wwPDB X-ray Structure Validation Summary Report (i)

Mar 12, 2024 – 01:05 PM JST

PDB ID	:	8IR5
Title	:	XFEL structure of cyanobacterial photosystem II under dark conditions
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.15 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:

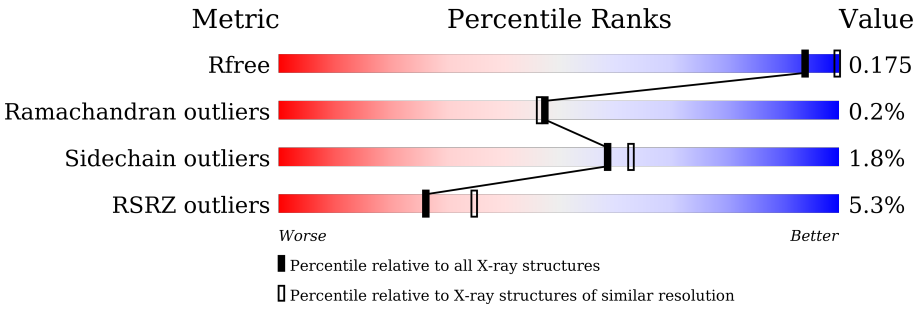
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	2% 97%
1	a	344	2% 97%
2	B	505	3% 99%
2	b	505	8% 99%
3	C	455	2% 98%
3	c	455	3% 99%
4	D	342	% 99%

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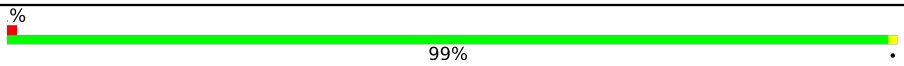
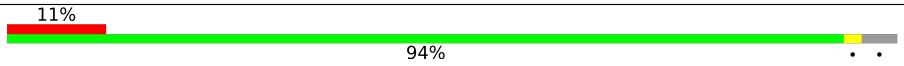
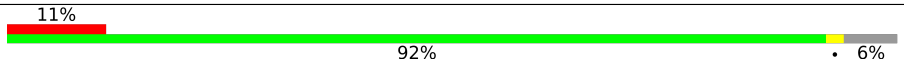
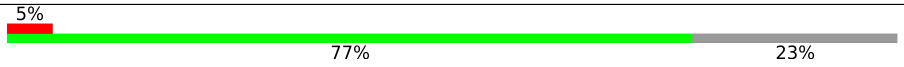
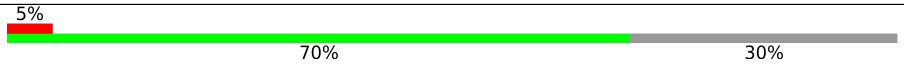
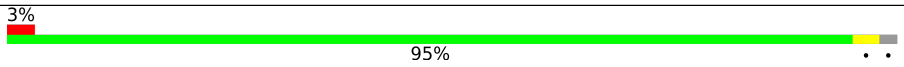
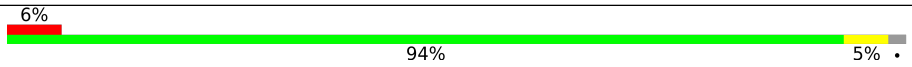
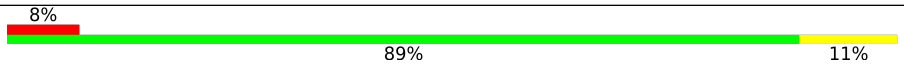
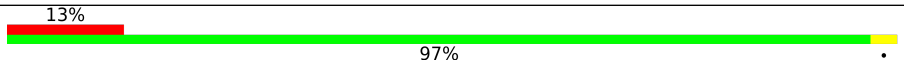
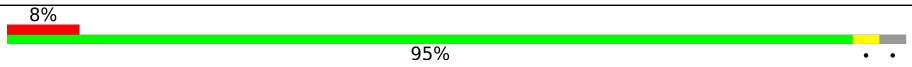
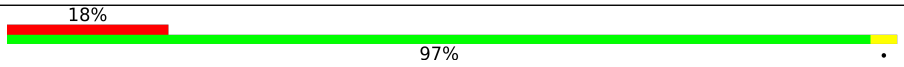
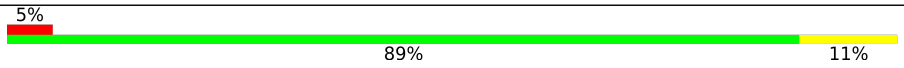
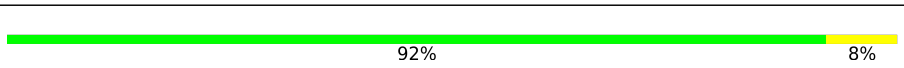
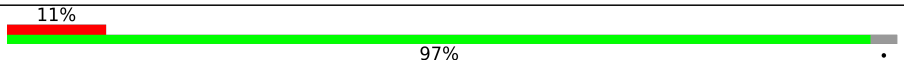
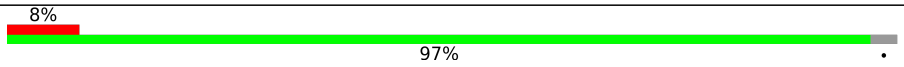
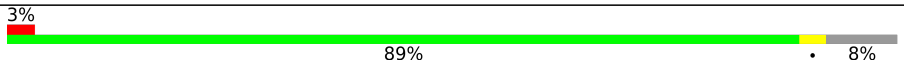
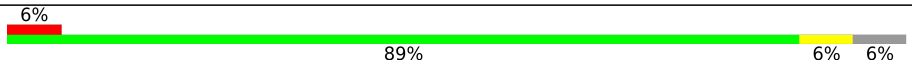
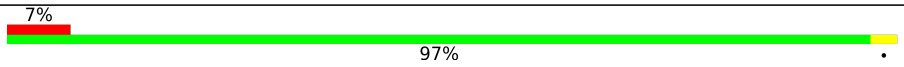
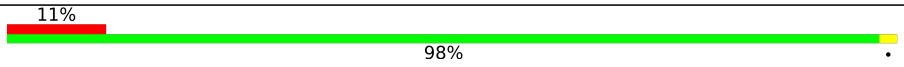
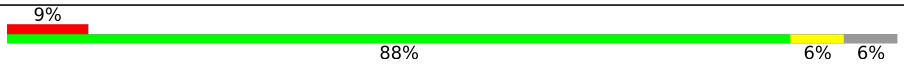
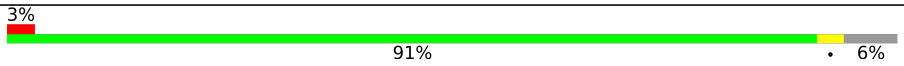
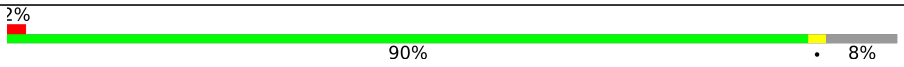
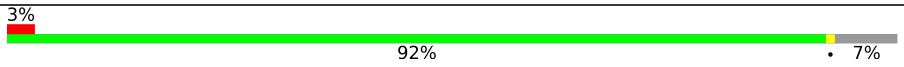
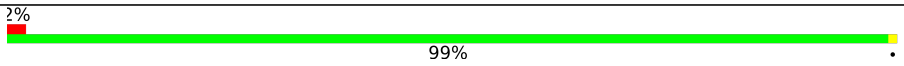
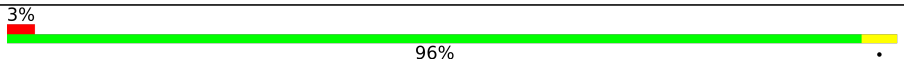
Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	X	40	10% 95% 5%
17	x	40	12% 95% 5%
18	Y	30	23% 97%
18	y	30	17% 87% 10%
19	Z	62	15% 98%
19	z	62	21% 89% 11%
20	R	34	59% 94% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	402	X	-	-	-
27	GOL	A	418	-	-	-	X
27	GOL	a	419	-	-	-	X
27	GOL	a	420	-	-	-	X
27	GOL	l	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	UNL	B	626	-	-	-	X
31	LMT	F	101	-	-	-	X
31	LMT	e	101	-	-	-	X
34	HTG	b	623	-	-	-	X

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 52978 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 II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2628	1722	432	459	15			
1	a	334	Total	C	N	O	S	0	2	0
			2629	1721	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	7	0
			4029	2639	674	703	13			
2	b	504	Total	C	N	O	S	0	6	0
			4017	2636	669	699	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	1	0
			3497	2287	588	609	13			
3	c	455	Total	C	N	O	S	0	5	0
			3555	2327	595	620	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

- 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
			2732	1808	446	466	12			
4	d	341	Total	C	N	O	S	0	2	0
			2732	1808	447	465	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			

- 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 277	C 185	N 43	O 48	S 1	0	0	0

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 268	C 179	N 39	O 49	S 1	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	3	0
			1894	1181	321	388	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			267	186	37	42	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	1	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	1	0
			781	496	130	155			

- 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	2	0
			1082	685	179	214	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 X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total 289	C 194	N 46	O 49	0	1	0
17	x	38	Total 281	C 188	N 45	O 48	0	0	0

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total 479	C 328	N 72	O 77	S 2	0	0	0
19	z	62	Total 479	C 328	N 72	O 77	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total 273	C 186	N 47	O 40	0	0	0

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

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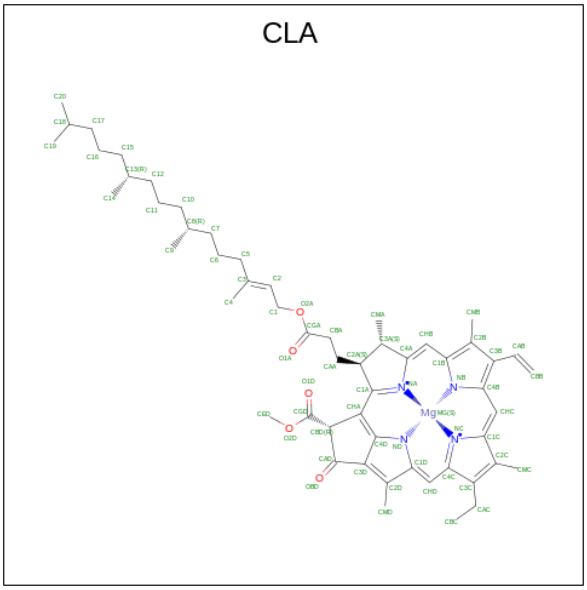
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 2 2	0	0

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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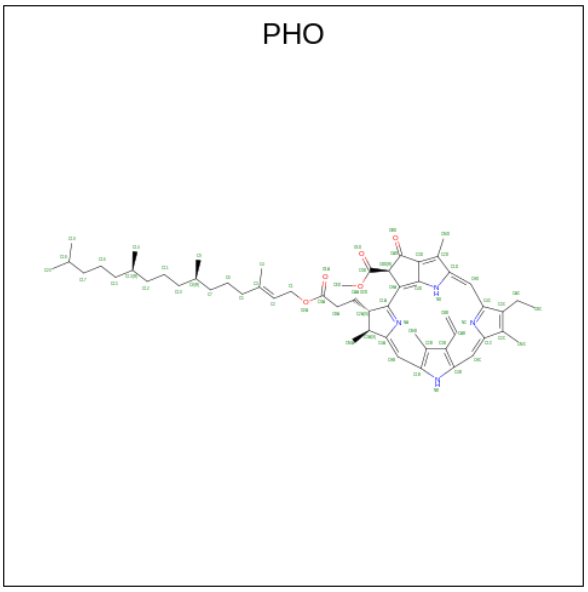
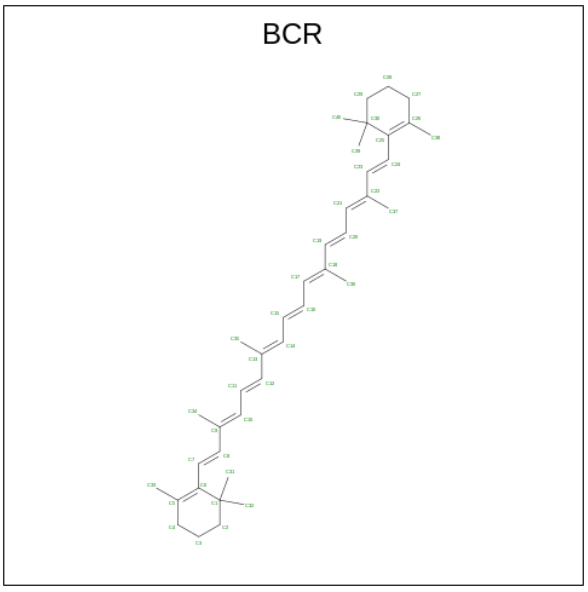
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



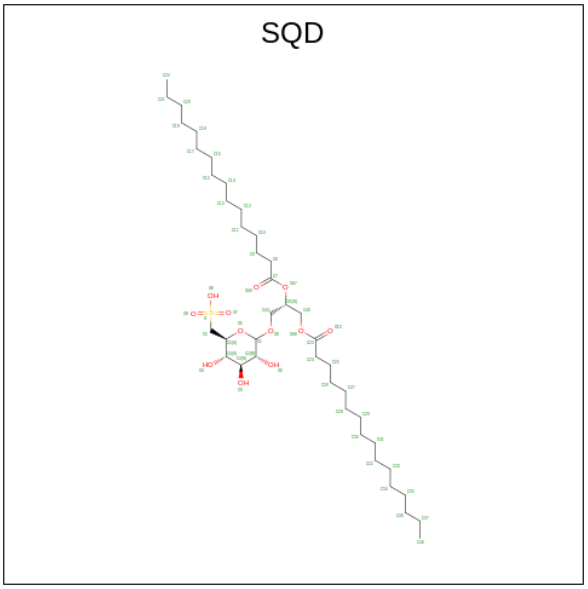
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



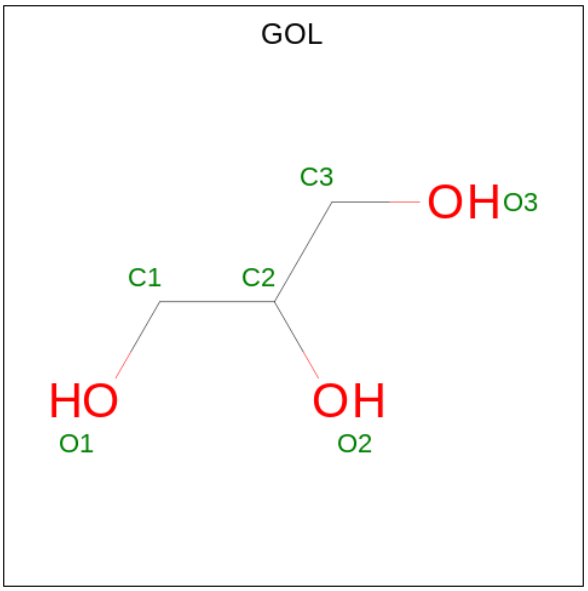
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 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
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0

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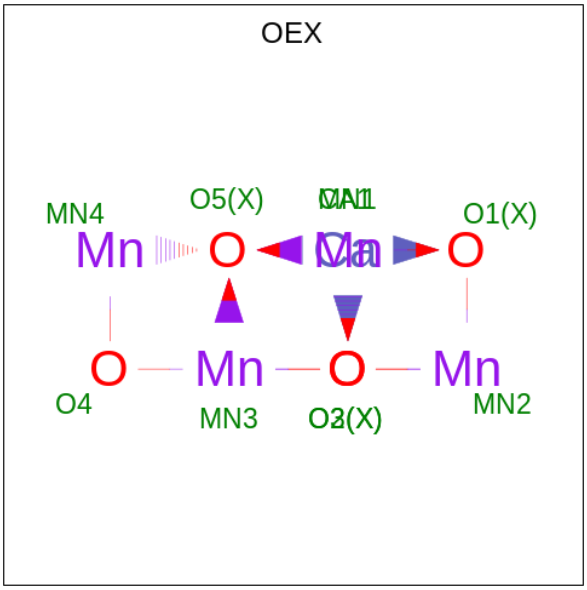
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C O 6 3 3	0	0
27	c	1	Total C O 6 3 3	0	0
27	c	1	Total C O 6 3 3	0	0
27	l	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	v	1	Total C O 6 3 3	0	0

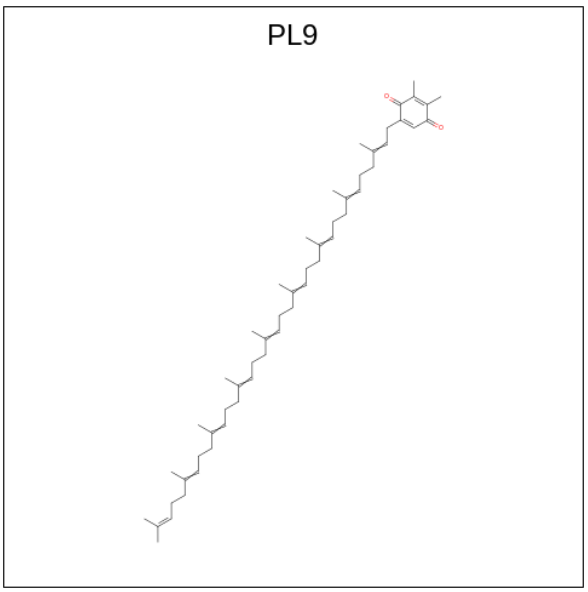
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 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:

$C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

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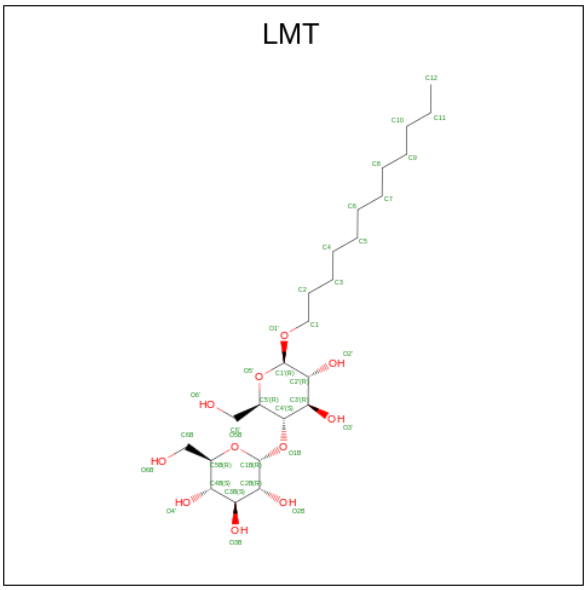
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0
31	A	1	Total C O 35 24 11	0	0

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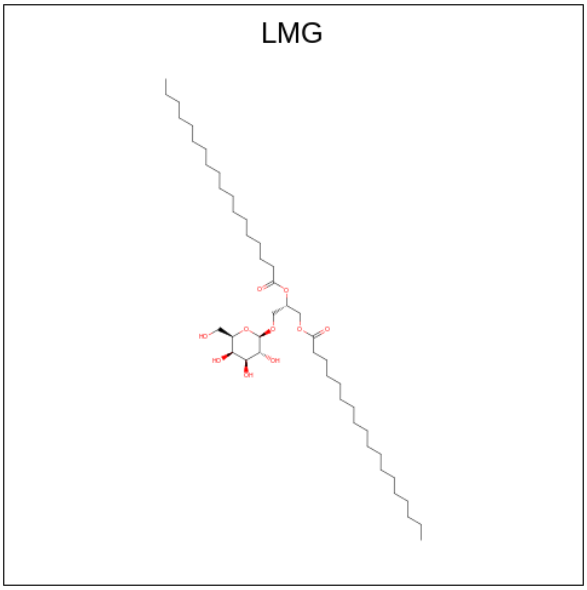
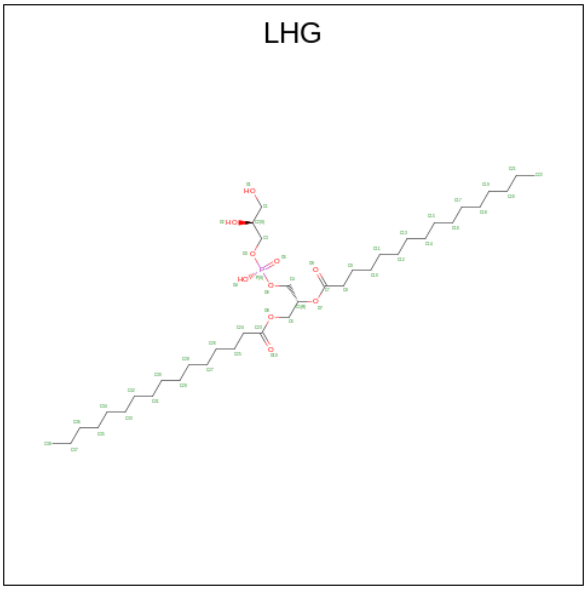
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 25 19 6	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	T	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 6	0	0
31	c	1	Total C O 35 24 11	0	0
31	e	1	Total C O 35 24 11	0	0
31	m	1	Total C O 35 24 11	0	0
31	t	1	Total C O 26 19 7	0	0

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



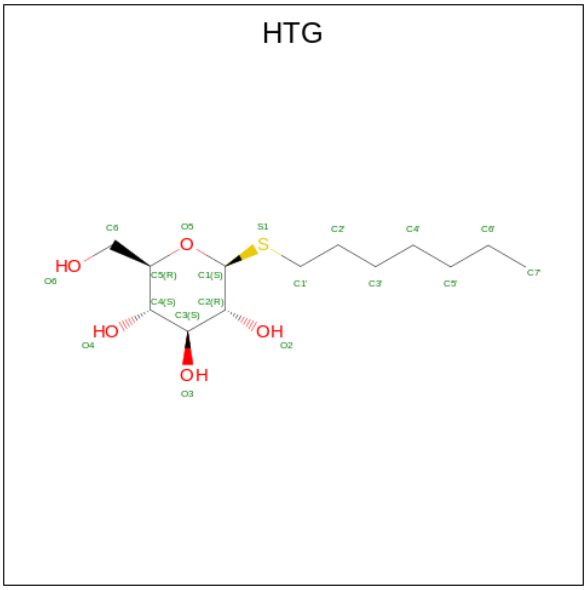
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	m	1	Total	C	O	0	0
			51	41	10		
32	Z	1	Total	C	O	0	0
			37	27	10		
32	z	1	Total	C	O	0	0
			39	29	10		

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



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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

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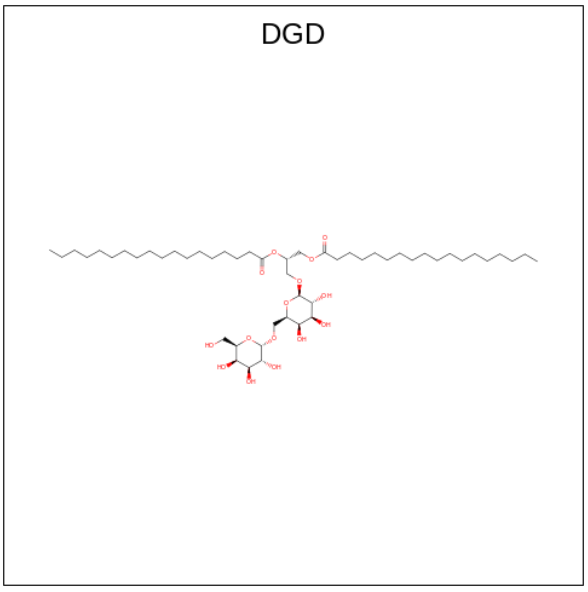
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	d	1	Total C O S 16 10 5 1	0	0

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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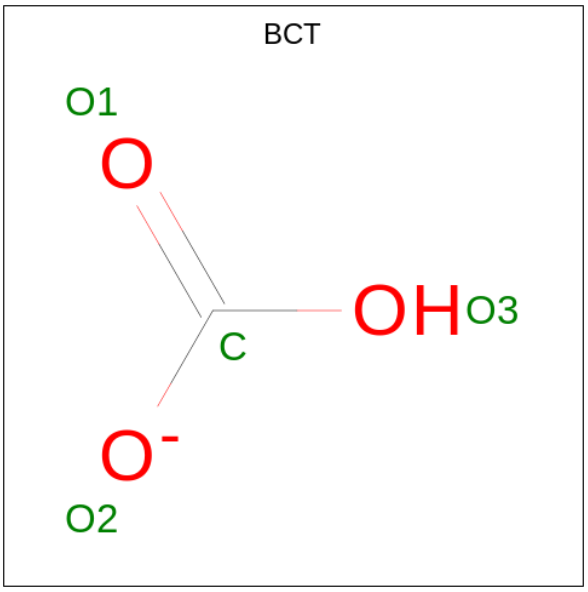
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

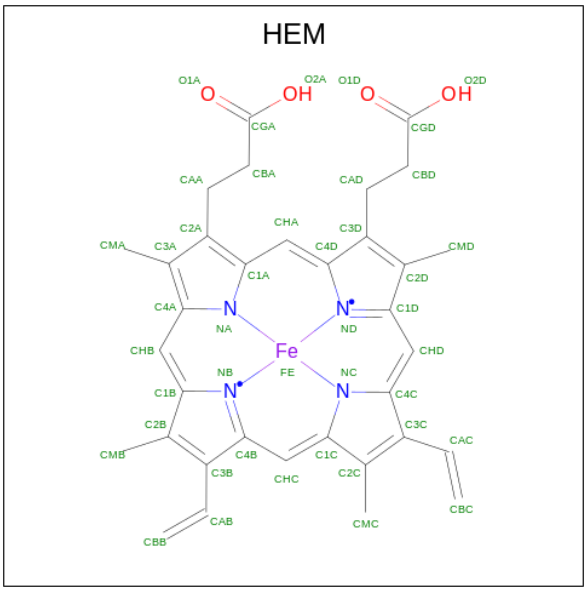
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 4 1 3	0	0
37	a	1	Total C O 4 1 3	0	0

- 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	F	1	Total C Fe N O 43 34 1 4 4	0	0

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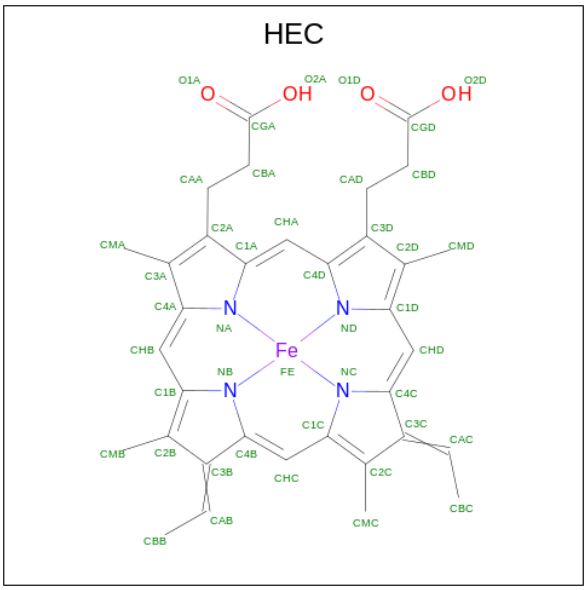
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	139	Total	O	0	1
			140	140		
41	B	188	Total	O	0	0
			188	188		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	167	Total O 167 167	0	0
41	D	123	Total O 123 123	0	0
41	E	13	Total O 13 13	0	0
41	F	7	Total O 7 7	0	0
41	H	21	Total O 21 21	0	0
41	I	5	Total O 5 5	0	0
41	J	8	Total O 8 8	0	0
41	K	5	Total O 5 5	0	0
41	L	9	Total O 9 9	0	0
41	M	5	Total O 5 5	0	0
41	O	105	Total O 105 105	0	0
41	T	10	Total O 10 10	0	0
41	U	44	Total O 44 44	0	0
41	V	82	Total O 82 82	0	0
41	X	7	Total O 7 7	0	0
41	a	130	Total O 130 130	0	0
41	b	202	Total O 202 202	0	0
41	c	161	Total O 161 161	0	0
41	d	111	Total O 111 111	0	0
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0

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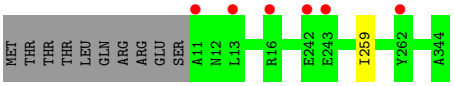
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 8 8	0	0
41	m	13	Total O 13 13	0	0
41	o	103	Total O 103 103	0	0
41	t	7	Total O 7 7	0	0
41	u	49	Total O 49 49	0	0
41	v	57	Total O 57 57	0	0
41	x	8	Total O 8 8	0	0
41	y	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

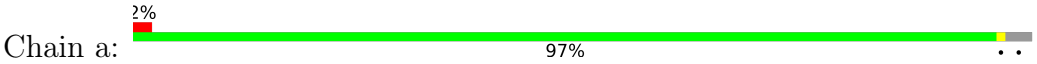
• Molecule 1: Photosystem II protein D1

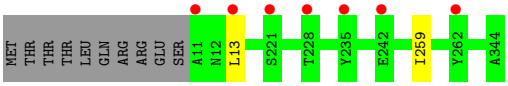
Chain A:



• Molecule 1: Photosystem II protein D1

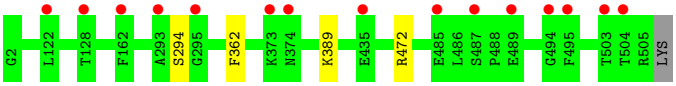
Chain a:





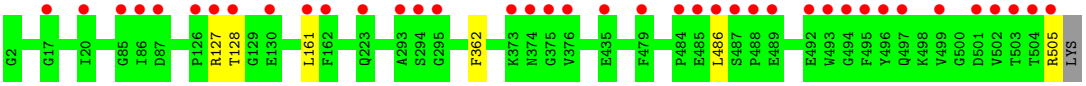
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



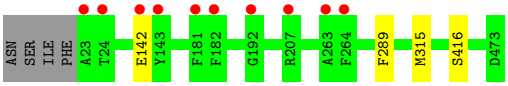
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



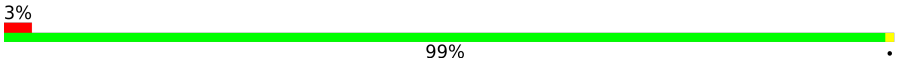
• Molecule 3: Photosystem II CP43 reaction center protein

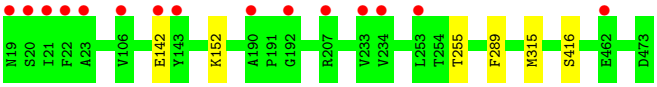
Chain C:



• Molecule 3: Photosystem II CP43 reaction center protein

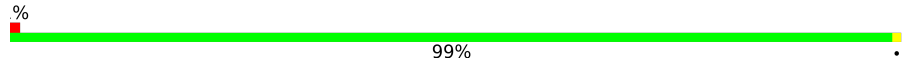
Chain c:

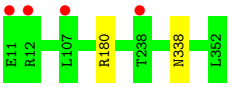




• Molecule 4: Photosystem II D2 protein

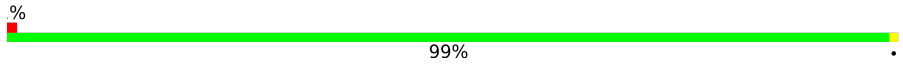
Chain D:

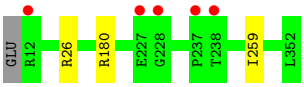




• Molecule 4: Photosystem II D2 protein

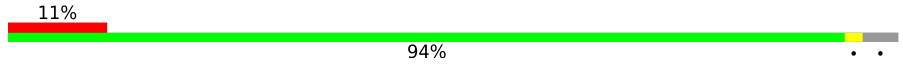
Chain d:

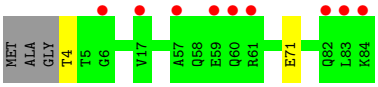




• Molecule 5: Cytochrome b559 subunit alpha

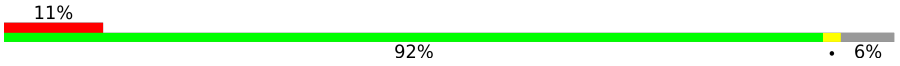
Chain E:

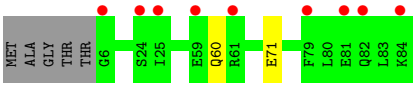




• Molecule 5: Cytochrome b559 subunit alpha

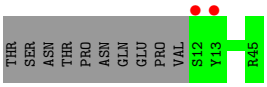
Chain e:





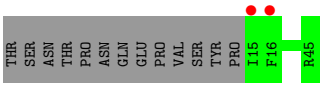
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



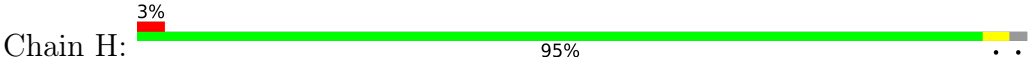
• Molecule 6: Cytochrome b559 subunit beta

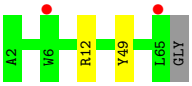
Chain f:



• Molecule 7: Photosystem II reaction center protein H

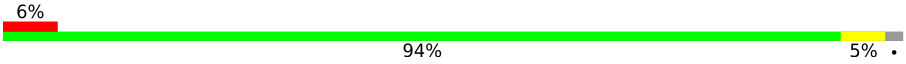
Chain H:

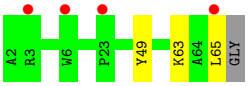




• Molecule 7: Photosystem II reaction center protein H

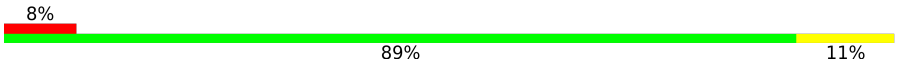
Chain h:

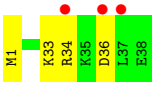




• Molecule 8: Photosystem II reaction center protein I

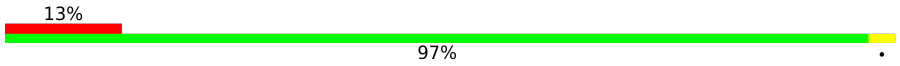
Chain I:

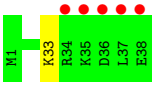




• Molecule 8: Photosystem II reaction center protein I

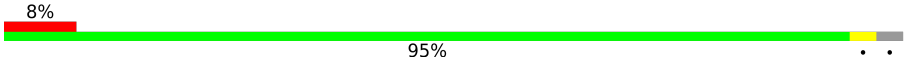
Chain i:

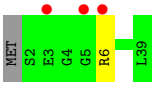




• Molecule 9: Photosystem II reaction center protein J

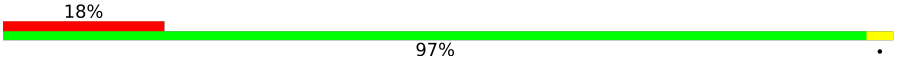
Chain J:

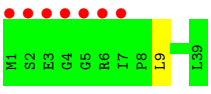




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

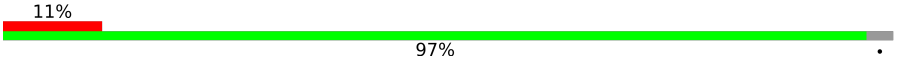
Chain K:

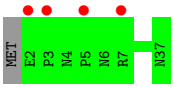
• Molecule 10: Photosystem II reaction center protein K

Chain k:

• Molecule 11: Photosystem II reaction center protein L

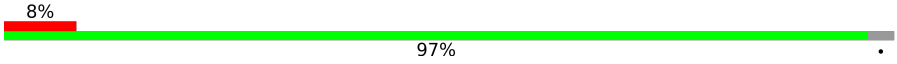
Chain L:

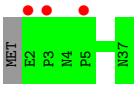




• Molecule 11: Photosystem II reaction center protein L

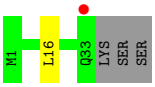
Chain l:





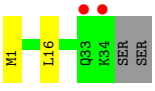
• Molecule 12: Photosystem II reaction center protein M

Chain M:



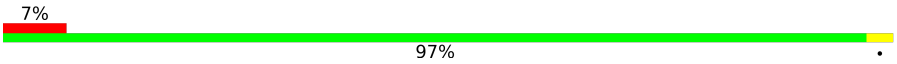
• Molecule 12: Photosystem II reaction center protein M

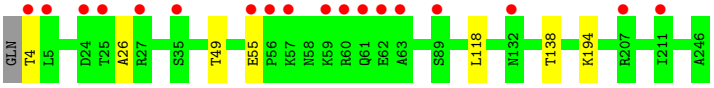
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

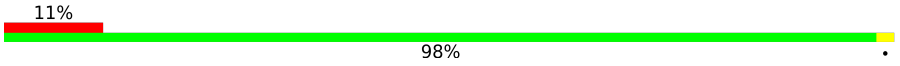
Chain O:

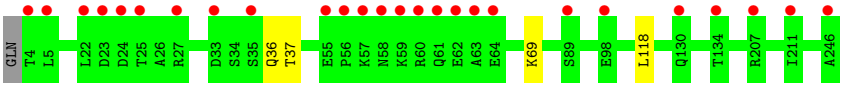




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

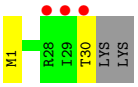
Chain o:





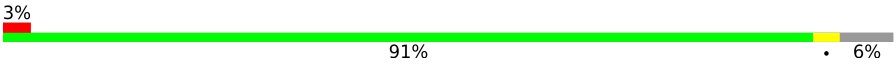
• Molecule 14: Photosystem II reaction center protein T

Chain T:



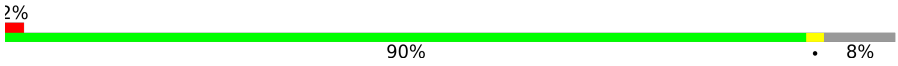
• Molecule 14: Photosystem II reaction center protein T

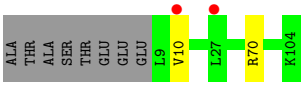
Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

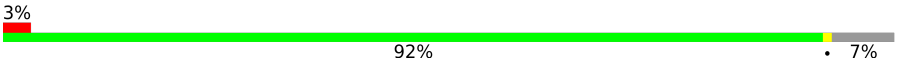
Chain U:

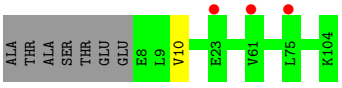




• Molecule 15: Photosystem II 12 kDa extrinsic protein

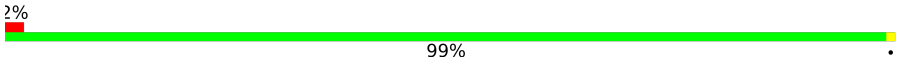
Chain u:

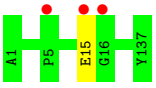




• Molecule 16: Cytochrome c-550

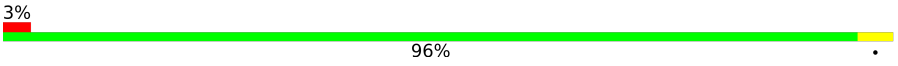
Chain V:

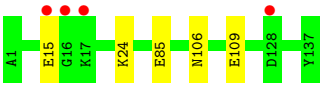




• Molecule 16: Cytochrome c-550

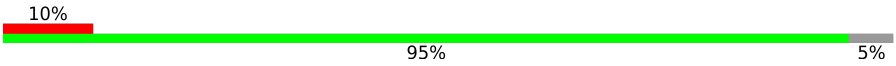
Chain v:

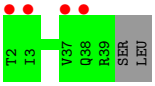




• Molecule 17: Photosystem II reaction center protein X

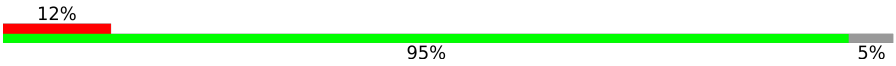
Chain X:

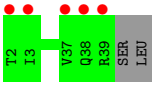




• Molecule 17: Photosystem II reaction center protein X

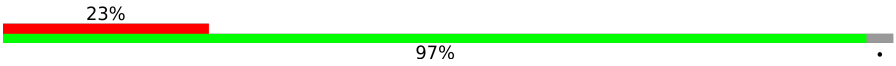
Chain x:

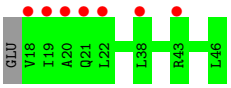




• Molecule 18: Photosystem II reaction center protein Ycf12

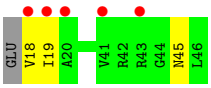
Chain Y:





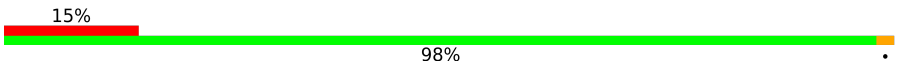
• Molecule 18: Photosystem II reaction center protein Ycf12

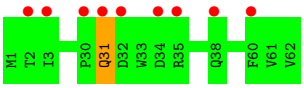
Chain y:



• Molecule 19: Photosystem II reaction center protein Z

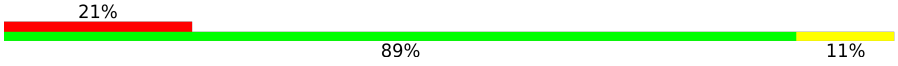
Chain Z:

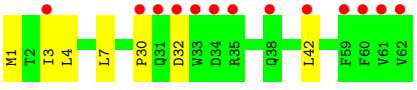




• Molecule 19: Photosystem II reaction center protein Z

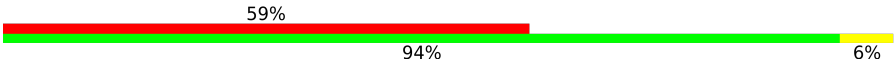
Chain z:

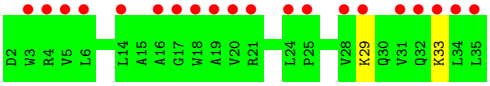




• Molecule 20: Photosystem II protein Y

Chain R:




D2
W3
R4
V5
L6
L14
A15
A16
G17
W18
A19
V20
R21
L24
P25
V28
K29
Q30
V31
Q32
K33
L34
L35

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.15) 99.9 (19.98-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.15Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.144 , 0.175 0.144 , 0.175	Depositor DCC
R_{free} test set	22612 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	52978	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: CLA, CA, LMT, LHG, FE2, HTG, LMG, SQD, MG, UNL, HEM, GOL, BCR, CL, BCT, PHO, OEX, DGD, PL9, HEC, FME

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	0.42	0/2713	0.57	0/3700
1	a	0.41	0/2717	0.55	0/3705
2	B	0.41	0/4169	0.57	0/5679
2	b	0.38	0/4161	0.56	0/5669
3	C	0.37	0/3610	0.54	0/4914
3	c	0.37	0/3675	0.52	0/5002
4	D	0.44	0/2827	0.59	0/3852
4	d	0.43	0/2827	0.56	0/3852
5	E	0.36	0/681	0.56	0/928
5	e	0.36	0/690	0.53	0/939
6	F	0.37	0/284	0.52	0/387
6	f	0.34	0/269	0.51	0/365
7	H	0.36	0/519	0.58	0/708
7	h	0.35	0/530	0.55	0/722
8	I	0.33	0/311	0.53	0/419
8	i	0.38	0/311	0.53	0/419
9	J	0.37	0/278	0.51	0/376
9	j	0.32	0/283	0.52	0/383
10	K	0.36	0/303	0.49	0/416
10	k	0.35	0/303	0.49	0/416
11	L	0.37	0/303	0.53	0/412
11	l	0.40	0/303	0.52	0/412
12	M	0.39	0/261	0.48	0/357
12	m	0.37	0/279	0.49	0/380
13	O	0.38	0/1925	0.61	0/2609
13	o	0.37	0/1896	0.61	0/2571
14	T	0.45	0/266	0.54	0/362
14	t	0.43	0/257	0.51	0/349
15	U	0.40	0/785	0.59	0/1064
15	u	0.39	0/792	0.60	0/1074
16	V	0.37	0/1103	0.56	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.33	0/1085	0.53	0/1473
17	X	0.31	0/292	0.47	0/395
17	x	0.30	0/284	0.46	0/384
18	Y	0.31	0/216	0.51	0/289
18	y	0.28	0/216	0.48	0/289
19	Z	0.29	0/490	0.43	0/669
19	z	0.30	0/490	0.41	0/669
20	R	0.29	0/279	0.52	0/383
All	All	0.39	0/42983	0.55	0/58489

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	333/344 (97%)	328 (98%)	4 (1%)	1 (0%)	41	37
1	a	334/344 (97%)	327 (98%)	6 (2%)	1 (0%)	41	37
2	B	509/505 (101%)	501 (98%)	8 (2%)	0	100	100
2	b	508/505 (101%)	496 (98%)	12 (2%)	0	100	100
3	C	450/455 (99%)	443 (98%)	6 (1%)	1 (0%)	47	46
3	c	458/455 (101%)	449 (98%)	8 (2%)	1 (0%)	47	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	327 (96%)	14 (4%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	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	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	9	4
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	1
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	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	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	244/244 (100%)	237 (97%)	5 (2%)	2 (1%)	19	12
13	o	241/244 (99%)	237 (98%)	4 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	94 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9 3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	5252/5384 (98%)	5138 (98%)	104 (2%)	10 (0%)	47 46

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/279 (97%)	270 (100%)	0	100 100
1	a	271/279 (97%)	270 (100%)	1 (0%)	91 93
2	B	409/403 (102%)	405 (99%)	4 (1%)	76 81
2	b	408/403 (101%)	402 (98%)	6 (2%)	65 69
3	C	353/356 (99%)	350 (99%)	3 (1%)	81 86
3	c	361/356 (101%)	356 (99%)	5 (1%)	67 72
4	D	278/277 (100%)	276 (99%)	2 (1%)	84 89
4	d	278/277 (100%)	275 (99%)	3 (1%)	73 78
5	E	72/73 (99%)	70 (97%)	2 (3%)	43 44
5	e	72/73 (99%)	70 (97%)	2 (3%)	43 44
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	34 32
7	h	55/54 (102%)	53 (96%)	2 (4%)	35 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	I	34/34 (100%)	32 (94%)	2 (6%)	19 15
8	i	34/34 (100%)	33 (97%)	1 (3%)	42 42
9	J	26/27 (96%)	25 (96%)	1 (4%)	33 31
9	j	26/27 (96%)	25 (96%)	1 (4%)	33 31
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 1
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 4
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	34/35 (97%)	34 (100%)	0	100 100
12	M	30/32 (94%)	28 (93%)	2 (7%)	16 11
12	m	32/32 (100%)	30 (94%)	2 (6%)	18 13
13	O	209/207 (101%)	204 (98%)	5 (2%)	49 51
13	o	206/207 (100%)	202 (98%)	4 (2%)	57 61
14	T	27/28 (96%)	26 (96%)	1 (4%)	34 32
14	t	26/28 (93%)	26 (100%)	0	100 100
15	U	84/89 (94%)	82 (98%)	2 (2%)	49 51
15	u	85/89 (96%)	83 (98%)	2 (2%)	49 51
16	V	119/117 (102%)	118 (99%)	1 (1%)	81 86
16	v	117/117 (100%)	112 (96%)	5 (4%)	29 27
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3 1
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57 61
19	z	52/52 (100%)	46 (88%)	6 (12%)	5 2
20	R	29/29 (100%)	27 (93%)	2 (7%)	15 10
All	All	4358/4403 (99%)	4278 (98%)	80 (2%)	59 63

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

Mol	Chain	Res	Type
13	o	36	GLN
19	Z	31	GLN
13	o	69	LYS

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Mol	Chain	Res	Type
16	v	85	GLU
19	z	3	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
5	E	60	GLN
13	o	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.38	1 (14%)
14	FME	t	1	14	8,9,10	0.62	0	7,9,11	1.63	2 (28%)
12	FME	M	1	12	8,9,10	0.66	0	7,9,11	1.24	0
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.28	0
8	FME	I	1	8	8,9,10	0.55	0	7,9,11	1.24	1 (14%)
14	FME	T	1	14	8,9,10	0.71	0	7,9,11	1.68	2 (28%)

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
12	FME	m	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-2.69	118.69	122.82
14	T	1	FME	CG-CB-CA	2.51	119.91	112.95
14	T	1	FME	CA-N-CN	2.43	126.55	122.82
14	t	1	FME	O-C-CA	-2.42	118.42	124.78
12	m	1	FME	O1-CN-N	-2.26	119.31	125.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA

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 225 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 192 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	b	616	-	65,73,73	1.99	15 (23%)	76,113,113	2.90	26 (34%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.36	8 (14%)
23	CLA	B	604	-	65,73,73	2.00	18 (27%)	76,113,113	2.67	28 (36%)
24	PHO	A	416	-	51,69,69	1.87	8 (15%)	47,99,99	1.93	12 (25%)
27	GOL	b	628	-	5,5,5	0.40	0	5,5,5	1.38	1 (20%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	9 (16%)
32	LMG	c	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.36	7 (11%)
23	CLA	B	601	41	65,73,73	2.09	17 (26%)	76,113,113	2.76	27 (35%)
26	SQD	A	410	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
25	BCR	C	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.38	8 (14%)
33	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	C	513	-	65,73,73	2.07	15 (23%)	76,113,113	2.72	28 (36%)
23	CLA	c	507	-	65,73,73	2.05	17 (26%)	76,113,113	2.77	28 (36%)
31	LMT	c	501	-	36,36,36	1.03	1 (2%)	47,47,47	1.02	1 (2%)
33	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
32	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.42	5 (11%)
23	CLA	b	612	-	65,73,73	2.00	15 (23%)	76,113,113	2.79	27 (35%)
31	LMT	B	630	-	36,36,36	1.00	3 (8%)	47,47,47	1.14	3 (6%)
33	LHG	d	411	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
35	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	a	409	-	65,73,73	1.97	16 (24%)	76,113,113	2.84	28 (36%)
34	HTG	d	409	-	16,16,19	0.98	1 (6%)	20,21,24	1.59	1 (5%)
23	CLA	D	403	-	65,73,73	2.07	16 (24%)	76,113,113	2.75	29 (38%)
35	DGD	C	517	-	63,63,67	0.87	3 (4%)	77,77,81	0.93	3 (3%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.32	8 (14%)
32	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.43	8 (13%)
34	HTG	B	622	-	19,19,19	1.16	2 (10%)	23,24,24	1.52	5 (21%)
27	GOL	a	419	-	5,5,5	1.02	0	5,5,5	0.97	0
29	PL9	a	415	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
27	GOL	B	624	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
27	GOL	v	202	-	5,5,5	1.27	0	5,5,5	0.72	0
23	CLA	B	606	-	65,73,73	1.98	16 (24%)	76,113,113	2.93	28 (36%)
31	LMT	b	627	-	25,25,36	0.89	2 (8%)	30,30,47	1.10	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	506	-	65,73,73	2.05	17 (26%)	76,113,113	2.73	29 (38%)
31	LMT	F	101	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.72	14 (25%)
23	CLA	B	607	41	65,73,73	1.93	17 (26%)	76,113,113	2.80	26 (34%)
27	GOL	l	102	-	5,5,5	0.96	0	5,5,5	0.97	0
28	OEX	a	414	41,1,3	0,15,15	-	-	-		
26	SQD	a	413	-	53,54,54	1.05	3 (5%)	62,65,65	1.19	8 (12%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.30	7 (12%)
35	DGD	H	102	-	63,63,67	0.85	4 (6%)	77,77,81	0.97	6 (7%)
27	GOL	A	418	-	5,5,5	1.58	2 (40%)	5,5,5	1.02	1 (20%)
23	CLA	b	601	41	65,73,73	2.12	16 (24%)	76,113,113	2.75	27 (35%)
23	CLA	c	504	-	65,73,73	2.00	16 (24%)	76,113,113	2.79	25 (32%)
23	CLA	b	615	-	65,73,73	1.99	16 (24%)	76,113,113	2.77	28 (36%)
23	CLA	B	613	-	65,73,73	2.02	15 (23%)	76,113,113	2.76	29 (38%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.02	0
27	GOL	b	629	-	5,5,5	1.07	0	5,5,5	0.91	0
33	LHG	a	421	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
35	DGD	c	519	-	63,63,67	0.87	3 (4%)	77,77,81	1.00	5 (6%)
27	GOL	C	521	-	5,5,5	1.18	0	5,5,5	0.83	0
23	CLA	c	512	3	65,73,73	2.10	16 (24%)	76,113,113	2.74	30 (39%)
31	LMT	T	101	-	36,36,36	1.09	3 (8%)	47,47,47	1.07	2 (4%)
32	LMG	a	418	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	b	610	41	65,73,73	2.02	16 (24%)	76,113,113	2.80	28 (36%)
23	CLA	b	607	41	65,73,73	1.95	19 (29%)	76,113,113	2.76	27 (35%)
25	BCR	k	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.52	12 (21%)
32	LMG	C	519	-	51,51,55	1.05	3 (5%)	59,59,63	1.31	5 (8%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.29	6 (10%)
27	GOL	O	303	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.07	6 (7%)
23	CLA	b	602	-	65,73,73	2.04	16 (24%)	76,113,113	2.87	35 (46%)
23	CLA	c	511	-	65,73,73	1.99	16 (24%)	76,113,113	2.82	30 (39%)
37	BCT	a	404	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	A	408	-	65,73,73	2.00	16 (24%)	76,113,113	2.87	34 (44%)
23	CLA	b	613	-	65,73,73	1.96	15 (23%)	76,113,113	2.76	29 (38%)
23	CLA	C	503	-	65,73,73	1.98	16 (24%)	76,113,113	2.82	27 (35%)
27	GOL	c	526	-	5,5,5	0.94	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	D	404	-	41,41,41	1.07	1 (2%)	56,56,56	1.80	15 (26%)
23	CLA	B	611	-	65,73,73	2.61	18 (27%)	76,113,113	3.13	27 (35%)
23	CLA	D	402	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	29 (38%)
38	HEM	f	101	6,5	41,50,50	1.30	5 (12%)	45,82,82	1.78	10 (22%)
23	CLA	B	608	-	65,73,73	1.93	15 (23%)	76,113,113	2.78	31 (40%)
31	LMT	A	421	-	36,36,36	1.06	4 (11%)	47,47,47	1.14	4 (8%)
23	CLA	a	407	41	65,73,73	1.94	16 (24%)	76,113,113	2.81	27 (35%)
25	BCR	a	410	-	41,41,41	1.03	1 (2%)	56,56,56	1.39	9 (16%)
26	SQD	F	103	-	42,43,54	1.19	4 (9%)	51,54,65	2.02	12 (23%)
23	CLA	b	614	-	65,73,73	1.99	16 (24%)	76,113,113	2.85	28 (36%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.61	11 (17%)
23	CLA	c	506	-	65,73,73	1.98	16 (24%)	76,113,113	2.69	26 (34%)
32	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	6 (10%)
23	CLA	B	605	-	65,73,73	1.96	15 (23%)	76,113,113	2.92	28 (36%)
23	CLA	a	405	-	65,73,73	1.99	15 (23%)	76,113,113	2.87	32 (42%)
23	CLA	C	512	-	65,73,73	2.06	16 (24%)	76,113,113	2.78	32 (42%)
23	CLA	B	610	41	65,73,73	2.06	16 (24%)	76,113,113	2.90	28 (36%)
23	CLA	C	505	-	65,73,73	1.97	16 (24%)	76,113,113	2.73	28 (36%)
27	GOL	o	302	-	5,5,5	0.94	0	5,5,5	0.95	0
32	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.22	5 (8%)
38	HEM	F	102	6,5	41,50,50	1.29	6 (14%)	45,82,82	2.00	13 (28%)
23	CLA	c	514	-	65,73,73	2.11	17 (26%)	76,113,113	2.77	28 (36%)
31	LMT	t	101	-	26,26,36	0.93	2 (7%)	31,31,47	1.31	2 (6%)
23	CLA	b	611	-	65,73,73	1.93	16 (24%)	76,113,113	2.86	27 (35%)
23	CLA	C	507	41	65,73,73	2.00	15 (23%)	76,113,113	2.77	27 (35%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.22	3 (13%)
27	GOL	o	303	-	5,5,5	1.04	0	5,5,5	1.04	0
23	CLA	b	608	-	65,73,73	1.98	16 (24%)	76,113,113	2.84	31 (40%)
27	GOL	O	302	-	5,5,5	0.92	0	5,5,5	0.95	0
34	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.33	2 (8%)
33	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
27	GOL	B	629	-	5,5,5	1.32	1 (20%)	5,5,5	0.90	0
27	GOL	a	420	-	5,5,5	1.26	1 (20%)	5,5,5	0.87	0
23	CLA	c	509	-	65,73,73	2.11	16 (24%)	76,113,113	2.71	26 (34%)
34	HTG	B	623	-	19,19,19	0.79	1 (5%)	23,24,24	1.47	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	B	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.25	3 (5%)
35	DGD	C	516	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
40	HEC	V	201	16	32,50,50	2.00	4 (12%)	24,82,82	2.02	6 (25%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.35	11 (19%)
23	CLA	b	605	-	65,73,73	1.96	17 (26%)	76,113,113	3.00	25 (32%)
33	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	614	-	65,73,73	2.00	17 (26%)	76,113,113	2.91	30 (39%)
23	CLA	B	612	-	65,73,73	2.03	16 (24%)	76,113,113	2.87	30 (39%)
23	CLA	c	502	-	65,73,73	2.00	17 (26%)	76,113,113	2.78	27 (35%)
23	CLA	c	503	-	65,73,73	2.01	15 (23%)	76,113,113	2.70	24 (31%)
23	CLA	B	602	-	65,73,73	2.03	16 (24%)	76,113,113	2.83	27 (35%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.66	12 (21%)
23	CLA	A	405	41	65,73,73	1.90	16 (24%)	76,113,113	2.85	30 (39%)
34	HTG	b	625	-	19,19,19	1.01	2 (10%)	23,24,24	1.61	5 (21%)
23	CLA	A	406	41	65,73,73	1.96	16 (24%)	76,113,113	2.81	29 (38%)
27	GOL	b	624	-	5,5,5	1.15	1 (20%)	5,5,5	0.81	0
23	CLA	C	510	-	65,73,73	2.09	17 (26%)	76,113,113	2.85	30 (39%)
24	PHO	a	417	-	51,69,69	1.86	9 (17%)	47,99,99	1.99	13 (27%)
31	LMT	m	103	-	36,36,36	1.10	4 (11%)	47,47,47	1.06	3 (6%)
23	CLA	A	404	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	32 (42%)
31	LMT	A	417	-	36,36,36	0.96	3 (8%)	47,47,47	1.01	1 (2%)
34	HTG	b	623	-	19,19,19	1.05	1 (5%)	23,24,24	1.87	2 (8%)
25	BCR	d	403	-	41,41,41	1.11	1 (2%)	56,56,56	1.89	18 (32%)
25	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	12 (21%)
25	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	9 (16%)
31	LMT	e	101	-	36,36,36	1.04	4 (11%)	47,47,47	0.97	1 (2%)
27	GOL	c	527	-	5,5,5	0.97	0	5,5,5	0.98	0
35	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
35	DGD	C	515	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
34	HTG	c	522	-	19,19,19	0.97	2 (10%)	23,24,24	1.54	2 (8%)
26	SQD	B	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.75	14 (22%)
25	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.23	7 (12%)
25	BCR	t	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	12 (21%)
23	CLA	B	615	-	65,73,73	2.01	17 (26%)	76,113,113	2.79	27 (35%)
29	PL9	D	405	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	504	41	65,73,73	2.02	16 (24%)	76,113,113	2.74	27 (35%)
23	CLA	C	509	-	65,73,73	2.08	17 (26%)	76,113,113	2.88	28 (36%)
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.28	4 (6%)
33	LHG	b	630	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
23	CLA	d	401	-	65,73,73	1.94	17 (26%)	76,113,113	2.79	29 (38%)
37	BCT	D	401	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	c	508	41	65,73,73	2.02	15 (23%)	76,113,113	2.79	26 (34%)
33	LHG	d	405	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	5 (8%)
23	CLA	d	402	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	29 (38%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	10 (19%)
27	GOL	B	627	-	5,5,5	0.95	0	5,5,5	0.99	0
27	GOL	A	411	-	5,5,5	1.14	0	5,5,5	0.71	0
29	PL9	d	404	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
25	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.55	12 (21%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	6 (9%)
32	LMG	C	518	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	4 (6%)
32	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	3 (5%)
23	CLA	b	604	-	65,73,73	2.02	15 (23%)	76,113,113	2.73	25 (32%)
23	CLA	B	609	-	65,73,73	2.02	16 (24%)	76,113,113	2.75	26 (34%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
33	LHG	E	101	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
33	LHG	A	420	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
25	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
23	CLA	c	510	-	65,73,73	2.06	15 (23%)	76,113,113	2.79	29 (38%)
23	CLA	a	406	41	65,73,73	2.00	14 (21%)	76,113,113	2.75	26 (34%)
31	LMT	b	621	-	25,25,36	0.97	2 (8%)	30,30,47	1.17	1 (3%)
23	CLA	B	603	-	65,73,73	2.02	16 (24%)	76,113,113	2.96	27 (35%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.33	7 (12%)
23	CLA	C	511	3	65,73,73	2.03	16 (24%)	76,113,113	2.71	24 (31%)
23	CLA	b	603	-	65,73,73	1.99	15 (23%)	76,113,113	2.86	29 (38%)
31	LMT	B	631	-	25,25,36	0.90	2 (8%)	30,30,47	1.12	3 (10%)
23	CLA	B	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	25 (32%)
23	CLA	c	513	-	65,73,73	2.06	16 (24%)	76,113,113	2.72	29 (38%)
31	LMT	M	101	-	36,36,36	1.15	3 (8%)	47,47,47	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PHO	A	407	-	51,69,69	1.78	8 (15%)	47,99,99	1.77	11 (23%)
23	CLA	b	609	-	65,73,73	2.01	16 (24%)	76,113,113	2.72	29 (38%)
28	OEX	A	413	41,1,3	0,15,15	-	-	-		
32	LMG	d	410	39	51,51,55	0.90	2 (3%)	59,59,63	1.10	5 (8%)
29	PL9	A	414	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
24	PHO	a	408	-	51,69,69	1.83	8 (15%)	47,99,99	1.71	10 (21%)
27	GOL	V	203	-	5,5,5	1.22	0	5,5,5	0.91	0
34	HTG	V	202	-	11,11,19	0.23	0	15,15,24	1.08	1 (6%)
34	HTG	D	410	-	16,16,19	1.08	2 (12%)	20,21,24	1.50	1 (5%)
23	CLA	c	505	41	65,73,73	2.07	17 (26%)	76,113,113	2.74	26 (34%)
23	CLA	C	508	-	65,73,73	2.11	15 (23%)	76,113,113	2.72	26 (34%)
34	HTG	b	622	-	19,19,19	1.20	2 (10%)	23,24,24	1.94	7 (30%)
40	HEC	v	201	16	32,50,50	2.02	3 (9%)	24,82,82	1.94	6 (25%)
32	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.07	3 (6%)
23	CLA	C	502	-	65,73,73	2.04	16 (24%)	76,113,113	2.64	25 (32%)
31	LMT	B	628	-	36,36,36	1.17	4 (11%)	47,47,47	1.30	5 (10%)
23	CLA	C	501	-	65,73,73	1.98	16 (24%)	76,113,113	2.78	27 (35%)
23	CLA	b	606	-	65,73,73	2.01	15 (23%)	76,113,113	2.84	29 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	616	-	1/1/15/20	10/37/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	2/37/115/115	-
24	PHO	A	416	-	-	1/37/103/103	0/5/6/6
27	GOL	b	628	-	-	0/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
32	LMG	c	521	-	-	7/46/66/70	0/1/1/1
23	CLA	B	601	41	1/1/15/20	12/37/115/115	-
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
33	LHG	d	406	-	-	11/53/53/53	-
23	CLA	C	513	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	507	-	1/1/15/20	8/37/115/115	-
31	LMT	c	501	-	-	11/21/61/61	0/2/2/2
33	LHG	L	101	-	-	19/53/53/53	-
32	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
23	CLA	b	612	-	1/1/15/20	2/37/115/115	-
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
33	LHG	d	411	-	-	13/53/53/53	-
35	DGD	c	518	-	-	17/51/91/95	0/2/2/2
23	CLA	a	409	-	1/1/15/20	9/37/115/115	-
34	HTG	d	409	-	-	1/7/27/30	0/1/1/1
23	CLA	D	403	-	1/1/15/20	14/37/115/115	-
35	DGD	C	517	-	-	16/51/91/95	0/2/2/2
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
32	LMG	A	419	-	-	13/46/66/70	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
27	GOL	a	419	-	-	2/4/4/4	-
29	PL9	a	415	-	-	14/53/73/73	0/1/1/1
27	GOL	B	624	-	-	4/4/4/4	-
27	GOL	v	202	-	-	1/4/4/4	-
23	CLA	B	606	-	1/1/15/20	10/37/115/115	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	C	506	-	1/1/15/20	11/37/115/115	-
31	LMT	F	101	-	-	9/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	607	41	1/1/15/20	5/37/115/115	-
27	GOL	l	102	-	-	2/4/4/4	-
26	SQD	a	413	-	-	15/49/69/69	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
27	GOL	A	418	-	-	2/4/4/4	-
23	CLA	b	601	41	1/1/15/20	19/37/115/115	-
23	CLA	c	504	-	1/1/15/20	1/37/115/115	-
23	CLA	b	615	-	1/1/15/20	7/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
27	GOL	a	412	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	b	629	-	-	1/4/4/4	-
33	LHG	a	421	-	-	16/46/46/53	-
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
27	GOL	C	521	-	-	0/4/4/4	-
23	CLA	c	512	3	1/1/15/20	4/37/115/115	-
31	LMT	T	101	-	-	8/21/61/61	0/2/2/2
32	LMG	a	418	-	-	13/46/66/70	0/1/1/1
23	CLA	b	610	41	1/1/15/20	7/37/115/115	-
23	CLA	b	607	41	1/1/15/20	2/37/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LMG	C	519	-	-	11/46/66/70	0/1/1/1
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
27	GOL	O	303	-	-	2/4/4/4	-
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	b	602	-	1/1/15/20	5/37/115/115	-
23	CLA	c	511	-	1/1/15/20	11/37/115/115	-
23	CLA	A	408	-	1/1/15/20	8/37/115/115	-
23	CLA	b	613	-	1/1/15/20	3/37/115/115	-
23	CLA	C	503	-	-	3/37/115/115	-
27	GOL	c	526	-	-	0/4/4/4	-
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	B	611	-	1/1/15/20	3/37/115/115	-
23	CLA	D	402	-	1/1/15/20	0/37/115/115	-
38	HEM	f	101	6,5	-	4/12/54/54	-
23	CLA	B	608	-	-	3/37/115/115	-
31	LMT	A	421	-	-	15/21/61/61	0/2/2/2
23	CLA	a	407	41	-	5/37/115/115	-
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
23	CLA	b	614	-	1/1/15/20	15/37/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
32	LMG	c	520	-	-	11/46/66/70	0/1/1/1
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
23	CLA	a	405	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	512	-	1/1/15/20	11/37/115/115	-
23	CLA	B	610	41	1/1/15/20	7/37/115/115	-
23	CLA	C	505	-	1/1/15/20	6/37/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-
32	LMG	m	101	-	-	10/46/66/70	0/1/1/1
38	HEM	F	102	6,5	-	4/12/54/54	-
23	CLA	c	514	-	1/1/15/20	8/37/115/115	-
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
23	CLA	C	507	41	1/1/15/20	6/37/115/115	-
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
27	GOL	o	303	-	-	4/4/4/4	-
23	CLA	b	608	-	-	5/37/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
34	HTG	C	520	-	-	0/10/30/30	0/1/1/1
33	LHG	D	407	-	-	14/53/53/53	-
27	GOL	B	629	-	-	4/4/4/4	-
27	GOL	a	420	-	-	0/4/4/4	-
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
34	HTG	B	623	-	-	1/10/30/30	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
35	DGD	C	516	-	-	15/51/91/95	0/2/2/2
40	HEC	V	201	16	-	2/10/54/54	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	b	605	-	1/1/15/20	7/37/115/115	-
33	LHG	D	406	-	-	16/53/53/53	-
23	CLA	B	614	-	1/1/15/20	14/37/115/115	-
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
23	CLA	c	502	-	1/1/15/20	1/37/115/115	-
23	CLA	c	503	-	1/1/15/20	7/37/115/115	-
23	CLA	B	602	-	1/1/15/20	8/37/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	A	405	41	-	4/37/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	A	406	41	-	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	C	510	-	1/1/15/20	13/37/115/115	-
24	PHO	a	417	-	-	2/37/103/103	0/5/6/6
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2
23	CLA	A	404	-	1/1/15/20	5/37/115/115	-
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
25	BCR	d	403	-	-	5/29/63/63	0/2/2/2
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
31	LMT	e	101	-	-	14/21/61/61	0/2/2/2
27	GOL	c	527	-	-	4/4/4/4	-
35	DGD	c	517	-	-	20/51/91/95	0/2/2/2
35	DGD	C	515	-	-	11/51/91/95	0/2/2/2
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	5/37/115/115	-
29	PL9	D	405	-	-	8/53/73/73	0/1/1/1
23	CLA	C	504	41	1/1/15/20	6/37/115/115	-
23	CLA	C	509	-	1/1/15/20	2/37/115/115	-
32	LMG	B	621	-	-	19/46/66/70	0/1/1/1
33	LHG	b	630	-	-	20/53/53/53	-
23	CLA	d	401	-	1/1/15/20	2/37/115/115	-
23	CLA	c	508	41	1/1/15/20	7/37/115/115	-
33	LHG	d	405	-	-	13/53/53/53	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	d	402	-	1/1/15/20	8/37/115/115	-
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
27	GOL	B	627	-	-	2/4/4/4	-
27	GOL	A	411	-	-	2/4/4/4	-
29	PL9	d	404	-	-	6/53/73/73	0/1/1/1
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	C	518	-	-	8/46/66/70	0/1/1/1
32	LMG	D	411	39	-	10/46/66/70	0/1/1/1
23	CLA	b	604	-	1/1/15/20	8/37/115/115	-
23	CLA	B	609	-	1/1/15/20	1/37/115/115	-
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
33	LHG	E	101	-	-	22/46/46/53	-
33	LHG	A	420	-	-	10/53/53/53	-
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/15/20	14/37/115/115	-
23	CLA	a	406	41	1/1/15/20	8/37/115/115	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	B	603	-	1/1/15/20	8/37/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	C	511	3	1/1/15/20	3/37/115/115	-
23	CLA	b	603	-	1/1/15/20	5/37/115/115	-
31	LMT	B	631	-	-	10/17/37/61	0/1/1/2
23	CLA	B	616	-	1/1/15/20	5/37/115/115	-
23	CLA	c	513	-	1/1/15/20	11/37/115/115	-
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	PHO	A	407	-	-	4/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	3/37/115/115	-
32	LMG	d	410	39	-	11/46/66/70	0/1/1/1
29	PL9	A	414	-	-	15/53/73/73	0/1/1/1
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6
27	GOL	V	203	-	-	2/4/4/4	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	c	505	41	1/1/15/20	7/37/115/115	-
23	CLA	C	508	-	-	3/37/115/115	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
40	HEC	v	201	16	-	2/10/54/54	-
32	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	C	502	-	1/1/15/20	9/37/115/115	-
31	LMT	B	628	-	-	11/21/61/61	0/2/2/2
23	CLA	C	501	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	-	1/1/15/20	12/37/115/115	-

The worst 5 of 1356 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	10.63	1.55	1.40
23	B	611	CLA	CMB-C2B	6.82	1.65	1.51
23	B	616	CLA	C3B-C2B	6.65	1.49	1.40
23	B	612	CLA	C3B-C2B	6.62	1.49	1.40
23	b	612	CLA	C3B-C2B	6.57	1.49	1.40

The worst 5 of 2626 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C1D-ND-C4D	-11.66	98.05	106.33
23	B	612	CLA	C1D-ND-C4D	-10.41	98.94	106.33
23	b	605	CLA	C1D-ND-C4D	-10.31	99.01	106.33
23	B	611	CLA	C2D-C1D-ND	9.92	117.42	110.10
23	a	409	CLA	C1D-ND-C4D	-9.84	99.34	106.33

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 1274 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D

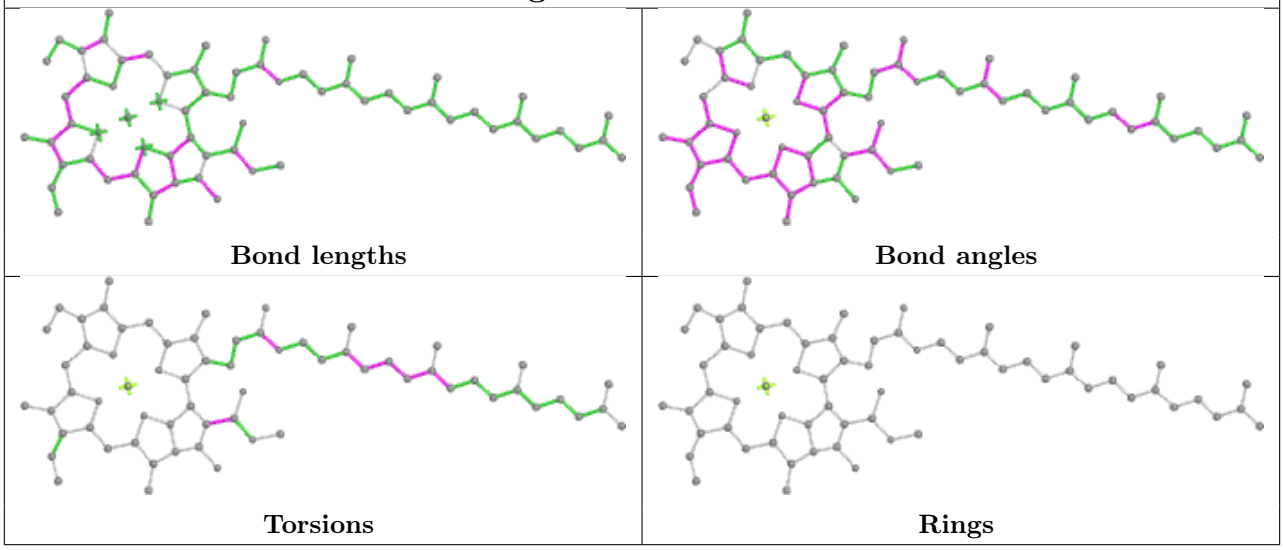
There are no ring outliers.

No monomer is involved in short contacts.

