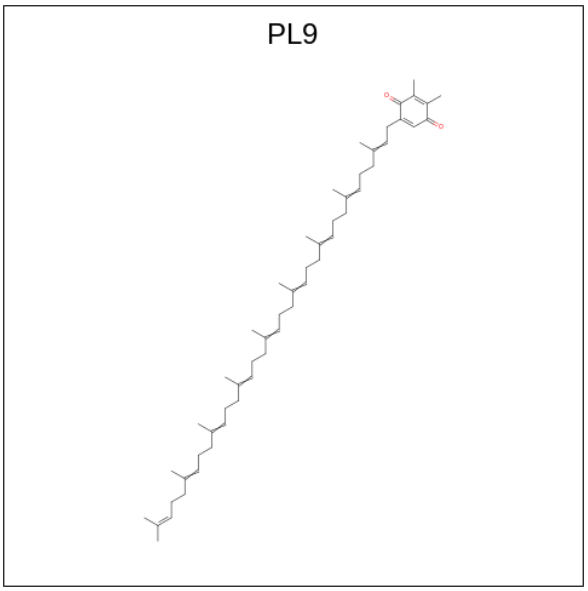
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 35 24 11	0	0
29	f	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 31 is 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
31	A	1	Total C O 55 53 2	0	0
31	D	1	Total C O 55 53 2	0	0
31	a	1	Total C O 55 53 2	0	0
31	d	1	Total C O 55 53 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	I	1	Total C O 40 35 5	0	0
32	J	1	Total C 10 10	0	0
32	K	1	Total C O 34 29 5	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0

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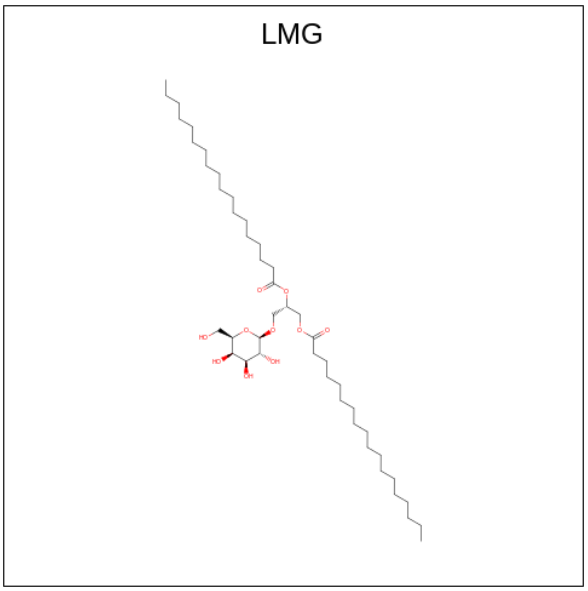
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

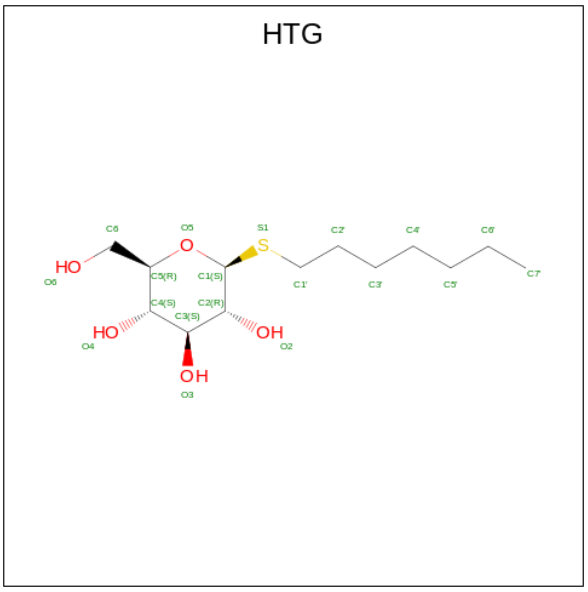
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	J	1	Total C O 51 41 10	0	0
34	Z	1	Total C O 37 27 10	0	0
34	a	1	Total C O 51 41 10	0	0
34	b	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	j	1	Total C O 51 41 10	0	0
34	z	1	Total C O 39 29 10	0	0

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

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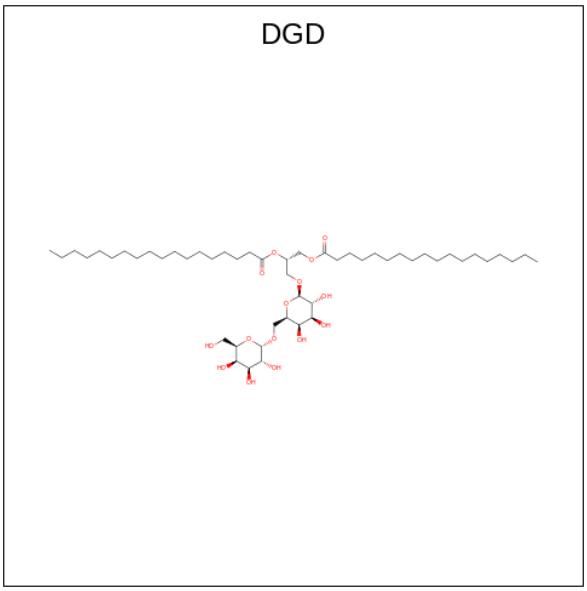
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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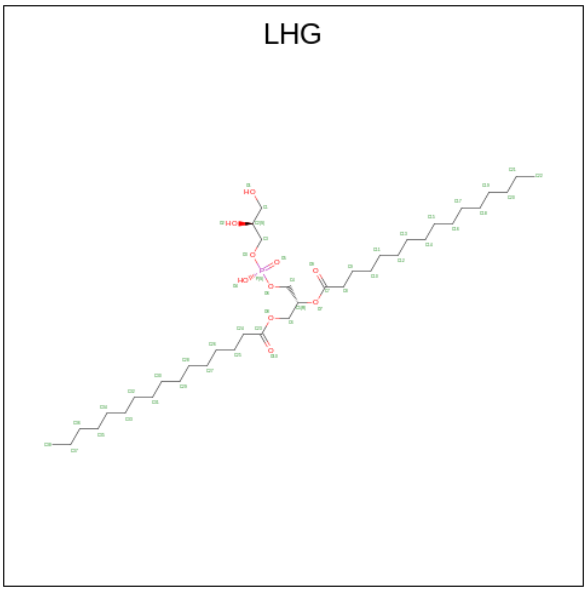
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	e	1	Total C O P 42 31 10 1	0	0

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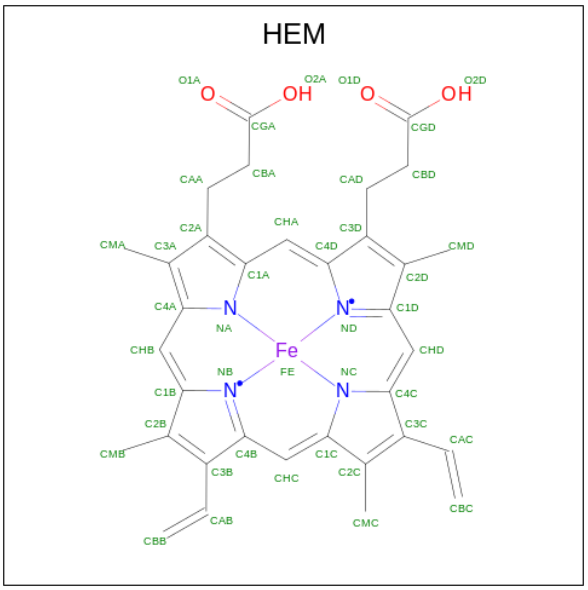
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

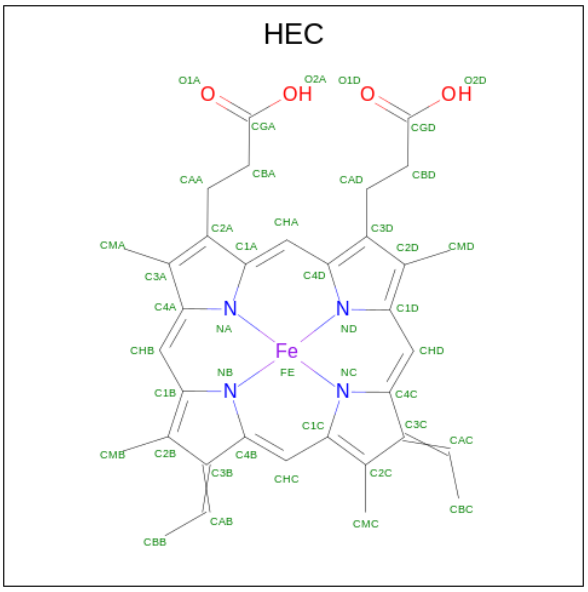


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	165	Total	O	0	2
			167	167		
41	B	289	Total	O	0	4
			293	293		
41	C	233	Total	O	0	2
			235	235		
41	D	138	Total	O	0	5
			143	143		
41	E	31	Total	O	0	0
			31	31		
41	F	9	Total	O	0	0
			9	9		
41	H	48	Total	O	0	1
			49	49		
41	I	4	Total	O	0	0
			4	4		
41	J	13	Total	O	0	0
			13	13		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	16	Total O 17 17	0	1
41	M	8	Total O 8 8	0	0
41	O	188	Total O 191 191	0	3
41	T	16	Total O 17 17	0	1
41	U	81	Total O 81 81	0	0
41	V	116	Total O 118 118	0	2
41	Y	4	Total O 4 4	0	0
41	X	9	Total O 9 9	0	0
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 154 154	0	1
41	b	261	Total O 264 264	0	3
41	c	197	Total O 199 199	0	2
41	d	132	Total O 137 137	0	5
41	e	17	Total O 17 17	0	0
41	f	5	Total O 5 5	0	0
41	h	41	Total O 41 41	0	0
41	i	6	Total O 6 6	0	0
41	j	7	Total O 7 7	0	0
41	k	6	Total O 6 6	0	0
41	l	10	Total O 10 10	0	0
41	m	18	Total O 18 18	0	0

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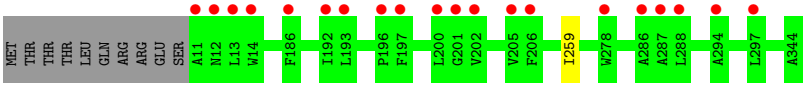
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	154	Total O 155 155	0	1
41	t	12	Total O 12 12	0	0
41	u	97	Total O 97 97	0	0
41	v	89	Total O 90 90	0	1
41	y	4	Total O 4 4	0	0
41	x	4	Total O 4 4	0	0

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.

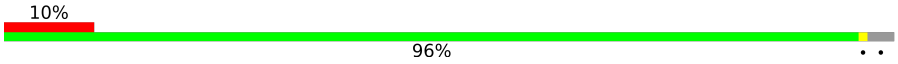
• Molecule 1: Photosystem Q(B) protein

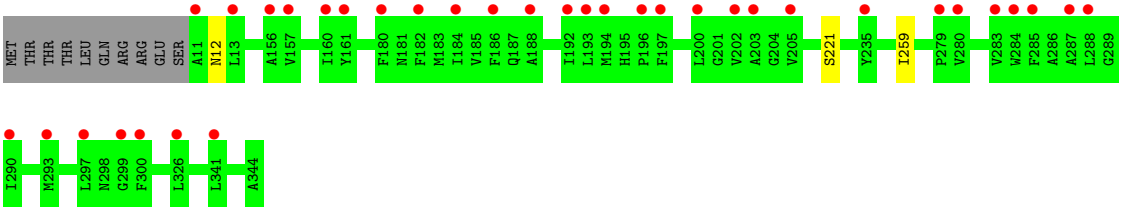
Chain A:



• Molecule 1: Photosystem Q(B) protein

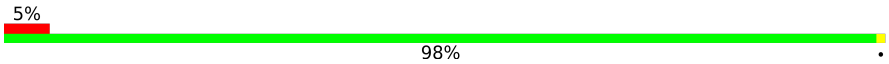
Chain a:

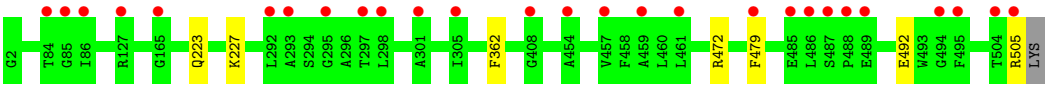




• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

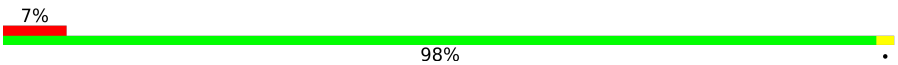
Chain B:

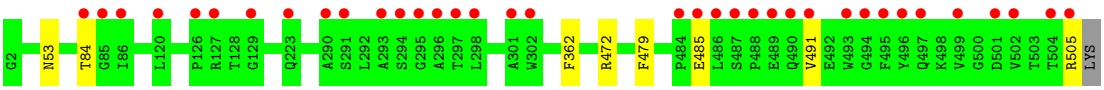




• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

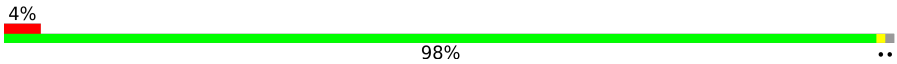
Chain b:

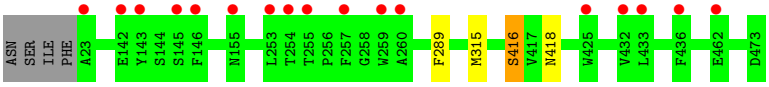




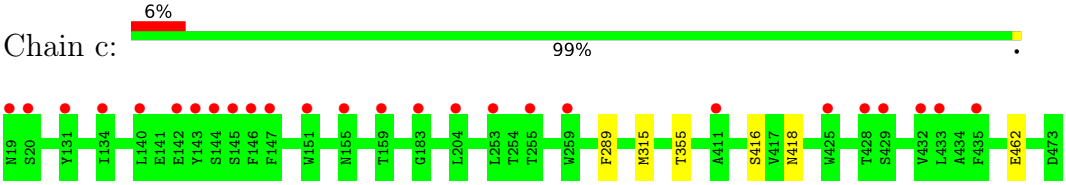
• Molecule 3: Photosystem II 44 kDa reaction center protein

Chain C:

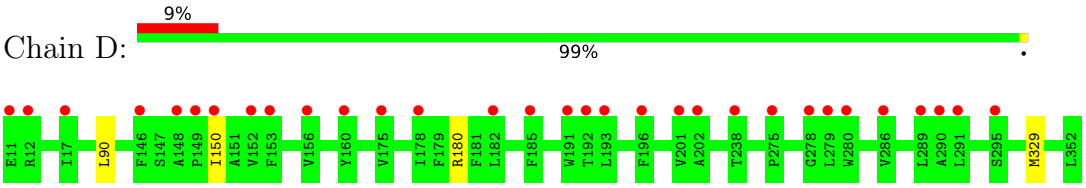




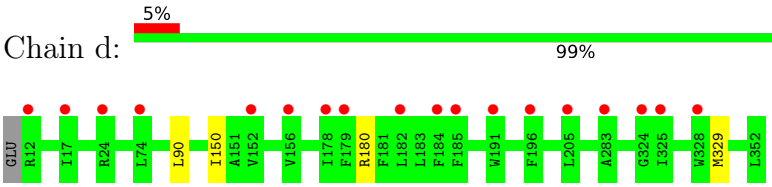
• Molecule 3: Photosystem II 44 kDa reaction center protein



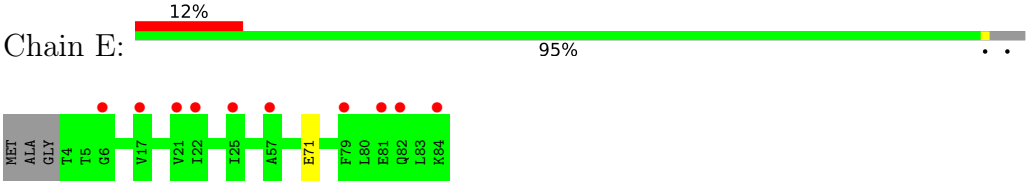
• Molecule 4: Photosystem II D2 protein



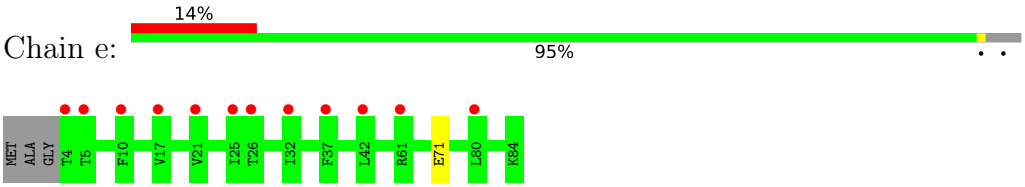
• Molecule 4: Photosystem II D2 protein



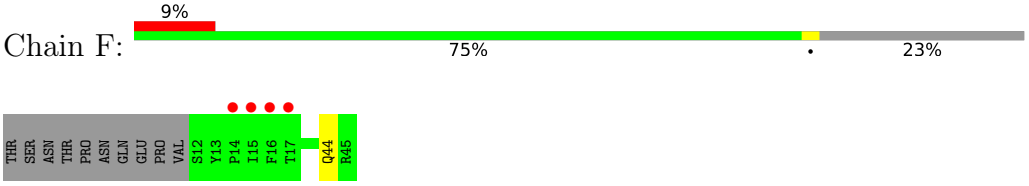
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

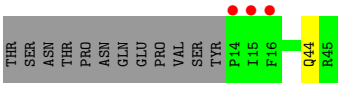


• Molecule 6: Cytochrome b559 subunit beta



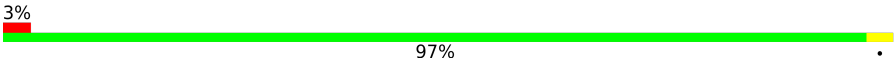
• Molecule 6: Cytochrome b559 subunit beta

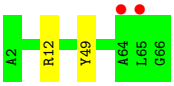
Chain f:



• Molecule 7: Photosystem II reaction center protein H

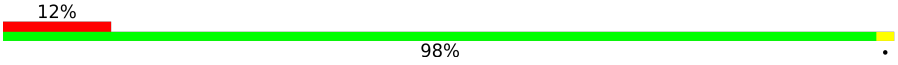
Chain H:

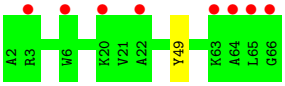




• Molecule 7: Photosystem II reaction center protein H

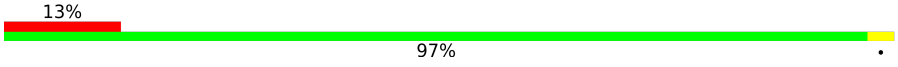
Chain h:

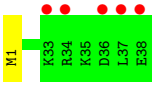




• Molecule 8: Photosystem II reaction center protein I

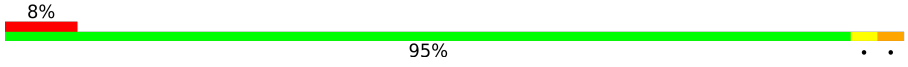
Chain I:





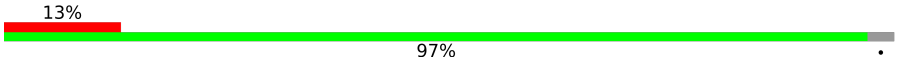
• Molecule 8: Photosystem II reaction center protein I

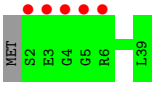
Chain i:



• Molecule 9: Photosystem II reaction center protein J

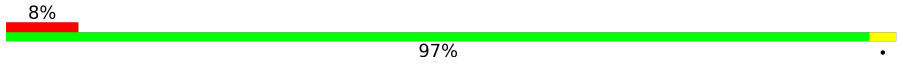
Chain J:

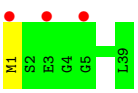




• Molecule 9: Photosystem II reaction center protein J

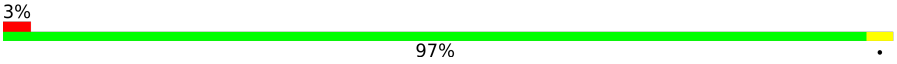
Chain j:

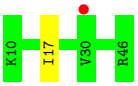




• Molecule 10: Photosystem II reaction center protein K

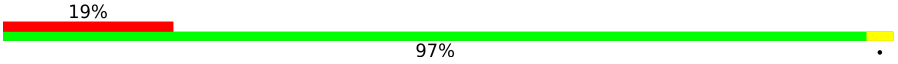
Chain K:

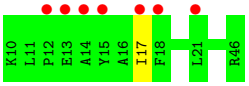




• Molecule 10: Photosystem II reaction center protein K

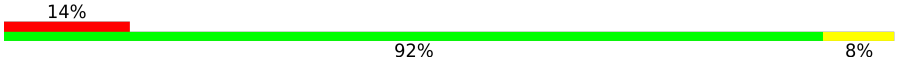
Chain k:

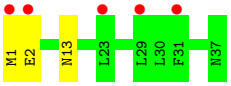




• Molecule 11: Photosystem II reaction center protein L

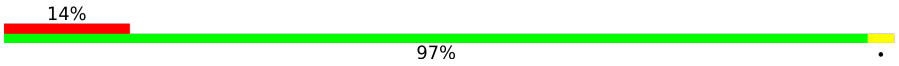
Chain L:

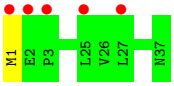




• Molecule 11: Photosystem II reaction center protein L

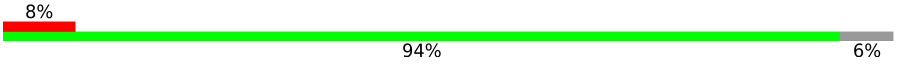
Chain l:

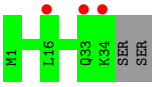




• Molecule 12: Photosystem II reaction center protein M

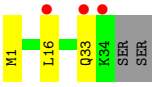
Chain M:





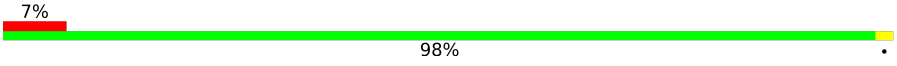
• Molecule 12: Photosystem II reaction center protein M

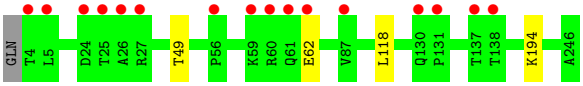
Chain m:



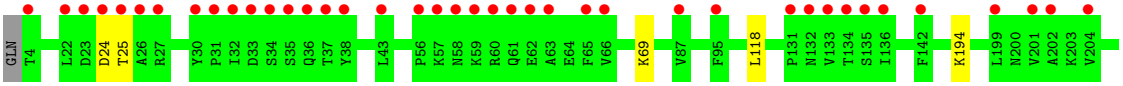
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

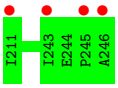
Chain O:



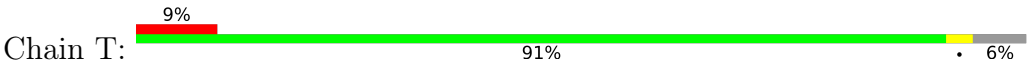


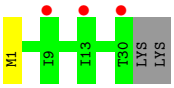
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



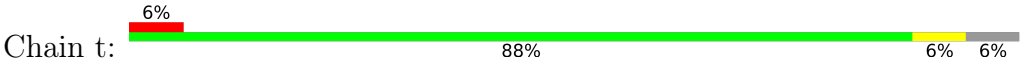


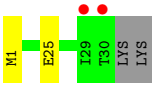
• Molecule 14: Photosystem II reaction center protein T



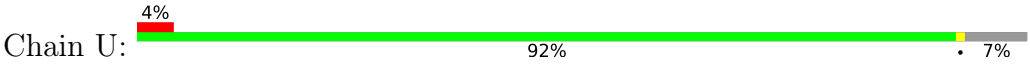


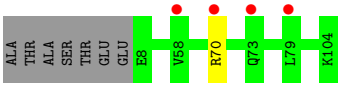
• Molecule 14: Photosystem II reaction center protein T



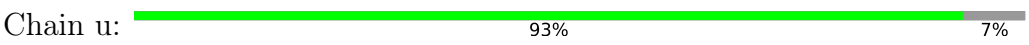


• Molecule 15: Photosystem II 12 kDa extrinsic protein





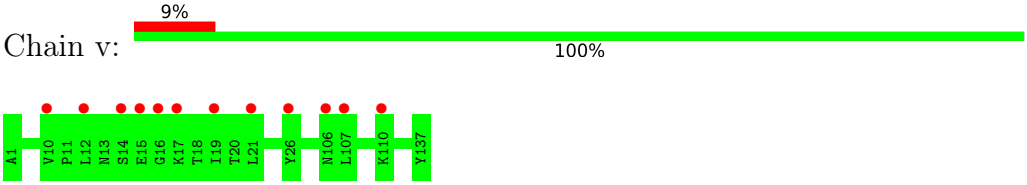
• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 16: Cytochrome c-550

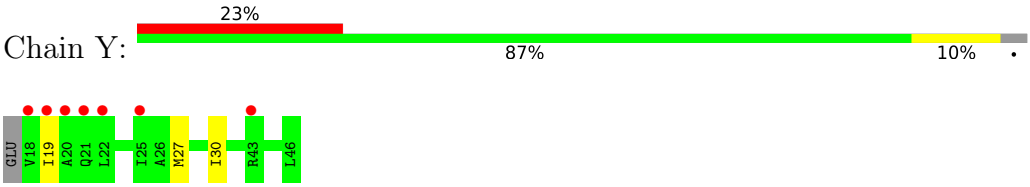
• Molecule 16: Cytochrome c-550

Chain v:



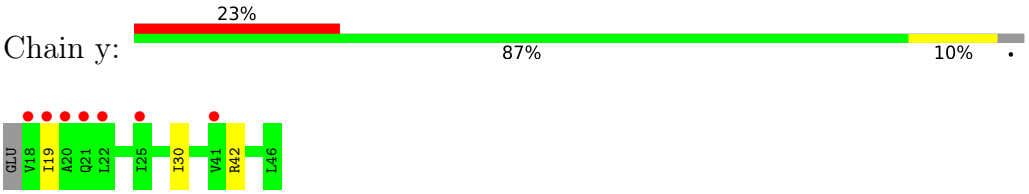
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



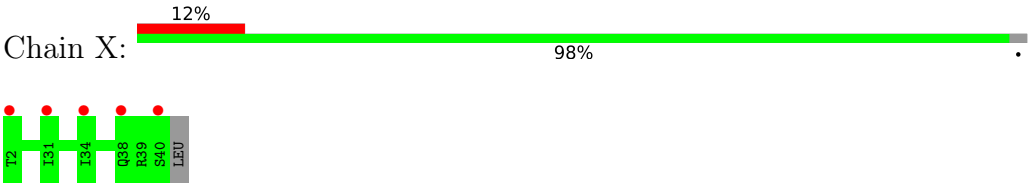
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



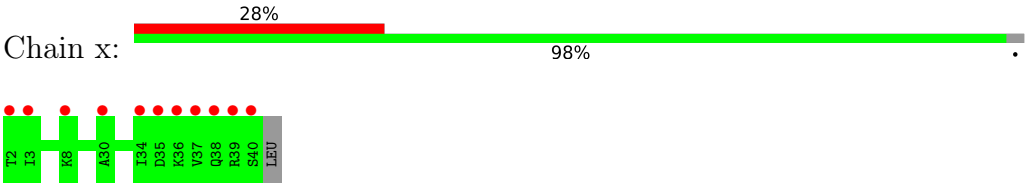
• Molecule 18: Photosystem II reaction center protein X

Chain X:



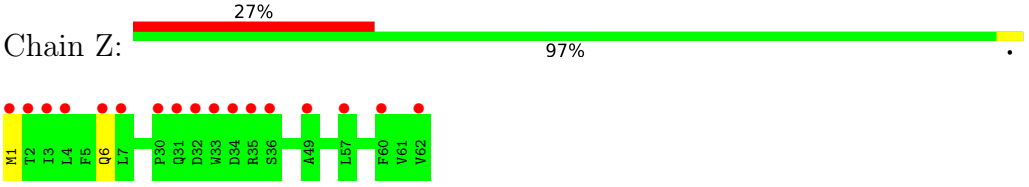
• Molecule 18: Photosystem II reaction center protein X

Chain x:



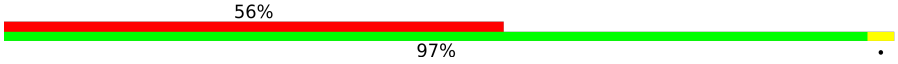
• Molecule 19: Photosystem II reaction center protein Z

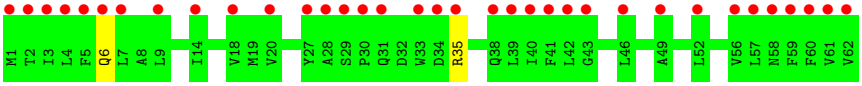
Chain Z:



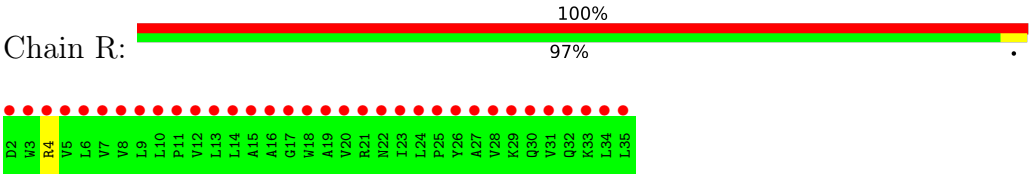
• Molecule 19: Photosystem II reaction center protein Z

Chain z:





• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.74Å 229.99Å 288.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.29 – 1.95 62.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.29-1.95) 92.0 (62.29-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.67 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	29338 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	54195	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.52	0/2728	0.59	0/3719
1	a	0.52	0/2748	0.57	0/3746
2	B	0.49	0/4200	0.56	0/5721
2	b	0.47	0/4209	0.56	0/5734
3	C	0.45	0/3626	0.54	0/4936
3	c	0.45	0/3676	0.53	0/5004
4	D	0.53	0/2827	0.57	0/3852
4	d	0.51	0/2818	0.56	0/3840
5	E	0.37	0/693	0.54	0/944
5	e	0.35	0/695	0.50	0/948
6	F	0.40	0/284	0.52	0/387
6	f	0.39	0/265	0.52	0/360
7	H	0.37	0/535	0.53	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.38	0/311	0.55	0/419
8	i	0.38	0/311	0.51	0/419
9	J	0.42	0/278	0.47	0/376
9	j	0.41	0/286	0.47	0/386
10	K	0.33	0/303	0.52	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.47	0/319	0.51	0/433
11	l	0.45	0/319	0.50	0/433
12	M	0.45	0/270	0.58	0/368
12	m	0.55	0/262	0.63	0/357
13	O	0.40	0/1958	0.58	0/2654
13	o	0.39	0/1937	0.58	0/2625
14	T	0.55	0/266	0.54	0/362
14	t	0.56	0/266	0.57	0/362
15	U	0.45	0/785	0.58	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.42	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.39	0/1085	0.52	0/1473
17	Y	0.32	0/216	0.46	0/289
17	y	0.33	0/216	0.51	0/289
18	X	0.37	0/290	0.42	0/392
18	x	0.35	0/290	0.46	0/392
19	Z	0.33	0/490	0.43	0/669
19	z	0.33	0/490	0.45	0/669
20	R	0.26	0/279	0.38	0/383
All	All	0.46	0/43239	0.55	0/58829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	30
1	a	338/344 (98%)	333 (98%)	4 (1%)	1 (0%)	41	30
2	B	513/505 (102%)	506 (99%)	7 (1%)	0	100	100
2	b	514/505 (102%)	506 (98%)	8 (2%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	34	22
3	c	459/455 (101%)	445 (97%)	12 (3%)	2 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	240 (96%)	8 (3%)	1 (0%)	34	22
13	o	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100 100
20	R	32/34 (94%)	32 (100%)	0	0	100 100
All	All	5290/5384 (98%)	5170 (98%)	112 (2%)	8 (0%)	51 38

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
13	O	62	GLU

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	272/279 (98%)	272 (100%)	0	100 100
1	a	275/279 (99%)	272 (99%)	3 (1%)	73 71
2	B	413/403 (102%)	405 (98%)	8 (2%)	57 50
2	b	414/403 (103%)	406 (98%)	8 (2%)	57 50
3	C	356/356 (100%)	351 (99%)	5 (1%)	67 62
3	c	362/356 (102%)	356 (98%)	6 (2%)	60 55
4	D	278/277 (100%)	274 (99%)	4 (1%)	67 62
4	d	277/277 (100%)	273 (99%)	4 (1%)	67 62
5	E	74/73 (101%)	73 (99%)	1 (1%)	67 62
5	e	74/73 (101%)	73 (99%)	1 (1%)	67 62
6	F	28/38 (74%)	27 (96%)	1 (4%)	35 23
6	f	26/38 (68%)	25 (96%)	1 (4%)	33 21
7	H	55/54 (102%)	52 (94%)	3 (6%)	21 9
7	h	54/54 (100%)	53 (98%)	1 (2%)	57 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42 31
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34 22
10	K	30/30 (100%)	29 (97%)	1 (3%)	38 26
10	k	30/30 (100%)	29 (97%)	1 (3%)	38 26
11	L	36/35 (103%)	33 (92%)	3 (8%)	11 3
11	l	36/35 (103%)	35 (97%)	1 (3%)	43 33
12	M	31/32 (97%)	31 (100%)	0	100 100
12	m	30/32 (94%)	28 (93%)	2 (7%)	16 5
13	O	214/207 (103%)	210 (98%)	4 (2%)	57 50
13	o	211/207 (102%)	206 (98%)	5 (2%)	49 40
14	T	27/28 (96%)	27 (100%)	0	100 100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13 4
15	U	84/89 (94%)	83 (99%)	1 (1%)	71 68
15	u	84/89 (94%)	84 (100%)	0	100 100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81 80
16	v	117/117 (100%)	117 (100%)	0	100 100
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3 0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 0
18	X	32/33 (97%)	32 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33 21
19	z	52/52 (100%)	50 (96%)	2 (4%)	33 21
20	R	29/29 (100%)	28 (97%)	1 (3%)	37 25
All	All	4395/4403 (100%)	4315 (98%)	80 (2%)	60 53

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	180	ARG
13	o	118	LEU
5	e	71	GLU

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Mol	Chain	Res	Type
11	l	1	MET
17	y	19	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	289	GLN
19	z	31	GLN
3	c	201	ASN
13	o	147	ASN
2	b	490	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.56	1 (14%)
12	FME	m	1	12	8,9,10	0.72	0	7,9,11	1.11	1 (14%)
8	FME	i	1	8	8,9,10	0.69	0	7,9,11	1.37	1 (14%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.11	0
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.32	2 (28%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	2.10	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	3.07	115.27	109.73
14	T	1	FME	C-CA-N	2.67	114.55	109.73
14	t	1	FME	O-C-CA	-2.63	117.88	124.78
14	t	1	FME	CA-N-CN	-2.56	118.89	122.82
8	I	1	FME	O-C-CA	-2.36	118.59	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 251 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 216 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	$\#\|Z\| > 2$
24	CLA	B	615	-	65,73,73	2.04	16 (24%)	76,113,113	2.95	31 (40%)
34	LMG	C	501	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
24	CLA	C	505	41	65,73,73	2.07	16 (24%)	76,113,113	2.87	27 (35%)
28	GOL	a	414	-	5,5,5	0.39	0	5,5,5	0.43	0
26	BCR	k	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.46	10 (17%)
34	LMG	B	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.16	3 (5%)
35	HTG	d	412	-	16,16,19	1.11	2 (12%)	20,21,24	1.38	1 (5%)
26	BCR	D	403	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	14 (25%)
25	PHO	A	408	-	51,69,69	1.83	7 (13%)	47,99,99	1.97	8 (17%)
24	CLA	B	609	-	65,73,73	2.11	16 (24%)	76,113,113	2.71	30 (39%)
28	GOL	O	302	-	5,5,5	0.32	0	5,5,5	0.44	0
24	CLA	C	508	41	65,73,73	2.01	16 (24%)	76,113,113	2.61	26 (34%)
25	PHO	a	408	-	51,69,69	1.75	7 (13%)	47,99,99	1.58	6 (12%)
27	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.45	8 (15%)
24	CLA	b	610	-	65,73,73	1.99	15 (23%)	76,113,113	2.84	28 (36%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.00	1 (5%)
29	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.86	0
24	CLA	B	605	-	65,73,73	1.98	15 (23%)	76,113,113	2.70	25 (32%)
24	CLA	b	611	41	65,73,73	2.06	17 (26%)	76,113,113	2.87	28 (36%)
34	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.31	6 (13%)
35	HTG	b	602	-	19,19,19	1.14	2 (10%)	23,24,24	1.22	1 (4%)
28	GOL	A	413	-	5,5,5	0.25	0	5,5,5	0.52	0
24	CLA	d	403	-	65,73,73	2.05	16 (24%)	76,113,113	2.74	27 (35%)
35	HTG	c	923	-	19,19,19	1.14	2 (10%)	23,24,24	1.84	5 (21%)
38	HEM	E	103	6,5	41,50,50	1.29	5 (12%)	45,82,82	1.93	13 (28%)
24	CLA	a	407	41	65,73,73	2.07	16 (24%)	76,113,113	2.78	32 (42%)
34	LMG	j	101	39	51,51,55	0.89	2 (3%)	59,59,63	0.99	4 (6%)
29	LMT	a	401	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.34	0
26	BCR	B	620	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	612	-	65,73,73	2.05	16 (24%)	76,113,113	2.81	28 (36%)
29	LMT	B	636	-	25,25,36	0.43	0	30,30,47	0.65	0
29	LMT	m	102	-	36,36,36	0.48	0	47,47,47	0.91	1 (2%)
28	GOL	v	205	-	5,5,5	0.39	0	5,5,5	0.35	0
24	CLA	B	602	41	65,73,73	2.04	17 (26%)	76,113,113	2.75	29 (38%)
34	LMG	c	919	-	51,51,55	0.97	3 (5%)	59,59,63	1.01	2 (3%)
24	CLA	b	619	-	65,73,73	2.05	15 (23%)	76,113,113	2.68	28 (36%)
24	CLA	C	503	-	65,73,73	2.07	16 (24%)	76,113,113	2.60	27 (35%)
29	LMT	b	601	-	25,25,36	0.46	0	30,30,47	1.35	3 (10%)
28	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.37	0
24	CLA	c	911	-	65,73,73	2.07	16 (24%)	76,113,113	2.60	28 (36%)
23	BCT	A	404	21	2,3,3	0.88	0	2,3,3	0.45	0
24	CLA	c	909	-	65,73,73	2.06	16 (24%)	76,113,113	2.67	25 (32%)
35	HTG	B	633	-	19,19,19	1.12	2 (10%)	23,24,24	1.30	1 (4%)
29	LMT	C	522	-	36,36,36	0.48	0	47,47,47	1.27	5 (10%)
27	SQD	A	412	-	53,54,54	0.99	3 (5%)	62,65,65	1.77	12 (19%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	2 (3%)
24	CLA	B	617	-	65,73,73	2.04	17 (26%)	76,113,113	2.73	26 (34%)
37	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.23	5 (8%)
24	CLA	c	902	-	65,73,73	2.02	15 (23%)	76,113,113	2.72	26 (34%)
28	GOL	T	103	-	5,5,5	0.39	0	5,5,5	0.19	0
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	4 (7%)
29	LMT	A	417	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	2 (4%)
40	HEC	V	201	16	32,50,50	1.47	4 (12%)	24,82,82	1.47	6 (25%)
36	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	2 (2%)
28	GOL	f	101	33	5,5,5	0.37	0	5,5,5	0.40	0
24	CLA	b	614	41	65,73,73	2.09	16 (24%)	76,113,113	2.72	31 (40%)
29	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.40	5 (10%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
24	CLA	c	914	-	65,73,73	2.06	17 (26%)	76,113,113	2.76	28 (36%)
28	GOL	B	630	-	5,5,5	0.33	0	5,5,5	0.36	0
24	CLA	c	908	41	65,73,73	2.03	16 (24%)	76,113,113	2.75	28 (36%)
31	PL9	A	419	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	b	632	-	5,5,5	0.37	0	5,5,5	0.56	0
26	BCR	B	618	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	8 (14%)
35	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.37	2 (8%)
37	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	4 (7%)
30	OEX	A	418	41,1,3	0,15,15	-	-	-		
24	CLA	B	613	-	65,73,73	2.04	16 (24%)	76,113,113	2.63	23 (30%)
24	CLA	B	606	-	65,73,73	2.00	16 (24%)	76,113,113	2.68	26 (34%)
24	CLA	b	607	-	65,73,73	2.08	16 (24%)	76,113,113	2.80	31 (40%)
24	CLA	c	907	-	65,73,73	2.06	17 (26%)	76,113,113	2.69	30 (39%)
29	LMT	m	104	-	36,36,36	0.51	0	47,47,47	1.01	2 (4%)
31	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.55	14 (20%)
28	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.61	0
24	CLA	C	504	-	65,73,73	2.05	16 (24%)	76,113,113	2.78	26 (34%)
24	CLA	b	609	-	65,73,73	2.03	15 (23%)	76,113,113	2.86	27 (35%)
28	GOL	a	415	-	5,5,5	0.40	0	5,5,5	0.46	0
24	CLA	b	606	-	65,73,73	2.04	17 (26%)	76,113,113	2.80	28 (36%)
28	GOL	c	925	-	5,5,5	0.36	0	5,5,5	0.56	0
24	CLA	B	616	-	65,73,73	1.99	16 (24%)	76,113,113	2.74	29 (38%)
35	HTG	O	303	-	19,19,19	0.95	1 (5%)	23,24,24	0.71	0
24	CLA	C	513	-	65,73,73	2.02	15 (23%)	76,113,113	2.77	30 (39%)
35	HTG	b	626	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	3 (13%)
29	LMT	b	625	-	25,25,36	0.52	1 (4%)	30,30,47	0.60	0
24	CLA	B	611	41	65,73,73	2.09	16 (24%)	76,113,113	2.69	29 (38%)
36	DGD	D	405	-	63,63,67	0.98	3 (4%)	77,77,81	1.24	7 (9%)
40	HEC	v	202	16	32,50,50	1.50	4 (12%)	24,82,82	1.32	5 (20%)
28	GOL	F	103	33	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	C	502	-	65,73,73	2.05	16 (24%)	76,113,113	2.79	28 (36%)
28	GOL	B	627	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	c	904	-	65,73,73	2.04	16 (24%)	76,113,113	2.68	27 (35%)
26	BCR	b	621	-	41,41,41	1.12	1 (2%)	56,56,56	1.19	2 (3%)
35	HTG	B	634	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
34	LMG	J	101	39	51,51,55	0.88	2 (3%)	59,59,63	0.89	3 (5%)
25	PHO	a	420	-	51,69,69	1.87	8 (15%)	47,99,99	1.88	8 (17%)
24	CLA	c	913	-	65,73,73	1.99	16 (24%)	76,113,113	2.80	29 (38%)
37	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	B	604	-	65,73,73	2.08	16 (24%)	76,113,113	2.84	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	A	410	-	65,73,73	2.08	14 (21%)	76,113,113	2.70	28 (36%)
36	DGD	C	519	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	5 (6%)
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.31	0
26	BCR	A	411	-	41,41,41	1.02	1 (2%)	56,56,56	1.22	5 (8%)
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.27	0
36	DGD	c	918	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
24	CLA	d	402	-	65,73,73	1.96	17 (26%)	76,113,113	2.88	26 (34%)
29	LMT	m	103	-	36,36,36	0.48	0	47,47,47	0.99	1 (2%)
24	CLA	b	615	-	65,73,73	2.01	16 (24%)	76,113,113	2.82	25 (32%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	12 (21%)
24	CLA	b	617	-	65,73,73	2.06	17 (26%)	76,113,113	2.67	31 (40%)
24	CLA	B	610	-	65,73,73	1.98	16 (24%)	76,113,113	2.78	29 (38%)
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.21	6 (9%)
24	CLA	B	608	41	65,73,73	2.04	16 (24%)	76,113,113	2.67	26 (34%)
28	GOL	T	101	-	5,5,5	0.41	0	5,5,5	0.31	0
28	GOL	C	526	-	5,5,5	0.22	0	5,5,5	0.43	0
36	DGD	C	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
34	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
25	PHO	A	409	-	51,69,69	1.96	9 (17%)	47,99,99	1.75	8 (17%)
24	CLA	C	511	-	65,73,73	2.09	16 (24%)	76,113,113	2.63	27 (35%)
35	HTG	B	624	-	19,19,19	1.13	1 (5%)	23,24,24	1.39	1 (4%)
26	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	7 (12%)
24	CLA	c	912	3	65,73,73	2.08	17 (26%)	76,113,113	2.66	27 (35%)
26	BCR	c	915	-	41,41,41	1.07	1 (2%)	56,56,56	1.43	9 (16%)
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	6 (7%)
36	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	1.22	6 (7%)
28	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.61	0
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
28	GOL	V	206	-	5,5,5	0.32	0	5,5,5	0.30	0
28	GOL	B	637	-	5,5,5	0.40	0	5,5,5	0.30	0
28	GOL	B	631	-	5,5,5	0.42	0	5,5,5	0.47	0
24	CLA	b	605	41	65,73,73	2.08	15 (23%)	76,113,113	2.73	24 (31%)
24	CLA	b	620	-	65,73,73	2.07	17 (26%)	76,113,113	2.70	25 (32%)
24	CLA	A	407	41	65,73,73	2.06	16 (24%)	76,113,113	2.78	29 (38%)
28	GOL	V	205	-	5,5,5	0.36	0	5,5,5	0.38	0
28	GOL	a	413	-	5,5,5	0.31	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.57	11 (17%)
27	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.60	10 (16%)
24	CLA	b	613	-	65,73,73	2.02	16 (24%)	76,113,113	2.81	29 (38%)
28	GOL	b	630	-	5,5,5	0.32	0	5,5,5	0.52	0
28	GOL	V	203	-	5,5,5	0.38	0	5,5,5	0.15	0
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	7 (12%)
26	BCR	T	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.38	11 (19%)
28	GOL	V	204	-	5,5,5	0.43	0	5,5,5	0.44	0
24	CLA	c	905	41	65,73,73	2.04	16 (24%)	76,113,113	2.76	29 (38%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)
28	GOL	o	302	-	5,5,5	0.39	0	5,5,5	0.48	0
24	CLA	b	616	-	65,73,73	2.00	16 (24%)	76,113,113	2.75	26 (34%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.07	4 (6%)
35	HTG	b	603	-	19,19,19	1.03	2 (10%)	23,24,24	1.47	3 (13%)
24	CLA	c	903	-	65,73,73	2.01	16 (24%)	76,113,113	2.68	25 (32%)
24	CLA	C	514	-	65,73,73	2.07	16 (24%)	76,113,113	2.75	27 (35%)
28	GOL	B	632	-	5,5,5	0.35	0	5,5,5	0.36	0
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
37	LHG	e	101	-	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
28	GOL	b	631	-	5,5,5	0.33	0	5,5,5	0.46	0
34	LMG	b	624	-	51,51,55	0.91	3 (5%)	59,59,63	1.05	3 (5%)
24	CLA	b	618	-	65,73,73	2.03	16 (24%)	76,113,113	2.90	30 (39%)
26	BCR	K	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
23	BCT	a	419	21	2,3,3	0.96	0	2,3,3	0.22	0
24	CLA	A	406	41	65,73,73	2.03	14 (21%)	76,113,113	2.97	31 (40%)
24	CLA	D	401	-	65,73,73	2.00	16 (24%)	76,113,113	2.74	26 (34%)
35	HTG	V	202	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	3 (13%)
24	CLA	d	401	41	65,73,73	2.06	16 (24%)	76,113,113	2.76	28 (36%)
37	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.09	3 (6%)
26	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.37	7 (12%)
31	PL9	D	404	-	55,55,55	0.73	2 (3%)	68,69,69	1.58	14 (20%)
38	HEM	e	102	6,5	41,50,50	1.31	6 (14%)	45,82,82	1.89	11 (24%)
24	CLA	C	510	-	65,73,73	2.14	16 (24%)	76,113,113	2.74	31 (40%)
24	CLA	C	512	3	65,73,73	2.07	19 (29%)	76,113,113	2.68	26 (34%)
35	HTG	c	922	-	19,19,19	0.90	1 (5%)	23,24,24	1.34	1 (4%)
35	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.18	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	a	409	-	65,73,73	2.01	16 (24%)	76,113,113	2.64	32 (42%)
35	HTG	b	627	-	19,19,19	1.09	2 (10%)	23,24,24	1.97	4 (17%)
26	BCR	b	623	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	9 (16%)
27	SQD	a	402	-	53,54,54	1.06	3 (5%)	62,65,65	1.16	7 (11%)
24	CLA	c	910	-	65,73,73	2.13	16 (24%)	76,113,113	2.73	28 (36%)
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.96	10 (19%)
28	GOL	B	629	-	5,5,5	0.41	0	5,5,5	0.56	0
31	PL9	a	417	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	18 (26%)
29	LMT	c	921	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
24	CLA	B	603	-	65,73,73	2.08	16 (24%)	76,113,113	2.87	32 (42%)
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.46	7 (14%)
28	GOL	b	629	-	5,5,5	0.34	0	5,5,5	0.15	0
28	GOL	t	102	-	5,5,5	0.40	0	5,5,5	0.23	0
27	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.48	9 (14%)
24	CLA	C	507	-	65,73,73	2.09	16 (24%)	76,113,113	2.69	29 (38%)
36	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	6 (7%)
24	CLA	B	614	-	65,73,73	2.09	15 (23%)	76,113,113	2.77	28 (36%)
24	CLA	c	906	-	65,73,73	2.01	15 (23%)	76,113,113	2.64	23 (30%)
24	CLA	C	506	-	65,73,73	2.07	17 (26%)	76,113,113	2.66	26 (34%)
24	CLA	b	608	-	65,73,73	2.09	16 (24%)	76,113,113	2.64	25 (32%)
26	BCR	d	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	16 (28%)
34	LMG	a	412	-	51,51,55	0.91	2 (3%)	59,59,63	1.15	6 (10%)
26	BCR	b	622	-	41,41,41	1.06	1 (2%)	56,56,56	1.27	5 (8%)
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.06	4 (7%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.29	5 (8%)
30	OEX	a	416	41,1,3	0,15,15	-	-	-		
24	CLA	D	402	-	65,73,73	2.03	16 (24%)	76,113,113	2.70	25 (32%)
35	HTG	C	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.64	4 (17%)
24	CLA	a	406	-	65,73,73	2.10	16 (24%)	76,113,113	2.76	33 (43%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.90	1 (2%)
24	CLA	A	405	-	65,73,73	2.03	15 (23%)	76,113,113	2.75	23 (30%)
24	CLA	b	612	-	65,73,73	2.09	16 (24%)	76,113,113	2.67	27 (35%)
24	CLA	B	607	-	65,73,73	2.08	17 (26%)	76,113,113	2.88	30 (39%)
26	BCR	t	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
28	GOL	B	628	-	5,5,5	0.27	0	5,5,5	0.42	0
29	LMT	f	103	-	36,36,36	0.54	1 (2%)	47,47,47	0.93	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	0.93	4 (5%)
37	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	4 (7%)
28	GOL	b	628	-	5,5,5	0.36	0	5,5,5	0.30	0
24	CLA	C	509	-	65,73,73	2.06	16 (24%)	76,113,113	2.81	28 (36%)
35	HTG	B	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	2 (8%)

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
24	CLA	B	615	-	1/1/15/20	18/37/115/115	-
34	LMG	C	501	-	-	19/46/66/70	0/1/1/1
24	CLA	C	505	41	1/1/15/20	5/37/115/115	-
28	GOL	a	414	-	-	2/4/4/4	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
35	HTG	d	412	-	-	0/7/27/30	0/1/1/1
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2
25	PHO	A	408	-	-	5/37/103/103	0/5/6/6
24	CLA	B	609	-	-	0/37/115/115	-
28	GOL	O	302	-	-	2/4/4/4	-
24	CLA	C	508	41	1/1/15/20	6/37/115/115	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
24	CLA	b	610	-	1/1/15/20	16/37/115/115	-
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
29	LMT	E	102	-	-	7/21/61/61	0/2/2/2
24	CLA	B	605	-	1/1/15/20	4/37/115/115	-
24	CLA	b	611	41	1/1/15/20	2/37/115/115	-
34	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
35	HTG	b	602	-	-	1/10/30/30	0/1/1/1
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	d	403	-	-	7/37/115/115	-
35	HTG	c	923	-	-	0/10/30/30	0/1/1/1
38	HEM	E	103	6,5	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	407	41	-	6/37/115/115	-
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
29	LMT	a	401	-	-	11/21/61/61	0/2/2/2
28	GOL	A	414	-	-	2/4/4/4	-
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
24	CLA	B	612	-	1/1/15/20	2/37/115/115	-
29	LMT	B	636	-	-	8/17/37/61	0/1/1/2
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
28	GOL	v	205	-	-	2/4/4/4	-
24	CLA	B	602	41	1/1/15/20	16/37/115/115	-
34	LMG	c	919	-	-	16/46/66/70	0/1/1/1
24	CLA	b	619	-	1/1/15/20	4/37/115/115	-
24	CLA	C	503	-	-	4/37/115/115	-
29	LMT	b	601	-	-	8/17/37/61	0/1/1/2
28	GOL	b	633	-	-	2/4/4/4	-
28	GOL	v	204	-	-	3/4/4/4	-
24	CLA	c	911	-	1/1/15/20	9/37/115/115	-
24	CLA	c	909	-	1/1/15/20	3/37/115/115	-
35	HTG	B	633	-	-	3/10/30/30	0/1/1/1
29	LMT	C	522	-	-	9/21/61/61	0/2/2/2
27	SQD	A	412	-	-	11/49/69/69	0/1/1/1
37	LHG	D	407	-	-	5/53/53/53	-
24	CLA	B	617	-	1/1/15/20	9/37/115/115	-
37	LHG	D	406	-	-	6/53/53/53	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	c	902	-	1/1/15/20	4/37/115/115	-
28	GOL	T	103	-	-	4/4/4/4	-
37	LHG	d	408	-	-	11/53/53/53	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
40	HEC	V	201	16	-	2/10/54/54	-
36	DGD	c	917	-	-	14/51/91/95	0/2/2/2
28	GOL	f	101	33	-	4/4/4/4	-
24	CLA	b	614	41	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	B	623	-	-	7/21/61/61	0/2/2/2
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	CLA	c	914	-	1/1/15/20	10/37/115/115	-
28	GOL	B	630	-	-	0/4/4/4	-
24	CLA	c	908	41	1/1/15/20	2/37/115/115	-
31	PL9	A	419	-	-	7/53/73/73	0/1/1/1
28	GOL	b	632	-	-	2/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
37	LHG	d	409	-	-	12/53/53/53	-
24	CLA	B	613	-	1/1/15/20	4/37/115/115	-
24	CLA	B	606	-	1/1/15/20	7/37/115/115	-
24	CLA	b	607	-	1/1/15/20	8/37/115/115	-
24	CLA	c	907	-	1/1/15/20	9/37/115/115	-
29	LMT	m	104	-	-	7/21/61/61	0/2/2/2
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
24	CLA	C	504	-	1/1/15/20	5/37/115/115	-
24	CLA	b	609	-	1/1/15/20	9/37/115/115	-
28	GOL	a	415	-	-	2/4/4/4	-
24	CLA	b	606	-	1/1/15/20	3/37/115/115	-
28	GOL	c	925	-	-	0/4/4/4	-
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
24	CLA	C	513	-	1/1/15/20	10/37/115/115	-
35	HTG	b	626	-	-	1/10/30/30	0/1/1/1
29	LMT	b	625	-	-	4/17/37/61	0/1/1/2
24	CLA	B	611	41	1/1/15/20	7/37/115/115	-
36	DGD	D	405	-	-	22/51/91/95	0/2/2/2
40	HEC	v	202	16	-	2/10/54/54	-
28	GOL	F	103	33	-	2/4/4/4	-
24	CLA	C	502	-	1/1/15/20	9/37/115/115	-
28	GOL	B	627	-	-	1/4/4/4	-
24	CLA	c	904	-	1/1/15/20	3/37/115/115	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	B	634	-	-	2/10/30/30	0/1/1/1
34	LMG	J	101	39	-	13/46/66/70	0/1/1/1
25	PHO	a	420	-	-	1/37/103/103	0/5/6/6
24	CLA	c	913	-	1/1/15/20	7/37/115/115	-
37	LHG	L	101	-	-	15/53/53/53	-
24	CLA	B	604	-	1/1/15/20	6/37/115/115	-
24	CLA	A	410	-	-	9/37/115/115	-
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
28	GOL	c	924	-	-	0/4/4/4	-
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
28	GOL	A	415	-	-	2/4/4/4	-
36	DGD	c	918	-	-	17/51/91/95	0/2/2/2
37	LHG	l	101	-	-	15/53/53/53	-
24	CLA	d	402	-	1/1/15/20	0/37/115/115	-
29	LMT	m	103	-	-	3/21/61/61	0/2/2/2
24	CLA	b	615	-	1/1/15/20	5/37/115/115	-
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2
24	CLA	b	617	-	1/1/15/20	4/37/115/115	-
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
24	CLA	B	608	41	1/1/15/20	2/37/115/115	-
28	GOL	T	101	-	-	0/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
34	LMG	c	920	-	-	4/46/66/70	0/1/1/1
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6
24	CLA	C	511	-	1/1/15/20	9/37/115/115	-
35	HTG	B	624	-	-	1/10/30/30	0/1/1/1
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
24	CLA	c	912	3	1/1/15/20	5/37/115/115	-
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
36	DGD	d	406	-	-	28/51/91/95	0/2/2/2
28	GOL	v	203	-	-	4/4/4/4	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
28	GOL	V	206	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	637	-	-	2/4/4/4	-
28	GOL	B	631	-	-	4/4/4/4	-
24	CLA	b	605	41	1/1/15/20	12/37/115/115	-
24	CLA	b	620	-	1/1/15/20	8/37/115/115	-
24	CLA	A	407	41	-	2/37/115/115	-
28	GOL	V	205	-	-	1/4/4/4	-
28	GOL	a	413	-	-	0/4/4/4	-
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
27	SQD	a	411	-	-	11/49/69/69	0/1/1/1
24	CLA	b	613	-	1/1/15/20	2/37/115/115	-
28	GOL	b	630	-	-	0/4/4/4	-
28	GOL	V	203	-	-	4/4/4/4	-
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
28	GOL	V	204	-	-	2/4/4/4	-
24	CLA	c	905	41	1/1/15/20	5/37/115/115	-
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
28	GOL	o	302	-	-	2/4/4/4	-
24	CLA	b	616	-	1/1/15/20	1/37/115/115	-
34	LMG	C	521	-	-	12/46/66/70	0/1/1/1
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
24	CLA	c	903	-	1/1/15/20	4/37/115/115	-
24	CLA	C	514	-	-	2/37/115/115	-
28	GOL	B	632	-	-	2/4/4/4	-
36	DGD	C	518	-	-	15/51/91/95	0/2/2/2
37	LHG	e	101	-	-	10/46/46/53	-
28	GOL	b	631	-	-	2/4/4/4	-
34	LMG	b	624	-	-	14/46/66/70	0/1/1/1
24	CLA	b	618	-	1/1/15/20	17/37/115/115	-
26	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	CLA	A	406	41	1/1/15/20	4/37/115/115	-
24	CLA	D	401	-	1/1/15/20	0/37/115/115	-
35	HTG	V	202	-	-	5/10/30/30	0/1/1/1
24	CLA	d	401	41	1/1/15/20	7/37/115/115	-
37	LHG	E	101	-	-	21/46/46/53	-
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	D	404	-	-	3/53/73/73	0/1/1/1
38	HEM	e	102	6,5	-	4/12/54/54	-
24	CLA	C	510	-	1/1/15/20	7/37/115/115	-
24	CLA	C	512	3	1/1/15/20	2/37/115/115	-
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	a	409	-	1/1/15/20	7/37/115/115	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
26	BCR	b	623	-	-	3/29/63/63	0/2/2/2
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
24	CLA	c	910	-	1/1/15/20	9/37/115/115	-
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
28	GOL	B	629	-	-	2/4/4/4	-
31	PL9	a	417	-	-	12/53/73/73	0/1/1/1
29	LMT	c	921	-	-	4/21/61/61	0/2/2/2
24	CLA	B	603	-	1/1/15/20	5/37/115/115	-
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
28	GOL	b	629	-	-	0/4/4/4	-
28	GOL	t	102	-	-	0/4/4/4	-
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
24	CLA	C	507	-	1/1/15/20	11/37/115/115	-
36	DGD	c	916	-	-	10/51/91/95	0/2/2/2
24	CLA	B	614	-	1/1/15/20	9/37/115/115	-
24	CLA	c	906	-	1/1/15/20	4/37/115/115	-
24	CLA	C	506	-	1/1/15/20	6/37/115/115	-
24	CLA	b	608	-	1/1/15/20	7/37/115/115	-
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
34	LMG	a	412	-	-	10/46/66/70	0/1/1/1
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
37	LHG	D	408	-	-	11/53/53/53	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
24	CLA	D	402	-	1/1/15/20	9/37/115/115	-
35	HTG	C	524	-	-	2/10/30/30	0/1/1/1
24	CLA	a	406	-	1/1/15/20	2/37/115/115	-
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	405	-	1/1/15/20	2/37/115/115	-
24	CLA	b	612	-	-	4/37/115/115	-
24	CLA	B	607	-	1/1/15/20	7/37/115/115	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
36	DGD	H	102	-	-	9/51/91/95	0/2/2/2
37	LHG	d	407	-	-	9/53/53/53	-
28	GOL	b	628	-	-	2/4/4/4	-
24	CLA	C	509	-	-	7/37/115/115	-
35	HTG	B	626	-	-	4/10/30/30	0/1/1/1

The worst 5 of 1331 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-C2B	6.98	1.50	1.40
24	b	620	CLA	C3B-C2B	6.75	1.49	1.40
24	a	406	CLA	C3B-C2B	6.74	1.49	1.40
24	B	617	CLA	C3B-C2B	6.73	1.49	1.40
25	a	420	PHO	C3B-C2B	6.72	1.49	1.40

The worst 5 of 2513 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C1D-ND-C4D	-10.00	99.23	106.33
24	C	505	CLA	C1D-ND-C4D	-9.97	99.26	106.33
24	B	615	CLA	C1D-ND-C4D	-9.86	99.33	106.33
24	c	914	CLA	C1D-ND-C4D	-9.84	99.34	106.33
24	C	504	CLA	C1D-ND-C4D	-9.73	99.43	106.33

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND

5 of 1251 torsion outliers are listed below:

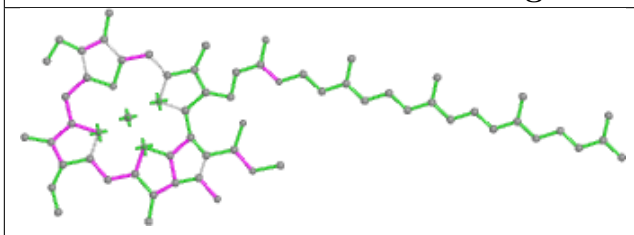
Mol	Chain	Res	Type	Atoms
24	A	410	CLA	C2-C3-C5-C6
24	A	410	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

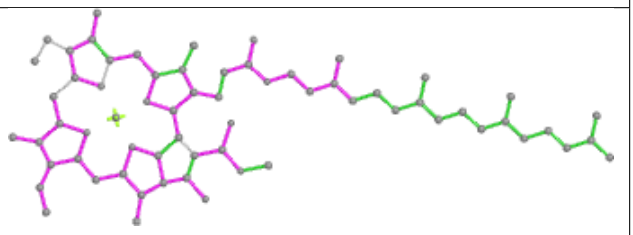
No monomer is involved in short contacts.

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

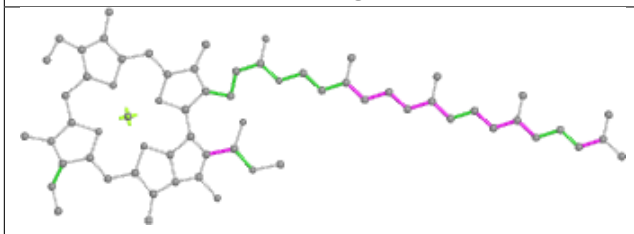
Ligand CLA B 615



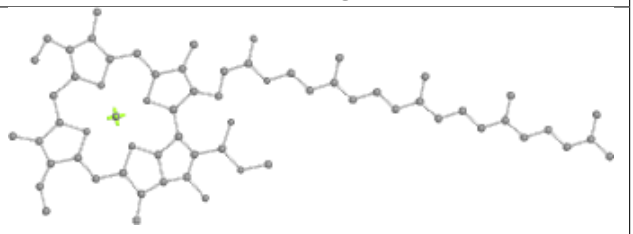
Bond lengths



Bond angles

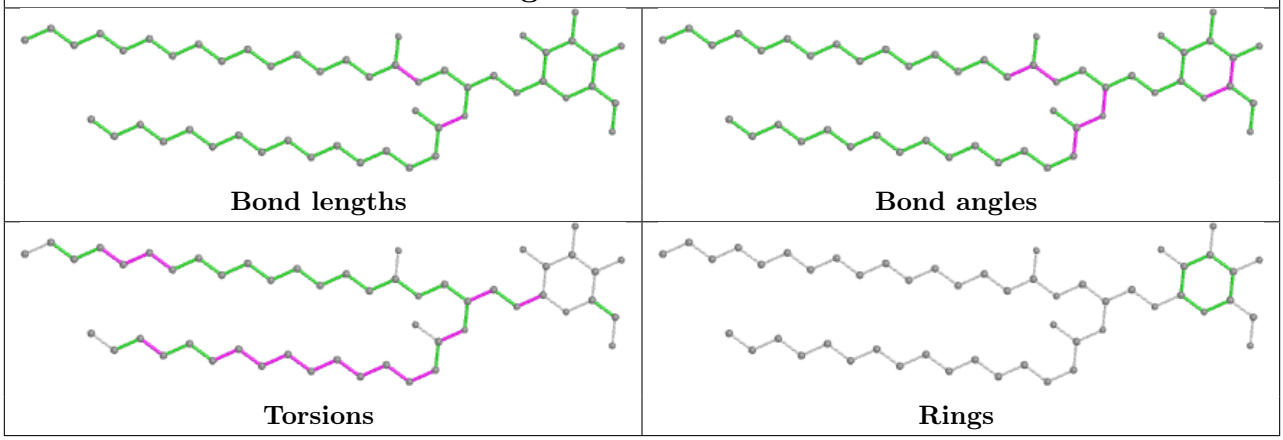


Torsions

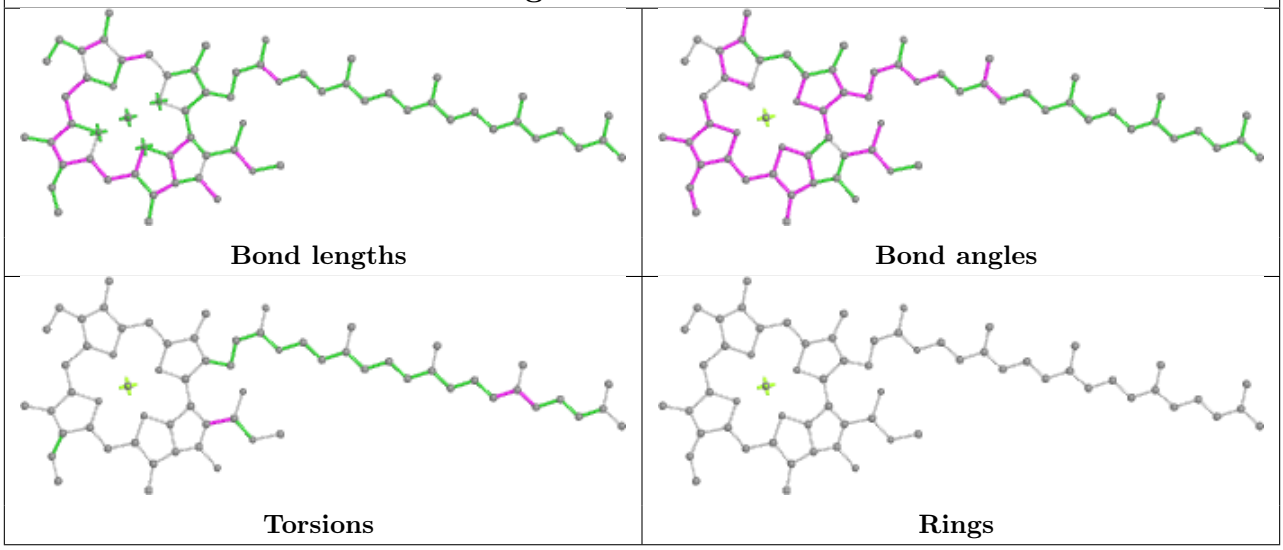


Rings

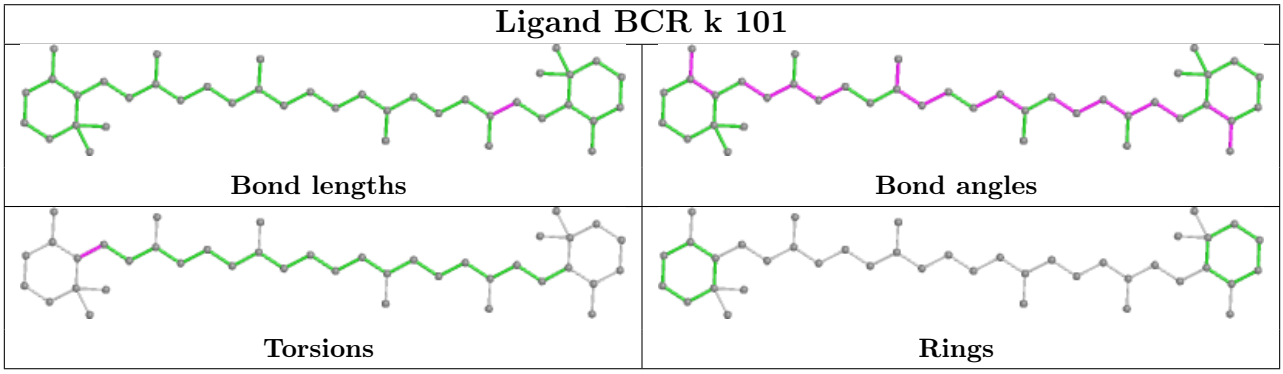
Ligand LMG C 501



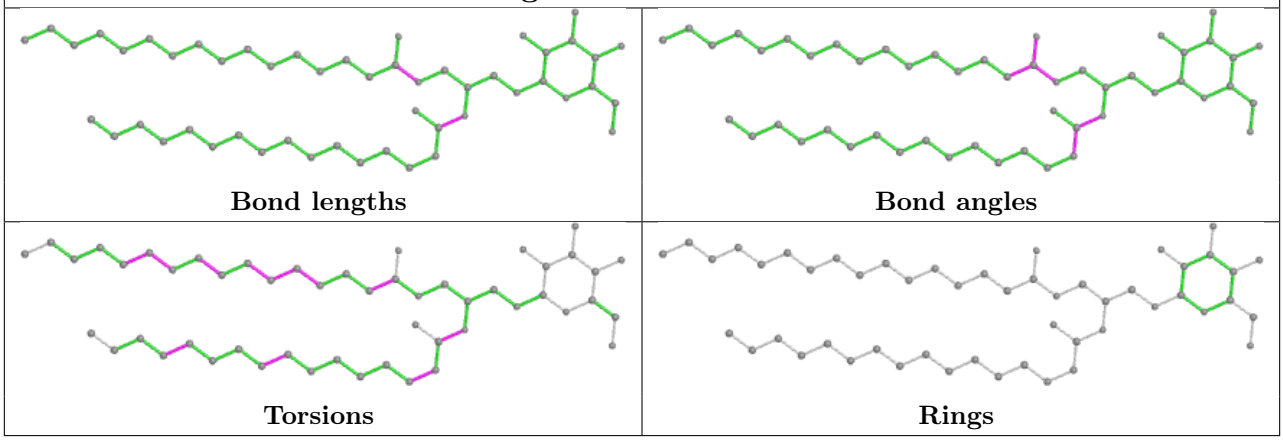
Ligand CLA C 505



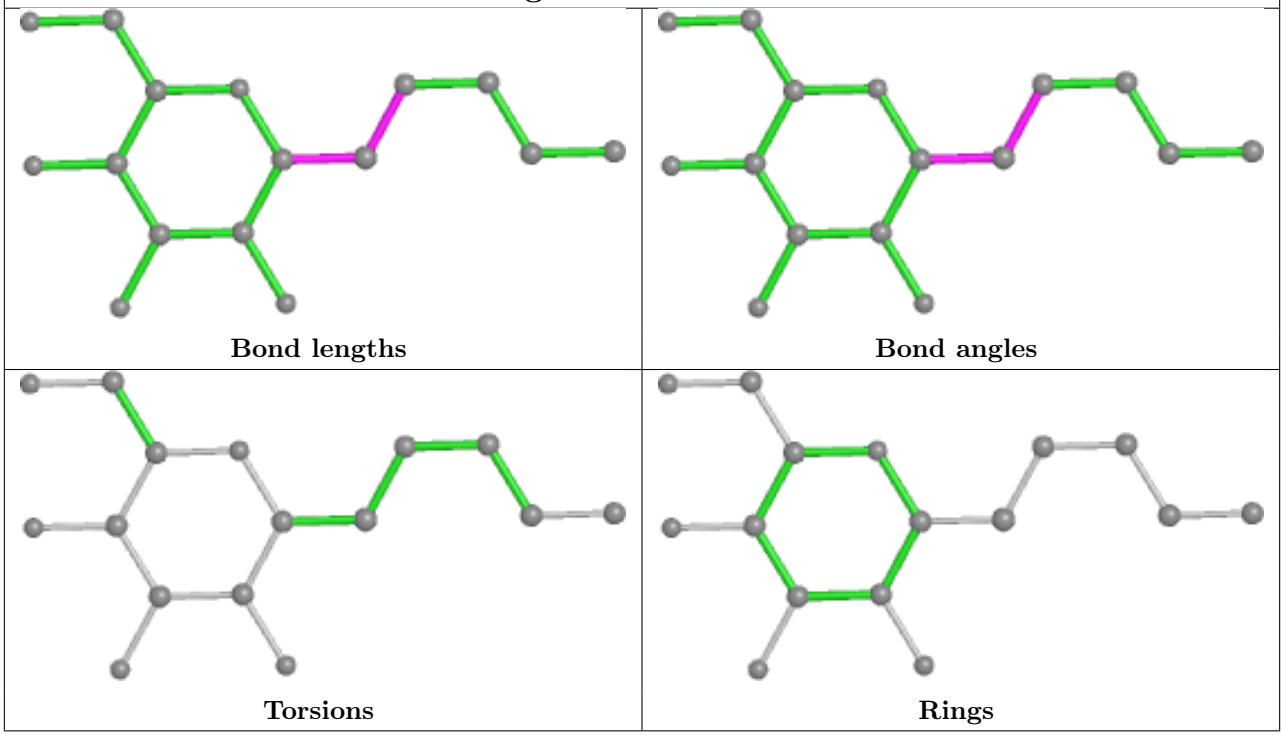
Ligand BCR k 101



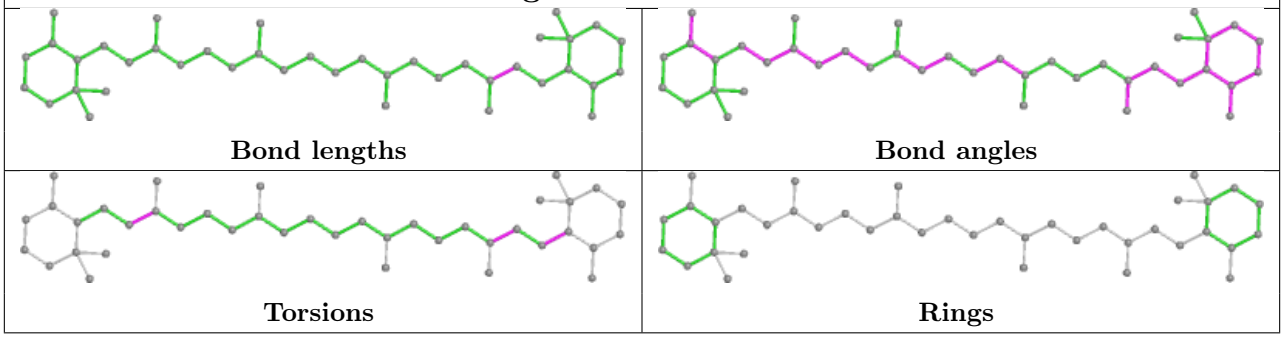
Ligand LMG B 622



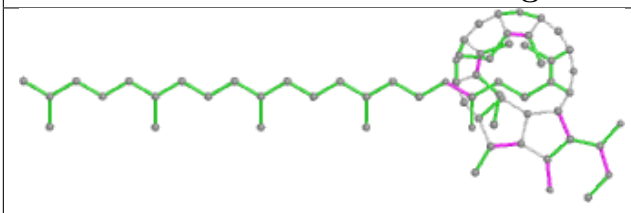
Ligand HTG d 412



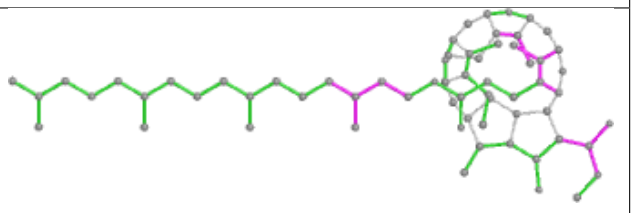
Ligand BCR D 403



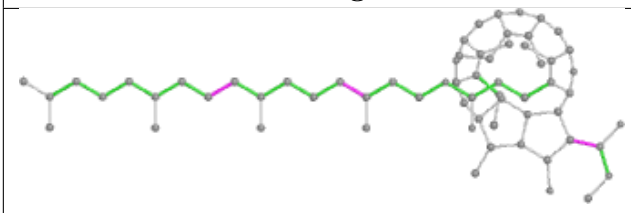
Ligand PHO A 408



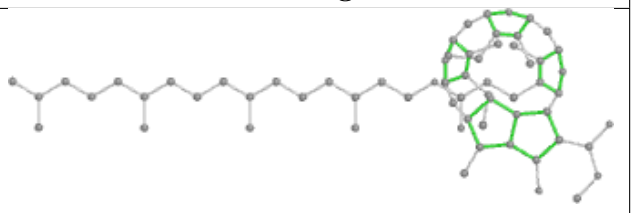
Bond lengths



Bond angles

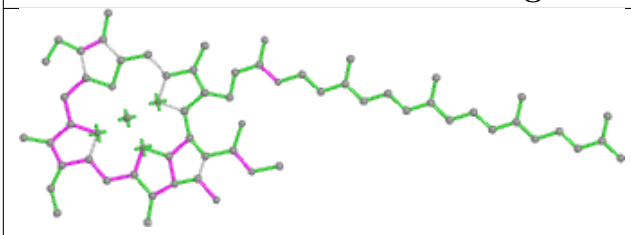


Torsions

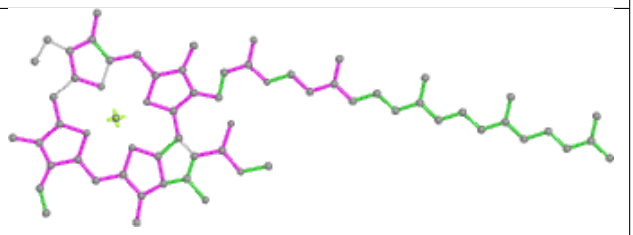


Rings

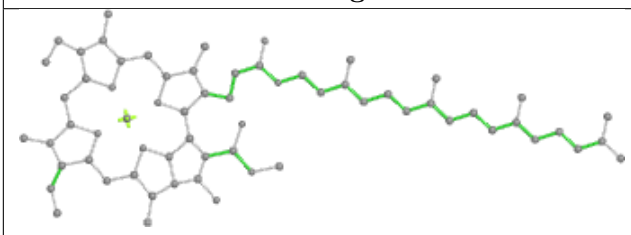
Ligand CLA B 609



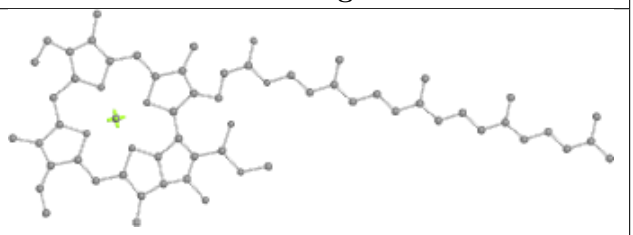
Bond lengths



Bond angles

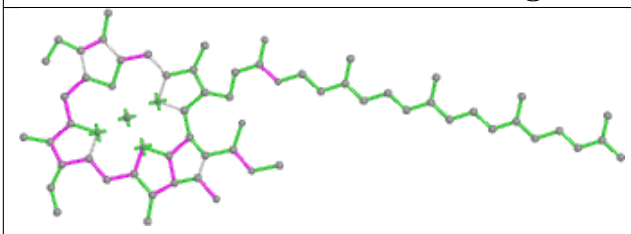


Torsions

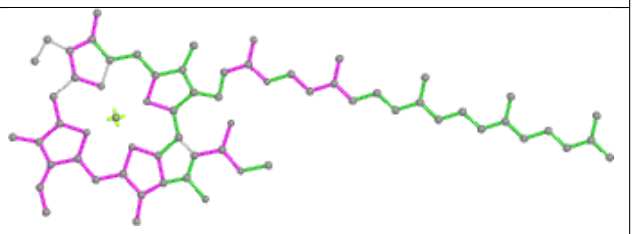


Rings

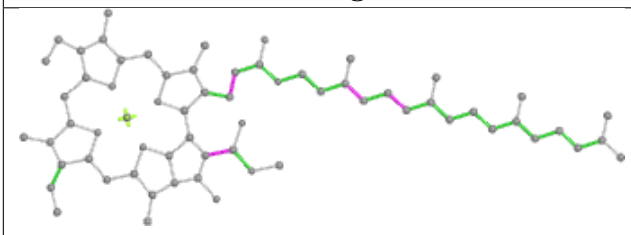
Ligand CLA C 508



Bond lengths



Bond angles



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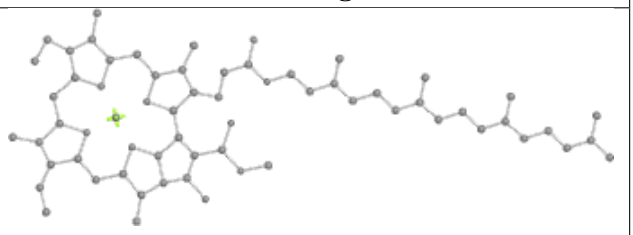
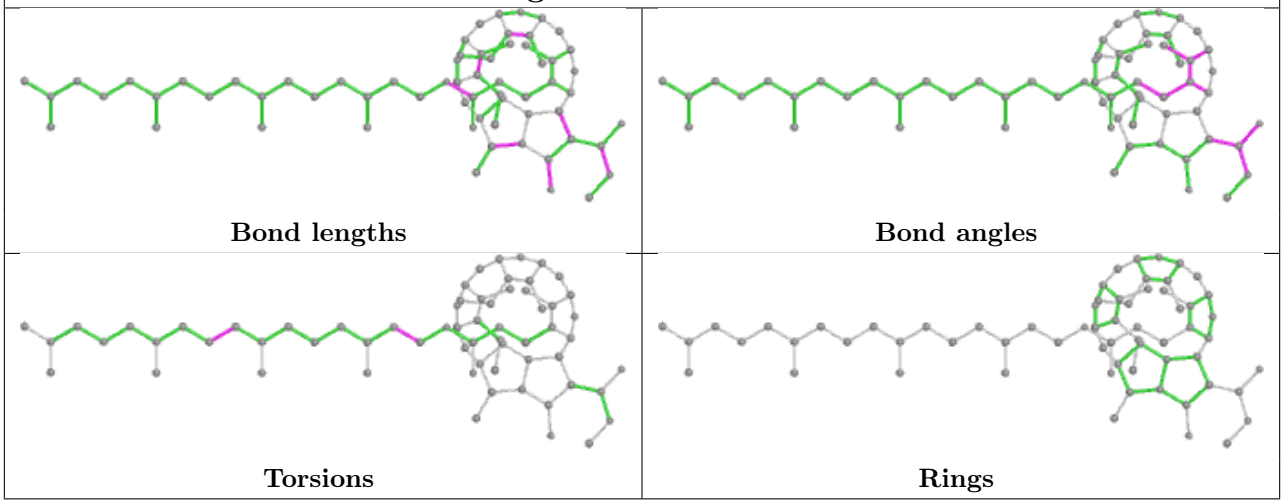
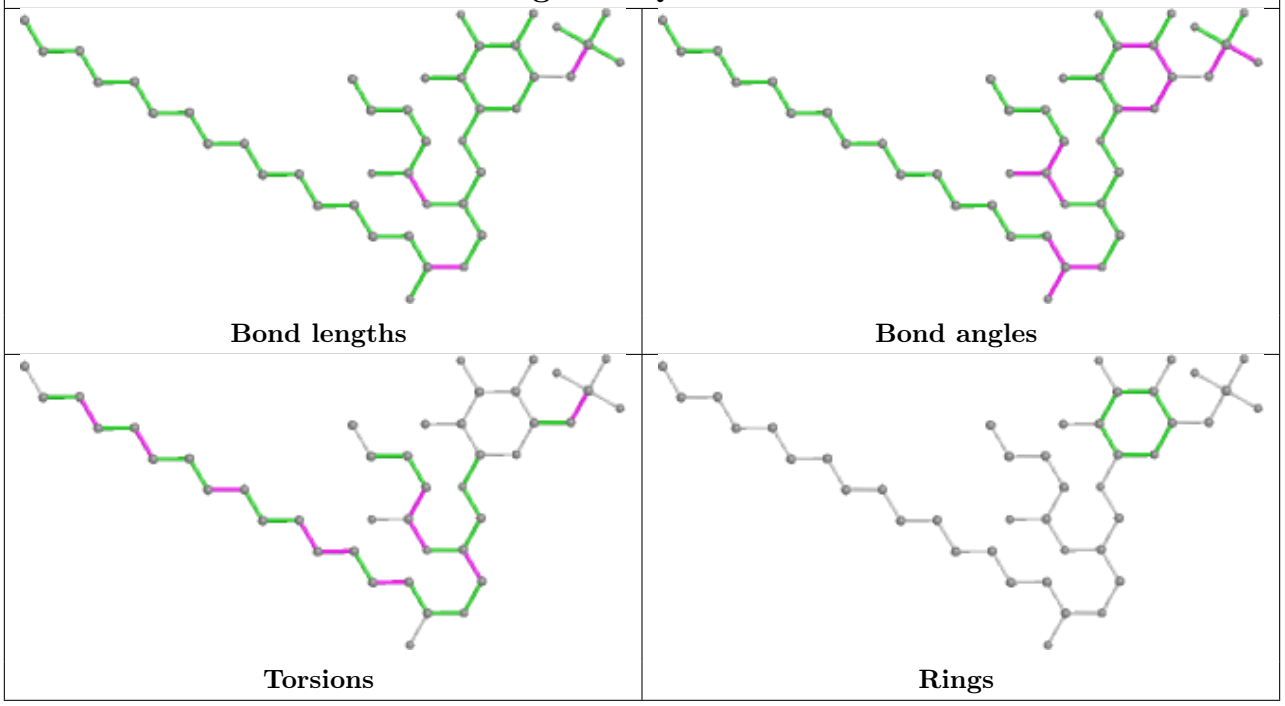


Rings

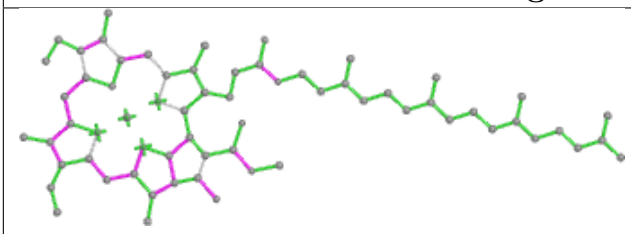
Ligand PHO a 408



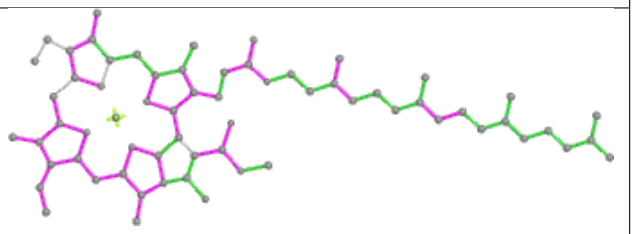
Ligand SQD f 102



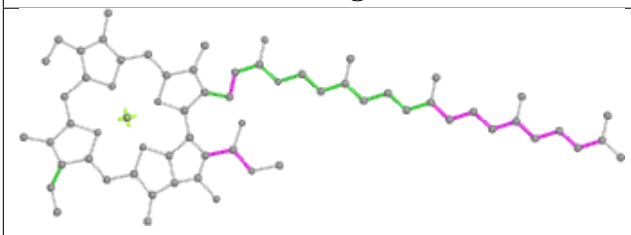
Ligand CLA b 610



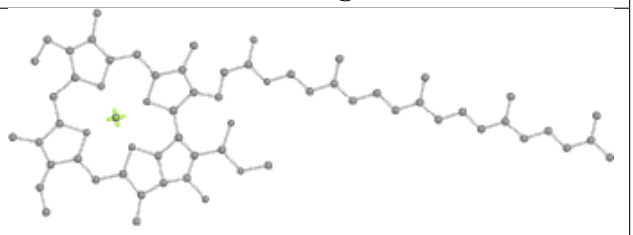
Bond lengths



Bond angles

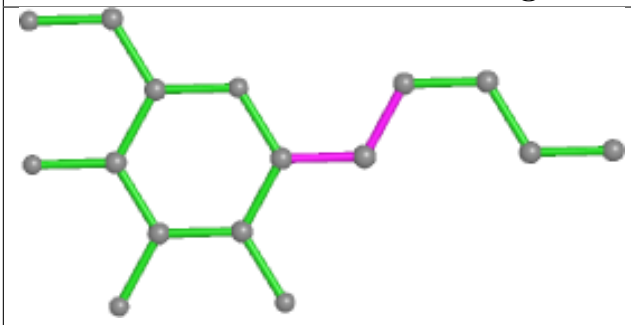


Torsions

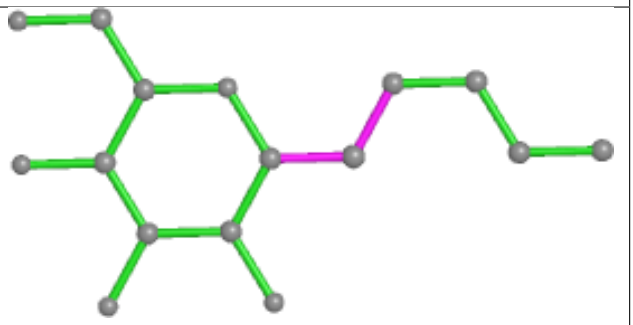


Rings

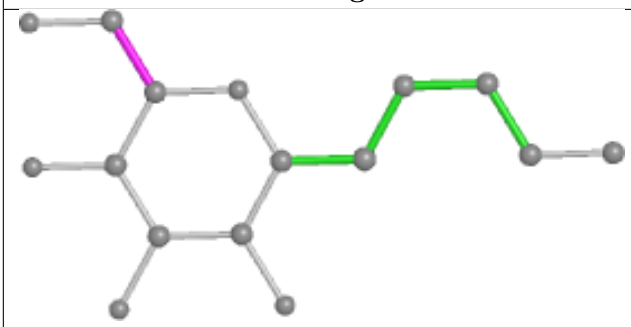
Ligand HTG D 411



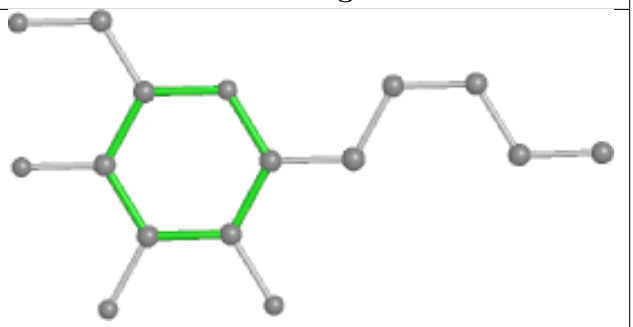
Bond lengths



Bond angles

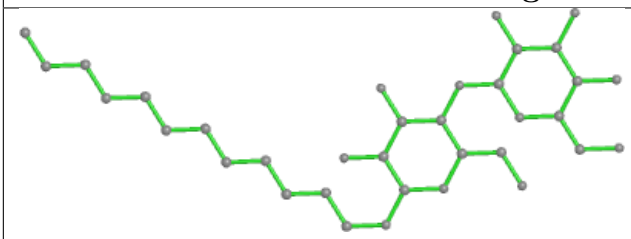


Torsions

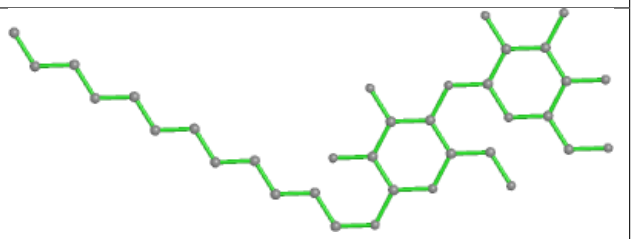


Rings

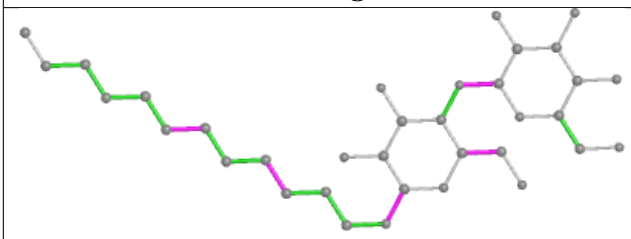
Ligand LMT E 102



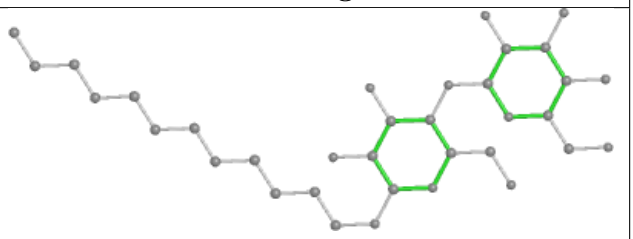
Bond lengths



Bond angles

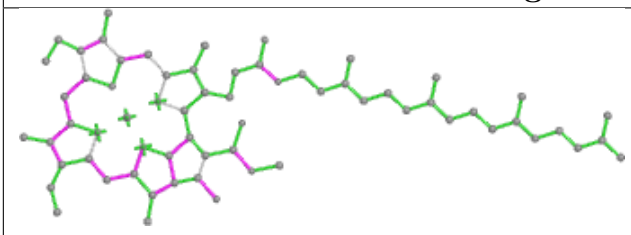


Torsions

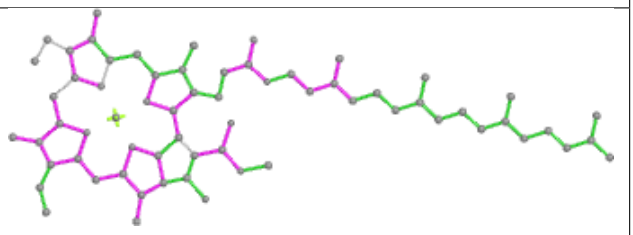


Rings

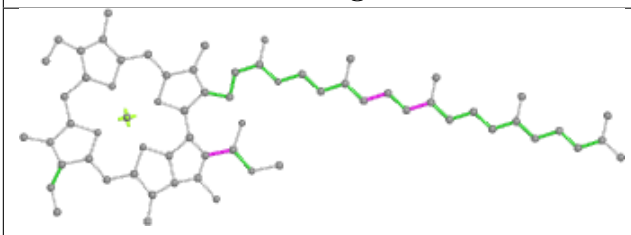
Ligand CLA B 605



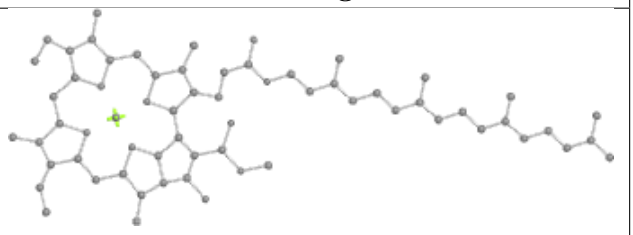
Bond lengths



Bond angles

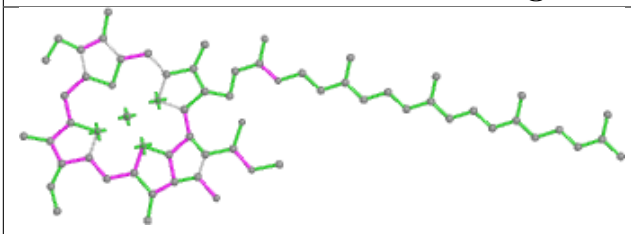


Torsions

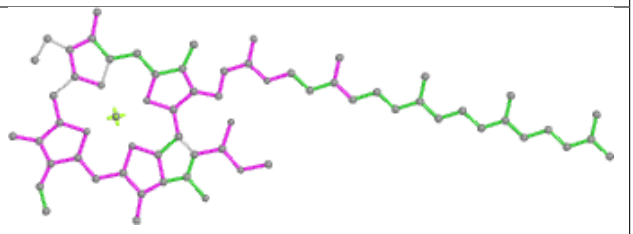


Rings

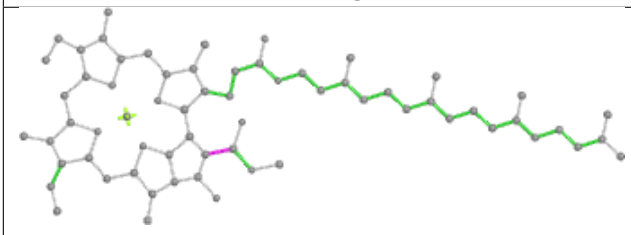
Ligand CLA b 611



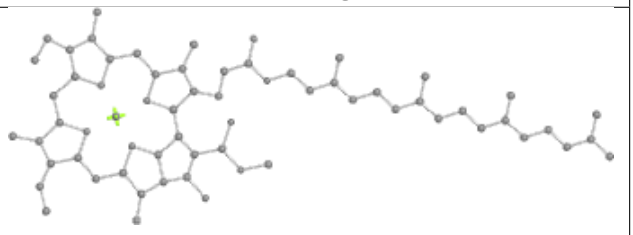
Bond lengths



Bond angles

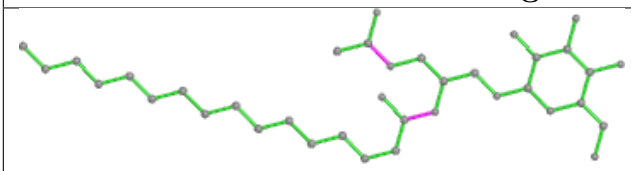


Torsions

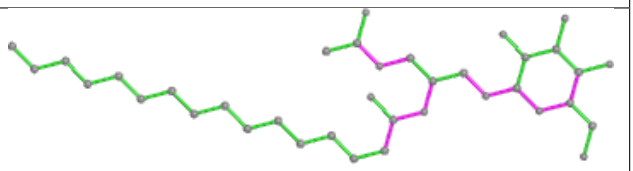


Rings

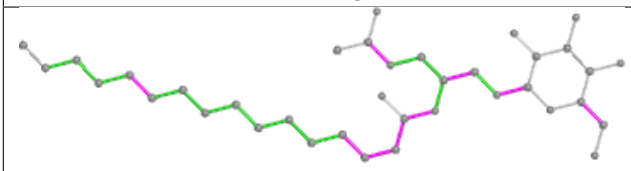
Ligand LMG Z 101



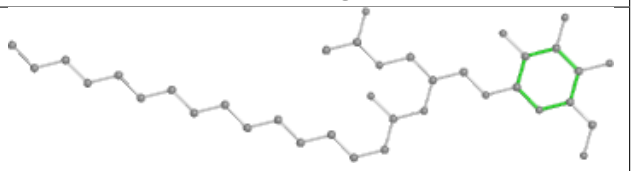
Bond lengths



Bond angles

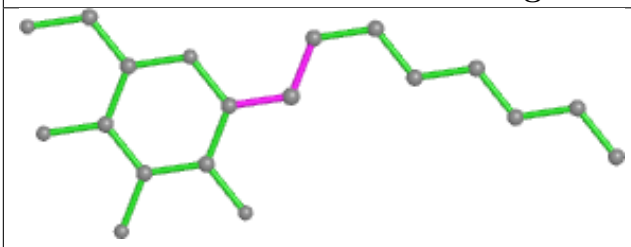


Torsions

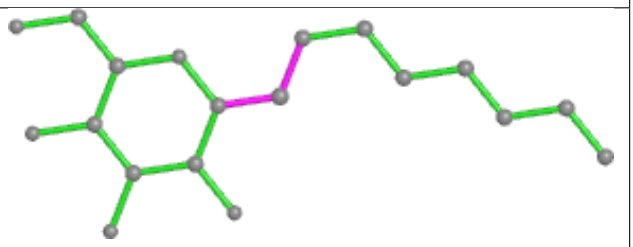


Rings

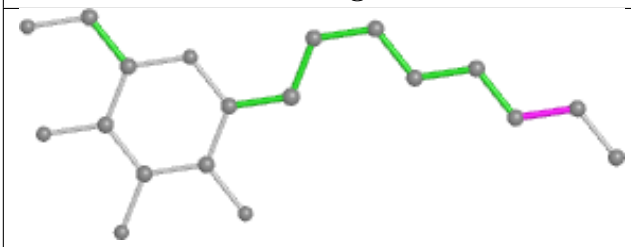
Ligand HTG b 602



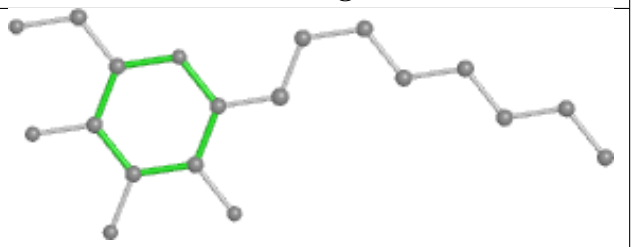
Bond lengths



Bond angles

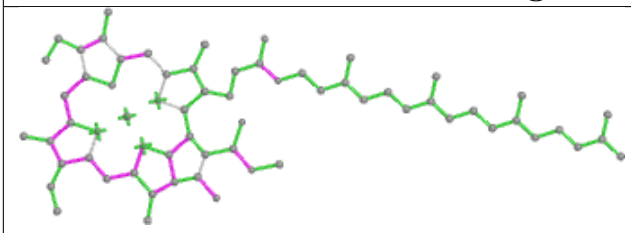


Torsions

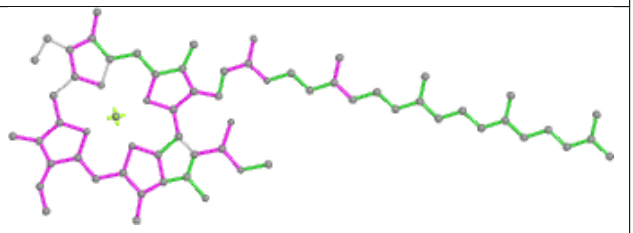


Rings

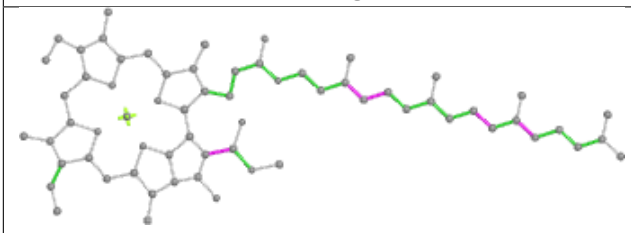
Ligand CLA d 403



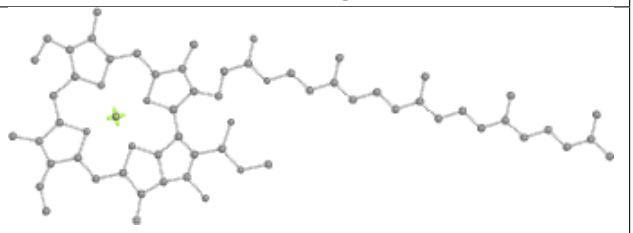
Bond lengths



Bond angles

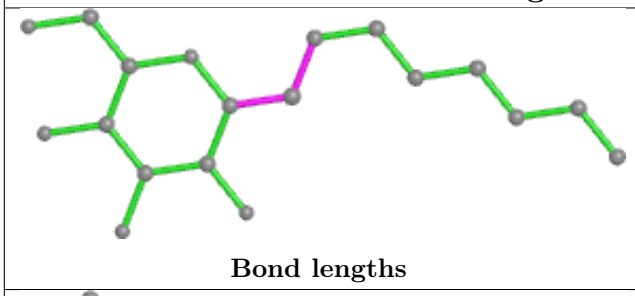


Torsions

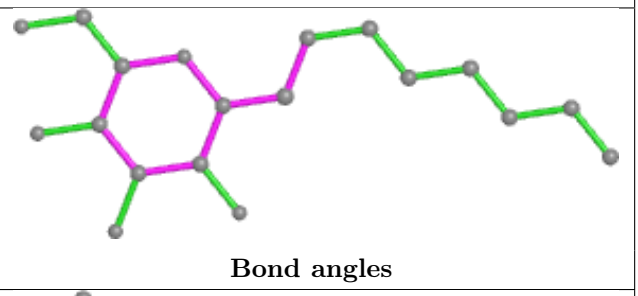


Rings

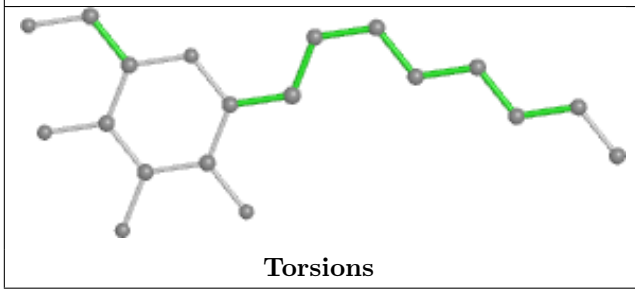
Ligand HTG c 923



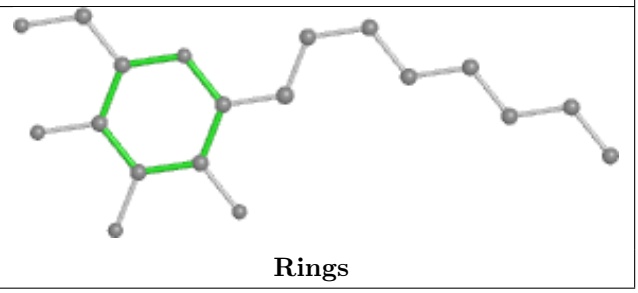
Bond lengths



Bond angles

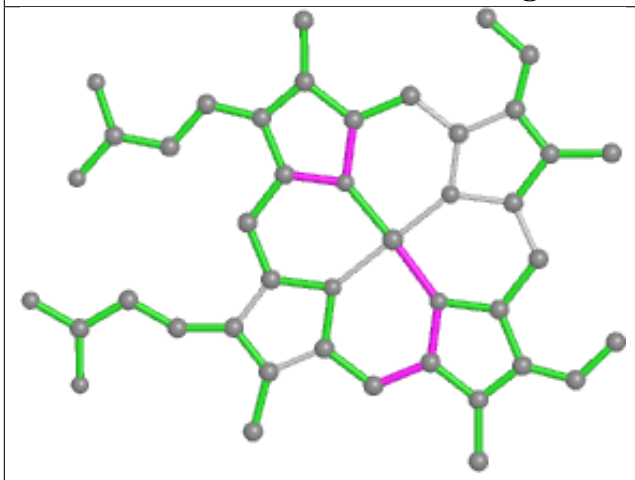


Torsions

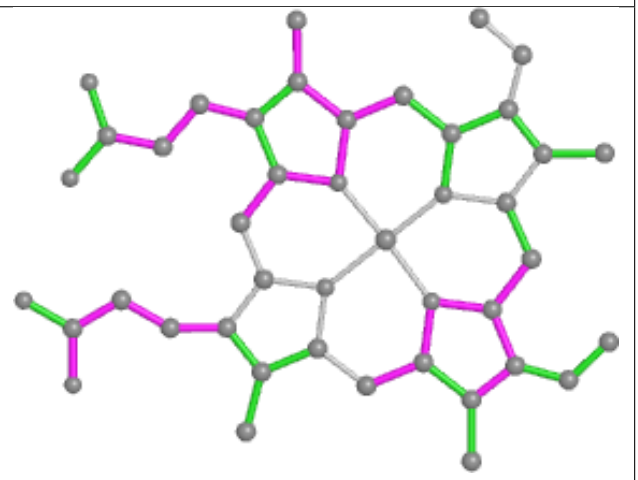


Rings

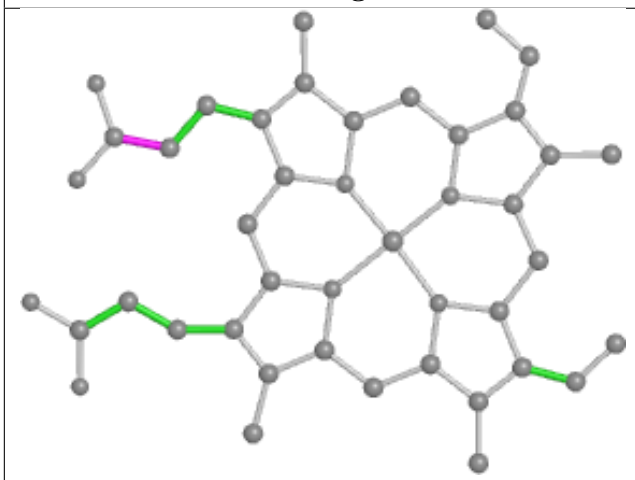
Ligand HEM E 103



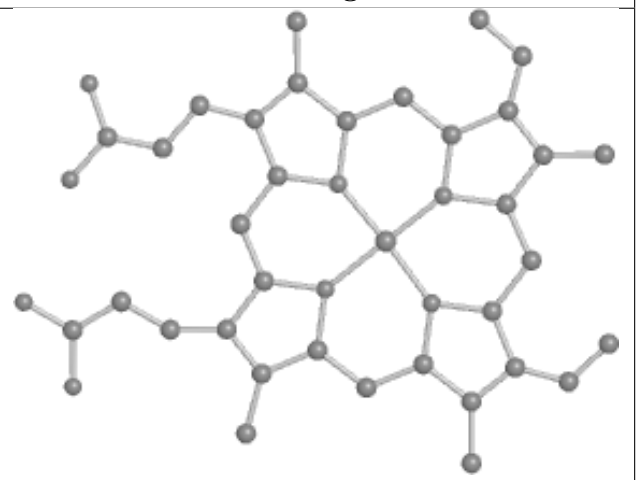
Bond lengths



Bond angles

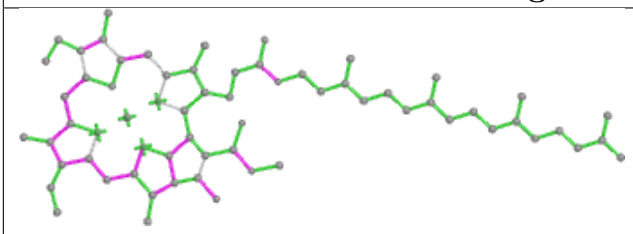


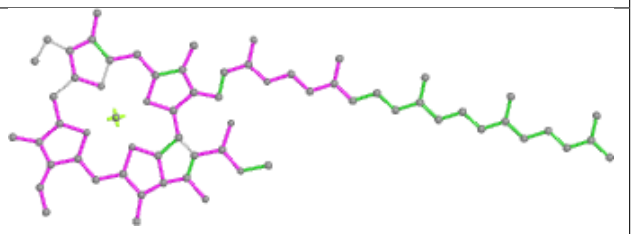
Torsions

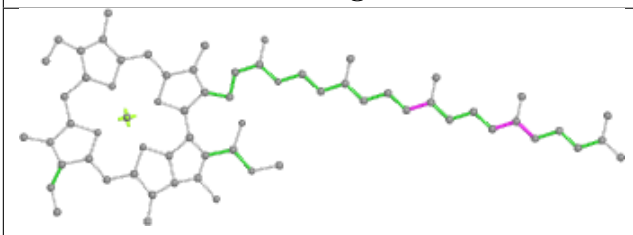


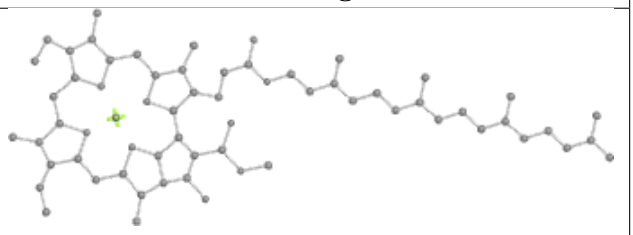
Rings

Ligand CLA a 407

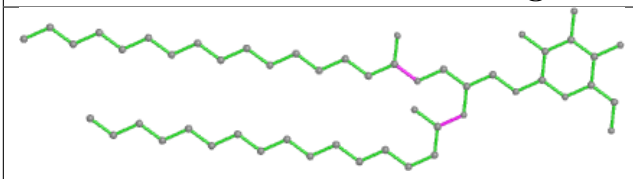

Bond lengths

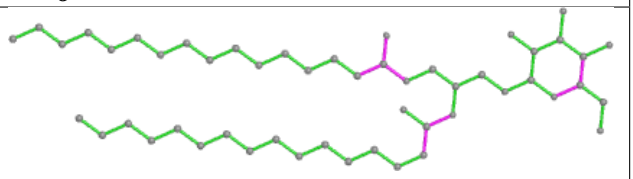

Bond angles

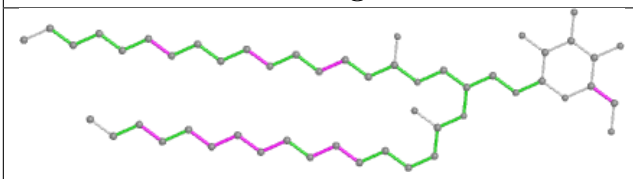

Torsions

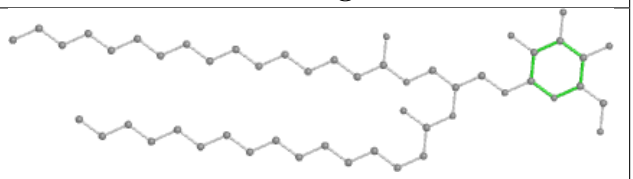

Rings

Ligand LMG j 101

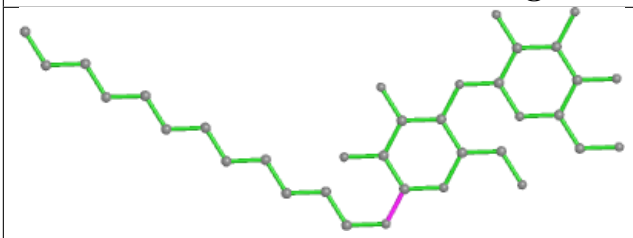

Bond lengths

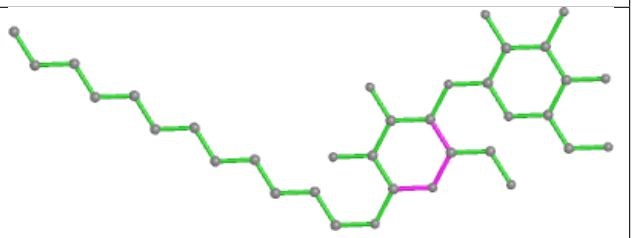

Bond angles

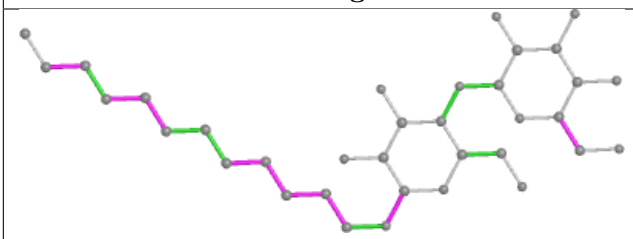

Torsions

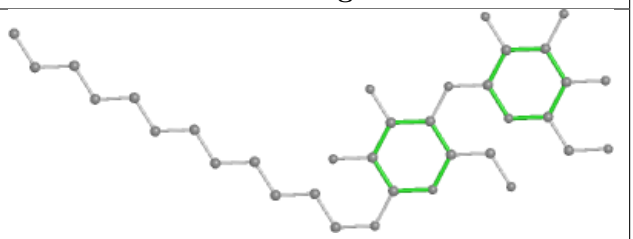

Rings

Ligand LMT a 401

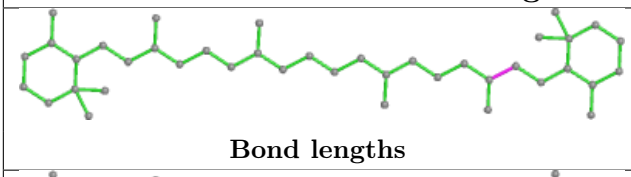

Bond lengths


Bond angles

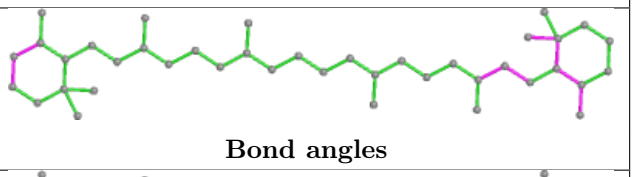

Torsions


Rings

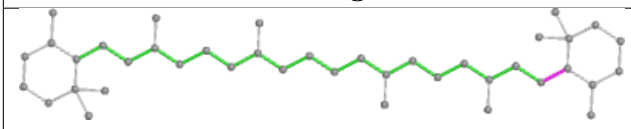
Ligand BCR B 620



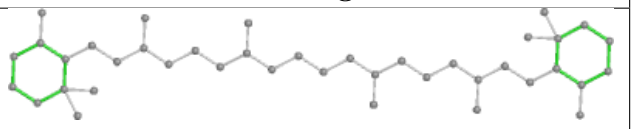
Bond lengths



Bond angles

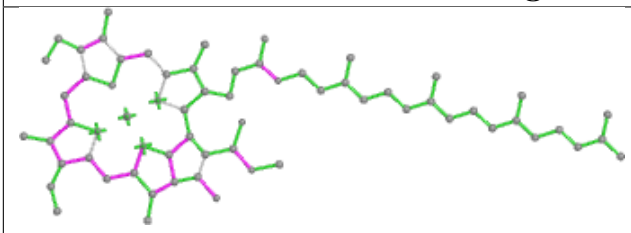


Torsions

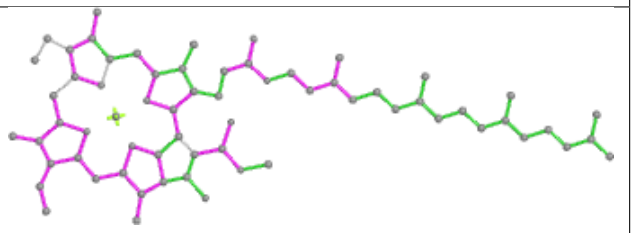


Rings

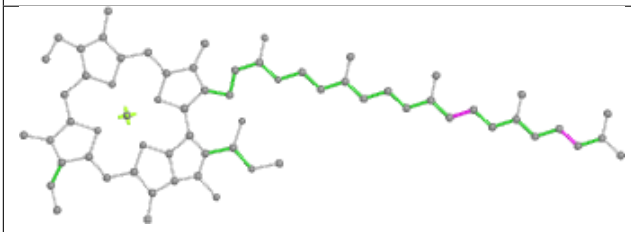
Ligand CLA B 612



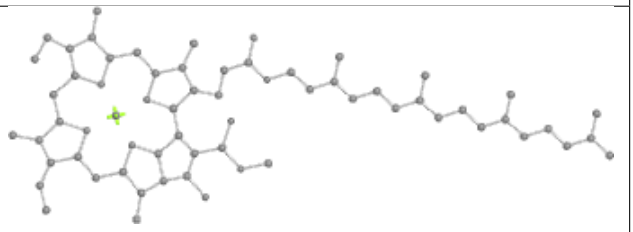
Bond lengths



Bond angles

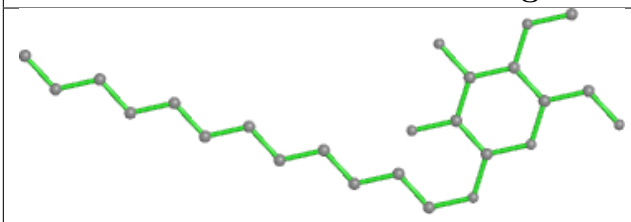


Torsions

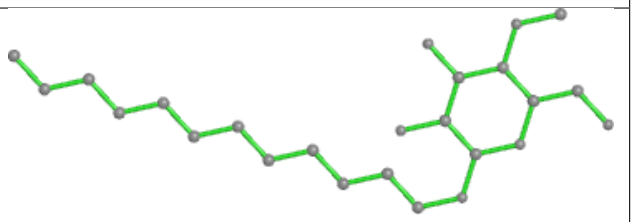


Rings

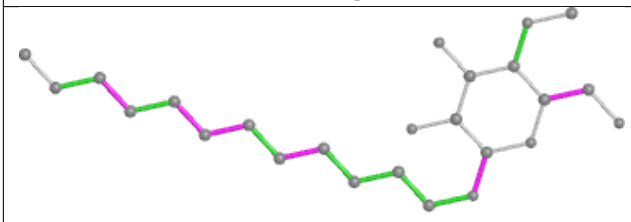
Ligand LMT B 636



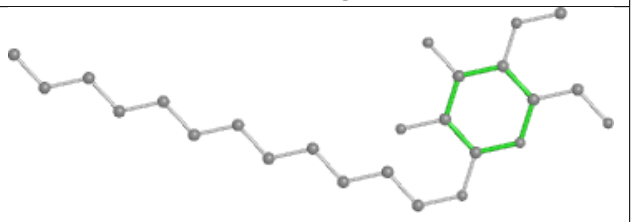
Bond lengths



Bond angles

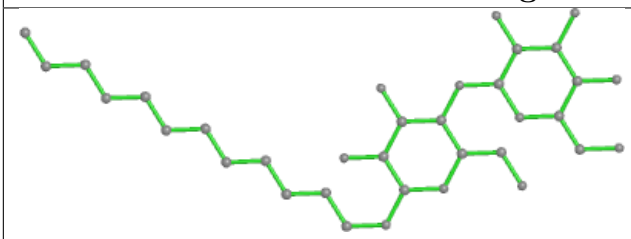


Torsions

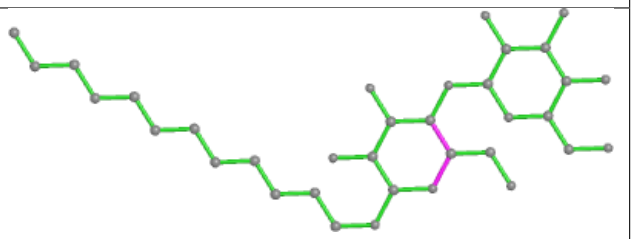


Rings

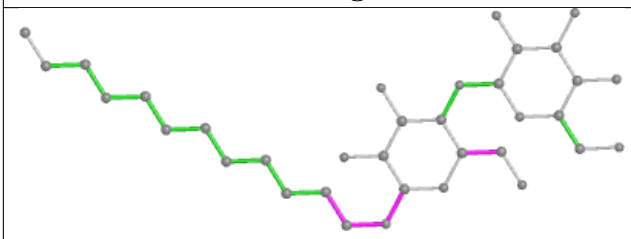
Ligand LMT m 102



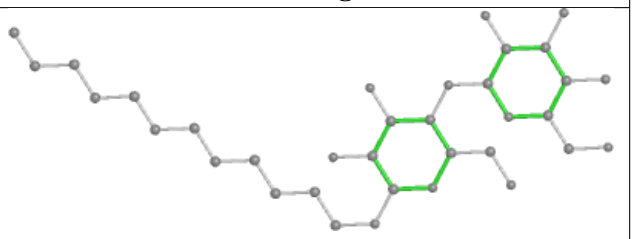
Bond lengths



Bond angles

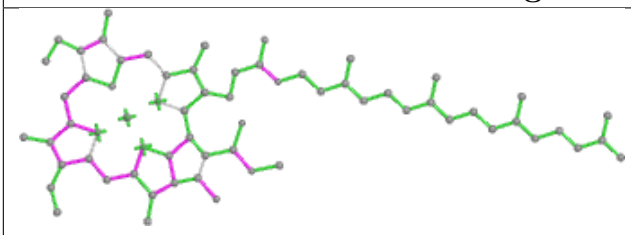


Torsions

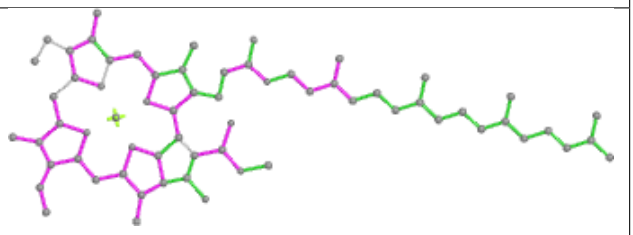


Rings

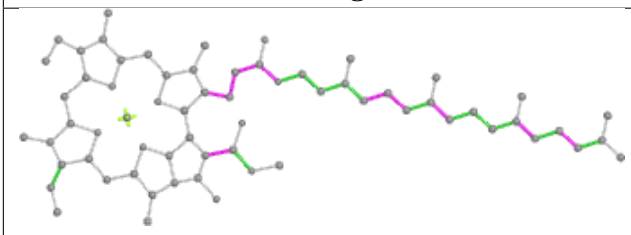
Ligand CLA B 602



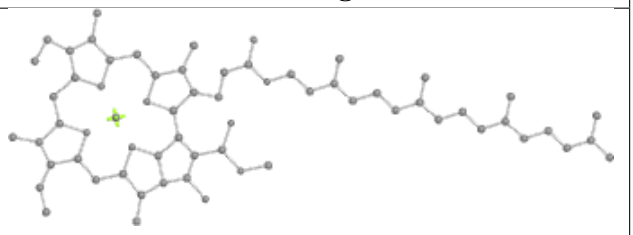
Bond lengths



Bond angles

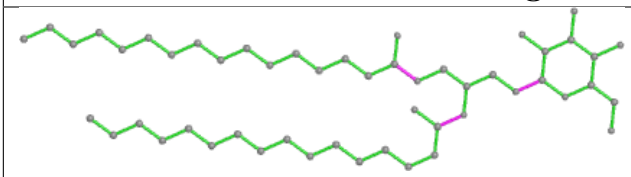


Torsions

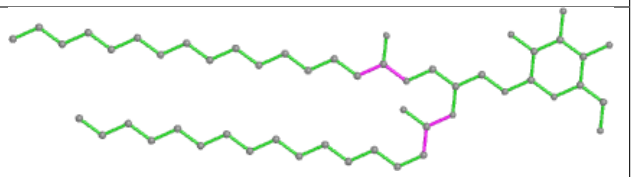


Rings

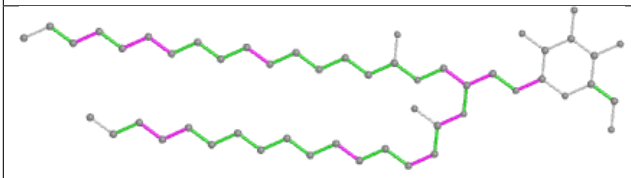
Ligand LMG c 919



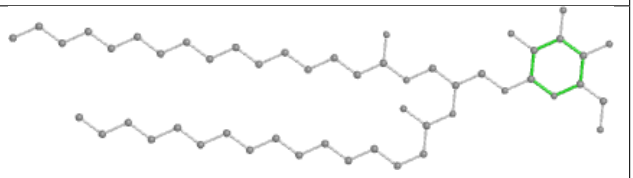
Bond lengths



Bond angles

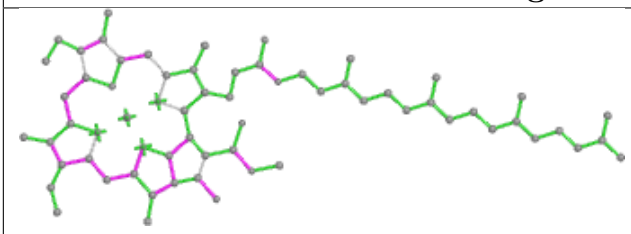


Torsions

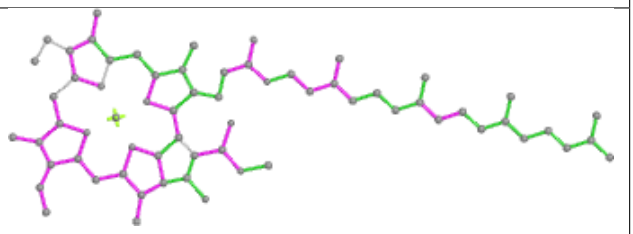


Rings

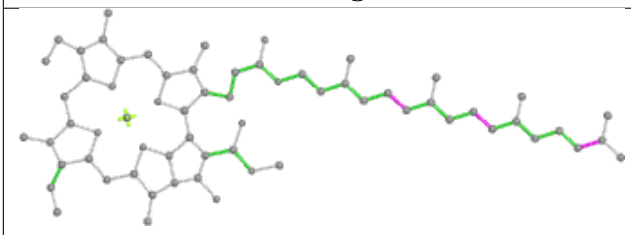
Ligand CLA b 619



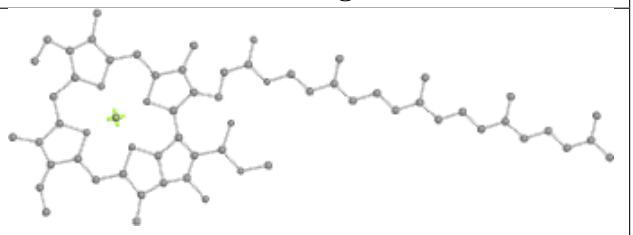
Bond lengths



Bond angles

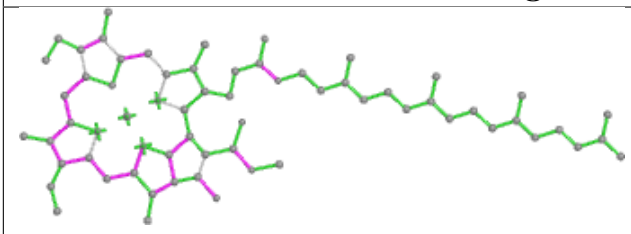


Torsions

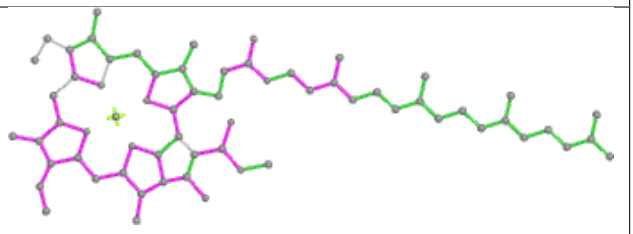


Rings

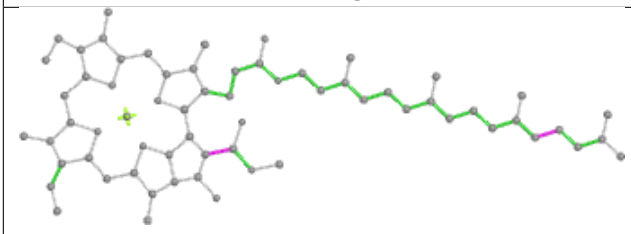
Ligand CLA C 503



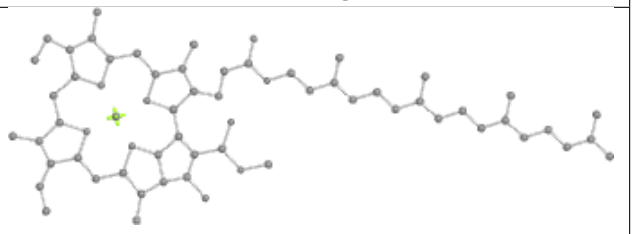
Bond lengths



Bond angles

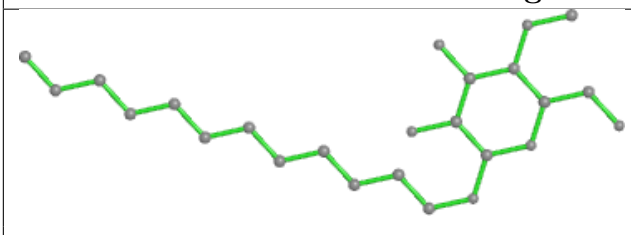


Torsions

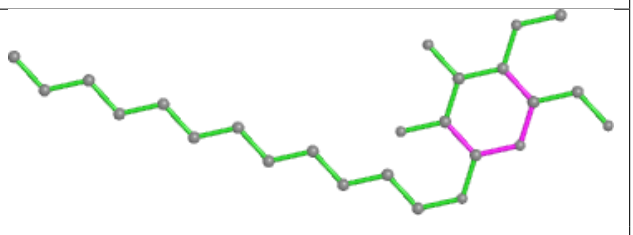


Rings

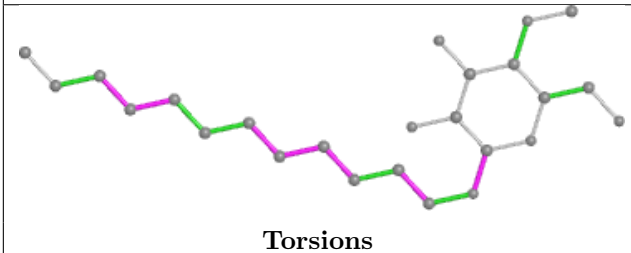
Ligand LMT b 601



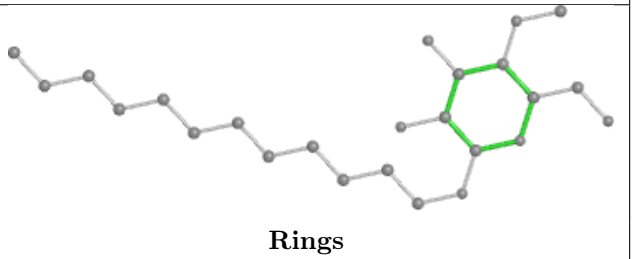
Bond lengths



Bond angles

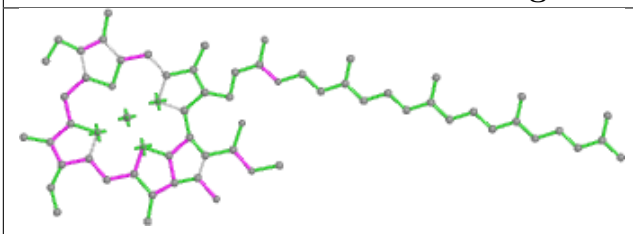


Torsions

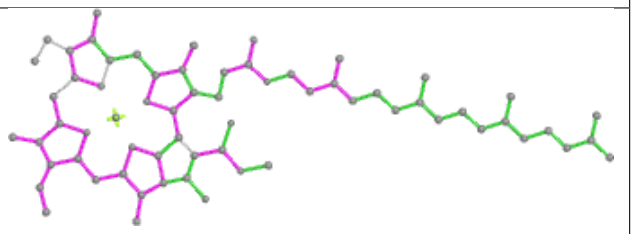


Rings

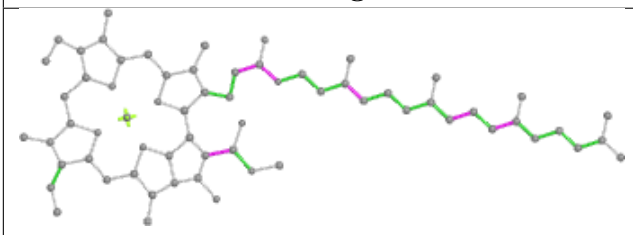
Ligand CLA c 911



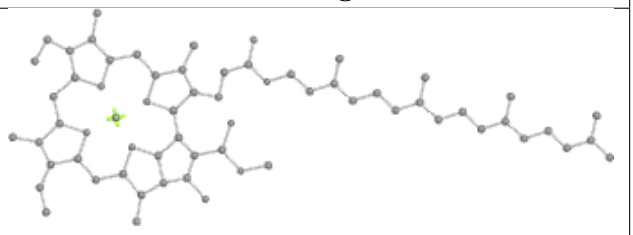
Bond lengths



Bond angles

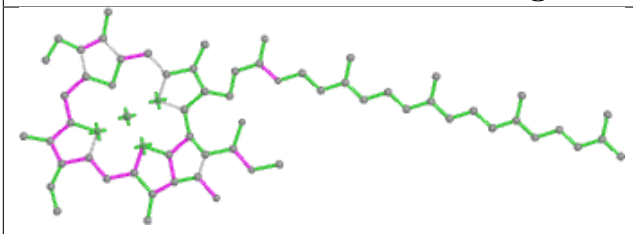


Torsions



Rings

Ligand CLA c 909



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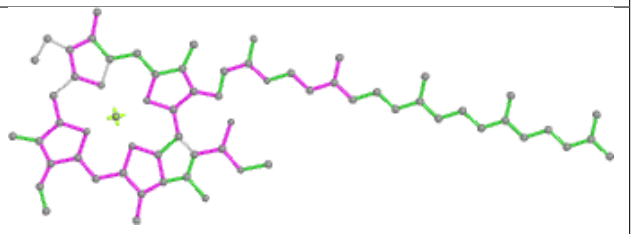