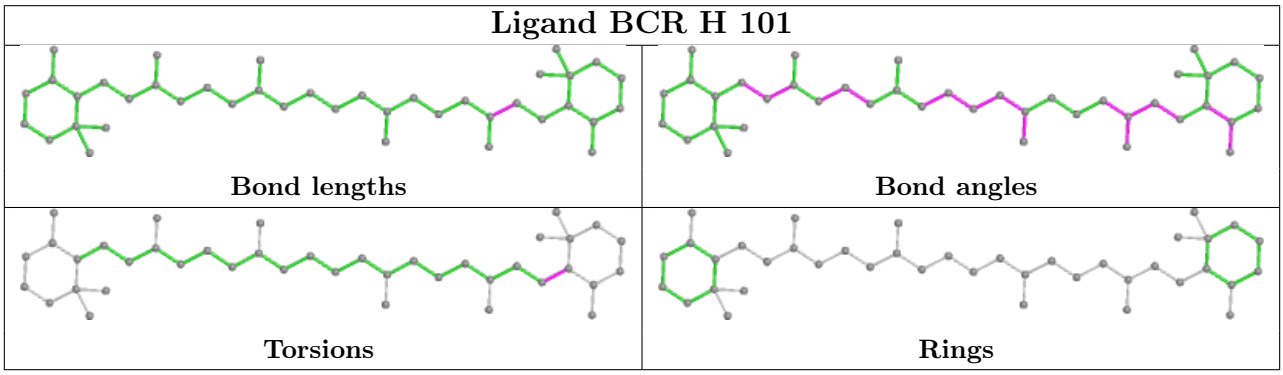
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

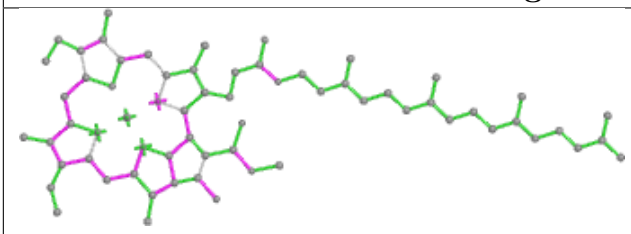
Ligand CLA b 616



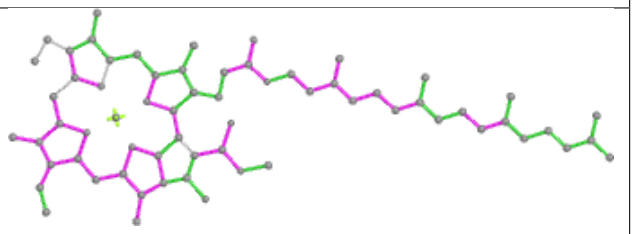
Ligand BCR H 101



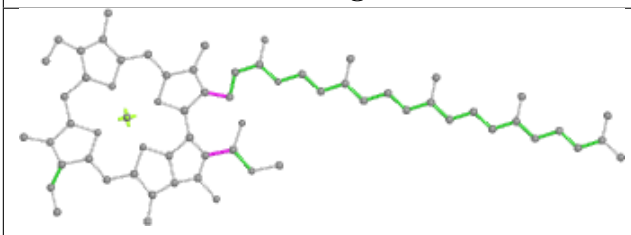
Ligand CLA B 604



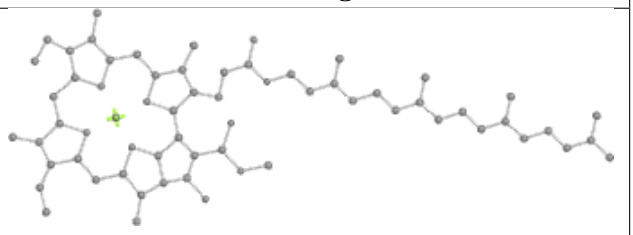
Bond lengths



Bond angles

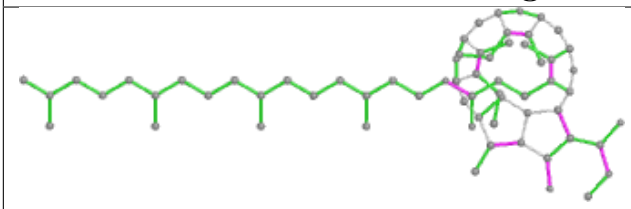


Torsions

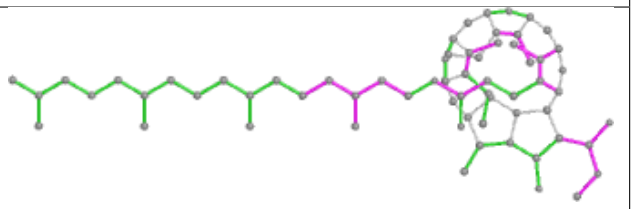


Rings

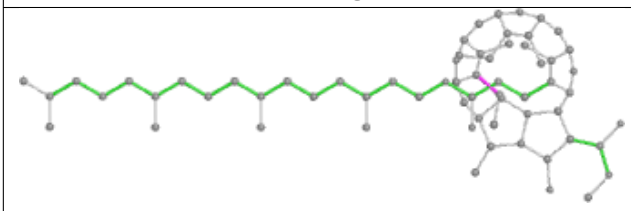
Ligand PHO A 416



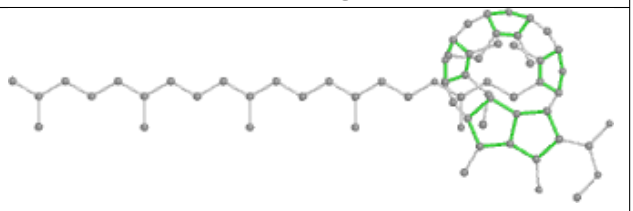
Bond lengths



Bond angles

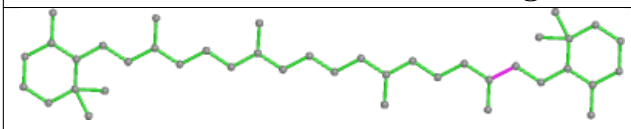


Torsions

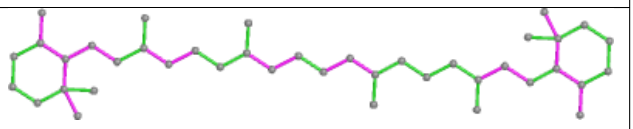


Rings

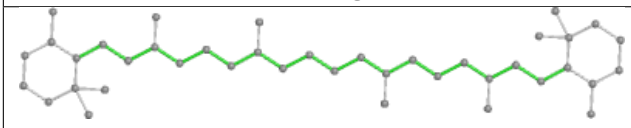
Ligand BCR A 409



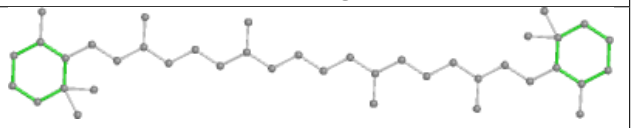
Bond lengths



Bond angles

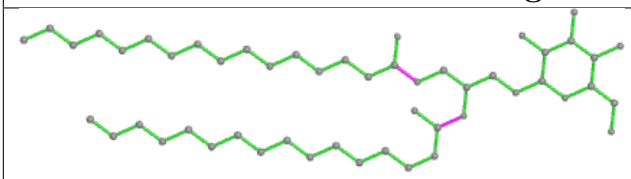


Torsions

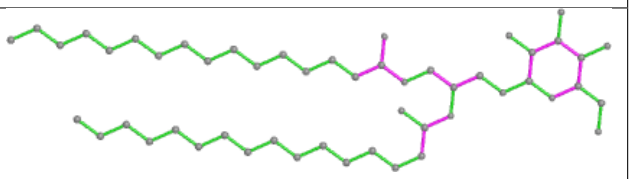


Rings

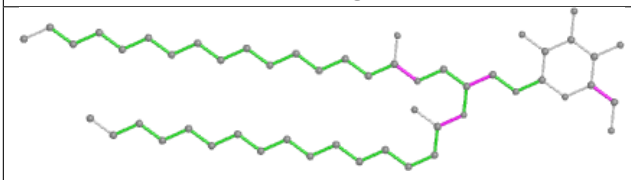
Ligand LMG c 521



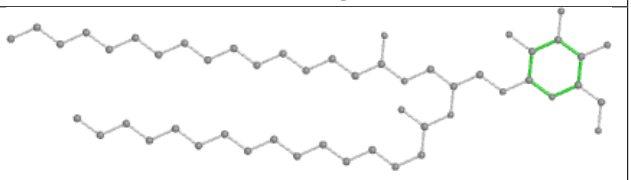
Bond lengths



Bond angles

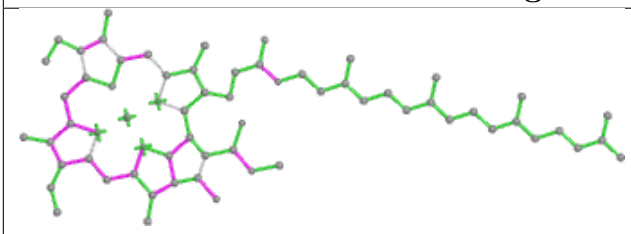


Torsions

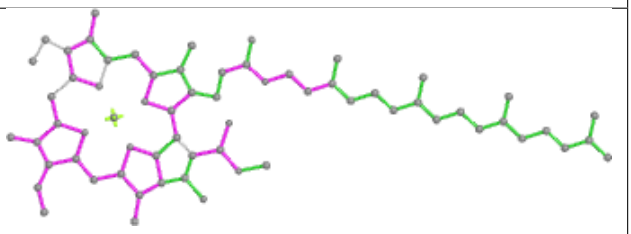


Rings

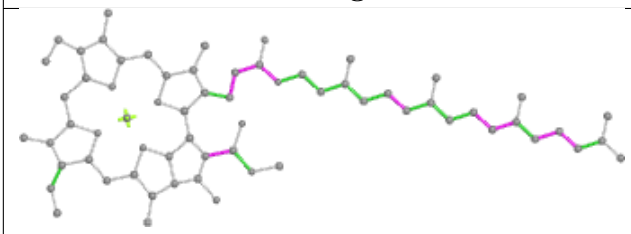
Ligand CLA B 601



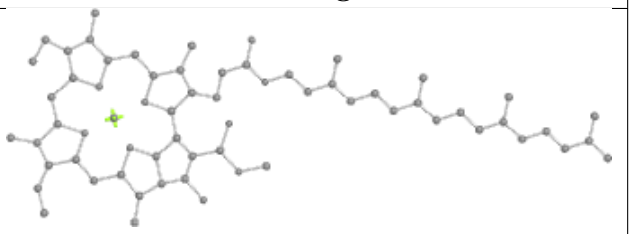
Bond lengths



Bond angles

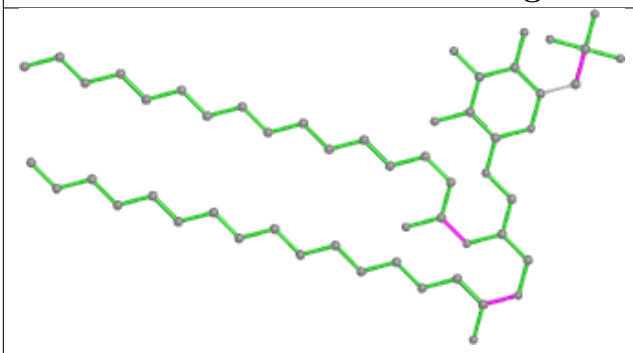


Torsions

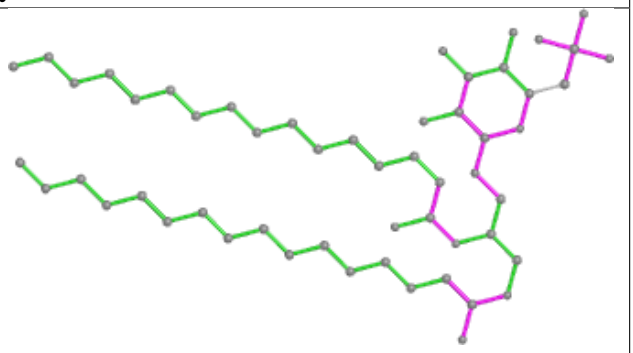


Rings

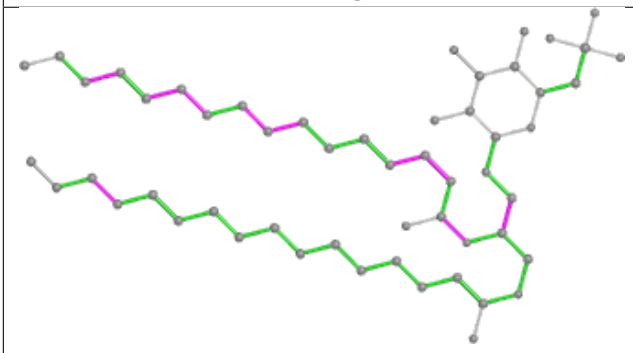
Ligand SQD A 410



Bond lengths



Bond angles



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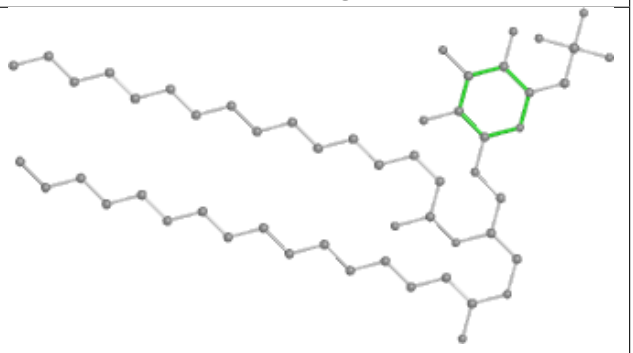
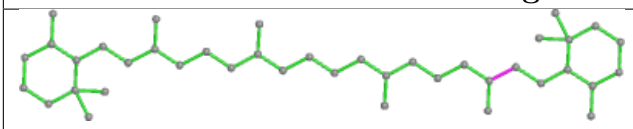
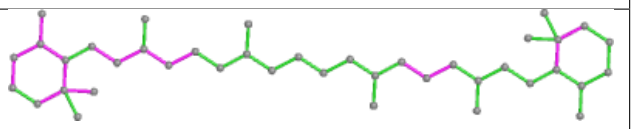


Rings

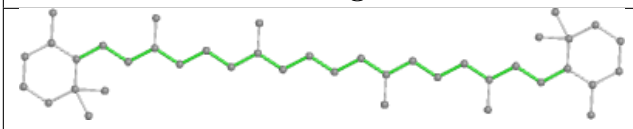
Ligand BCR C 514



Bond lengths



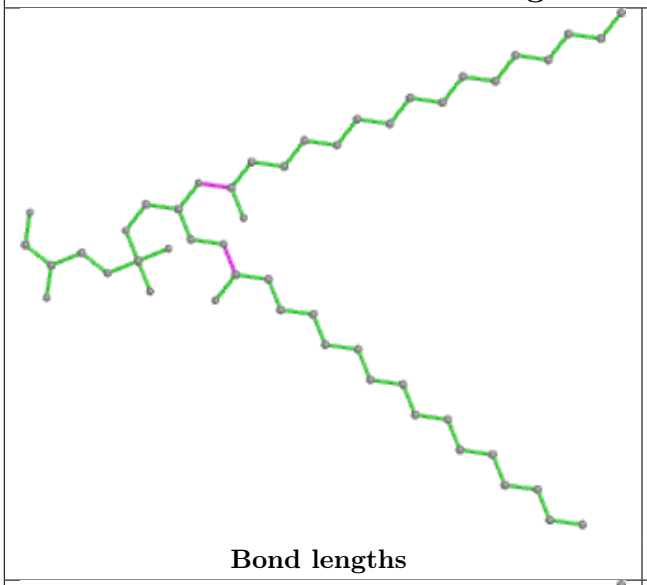
Bond angles



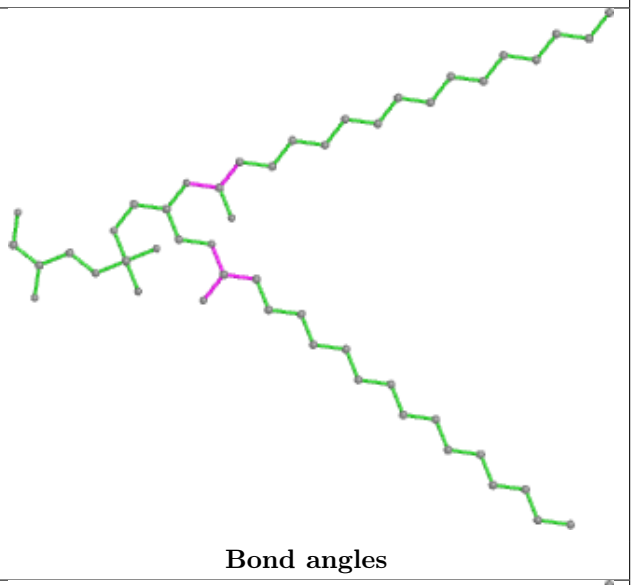
Torsions

Rings

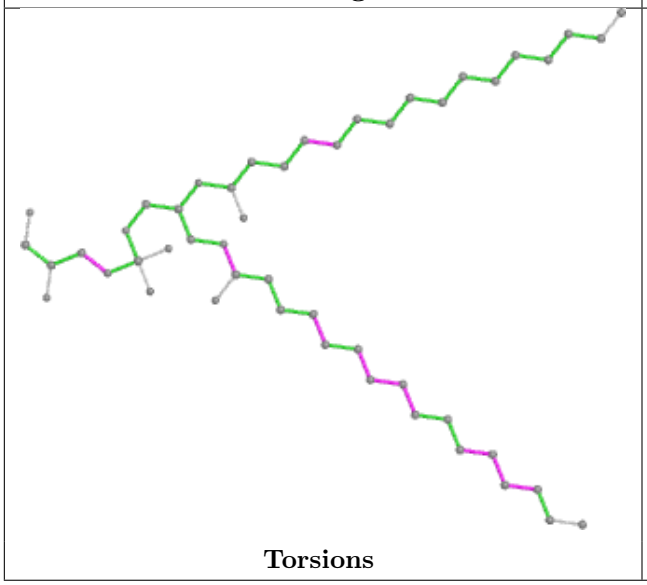
Ligand LHG d 406



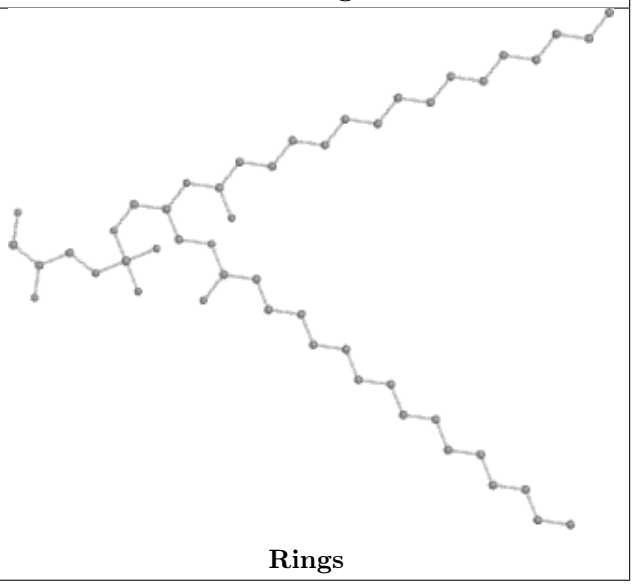
Bond lengths



Bond angles

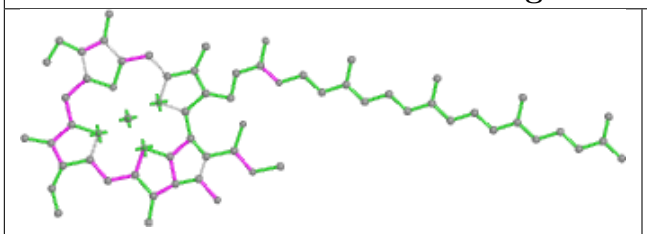


Torsions

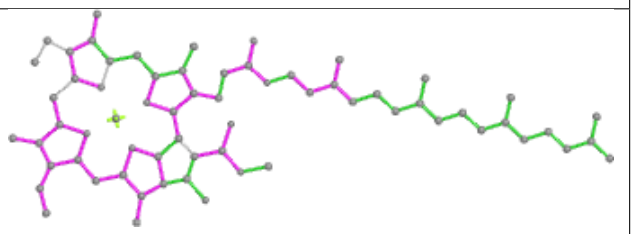


Rings

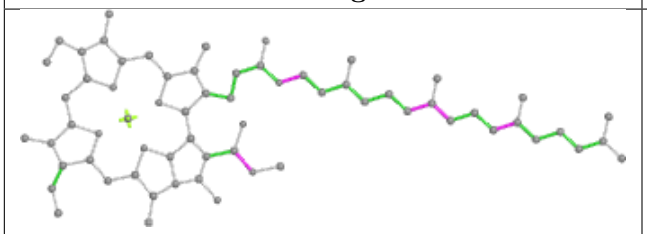
Ligand CLA C 513



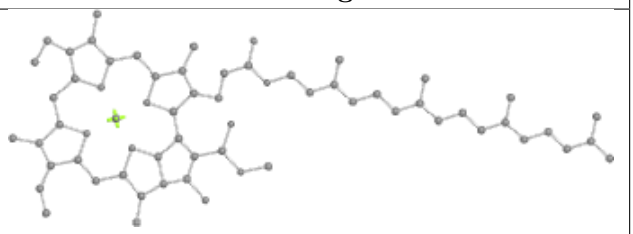
Bond lengths



Bond angles

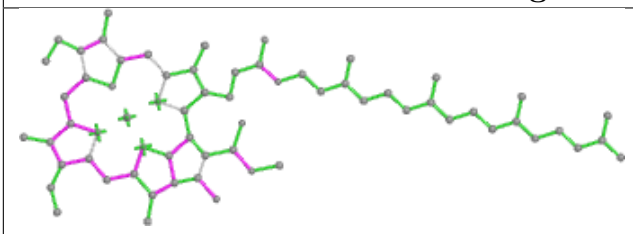


Torsions

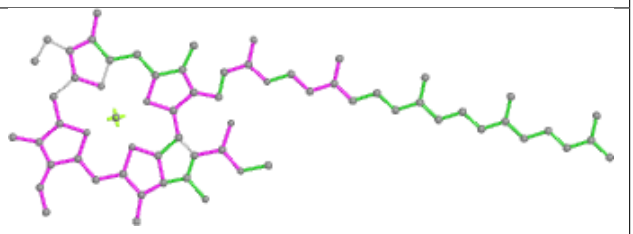


Rings

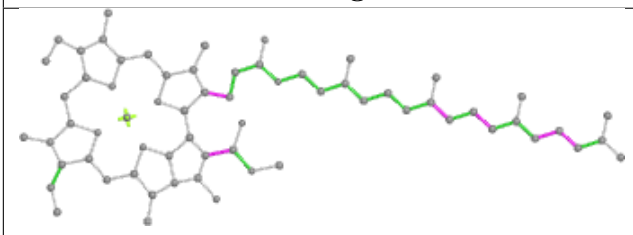
Ligand CLA c 507



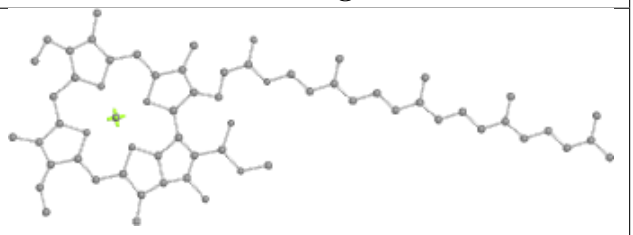
Bond lengths



Bond angles

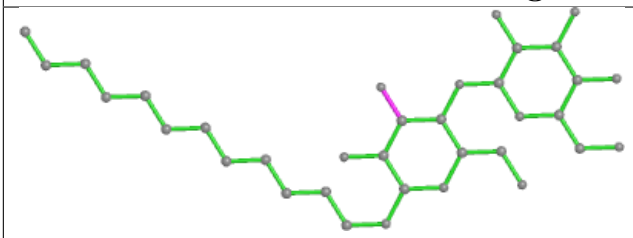


Torsions



Rings

Ligand LMT c 501



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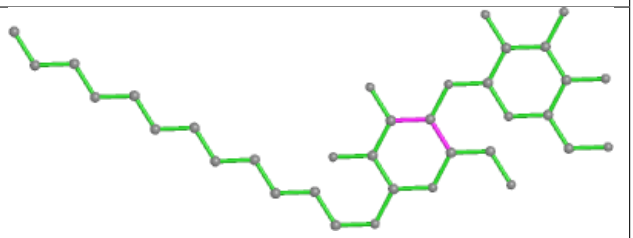
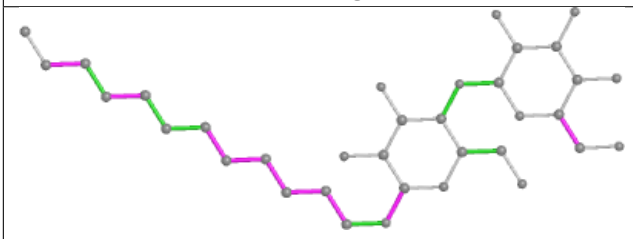
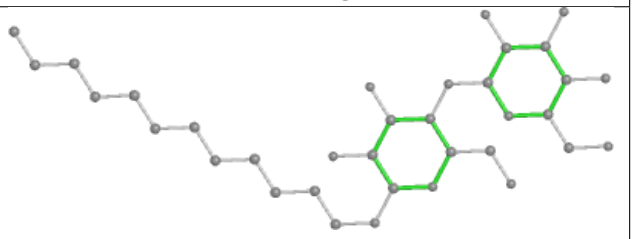


Bond angles

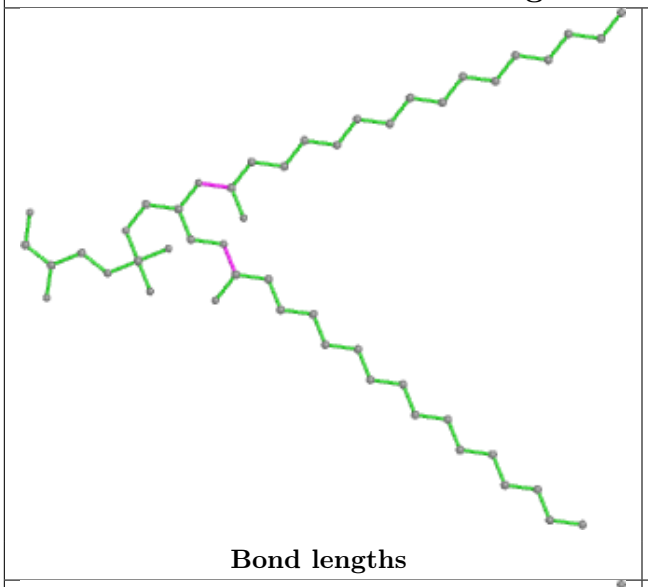


Torsions

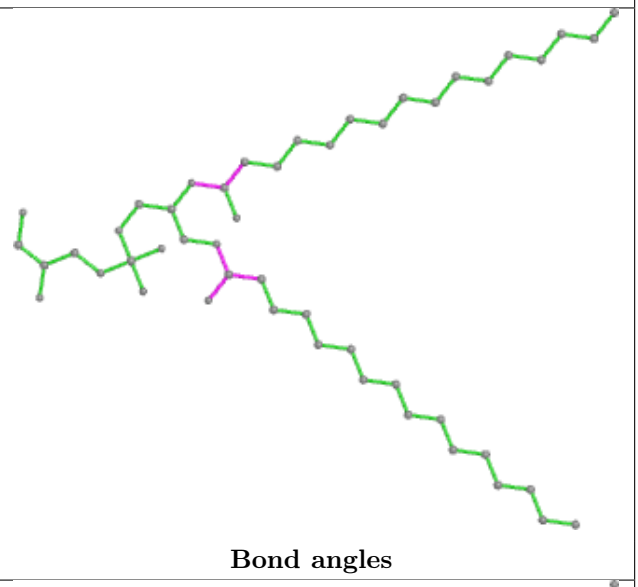


Rings

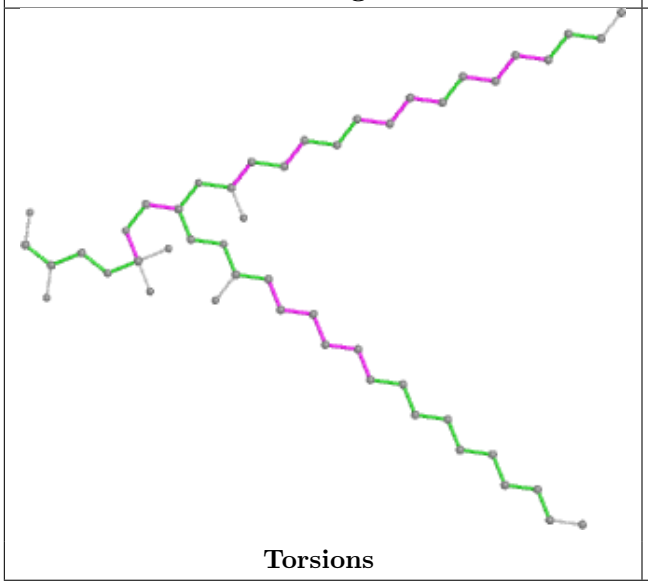
Ligand LHG L 101



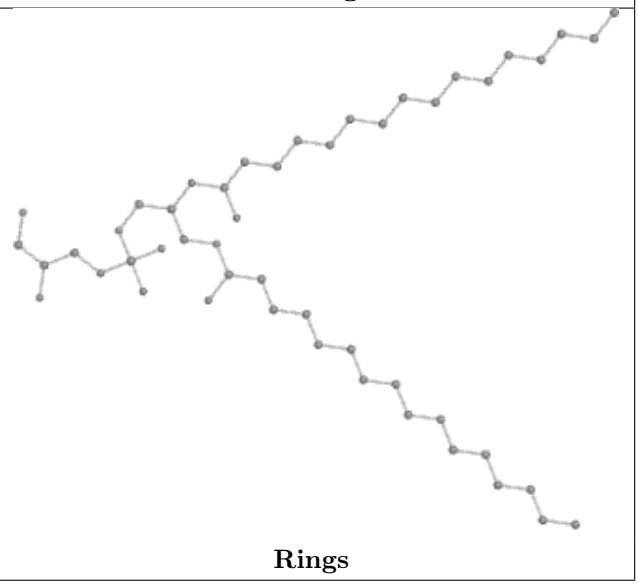
Bond lengths



Bond angles

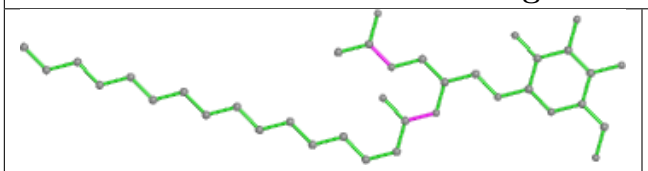


Torsions

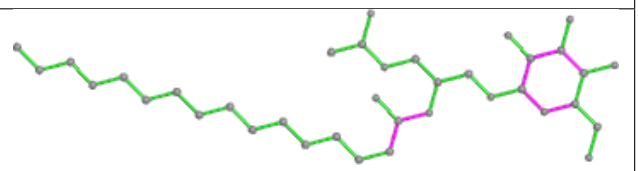


Rings

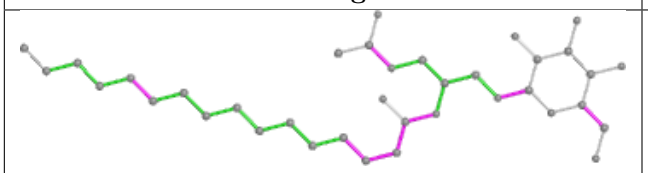
Ligand LMG Z 101



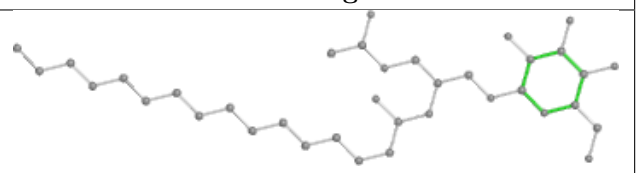
Bond lengths



Bond angles

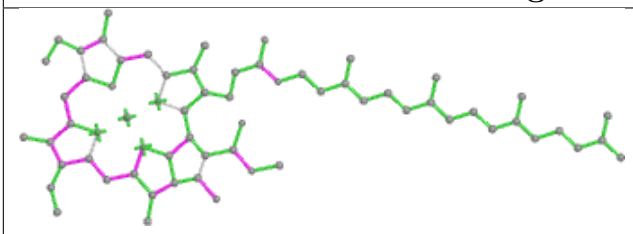


Torsions

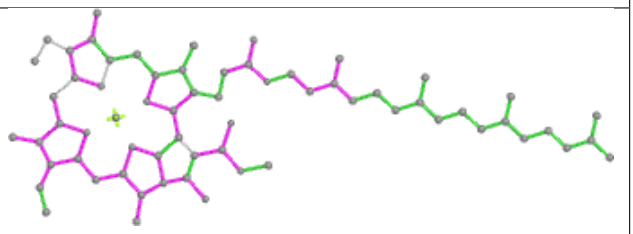


Rings

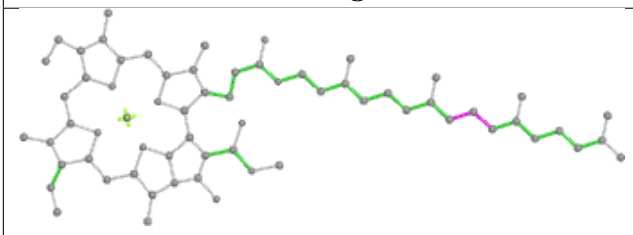
Ligand CLA b 612



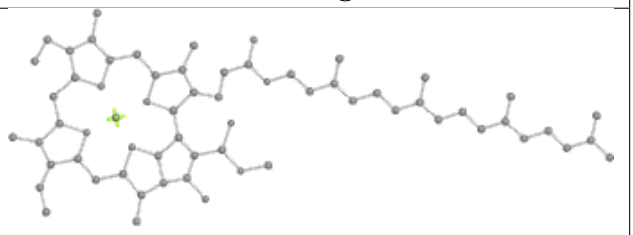
Bond lengths



Bond angles

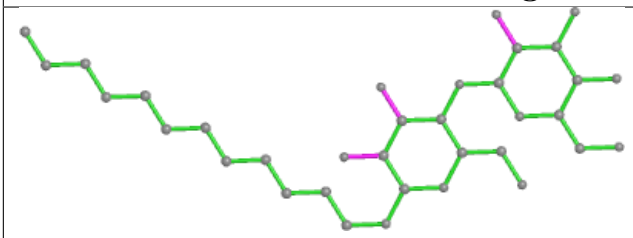


Torsions

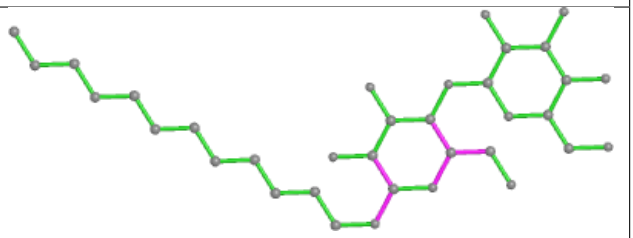


Rings

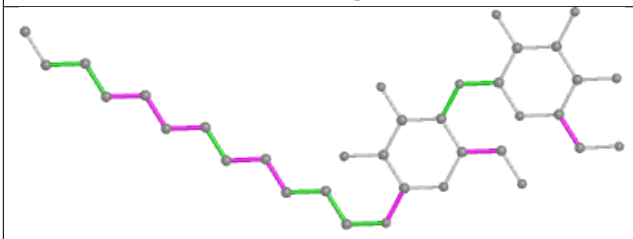
Ligand LMT B 630



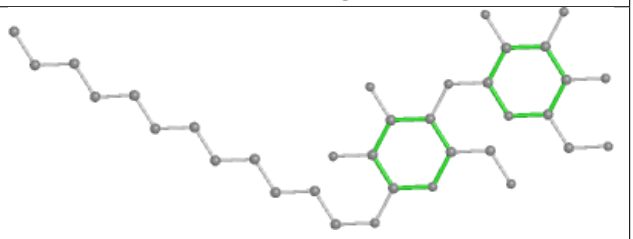
Bond lengths



Bond angles

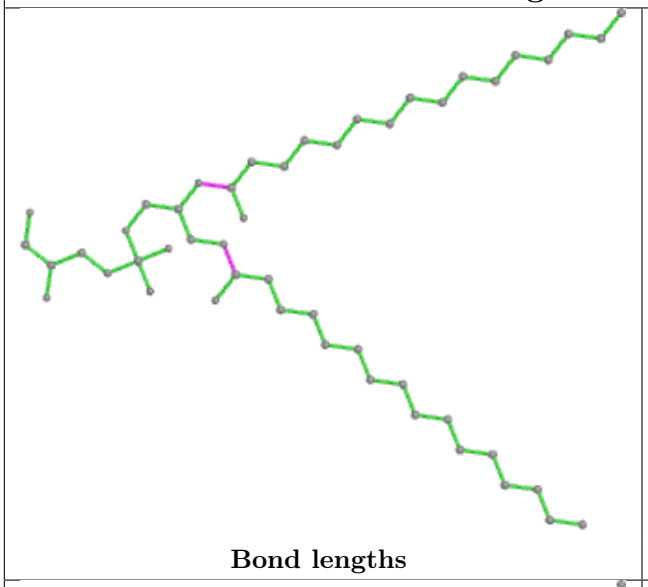


Torsions

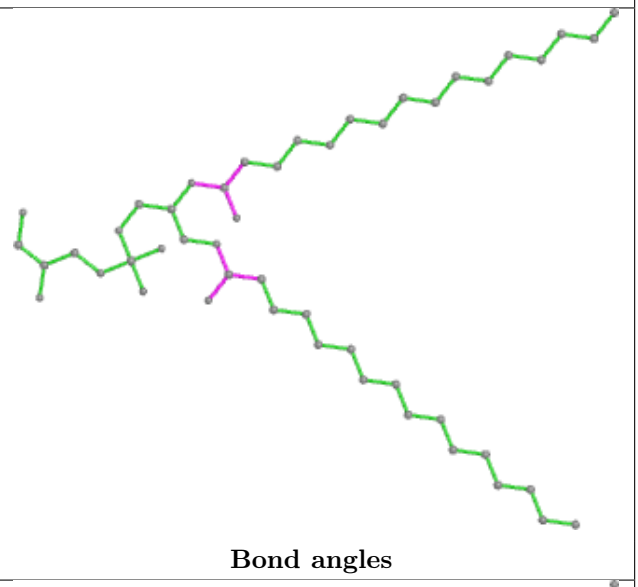


Rings

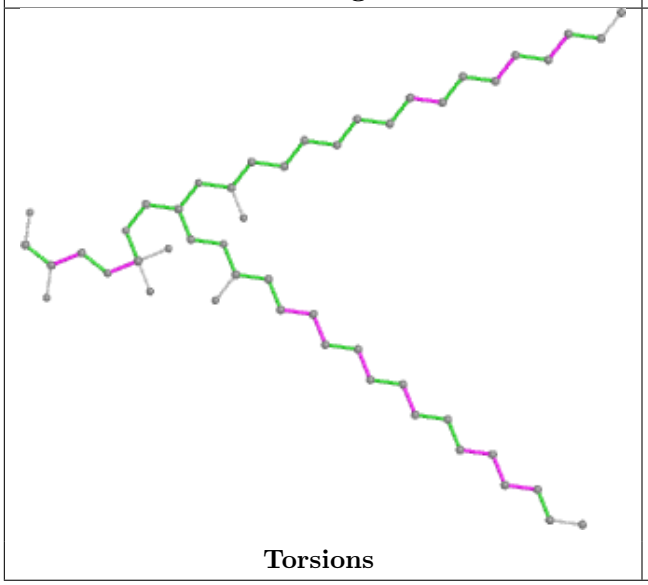
Ligand LHG d 411



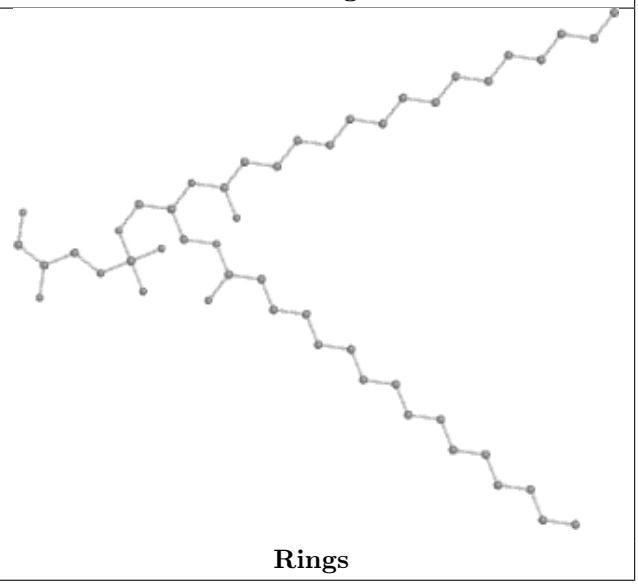
Bond lengths



Bond angles

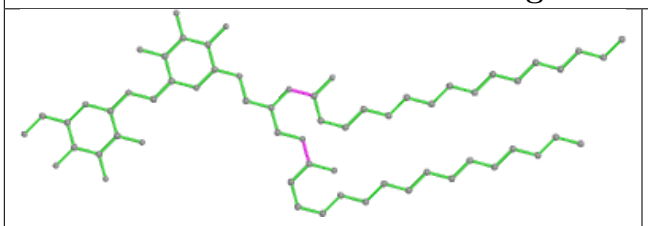


Torsions

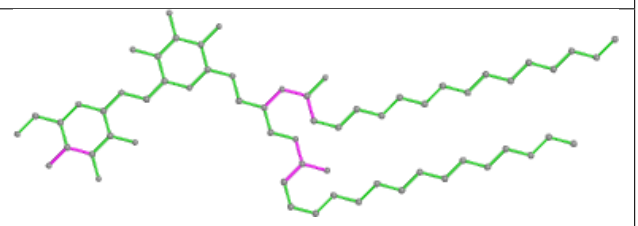


Rings

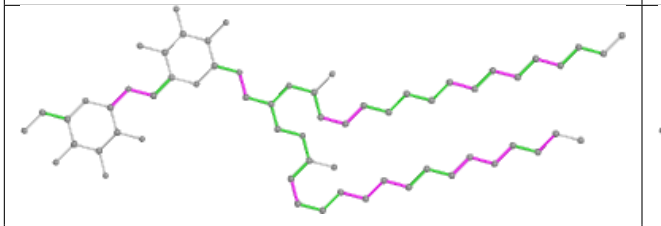
Ligand DGD c 518



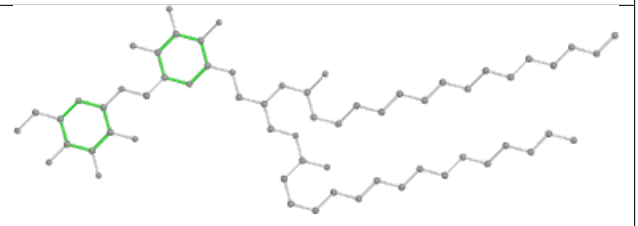
Bond lengths



Bond angles

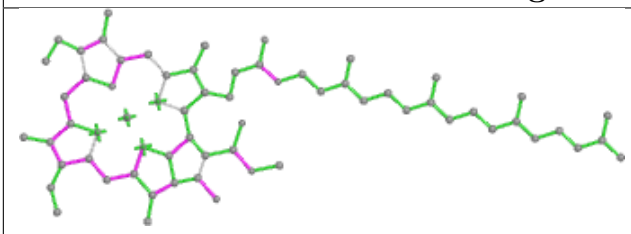


Torsions

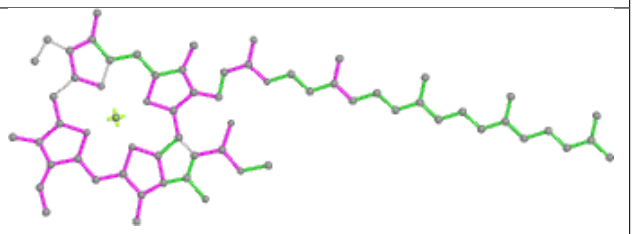


Rings

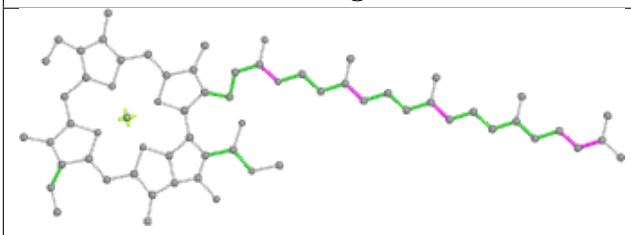
Ligand CLA a 409



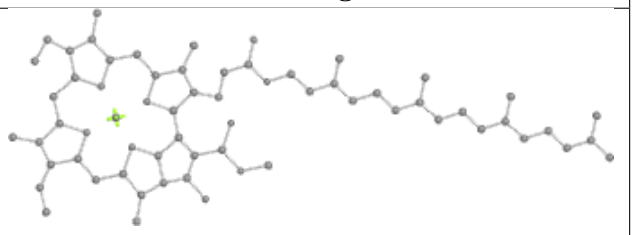
Bond lengths



Bond angles

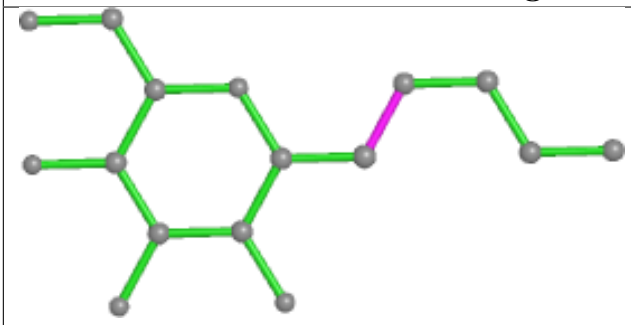


Torsions



Rings

Ligand HTG d 409



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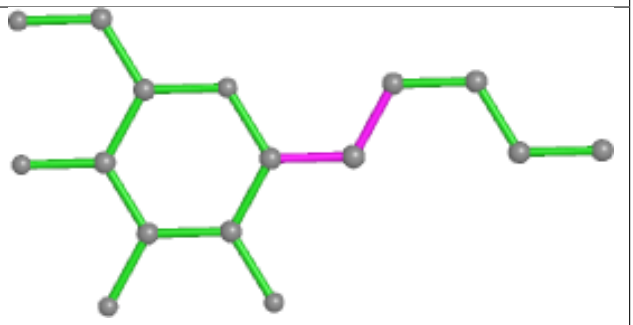
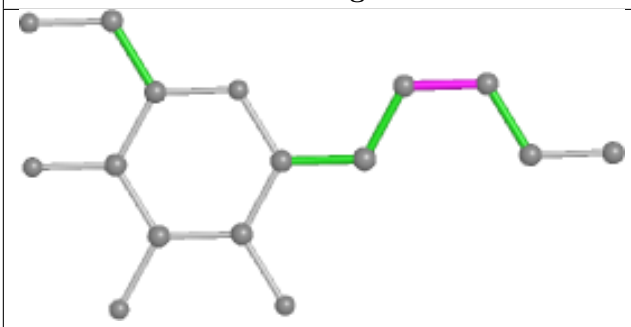
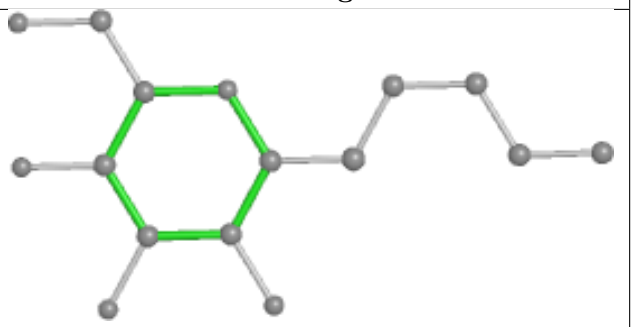


Bond angles

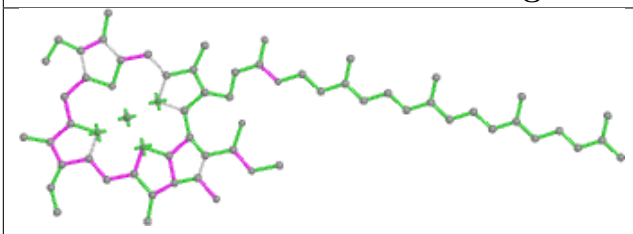


Torsions



Rings

Ligand CLA D 403



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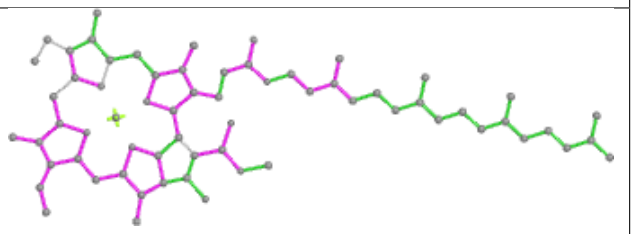
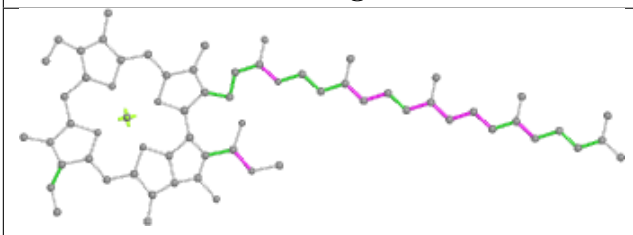
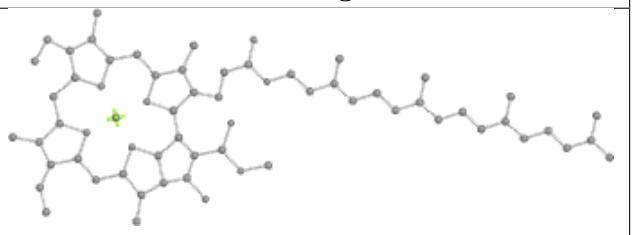


Bond angles

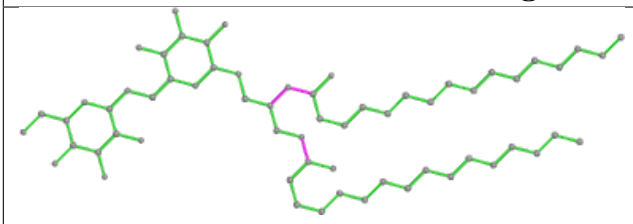


Torsions

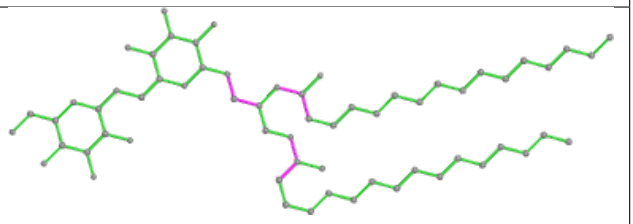


Rings

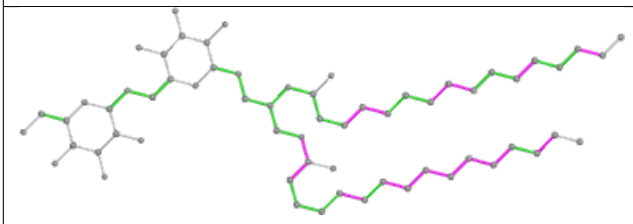
Ligand DGD C 517



Bond lengths



Bond angles



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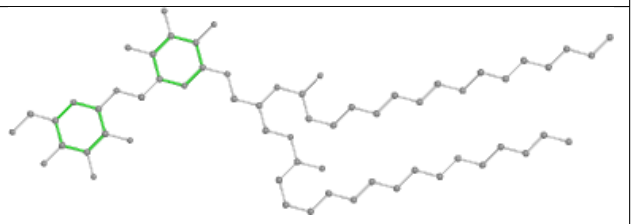
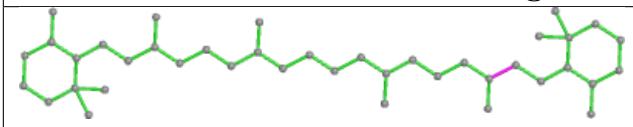
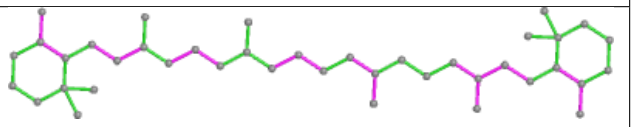


Rings

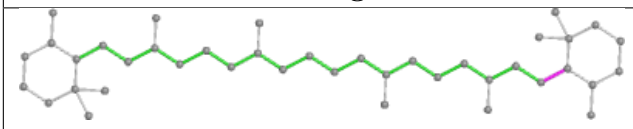
Ligand BCR h 101



Bond lengths



Bond angles



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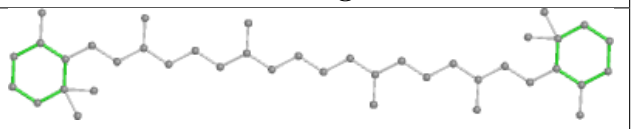
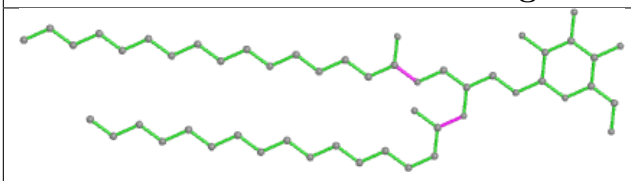
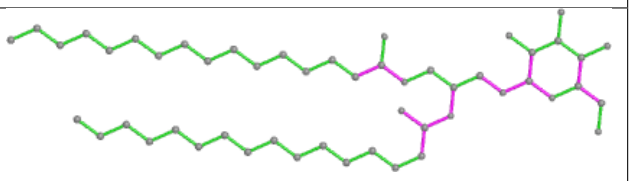


Rings

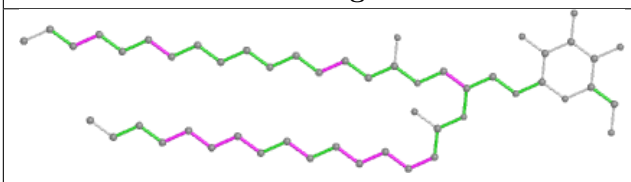
Ligand LMG A 419



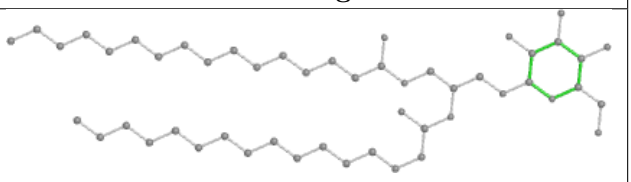
Bond lengths



Bond angles

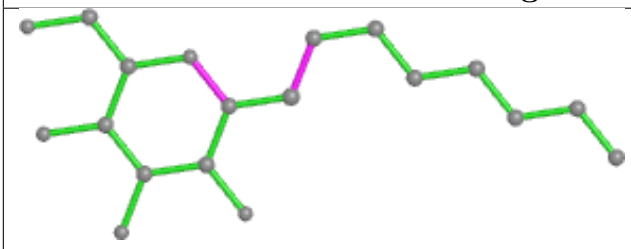


Torsions

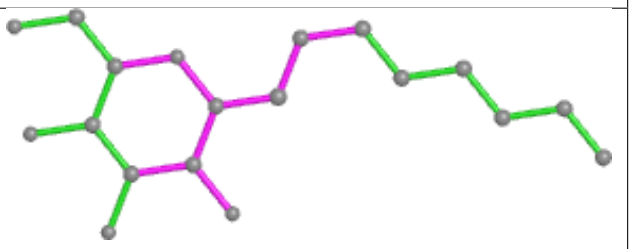


Rings

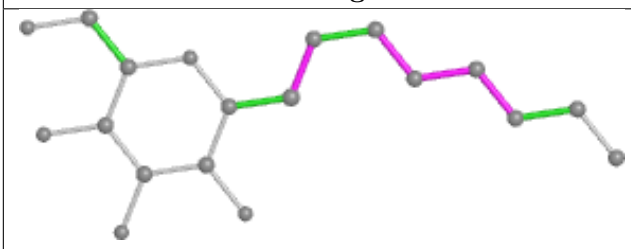
Ligand HTG B 622



Bond lengths



Bond angles



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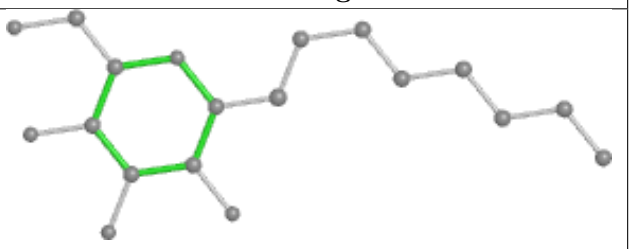
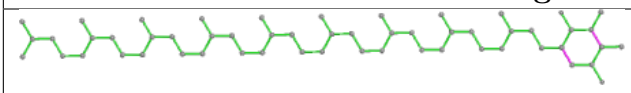
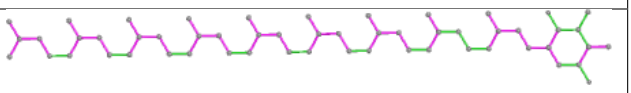


Rings

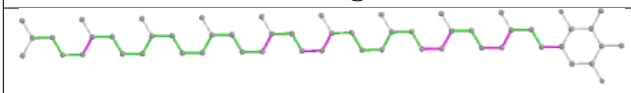
Ligand PL9 a 415



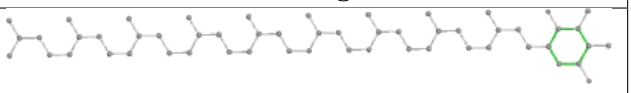
Bond lengths



Bond angles

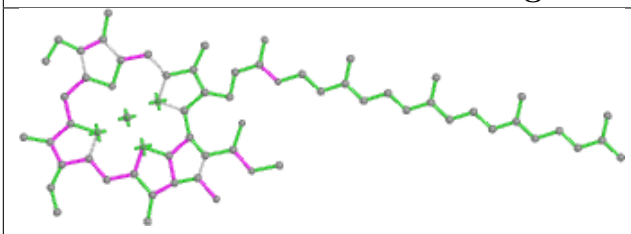


Torsions

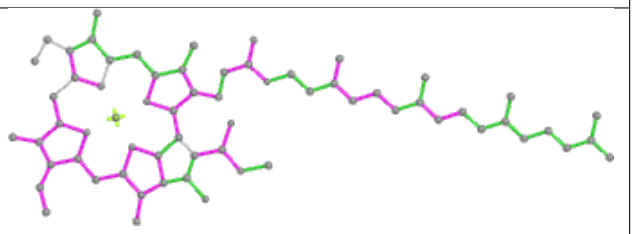


Rings

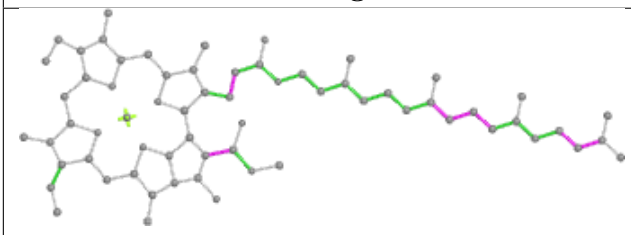
Ligand CLA B 606



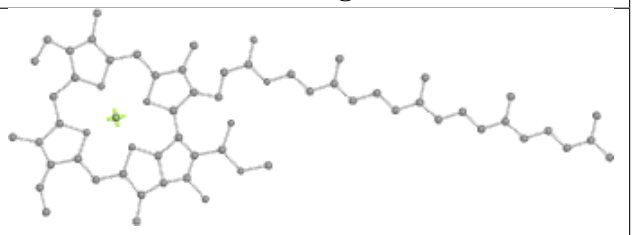
Bond lengths



Bond angles

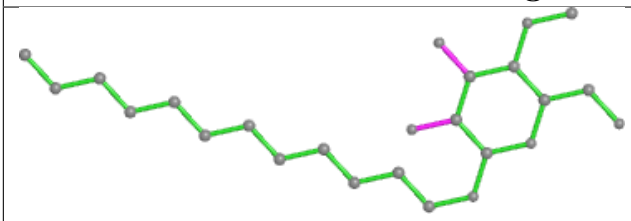


Torsions

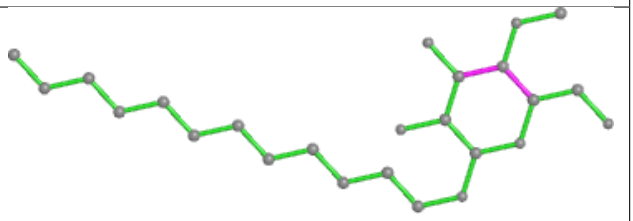


Rings

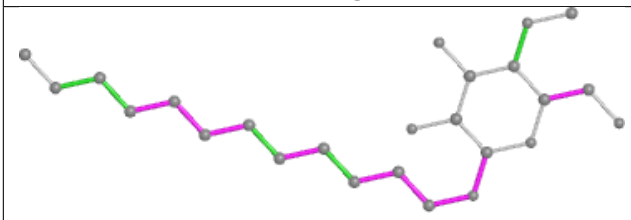
Ligand LMT b 627



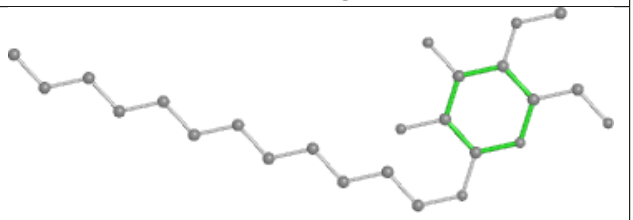
Bond lengths



Bond angles

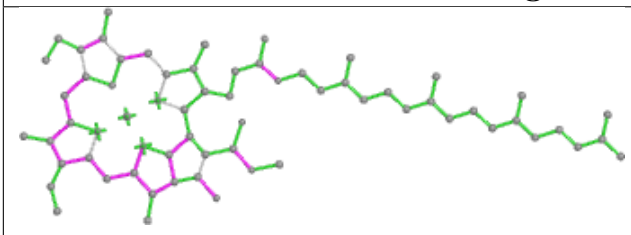


Torsions

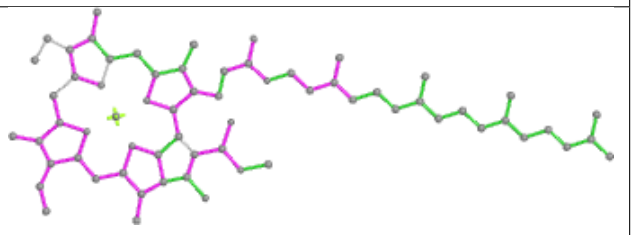


Rings

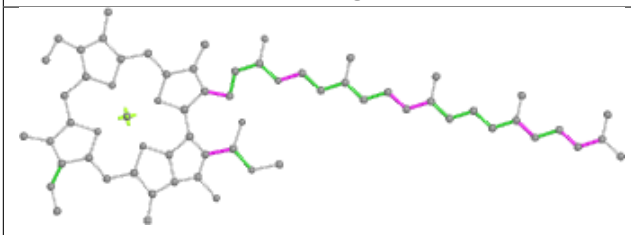
Ligand CLA C 506



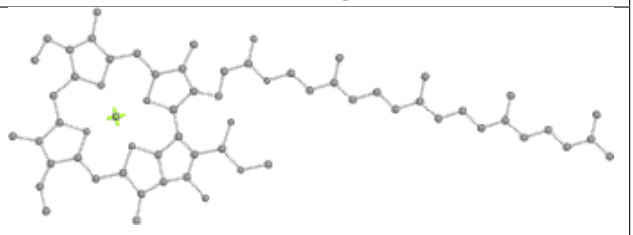
Bond lengths



Bond angles

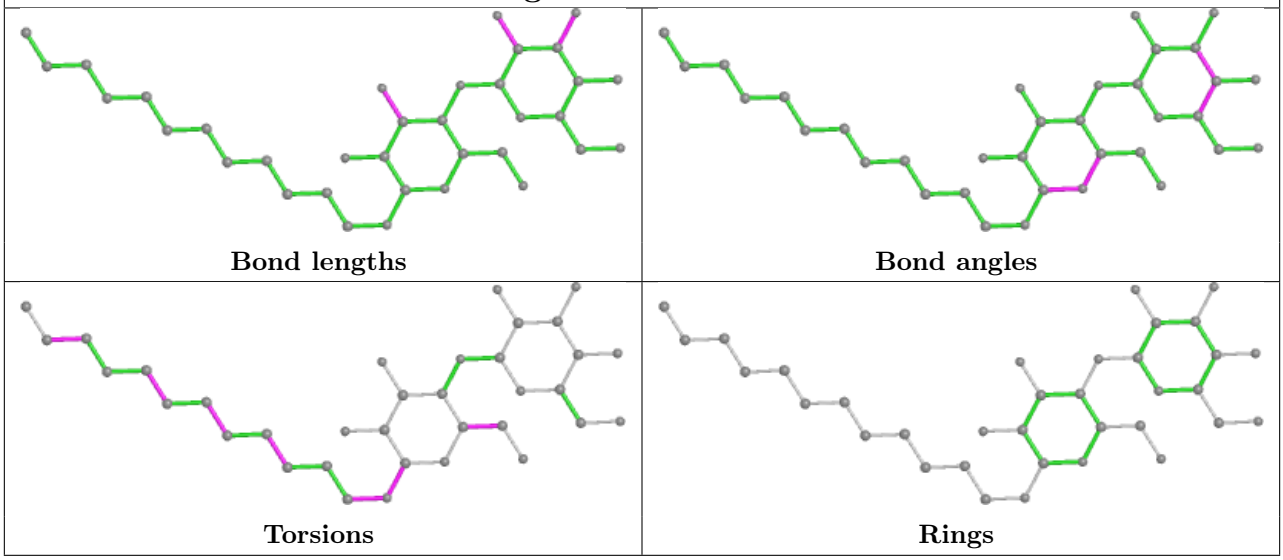


Torsions

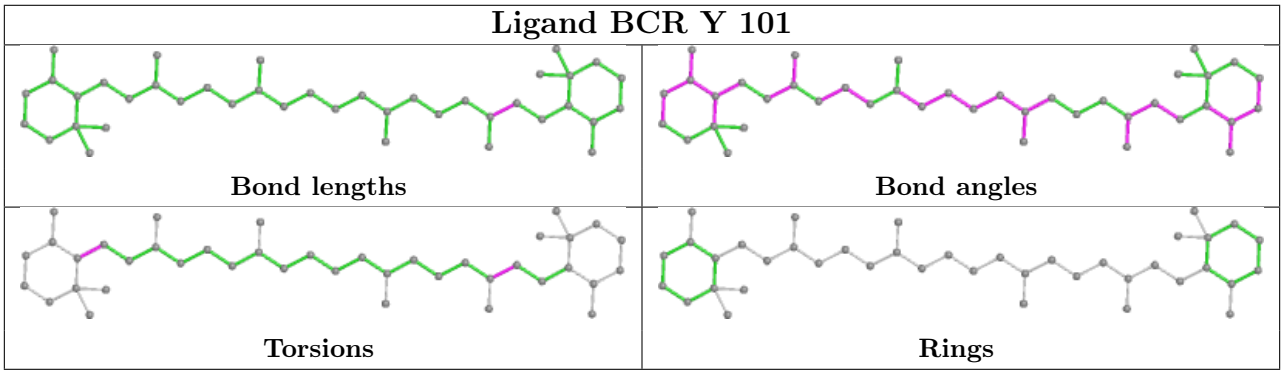


Rings

Ligand LMT F 101



Ligand BCR Y 101



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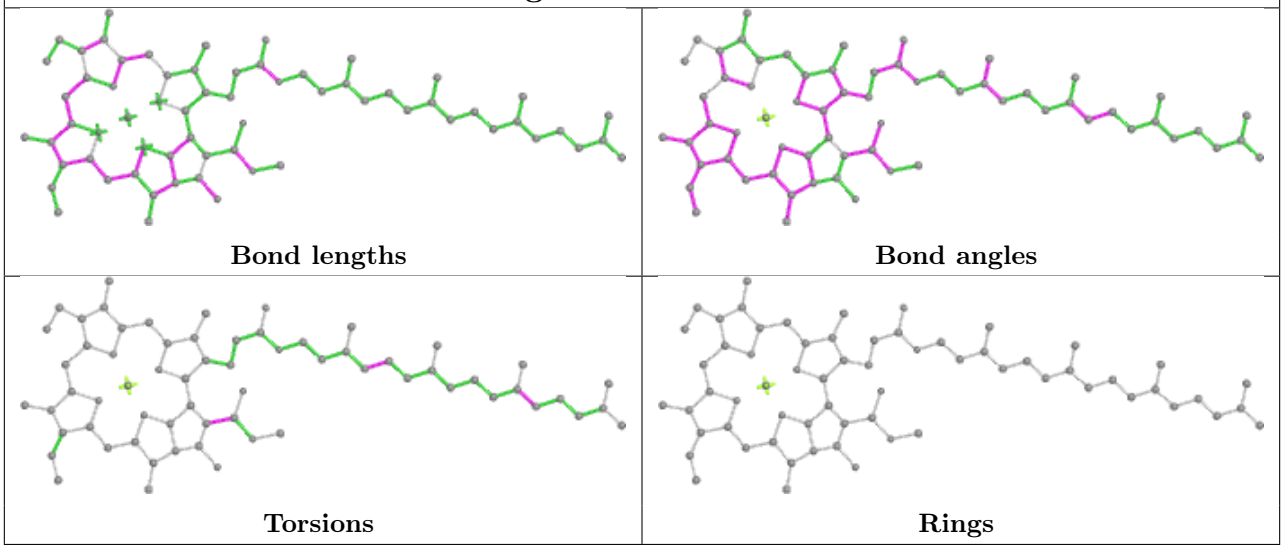
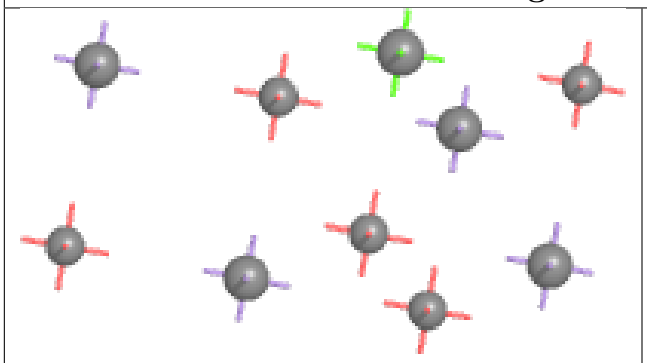
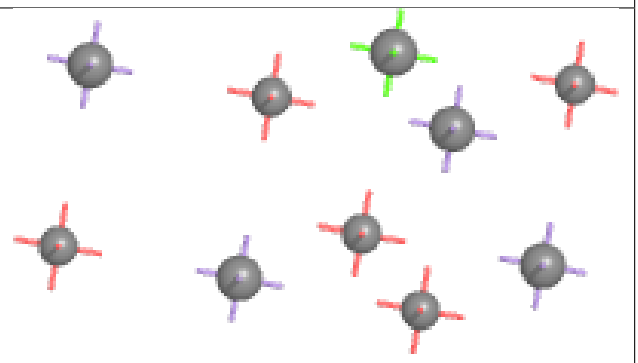


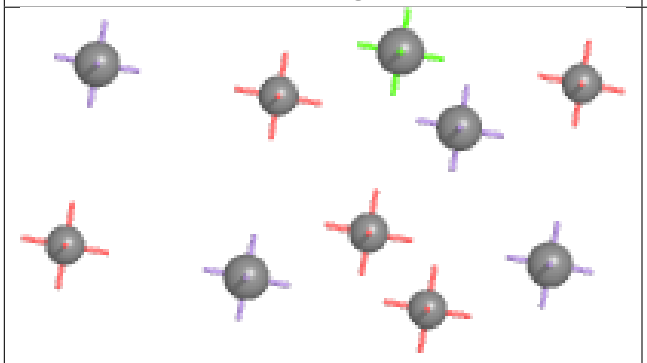
Ligand OEX a 414



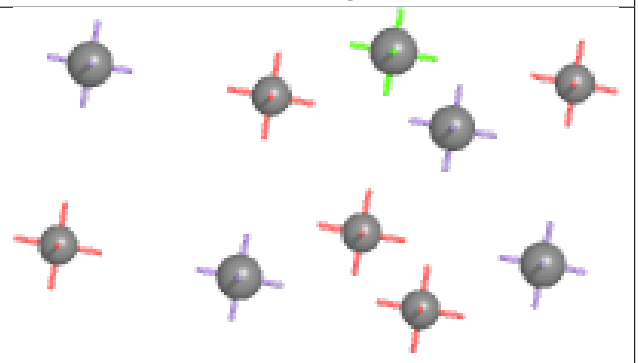
Bond lengths



Bond angles

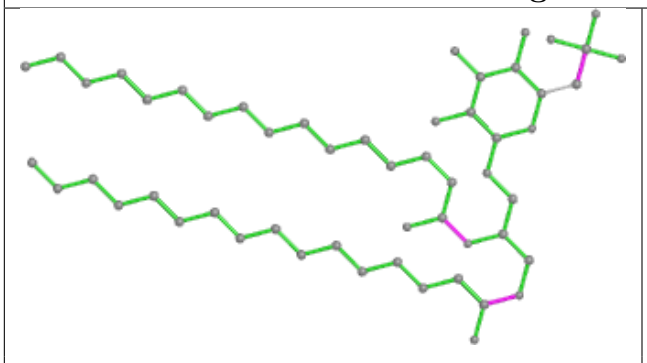


Torsions

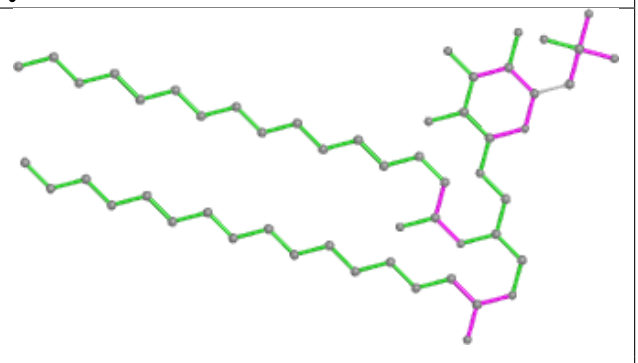


Rings

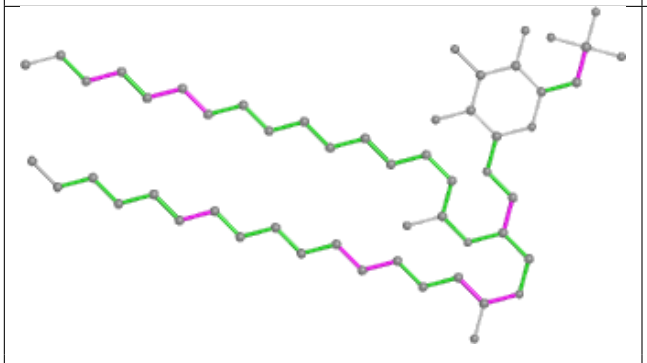
Ligand SQD a 413



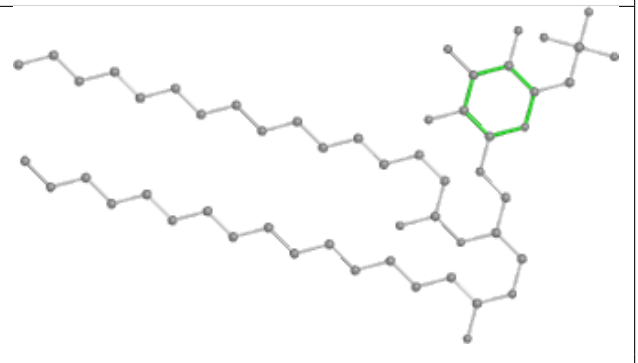
Bond lengths



Bond angles

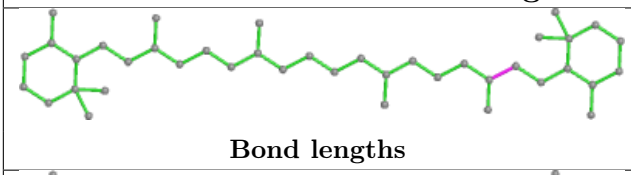


Torsions

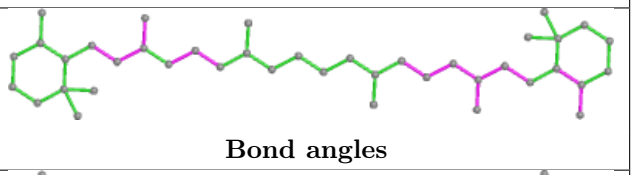


Rings

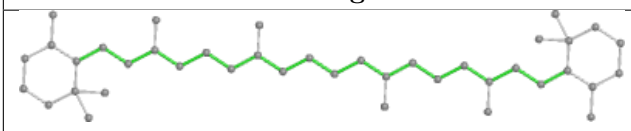
Ligand BCR B 619



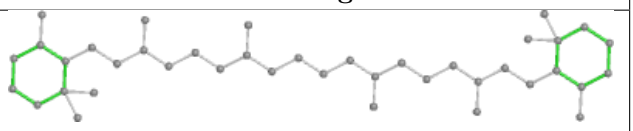
Bond lengths



Bond angles

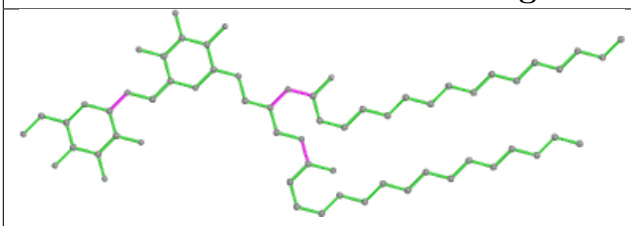


Torsions

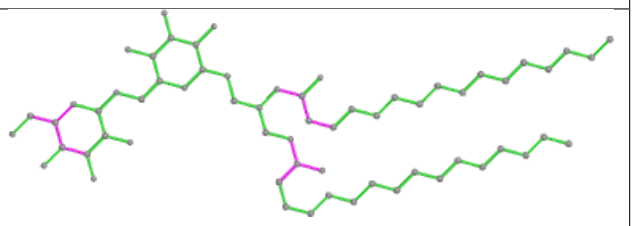


Rings

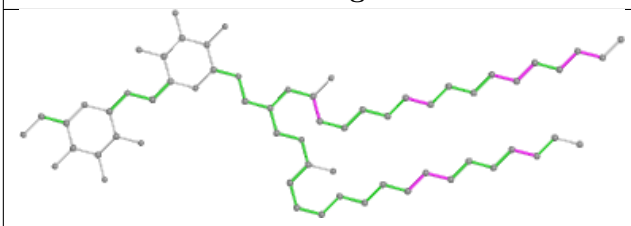
Ligand DGD H 102



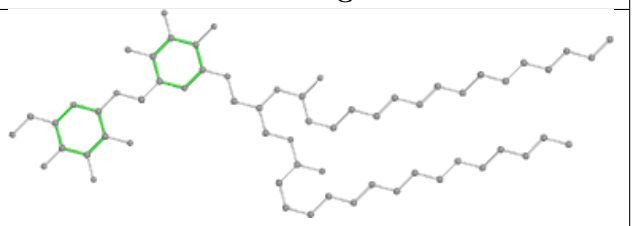
Bond lengths



Bond angles

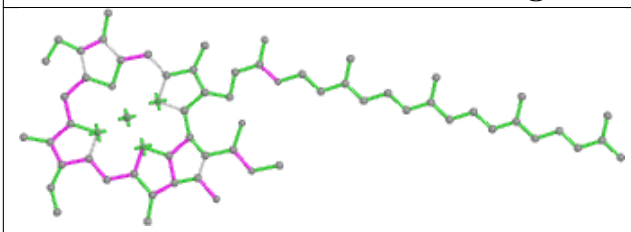


Torsions



Rings

Ligand CLA b 601



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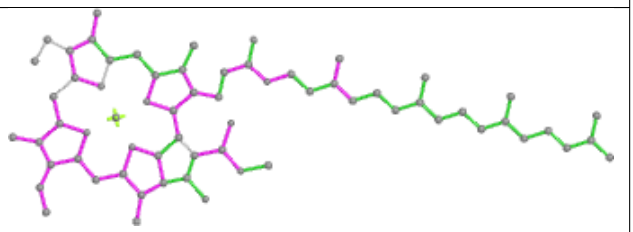
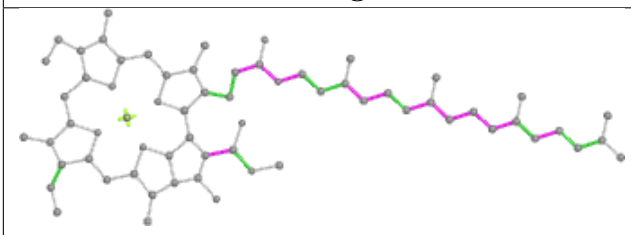
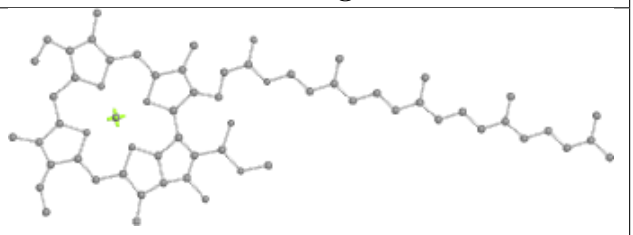


Bond angles

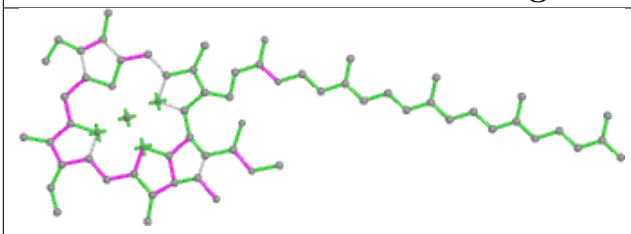


Torsions

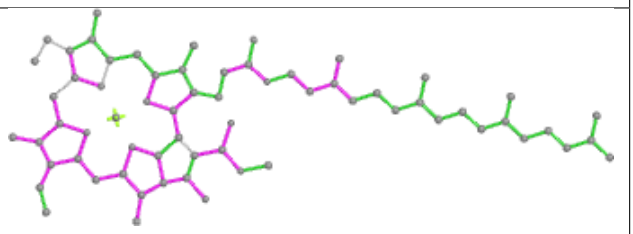


Rings

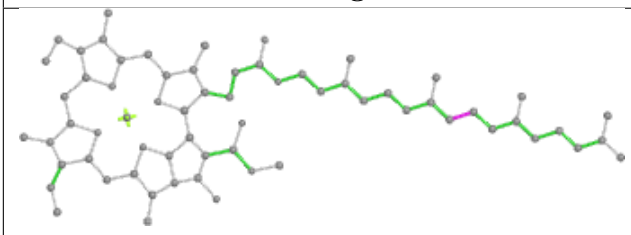
Ligand CLA c 504



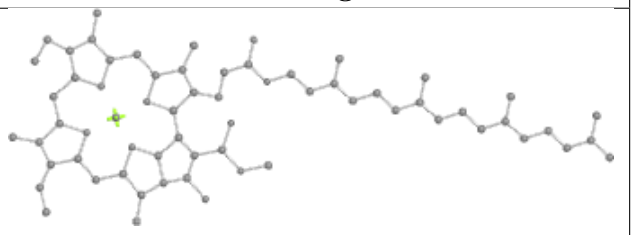
Bond lengths



Bond angles

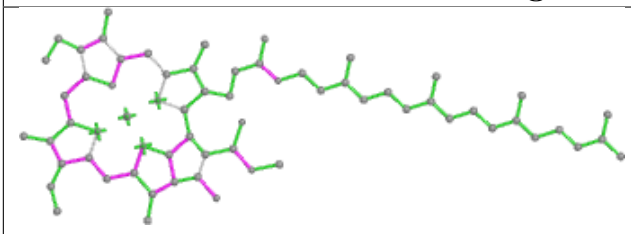


Torsions

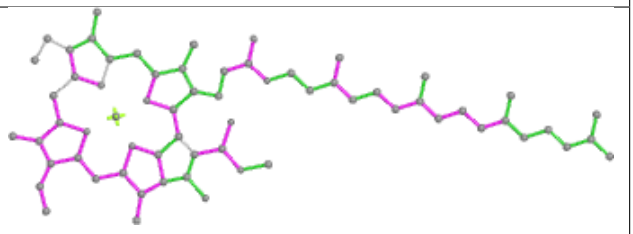


Rings

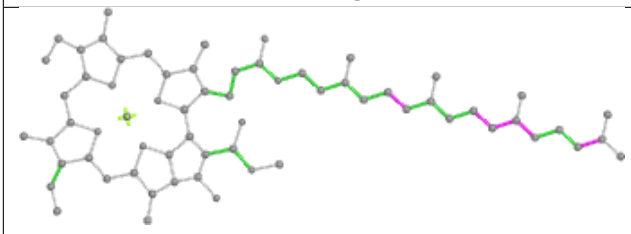
Ligand CLA b 615



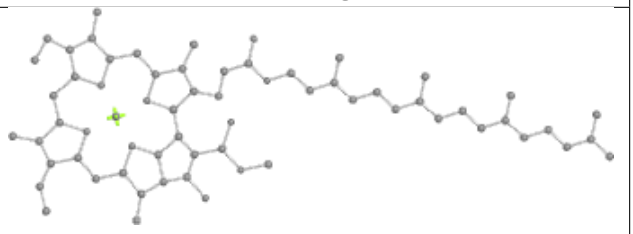
Bond lengths



Bond angles

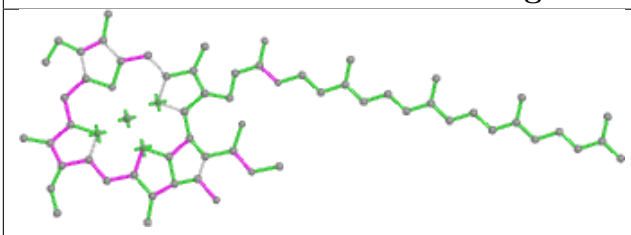


Torsions

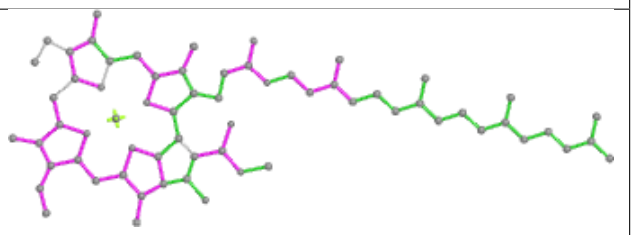


Rings

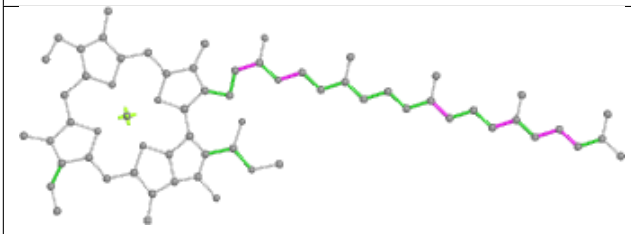
Ligand CLA B 613



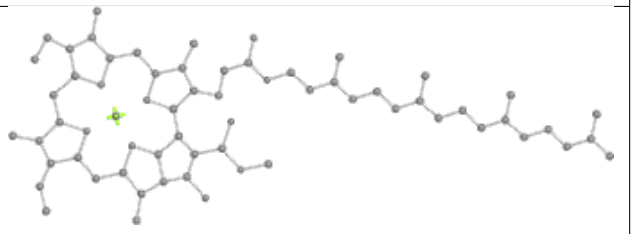
Bond lengths



Bond angles

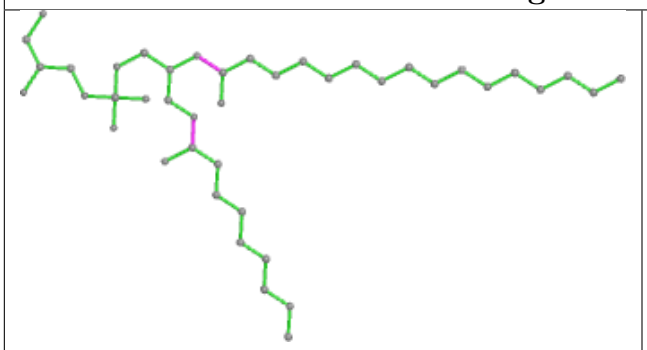


Torsions

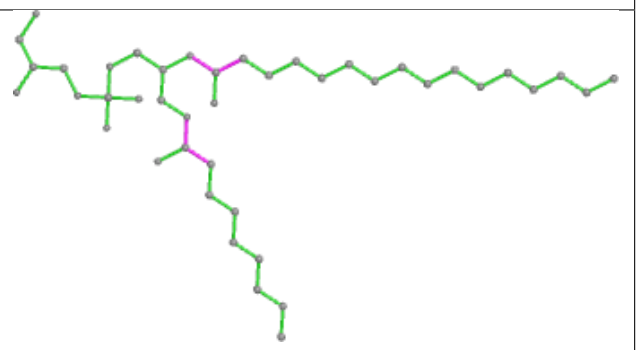


Rings

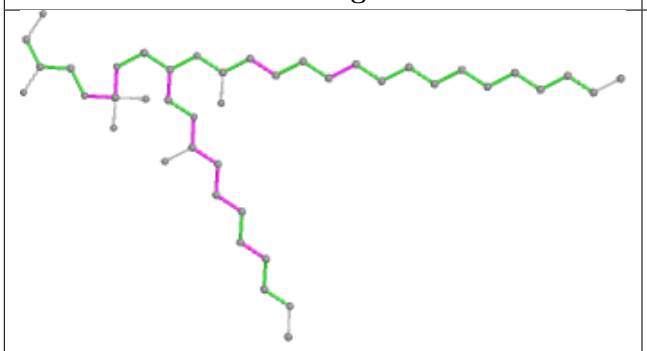
Ligand LHG a 421



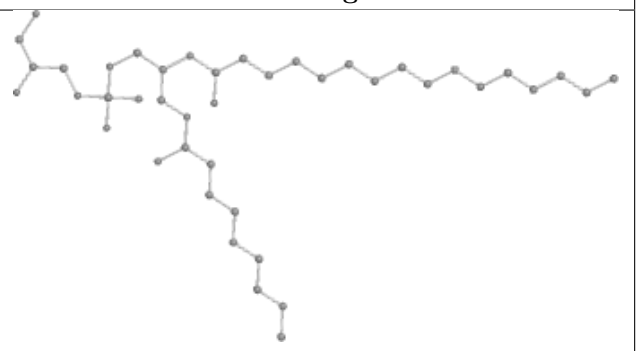
Bond lengths



Bond angles

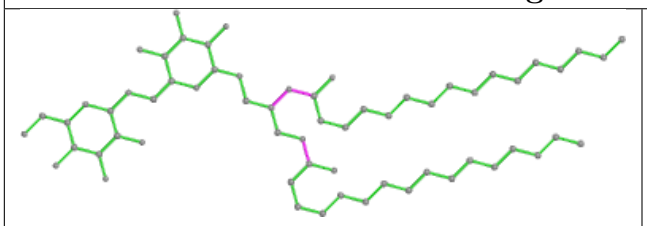


Torsions

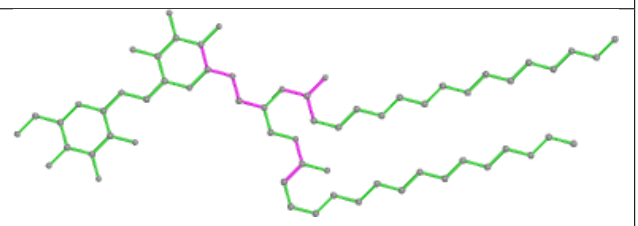


Rings

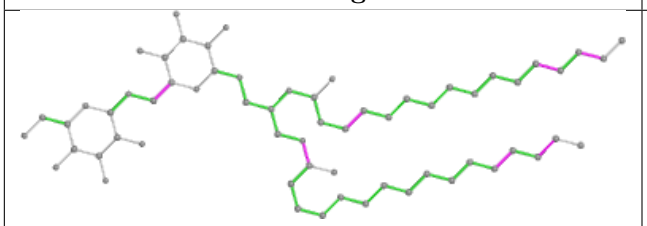
Ligand DGD c 519



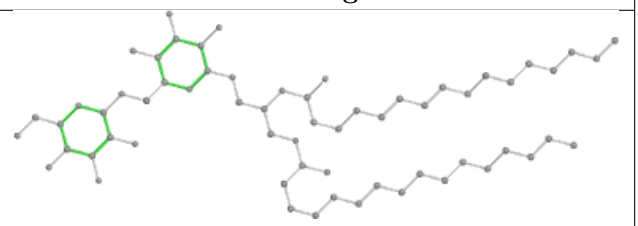
Bond lengths



Bond angles

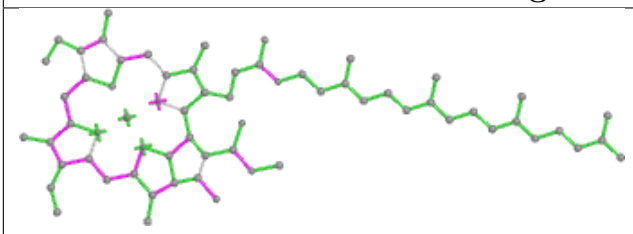


Torsions

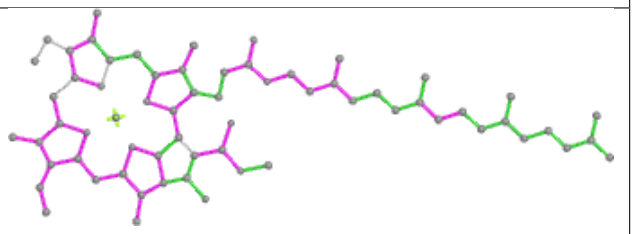


Rings

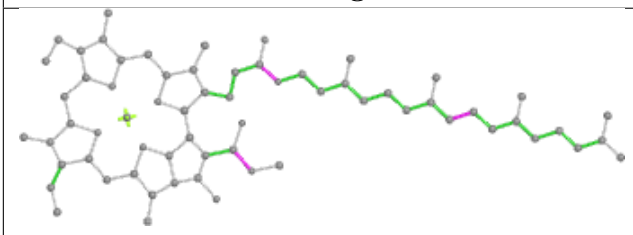
Ligand CLA c 512



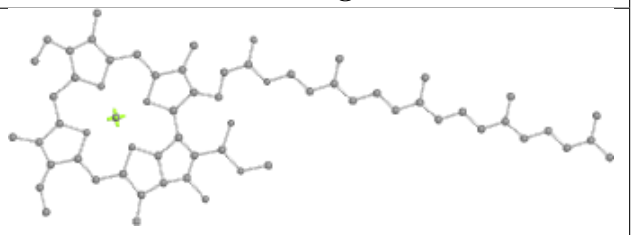
Bond lengths



Bond angles

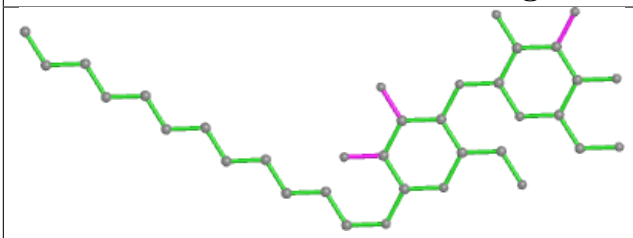


Torsions

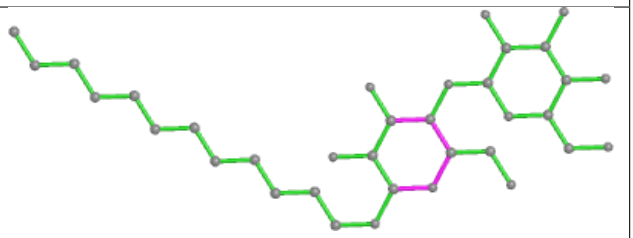


Rings

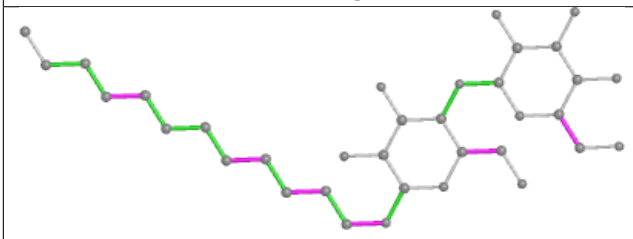
Ligand LMT T 101



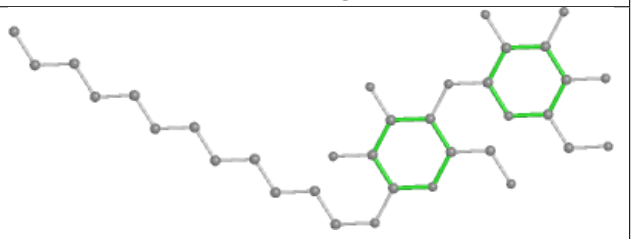
Bond lengths



Bond angles

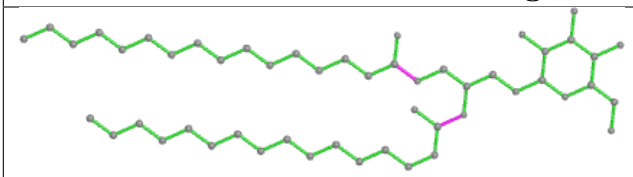


Torsions

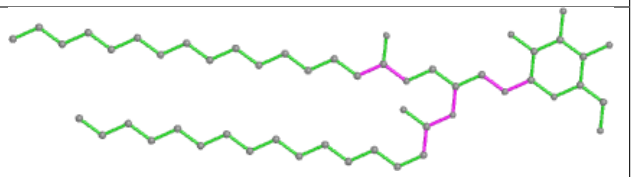


Rings

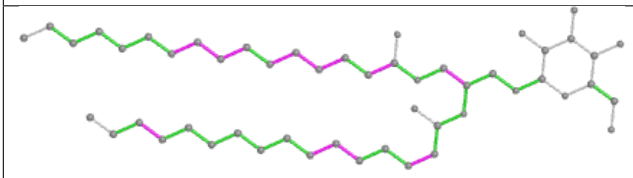
Ligand LMG a 418



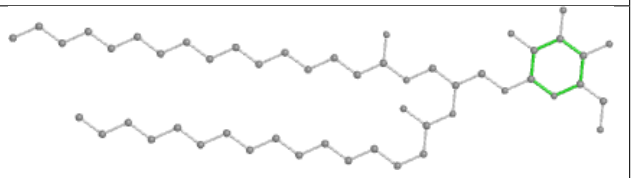
Bond lengths



Bond angles

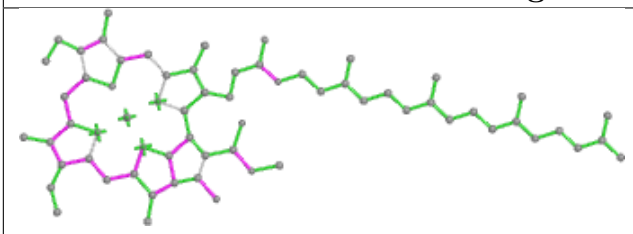


Torsions

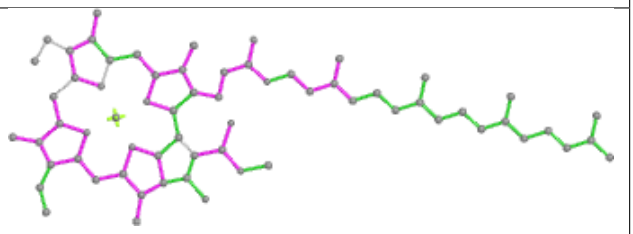


Rings

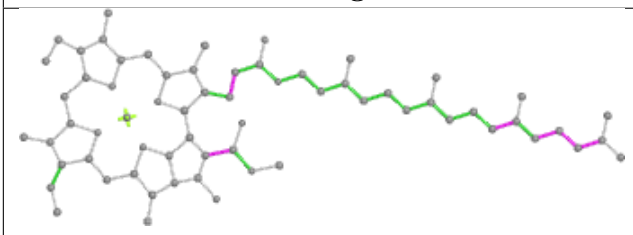
Ligand CLA b 610



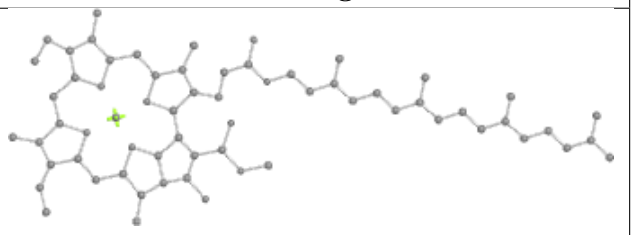
Bond lengths



Bond angles

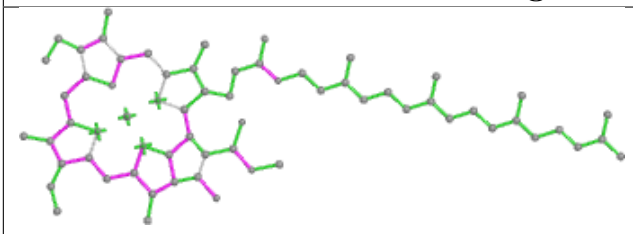


Torsions

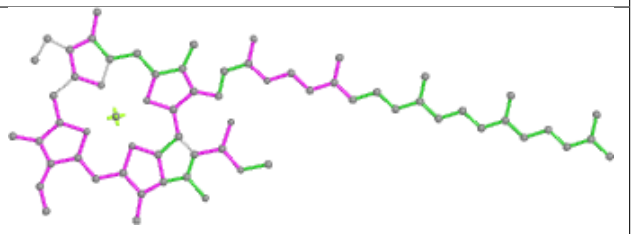


Rings

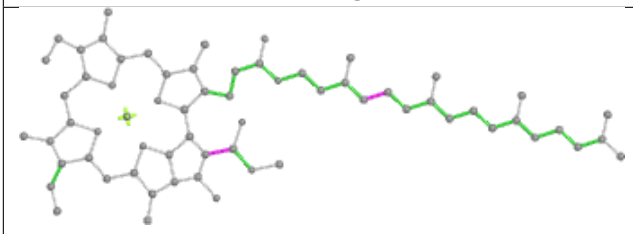
Ligand CLA b 607



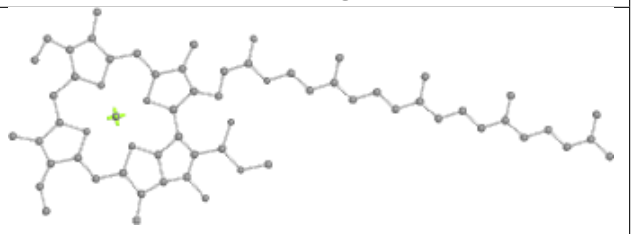
Bond lengths



Bond angles

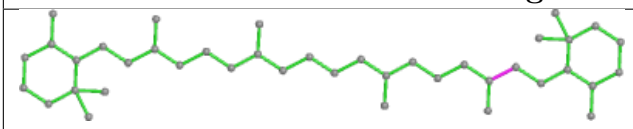


Torsions

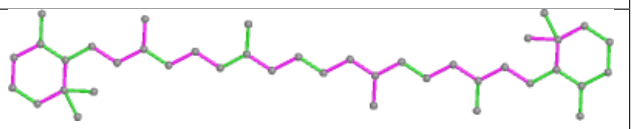


Rings

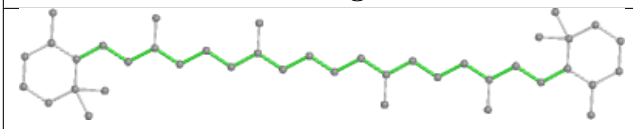
Ligand BCR k 101



Bond lengths



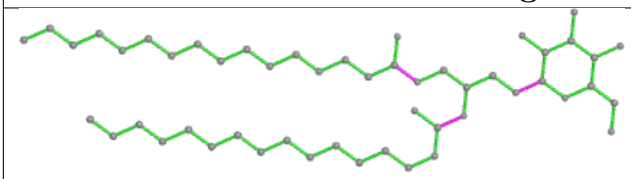
Bond angles



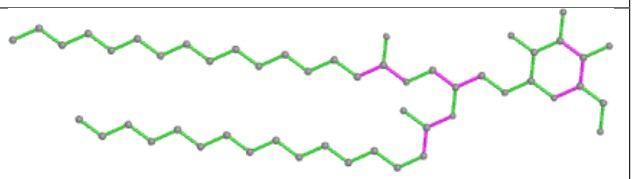
Torsions

Rings

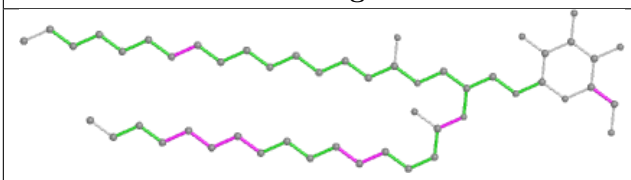
Ligand LMG C 519



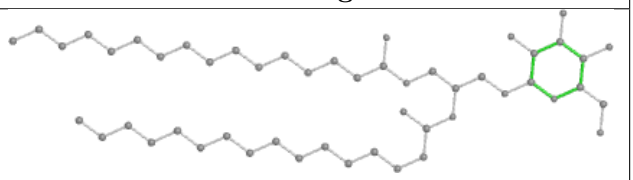
Bond lengths



Bond angles

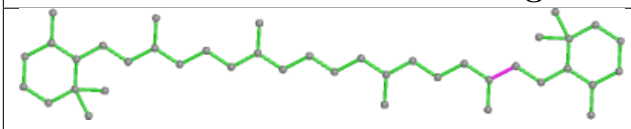


Torsions

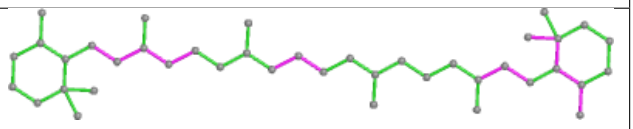


Rings

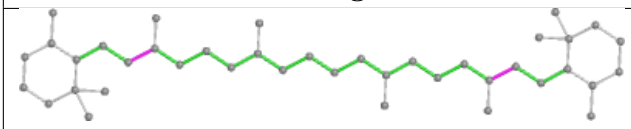
Ligand BCR b 619



Bond lengths



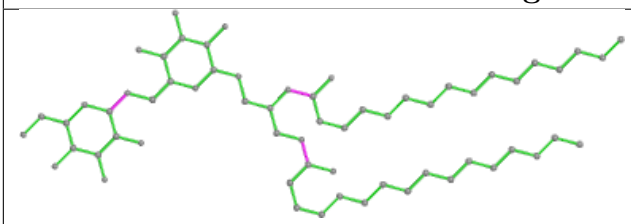
Bond angles



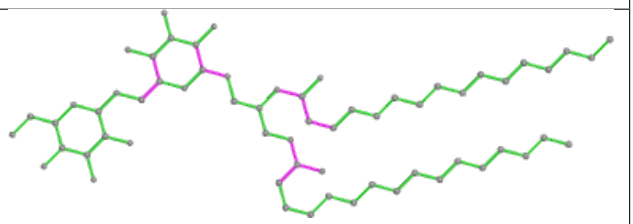
Torsions

Rings

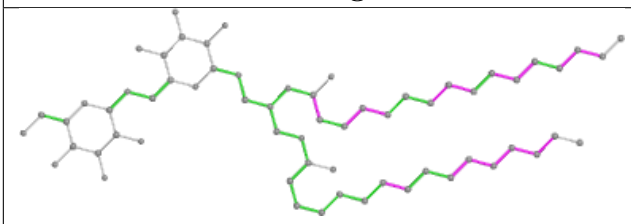
Ligand DGD h 102



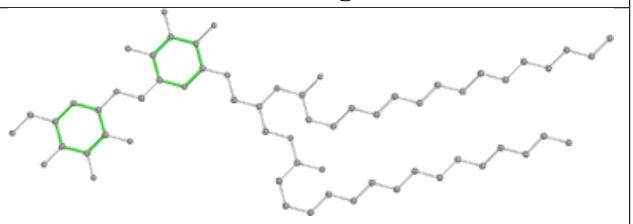
Bond lengths



Bond angles

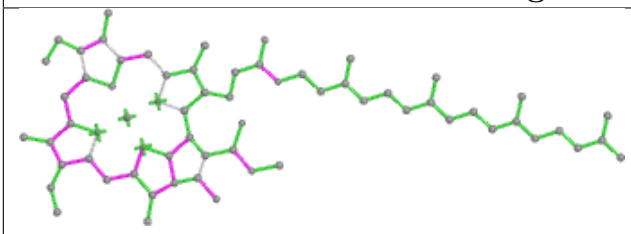


Torsions

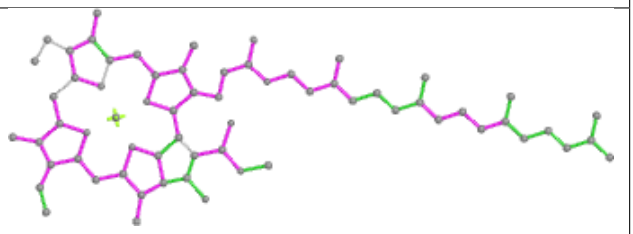


Rings

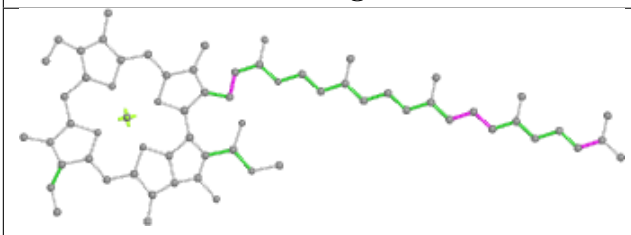
Ligand CLA b 602



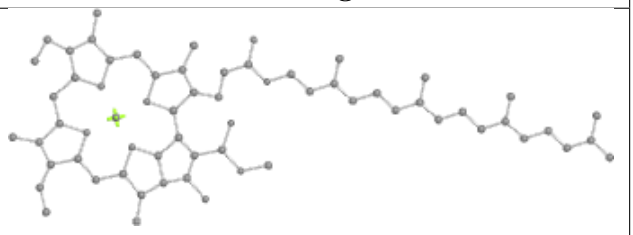
Bond lengths



Bond angles

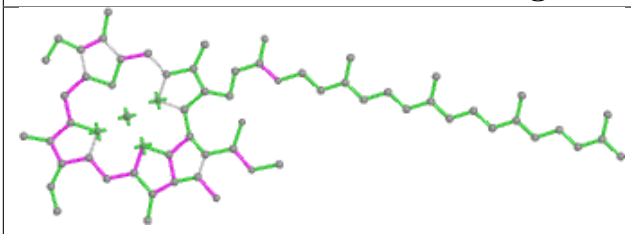


Torsions

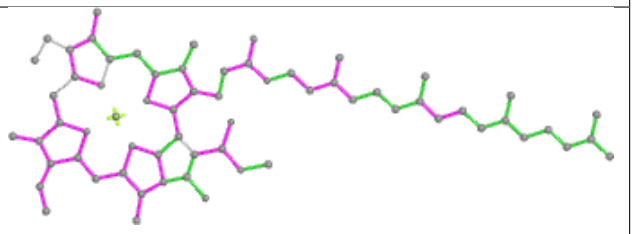


Rings

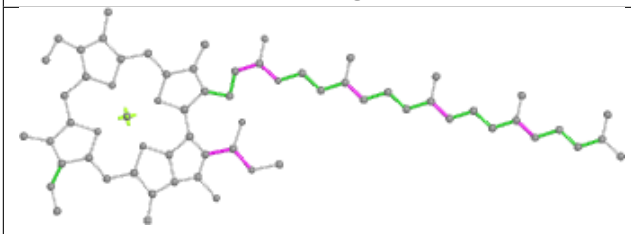
Ligand CLA c 511



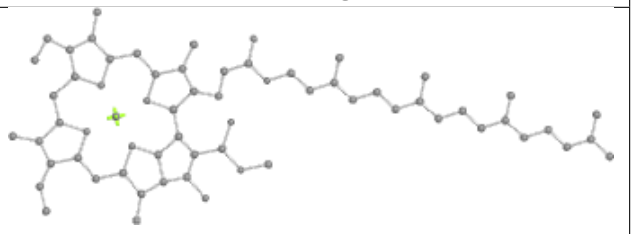
Bond lengths



Bond angles

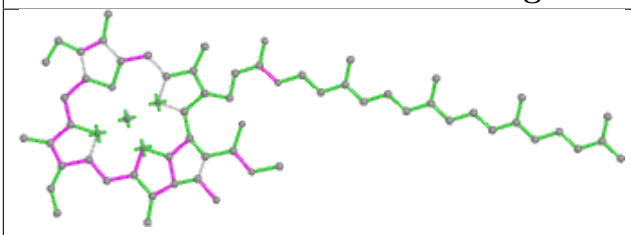


Torsions



Rings

Ligand CLA A 408



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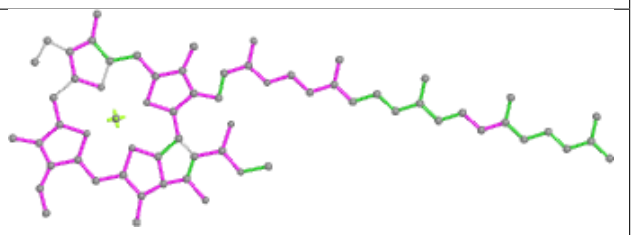
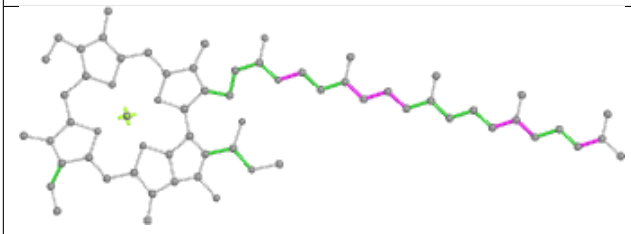
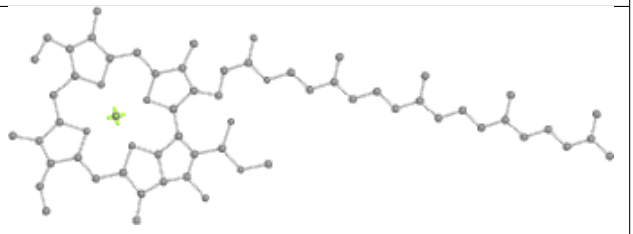


Bond angles

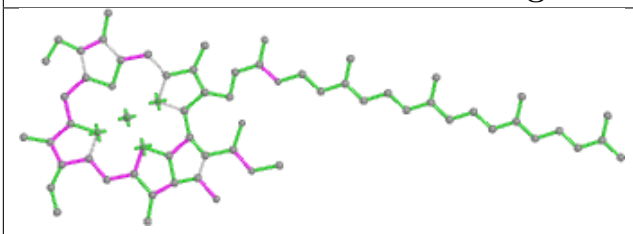


Torsions

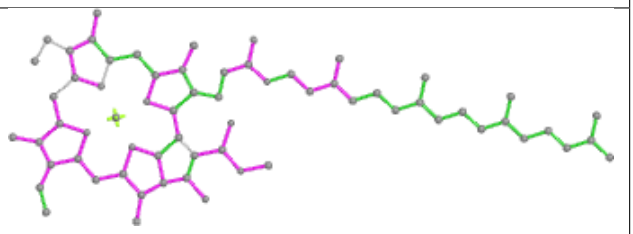


Rings

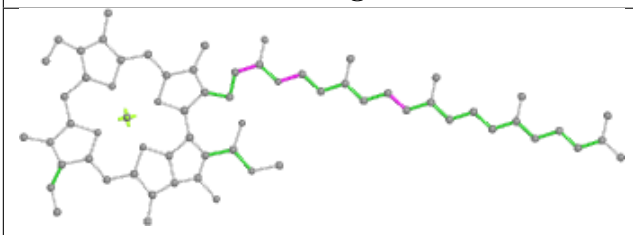
Ligand CLA b 613



Bond lengths



Bond angles



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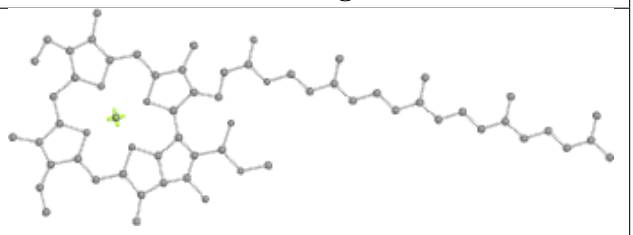
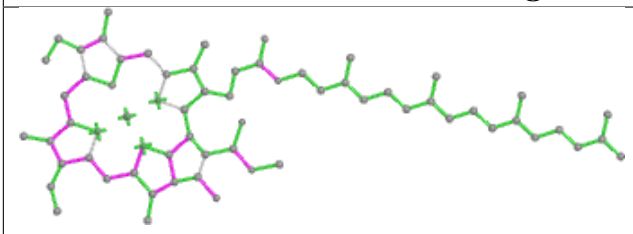
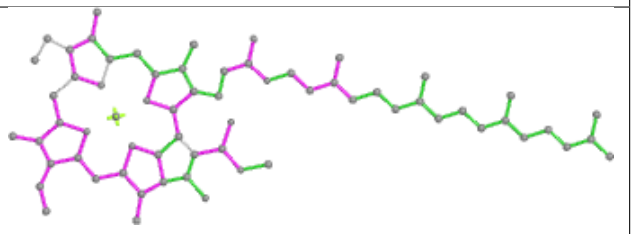


Rings

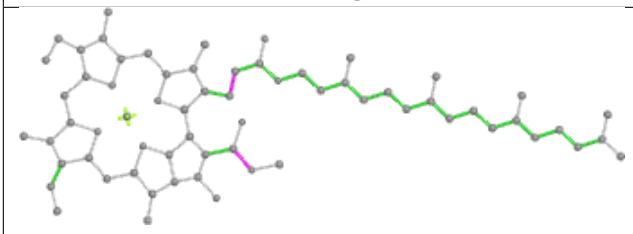
Ligand CLA C 503



Bond lengths



Bond angles



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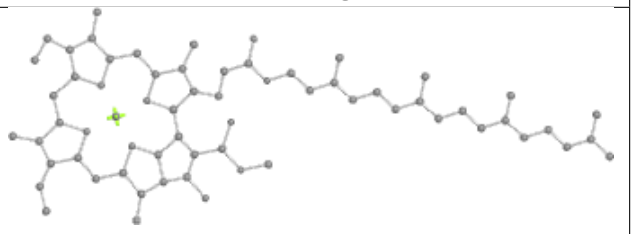
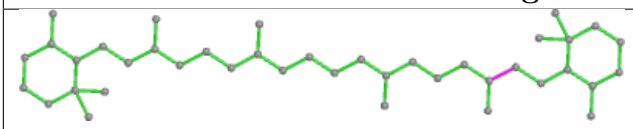
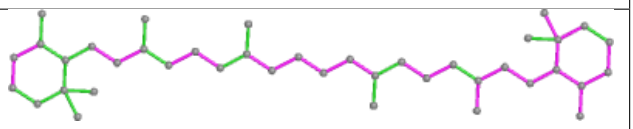


Rings

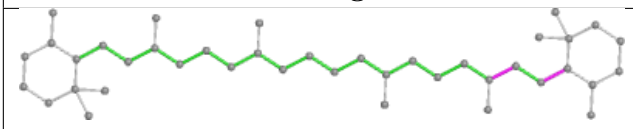
Ligand BCR D 404



Bond lengths



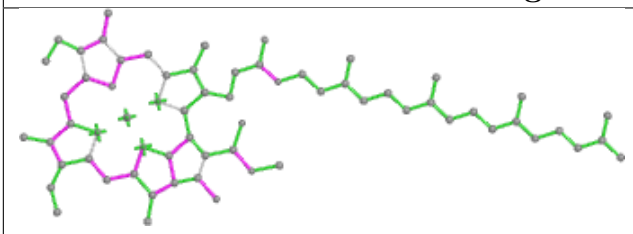
Bond angles



Torsions

Rings

Ligand CLA B 611



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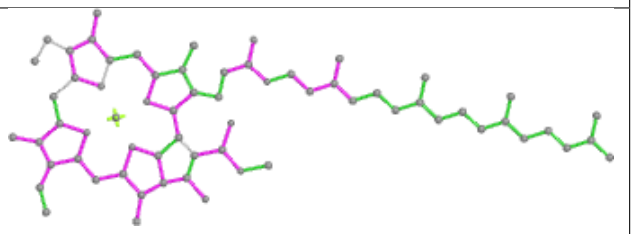
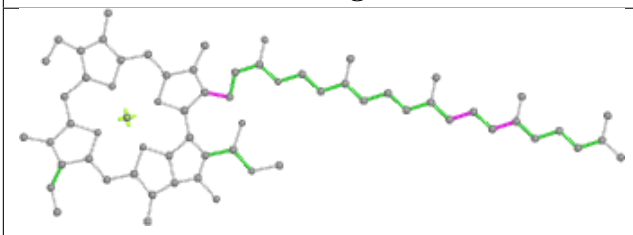


Bond angles



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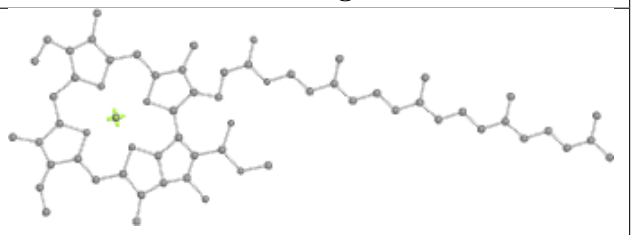
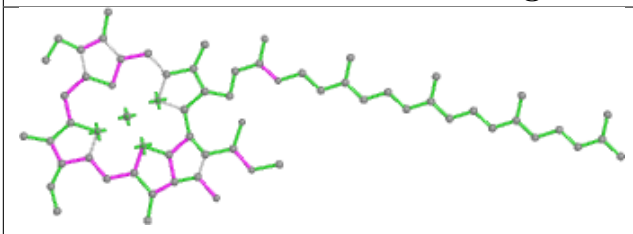


Rings

Ligand CLA D 402



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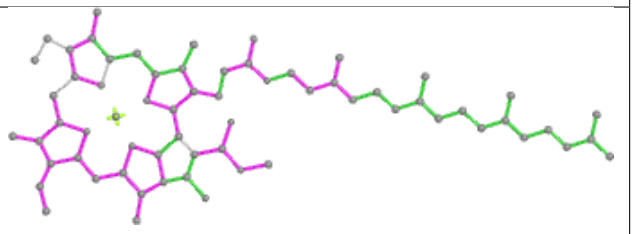
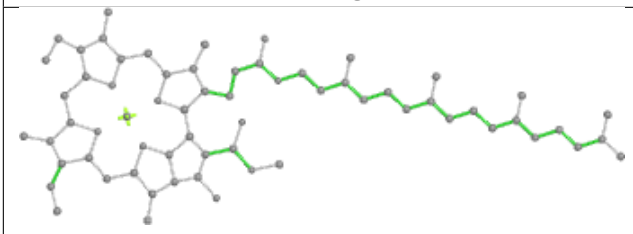
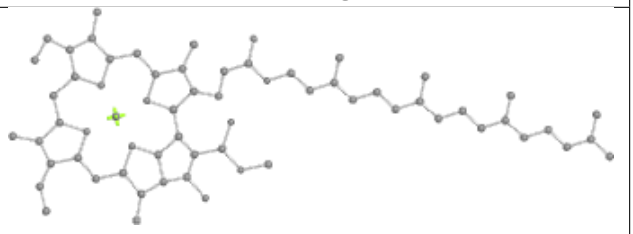


Bond angles

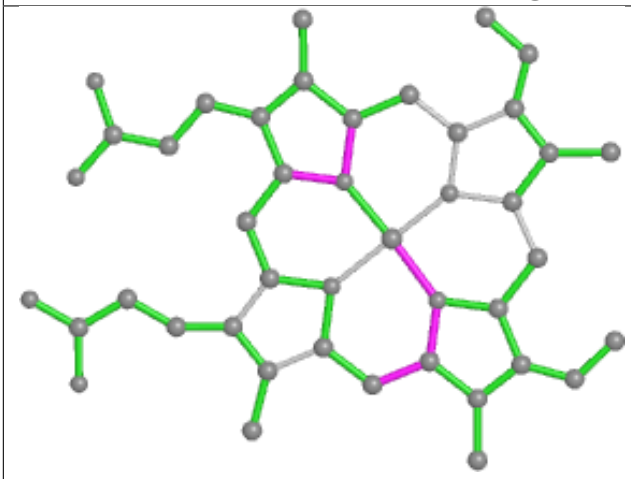


Torsions

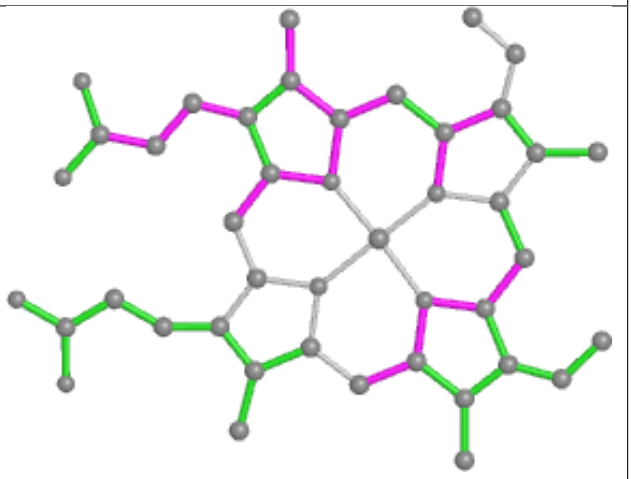


Rings

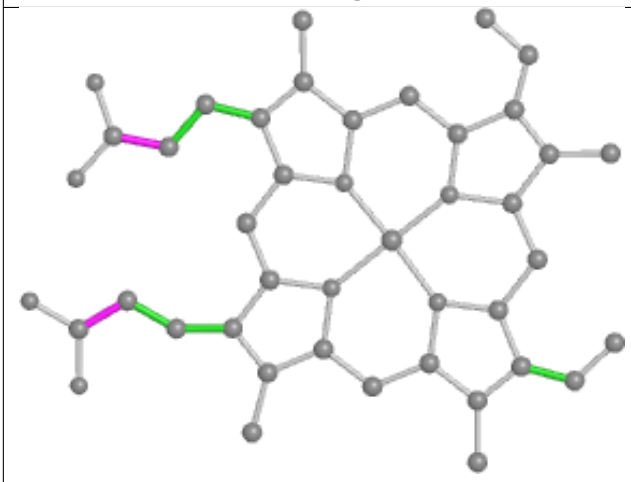
Ligand HEM f 101



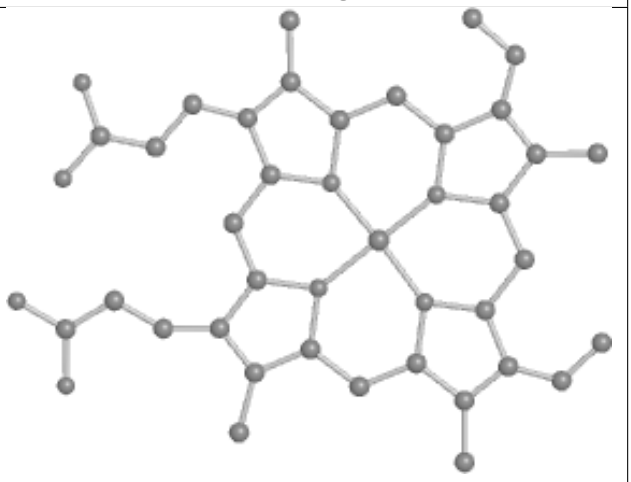
Bond lengths



Bond angles

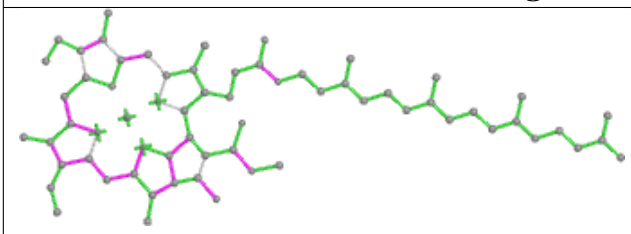


Torsions

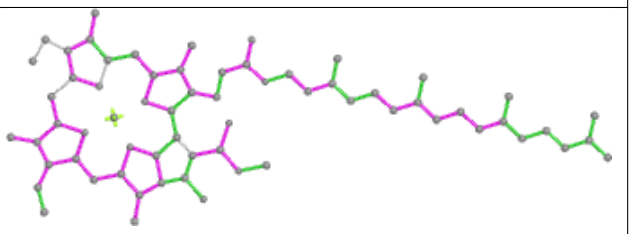


Rings

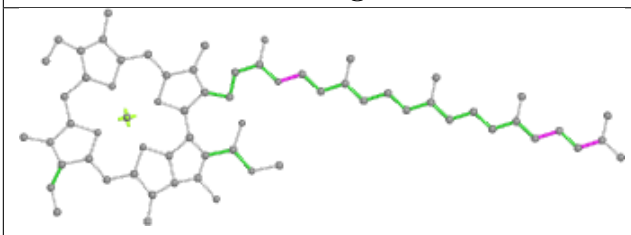
Ligand CLA B 608



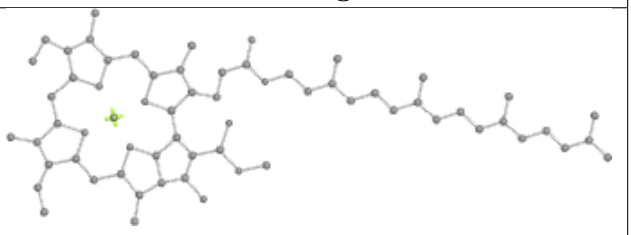
Bond lengths



Bond angles

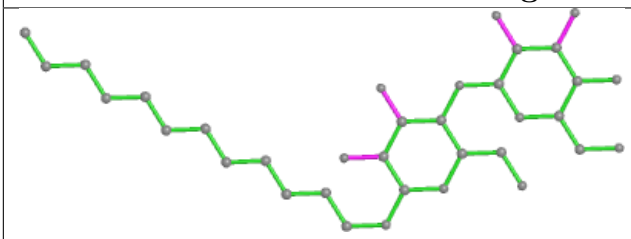


Torsions



Rings

Ligand LMT A 421



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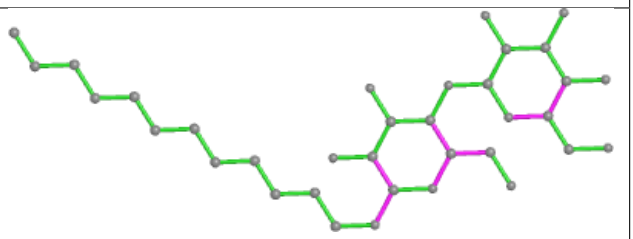
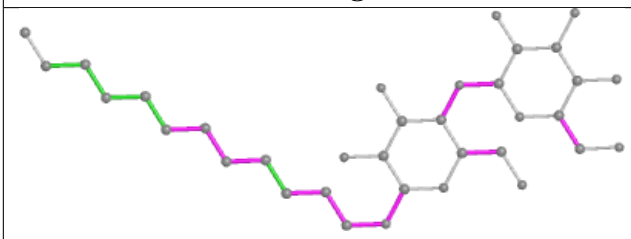


Bond angles



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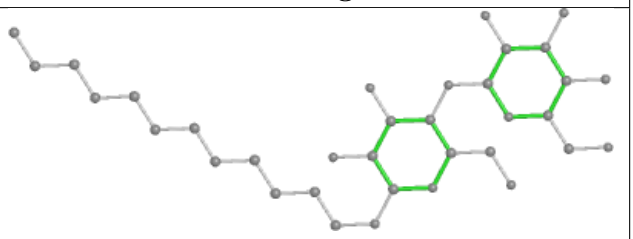
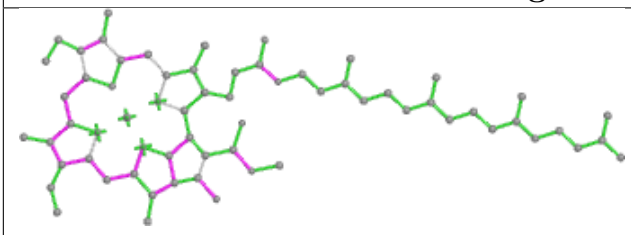
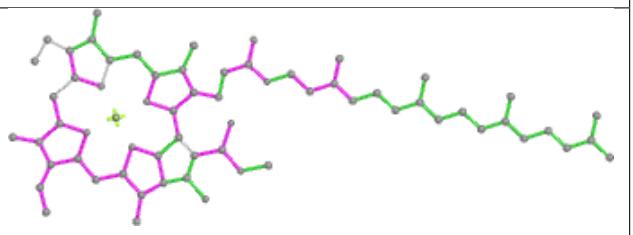


Rings

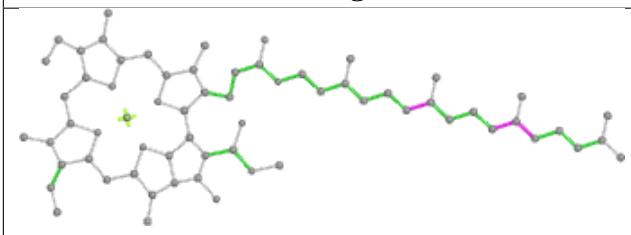
Ligand CLA a 407



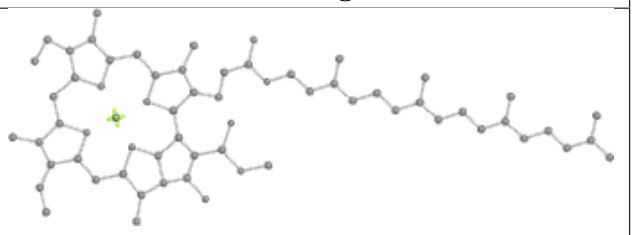
Bond lengths



Bond angles

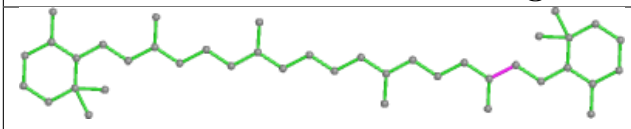


Torsions

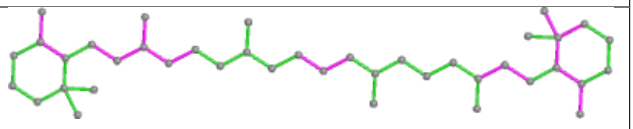


Rings

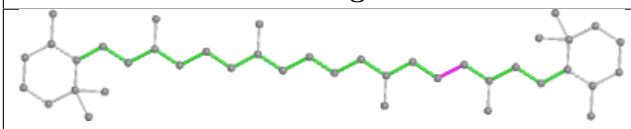
Ligand BCR a 410



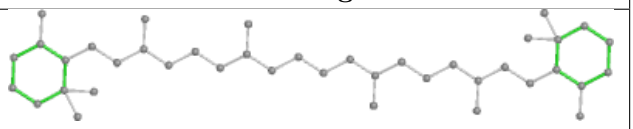
Bond lengths



Bond angles

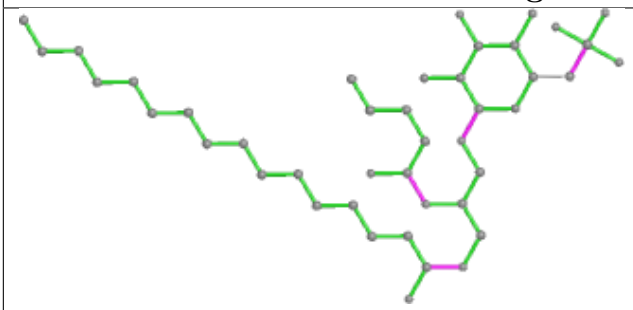


Torsions

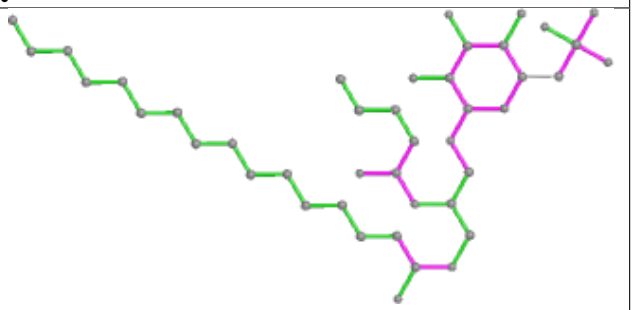


Rings

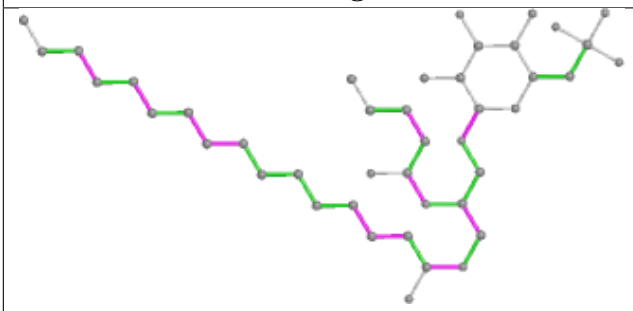
Ligand SQD F 103



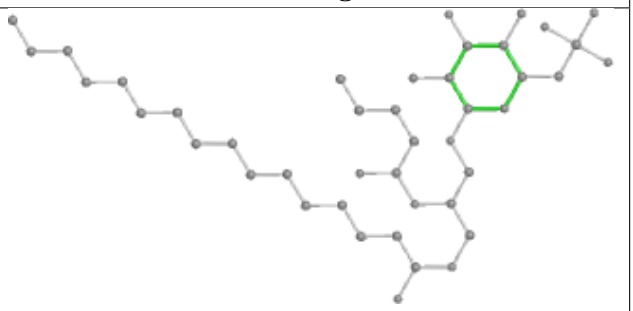
Bond lengths



Bond angles

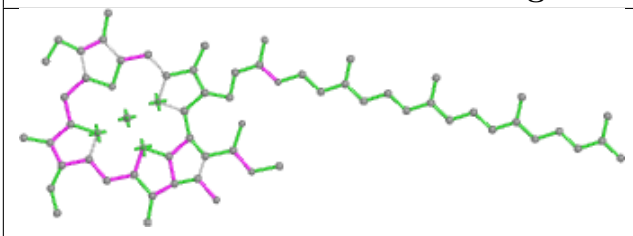


Torsions

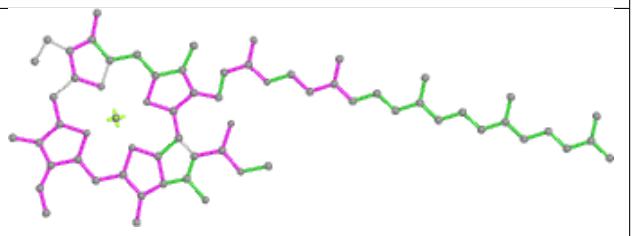


Rings

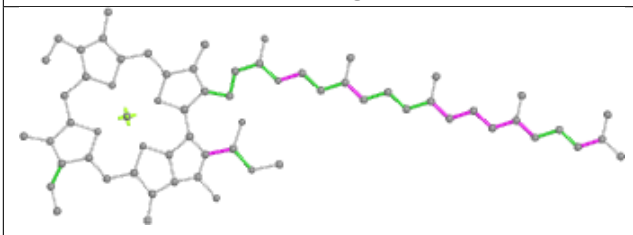
Ligand CLA b 614



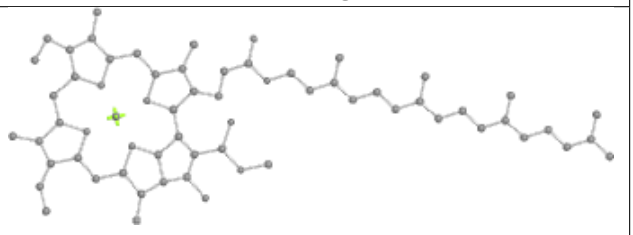
Bond lengths



Bond angles

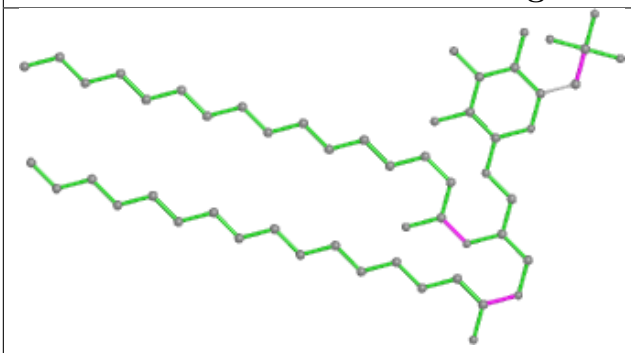


Torsions

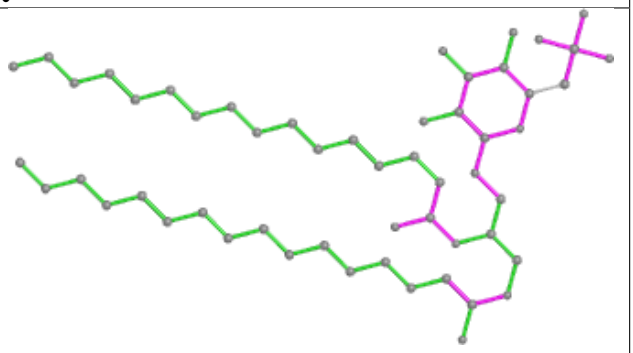


Rings

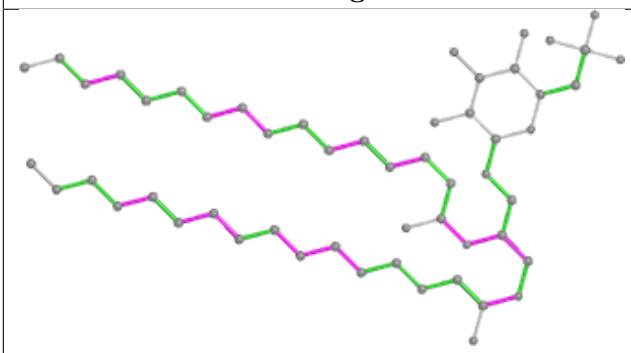
Ligand SQD b 620



Bond lengths



Bond angles



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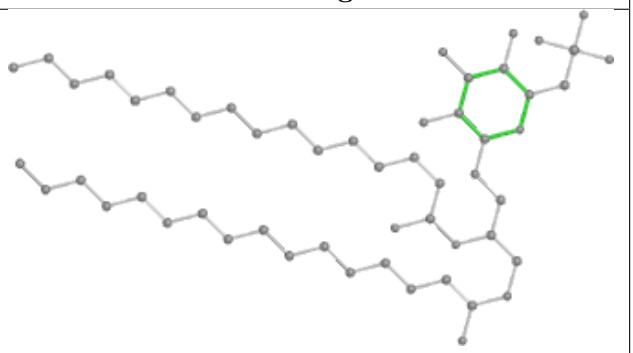
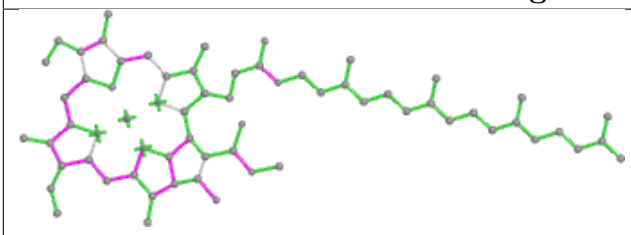
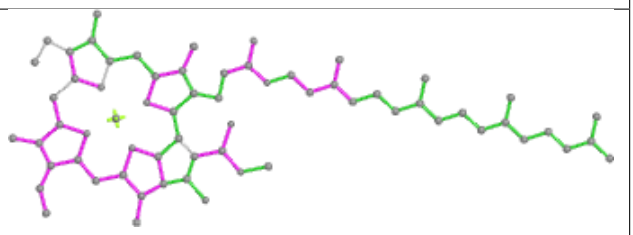


Rings

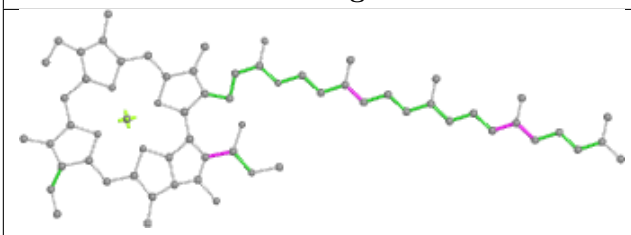
Ligand CLA c 506



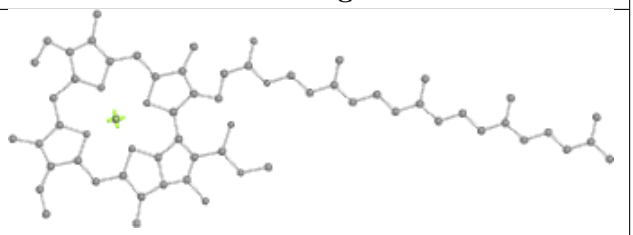
Bond lengths



Bond angles

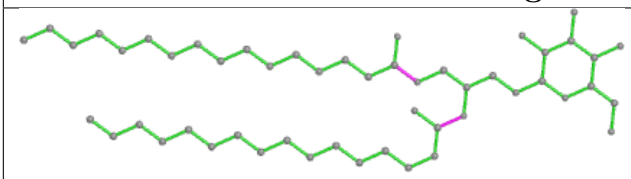


Torsions

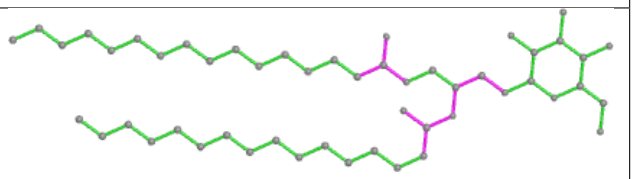


Rings

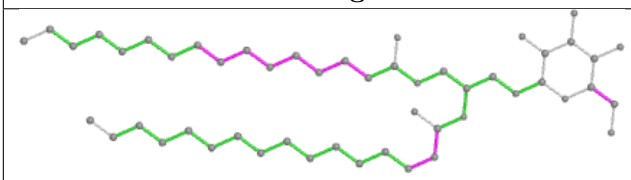
Ligand LMG c 520



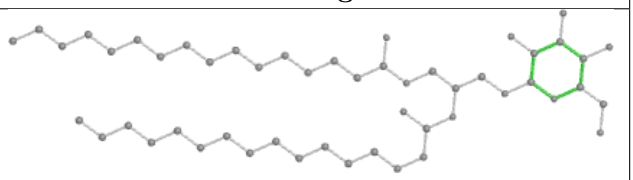
Bond lengths



Bond angles

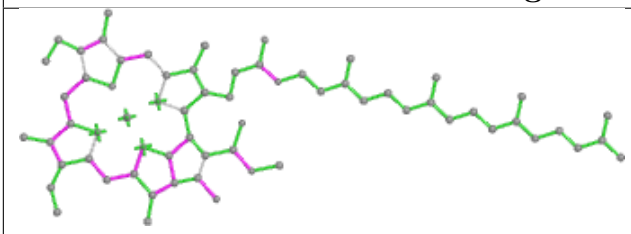


Torsions

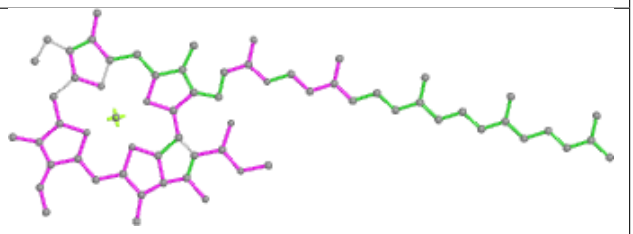


Rings

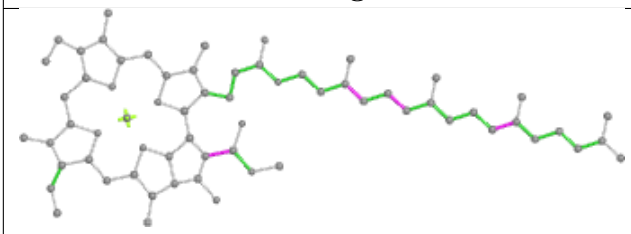
Ligand CLA B 605



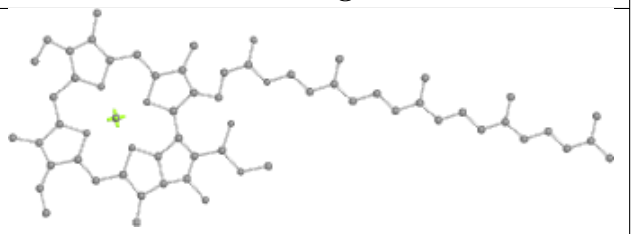
Bond lengths



Bond angles

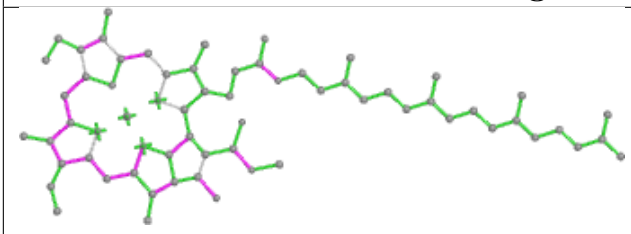


Torsions

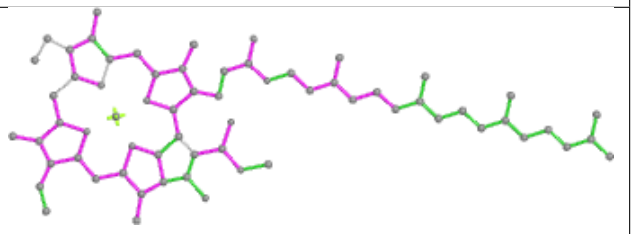


Rings

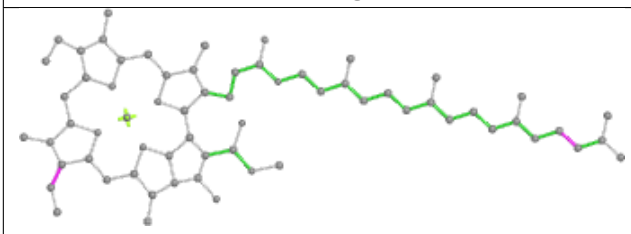
Ligand CLA a 405



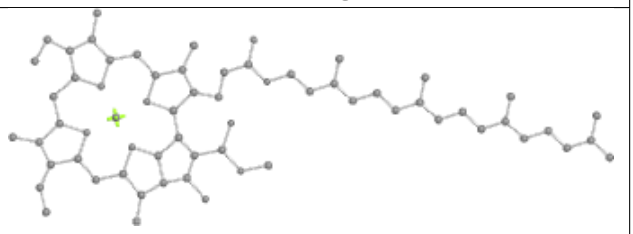
Bond lengths



Bond angles

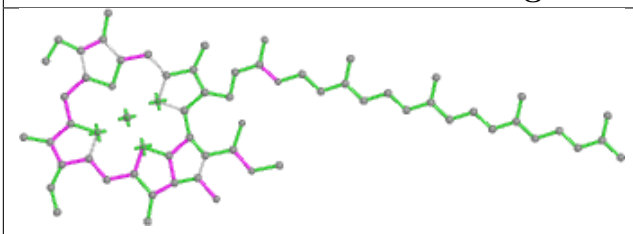


Torsions

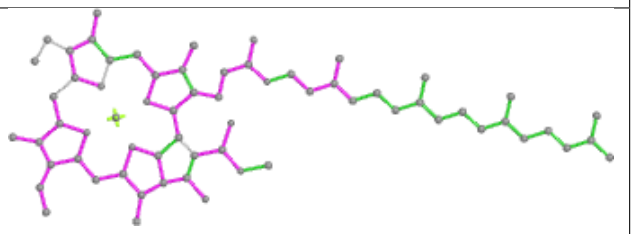


Rings

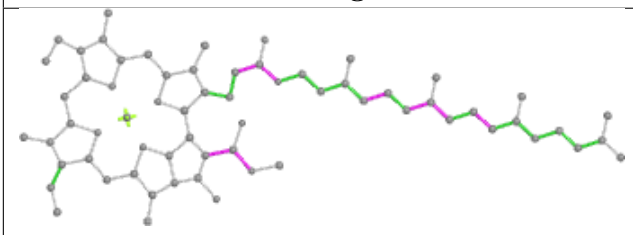
Ligand CLA C 512



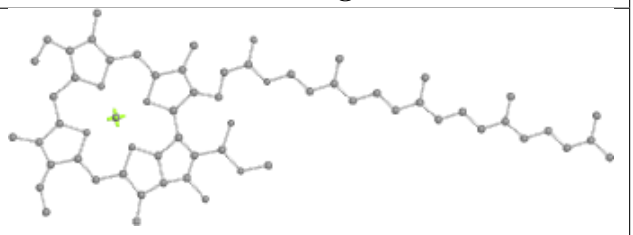
Bond lengths



Bond angles

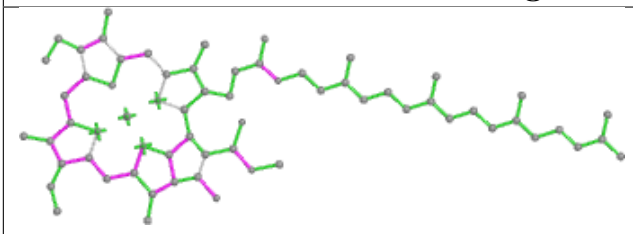


Torsions

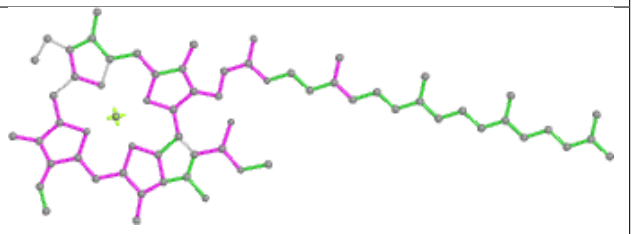


Rings

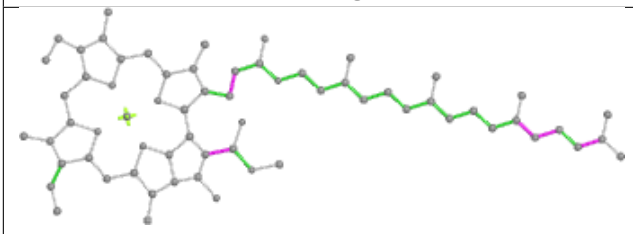
Ligand CLA B 610



Bond lengths



Bond angles



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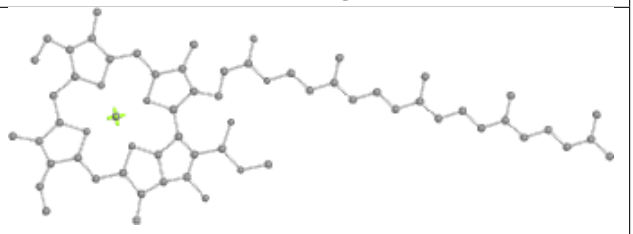
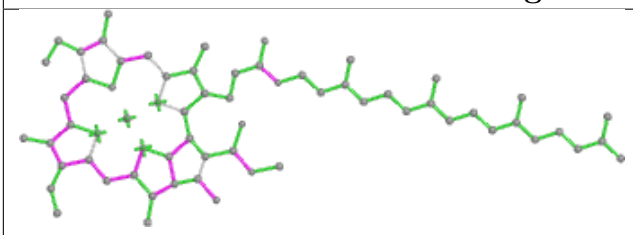
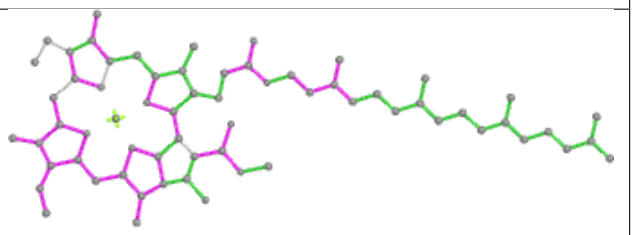


Rings

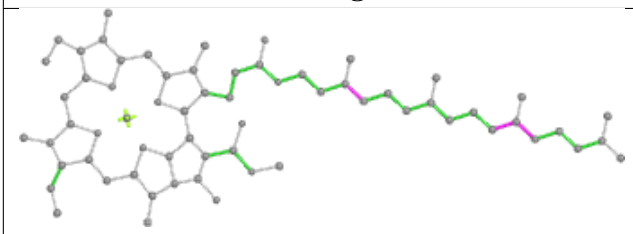
Ligand CLA C 505



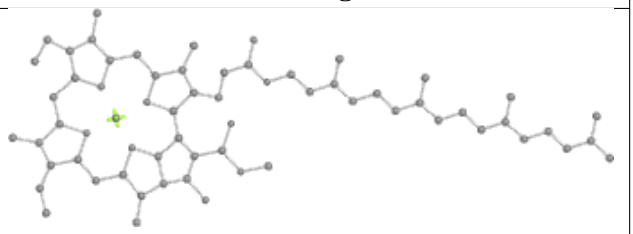
Bond lengths



Bond angles

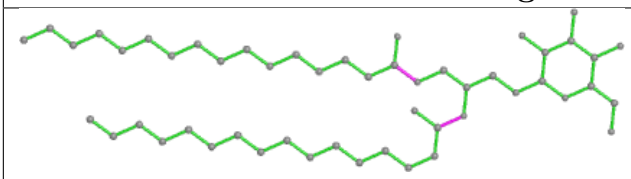


Torsions

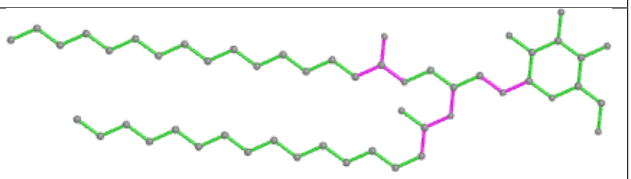


Rings

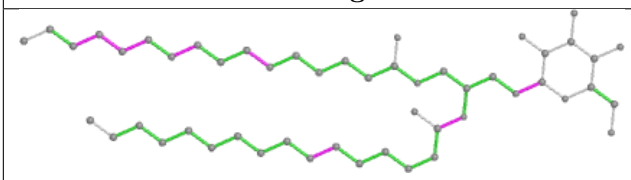
Ligand LMG m 101



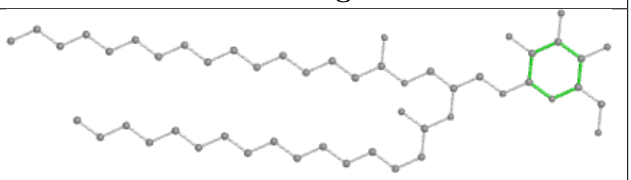
Bond lengths



Bond angles

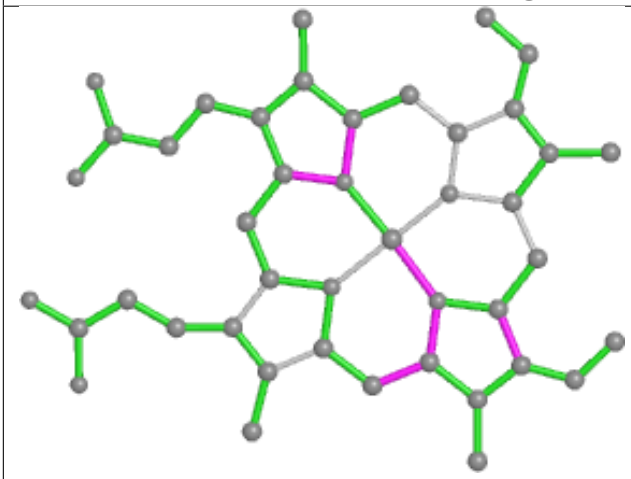


Torsions

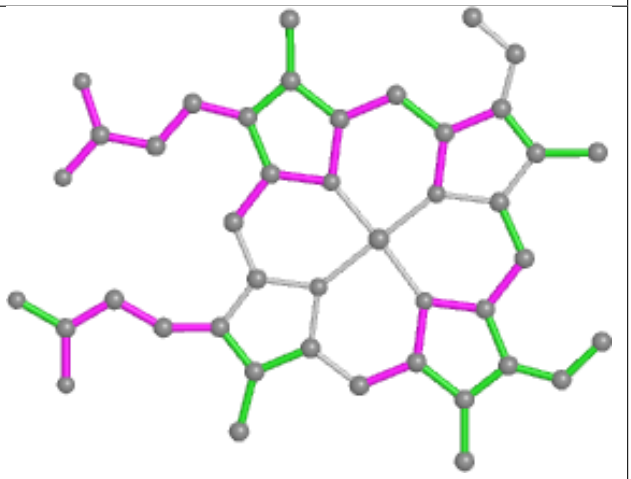


Rings

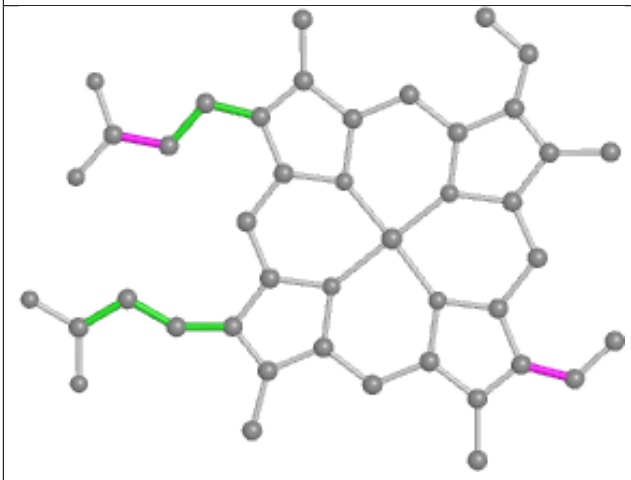
Ligand HEM F 102



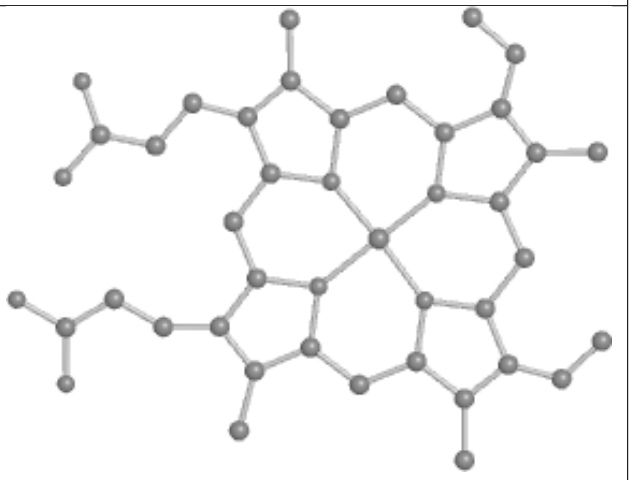
Bond lengths



Bond angles

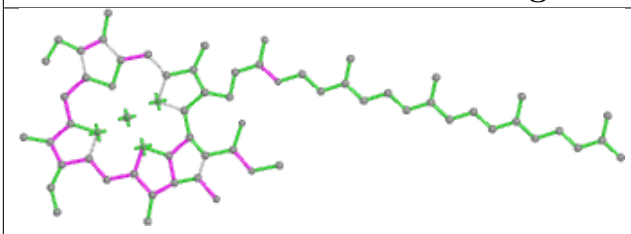


Torsions



Rings

Ligand CLA c 514



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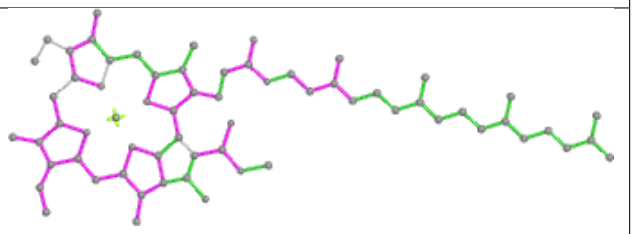
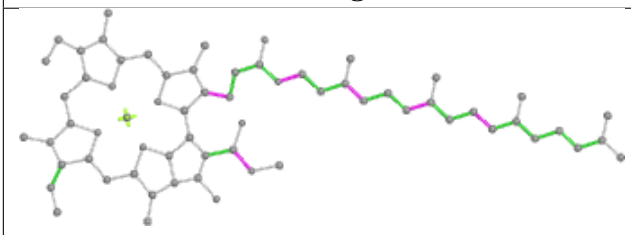


Bond angles



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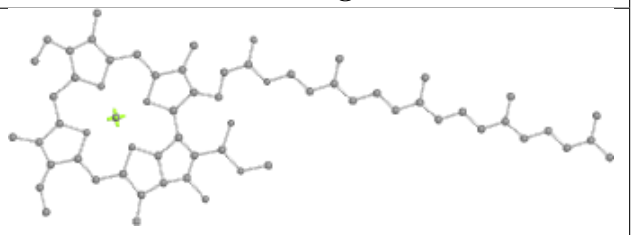
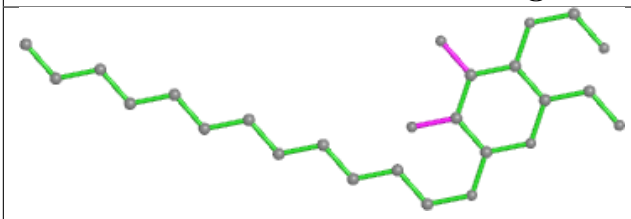
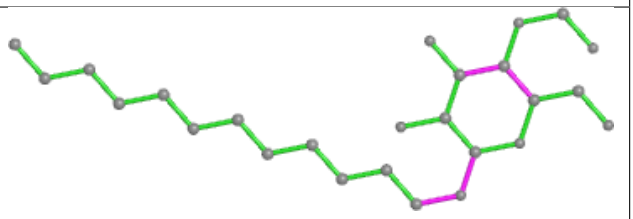