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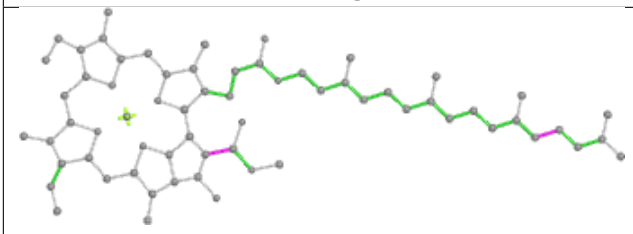
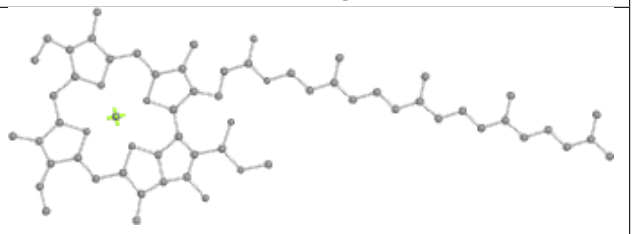
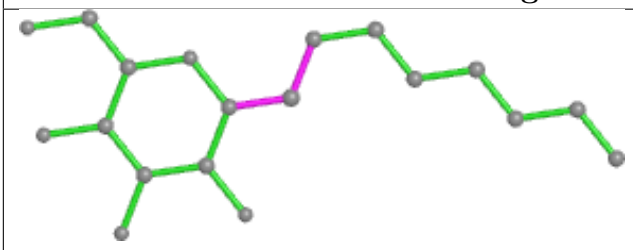


Torsions



Rings

Ligand HTG B 633



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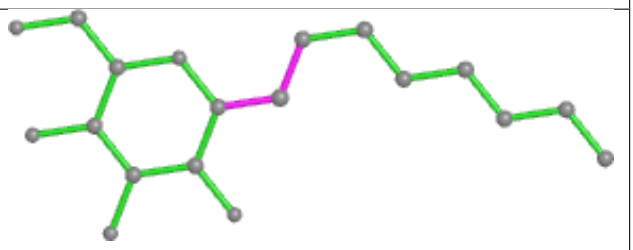
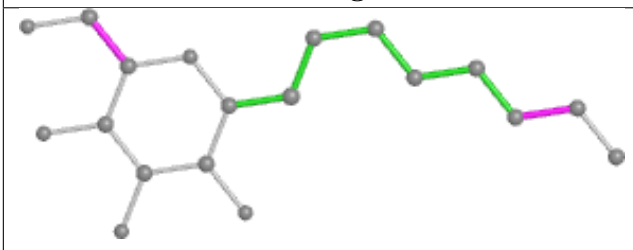
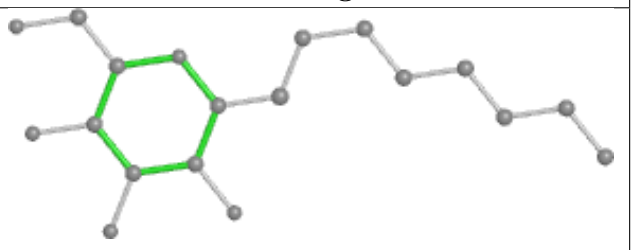


Bond angles

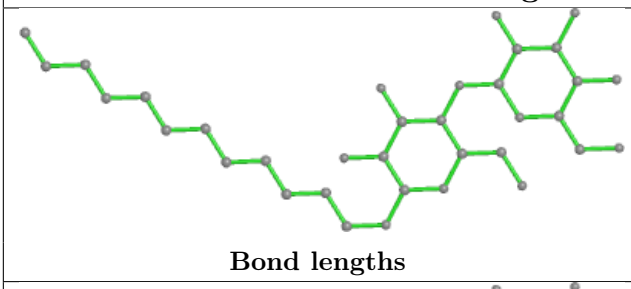


Torsions



Rings

Ligand LMT C 522



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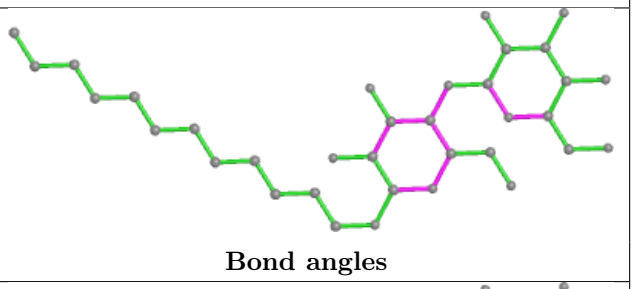
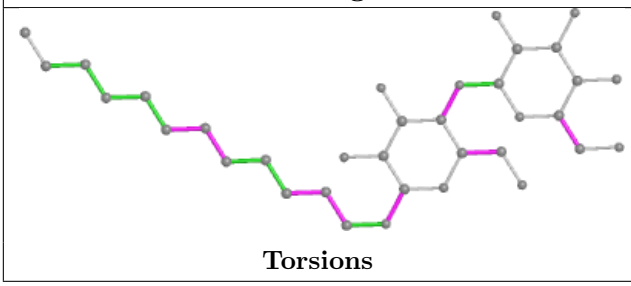


Bond angles



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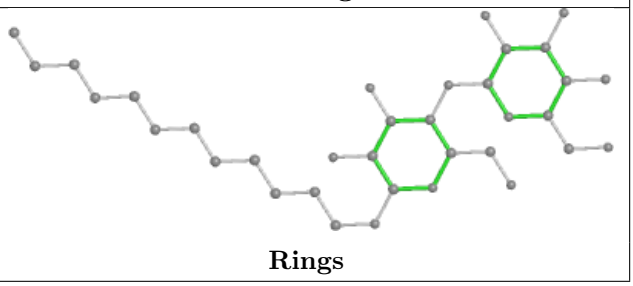
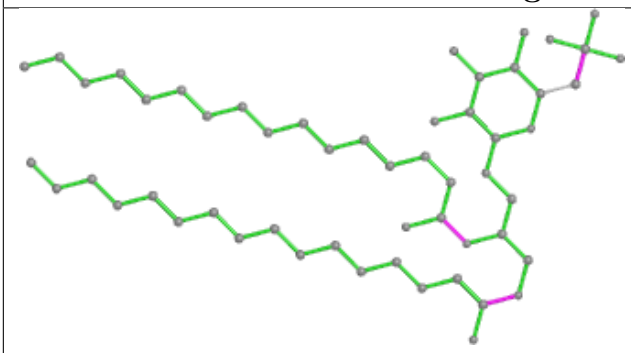
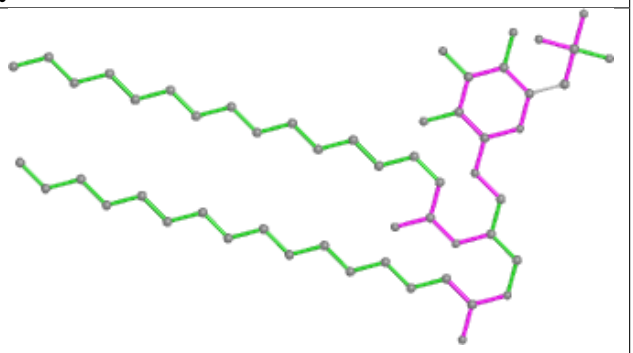


Rings

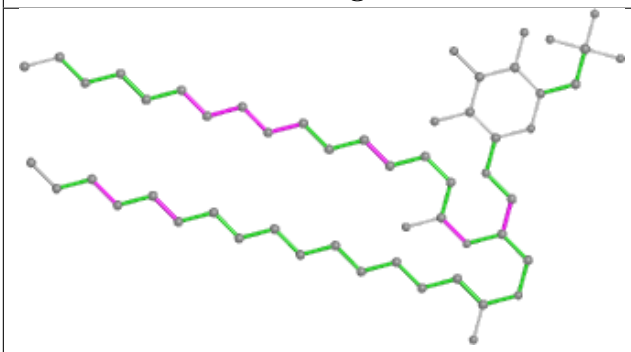
Ligand SQD A 412



Bond lengths



Bond angles



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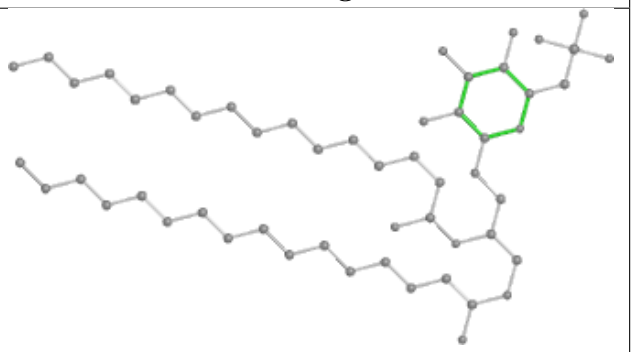
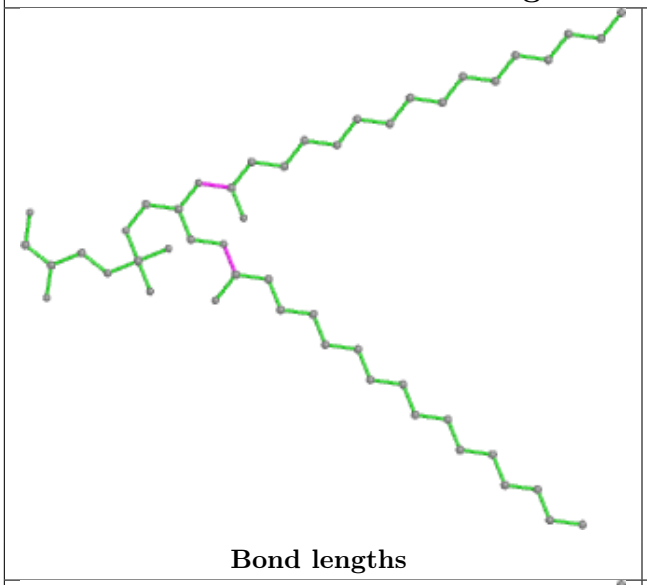


Rings

Ligand LHG D 407



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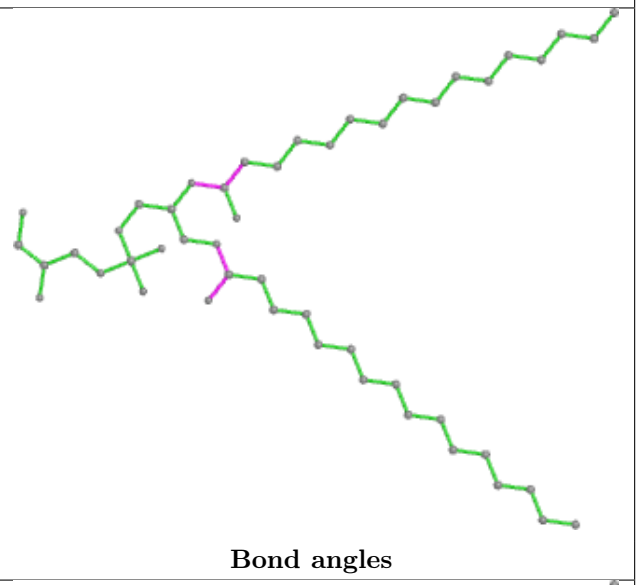
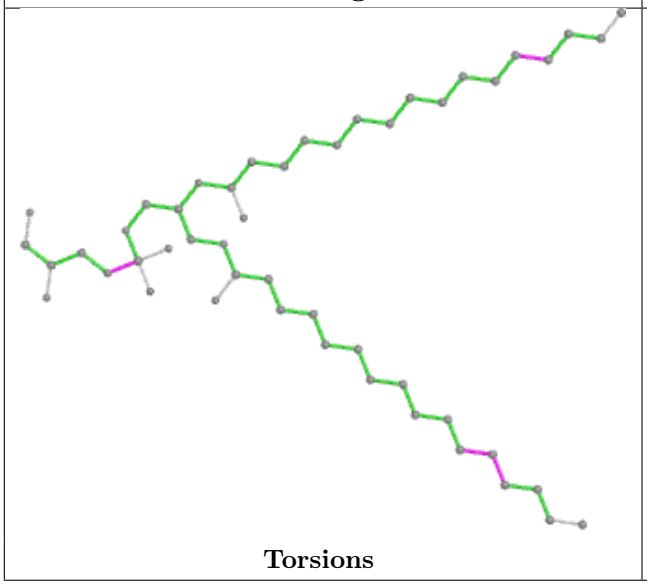


Bond angles



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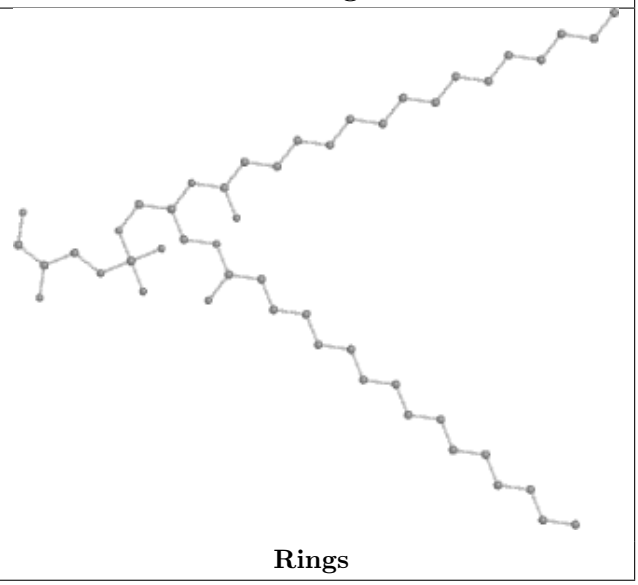
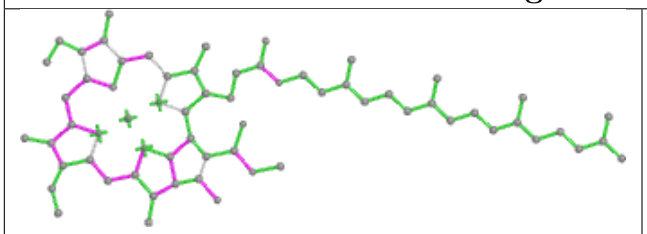


Rings

Ligand CLA B 617



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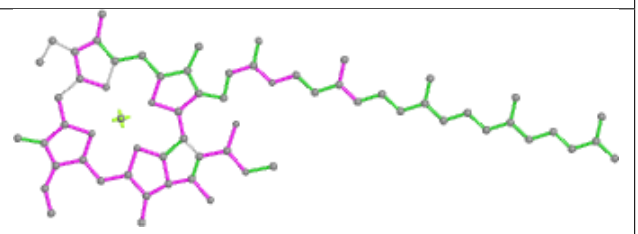
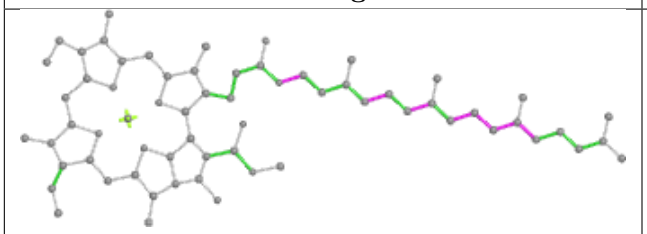


Bond angles



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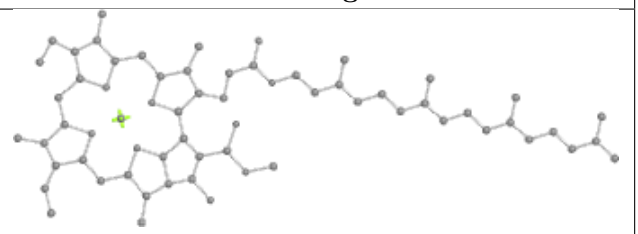
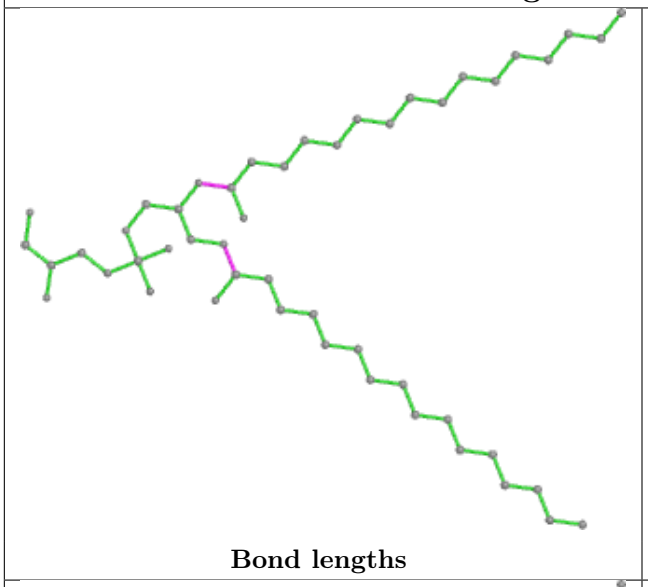
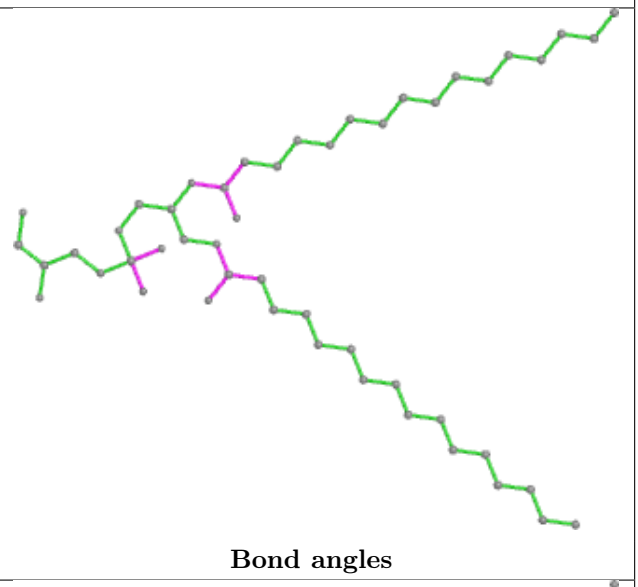


Rings

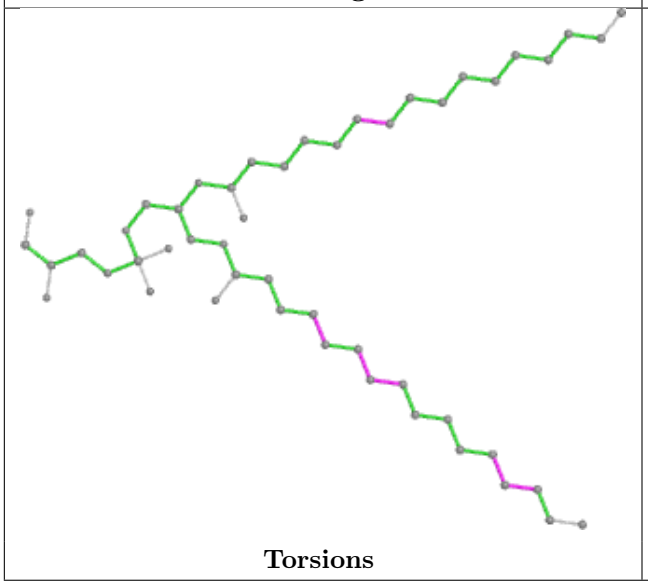
Ligand LHG D 406



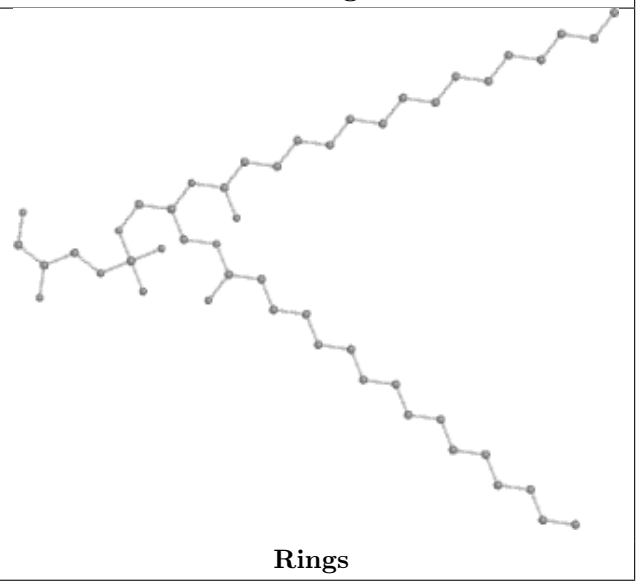
Bond lengths



Bond angles

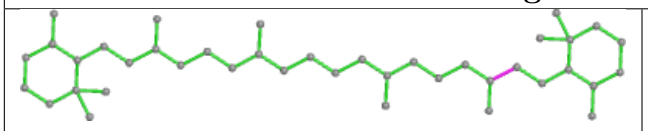


Torsions

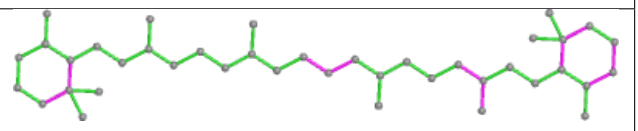


Rings

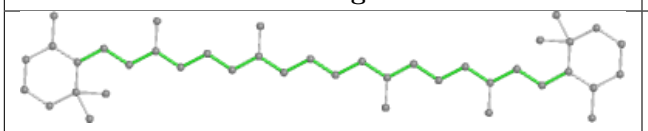
Ligand BCR B 619



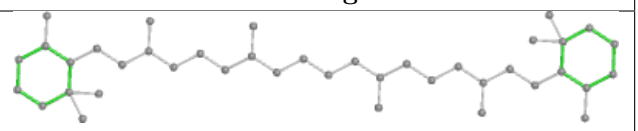
Bond lengths



Bond angles

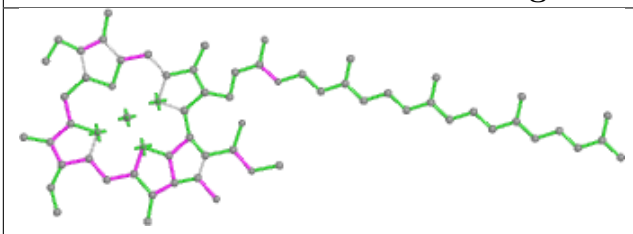


Torsions



Rings

Ligand CLA c 902



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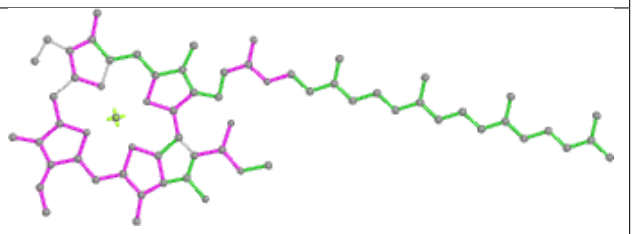
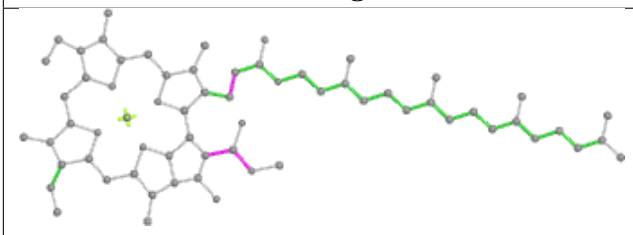
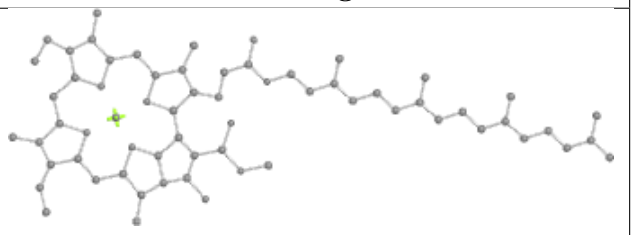


Bond angles

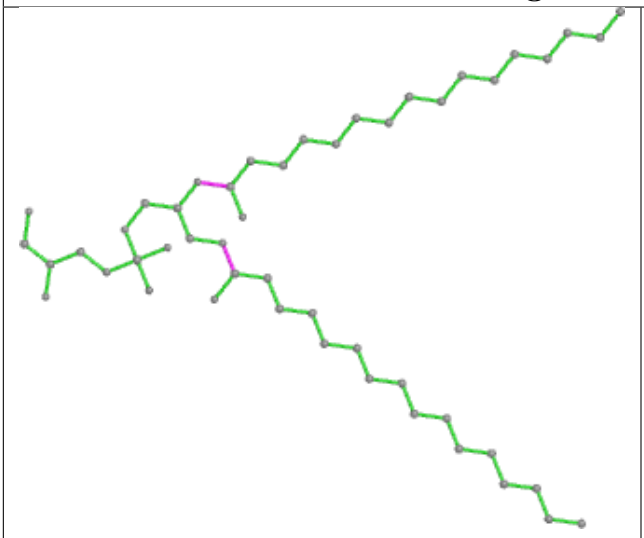


Torsions



Rings

Ligand LHG d 408



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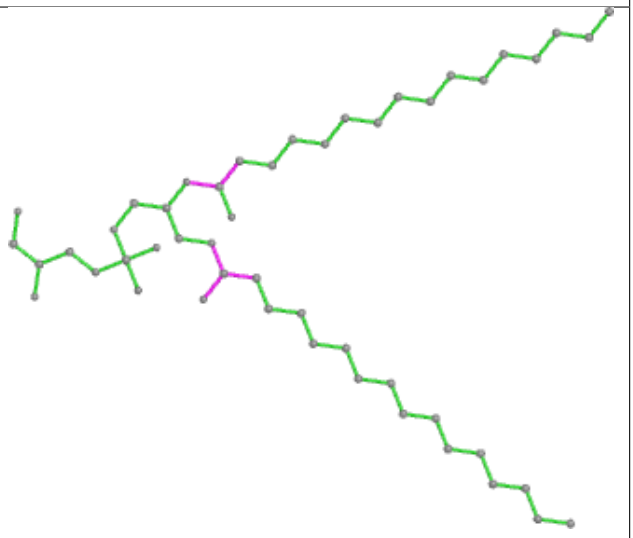
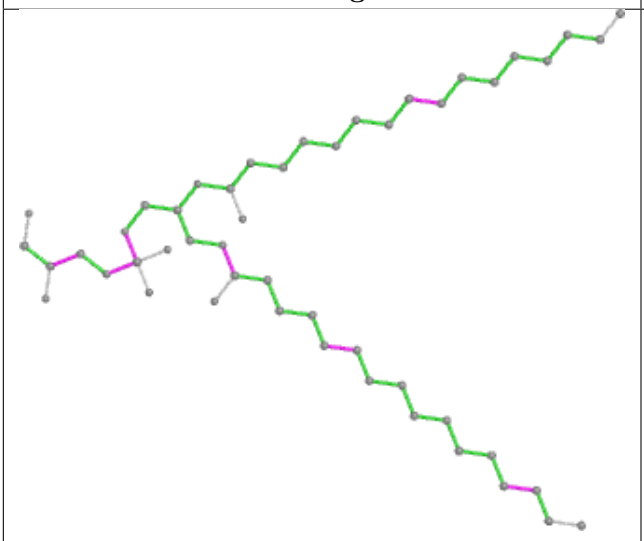
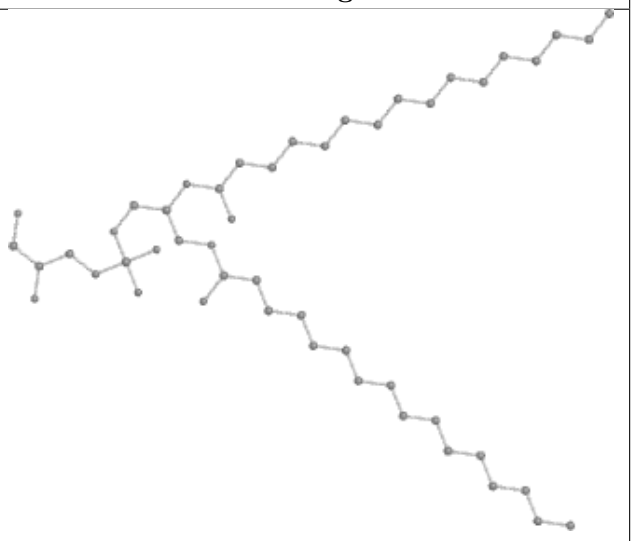


Bond angles

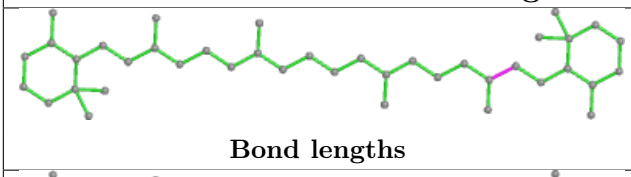


Torsions

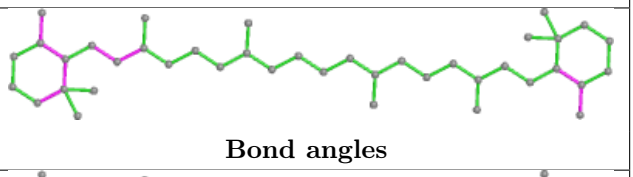


Rings

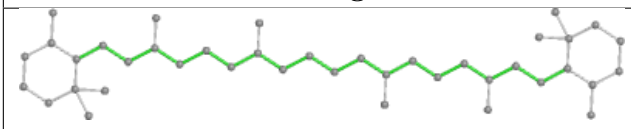
Ligand BCR C 515



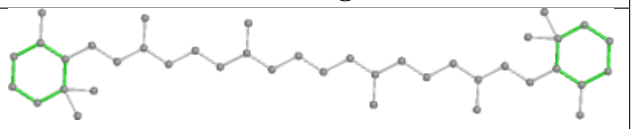
Bond lengths



Bond angles

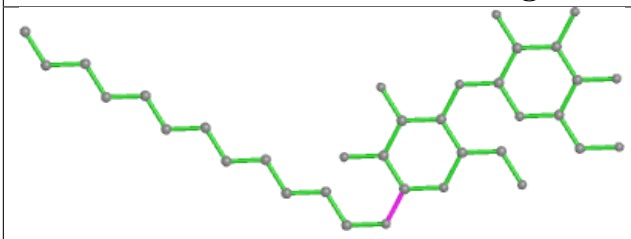


Torsions

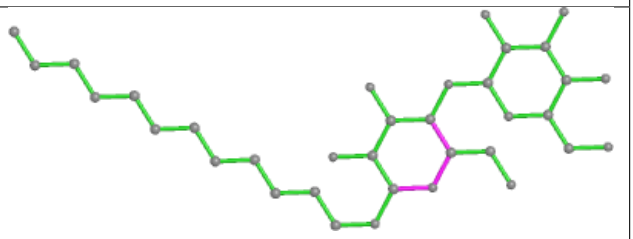


Rings

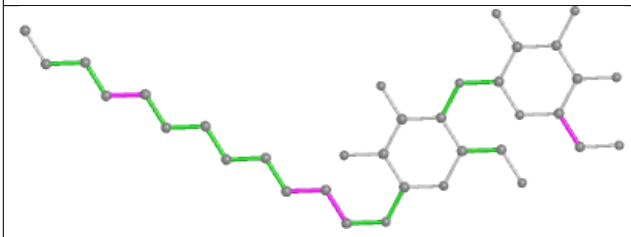
Ligand LMT A 417



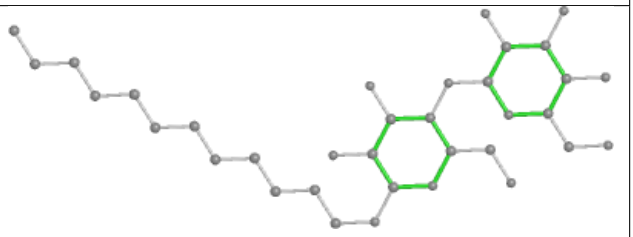
Bond lengths



Bond angles

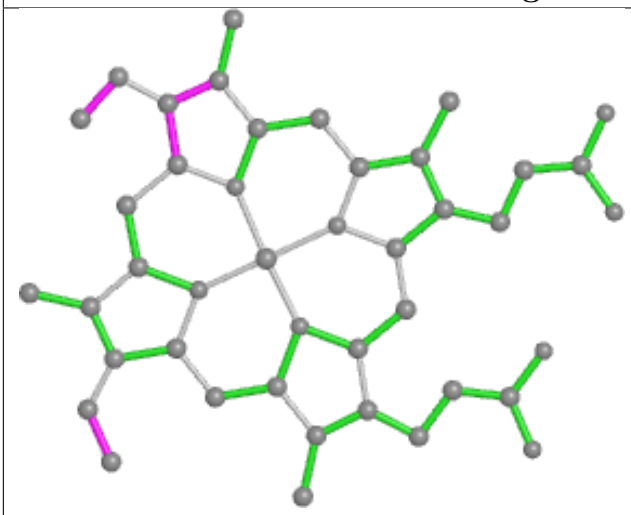


Torsions

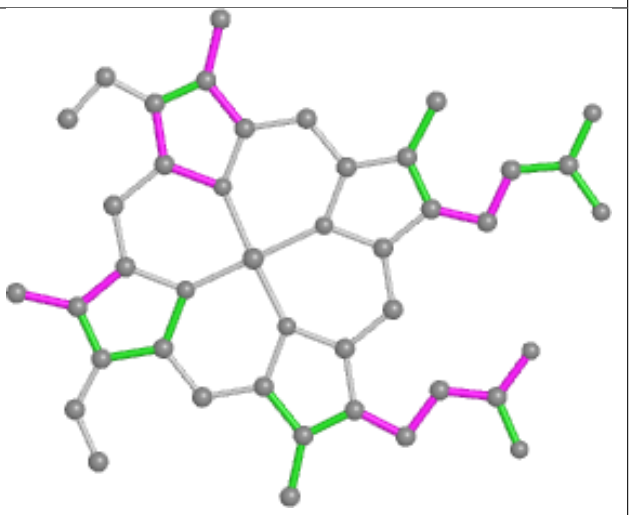


Rings

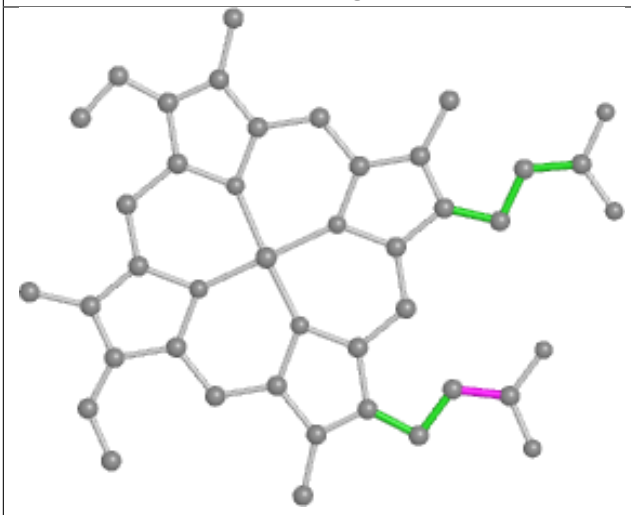
Ligand HEC V 201



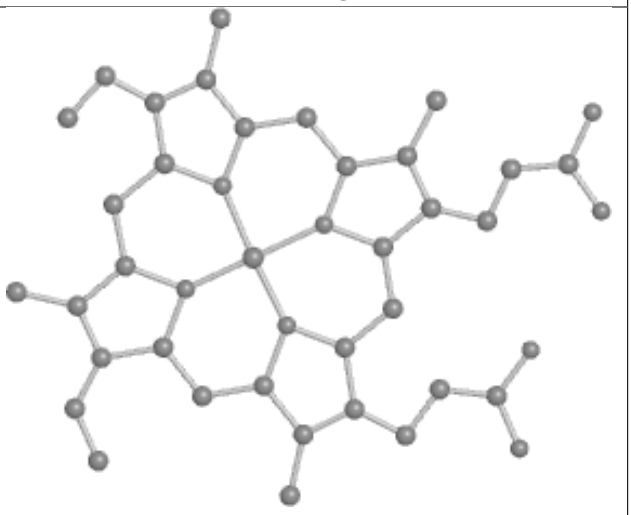
Bond lengths



Bond angles

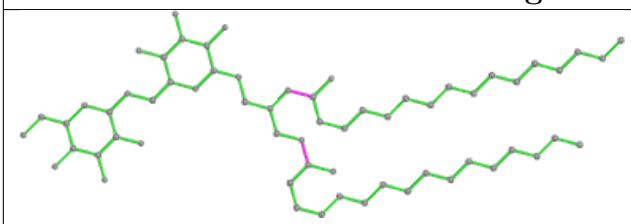


Torsions

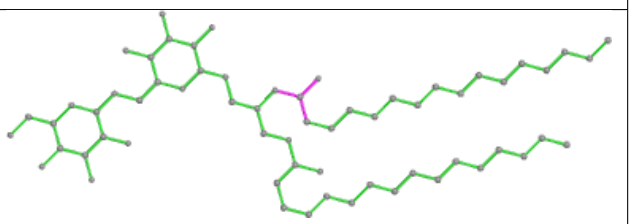


Rings

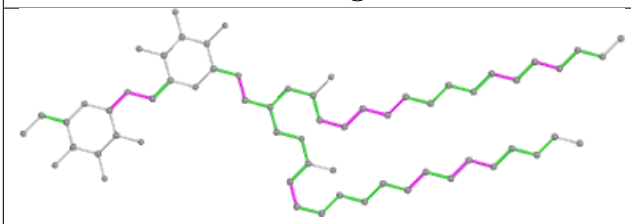
Ligand DGD c 917



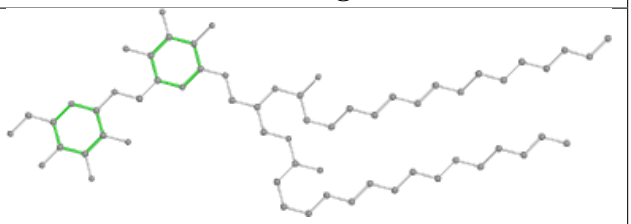
Bond lengths



Bond angles

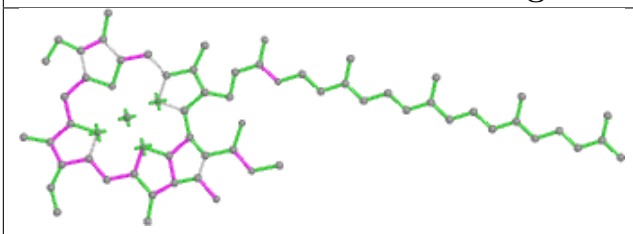


Torsions

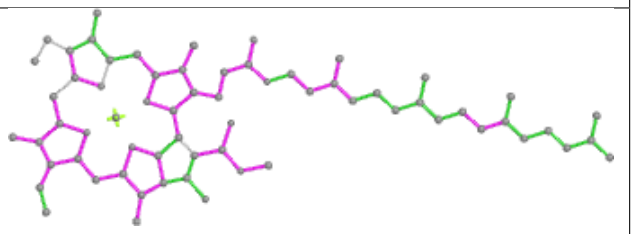


Rings

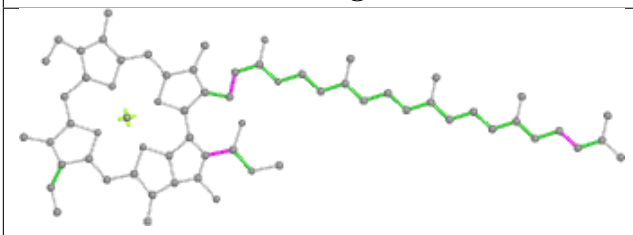
Ligand CLA b 614



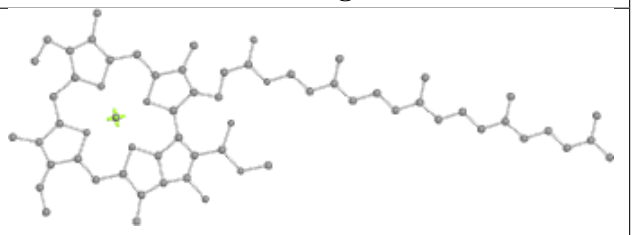
Bond lengths



Bond angles

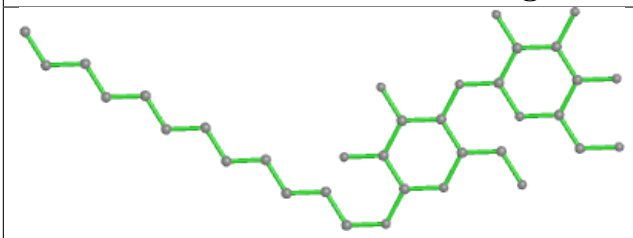


Torsions

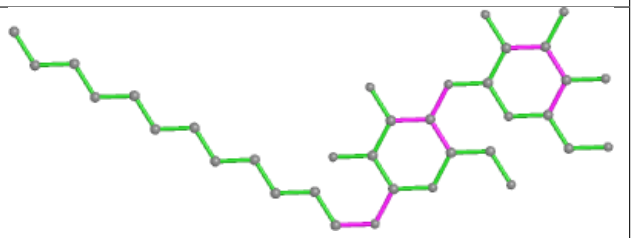


Rings

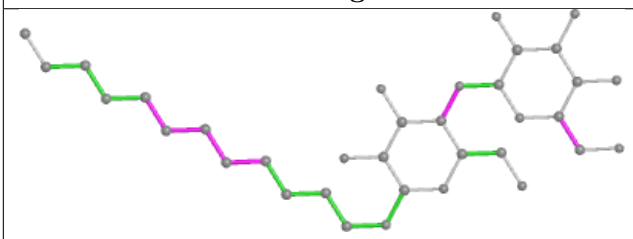
Ligand LMT B 623



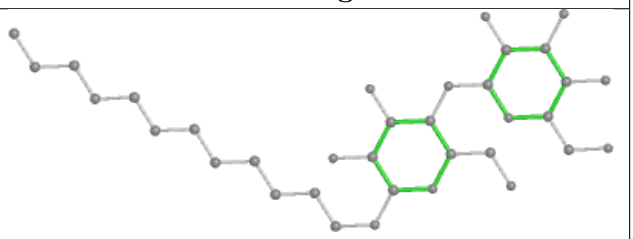
Bond lengths



Bond angles

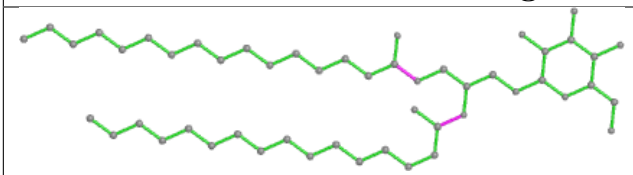


Torsions

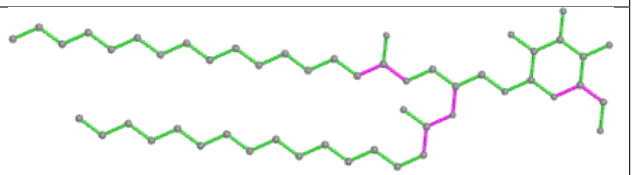


Rings

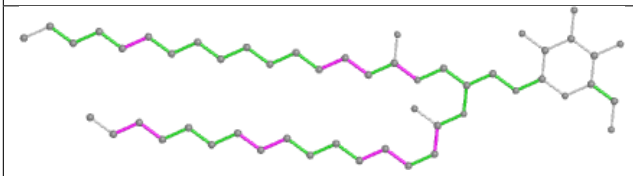
Ligand LMG C 520



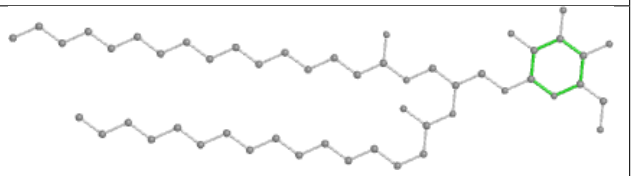
Bond lengths



Bond angles

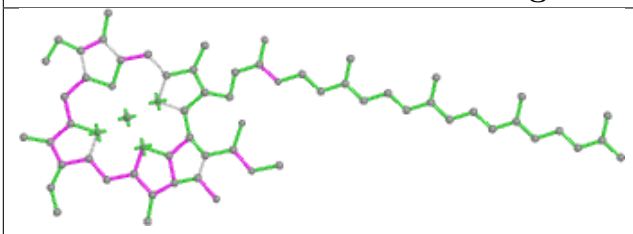


Torsions

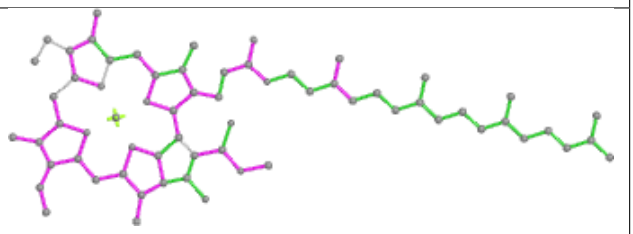


Rings

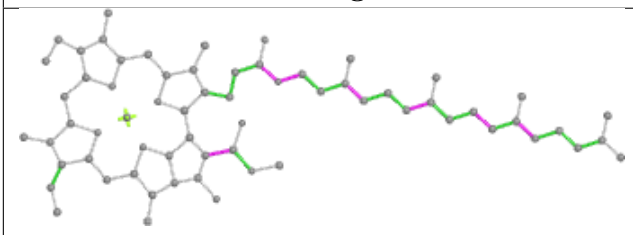
Ligand CLA c 914



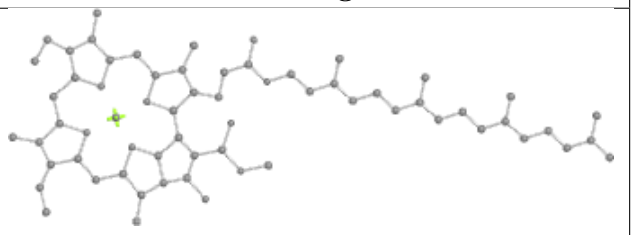
Bond lengths



Bond angles

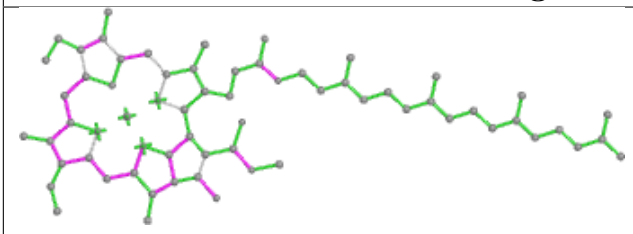


Torsions

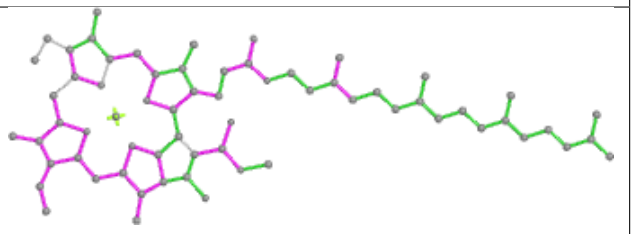


Rings

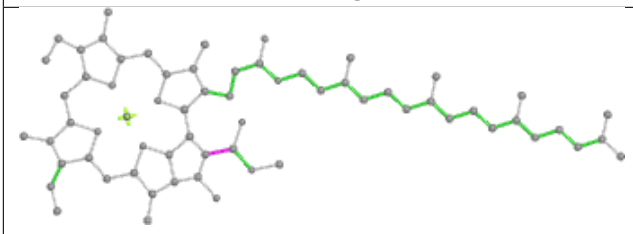
Ligand CLA c 908



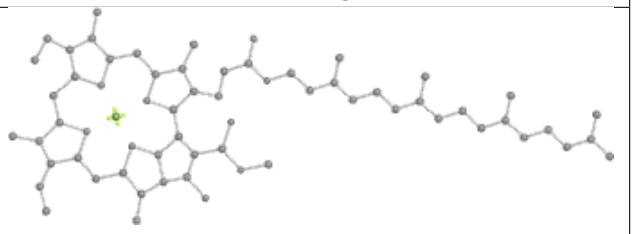
Bond lengths



Bond angles

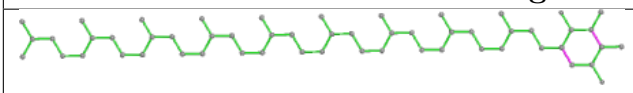


Torsions

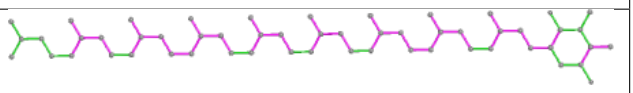


Rings

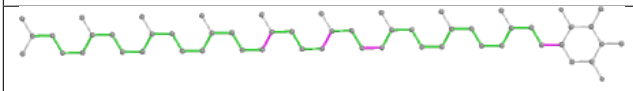
Ligand PL9 A 419



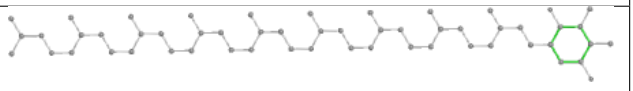
Bond lengths



Bond angles

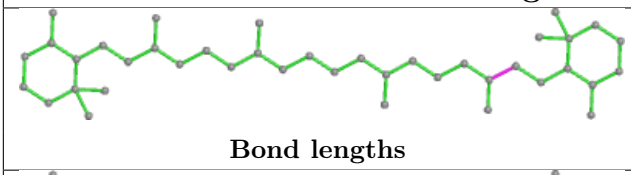


Torsions

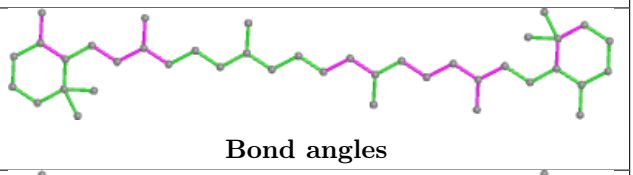


Rings

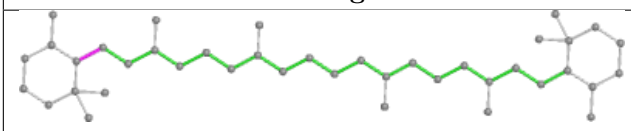
Ligand BCR B 618



Bond lengths



Bond angles



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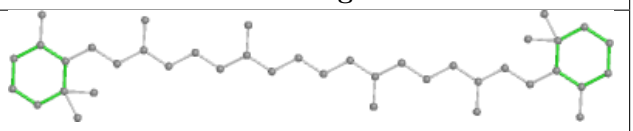
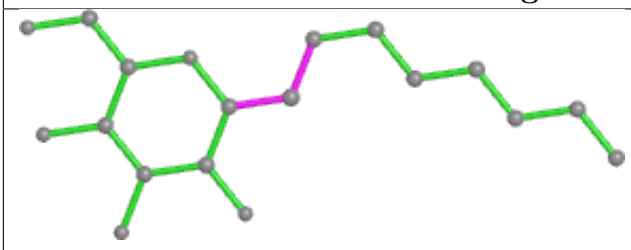


Rings

Ligand HTG C 523



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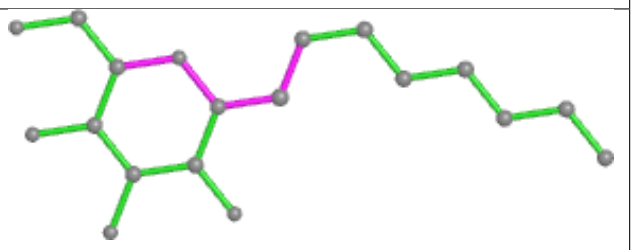
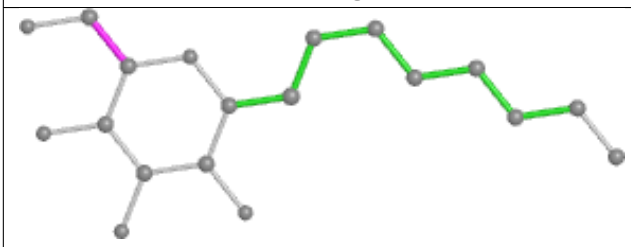
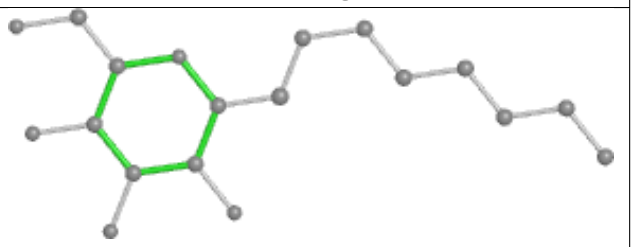


Bond angles

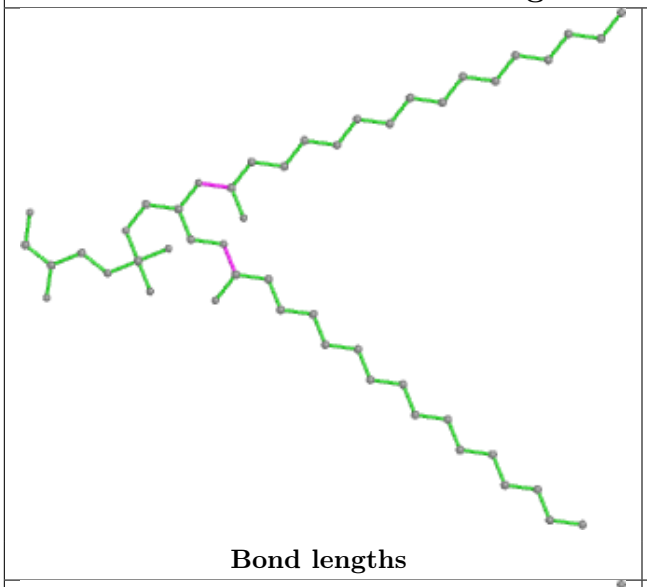


Torsions

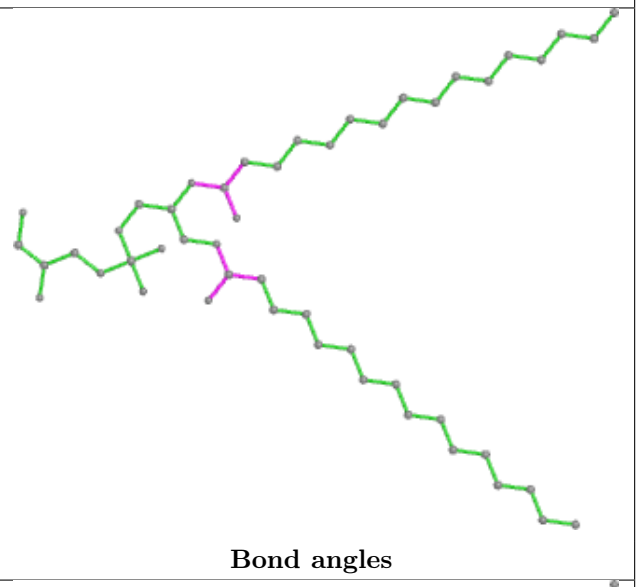


Rings

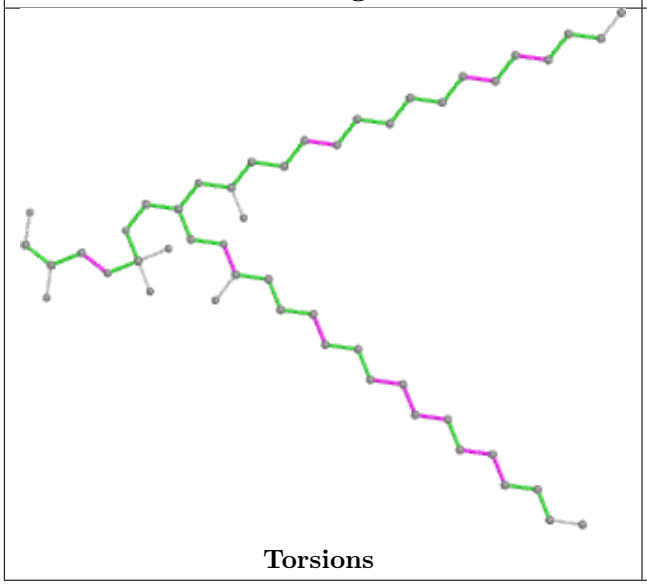
Ligand LHG d 409



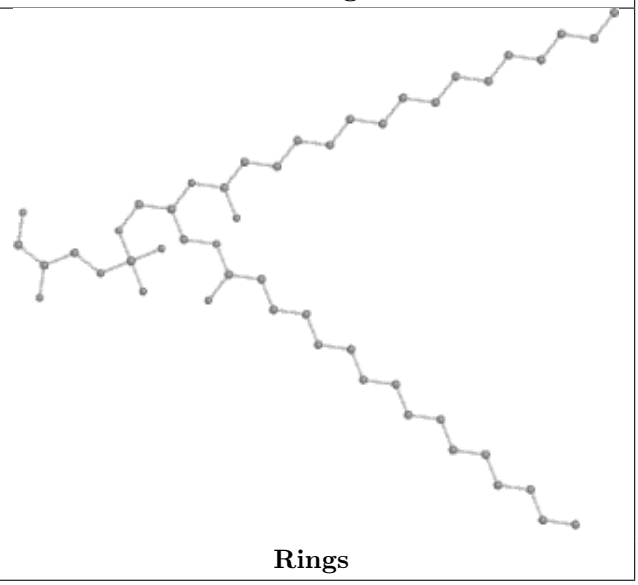
Bond lengths



Bond angles

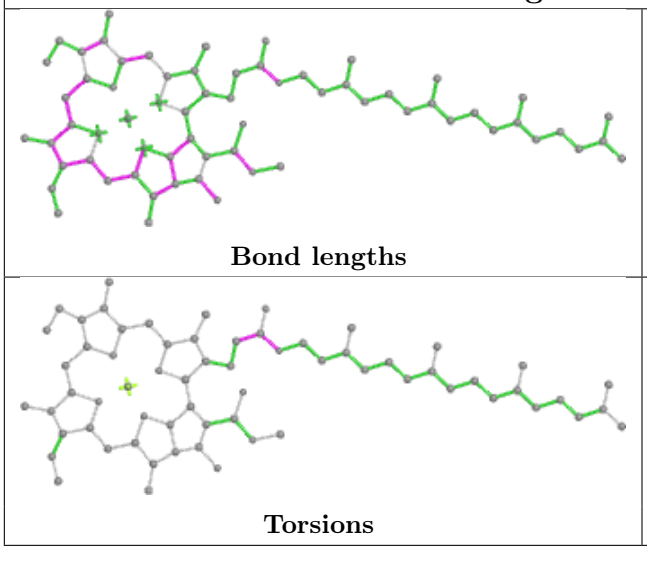


Torsions

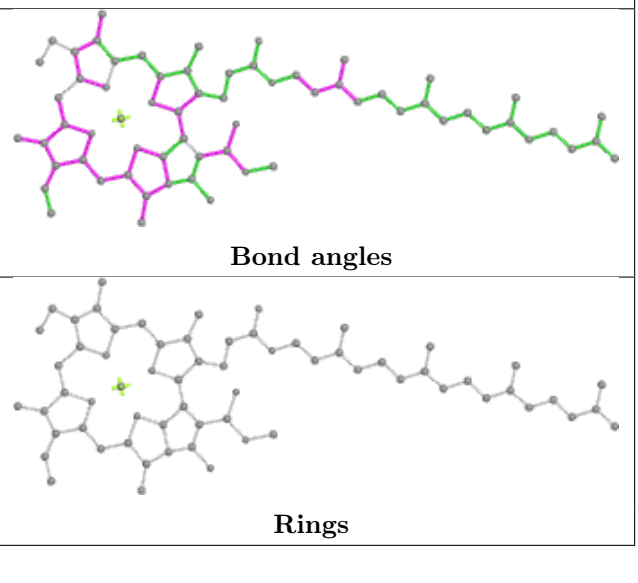


Rings

Ligand CLA B 613



Bond lengths

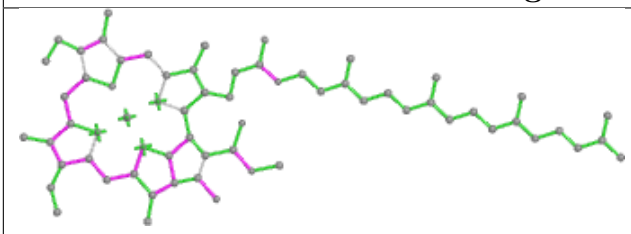


Bond angles

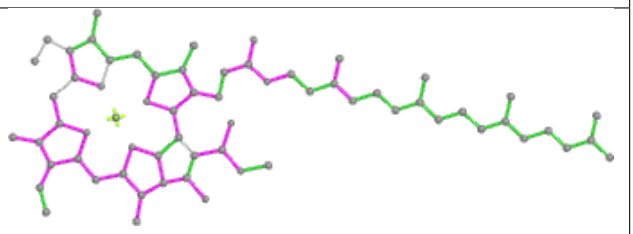
Torsions

Rings

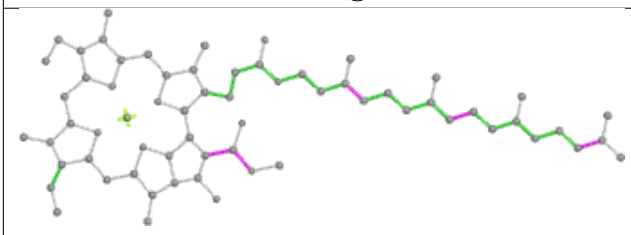
Ligand CLA B 606



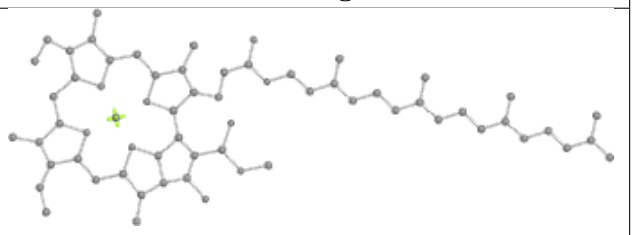
Bond lengths



Bond angles

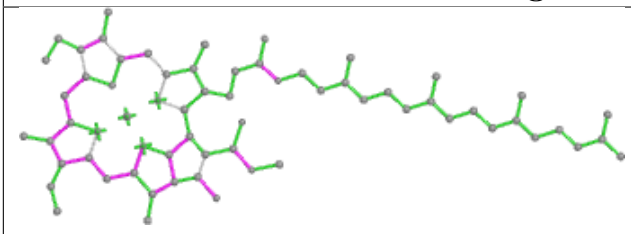


Torsions

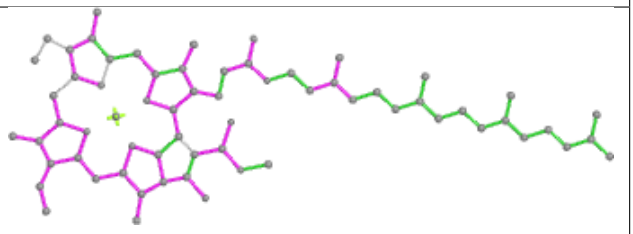


Rings

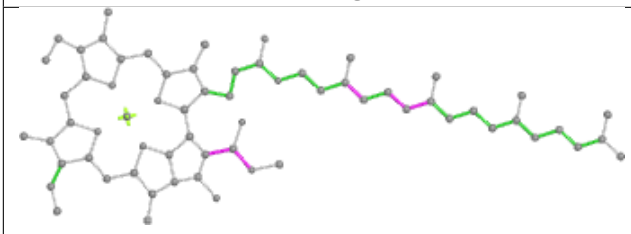
Ligand CLA b 607



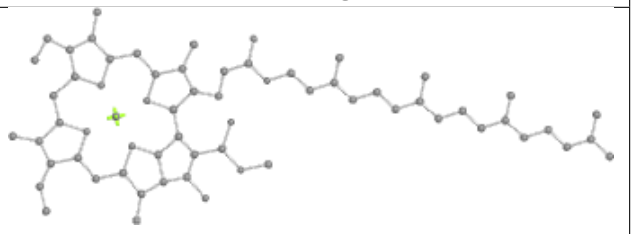
Bond lengths



Bond angles

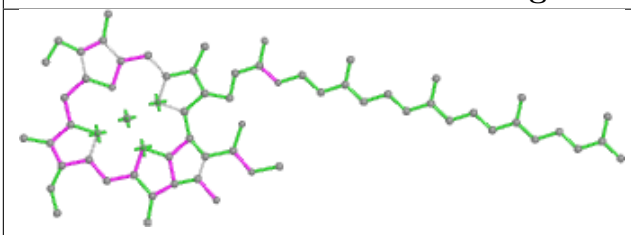


Torsions

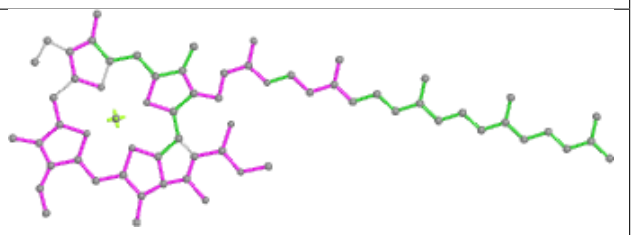


Rings

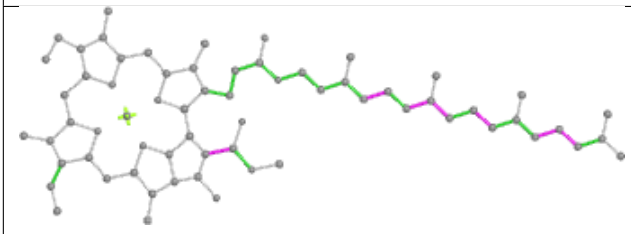
Ligand CLA c 907



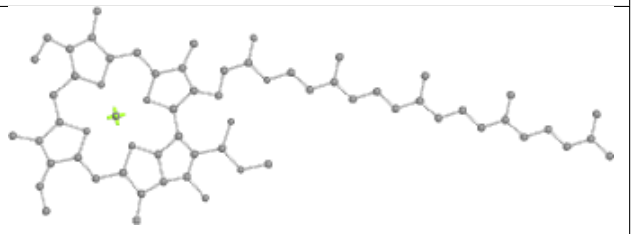
Bond lengths



Bond angles

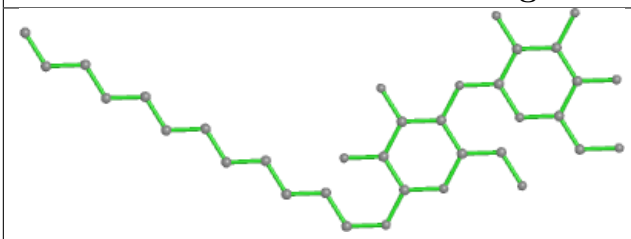


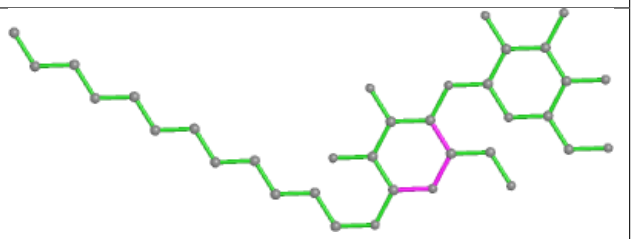
Torsions

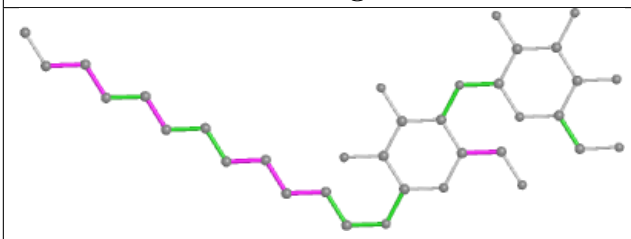


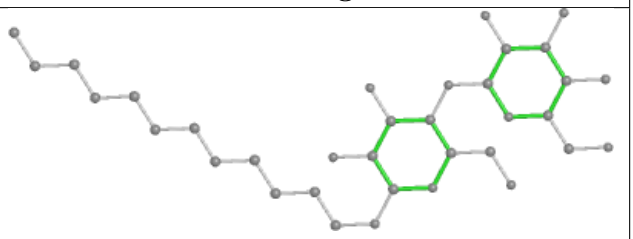
Rings

Ligand LMT m 104

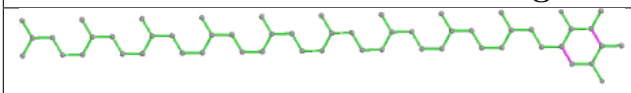

Bond lengths

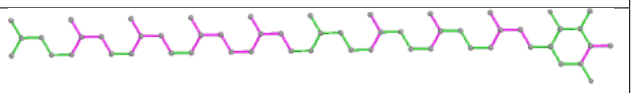

Bond angles

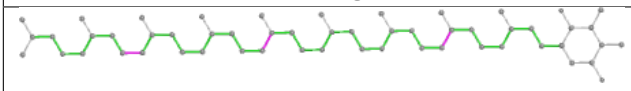

Torsions

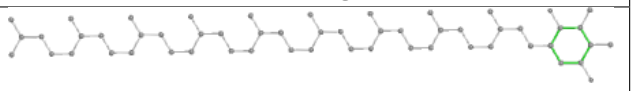

Rings

Ligand PL9 d 405

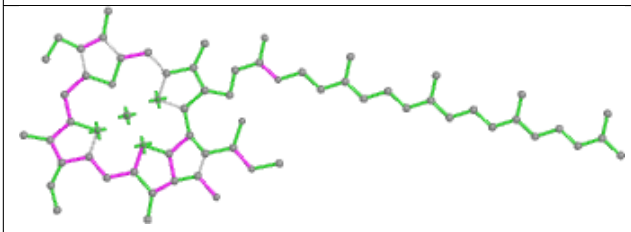

Bond lengths

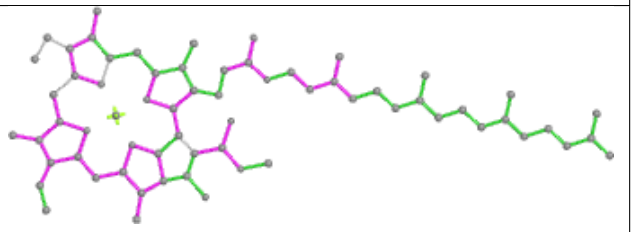

Bond angles

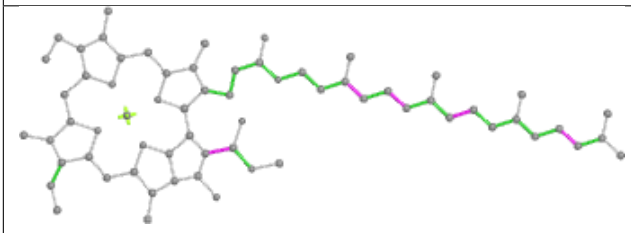

Torsions

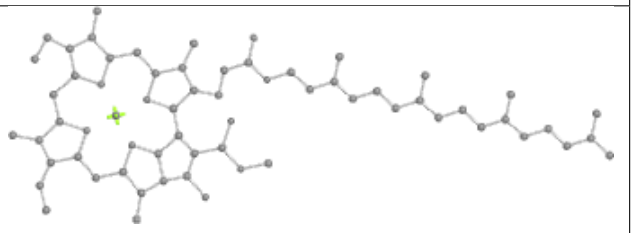

Rings

Ligand CLA C 504

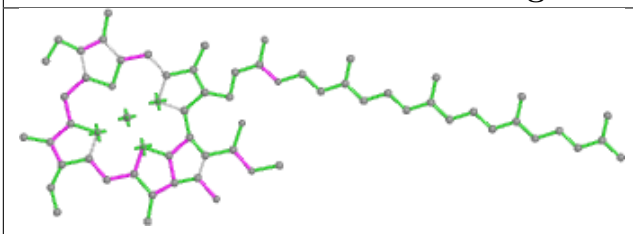

Bond lengths


Bond angles

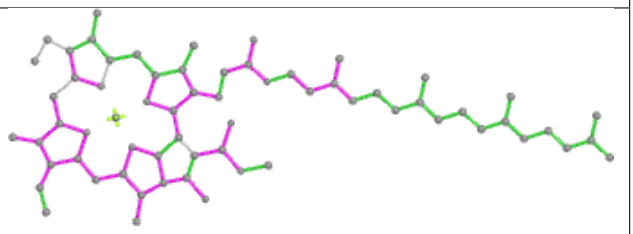

Torsions


Rings

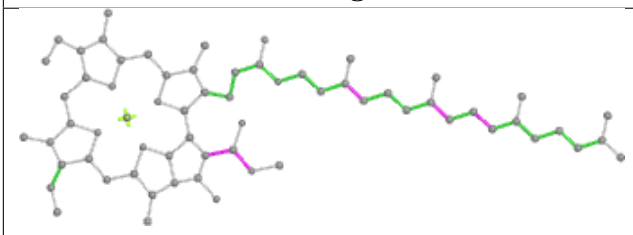
Ligand CLA b 609



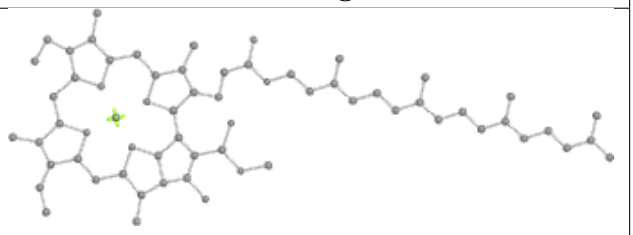
Bond lengths



Bond angles

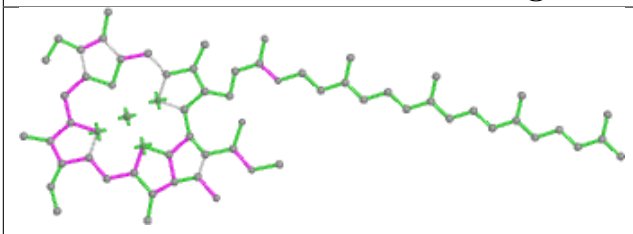


Torsions

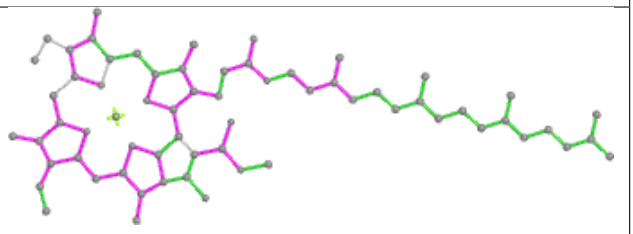


Rings

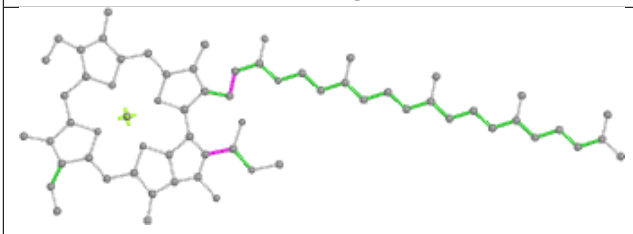
Ligand CLA b 606



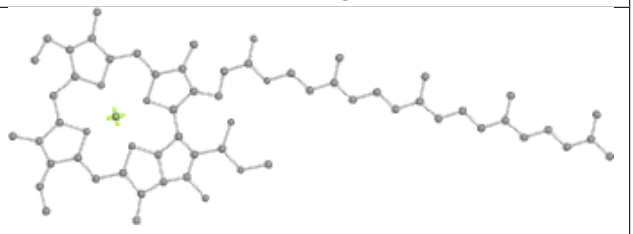
Bond lengths



Bond angles

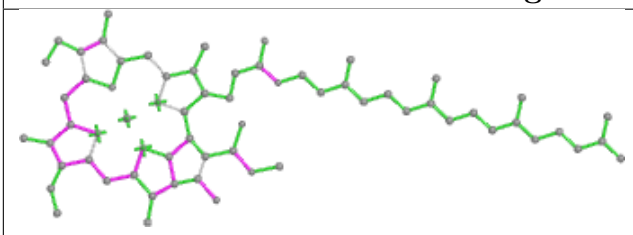


Torsions

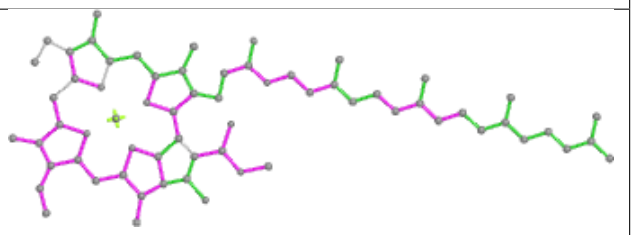


Rings

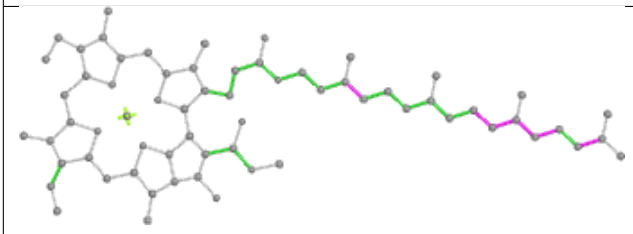
Ligand CLA B 616



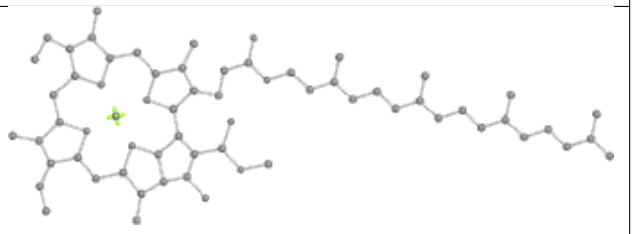
Bond lengths



Bond angles

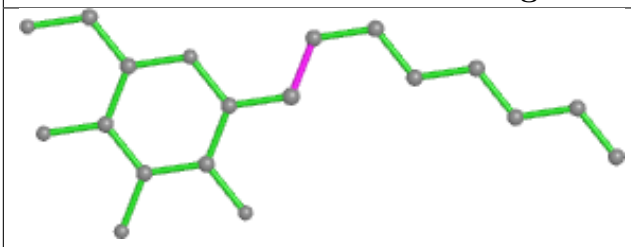


Torsions

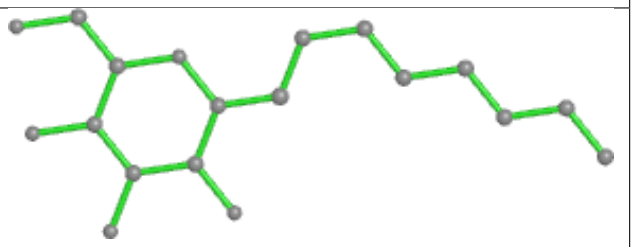


Rings

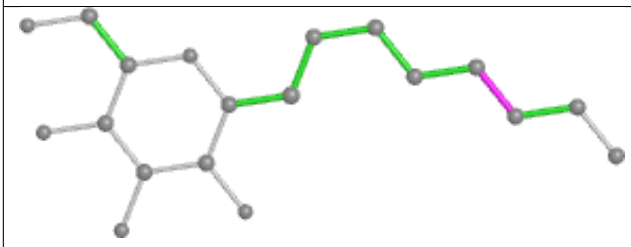
Ligand HTG O 303



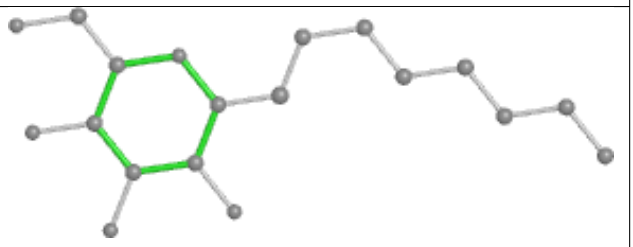
Bond lengths



Bond angles

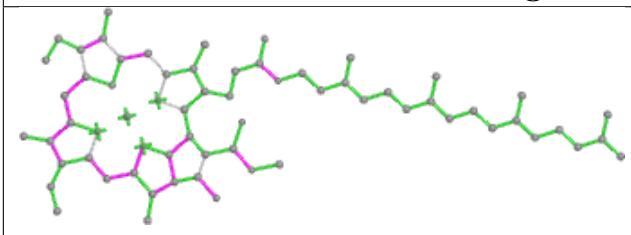


Torsions

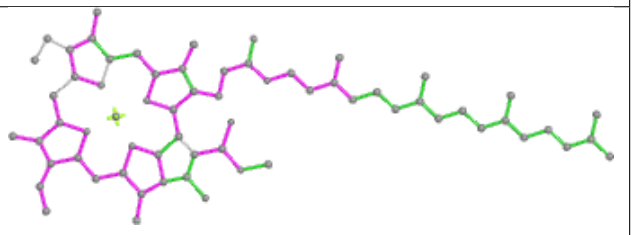


Rings

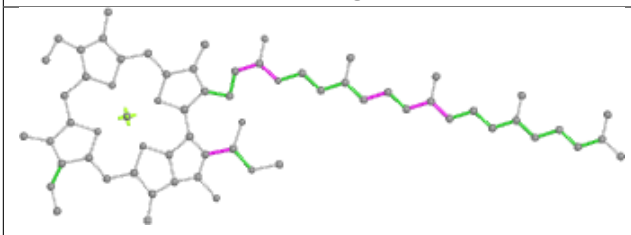
Ligand CLA C 513



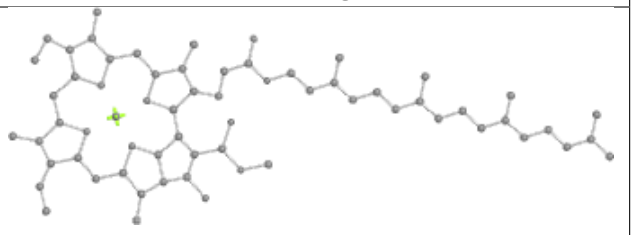
Bond lengths



Bond angles

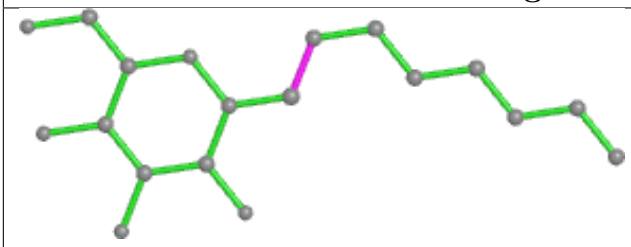


Torsions

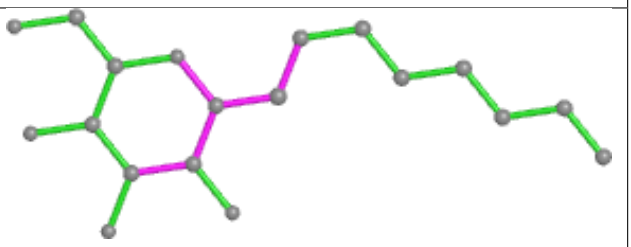


Rings

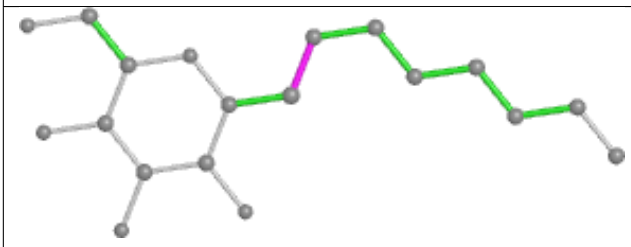
Ligand HTG b 626



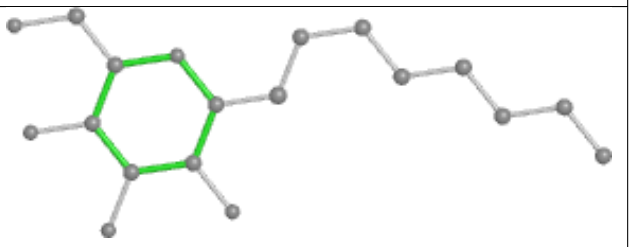
Bond lengths



Bond angles

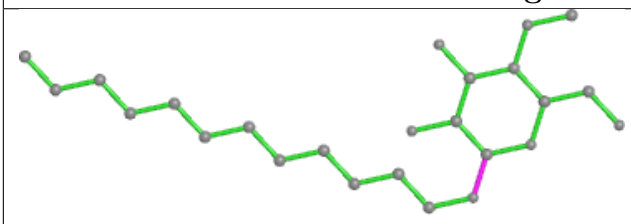


Torsions

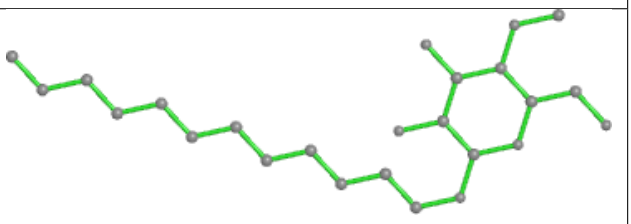


Rings

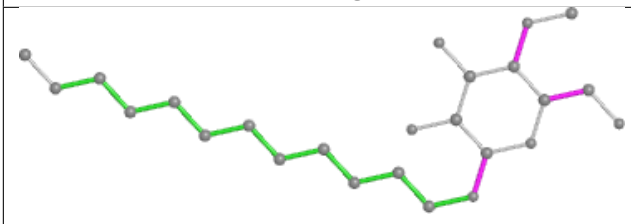
Ligand LMT b 625



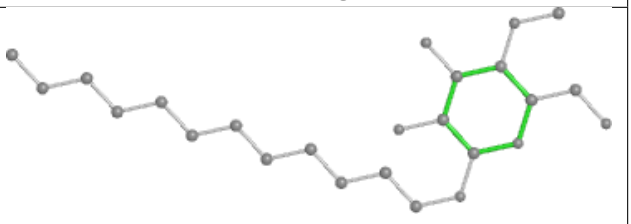
Bond lengths



Bond angles

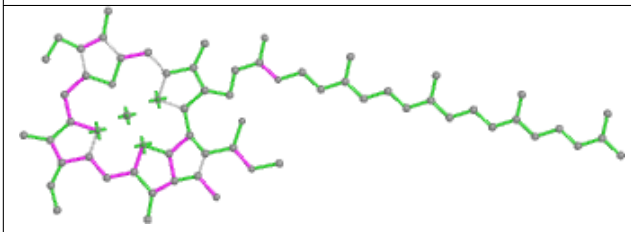


Torsions

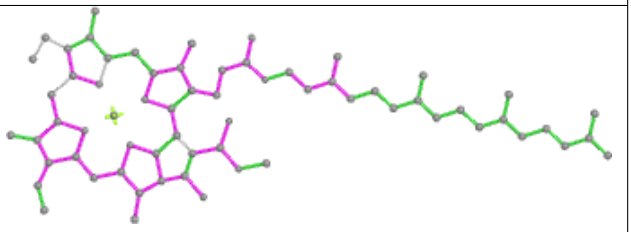


Rings

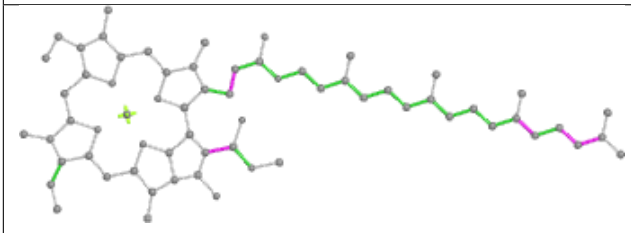
Ligand CLA B 611



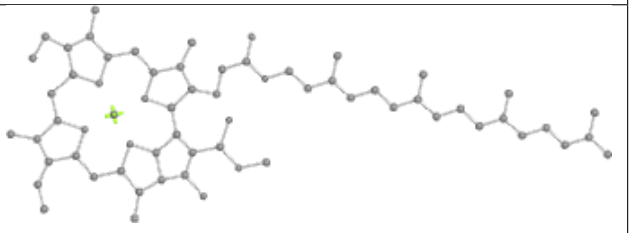
Bond lengths



Bond angles

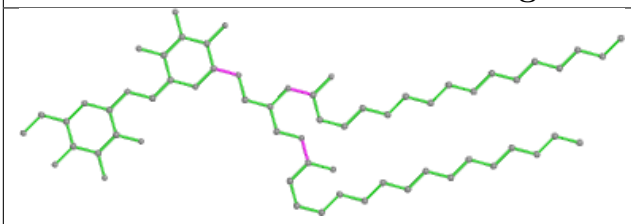


Torsions



Rings

Ligand DGD D 405



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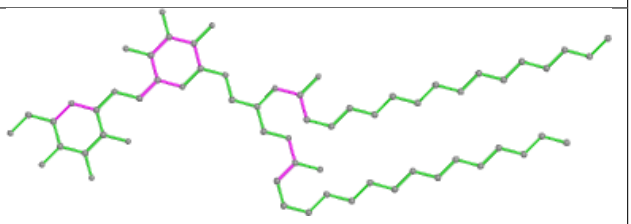
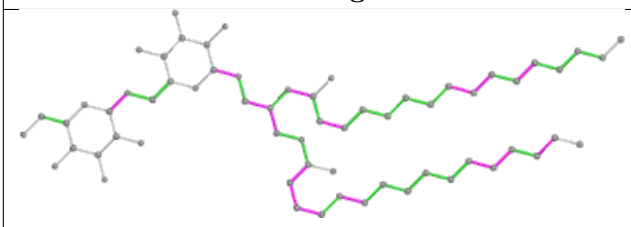


Bond angles



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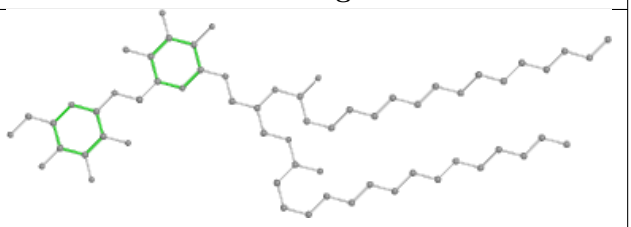
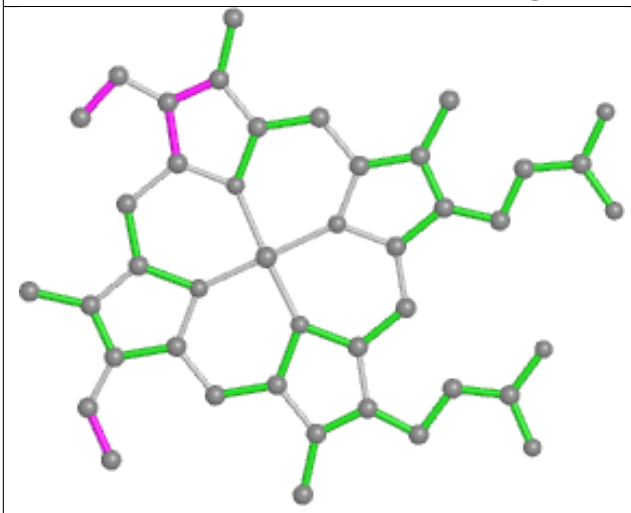
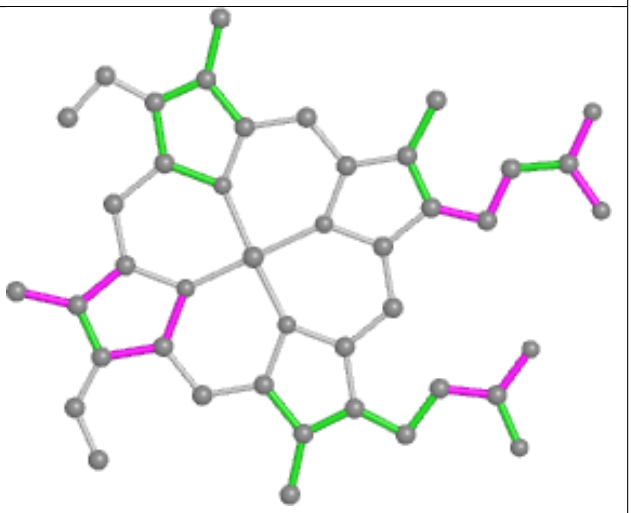


Rings

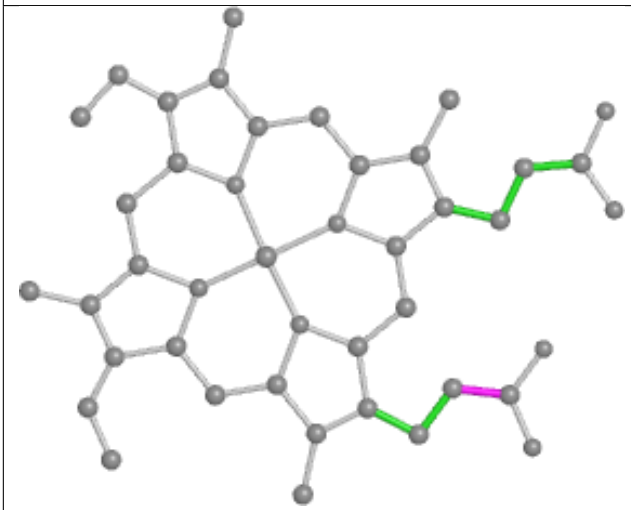
Ligand HEC v 202



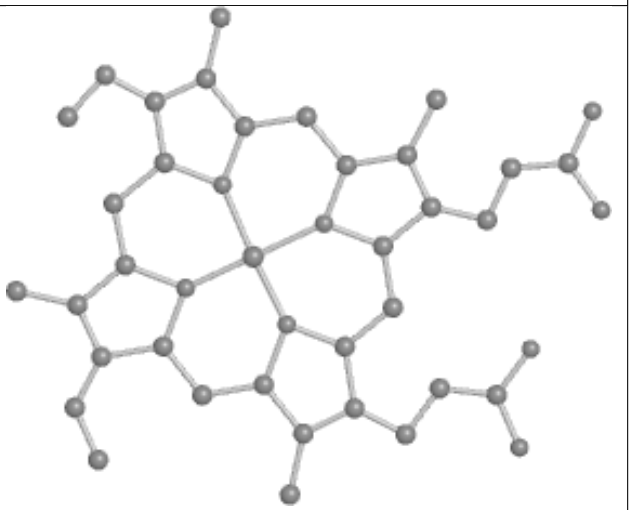
Bond lengths



Bond angles

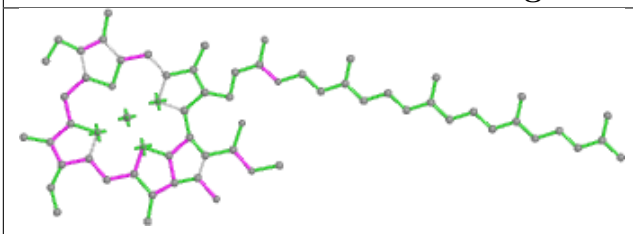


Torsions



Rings

Ligand CLA C 502



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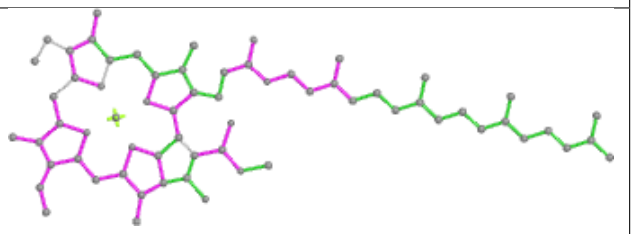
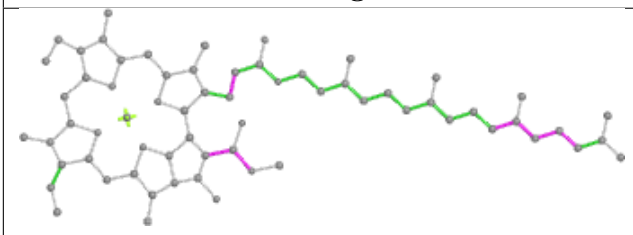
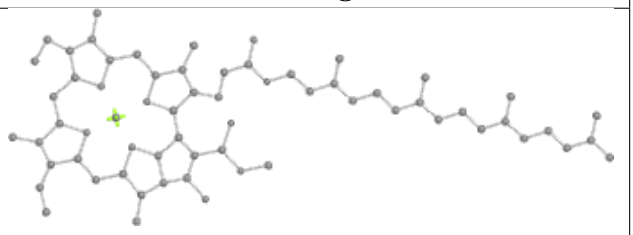


Bond angles

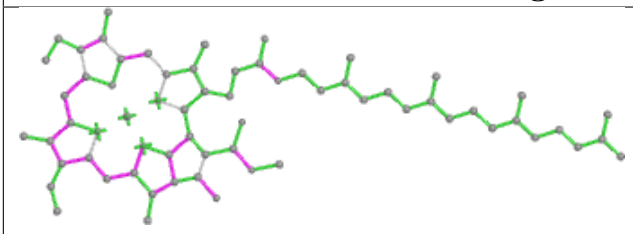


Torsions

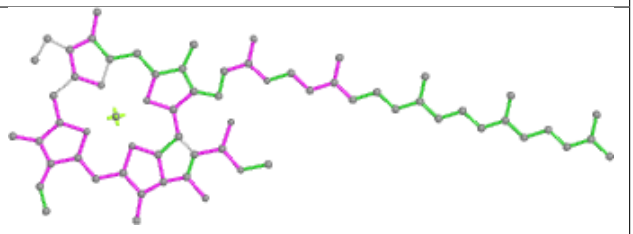


Rings

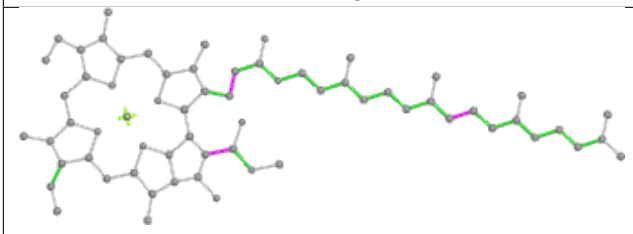
Ligand CLA c 904



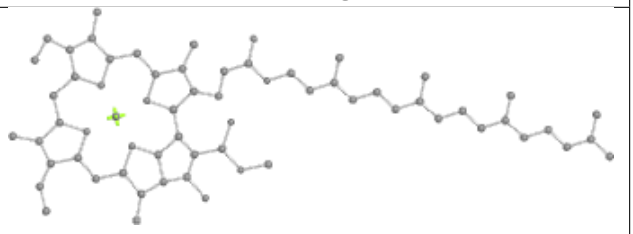
Bond lengths



Bond angles

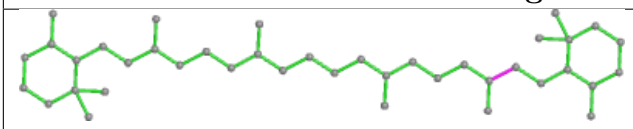


Torsions

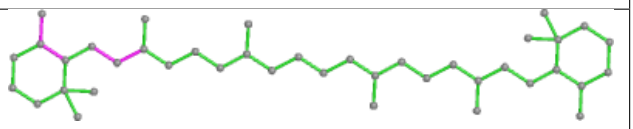


Rings

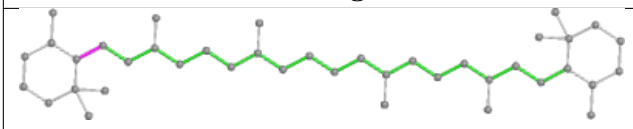
Ligand BCR b 621



Bond lengths



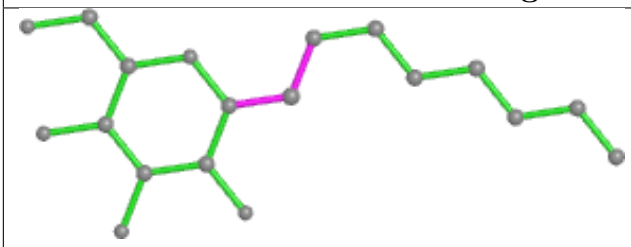
Bond angles



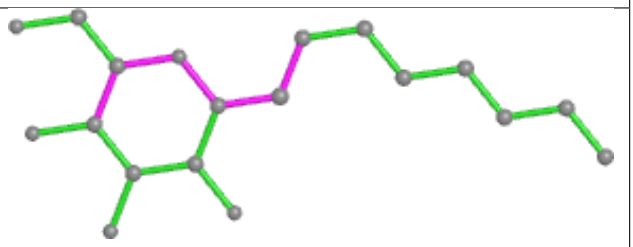
Torsions

Rings

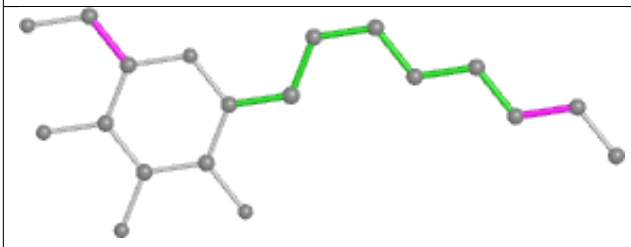
Ligand HTG B 634



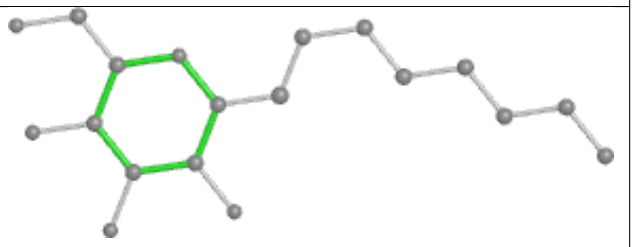
Bond lengths



Bond angles

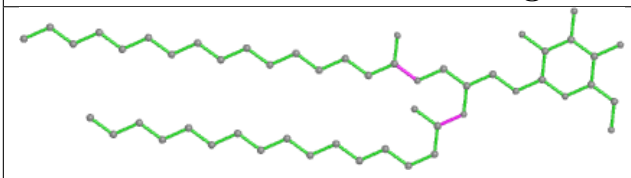


Torsions

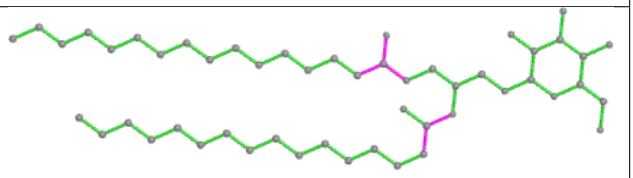


Rings

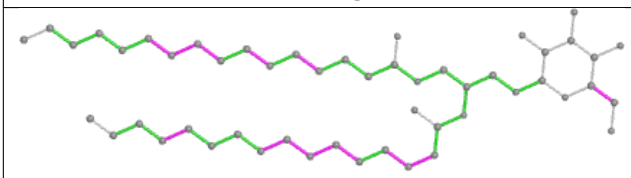
Ligand LMG J 101



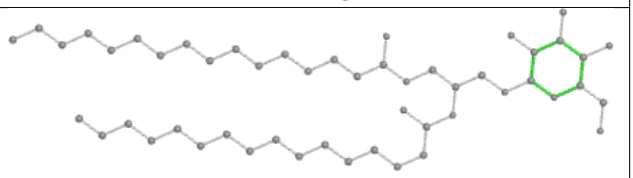
Bond lengths



Bond angles

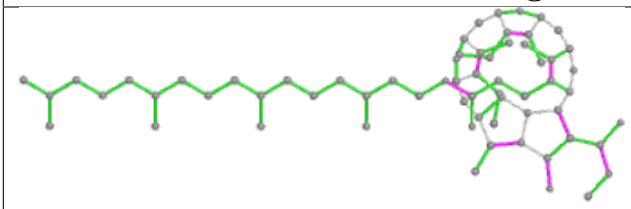


Torsions

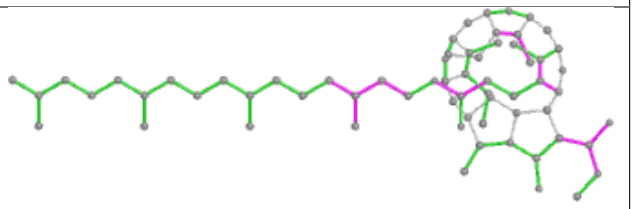


Rings

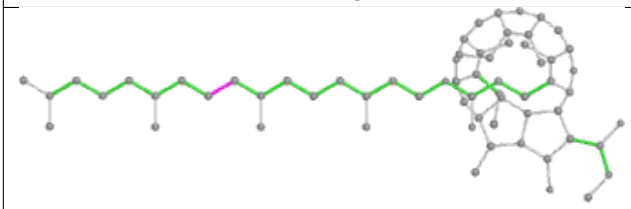
Ligand PHO a 420



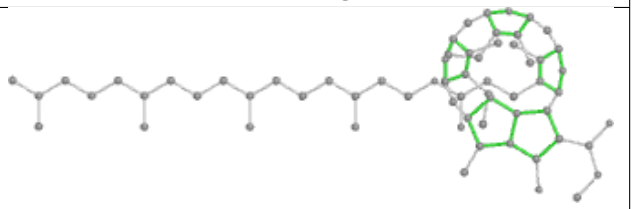
Bond lengths



Bond angles

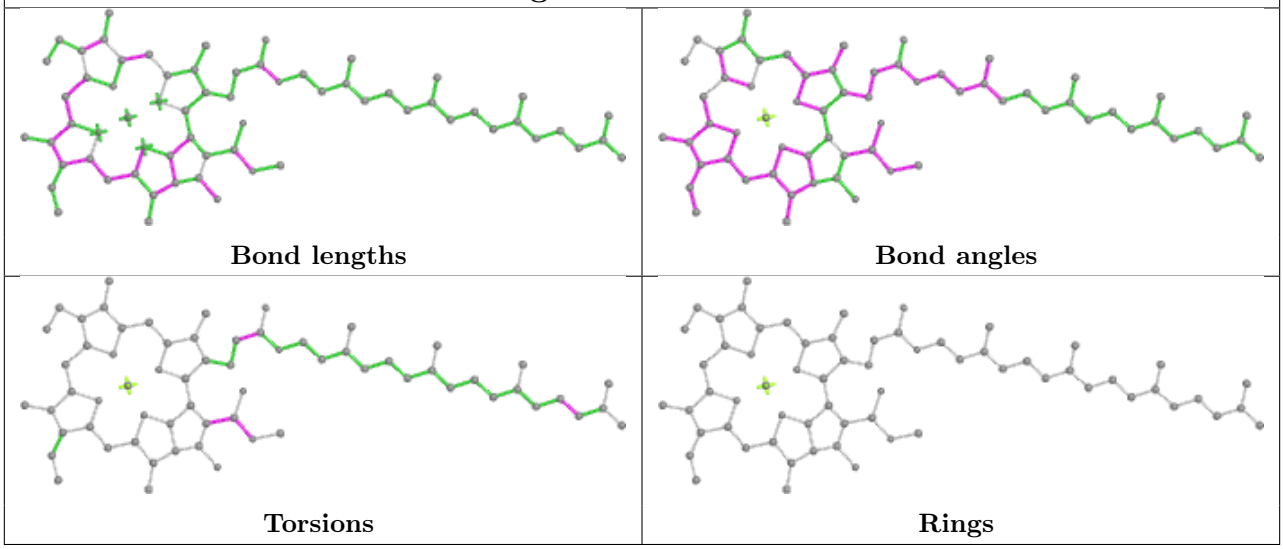


Torsions

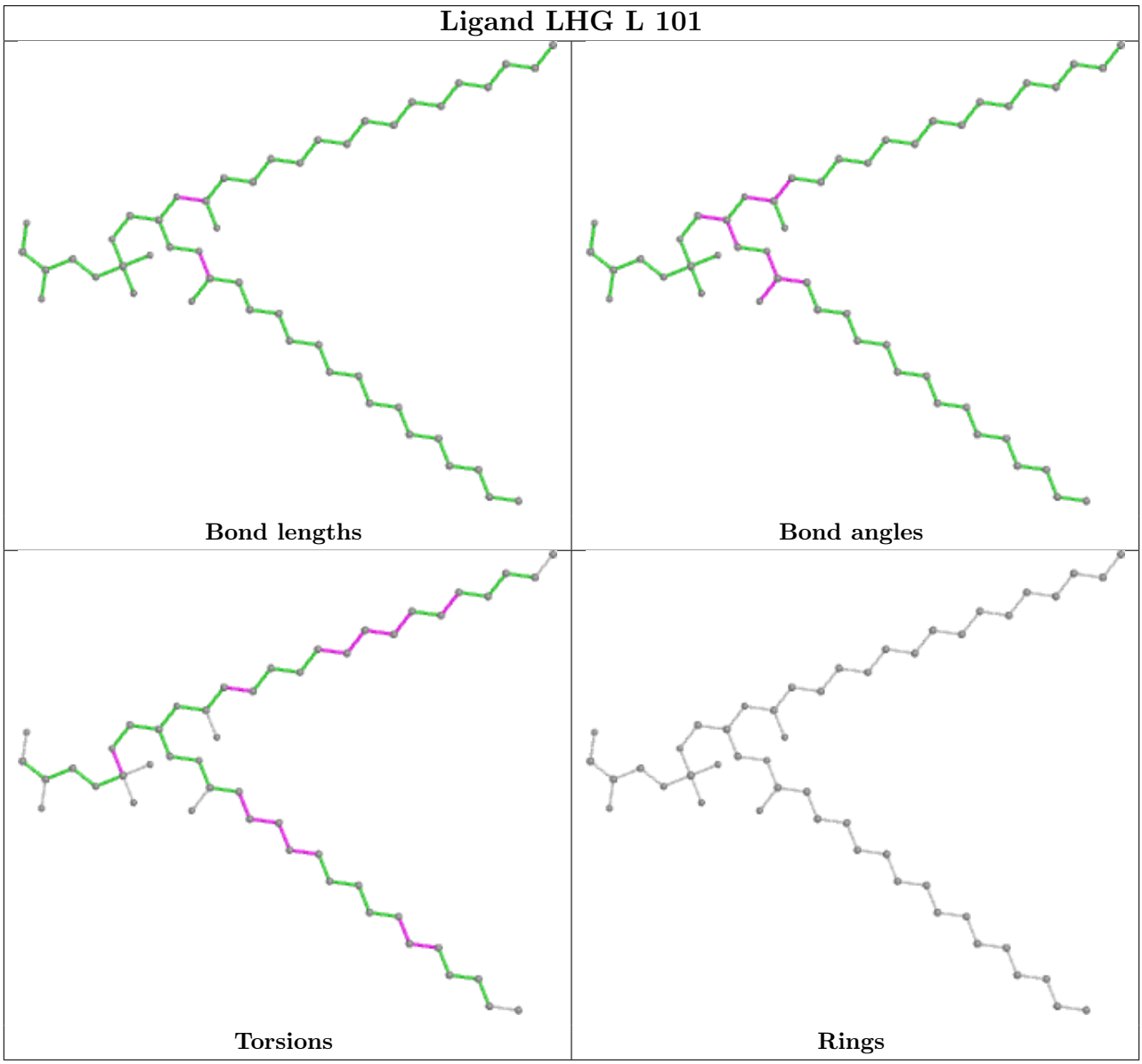


Rings

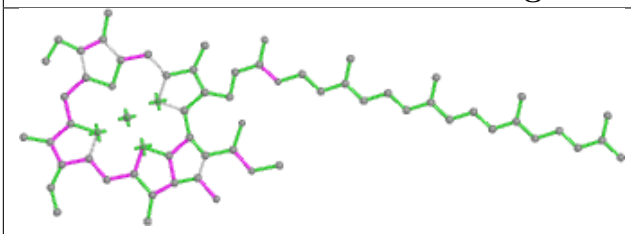
Ligand CLA c 913



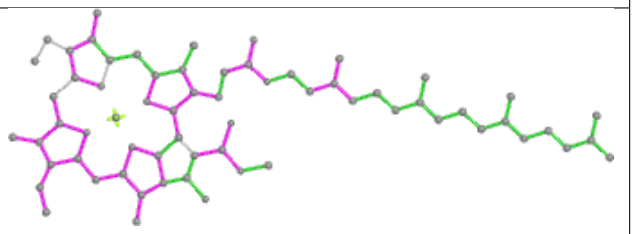
Ligand LHG L 101



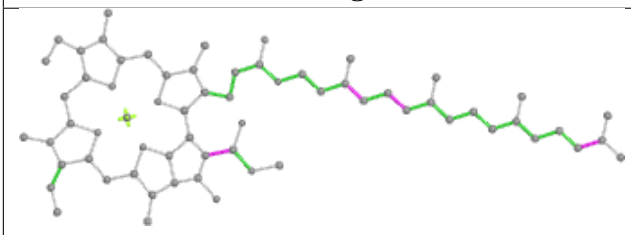
Ligand CLA B 604



Bond lengths



Bond angles



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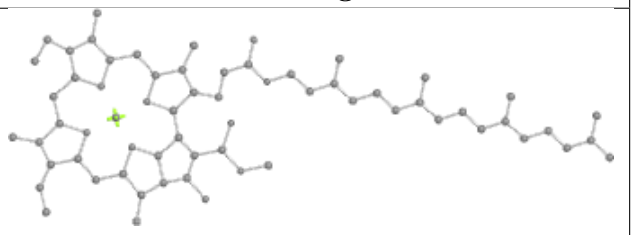
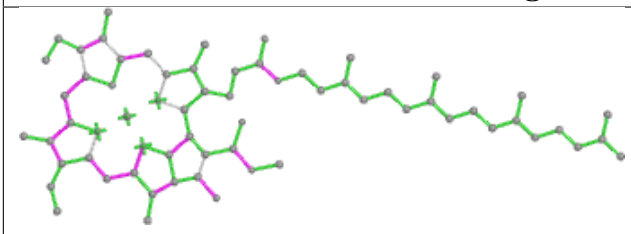