Rings

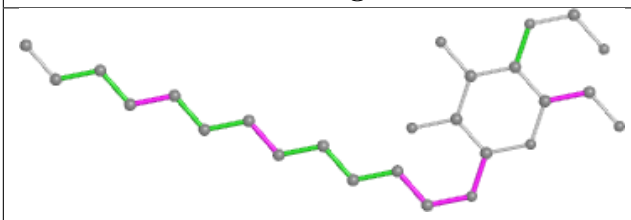
Ligand LMT t 101



Bond lengths



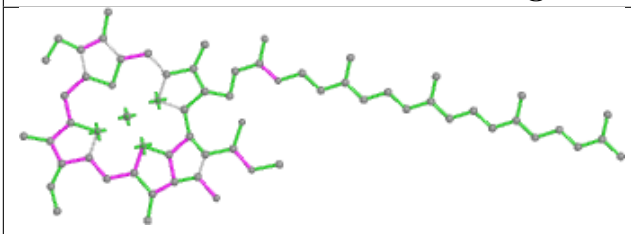
Bond angles



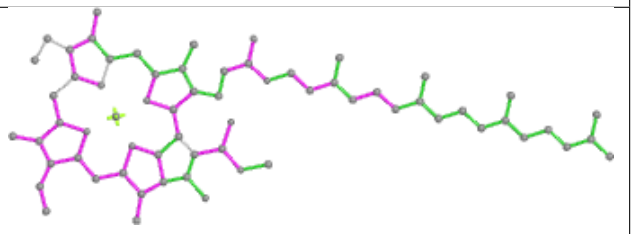
Torsions

Rings

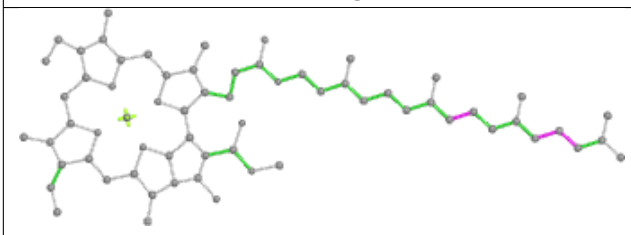
Ligand CLA b 611



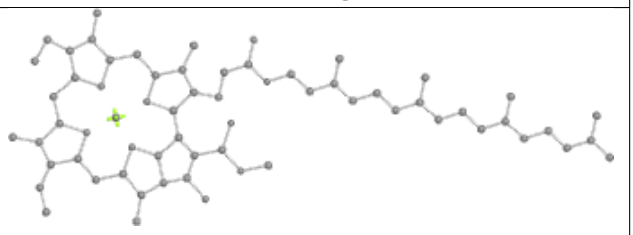
Bond lengths



Bond angles

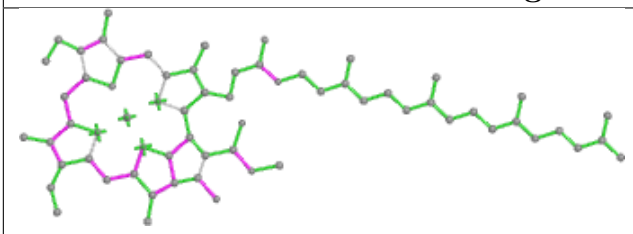


Torsions

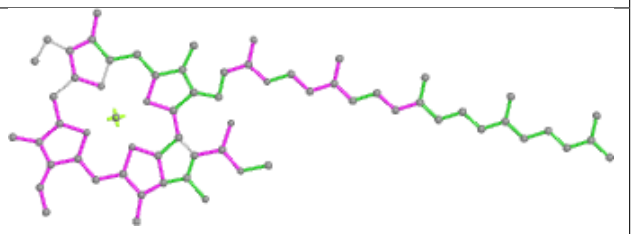


Rings

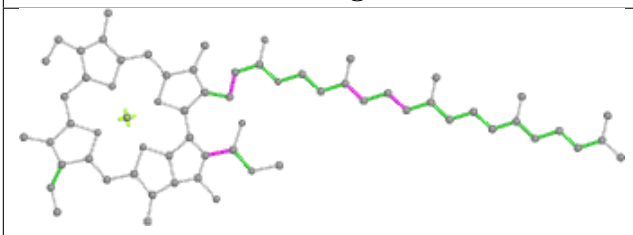
Ligand CLA C 507



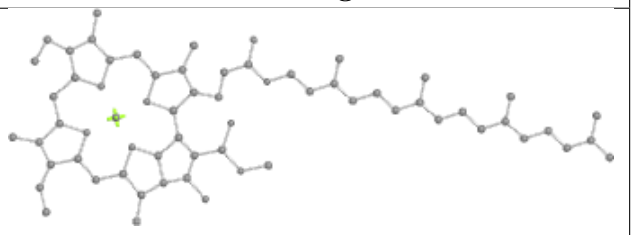
Bond lengths



Bond angles

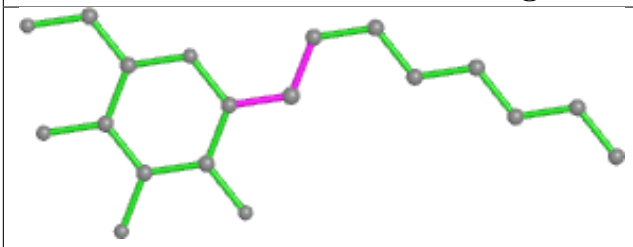


Torsions

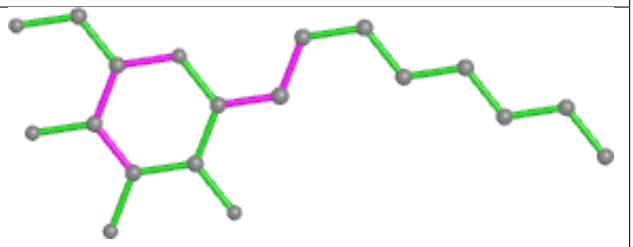


Rings

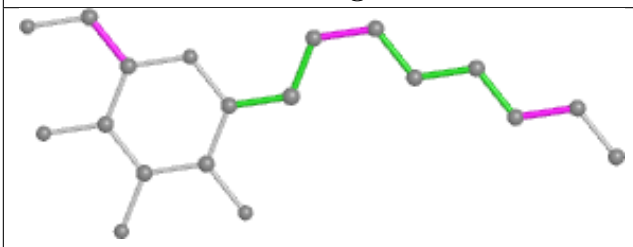
Ligand HTG B 625



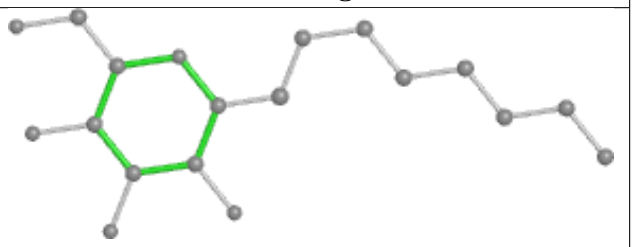
Bond lengths



Bond angles

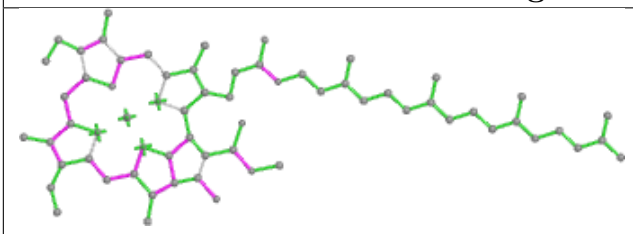


Torsions

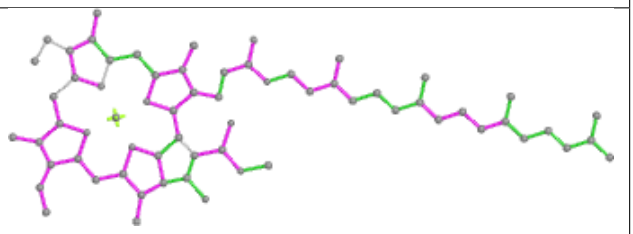


Rings

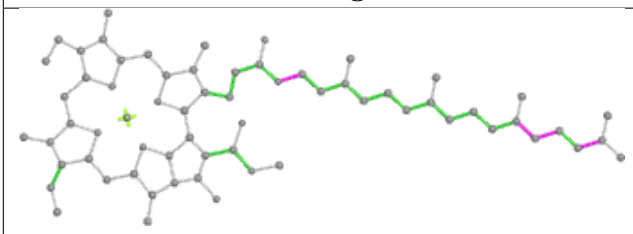
Ligand CLA b 608



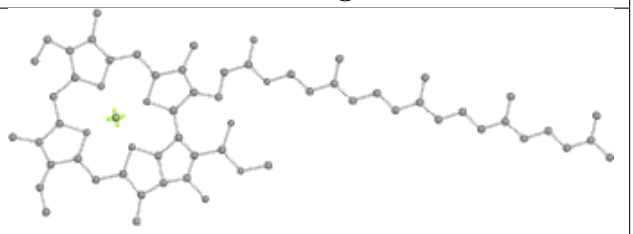
Bond lengths



Bond angles

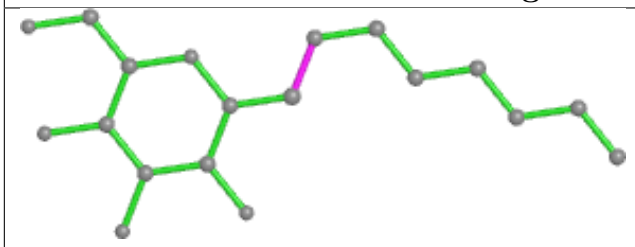


Torsions

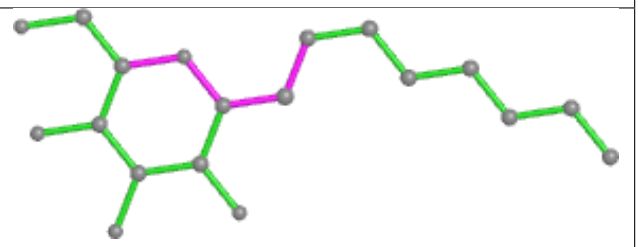


Rings

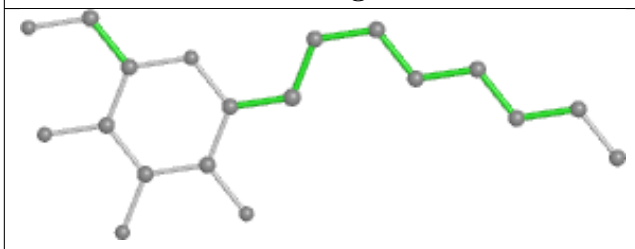
Ligand HTG C 520



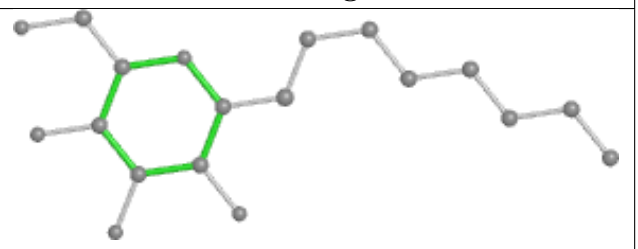
Bond lengths



Bond angles

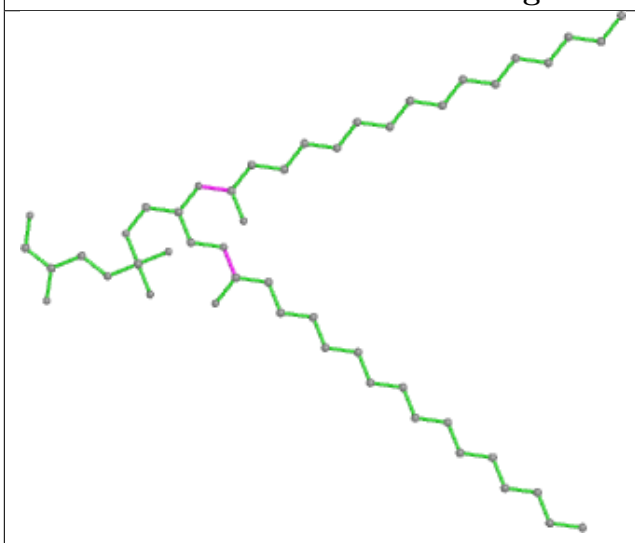


Torsions

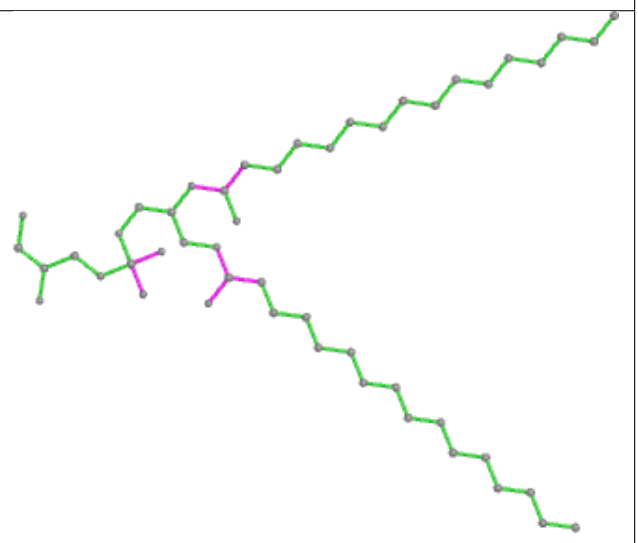


Rings

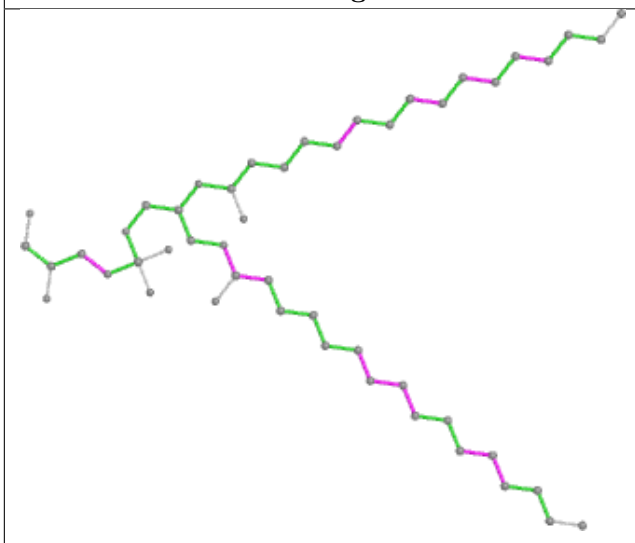
Ligand LHG D 407



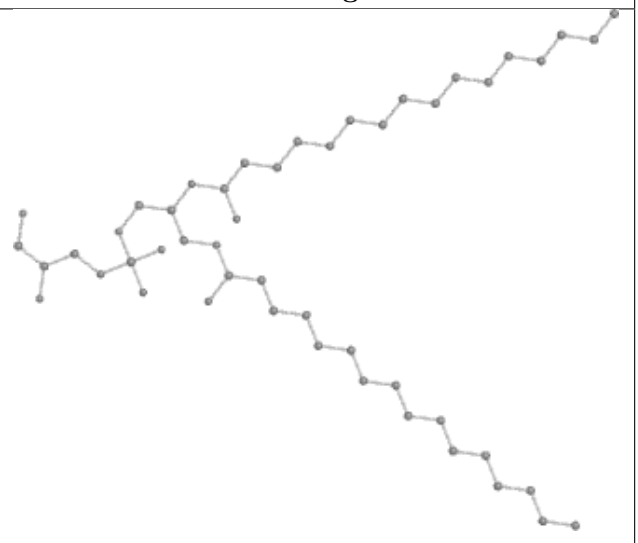
Bond lengths



Bond angles

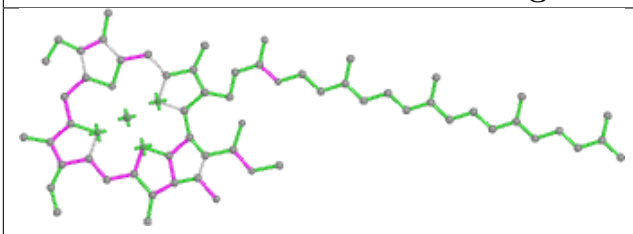


Torsions

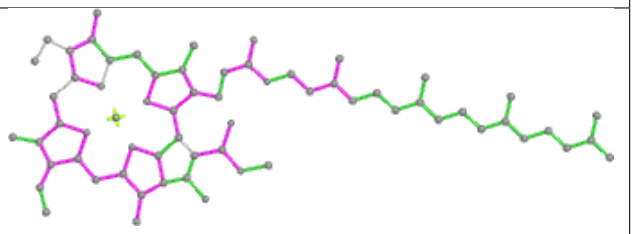


Rings

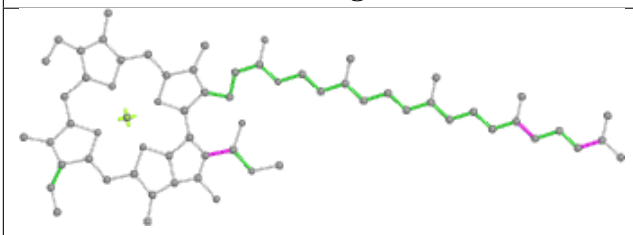
Ligand CLA c 509



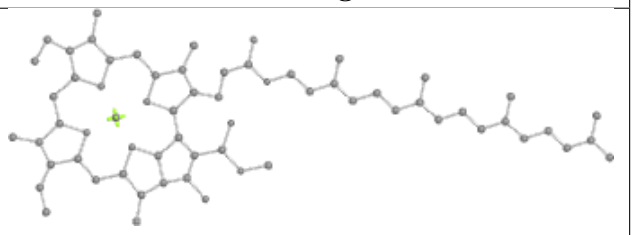
Bond lengths



Bond angles

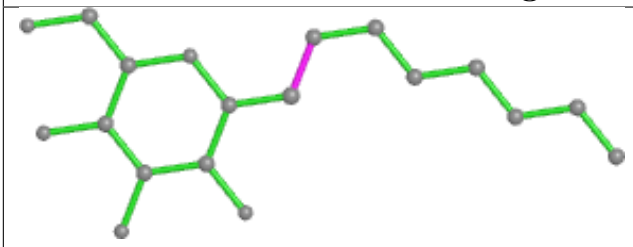


Torsions

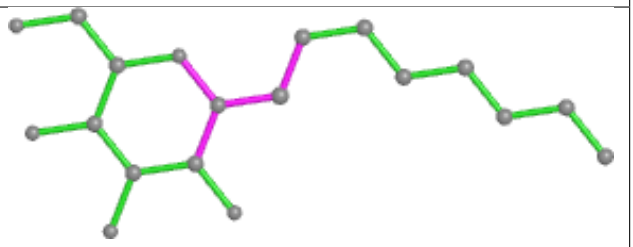


Rings

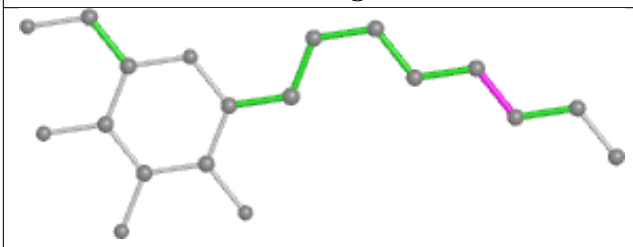
Ligand HTG B 623



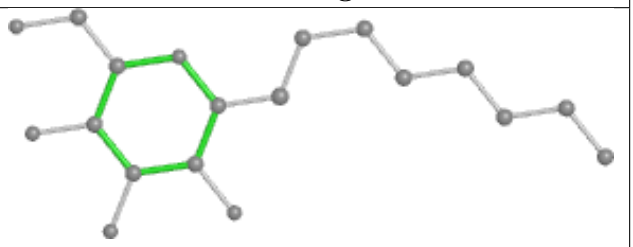
Bond lengths



Bond angles

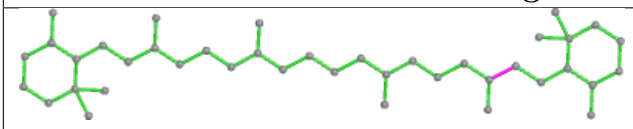


Torsions

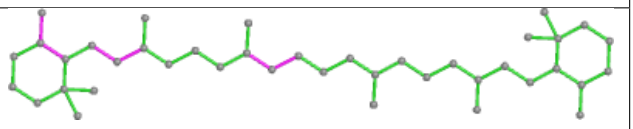


Rings

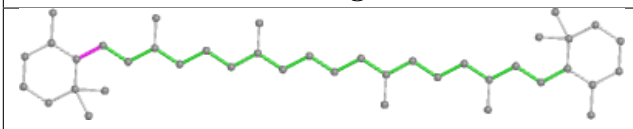
Ligand BCR B 617



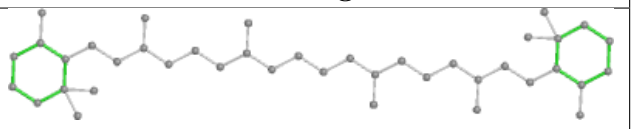
Bond lengths



Bond angles

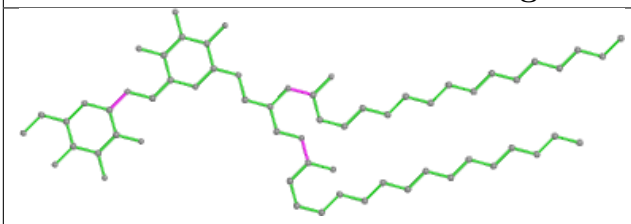


Torsions

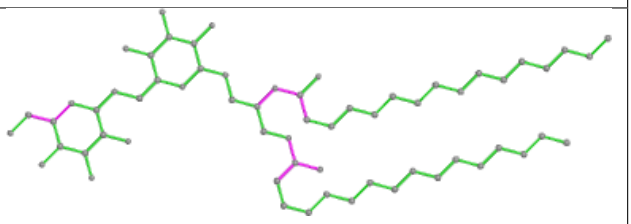


Rings

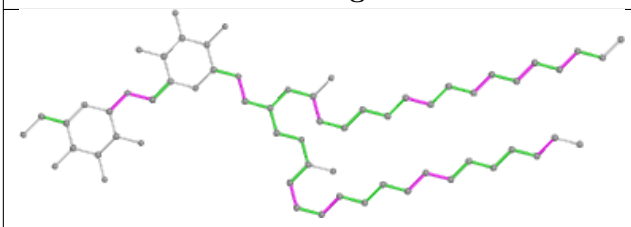
Ligand DGD C 516



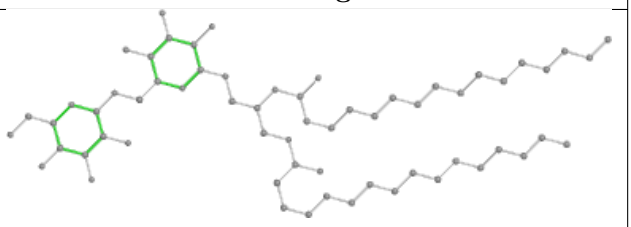
Bond lengths



Bond angles

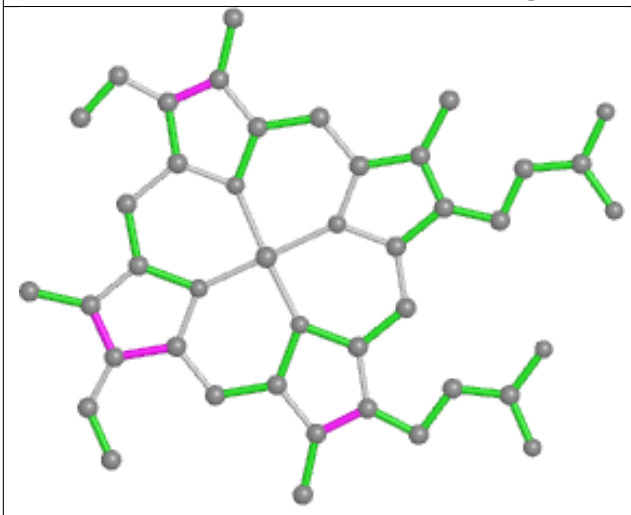


Torsions

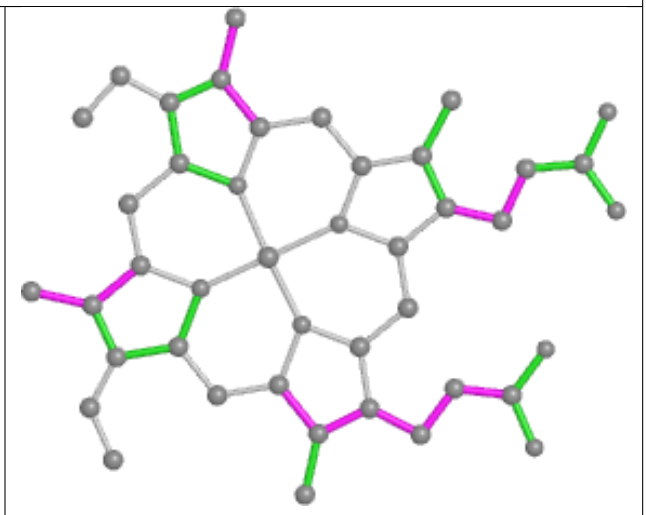


Rings

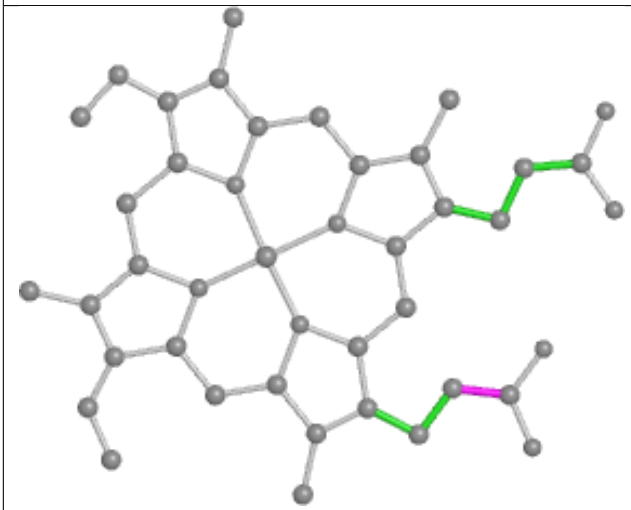
Ligand HEC V 201



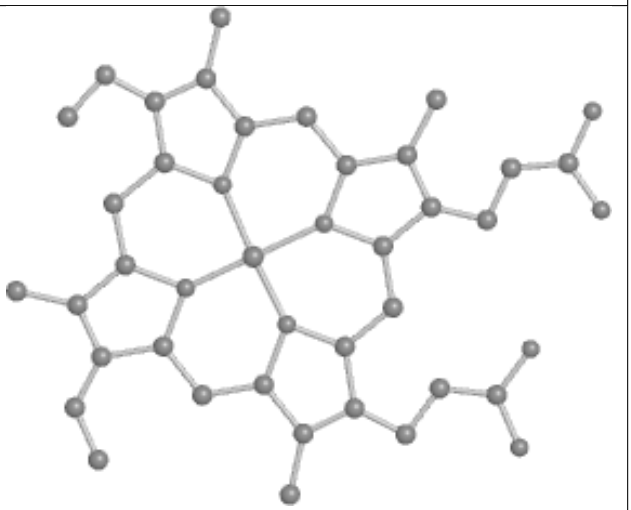
Bond lengths



Bond angles

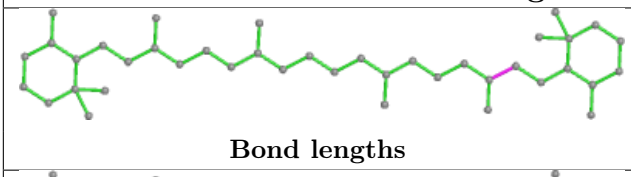


Torsions

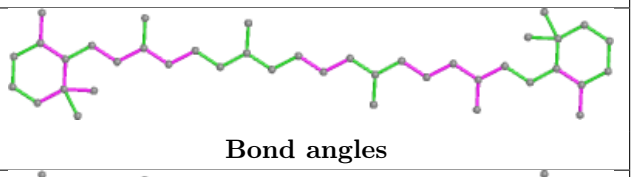


Rings

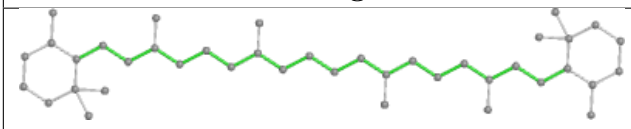
Ligand BCR c 516



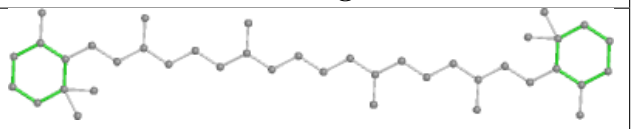
Bond lengths



Bond angles

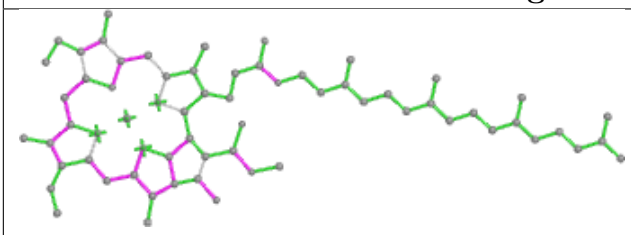


Torsions

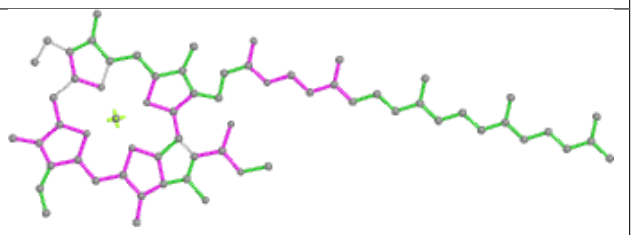


Rings

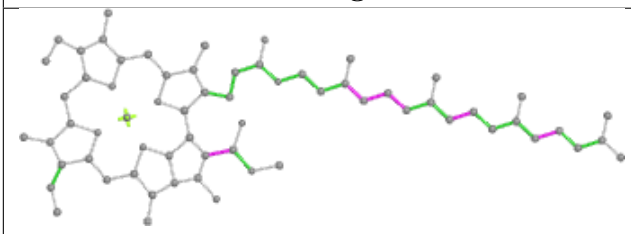
Ligand CLA b 605



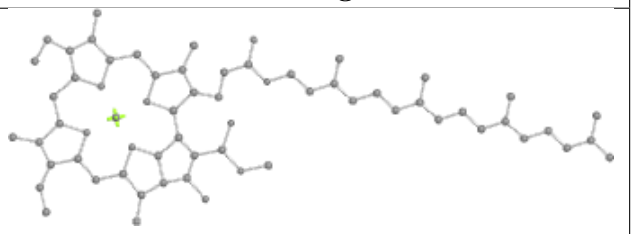
Bond lengths



Bond angles

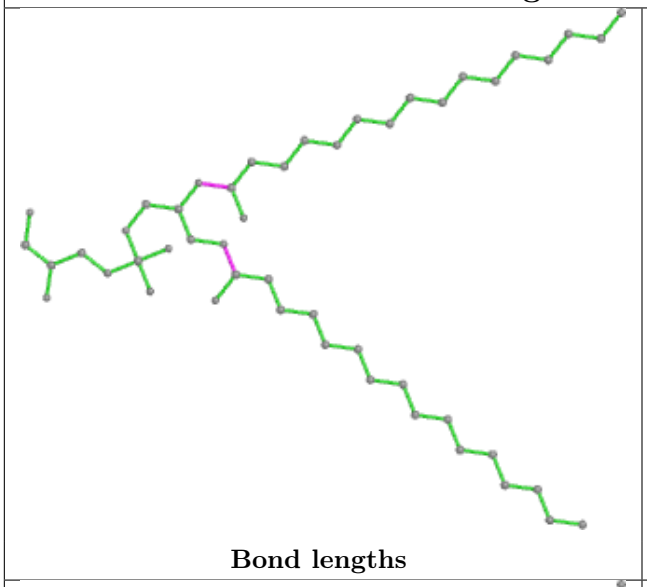


Torsions

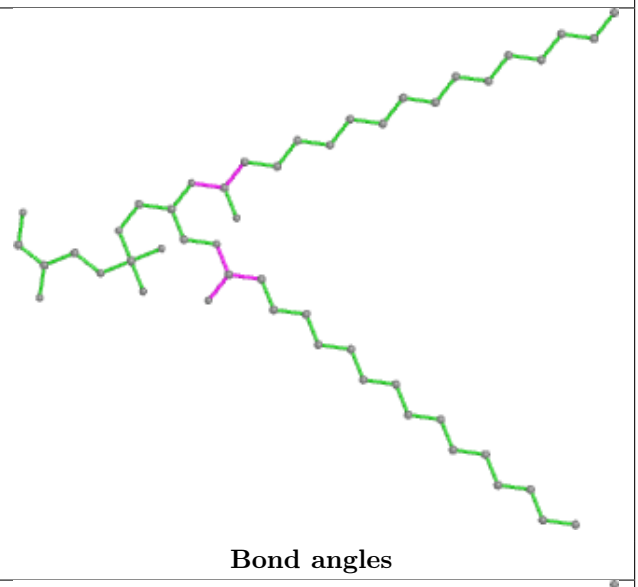


Rings

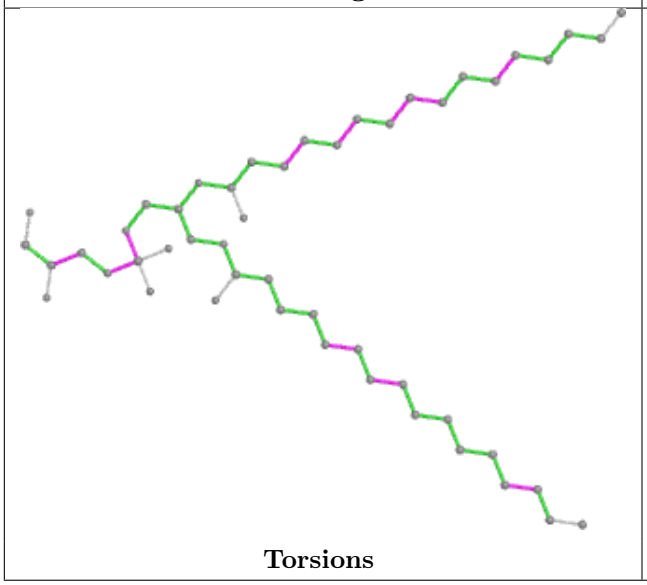
Ligand LHG D 406



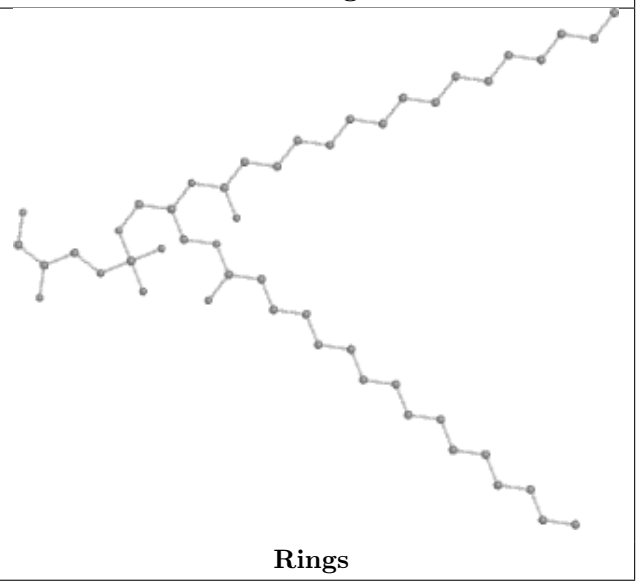
Bond lengths



Bond angles

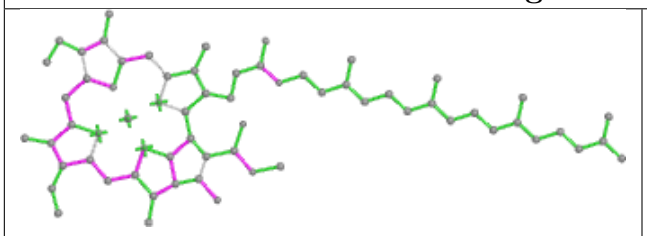


Torsions

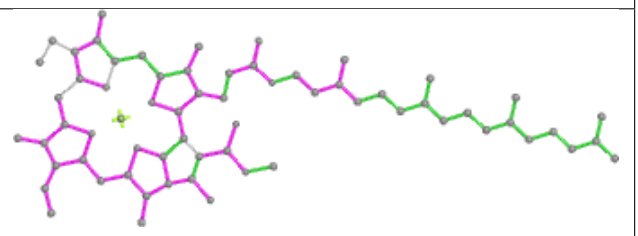


Rings

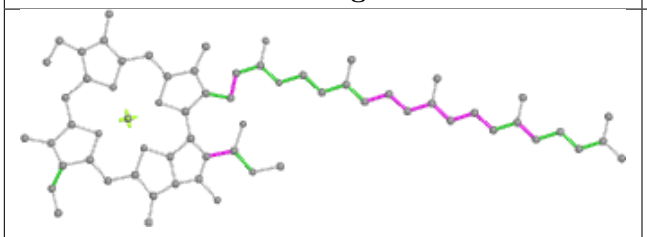
Ligand CLA B 614



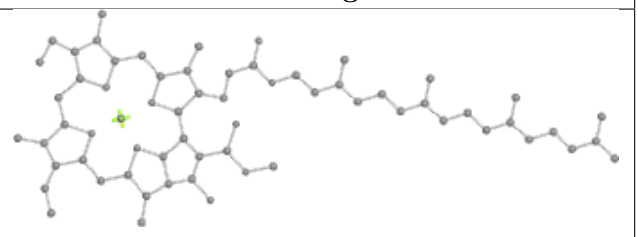
Bond lengths



Bond angles

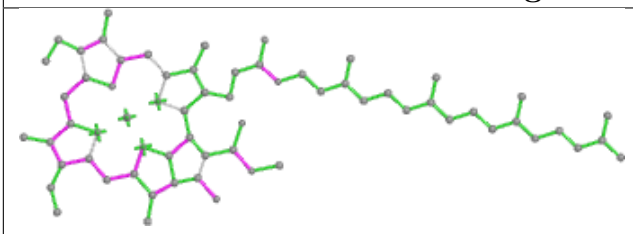


Torsions

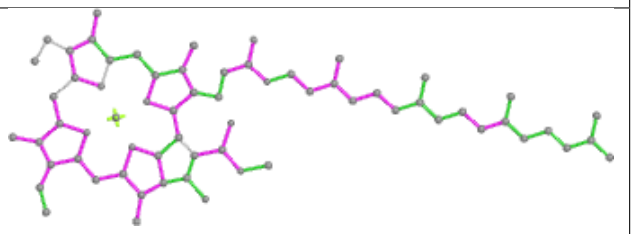


Rings

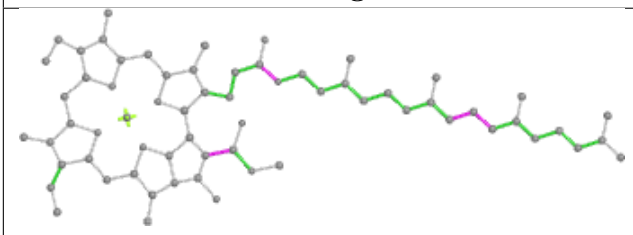
Ligand CLA B 612



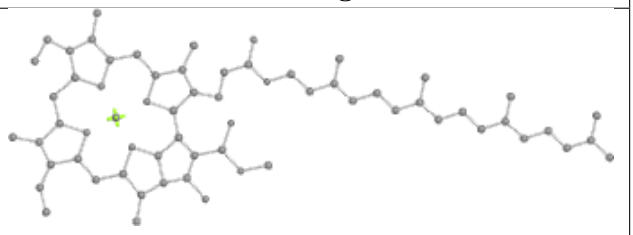
Bond lengths



Bond angles

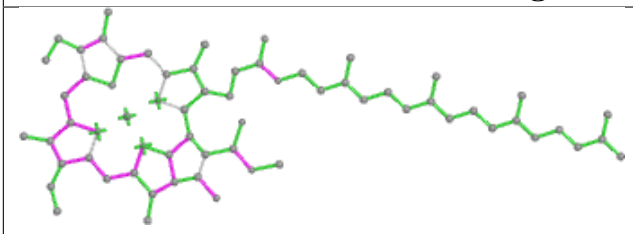


Torsions

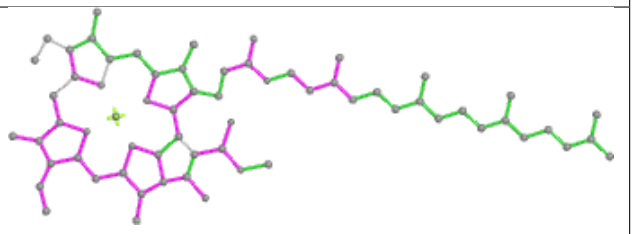


Rings

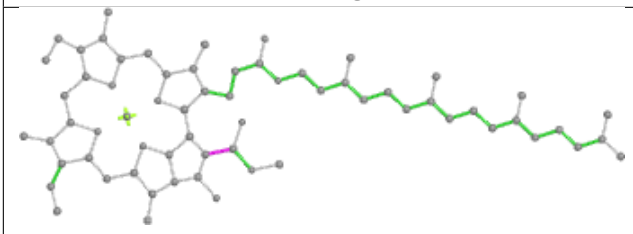
Ligand CLA c 502



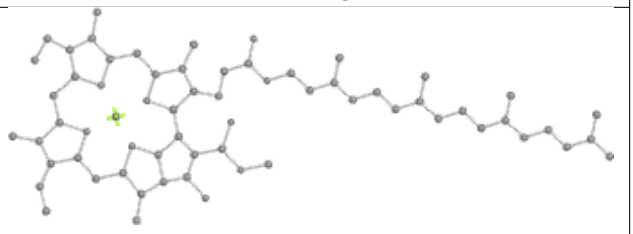
Bond lengths



Bond angles

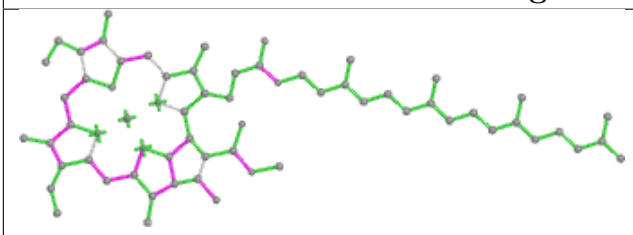


Torsions

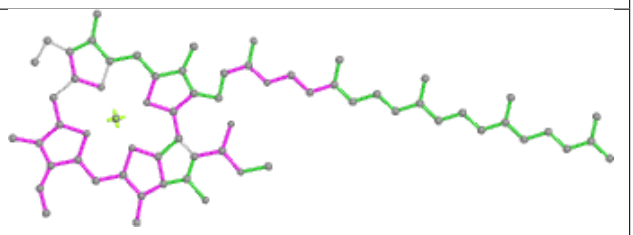


Rings

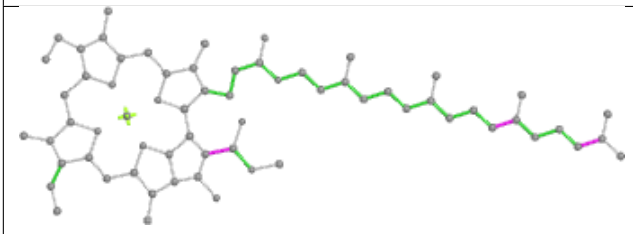
Ligand CLA c 503



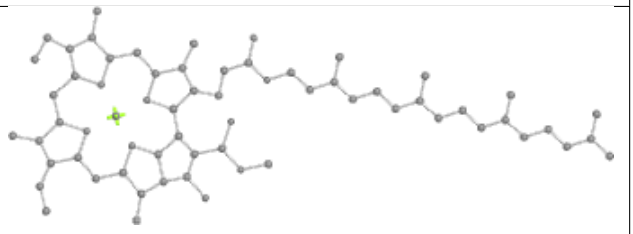
Bond lengths



Bond angles

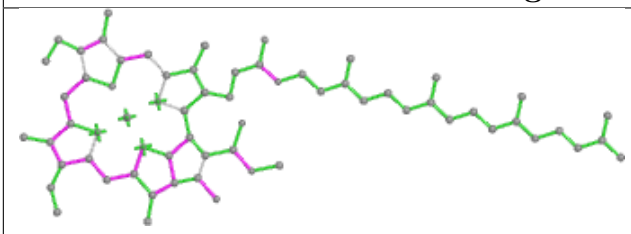


Torsions

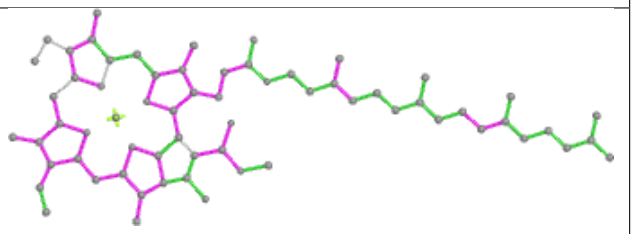


Rings

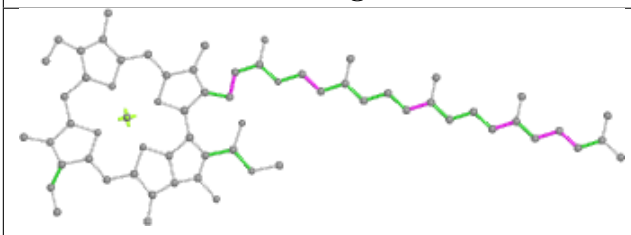
Ligand CLA B 602



Bond lengths



Bond angles



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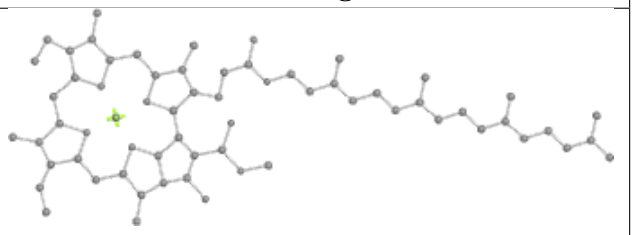
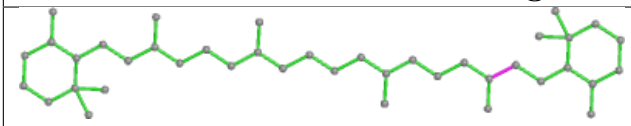


Rings

Ligand BCR y 101



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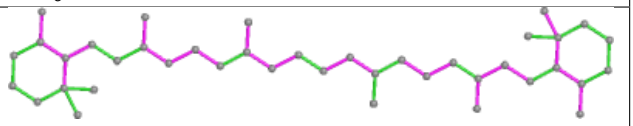

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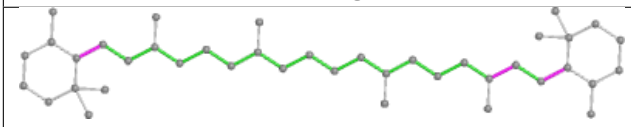
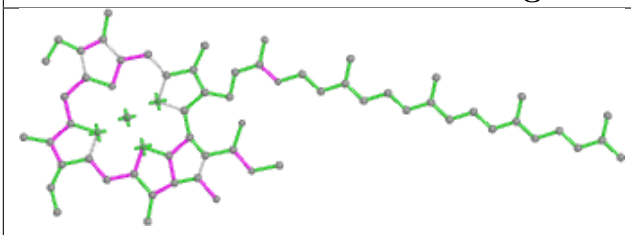


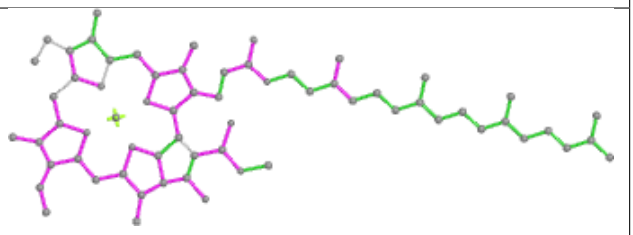
Torsions

Rings

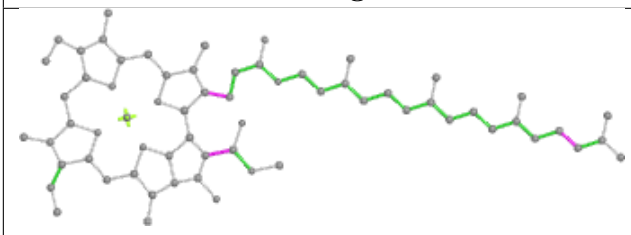
Ligand CLA A 405



Bond lengths



Bond angles



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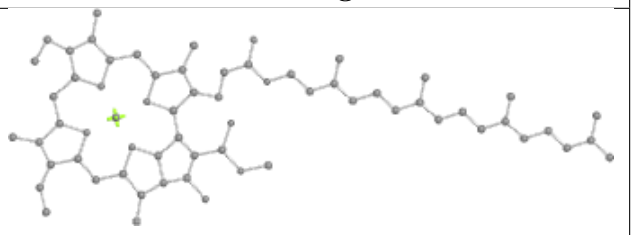
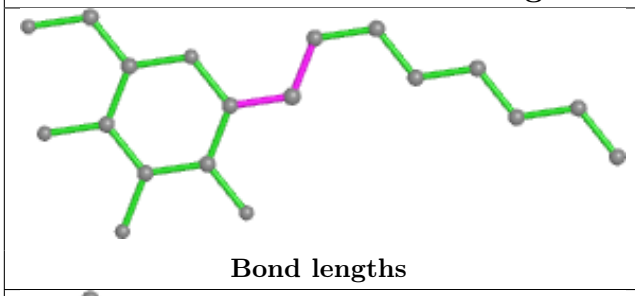


Rings

Ligand HTG b 625



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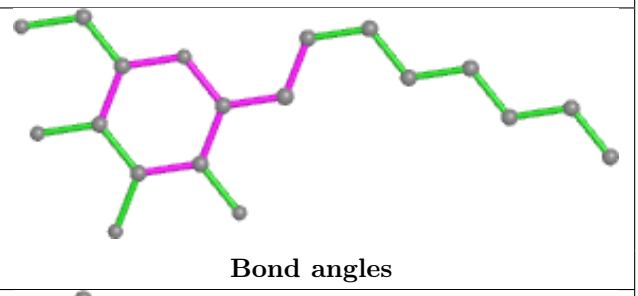
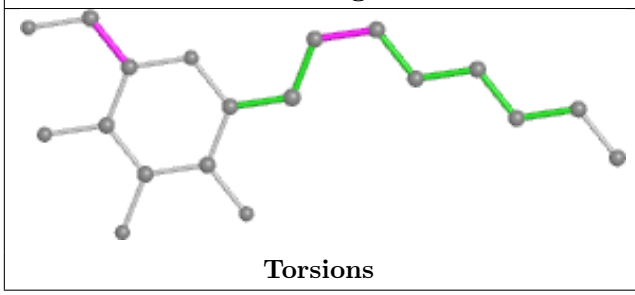


Bond angles



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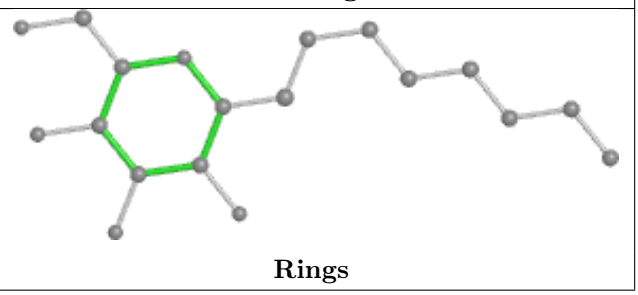
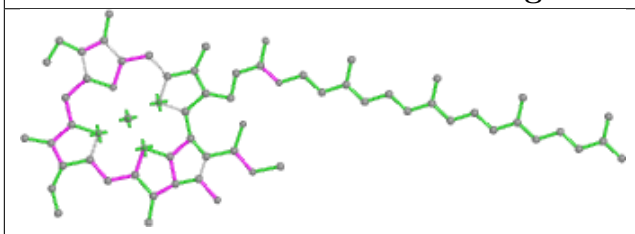


Rings

Ligand CLA A 406



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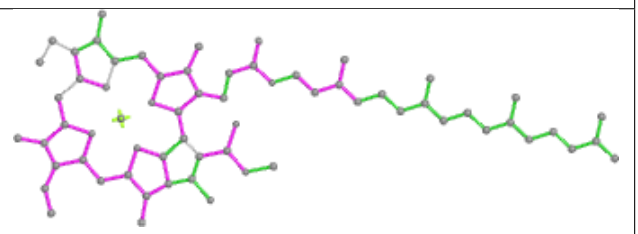
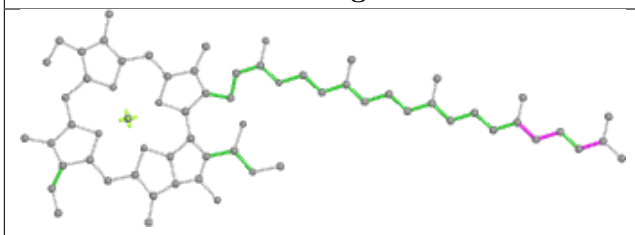


Bond angles



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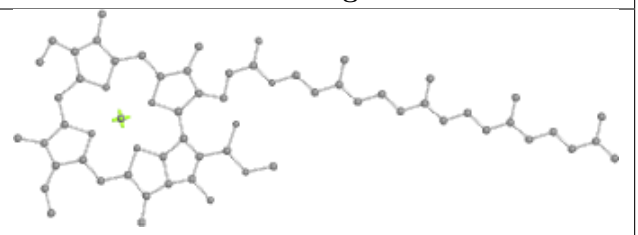
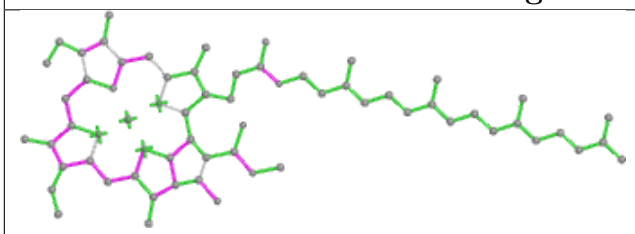
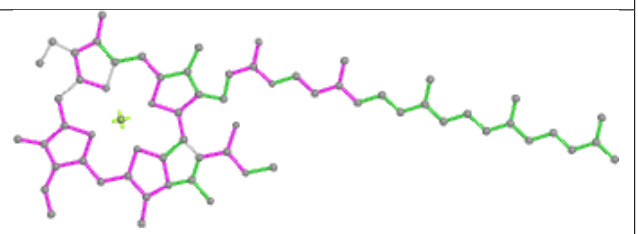


Rings

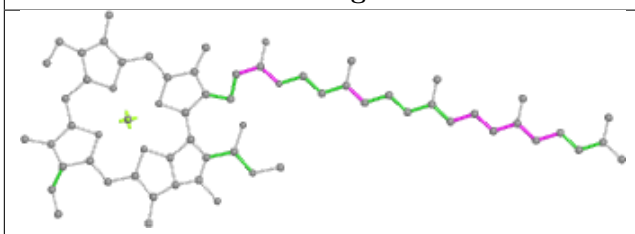
Ligand CLA C 510



Bond lengths



Bond angles



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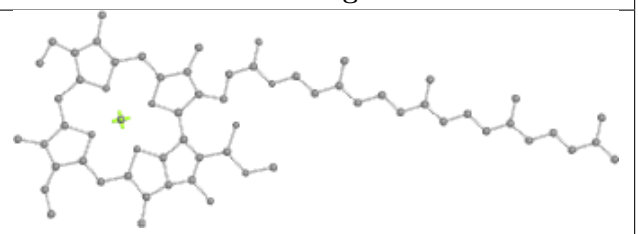
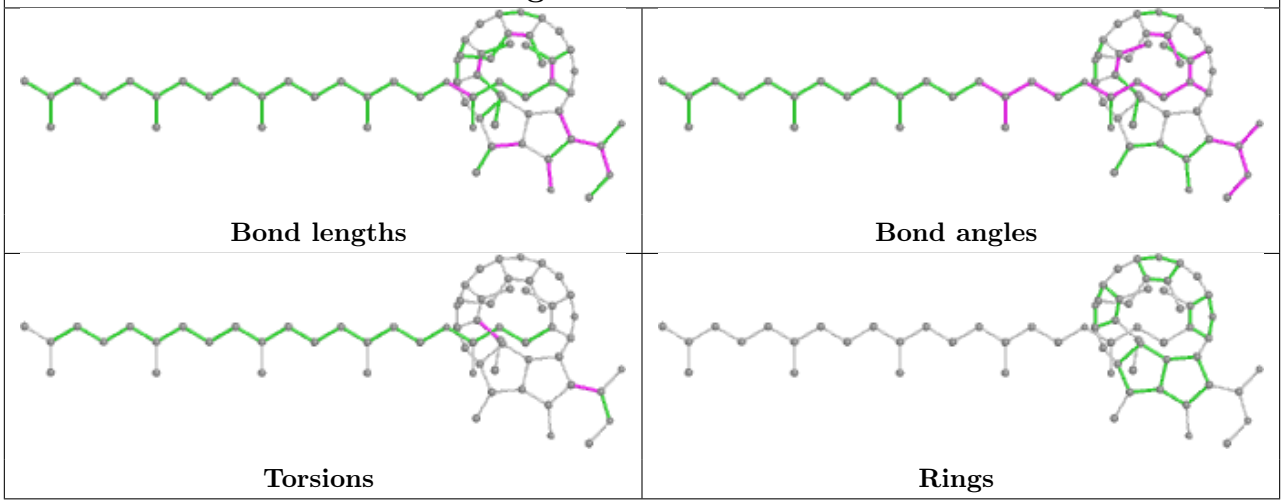
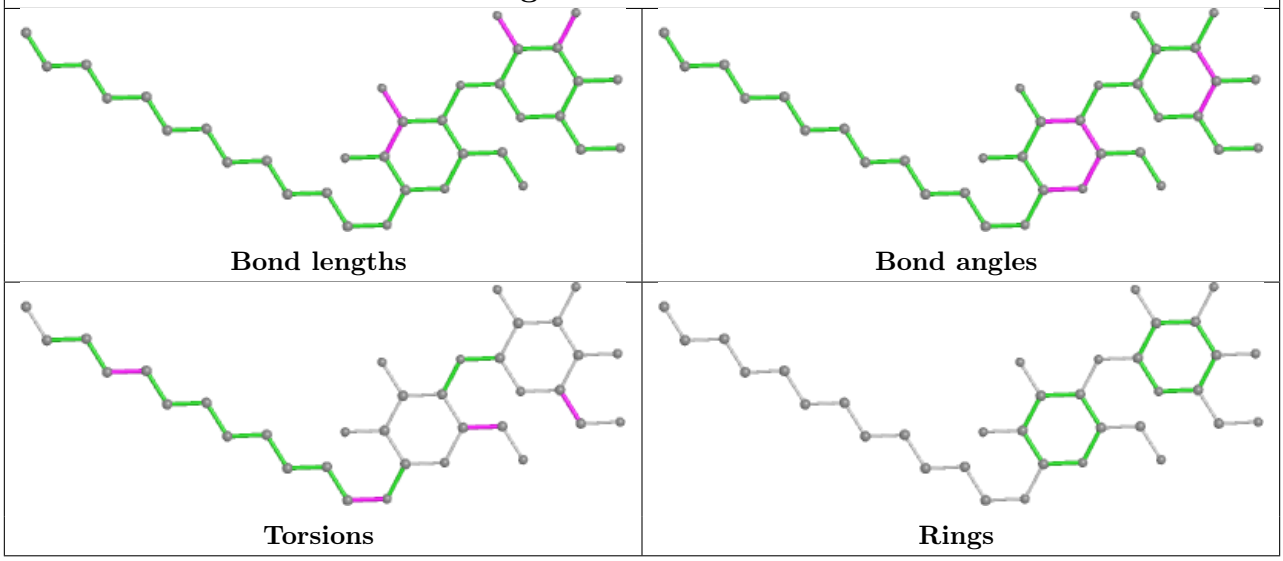


Rings

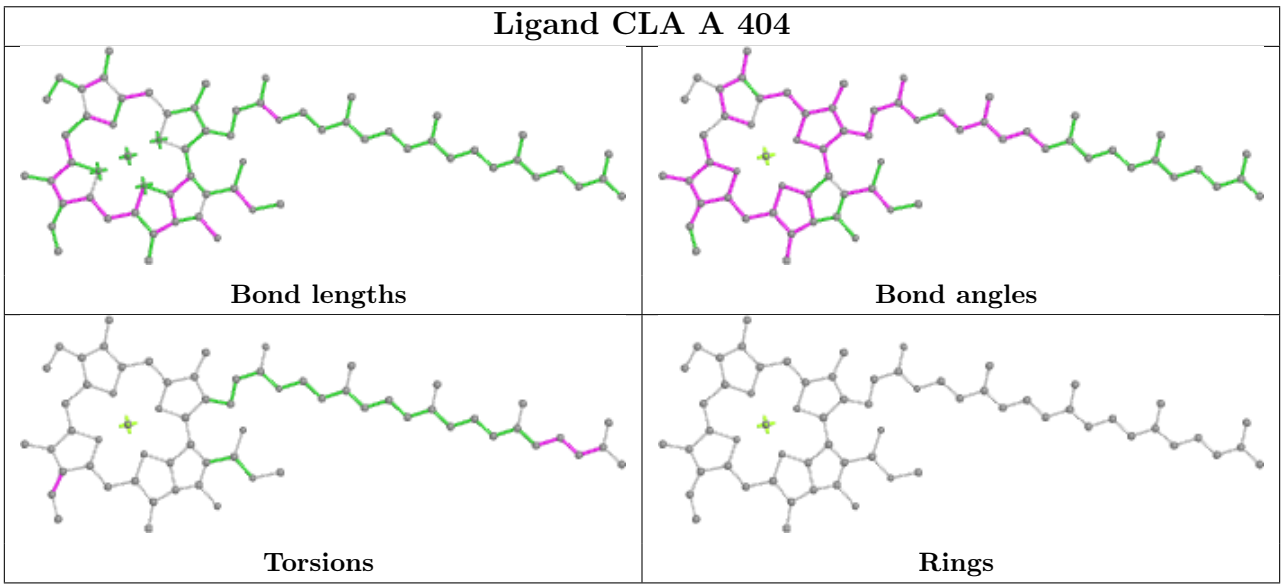
Ligand PHO a 417



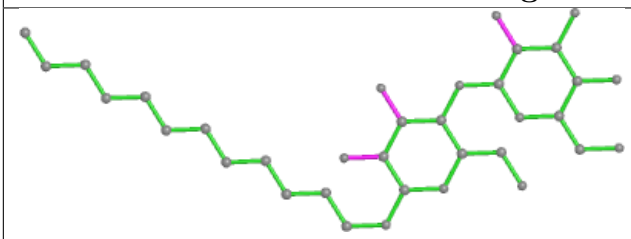
Ligand LMT m 103

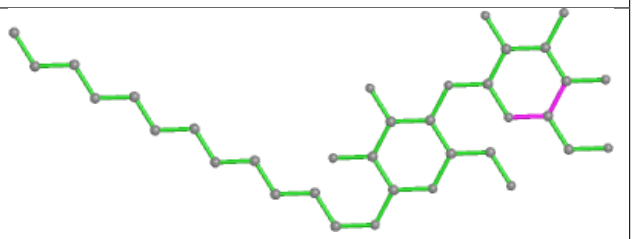


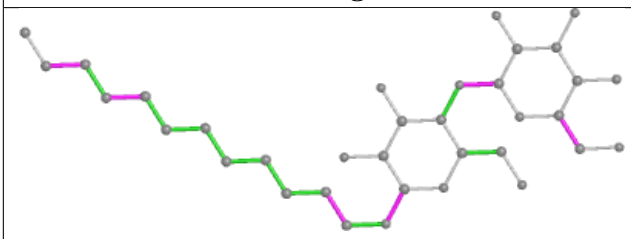
Ligand CLA A 404

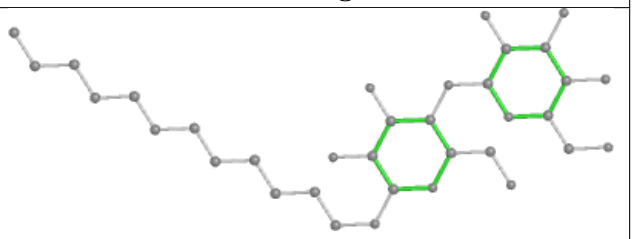


Ligand LMT A 417

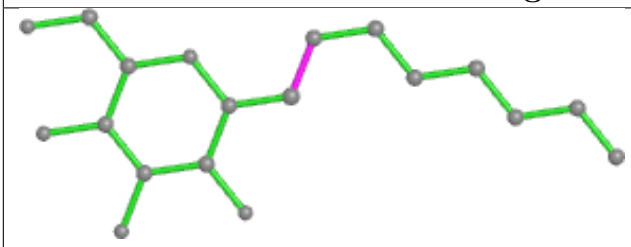

Bond lengths

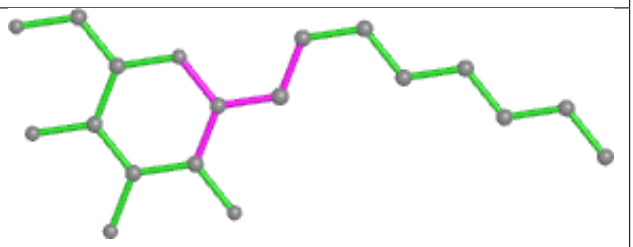

Bond angles

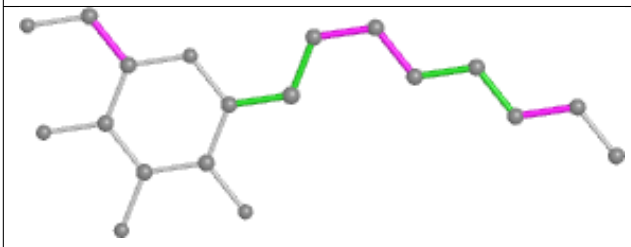

Torsions


Rings

Ligand HTG b 623


Bond lengths


Bond angles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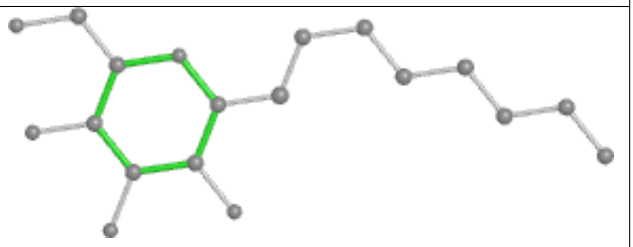
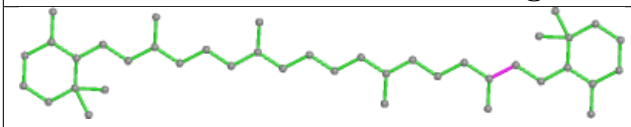
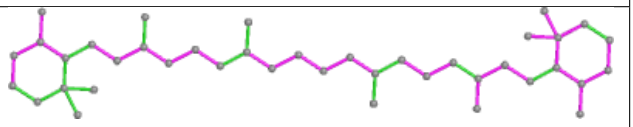
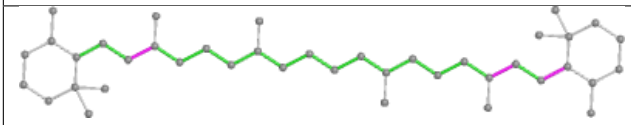

Rings

Ligand BCR d 403


Bond lengths


Bond angles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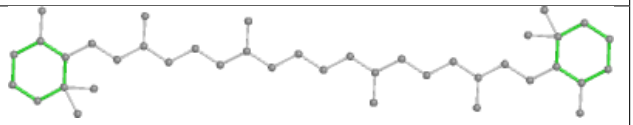
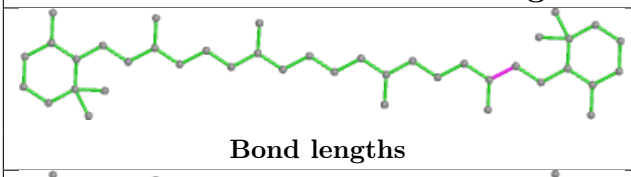
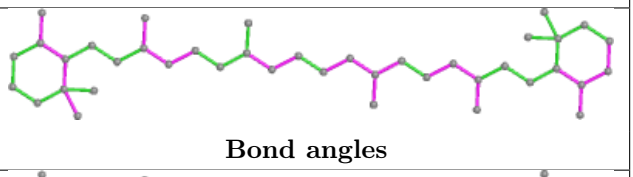

Rings

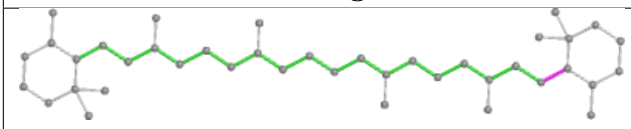
Ligand BCR c 515



Bond lengths



Bond angles



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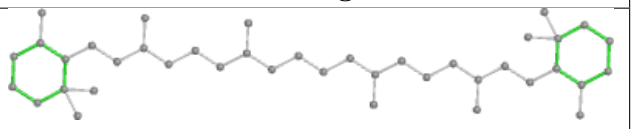
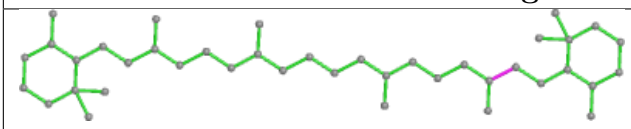
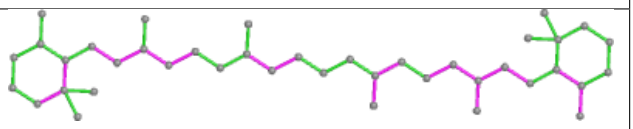


Rings

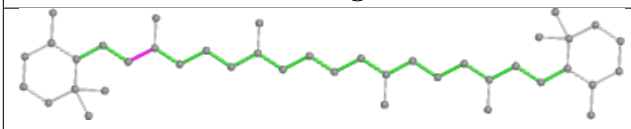
Ligand BCR K 103



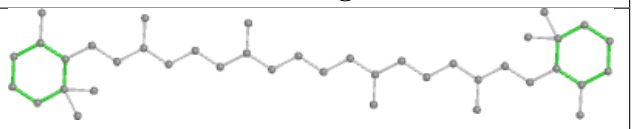
Bond lengths



Bond angles

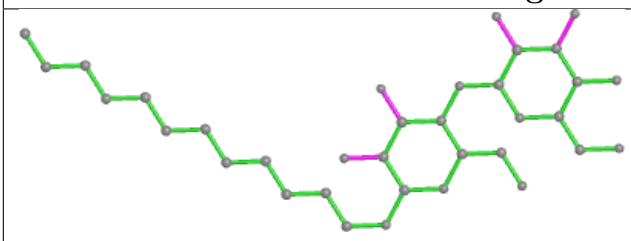


Torsions

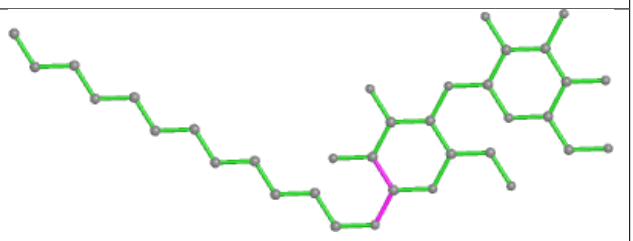


Rings

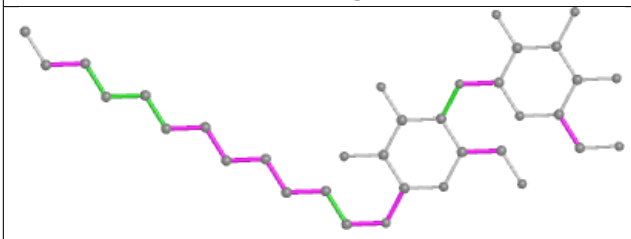
Ligand LMT e 101



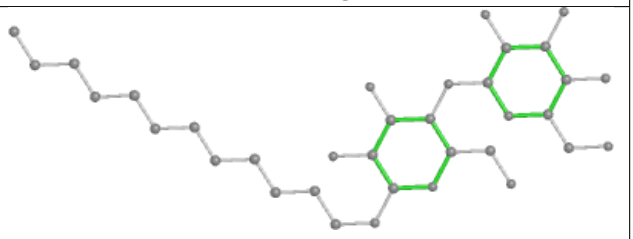
Bond lengths



Bond angles

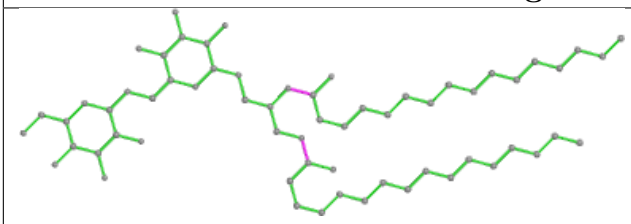


Torsions

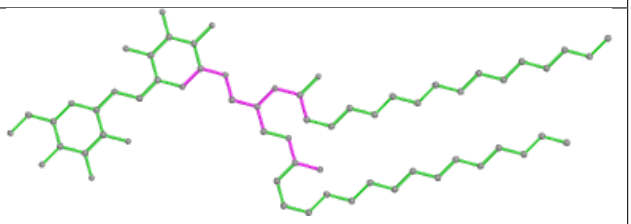


Rings

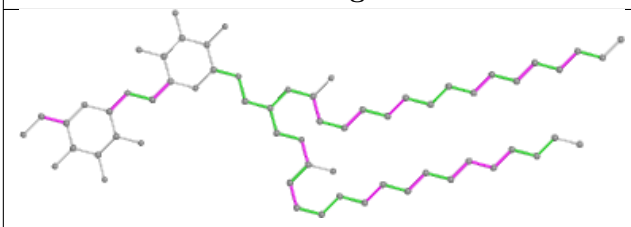
Ligand DGD c 517



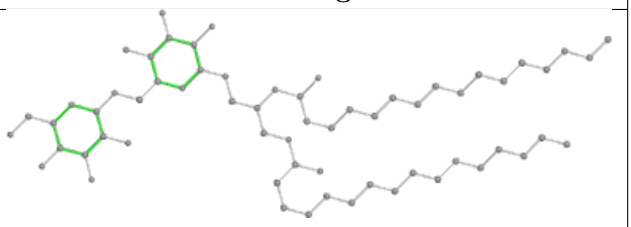
Bond lengths



Bond angles

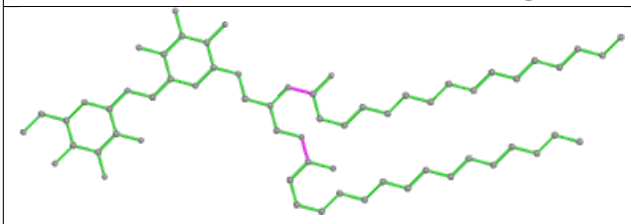


Torsions

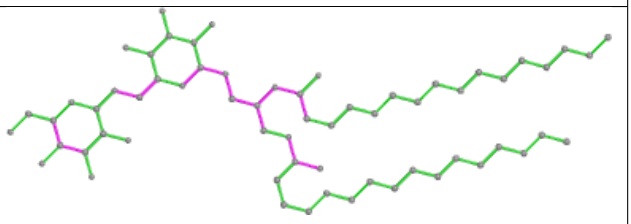


Rings

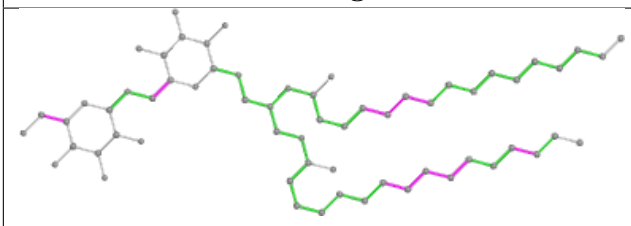
Ligand DGD C 515



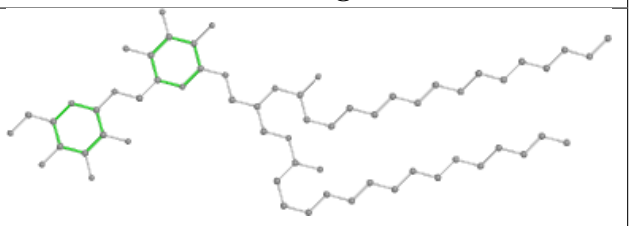
Bond lengths



Bond angles

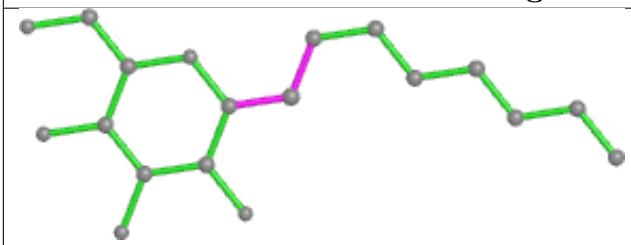


Torsions

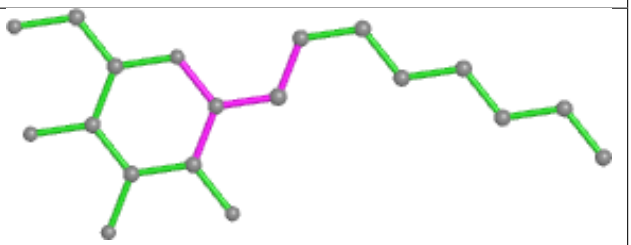


Rings

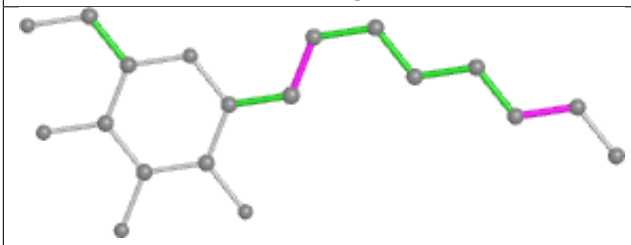
Ligand HTG c 522



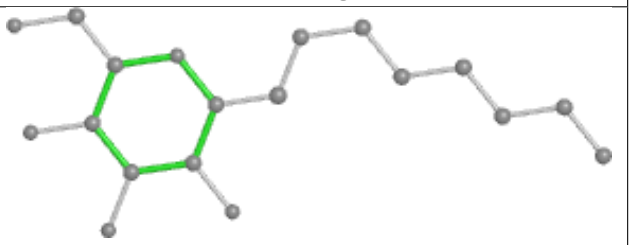
Bond lengths



Bond angles

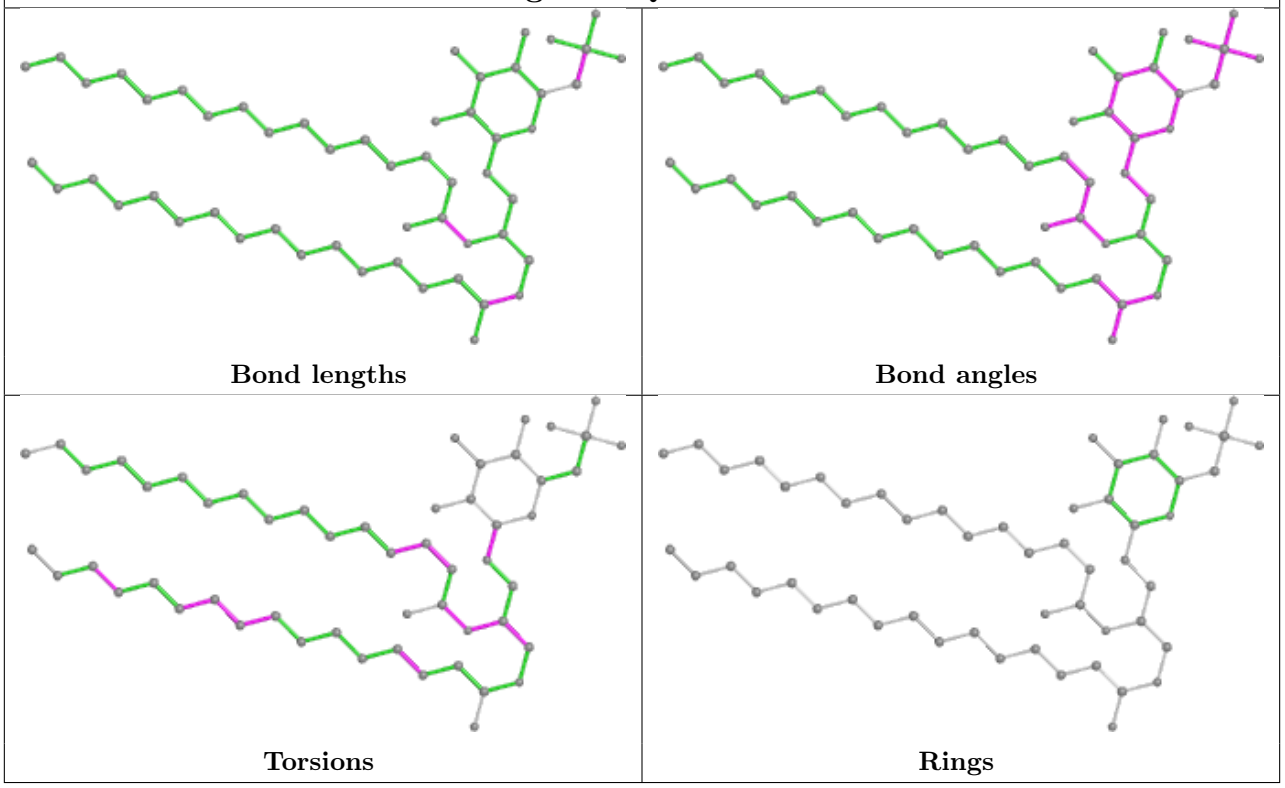


Torsions

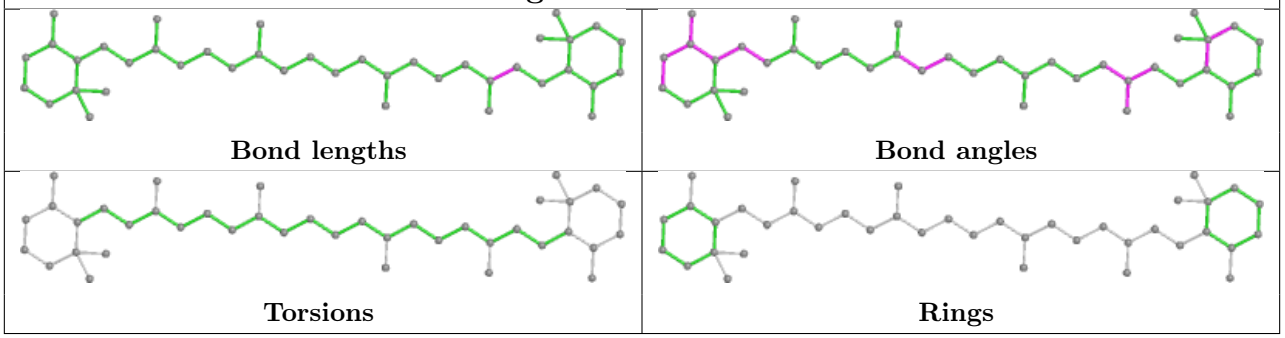


Rings

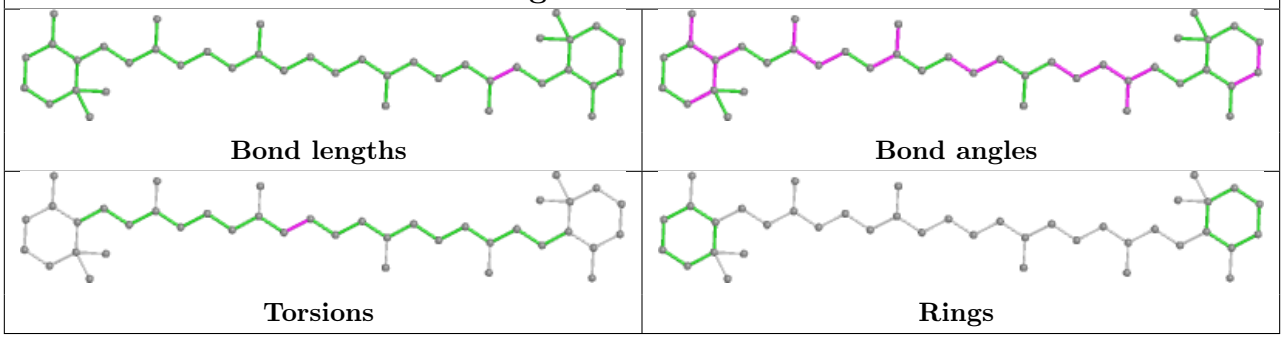
Ligand SQD B 620



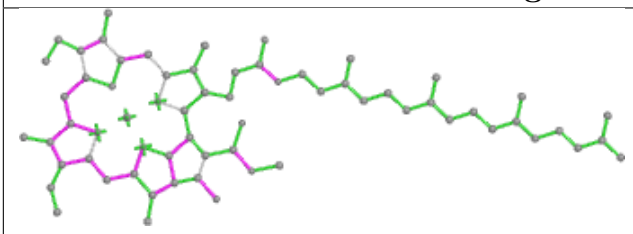
Ligand BCR b 618



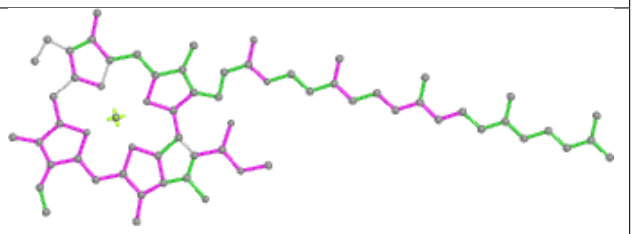
Ligand BCR t 102



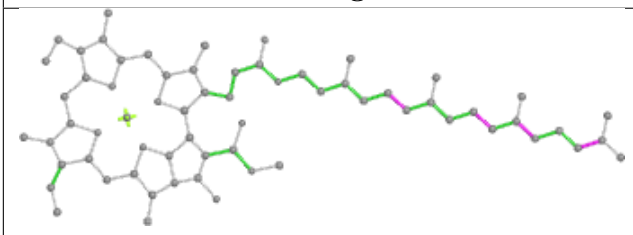
Ligand CLA B 615



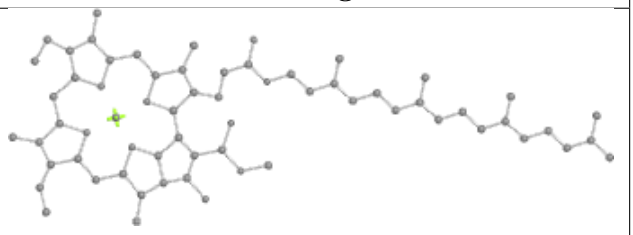
Bond lengths



Bond angles

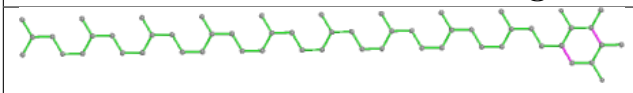


Torsions

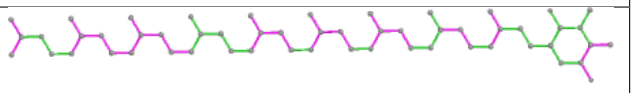


Rings

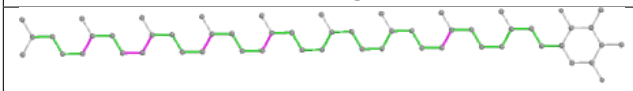
Ligand PL9 D 405



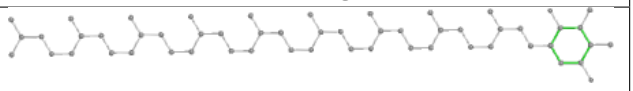
Bond lengths



Bond angles

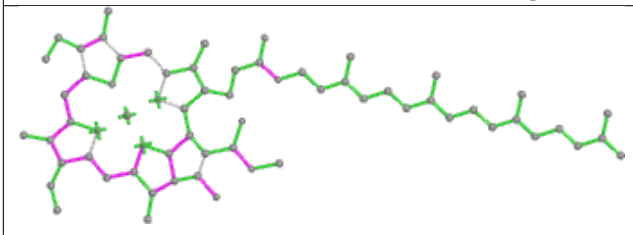


Torsions

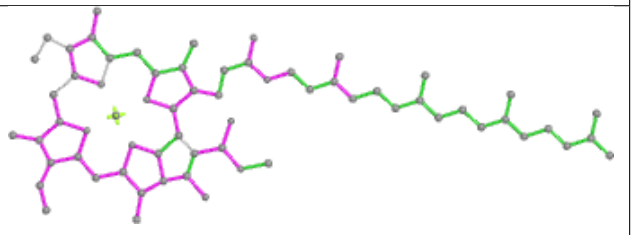


Rings

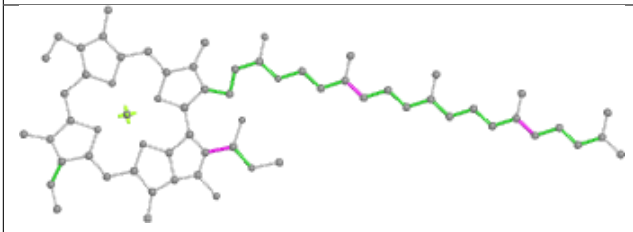
Ligand CLA C 504



Bond lengths



Bond angles



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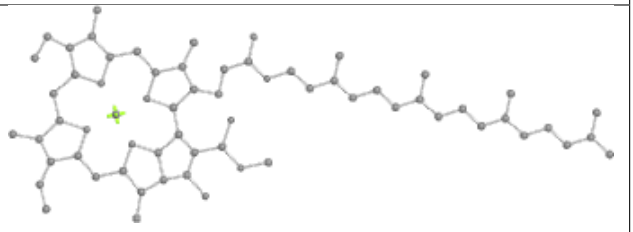
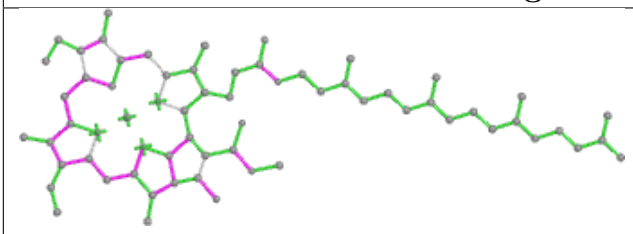
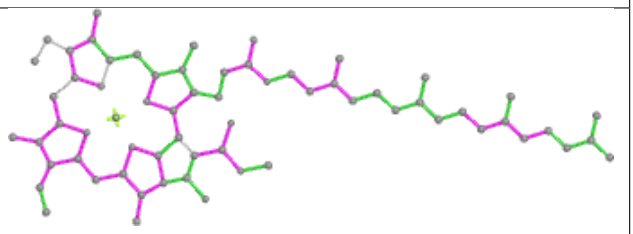


Rings

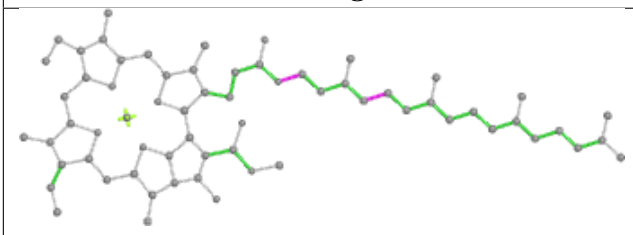
Ligand CLA C 509



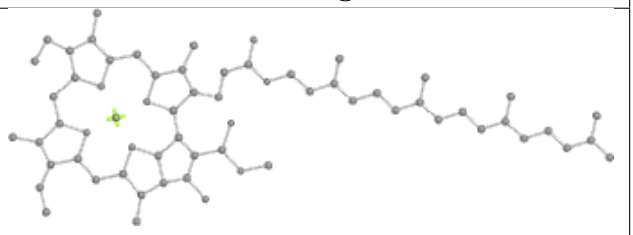
Bond lengths



Bond angles

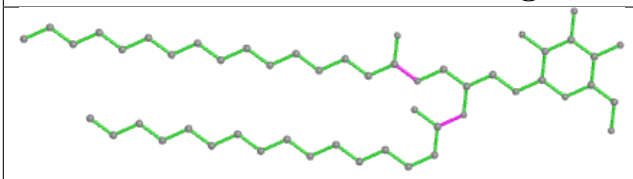


Torsions

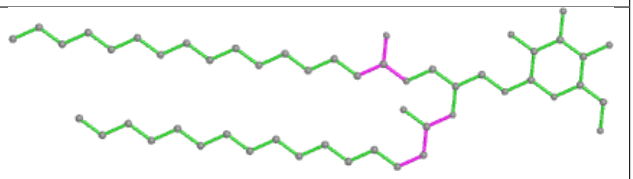


Rings

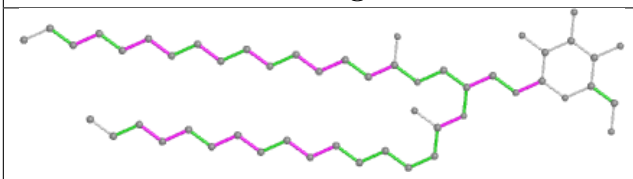
Ligand LMG B 621



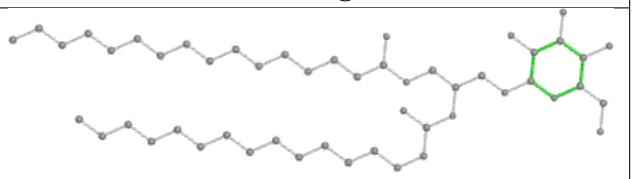
Bond lengths



Bond angles

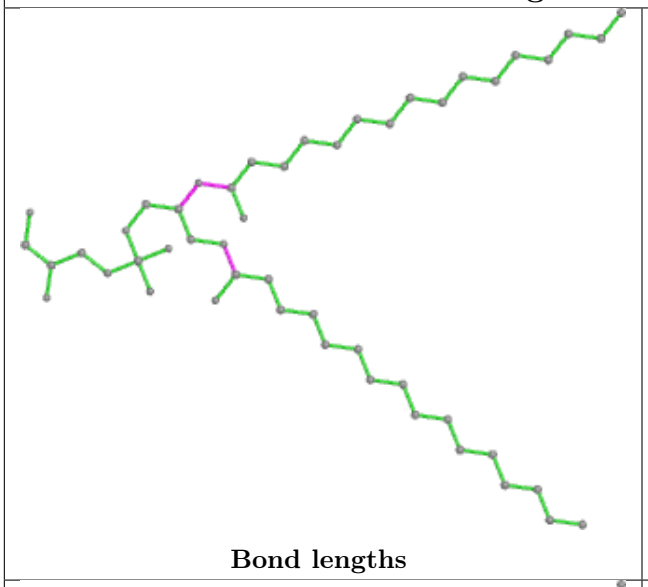


Torsions

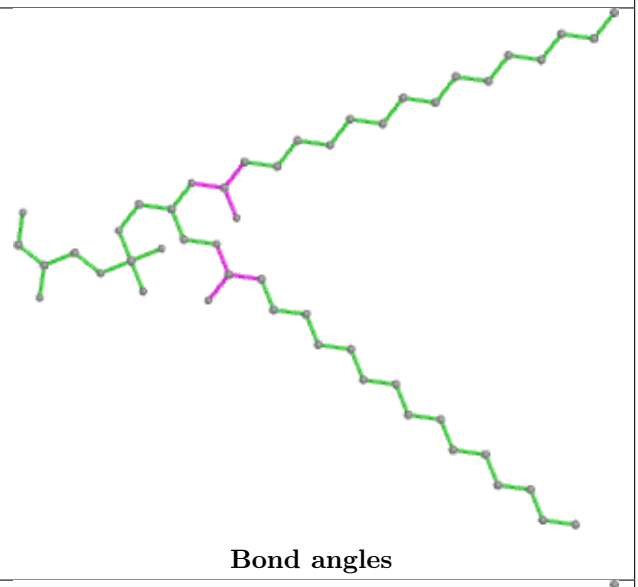


Rings

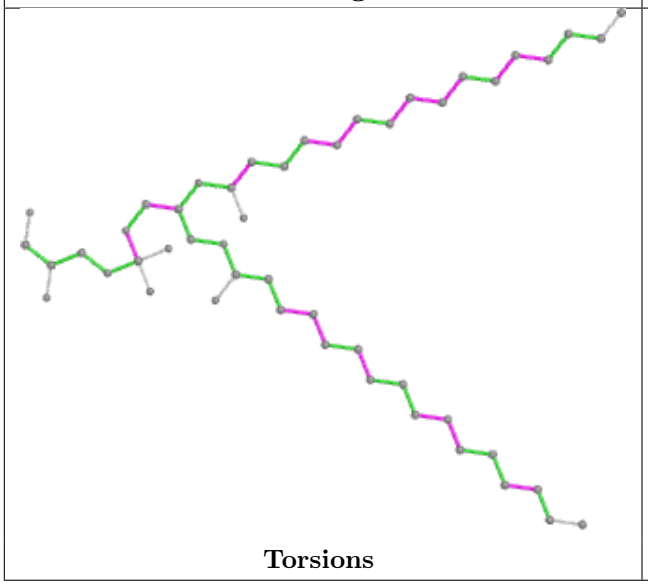
Ligand LHG b 630



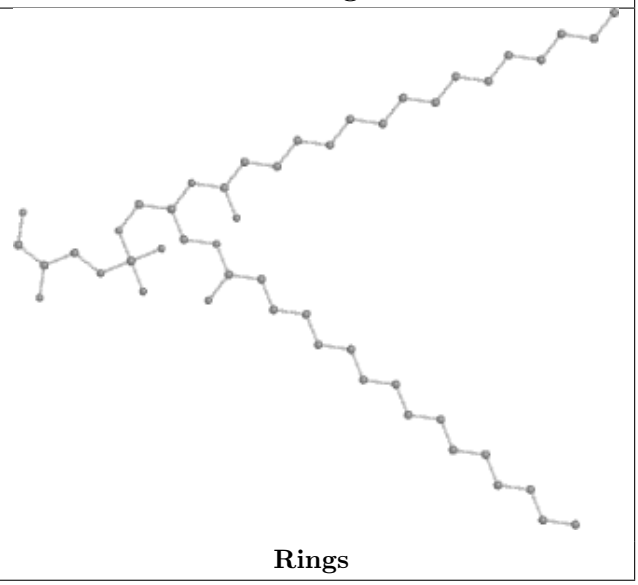
Bond lengths



Bond angles

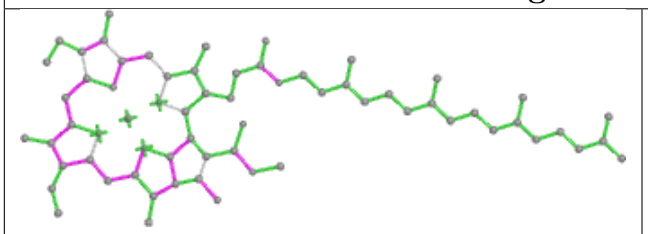


Torsions

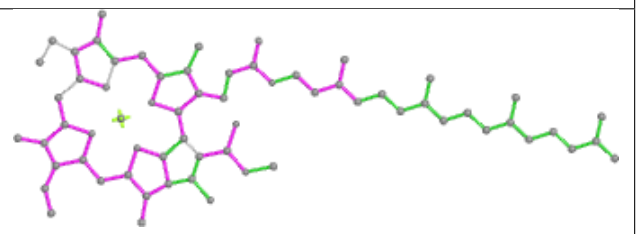


Rings

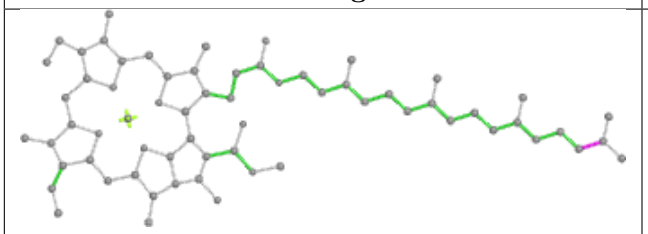
Ligand CLA d 401



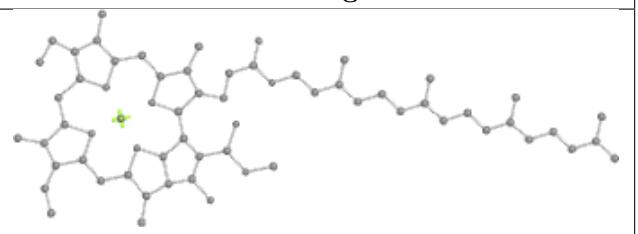
Bond lengths



Bond angles

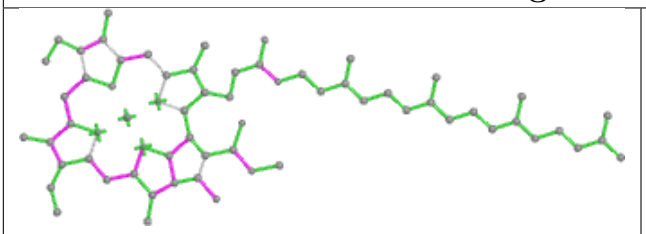


Torsions

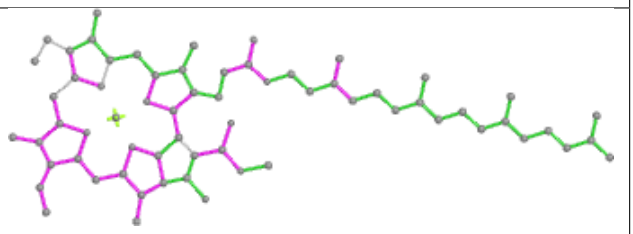


Rings

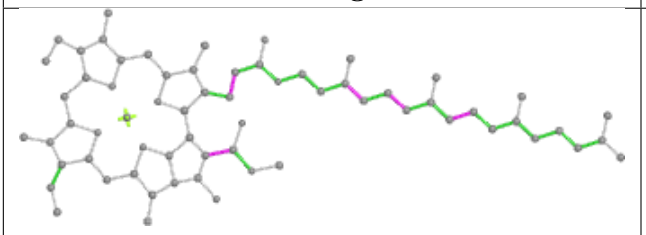
Ligand CLA c 508



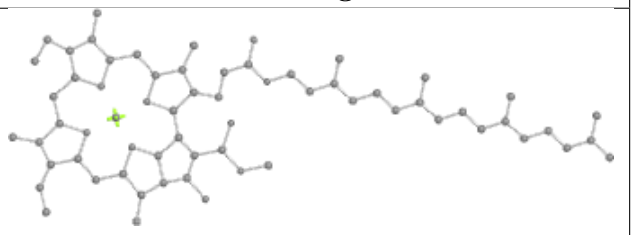
Bond lengths



Bond angles

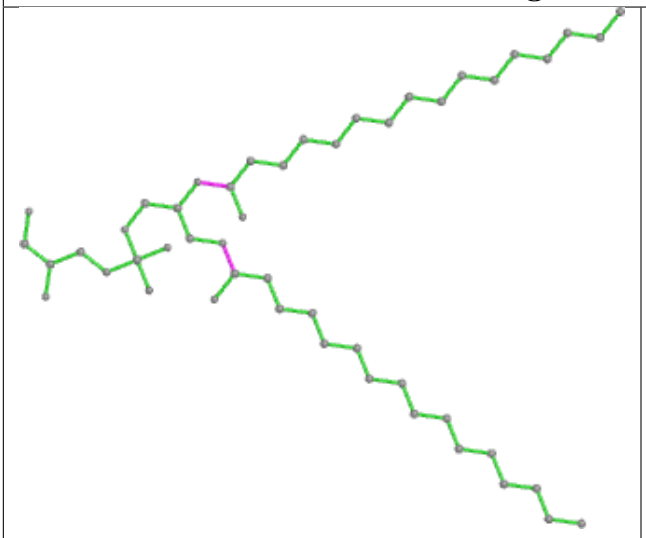


Torsions

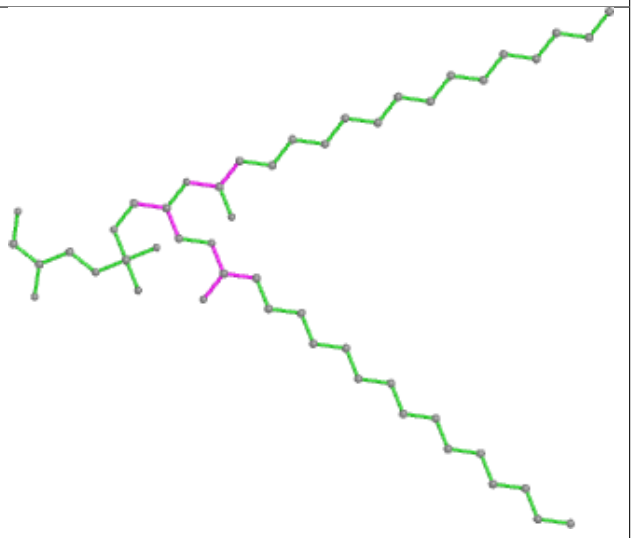


Rings

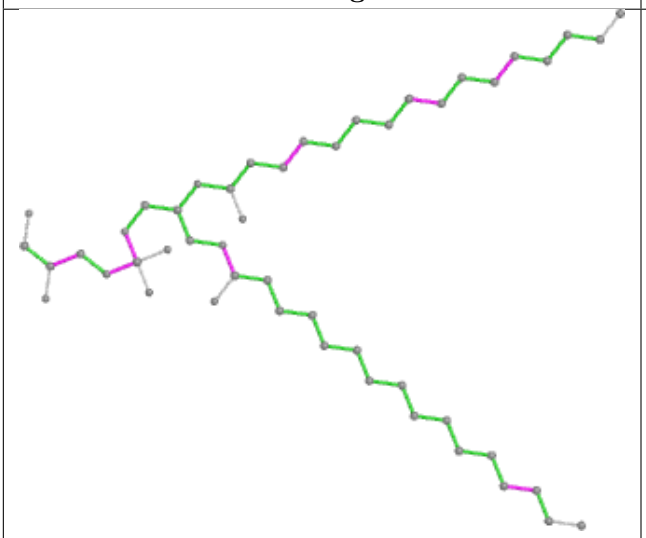
Ligand LHG d 405



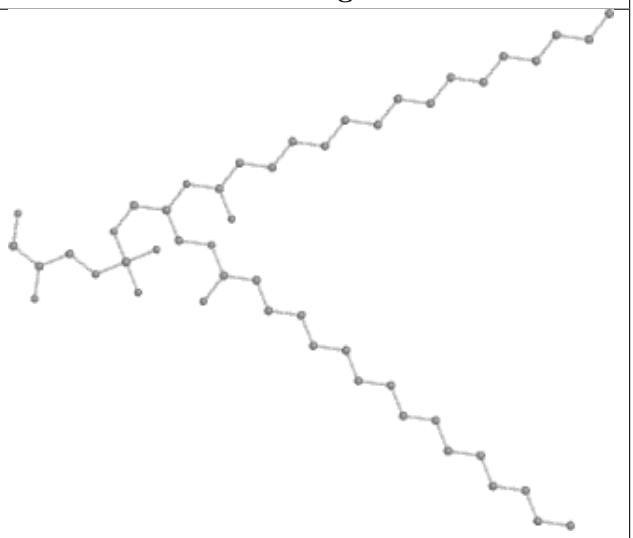
Bond lengths



Bond angles

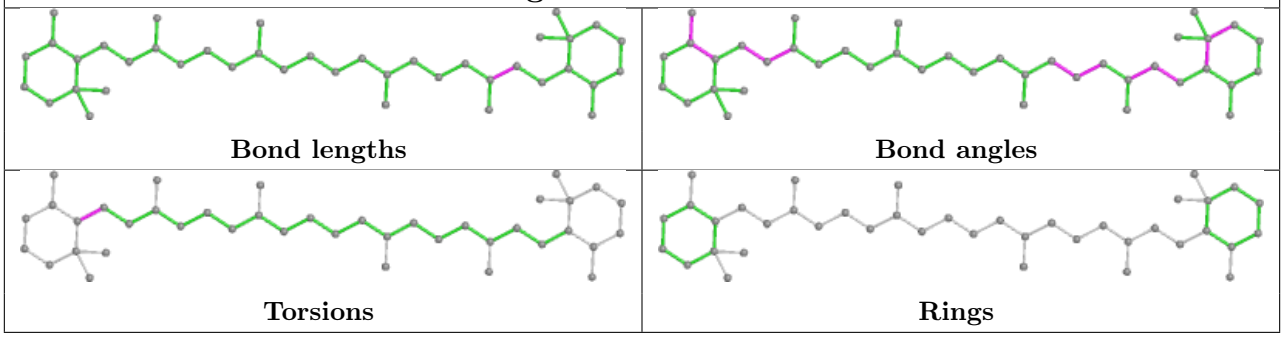


Torsions

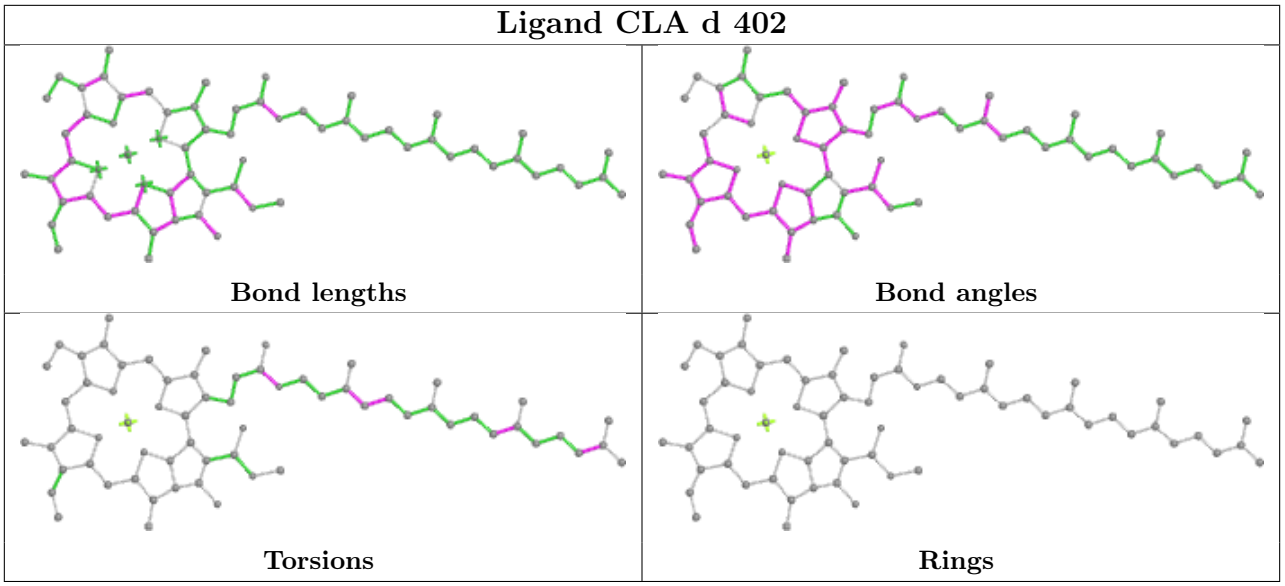


Rings

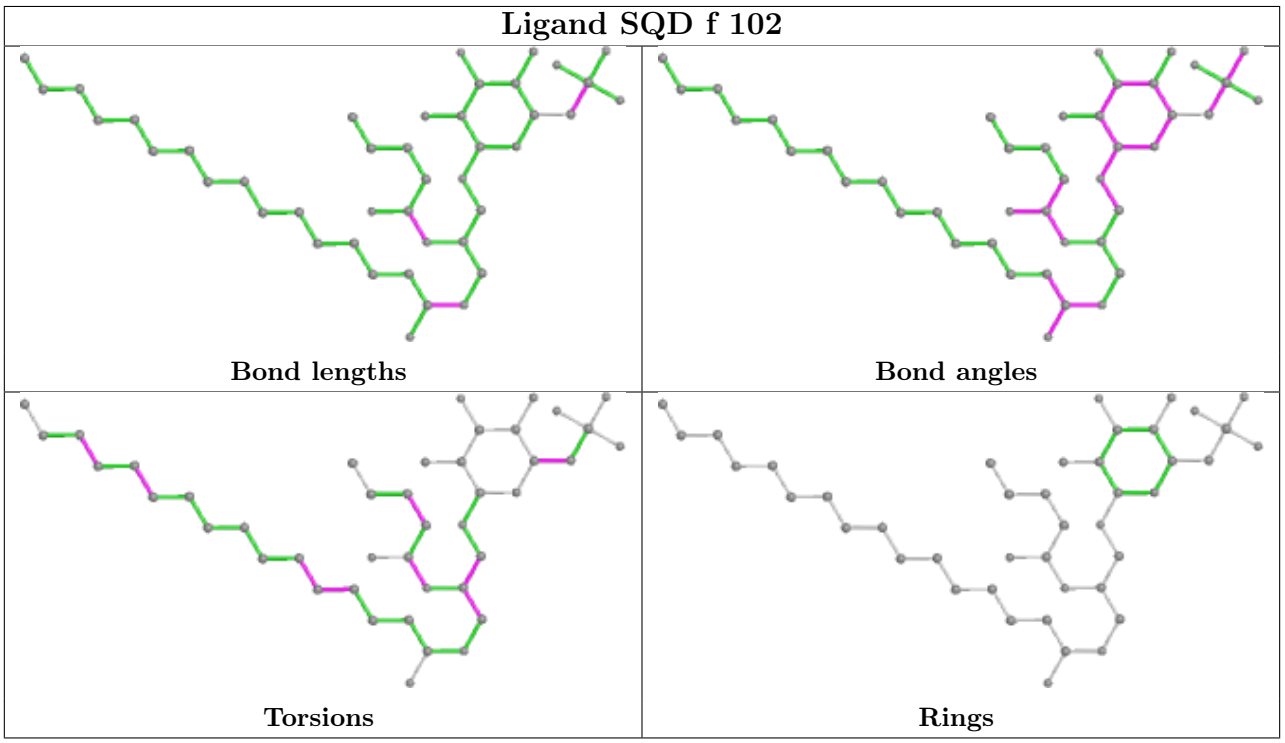
Ligand BCR b 617



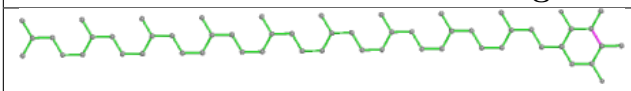
Ligand CLA d 402



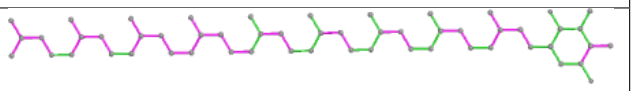
Ligand SQD f 102



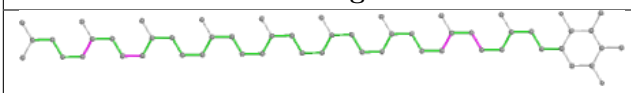
Ligand PL9 d 404



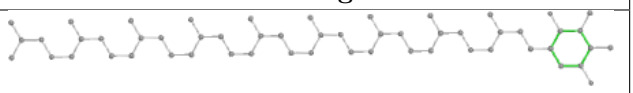
Bond lengths



Bond angles

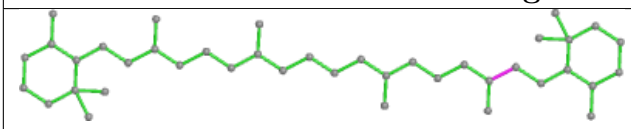


Torsions

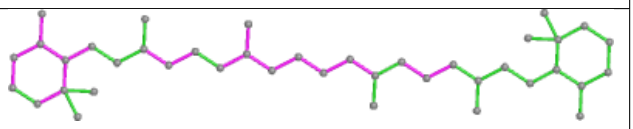


Rings

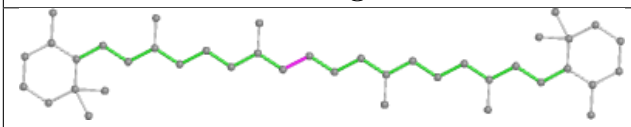
Ligand BCR T 102



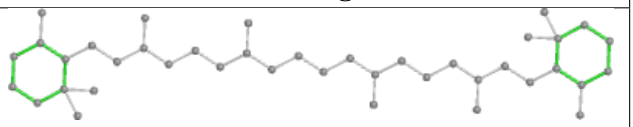
Bond lengths



Bond angles

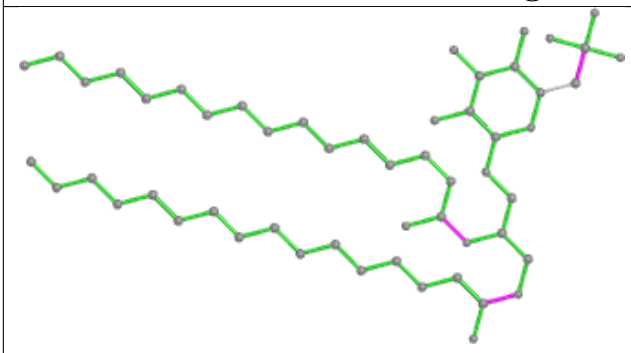


Torsions

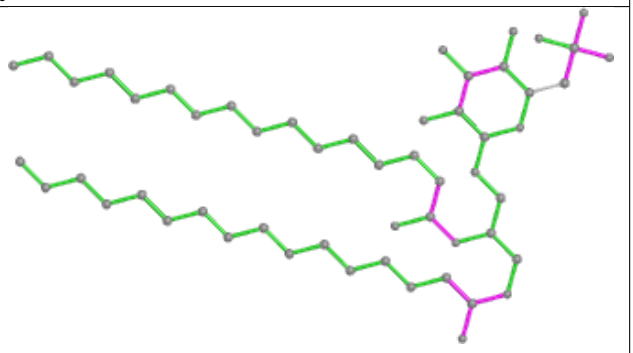


Rings

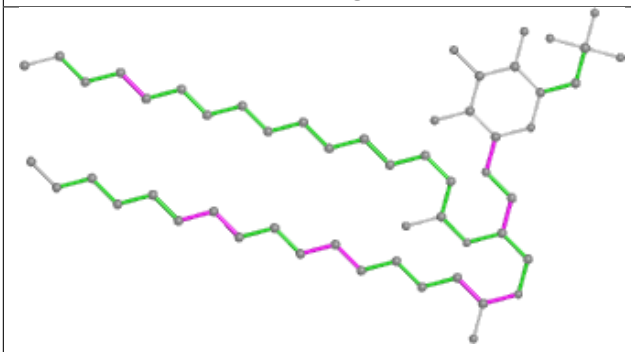
Ligand SQD A 412



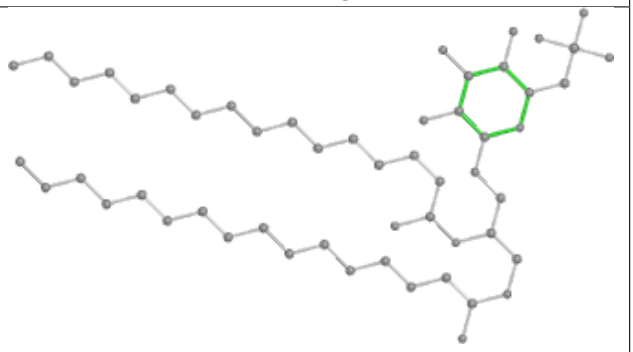
Bond lengths



Bond angles

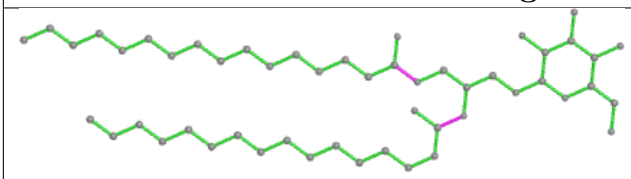


Torsions

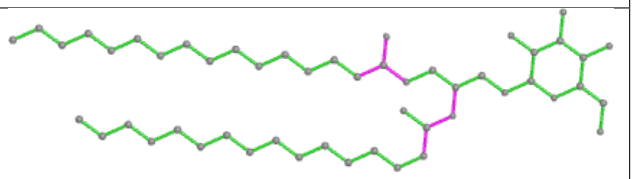


Rings

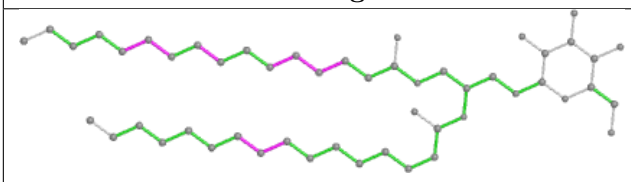
Ligand LMG C 518



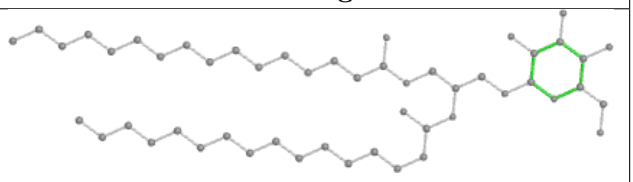
Bond lengths



Bond angles

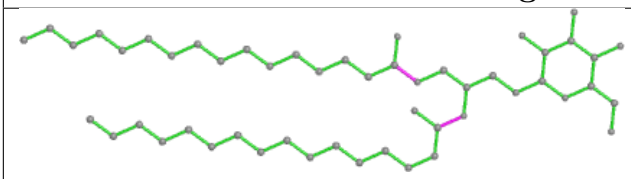


Torsions

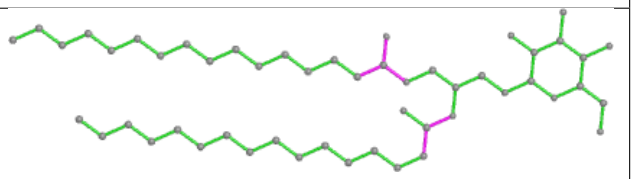


Rings

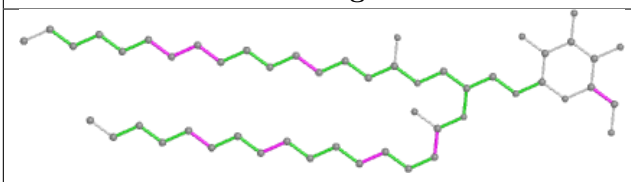
Ligand LMG D 411



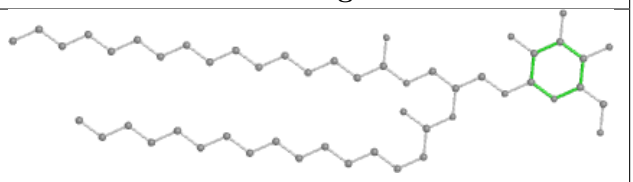
Bond lengths



Bond angles

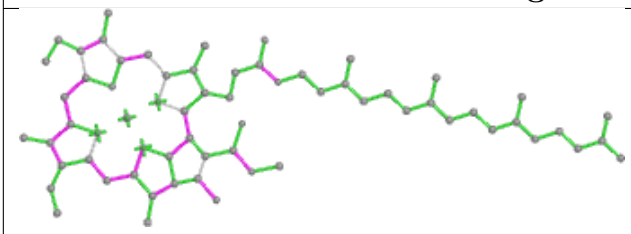


Torsions

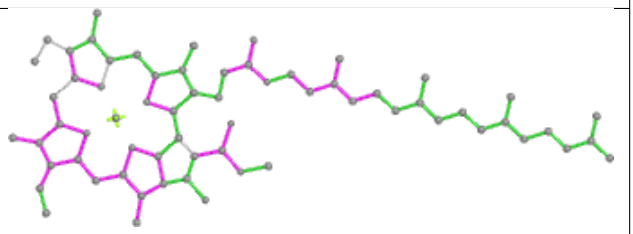


Rings

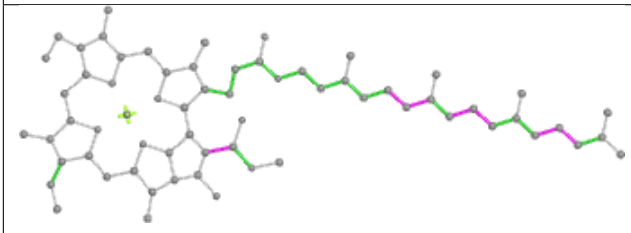
Ligand CLA b 604



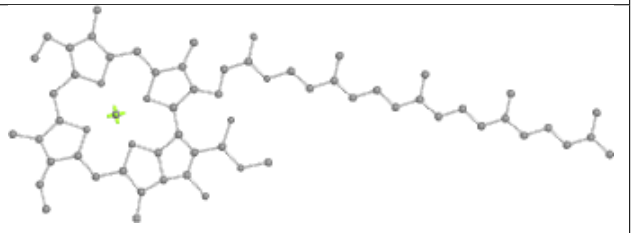
Bond lengths



Bond angles

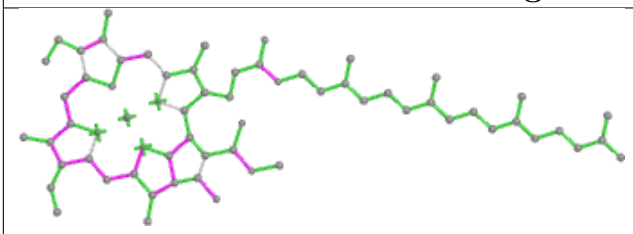


Torsions

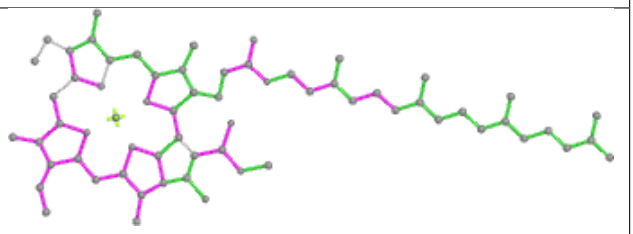


Rings

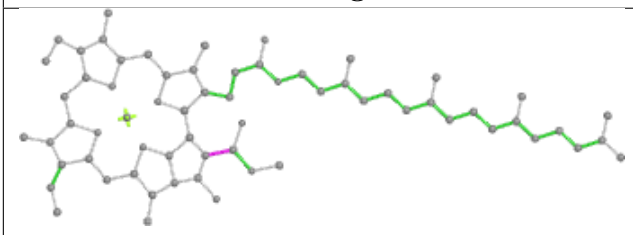
Ligand CLA B 609



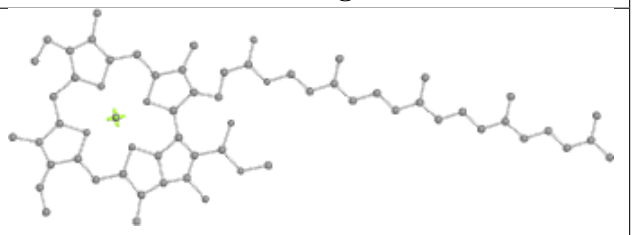
Bond lengths



Bond angles

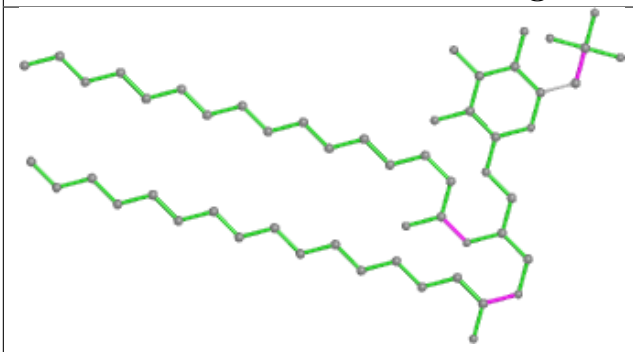


Torsions

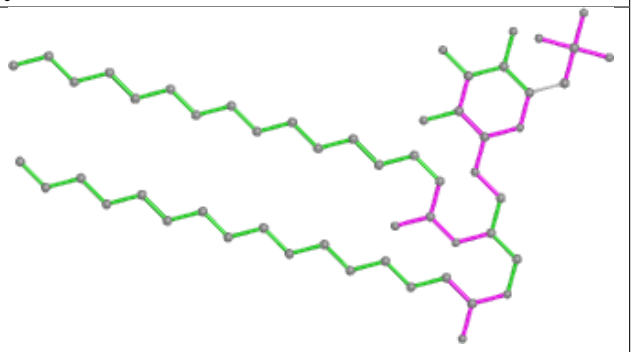


Rings

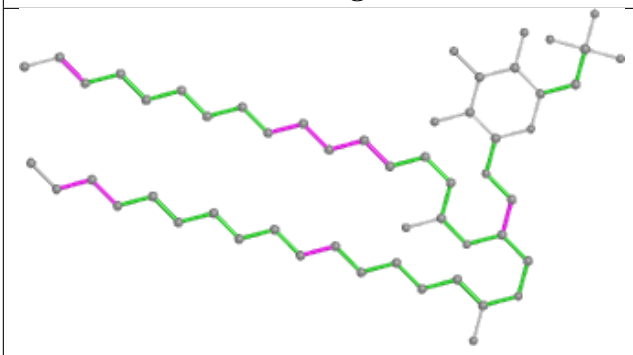
Ligand SQD a 411



Bond lengths



Bond angles



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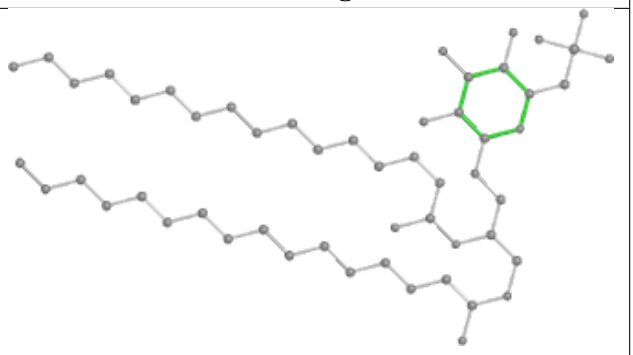
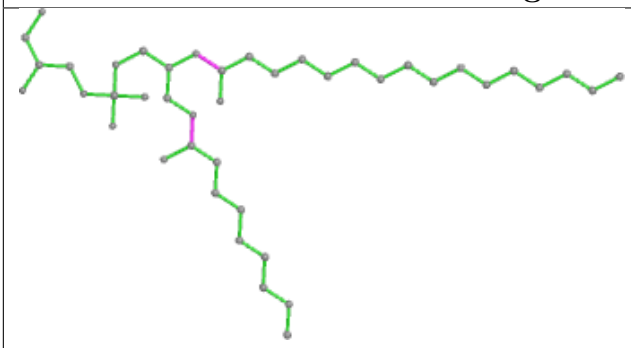
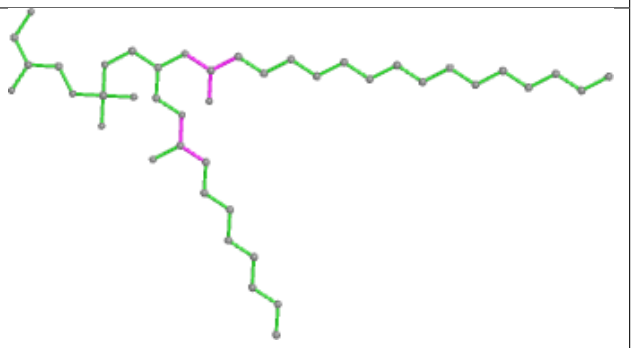


Rings

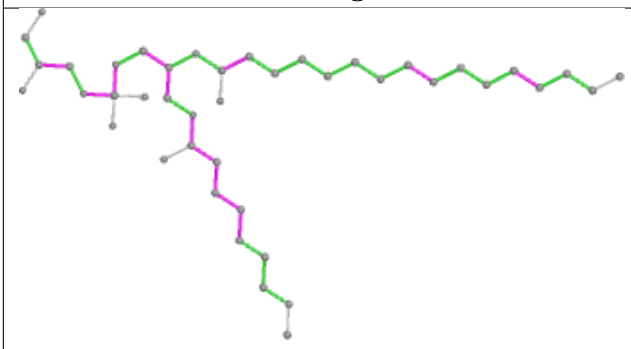
Ligand LHG E 101



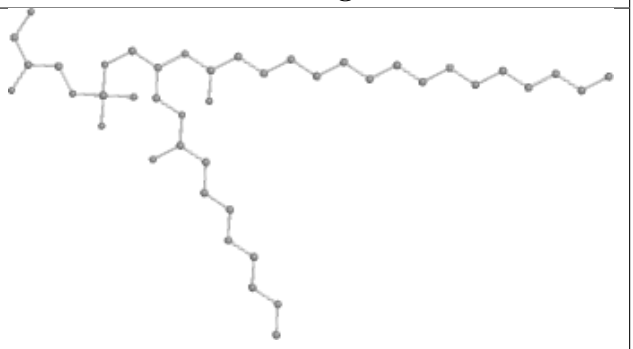
Bond lengths



Bond angles

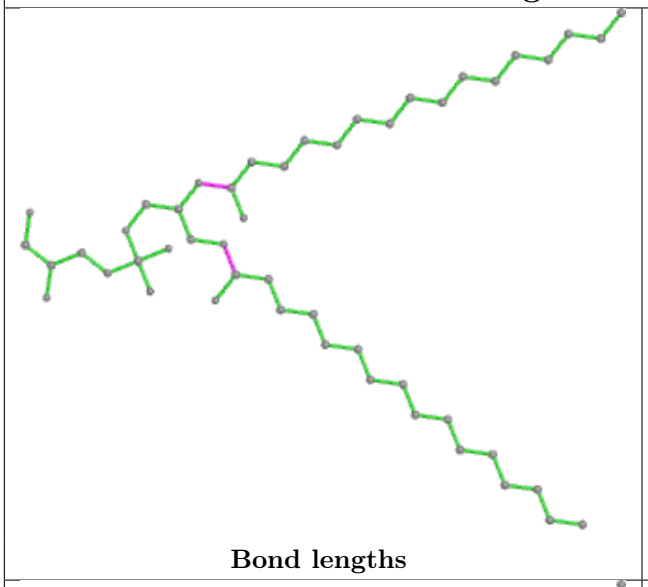


Torsions

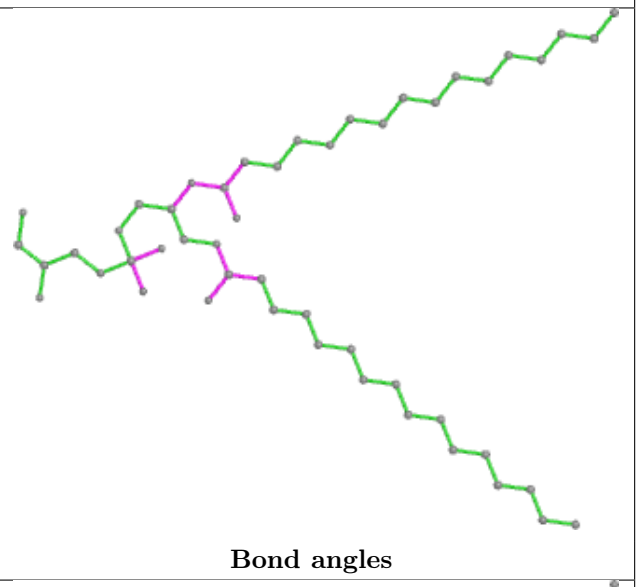


Rings

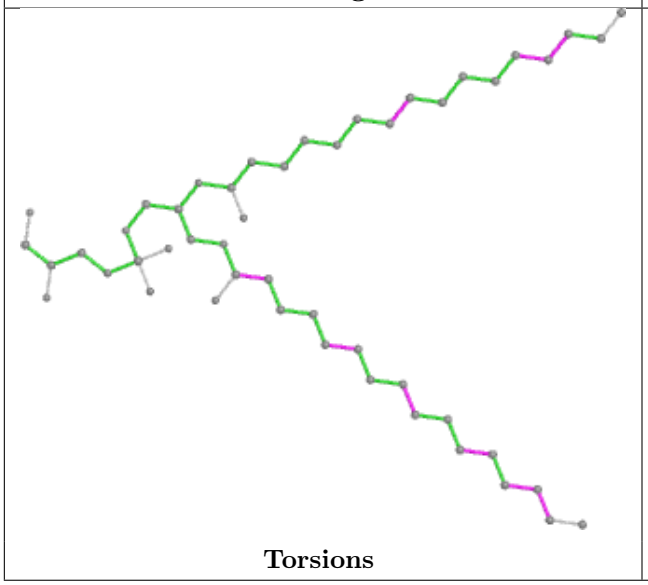
Ligand LHG A 420



Bond lengths



Bond angles



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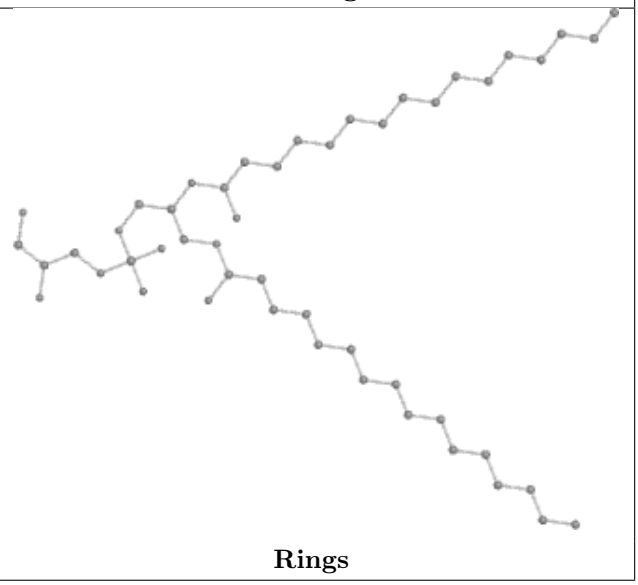
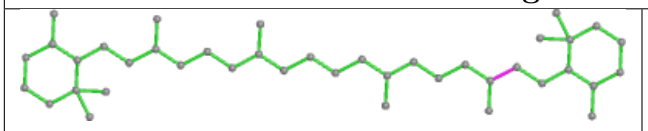
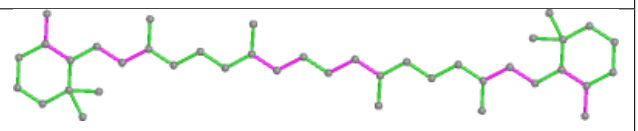


Rings

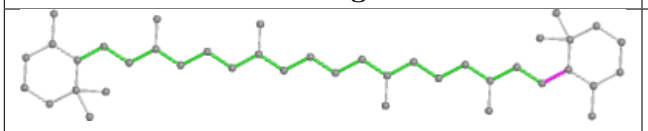
Ligand BCR K 101



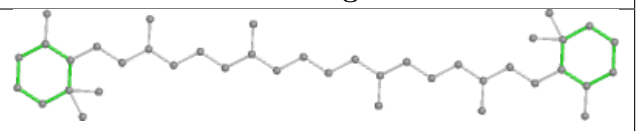
Bond lengths



Bond angles

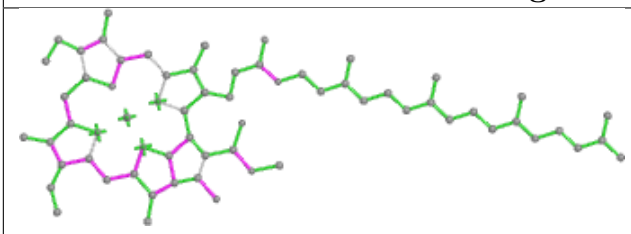


Torsions

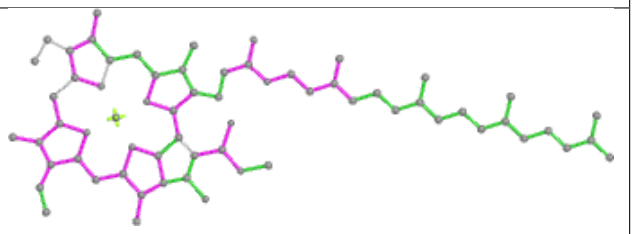


Rings

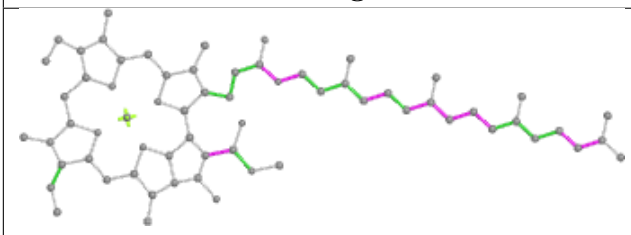
Ligand CLA c 510



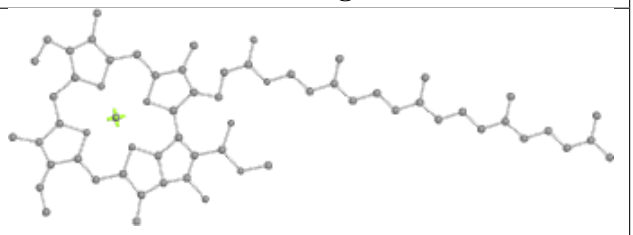
Bond lengths



Bond angles

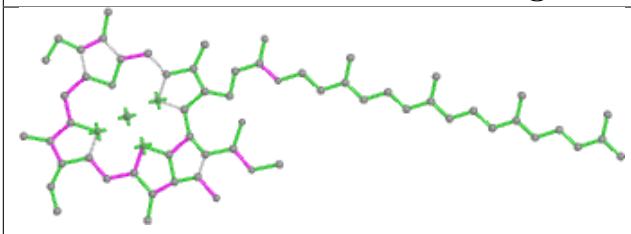


Torsions

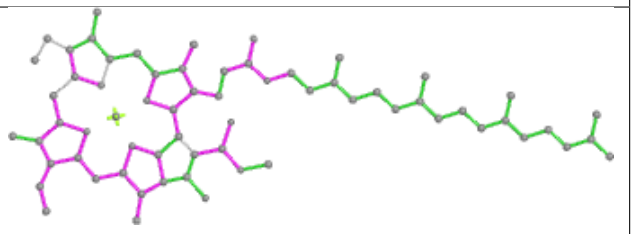


Rings

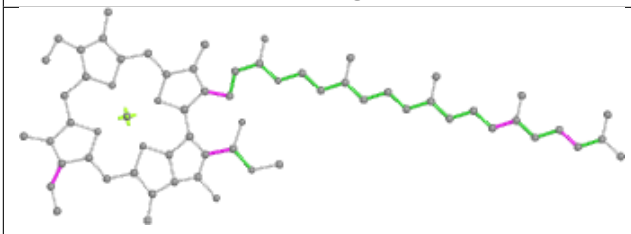
Ligand CLA a 406



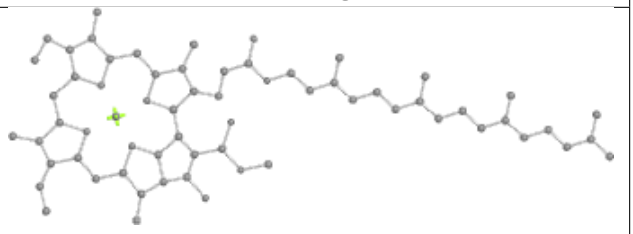
Bond lengths



Bond angles

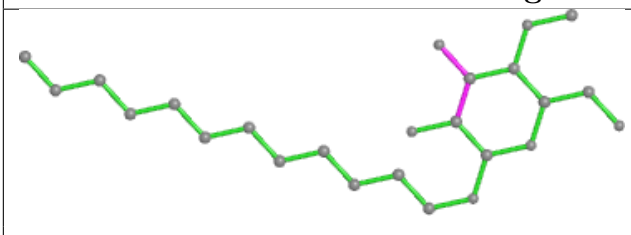


Torsions

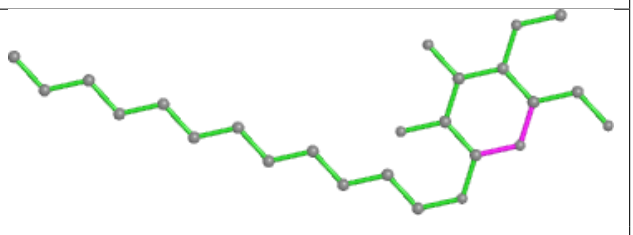


Rings

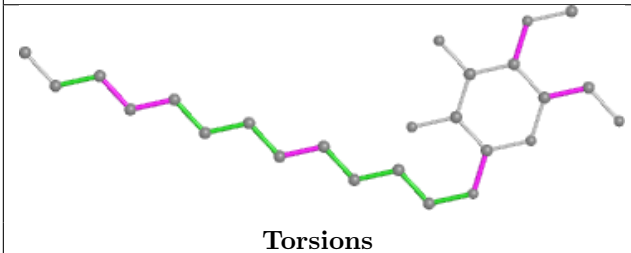
Ligand LMT b 621



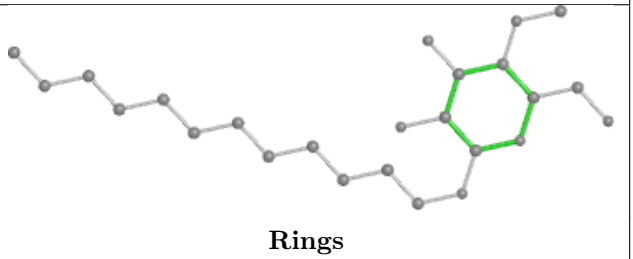
Bond lengths



Bond angles

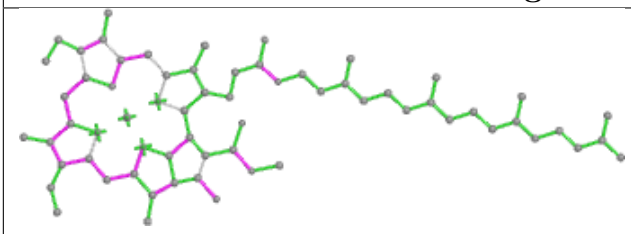


Torsions

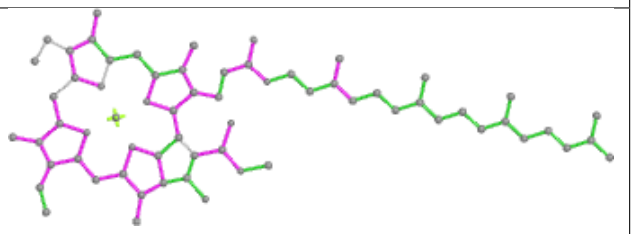


Rings

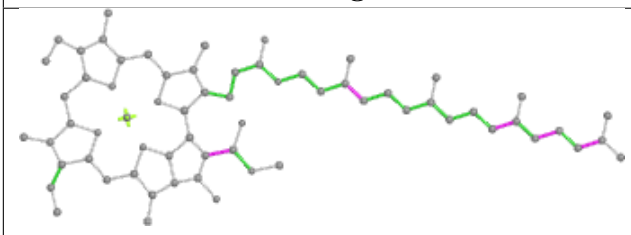
Ligand CLA B 603



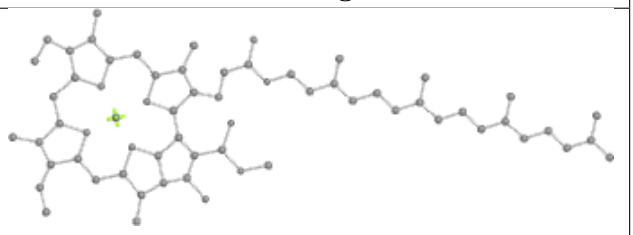
Bond lengths



Bond angles

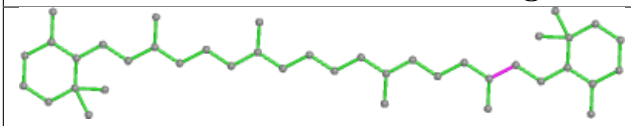


Torsions

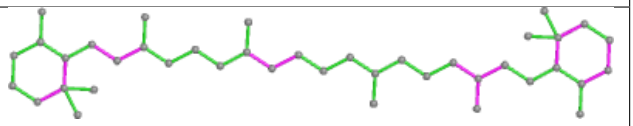


Rings

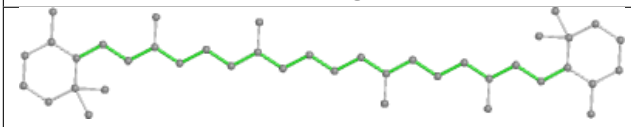
Ligand BCR B 618



Bond lengths



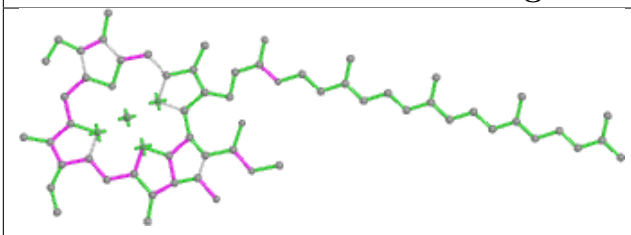
Bond angles



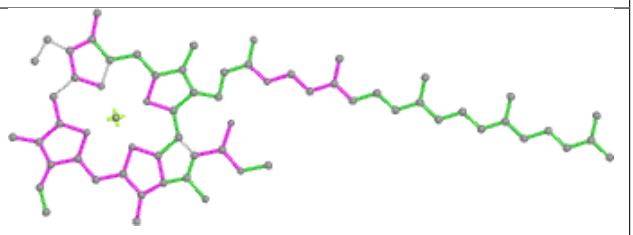
Torsions

Rings

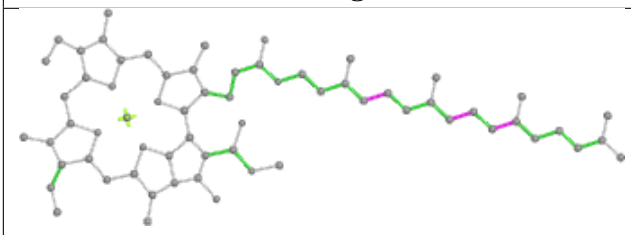
Ligand CLA C 511



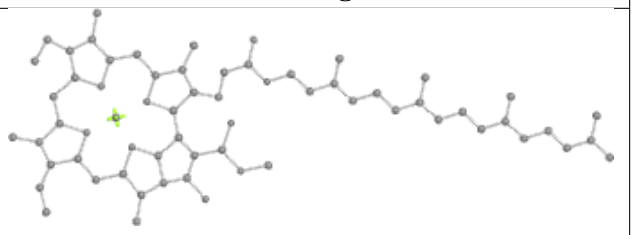
Bond lengths



Bond angles

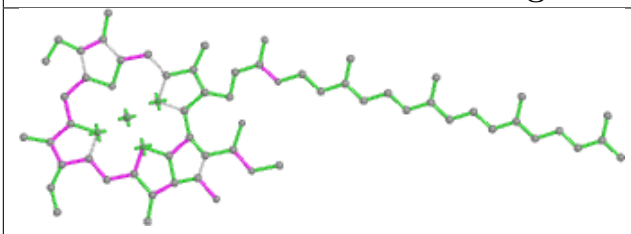


Torsions

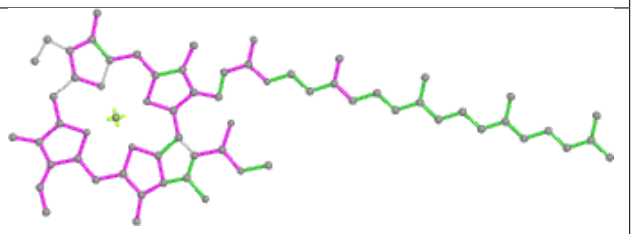


Rings

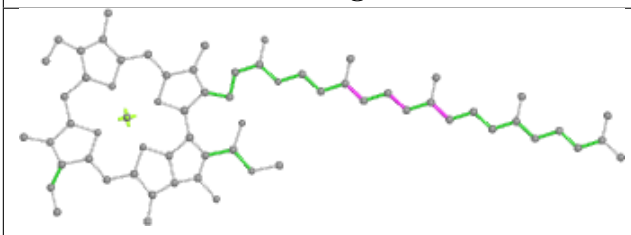
Ligand CLA b 603



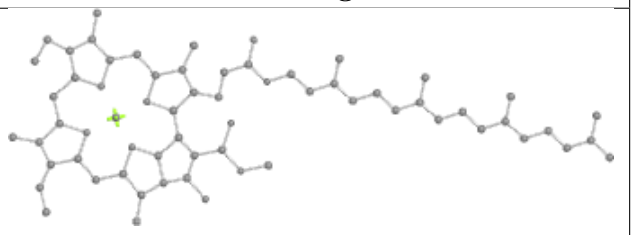
Bond lengths



Bond angles

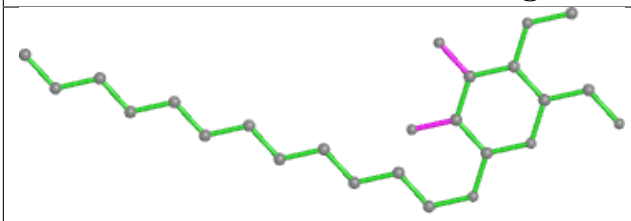


Torsions

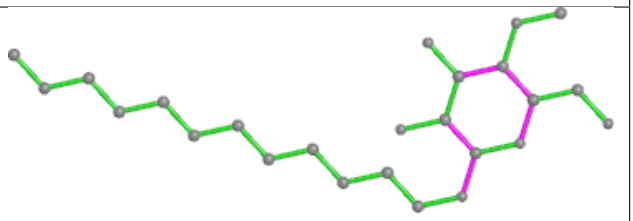


Rings

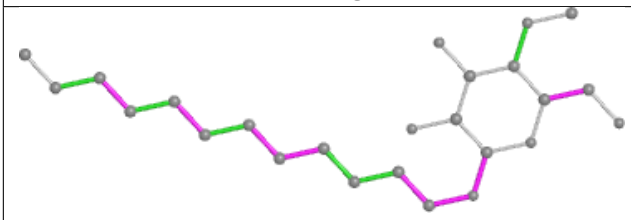
Ligand LMT B 631



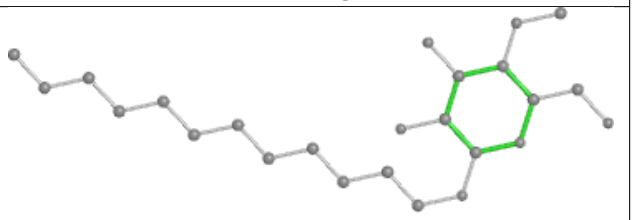
Bond lengths



Bond angles

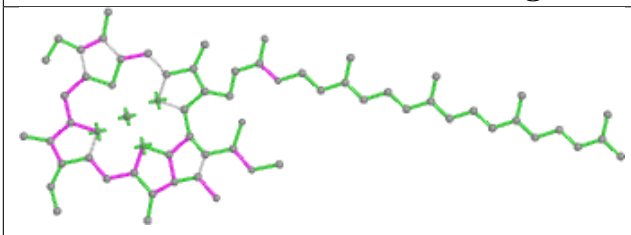


Torsions

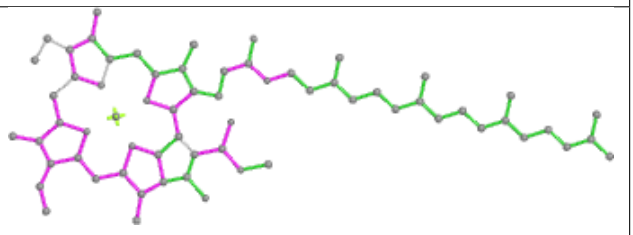


Rings

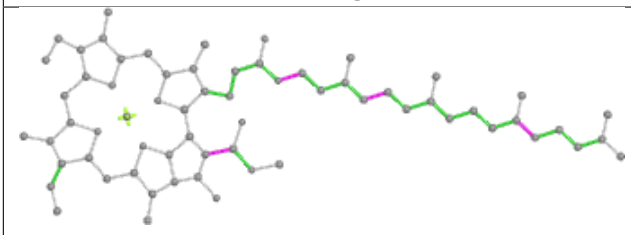
Ligand CLA B 616



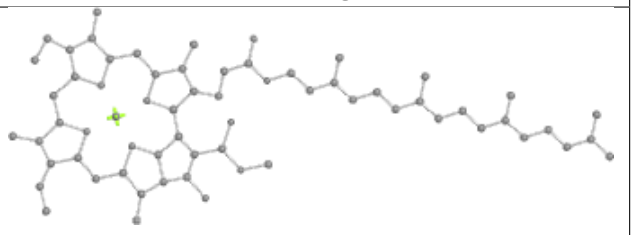
Bond lengths



Bond angles

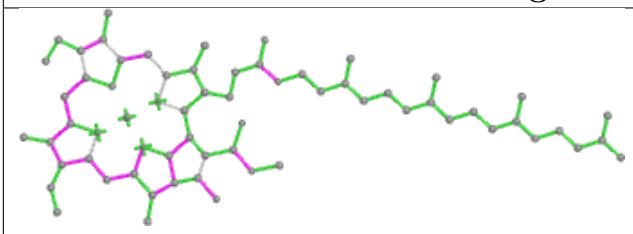


Torsions

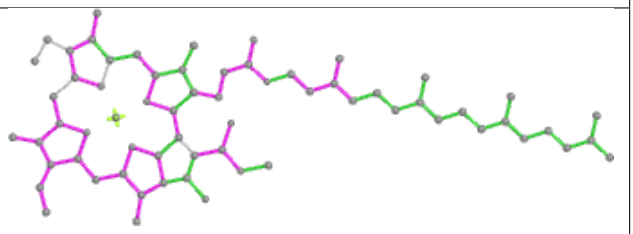


Rings

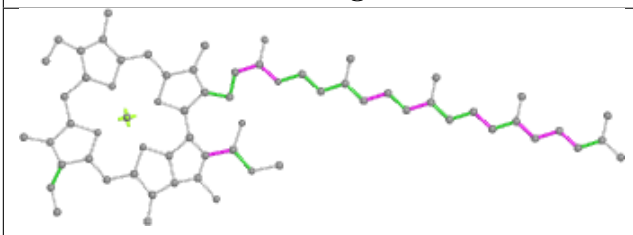
Ligand CLA c 513



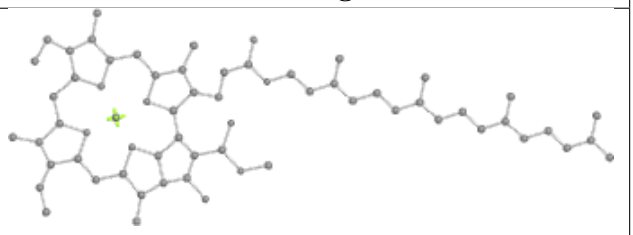
Bond lengths



Bond angles

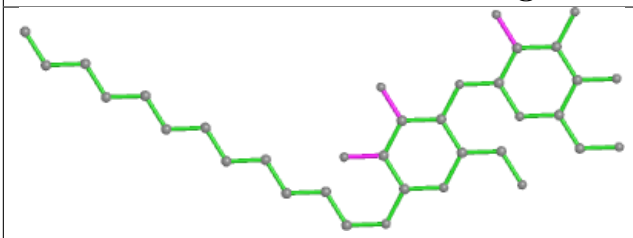


Torsions

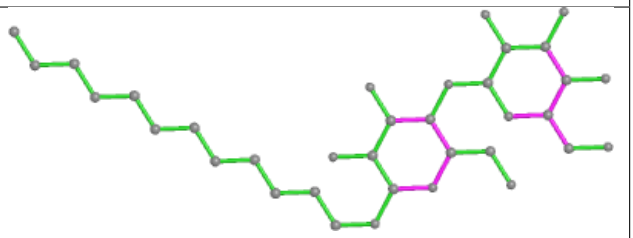


Rings

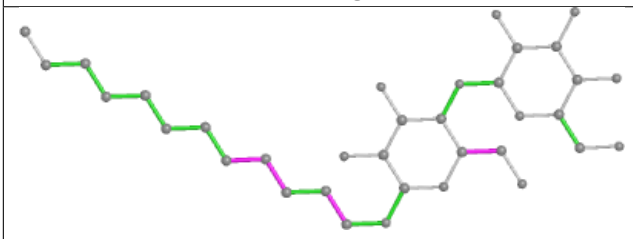
Ligand LMT M 101



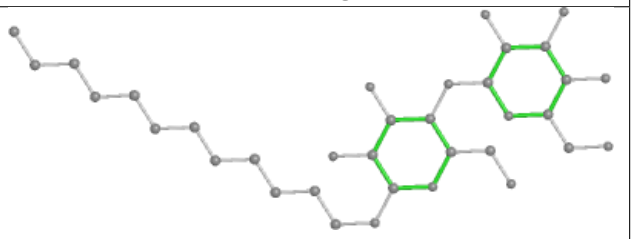
Bond lengths



Bond angles

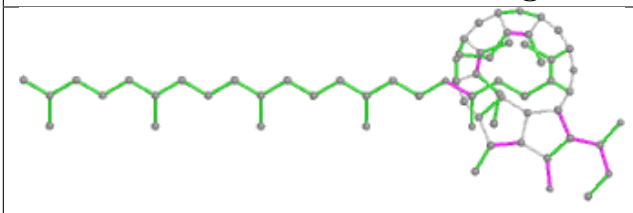


Torsions



Rings

Ligand PHO A 407



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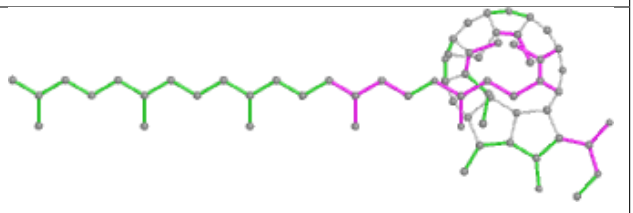
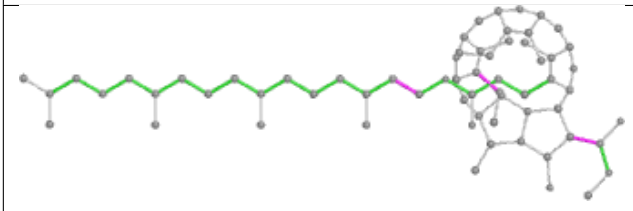


Bond angles



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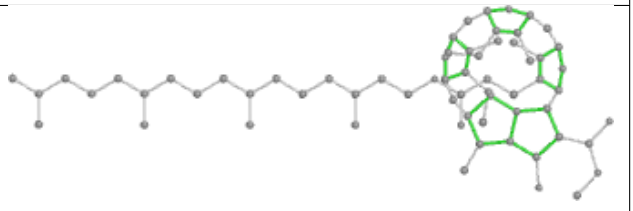
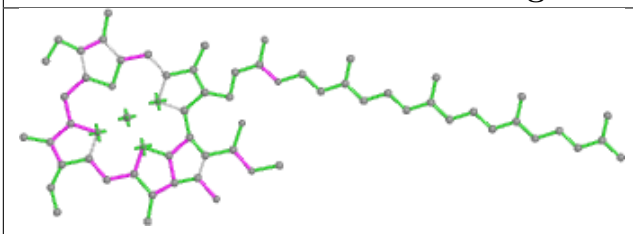


Rings

Ligand CLA b 609



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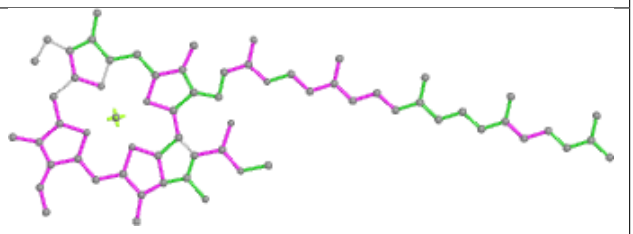
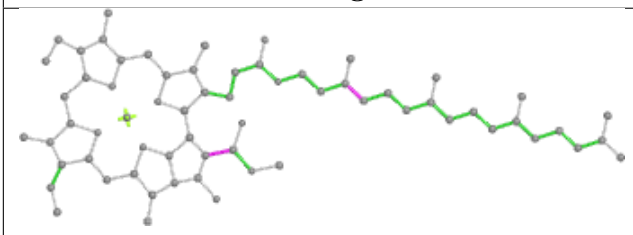
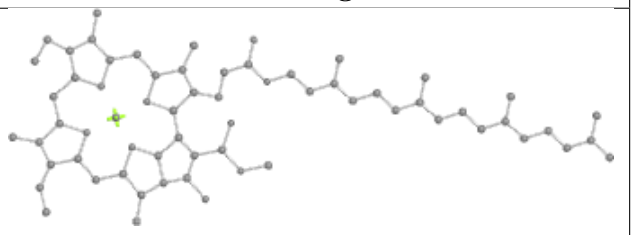


Bond angles

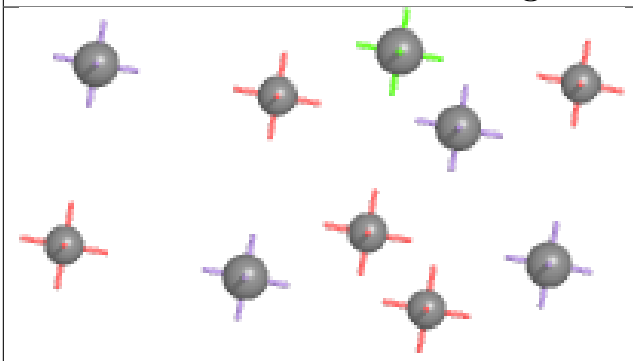


Torsions

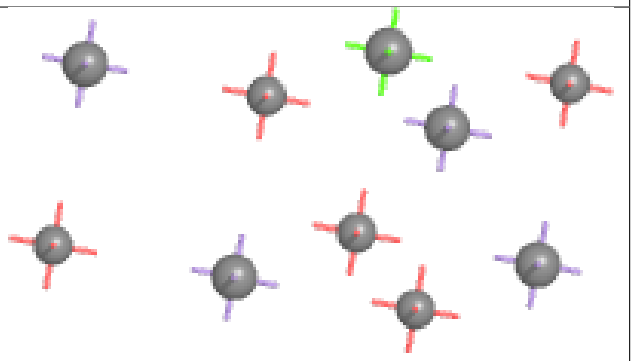


Rings

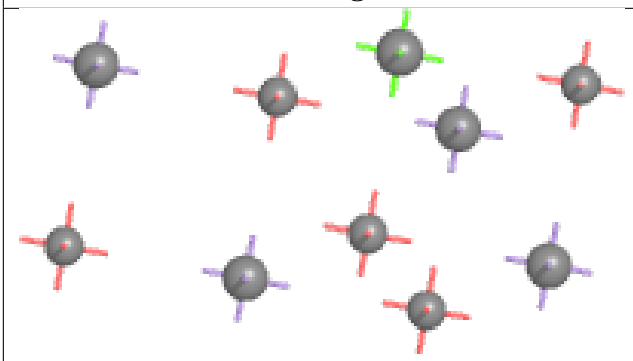
Ligand OEX A 413



Bond lengths



Bond angles



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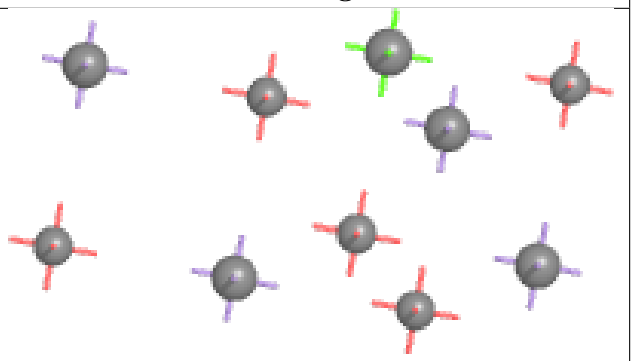
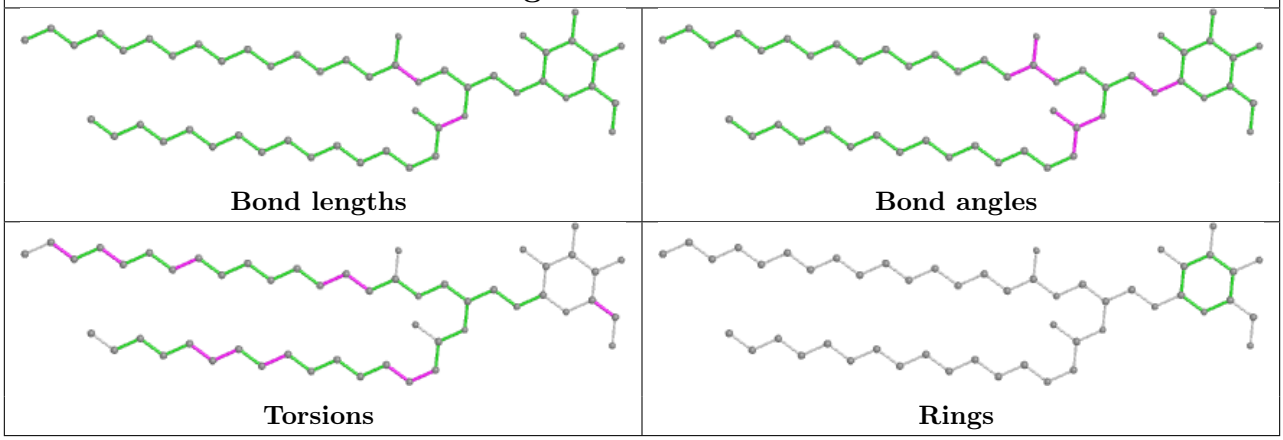
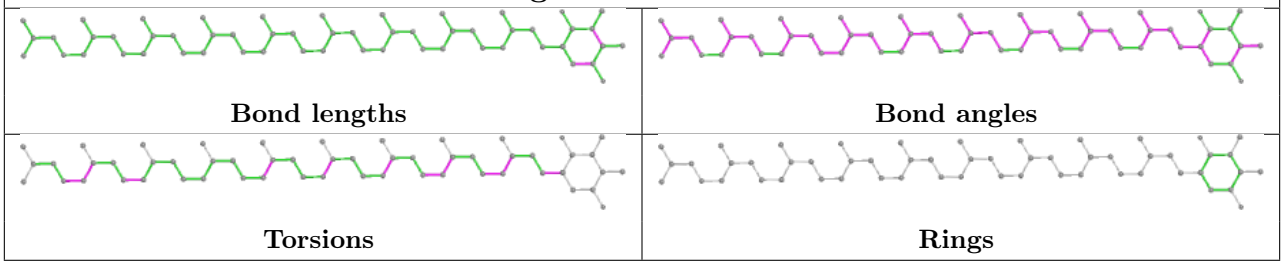


Rings

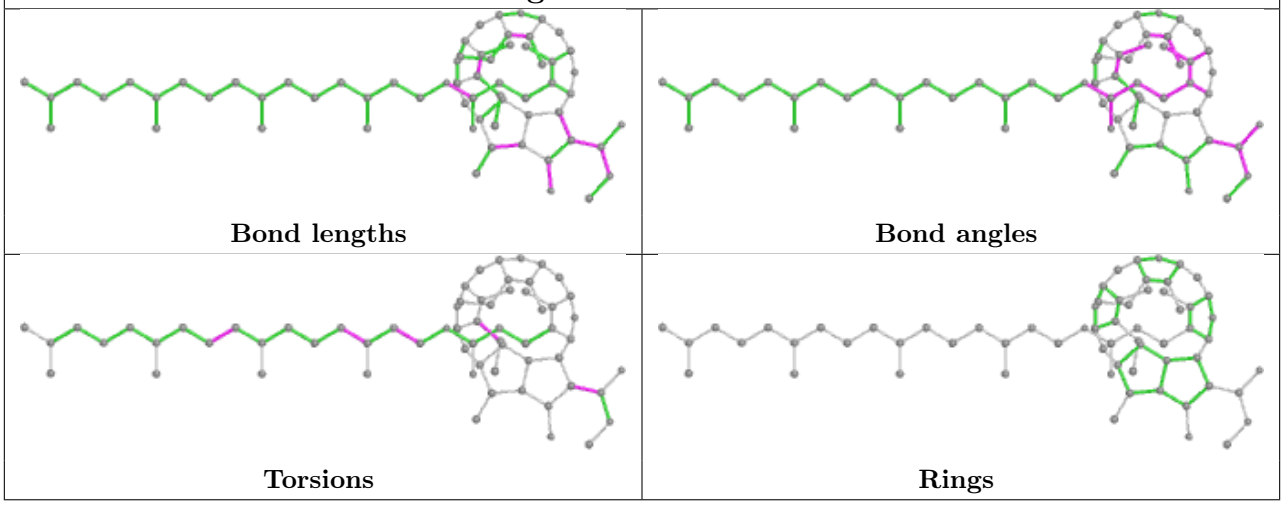
Ligand LMG d 410



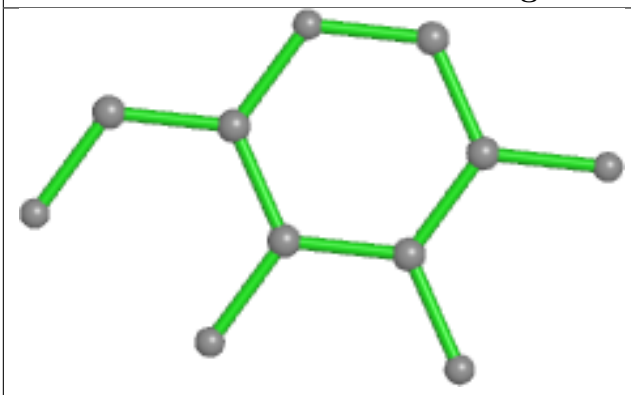
Ligand PL9 A 414



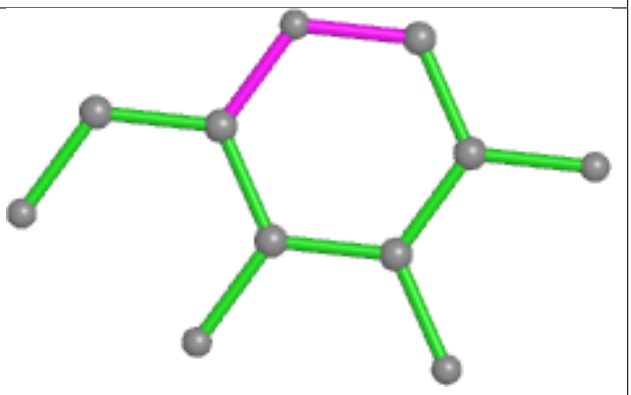
Ligand PHO a 408



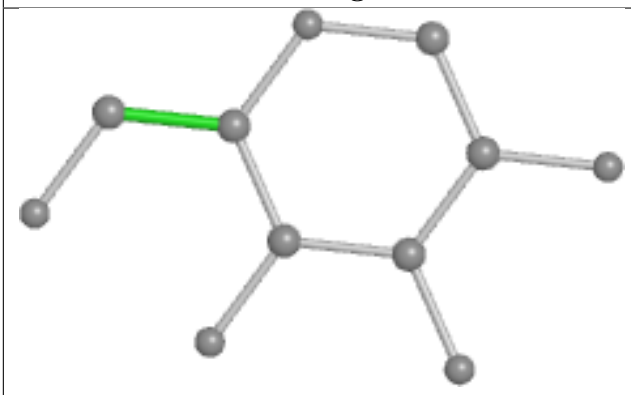
Ligand HTG V 202



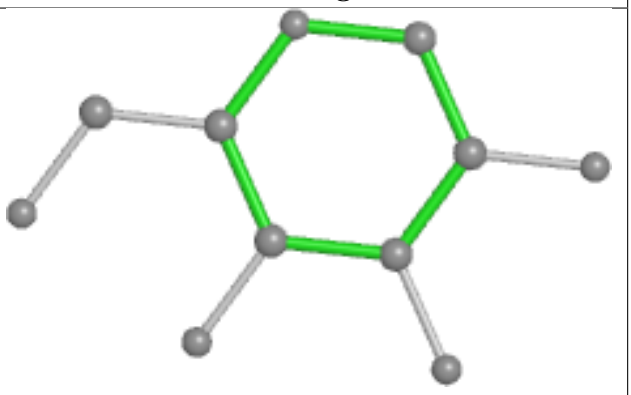
Bond lengths



Bond angles

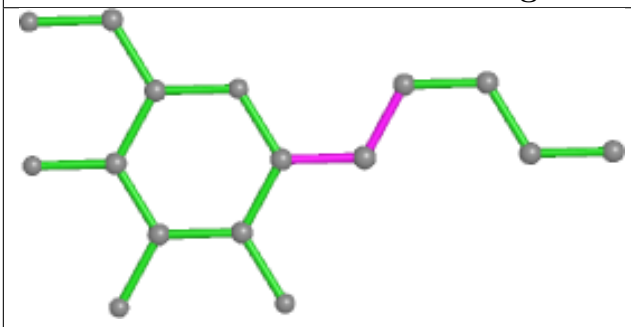


Torsions

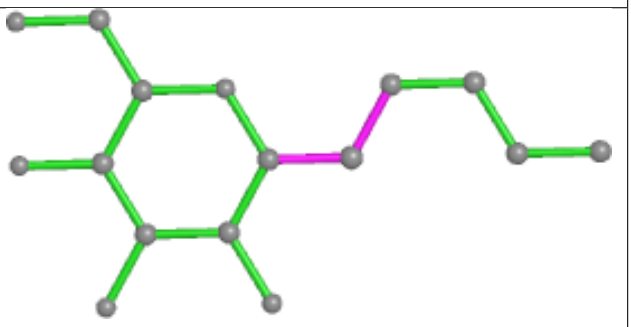


Rings

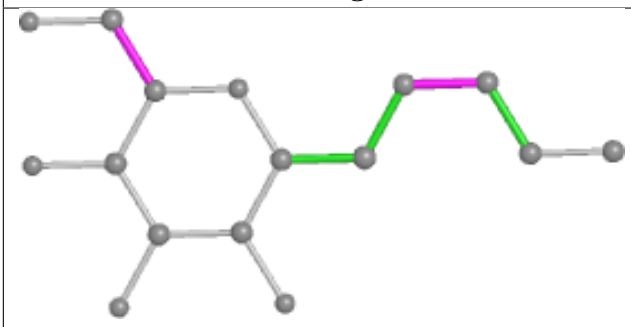
Ligand HTG D 410



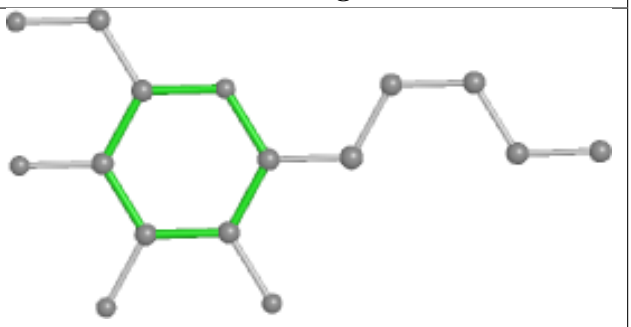
Bond lengths



Bond angles

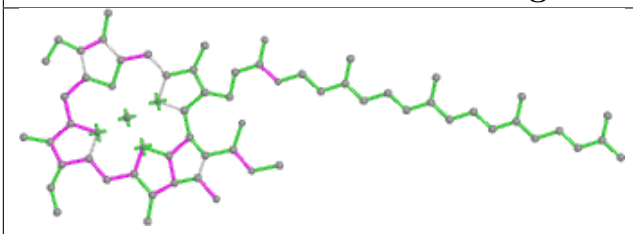


Torsions

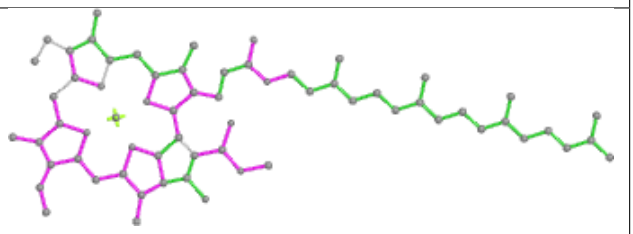


Rings

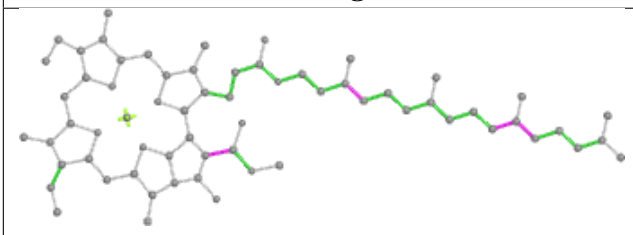
Ligand CLA c 505



Bond lengths



Bond angles



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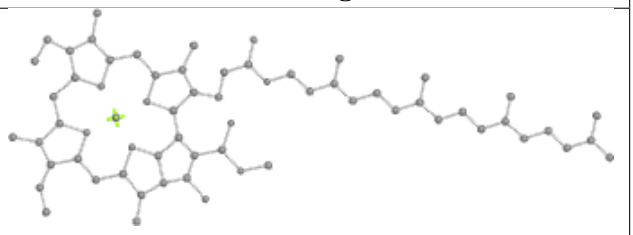
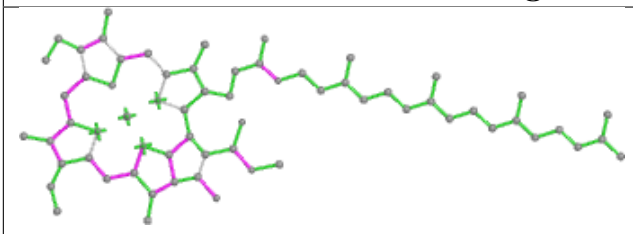
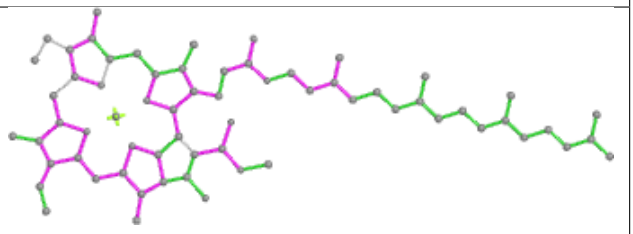