Rings

Ligand CLA A 410



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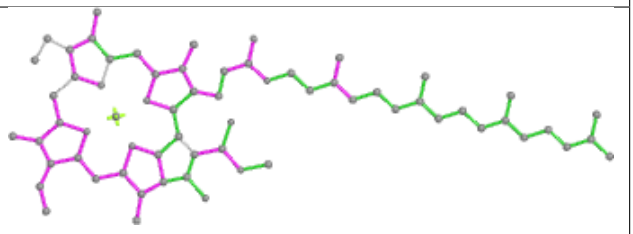
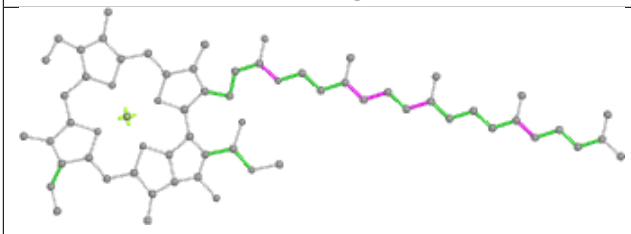


Bond angles



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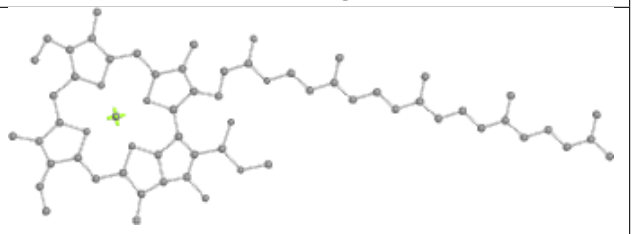
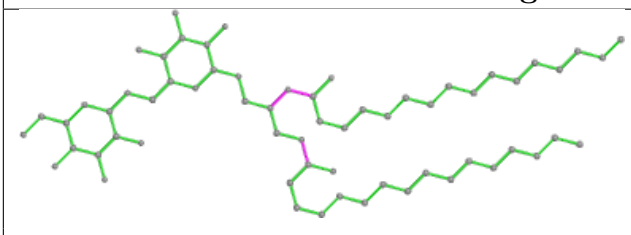


Rings

Ligand DGD C 519



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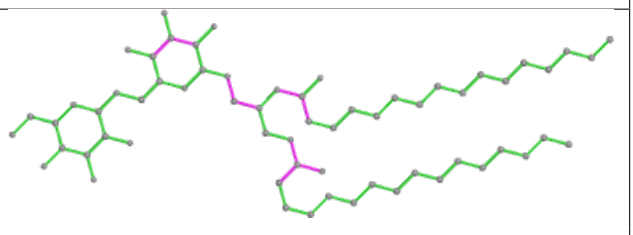
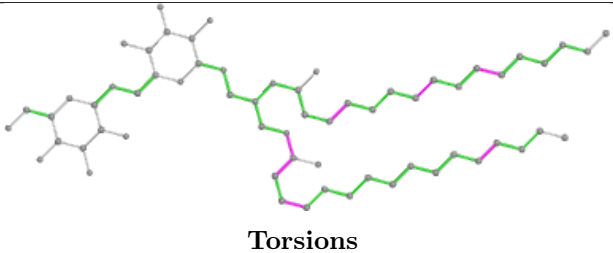


Bond angles



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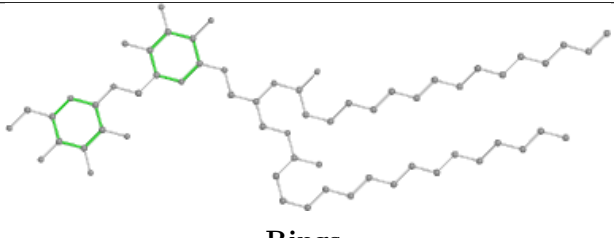
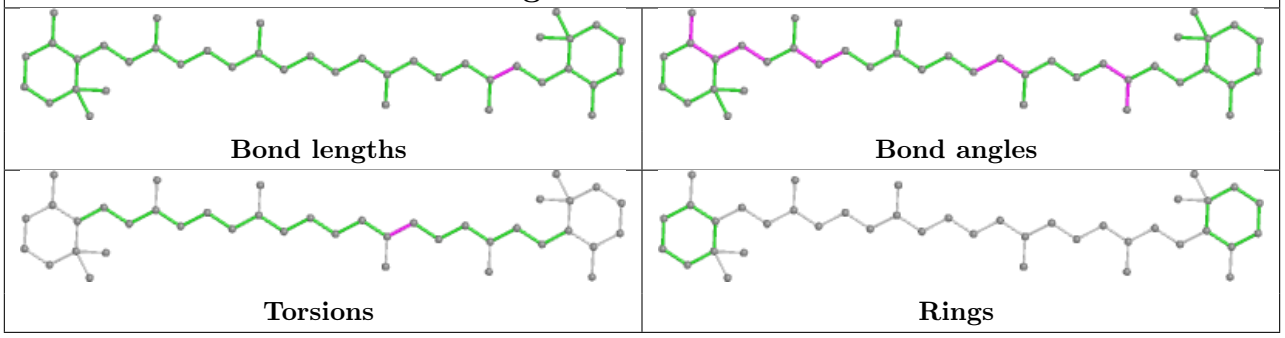
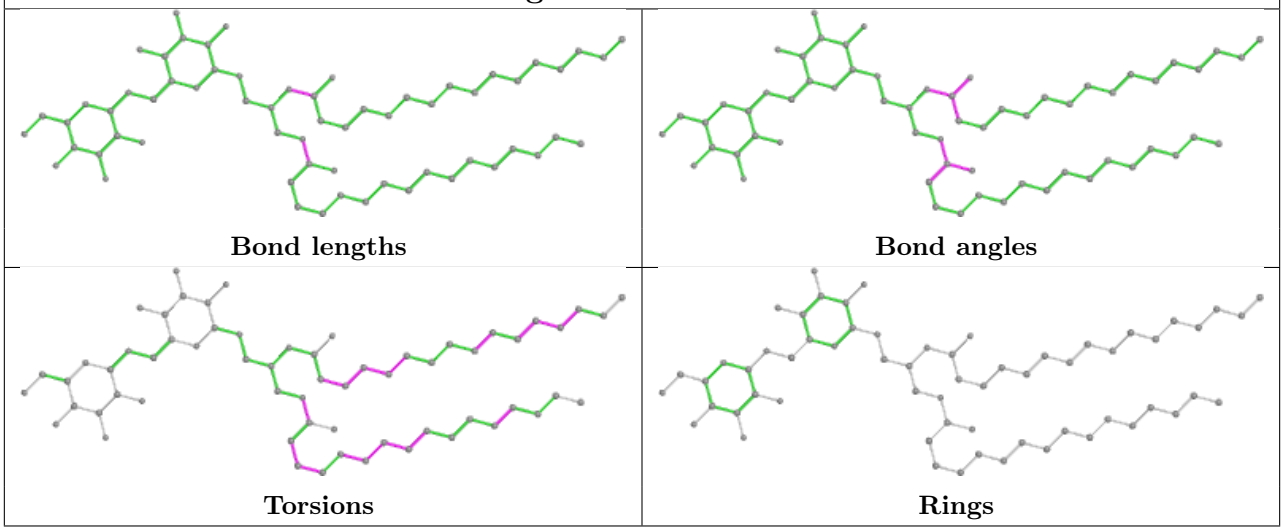


Rings

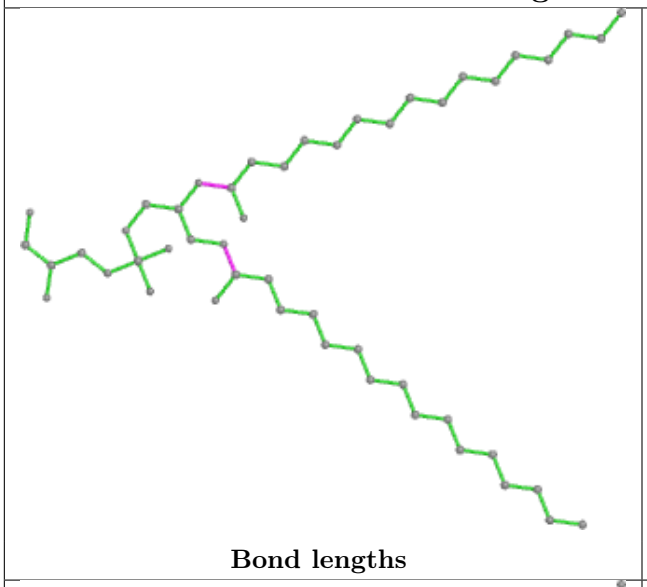
Ligand BCR A 411



Ligand DGD c 918



Ligand LHG l 101



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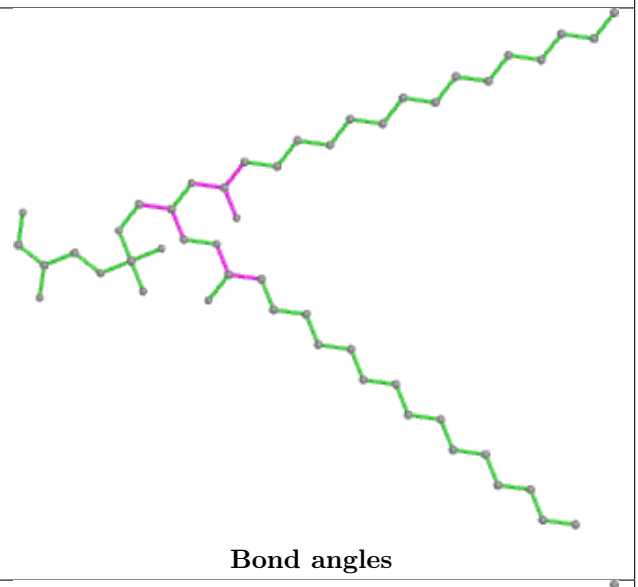
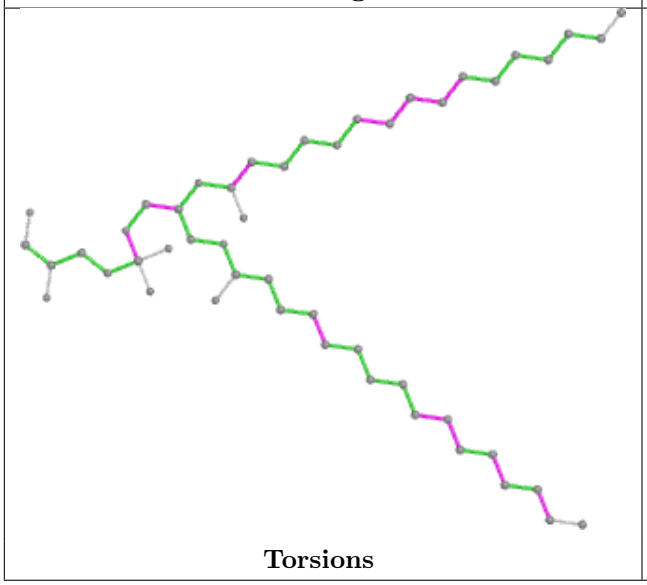


Bond angles



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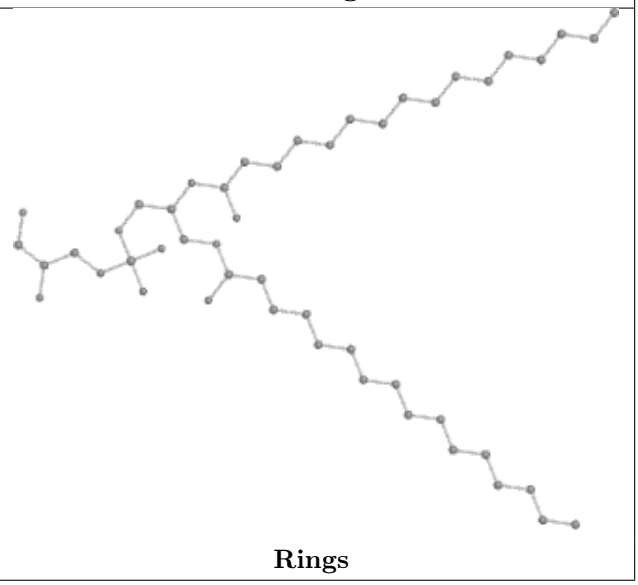
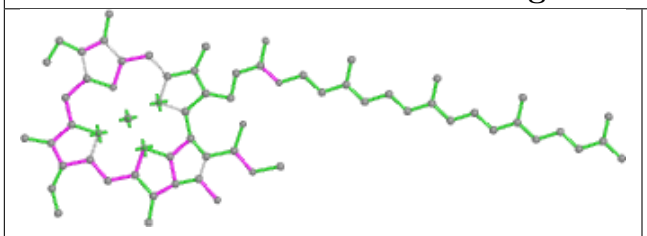
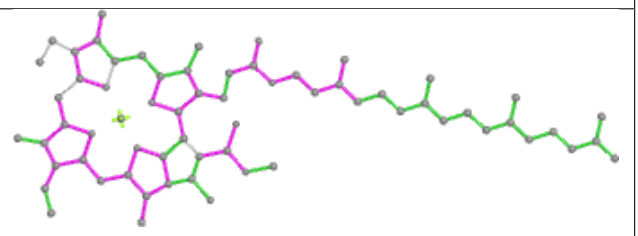


Rings

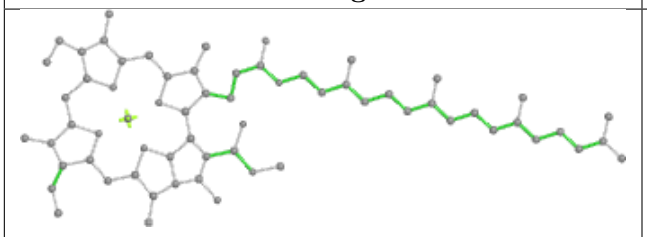
Ligand CLA d 402



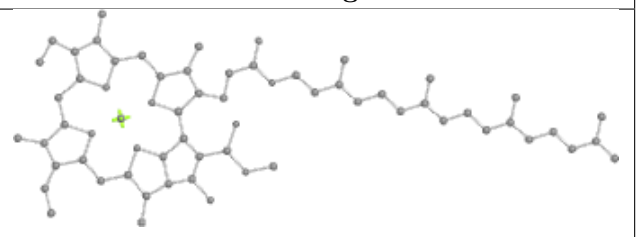
Bond lengths



Bond angles

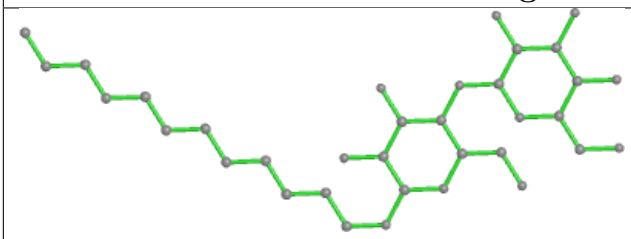


Torsions

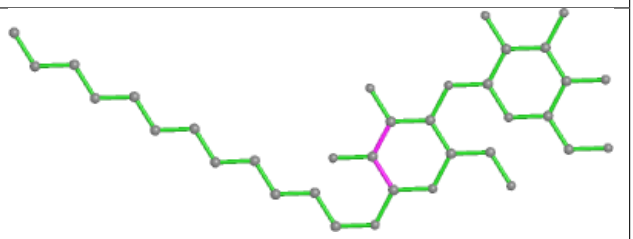


Rings

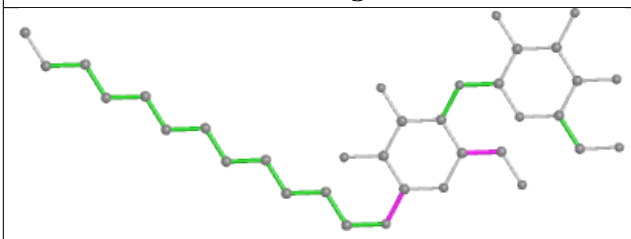
Ligand LMT m 103



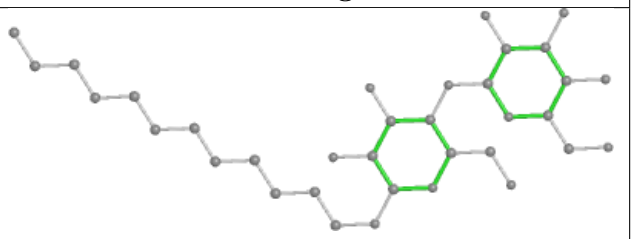
Bond lengths



Bond angles

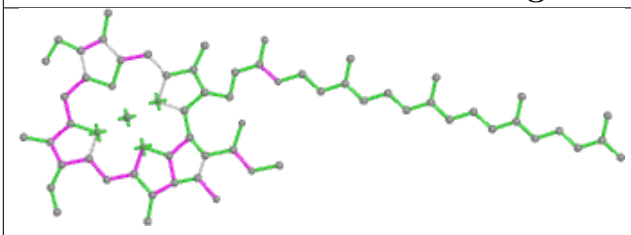


Torsions



Rings

Ligand CLA b 615



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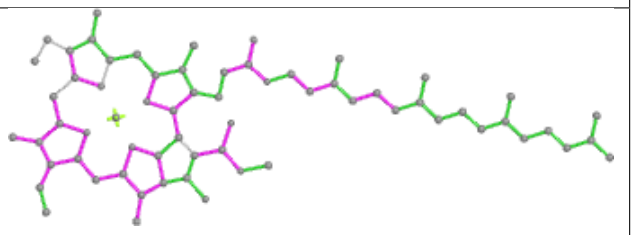
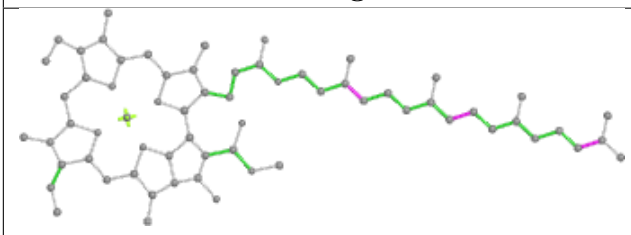
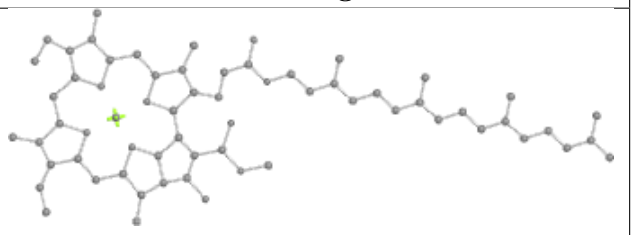


Bond angles

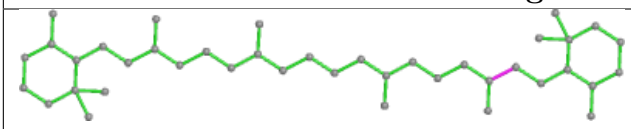


Torsions



Rings

Ligand BCR y 101



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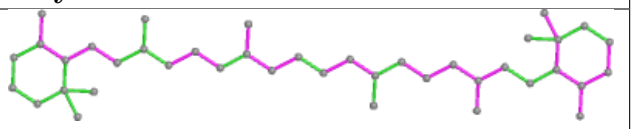
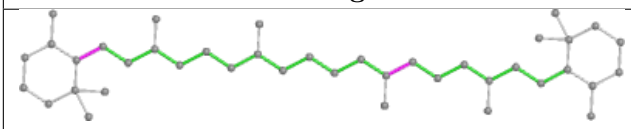
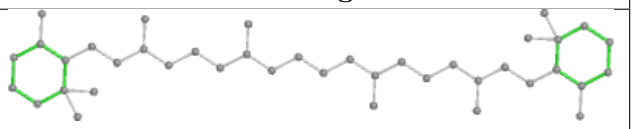


Bond angles

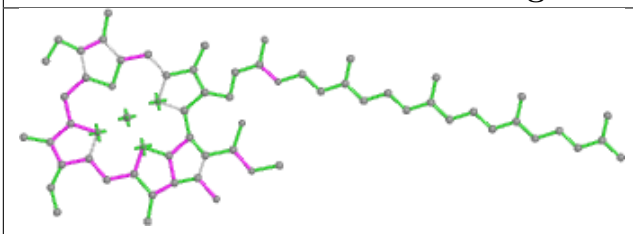


Torsions

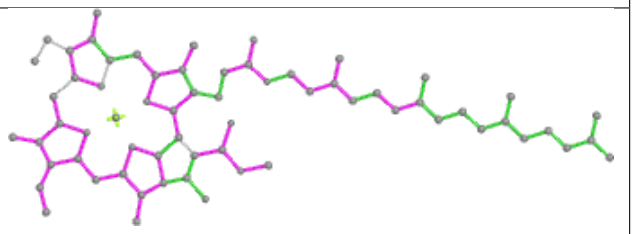


Rings

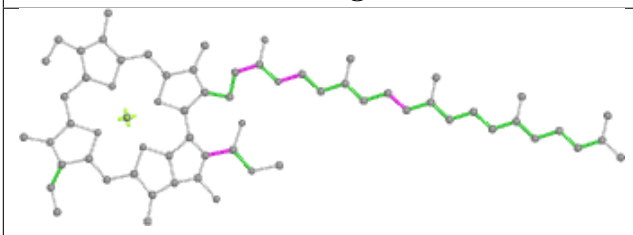
Ligand CLA b 617



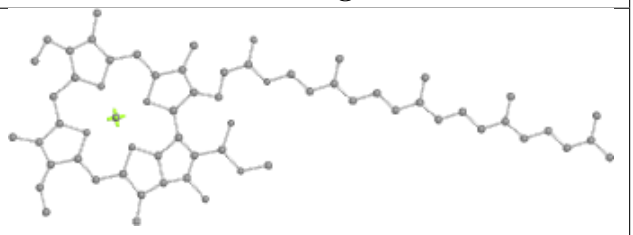
Bond lengths



Bond angles

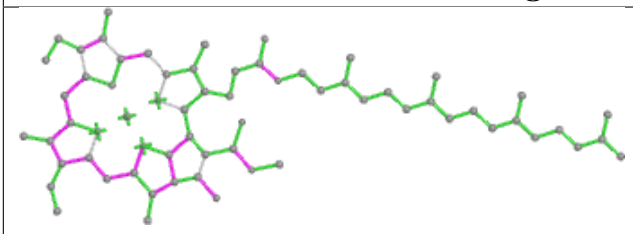


Torsions

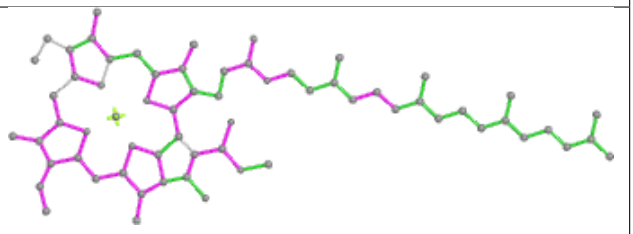


Rings

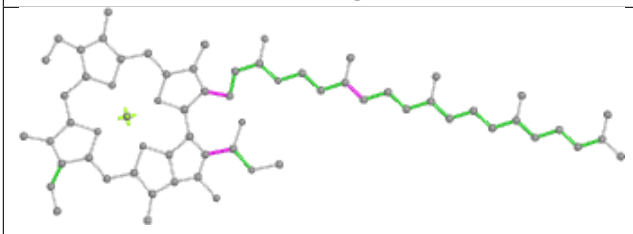
Ligand CLA B 610



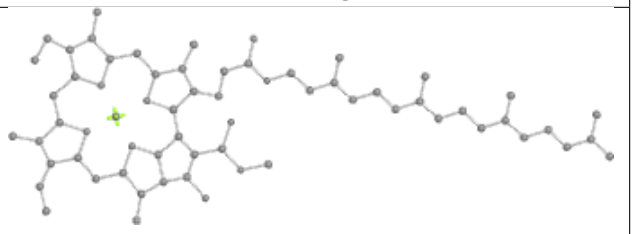
Bond lengths



Bond angles

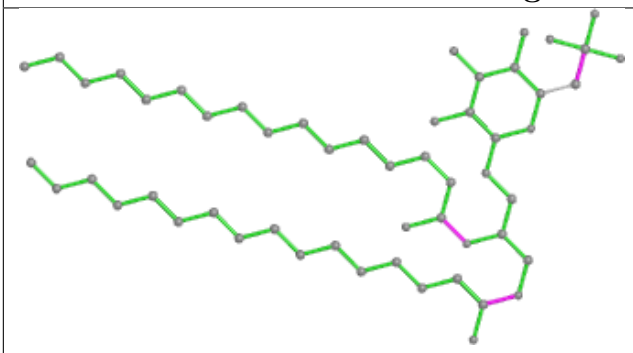


Torsions

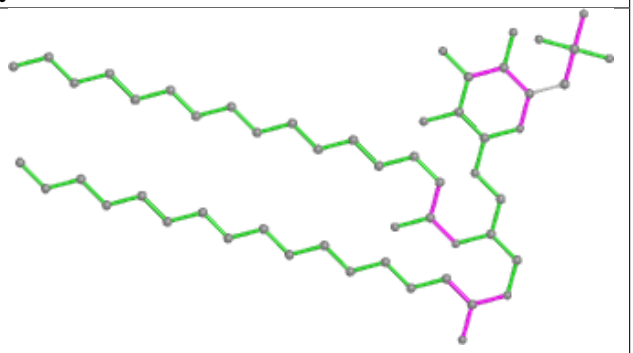


Rings

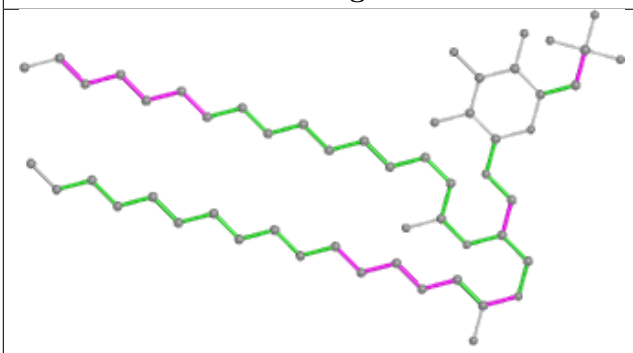
Ligand SQD A 416



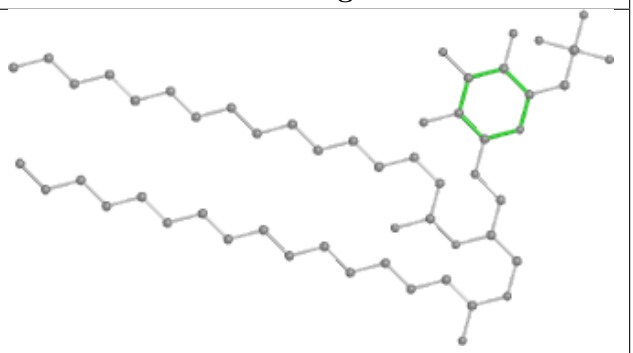
Bond lengths



Bond angles

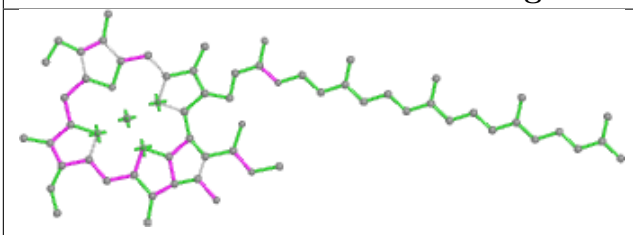


Torsions

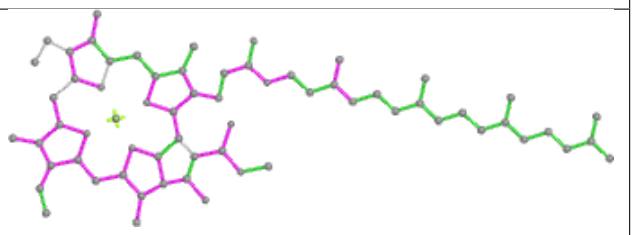


Rings

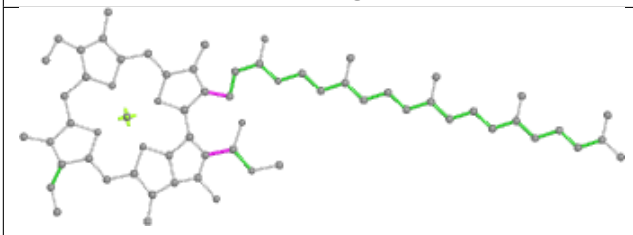
Ligand CLA B 608



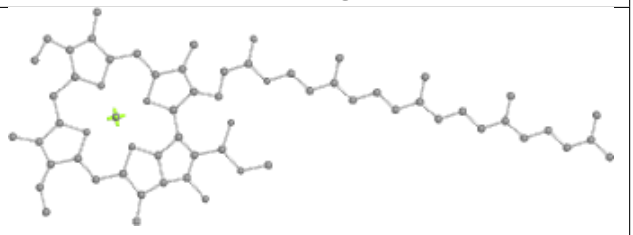
Bond lengths



Bond angles

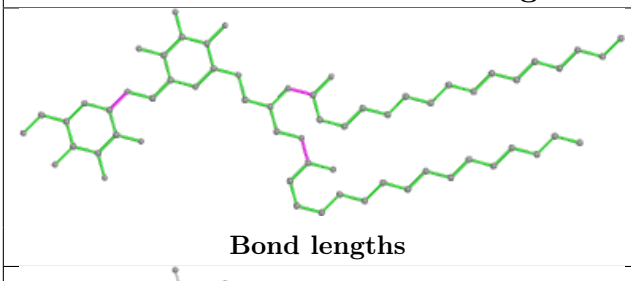


Torsions

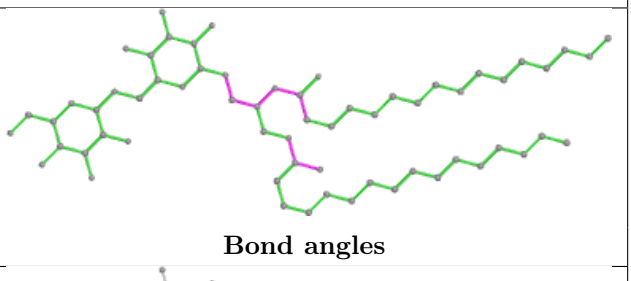


Rings

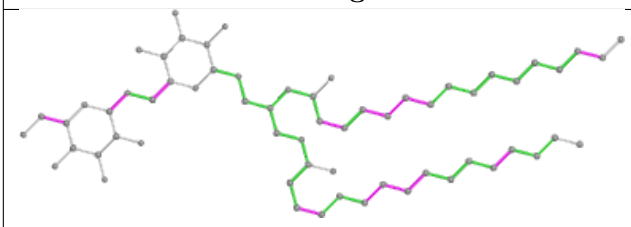
Ligand DGD C 517



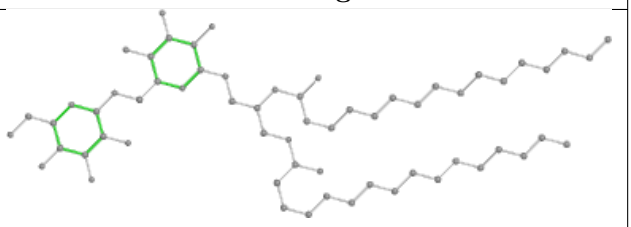
Bond lengths



Bond angles

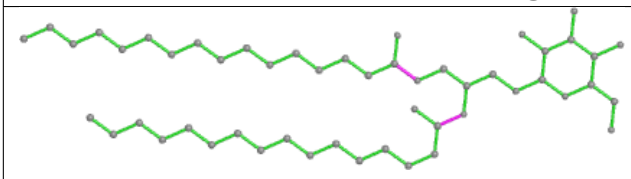


Torsions

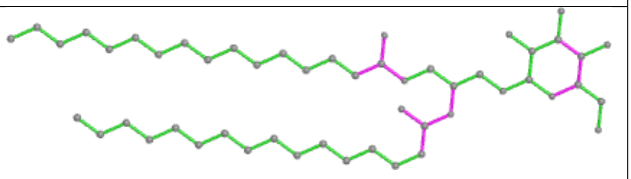


Rings

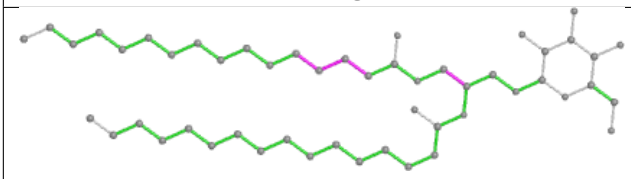
Ligand LMG c 920



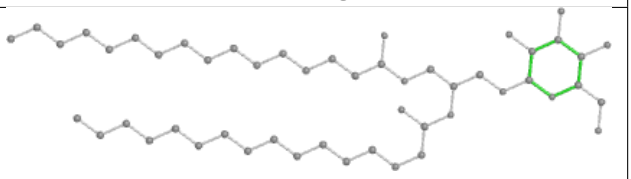
Bond lengths



Bond angles

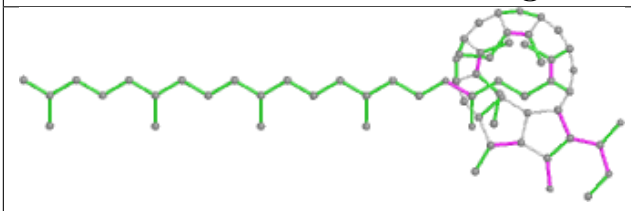


Torsions



Rings

Ligand PHO A 409



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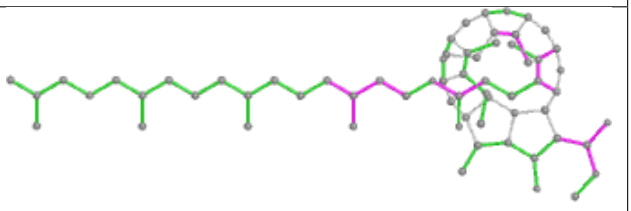
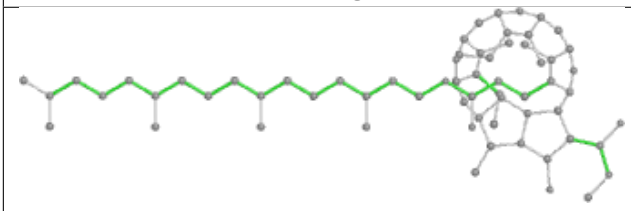
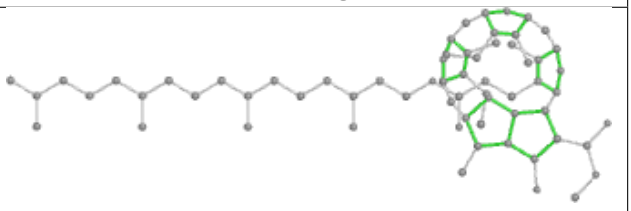


Bond angles

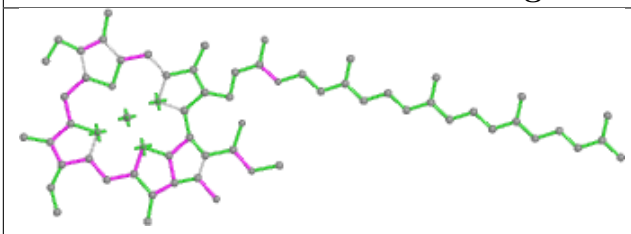


Torsions

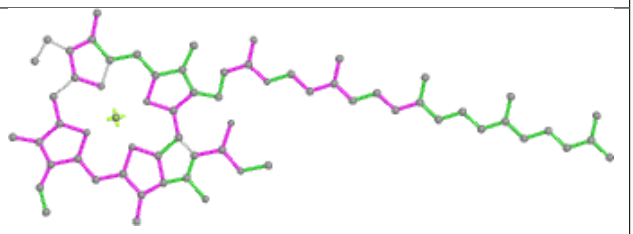


Rings

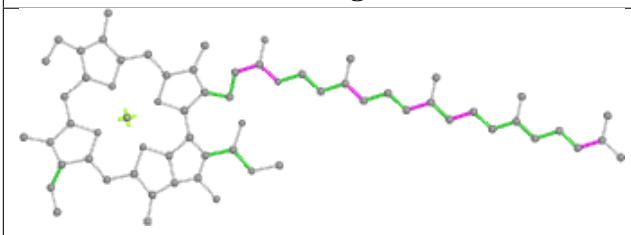
Ligand CLA C 511



Bond lengths



Bond angles



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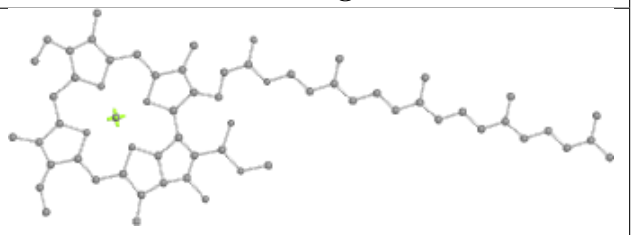
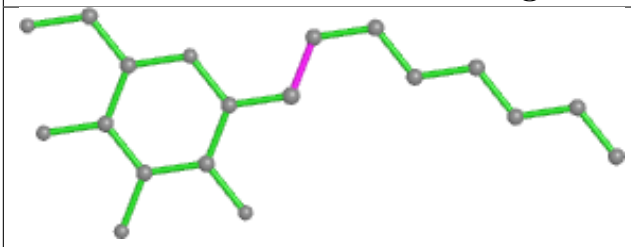


Rings

Ligand HTG B 624



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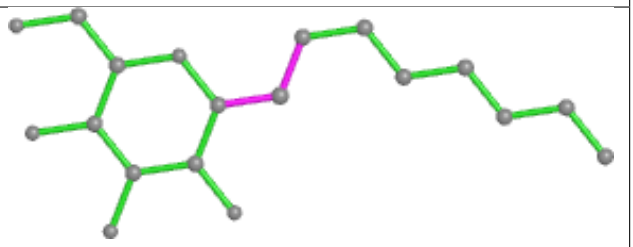
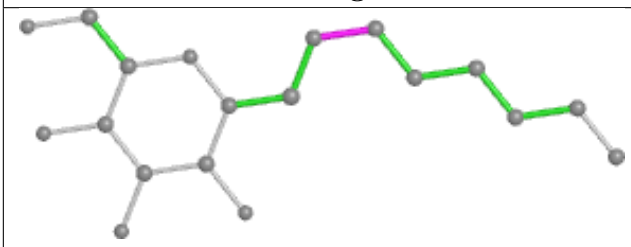
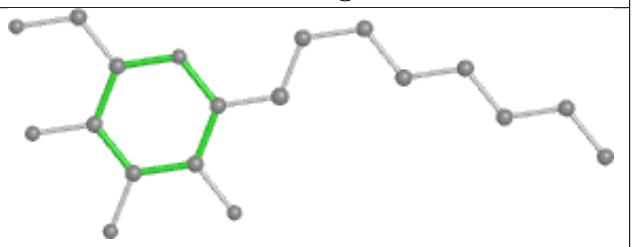


Bond angles

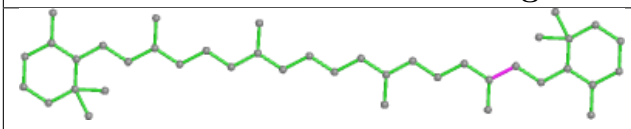


Torsions



Rings

Ligand BCR H 101



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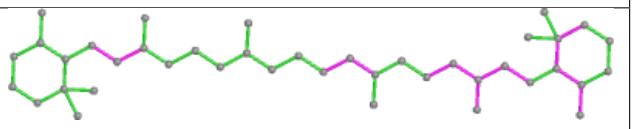
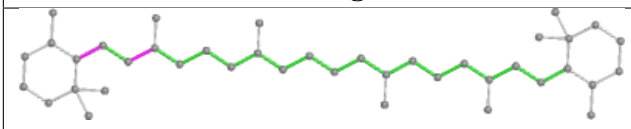
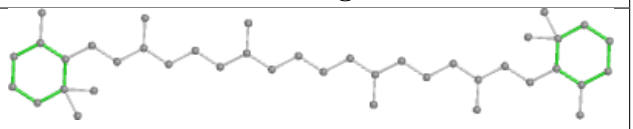


Bond angles

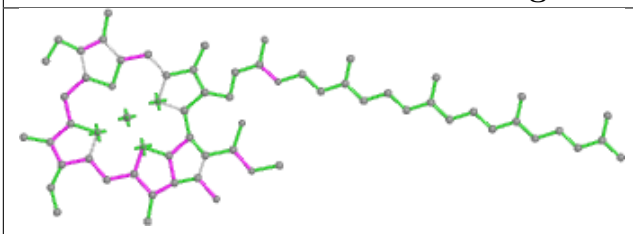


Torsions

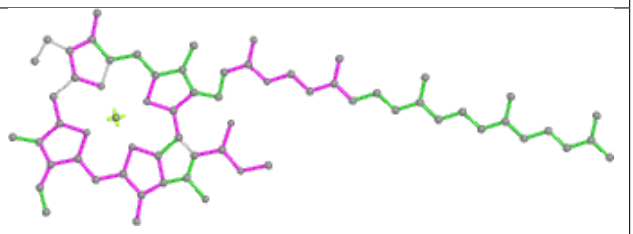


Rings

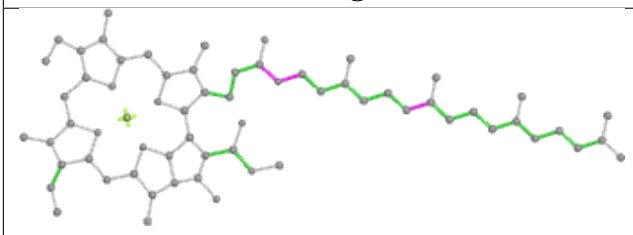
Ligand CLA c 912



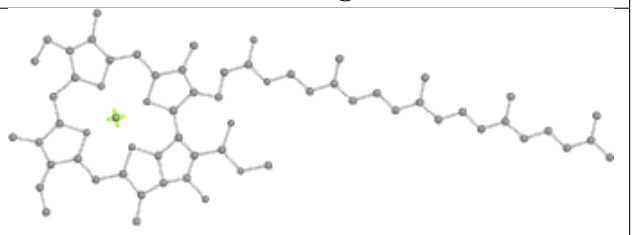
Bond lengths



Bond angles

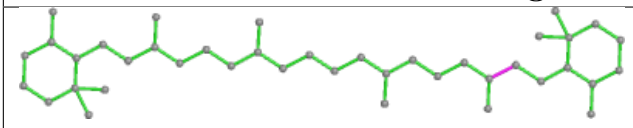


Torsions

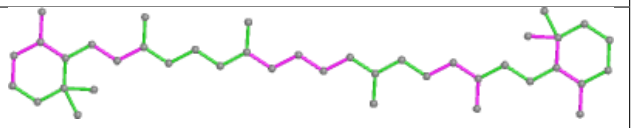


Rings

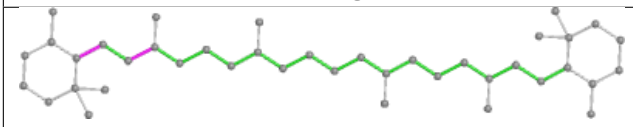
Ligand BCR c 915



Bond lengths



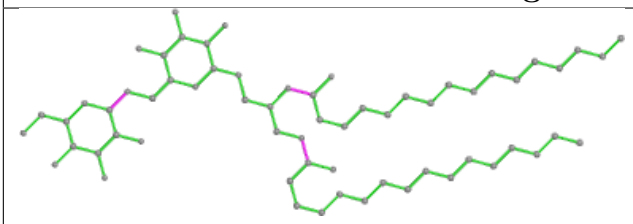
Bond angles



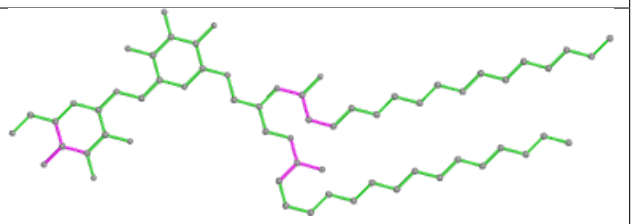
Torsions

Rings

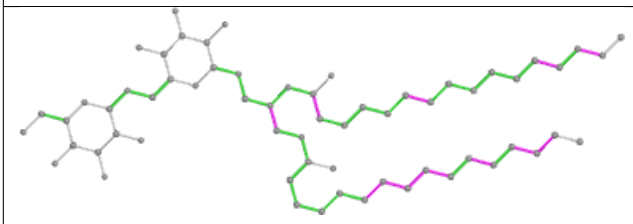
Ligand DGD h 102



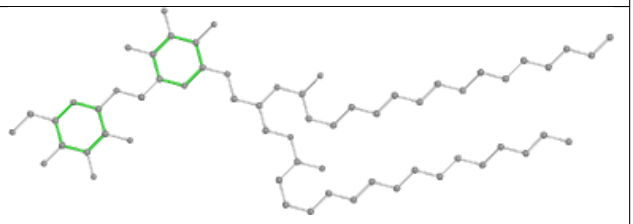
Bond lengths



Bond angles

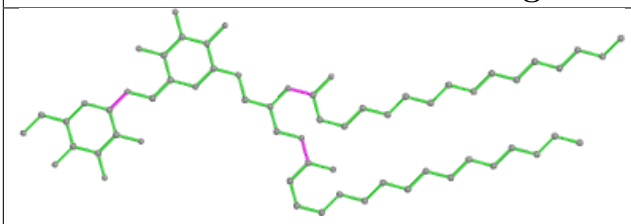


Torsions

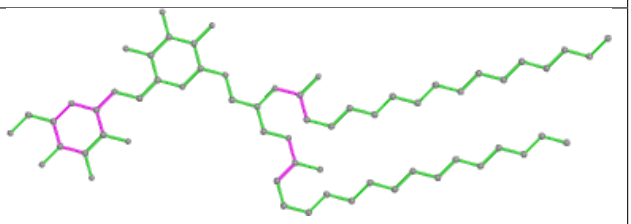


Rings

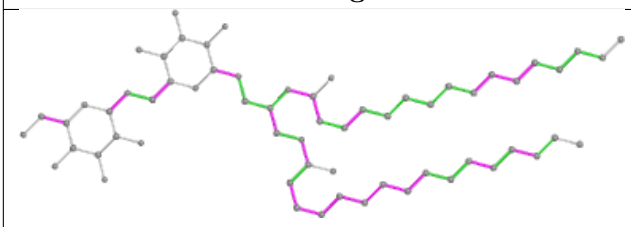
Ligand DGD d 406



Bond lengths



Bond angles



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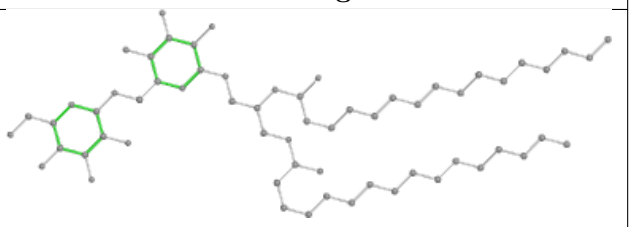
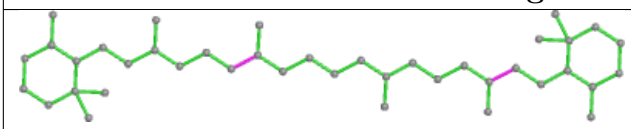
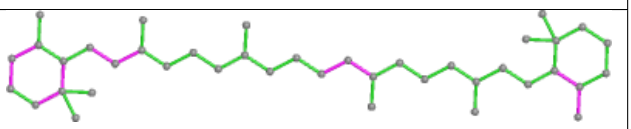


Rings

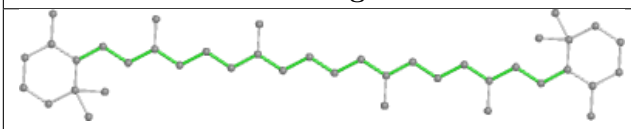
Ligand BCR a 410



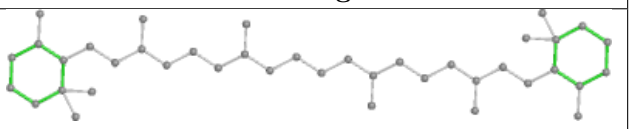
Bond lengths



Bond angles

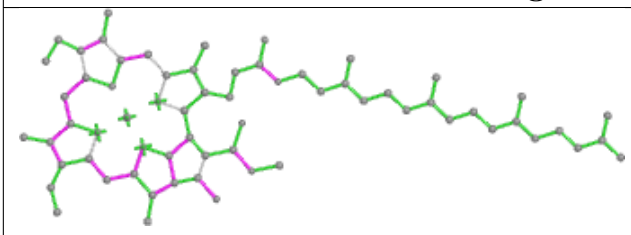


Torsions

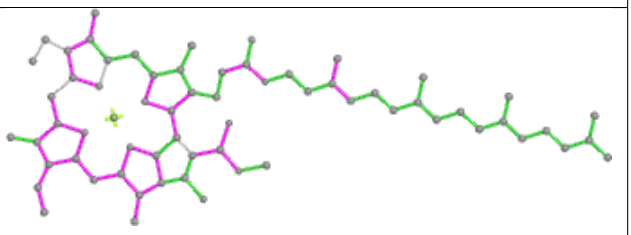


Rings

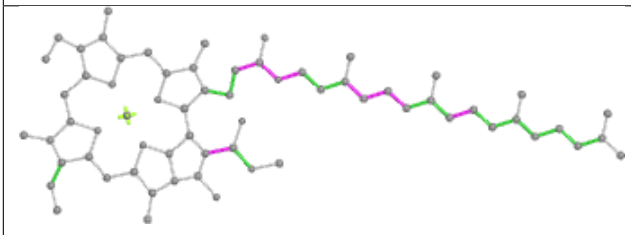
Ligand CLA b 605



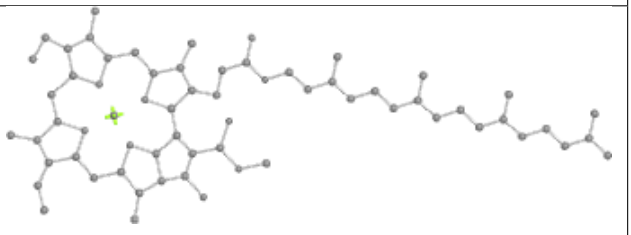
Bond lengths



Bond angles

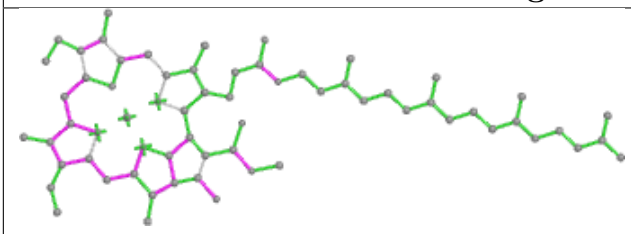


Torsions

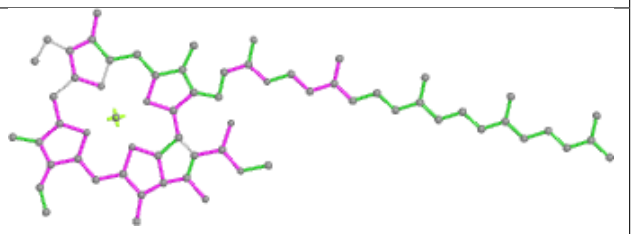


Rings

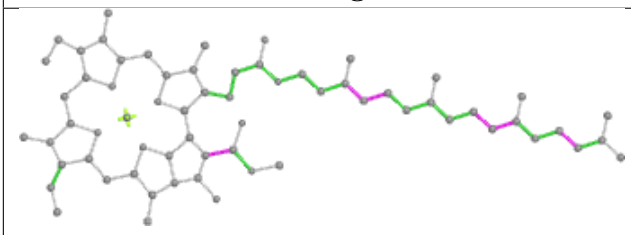
Ligand CLA b 620



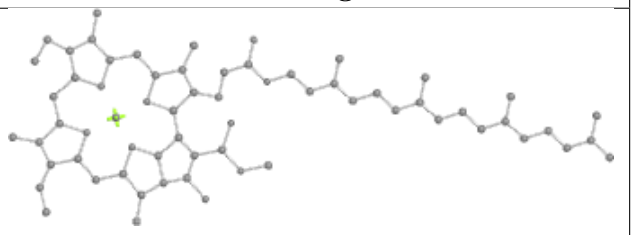
Bond lengths



Bond angles

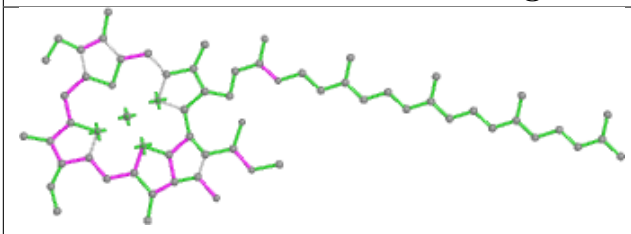


Torsions

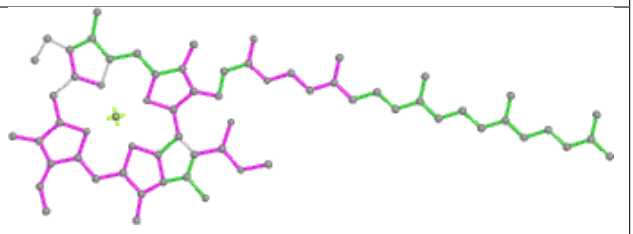


Rings

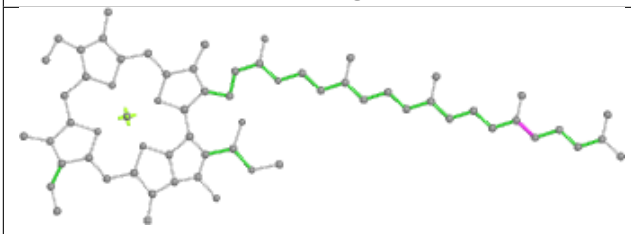
Ligand CLA A 407



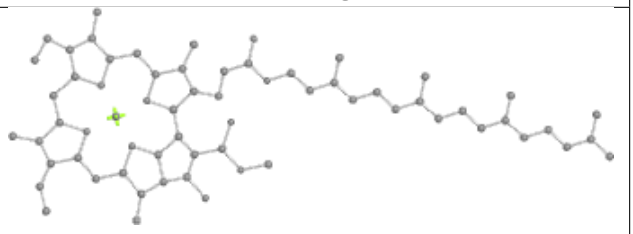
Bond lengths



Bond angles

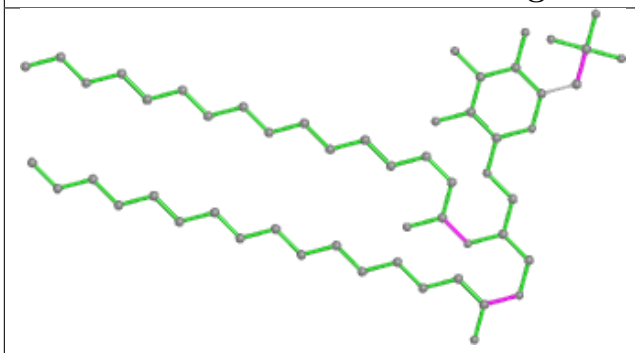


Torsions

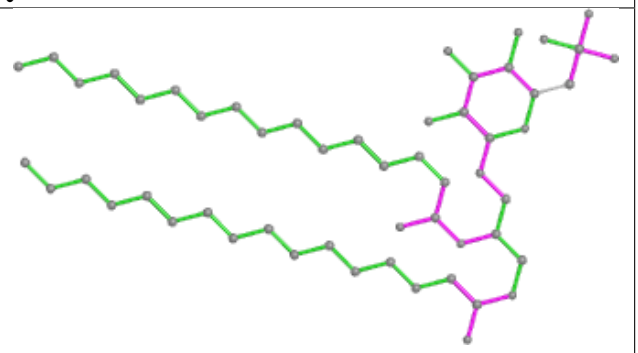


Rings

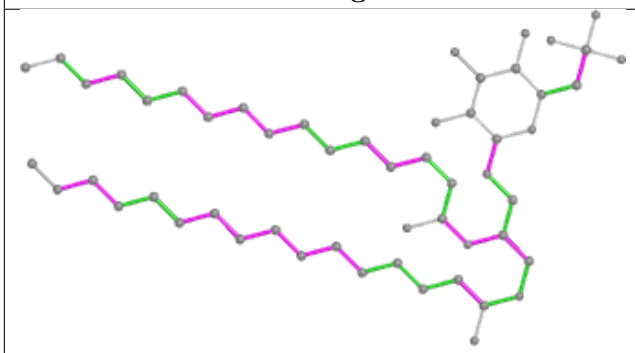
Ligand SQD L 102



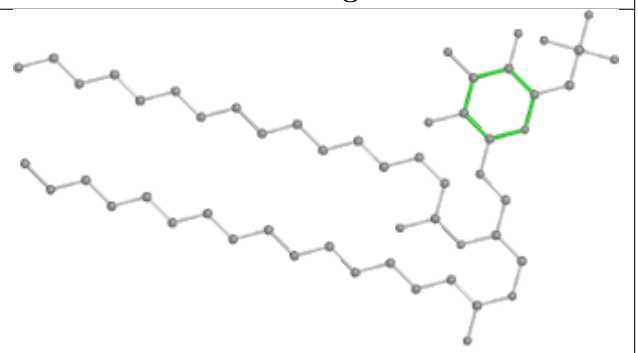
Bond lengths



Bond angles

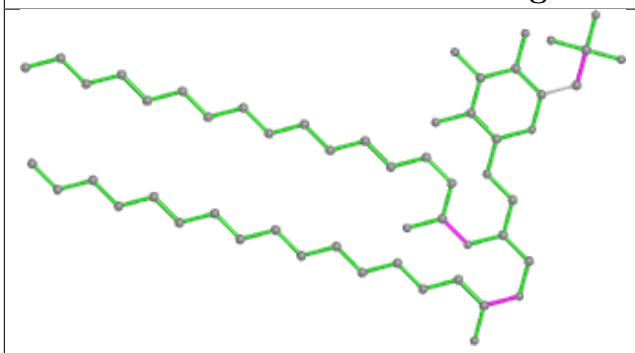


Torsions

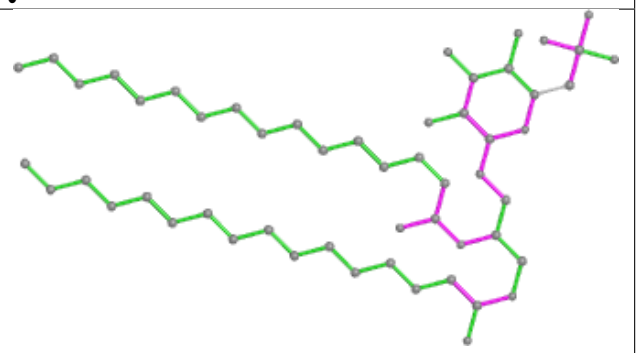


Rings

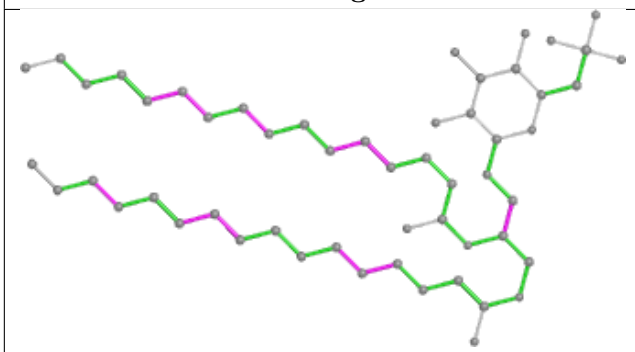
Ligand SQD a 411



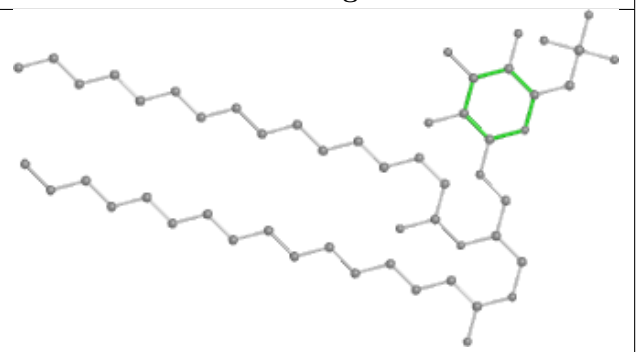
Bond lengths



Bond angles

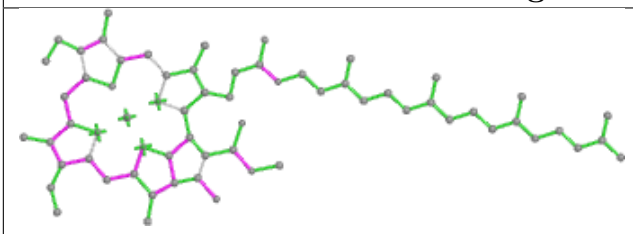


Torsions

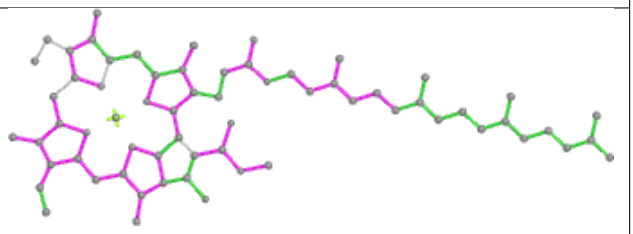


Rings

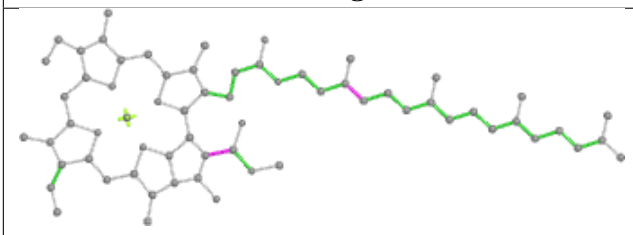
Ligand CLA b 613



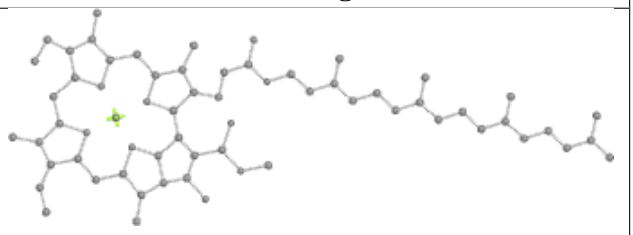
Bond lengths



Bond angles

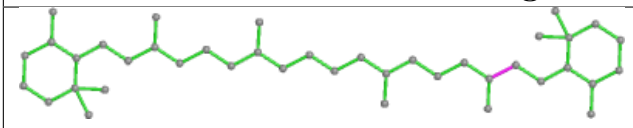


Torsions

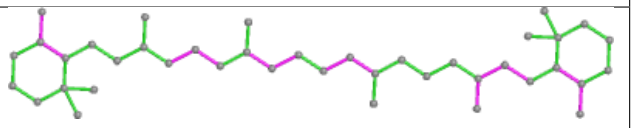


Rings

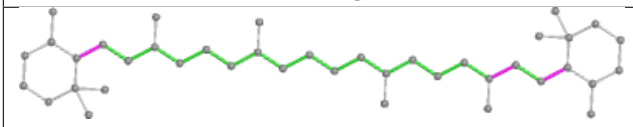
Ligand BCR K 102



Bond lengths



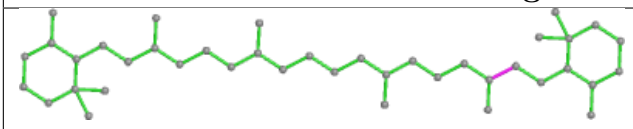
Bond angles



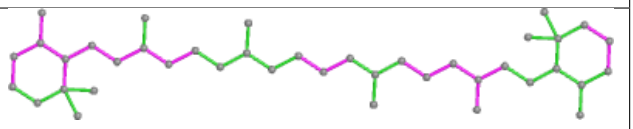
Torsions

Rings

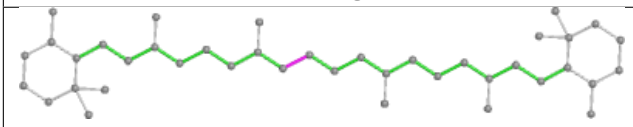
Ligand BCR T 102



Bond lengths



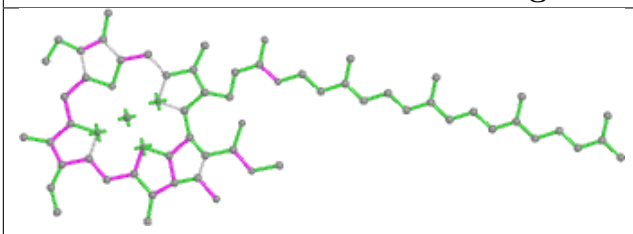
Bond angles



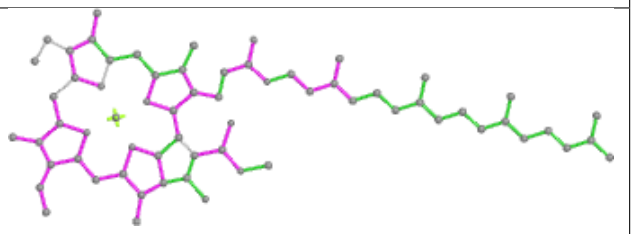
Torsions

Rings

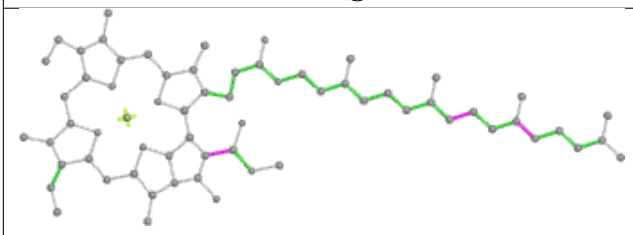
Ligand CLA c 905



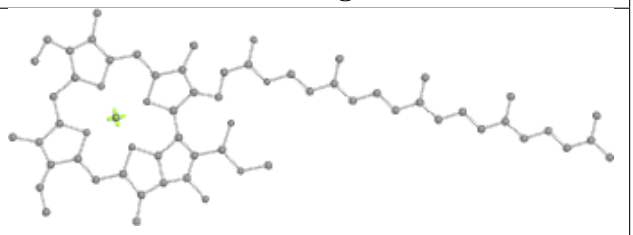
Bond lengths



Bond angles

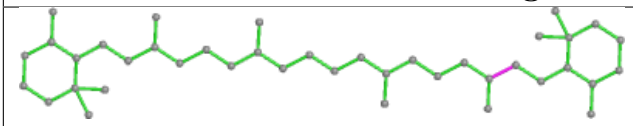


Torsions



Rings

Ligand BCR C 516



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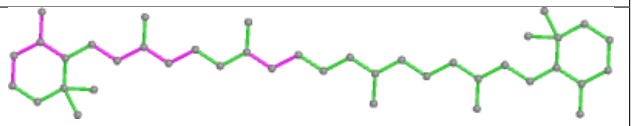
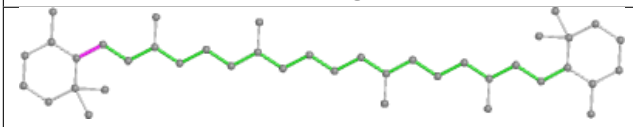


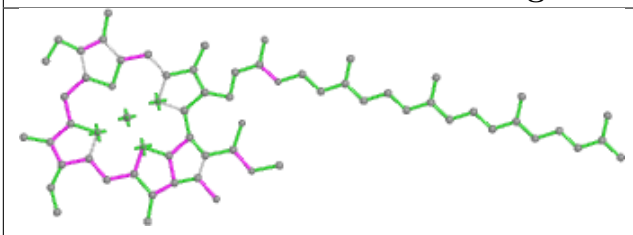
Bond angles



Torsions

Rings

Ligand CLA b 616



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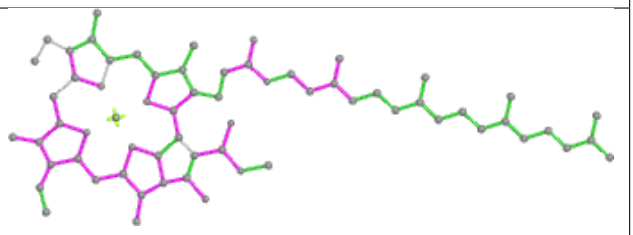
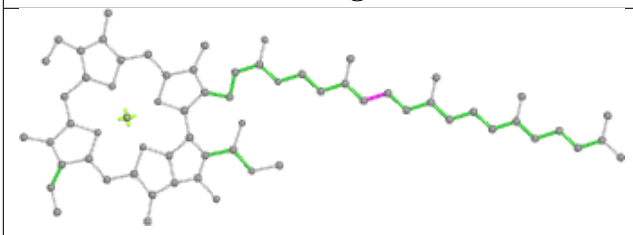
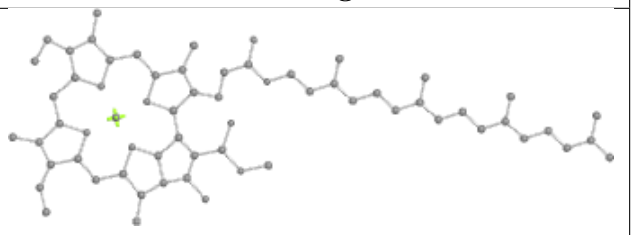


Bond angles

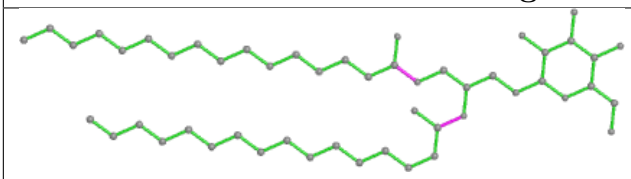


Torsions

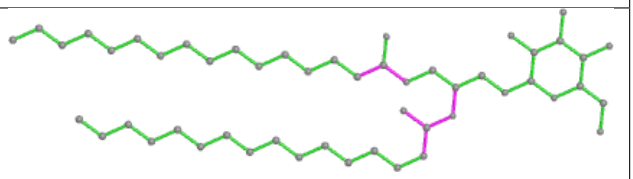


Rings

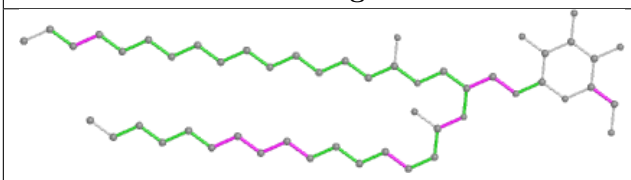
Ligand LMG C 521



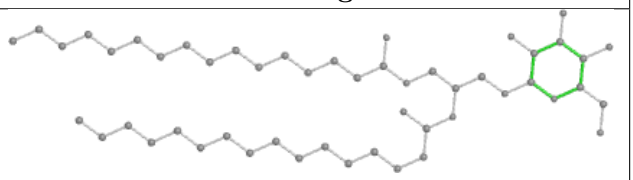
Bond lengths



Bond angles

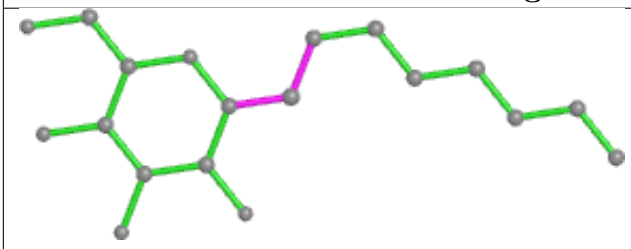


Torsions

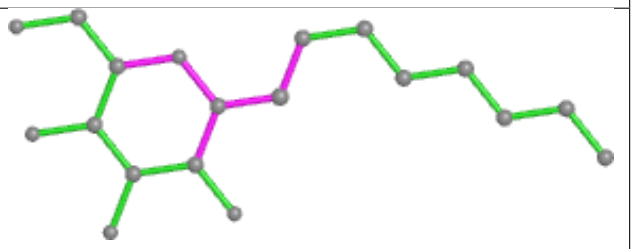


Rings

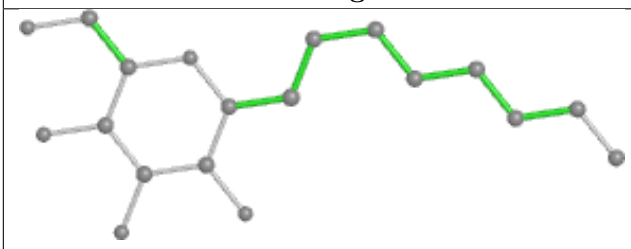
Ligand HTG b 603



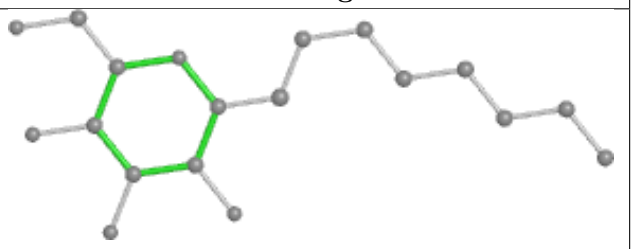
Bond lengths



Bond angles

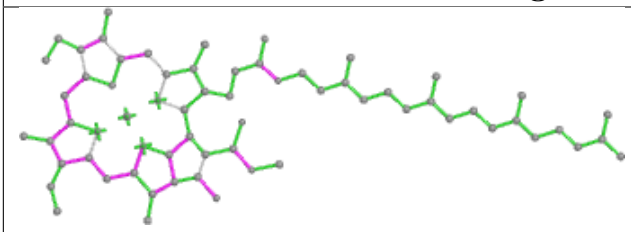


Torsions

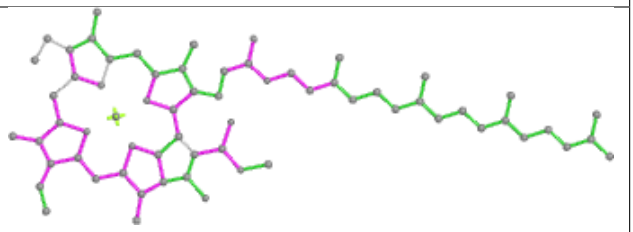


Rings

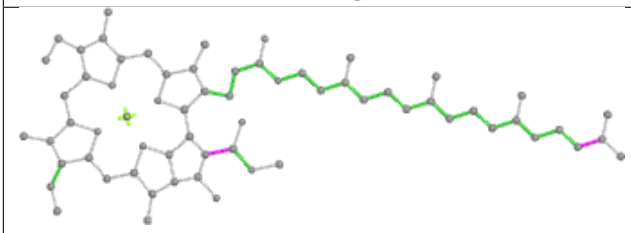
Ligand CLA c 903



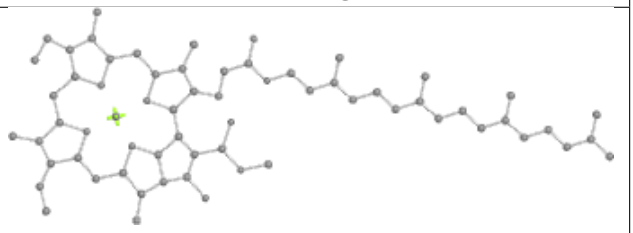
Bond lengths



Bond angles

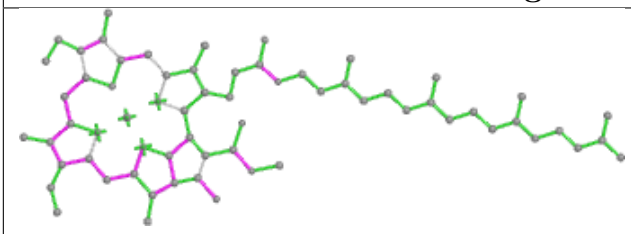


Torsions

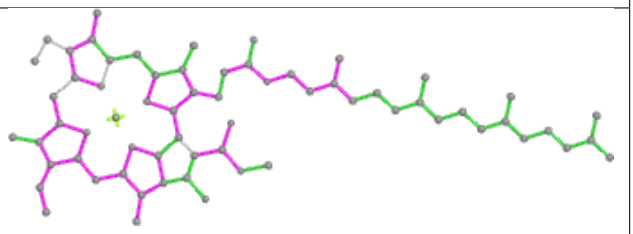


Rings

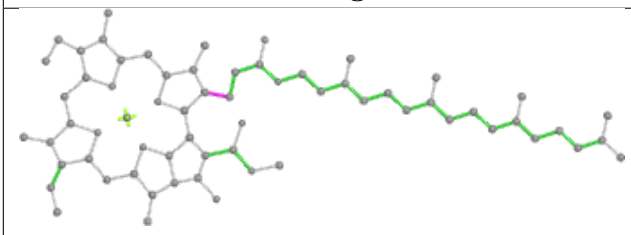
Ligand CLA C 514



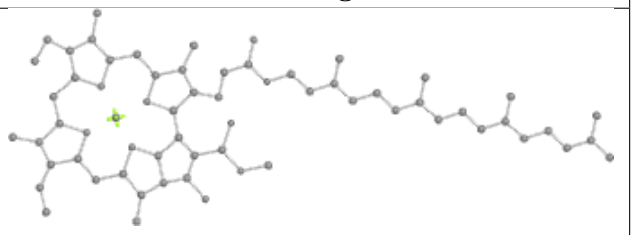
Bond lengths



Bond angles

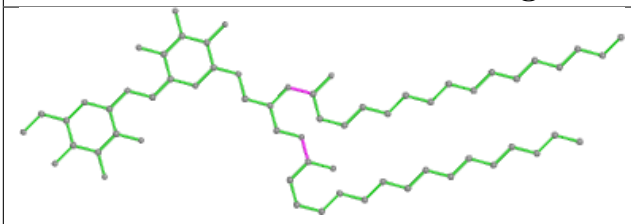


Torsions

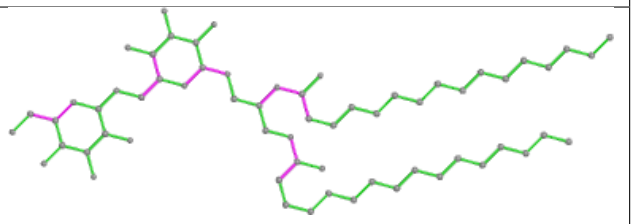


Rings

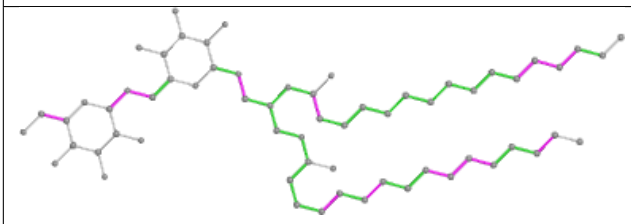
Ligand DGD C 518



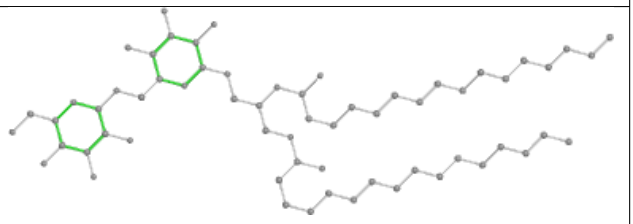
Bond lengths



Bond angles

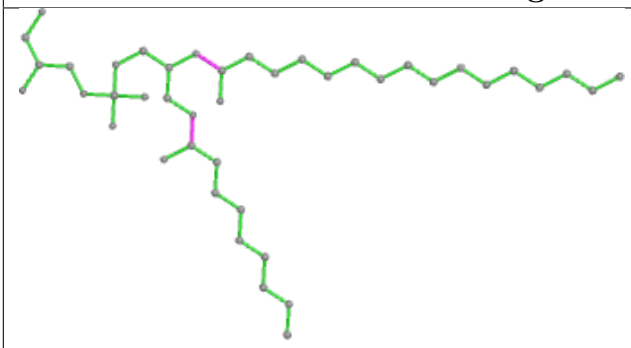


Torsions

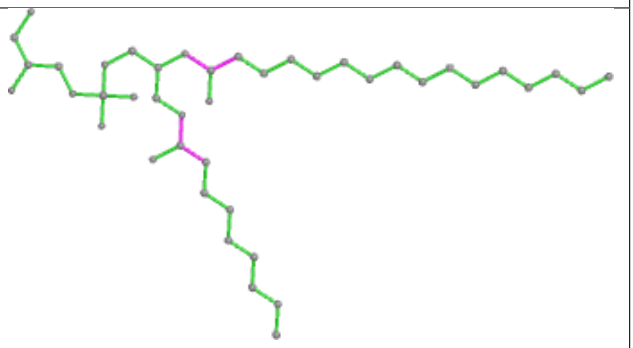


Rings

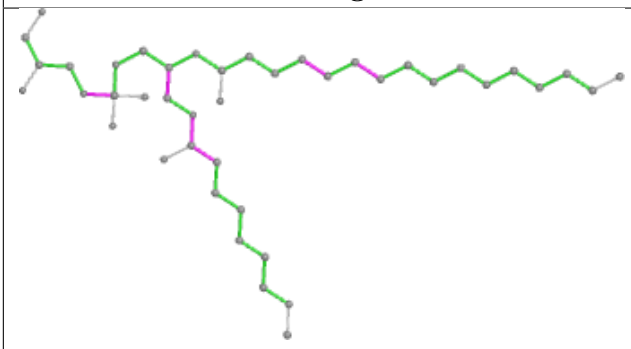
Ligand LHG e 101



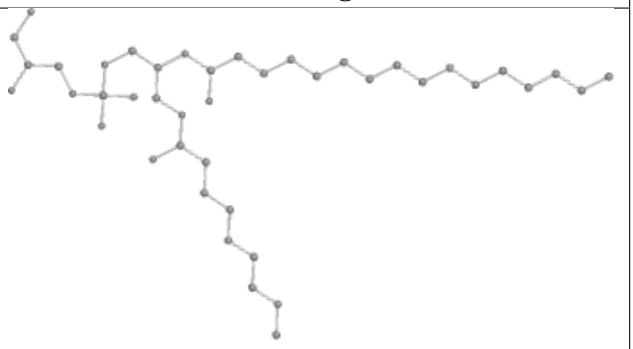
Bond lengths



Bond angles

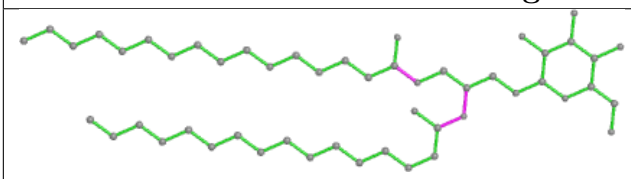


Torsions

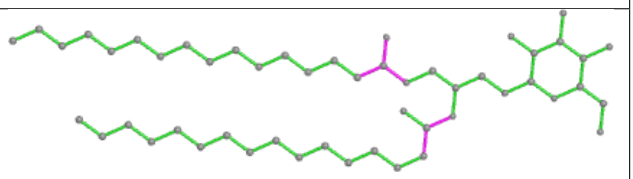


Rings

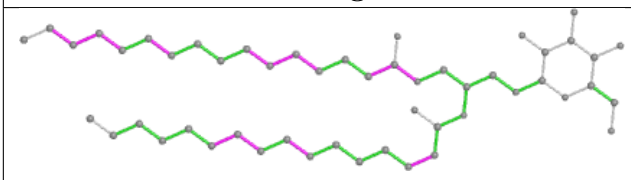
Ligand LMG b 624



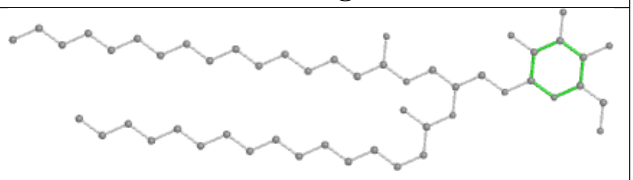
Bond lengths



Bond angles

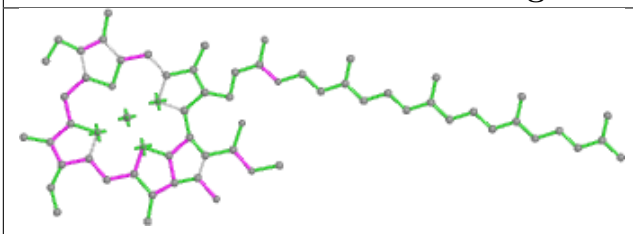


Torsions

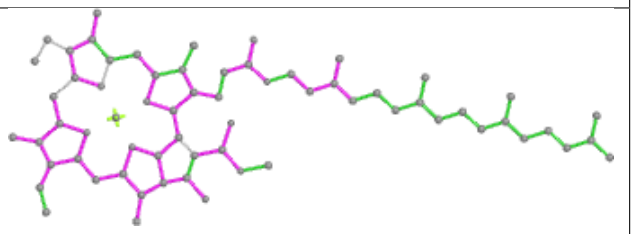


Rings

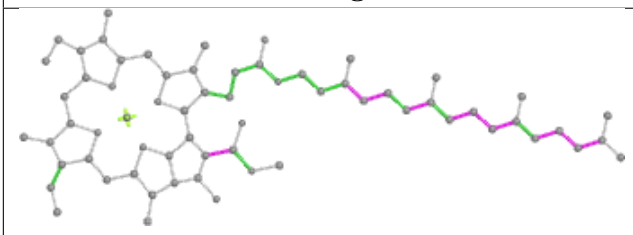
Ligand CLA b 618



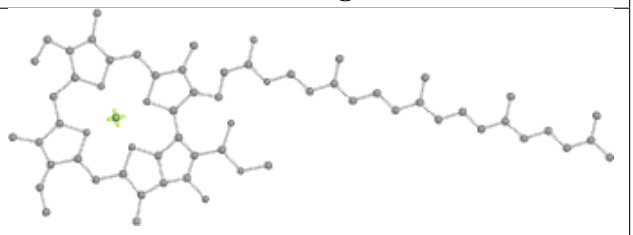
Bond lengths



Bond angles

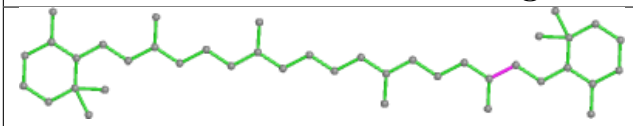


Torsions

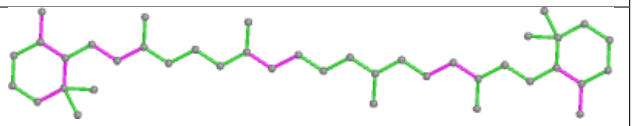


Rings

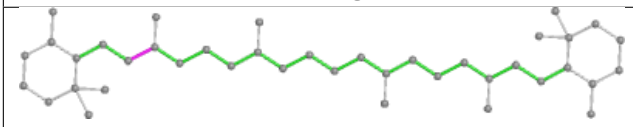
Ligand BCR K 103



Bond lengths



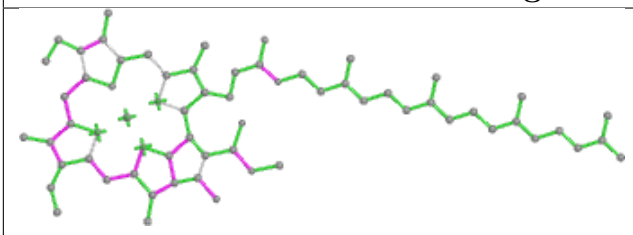
Bond angles



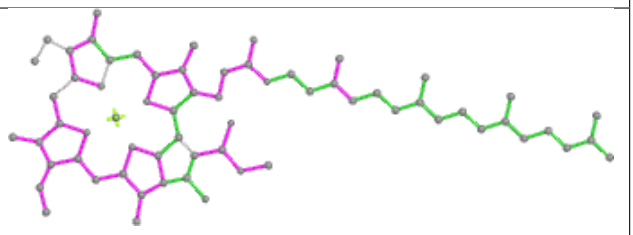
Torsions

Rings

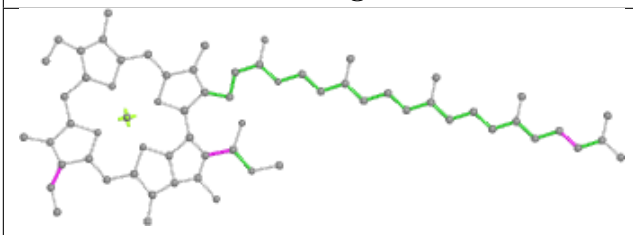
Ligand CLA A 406



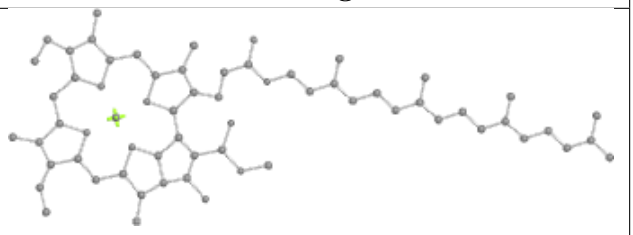
Bond lengths



Bond angles

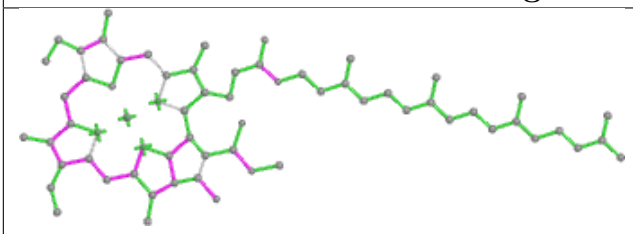


Torsions

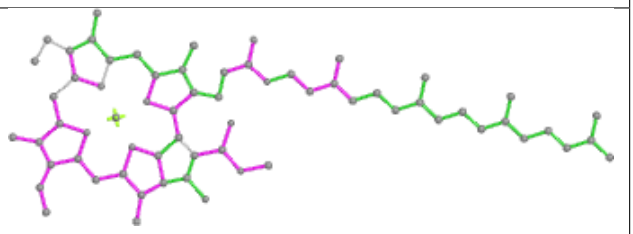


Rings

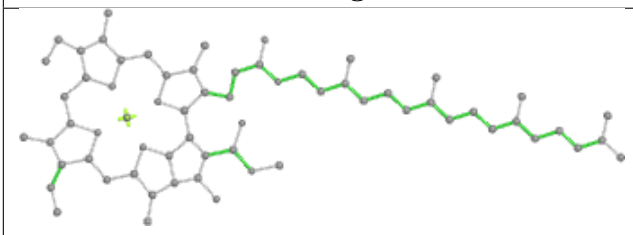
Ligand CLA D 401



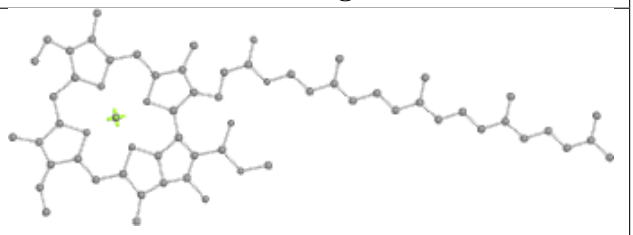
Bond lengths



Bond angles

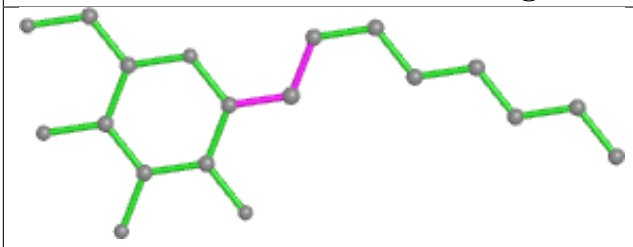


Torsions

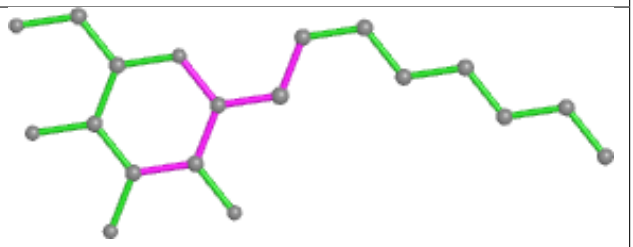


Rings

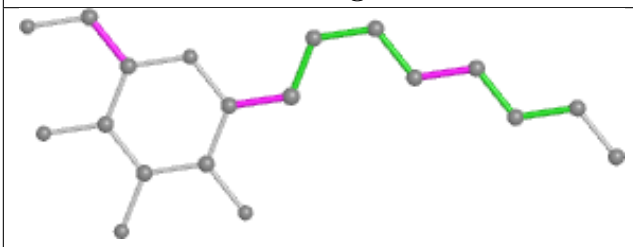
Ligand HTG V 202



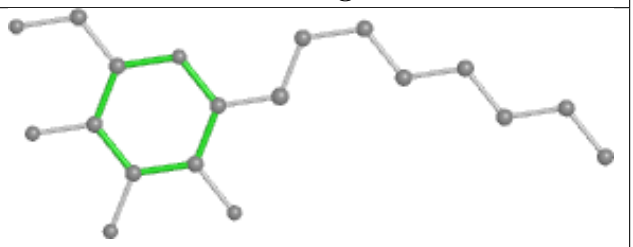
Bond lengths



Bond angles

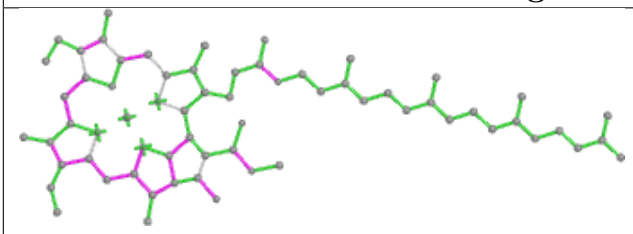


Torsions

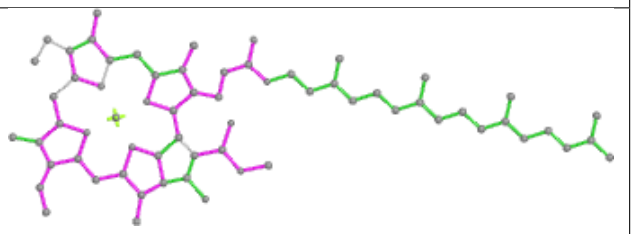


Rings

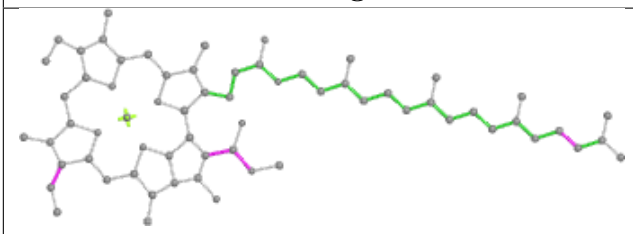
Ligand CLA d 401



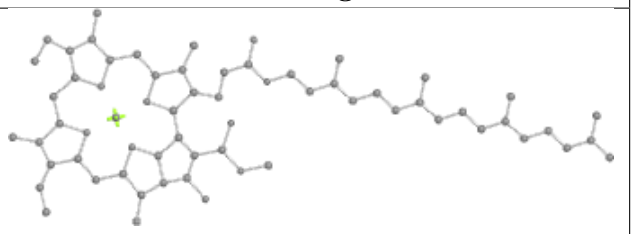
Bond lengths



Bond angles

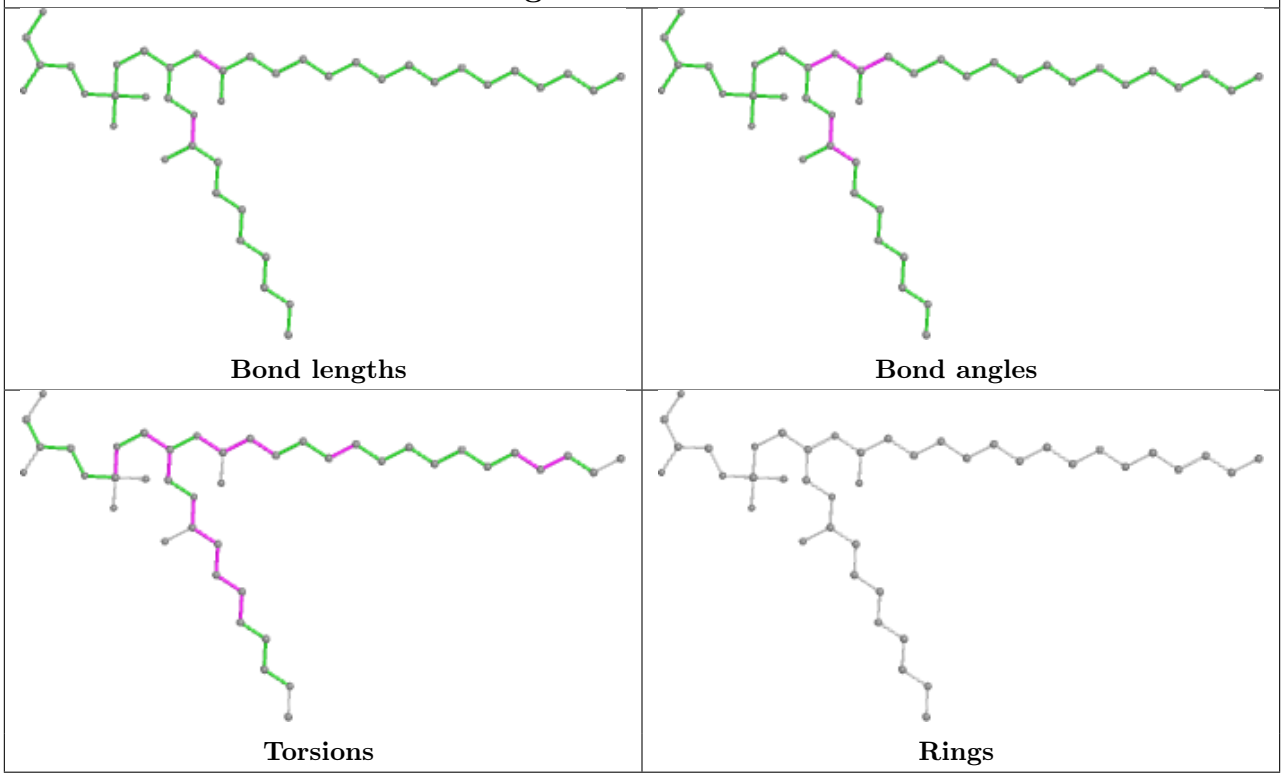


Torsions

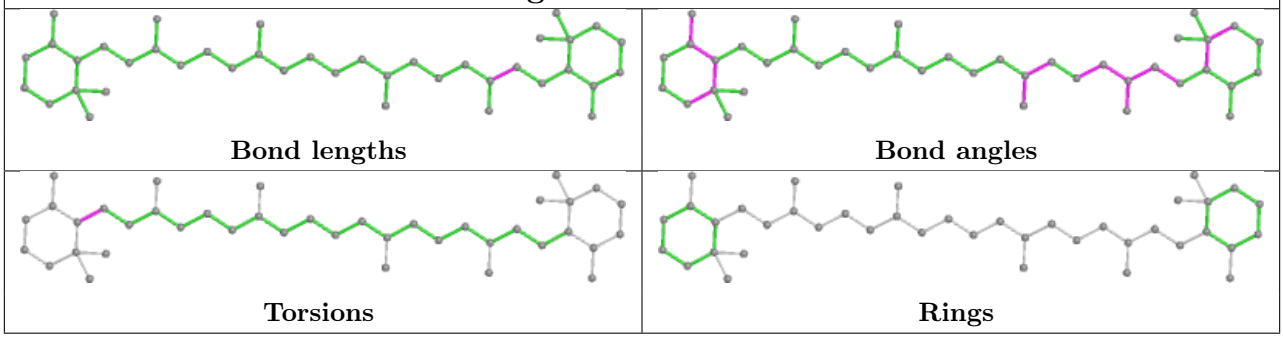


Rings

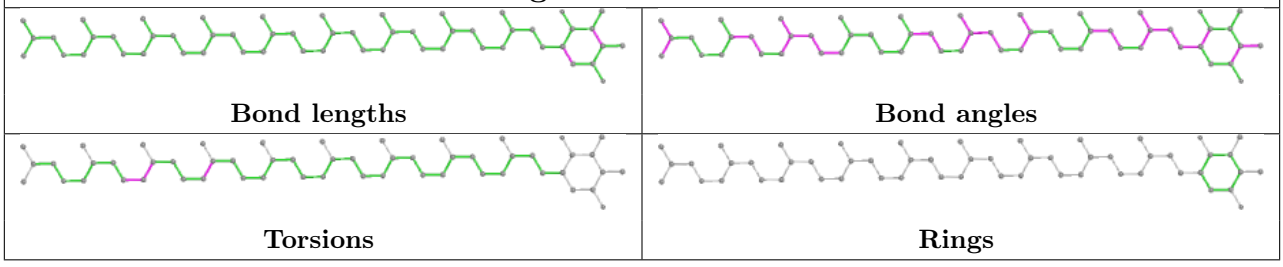
Ligand LHG E 101



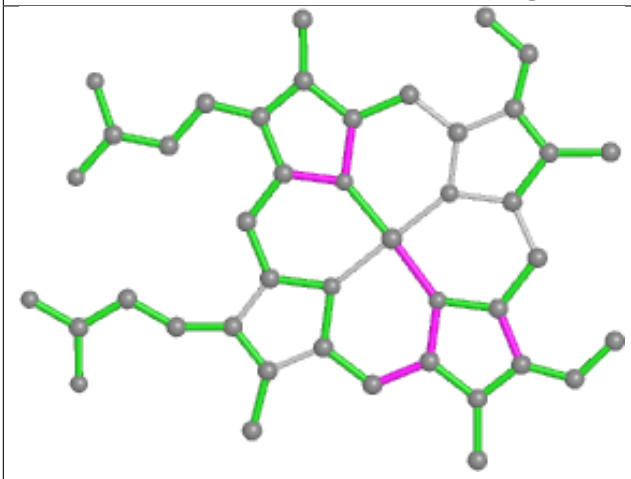
Ligand BCR k 102



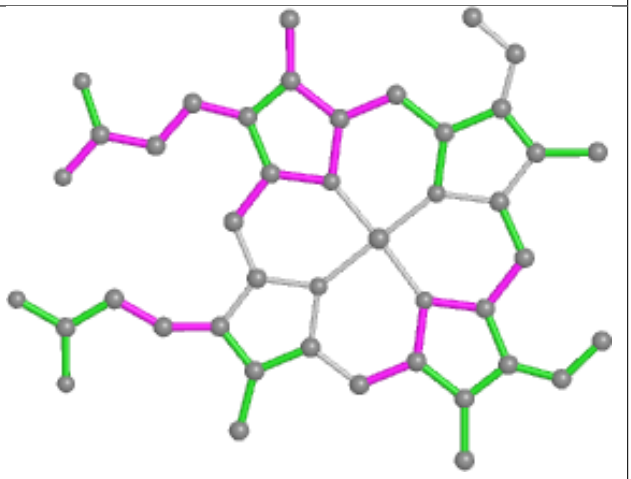
Ligand PL9 D 404



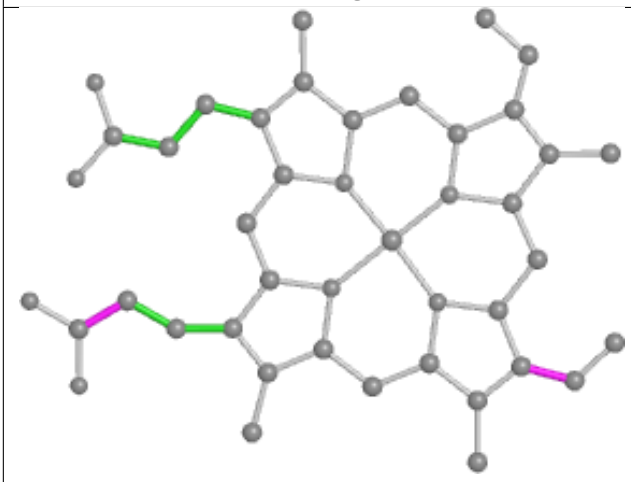
Ligand HEM e 102



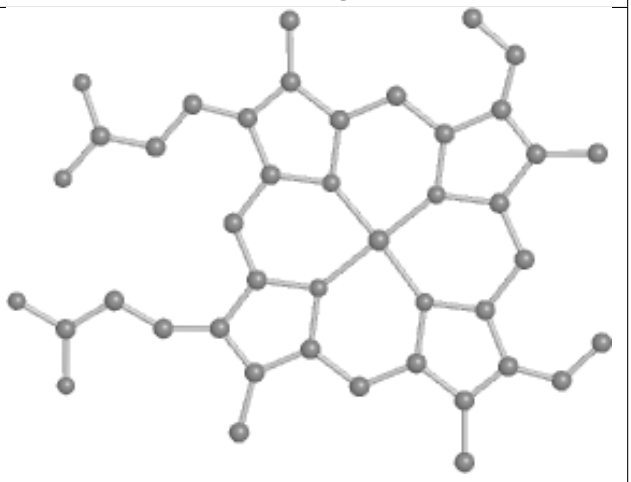
Bond lengths



Bond angles

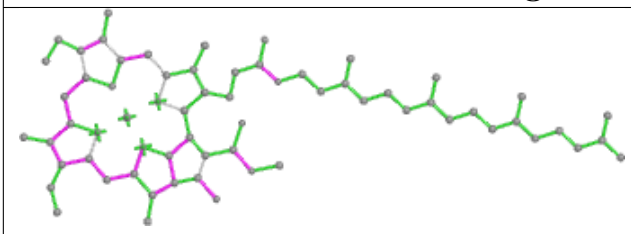


Torsions

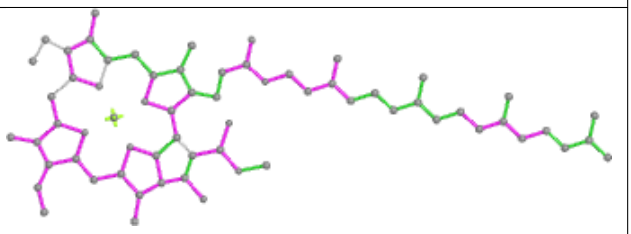


Rings

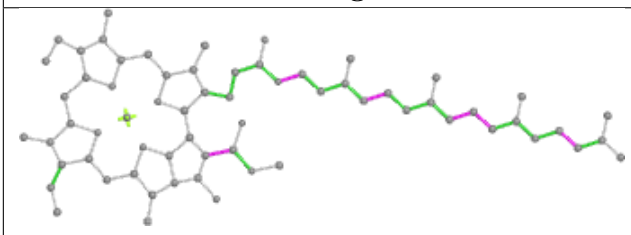
Ligand CLA C 510



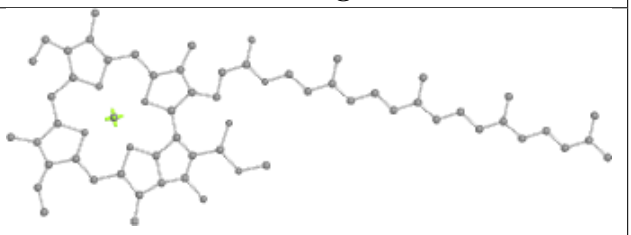
Bond lengths



Bond angles

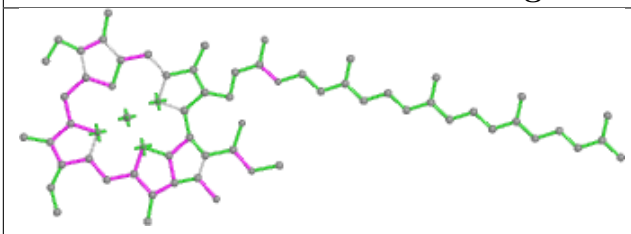


Torsions

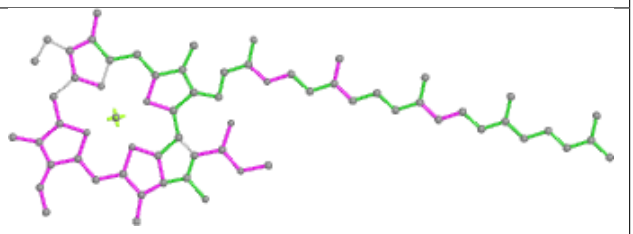


Rings

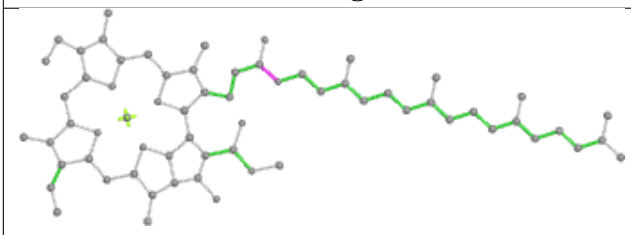
Ligand CLA C 512



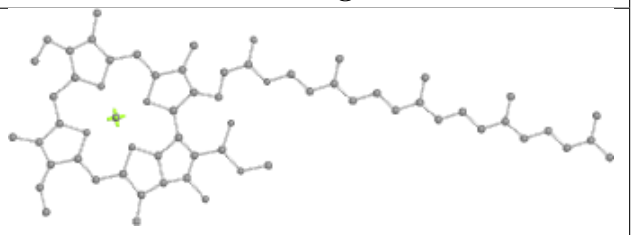
Bond lengths



Bond angles

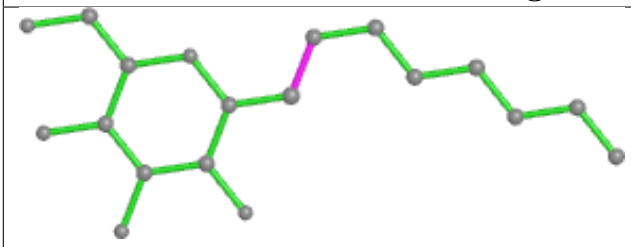


Torsions

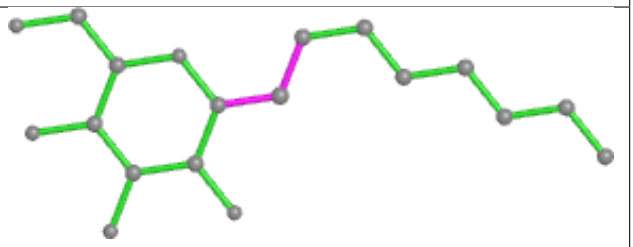


Rings

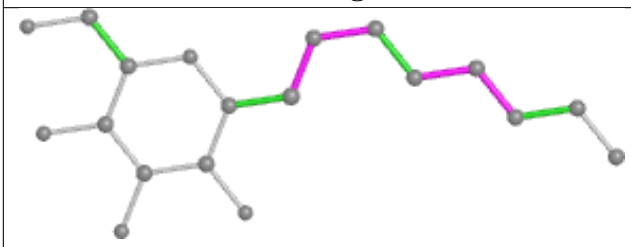
Ligand HTG c 922



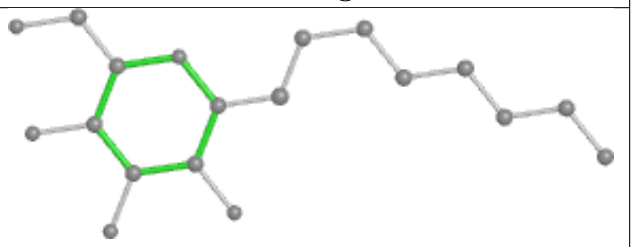
Bond lengths



Bond angles

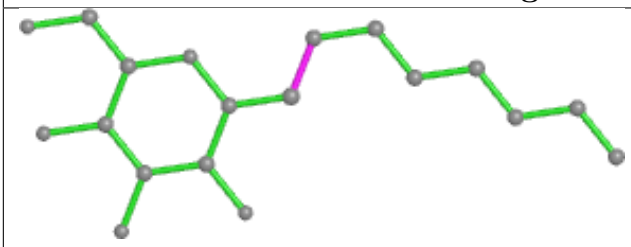


Torsions

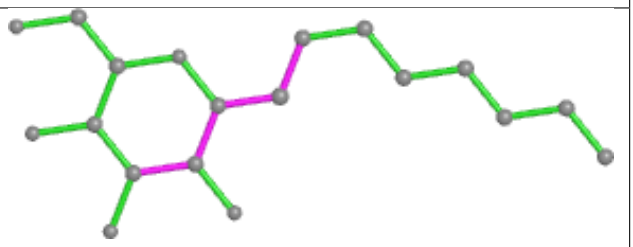


Rings

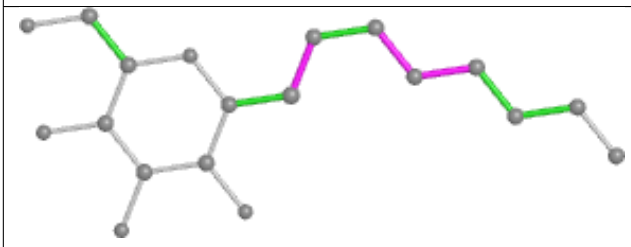
Ligand HTG B 625



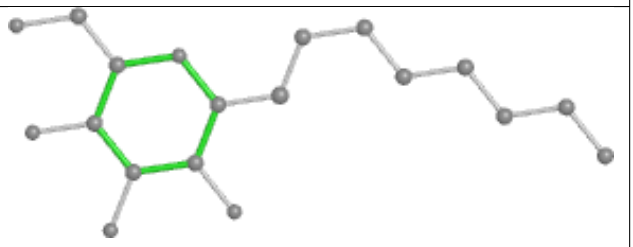
Bond lengths



Bond angles

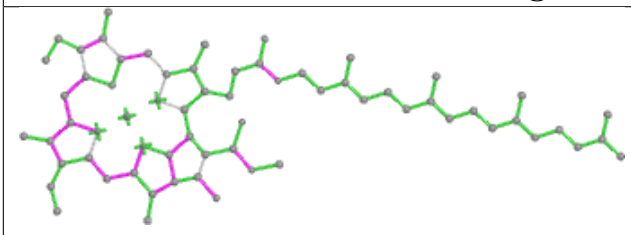


Torsions

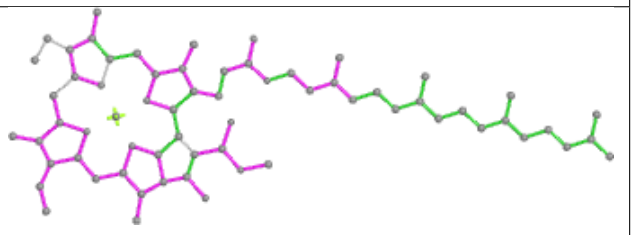


Rings

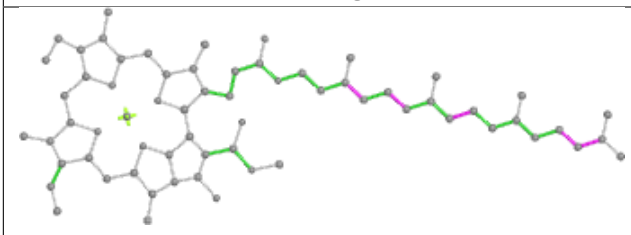
Ligand CLA a 409



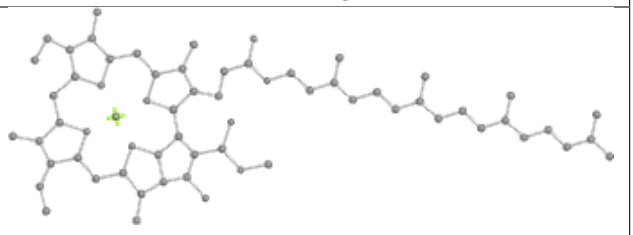
Bond lengths



Bond angles

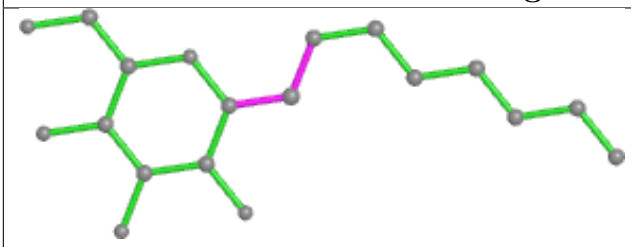


Torsions

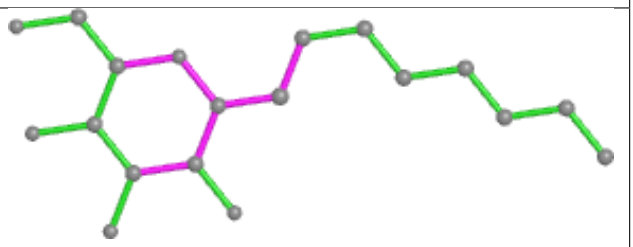


Rings

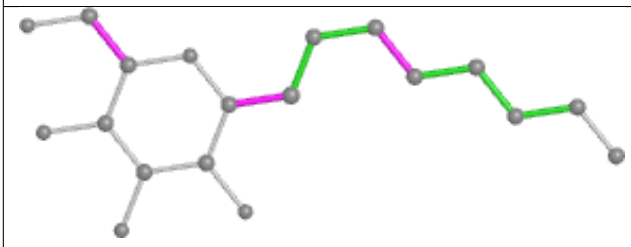
Ligand HTG b 627



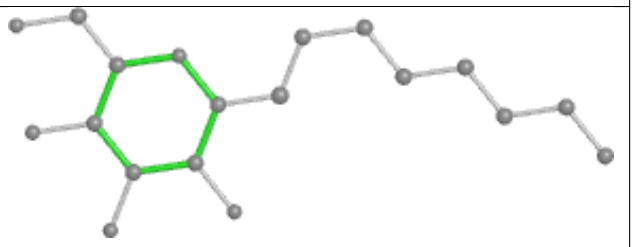
Bond lengths



Bond angles

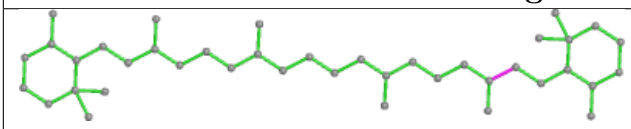


Torsions

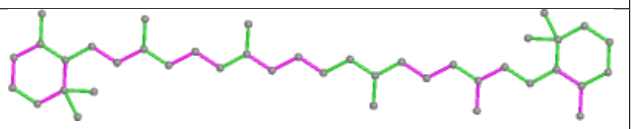


Rings

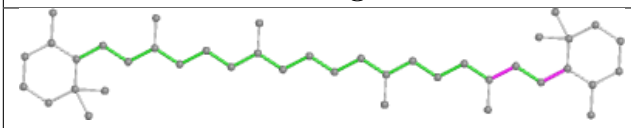
Ligand BCR b 623



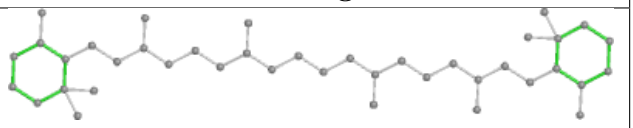
Bond lengths



Bond angles

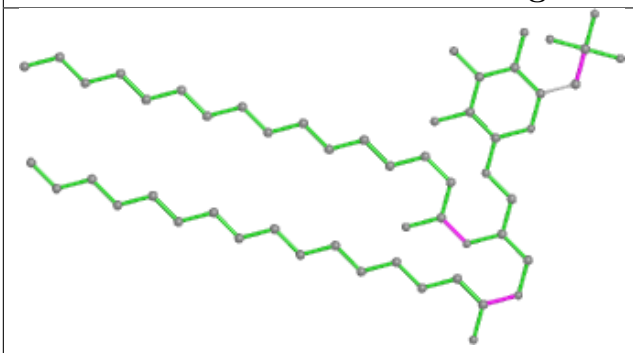


Torsions

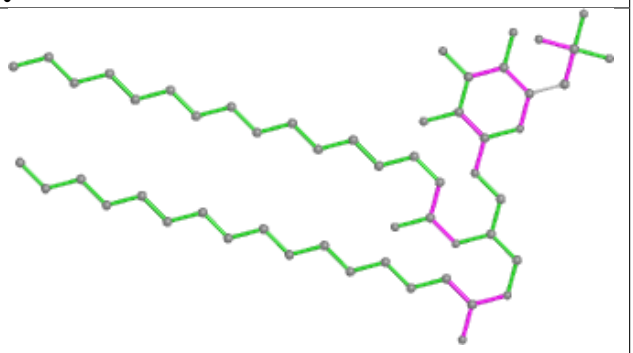


Rings

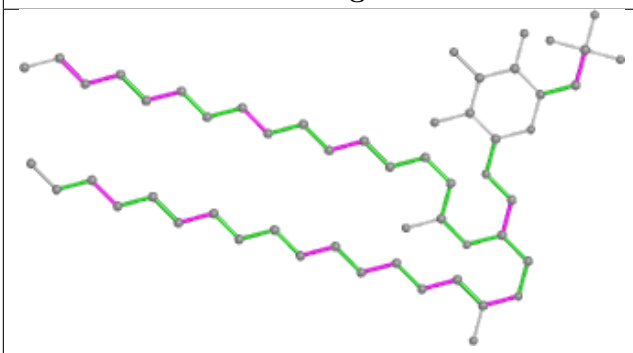
Ligand SQD a 402



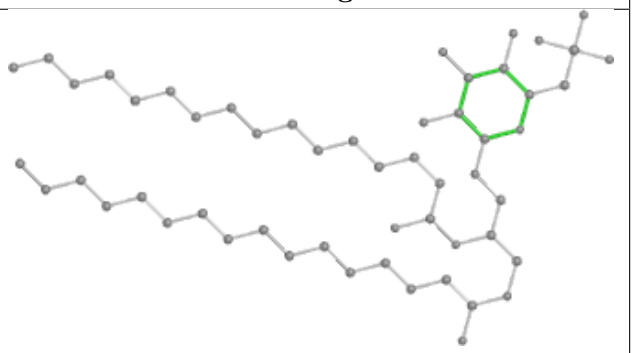
Bond lengths



Bond angles

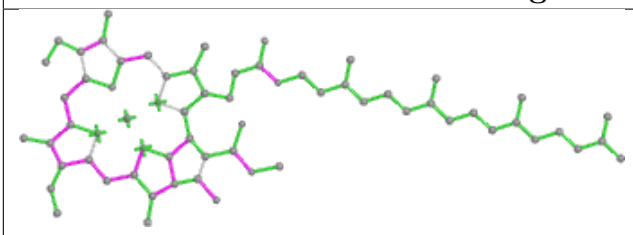


Torsions

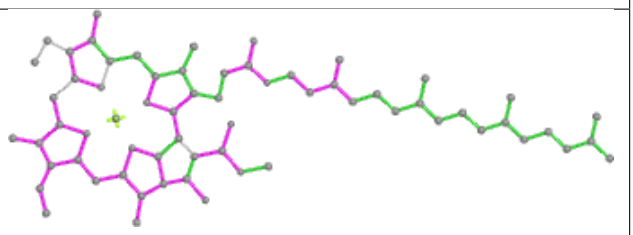


Rings

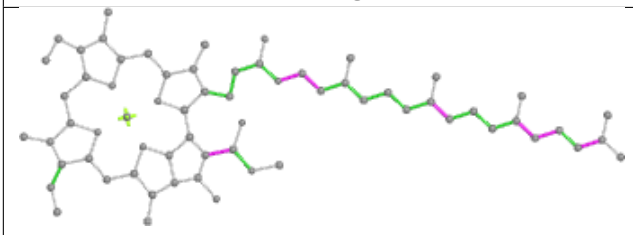
Ligand CLA c 910



Bond lengths



Bond angles



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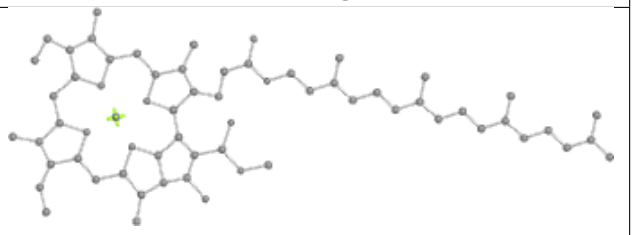
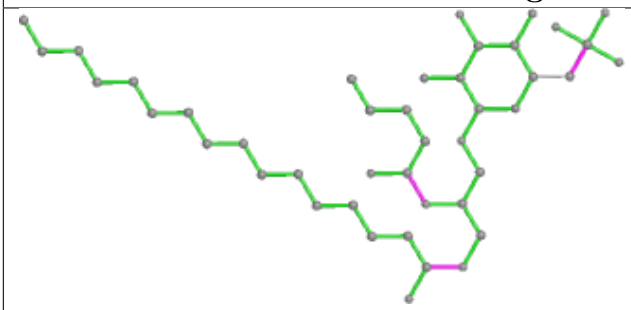


Rings

Ligand SQD F 101



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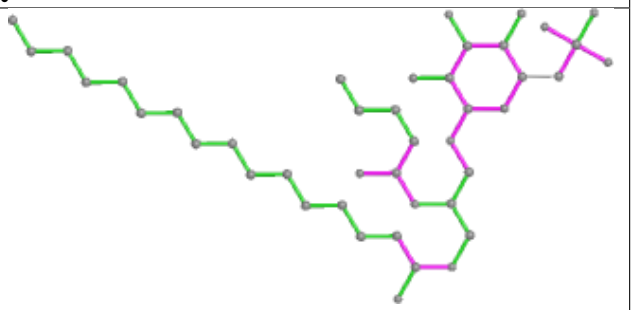
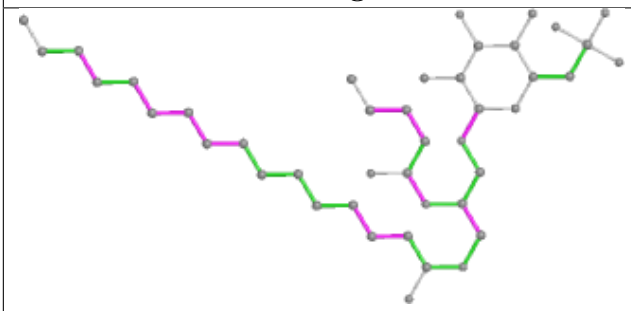
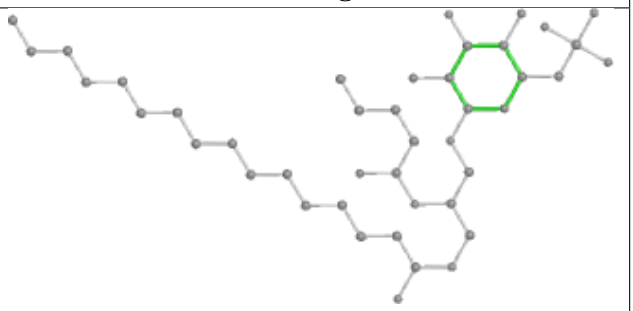


Bond angles

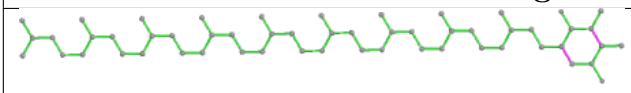


Torsions

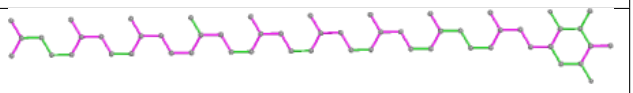


Rings

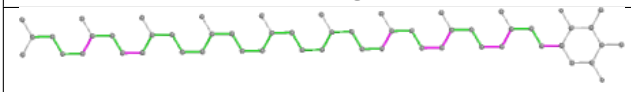
Ligand PL9 a 417



Bond lengths



Bond angles



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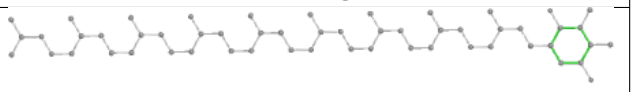
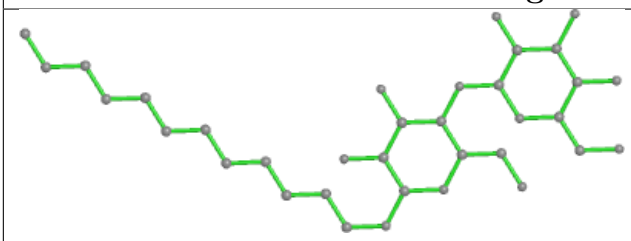


Rings

Ligand LMT c 921



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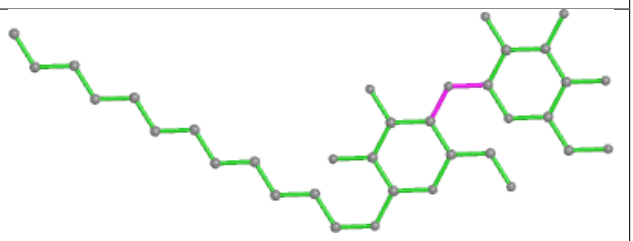
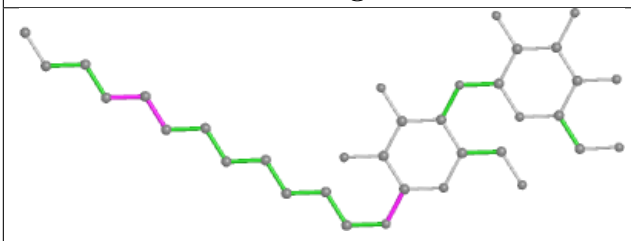


Bond angles



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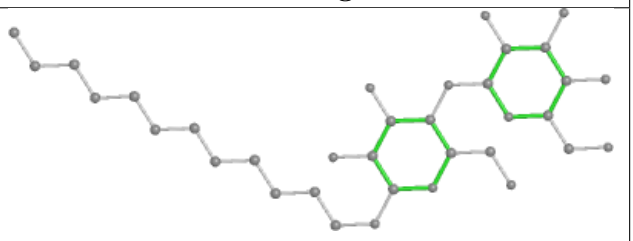
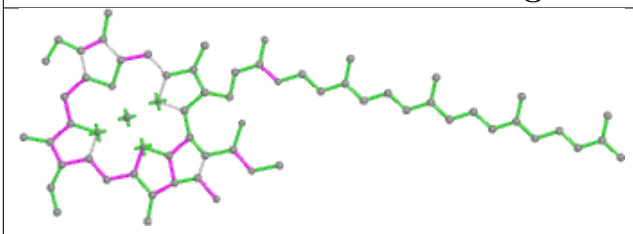
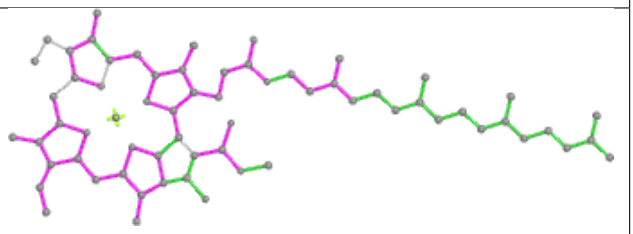


Rings

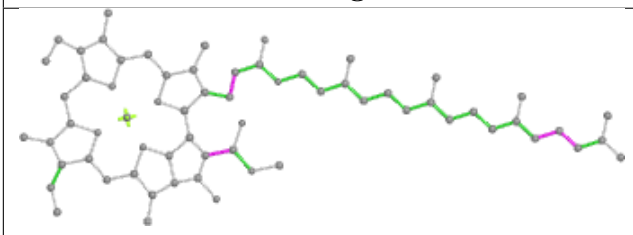
Ligand CLA B 603



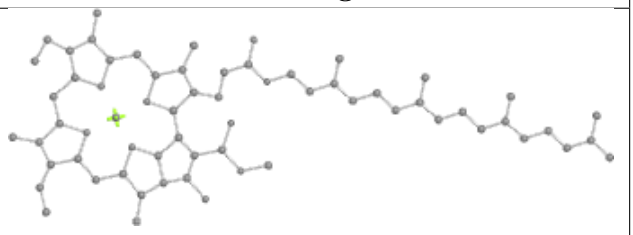
Bond lengths



Bond angles

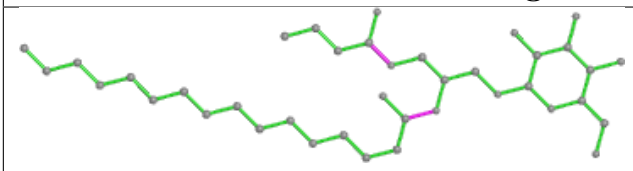


Torsions



Rings

Ligand LMG z 101



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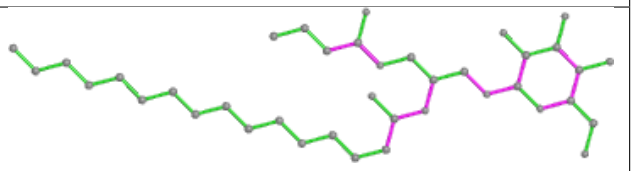
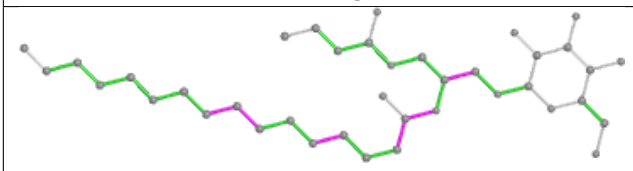


Bond angles



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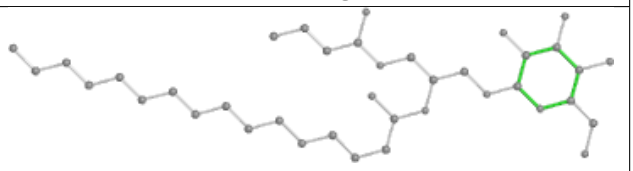
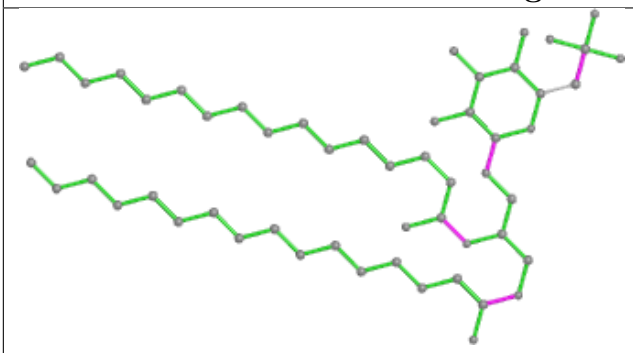
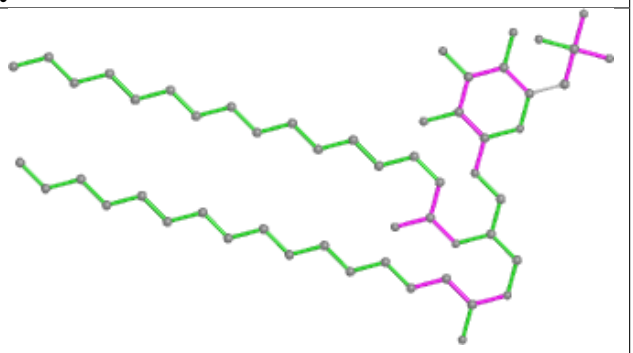


Rings

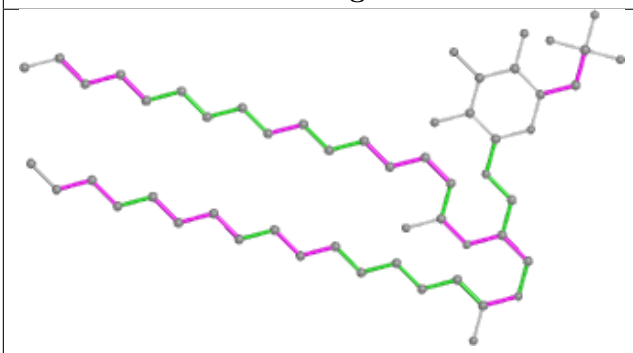
Ligand SQD B 621



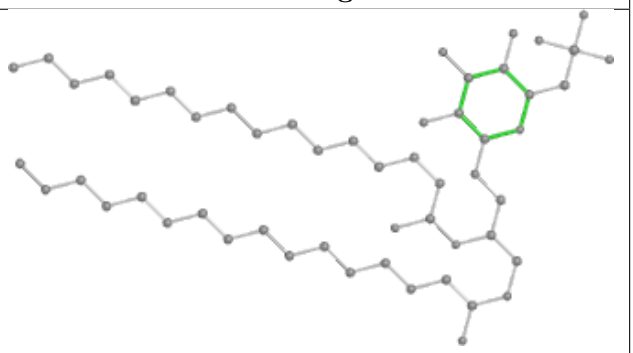
Bond lengths



Bond angles

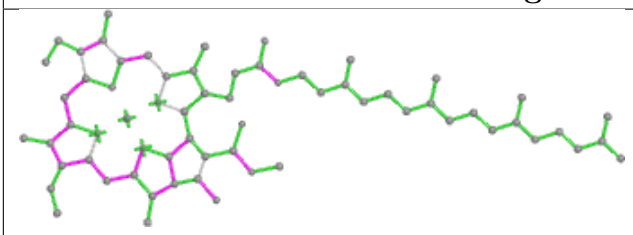


Torsions

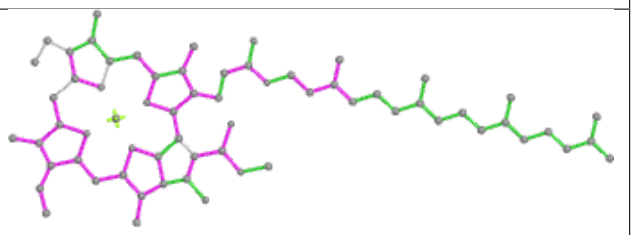


Rings

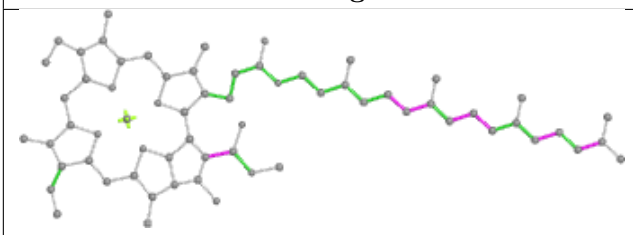
Ligand CLA C 507



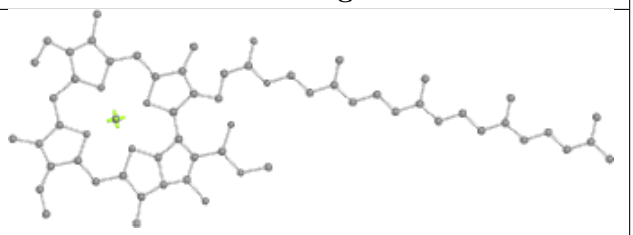
Bond lengths



Bond angles

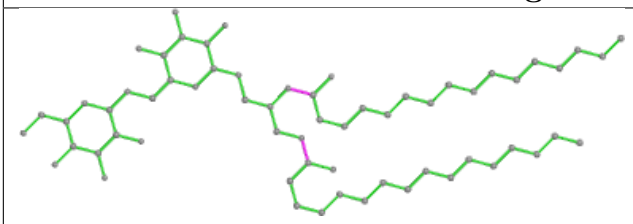


Torsions

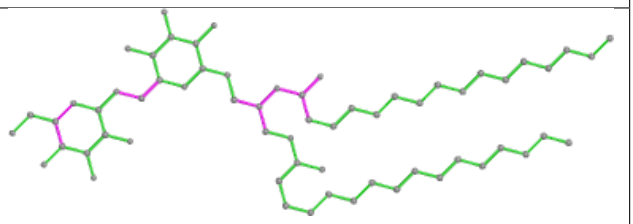


Rings

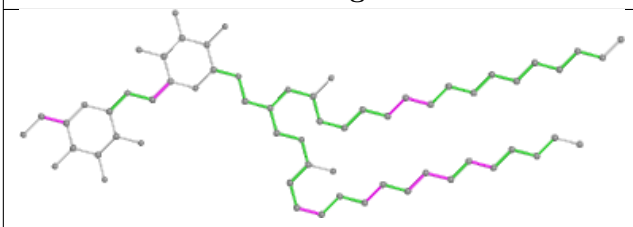
Ligand DGD c 916



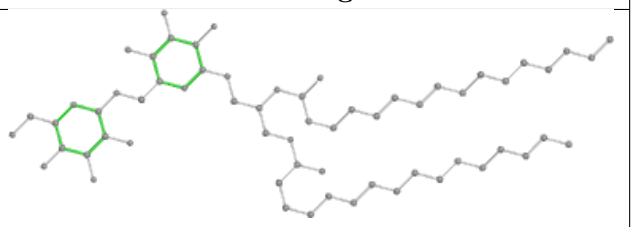
Bond lengths



Bond angles

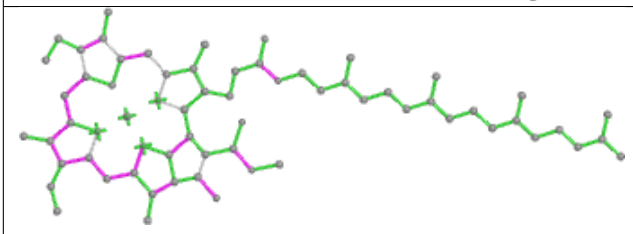


Torsions

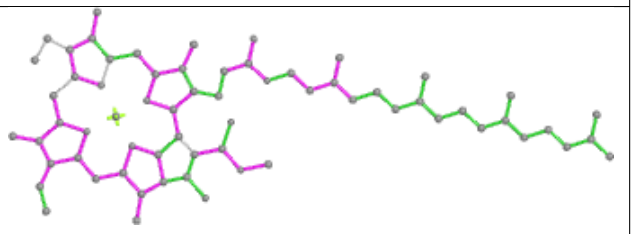


Rings

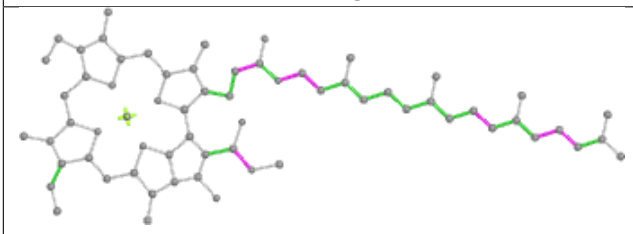
Ligand CLA B 614



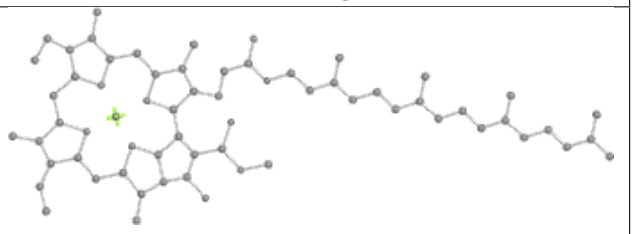
Bond lengths



Bond angles

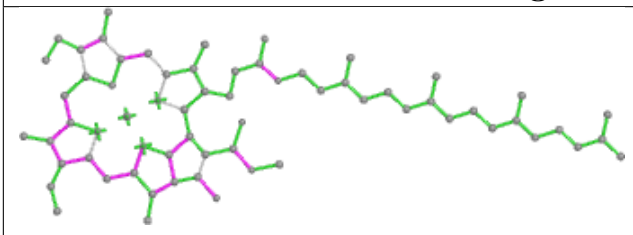


Torsions

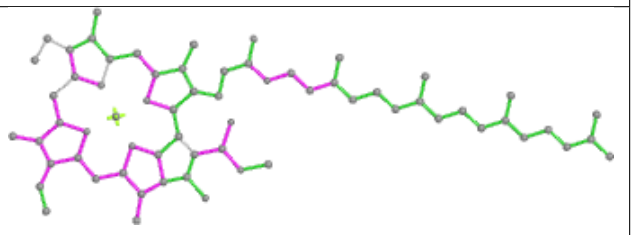


Rings

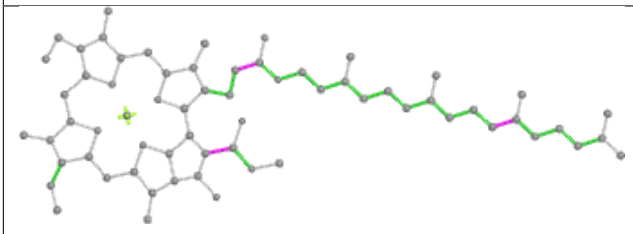
Ligand CLA c 906



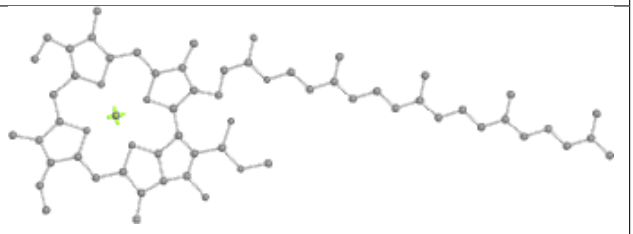
Bond lengths



Bond angles

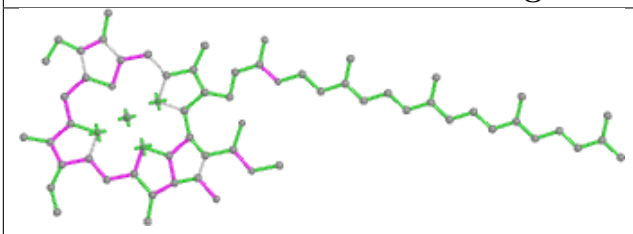


Torsions

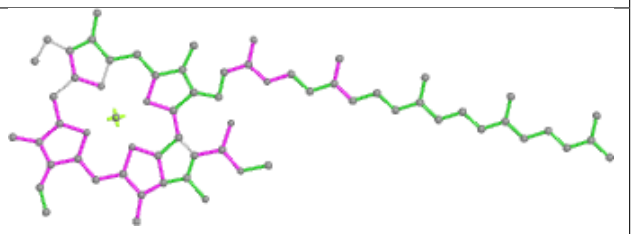


Rings

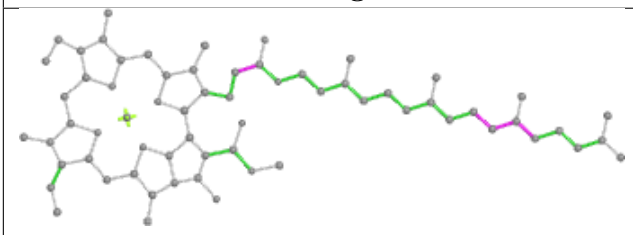
Ligand CLA C 506



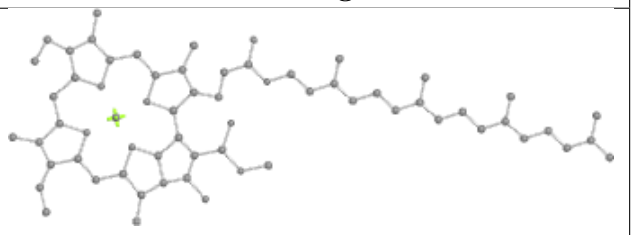
Bond lengths



Bond angles

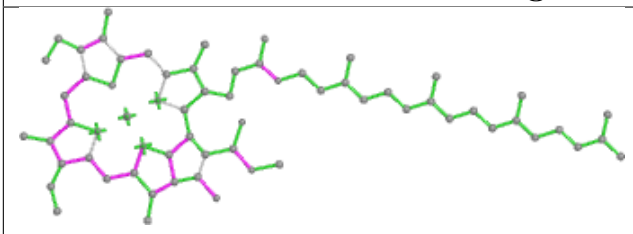


Torsions

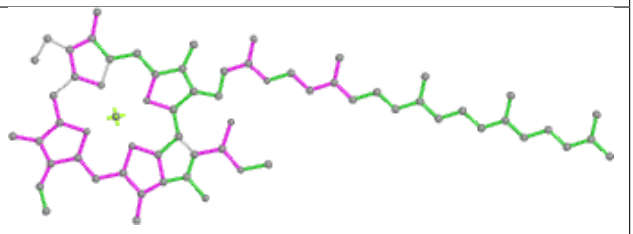


Rings

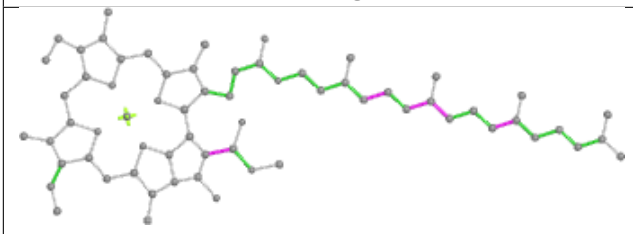
Ligand CLA b 608



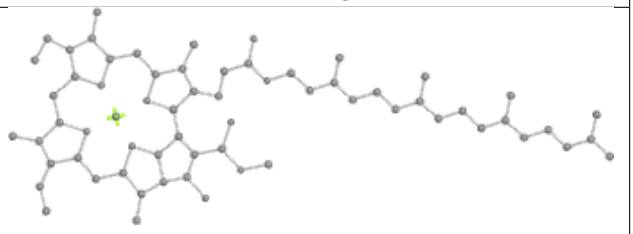
Bond lengths



Bond angles

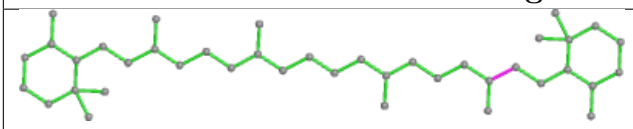


Torsions

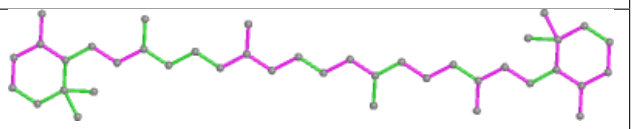


Rings

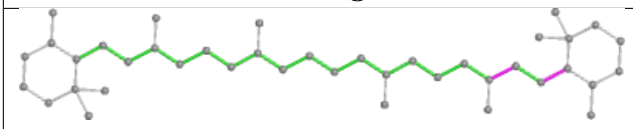
Ligand BCR d 404



Bond lengths



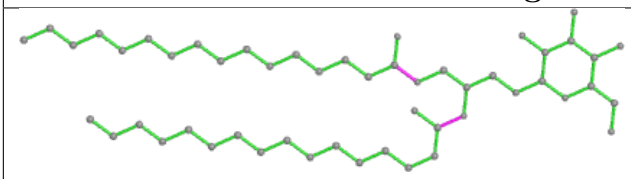
Bond angles



Torsions

Rings

Ligand LMG a 412



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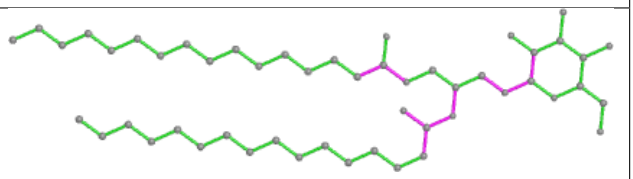
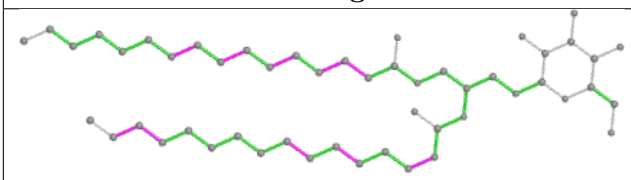
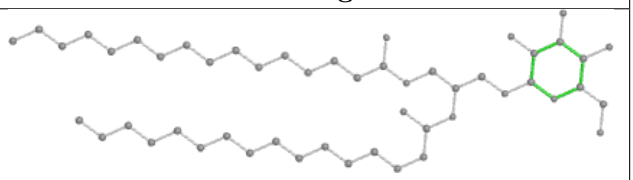


Bond angles

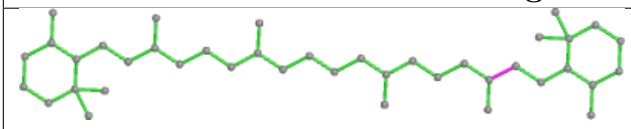


Torsions



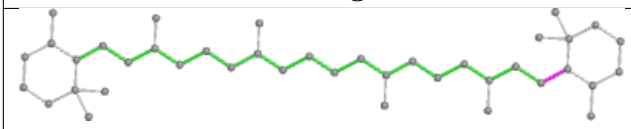
Rings

Ligand BCR b 622



Bond lengths

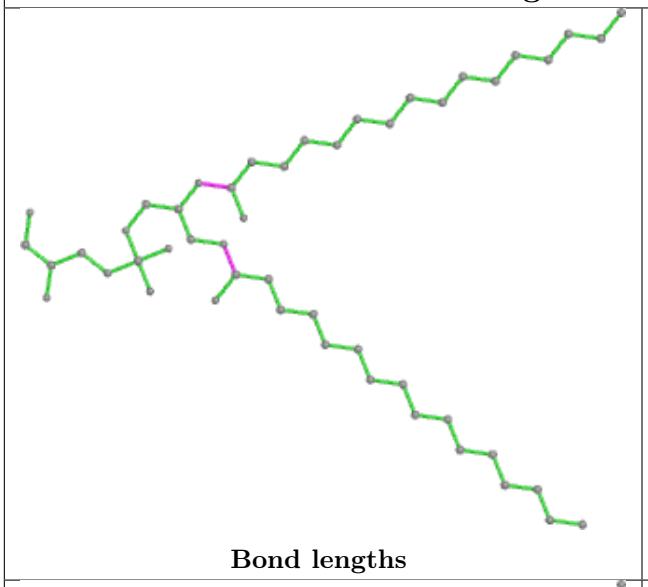
Bond angles



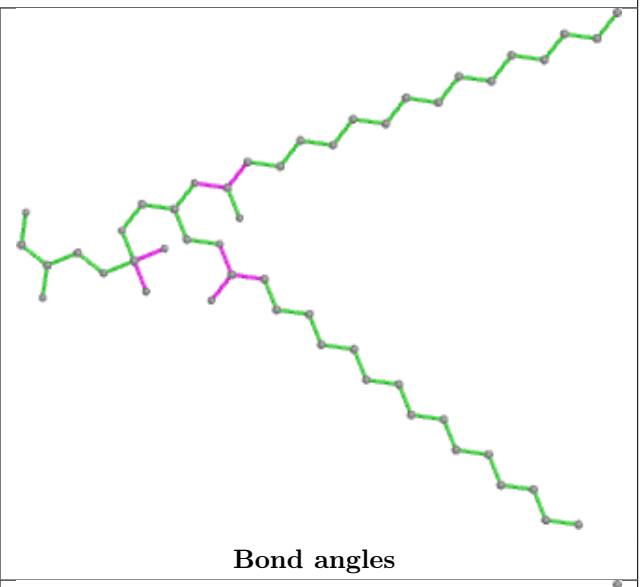
Torsions

Rings

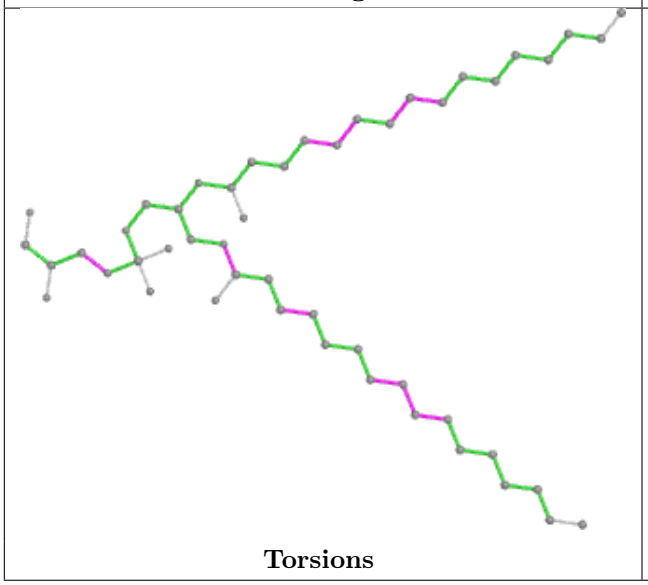
Ligand LHG D 408



Bond lengths



Bond angles



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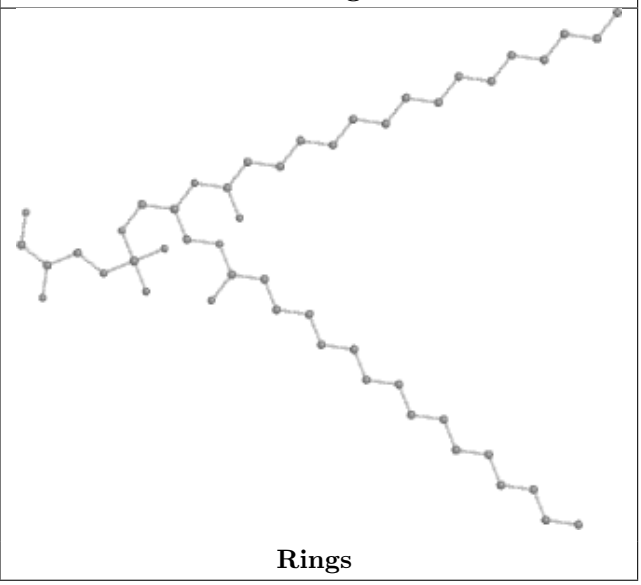
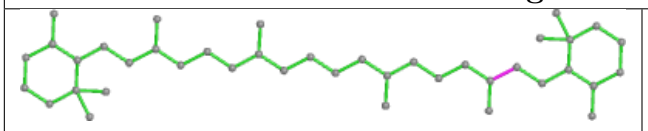


Rings

Ligand BCR h 101



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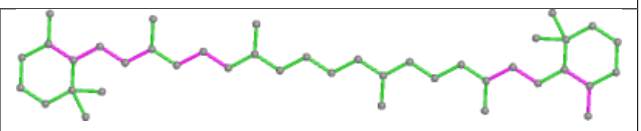
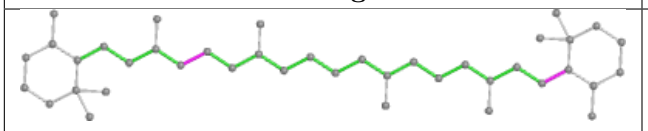


Bond angles



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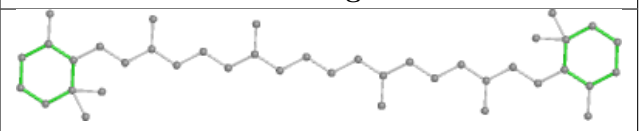
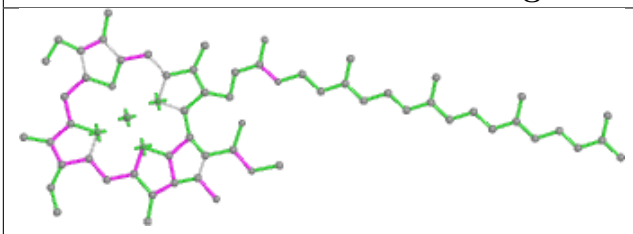


Rings

Ligand CLA D 402



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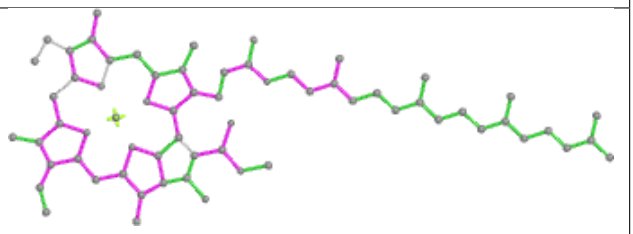
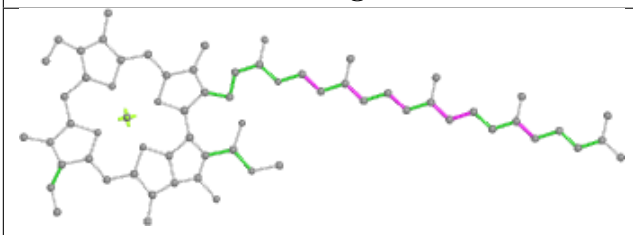


Bond angles



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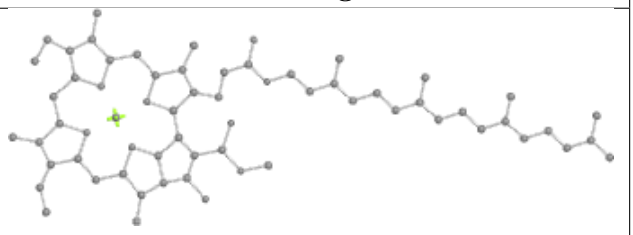
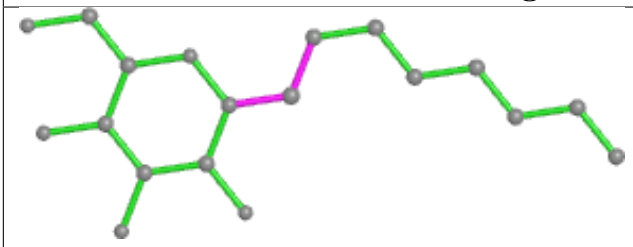


Rings

Ligand HTG C 524



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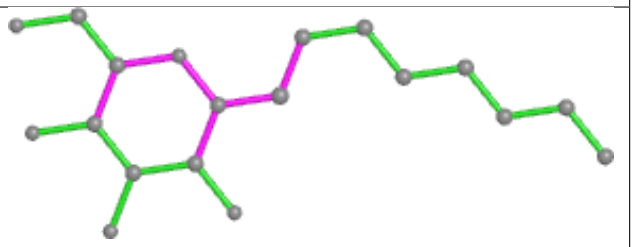
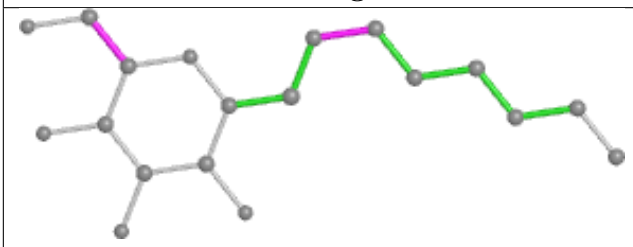
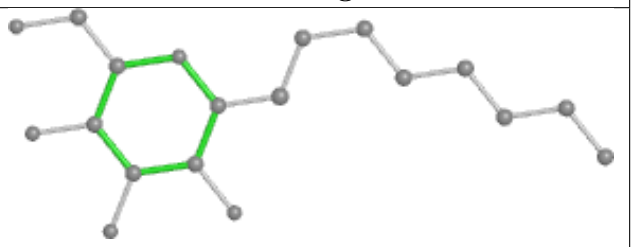


Bond angles

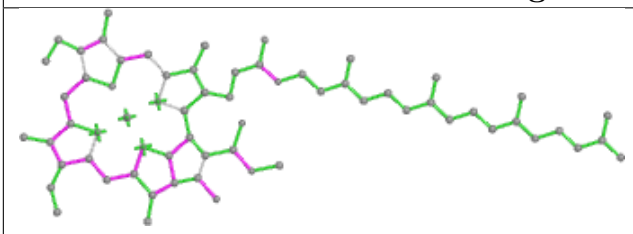


Torsions



Rings

Ligand CLA a 406



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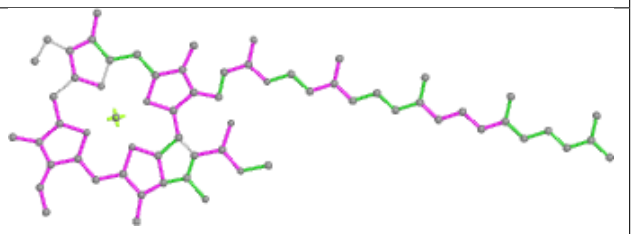
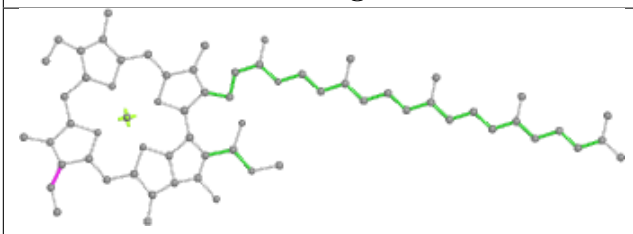
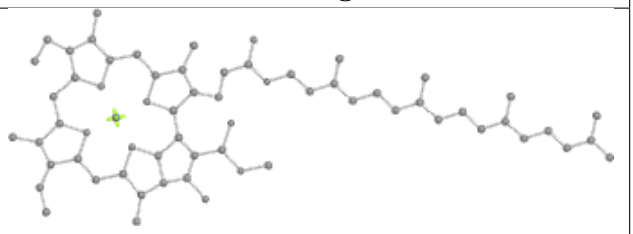


Bond angles

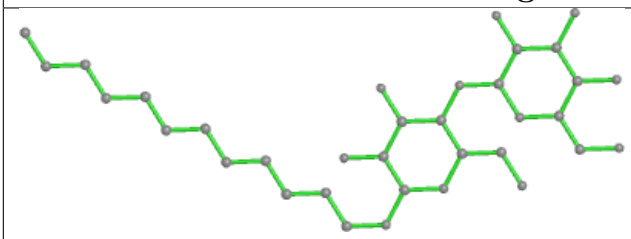


Torsions



Rings

Ligand LMT M 101



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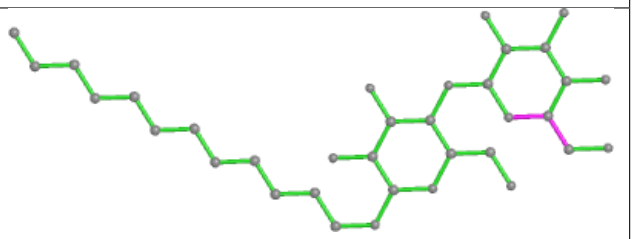
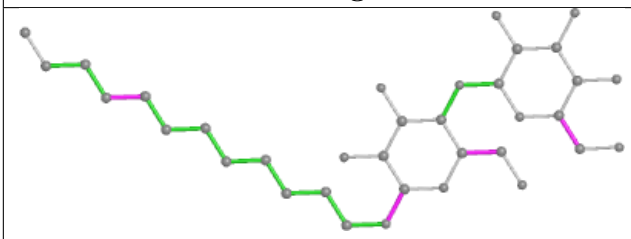
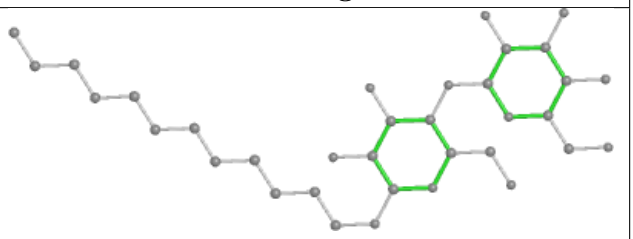


Bond angles

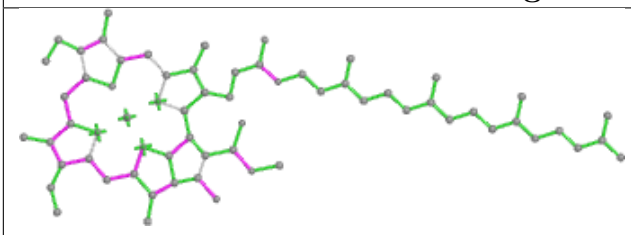


Torsions

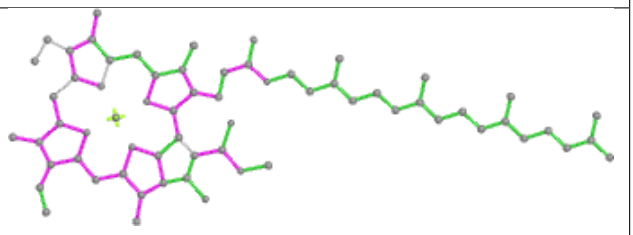


Rings

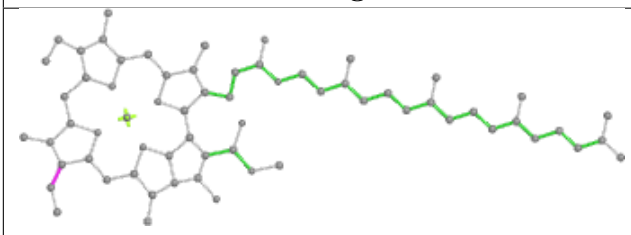
Ligand CLA A 405



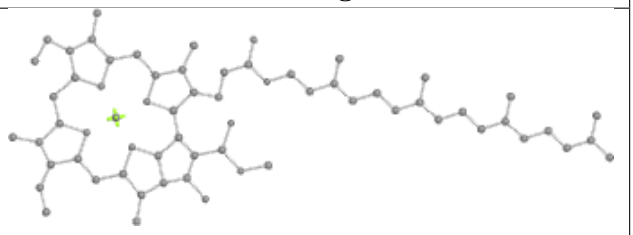
Bond lengths



Bond angles

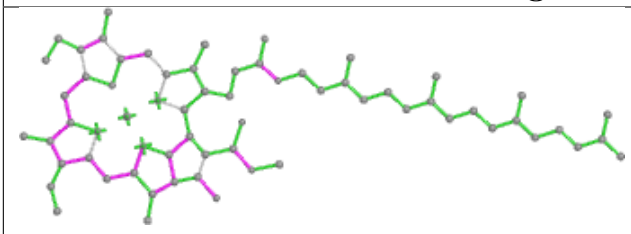


Torsions



Rings

Ligand CLA b 612



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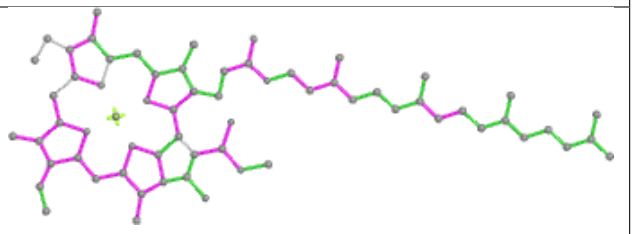
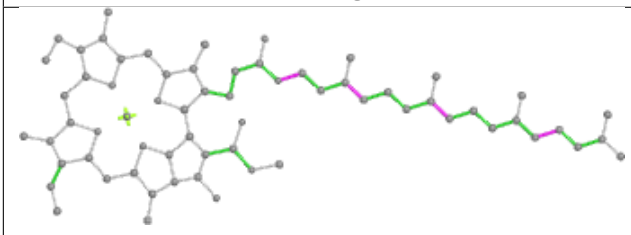


Bond angles



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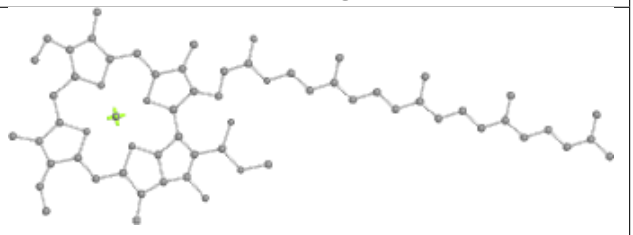
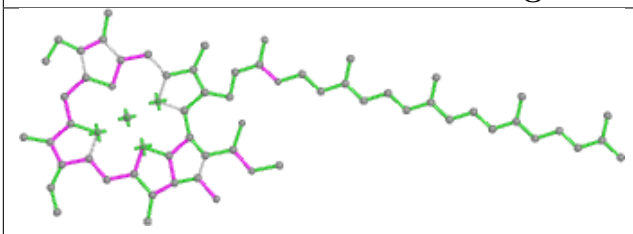
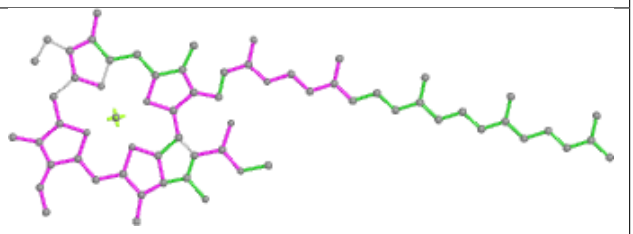


Rings

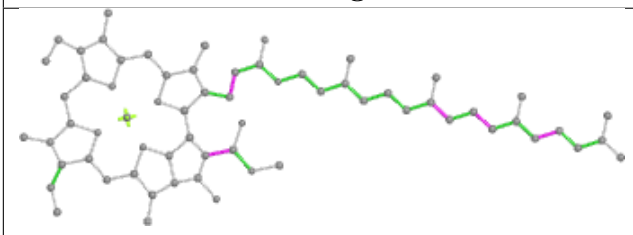
Ligand CLA B 607



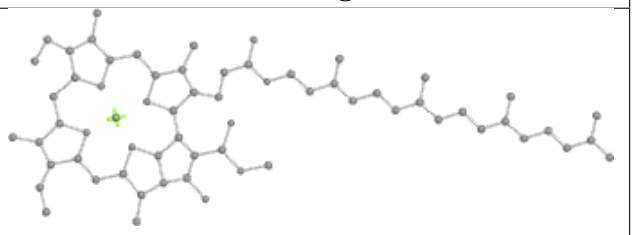
Bond lengths



Bond angles

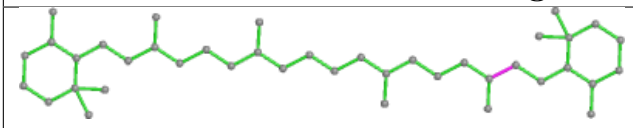


Torsions

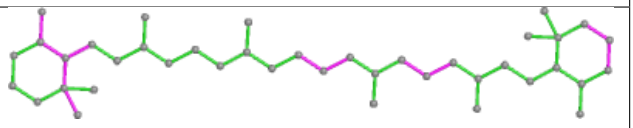


Rings

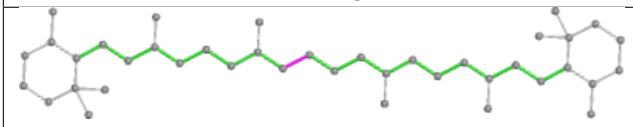
Ligand BCR t 101



Bond lengths



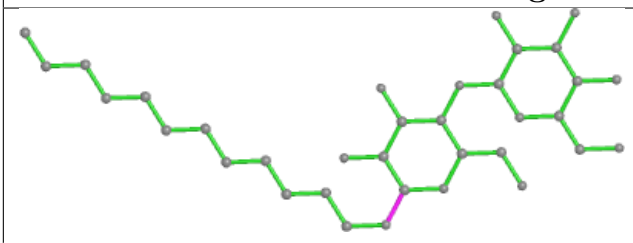
Bond angles



Torsions

Rings

Ligand LMT f 103



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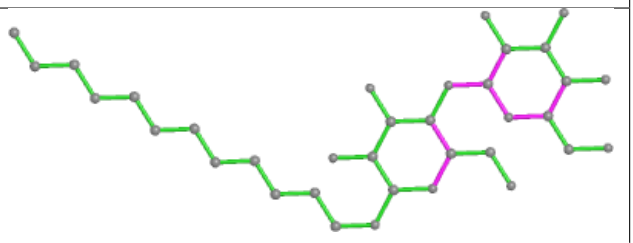
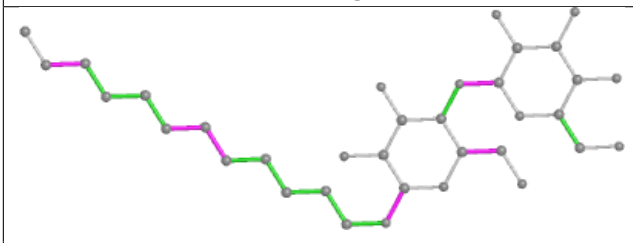
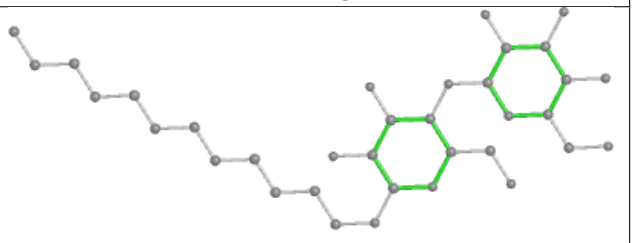


Bond angles

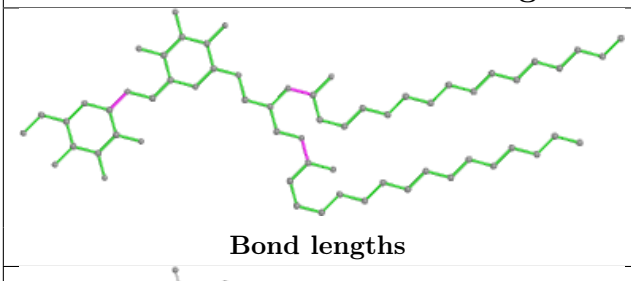


Torsions

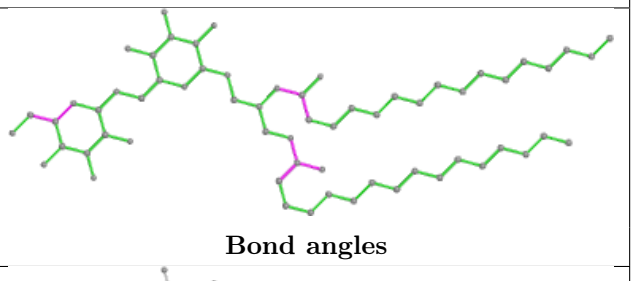


Rings

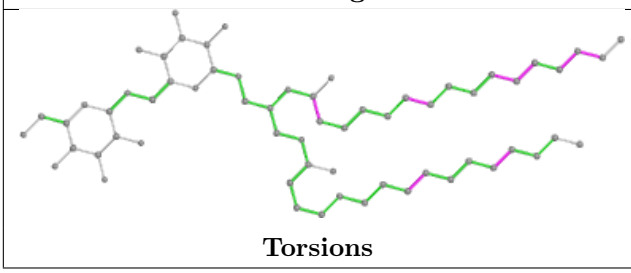
Ligand DGD H 102



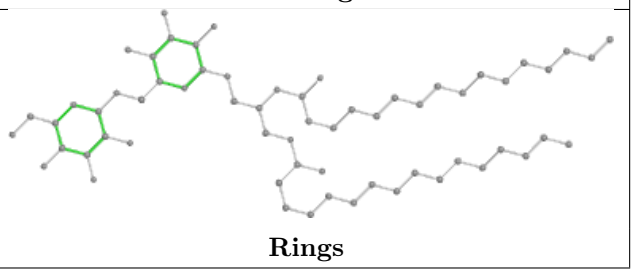
Bond lengths



Bond angles

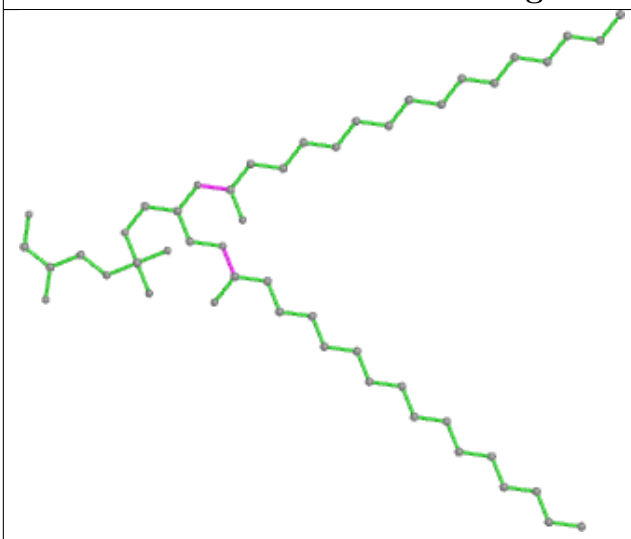


Torsions

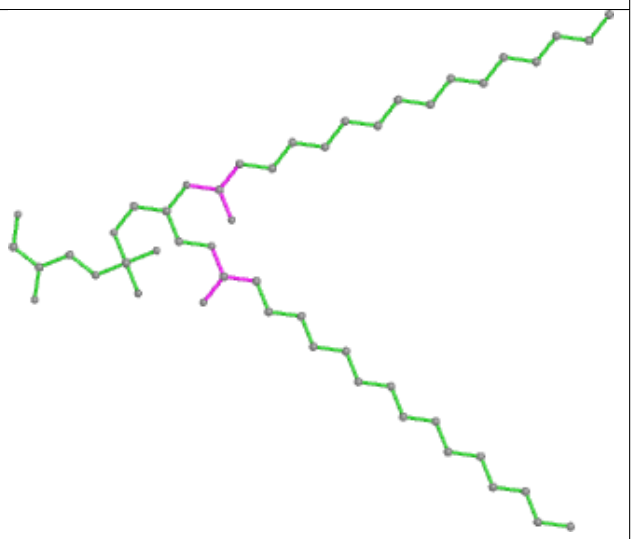


Rings

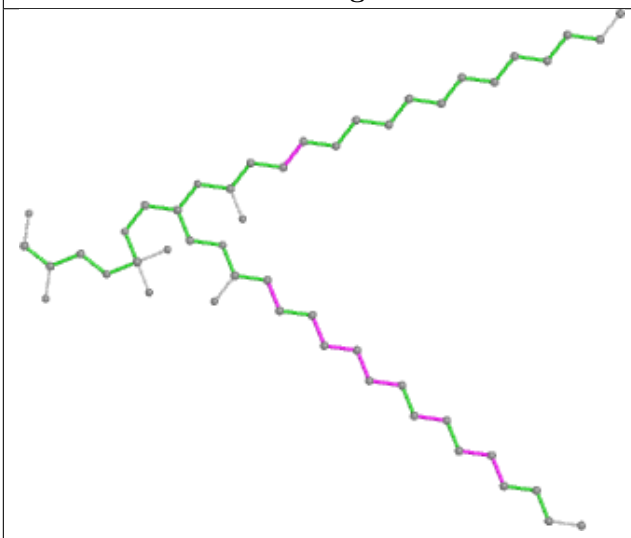
Ligand LHG d 407



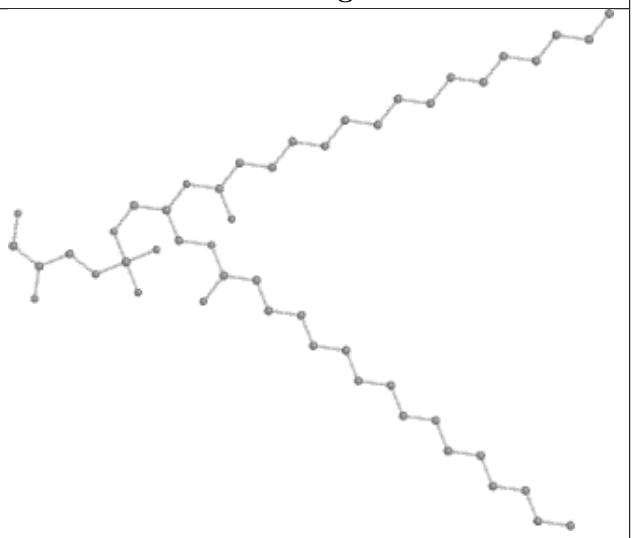
Bond lengths



Bond angles

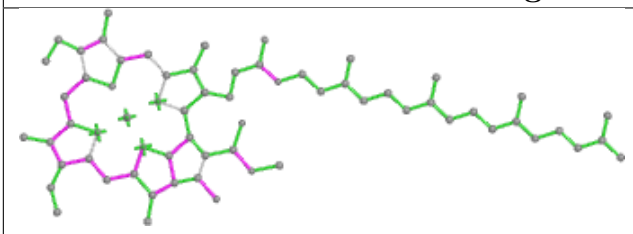


Torsions

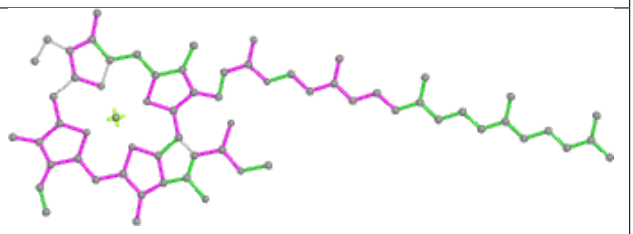


Rings

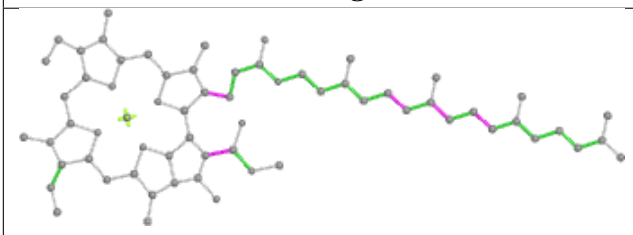
Ligand CLA C 509



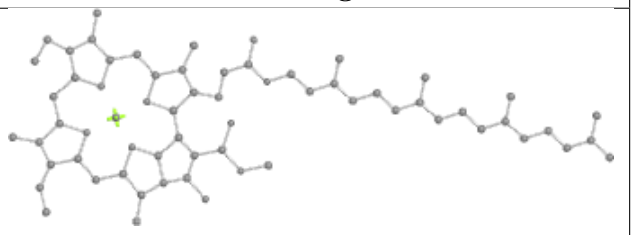
Bond lengths



Bond angles

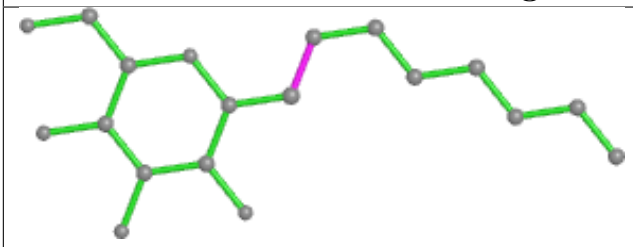


Torsions

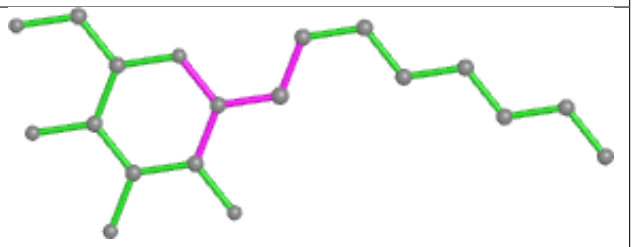


Rings

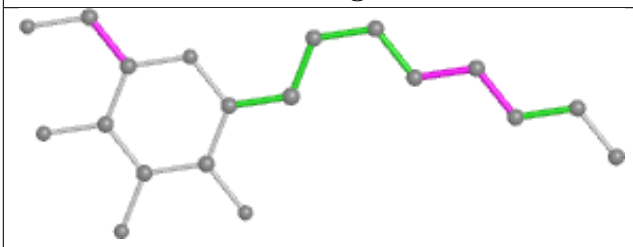
Ligand HTG B 626



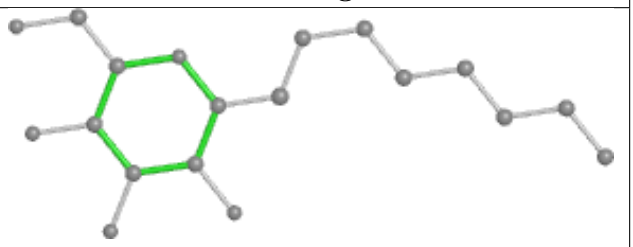
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	0.43	20 (5%) 21 30	13, 21, 38, 73	0
1	a	334/344 (97%)	0.58	35 (10%) 6 10	15, 23, 47, 90	0
2	B	504/505 (99%)	0.17	27 (5%) 25 34	15, 25, 48, 78	0
2	b	504/505 (99%)	0.26	36 (7%) 16 24	16, 27, 59, 92	0
3	C	451/455 (99%)	0.14	17 (3%) 40 50	18, 30, 46, 73	0
3	c	455/455 (100%)	0.29	26 (5%) 23 32	21, 33, 49, 92	0
4	D	342/342 (100%)	0.56	31 (9%) 9 15	14, 22, 37, 97	0
4	d	341/342 (99%)	0.36	18 (5%) 26 35	16, 25, 39, 90	0
5	E	81/84 (96%)	0.85	10 (12%) 4 6	26, 37, 66, 92	0
5	e	81/84 (96%)	1.10	12 (14%) 2 3	30, 42, 71, 92	0
6	F	34/44 (77%)	0.34	4 (11%) 4 7	23, 30, 50, 61	0
6	f	32/44 (72%)	0.27	3 (9%) 8 13	30, 34, 79, 84	0
7	H	65/65 (100%)	0.22	2 (3%) 49 58	23, 31, 46, 110	0
7	h	65/65 (100%)	0.72	8 (12%) 4 6	27, 35, 52, 105	0
8	I	37/38 (97%)	0.58	5 (13%) 3 5	26, 33, 88, 108	0
8	i	37/38 (97%)	0.52	3 (8%) 12 18	27, 33, 73, 102	0
9	J	38/39 (97%)	0.59	5 (13%) 3 5	24, 35, 84, 98	0
9	j	39/39 (100%)	0.37	3 (7%) 13 21	29, 38, 84, 96	0
10	K	37/37 (100%)	0.22	1 (2%) 54 63	27, 35, 54, 65	0
10	k	37/37 (100%)	0.85	7 (18%) 1 1	30, 38, 55, 68	0
11	L	37/37 (100%)	0.67	5 (13%) 3 5	15, 19, 56, 82	0
11	l	37/37 (100%)	0.79	5 (13%) 3 5	16, 20, 58, 83	0
12	M	33/36 (91%)	0.75	3 (9%) 9 15	15, 21, 45, 89	0
12	m	33/36 (91%)	0.67	3 (9%) 9 15	16, 21, 41, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.27	16 (6%) 18 26	16, 32, 66, 110	0
13	o	243/244 (99%)	0.71	44 (18%) 1 1	19, 33, 71, 125	0
14	T	29/32 (90%)	0.83	3 (10%) 6 10	16, 20, 43, 89	0
14	t	29/32 (90%)	0.45	2 (6%) 16 25	16, 20, 46, 89	0
15	U	97/104 (93%)	0.34	4 (4%) 37 46	21, 31, 54, 84	0
15	u	97/104 (93%)	-0.08	0 100 100	23, 33, 51, 84	0
16	V	137/137 (100%)	-0.09	0 100 100	20, 31, 51, 69	0
16	v	137/137 (100%)	0.47	12 (8%) 10 16	24, 36, 57, 70	0
17	Y	29/30 (96%)	1.56	7 (24%) 0 0	35, 47, 82, 101	0
17	y	29/30 (96%)	1.42	7 (24%) 0 0	38, 50, 83, 100	0
18	X	39/40 (97%)	0.60	5 (12%) 3 6	31, 38, 75, 102	0
18	x	39/40 (97%)	1.50	11 (28%) 0 0	33, 41, 83, 102	0
19	Z	62/62 (100%)	1.29	17 (27%) 0 0	36, 47, 83, 96	0
19	z	62/62 (100%)	2.79	35 (56%) 0 0	42, 49, 82, 96	0
20	R	34/34 (100%)	7.13	34 (100%) 0 0	54, 75, 98, 106	0
All	All	5294/5384 (98%)	0.48	486 (9%) 9 14	13, 29, 61, 125	0

The worst 5 of 486 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	15.8
20	R	18	TRP	11.3
7	H	65	LEU	11.1
17	Y	18	VAL	10.5
20	R	23	ILE	10.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	m	1	10/11	0.93	0.16	13,32,67,68	0
8	FME	I	1	10/11	0.95	0.12	22,34,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.96	0.17	18,26,40,49	0
14	FME	t	1	10/11	0.96	0.12	12,22,31,68	0
12	FME	M	1	10/11	0.97	0.12	23,36,70,74	0
8	FME	i	1	10/11	0.98	0.13	21,31,39,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	CA	b	604	1/1	0.47	0.25	117,117,117,117	0
36	DGD	D	405	62/66	0.55	0.40	48,79,113,122	0
29	LMT	E	102	35/35	0.57	0.34	43,80,109,115	0
29	LMT	f	103	35/35	0.59	0.37	43,86,107,111	0
35	HTG	B	626	19/19	0.61	0.36	48,81,94,95	0
28	GOL	B	637	6/6	0.61	0.26	51,72,83,86	0
36	DGD	d	406	62/66	0.61	0.45	38,89,122,130	0
35	HTG	B	634	19/19	0.65	0.29	32,76,109,127	0
32	UNL	A	420	28/-	0.66	0.28	50,71,78,86	0
35	HTG	b	603	19/19	0.67	0.24	46,84,110,111	0
29	LMT	m	102	35/35	0.68	0.25	33,61,79,95	0
32	UNL	b	634	33/-	0.68	0.29	29,62,111,117	0
37	LHG	e	101	42/49	0.69	0.28	52,89,118,129	0
35	HTG	d	412	16/19	0.70	0.31	38,78,97,98	0
32	UNL	K	101	34/-	0.70	0.30	37,61,83,88	0
29	LMT	b	625	25/35	0.71	0.29	44,67,109,119	0
32	UNL	c	926	32/-	0.71	0.36	39,79,98,105	0
29	LMT	M	101	35/35	0.72	0.21	23,52,69,77	0
35	HTG	b	627	19/19	0.72	0.27	49,86,110,116	0
32	UNL	B	635	33/-	0.72	0.25	33,58,102,102	0
34	LMG	z	101	39/55	0.73	0.33	45,82,99,107	0
32	UNL	a	418	30/-	0.73	0.31	42,66,98,106	0
31	PL9	a	417	55/55	0.73	0.26	41,73,92,99	0
29	LMT	C	522	35/35	0.74	0.40	52,81,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	v	203	6/6	0.75	0.31	39,74,86,87	0
28	GOL	a	415	6/6	0.76	0.22	48,62,65,66	0
34	LMG	Z	101	37/55	0.76	0.28	30,75,96,112	0
32	UNL	J	102	10/-	0.76	0.35	39,51,64,67	0
29	LMT	m	104	35/35	0.76	0.24	29,59,85,86	0
32	UNL	j	102	10/-	0.76	0.29	47,57,63,63	0
35	HTG	C	524	19/19	0.76	0.30	41,69,99,100	0
32	UNL	i	101	40/-	0.77	0.24	28,62,105,117	0
33	CA	B	601	1/1	0.77	0.10	83,83,83,83	0
27	SQD	B	621	54/54	0.78	0.20	26,55,94,104	0
28	GOL	O	302	6/6	0.78	0.23	49,55,57,61	0
35	HTG	D	411	16/19	0.78	0.26	38,102,111,112	0
28	GOL	V	203	6/6	0.78	0.43	50,64,71,72	0
34	LMG	C	521	51/55	0.78	0.25	32,69,88,108	0
35	HTG	c	923	19/19	0.78	0.30	45,80,94,97	0
32	UNL	I	101	40/-	0.78	0.24	27,62,110,120	0
34	LMG	a	412	51/55	0.78	0.21	33,62,84,90	0
32	UNL	d	413	18/-	0.78	0.19	30,52,81,84	0
27	SQD	L	102	54/54	0.78	0.22	24,52,86,91	0
34	LMG	C	501	51/55	0.80	0.21	34,56,76,85	0
32	UNL	d	411	36/-	0.80	0.23	32,56,104,111	0
28	GOL	A	415	6/6	0.81	0.19	36,49,64,64	0
31	PL9	A	419	55/55	0.81	0.23	28,56,91,98	0
27	SQD	a	402	54/54	0.81	0.20	29,55,76,90	0
29	LMT	B	623	35/35	0.81	0.22	26,74,96,101	0
35	HTG	c	922	19/19	0.81	0.21	43,67,84,95	0
32	UNL	m	101	10/-	0.82	0.21	35,50,55,61	0
34	LMG	c	919	51/55	0.82	0.21	29,57,78,81	0
34	LMG	c	920	51/55	0.82	0.25	33,74,88,93	0
28	GOL	f	101	6/6	0.82	0.25	44,50,62,64	0
27	SQD	A	416	54/54	0.82	0.20	26,51,78,85	0
32	UNL	M	102	10/-	0.82	0.21	28,38,57,58	0
32	UNL	D	410	40/-	0.82	0.20	24,54,93,101	0
37	LHG	E	101	42/49	0.82	0.22	22,63,78,93	0
28	GOL	T	103	6/6	0.82	0.23	52,68,70,79	0
29	LMT	b	601	25/35	0.83	0.27	18,55,104,111	0
29	LMT	a	401	35/35	0.83	0.20	21,53,74,80	0
29	LMT	c	921	35/35	0.83	0.40	46,76,97,104	0
28	GOL	V	206	6/6	0.84	0.27	47,63,66,66	0
34	LMG	C	520	51/55	0.84	0.22	22,52,72,90	0
29	LMT	m	103	35/35	0.84	0.17	19,48,62,74	0
29	LMT	B	636	25/35	0.85	0.23	24,61,106,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	b	632	6/6	0.85	0.20	38,52,59,59	0
29	LMT	A	417	35/35	0.85	0.19	22,57,79,97	0
28	GOL	B	629	6/6	0.85	0.21	28,42,50,56	0
27	SQD	f	102	43/54	0.86	0.24	41,75,103,108	0
28	GOL	B	628	6/6	0.86	0.31	33,42,54,72	0
32	UNL	X	101	18/-	0.87	0.15	29,44,62,79	0
28	GOL	A	414	6/6	0.87	0.18	30,40,43,49	0
28	GOL	v	204	6/6	0.87	0.17	54,66,71,80	0
32	UNL	D	409	17/-	0.87	0.16	30,40,63,66	0
32	UNL	d	410	17/-	0.87	0.18	34,48,82,82	0
28	GOL	B	631	6/6	0.87	0.24	30,48,62,65	0
34	LMG	B	622	51/55	0.87	0.23	19,32,49,71	0
35	HTG	b	602	19/19	0.88	0.15	29,45,65,68	0
35	HTG	B	633	19/19	0.88	0.16	28,54,70,76	0
24	CLA	c	914	65/65	0.88	0.26	35,48,81,87	0
28	GOL	T	101	6/6	0.88	0.27	54,60,61,69	0
28	GOL	t	102	6/6	0.88	0.25	22,59,67,67	0
26	BCR	k	102	40/40	0.89	0.15	30,37,50,61	0
28	GOL	c	925	6/6	0.89	0.23	34,52,63,66	0
26	BCR	d	404	40/40	0.89	0.15	27,36,54,60	0
34	LMG	b	624	51/55	0.89	0.23	21,36,57,81	0
35	HTG	V	202	19/19	0.89	0.19	40,59,77,163	0
26	BCR	H	101	40/40	0.90	0.13	19,32,45,59	0
27	SQD	F	101	43/54	0.90	0.24	34,59,81,90	0
28	GOL	F	103	6/6	0.90	0.19	60,65,71,71	0
26	BCR	h	101	40/40	0.90	0.12	25,35,48,52	0
36	DGD	H	102	62/66	0.90	0.16	16,28,46,59	0
33	CA	f	104	1/1	0.90	0.07	77,77,77,77	0
36	DGD	h	102	62/66	0.90	0.14	19,31,48,60	0
35	HTG	b	626	19/19	0.90	0.19	30,50,86,86	0
28	GOL	o	302	6/6	0.90	0.13	44,50,53,58	0
37	LHG	l	101	49/49	0.90	0.18	15,27,39,56	0
24	CLA	c	906	65/65	0.91	0.12	21,28,44,56	0
28	GOL	b	628	6/6	0.91	0.13	30,35,42,53	0
34	LMG	J	101	51/55	0.91	0.18	18,32,75,81	0
31	PL9	d	405	55/55	0.91	0.18	13,19,33,44	0
28	GOL	b	631	6/6	0.91	0.15	28,41,48,51	0
28	GOL	B	632	6/6	0.91	0.17	24,40,53,57	0
24	CLA	c	913	65/65	0.91	0.16	31,40,59,65	0
27	SQD	a	411	54/54	0.91	0.21	32,52,73,81	0
26	BCR	y	101	40/40	0.91	0.14	29,37,57,63	0
35	HTG	B	625	19/19	0.91	0.20	28,43,74,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	c	917	62/66	0.91	0.18	26,35,61,87	0
36	DGD	c	918	62/66	0.91	0.20	25,31,52,70	0
27	SQD	A	412	54/54	0.91	0.20	15,45,72,85	0
24	CLA	C	513	65/65	0.91	0.13	27,40,59,71	0
24	CLA	c	904	65/65	0.91	0.12	26,33,44,47	0
24	CLA	c	905	65/65	0.91	0.16	25,32,49,68	0
28	GOL	a	413	6/6	0.91	0.11	30,32,37,42	0
31	PL9	D	404	55/55	0.92	0.20	11,18,31,41	0
24	CLA	B	602	65/65	0.92	0.16	22,40,80,101	0
28	GOL	B	627	6/6	0.92	0.16	23,36,45,72	0
26	BCR	t	101	40/40	0.92	0.12	12,26,45,48	0
24	CLA	c	908	65/65	0.92	0.12	26,33,49,60	0
24	CLA	b	605	65/65	0.92	0.18	29,48,89,102	0
34	LMG	j	101	51/55	0.92	0.17	25,35,71,81	0
36	DGD	C	518	62/66	0.92	0.20	19,29,78,90	0
24	CLA	b	613	65/65	0.92	0.11	23,29,42,48	0
24	CLA	c	902	65/65	0.92	0.12	26,32,45,52	0
36	DGD	c	916	62/66	0.92	0.17	22,31,64,82	0
26	BCR	K	103	40/40	0.92	0.11	24,30,40,43	0
26	BCR	b	621	40/40	0.92	0.16	14,24,33,38	0
26	BCR	c	915	40/40	0.92	0.11	25,34,42,45	0
35	HTG	C	523	19/19	0.92	0.20	54,62,86,88	0
37	LHG	D	406	49/49	0.92	0.22	14,26,38,52	0
24	CLA	B	603	65/65	0.92	0.12	17,24,36,47	0
37	LHG	d	407	49/49	0.92	0.20	15,31,44,53	0
24	CLA	B	610	65/65	0.92	0.12	17,24,36,45	0
26	BCR	k	101	40/40	0.92	0.18	34,45,63,75	0
25	PHO	a	420	64/64	0.93	0.20	17,24,30,33	0
26	BCR	B	618	40/40	0.93	0.14	11,23,32,35	0
26	BCR	B	619	40/40	0.93	0.14	15,23,46,49	0
28	GOL	A	413	6/6	0.93	0.11	23,30,33,36	0
26	BCR	C	515	40/40	0.93	0.11	29,38,49,53	0
26	BCR	D	403	40/40	0.93	0.14	19,30,58,70	0
24	CLA	b	610	65/65	0.93	0.11	18,31,78,87	0
24	CLA	C	505	65/65	0.93	0.18	18,27,47,61	0
26	BCR	T	102	40/40	0.93	0.14	13,26,37,42	0
28	GOL	B	630	6/6	0.93	0.10	26,32,40,42	0
26	BCR	a	410	40/40	0.93	0.10	15,23,28,32	0
24	CLA	b	618	65/65	0.93	0.14	14,24,78,80	0
26	BCR	b	622	40/40	0.93	0.18	14,24,43,51	0
28	GOL	C	525	6/6	0.93	0.20	32,41,61,69	0
24	CLA	b	619	65/65	0.93	0.11	20,30,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	507	65/65	0.93	0.14	25,40,75,77	0
36	DGD	C	519	62/66	0.93	0.20	18,29,48,55	0
24	CLA	c	903	65/65	0.93	0.15	24,30,41,51	0
24	CLA	C	511	65/65	0.93	0.15	21,29,38,45	0
24	CLA	C	512	65/65	0.93	0.11	22,30,39,45	0
24	CLA	B	608	65/65	0.93	0.16	11,19,28,40	0
24	CLA	C	514	65/65	0.93	0.14	30,42,67,73	0
24	CLA	c	909	65/65	0.93	0.15	23,28,67,91	0
24	CLA	c	912	65/65	0.93	0.12	27,36,50,54	0
28	GOL	b	629	6/6	0.93	0.15	27,36,50,54	0
28	GOL	b	630	6/6	0.93	0.14	35,39,50,53	0
23	BCT	a	419	4/4	0.93	0.15	21,32,41,50	0
24	CLA	b	606	65/65	0.93	0.12	22,28,38,48	0
24	CLA	d	403	65/65	0.93	0.12	26,31,79,93	0
24	CLA	c	907	65/65	0.94	0.12	28,37,64,72	0
24	CLA	B	607	65/65	0.94	0.12	16,25,70,76	0
28	GOL	a	414	6/6	0.94	0.14	25,34,43,53	0
23	BCT	A	404	4/4	0.94	0.17	21,24,36,47	0
24	CLA	c	910	65/65	0.94	0.11	27,34,47,53	0
24	CLA	c	911	65/65	0.94	0.16	24,31,43,53	0
22	CL	v	201	1/1	0.94	0.08	62,62,62,62	0
24	CLA	D	402	65/65	0.94	0.12	18,27,68,84	0
24	CLA	a	407	65/65	0.94	0.23	18,23,72,84	0
28	GOL	b	633	6/6	0.94	0.36	34,60,65,65	0
24	CLA	B	614	65/65	0.94	0.16	12,20,43,55	0
25	PHO	a	408	64/64	0.94	0.15	15,18,27,30	0
24	CLA	B	615	65/65	0.94	0.12	12,21,66,79	0
26	BCR	A	411	40/40	0.94	0.11	15,22,29,31	0
24	CLA	C	502	65/65	0.94	0.11	22,30,42,54	0
24	CLA	C	503	65/65	0.94	0.12	20,25,39,63	0
26	BCR	B	620	40/40	0.94	0.09	16,26,39,49	0
24	CLA	b	614	65/65	0.94	0.10	20,29,39,42	0
24	CLA	b	615	65/65	0.94	0.14	17,22,38,46	0
24	CLA	b	616	65/65	0.94	0.10	16,23,32,44	0
26	BCR	K	102	40/40	0.94	0.11	22,30,39,47	0
24	CLA	C	504	65/65	0.94	0.11	22,28,40,45	0
24	CLA	B	604	65/65	0.94	0.11	16,25,32,38	0
24	CLA	b	620	65/65	0.94	0.14	19,33,77,78	0
24	CLA	B	605	65/65	0.94	0.13	13,19,44,57	0
24	CLA	C	508	65/65	0.94	0.12	23,35,47,54	0
26	BCR	b	623	40/40	0.94	0.09	18,31,42,48	0
24	CLA	C	509	65/65	0.94	0.14	18,25,67,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	LHG	D	408	49/49	0.94	0.18	17,29,88,100	0
24	CLA	C	510	65/65	0.94	0.10	23,30,45,62	0
37	LHG	L	101	49/49	0.94	0.21	12,26,38,46	0
24	CLA	B	606	65/65	0.94	0.10	13,20,31,41	0
37	LHG	d	408	49/49	0.94	0.13	15,23,41,54	0
28	GOL	V	204	6/6	0.94	0.14	19,26,30,37	0
28	GOL	V	205	6/6	0.94	0.16	34,41,45,52	0
35	HTG	O	303	19/19	0.95	0.10	23,32,46,55	0
24	CLA	b	609	65/65	0.95	0.10	16,24,37,44	0
24	CLA	B	617	65/65	0.95	0.15	16,28,79,88	0
24	CLA	b	611	65/65	0.95	0.16	13,20,31,34	0
24	CLA	b	612	65/65	0.95	0.10	21,28,40,43	0
24	CLA	A	407	65/65	0.95	0.25	13,20,71,73	0
24	CLA	B	611	65/65	0.95	0.10	17,25,33,50	0
24	CLA	B	612	65/65	0.95	0.15	12,18,30,37	0
24	CLA	B	613	65/65	0.95	0.11	13,20,27,33	0
36	DGD	C	517	62/66	0.95	0.12	19,28,60,72	0
24	CLA	d	401	65/65	0.95	0.19	14,18,27,47	0
24	CLA	d	402	65/65	0.95	0.23	16,20,36,46	0
24	CLA	b	617	65/65	0.95	0.15	14,22,44,52	0
25	PHO	A	408	64/64	0.95	0.16	12,16,23,24	0
28	GOL	C	526	6/6	0.95	0.18	17,21,26,26	0
28	GOL	v	205	6/6	0.95	0.16	23,35,46,50	0
25	PHO	A	409	64/64	0.95	0.21	13,20,29,35	0
24	CLA	D	401	65/65	0.95	0.24	12,16,32,36	0
24	CLA	C	506	65/65	0.95	0.10	18,27,47,54	0
35	HTG	B	624	19/19	0.95	0.10	20,32,43,46	0
37	LHG	D	407	49/49	0.95	0.15	13,22,44,57	0
24	CLA	a	406	65/65	0.95	0.22	15,17,32,38	0
24	CLA	A	405	65/65	0.95	0.23	13,17,27,52	0
24	CLA	a	409	65/65	0.95	0.12	18,26,79,83	0
24	CLA	B	609	65/65	0.95	0.14	15,24,30,36	0
24	CLA	B	616	65/65	0.95	0.11	16,23,42,45	0
37	LHG	d	409	49/49	0.95	0.17	21,32,85,88	0
26	BCR	C	516	40/40	0.95	0.09	23,32,42,43	0
24	CLA	b	608	65/65	0.95	0.13	15,23,51,62	0
38	HEM	e	102	43/43	0.95	0.18	37,46,76,95	0
33	CA	F	102	1/1	0.96	0.09	69,69,69,69	0
24	CLA	A	406	65/65	0.96	0.20	12,16,30,35	0
33	CA	c	901	1/1	0.96	0.04	44,44,44,44	0
22	CL	U	201	1/1	0.96	0.07	50,50,50,50	0
24	CLA	A	410	65/65	0.96	0.11	17,26,80,89	0

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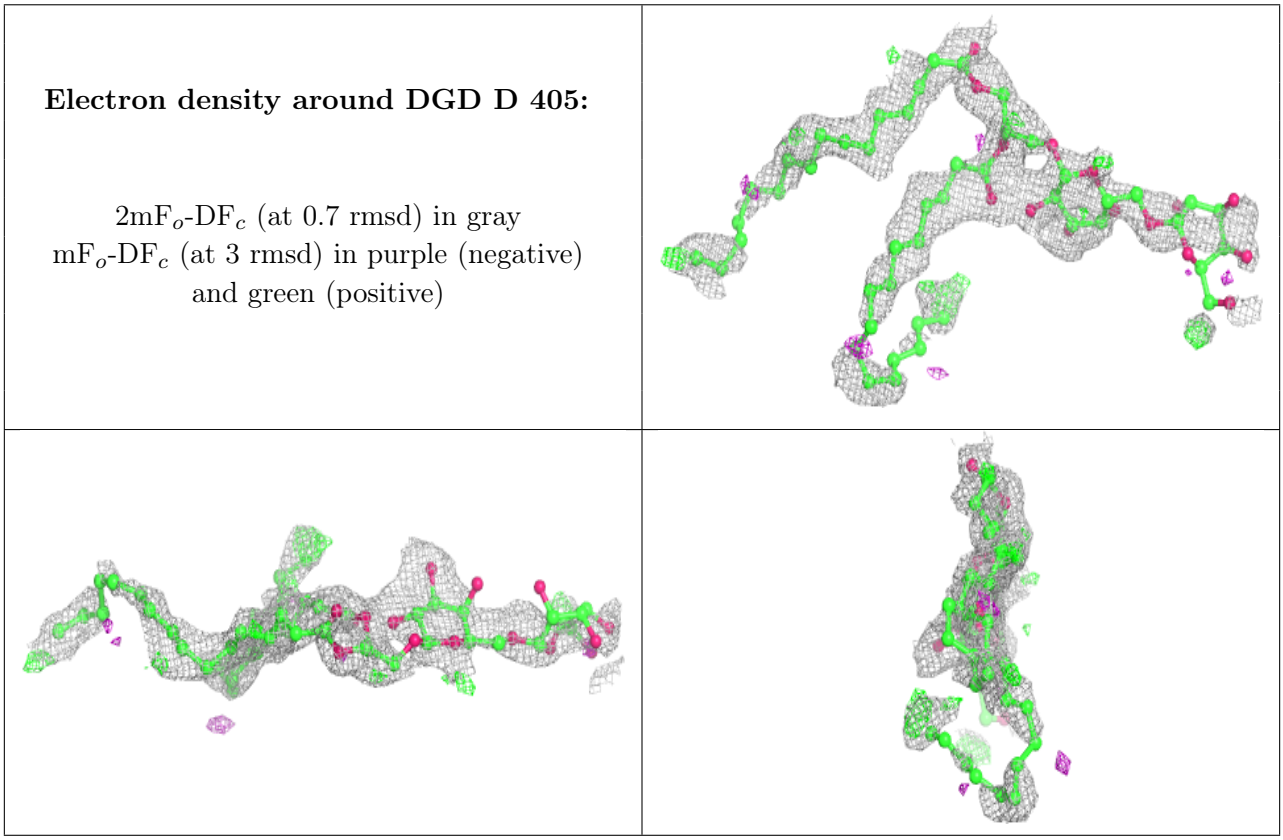
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
38	HEM	E	103	43/43	0.96	0.13	23,35,45,56	0
24	CLA	b	607	65/65	0.96	0.10	21,28,38,50	0
28	GOL	c	924	6/6	0.97	0.20	24,24,25,29	0
33	CA	O	301	1/1	0.97	0.14	53,53,53,53	0
39	MG	j	103	1/1	0.97	0.14	33,33,33,33	0
40	HEC	V	201	43/43	0.97	0.09	22,25,32,39	0
40	HEC	v	202	43/43	0.97	0.11	28,31,40,46	0
22	CL	a	404	1/1	0.98	0.07	20,20,20,20	0
30	OEX	a	416	10/10	0.98	0.10	18,21,24,34	0
33	CA	o	301	1/1	0.98	0.04	54,54,54,54	0
22	CL	a	405	1/1	0.99	0.09	26,26,26,26	0
39	MG	J	103	1/1	0.99	0.05	27,27,27,27	0
21	FE2	a	403	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	0.99	0.05	19,19,19,19	0
30	OEX	A	418	10/10	0.99	0.09	15,20,24,28	0
21	FE2	A	401	1/1	1.00	0.07	24,24,24,24	0
22	CL	A	402	1/1	1.00	0.07	18,18,18,18	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.

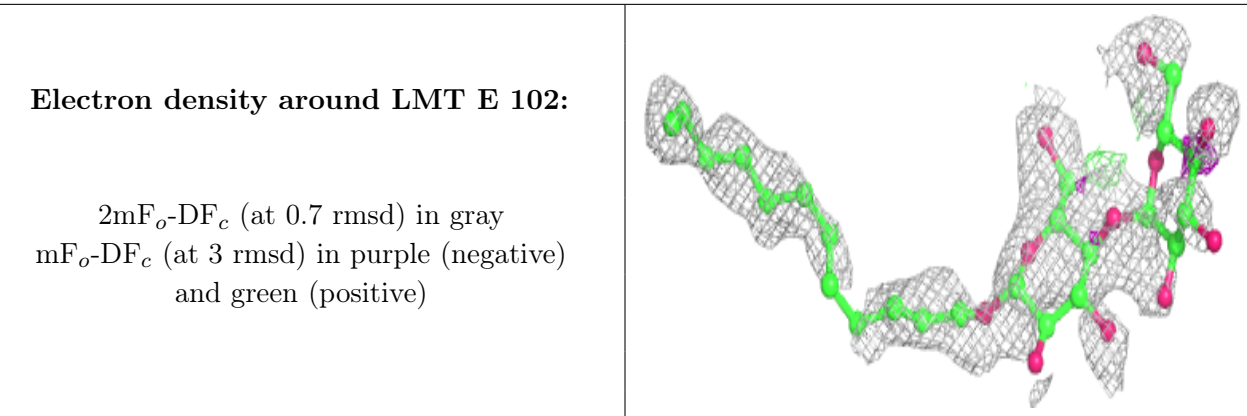
Electron density around DGD D 405:

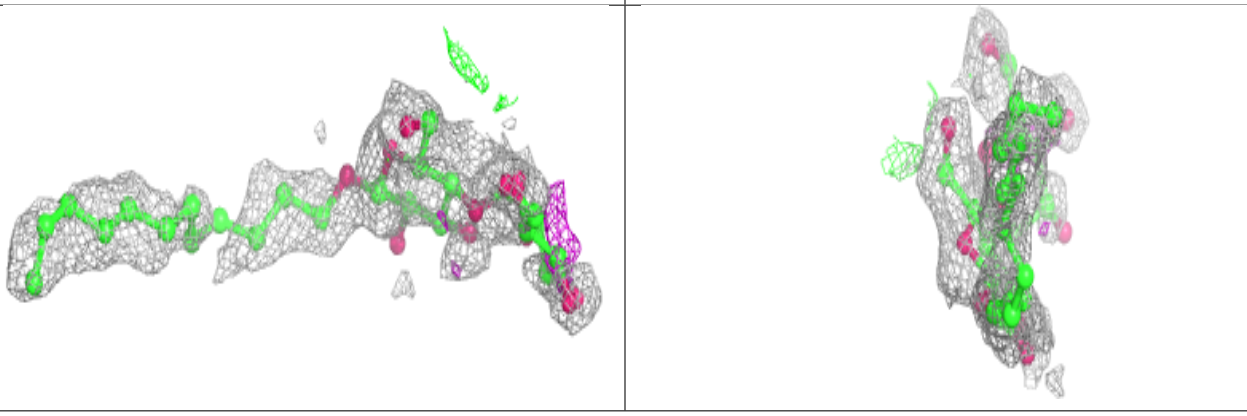
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT E 102:

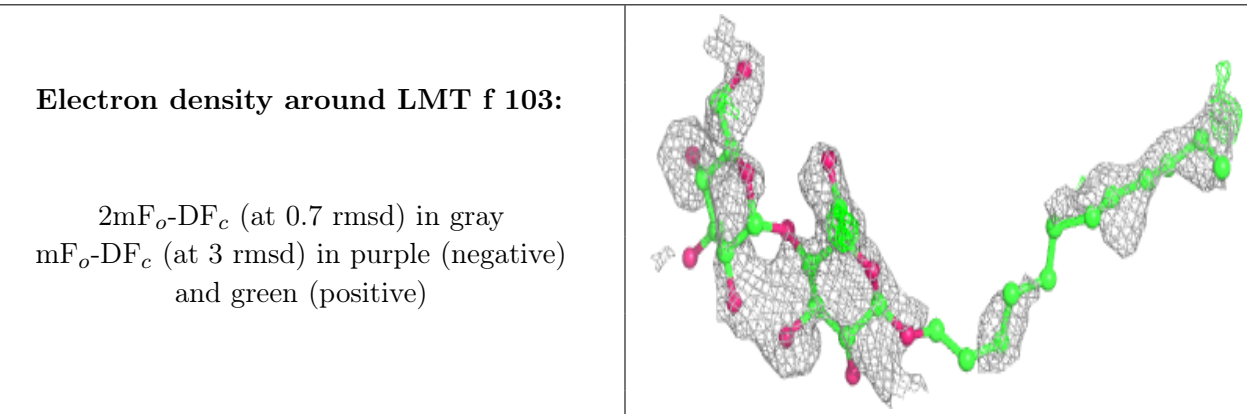
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

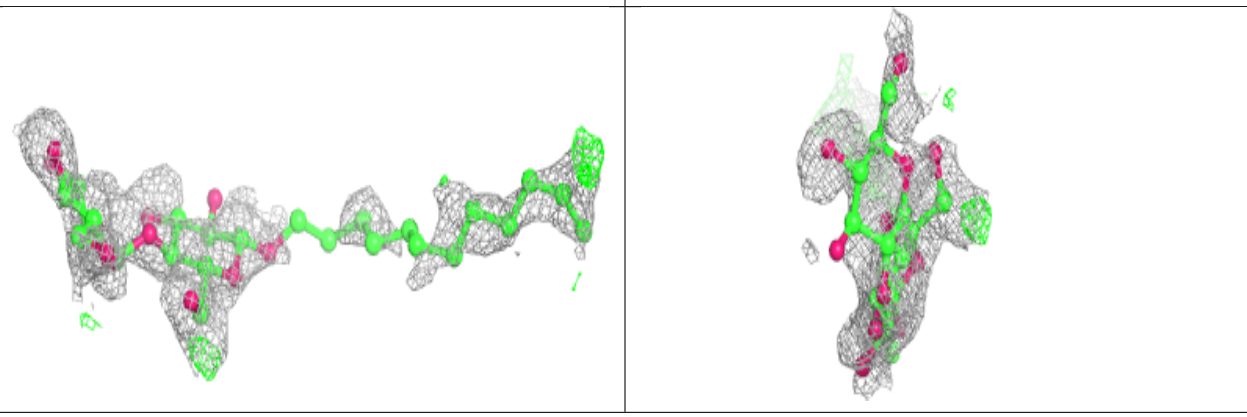




Electron density around LMT f 103:

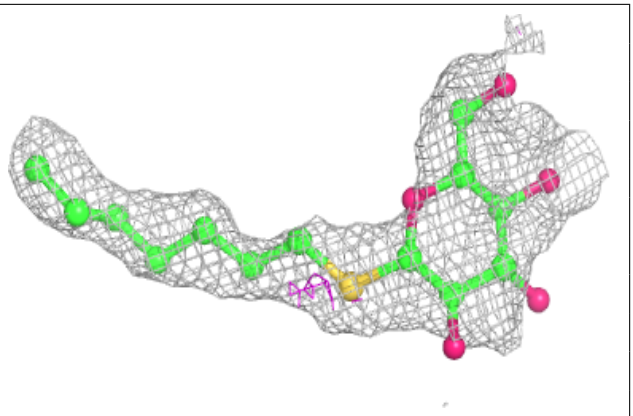
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

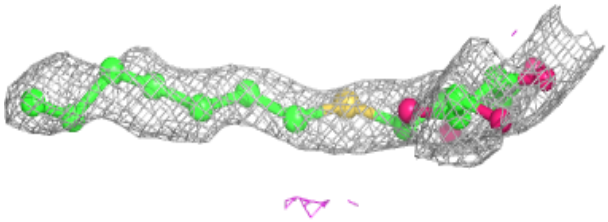


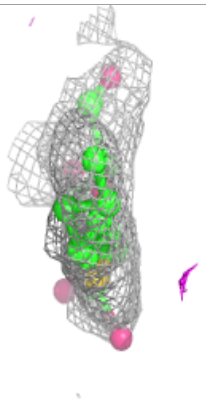


Electron density around HTG B 626:

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

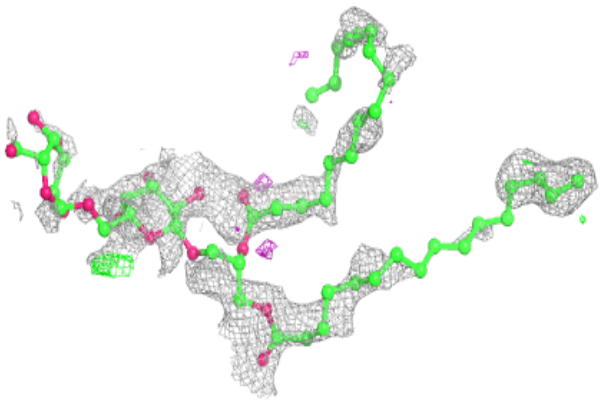


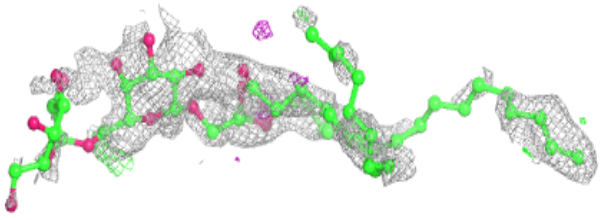


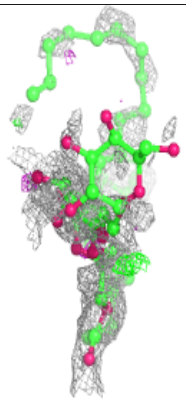


Electron density around DGD d 406:

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

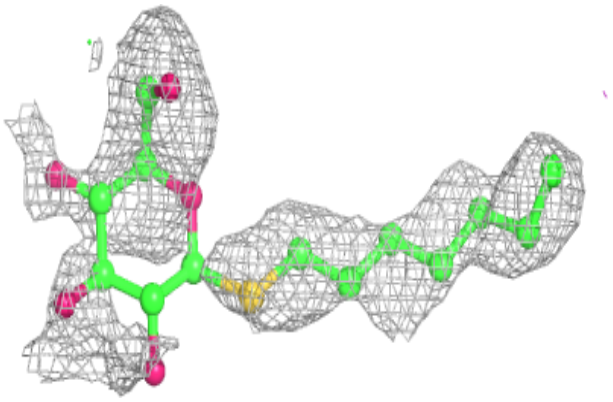


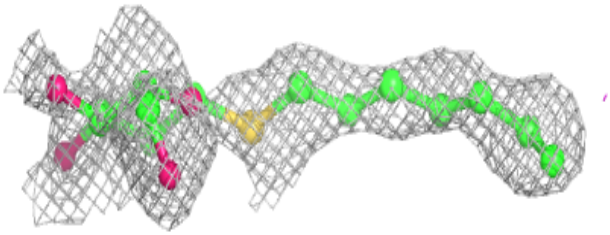


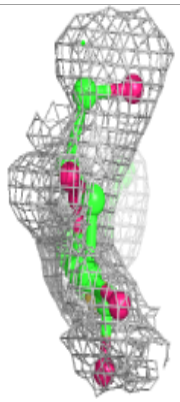


Electron density around HTG B 634:

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

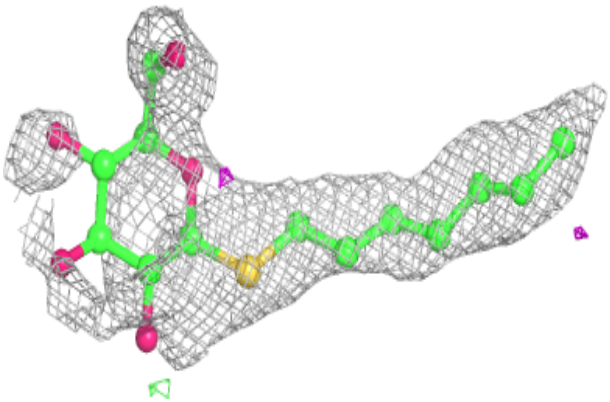


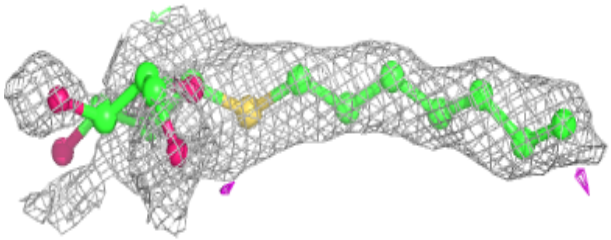


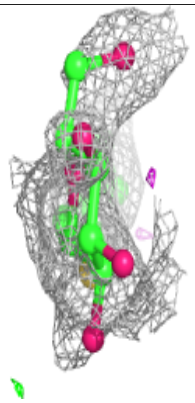


Electron density around HTG b 603:

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

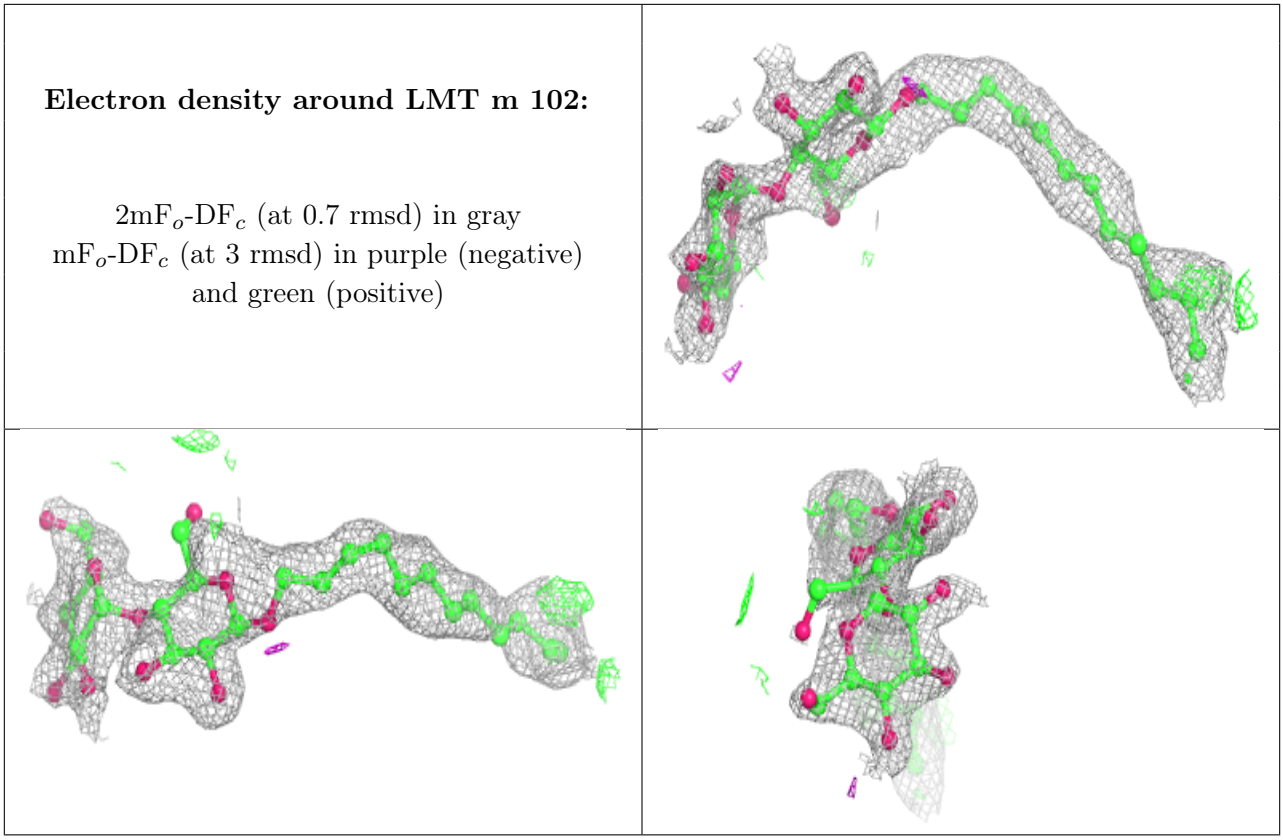






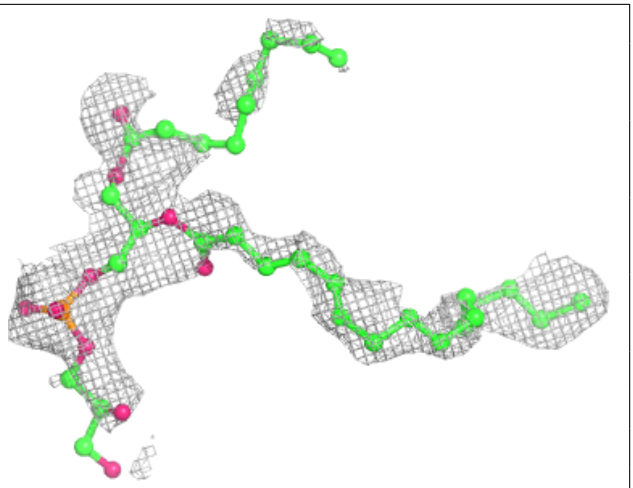
Electron density around LMT m 102:

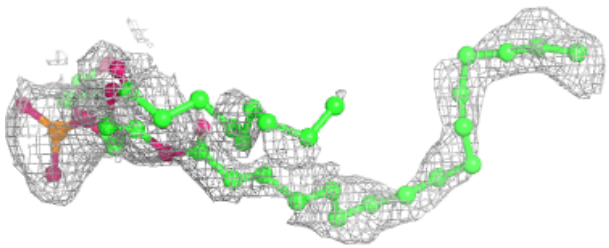
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG e 101:

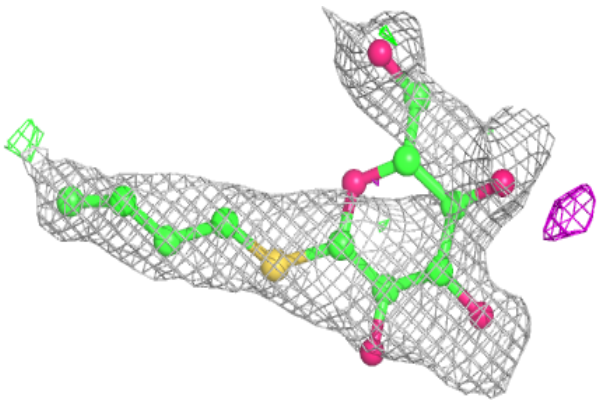
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

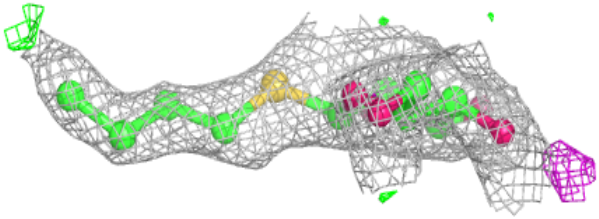


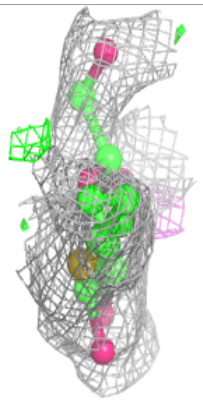


Electron density around HTG d 412:

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

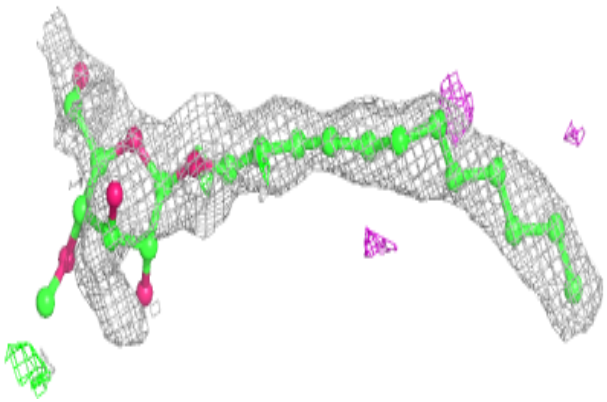


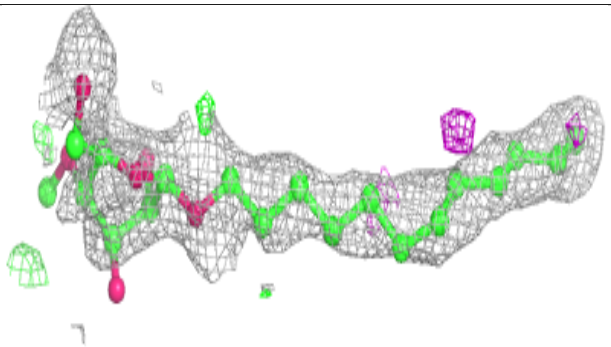


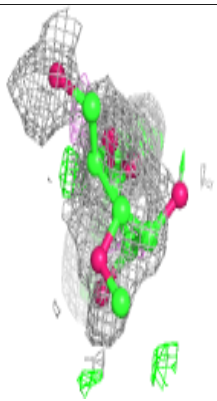


Electron density around LMT b 625:

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

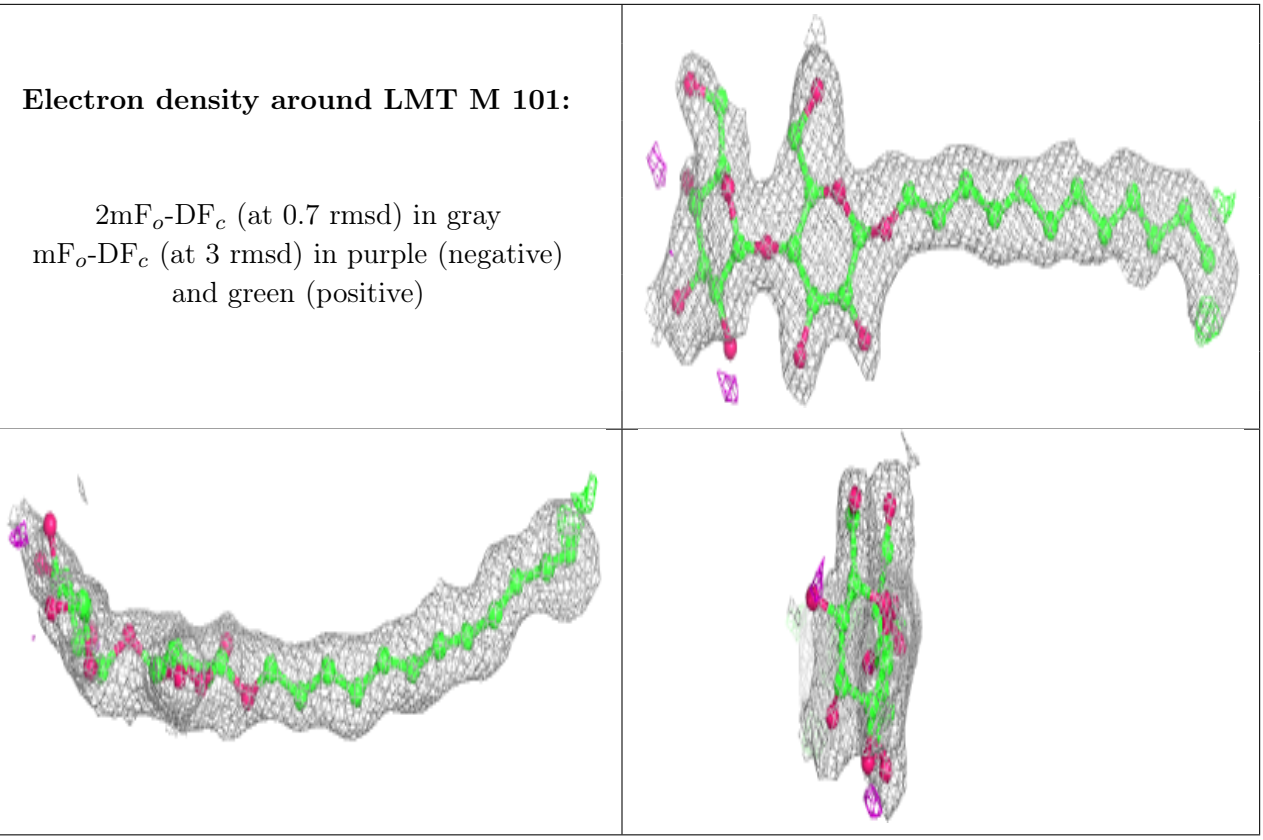






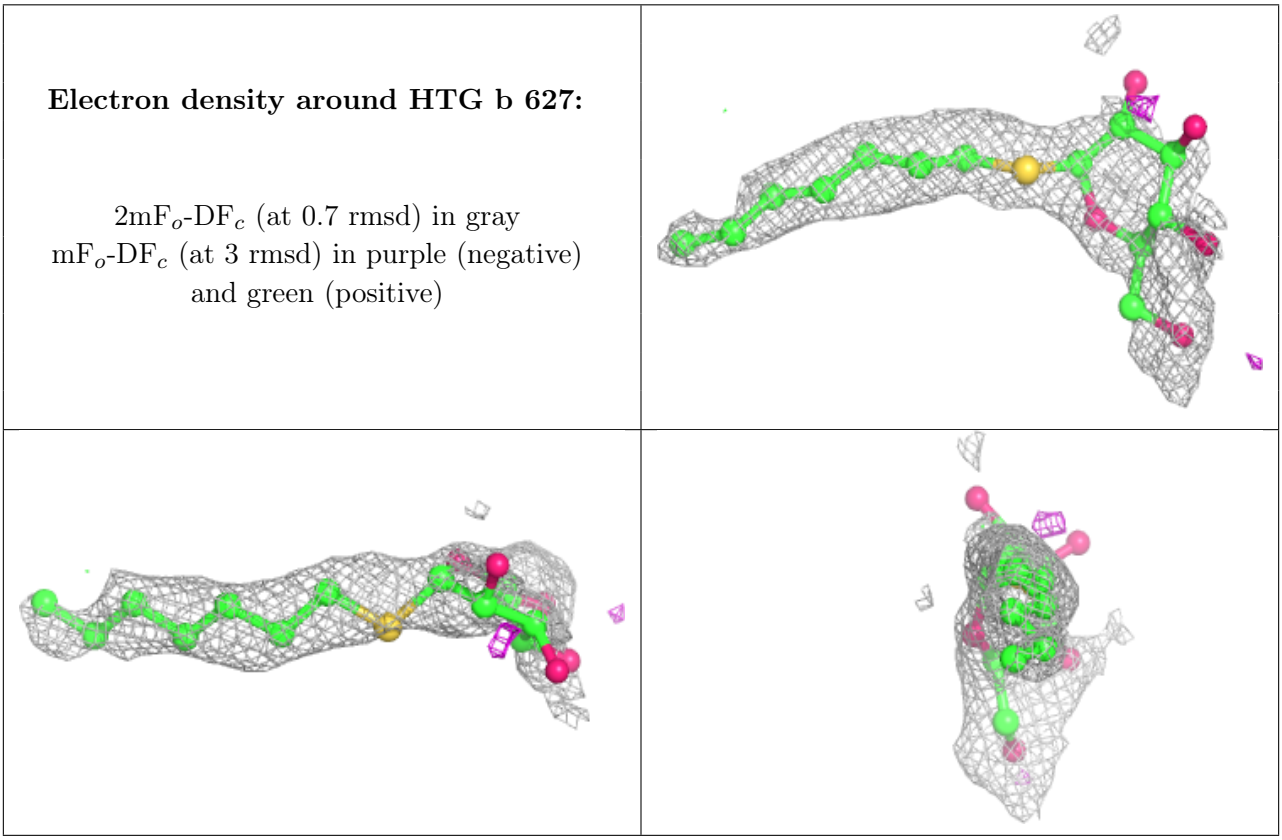
Electron density around LMT M 101:

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



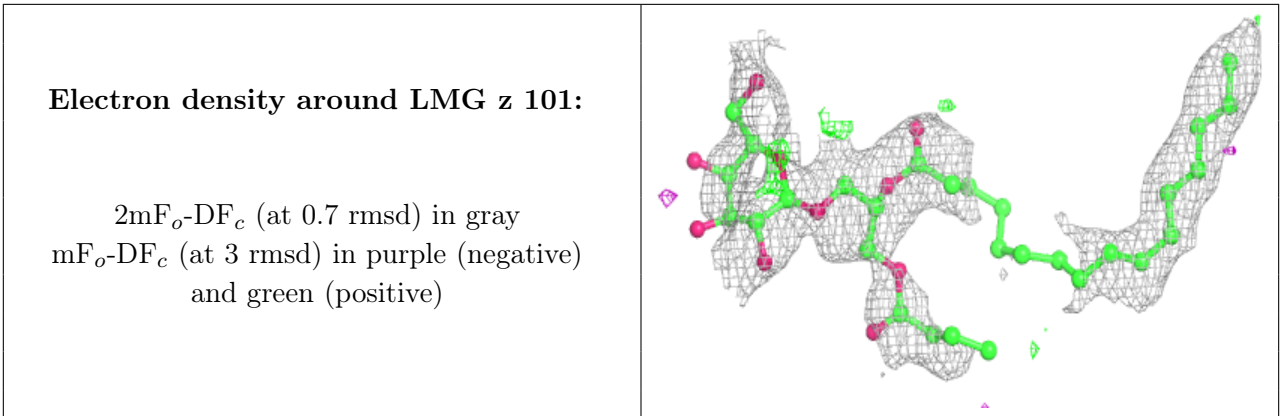
Electron density around HTG b 627:

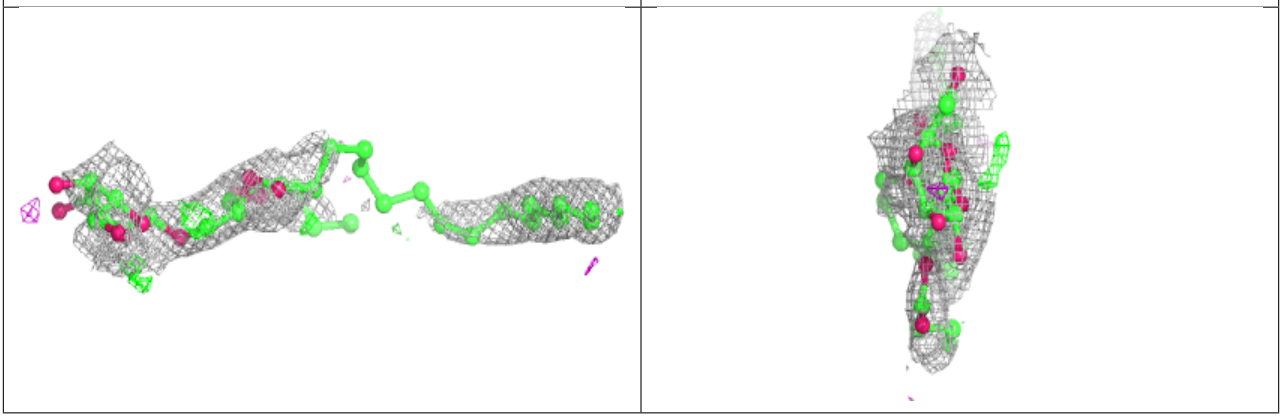
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG z 101:

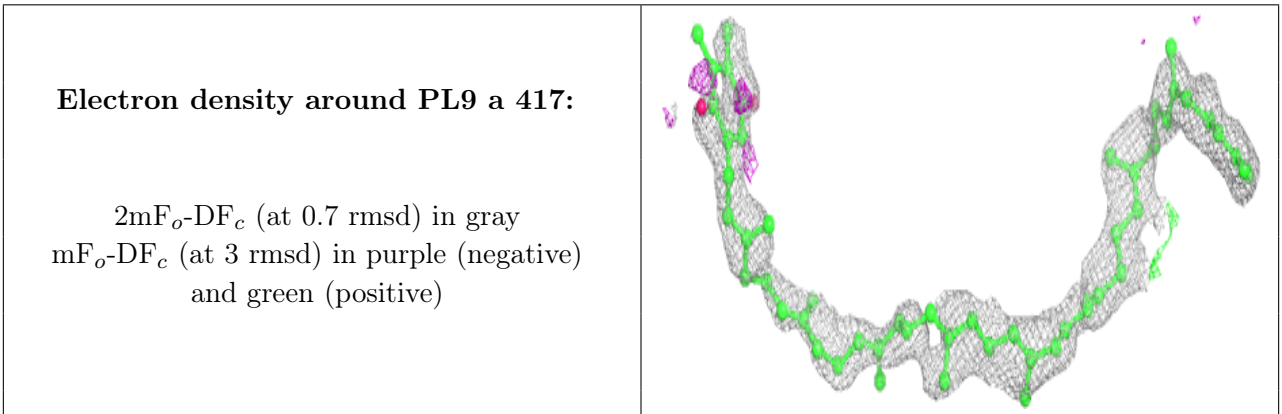
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

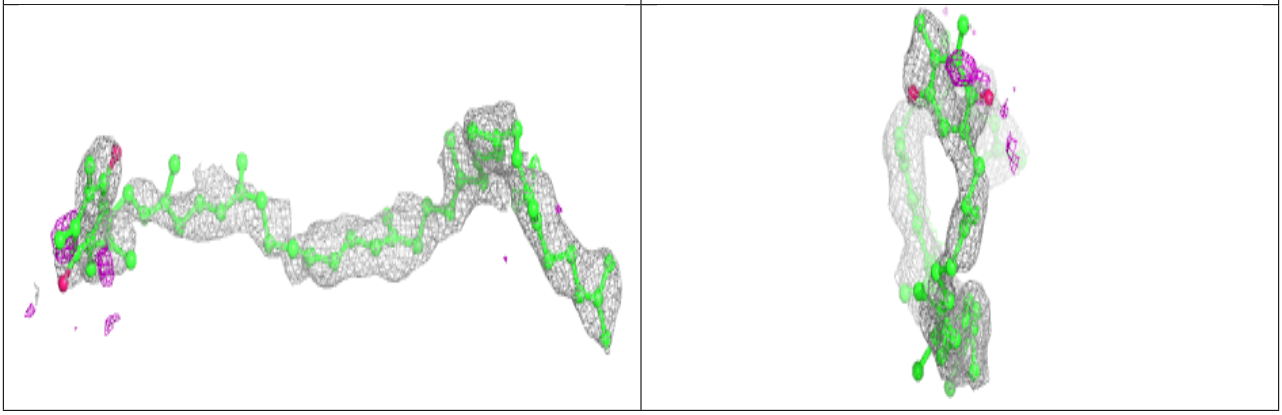




Electron density around PL9 a 417:

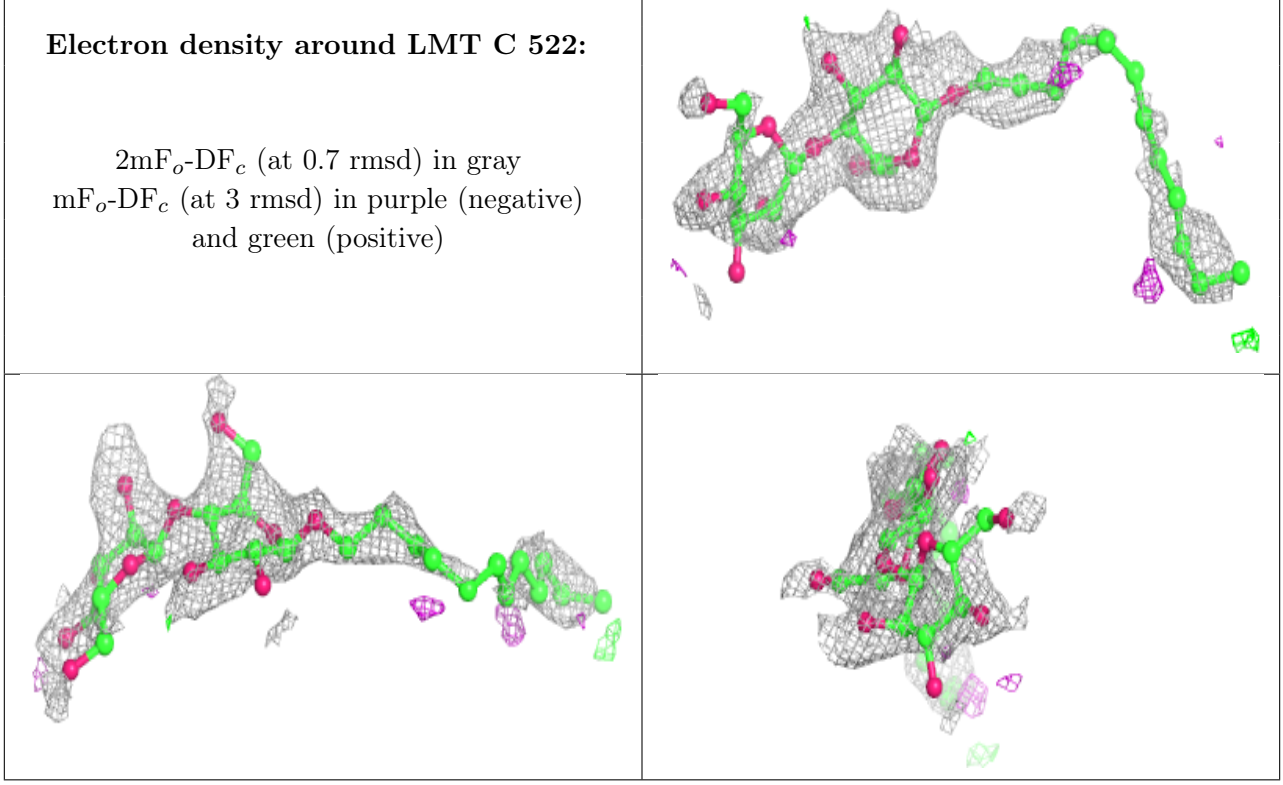
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





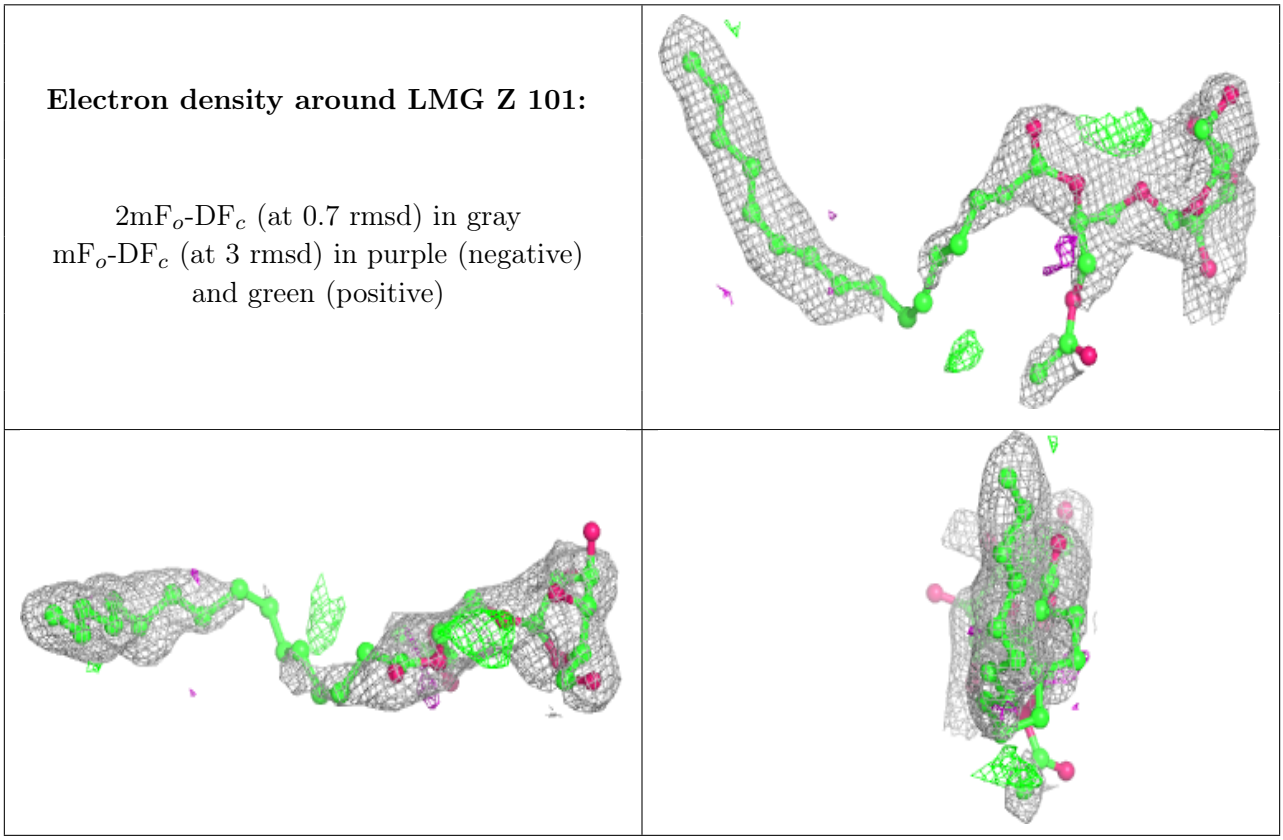
Electron density around LMT C 522:

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



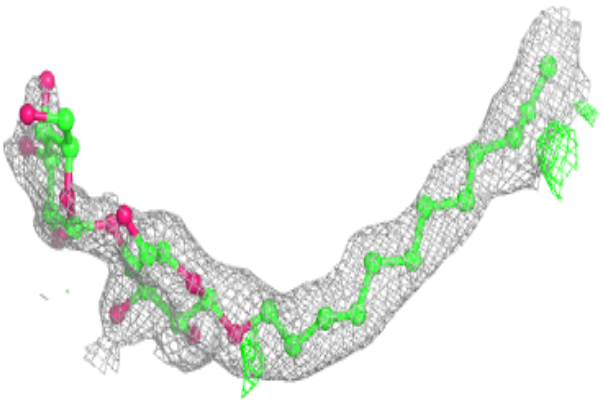
Electron density around LMG Z 101:

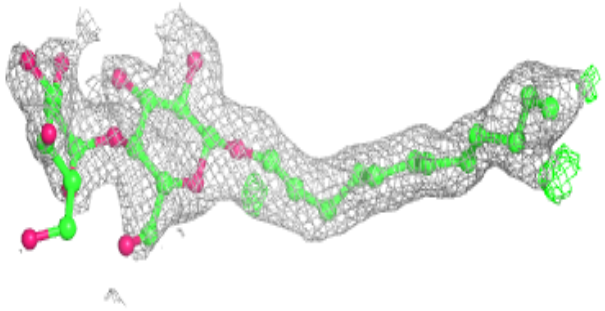
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

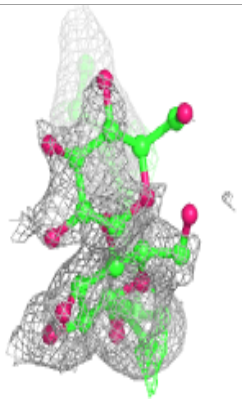


Electron density around LMT m 104:

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

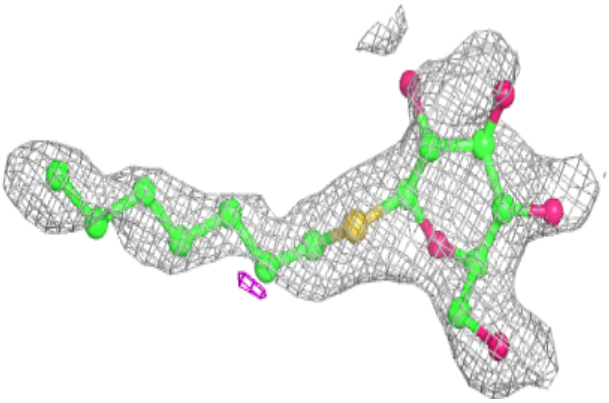


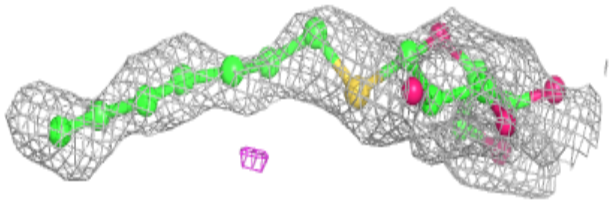


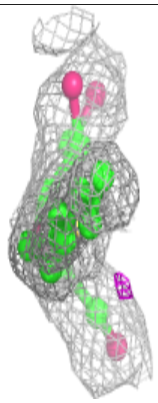


Electron density around HTG C 524:

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

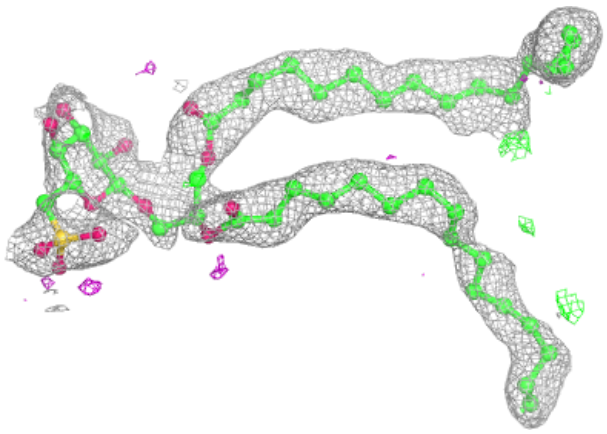


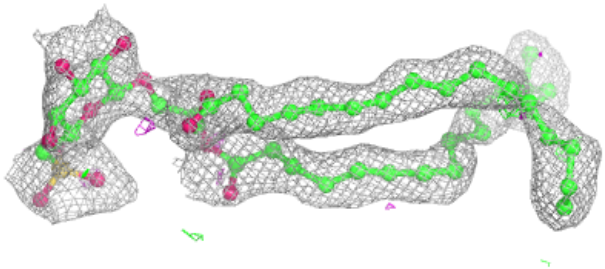


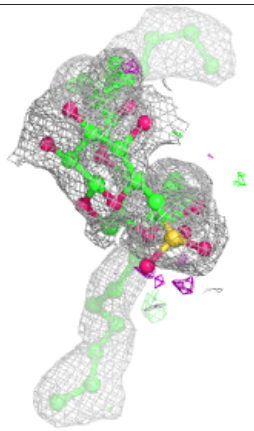


Electron density around SQD B 621:

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

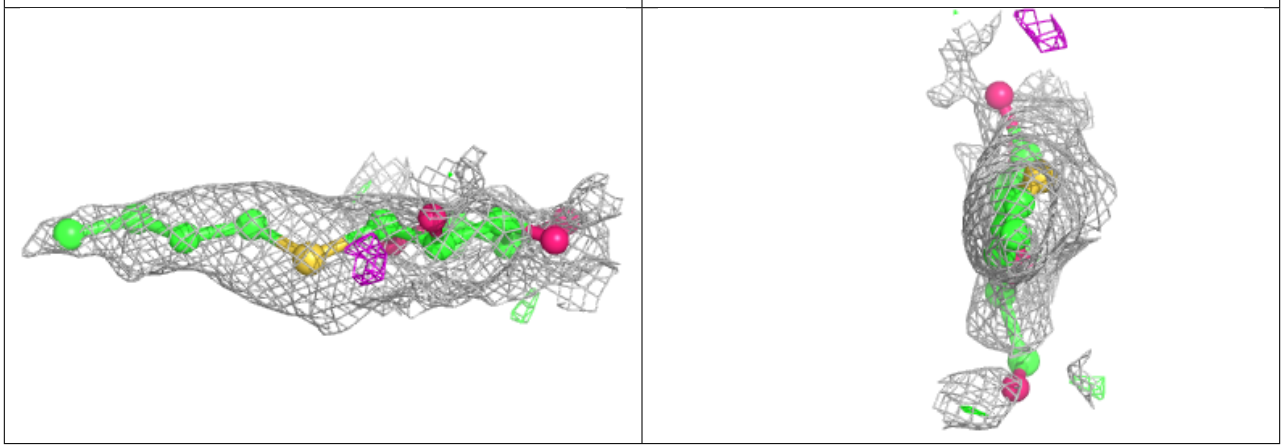






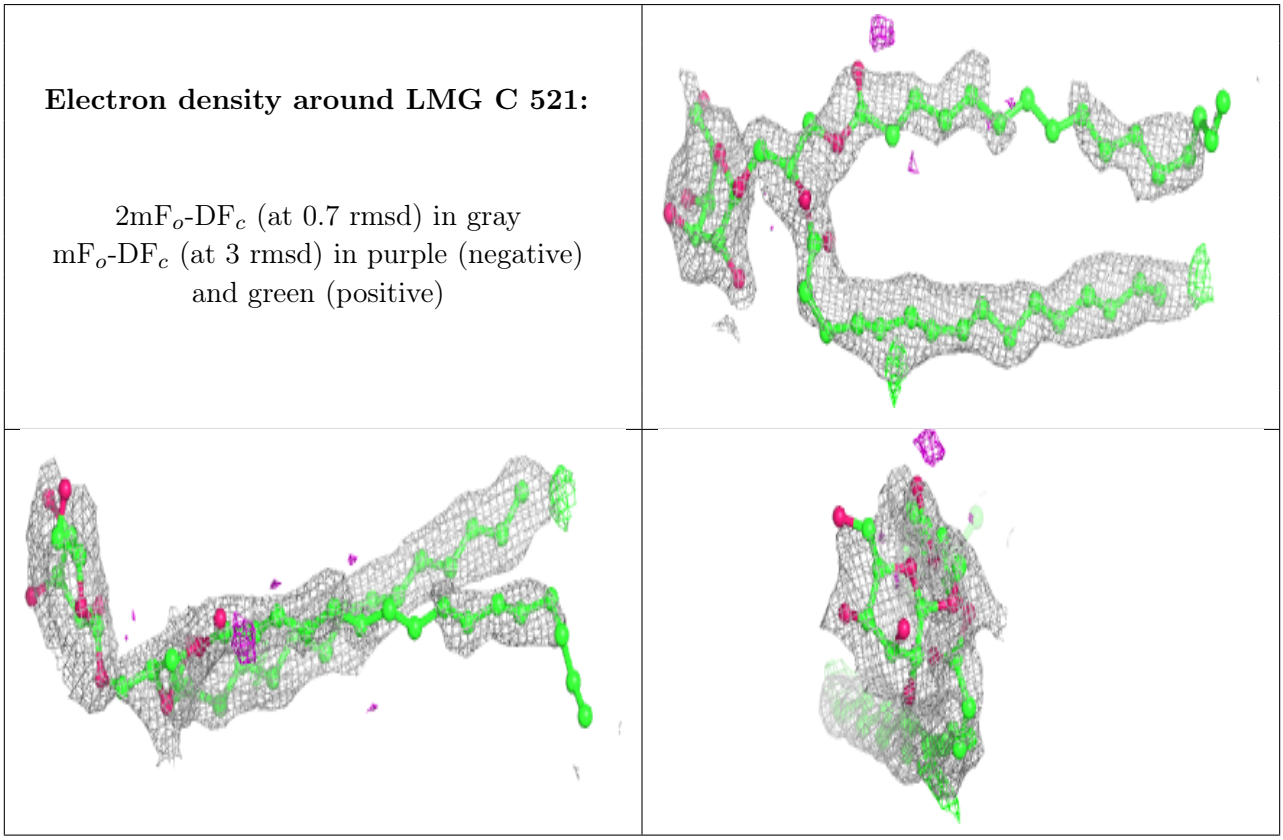
Electron density around HTG D 411:

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



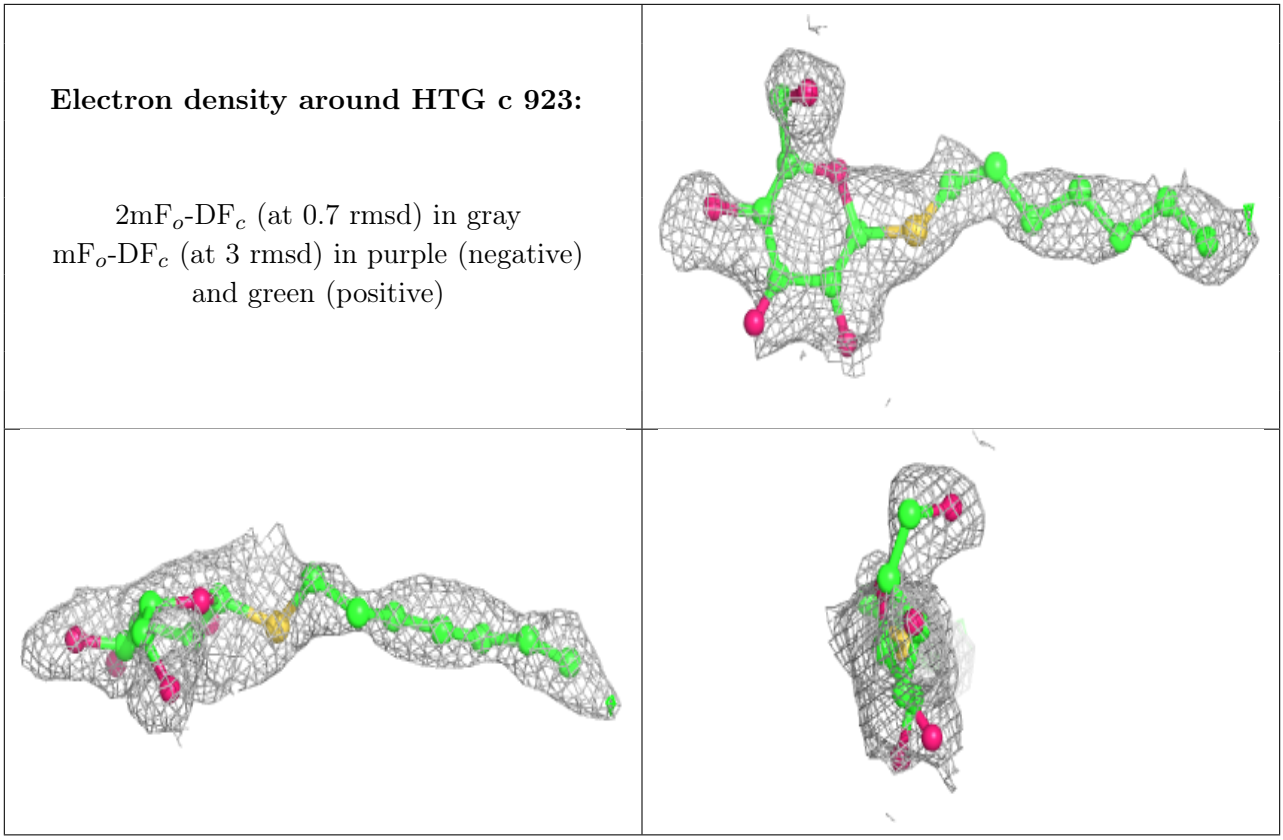
Electron density around LMG C 521:

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



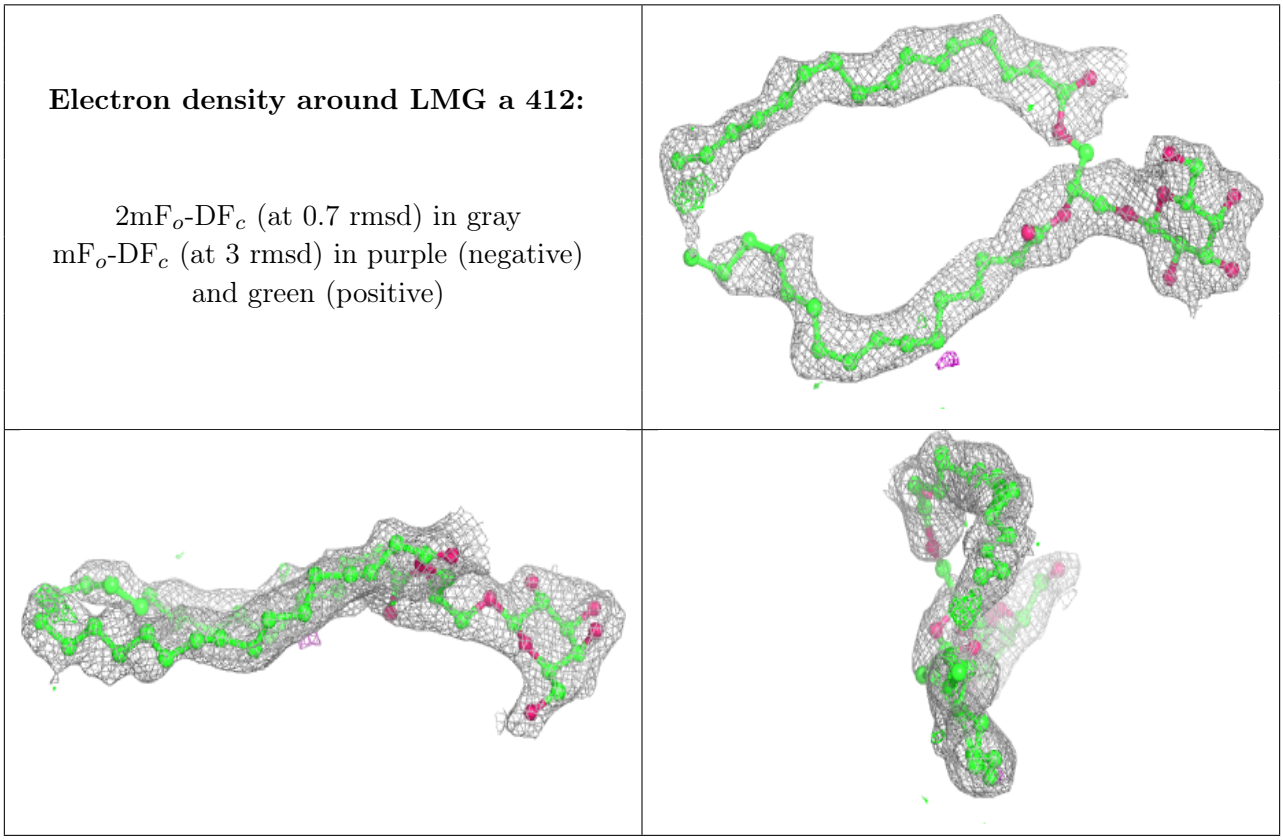
Electron density around HTG c 923:

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



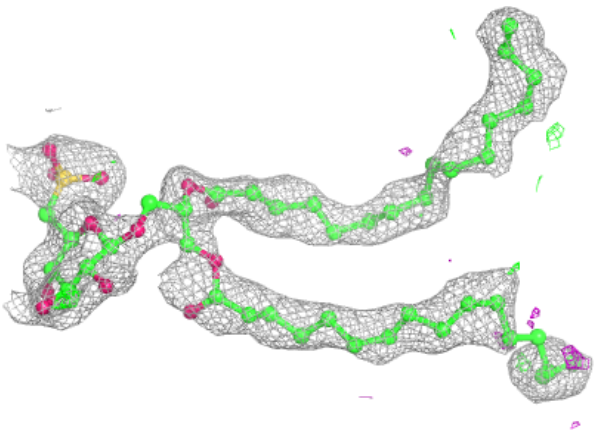
Electron density around LMG a 412:

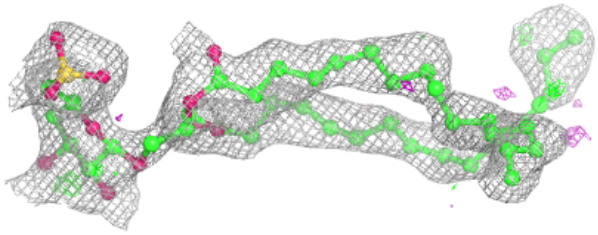
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

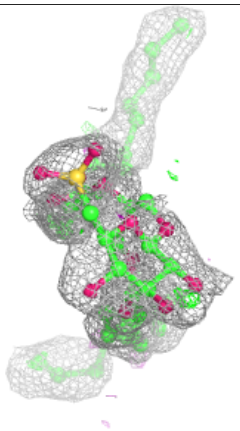


Electron density around SQD L 102:

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

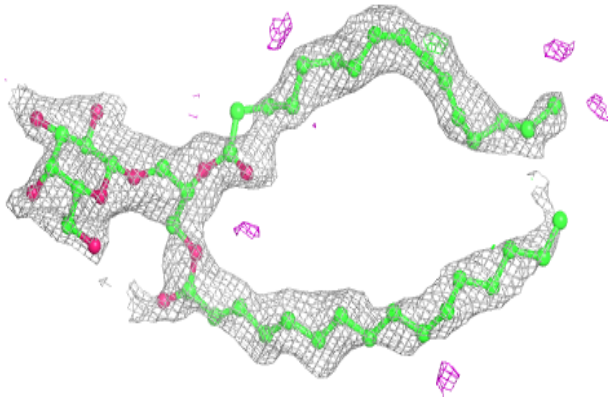


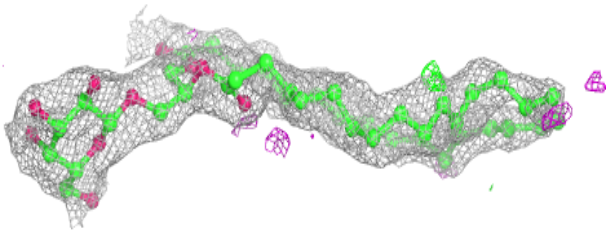


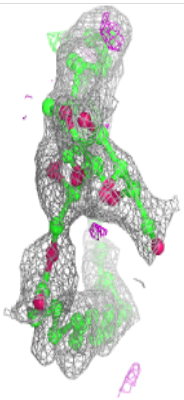


Electron density around LMG C 501:

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

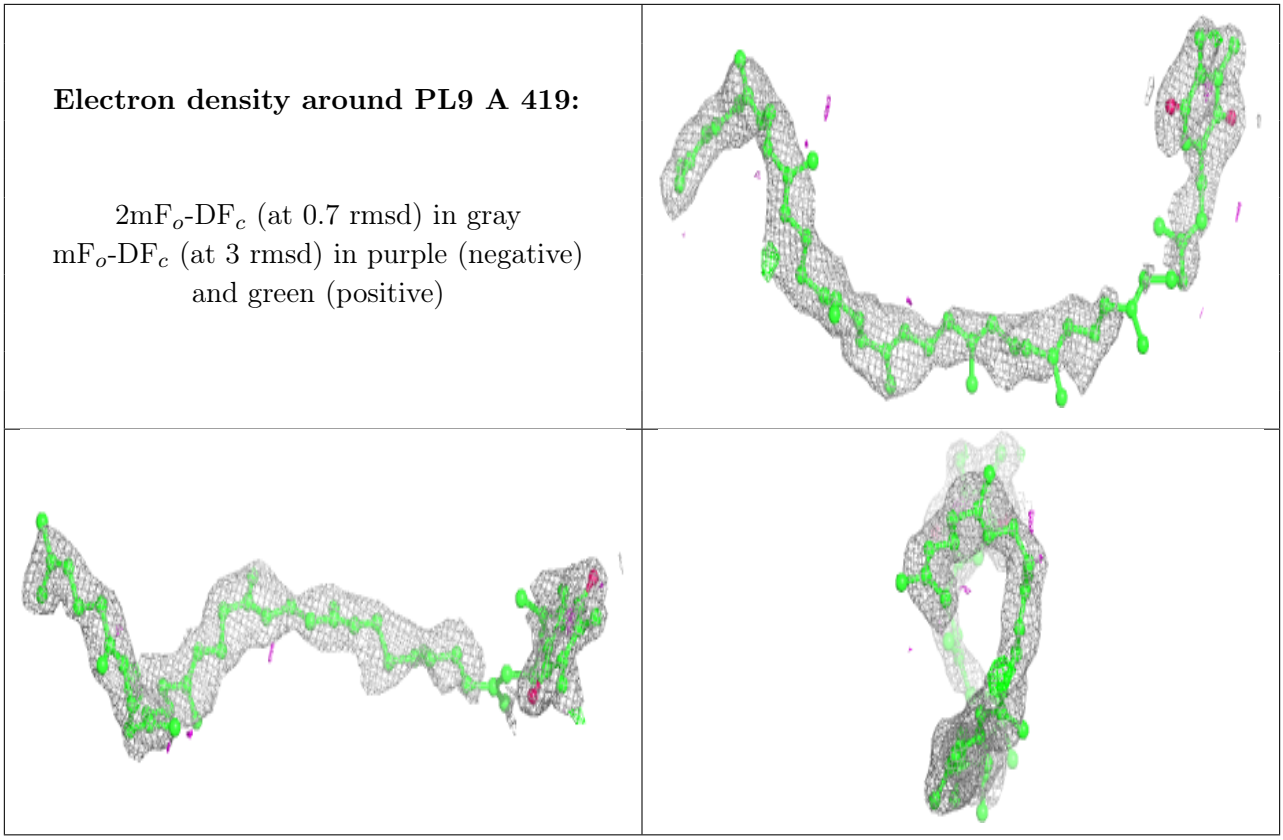






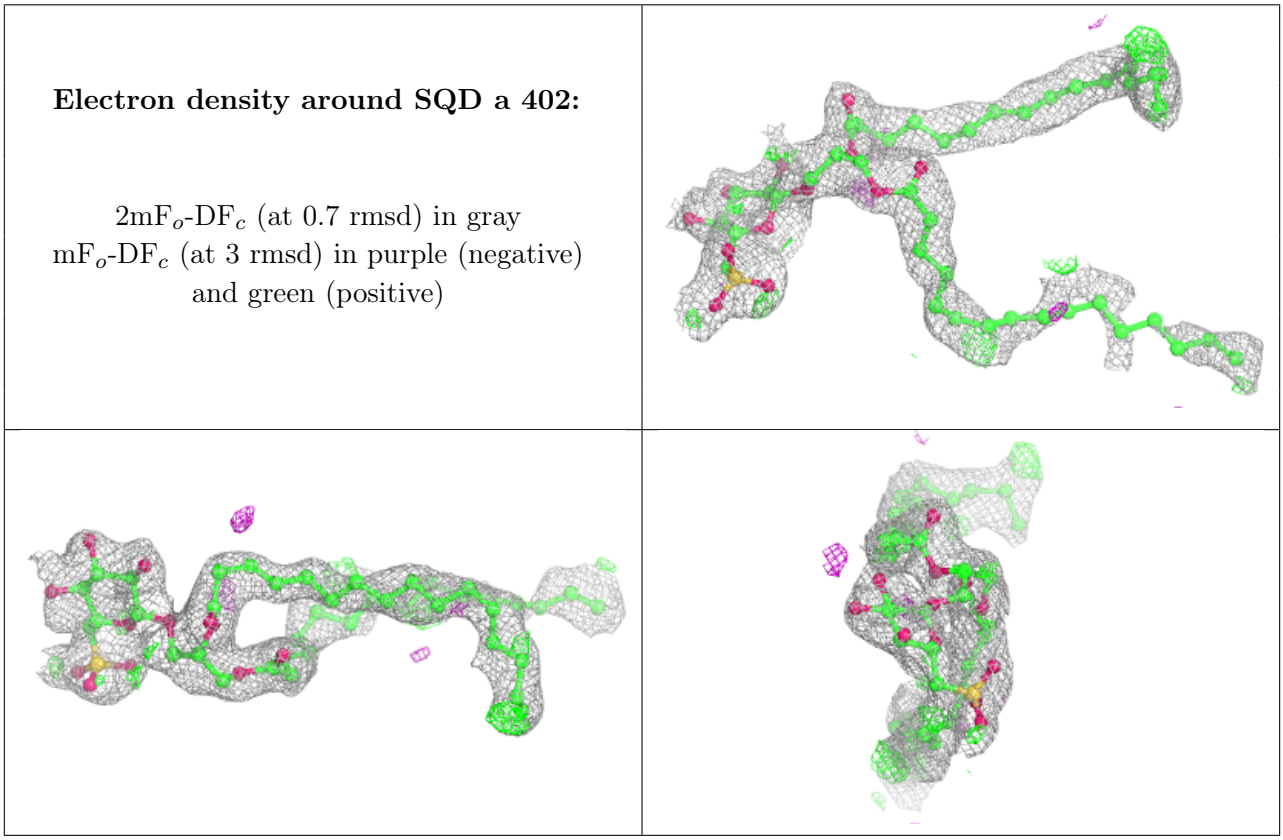
Electron density around PL9 A 419:

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



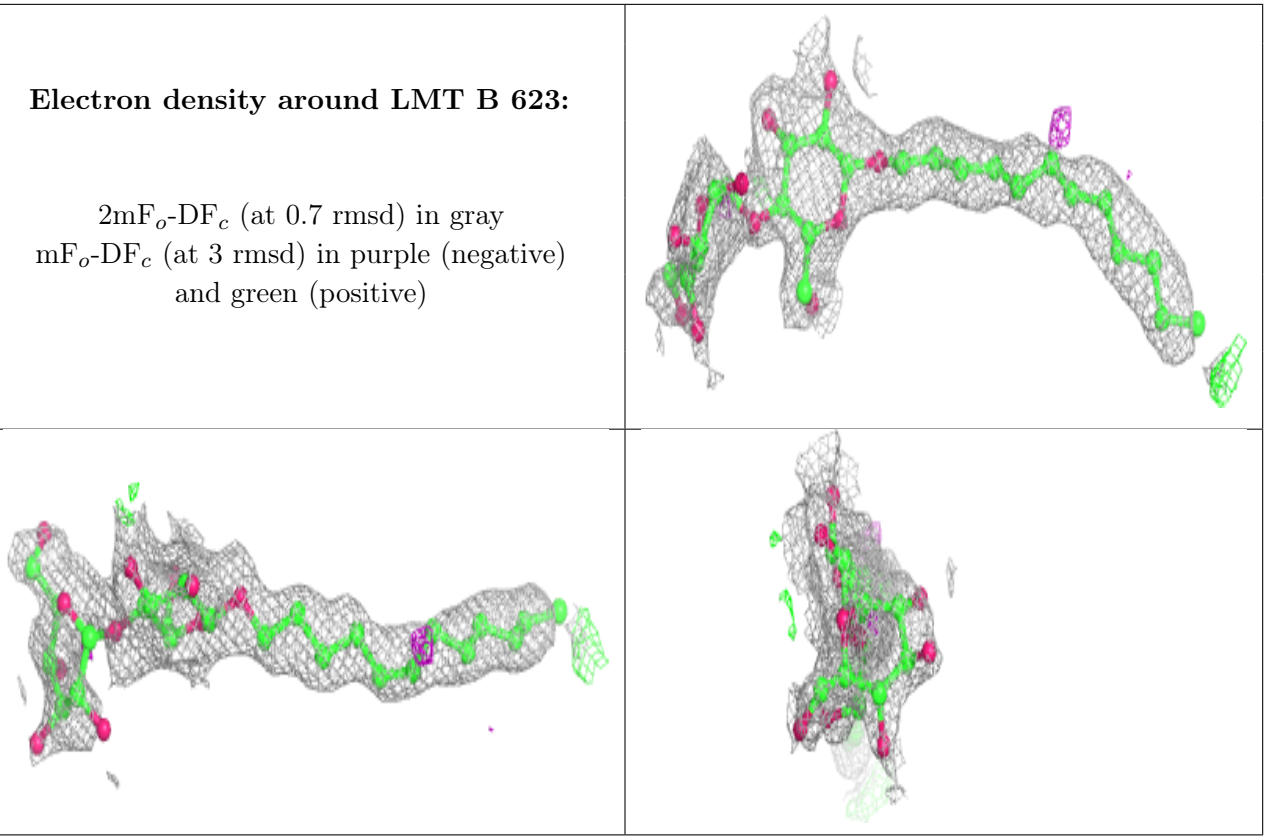
Electron density around SQD a 402:

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



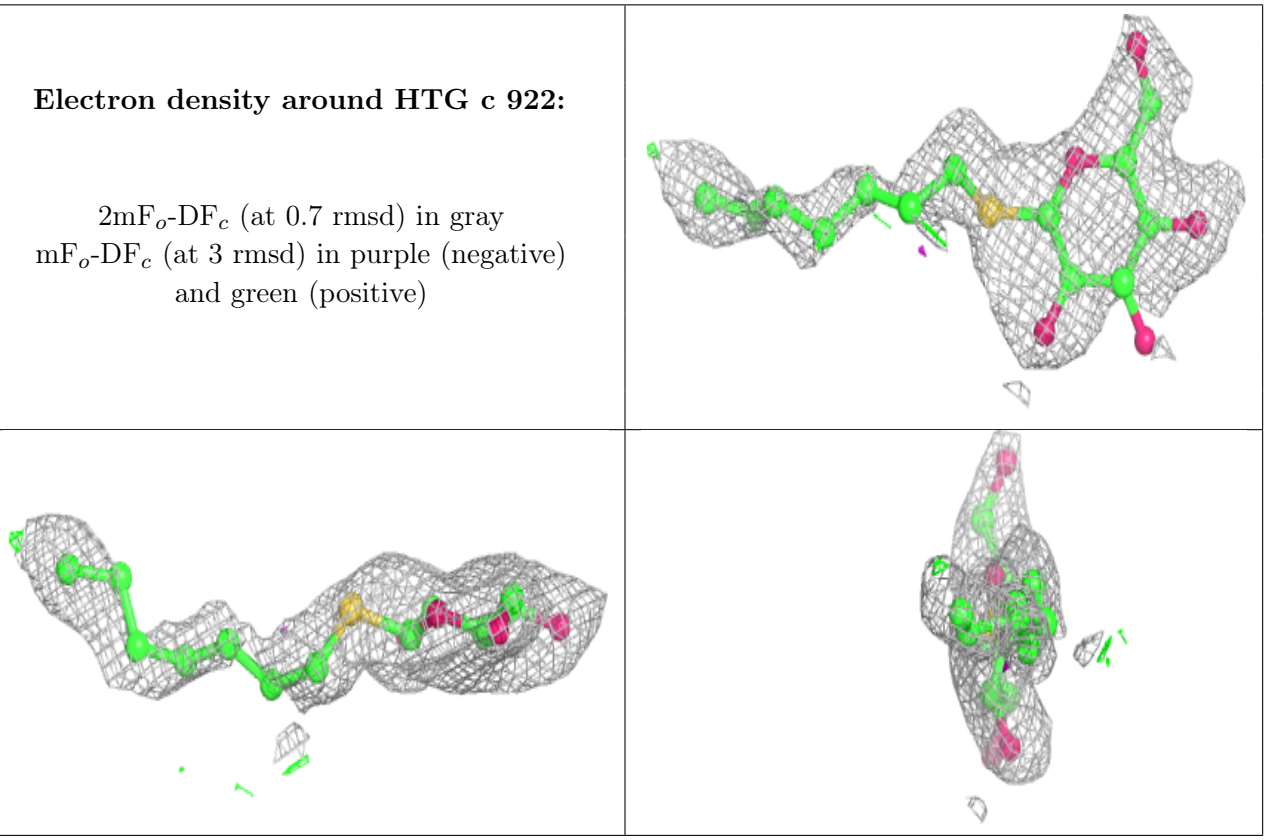
Electron density around LMT B 623:

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



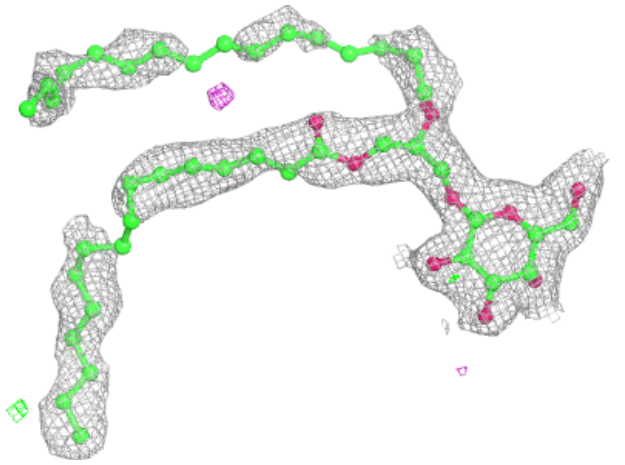
Electron density around HTG c 922:

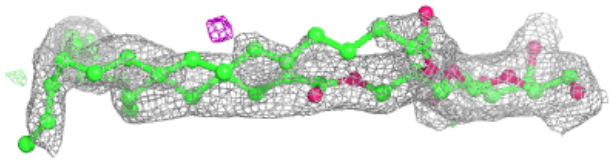
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

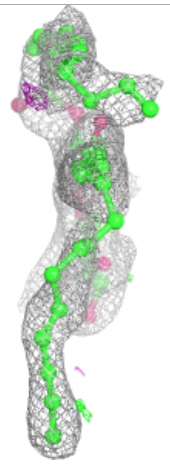


Electron density around LMG c 919:

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

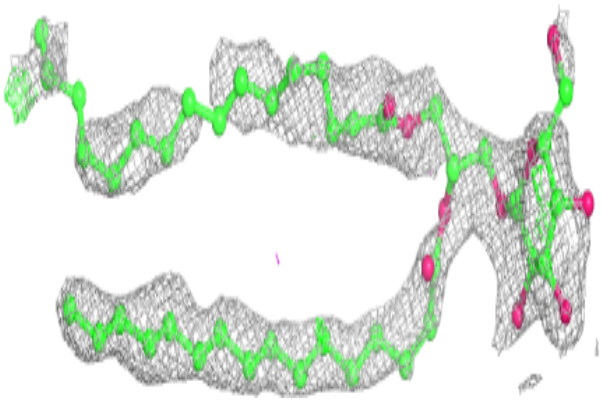


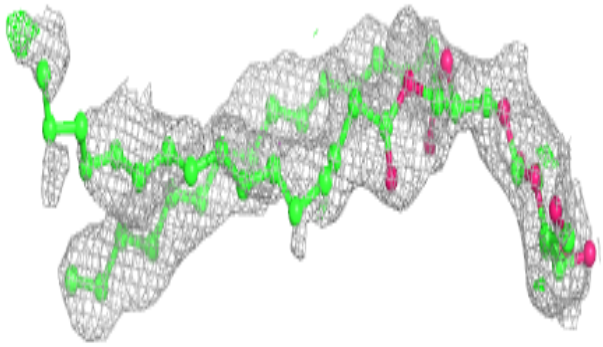


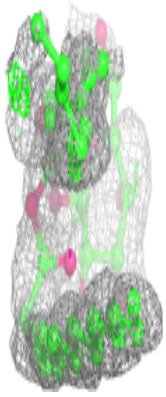


Electron density around LMG c 920:

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

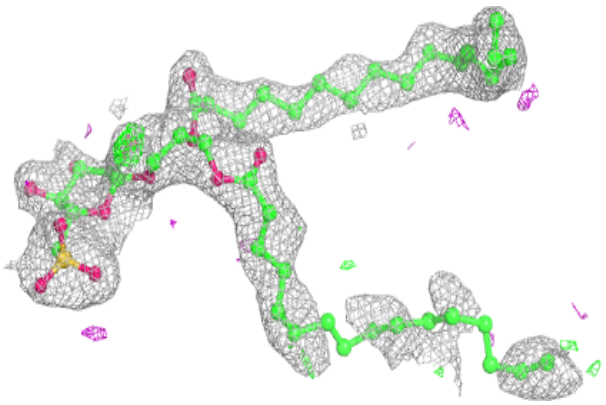


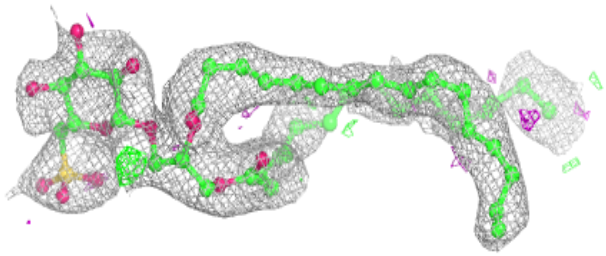


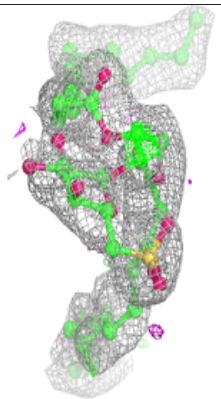


Electron density around SQD A 416:

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

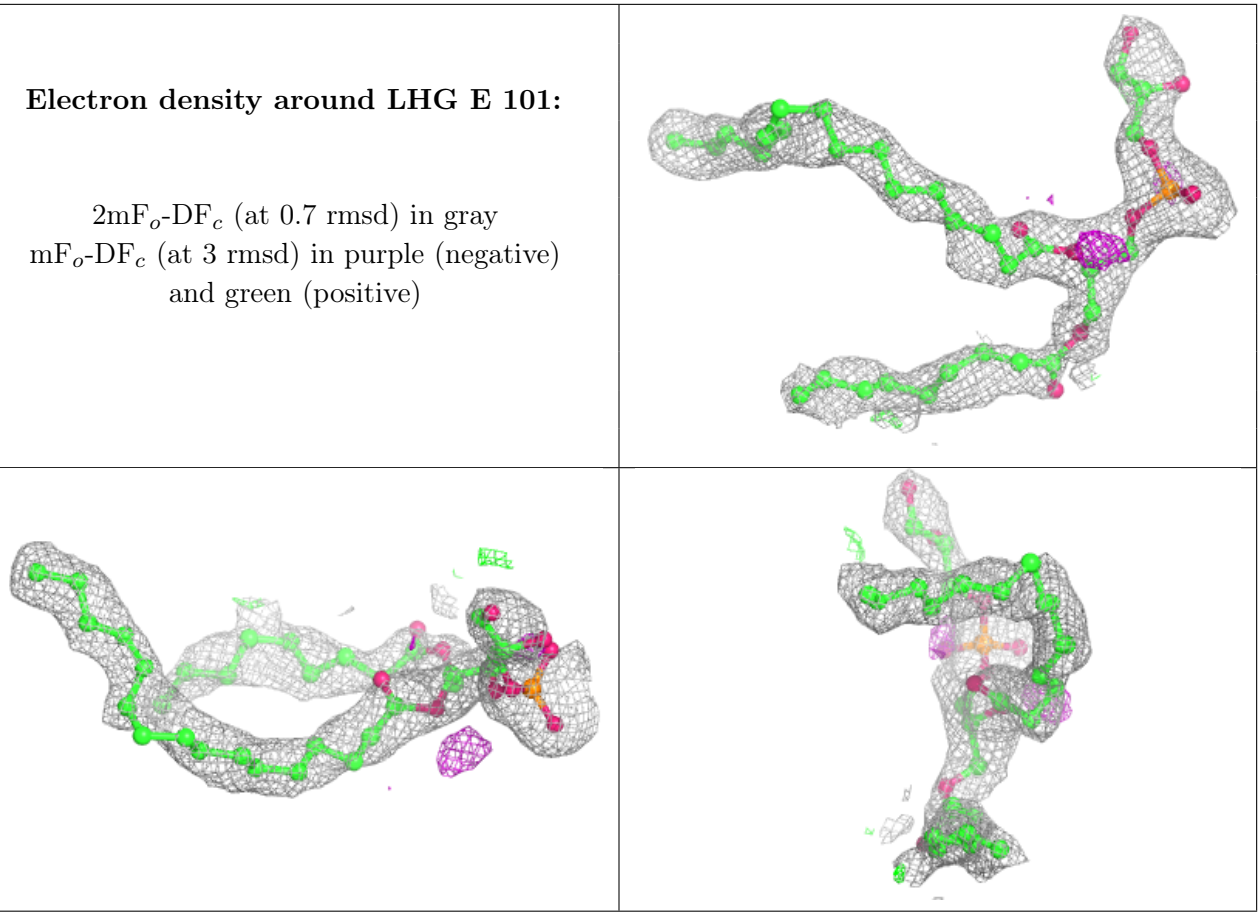






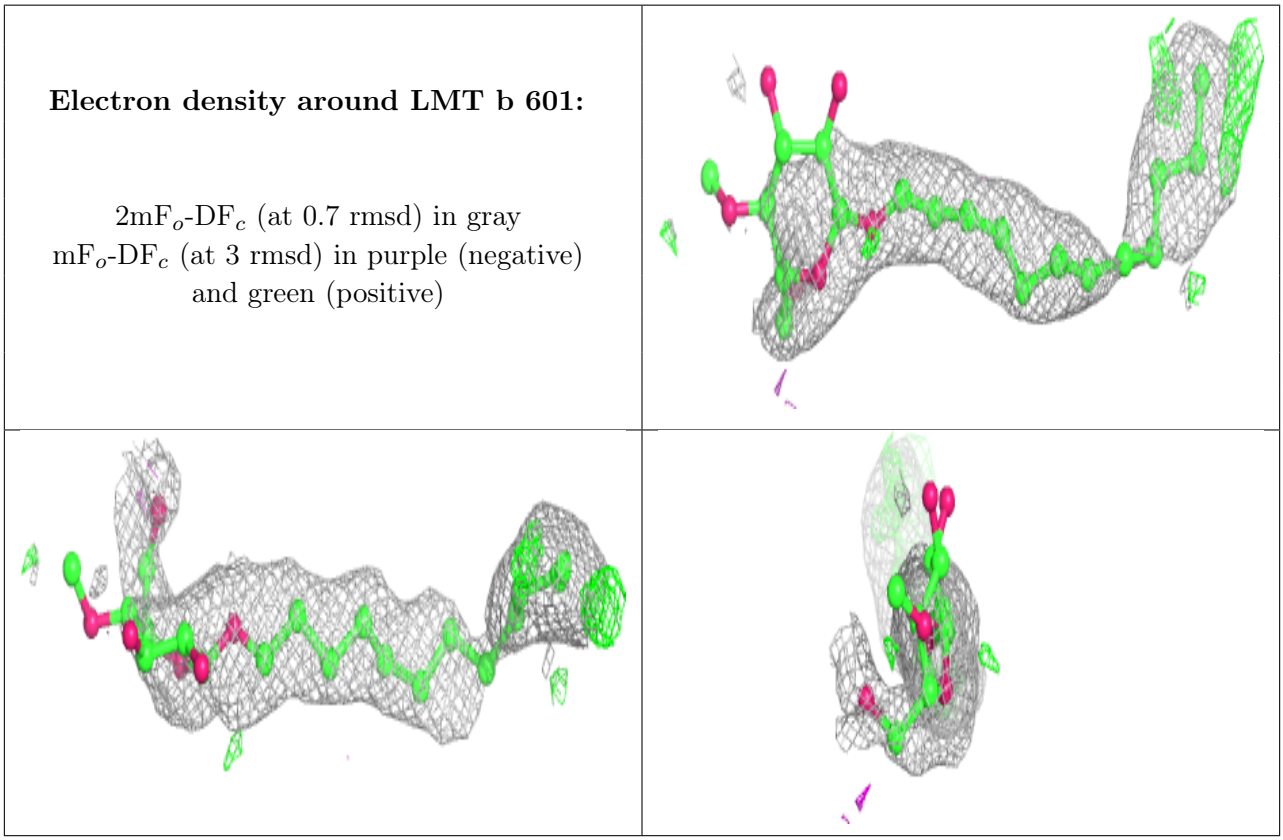
Electron density around LHG E 101:

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



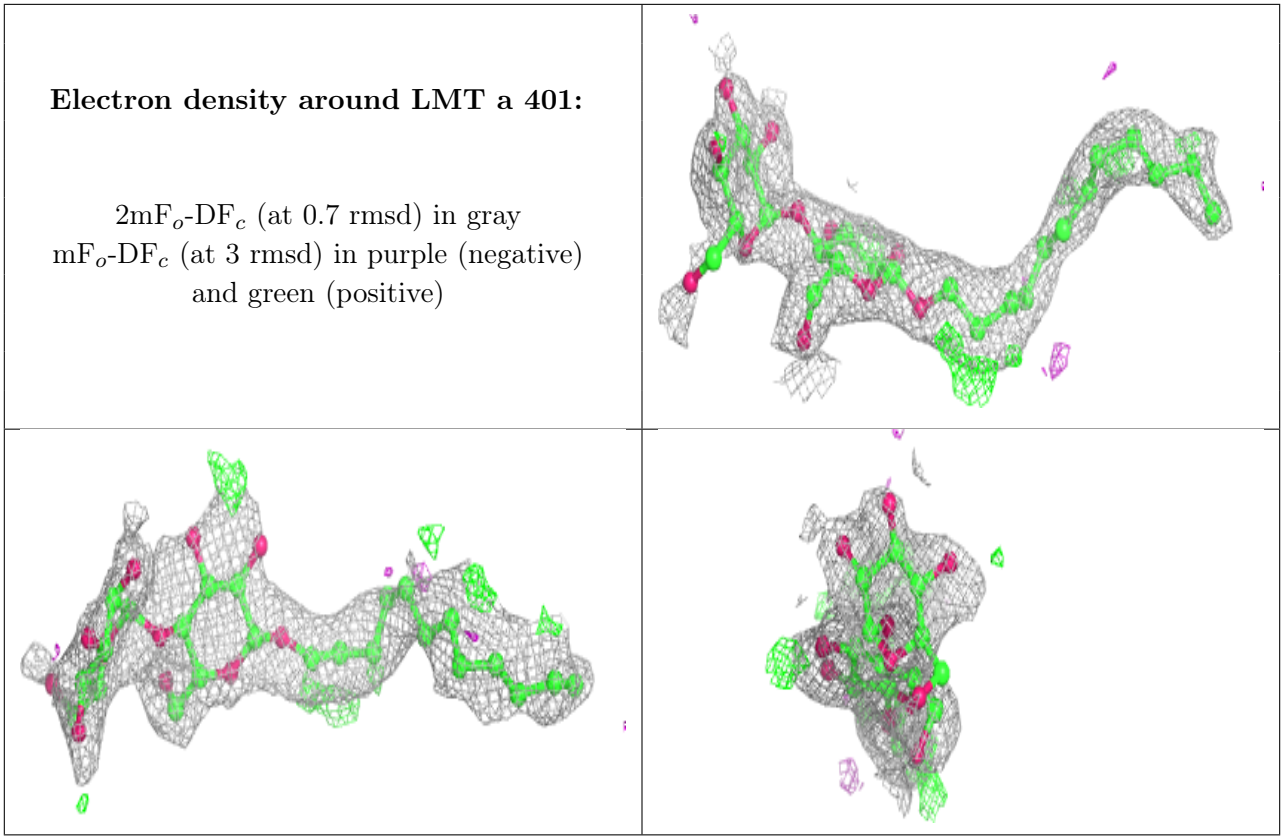
Electron density around LMT b 601:

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



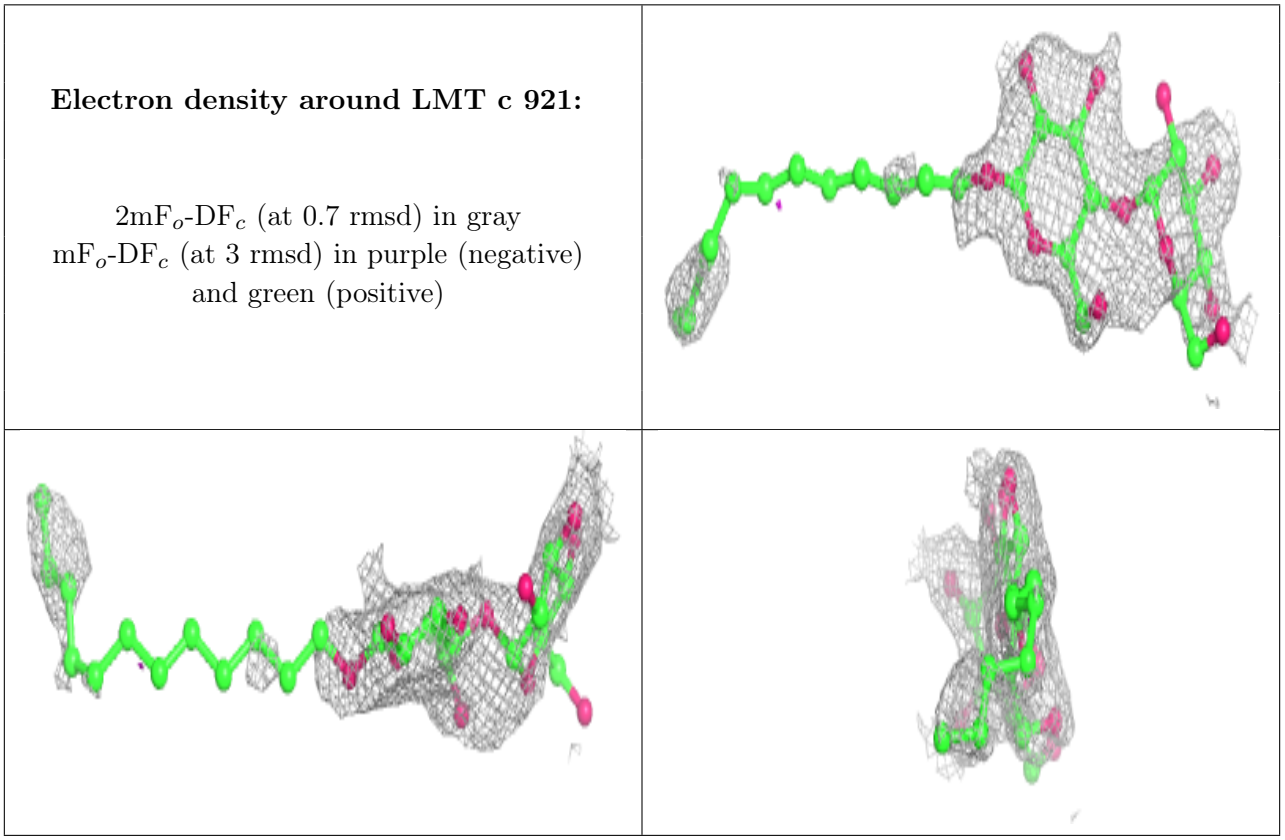
Electron density around LMT a 401:

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



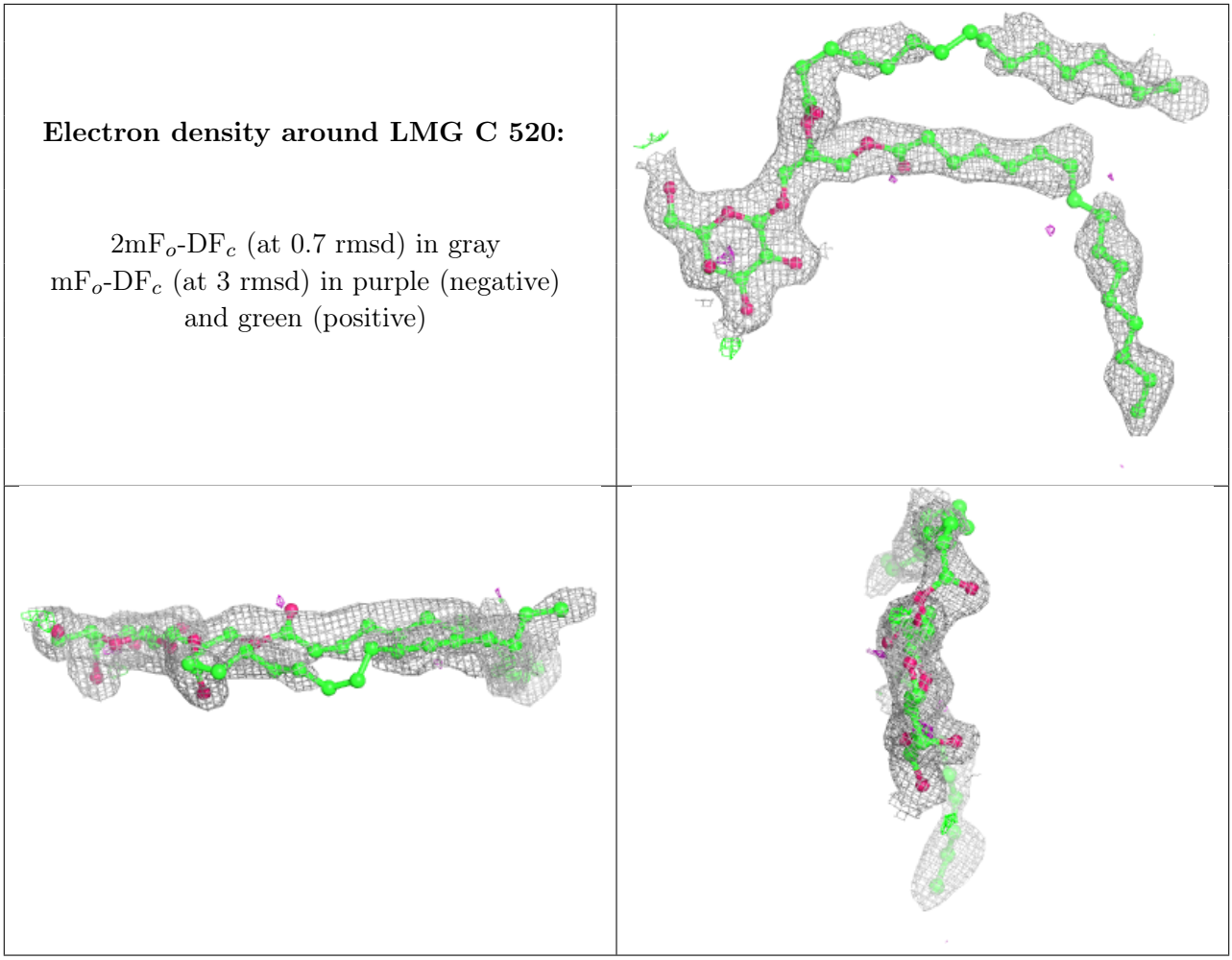
Electron density around LMT c 921:

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



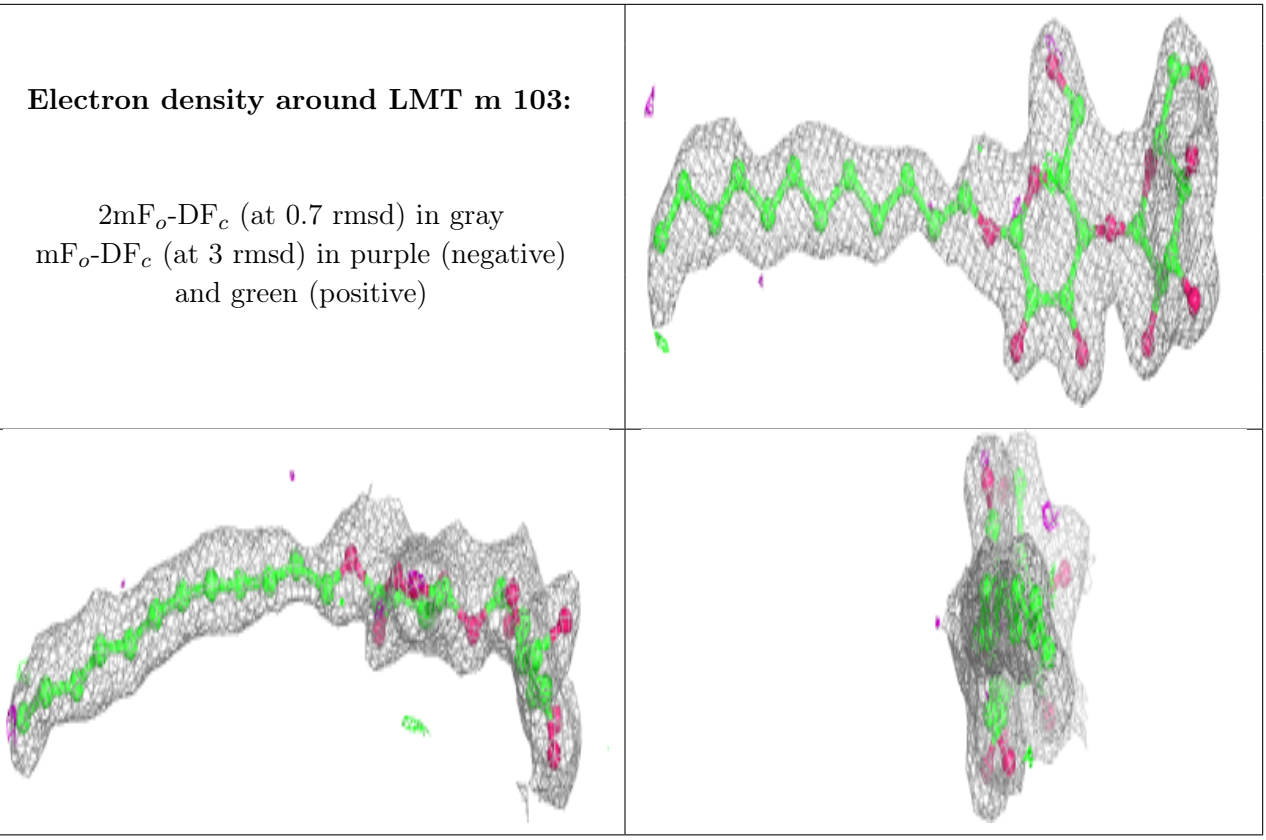
Electron density around LMG C 520:

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



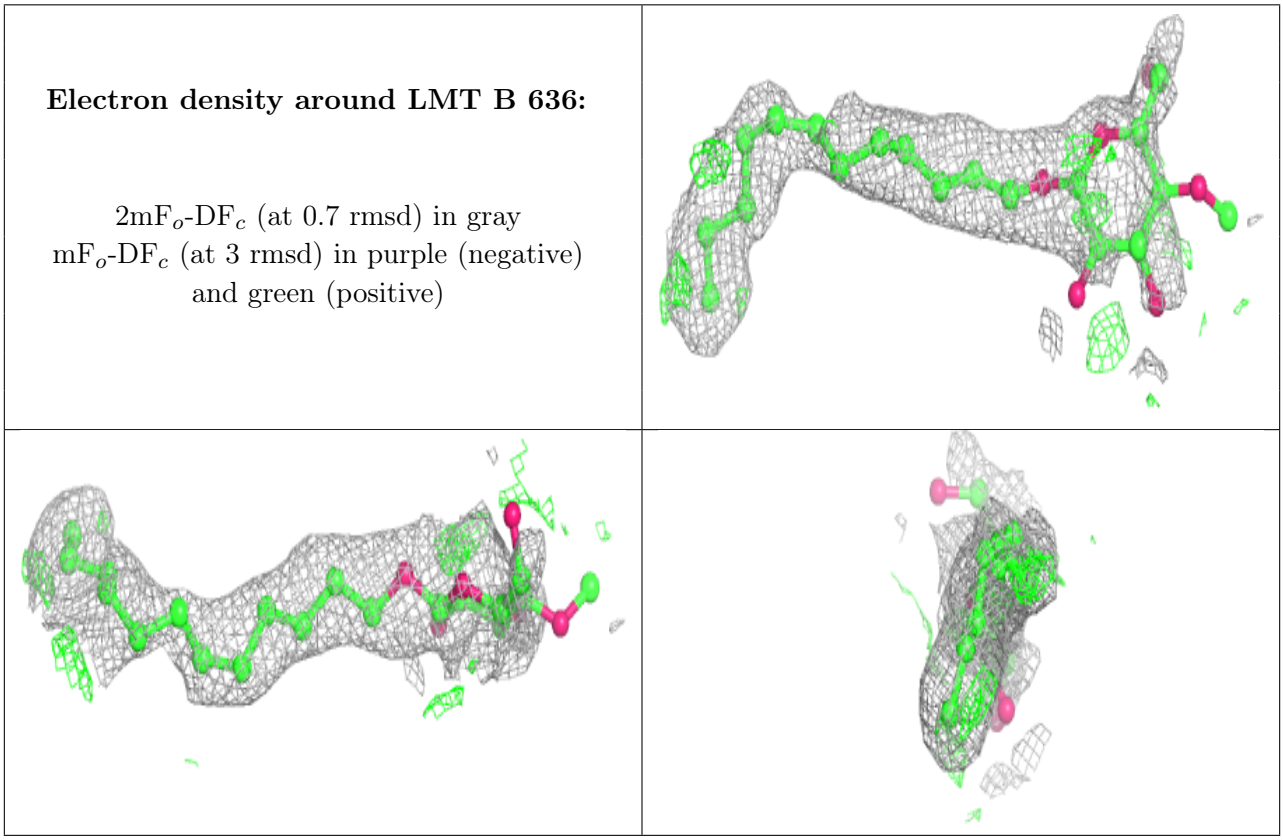
Electron density around LMT m 103:

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



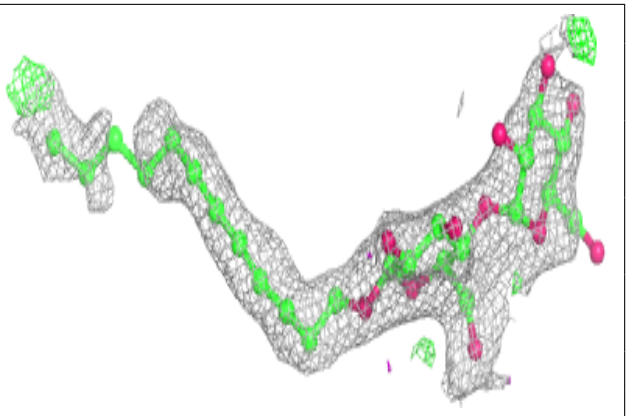
Electron density around LMT B 636:

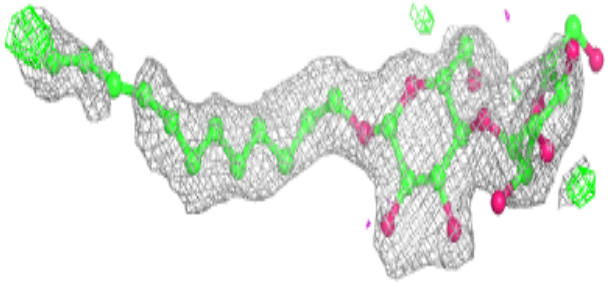
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT A 417:

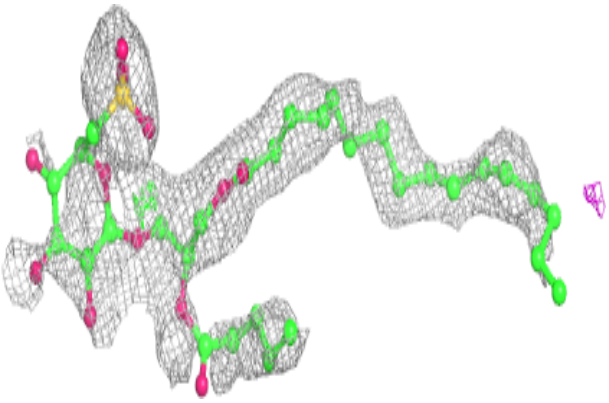
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

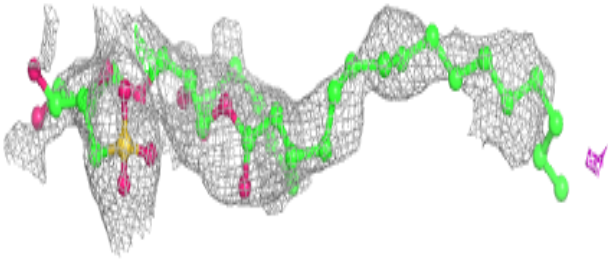


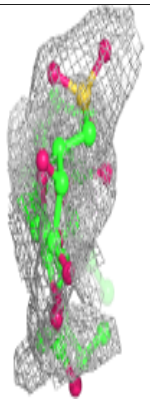


Electron density around SQD f 102:

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

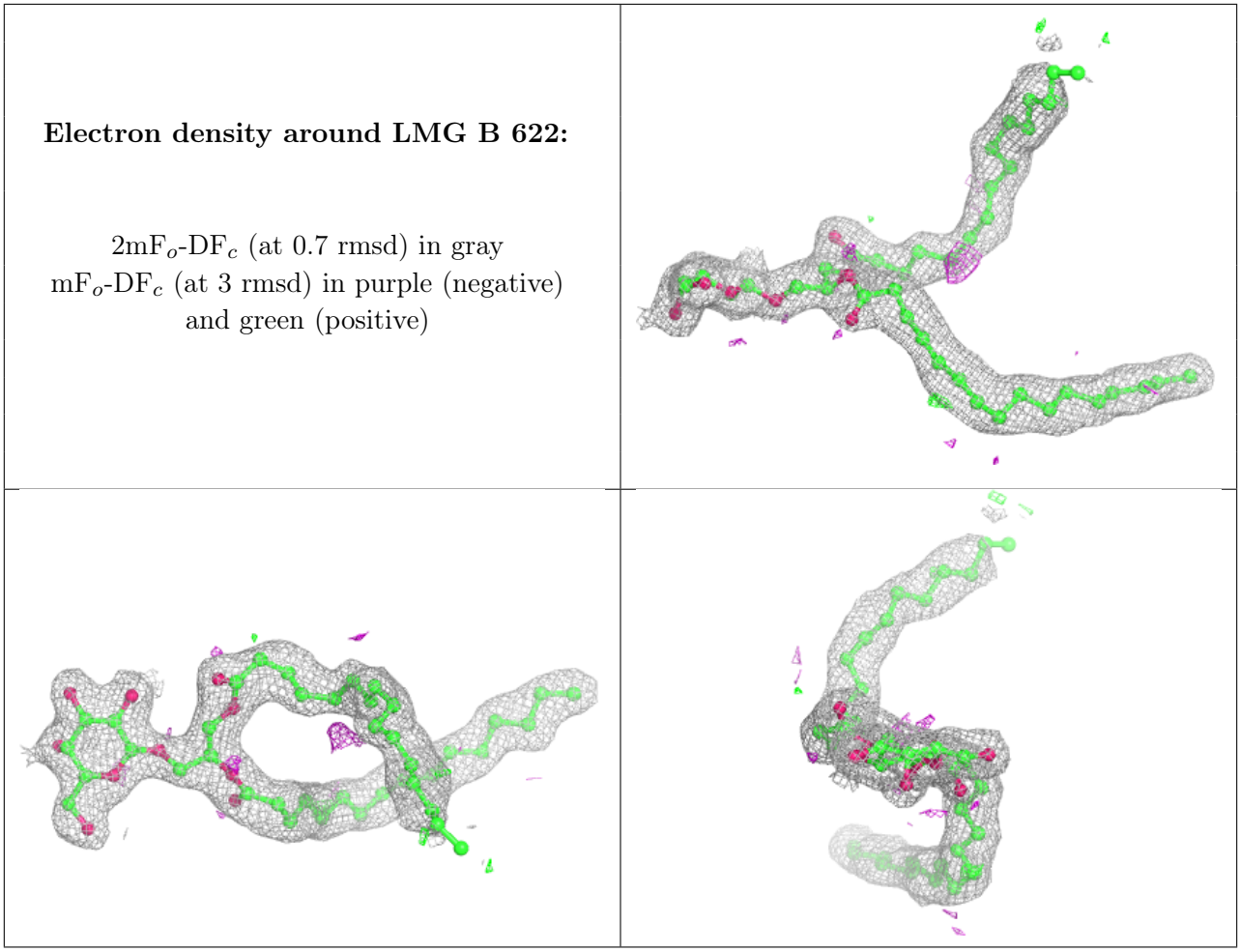






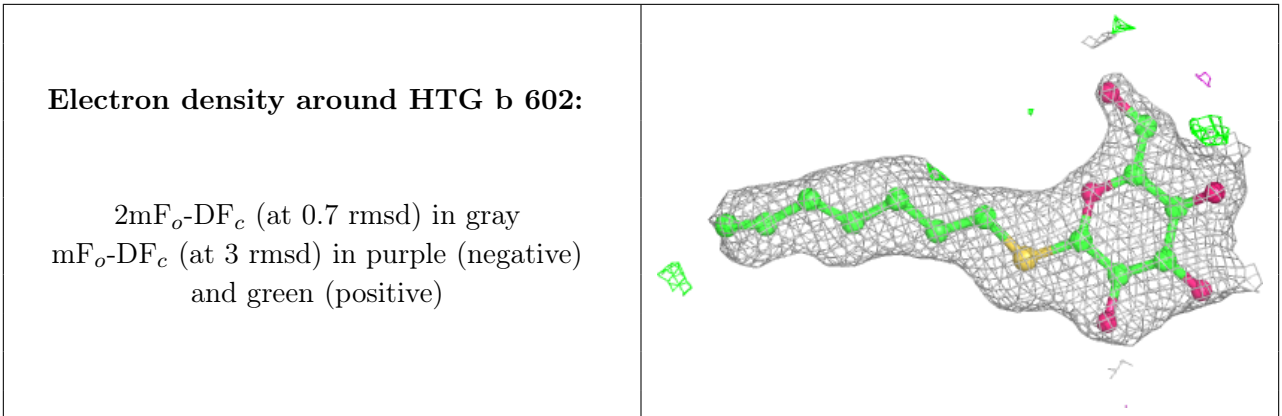
Electron density around LMG B 622:

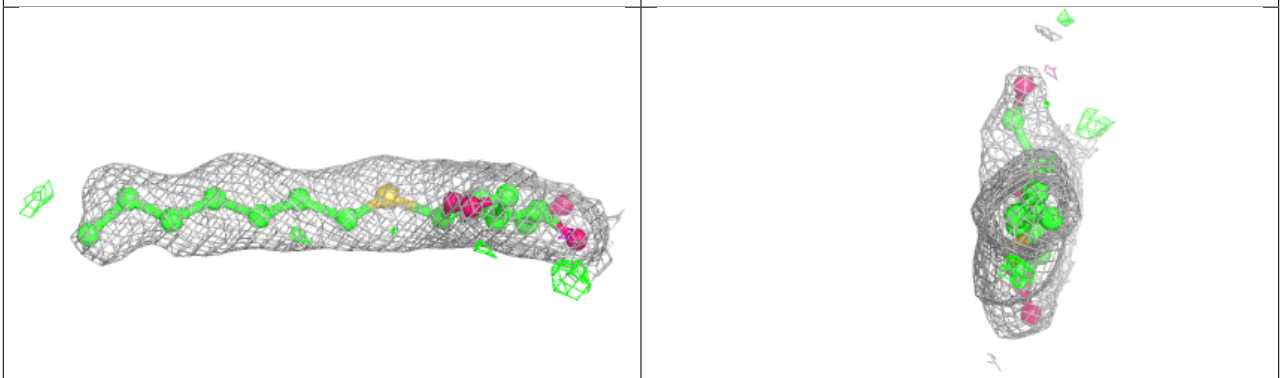
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HTG b 602:

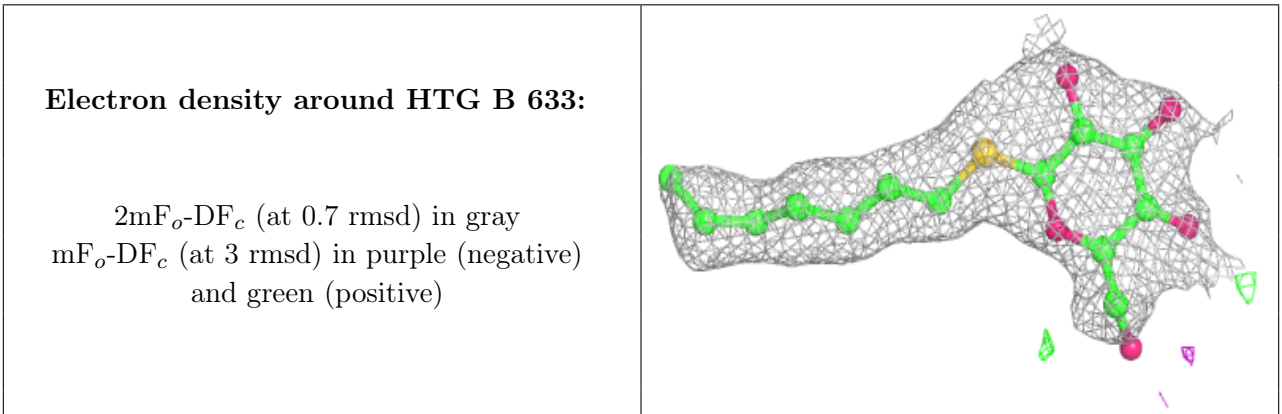
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

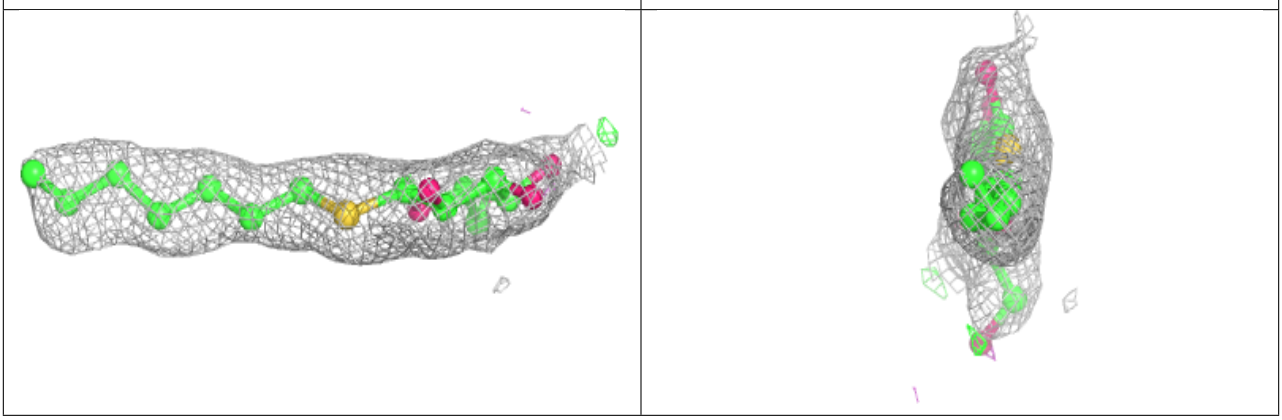




Electron density around HTG B 633:

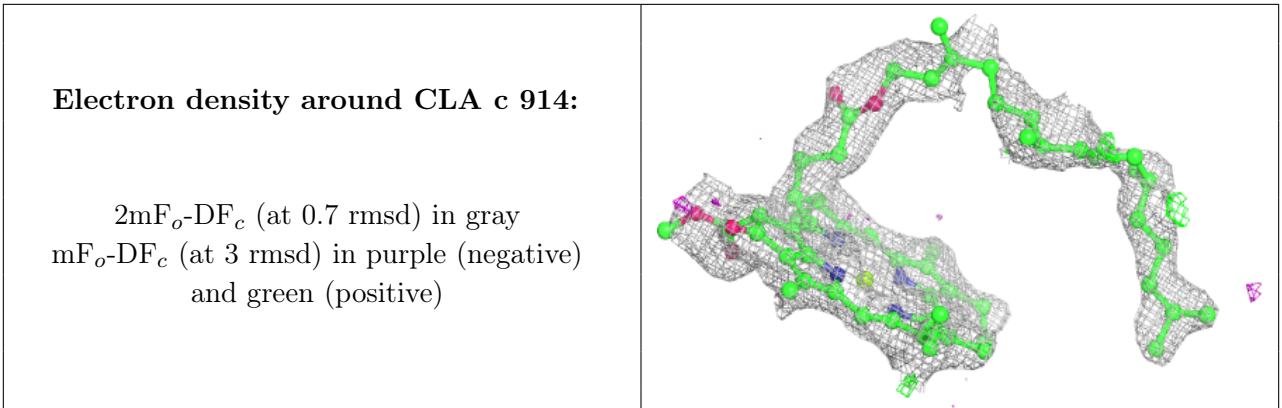
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

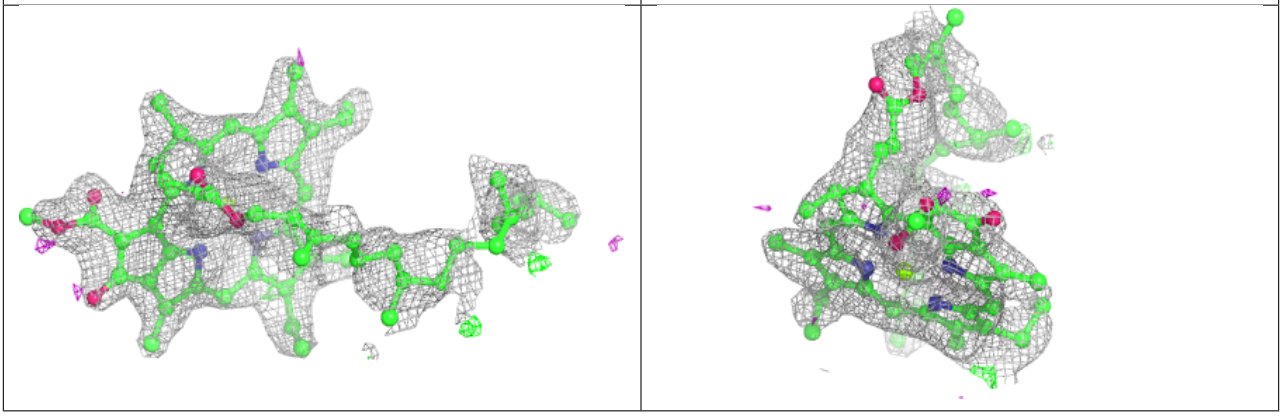




Electron density around CLA c 914:

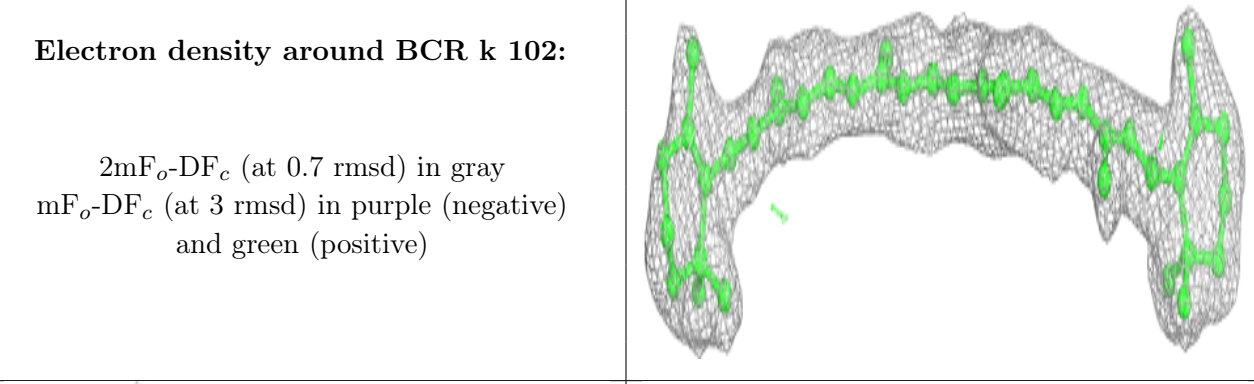
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

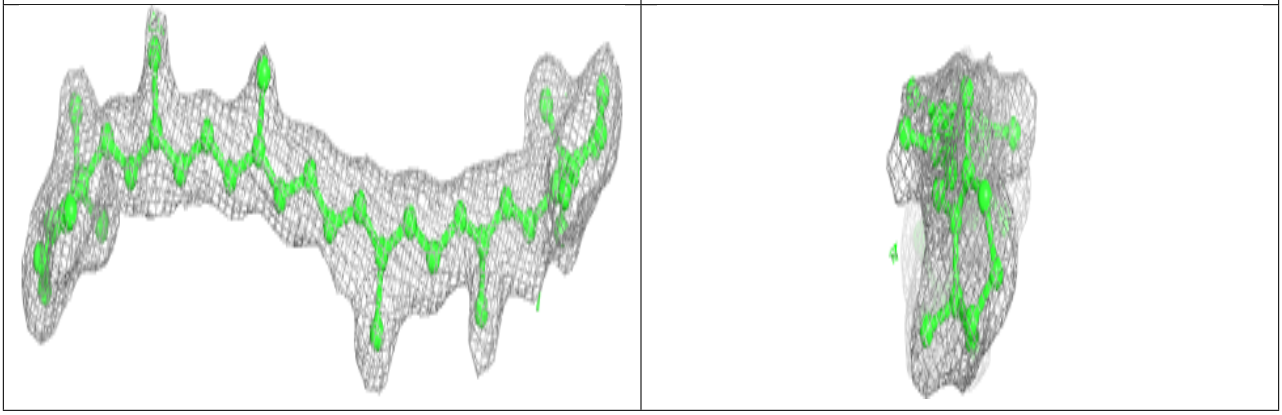




Electron density around BCR k 102:

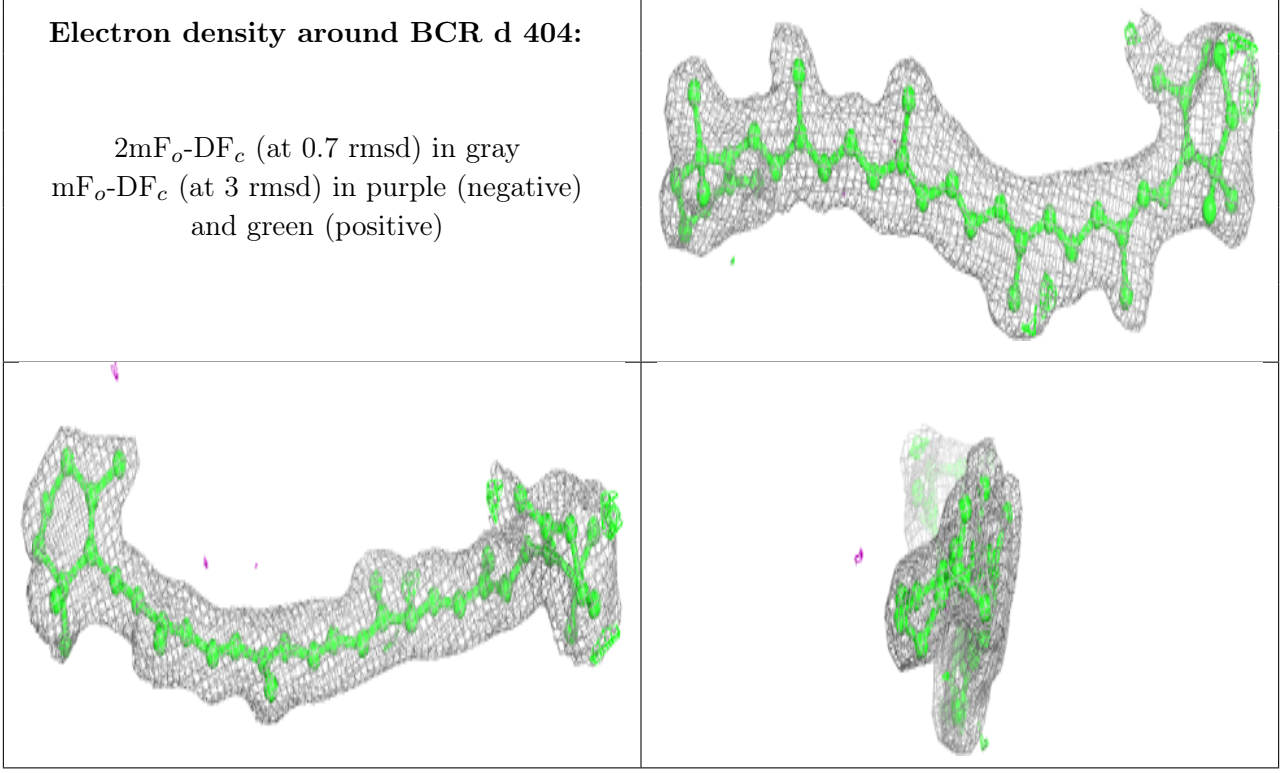
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





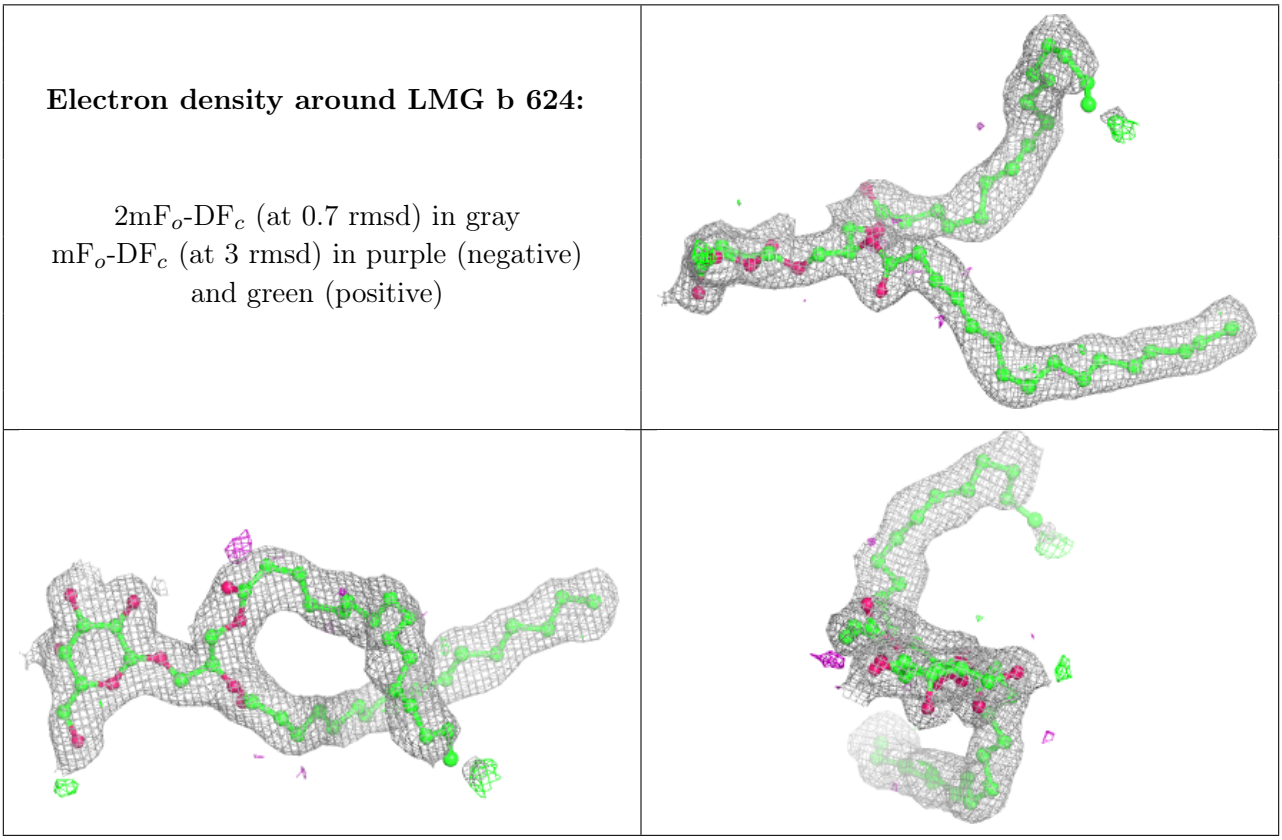
Electron density around BCR d 404:

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



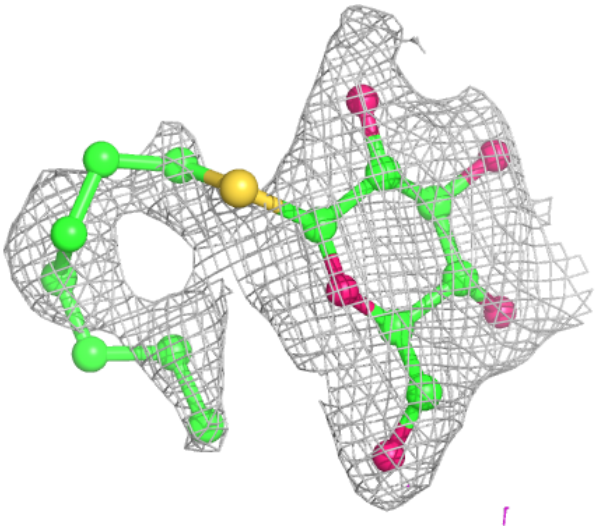
Electron density around LMG b 624:

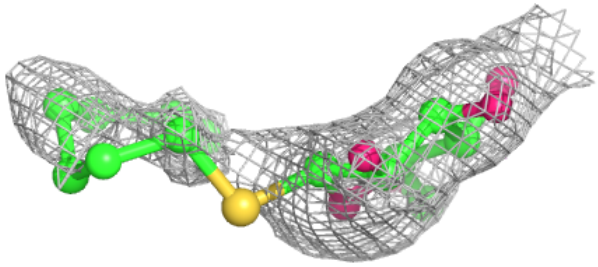
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

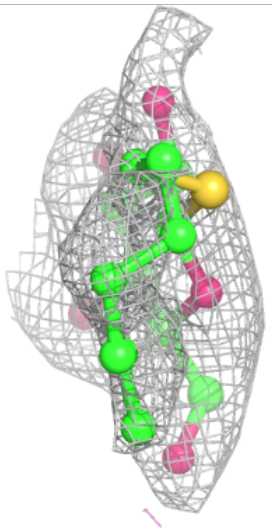


Electron density around HTG V 202:

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

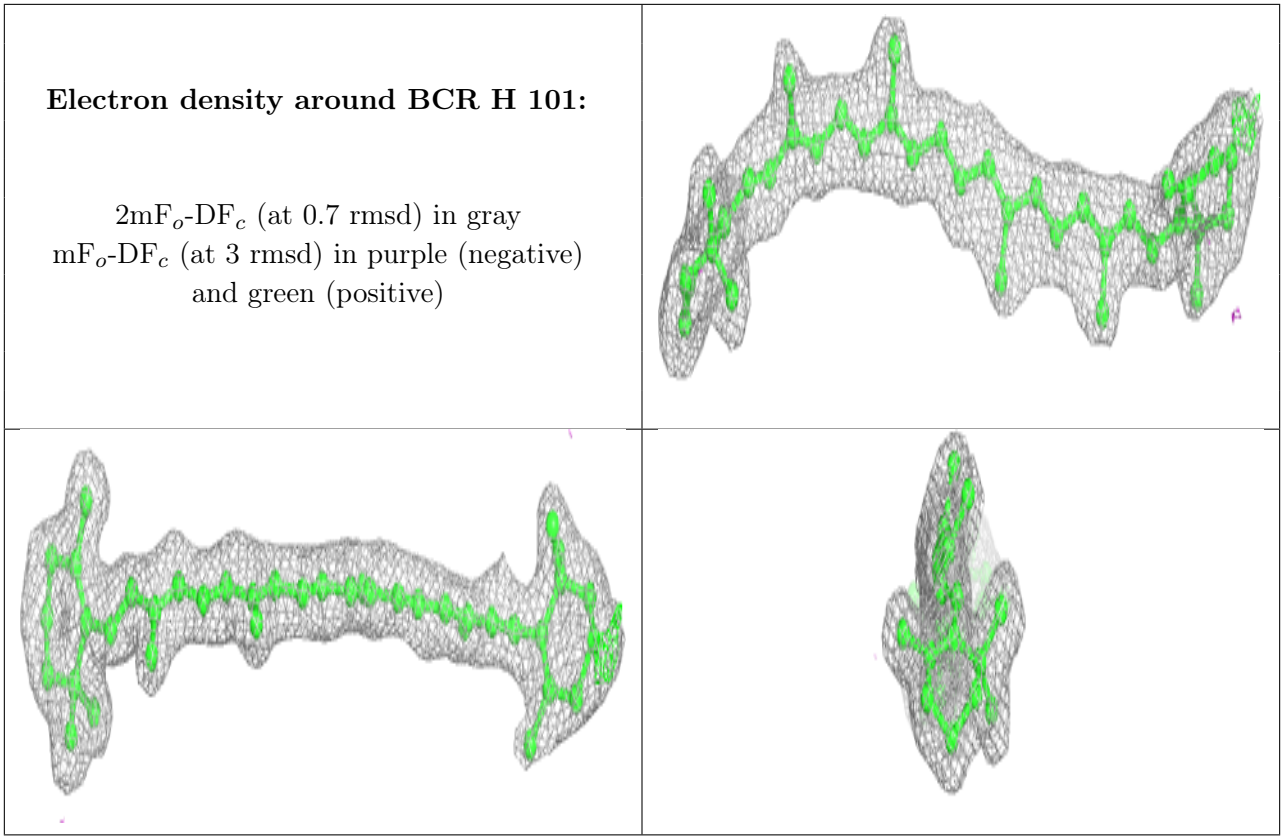






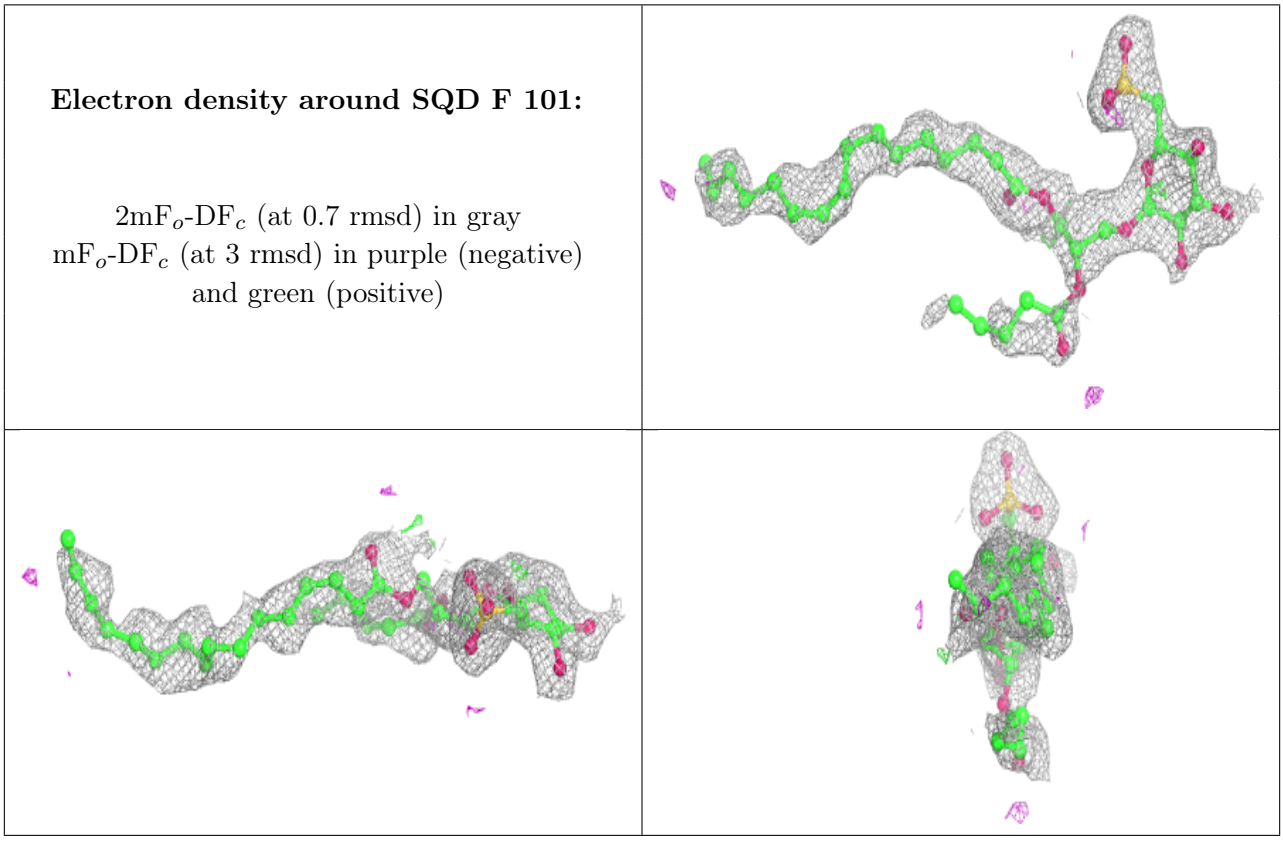
Electron density around BCR H 101:

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



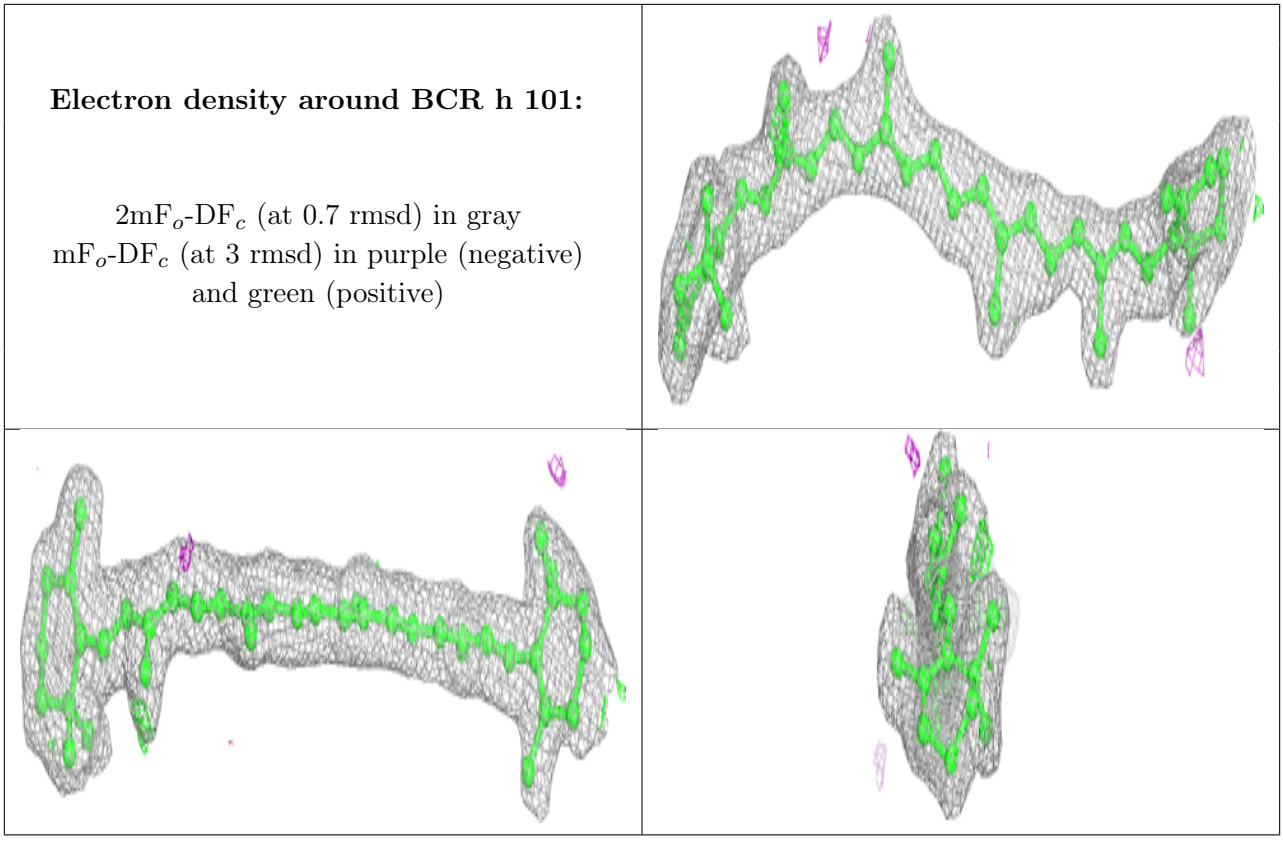
Electron density around SQD F 101:

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



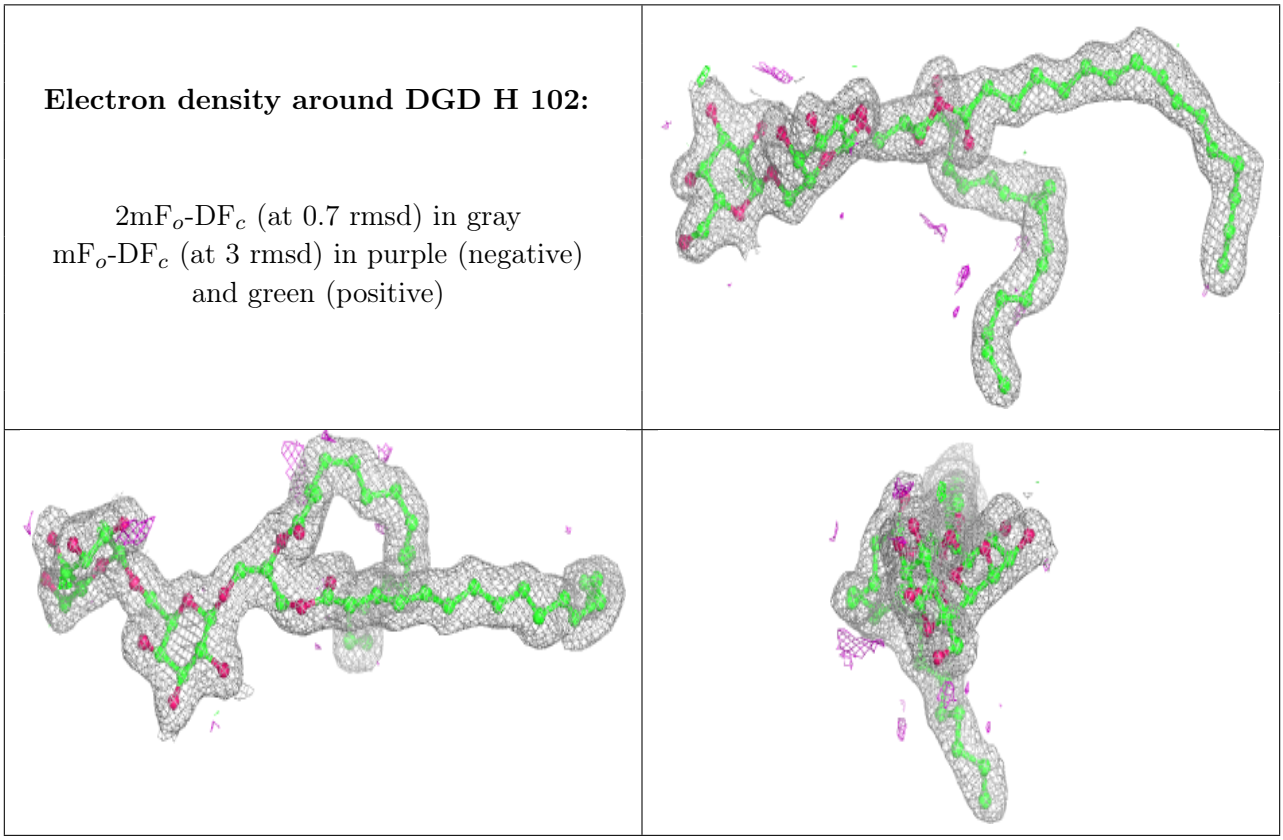
Electron density around BCR h 101:

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



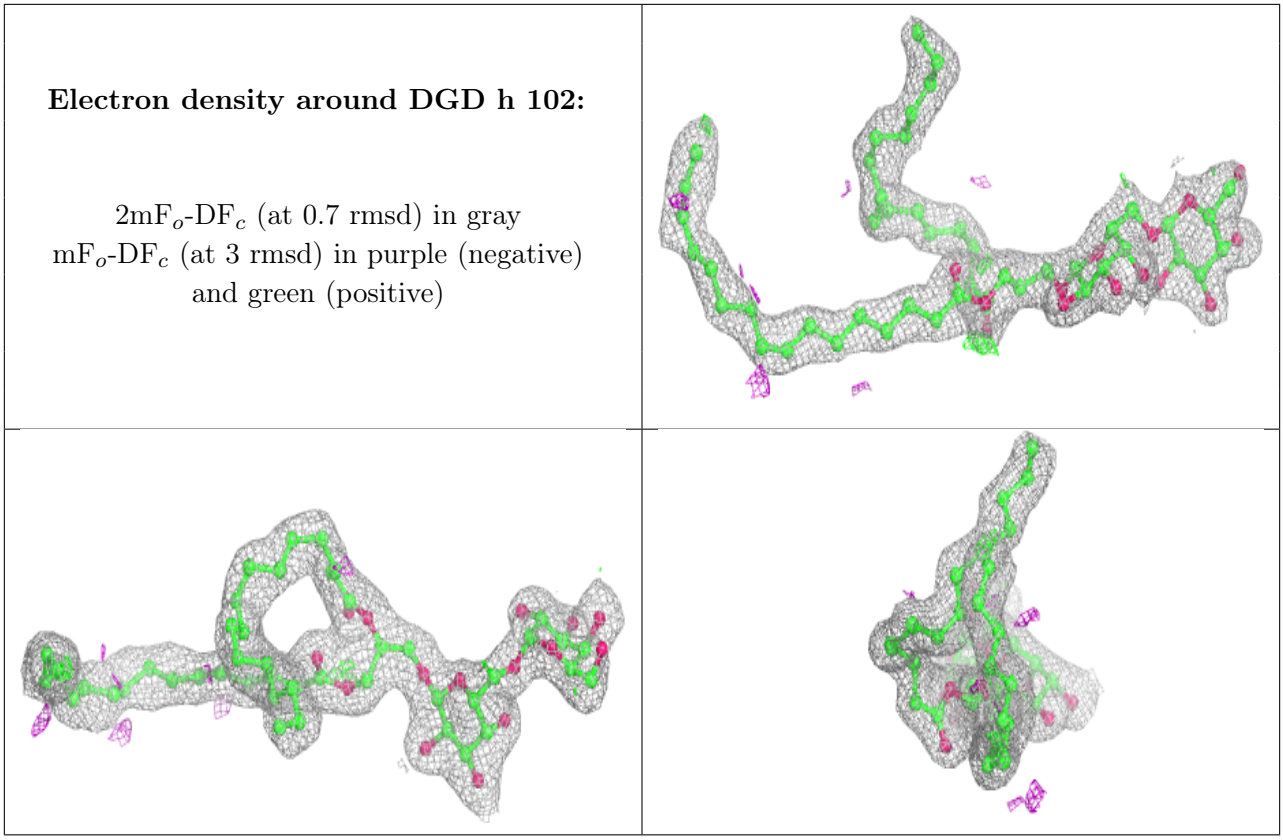
Electron density around DGD H 102:

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



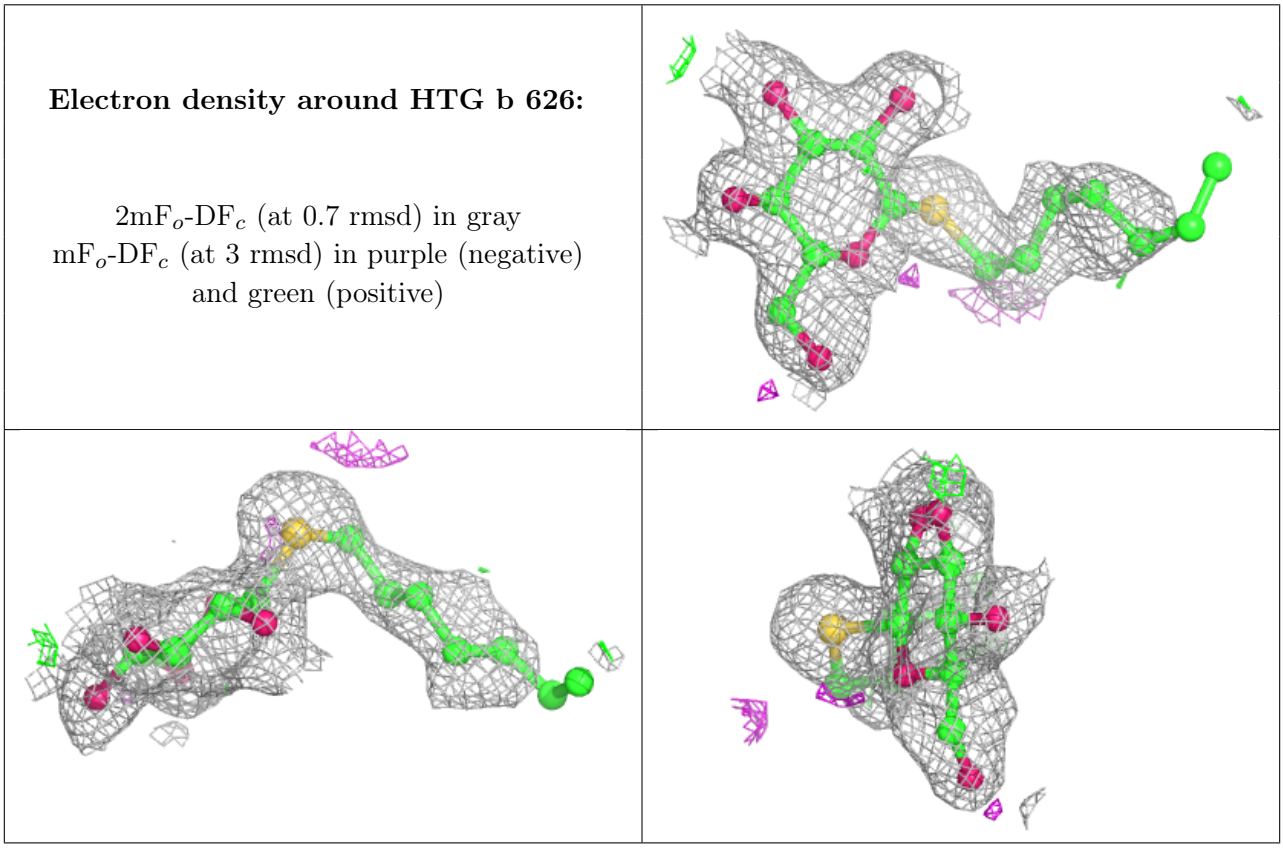
Electron density around DGD h 102:

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



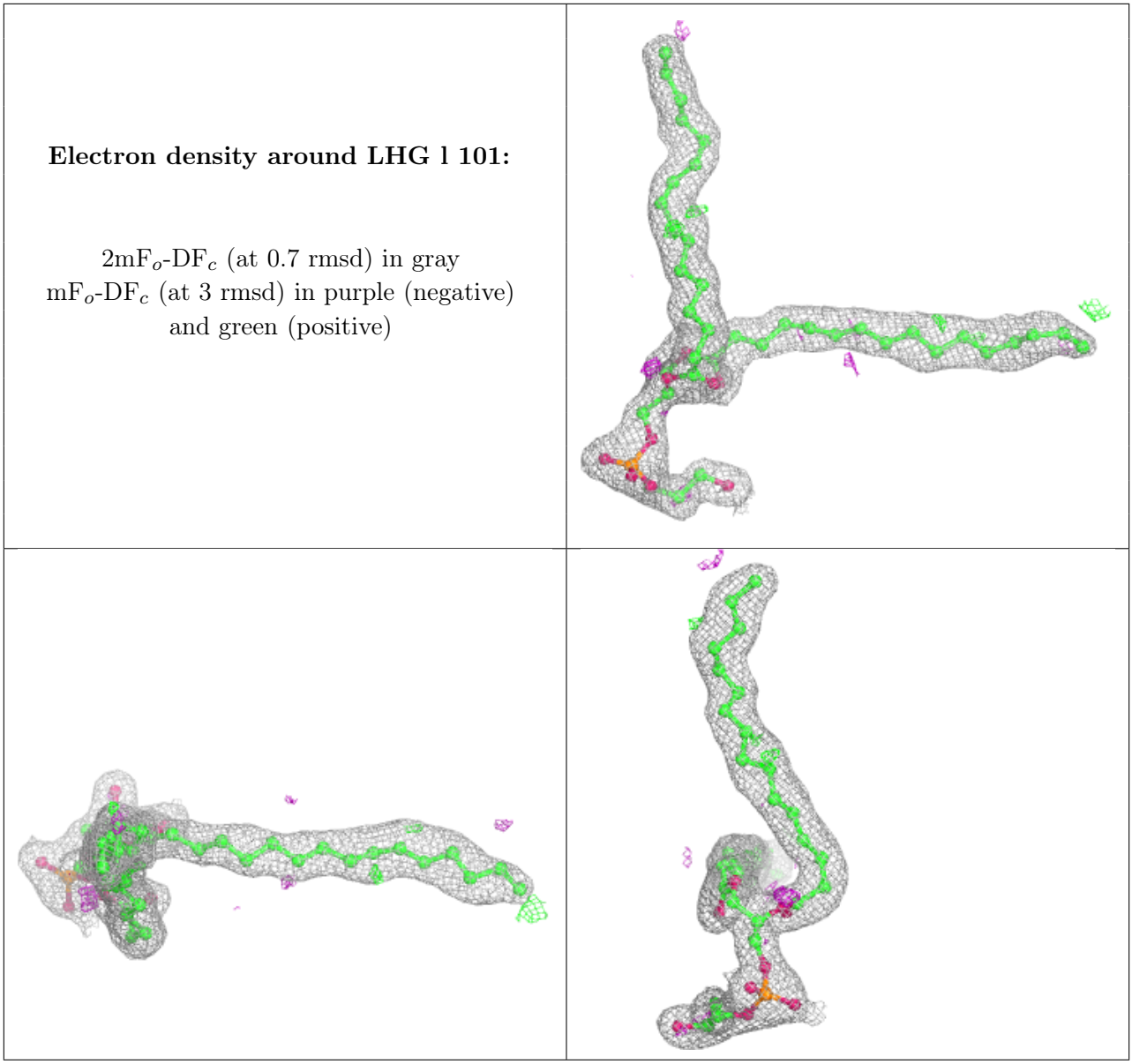
Electron density around HTG b 626:

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



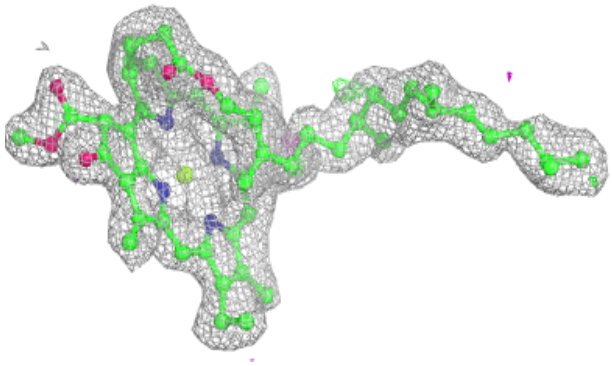
Electron density around LHG l 101:

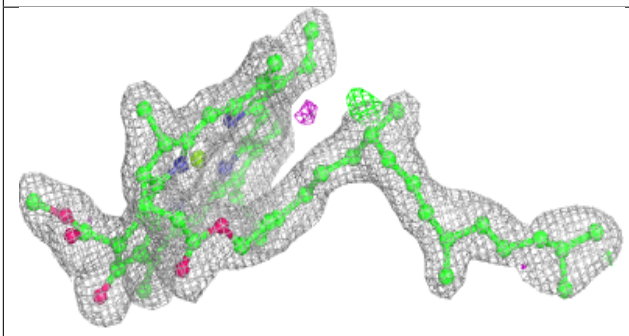
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

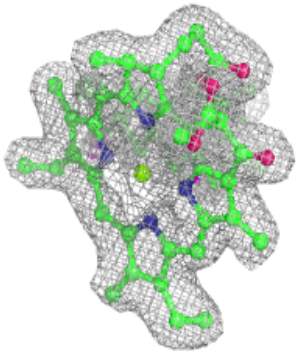


Electron density around CLA c 906:

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

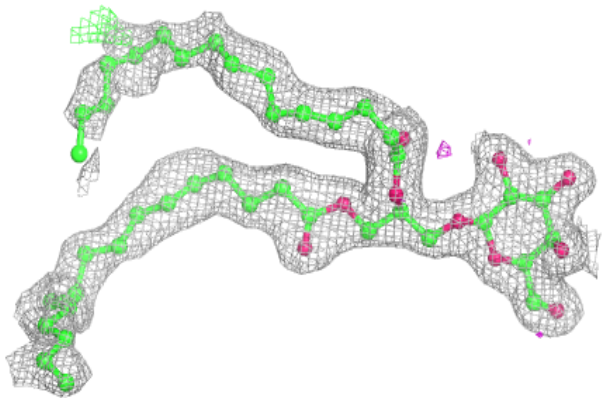


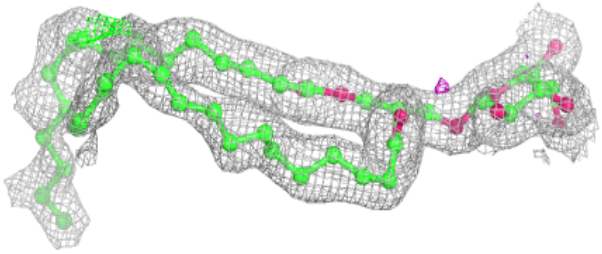


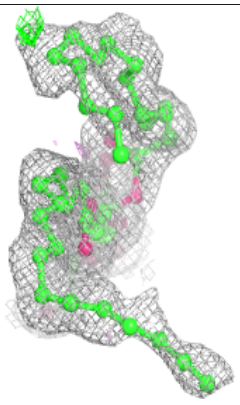


Electron density around LMG J 101:

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

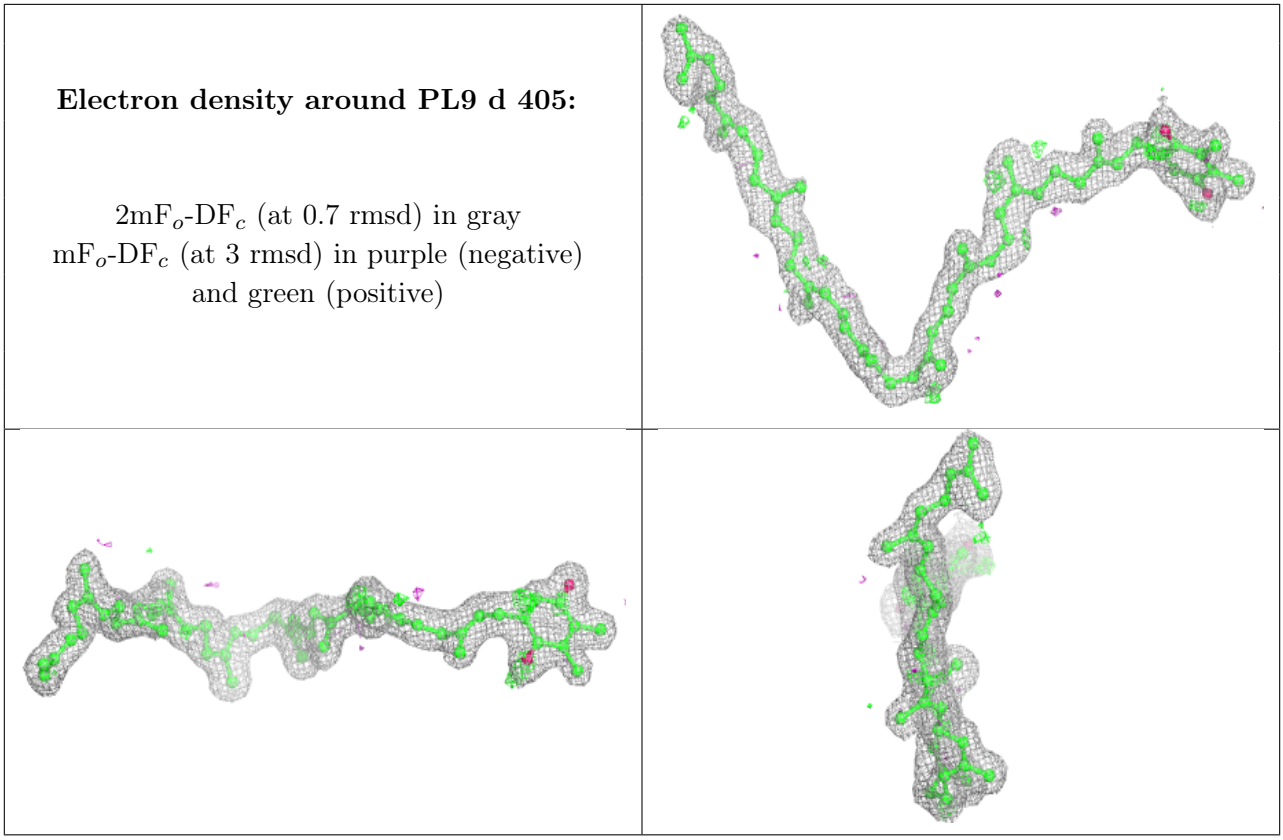






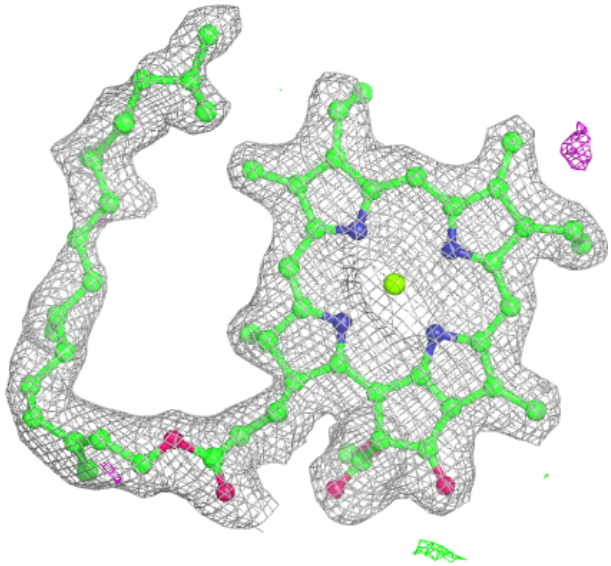
Electron density around PL9 d 405:

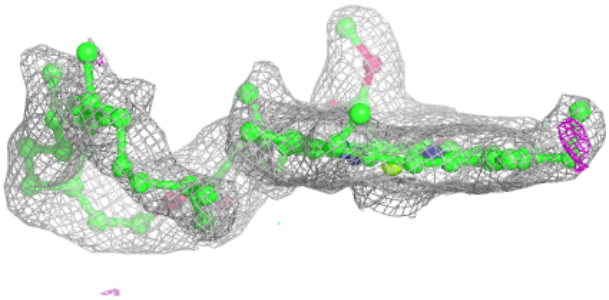
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

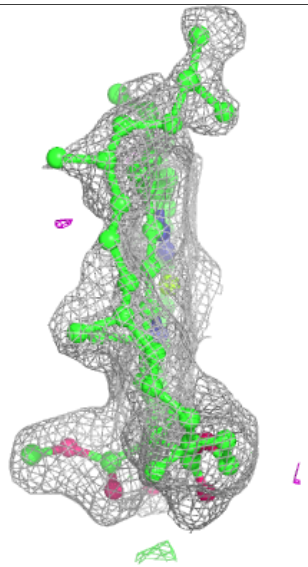


Electron density around CLA c 913:

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

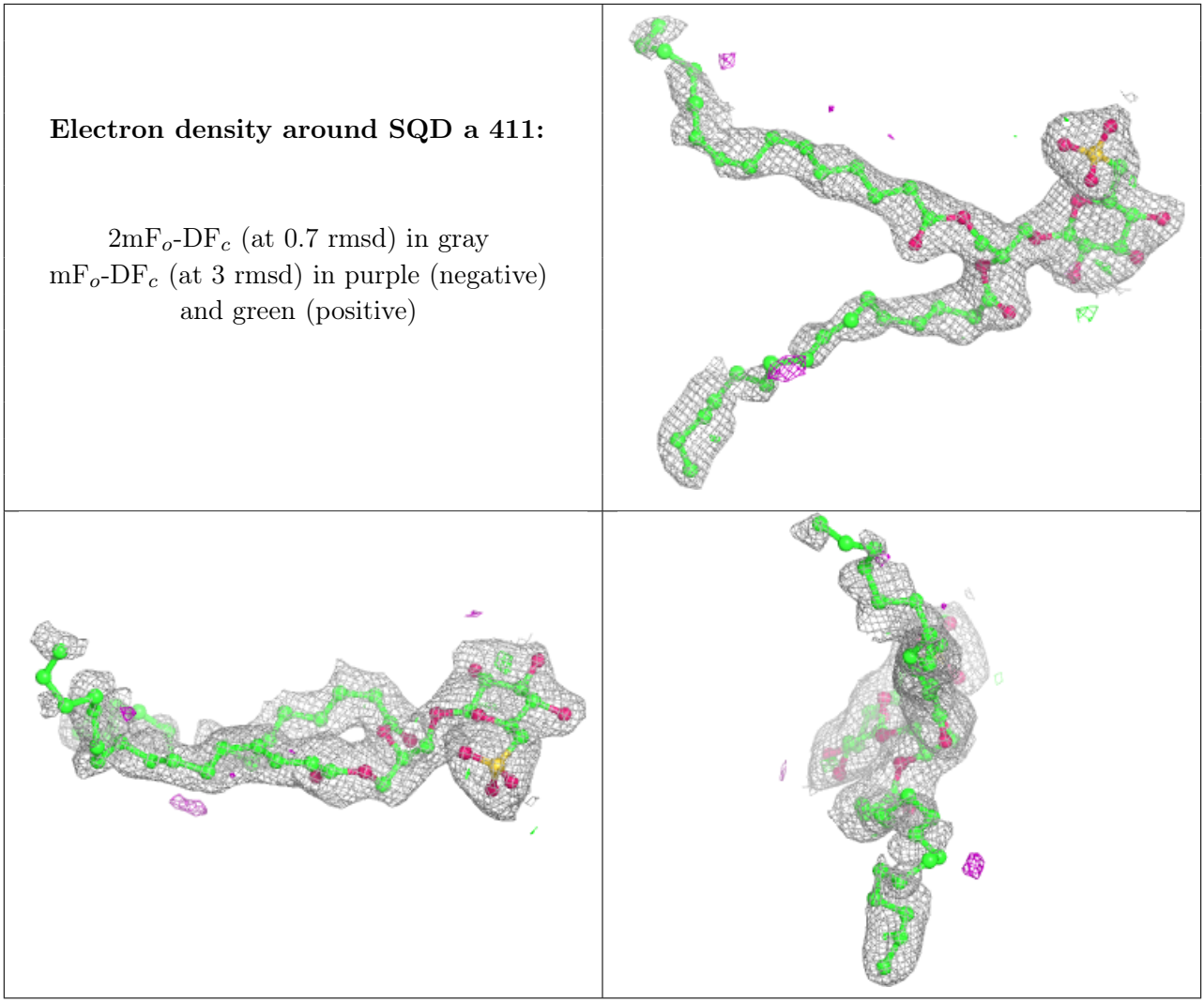






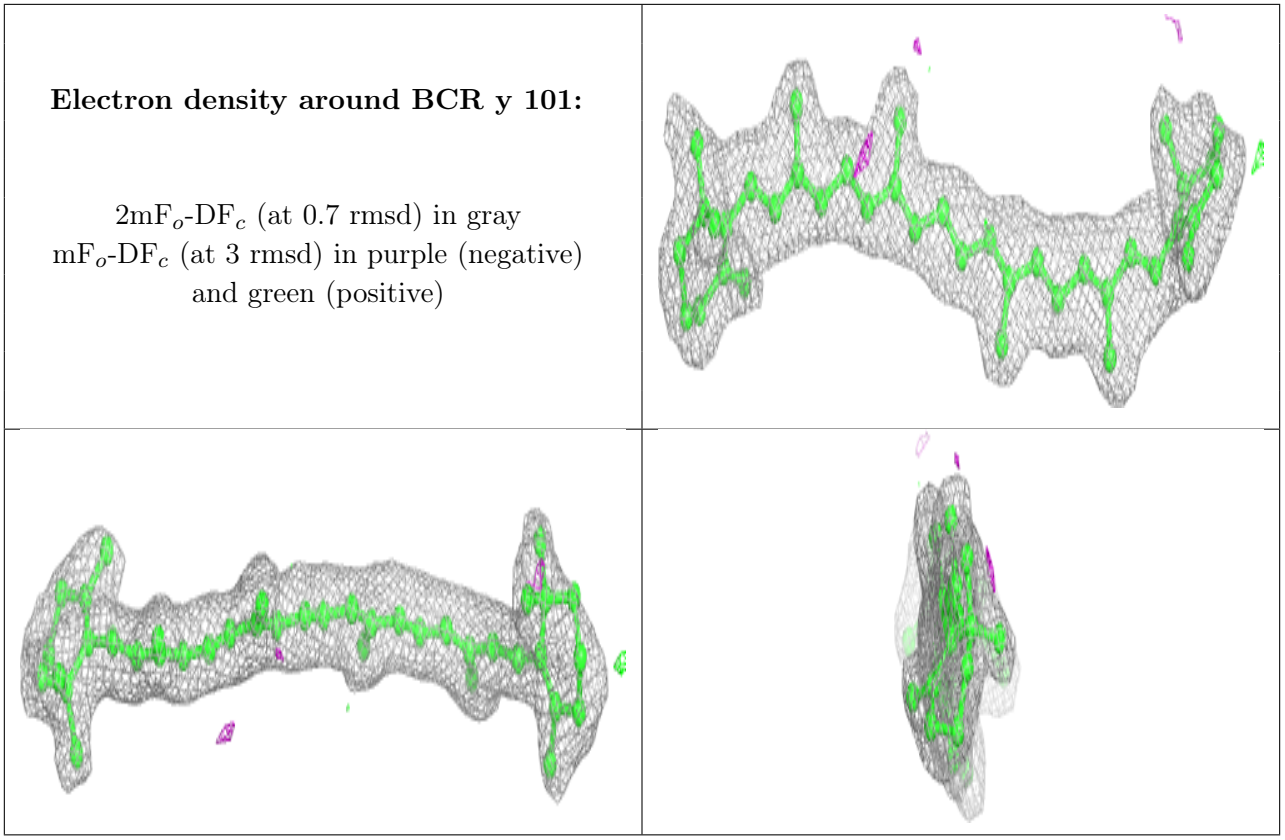
Electron density around SQD a 411:

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



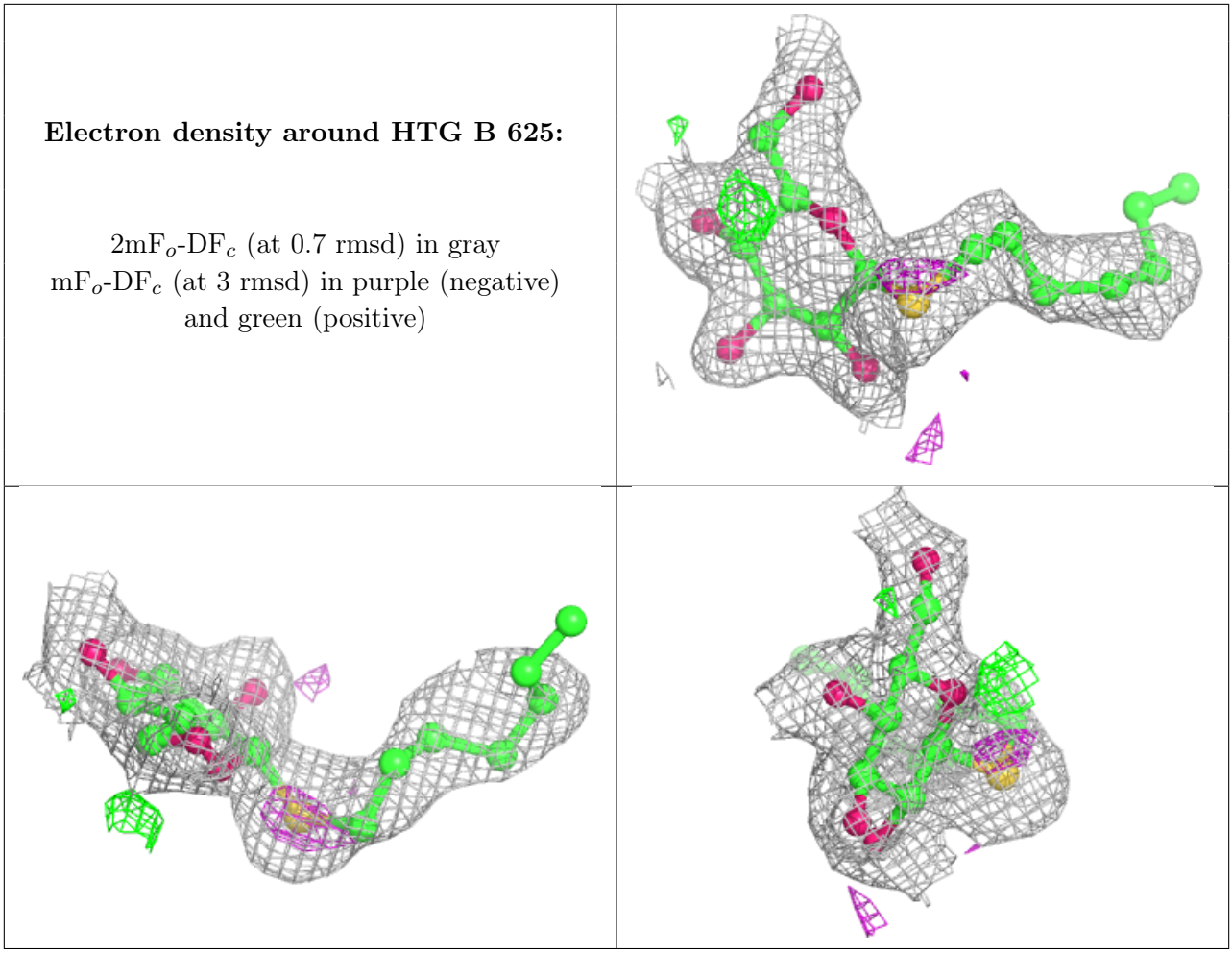
Electron density around BCR y 101:

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



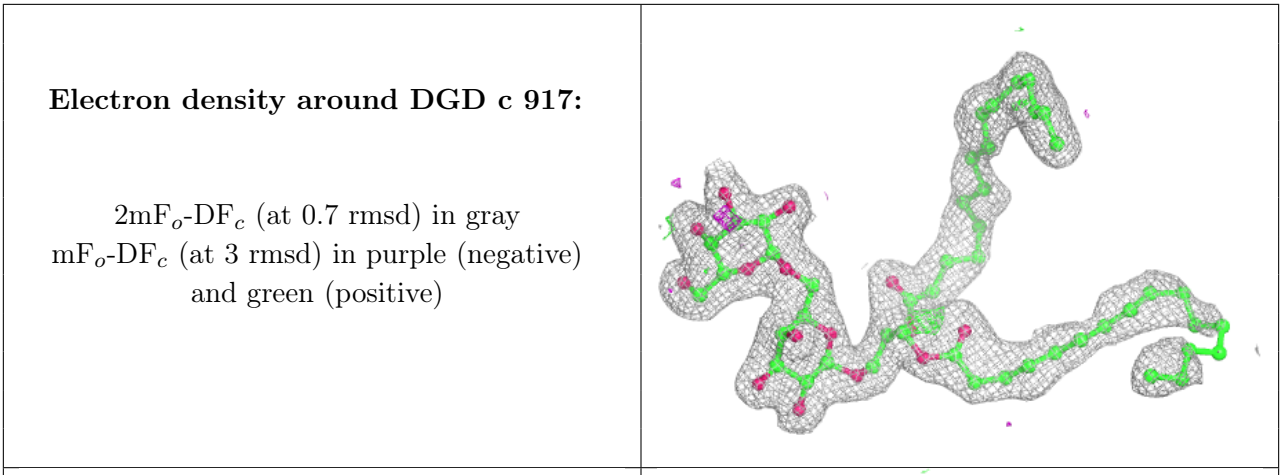
Electron density around HTG B 625:

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



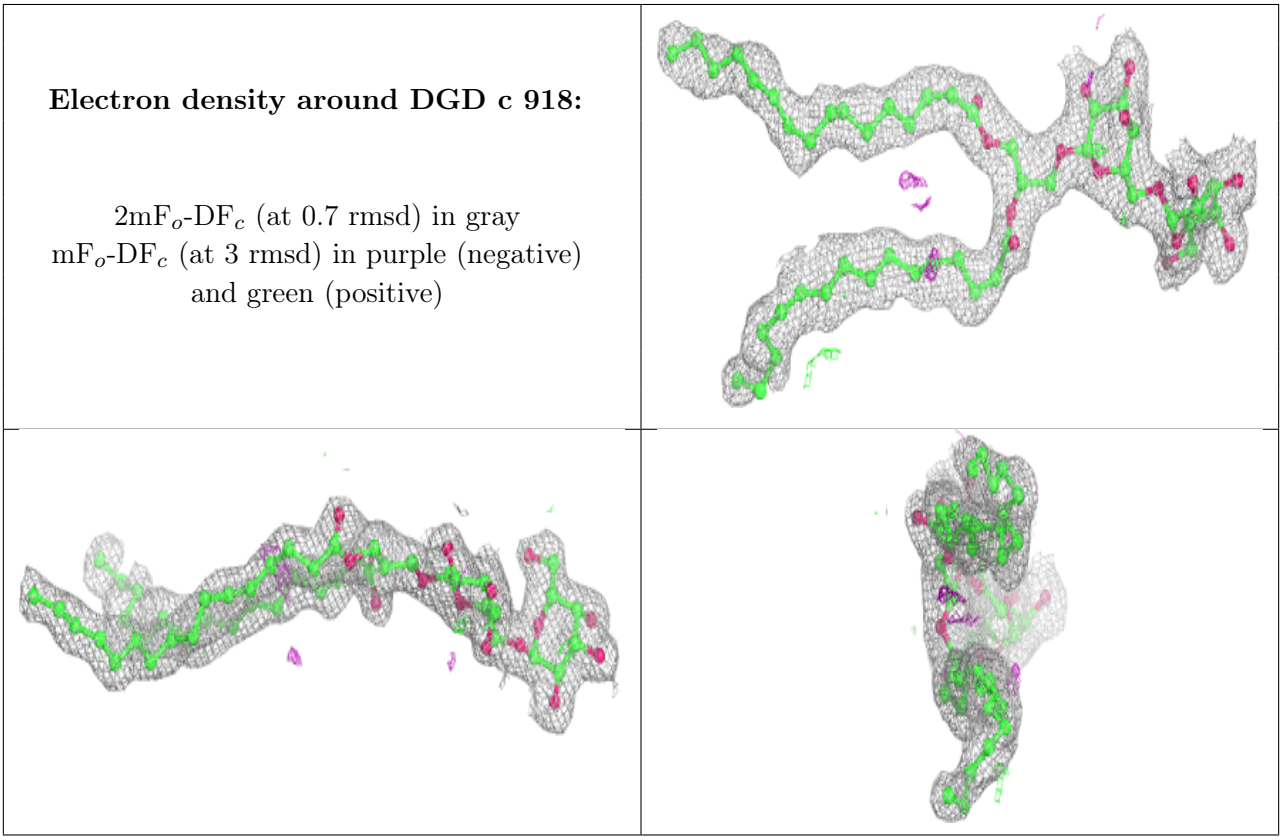
Electron density around DGD c 917:

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



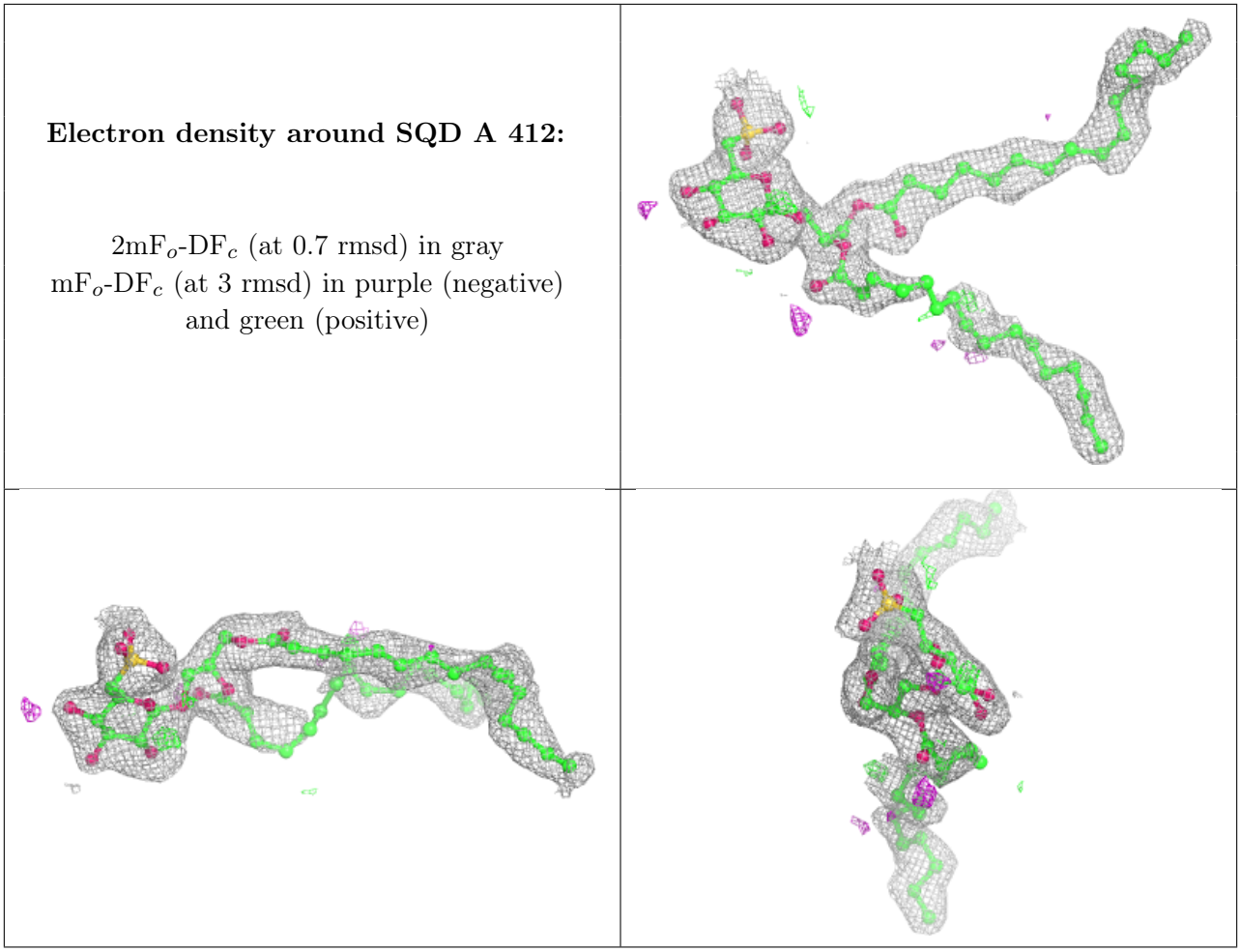
Electron density around DGD c 918:

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



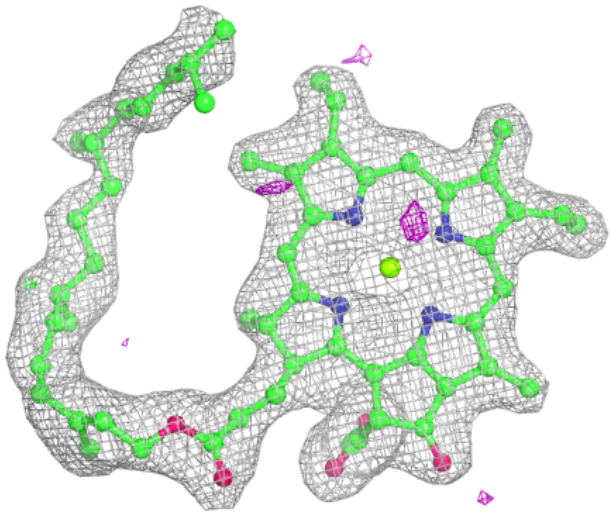
Electron density around SQD A 412:

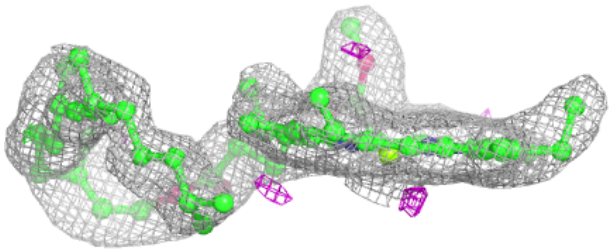
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

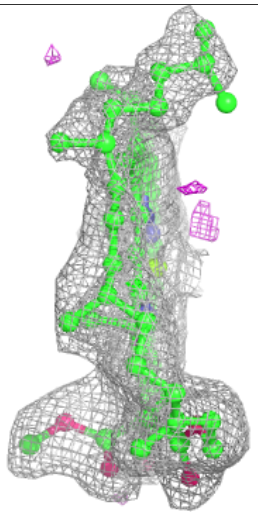


Electron density around CLA C 513:

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

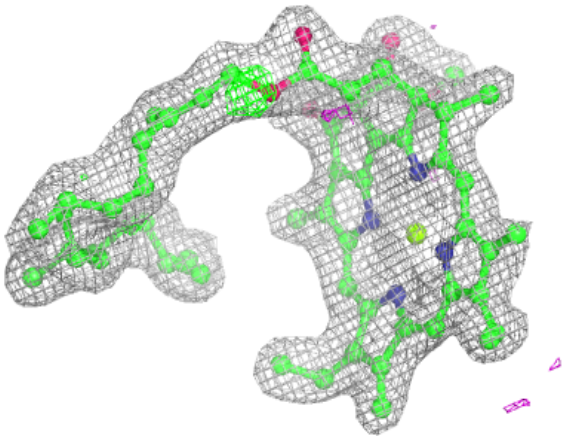


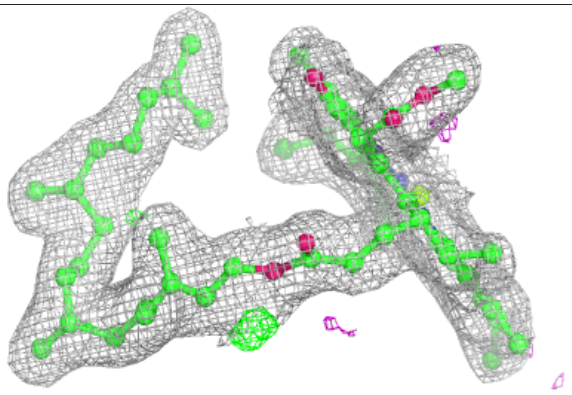


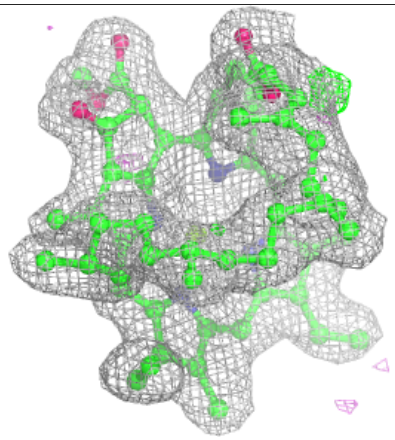


Electron density around CLA c 904:

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

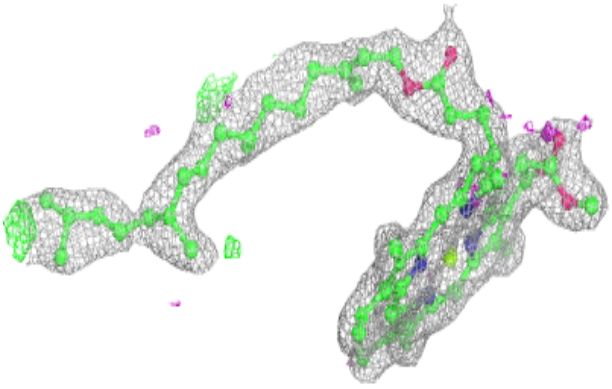


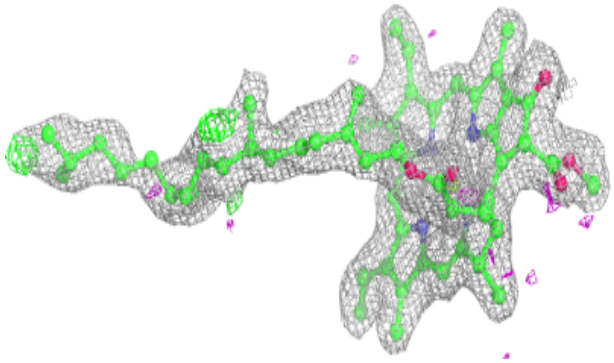


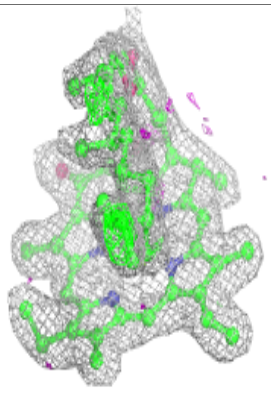


Electron density around CLA c 905:

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

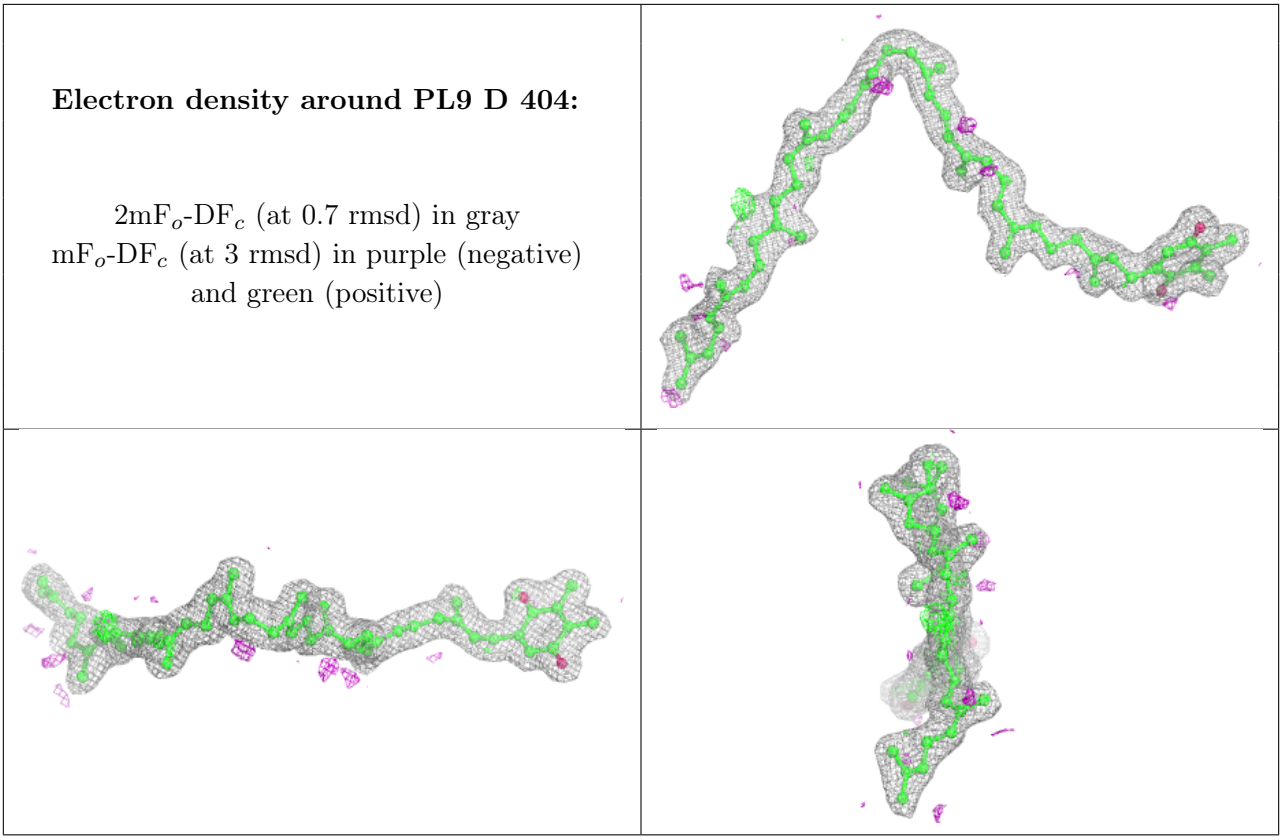






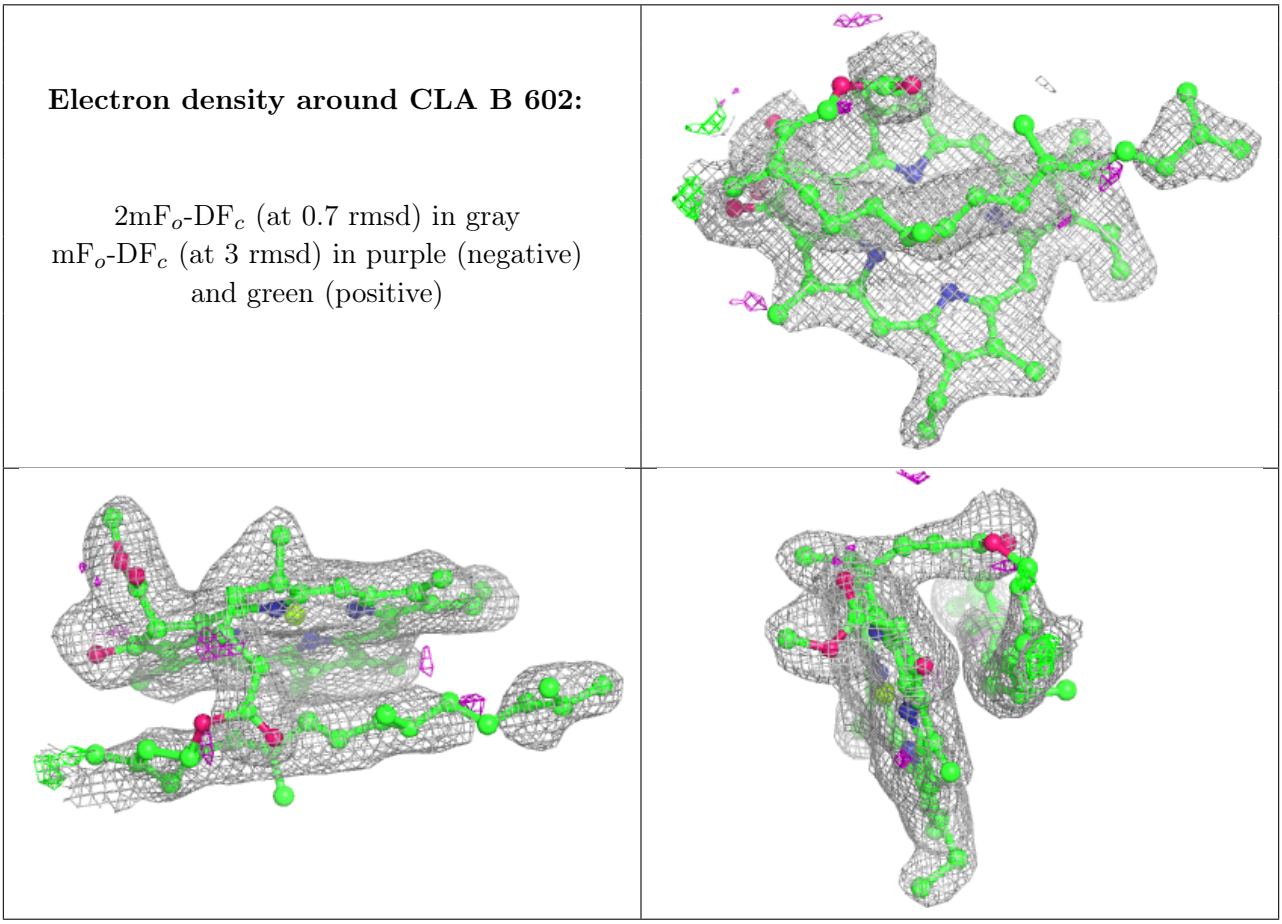
Electron density around PL9 D 404:

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



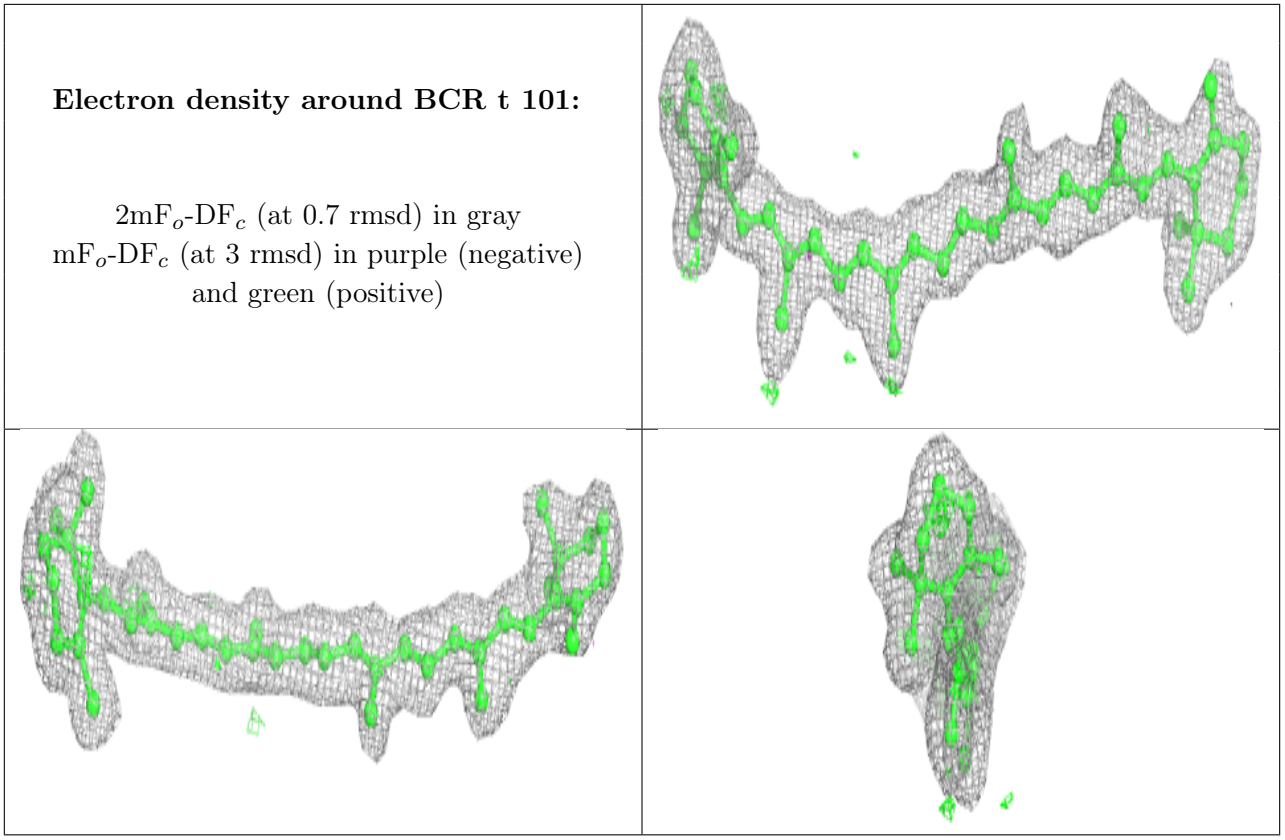
Electron density around CLA B 602:

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



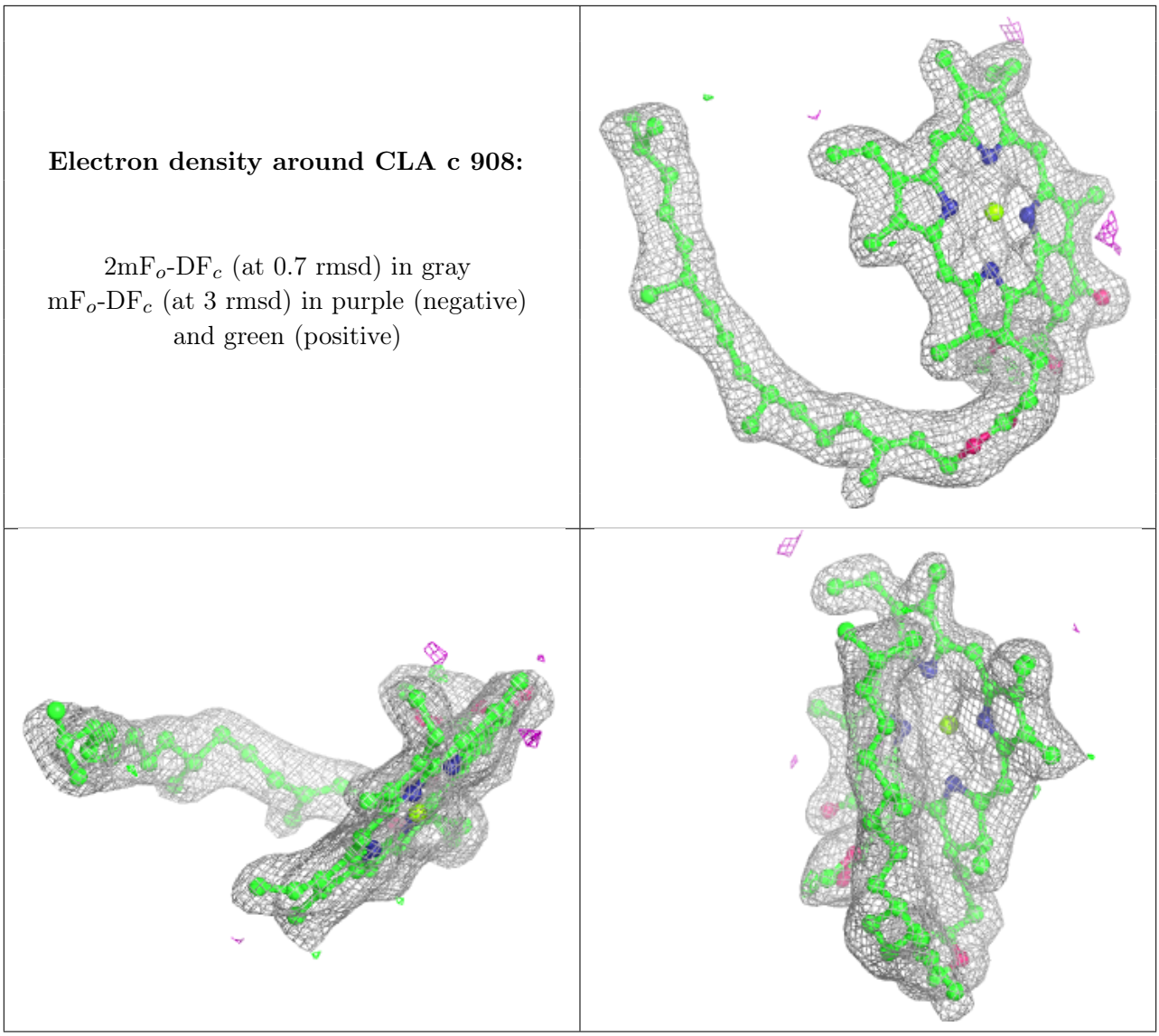
Electron density around BCR t 101:

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



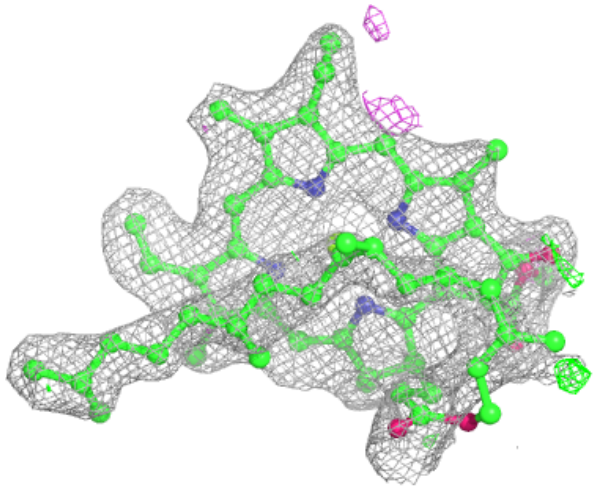
Electron density around CLA c 908:

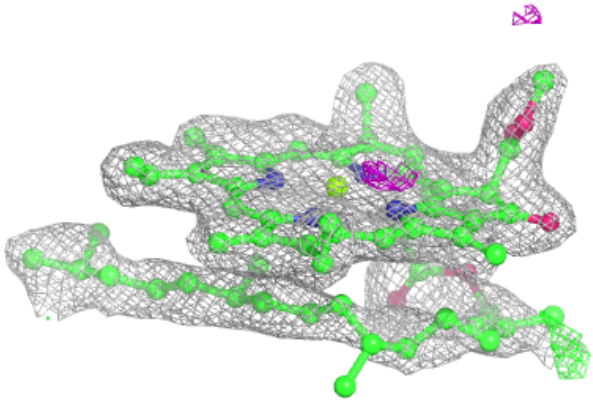
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

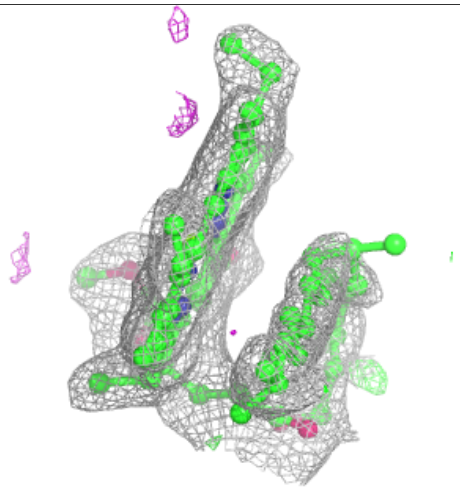


Electron density around CLA b 605:

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

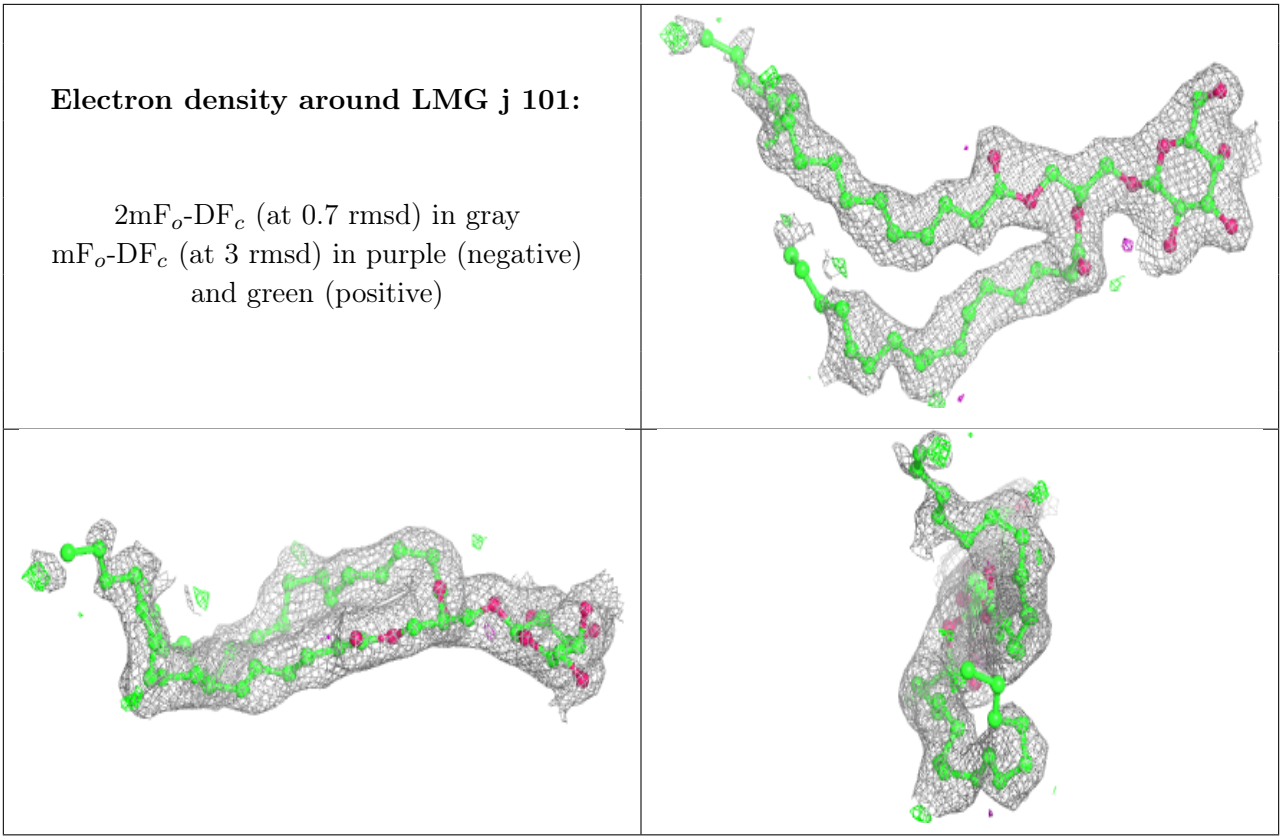






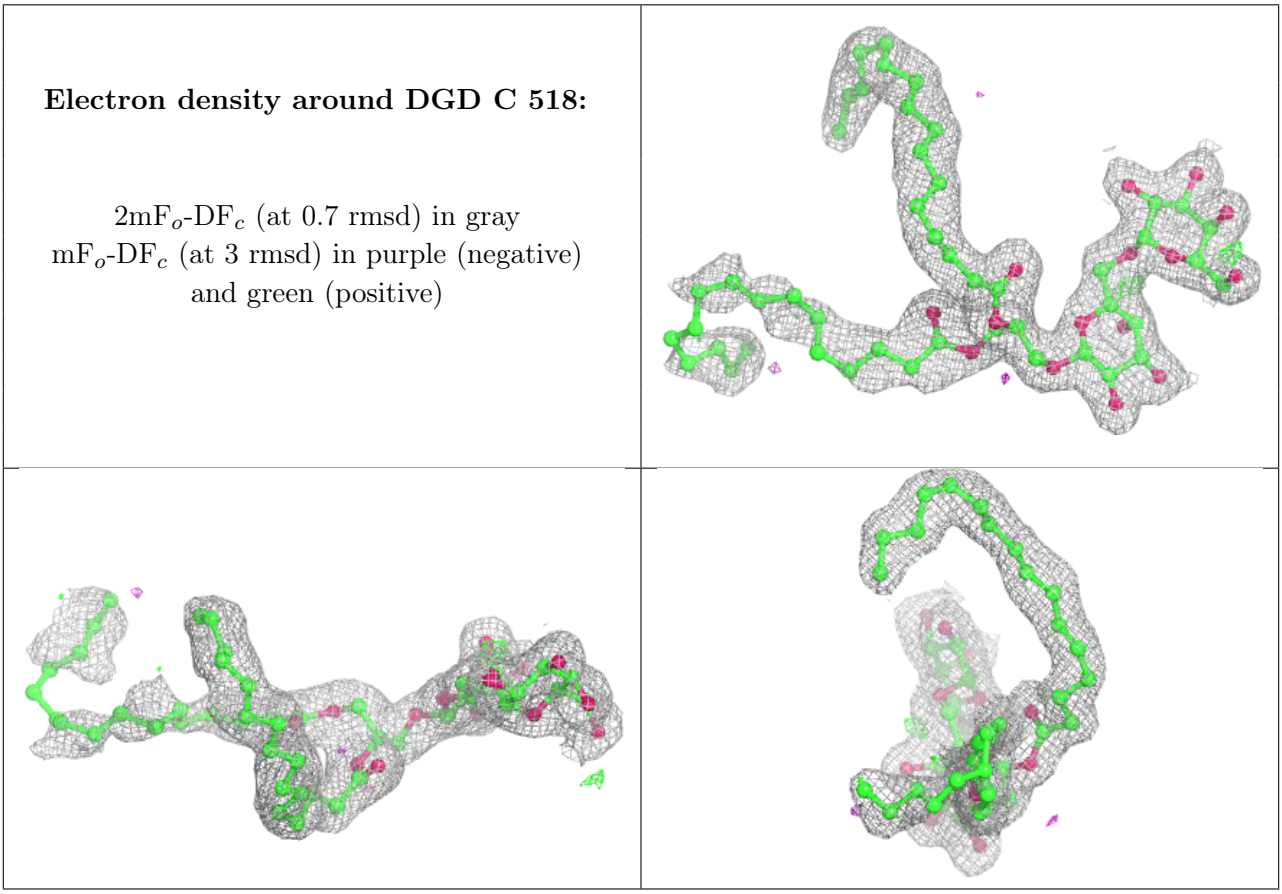
Electron density around LMG j 101:

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



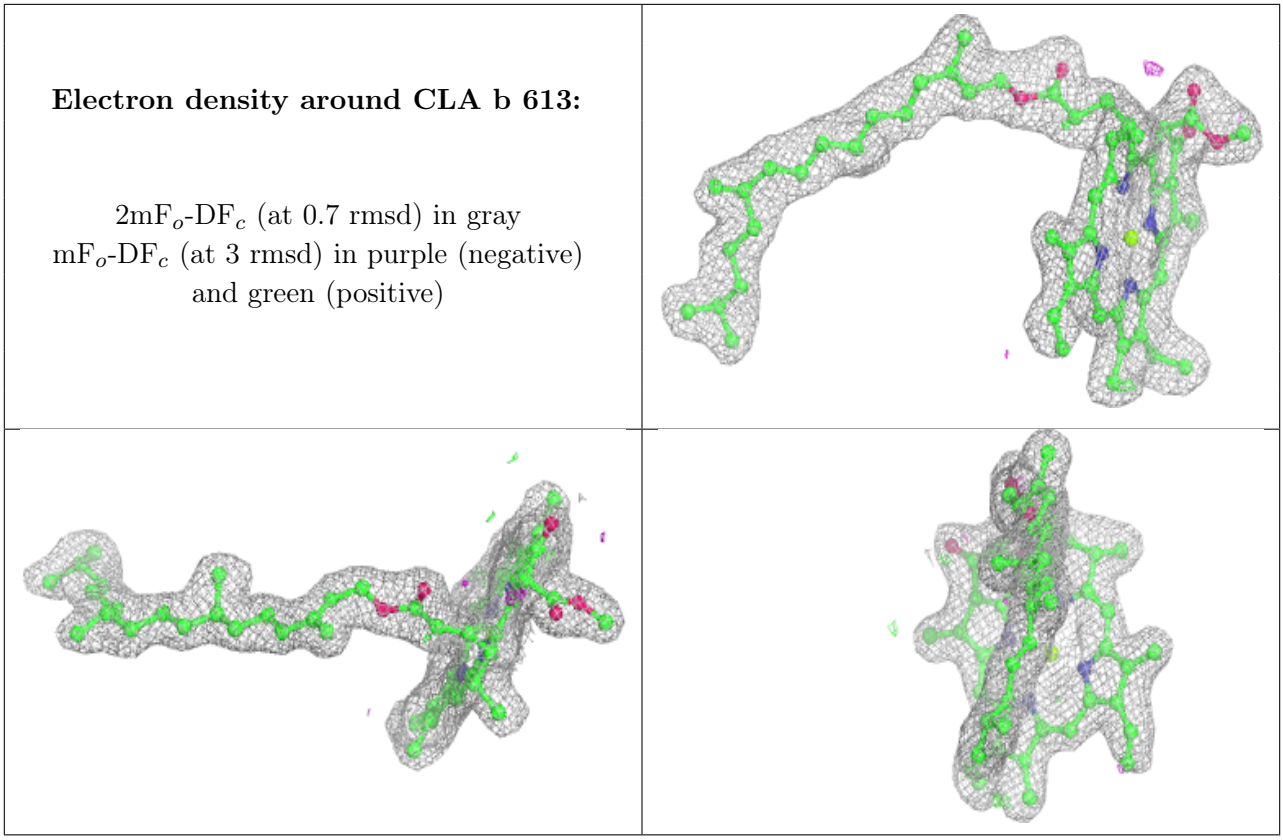
Electron density around DGD C 518:

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



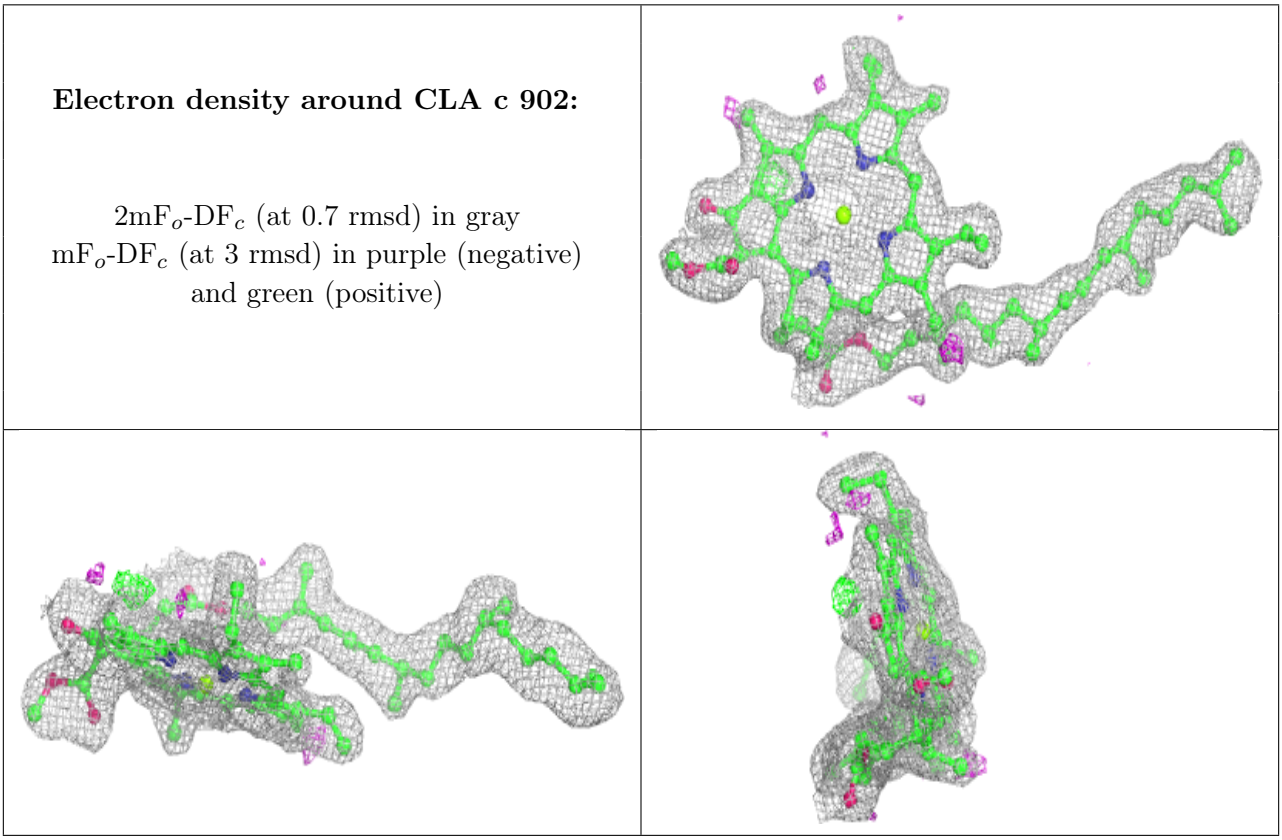
Electron density around CLA b 613:

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



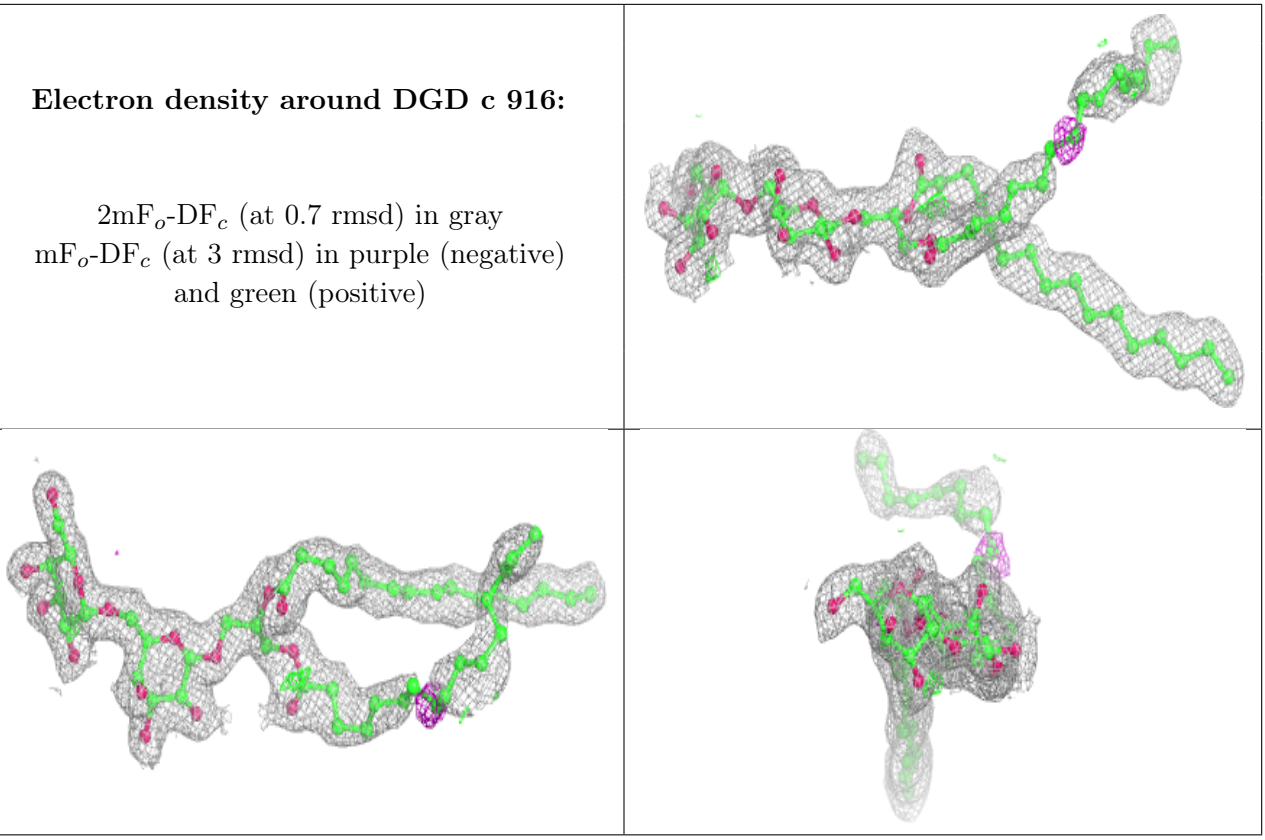
Electron density around CLA c 902:

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



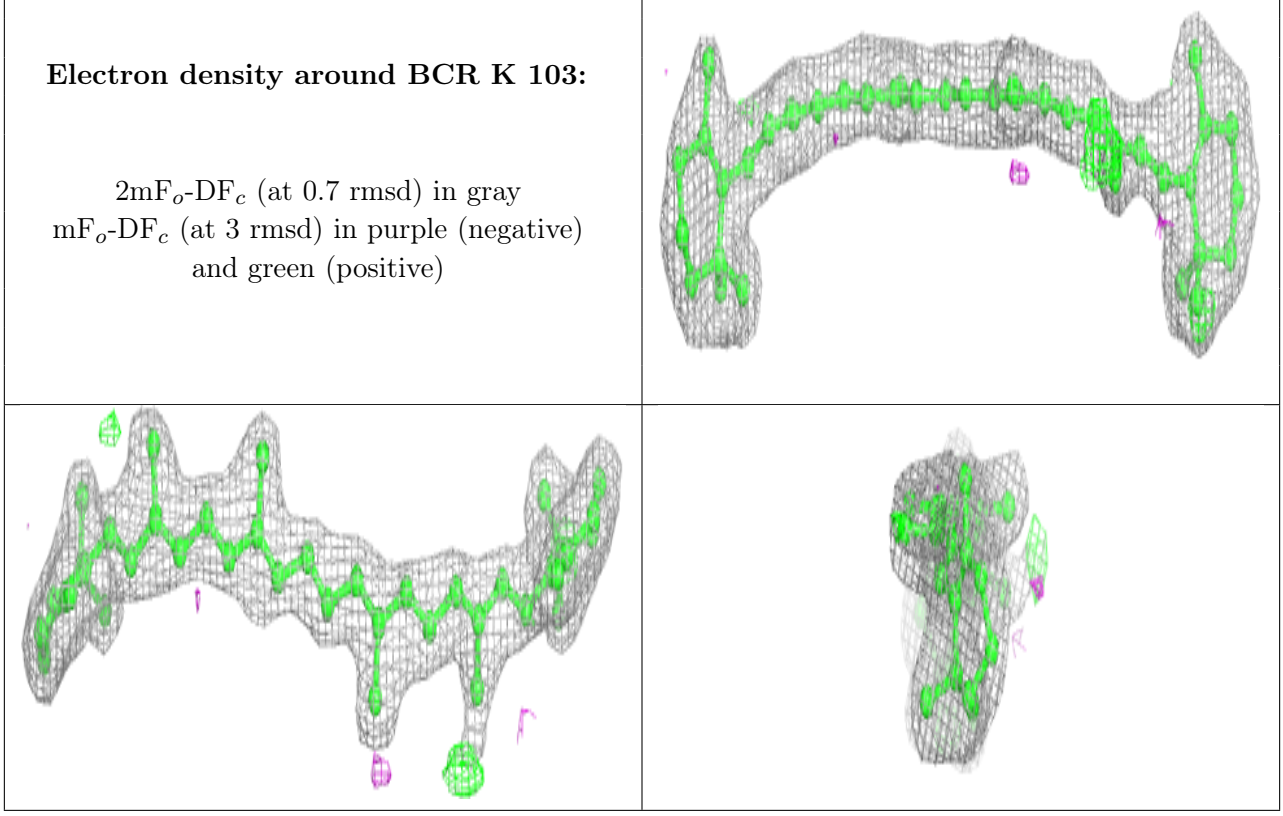
Electron density around DGD c 916:

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



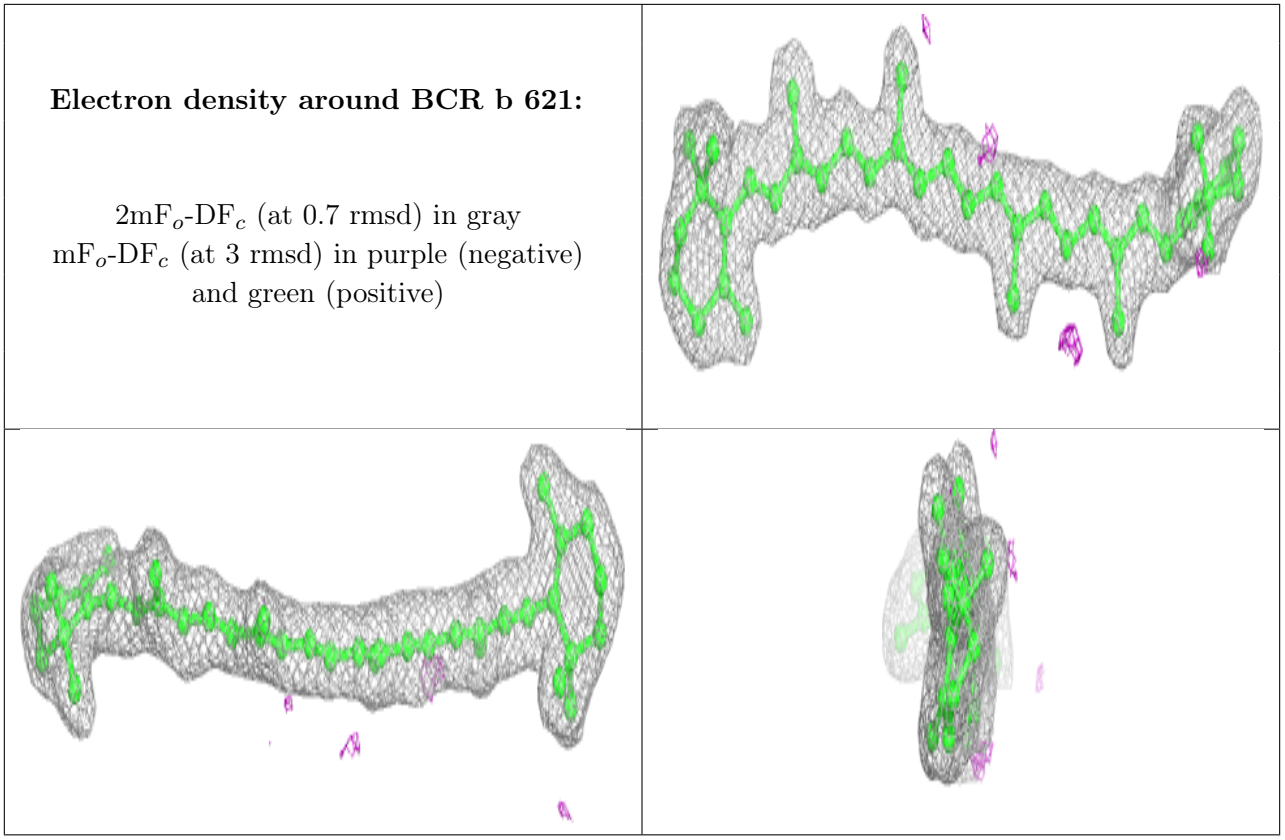
Electron density around BCR K 103:

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



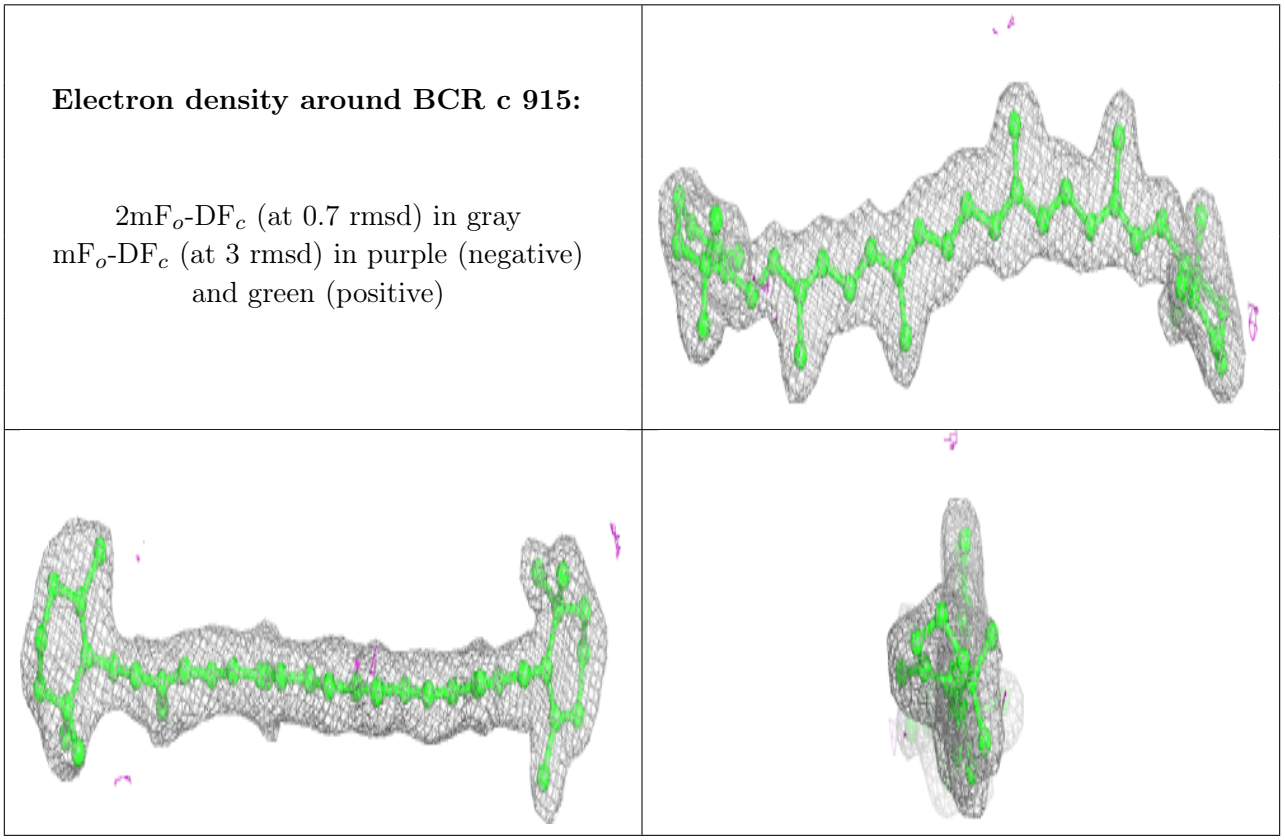
Electron density around BCR b 621:

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



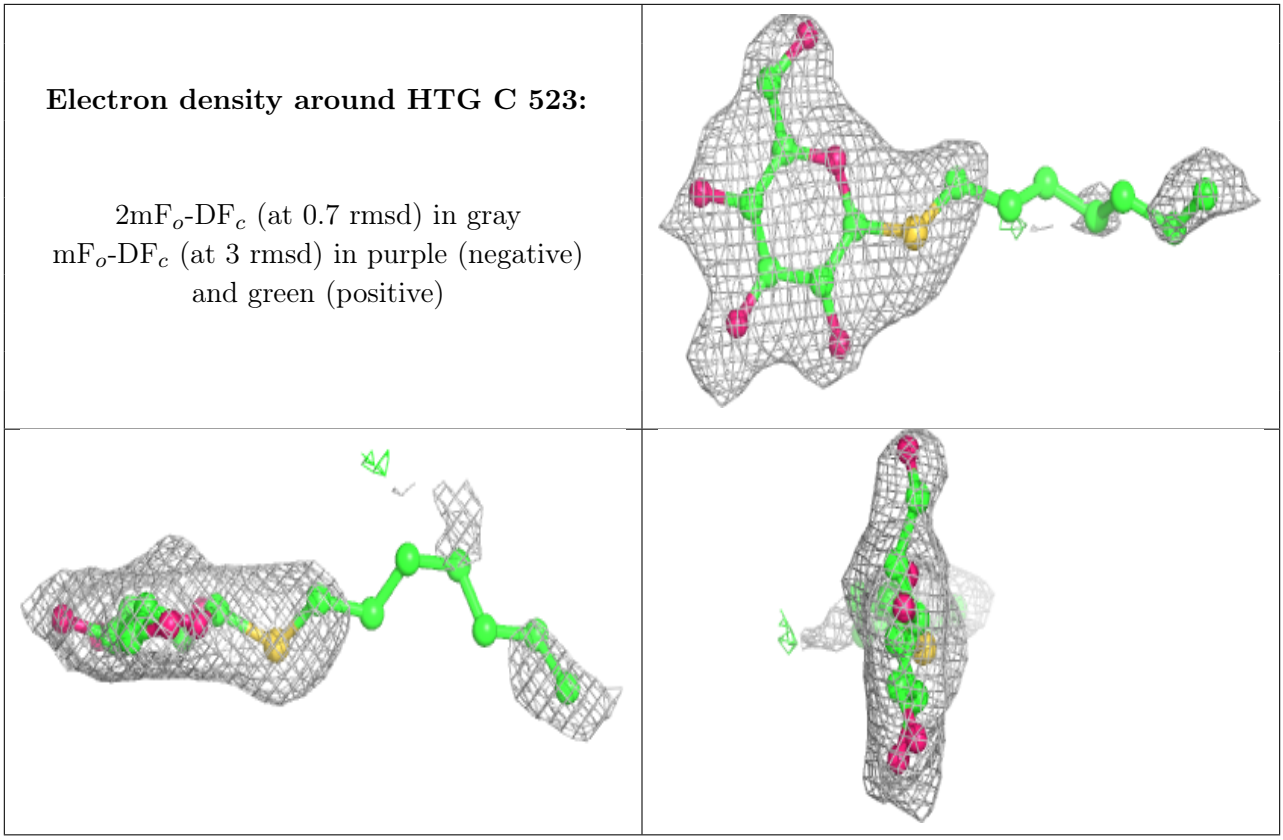
Electron density around BCR c 915:

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



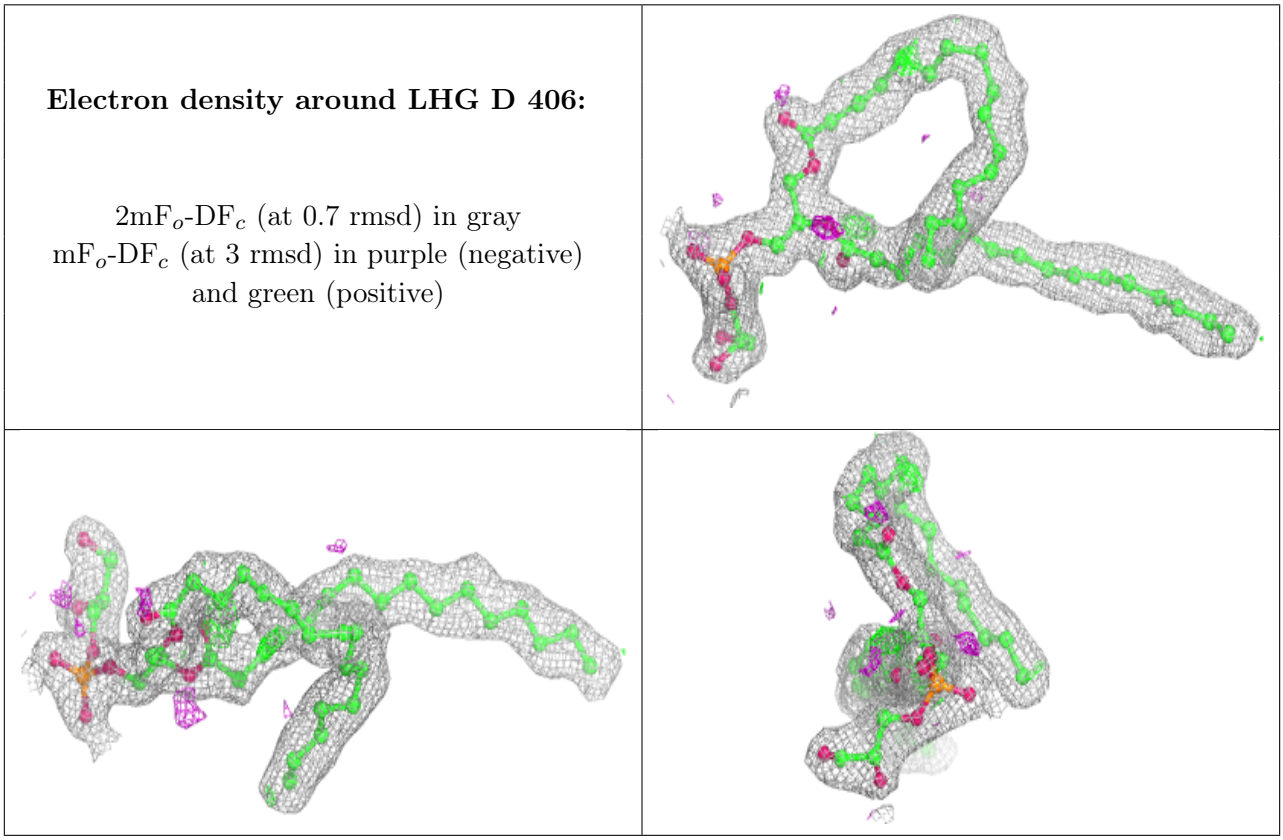
Electron density around HTG C 523:

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



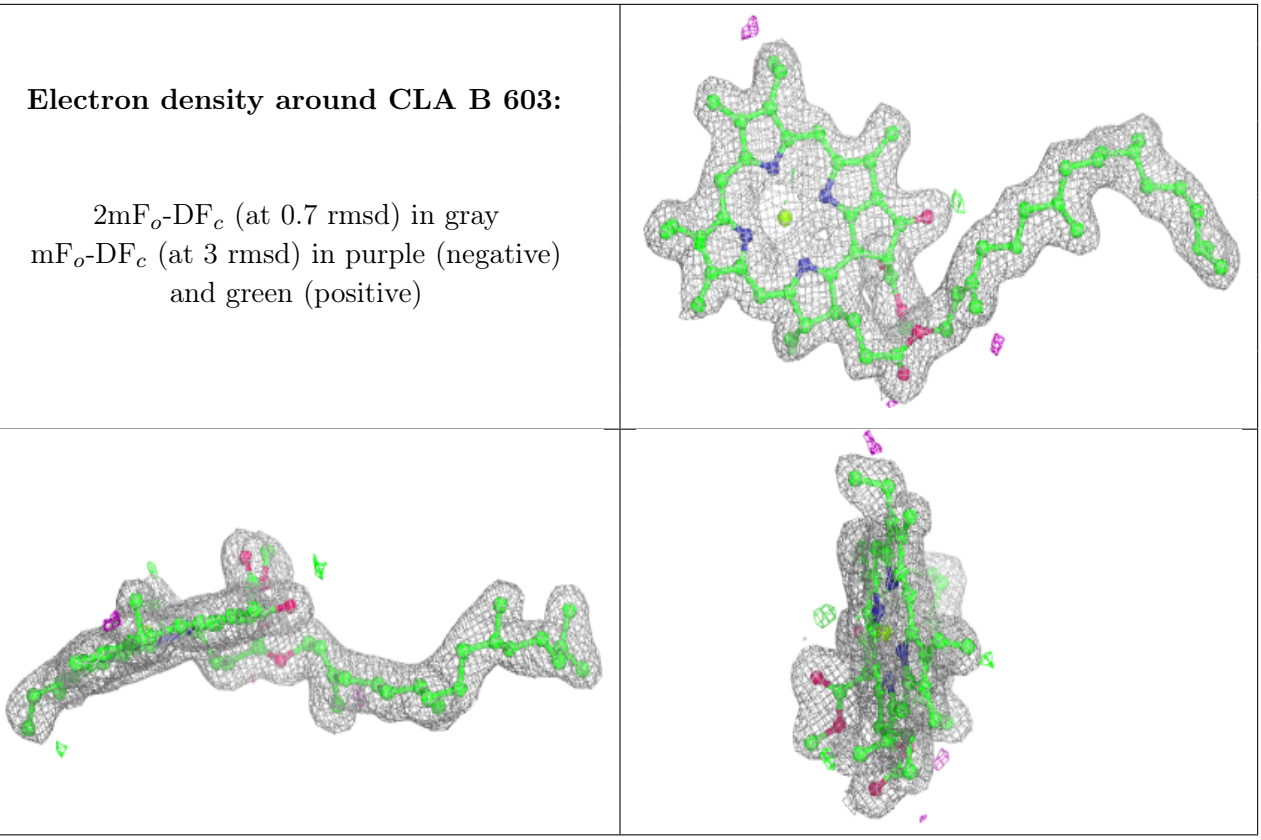
Electron density around LHG D 406:

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



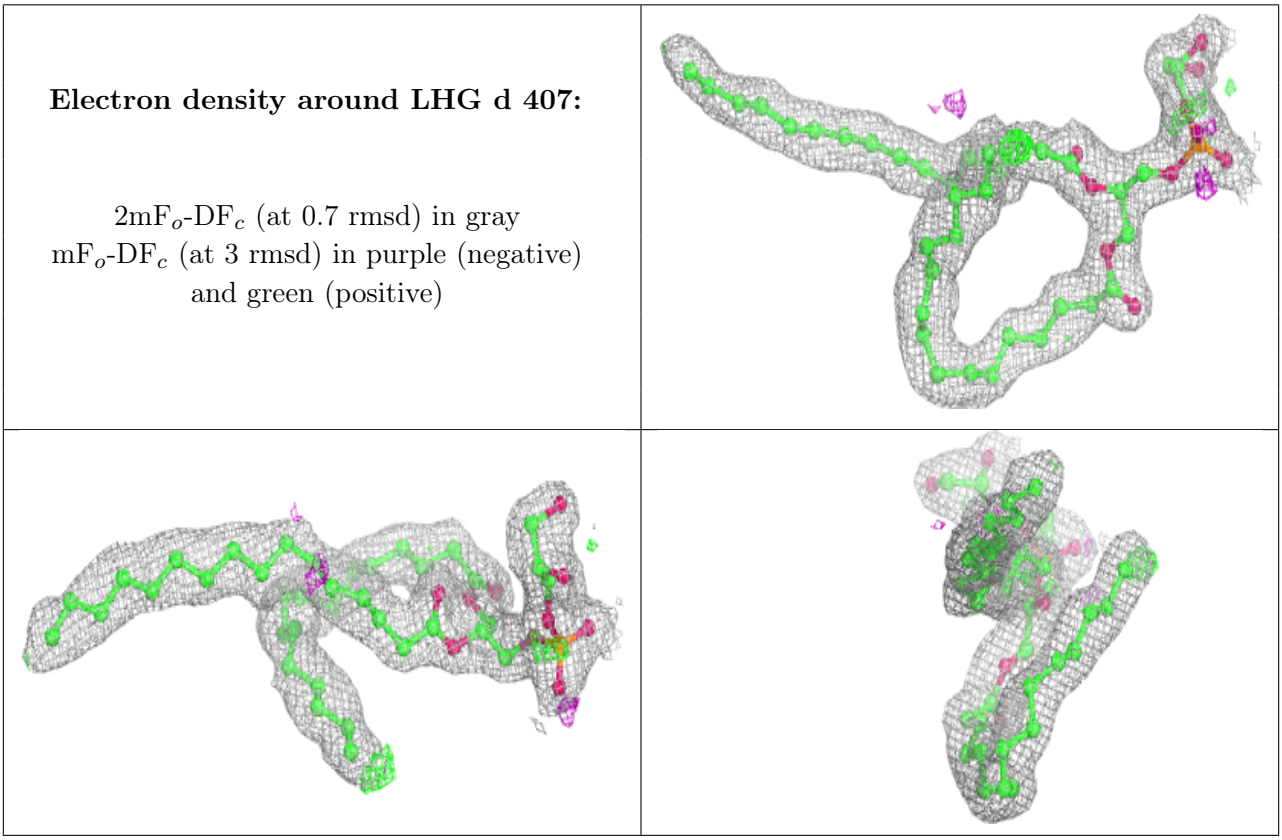
Electron density around CLA B 603:

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



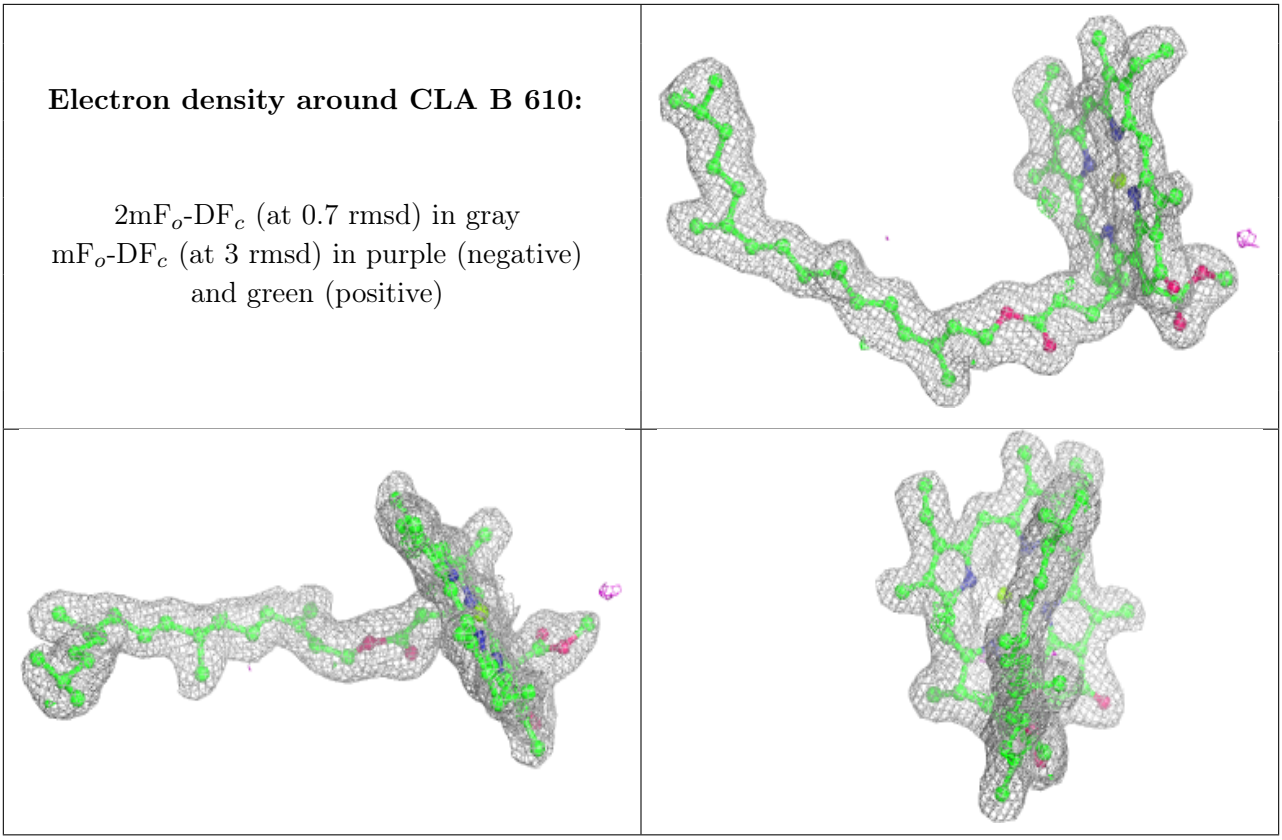
Electron density around LHG d 407:

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



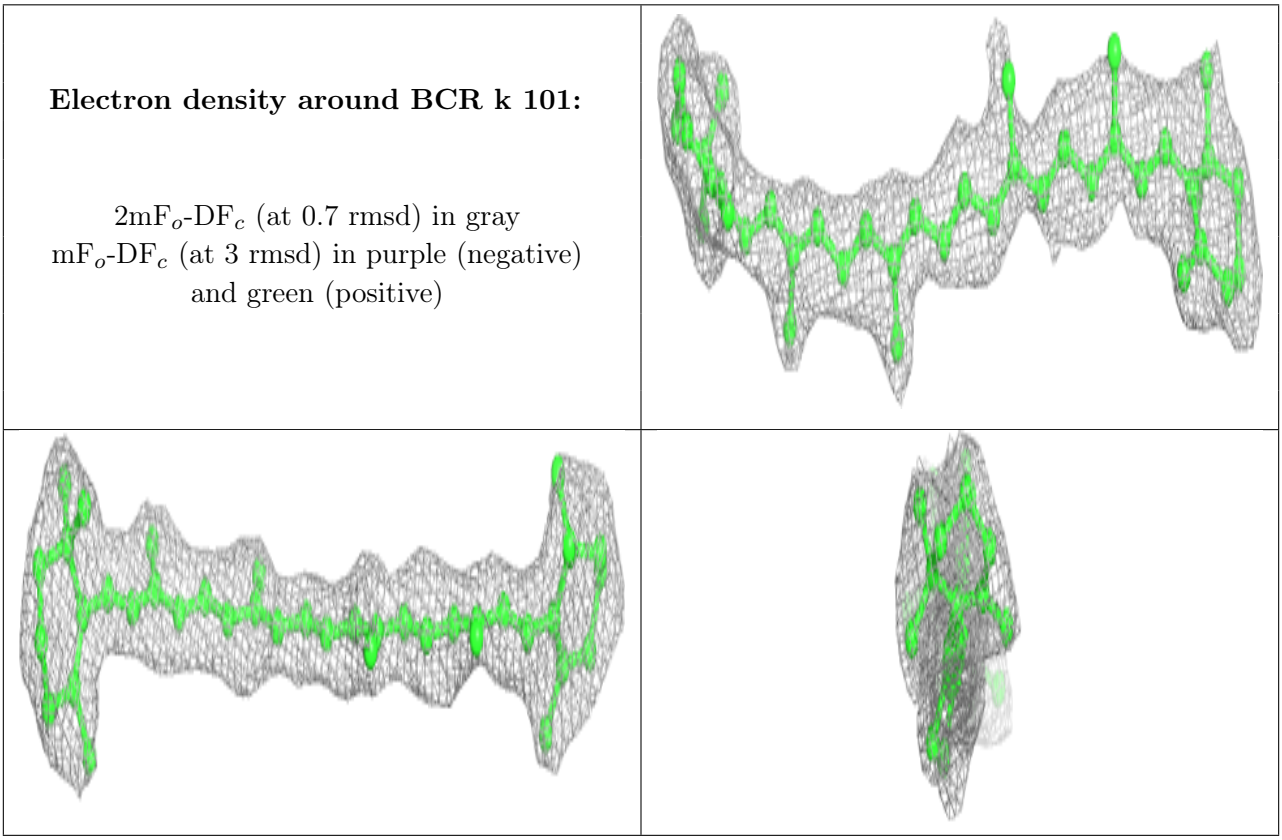
Electron density around CLA B 610:

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



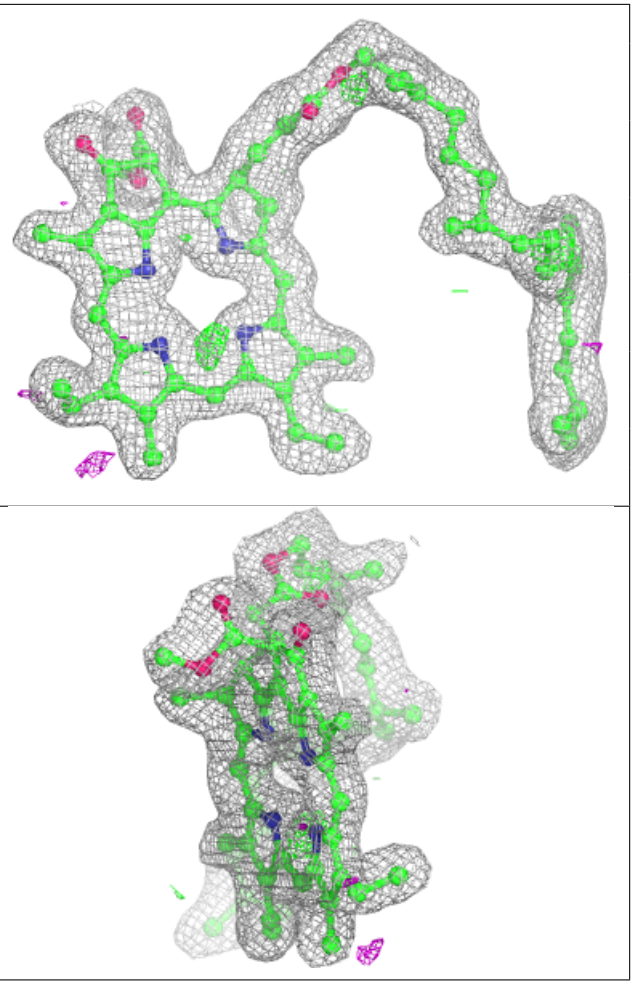
Electron density around BCR k 101:

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



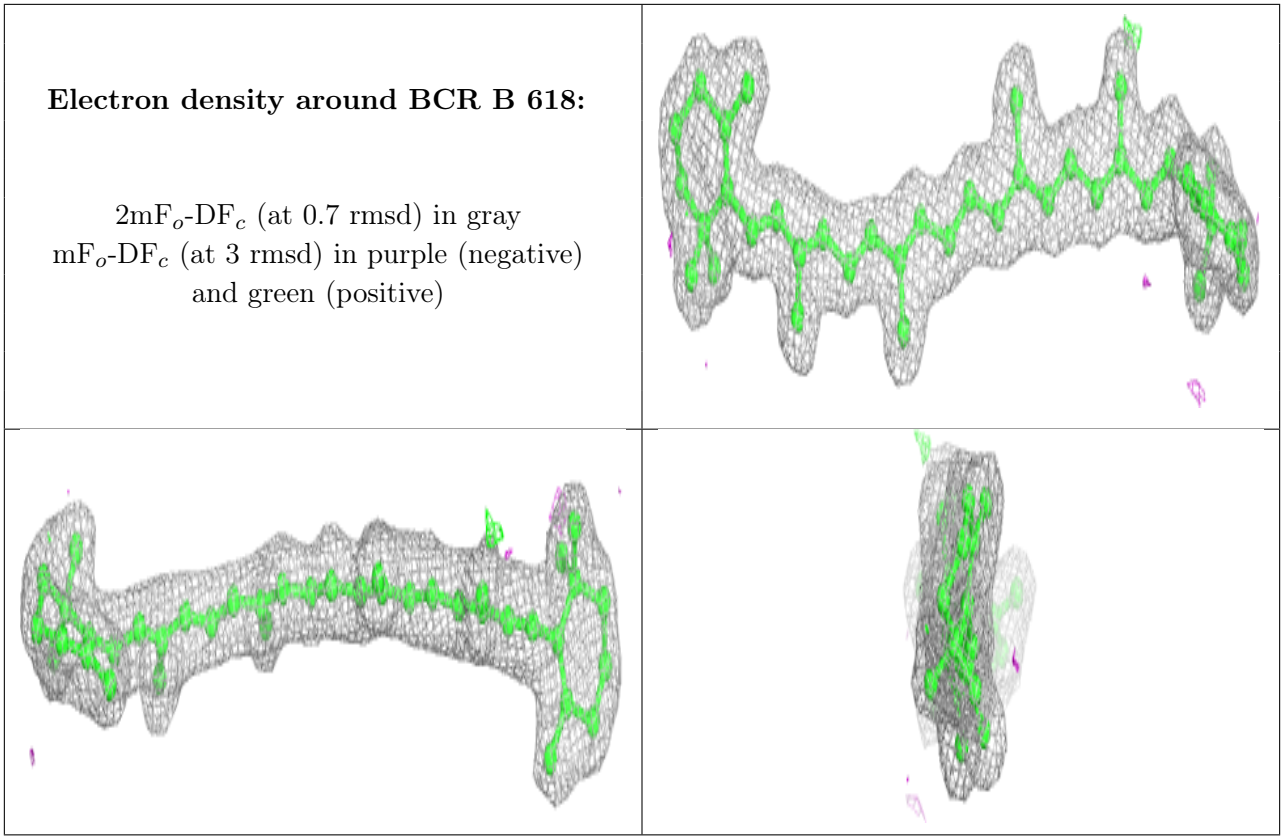
Electron density around PHO a 420:

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



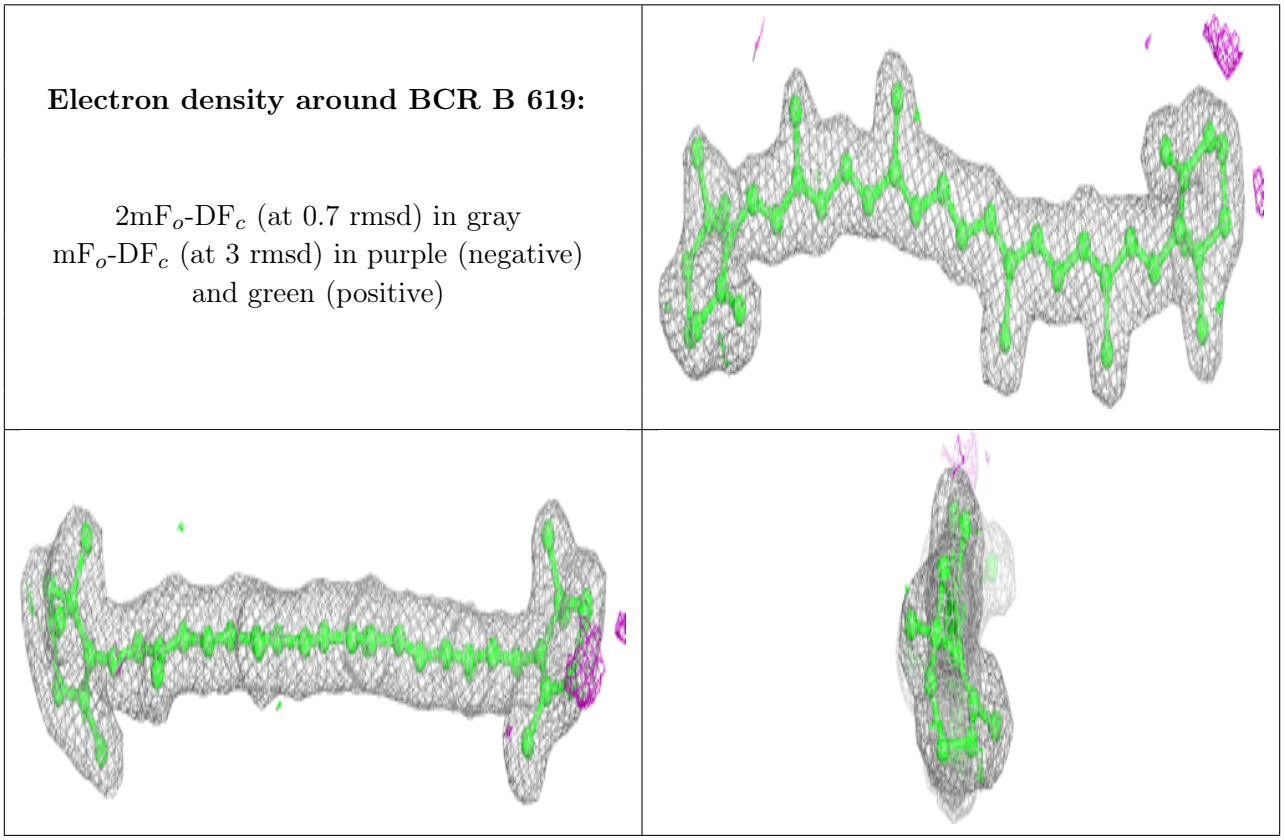
Electron density around BCR B 618:

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



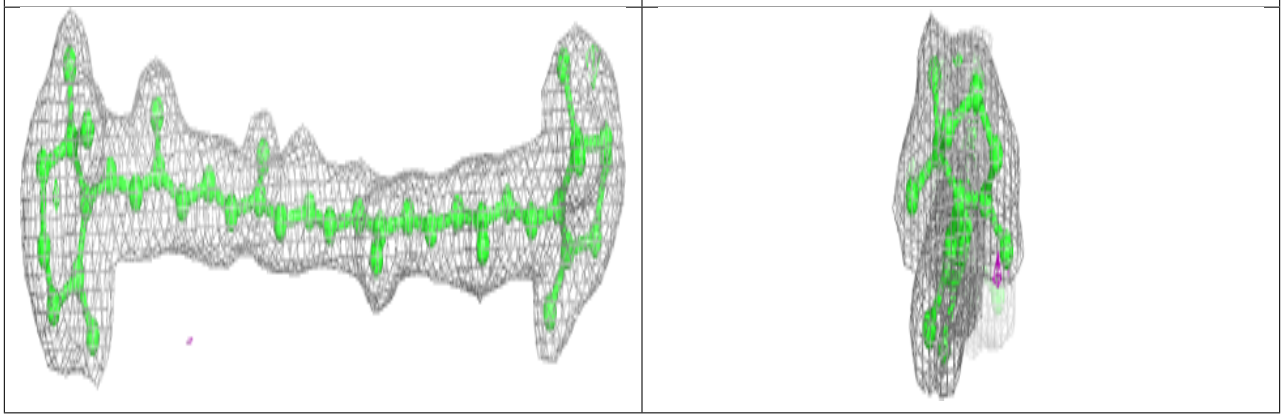
Electron density around BCR B 619:

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



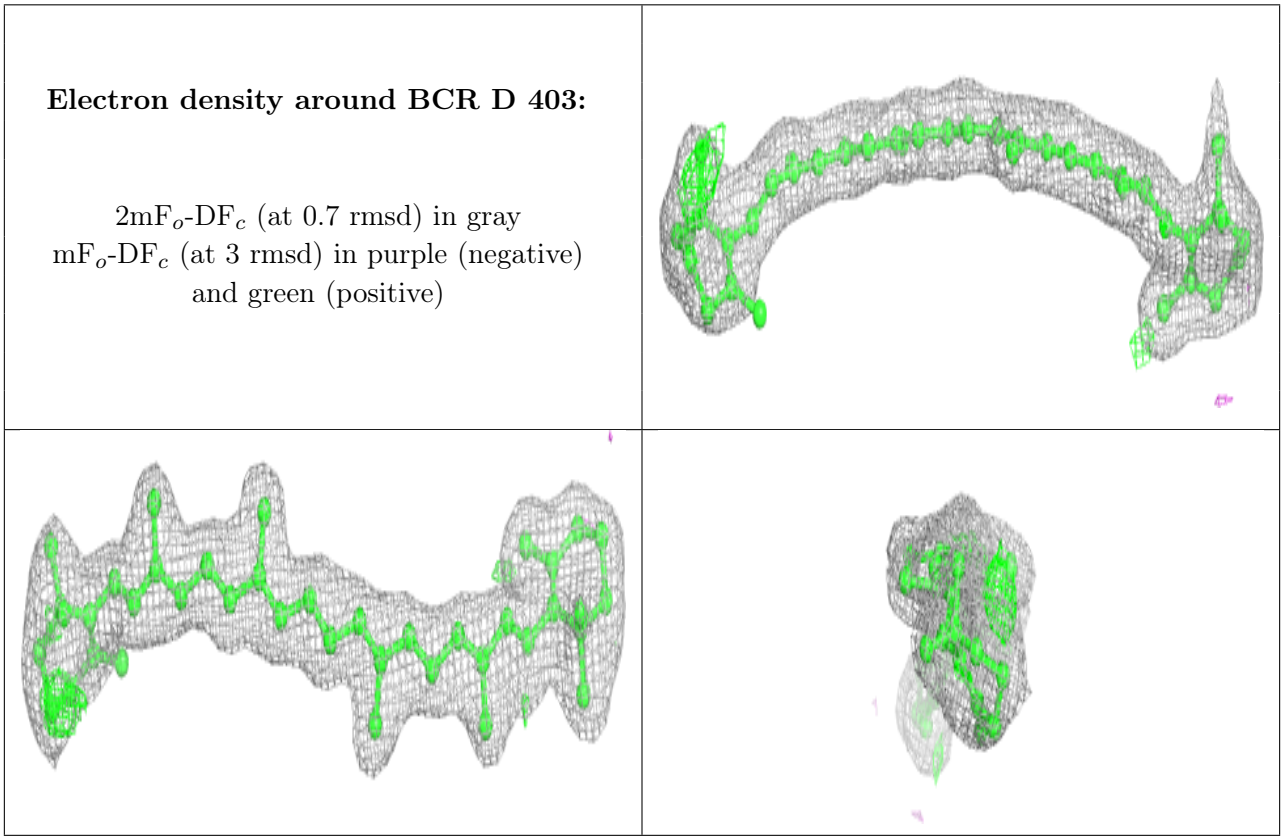
Electron density around BCR C 515:

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



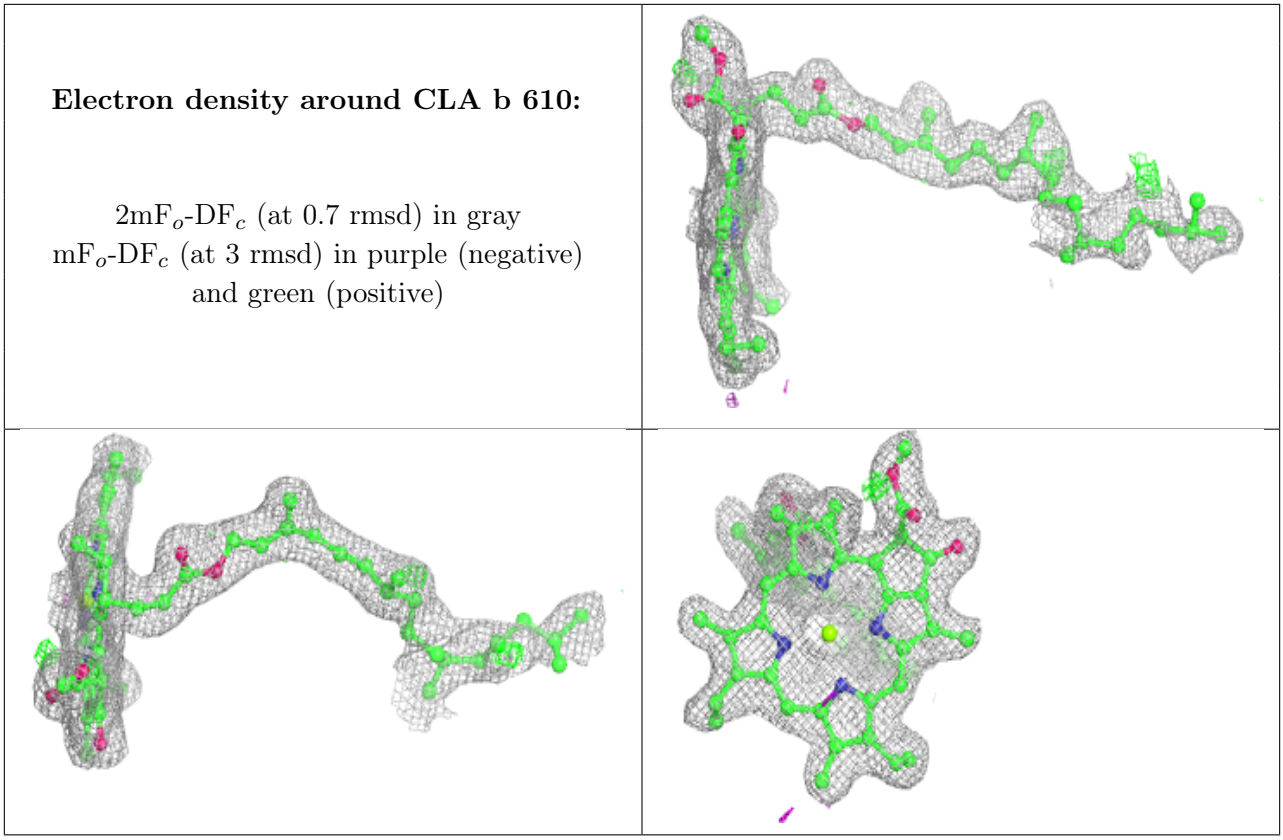
Electron density around BCR D 403:

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



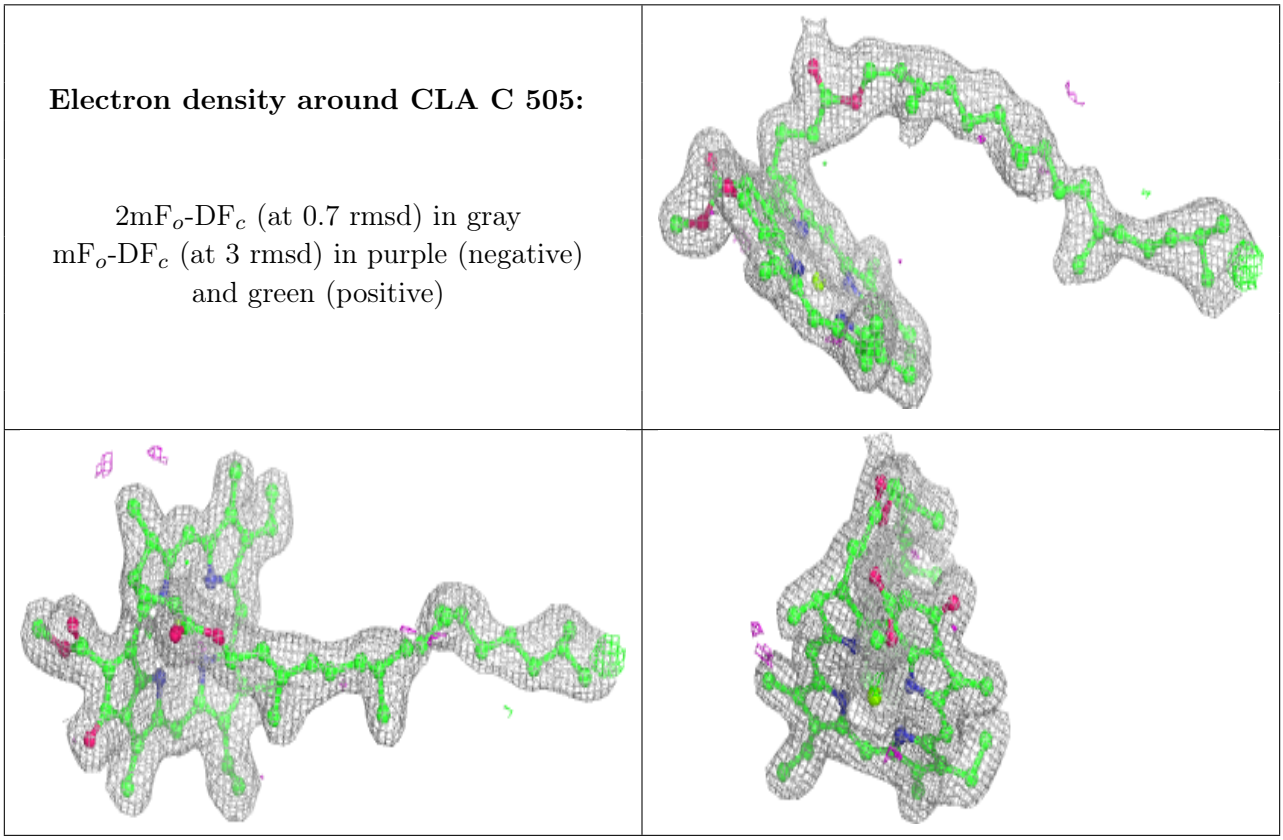
Electron density around CLA b 610:

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



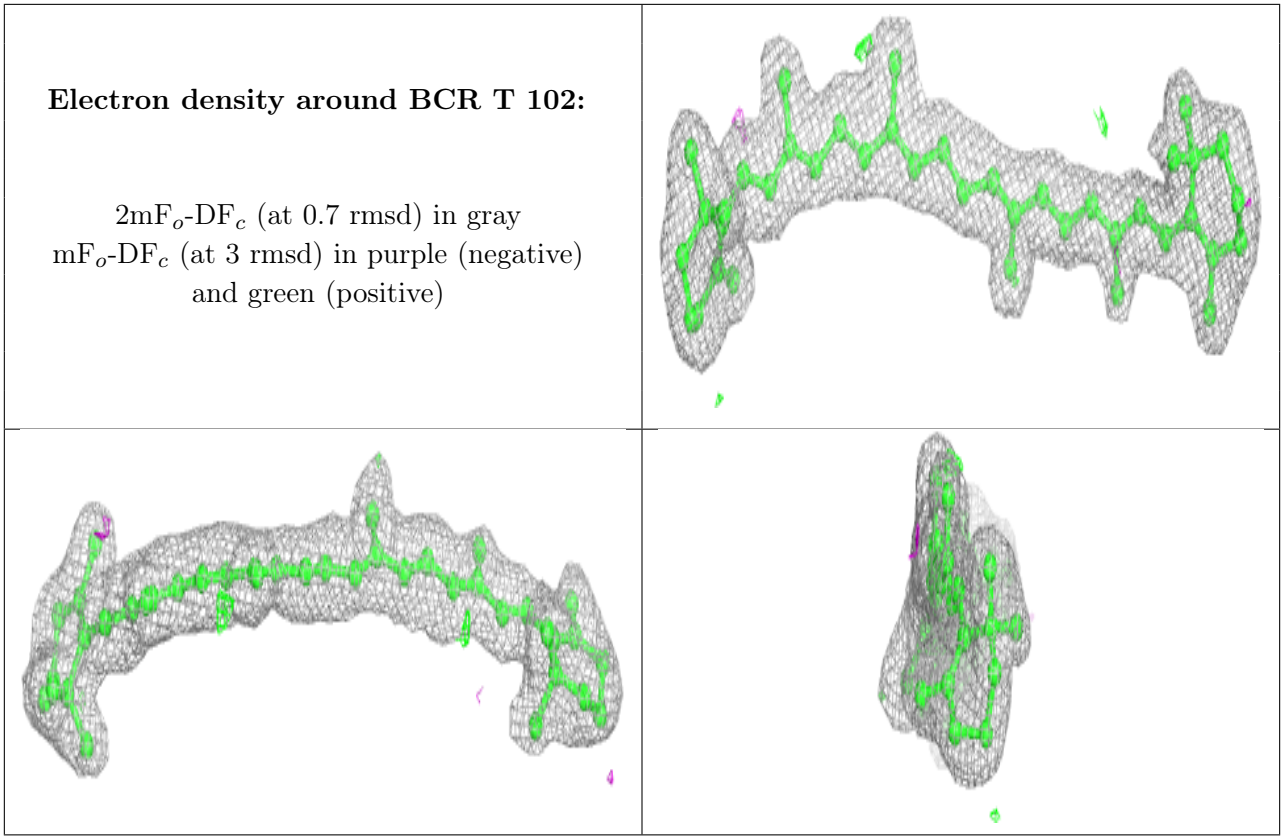
Electron density around CLA C 505:

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



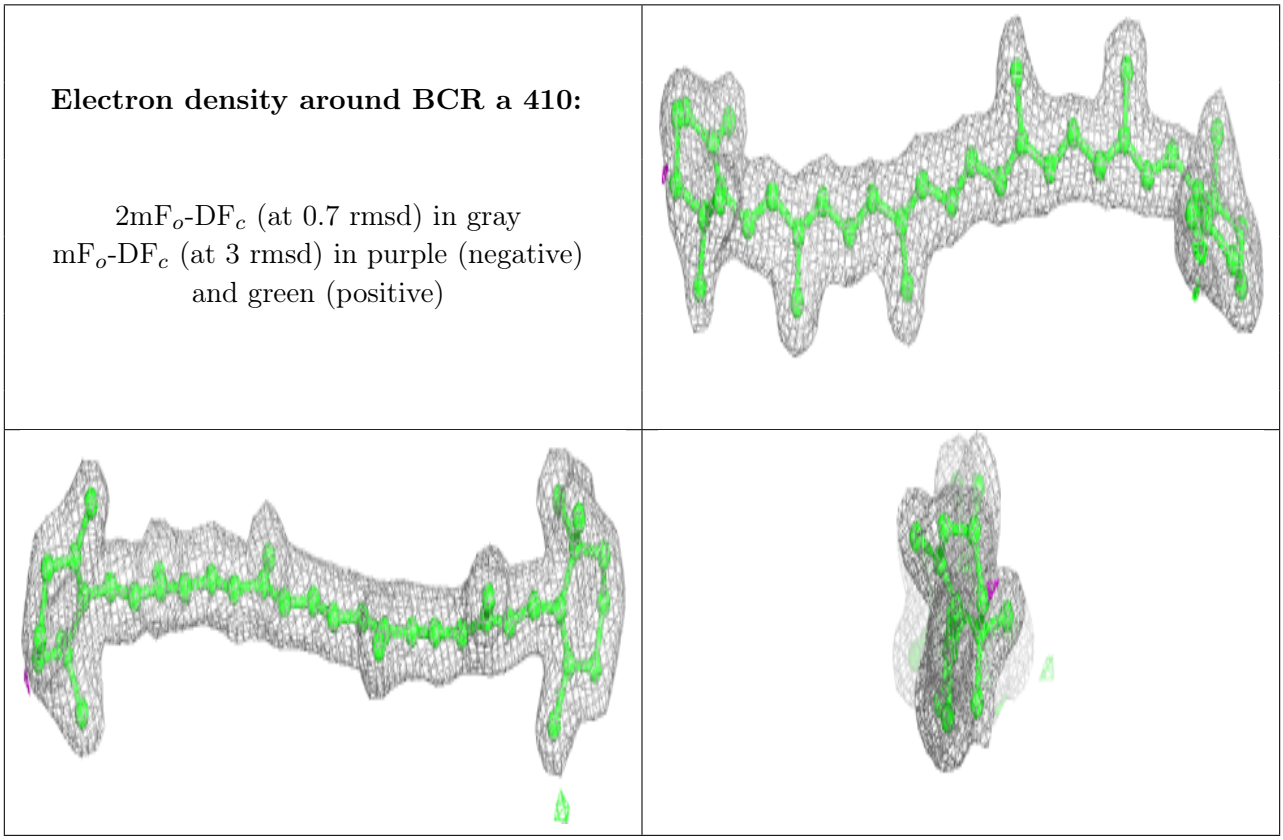
Electron density around BCR T 102:

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



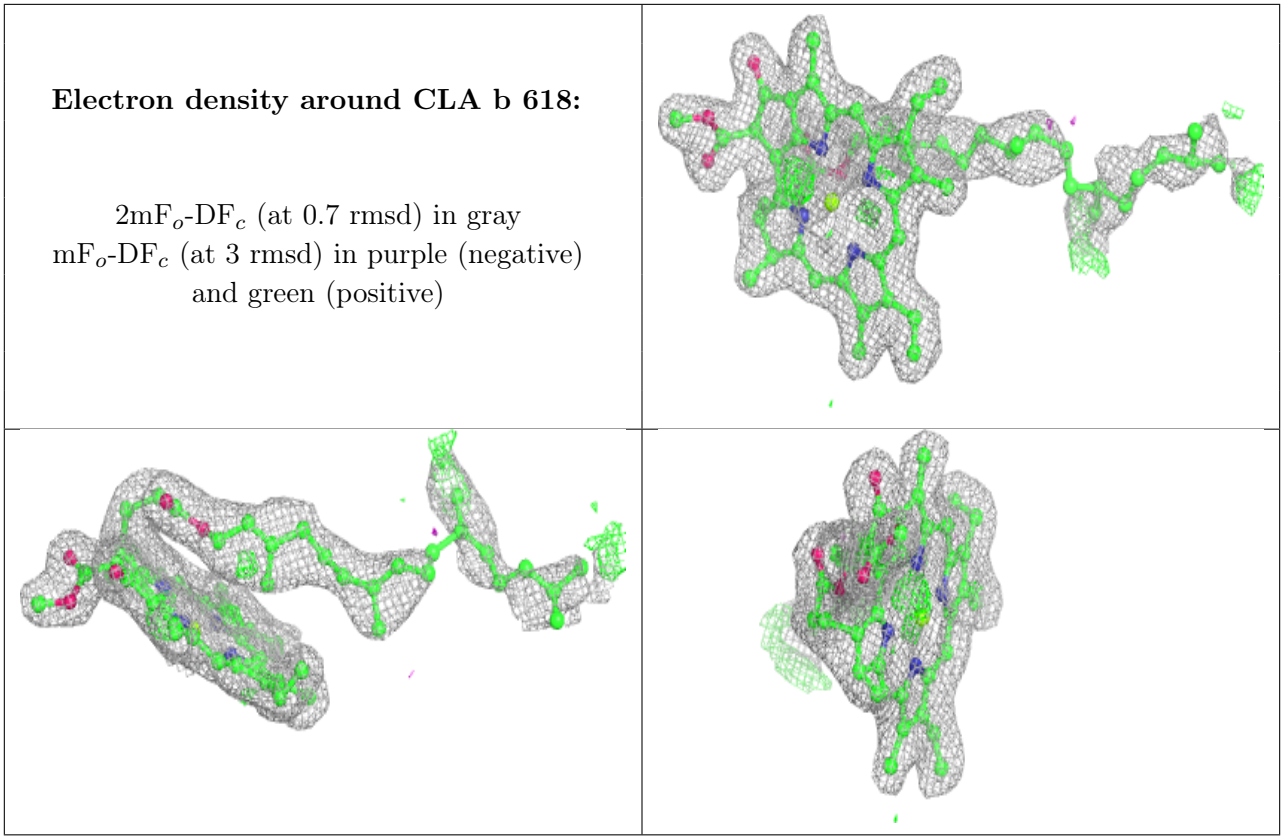
Electron density around BCR a 410:

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



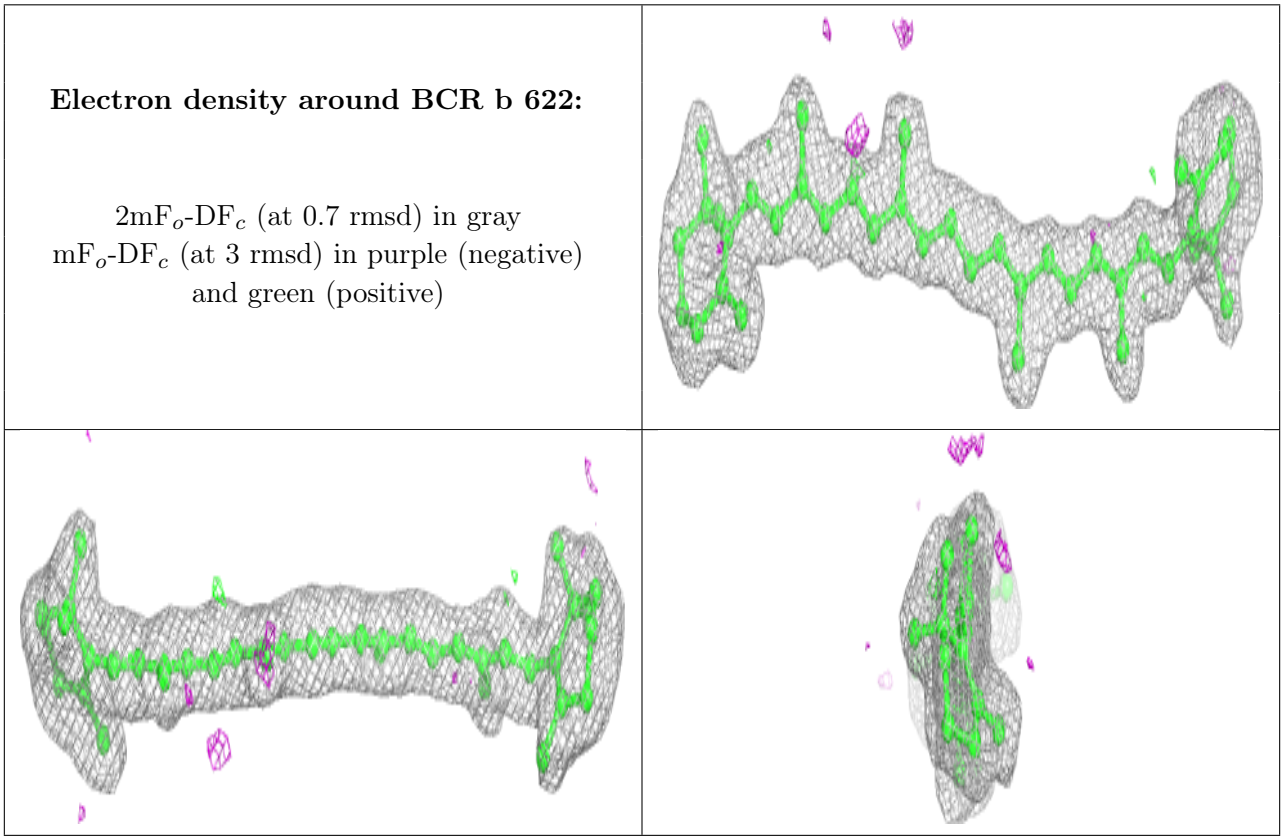
Electron density around CLA b 618:

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



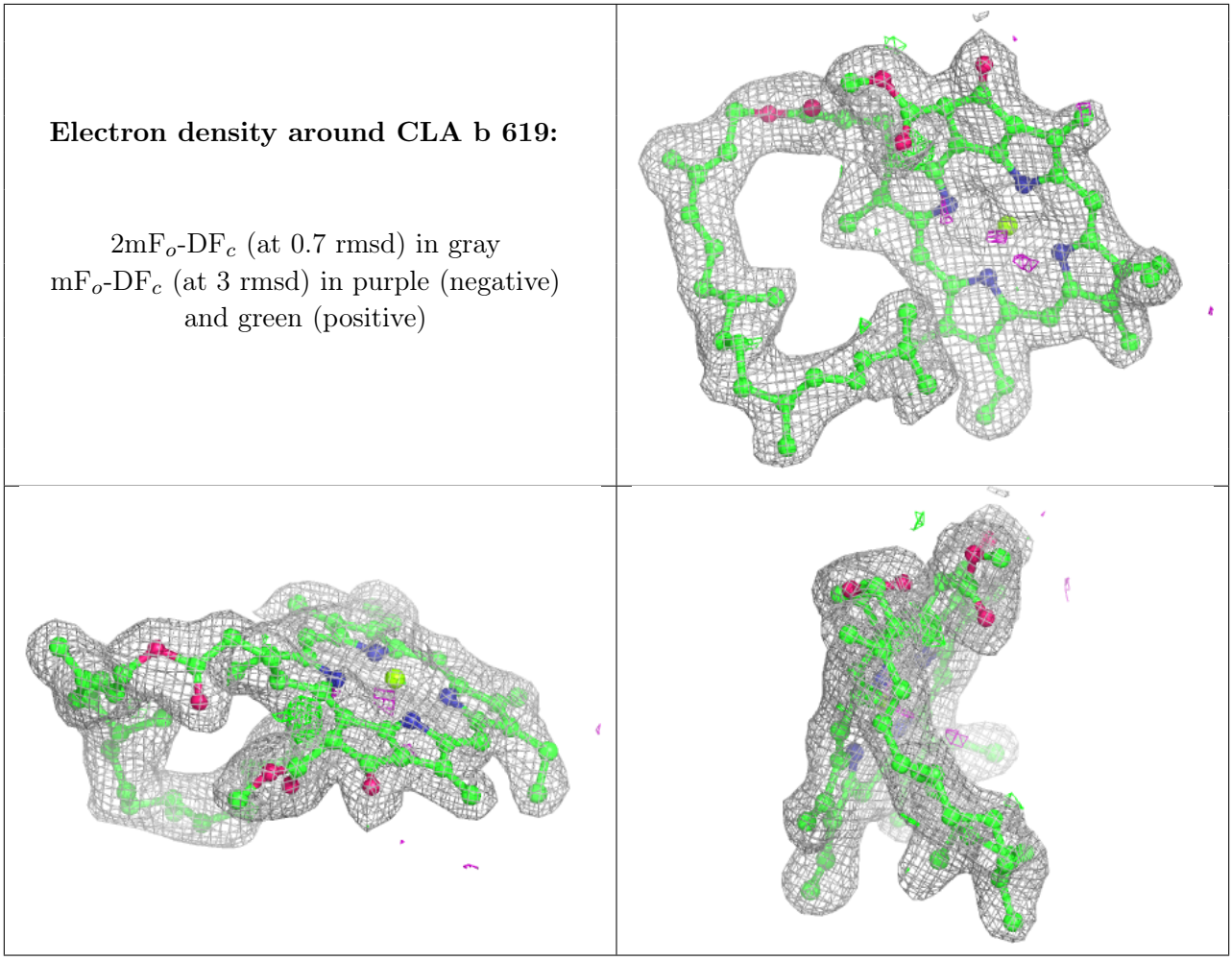
Electron density around BCR b 622:

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



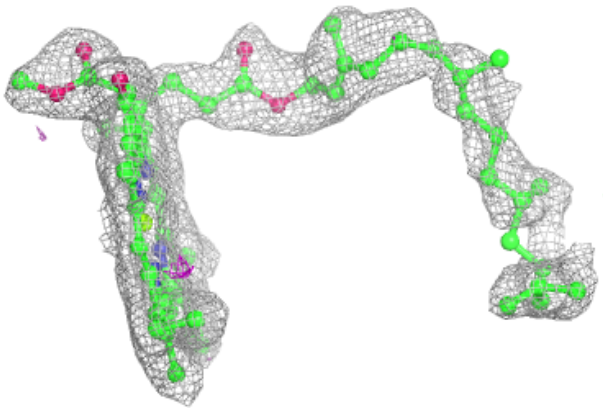
Electron density around CLA b 619:

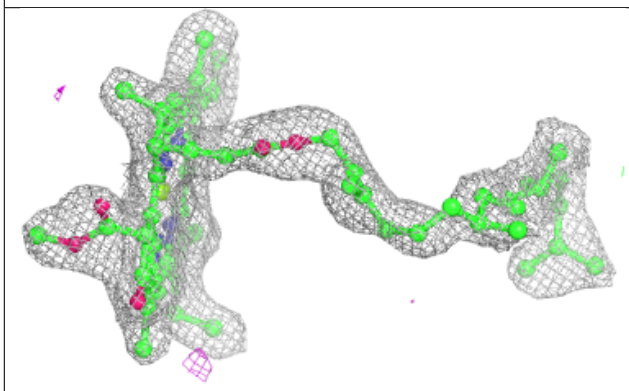
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

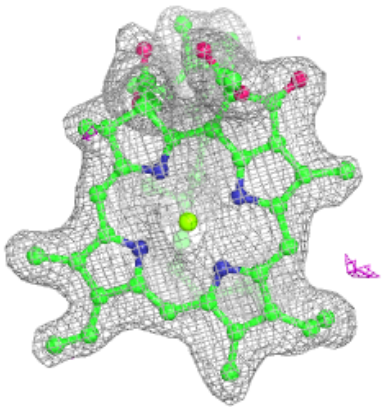


Electron density around CLA C 507:

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

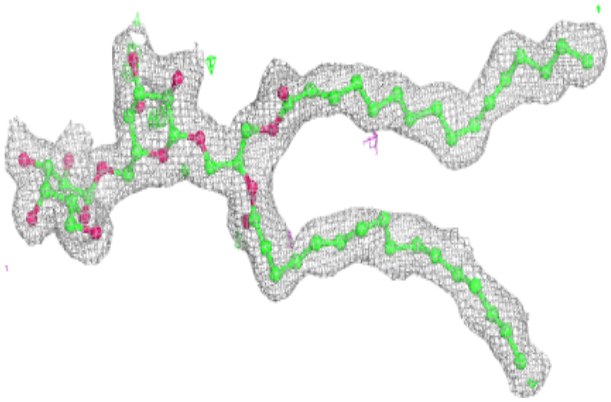


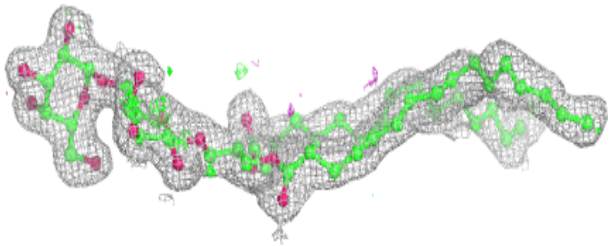


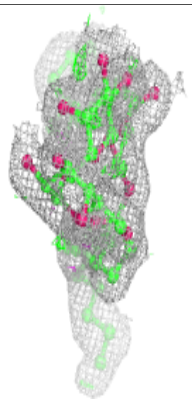


Electron density around DGD C 519:

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

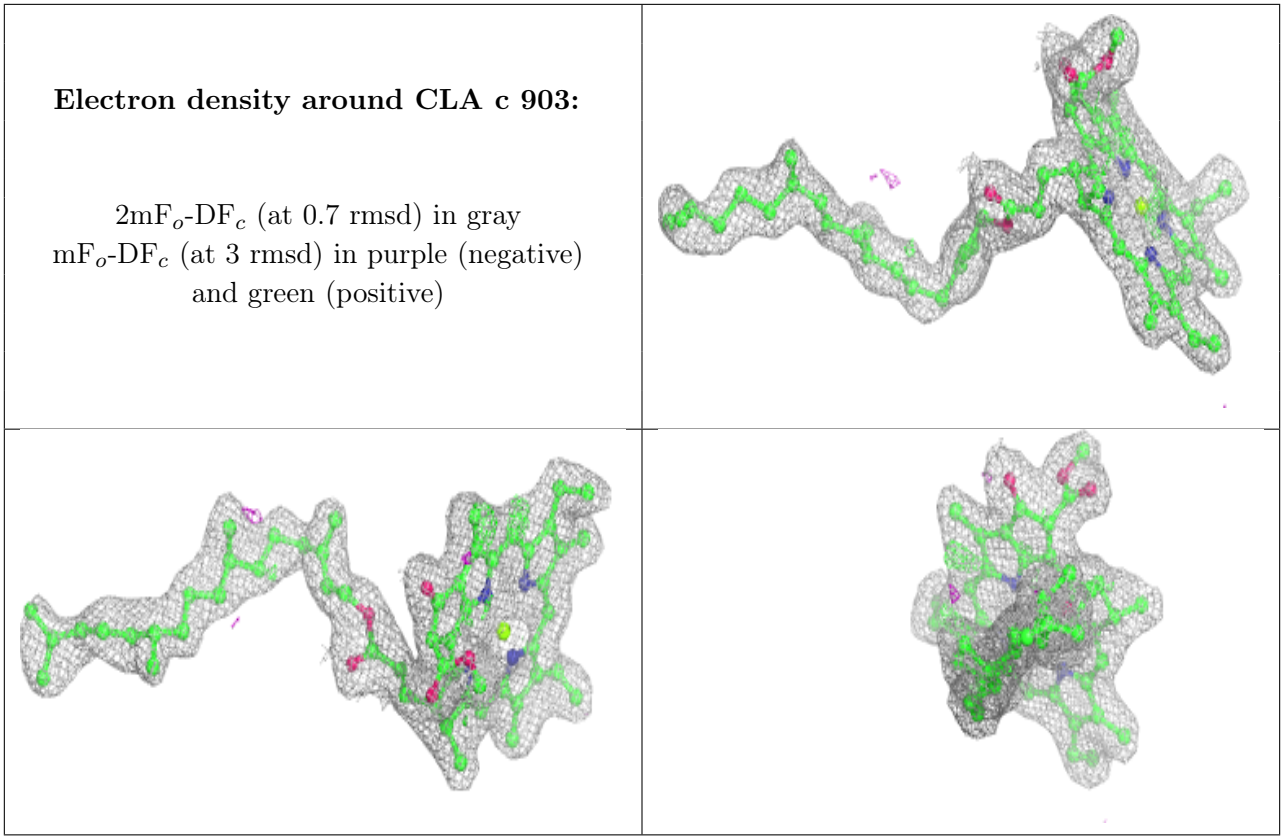






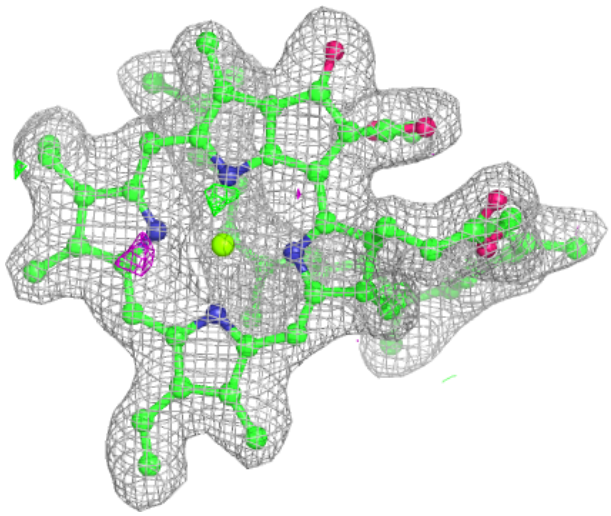
Electron density around CLA c 903:

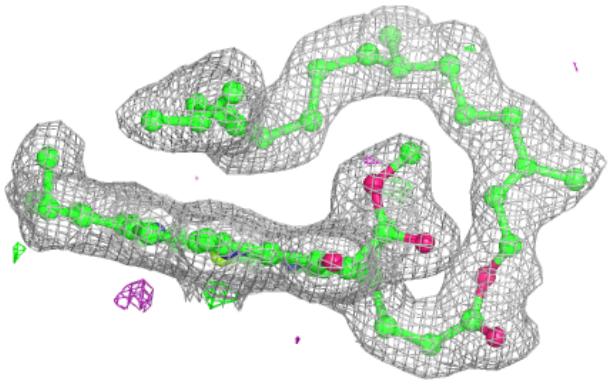
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

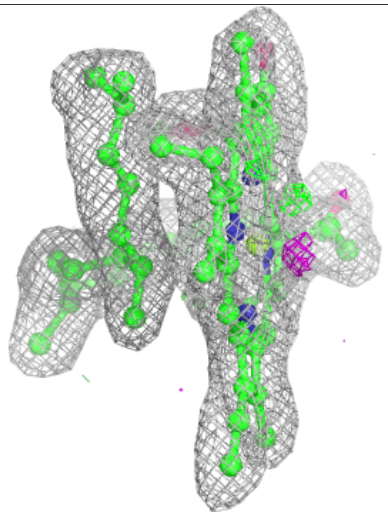


Electron density around CLA C 511:

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

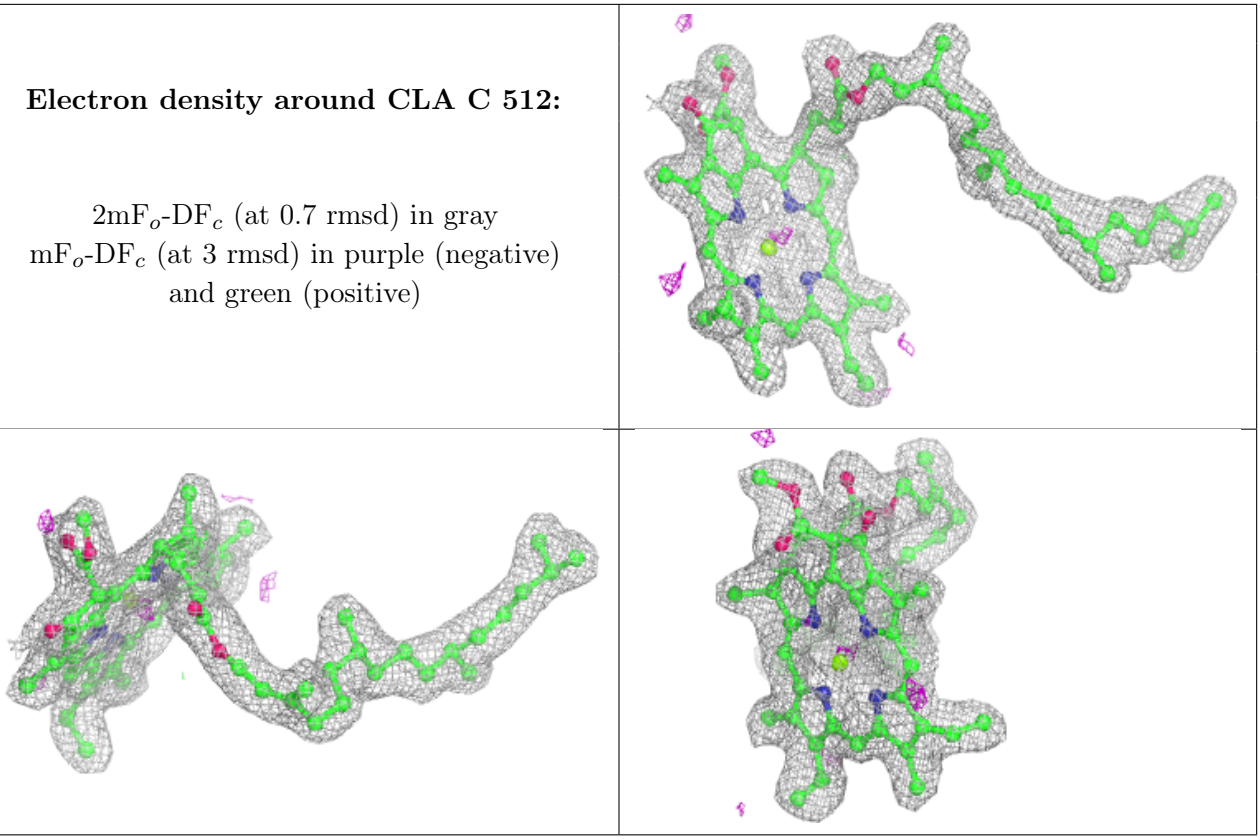






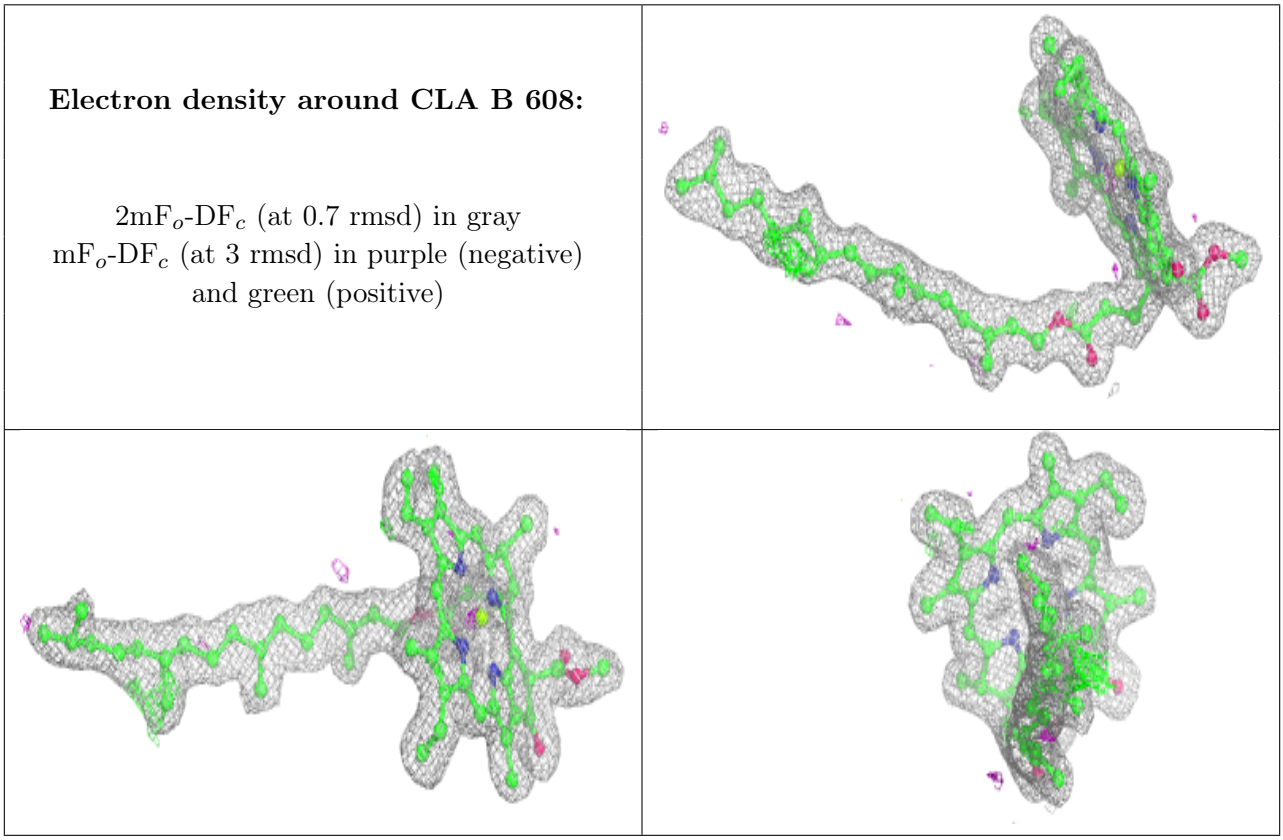
Electron density around CLA C 512:

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



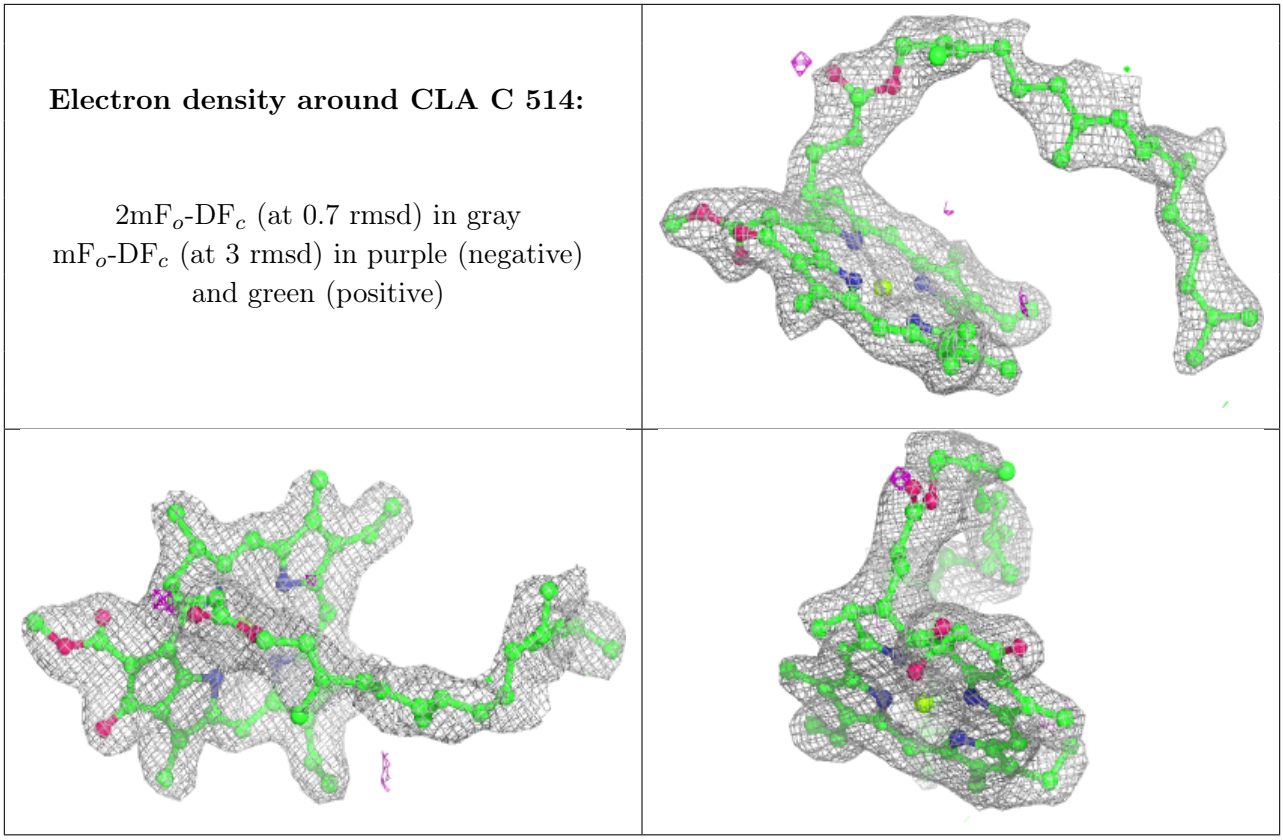
Electron density around CLA B 608:

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



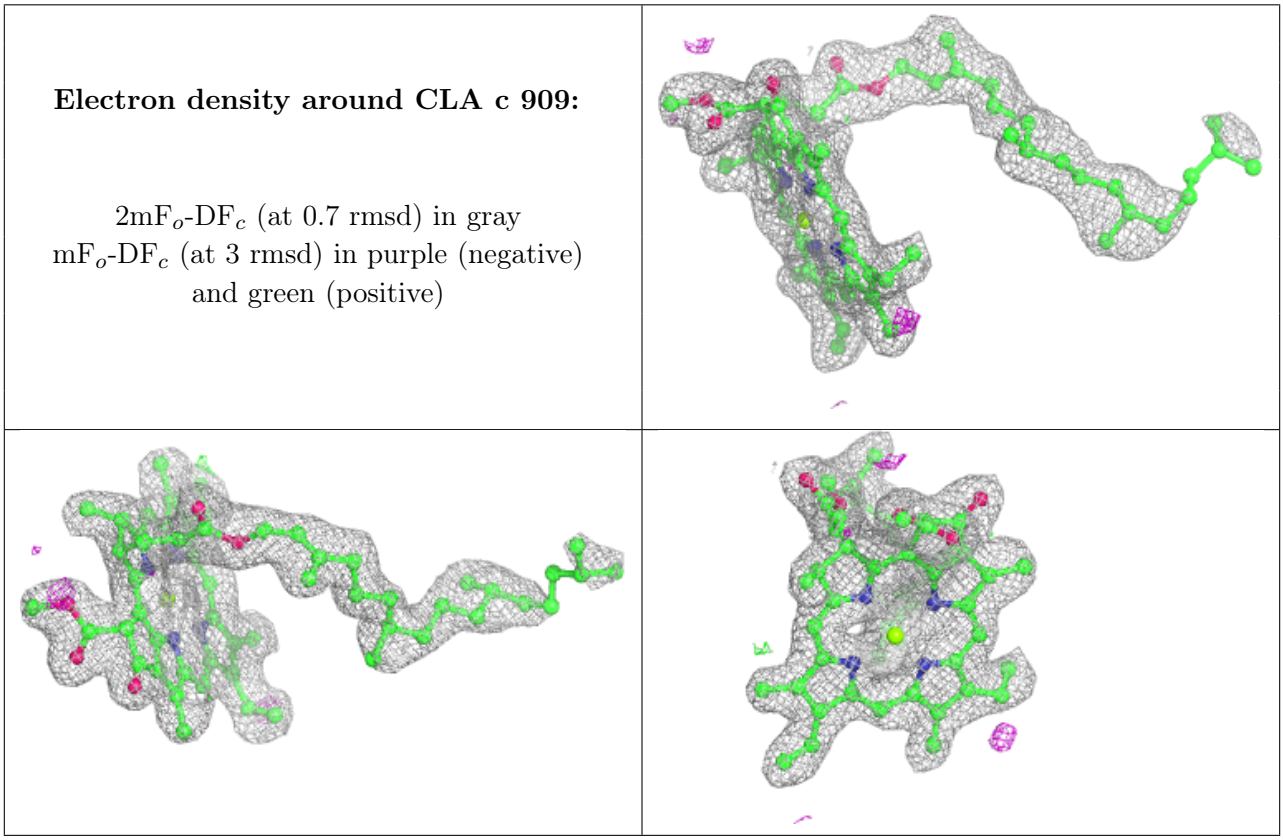
Electron density around CLA C 514:

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



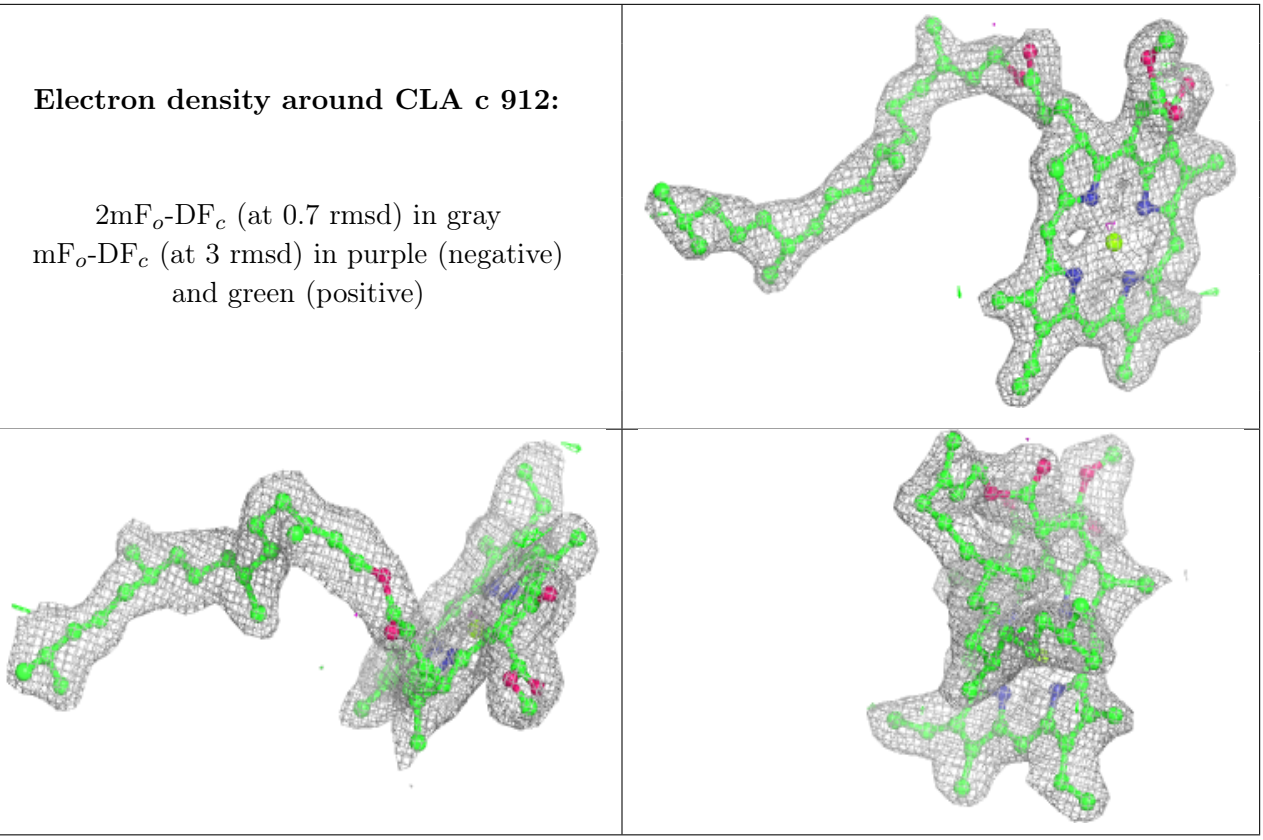
Electron density around CLA c 909:

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



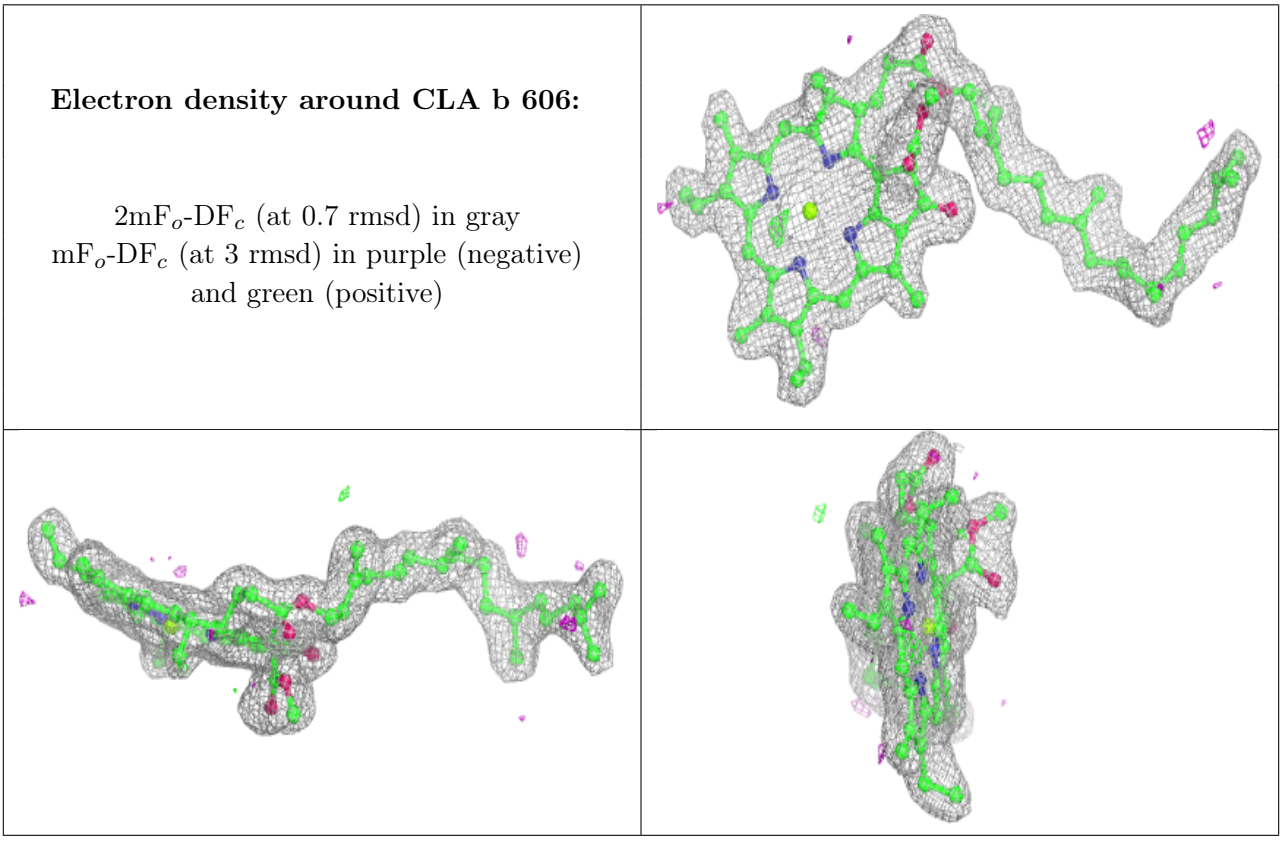
Electron density around CLA c 912:

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



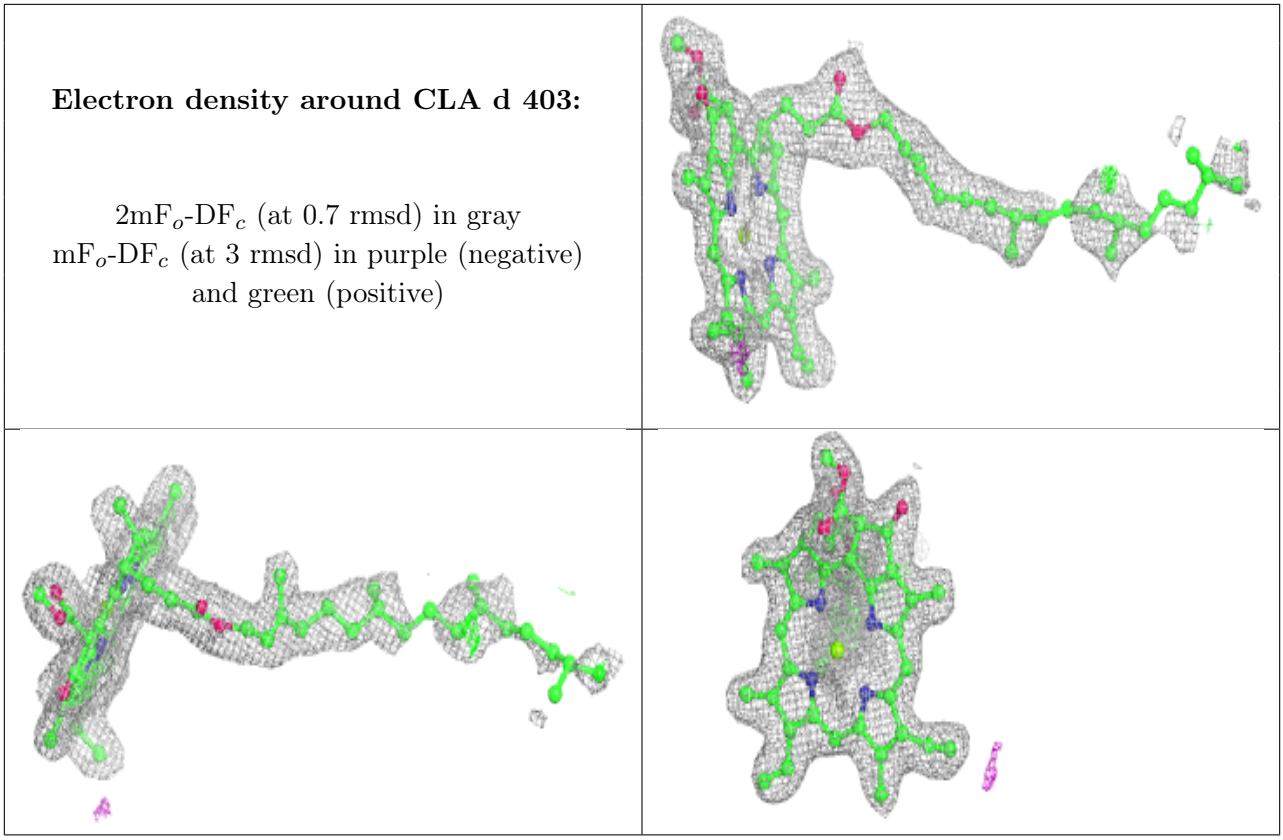
Electron density around CLA b 606:

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



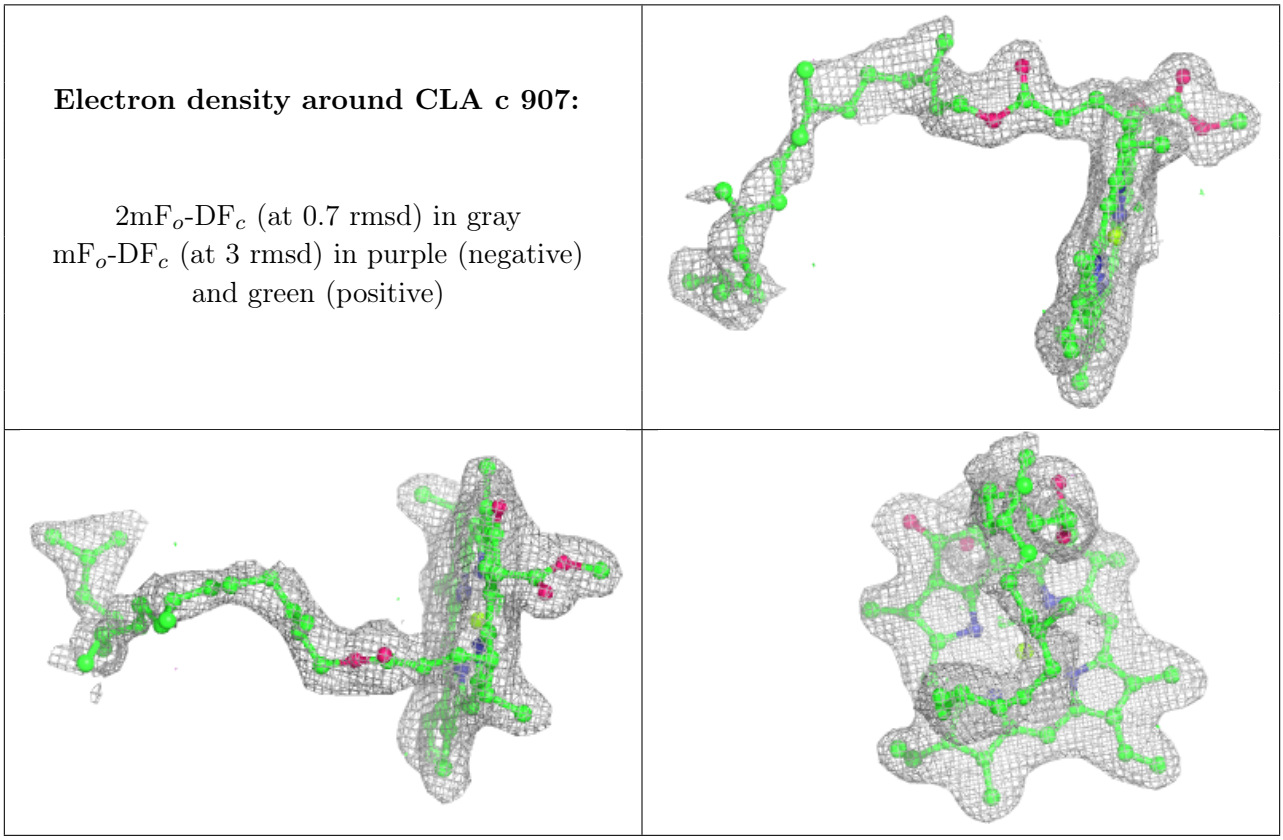
Electron density around CLA d 403:

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



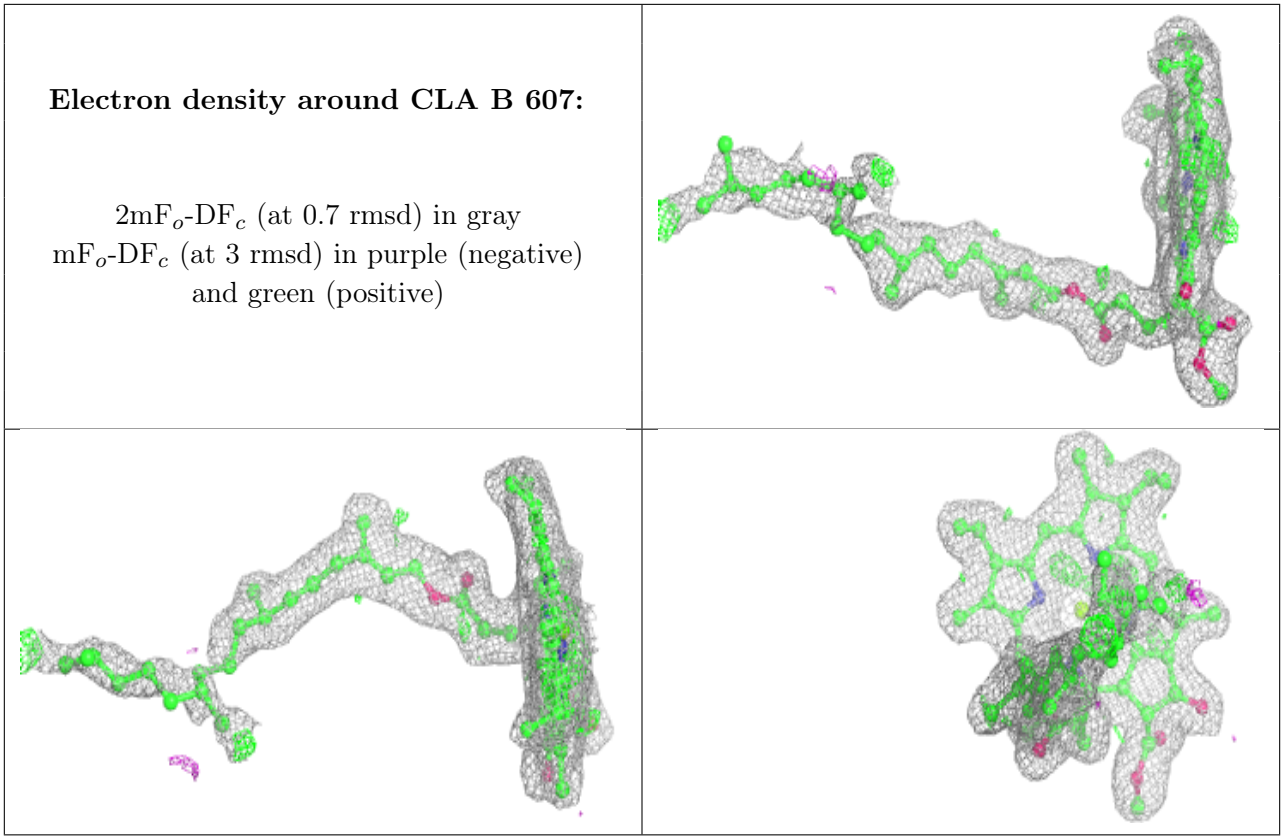
Electron density around CLA c 907:

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



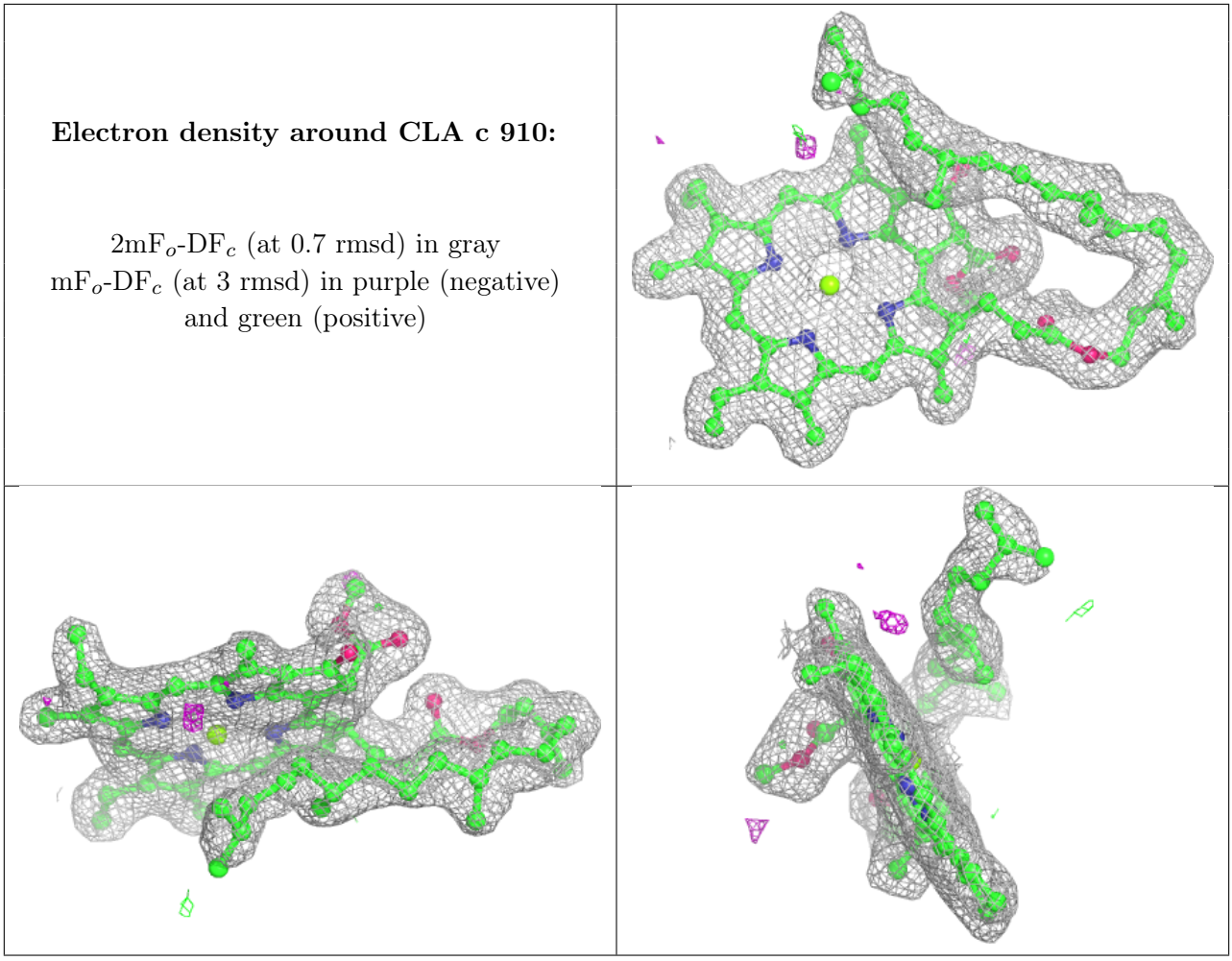
Electron density around CLA B 607:

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



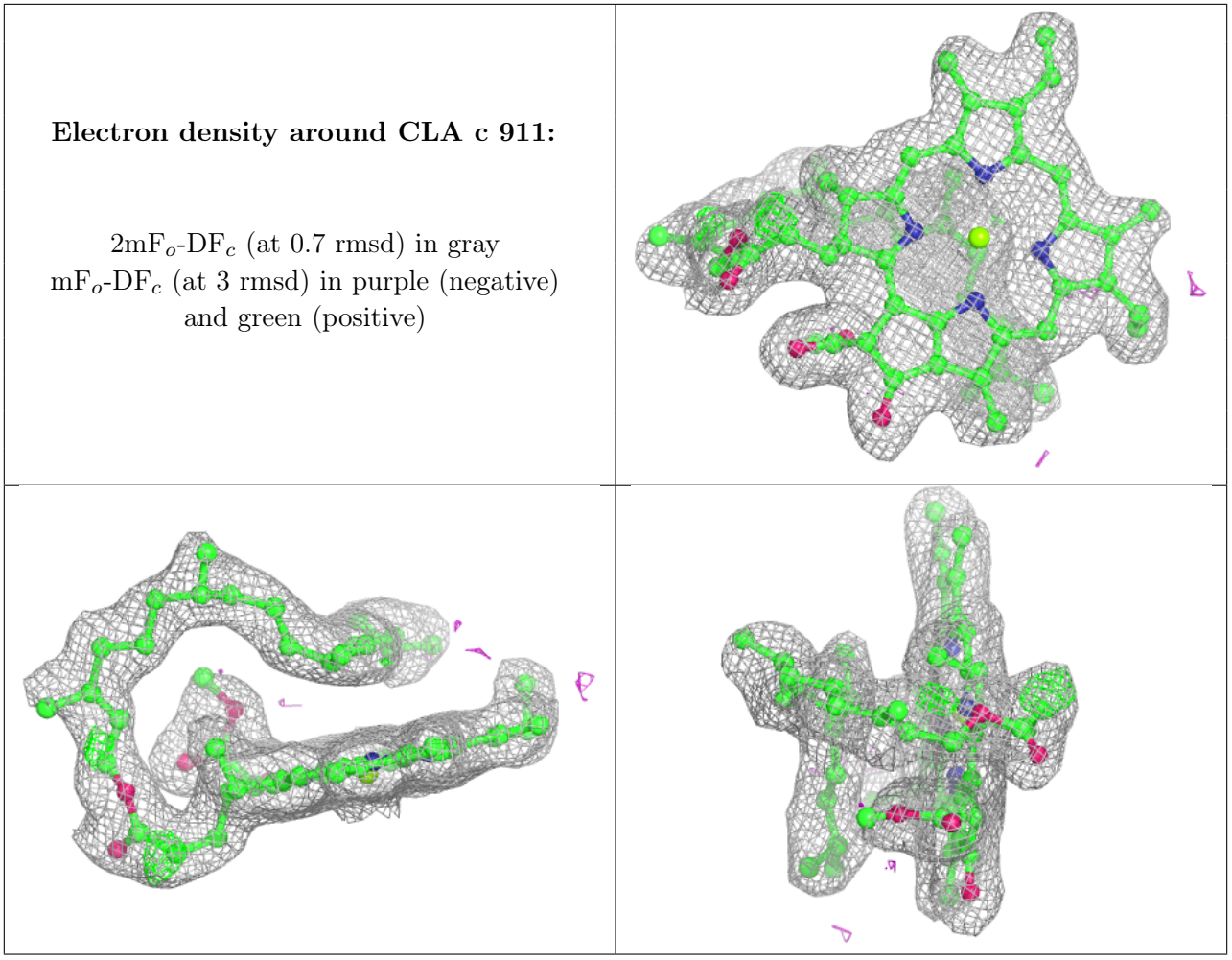
Electron density around CLA c 910:

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



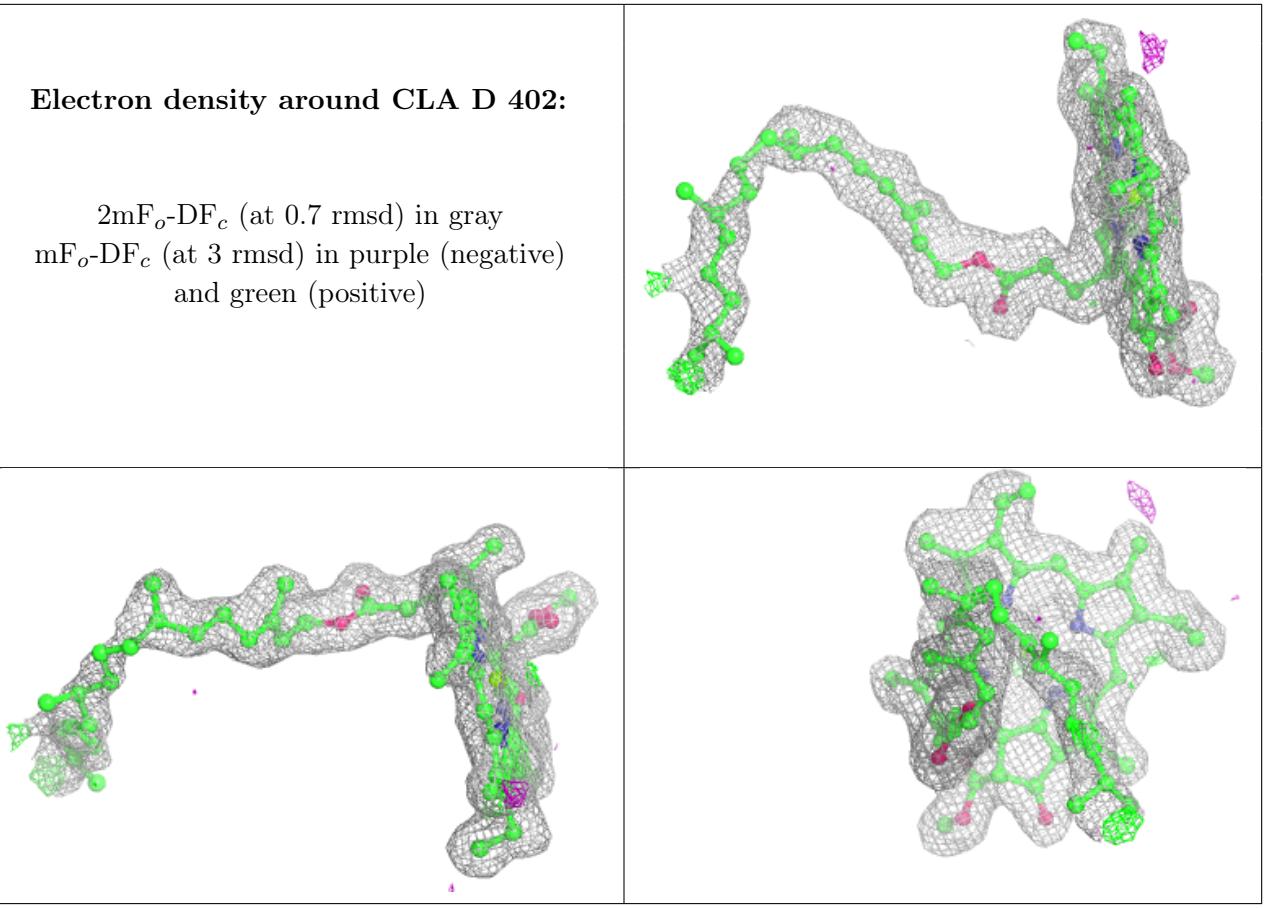
Electron density around CLA c 911:

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



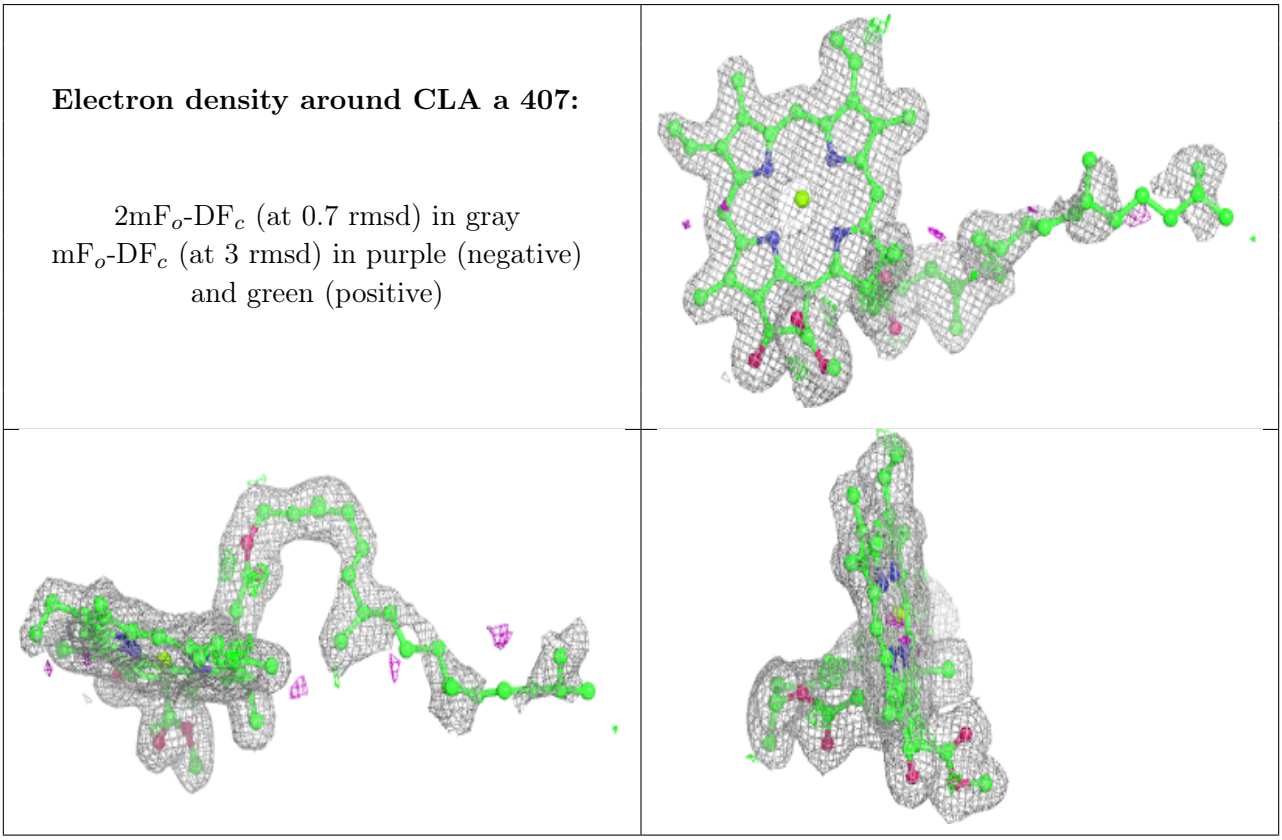
Electron density around CLA D 402:

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



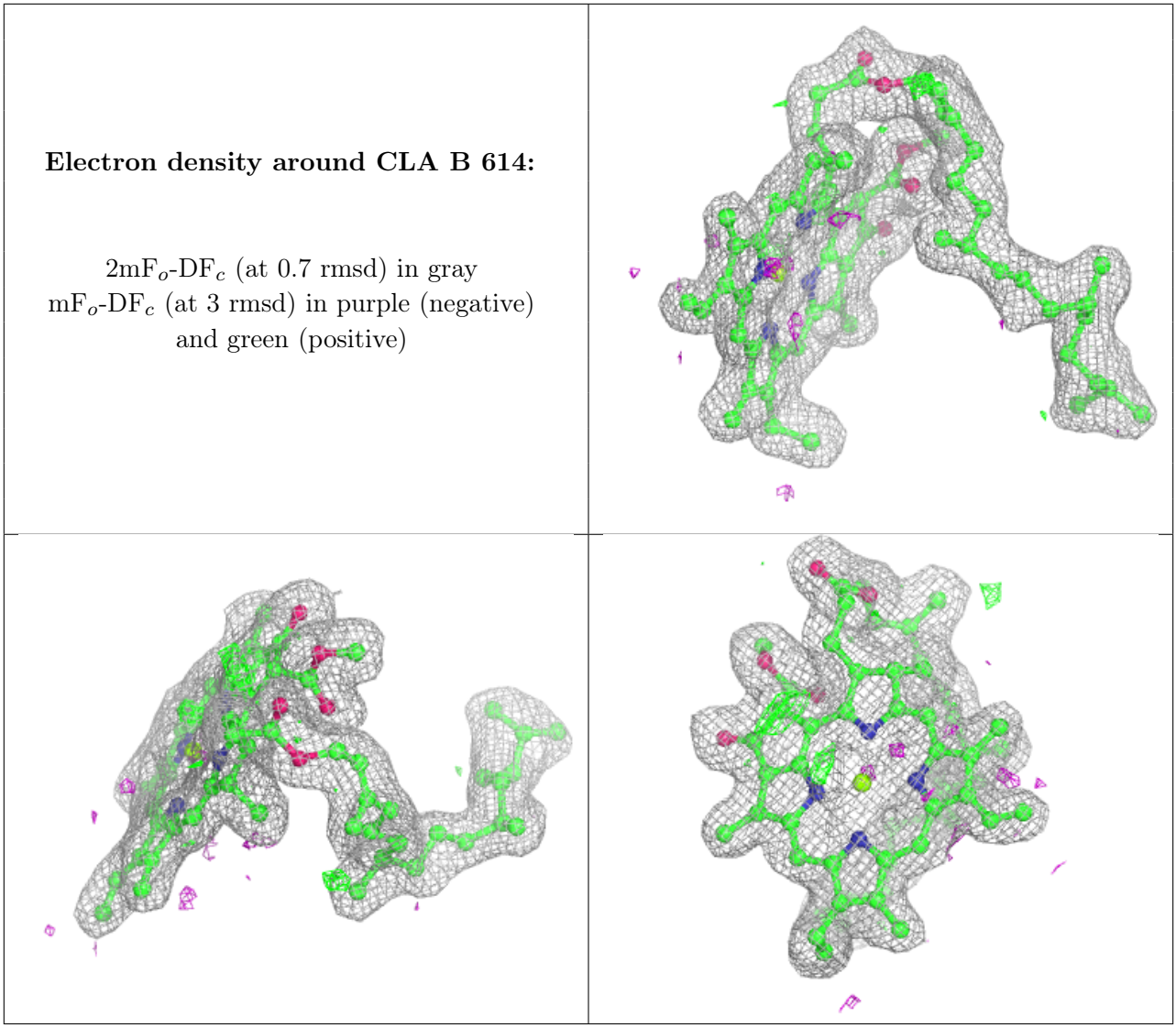
Electron density around CLA a 407:

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



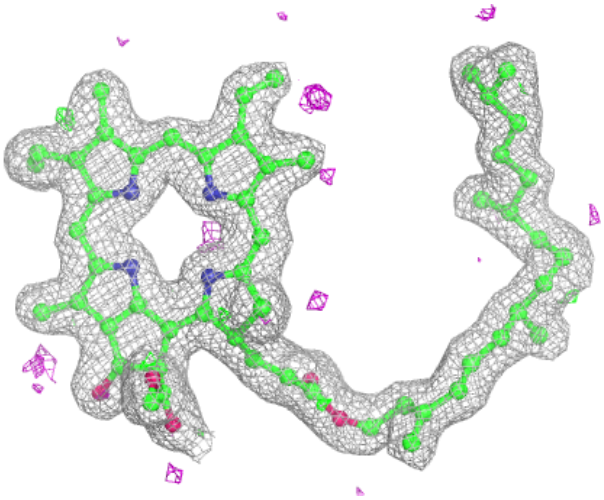
Electron density around CLA B 614:

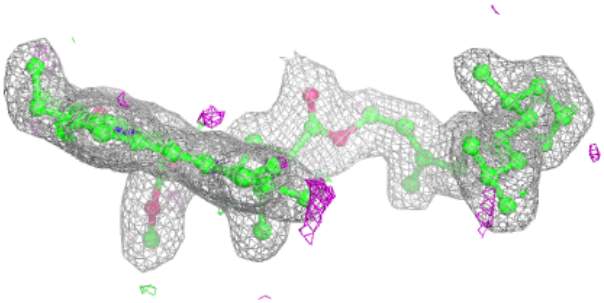
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

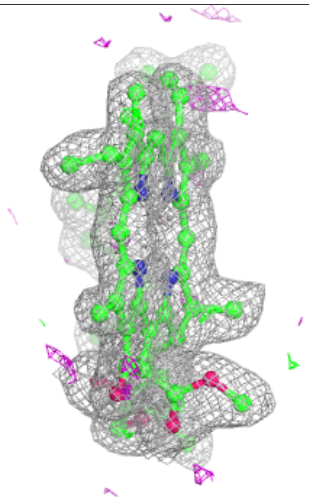


Electron density around PHO a 408:

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

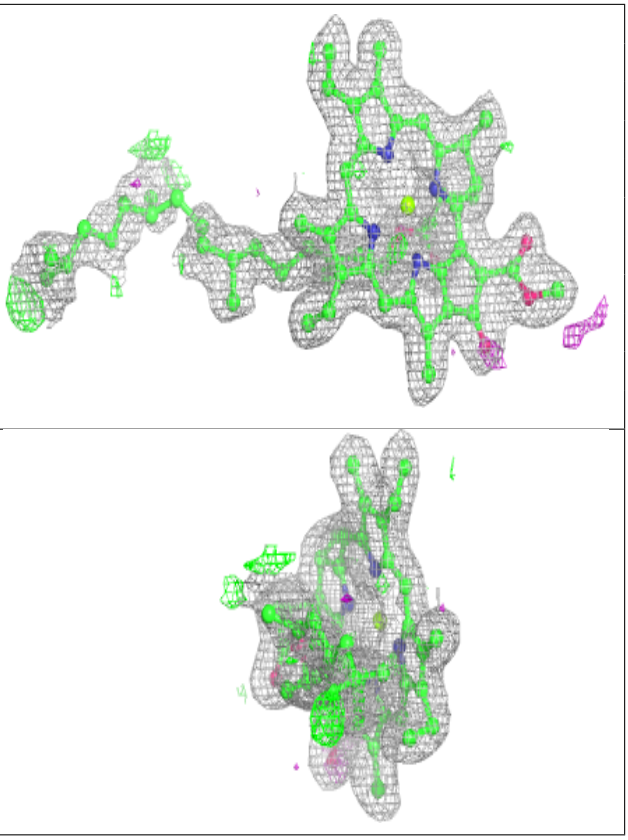






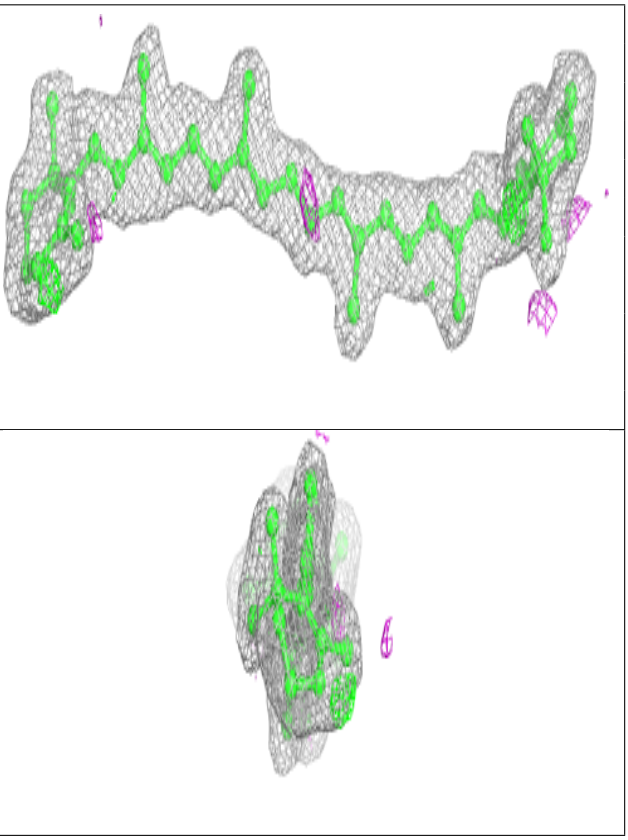
Electron density around CLA B 615:

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



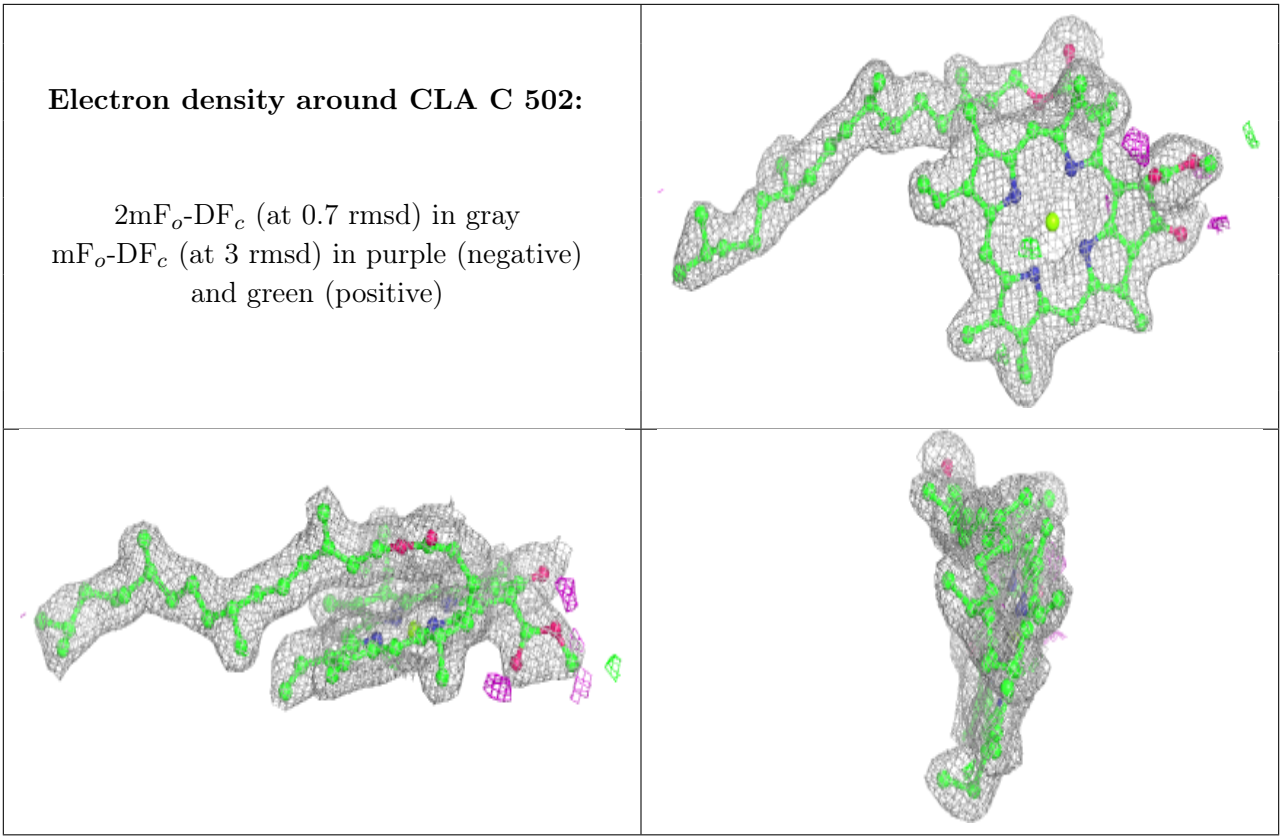
Electron density around BCR A 411:

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



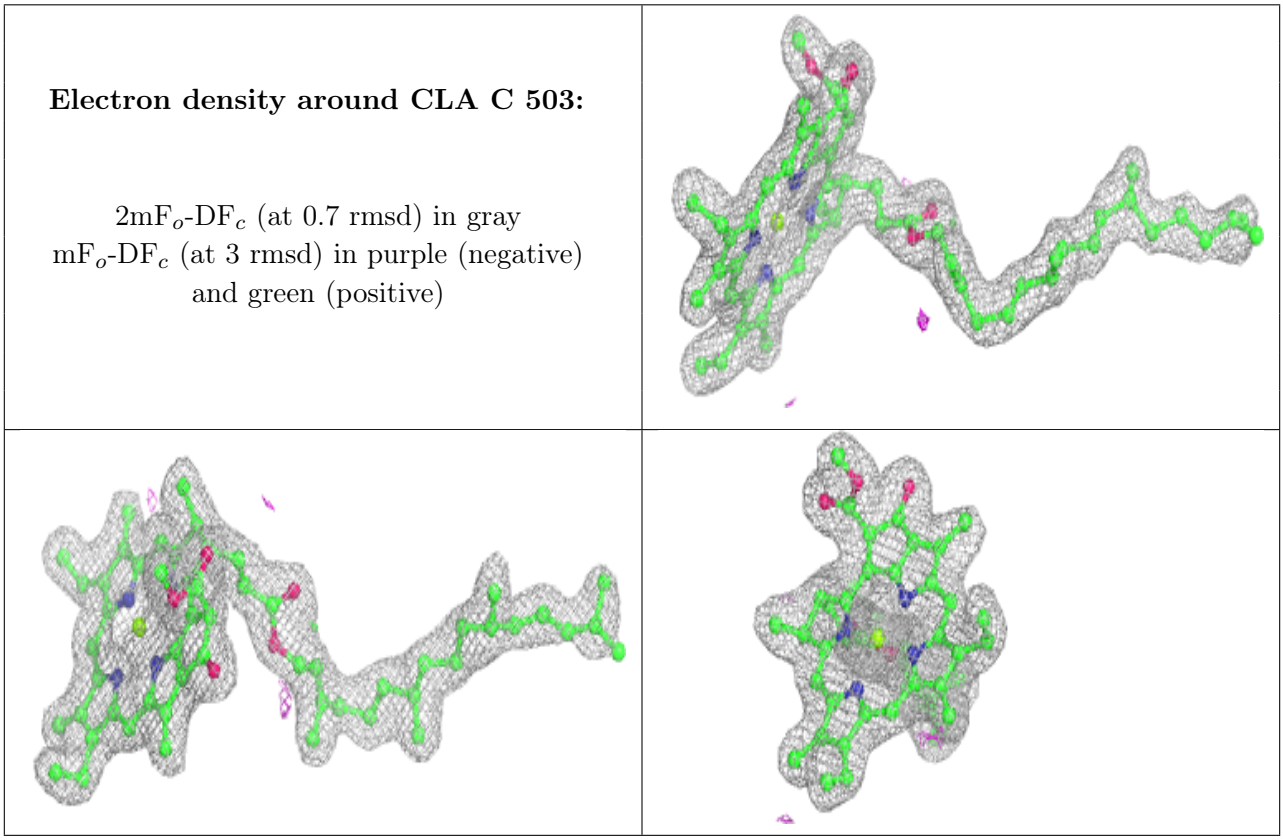
Electron density around CLA C 502:

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



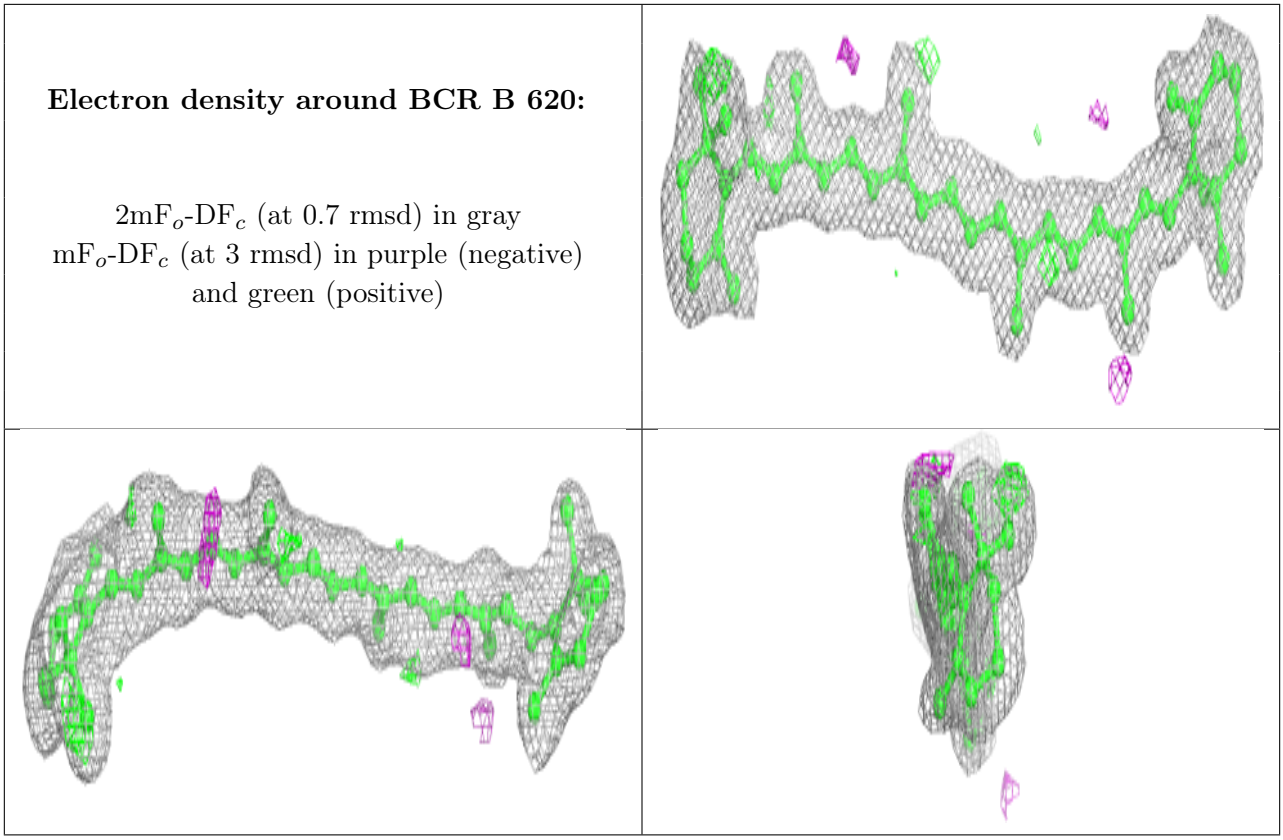
Electron density around CLA C 503:

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



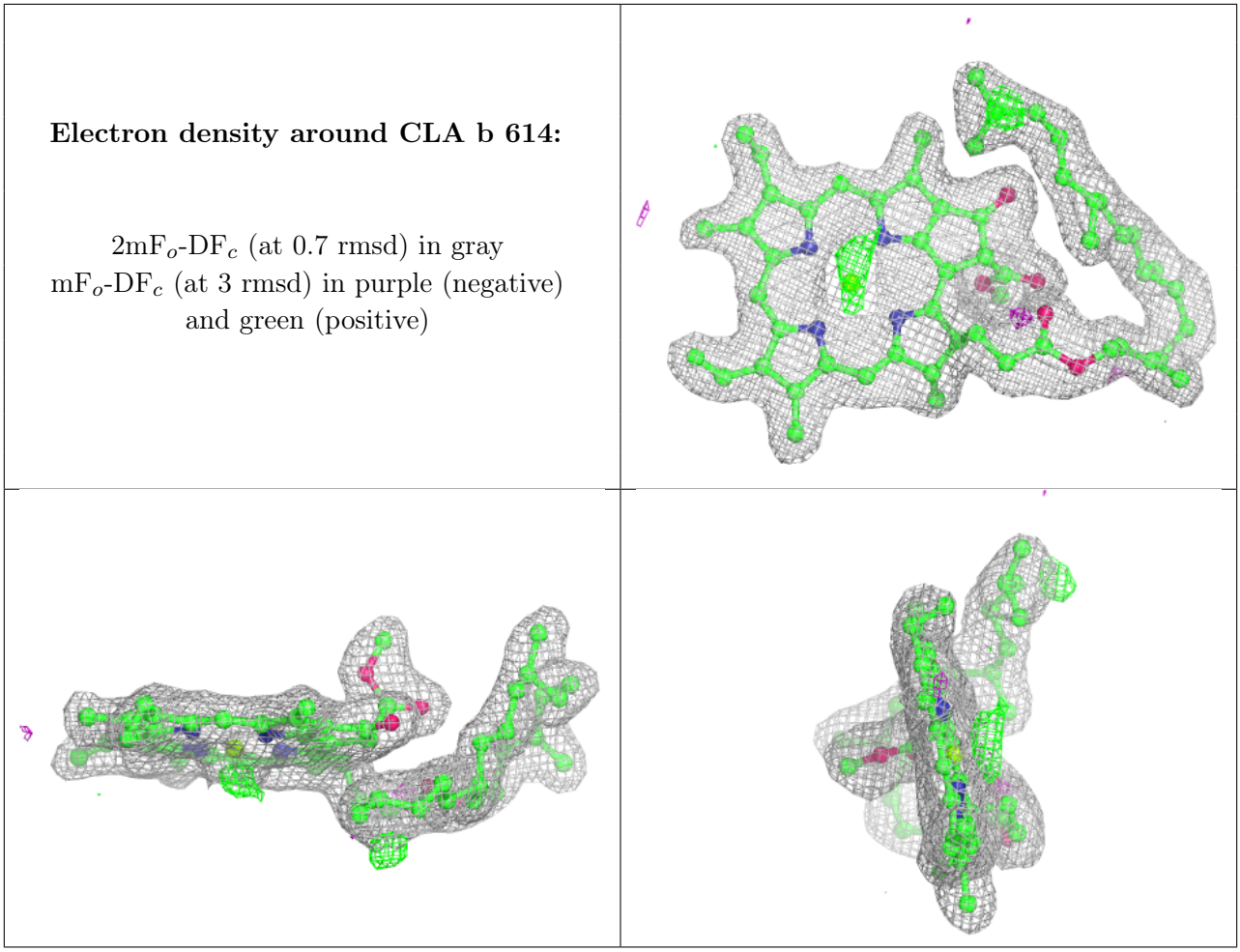
Electron density around BCR B 620:

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



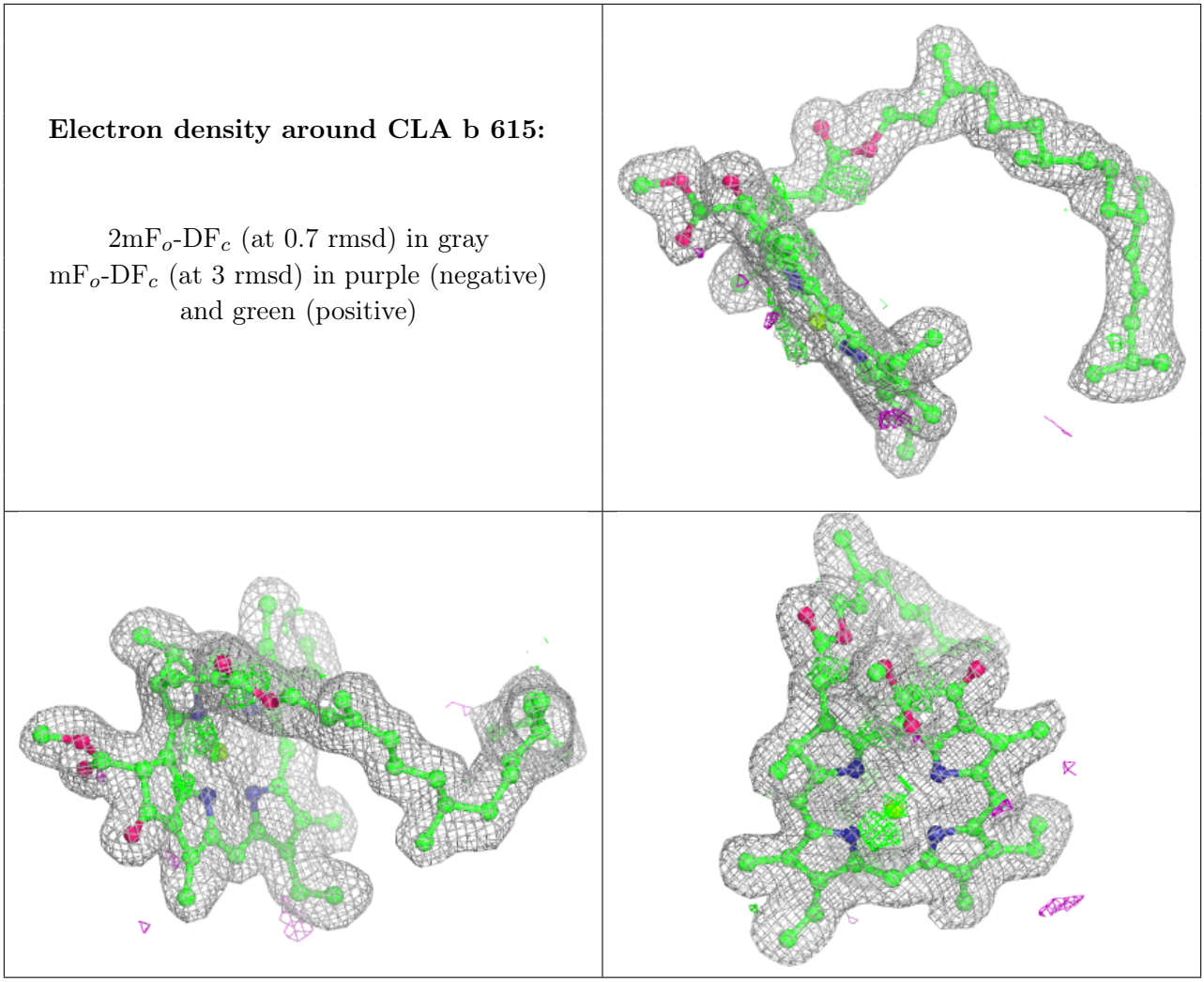
Electron density around CLA b 614:

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



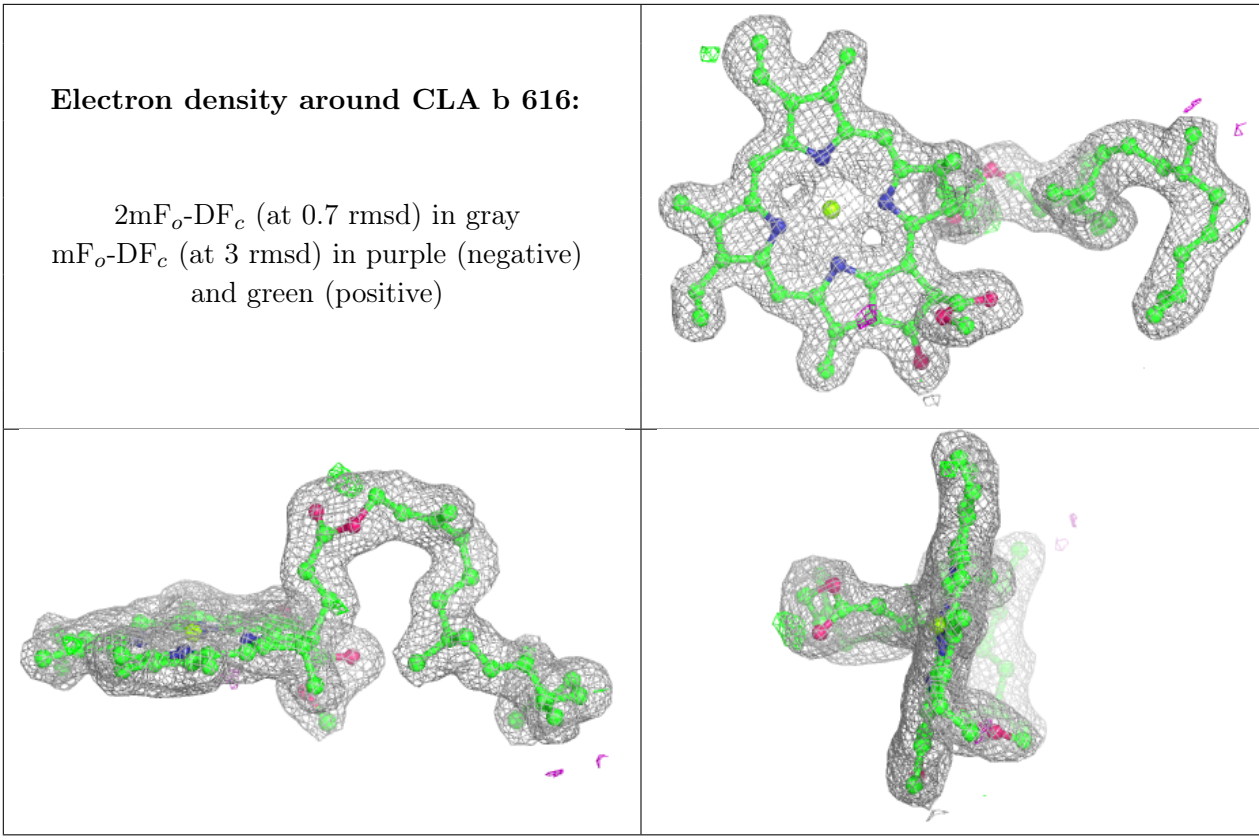
Electron density around CLA b 615:

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



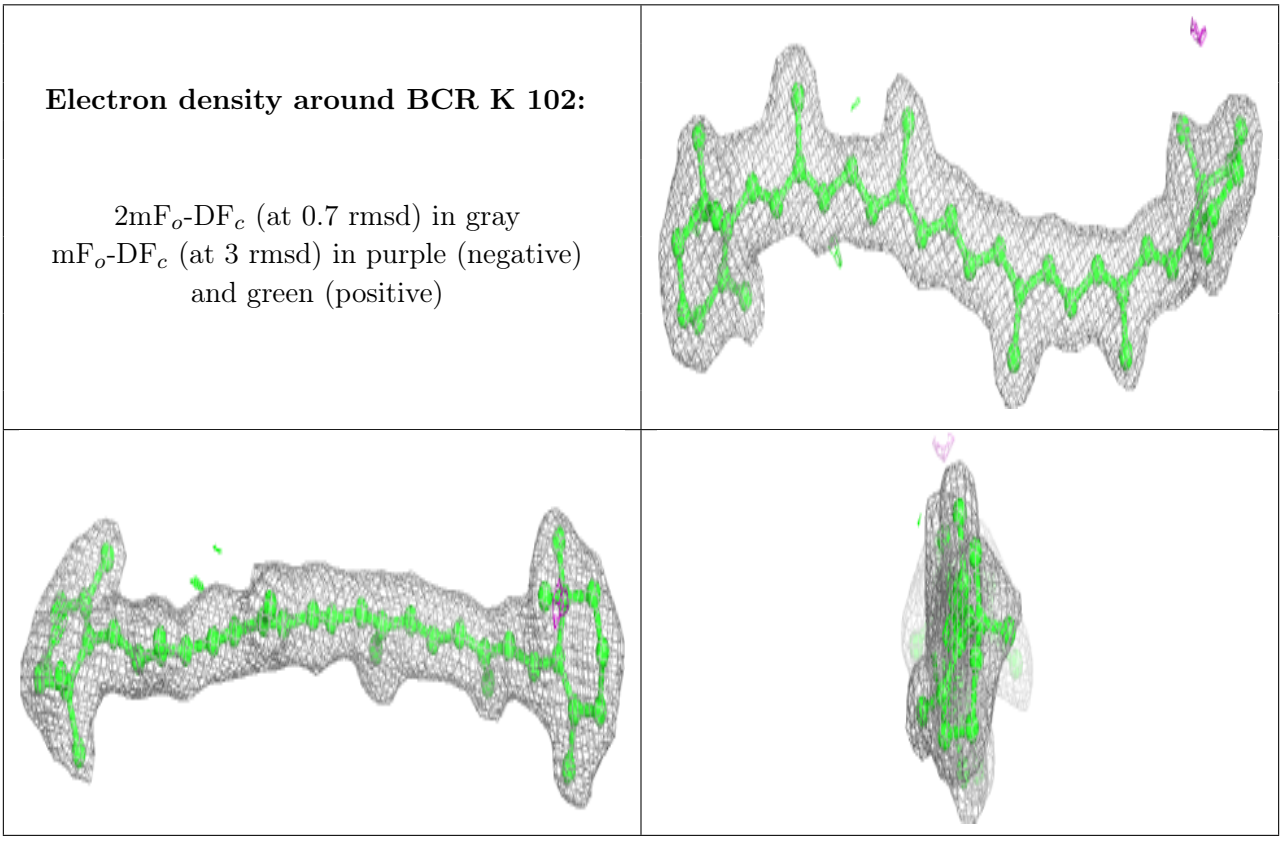
Electron density around CLA b 616:

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



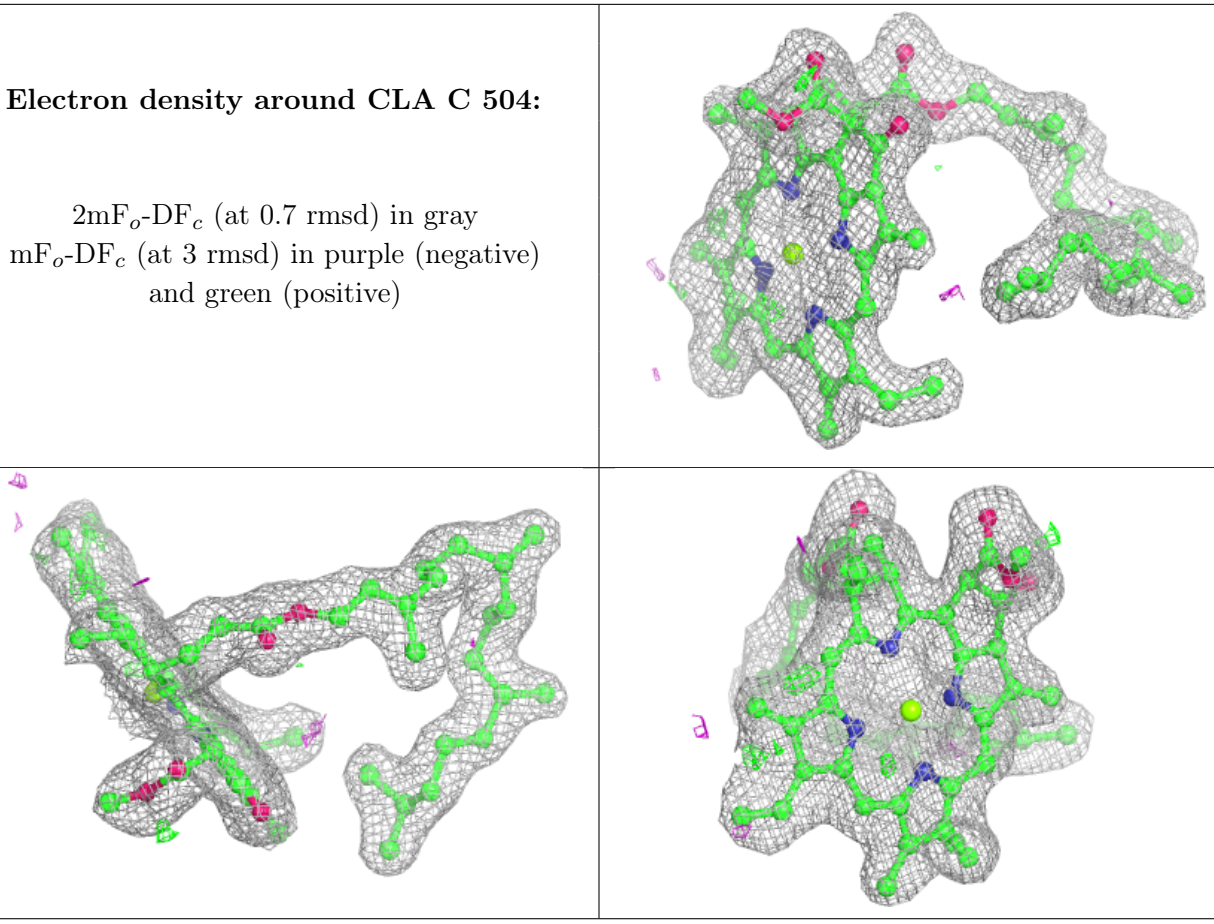
Electron density around BCR K 102:

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



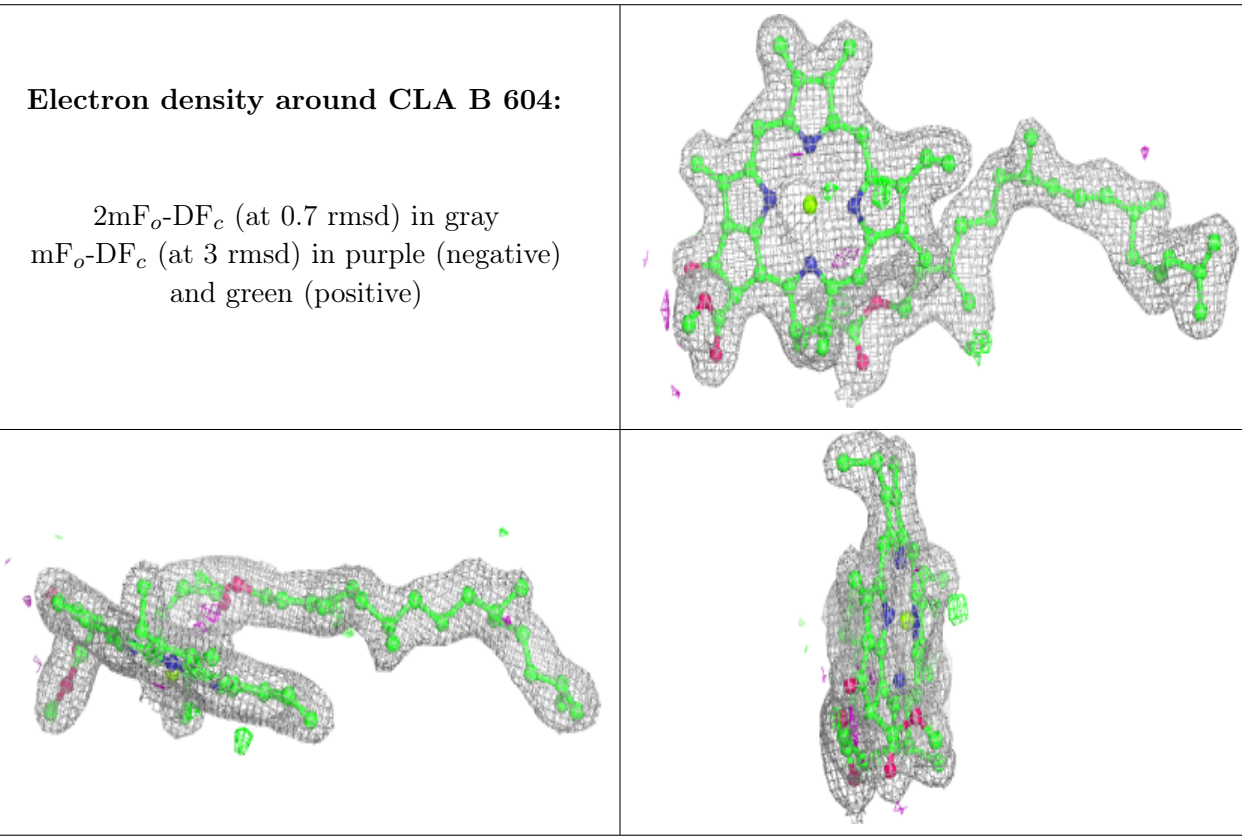
Electron density around CLA C 504:

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



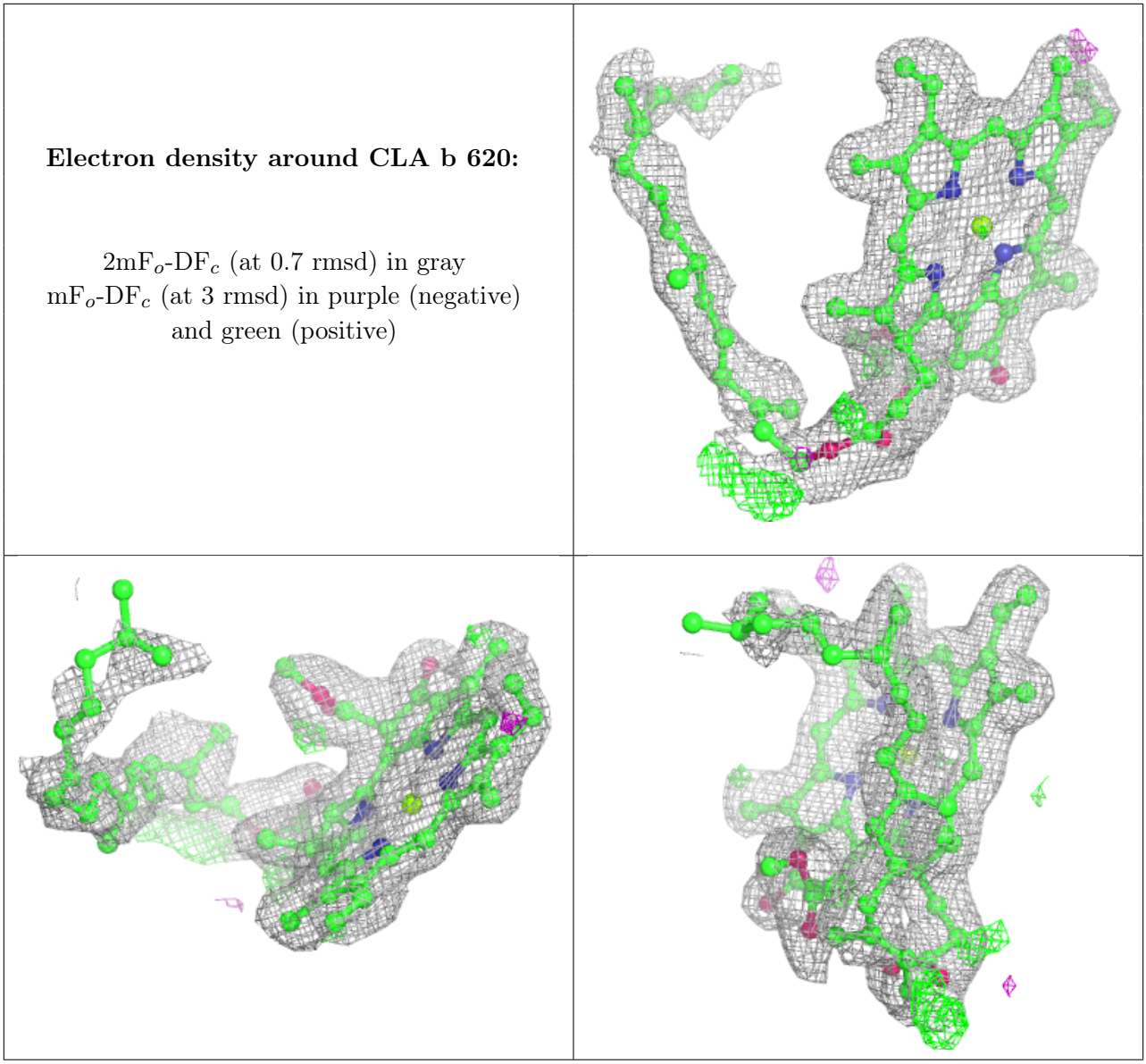
Electron density around CLA B 604:

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



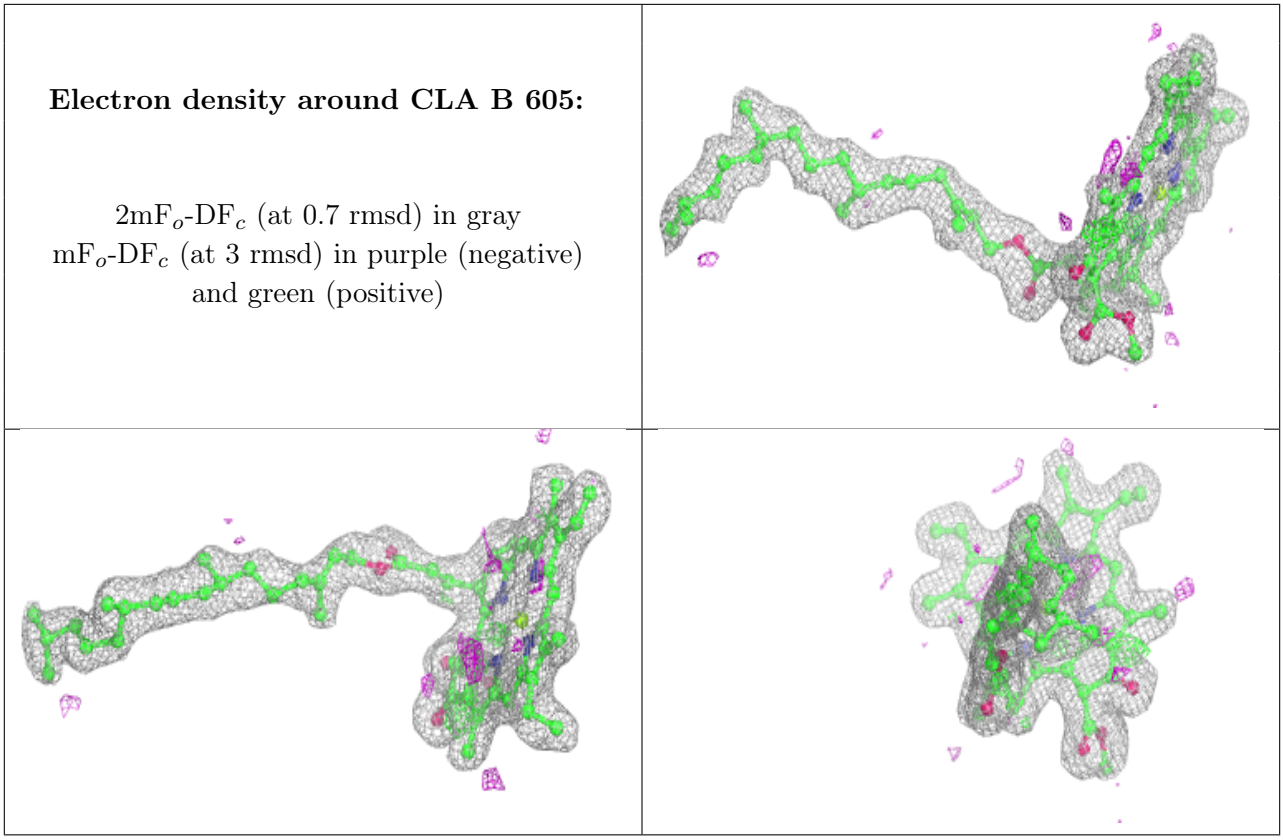
Electron density around CLA b 620:

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



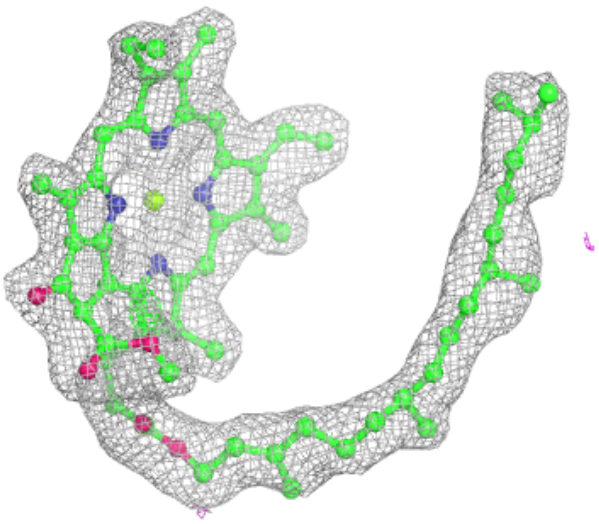
Electron density around CLA B 605:

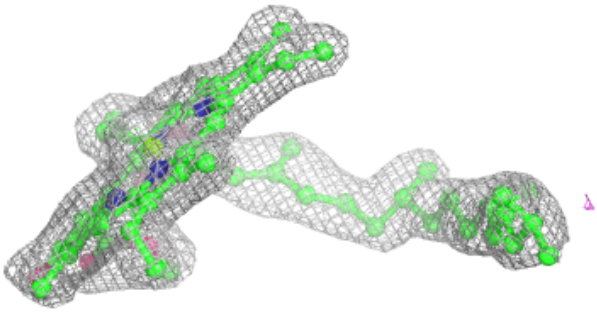
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

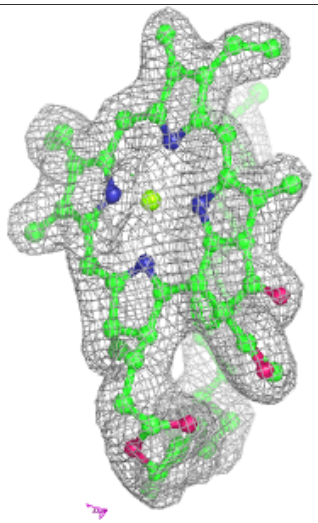


Electron density around CLA C 508:

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

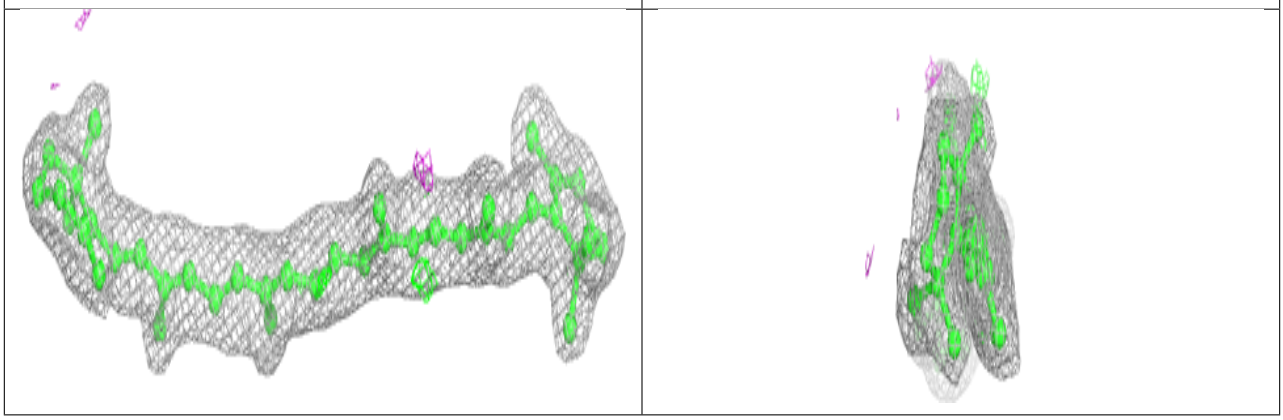






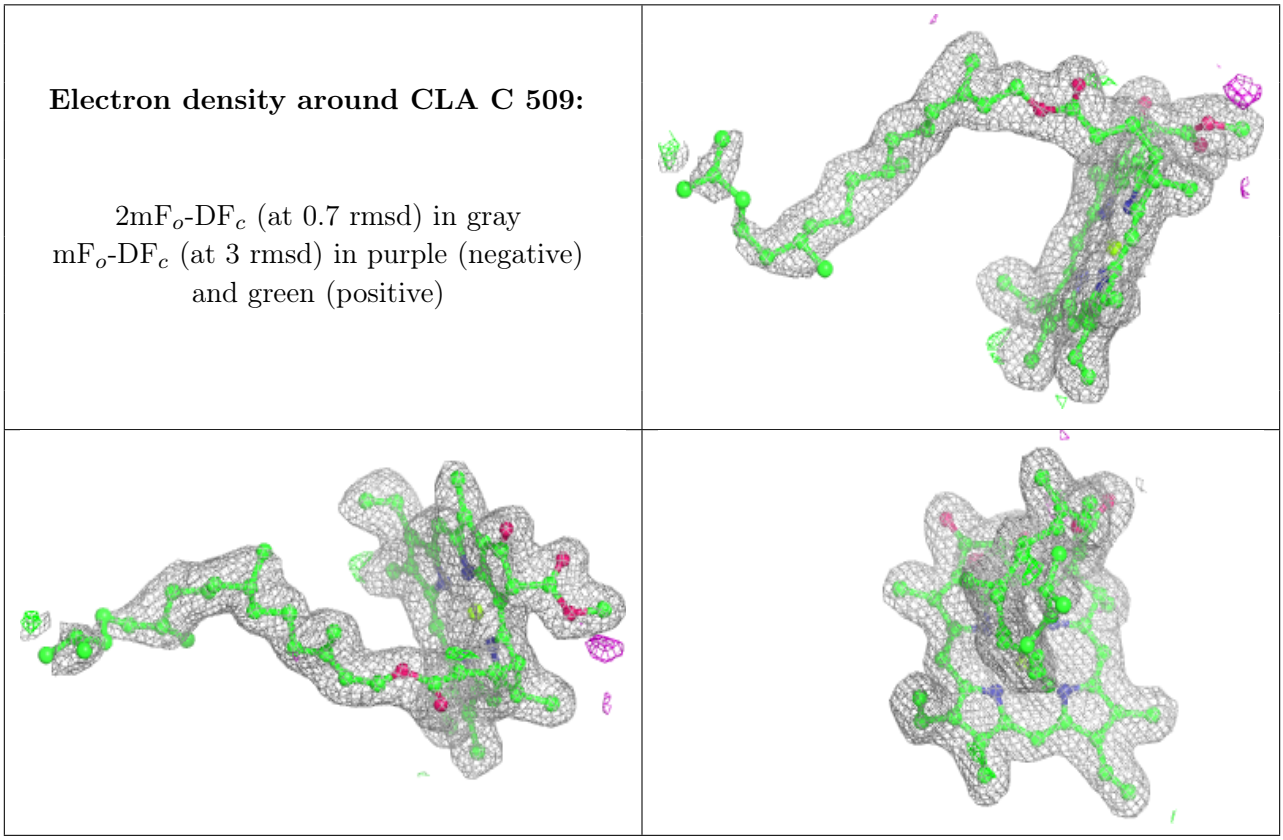
Electron density around BCR b 623:

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



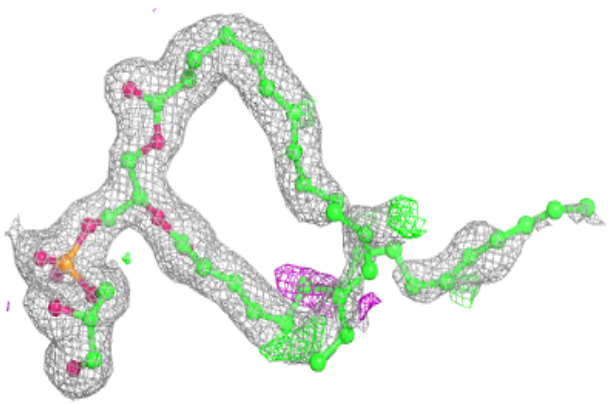
Electron density around CLA C 509:

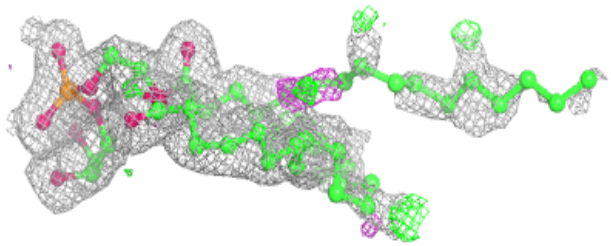
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

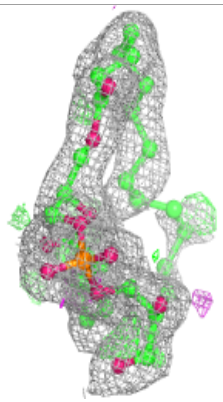


Electron density around LHG D 408:

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

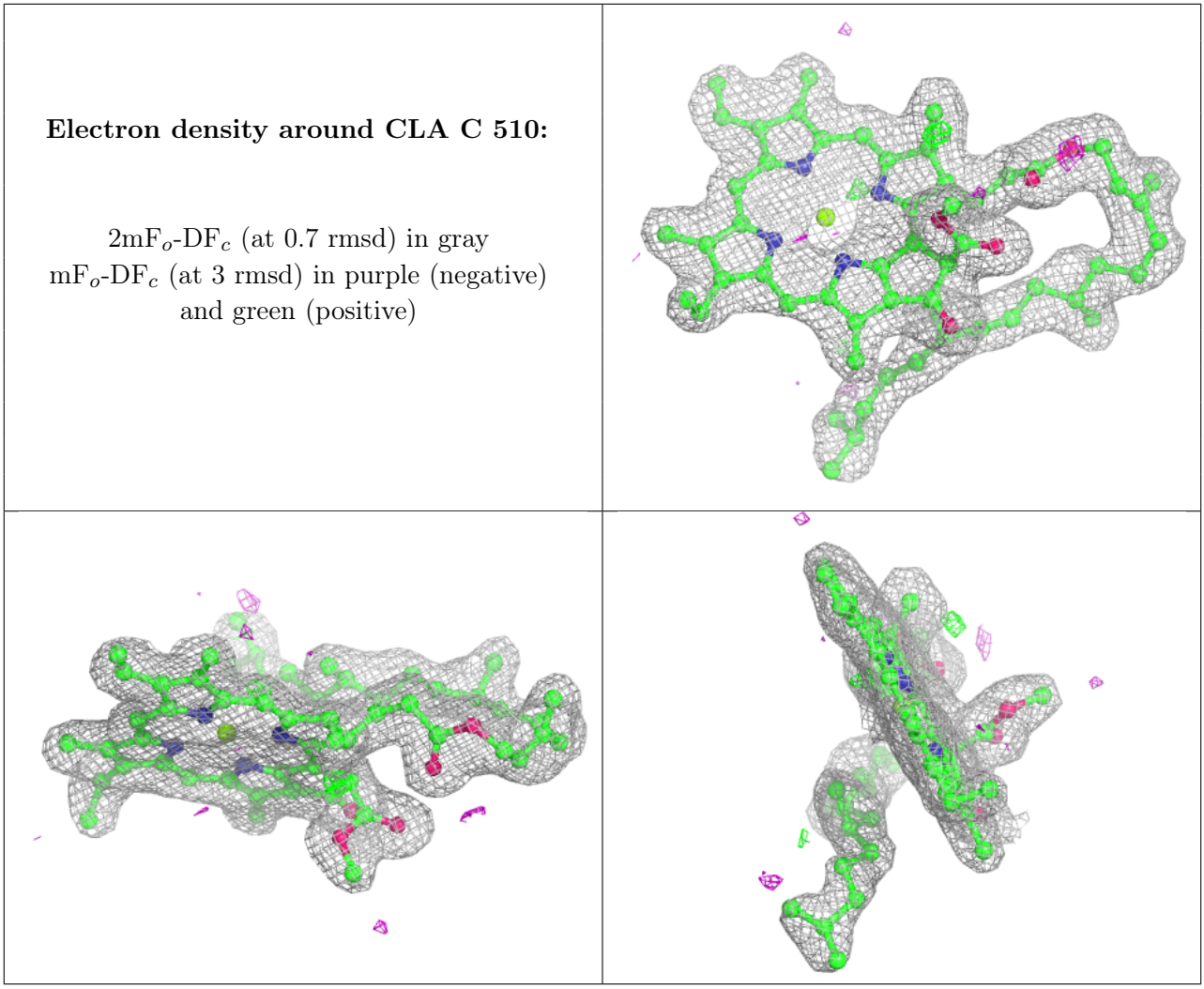






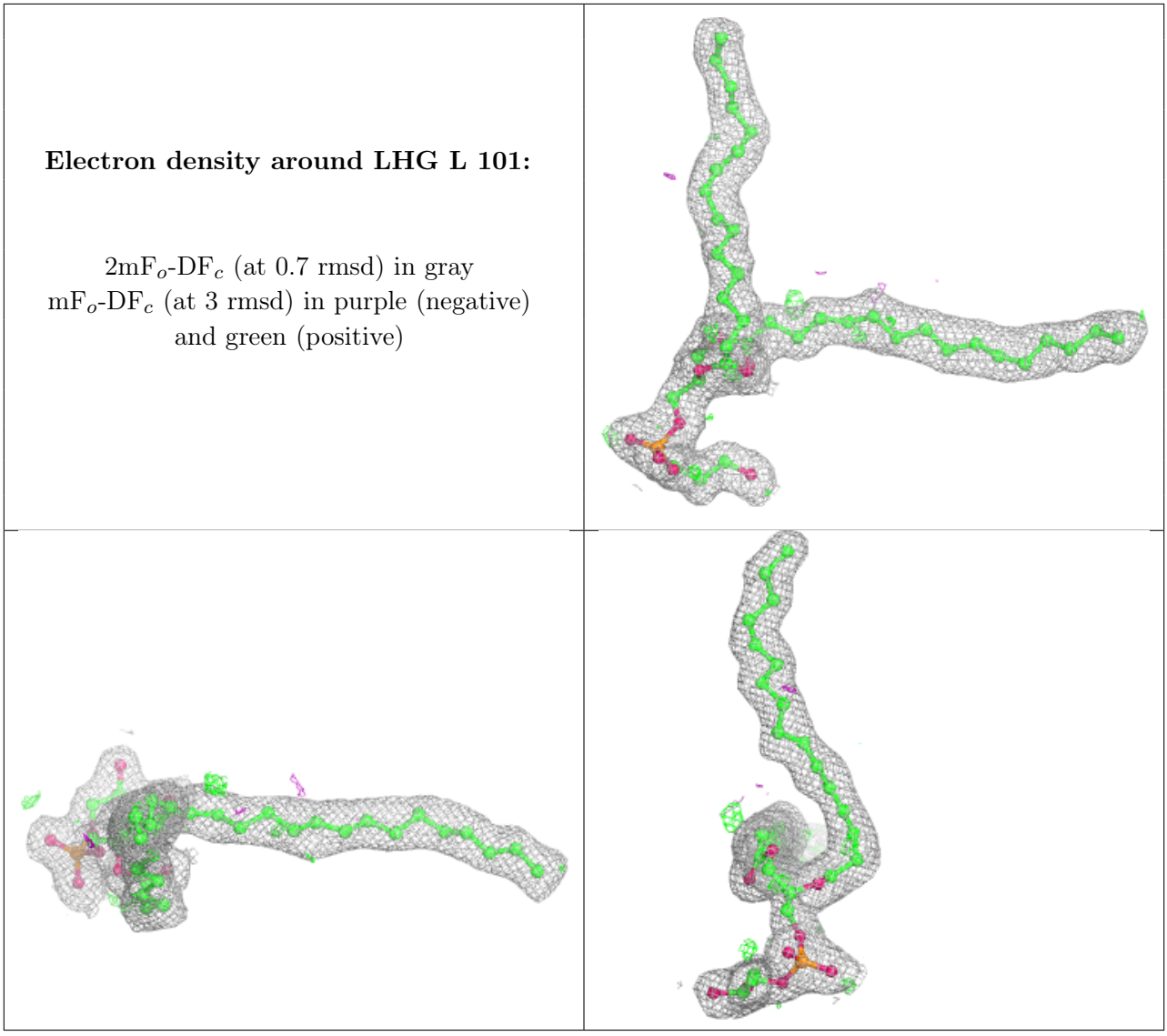
Electron density around CLA C 510:

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



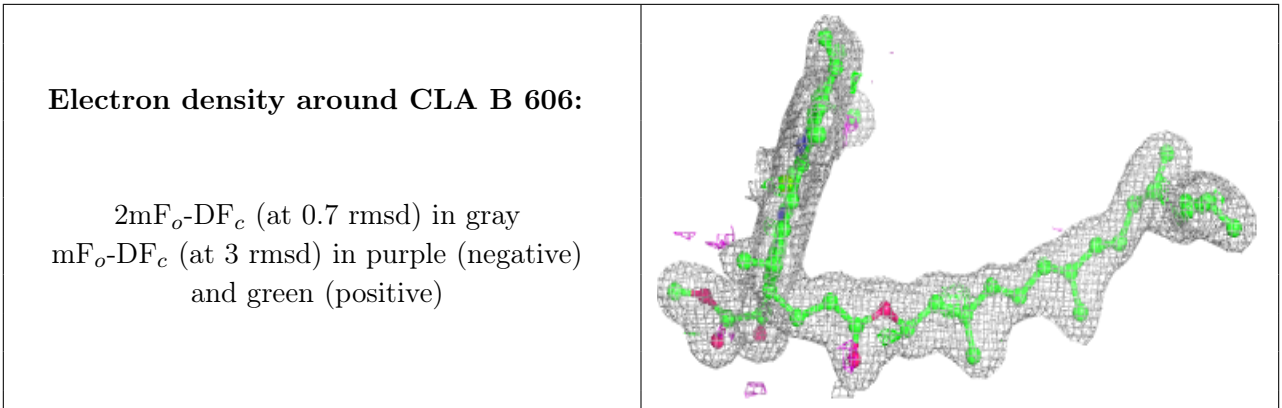
Electron density around LHG L 101:

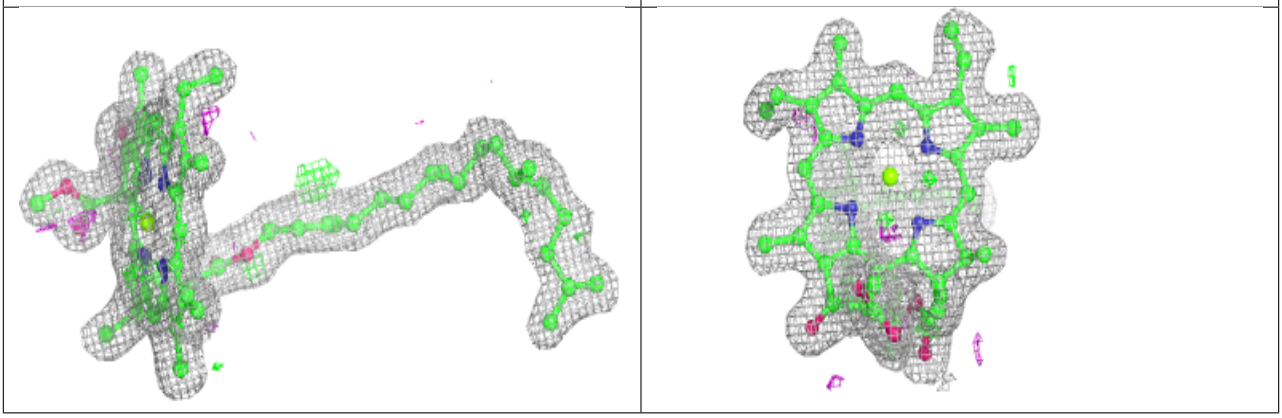
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 606:

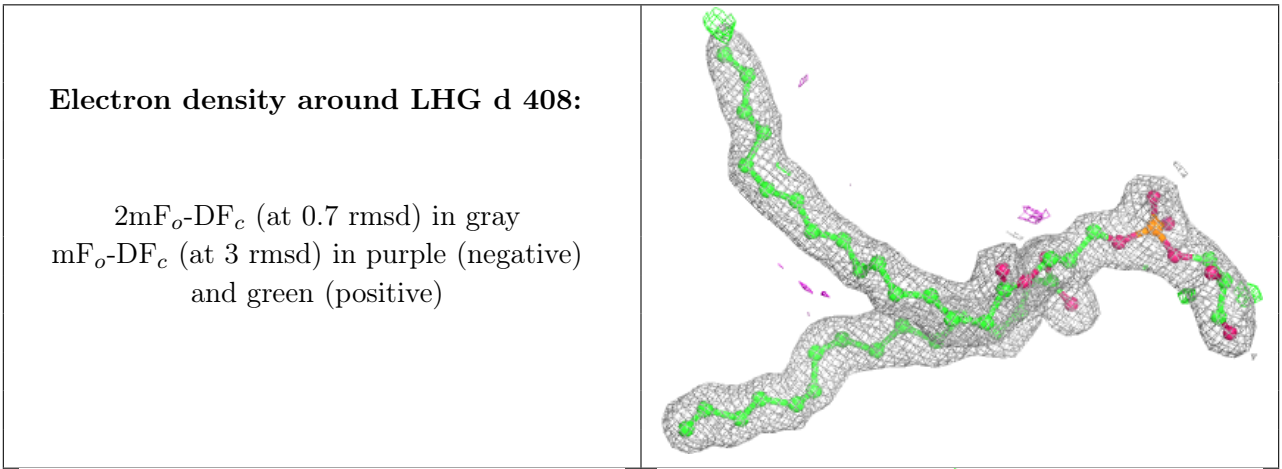
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

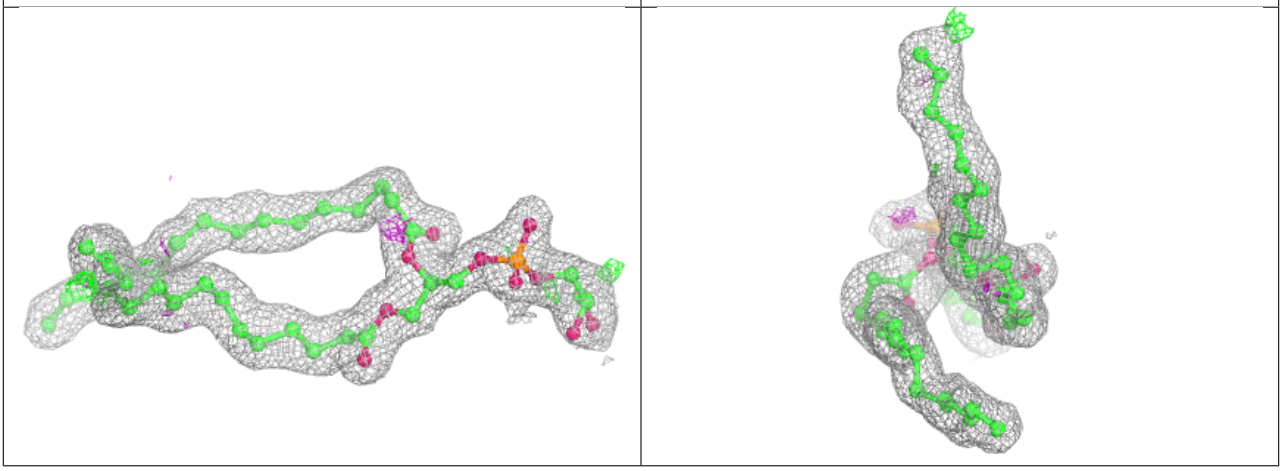




Electron density around LHG d 408:

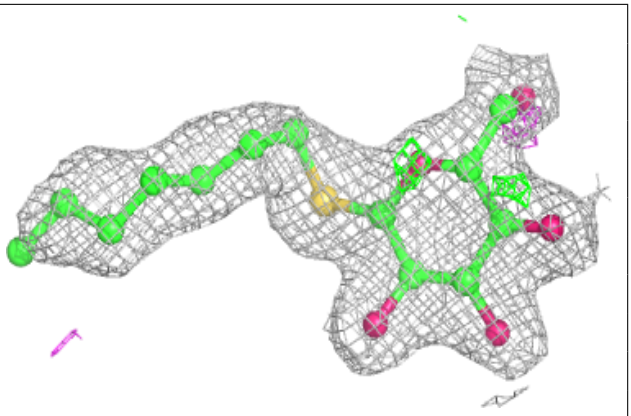
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

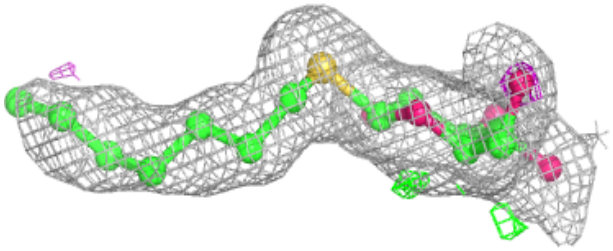


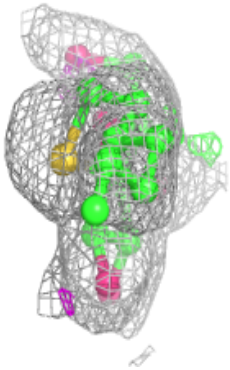


Electron density around HTG O 303:

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

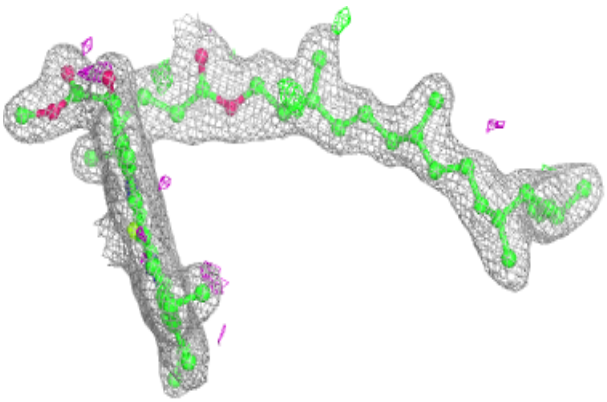


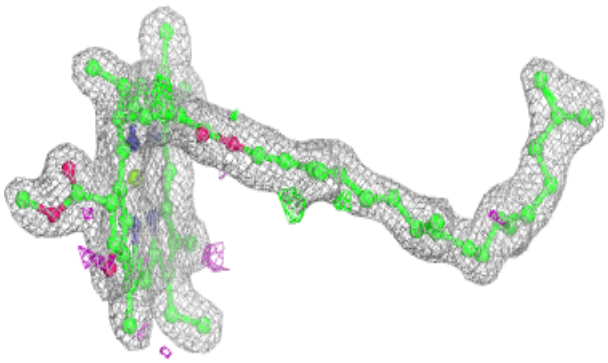


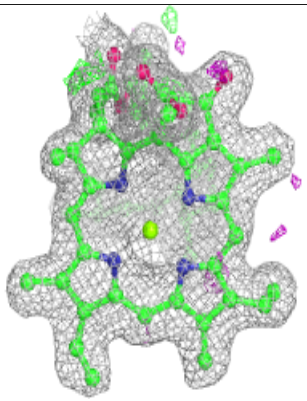


Electron density around CLA b 609:

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

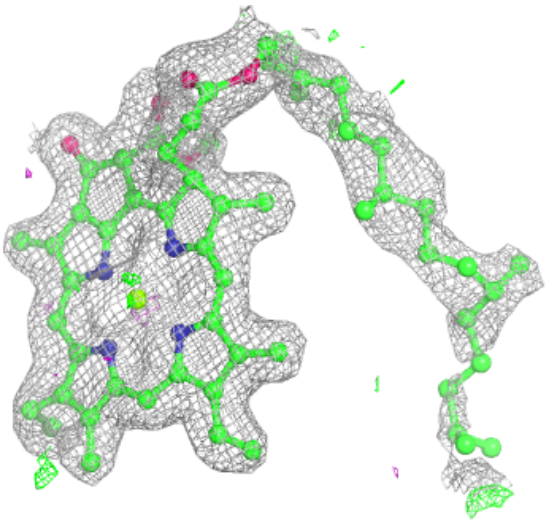


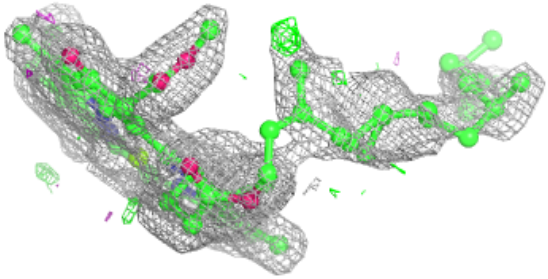


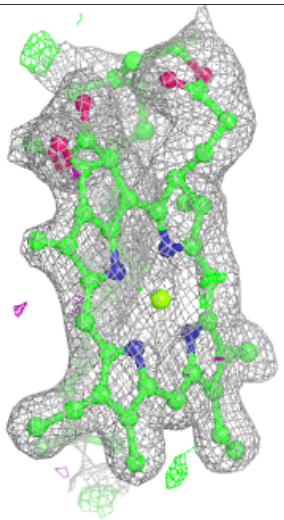


Electron density around CLA B 617:

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

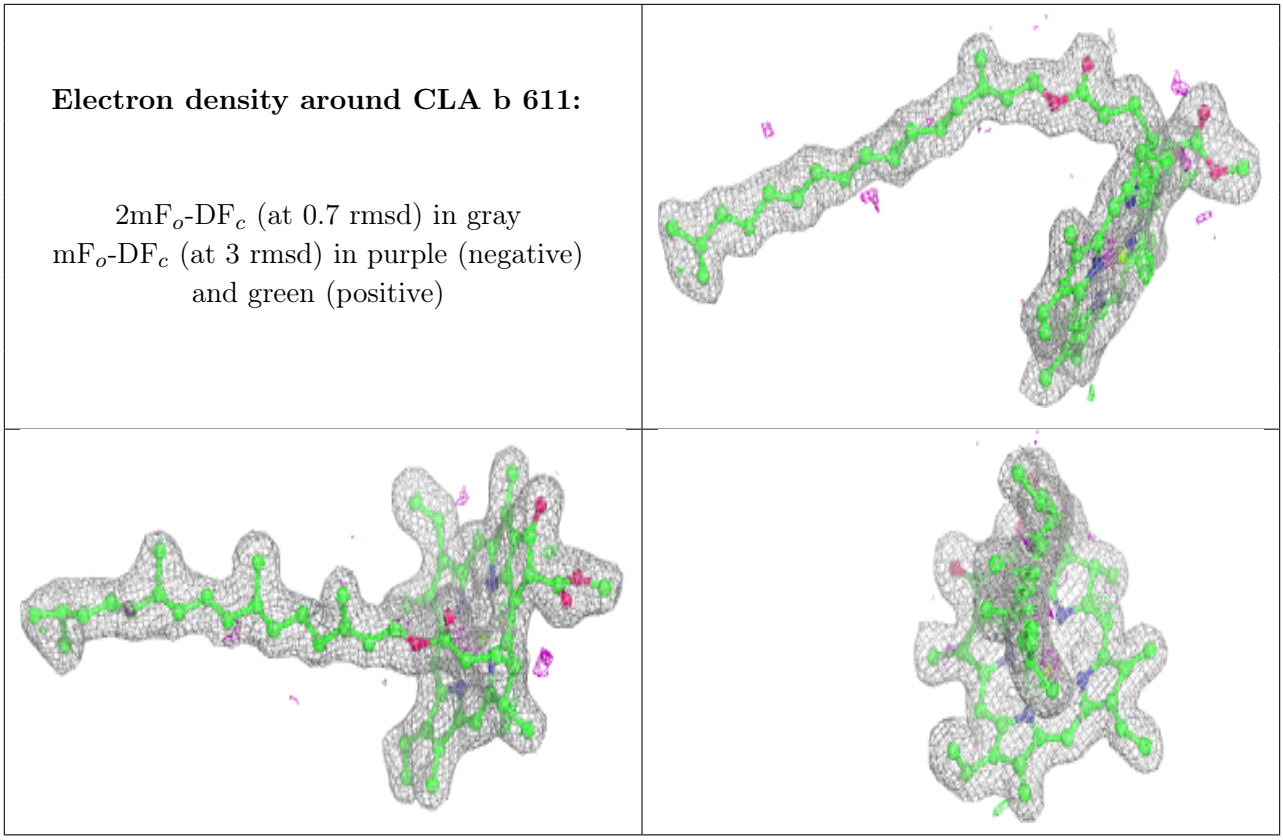






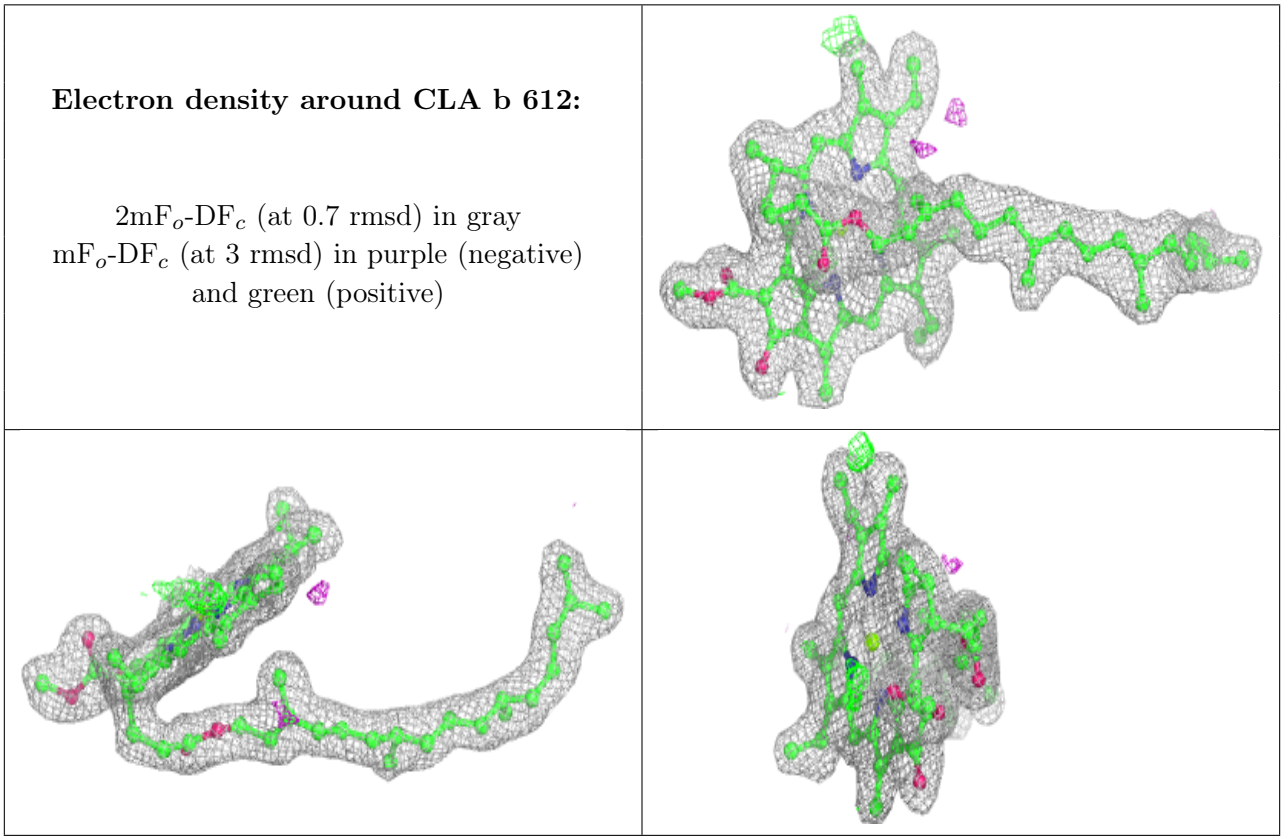
Electron density around CLA b 611:

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



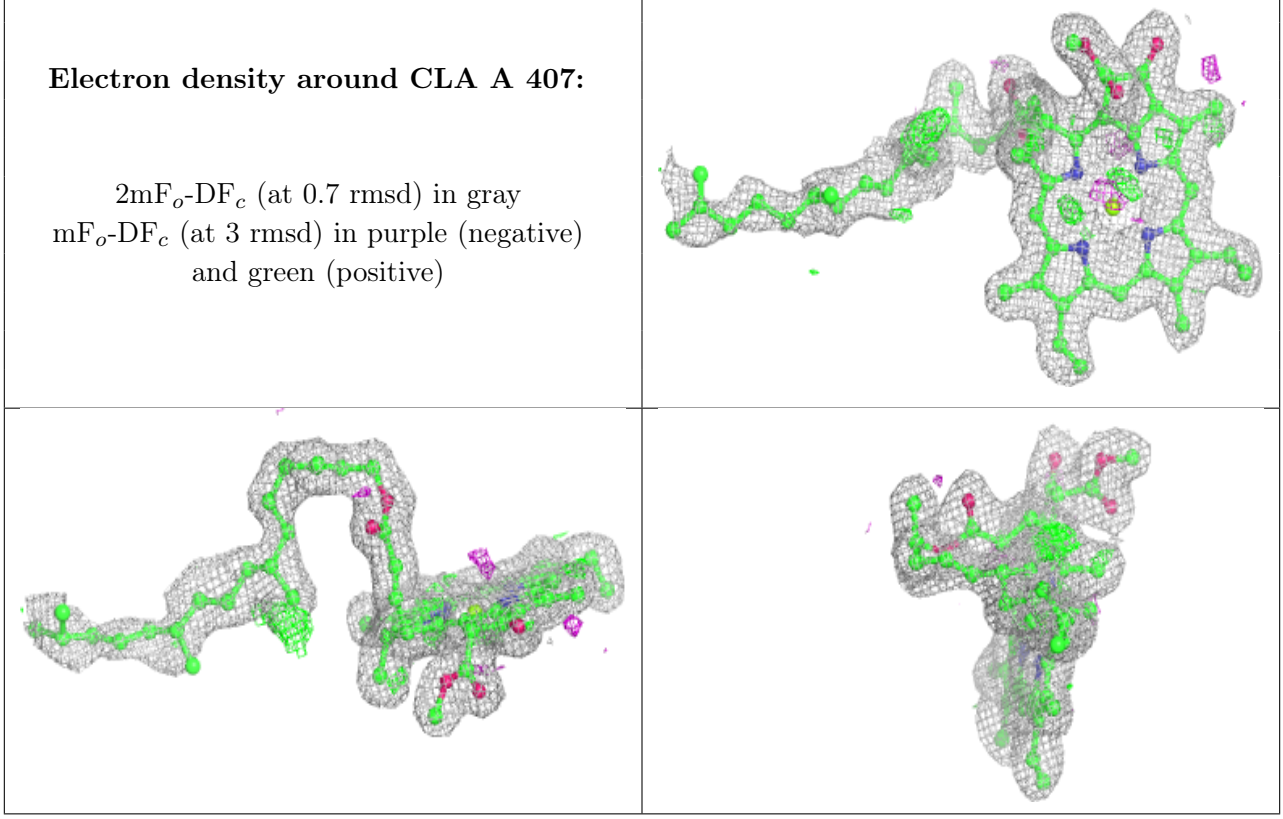
Electron density around CLA b 612:

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



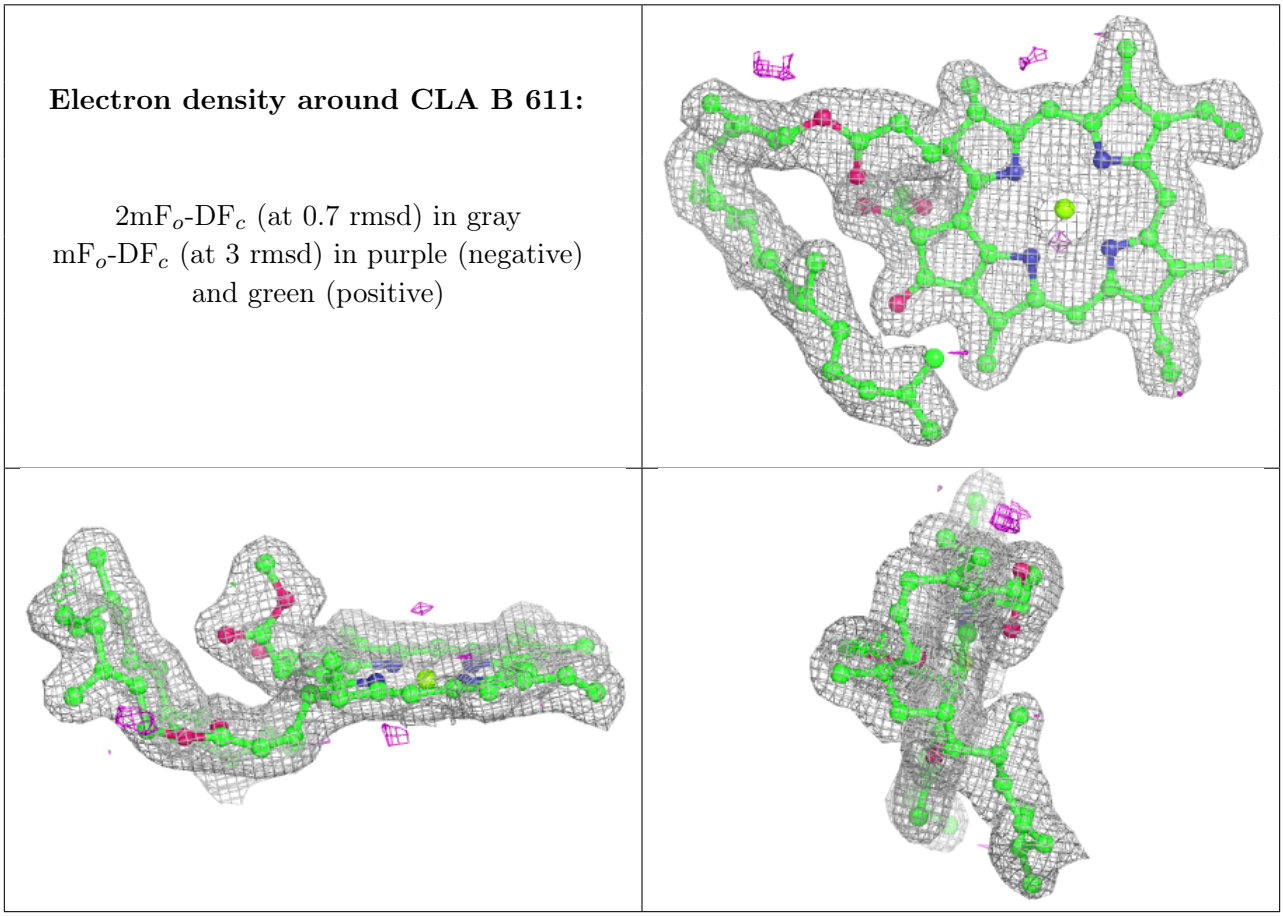
Electron density around CLA A 407:

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



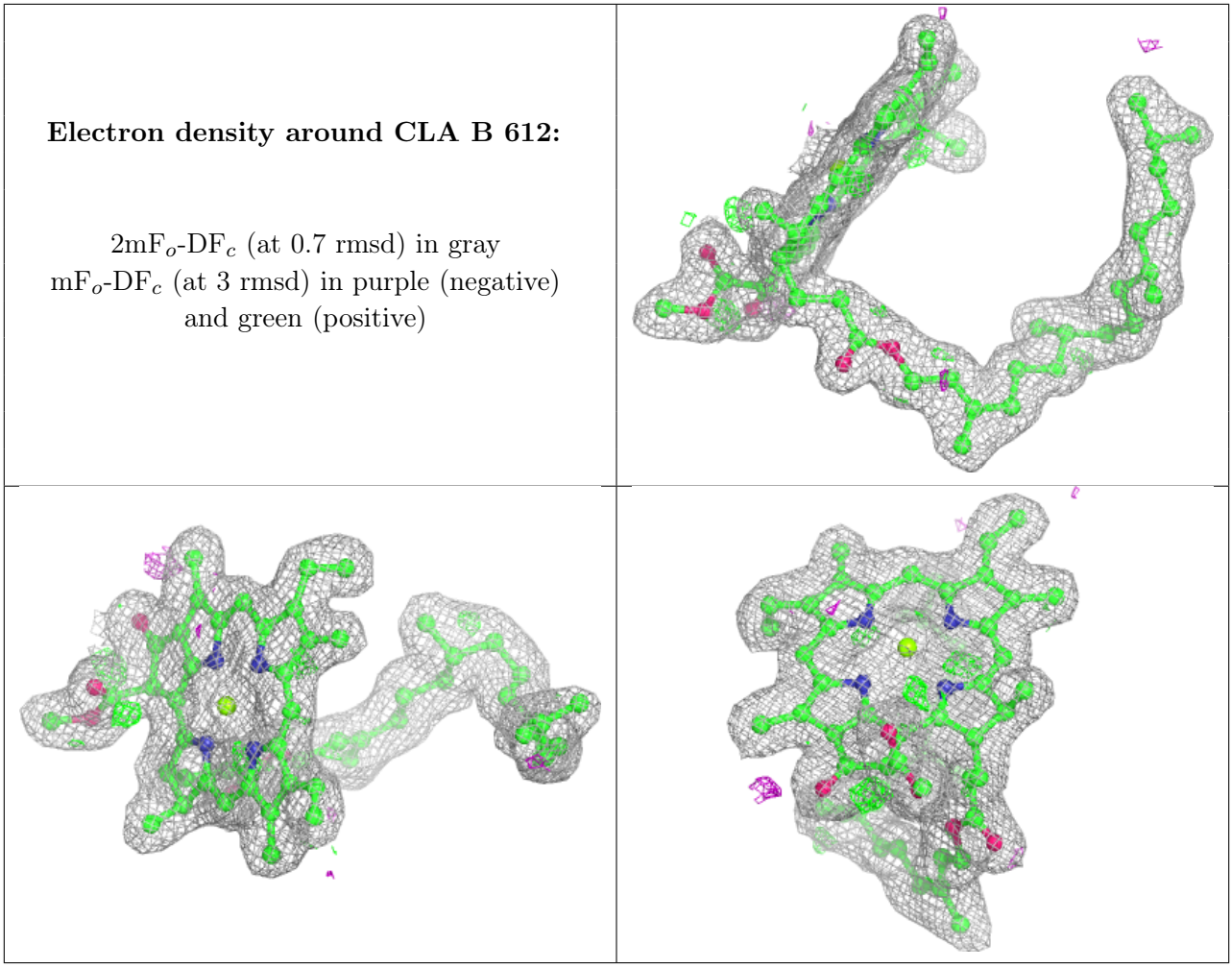
Electron density around CLA B 611:

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



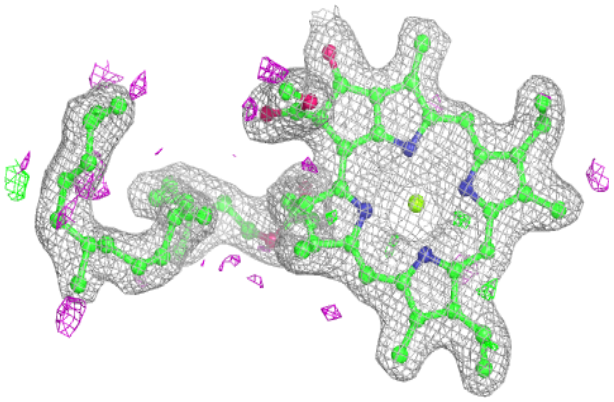
Electron density around CLA B 612:

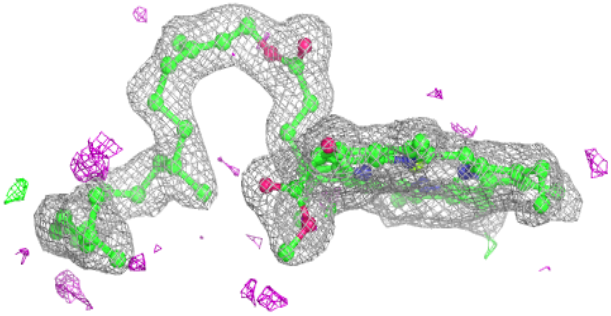
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

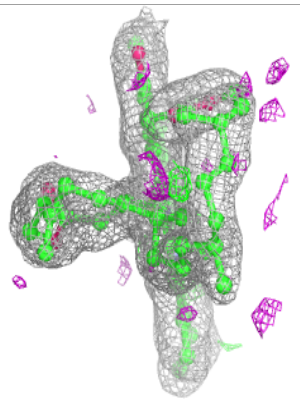


Electron density around CLA B 613:

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

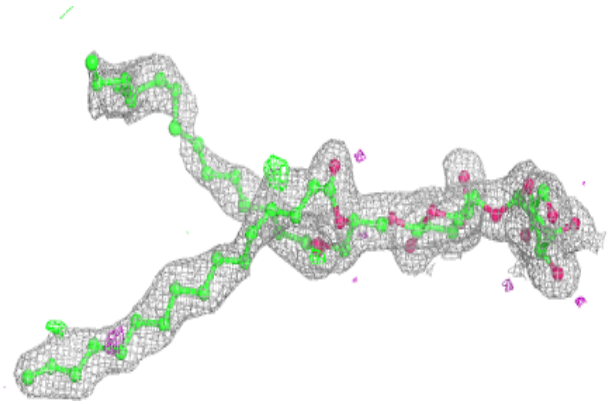


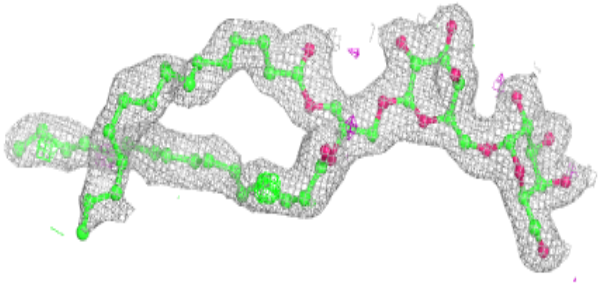


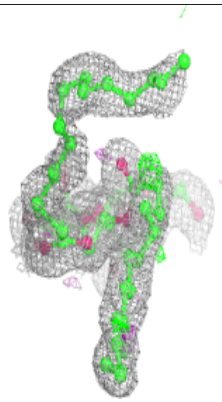


Electron density around DGD C 517:

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

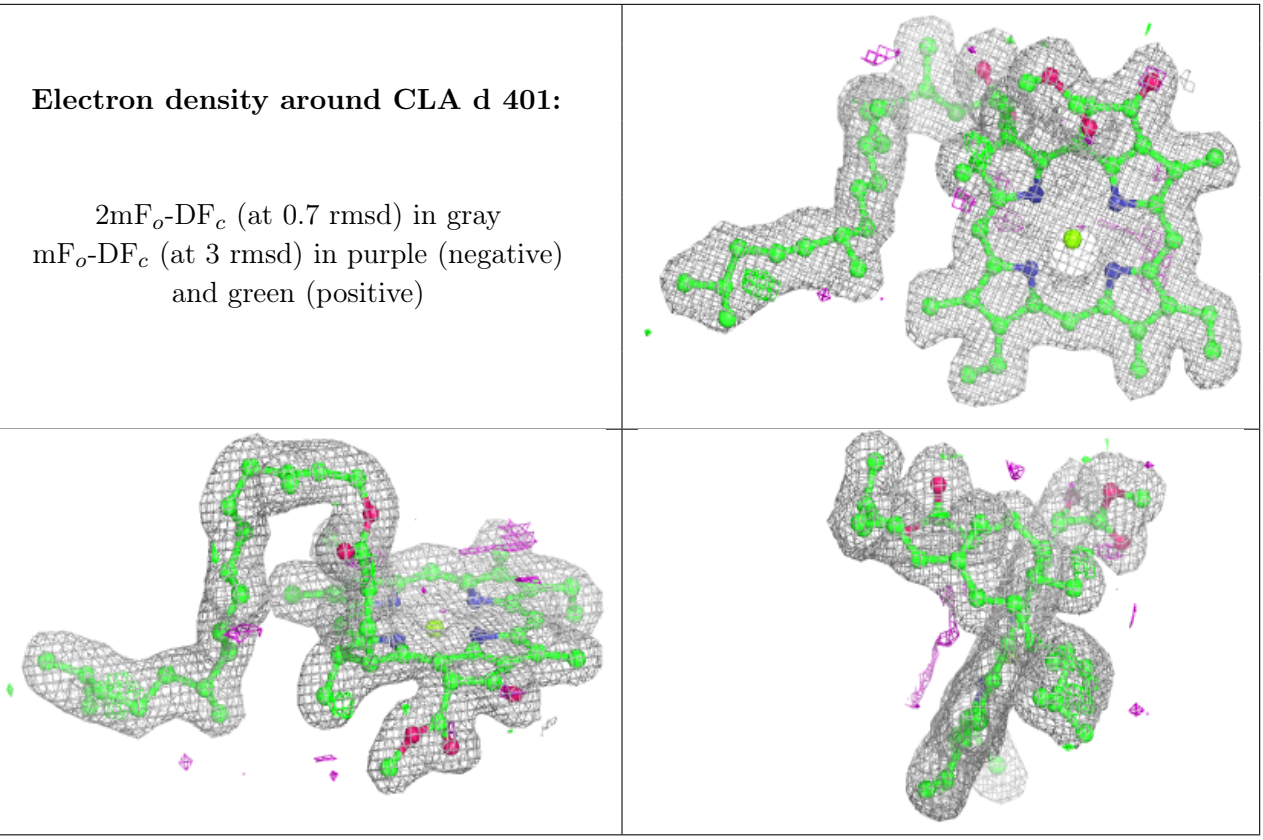






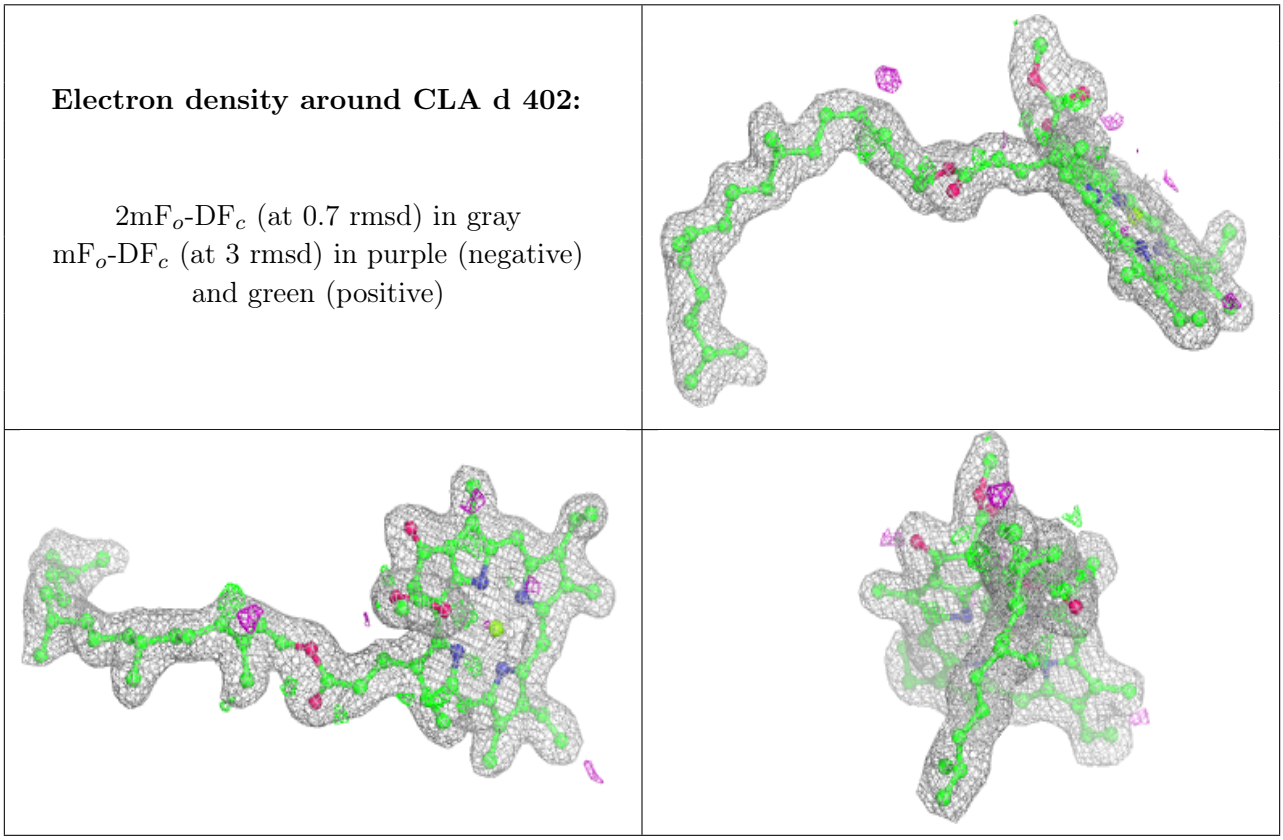
Electron density around CLA d 401:

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



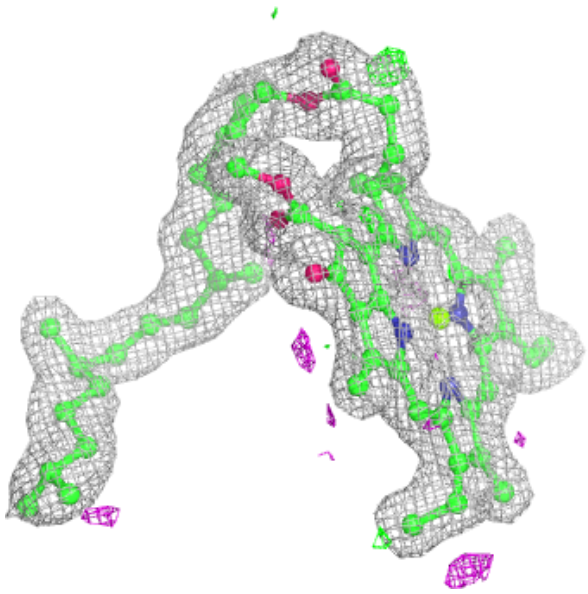
Electron density around CLA d 402:

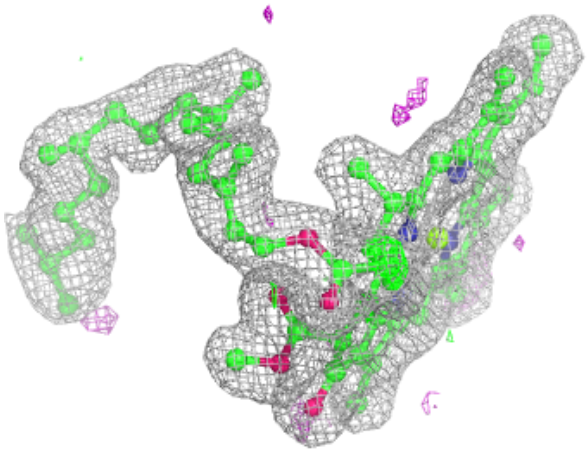
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

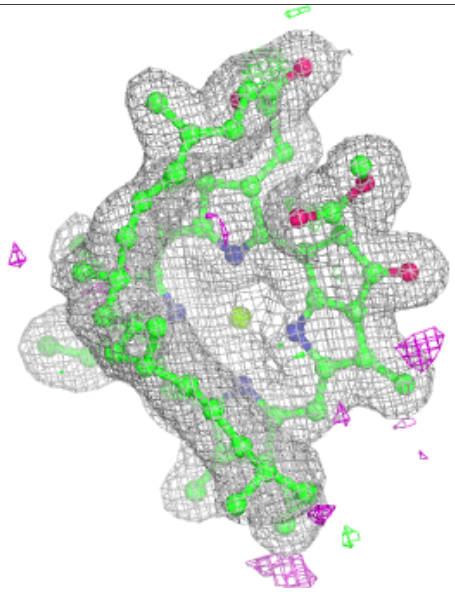


Electron density around CLA b 617:

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

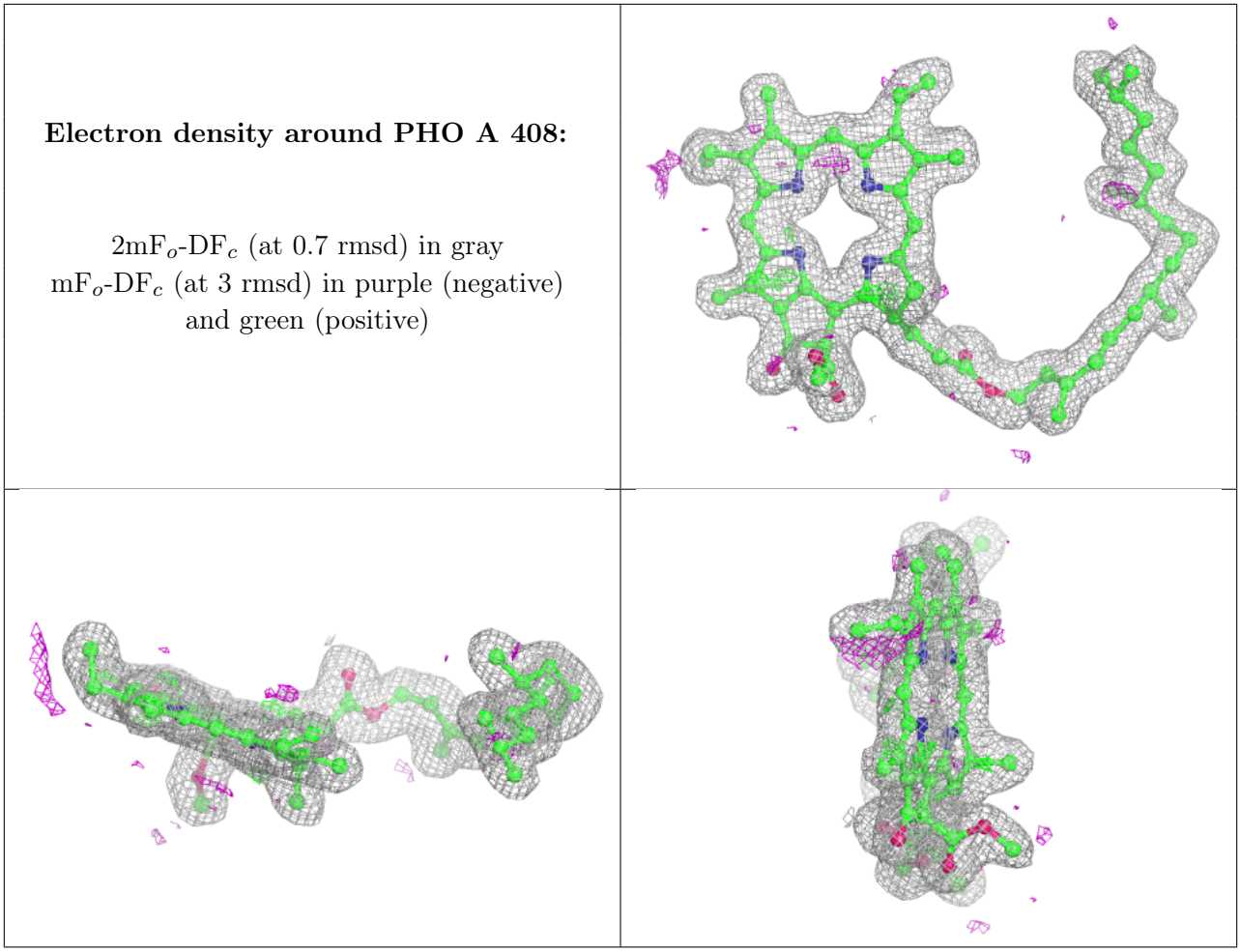






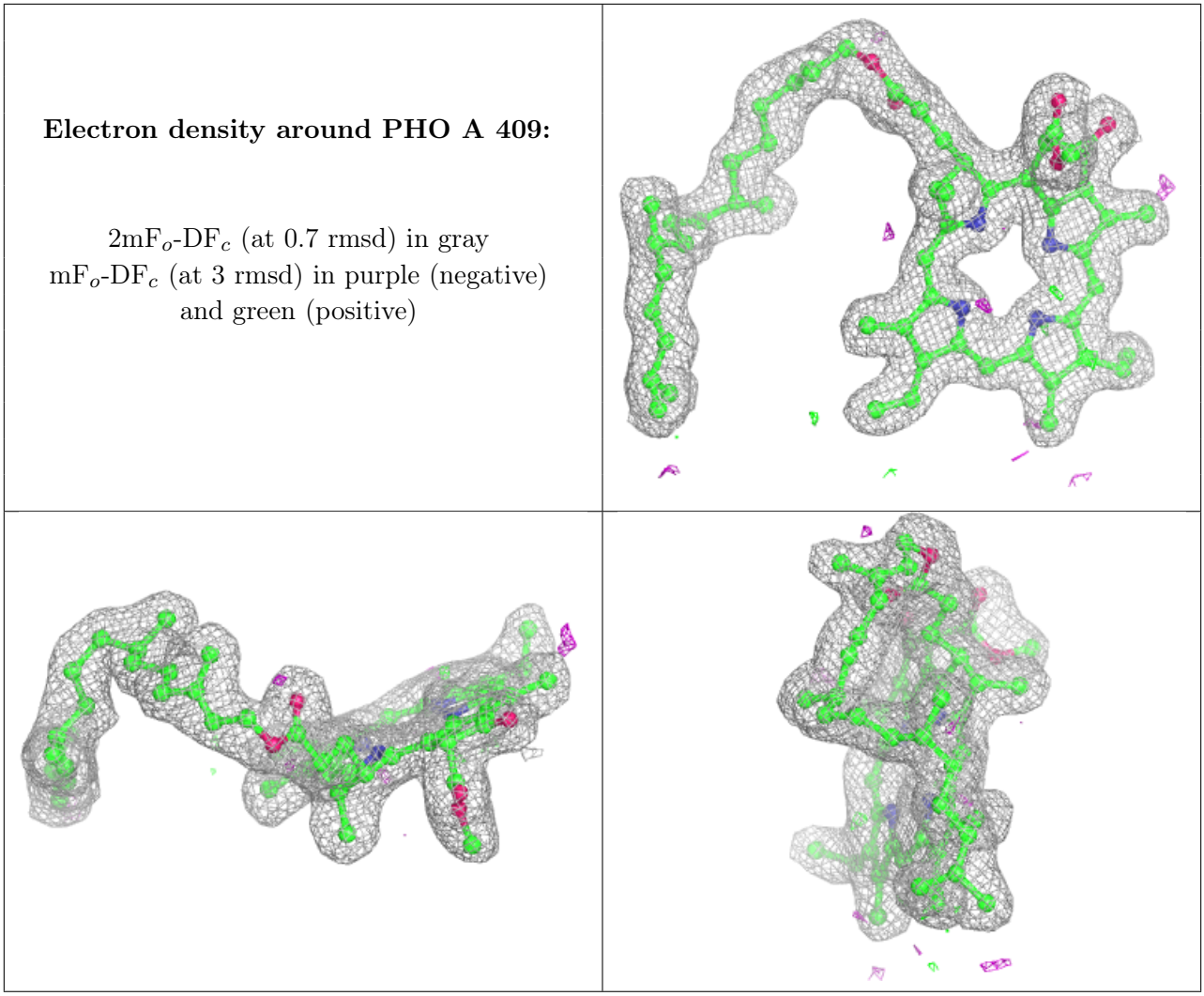
Electron density around PHO A 408:

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



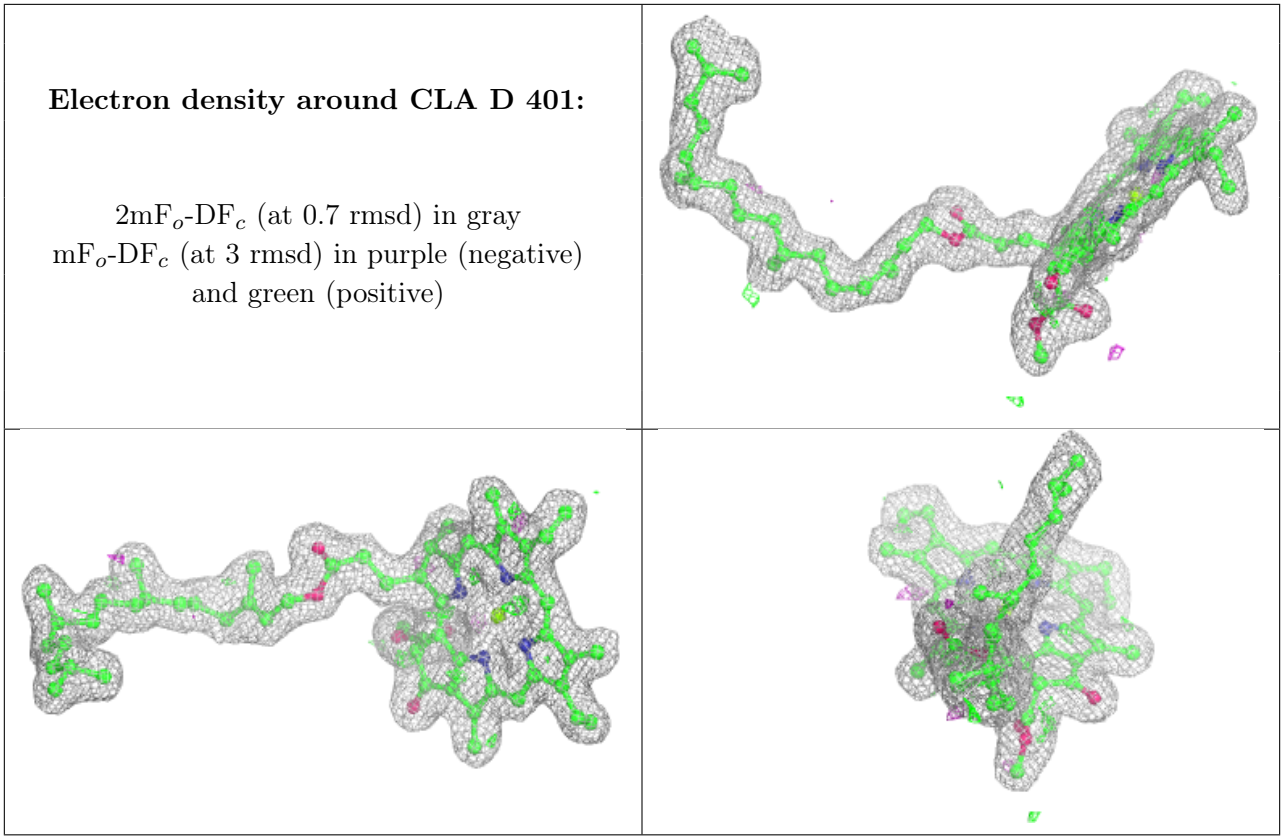
Electron density around PHO A 409:

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



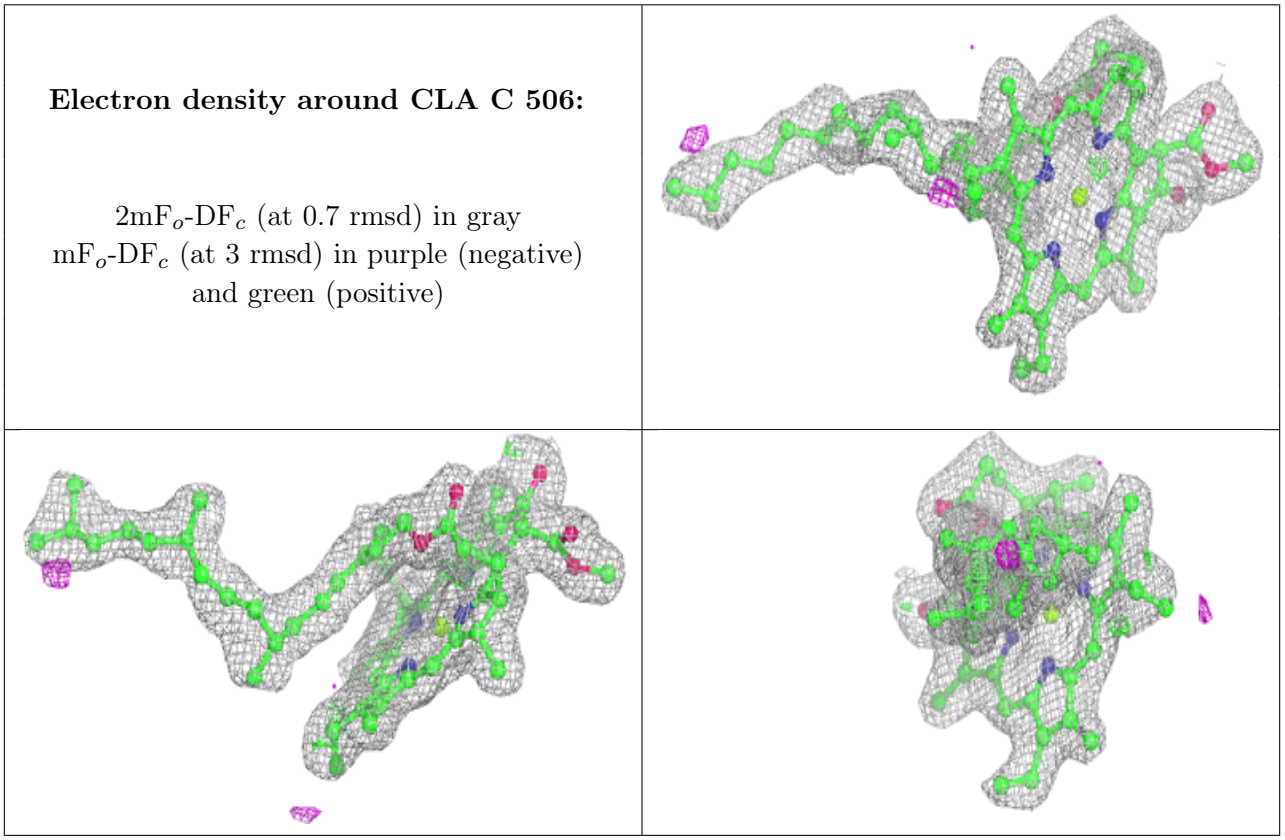
Electron density around CLA D 401:

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



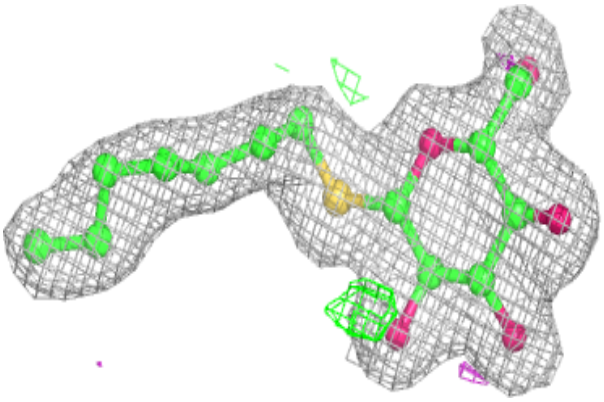
Electron density around CLA C 506:

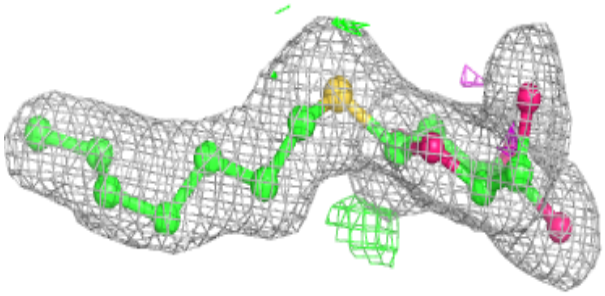
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

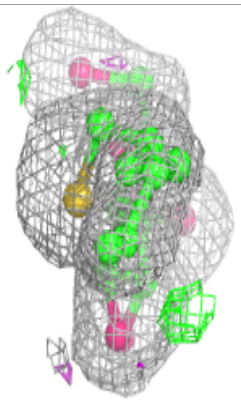


Electron density around HTG B 624:

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

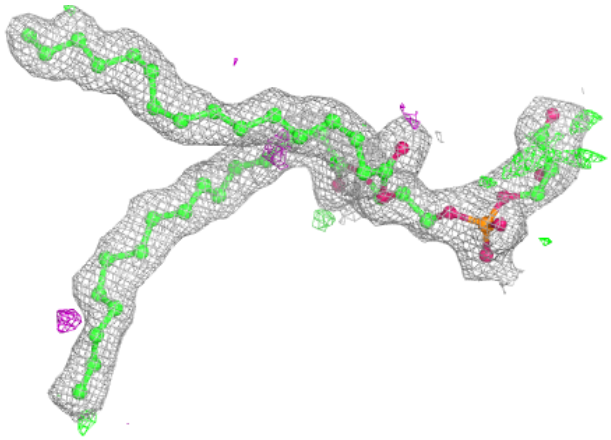


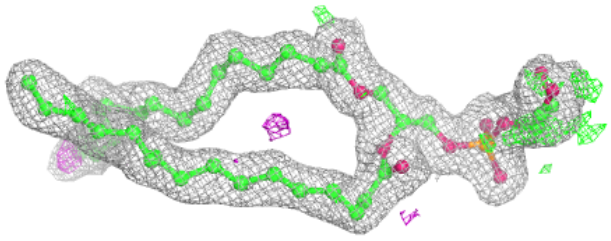


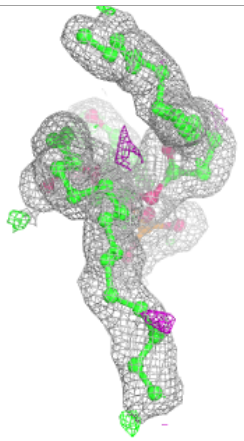


Electron density around LHG D 407:

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

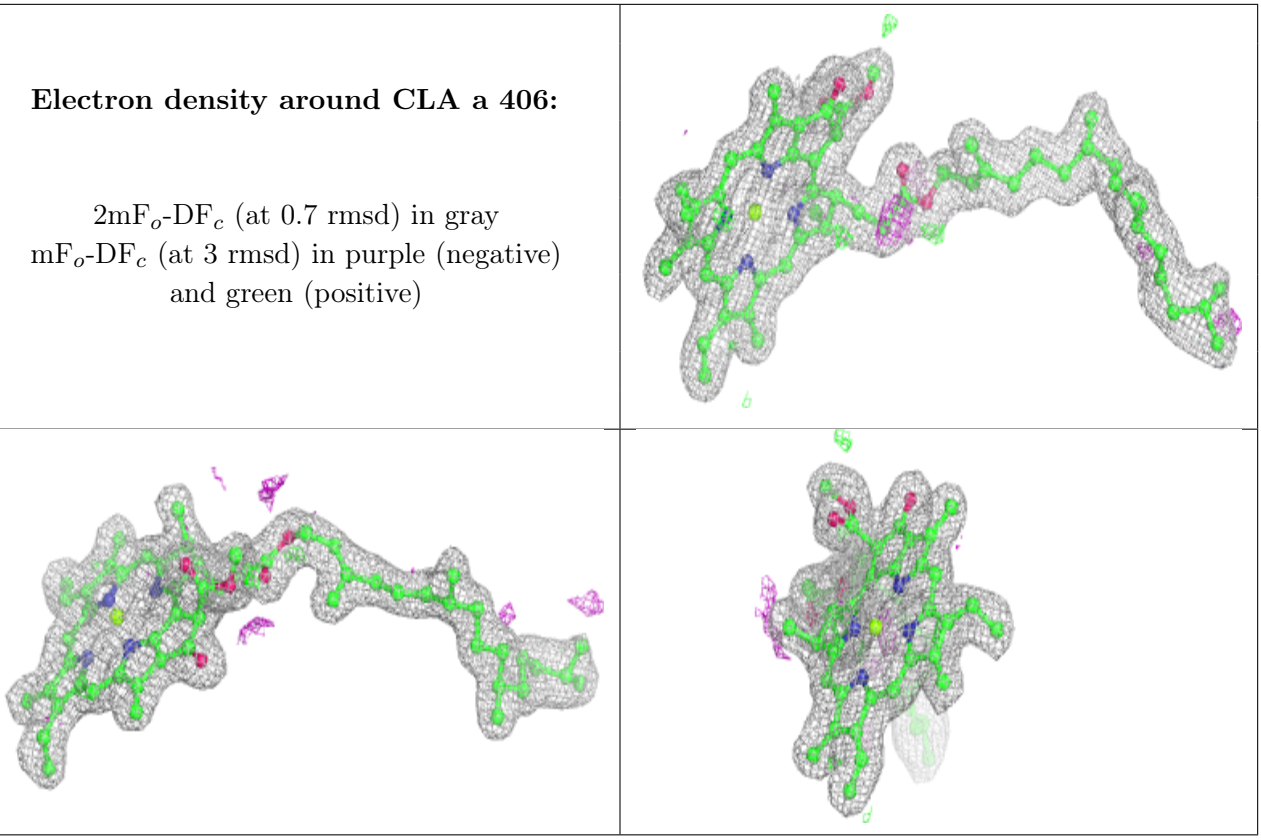






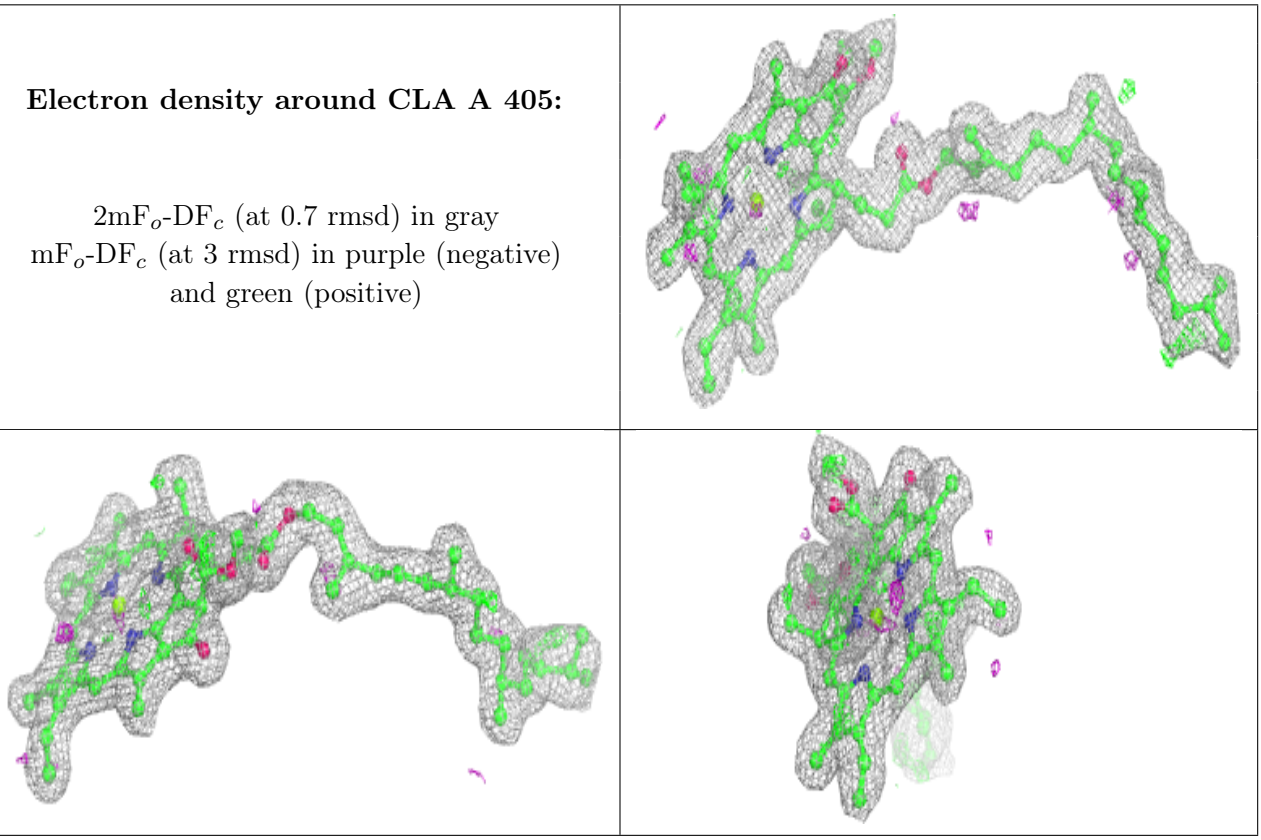
Electron density around CLA a 406:

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



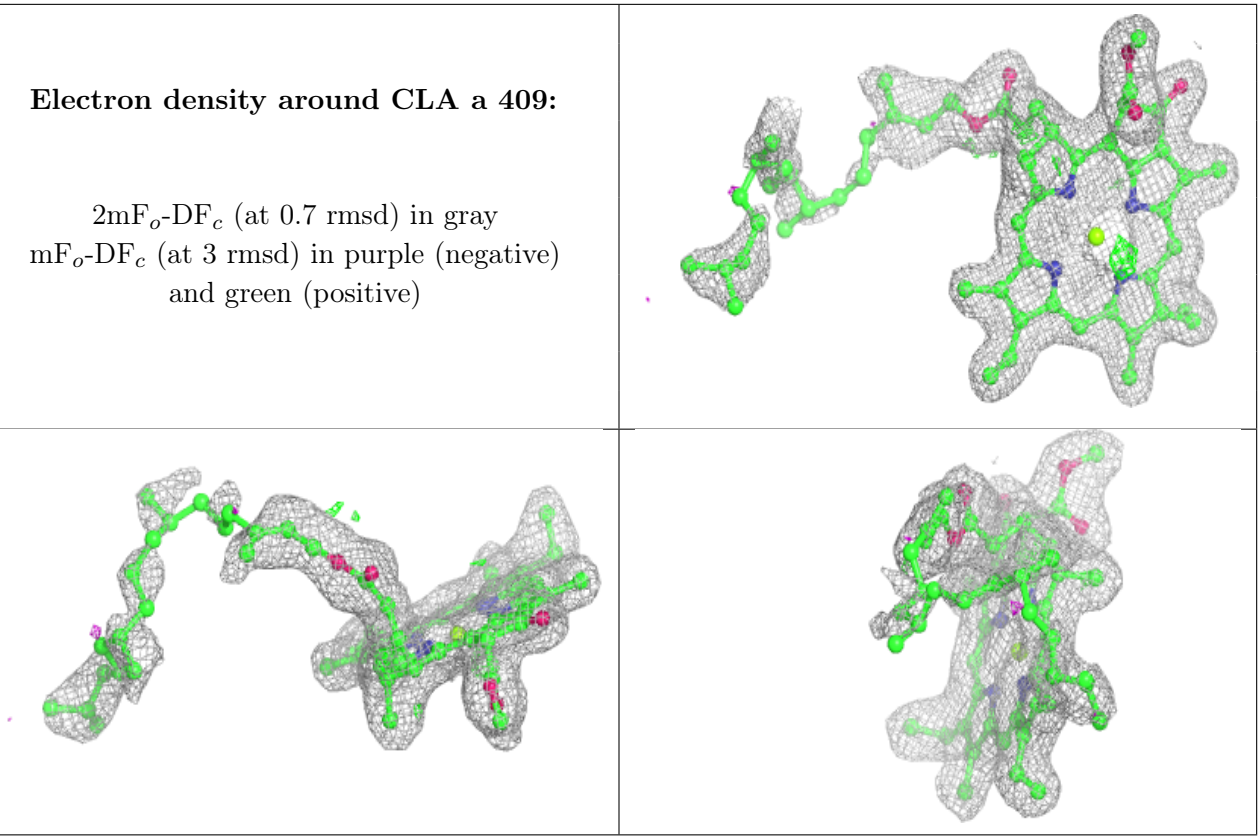
Electron density around CLA A 405:

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



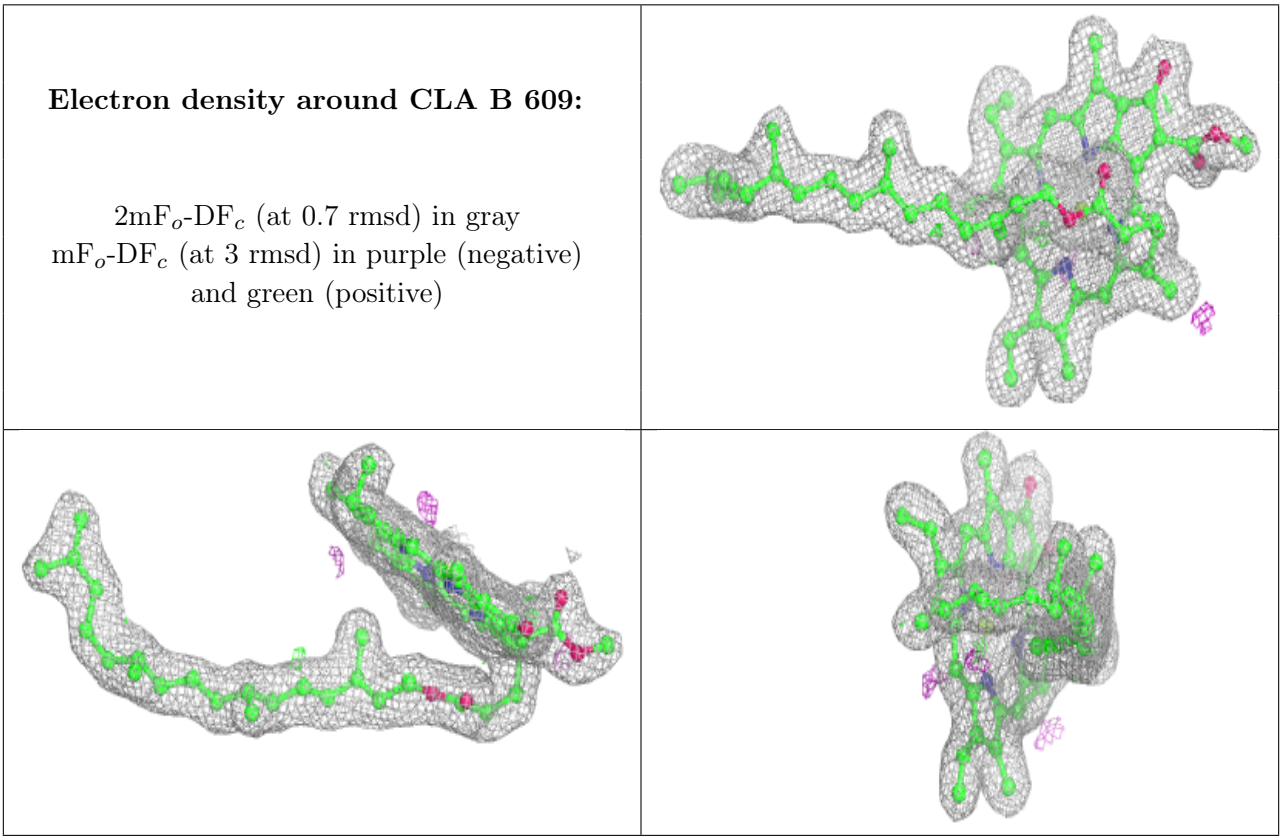
Electron density around CLA a 409:

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



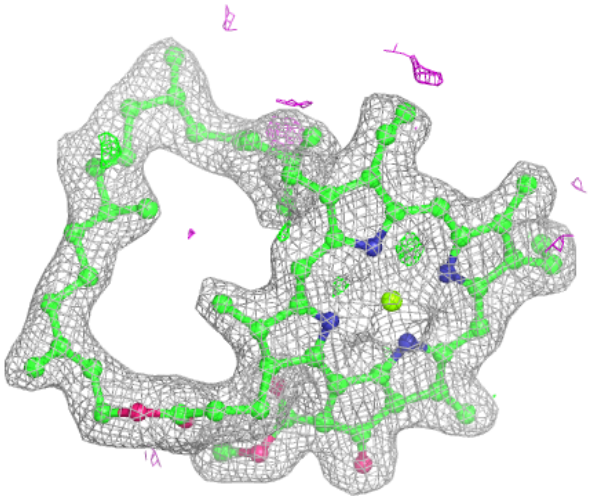
Electron density around CLA B 609:

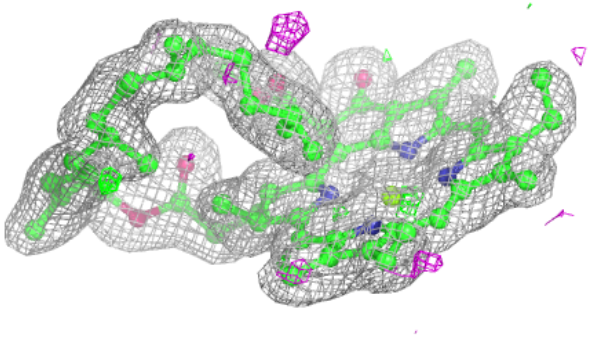
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

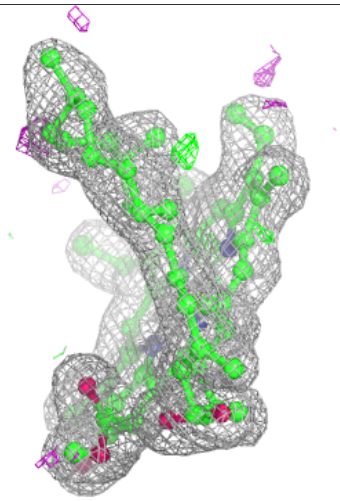


Electron density around CLA B 616:

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

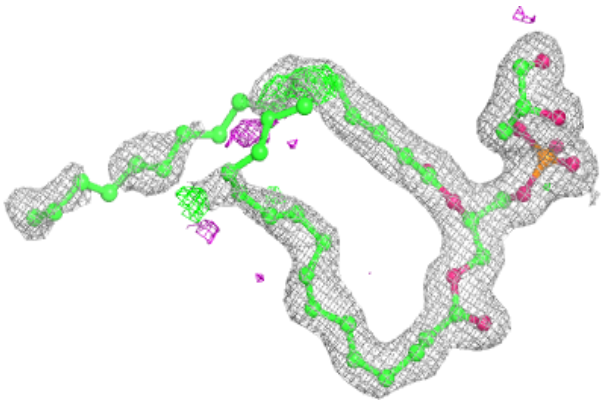


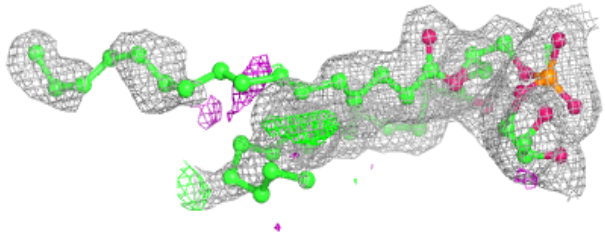


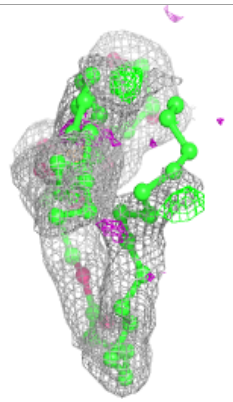


Electron density around LHG d 409:

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

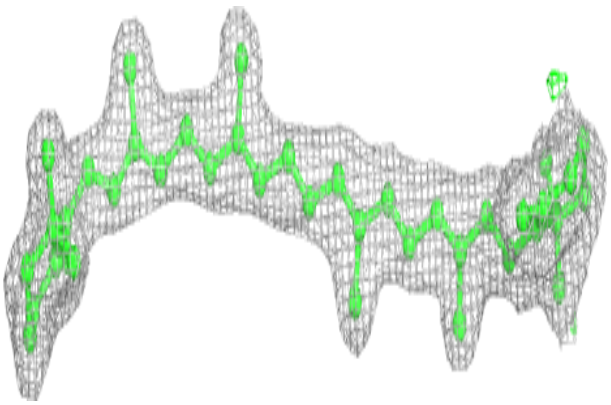


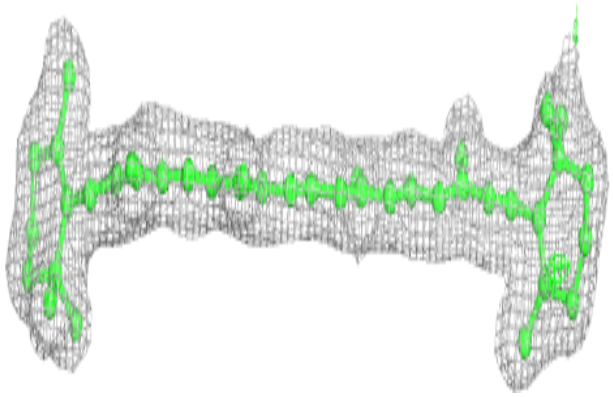


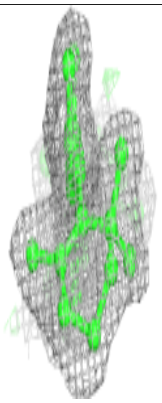


Electron density around BCR C 516:

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

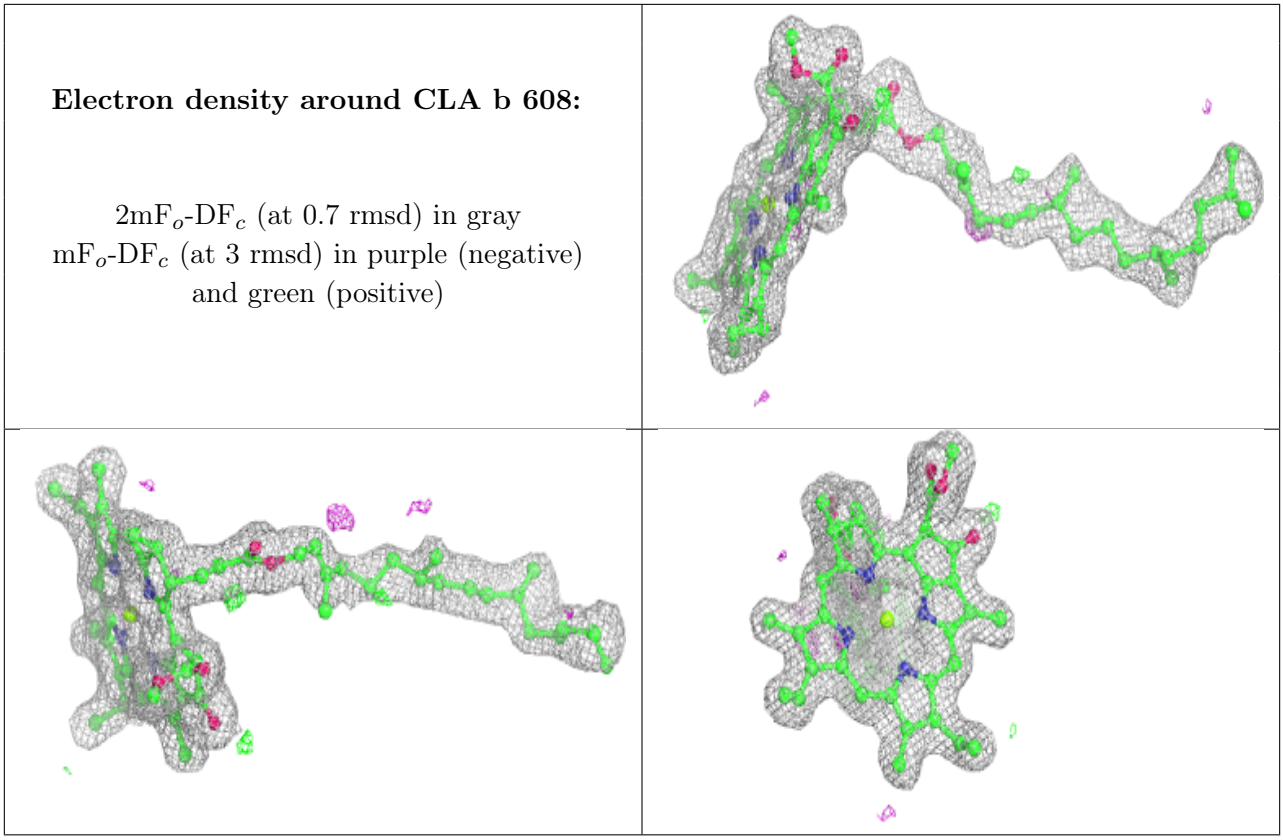






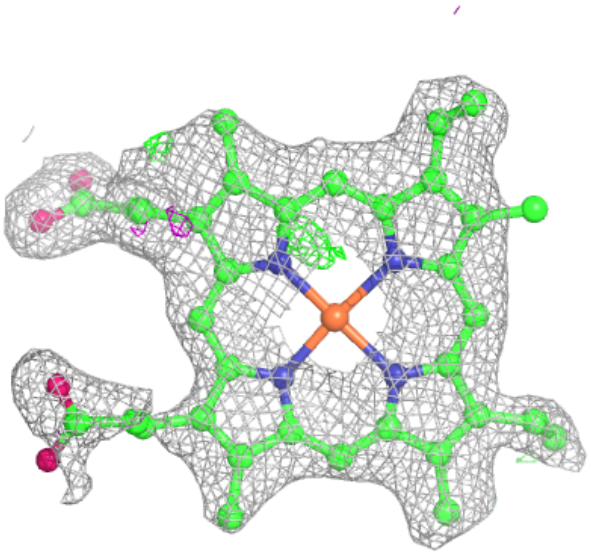
Electron density around CLA b 608:

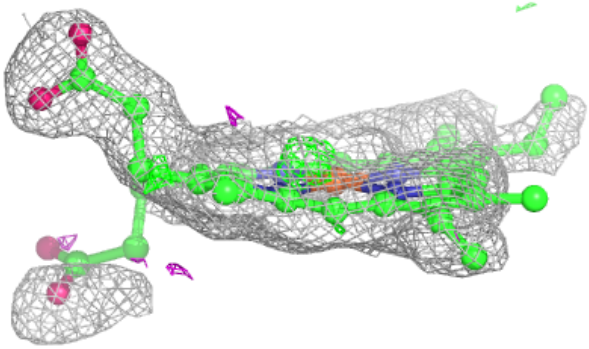
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

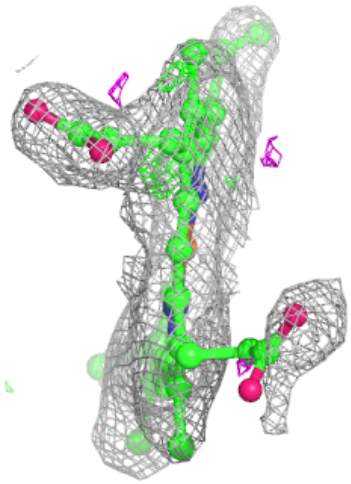


Electron density around HEM e 102:

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

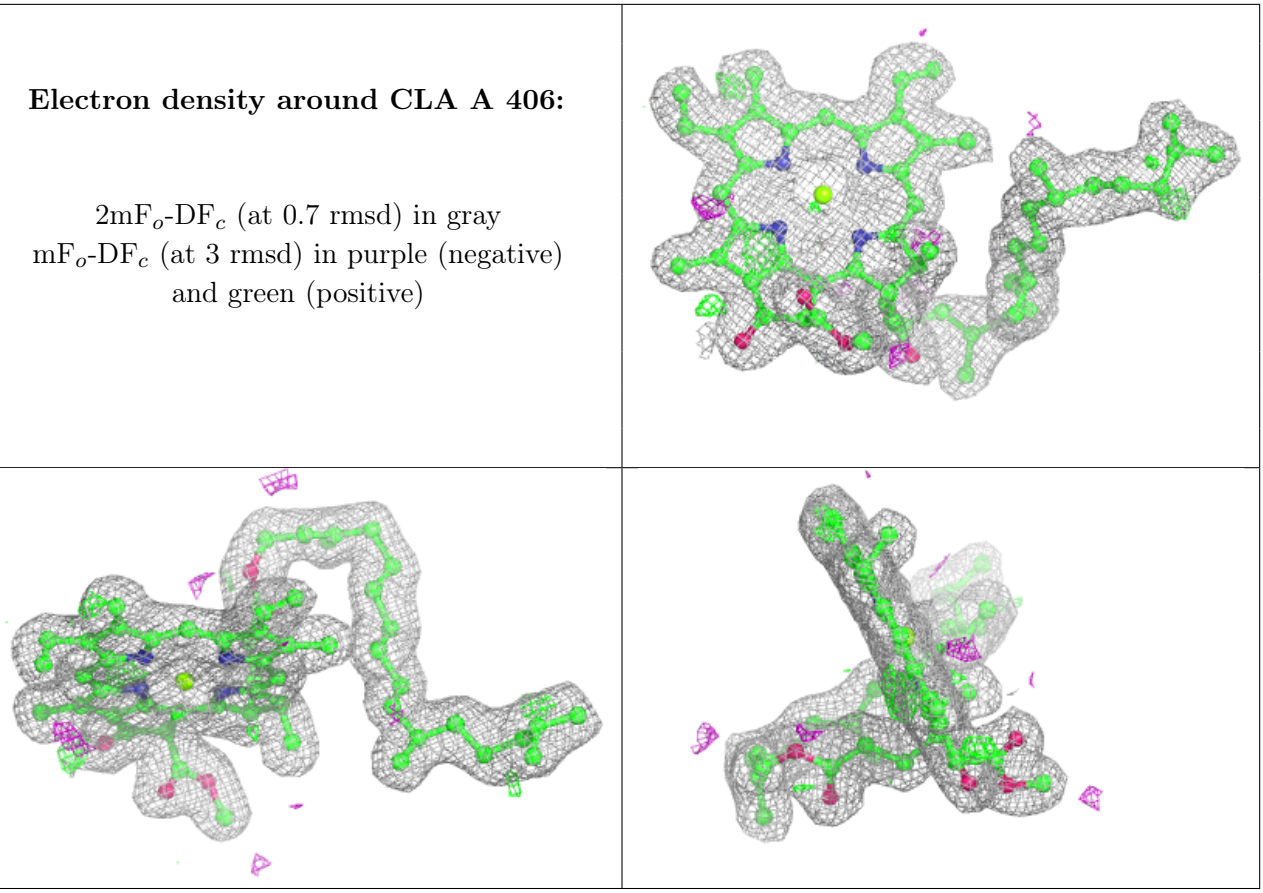






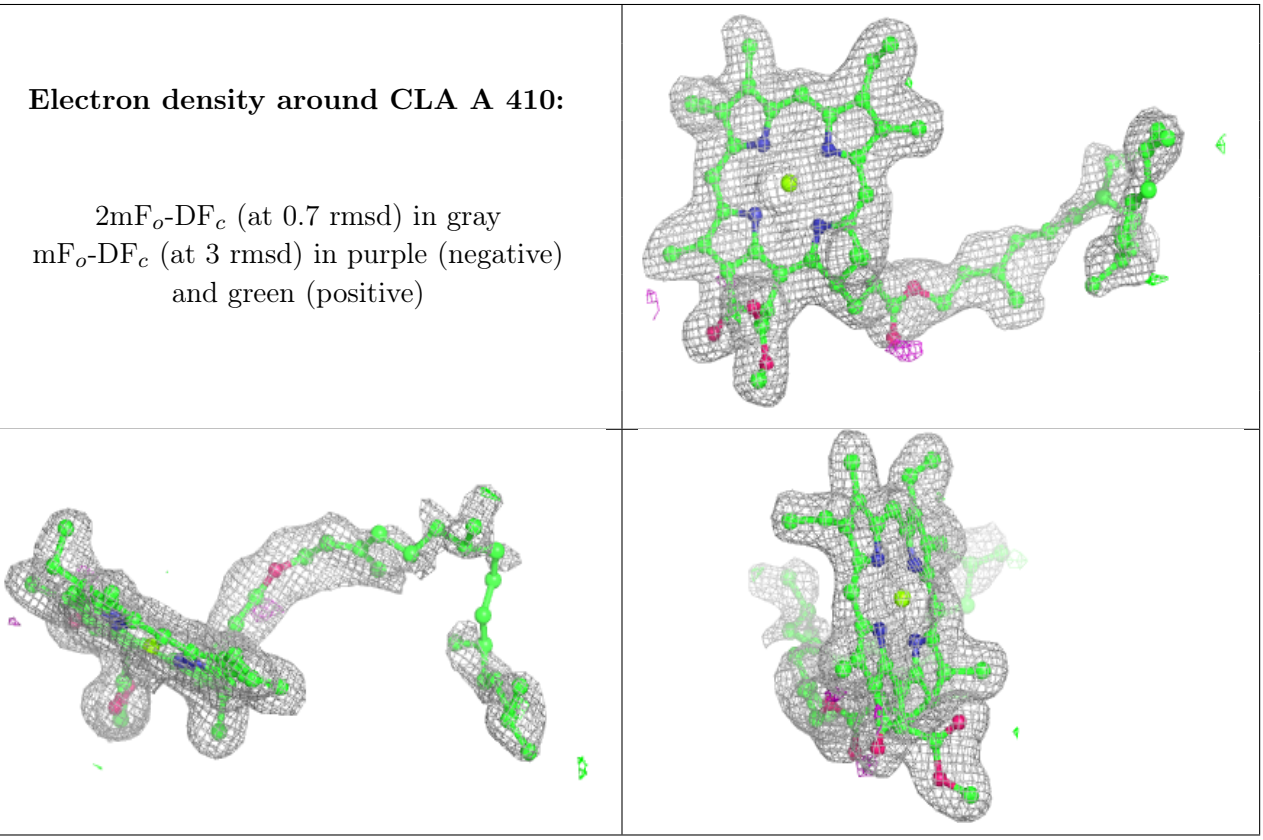
Electron density around CLA A 406:

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



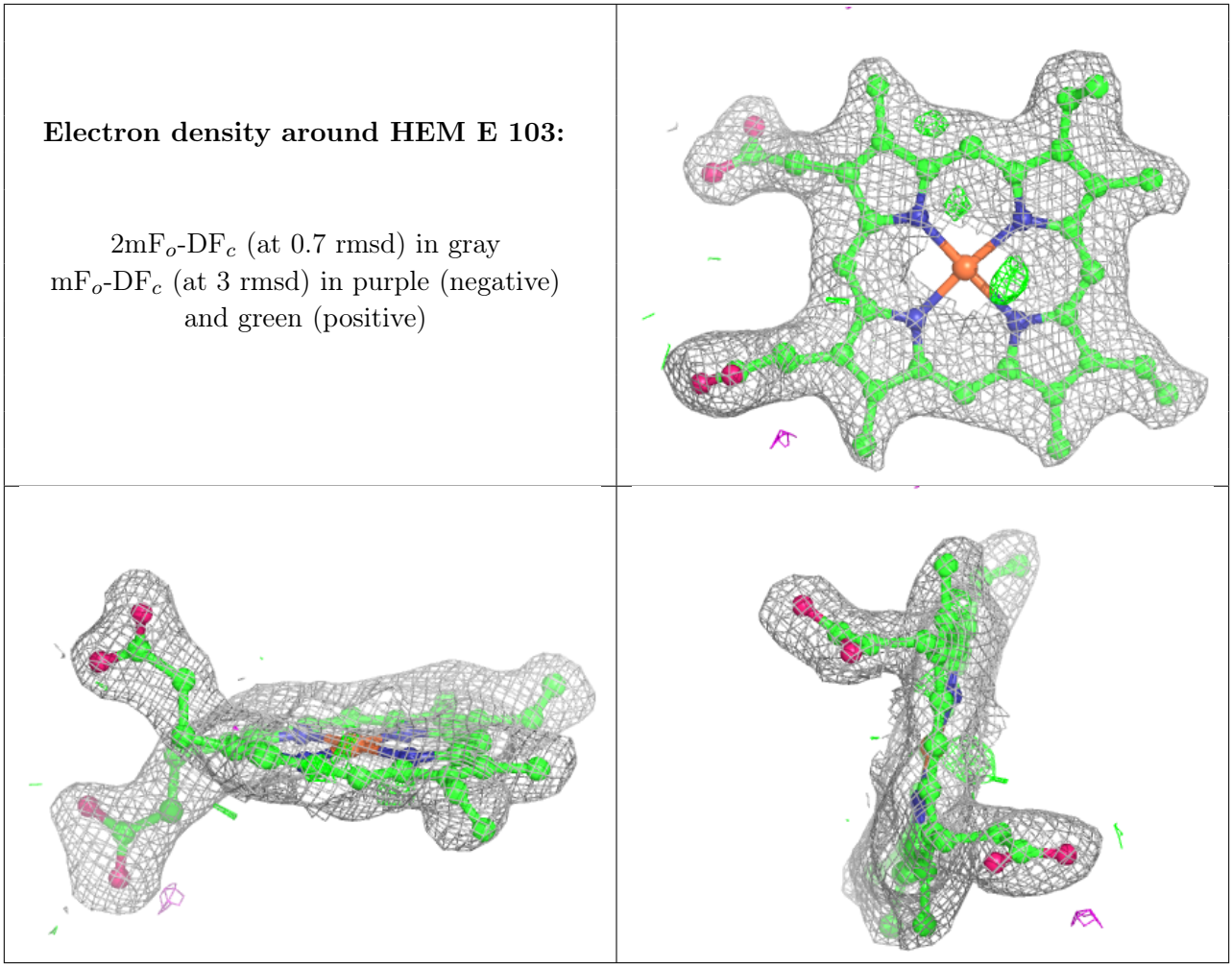
Electron density around CLA A 410:

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



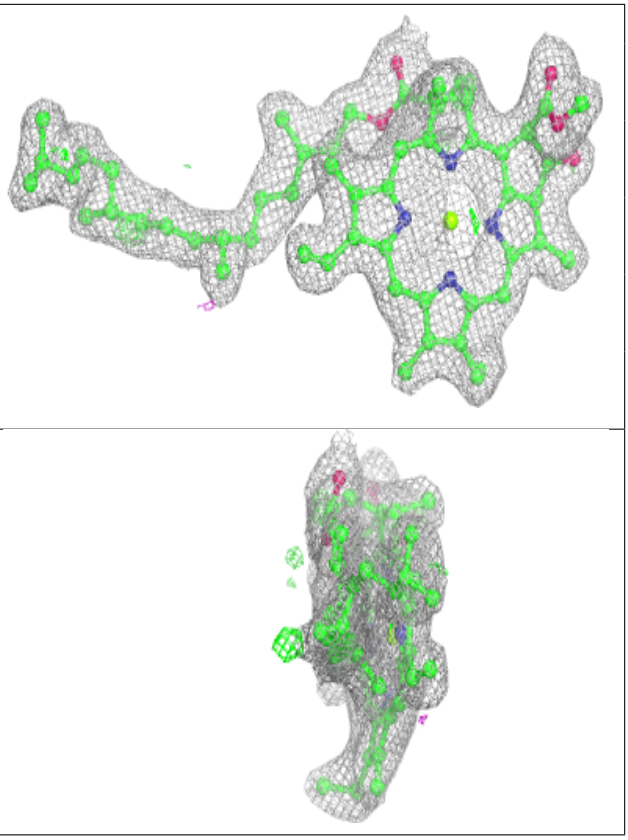
Electron density around HEM E 103:

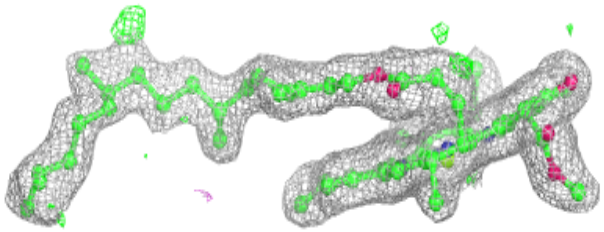
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 607:

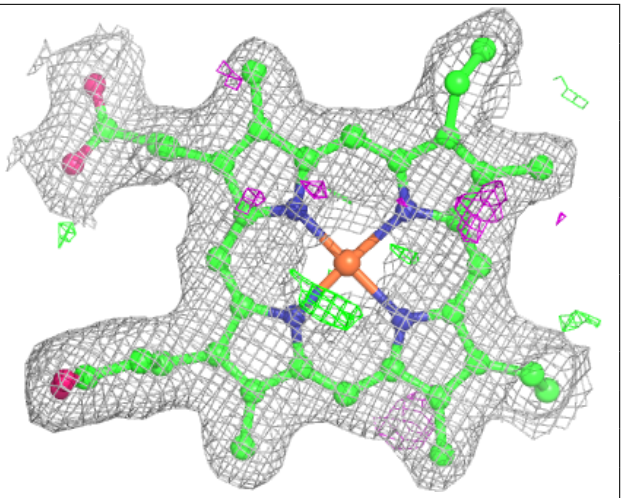
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

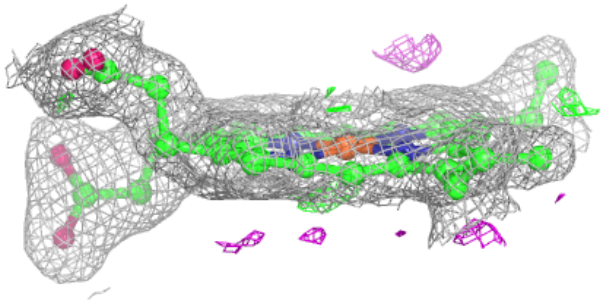




Electron density around HEC V 201:

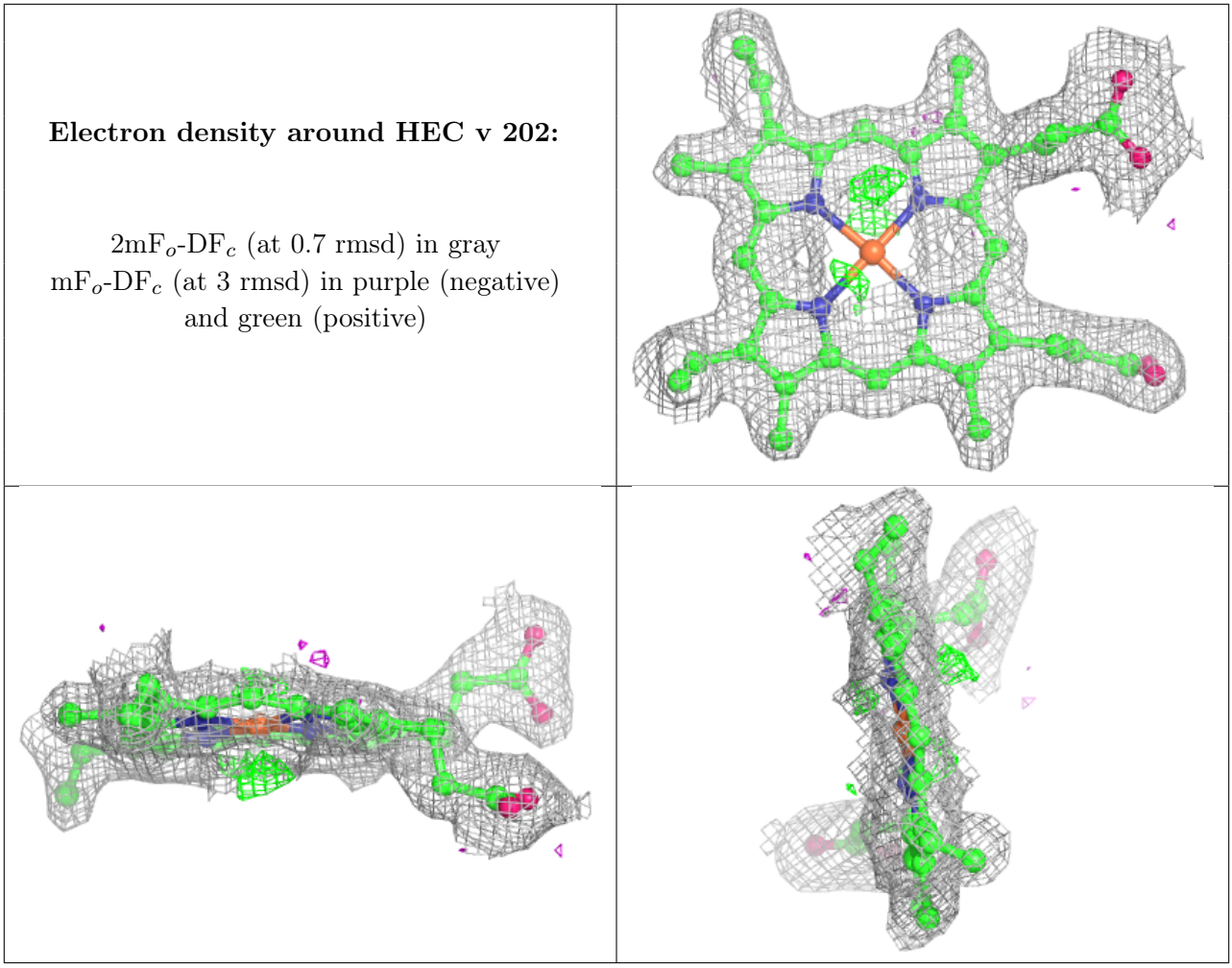
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC v 202:

$2mF_o$-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.