Rings

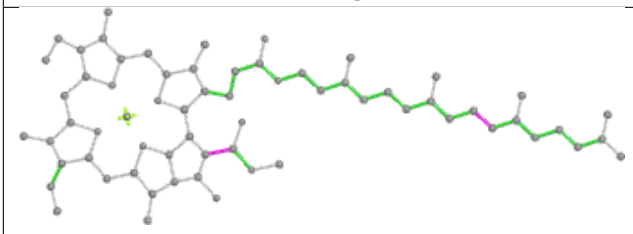
Ligand CLA C 508



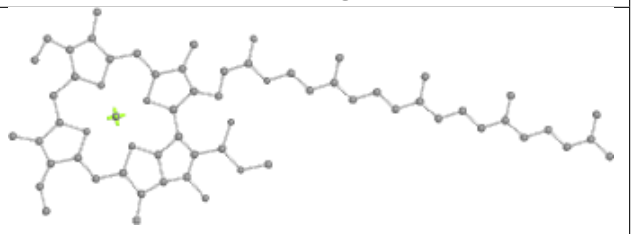
Bond lengths



Bond angles

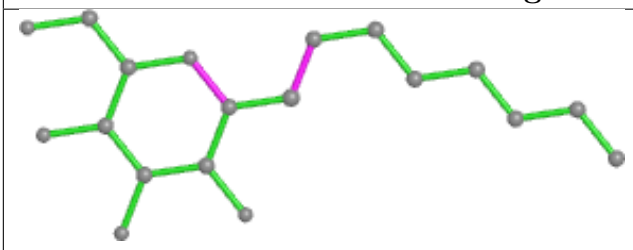


Torsions

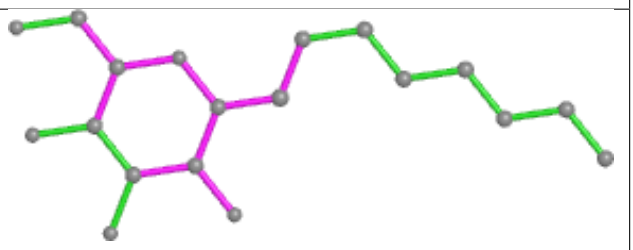


Rings

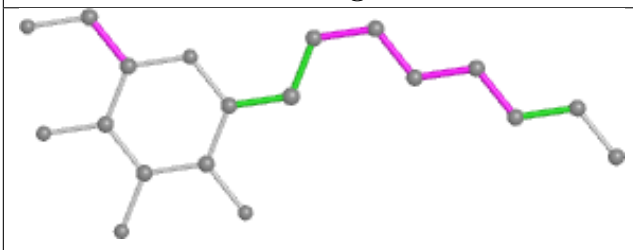
Ligand HTG b 622



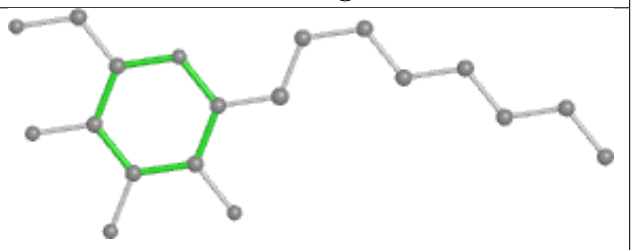
Bond lengths



Bond angles

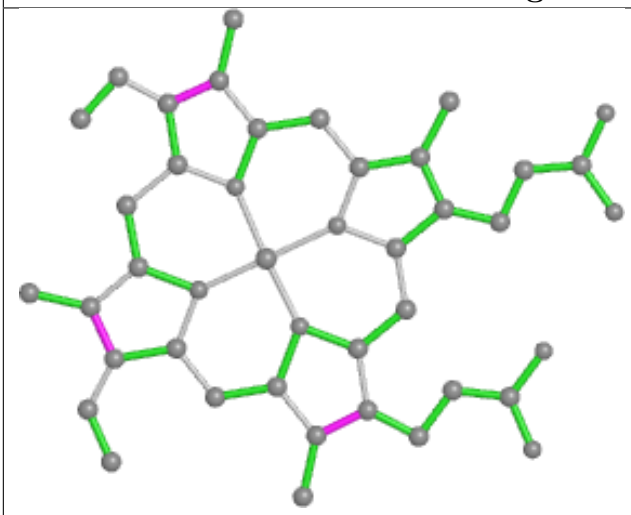


Torsions

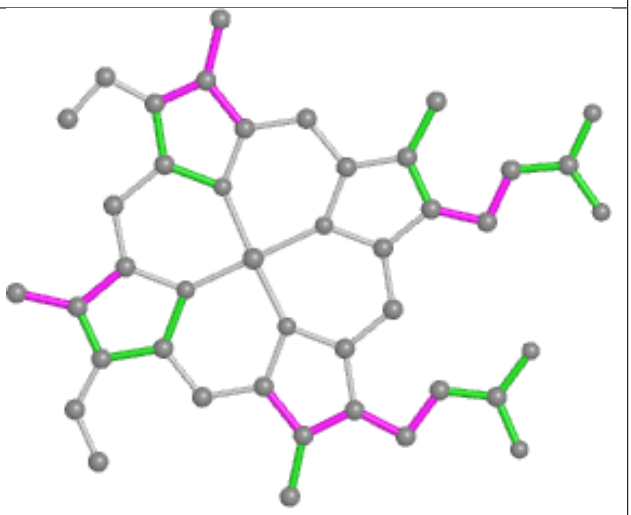


Rings

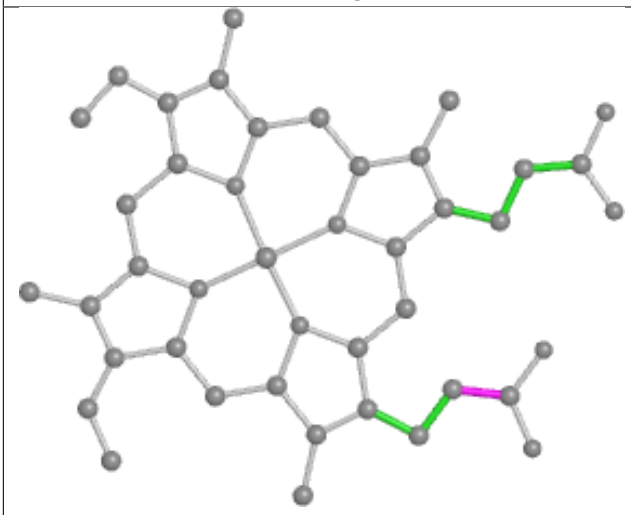
Ligand HEC v 201



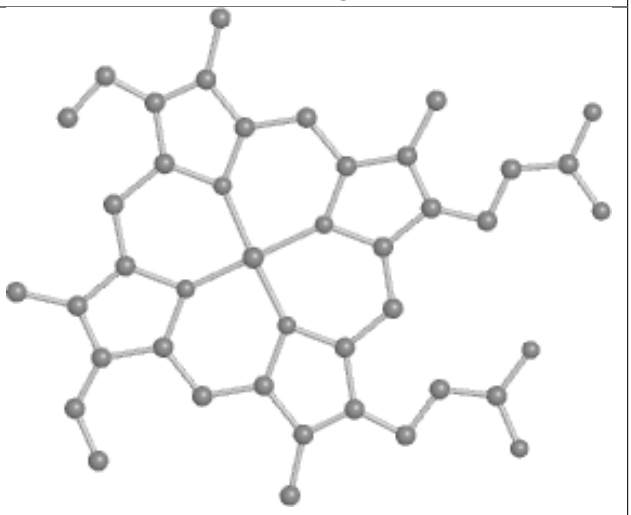
Bond lengths



Bond angles

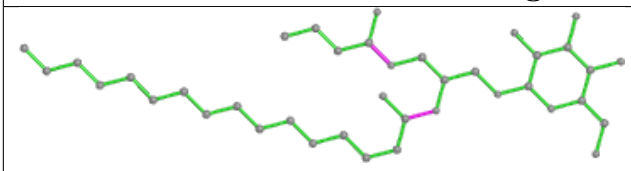


Torsions

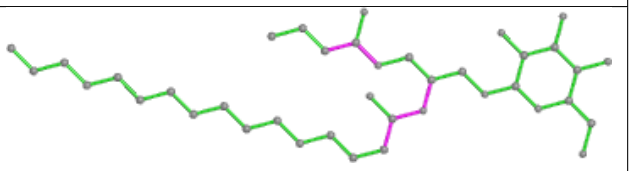


Rings

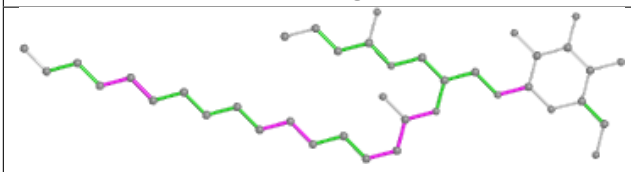
Ligand LMG z 101



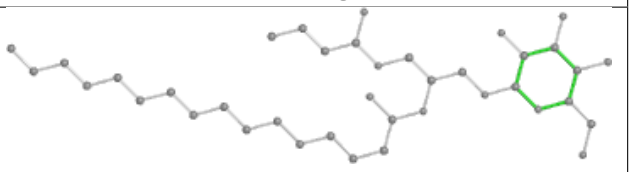
Bond lengths



Bond angles

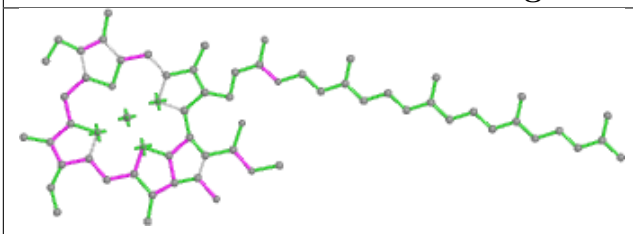


Torsions

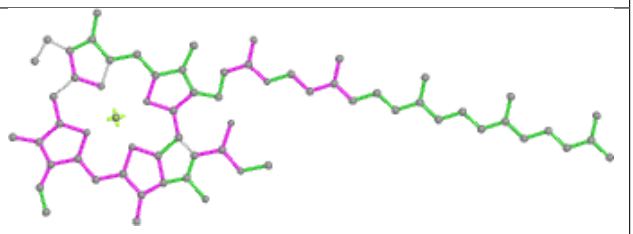


Rings

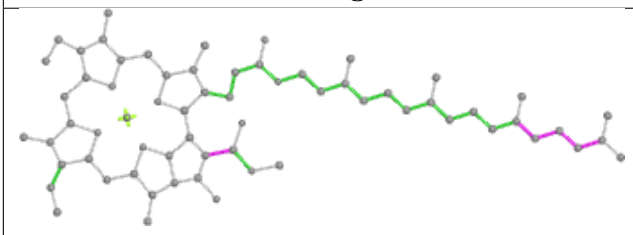
Ligand CLA C 502



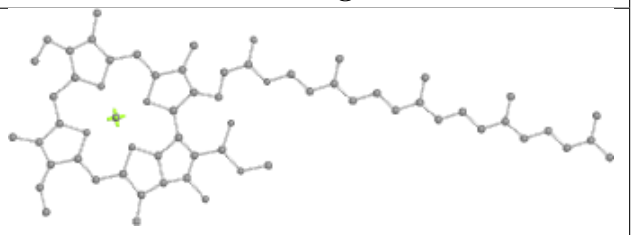
Bond lengths



Bond angles

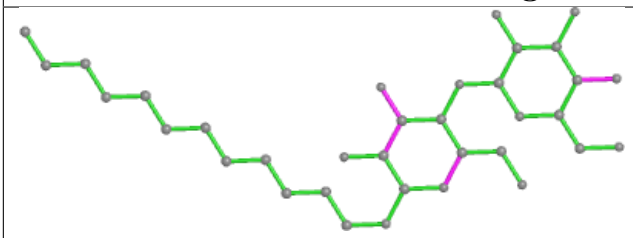


Torsions

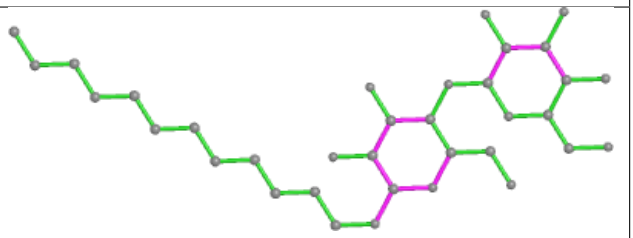


Rings

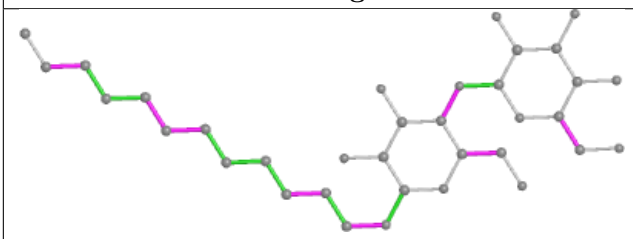
Ligand LMT B 628



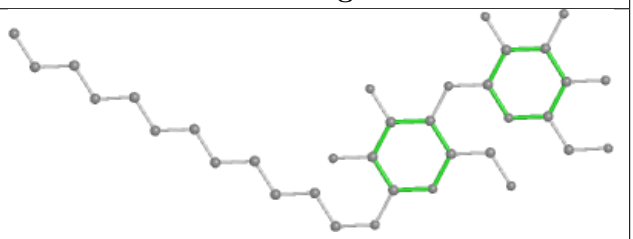
Bond lengths



Bond angles

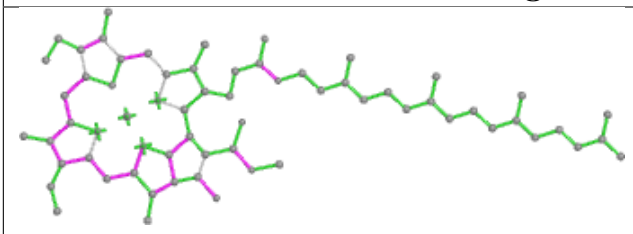


Torsions

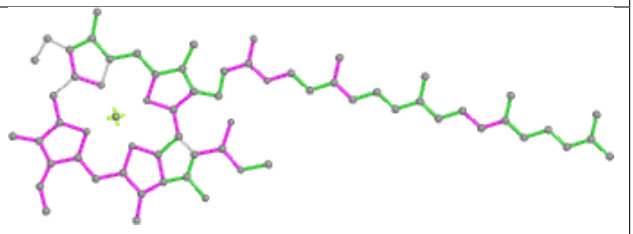


Rings

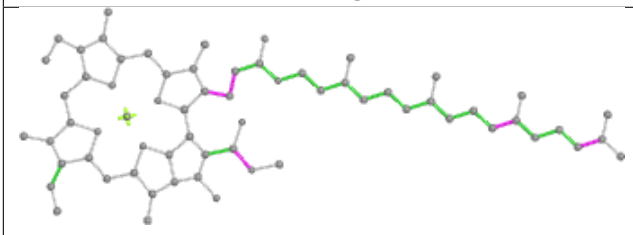
Ligand CLA C 501



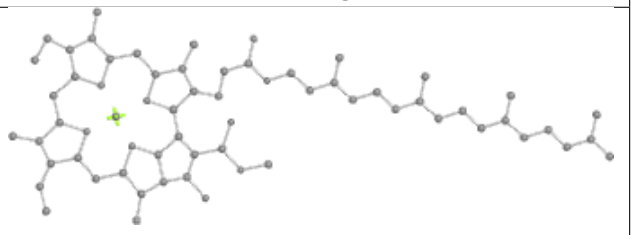
Bond lengths



Bond angles

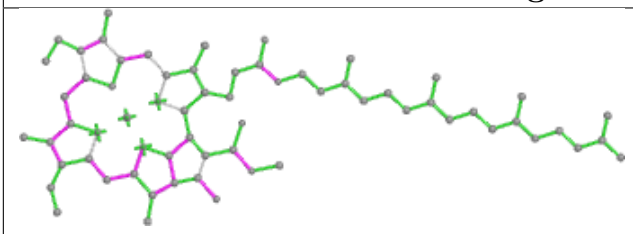


Torsions

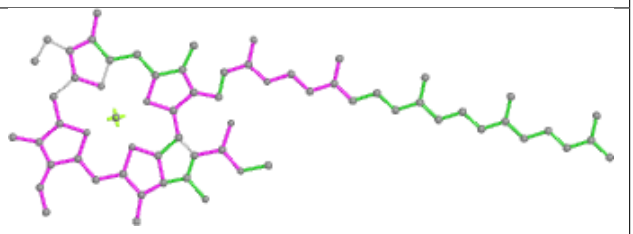


Rings

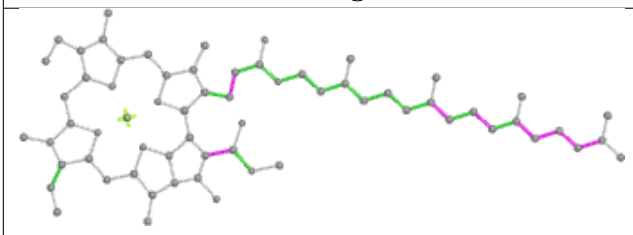
Ligand CLA b 606



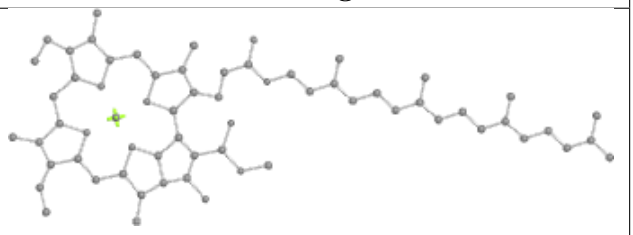
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.60	6 (1%) 68 75	41, 48, 69, 119	0
1	a	334/344 (97%)	-0.48	7 (2%) 63 71	43, 52, 79, 125	1 (0%)
2	B	504/505 (99%)	-0.33	15 (2%) 50 59	43, 54, 79, 111	0
2	b	504/505 (99%)	-0.15	39 (7%) 13 18	46, 58, 95, 164	1 (0%)
3	C	451/455 (99%)	-0.41	10 (2%) 62 69	45, 59, 79, 159	0
3	c	455/455 (100%)	-0.31	15 (3%) 46 55	49, 66, 85, 128	2 (0%)
4	D	342/342 (100%)	-0.51	4 (1%) 79 83	41, 50, 67, 137	0
4	d	341/342 (99%)	-0.51	5 (1%) 73 79	43, 54, 75, 131	0
5	E	81/84 (96%)	0.06	9 (11%) 5 7	53, 68, 94, 167	0
5	e	79/84 (94%)	0.42	9 (11%) 5 7	62, 75, 110, 146	0
6	F	34/44 (77%)	-0.28	2 (5%) 22 30	54, 62, 83, 114	0
6	f	31/44 (70%)	-0.11	2 (6%) 18 25	61, 68, 95, 155	0
7	H	64/65 (98%)	-0.11	2 (3%) 49 58	52, 61, 78, 106	0
7	h	64/65 (98%)	-0.15	4 (6%) 20 27	57, 69, 88, 110	0
8	I	37/38 (97%)	0.18	3 (8%) 12 16	55, 63, 122, 168	0
8	i	37/38 (97%)	0.18	5 (13%) 3 3	56, 64, 116, 142	0
9	J	38/39 (97%)	-0.10	3 (7%) 12 17	52, 70, 117, 179	0
9	j	39/39 (100%)	0.39	7 (17%) 1 1	59, 77, 125, 170	0
10	K	37/37 (100%)	-0.40	2 (5%) 25 34	60, 68, 88, 102	0
10	k	37/37 (100%)	-0.27	0 100 100	65, 74, 95, 105	0
11	L	36/37 (97%)	-0.16	4 (11%) 5 7	42, 47, 90, 145	0
11	l	36/37 (97%)	-0.20	3 (8%) 11 15	43, 49, 99, 122	0
12	M	32/36 (88%)	-0.44	1 (3%) 49 58	45, 50, 70, 139	0
12	m	33/36 (91%)	-0.19	2 (6%) 21 28	44, 50, 70, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.10	18 (7%) 14 20	42, 65, 113, 181	0
13	o	243/244 (99%)	0.20	26 (10%) 6 8	45, 66, 117, 166	0
14	T	29/32 (90%)	-0.37	3 (10%) 6 9	44, 49, 75, 116	0
14	t	29/32 (90%)	-0.49	1 (3%) 45 53	45, 51, 77, 126	0
15	U	96/104 (92%)	-0.25	2 (2%) 63 71	49, 59, 85, 91	0
15	u	97/104 (93%)	-0.19	3 (3%) 49 58	53, 63, 79, 135	0
16	V	137/137 (100%)	-0.43	3 (2%) 62 69	47, 58, 77, 101	0
16	v	137/137 (100%)	-0.08	4 (2%) 51 61	54, 71, 98, 133	0
17	X	38/40 (95%)	-0.11	4 (10%) 6 9	60, 71, 89, 113	0
17	x	38/40 (95%)	0.26	5 (13%) 3 4	63, 77, 117, 164	0
18	Y	29/30 (96%)	1.23	7 (24%) 0 0	68, 84, 120, 129	0
18	y	29/30 (96%)	0.60	5 (17%) 1 1	74, 90, 107, 113	0
19	Z	62/62 (100%)	0.29	9 (14%) 2 3	67, 80, 136, 162	0
19	z	62/62 (100%)	0.65	13 (20%) 1 1	80, 92, 140, 192	0
20	R	34/34 (100%)	2.41	20 (58%) 0 0	79, 101, 126, 136	0
All	All	5283/5384 (98%)	-0.22	282 (5%) 26 35	41, 59, 97, 192	4 (0%)

The worst 5 of 282 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	9.2
1	a	11	ALA	8.3
5	E	84	LYS	7.7
2	b	495	PHE	7.4
2	b	494	GLY	7.2

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
8	FME	i	1	10/11	0.91	0.16	59,69,77,78	0
14	FME	t	1	10/11	0.94	0.08	47,51,60,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.95	0.14	48,62,84,86	0
14	FME	T	1	10/11	0.95	0.09	47,54,66,71	0
12	FME	m	1	10/11	0.97	0.13	54,64,82,94	0
8	FME	I	1	10/11	0.97	0.07	61,69,78,79	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
30	UNL	b	626	33/-	0.27	0.36	72,99,138,140	0
30	UNL	B	626	33/-	0.30	0.40	67,102,124,131	0
30	UNL	I	101	40/-	0.34	0.35	85,110,133,135	0
31	LMT	b	621	25/35	0.41	0.35	94,115,138,141	0
32	LMG	C	519	51/55	0.41	0.34	69,116,136,139	0
31	LMT	T	101	35/35	0.42	0.35	85,118,145,149	0
30	UNL	i	101	40/-	0.45	0.32	82,104,130,136	0
27	GOL	a	419	6/6	0.48	0.58	80,92,94,96	0
31	LMT	b	627	25/35	0.53	0.29	69,89,123,125	0
31	LMT	B	630	35/35	0.53	0.40	82,106,122,128	0
30	UNL	x	101	18/-	0.55	0.27	75,83,119,121	0
31	LMT	B	631	25/35	0.55	0.29	70,91,121,130	0
32	LMG	Z	101	37/55	0.56	0.32	77,118,134,143	0
31	LMT	M	101	35/35	0.58	0.29	67,90,98,103	0
30	UNL	j	101	10/-	0.58	0.34	86,95,100,102	0
30	UNL	K	102	34/-	0.59	0.33	94,112,126,126	0
32	LMG	c	521	51/55	0.60	0.31	80,125,148,151	0
31	LMT	F	101	35/35	0.60	0.52	115,135,160,163	0
34	HTG	b	623	19/19	0.60	0.46	93,129,136,139	0
36	CA	f	103	1/1	0.60	0.09	125,125,125,125	0
31	LMT	m	103	35/35	0.61	0.28	69,89,99,104	0
30	UNL	A	415	28/-	0.62	0.33	103,117,125,134	0
30	UNL	d	408	36/-	0.63	0.23	73,97,115,119	0
31	LMT	t	101	26/35	0.64	0.24	89,110,127,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	c	525	32/-	0.65	0.37	100,115,126,133	0
31	LMT	e	101	35/35	0.65	0.54	124,145,169,174	0
31	LMT	A	417	35/35	0.65	0.35	86,110,122,126	0
31	LMT	B	628	35/35	0.66	0.28	79,103,120,123	0
31	LMT	A	421	35/35	0.67	0.35	121,134,154,156	0
34	HTG	D	410	16/19	0.67	0.29	94,109,119,129	0
30	UNL	D	409	40/-	0.68	0.21	74,93,114,120	0
33	LHG	a	421	42/49	0.69	0.37	99,144,155,158	0
30	UNL	m	102	10/-	0.69	0.31	80,83,89,95	0
36	CA	F	104	1/1	0.70	0.25	126,126,126,126	0
30	UNL	a	416	30/-	0.70	0.30	107,122,136,137	0
26	SQD	f	102	43/54	0.72	0.34	115,129,152,155	0
27	GOL	a	420	6/6	0.72	0.47	64,71,78,79	0
27	GOL	b	624	6/6	0.73	0.20	93,95,96,107	0
27	GOL	o	303	6/6	0.73	0.23	86,90,93,96	0
34	HTG	d	409	16/19	0.74	0.30	99,117,124,135	0
32	LMG	z	101	39/55	0.74	0.27	81,123,136,146	0
30	UNL	X	101	18/-	0.74	0.21	66,74,99,102	0
31	LMT	c	501	35/35	0.75	0.39	122,132,145,151	0
27	GOL	l	102	6/6	0.75	0.79	71,97,99,101	0
27	GOL	A	418	6/6	0.76	0.47	57,75,75,77	0
26	SQD	A	412	54/54	0.77	0.20	73,92,117,124	0
26	SQD	b	620	54/54	0.78	0.20	69,92,107,117	0
34	HTG	b	622	19/19	0.78	0.20	70,80,87,96	0
30	UNL	J	101	10/-	0.78	0.18	80,86,89,96	0
32	LMG	A	419	51/55	0.78	0.18	79,91,102,109	0
27	GOL	B	627	6/6	0.78	0.26	73,76,85,102	0
34	HTG	B	623	19/19	0.78	0.25	71,85,102,104	0
27	GOL	A	411	6/6	0.79	0.20	69,77,81,82	0
27	GOL	O	302	6/6	0.79	0.22	86,95,97,100	0
30	UNL	l	101	10/-	0.79	0.26	73,79,91,91	0
26	SQD	B	620	54/54	0.79	0.18	75,96,117,127	0
29	PL9	A	414	55/55	0.80	0.21	76,100,113,116	0
32	LMG	a	418	51/55	0.81	0.17	74,92,100,113	0
26	SQD	a	413	54/54	0.81	0.19	76,95,120,124	0
29	PL9	a	415	55/55	0.81	0.21	88,111,123,129	0
36	CA	o	301	1/1	0.81	0.06	102,102,102,102	0
27	GOL	o	302	6/6	0.82	0.28	88,101,106,109	0
27	GOL	b	629	6/6	0.82	0.29	58,69,75,76	0
33	LHG	E	101	42/49	0.82	0.23	79,104,117,122	0
34	HTG	C	520	19/19	0.84	0.31	121,127,141,144	0
32	LMG	D	411	51/55	0.84	0.18	51,67,103,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	HTG	B	622	19/19	0.84	0.18	66,83,92,93	0
27	GOL	V	203	6/6	0.84	0.14	60,68,74,76	0
32	LMG	d	410	51/55	0.85	0.18	58,71,102,107	0
34	HTG	c	522	19/19	0.85	0.27	123,132,138,140	0
27	GOL	c	527	6/6	0.85	0.24	107,114,117,121	0
23	CLA	b	616	65/65	0.86	0.17	54,62,117,125	0
27	GOL	O	303	6/6	0.86	0.20	86,95,97,100	0
23	CLA	B	616	65/65	0.86	0.18	49,59,106,115	0
27	GOL	a	412	6/6	0.86	0.25	75,79,87,88	0
23	CLA	b	601	65/65	0.86	0.16	66,85,114,125	0
27	GOL	v	202	6/6	0.87	0.12	66,78,83,85	0
23	CLA	B	601	65/65	0.87	0.14	57,77,100,115	0
23	CLA	d	402	65/65	0.87	0.14	55,65,113,123	0
30	UNL	D	408	17/-	0.88	0.13	66,75,99,104	0
23	CLA	C	513	65/65	0.88	0.14	65,83,103,109	0
25	BCR	K	101	40/40	0.88	0.14	62,76,85,89	0
25	BCR	K	103	40/40	0.88	0.17	57,64,72,74	0
23	CLA	c	514	65/65	0.88	0.17	71,89,112,120	0
23	CLA	c	513	65/65	0.89	0.17	66,80,114,117	0
32	LMG	C	518	51/55	0.89	0.17	58,84,102,108	0
32	LMG	c	520	51/55	0.89	0.19	63,91,116,123	0
30	UNL	d	407	17/-	0.89	0.13	74,83,97,98	0
25	BCR	d	403	40/40	0.90	0.11	53,67,92,95	0
25	BCR	h	101	40/40	0.90	0.13	57,68,87,93	0
34	HTG	b	625	19/19	0.90	0.11	71,82,88,96	0
23	CLA	B	606	65/65	0.90	0.14	44,57,97,104	0
32	LMG	B	621	51/55	0.90	0.13	61,74,87,95	0
23	CLA	C	506	65/65	0.90	0.14	59,69,103,104	0
32	LMG	m	101	51/55	0.90	0.13	62,77,90,99	0
23	CLA	b	606	65/65	0.90	0.14	48,60,97,106	0
25	BCR	Y	101	40/40	0.91	0.13	57,65,78,80	0
27	GOL	B	629	6/6	0.91	0.23	53,63,68,74	0
23	CLA	c	507	65/65	0.91	0.14	58,69,100,105	0
26	SQD	F	103	43/54	0.91	0.18	70,95,116,122	0
23	CLA	C	512	65/65	0.91	0.14	63,72,101,106	0
35	DGD	H	102	62/66	0.92	0.12	51,62,72,74	0
35	DGD	c	519	62/66	0.92	0.12	53,67,100,116	0
34	HTG	V	202	11/19	0.92	0.41	92,107,115,116	0
25	BCR	b	618	40/40	0.92	0.10	49,59,74,77	0
23	CLA	a	409	65/65	0.92	0.17	47,55,113,119	0
34	HTG	B	625	19/19	0.93	0.09	77,81,92,95	0
23	CLA	B	609	65/65	0.93	0.15	49,59,69,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	DGD	C	516	62/66	0.93	0.12	51,64,102,106	0
35	DGD	C	517	62/66	0.93	0.11	48,61,89,100	0
23	CLA	D	403	65/65	0.93	0.14	51,59,104,108	0
35	DGD	c	518	62/66	0.93	0.12	54,68,111,123	0
25	BCR	D	404	40/40	0.93	0.10	50,60,92,98	0
35	DGD	h	102	62/66	0.93	0.11	57,65,74,79	0
23	CLA	C	508	65/65	0.93	0.10	48,56,105,113	0
25	BCR	k	101	40/40	0.93	0.14	60,74,81,82	0
23	CLA	A	408	65/65	0.93	0.14	45,53,110,114	0
23	CLA	b	609	65/65	0.94	0.14	51,64,72,80	0
33	LHG	d	406	49/49	0.94	0.15	55,65,109,123	0
23	CLA	a	407	65/65	0.94	0.11	43,54,120,125	0
27	GOL	C	521	6/6	0.94	0.10	57,60,65,66	0
23	CLA	c	505	65/65	0.94	0.10	56,63,97,100	0
25	BCR	c	515	40/40	0.94	0.10	73,83,89,90	0
25	BCR	B	618	40/40	0.94	0.08	47,56,69,74	0
23	CLA	C	504	65/65	0.94	0.10	47,56,89,99	0
23	CLA	c	509	65/65	0.94	0.12	51,62,115,121	0
33	LHG	D	407	49/49	0.94	0.15	52,61,99,105	0
26	SQD	A	410	54/54	0.94	0.14	59,81,104,109	0
25	BCR	H	101	40/40	0.95	0.09	53,65,85,87	0
33	LHG	A	420	49/49	0.95	0.12	52,65,81,84	0
23	CLA	B	614	65/65	0.95	0.10	43,51,85,92	0
25	BCR	t	102	40/40	0.95	0.08	48,57,75,79	0
27	GOL	b	628	6/6	0.95	0.19	79,84,94,95	0
33	LHG	b	630	49/49	0.95	0.12	54,59,69,83	0
25	BCR	y	101	40/40	0.95	0.08	62,71,80,86	0
33	LHG	d	411	49/49	0.95	0.14	57,68,77,81	0
35	DGD	c	517	62/66	0.95	0.10	48,62,97,101	0
23	CLA	b	612	65/65	0.95	0.09	43,52,61,66	0
25	BCR	T	102	40/40	0.95	0.07	47,58,68,69	0
25	BCR	A	409	40/40	0.95	0.09	42,53,65,66	0
23	CLA	b	614	65/65	0.95	0.10	45,52,84,88	0
25	BCR	C	514	40/40	0.95	0.12	55,64,71,80	0
23	CLA	B	611	65/65	0.95	0.10	41,47,64,67	0
38	HEM	f	101	43/43	0.95	0.15	67,81,101,109	0
23	CLA	b	615	65/65	0.96	0.10	51,59,77,78	0
26	SQD	a	411	54/54	0.96	0.12	64,84,111,117	0
27	GOL	c	526	6/6	0.96	0.23	65,65,71,74	0
23	CLA	C	507	65/65	0.96	0.11	52,62,78,87	0
23	CLA	c	502	65/65	0.96	0.10	59,66,75,78	0
23	CLA	C	501	65/65	0.96	0.08	52,61,70,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	509	65/65	0.96	0.10	52,58,77,80	0
23	CLA	c	508	65/65	0.96	0.10	56,68,79,83	0
27	GOL	B	624	6/6	0.96	0.20	73,77,85,86	0
29	PL9	D	405	55/55	0.96	0.10	39,51,57,66	0
25	BCR	b	619	40/40	0.96	0.07	52,62,82,86	0
29	PL9	d	404	55/55	0.96	0.11	43,52,60,65	0
23	CLA	b	602	65/65	0.96	0.12	52,60,72,76	0
23	CLA	c	512	65/65	0.96	0.10	59,67,83,93	0
23	CLA	b	604	65/65	0.96	0.10	42,52,87,99	0
23	CLA	b	605	65/65	0.96	0.11	43,51,71,77	0
23	CLA	C	511	65/65	0.96	0.12	52,64,77,80	0
23	CLA	b	607	65/65	0.96	0.09	40,49,72,77	0
23	CLA	C	503	65/65	0.96	0.09	49,61,68,77	0
36	CA	O	301	1/1	0.96	0.09	100,100,100,100	0
33	LHG	d	405	49/49	0.96	0.15	49,58,72,76	0
23	CLA	B	610	65/65	0.96	0.12	46,56,61,75	0
23	CLA	A	406	65/65	0.96	0.10	40,49,109,115	0
23	CLA	c	511	65/65	0.97	0.09	53,63,74,89	0
23	CLA	B	613	65/65	0.97	0.08	41,47,84,90	0
23	CLA	B	605	65/65	0.97	0.11	43,49,66,73	0
23	CLA	C	510	65/65	0.97	0.07	52,60,75,76	0
23	CLA	B	615	65/65	0.97	0.10	46,54,74,80	0
24	PHO	A	416	64/64	0.97	0.09	39,51,58,64	0
24	PHO	a	417	64/64	0.97	0.11	46,54,62,68	0
23	CLA	A	404	65/65	0.97	0.12	38,45,62,66	0
25	BCR	B	617	40/40	0.97	0.08	45,53,61,64	0
23	CLA	b	610	65/65	0.97	0.08	51,58,64,69	0
25	BCR	B	619	40/40	0.97	0.07	51,60,83,88	0
23	CLA	b	611	65/65	0.97	0.08	43,51,66,70	0
23	CLA	B	607	65/65	0.97	0.09	40,47,68,73	0
23	CLA	b	613	65/65	0.97	0.07	43,50,81,87	0
23	CLA	D	402	65/65	0.97	0.11	36,44,69,76	0
23	CLA	B	602	65/65	0.97	0.11	48,56,67,77	0
35	DGD	C	515	62/66	0.97	0.09	48,56,95,100	0
23	CLA	a	405	65/65	0.97	0.12	42,48,63,74	0
23	CLA	B	603	65/65	0.97	0.09	44,52,70,74	0
25	BCR	a	410	40/40	0.97	0.07	46,55,62,64	0
23	CLA	c	504	65/65	0.97	0.09	53,69,78,88	0
23	CLA	C	505	65/65	0.97	0.08	51,59,83,90	0
23	CLA	c	506	65/65	0.97	0.09	52,63,84,92	0
25	BCR	c	516	40/40	0.97	0.10	60,66,73,78	0
36	CA	C	522	1/1	0.97	0.06	73,73,73,73	0

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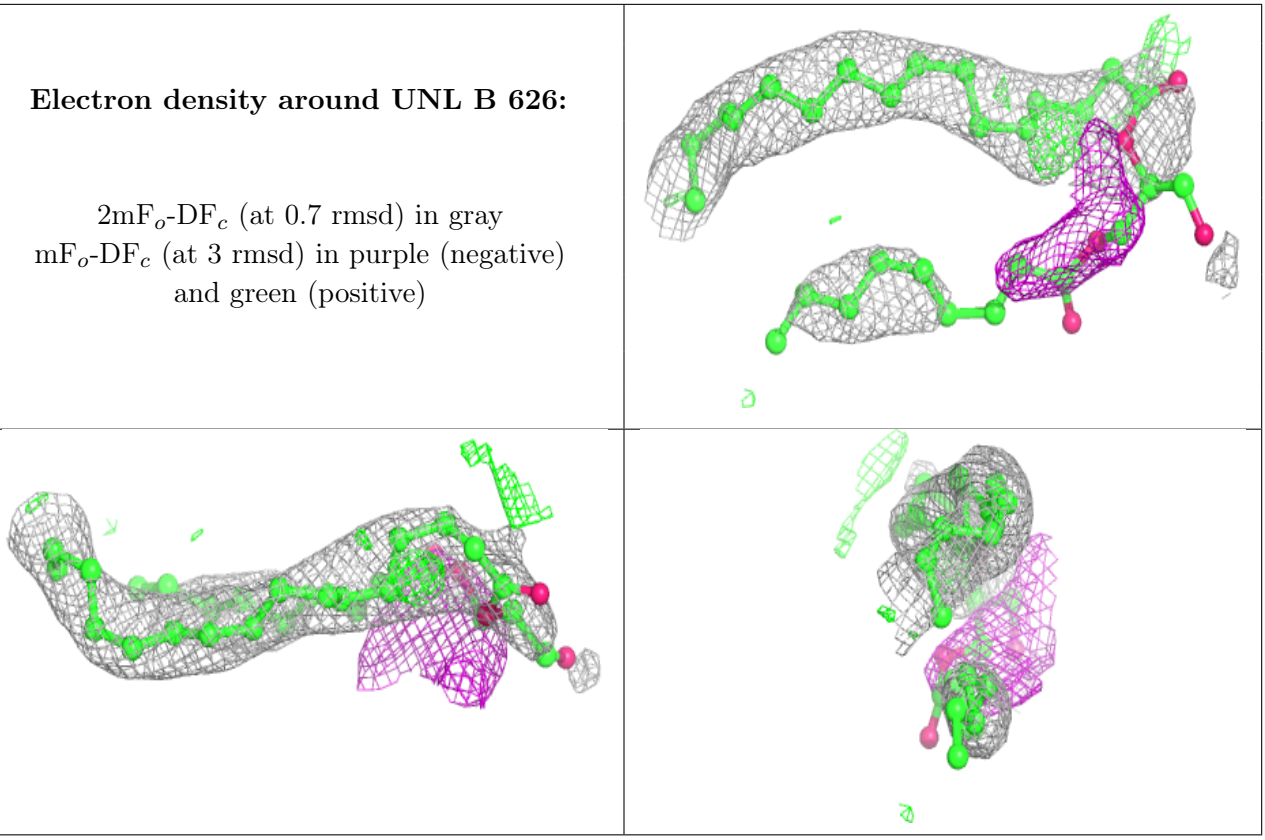
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	604	65/65	0.97	0.09	41,47,97,103	0
23	CLA	B	612	65/65	0.97	0.07	39,49,59,63	0
36	CA	c	524	1/1	0.97	0.07	76,76,76,76	0
23	CLA	b	603	65/65	0.97	0.08	47,58,78,84	0
23	CLA	c	510	65/65	0.97	0.08	49,64,83,85	0
33	LHG	L	101	49/49	0.97	0.11	52,58,70,87	0
39	MG	J	102	1/1	0.97	0.04	59,59,59,59	0
40	HEC	v	201	43/43	0.97	0.11	55,61,67,69	0
23	CLA	d	401	65/65	0.98	0.11	41,47,77,91	0
23	CLA	c	503	65/65	0.98	0.08	49,60,89,107	0
24	PHO	A	407	64/64	0.98	0.08	37,46,54,59	0
23	CLA	b	608	65/65	0.98	0.07	46,56,78,86	0
24	PHO	a	408	64/64	0.98	0.08	43,49,54,56	0
36	CA	c	523	1/1	0.98	0.06	75,75,75,75	0
23	CLA	B	608	65/65	0.98	0.07	44,51,69,77	0
23	CLA	A	405	65/65	0.98	0.09	37,44,58,70	0
33	LHG	D	406	49/49	0.98	0.13	48,56,68,73	0
37	BCT	a	404	4/4	0.98	0.07	58,60,68,77	0
38	HEM	F	102	43/43	0.98	0.10	60,68,75,85	0
23	CLA	a	406	65/65	0.98	0.08	41,46,63,69	0
23	CLA	C	502	65/65	0.98	0.08	48,56,78,85	0
40	HEC	V	201	43/43	0.98	0.11	44,51,56,57	0
25	BCR	b	617	40/40	0.98	0.07	48,54,61,61	0
28	OEX	a	414	10/10	0.99	0.06	47,50,51,55	0
22	CL	A	403	1/1	0.99	0.03	47,47,47,47	0
21	FE2	a	401	1/1	0.99	0.04	55,55,55,55	0
22	CL	A	402	1/1	0.99	0.03	43,43,43,43	0
39	MG	j	102	1/1	0.99	0.05	63,63,63,63	0
28	OEX	A	413	10/10	0.99	0.05	41,44,48,50	0
37	BCT	D	401	4/4	0.99	0.11	54,58,61,66	0
21	FE2	A	401	1/1	1.00	0.04	52,52,52,52	0
22	CL	a	402	1/1	1.00	0.03	50,50,50,50	0
22	CL	a	403	1/1	1.00	0.03	52,52,52,52	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.

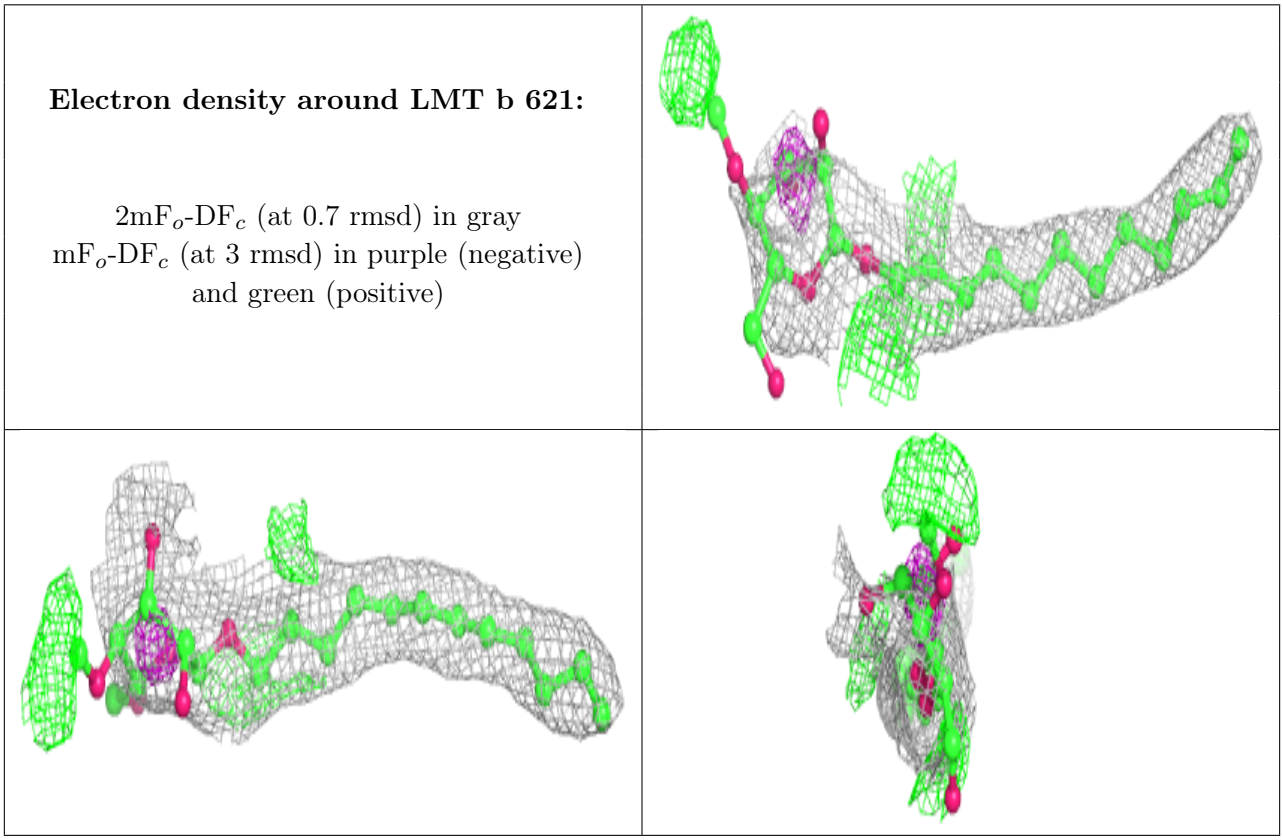
Electron density around UNL B 626:

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



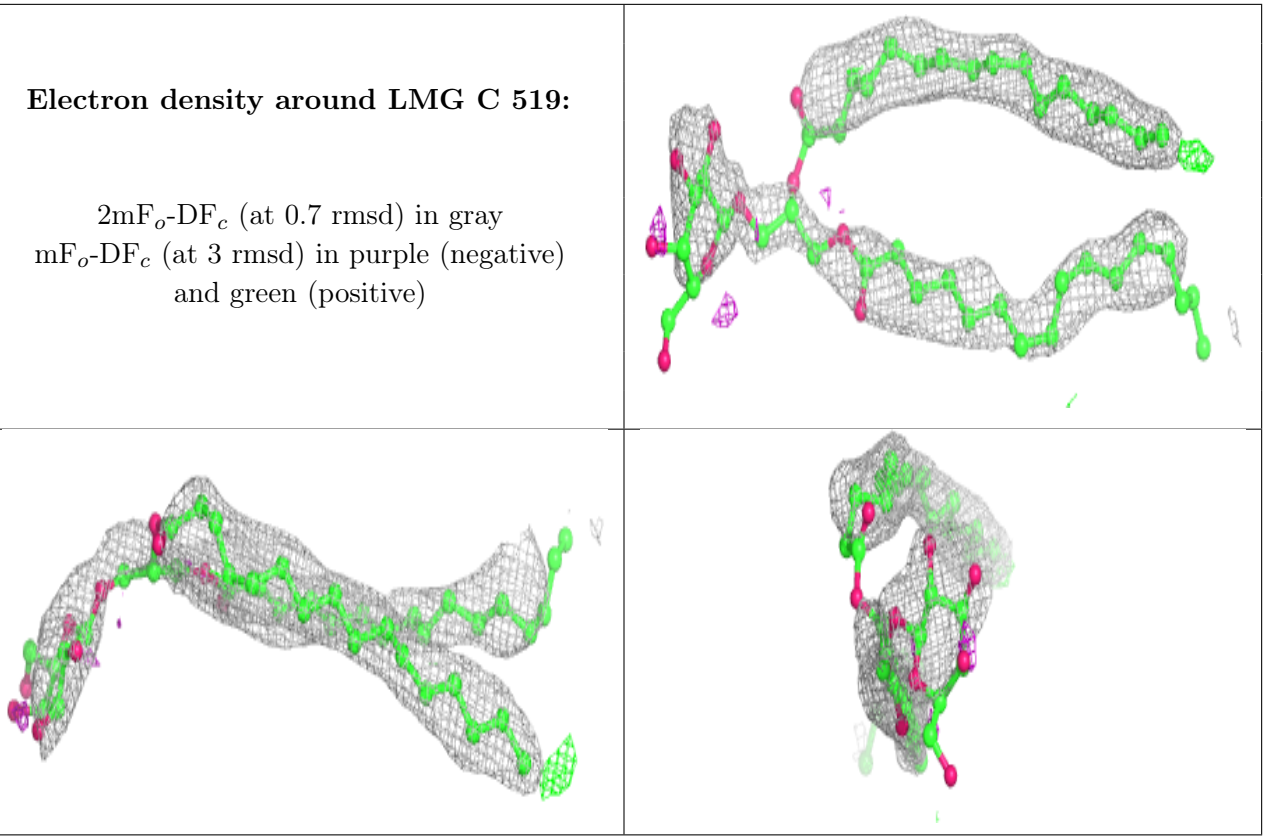
Electron density around LMT b 621:

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



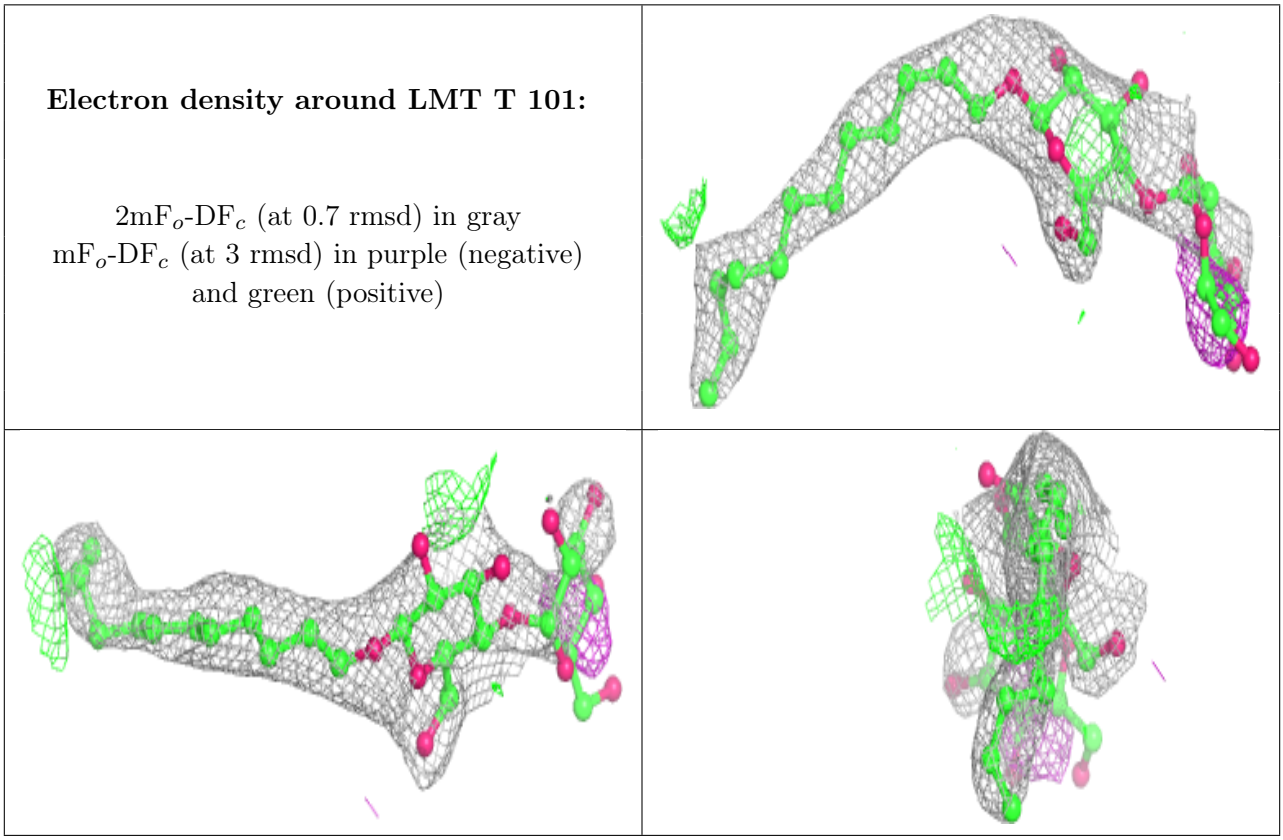
Electron density around LMG C 519:

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



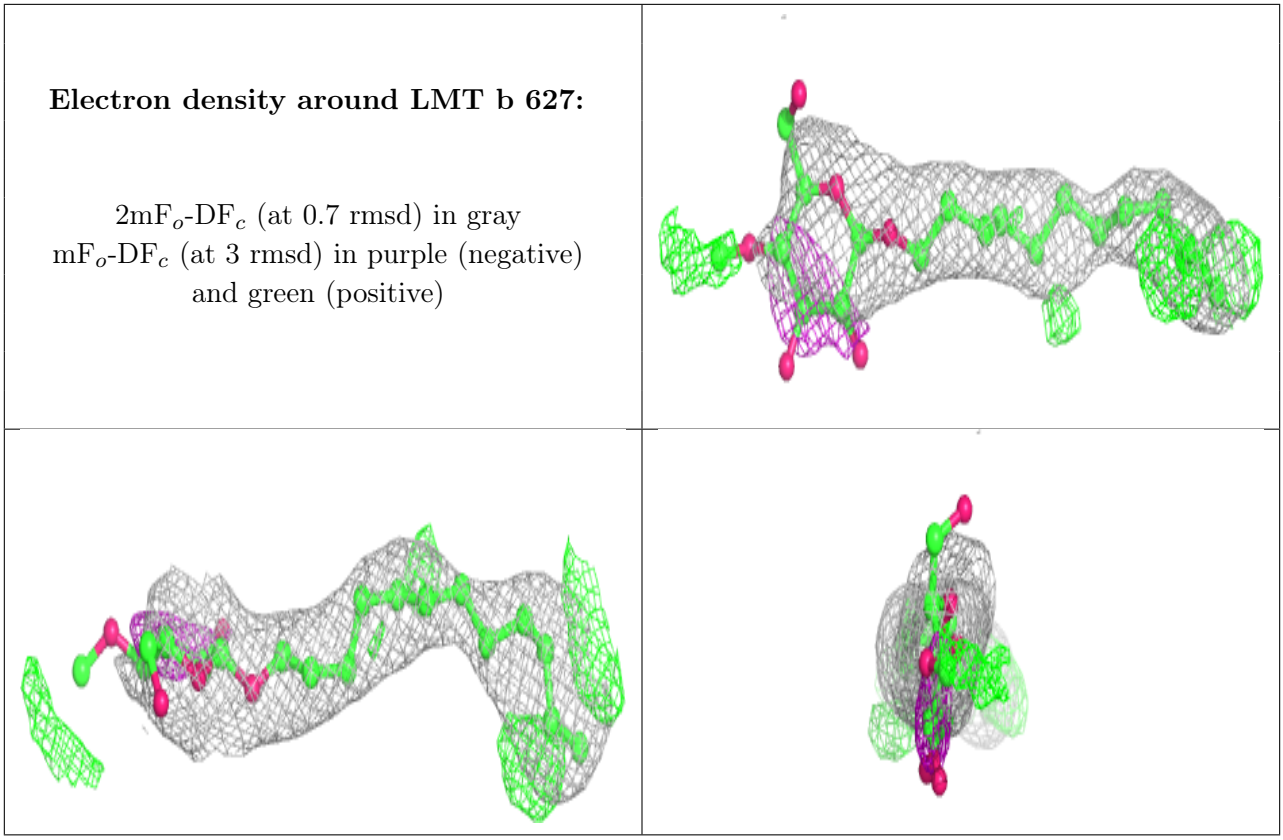
Electron density around LMT T 101:

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



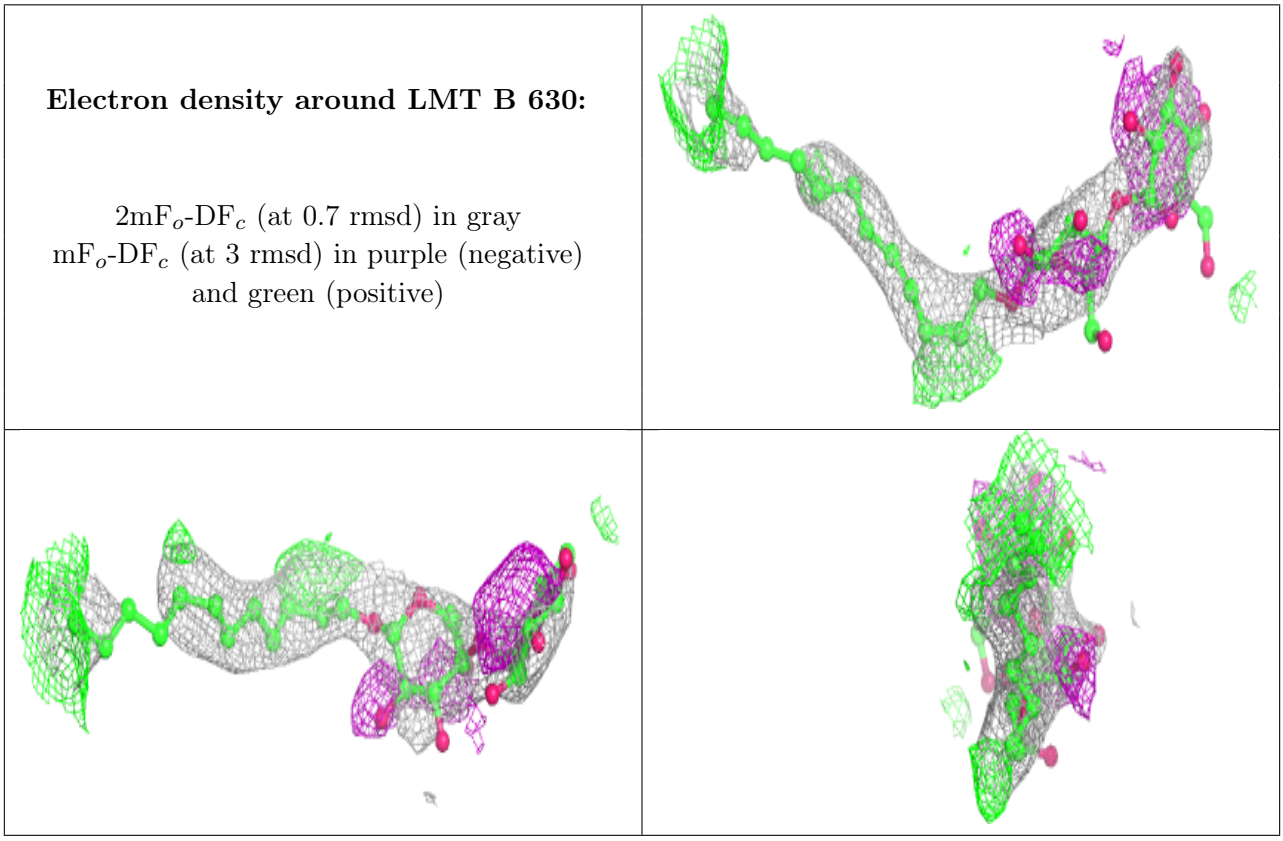
Electron density around LMT b 627:

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



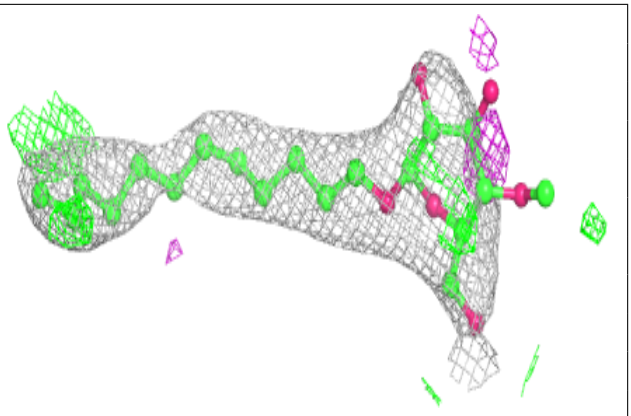
Electron density around LMT B 630:

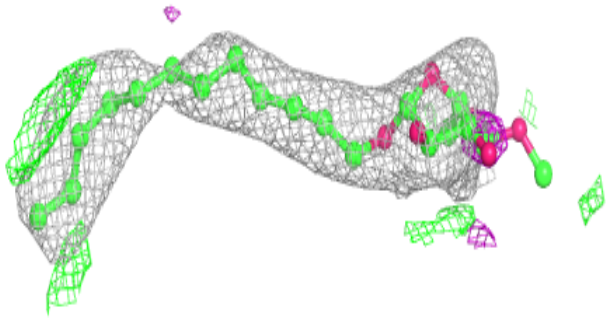
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

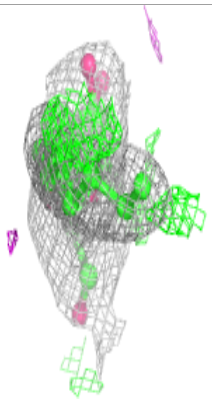


Electron density around LMT B 631:

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

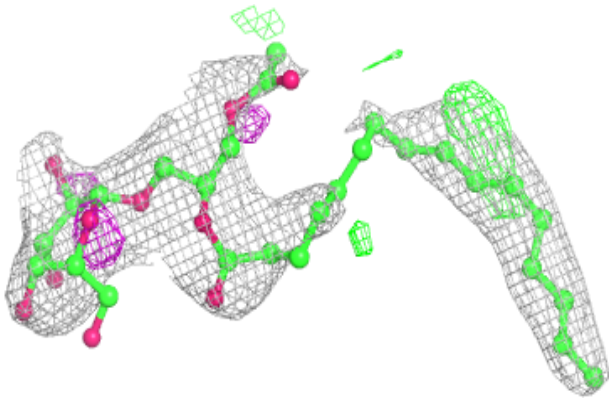


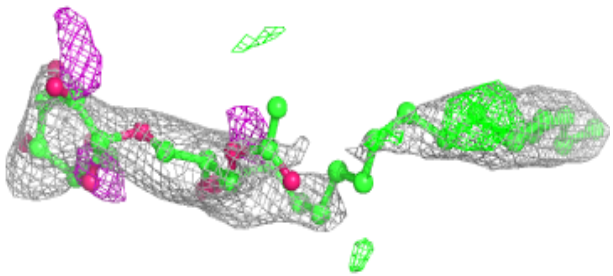


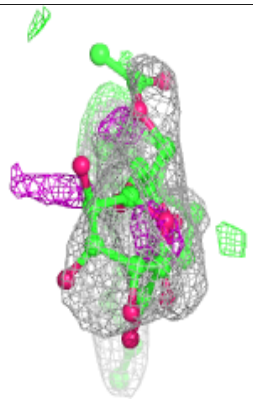


Electron density around LMG Z 101:

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

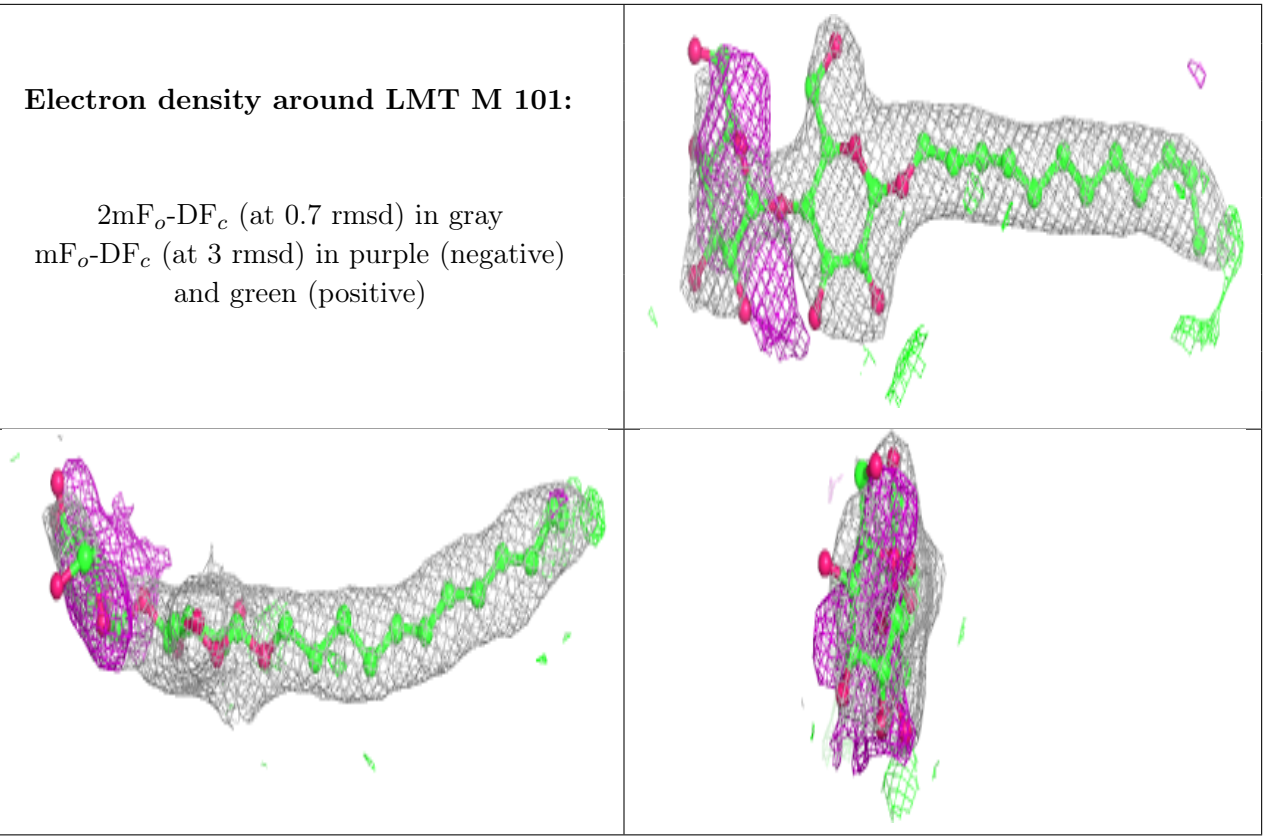






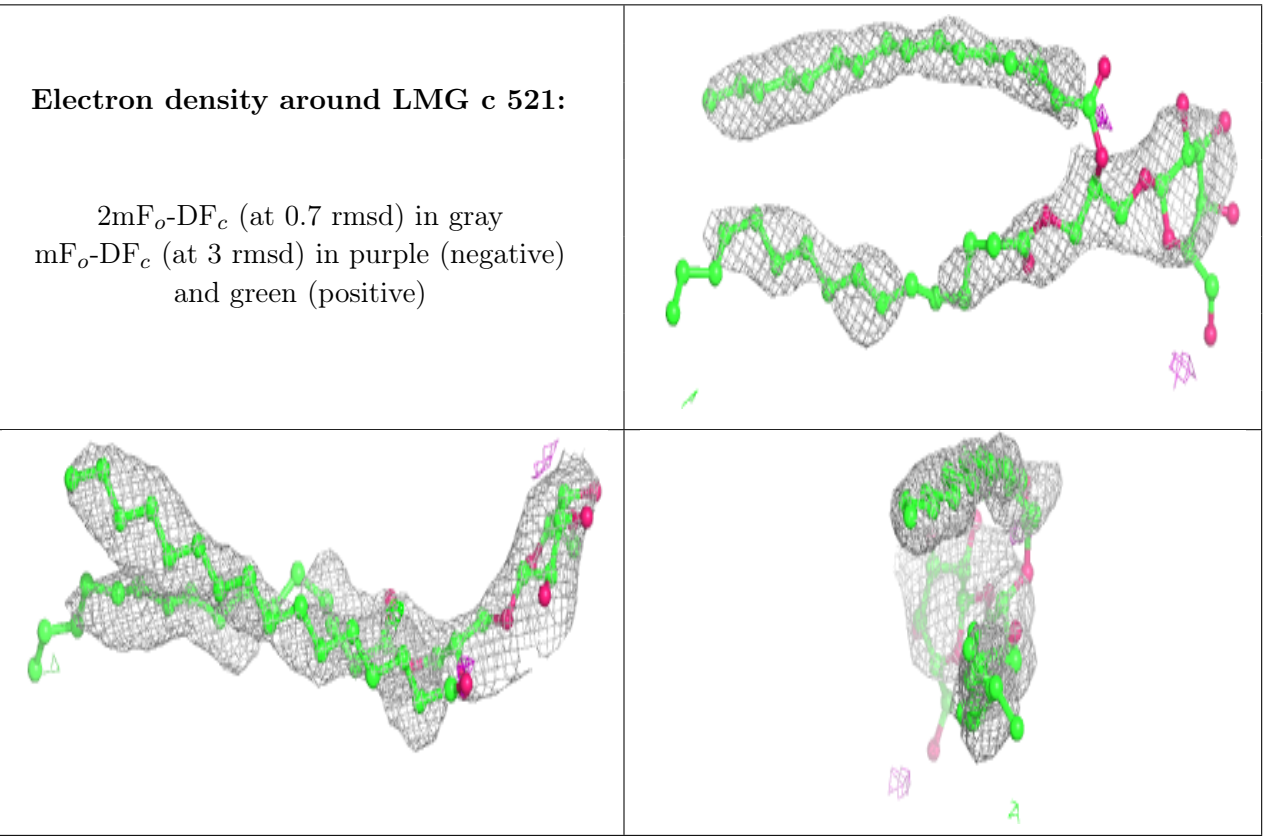
Electron density around LMT M 101:

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



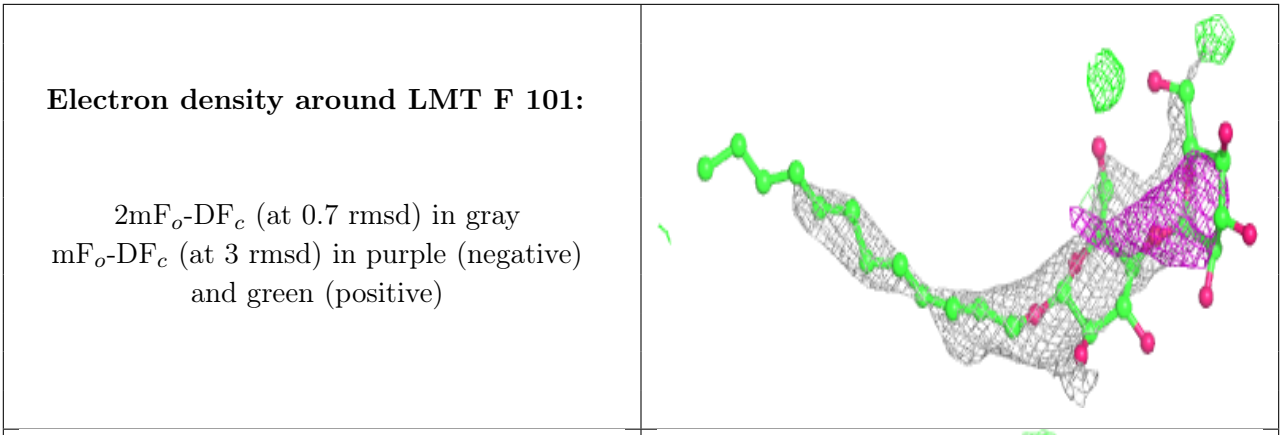
Electron density around LMG c 521:

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



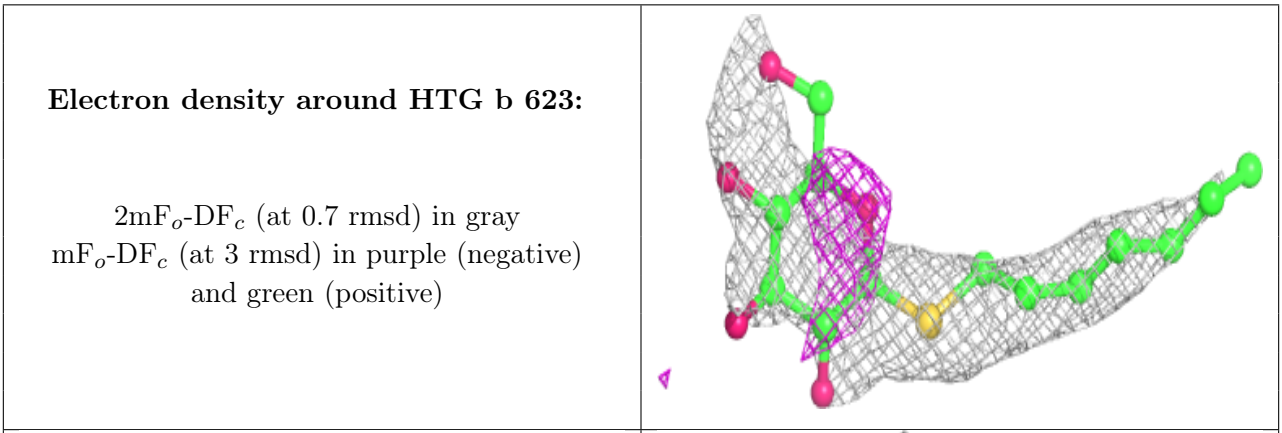
Electron density around LMT F 101:

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



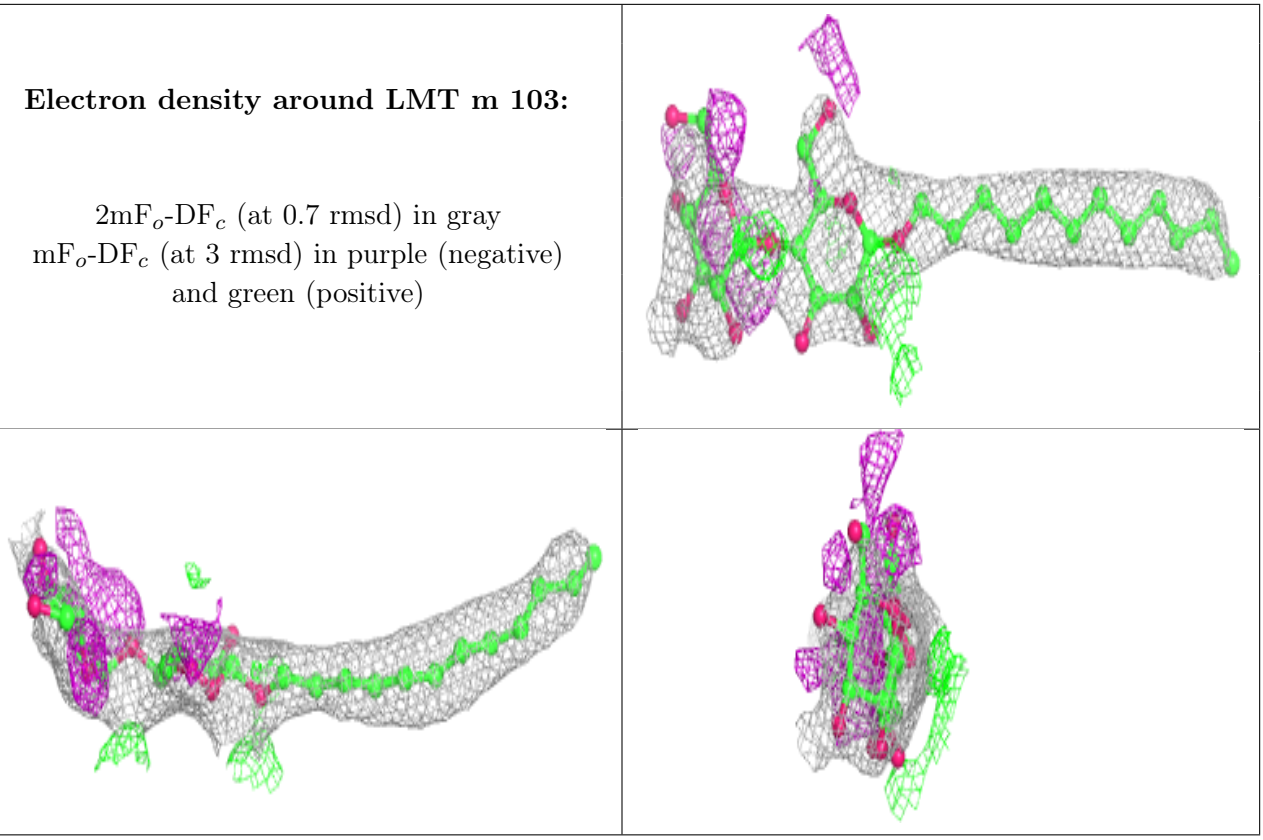
Electron density around HTG b 623:

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



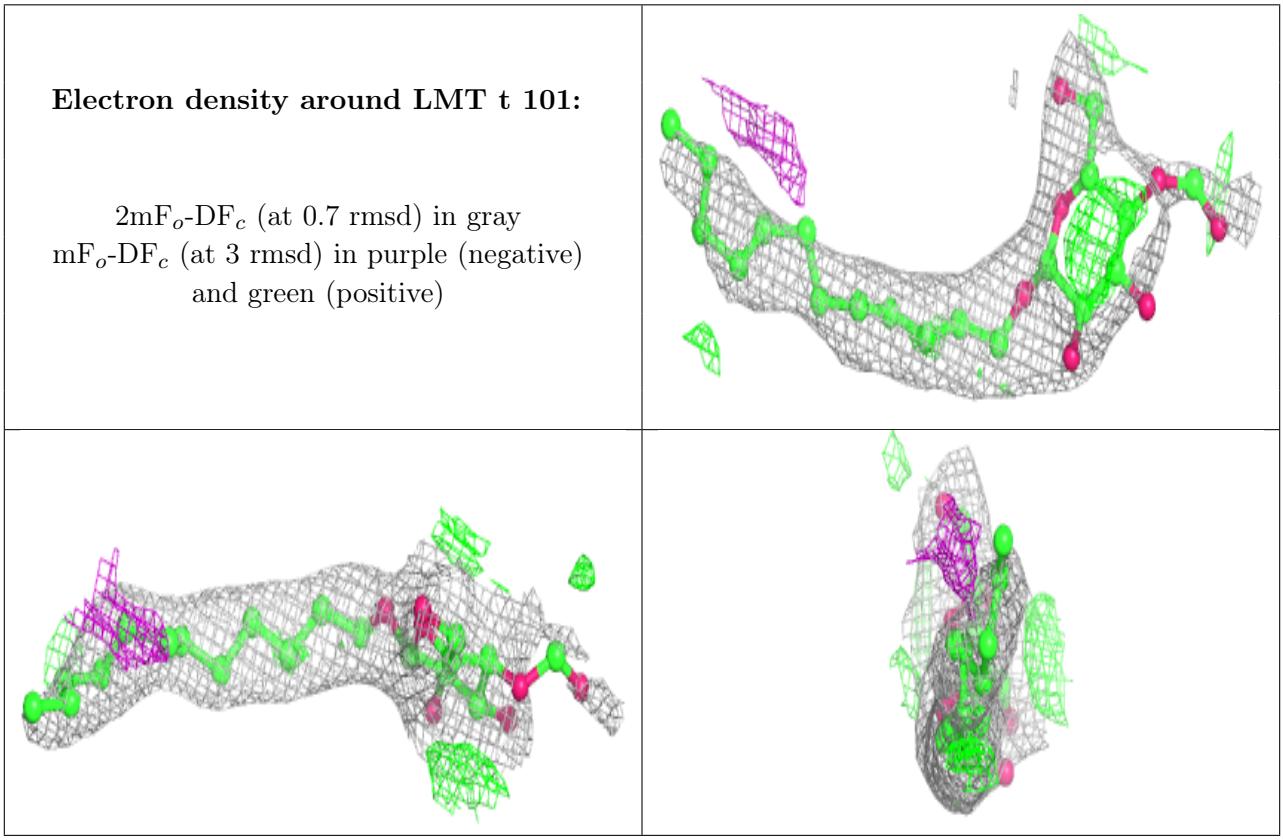
Electron density around LMT m 103:

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



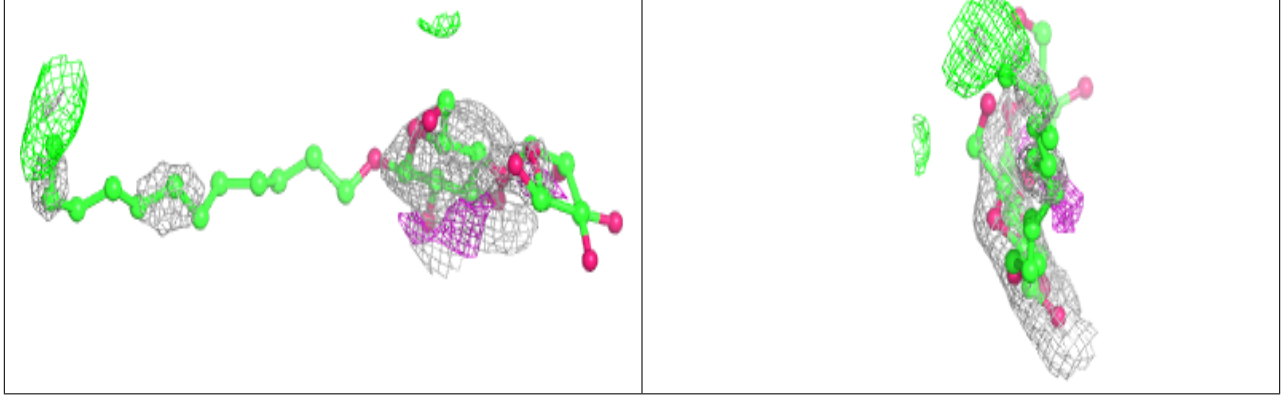
Electron density around LMT t 101:

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



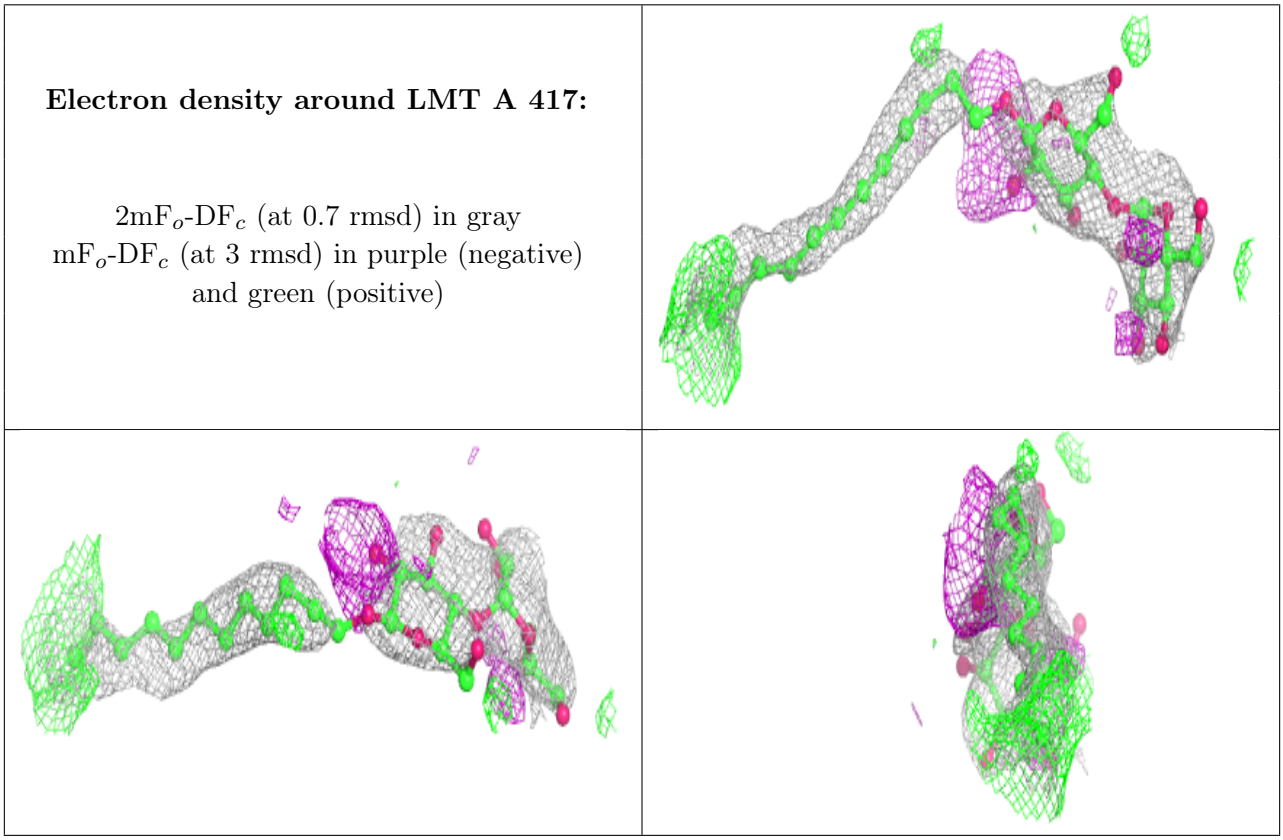
Electron density around LMT e 101:

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



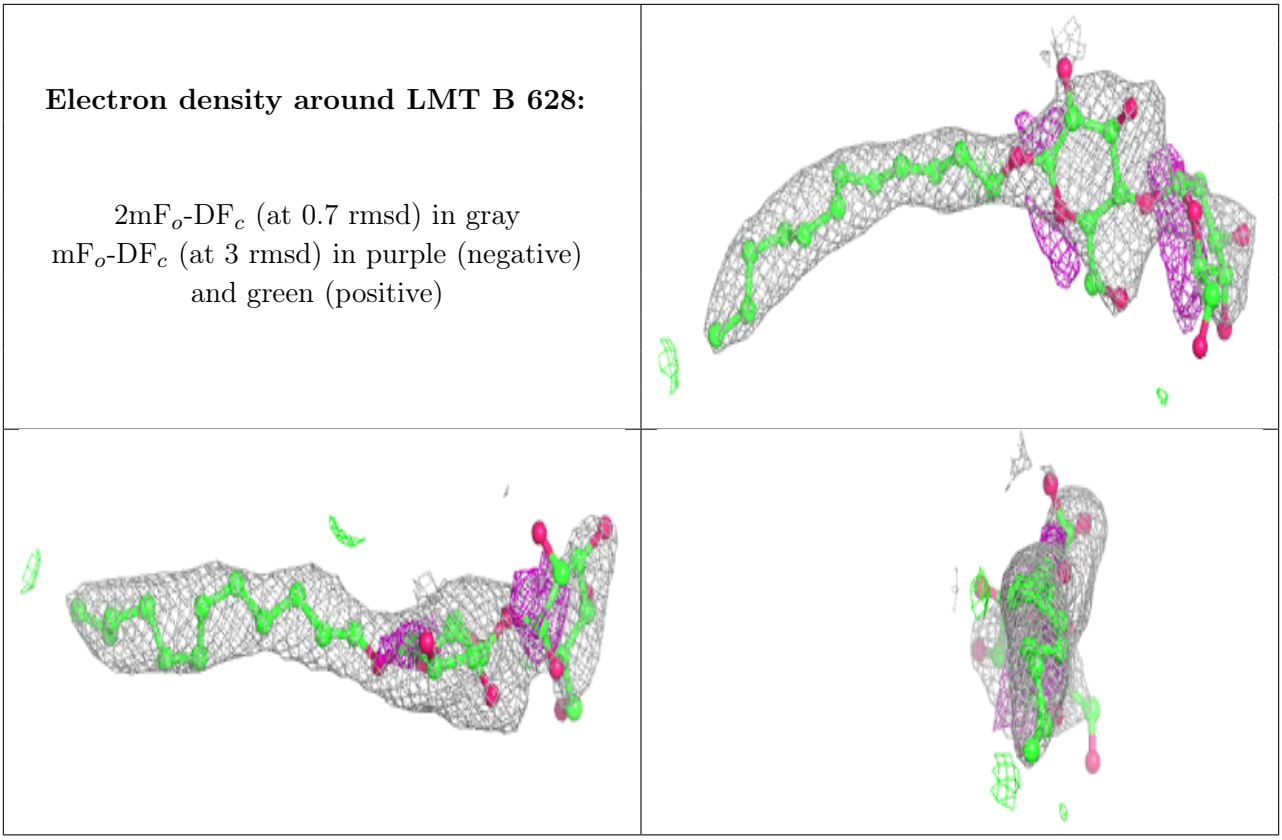
Electron density around LMT A 417:

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



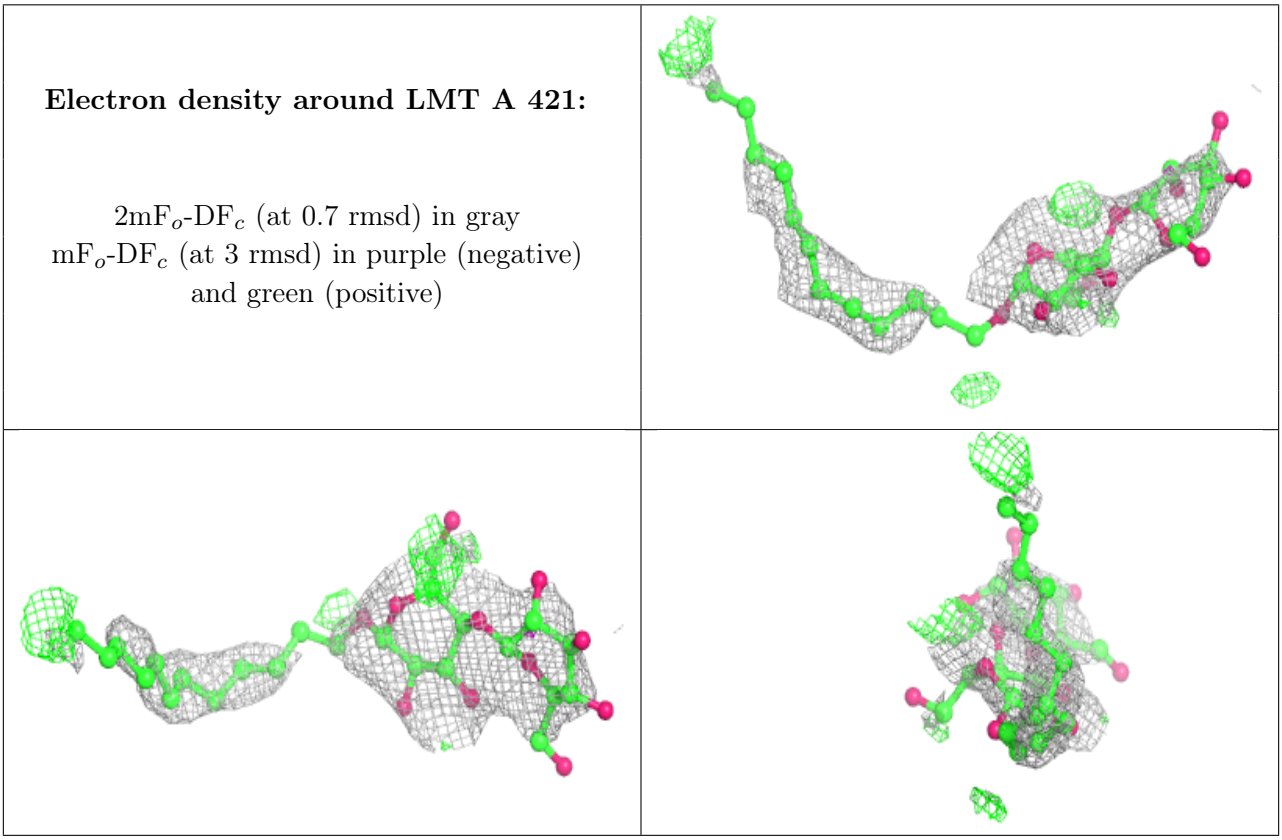
Electron density around LMT B 628:

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



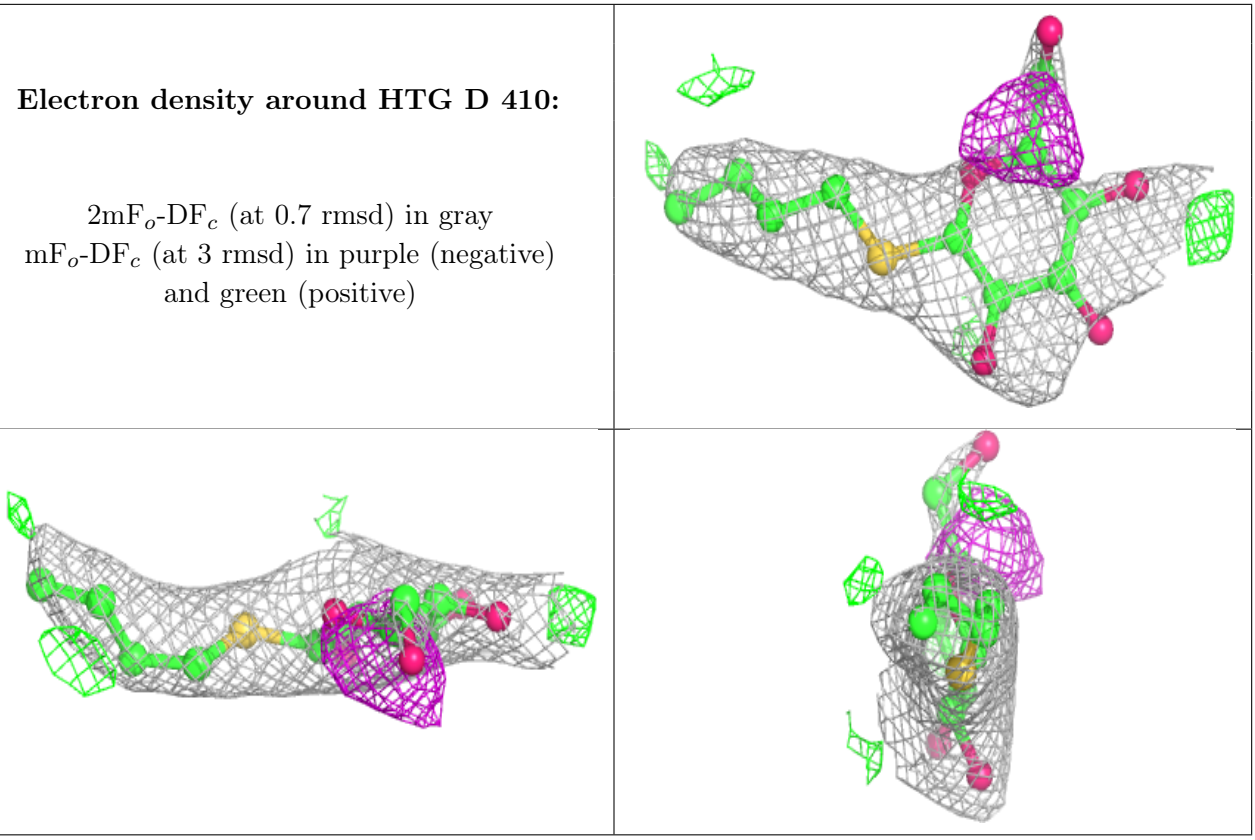
Electron density around LMT A 421:

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



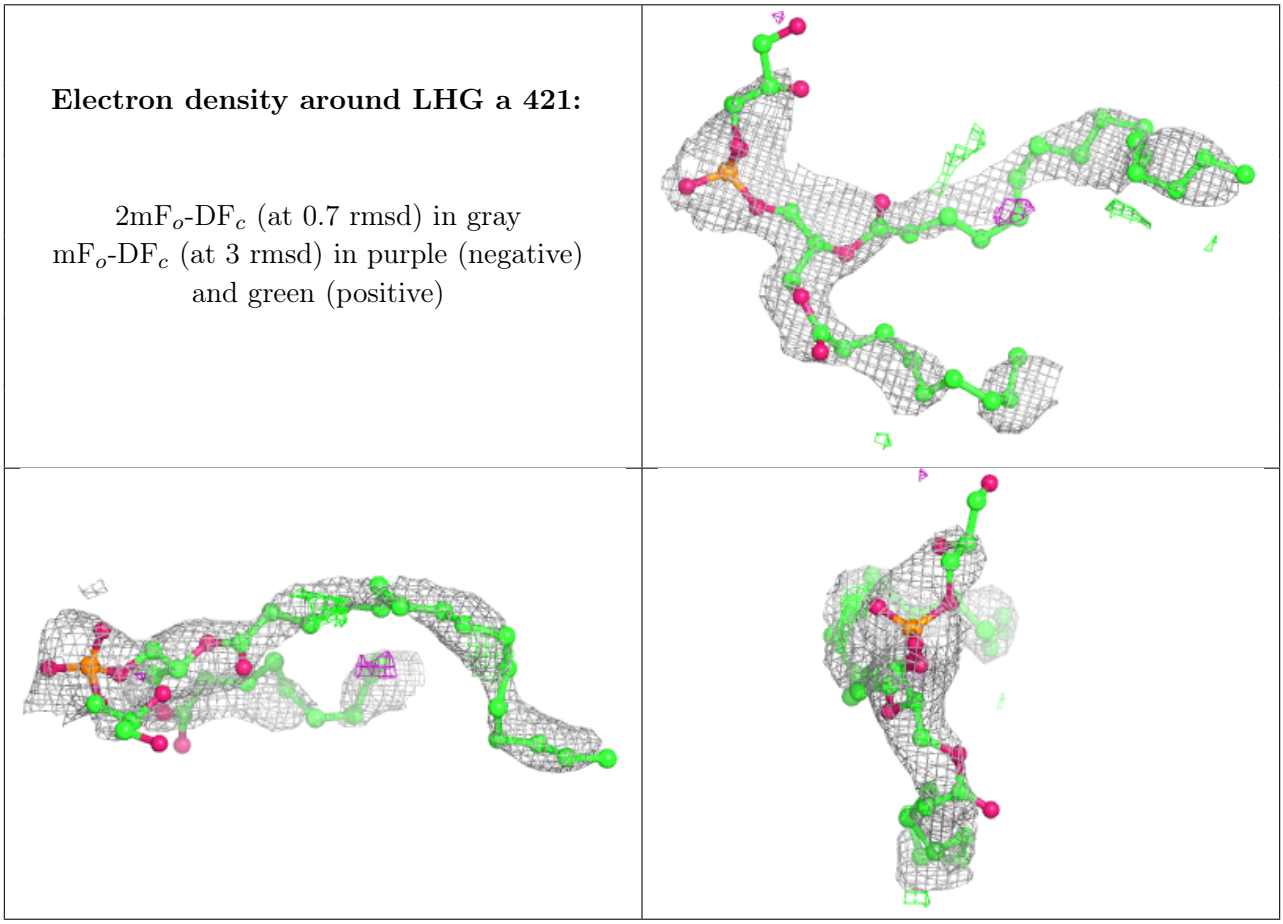
Electron density around HTG D 410:

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



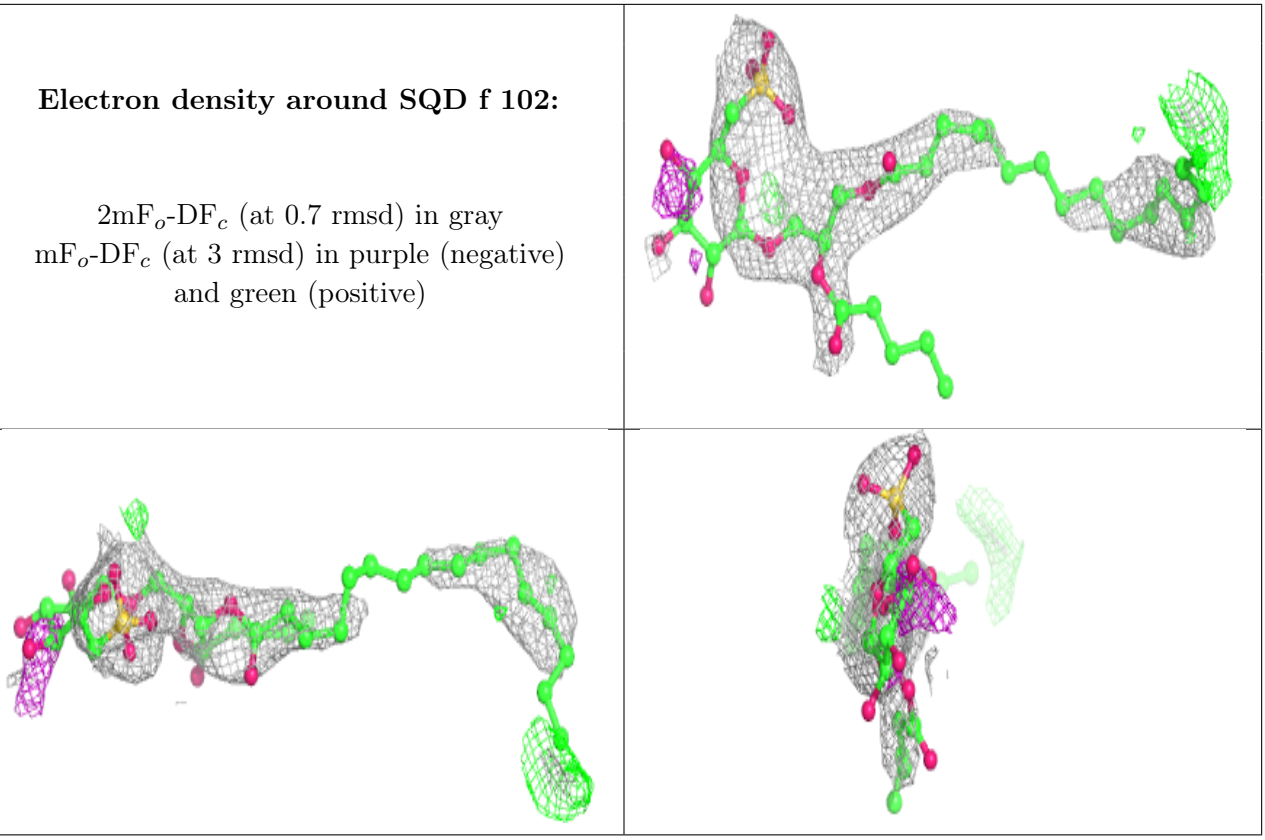
Electron density around LHG a 421:

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



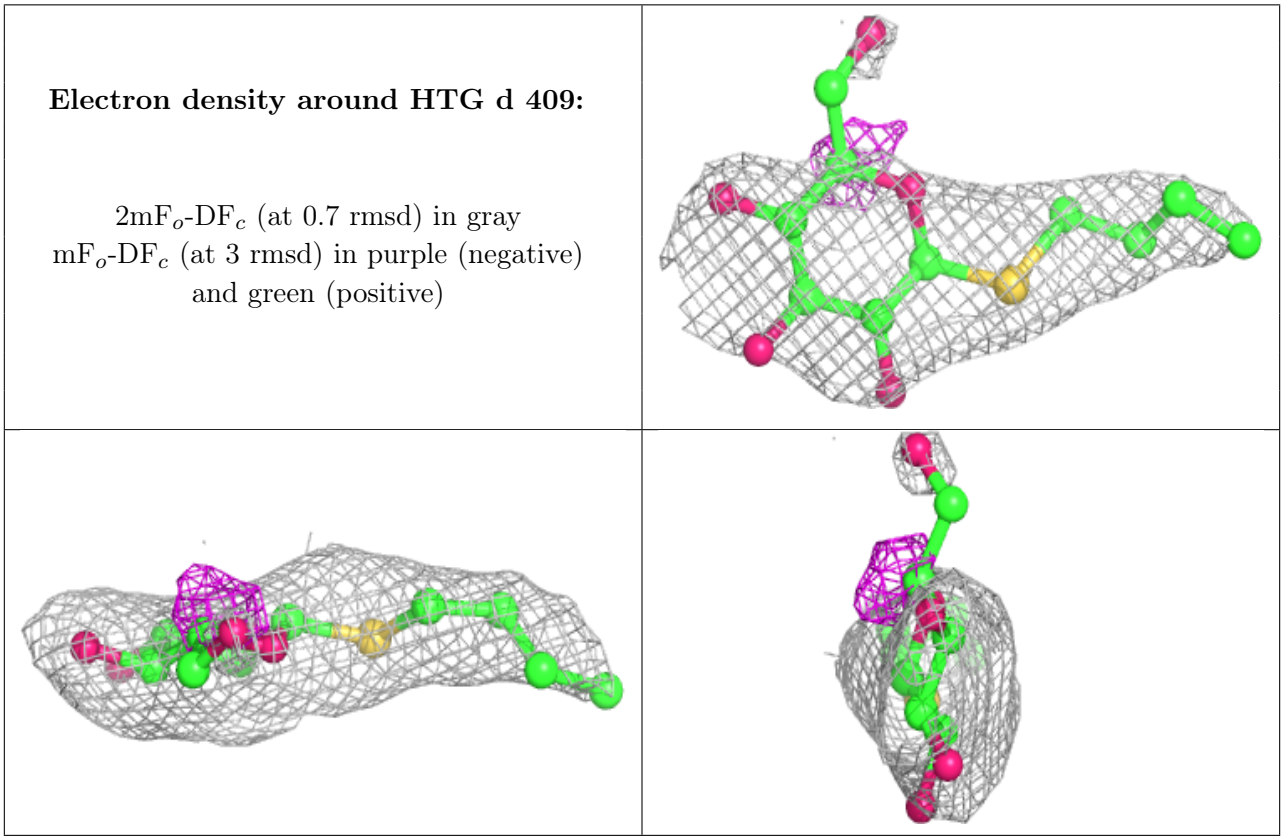
Electron density around SQD f 102:

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



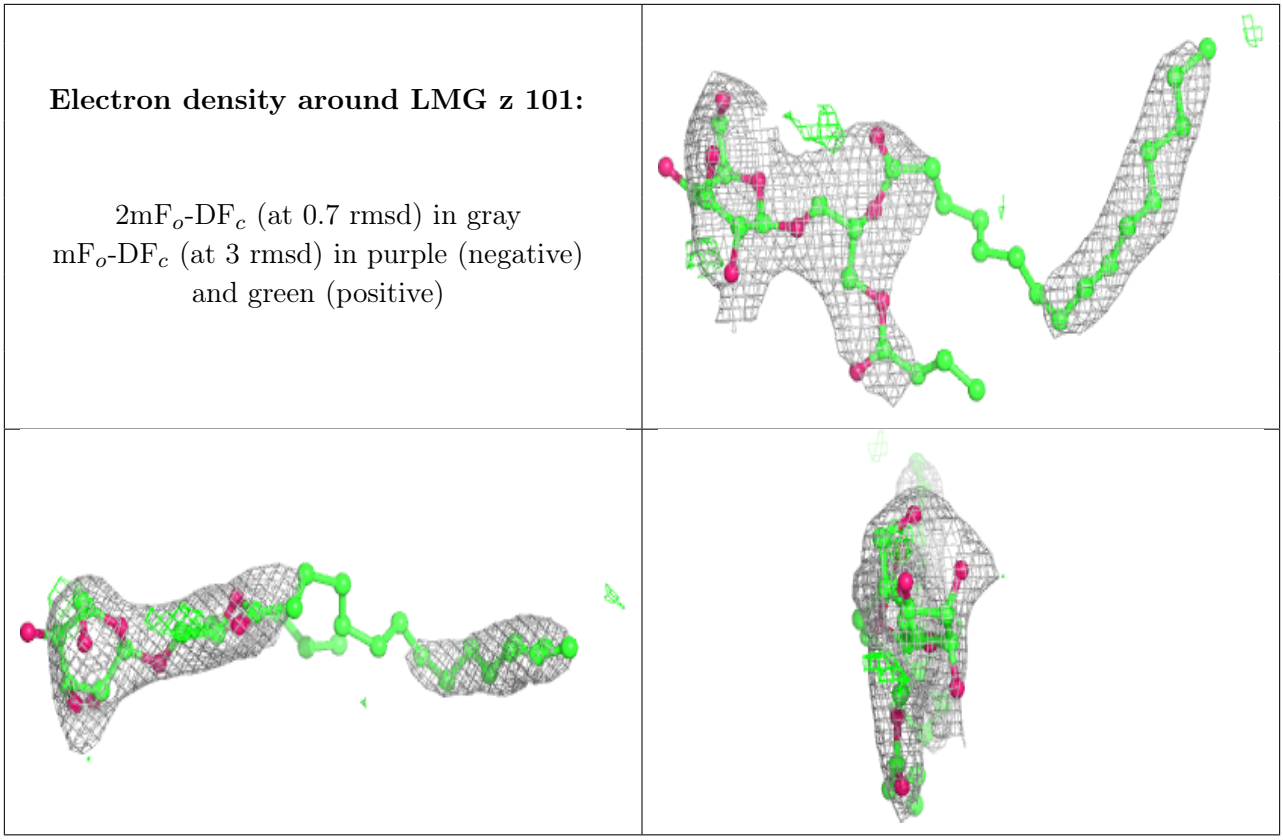
Electron density around HTG d 409:

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



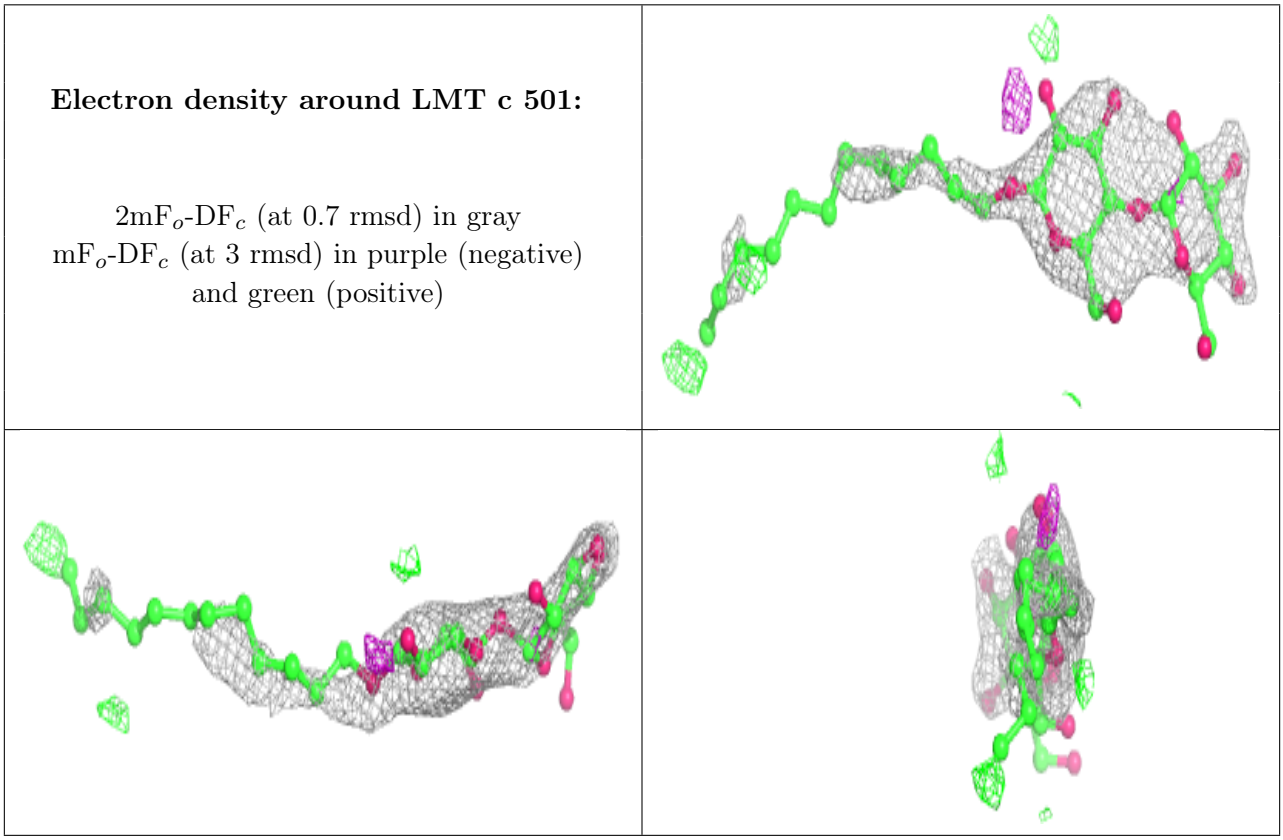
Electron density around LMG z 101:

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



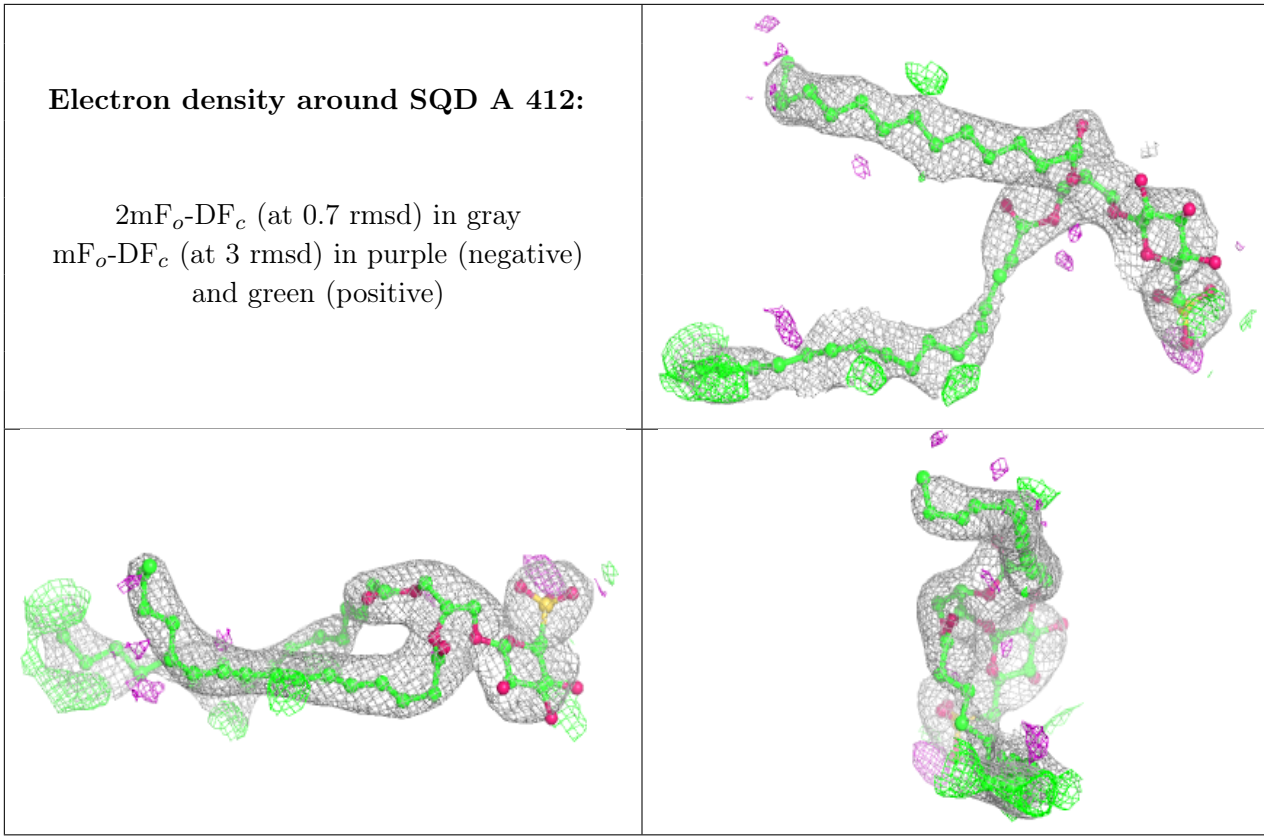
Electron density around LMT c 501:

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



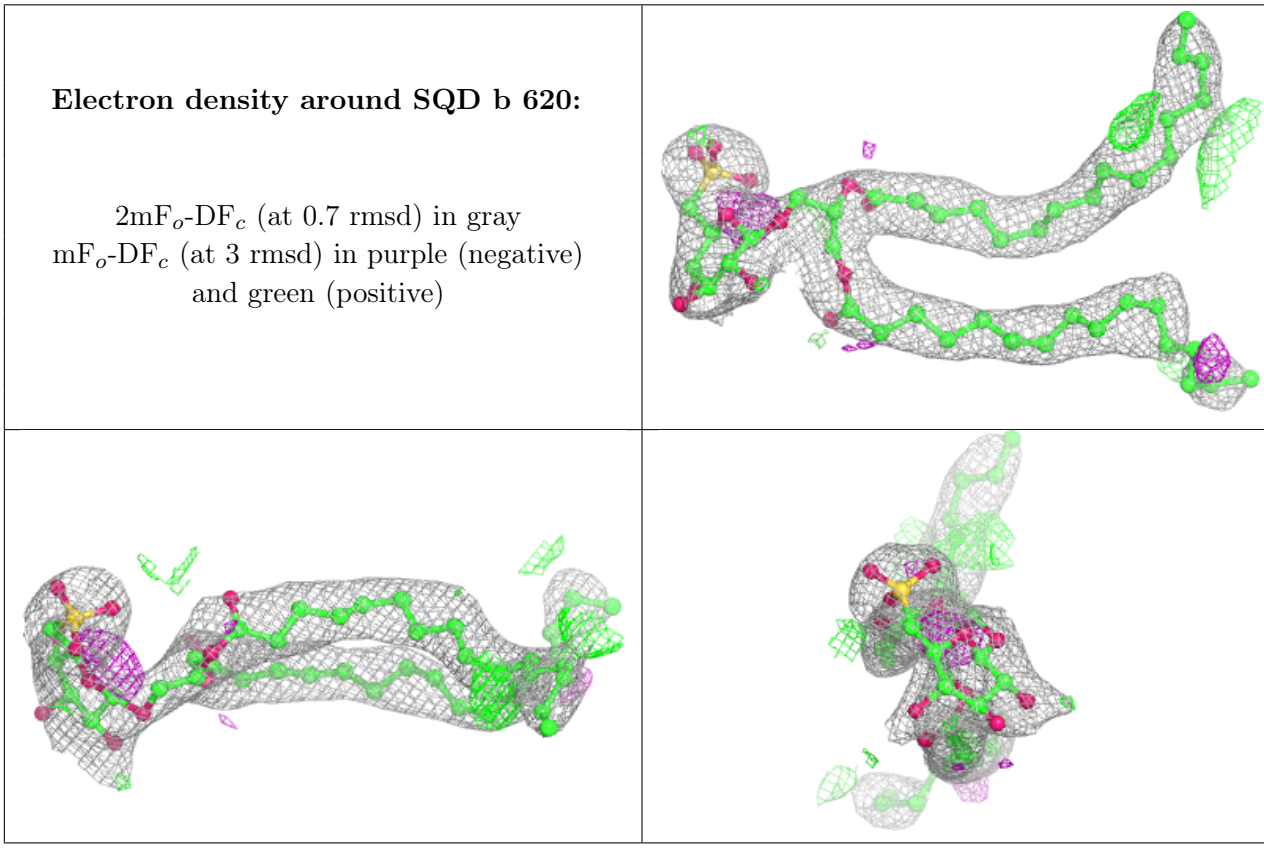
Electron density around SQD A 412:

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



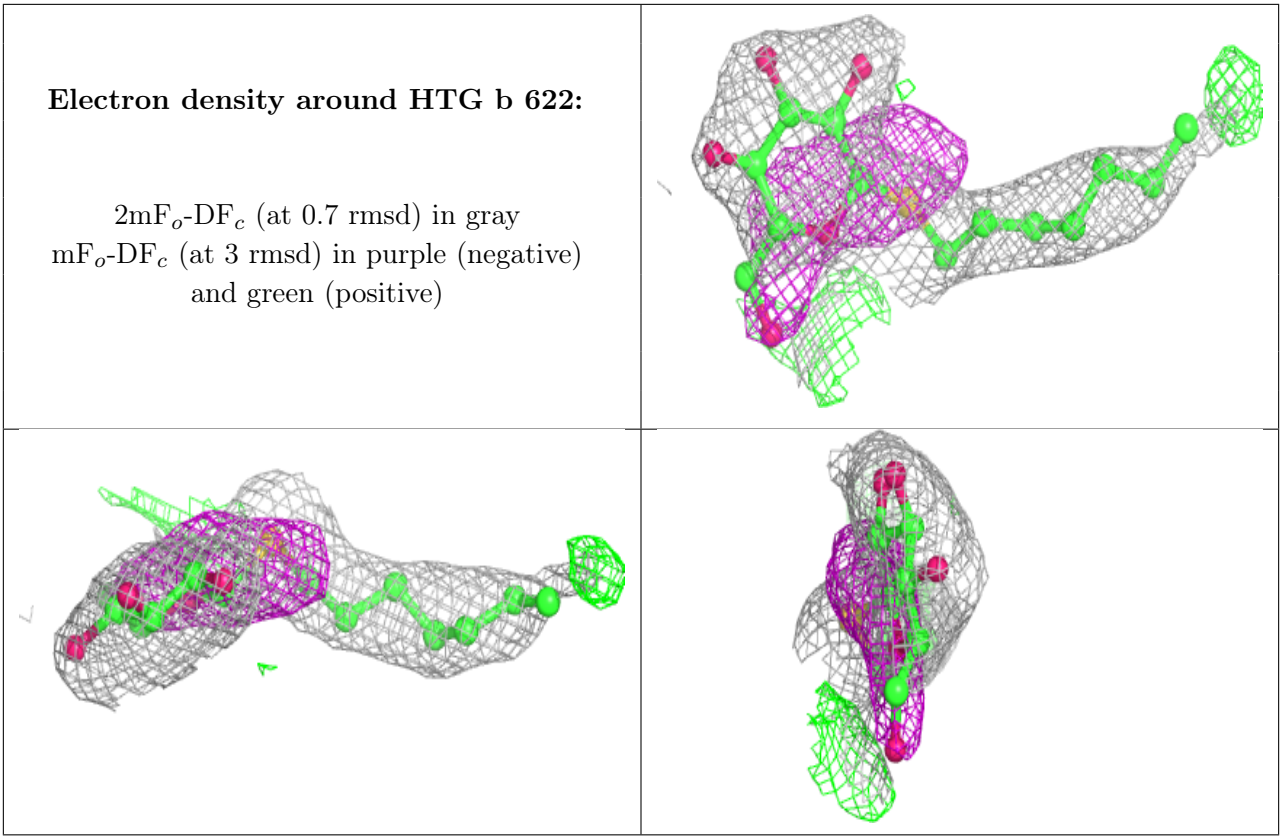
Electron density around SQD b 620:

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



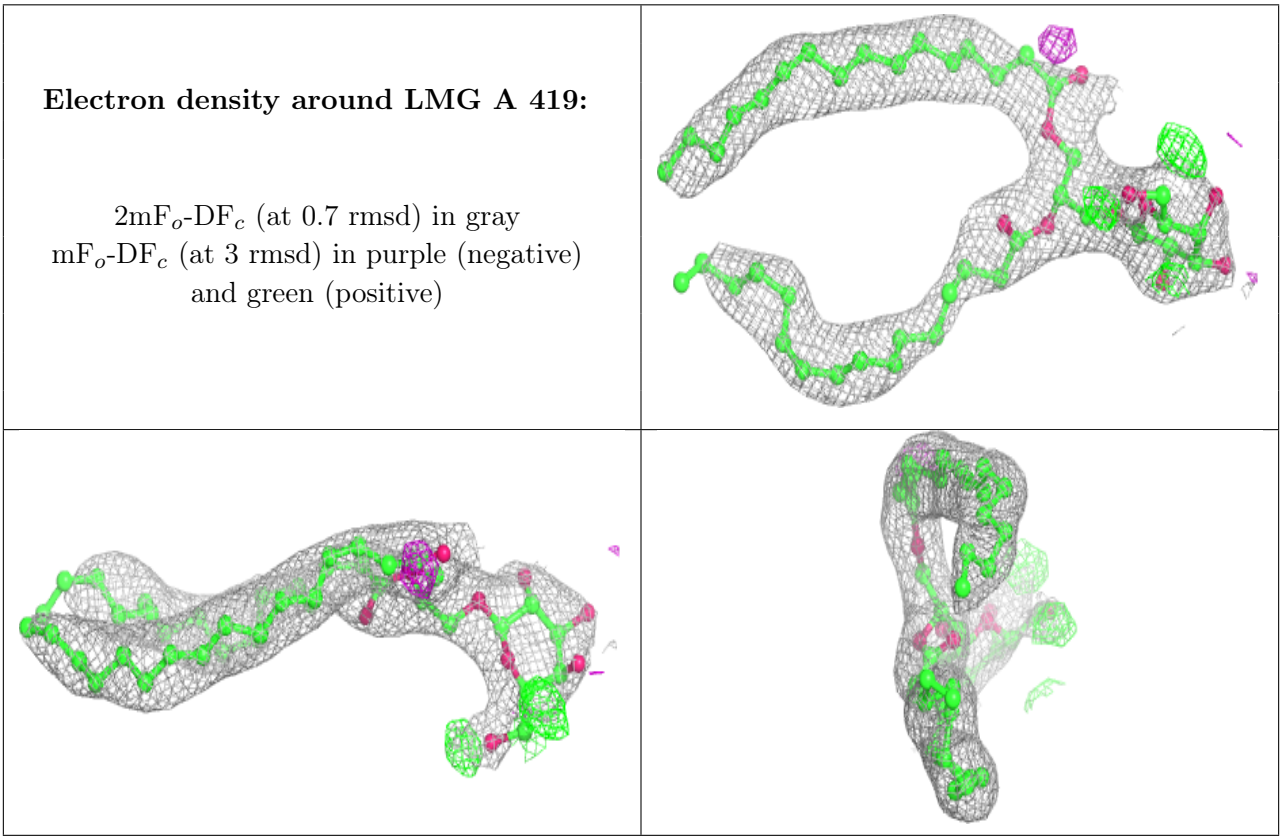
Electron density around HTG b 622:

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



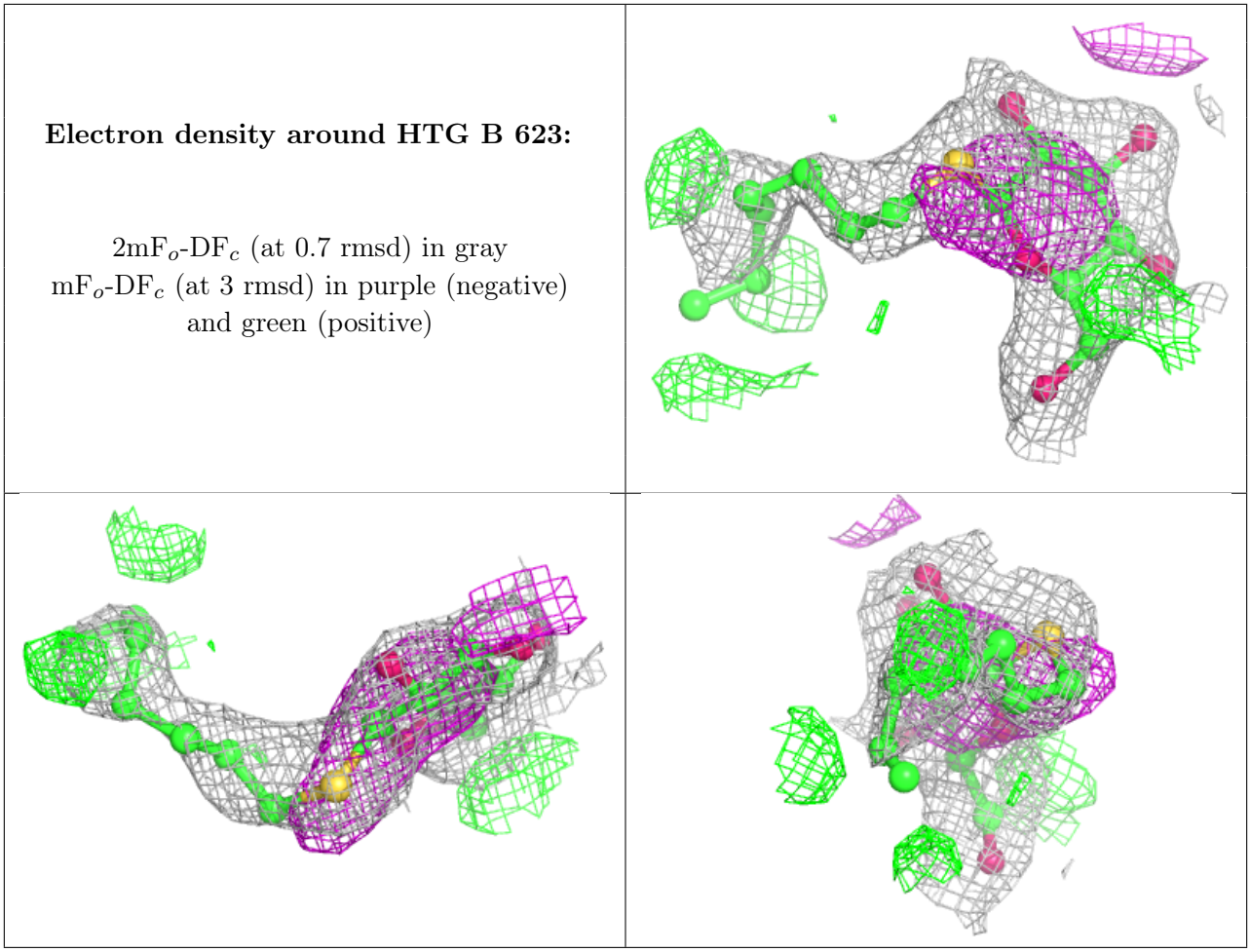
Electron density around LMG A 419:

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



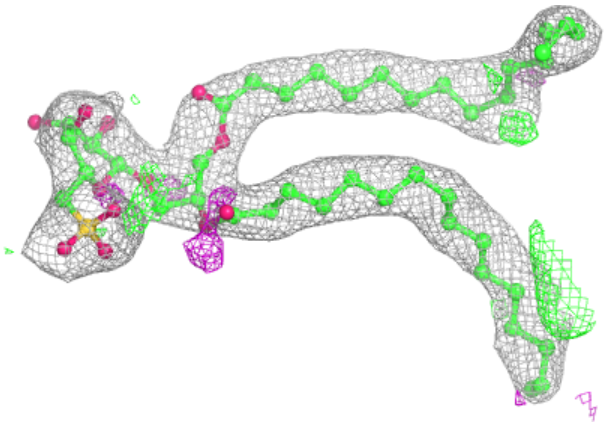
Electron density around HTG B 623:

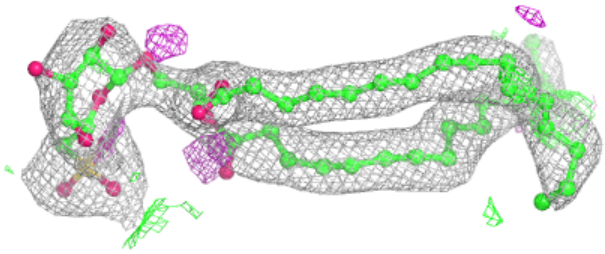
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

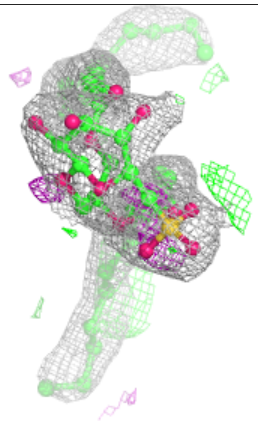


Electron density around SQD B 620:

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

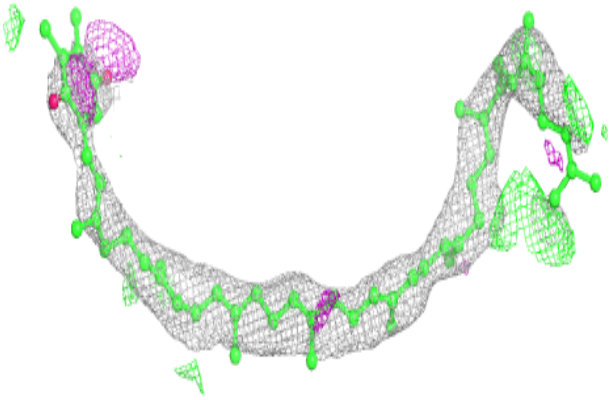


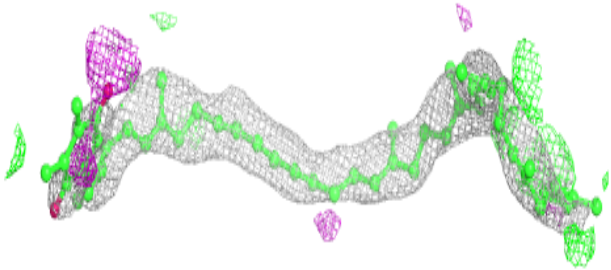


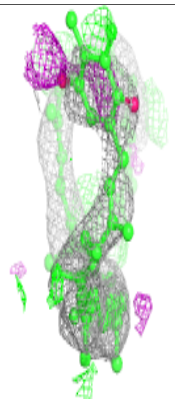


Electron density around PL9 A 414:

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

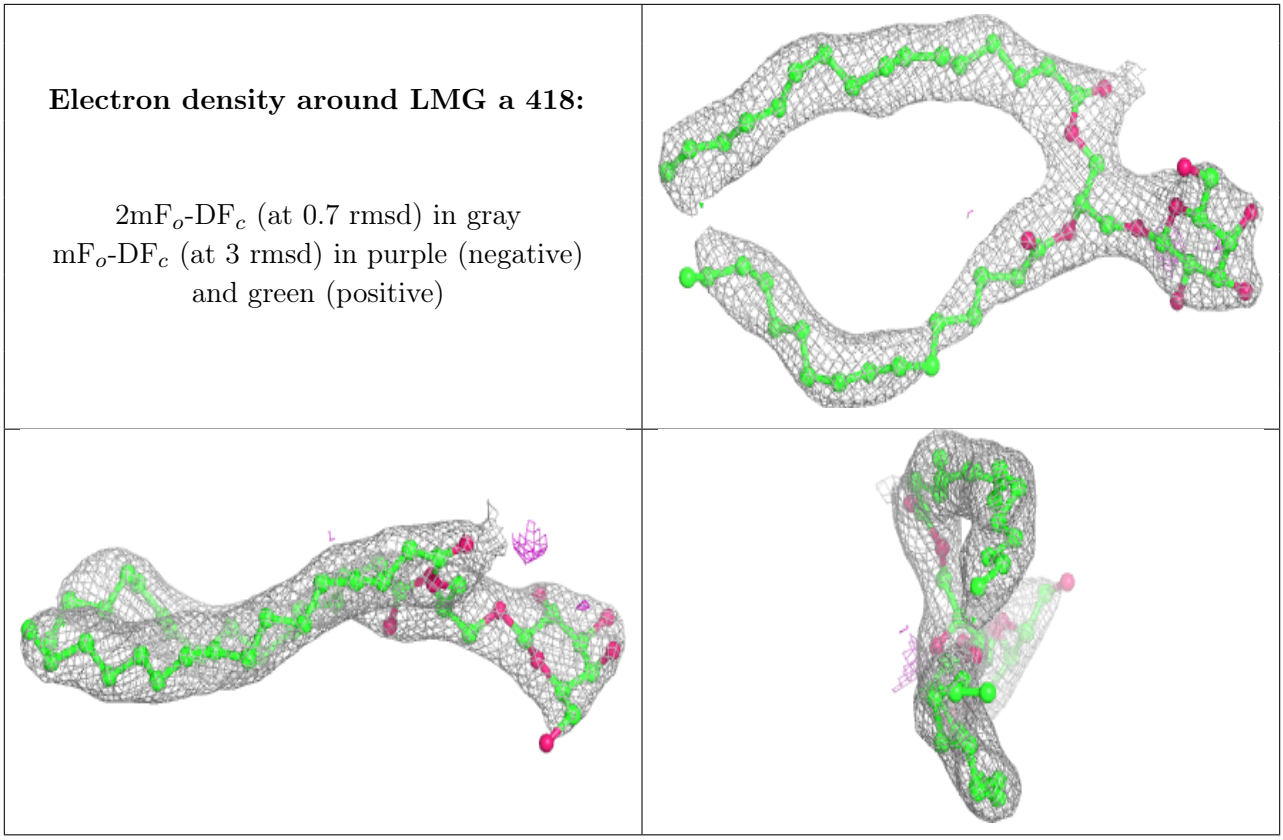






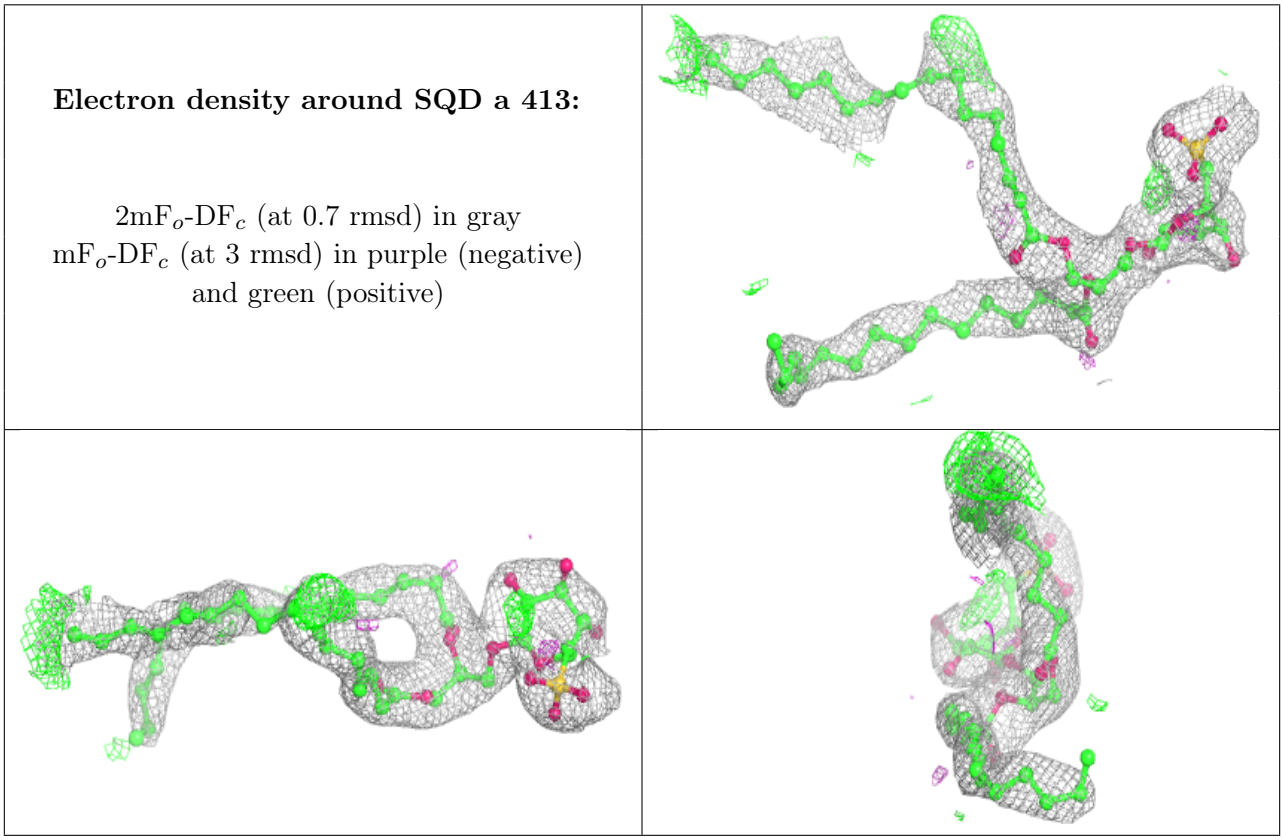
Electron density around LMG a 418:

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



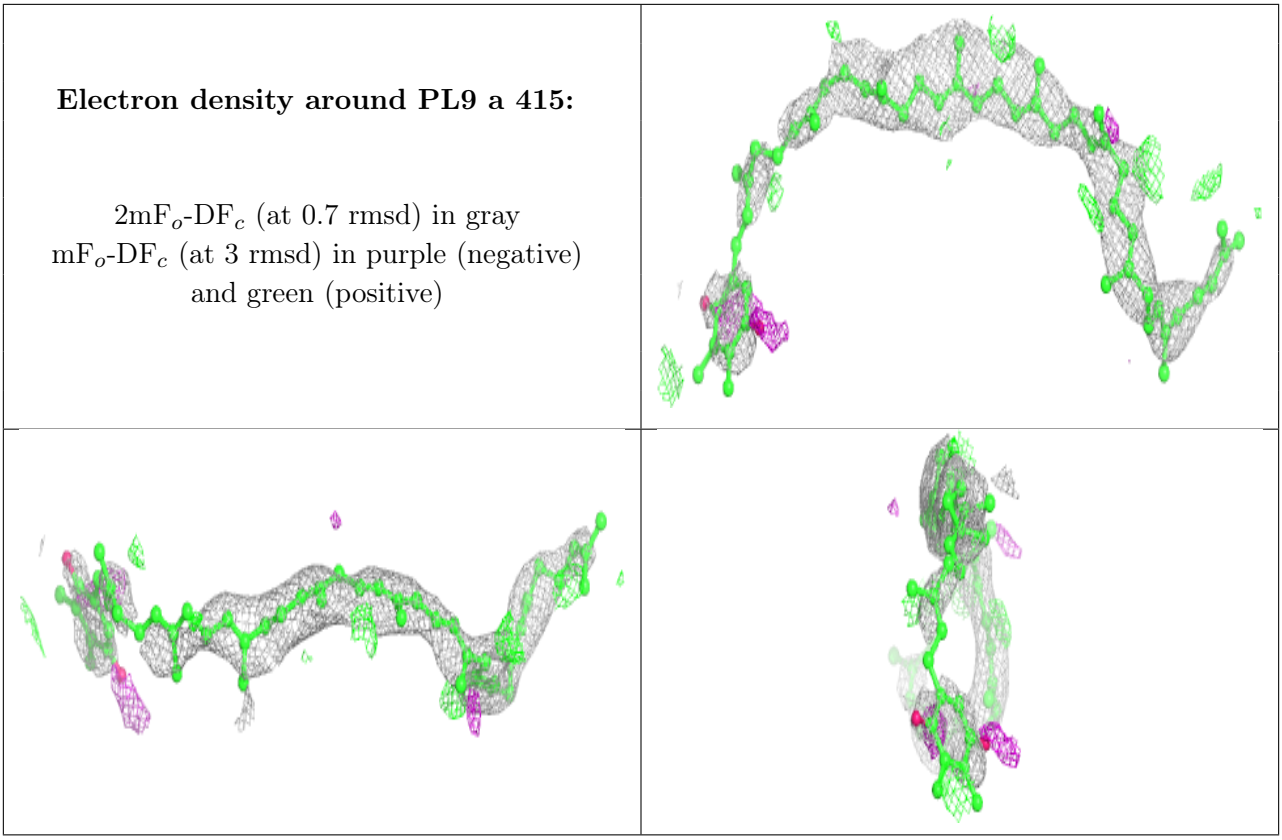
Electron density around SQD a 413:

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



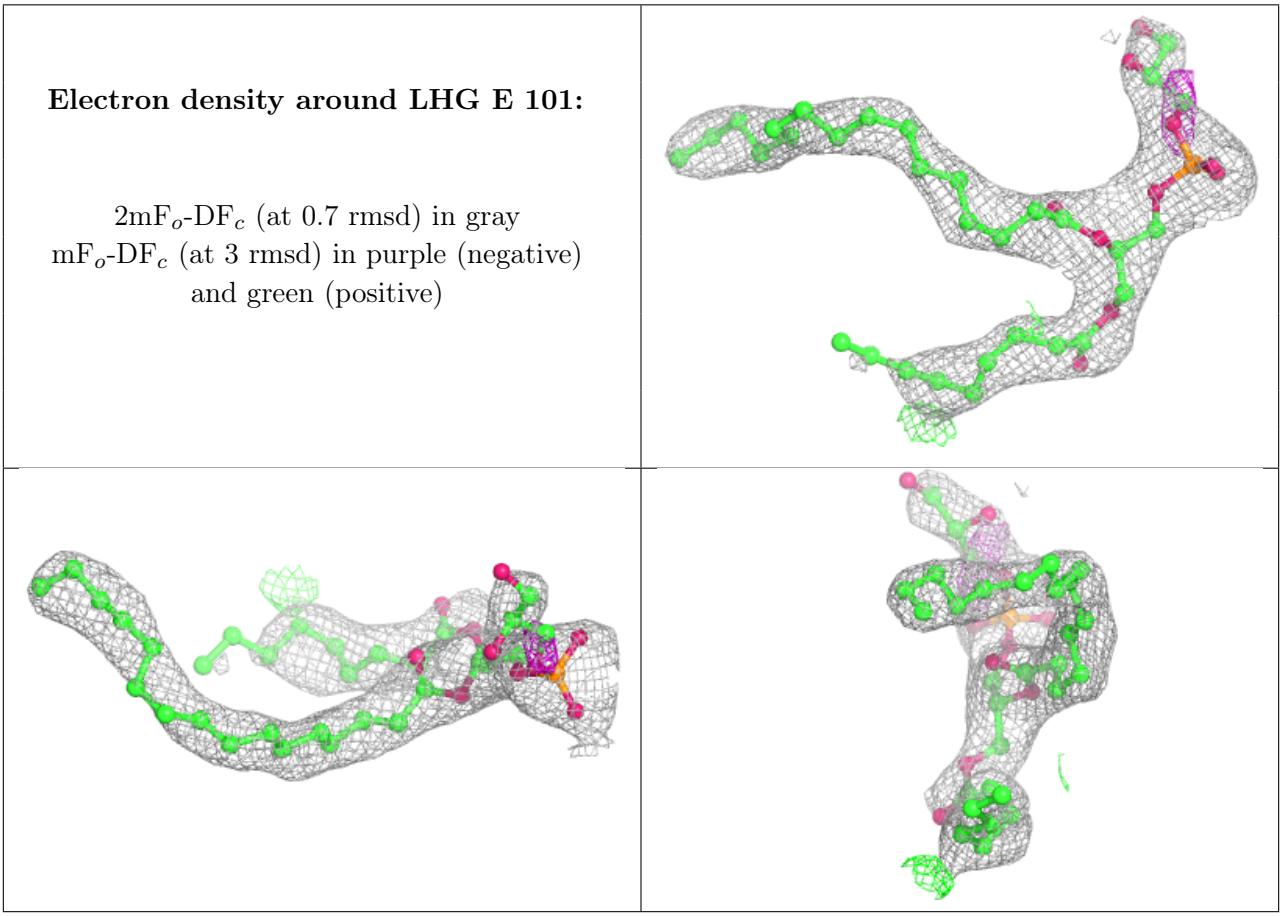
Electron density around PL9 a 415:

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



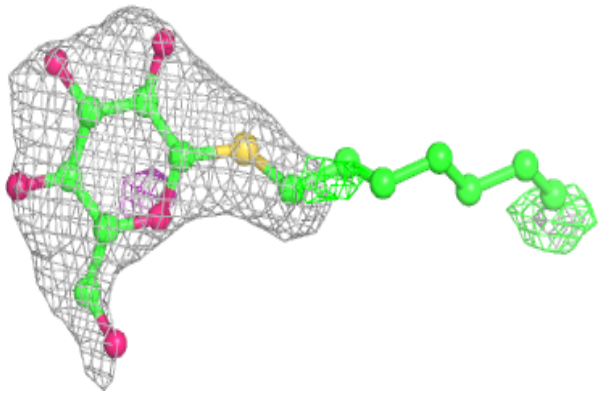
Electron density around LHG E 101:

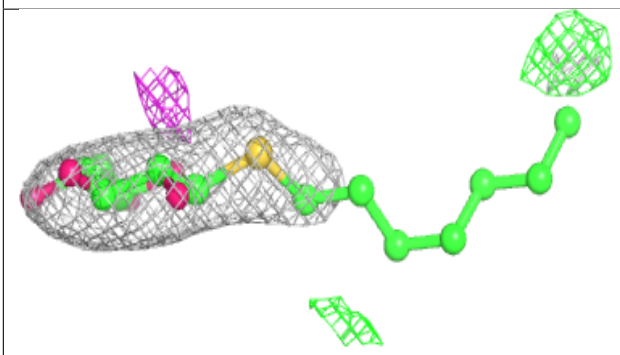
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

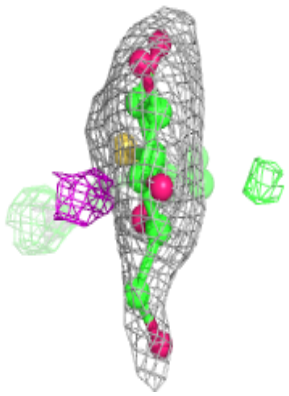


Electron density around HTG C 520:

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

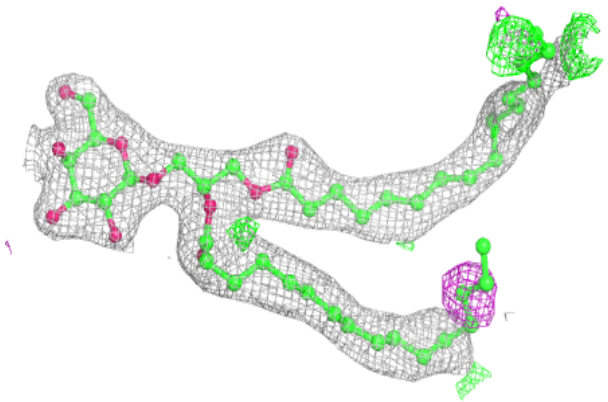


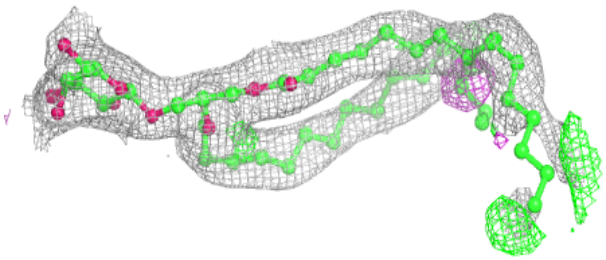


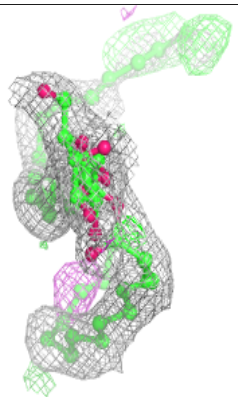


Electron density around LMG D 411:

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

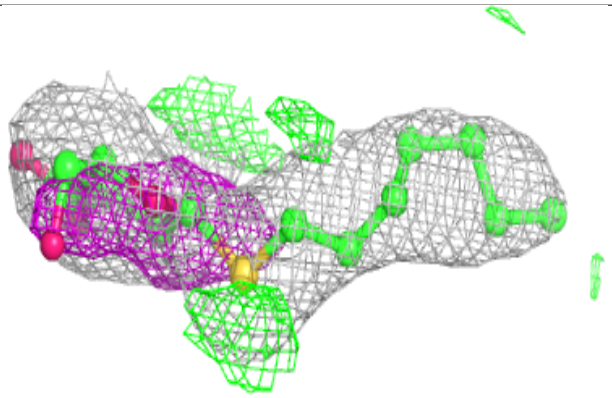


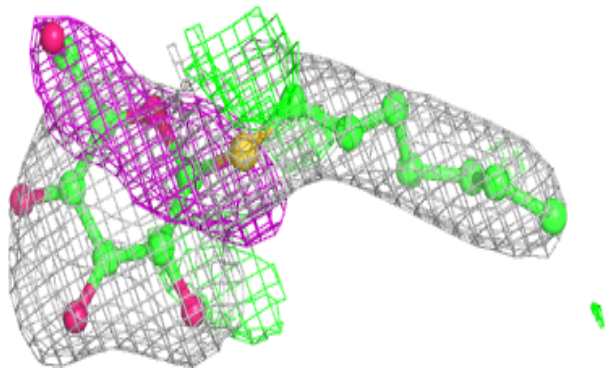


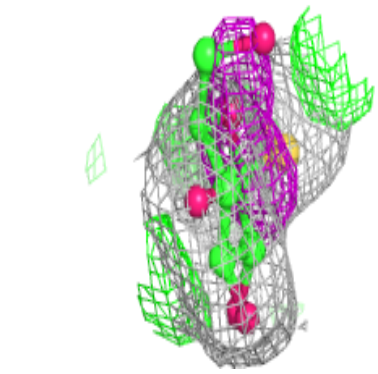


Electron density around HTG B 622:

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

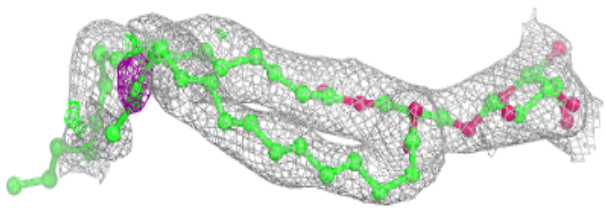


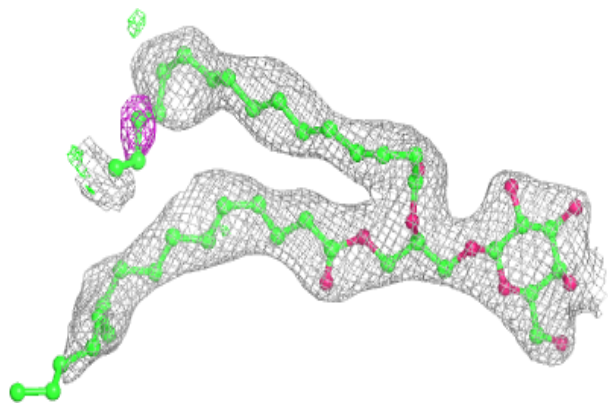


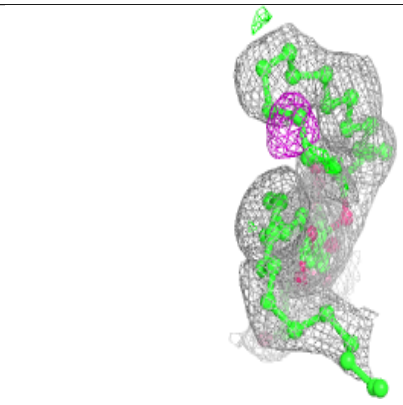


Electron density around LMG d 410:

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

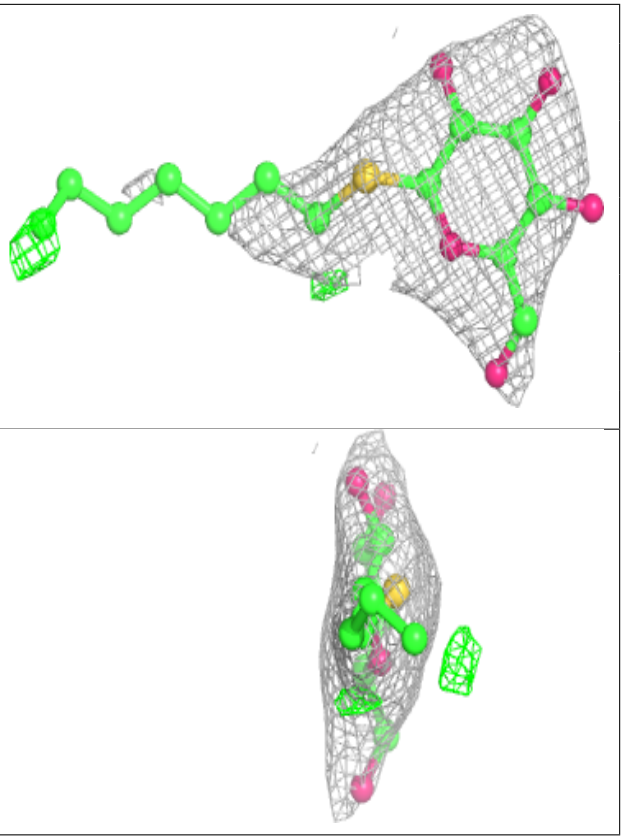


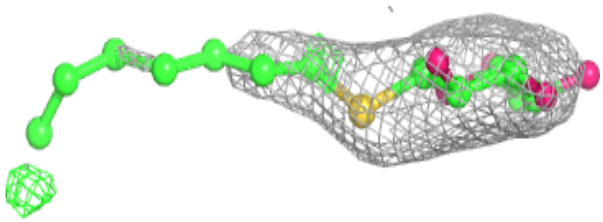




Electron density around HTG c 522:

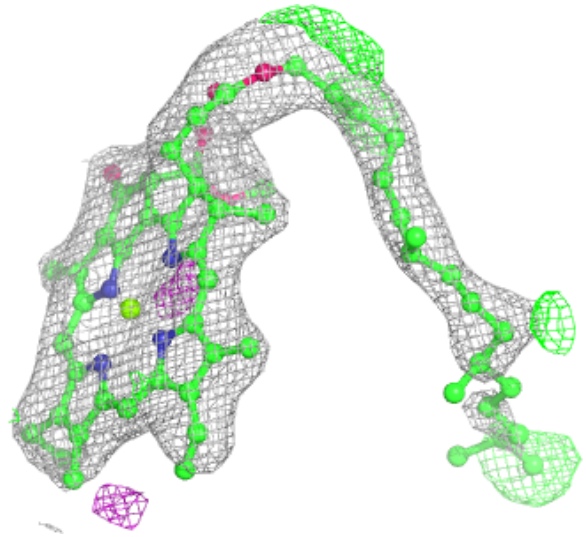
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

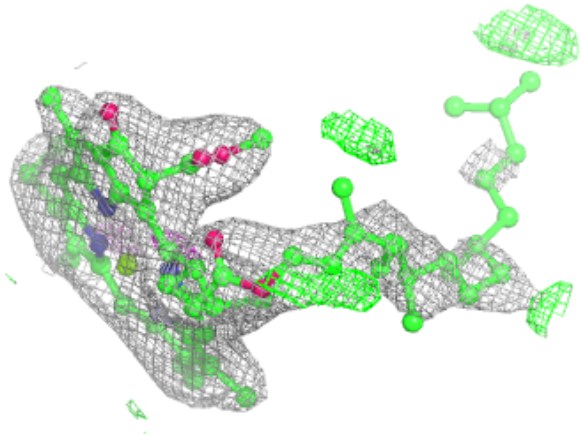


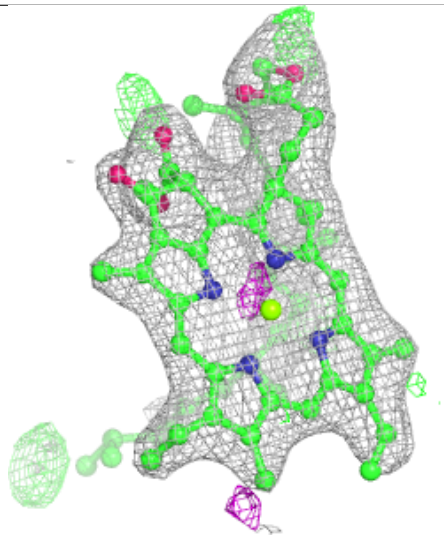


Electron density around CLA b 616:

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

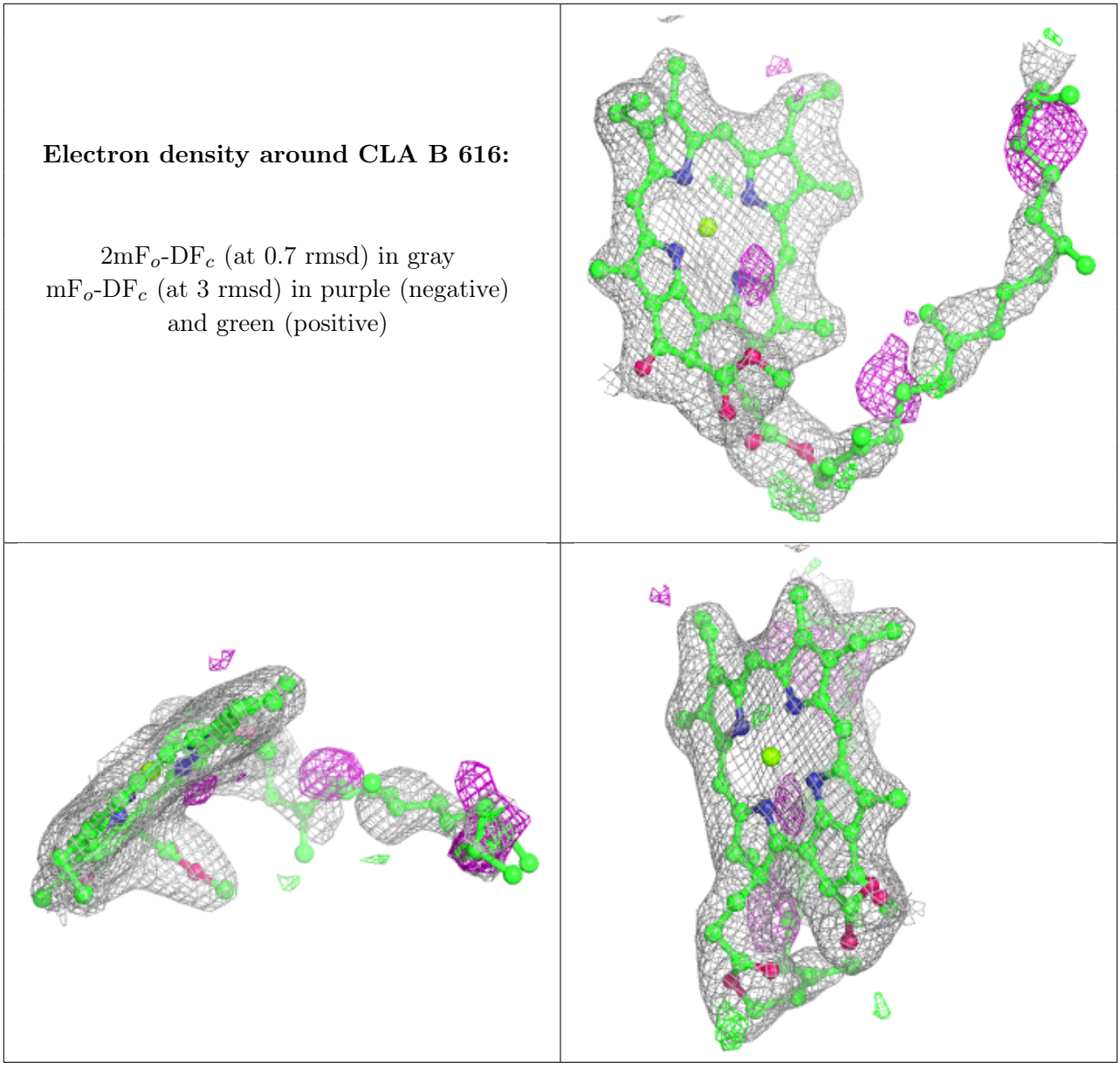






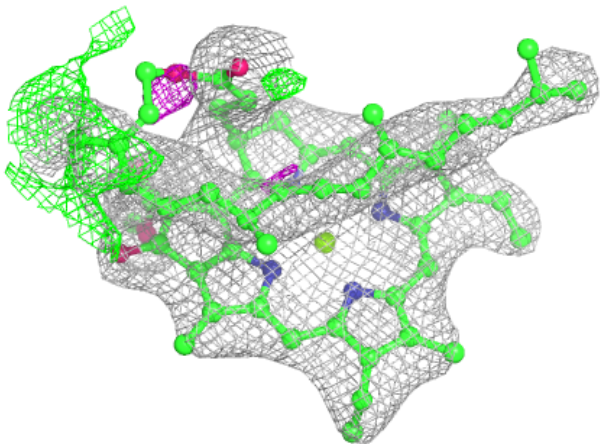
Electron density around CLA B 616:

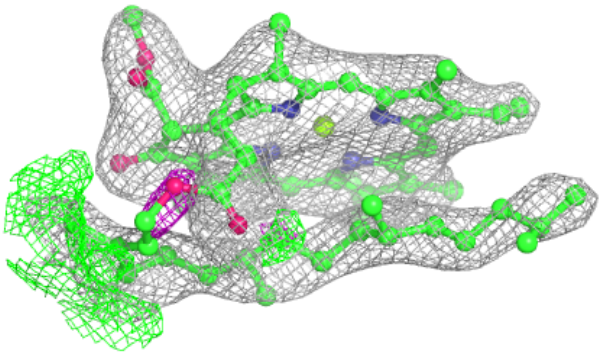
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

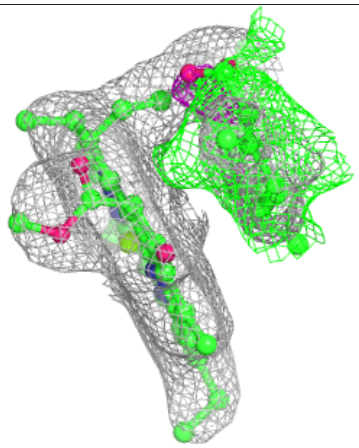


Electron density around CLA b 601:

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

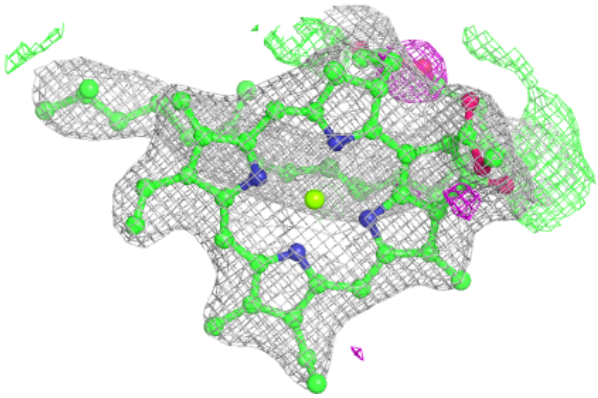


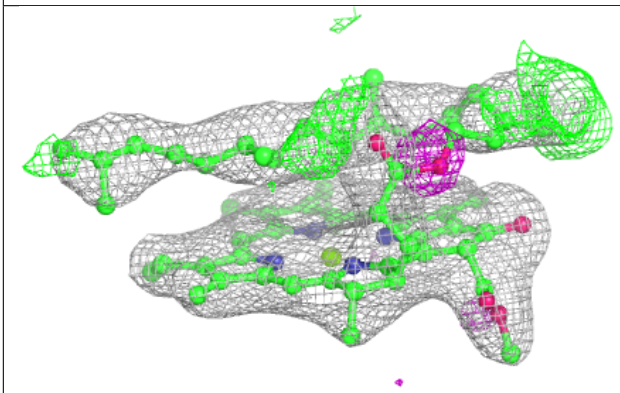


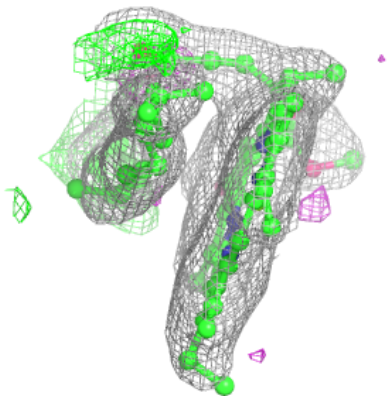


Electron density around CLA B 601:

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

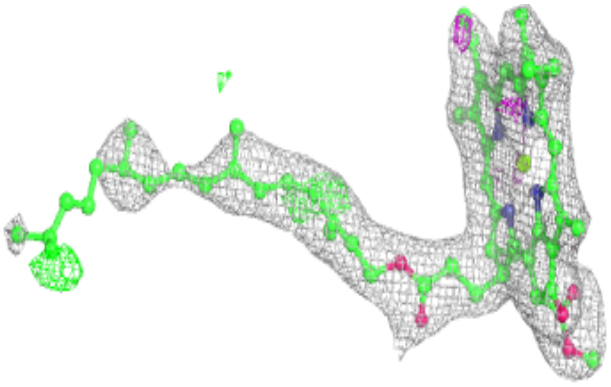


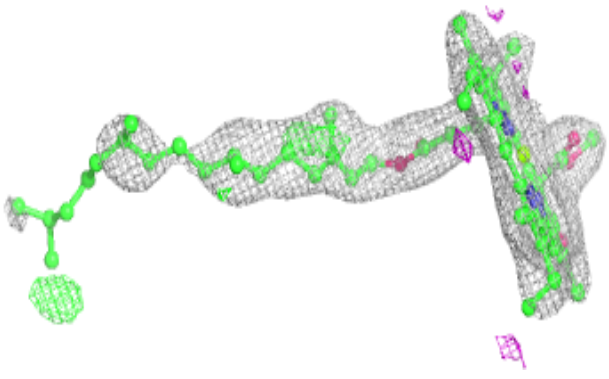


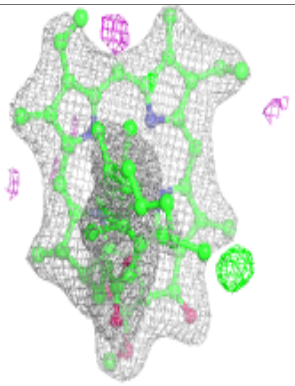


Electron density around CLA d 402:

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

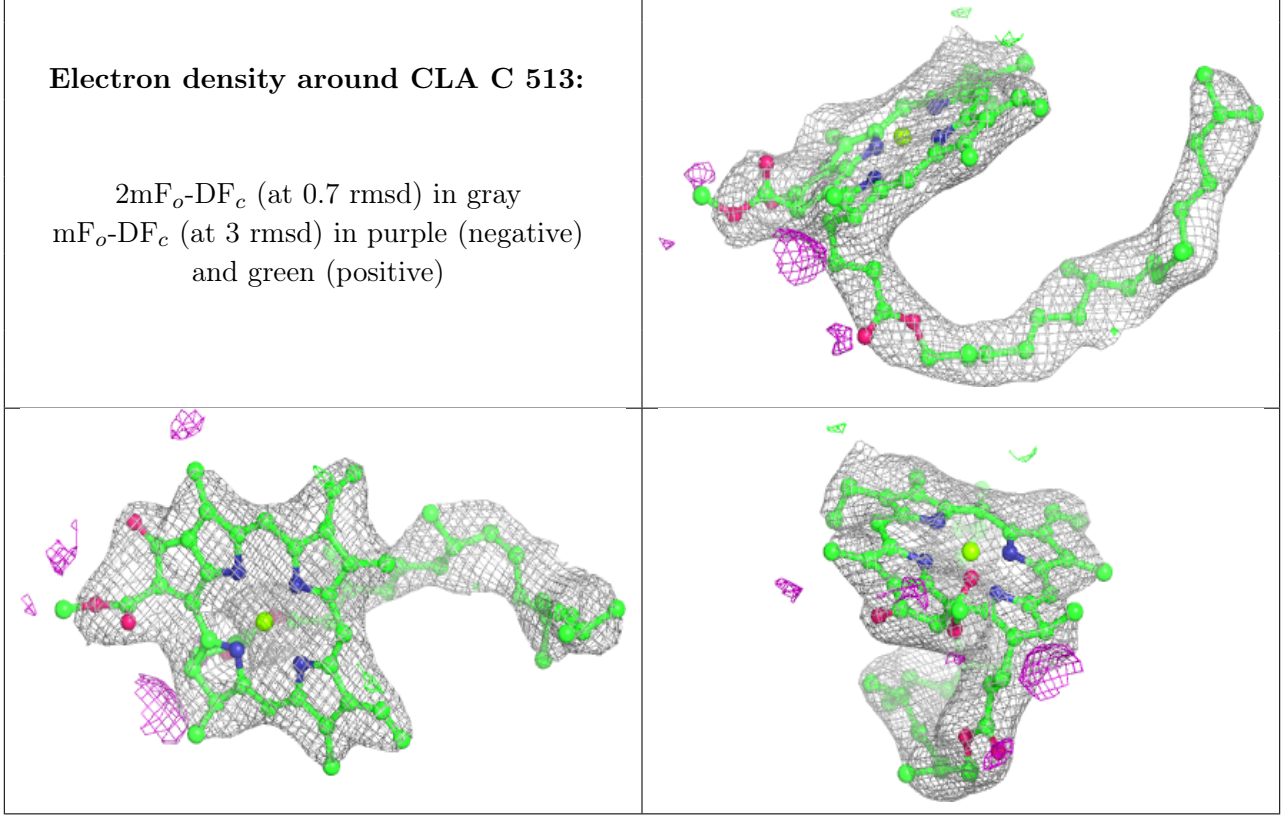






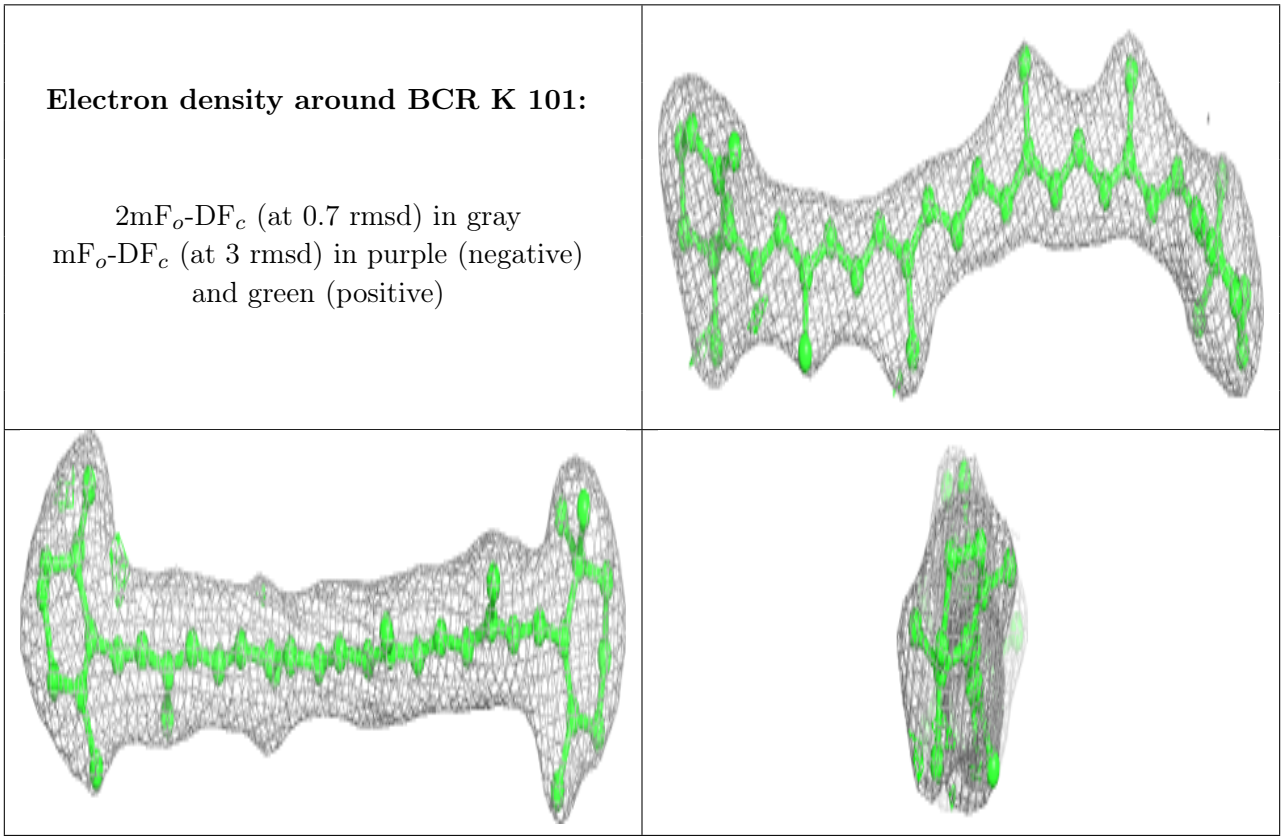
Electron density around CLA C 513:

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



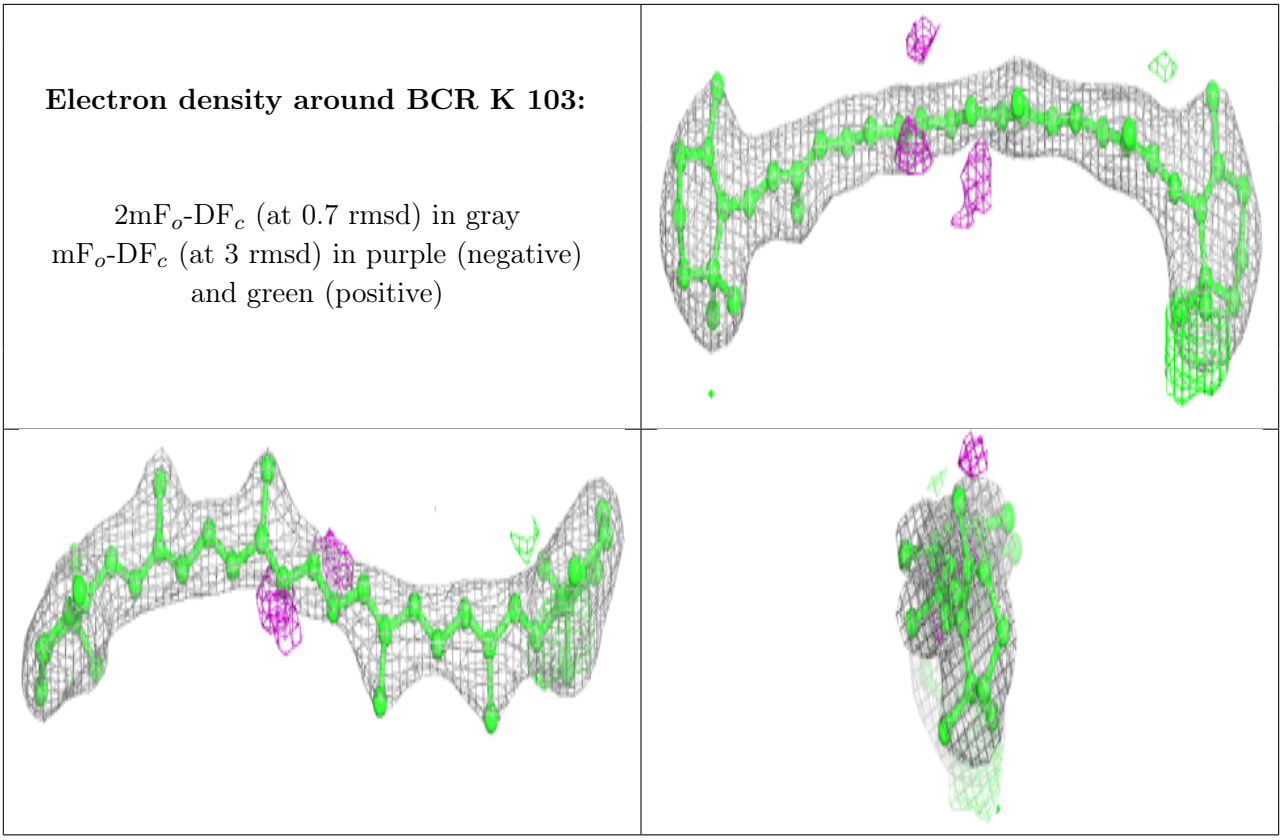
Electron density around BCR K 101:

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



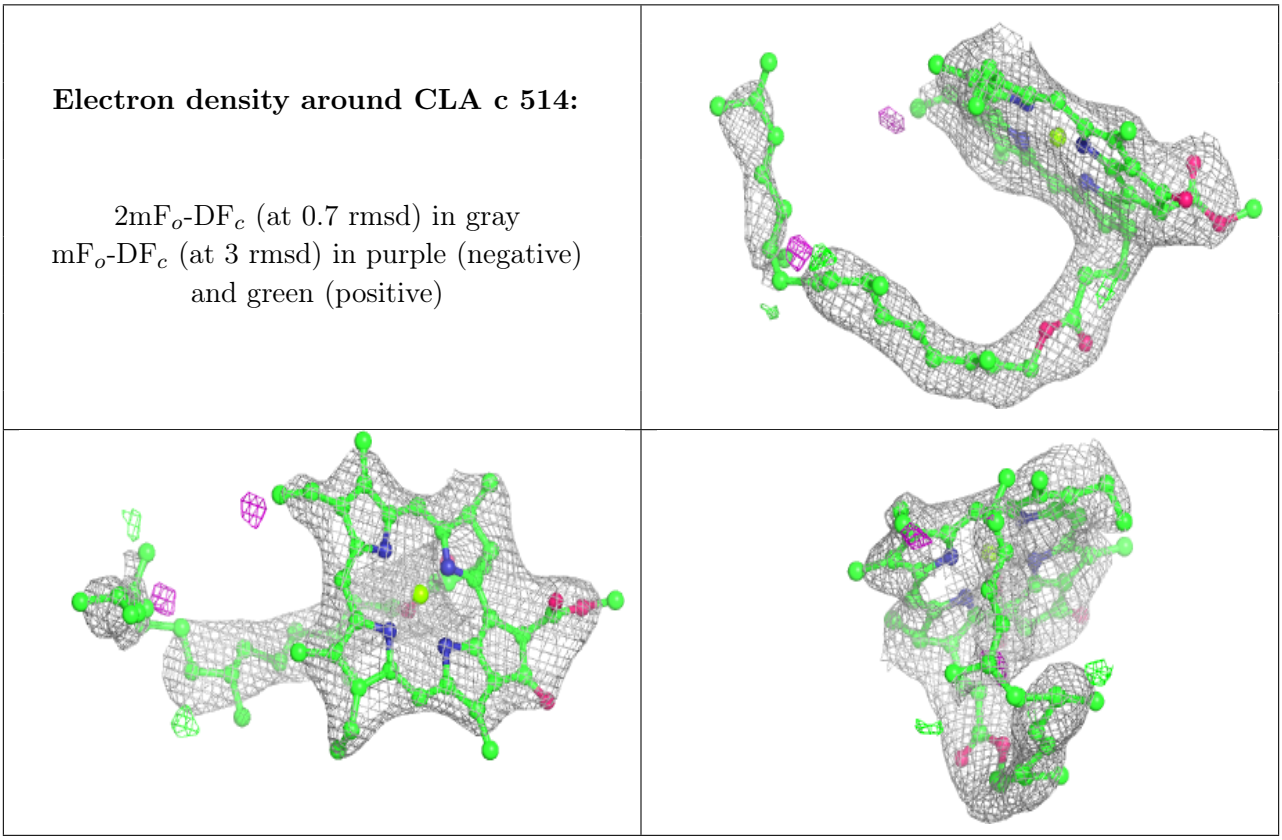
Electron density around BCR K 103:

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



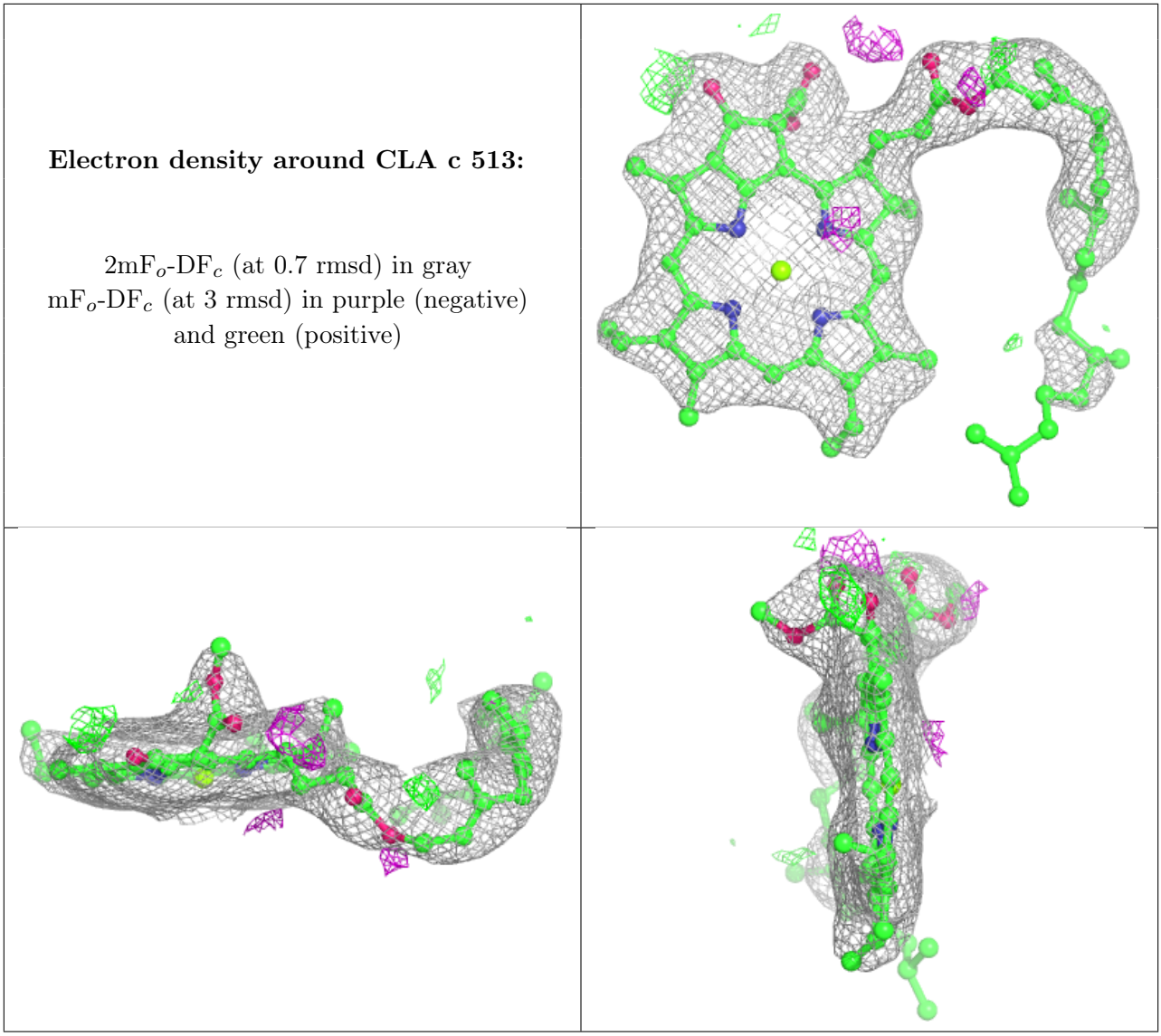
Electron density around CLA c 514:

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



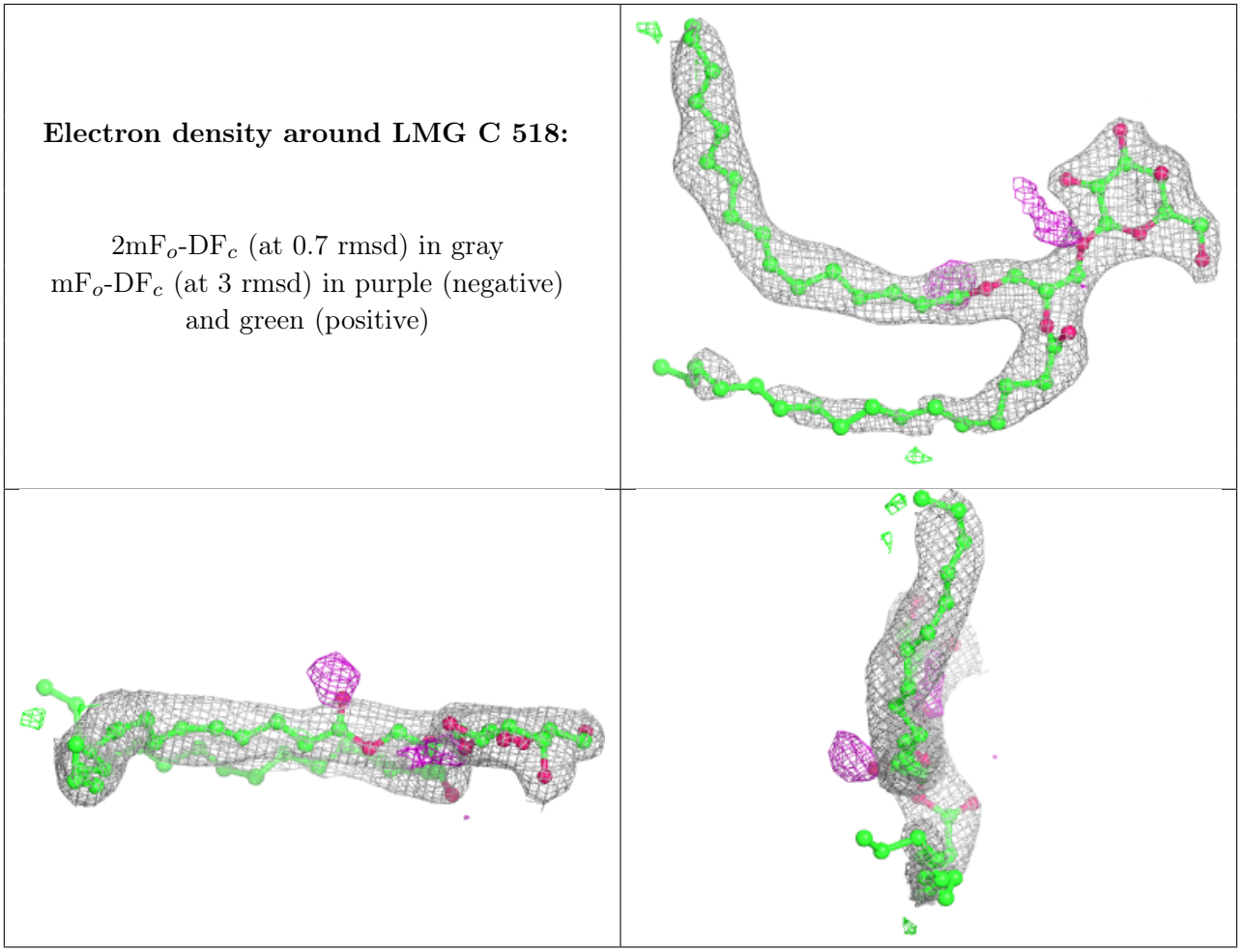
Electron density around CLA c 513:

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



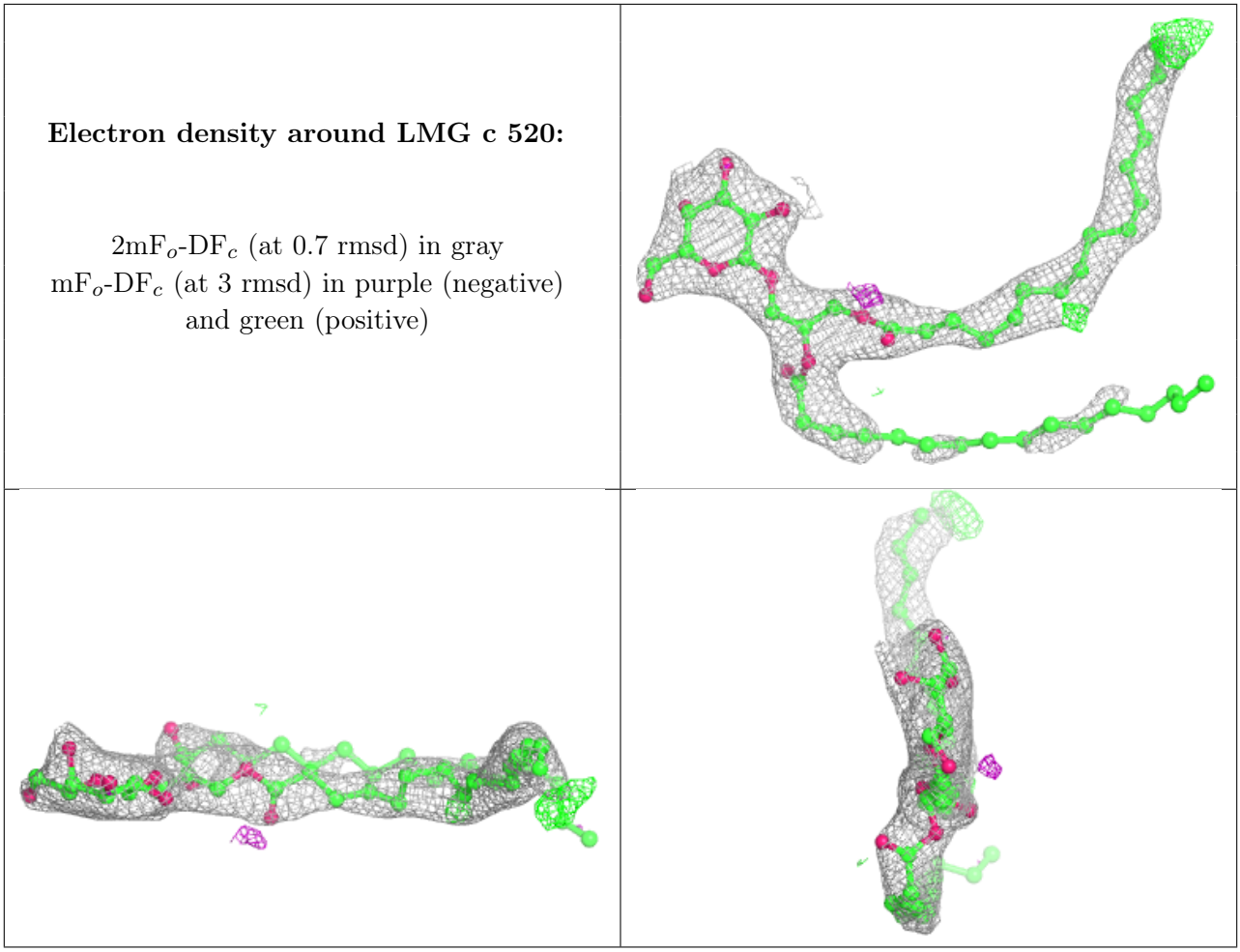
Electron density around LMG C 518:

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



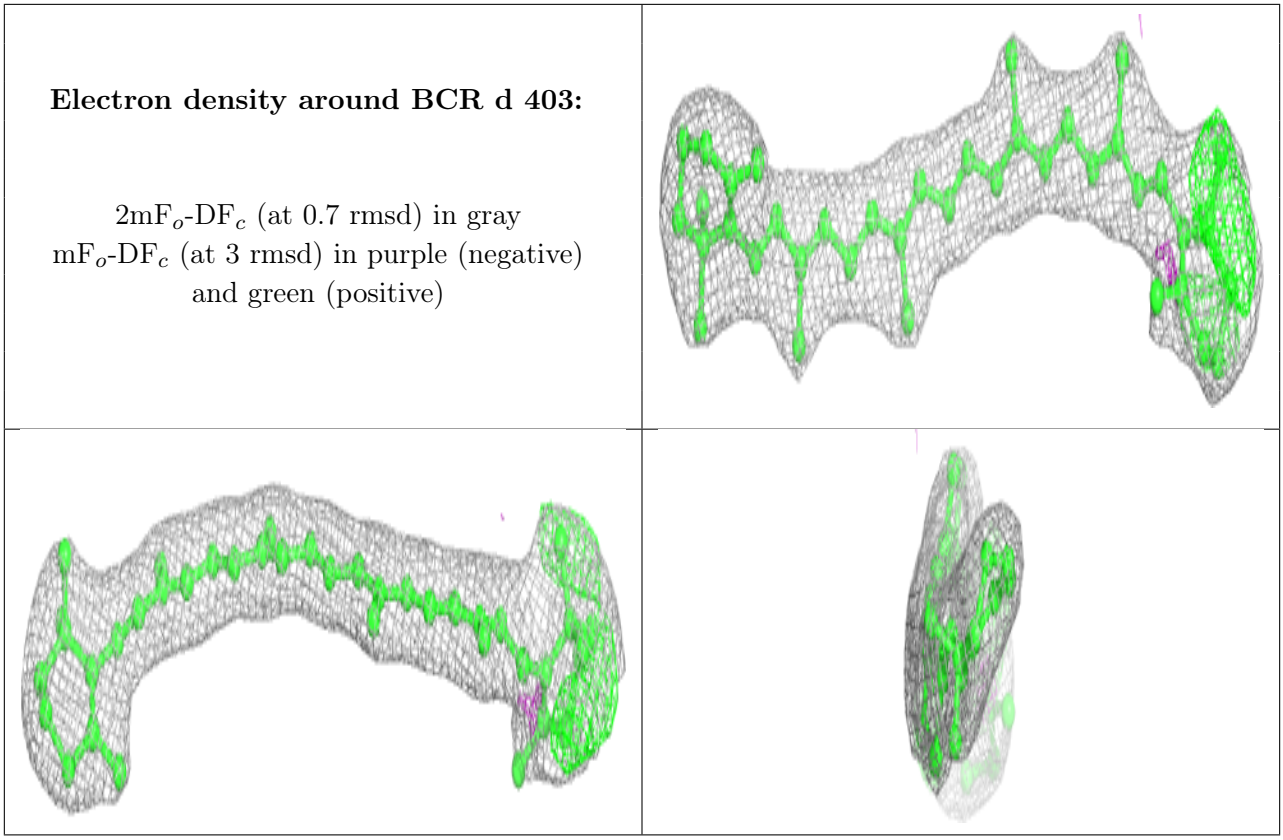
Electron density around LMG c 520:

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



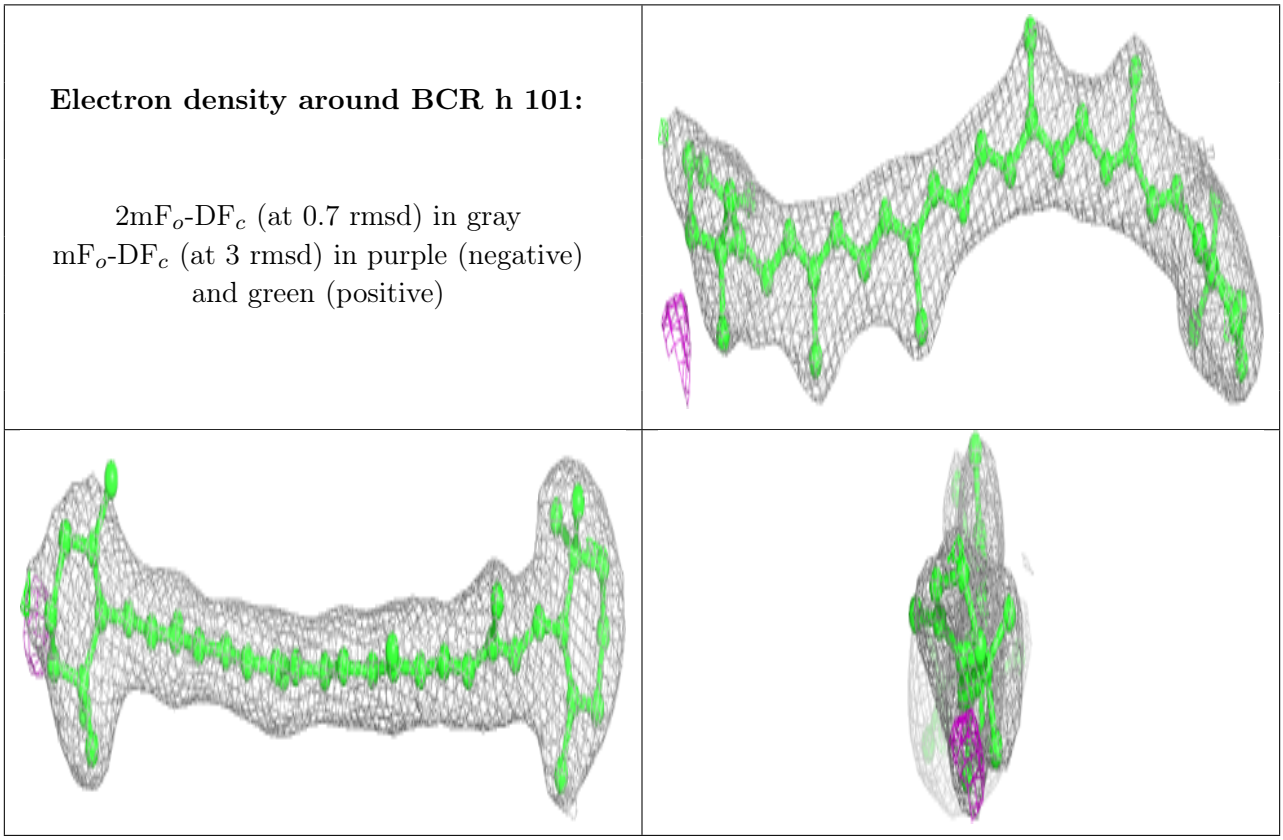
Electron density around BCR d 403:

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



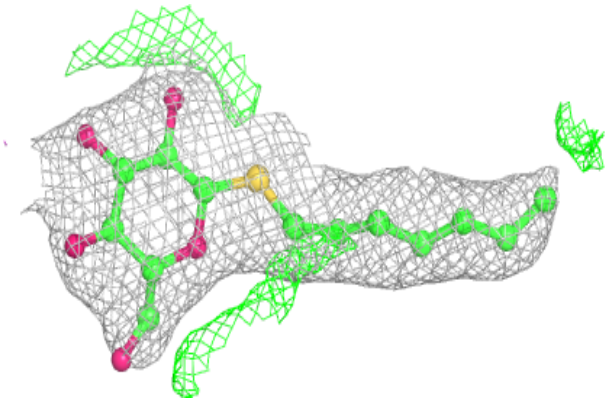
Electron density around BCR h 101:

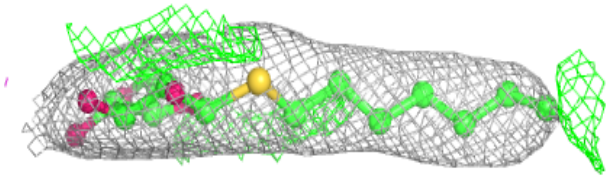
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

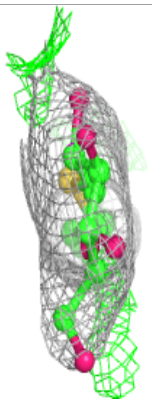


Electron density around HTG b 625:

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

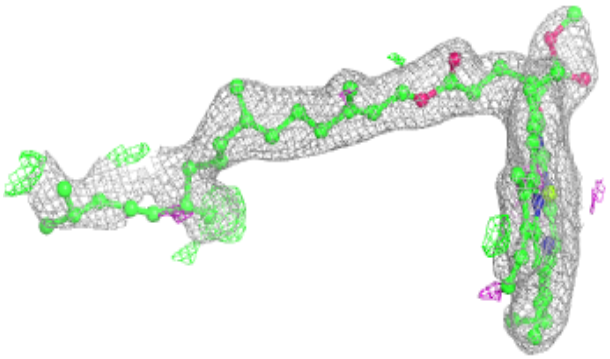


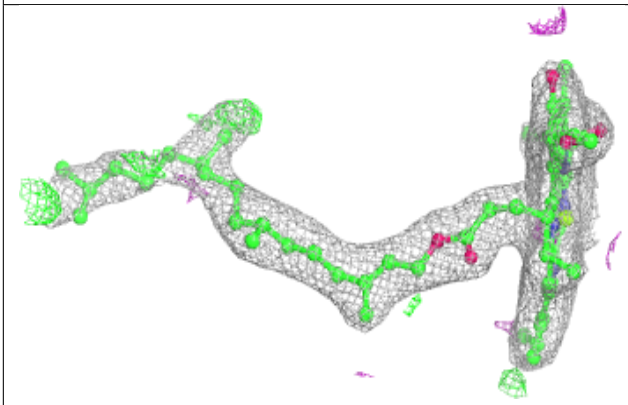


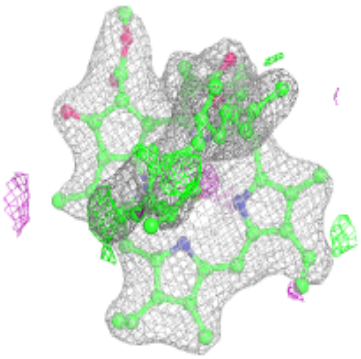


Electron density around CLA B 606:

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

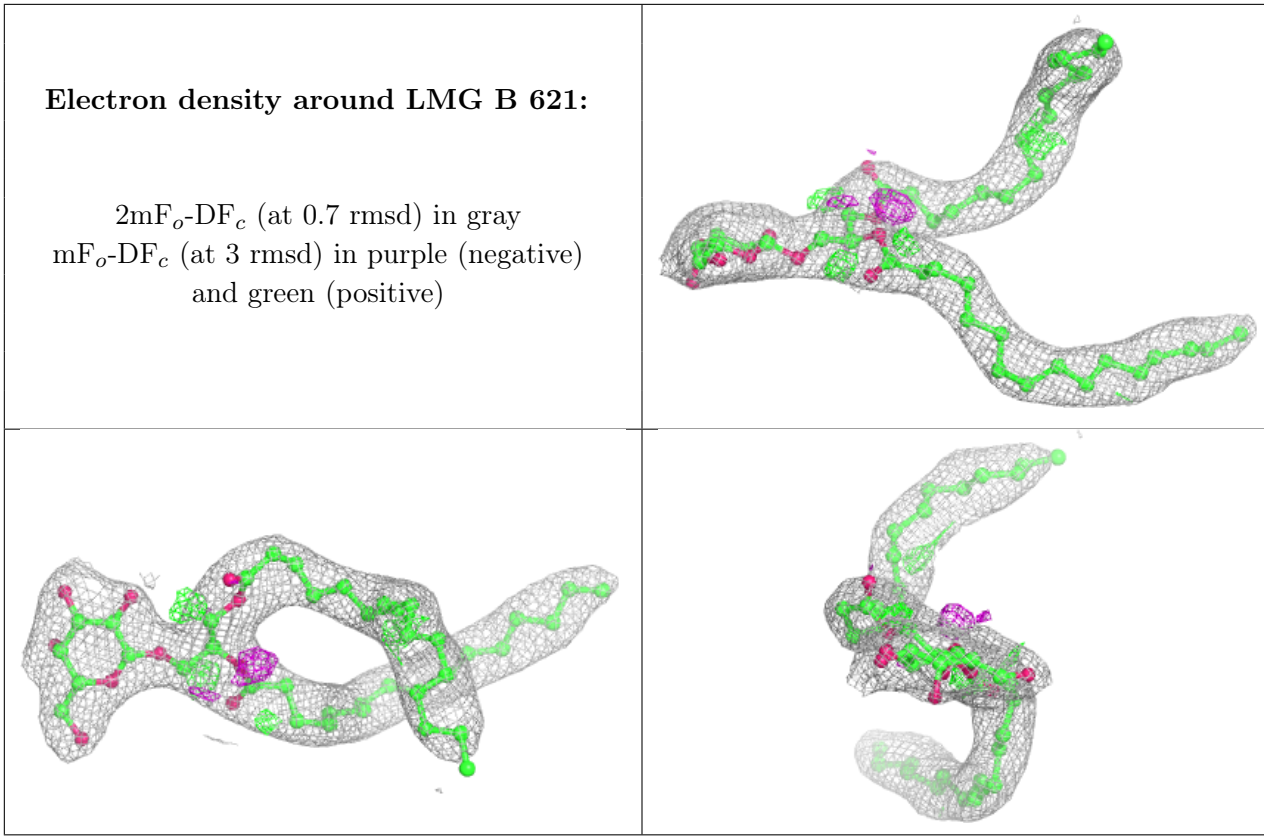






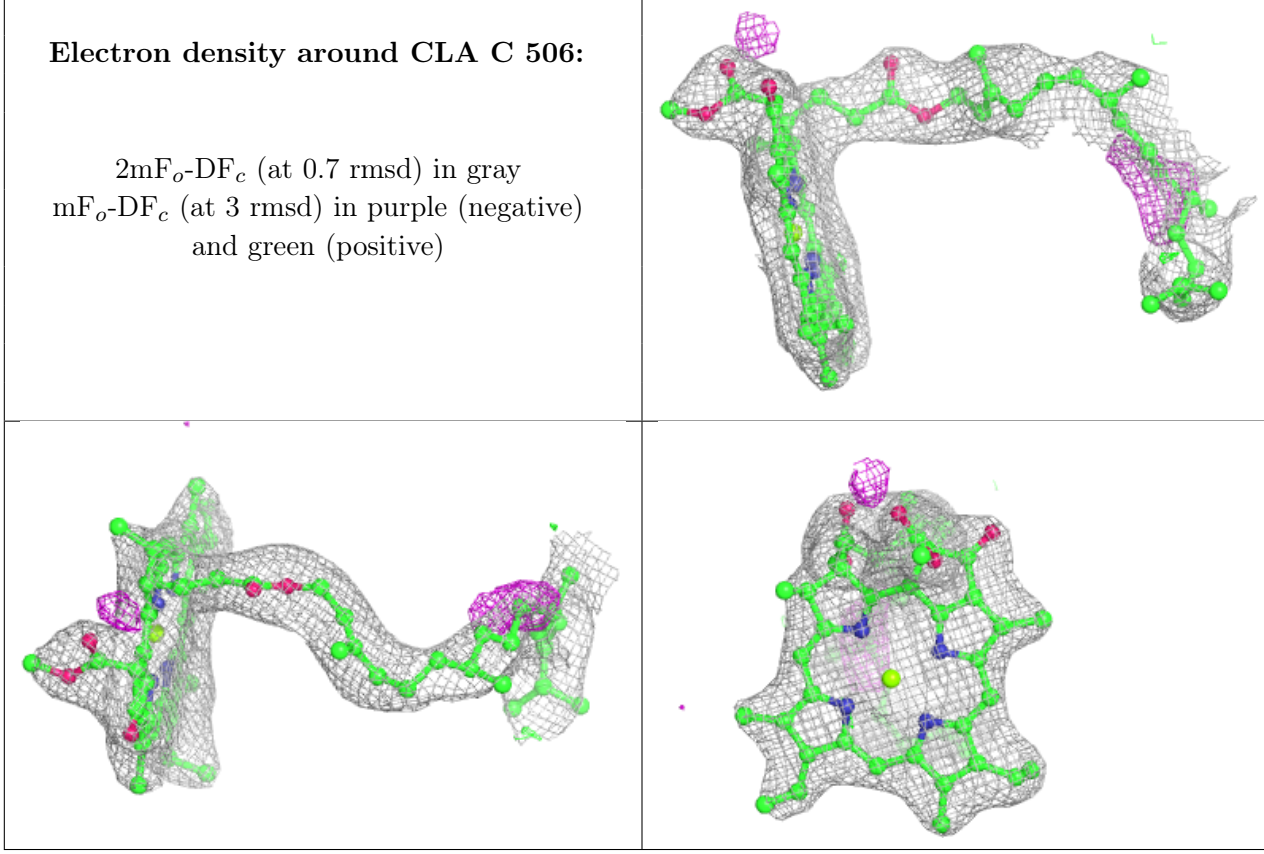
Electron density around LMG B 621:

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



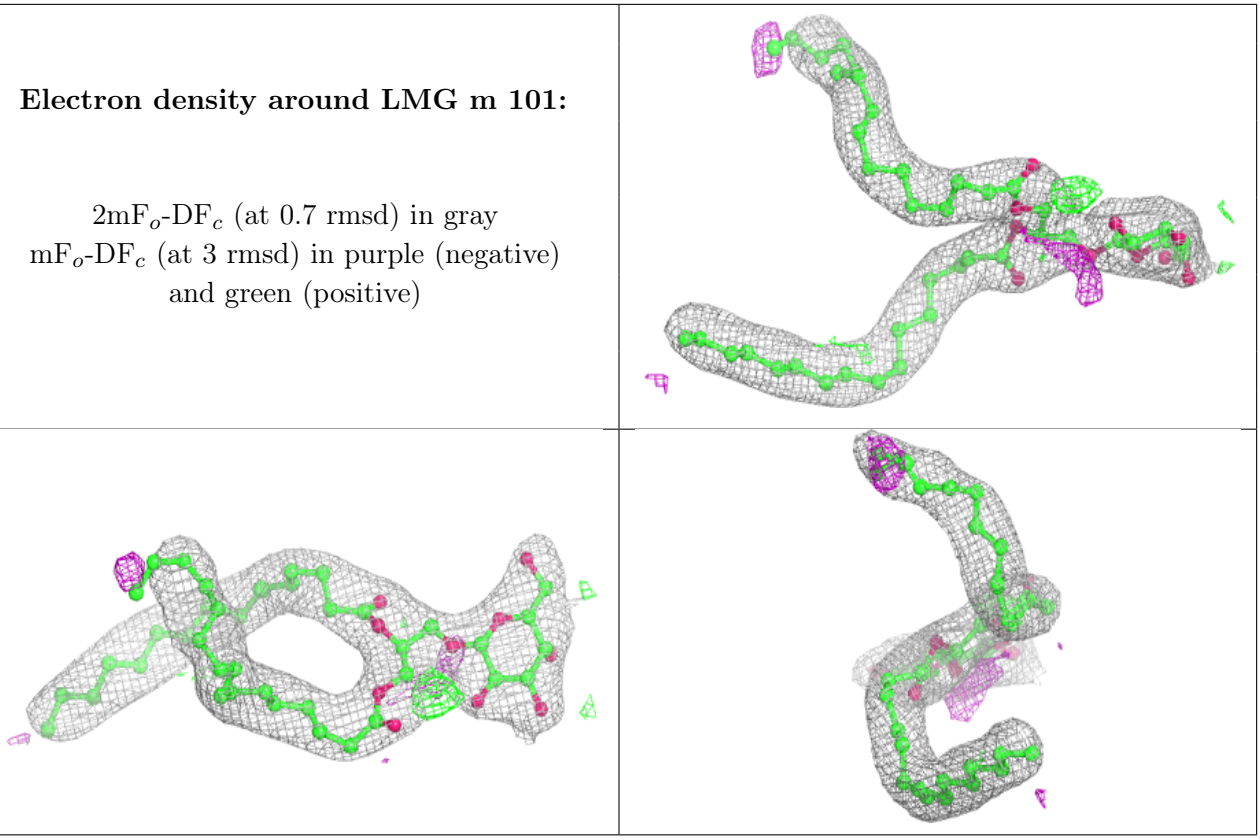
Electron density around CLA C 506:

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



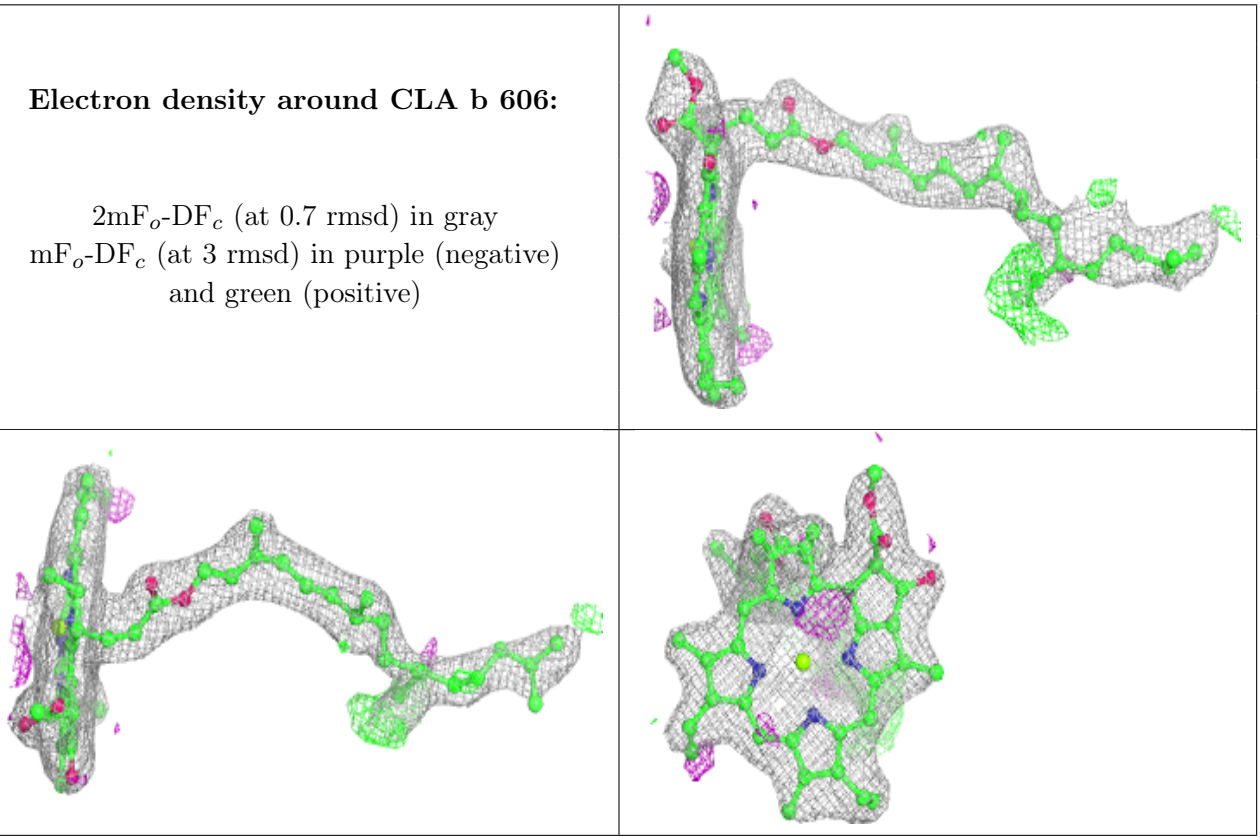
Electron density around LMG m 101:

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



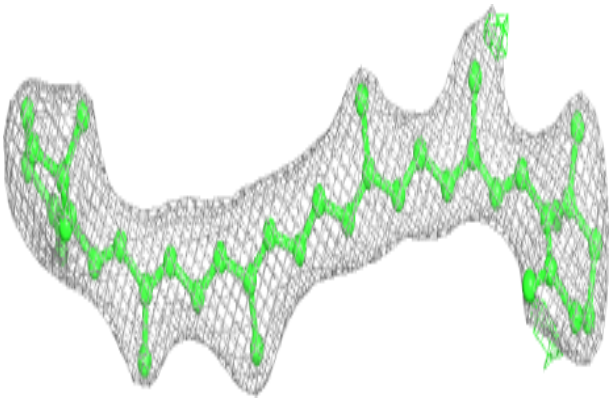
Electron density around CLA b 606:

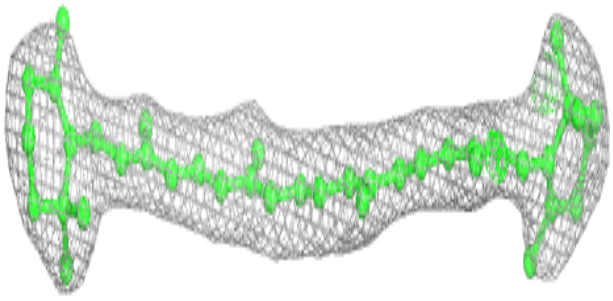
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

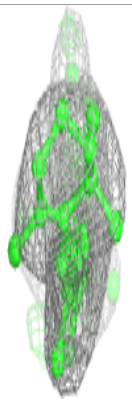


Electron density around BCR Y 101:

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

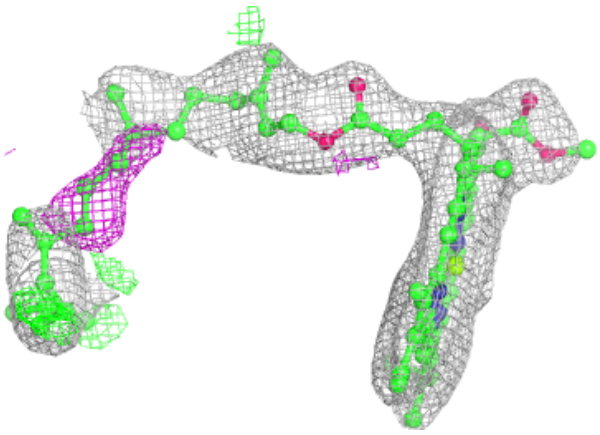


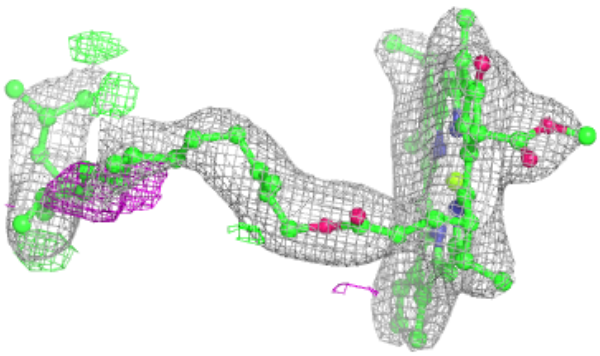


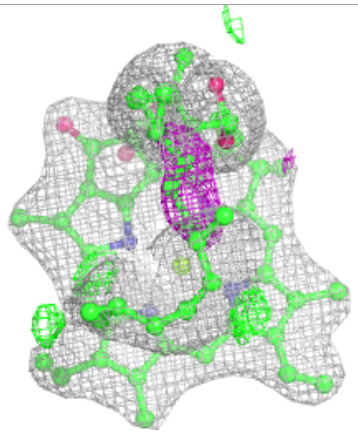


Electron density around CLA c 507:

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

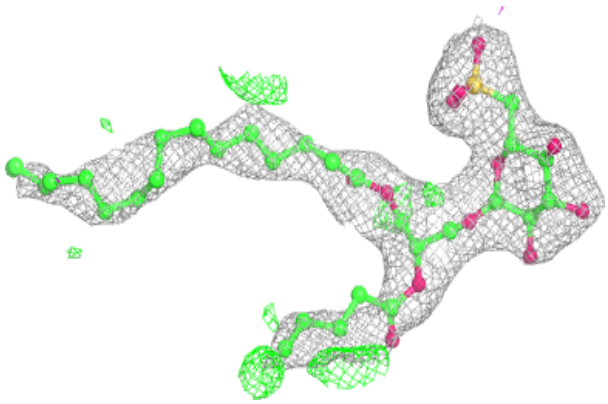


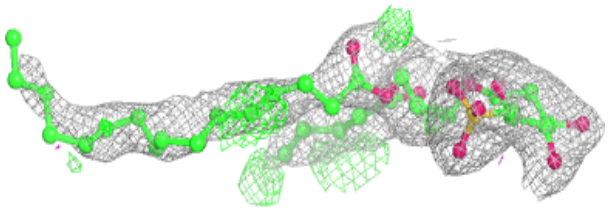


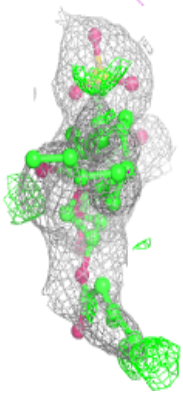


Electron density around SQD F 103:

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

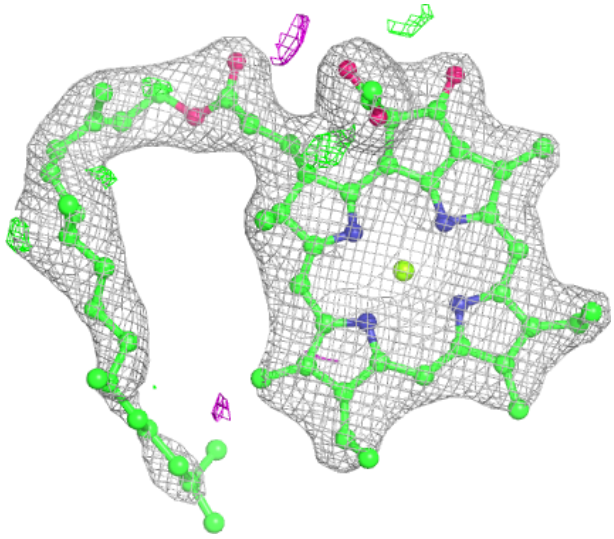


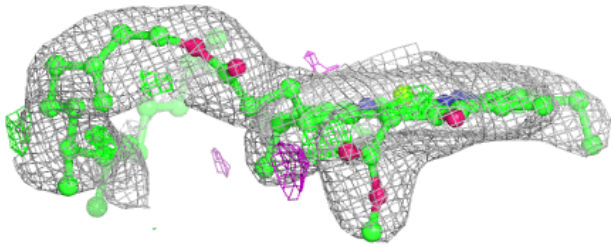


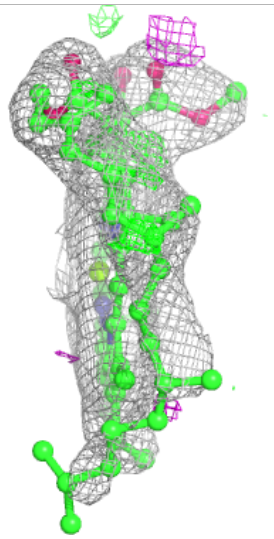


Electron density around CLA C 512:

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

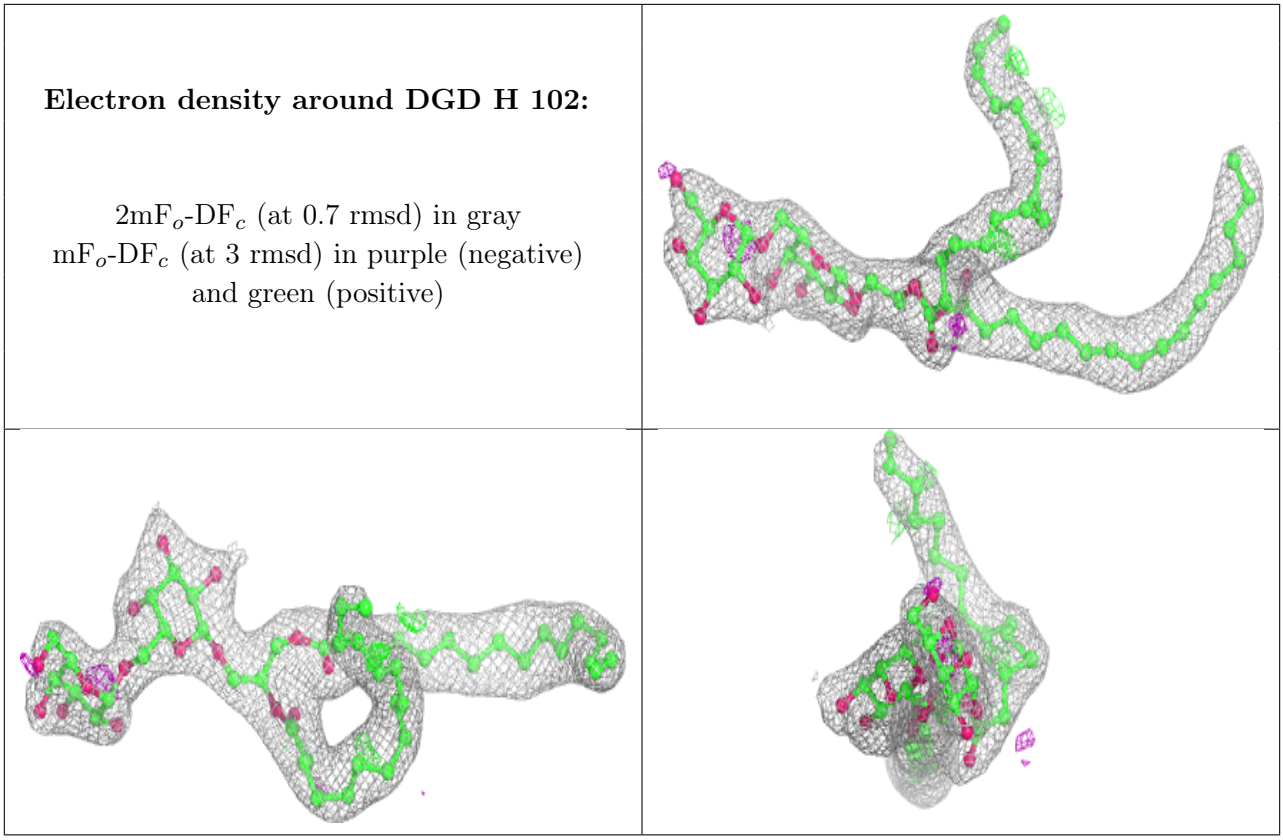






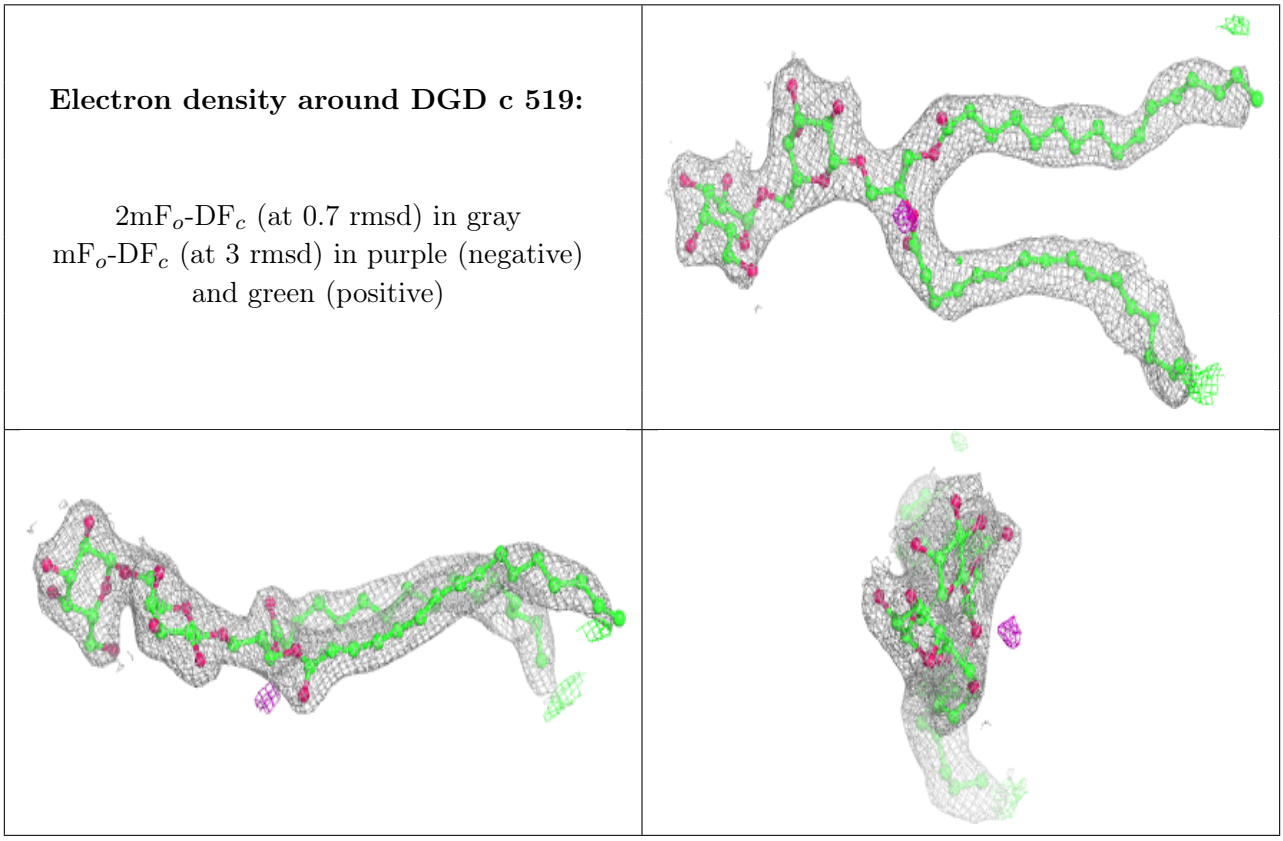
Electron density around DGD H 102:

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



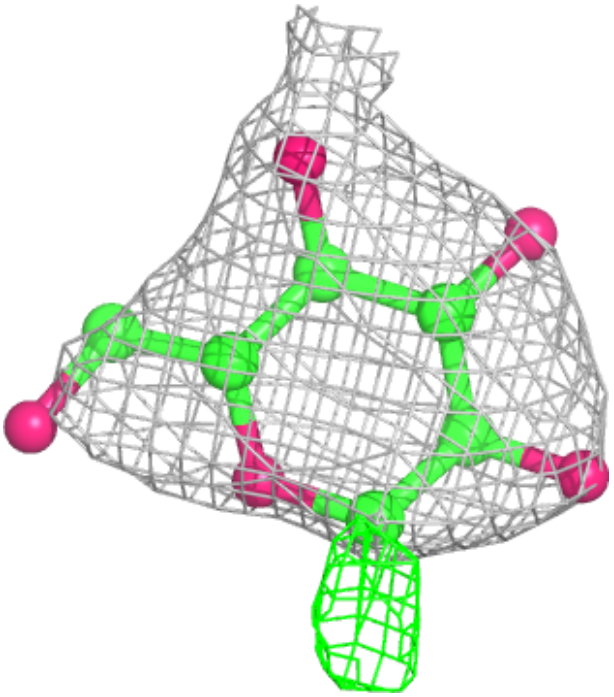
Electron density around DGD c 519:

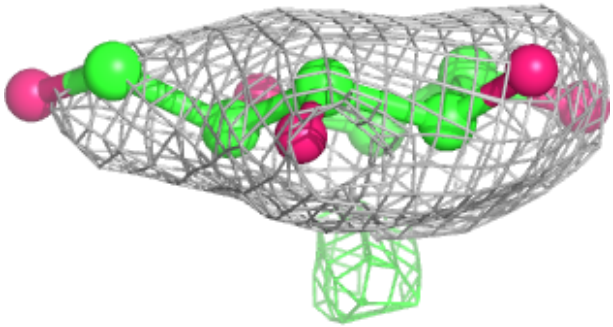
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

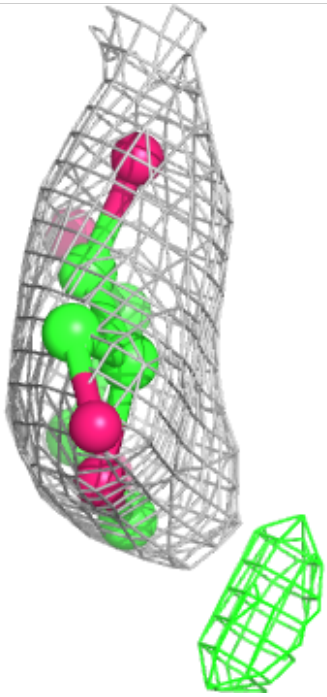


Electron density around HTG V 202:

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

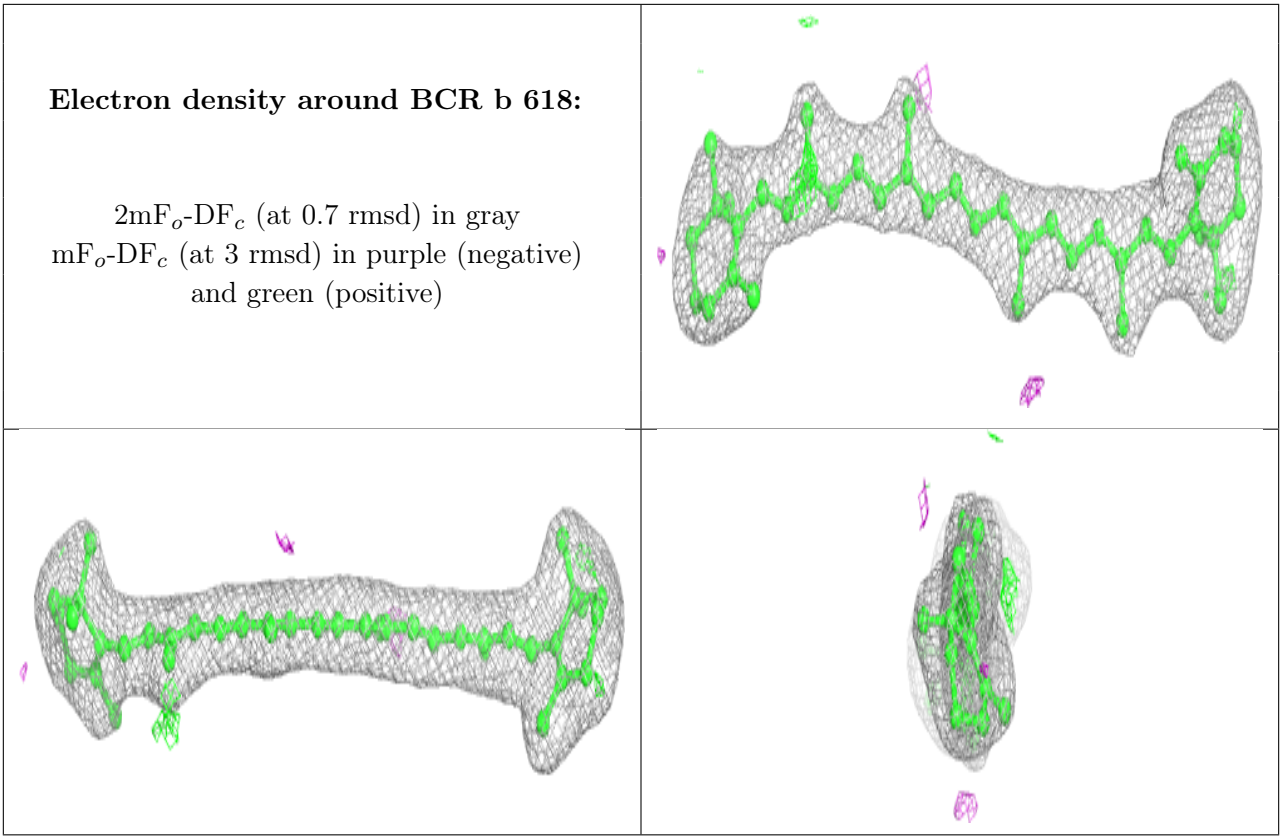






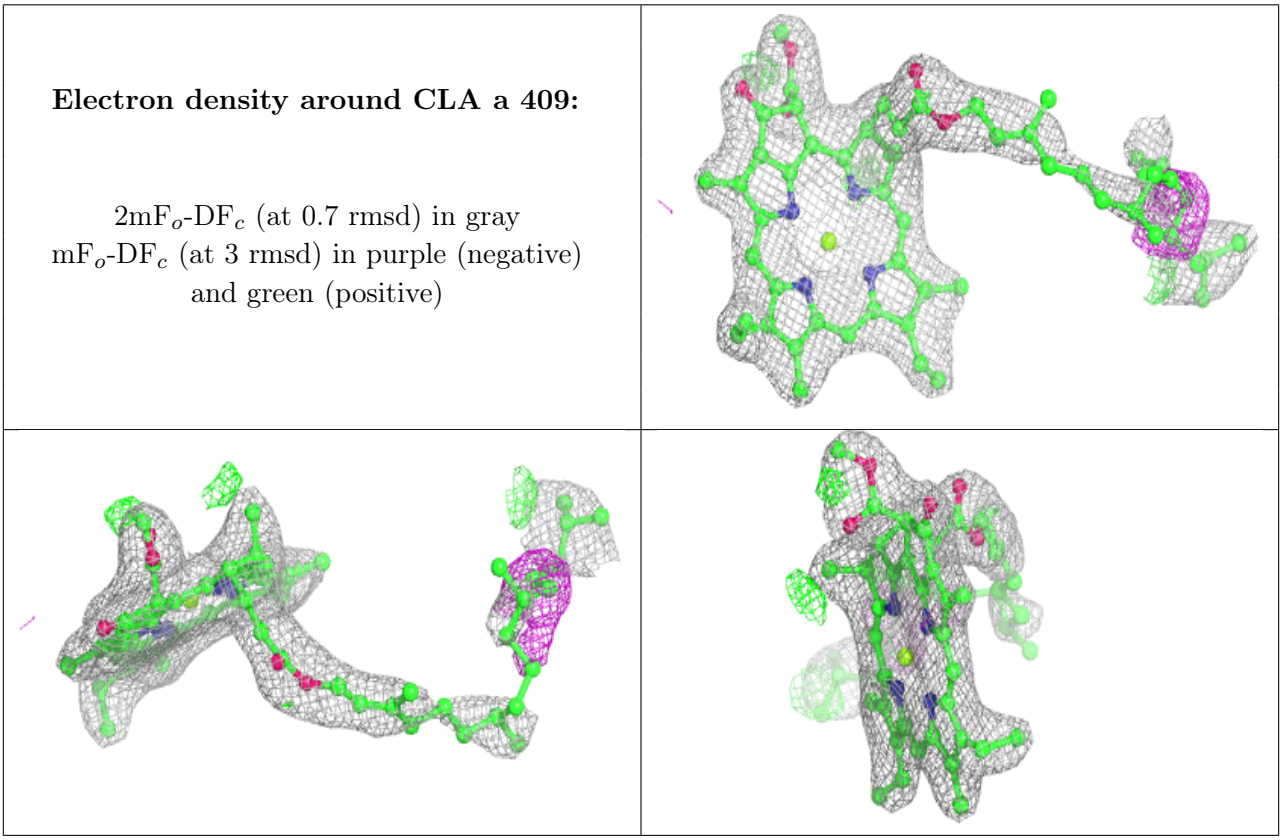
Electron density around BCR b 618:

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



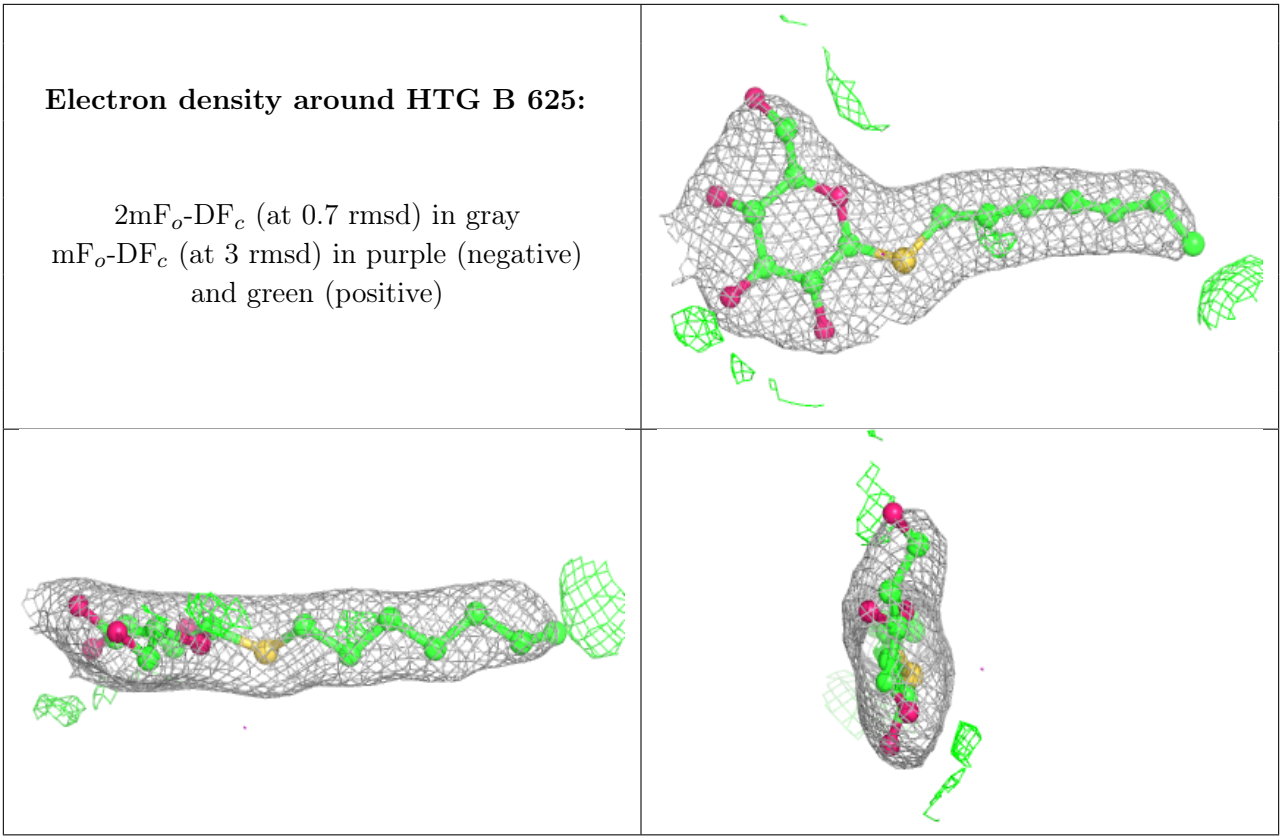
Electron density around CLA a 409:

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



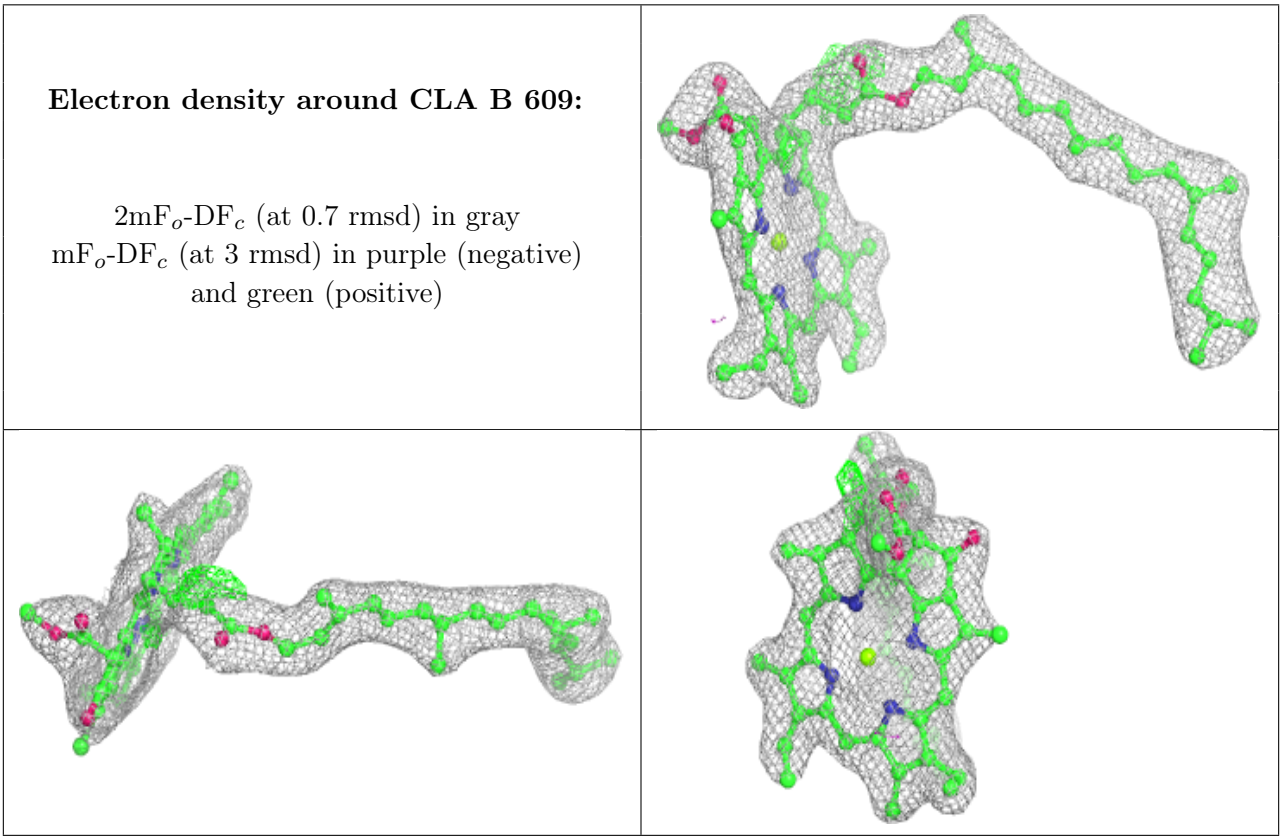
Electron density around HTG B 625:

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



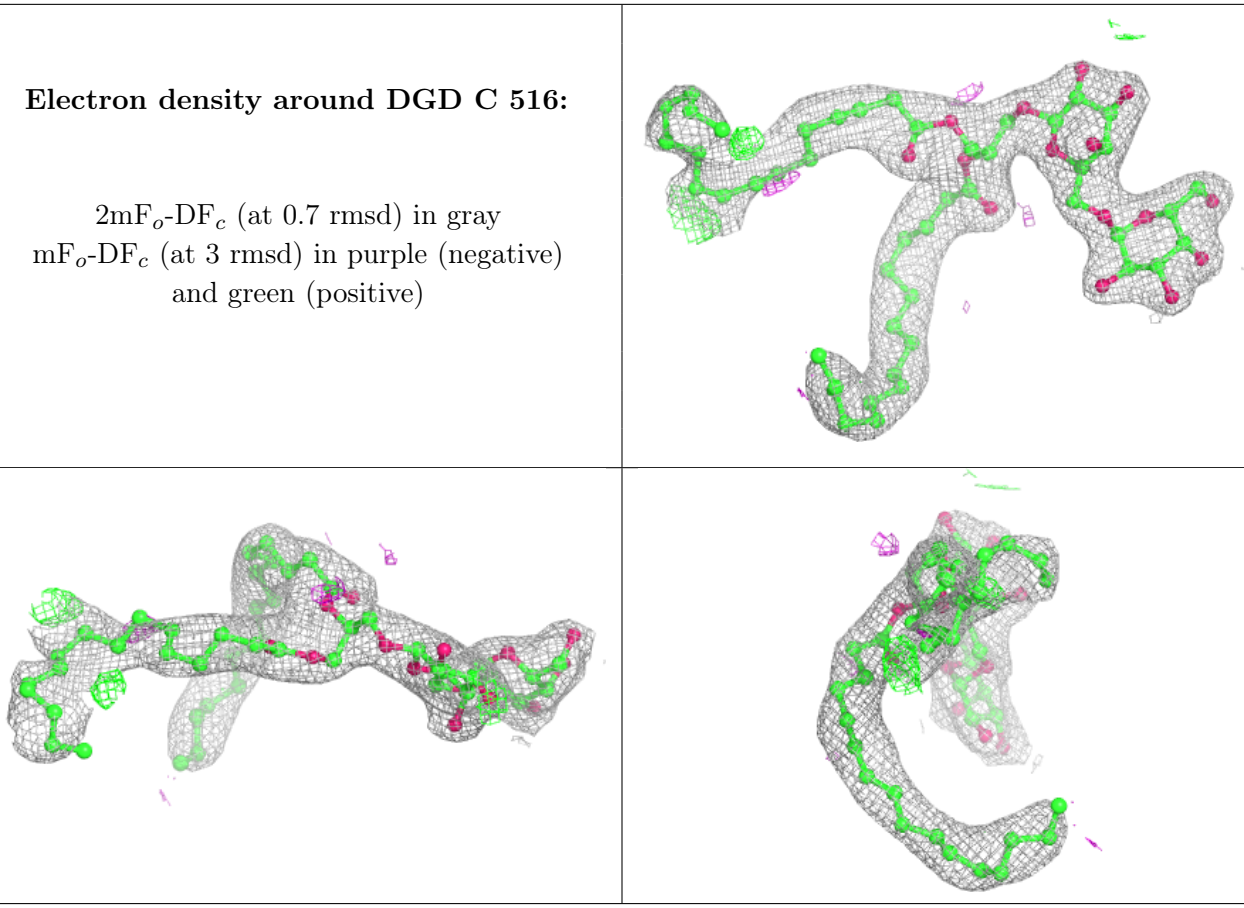
Electron density around CLA B 609:

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



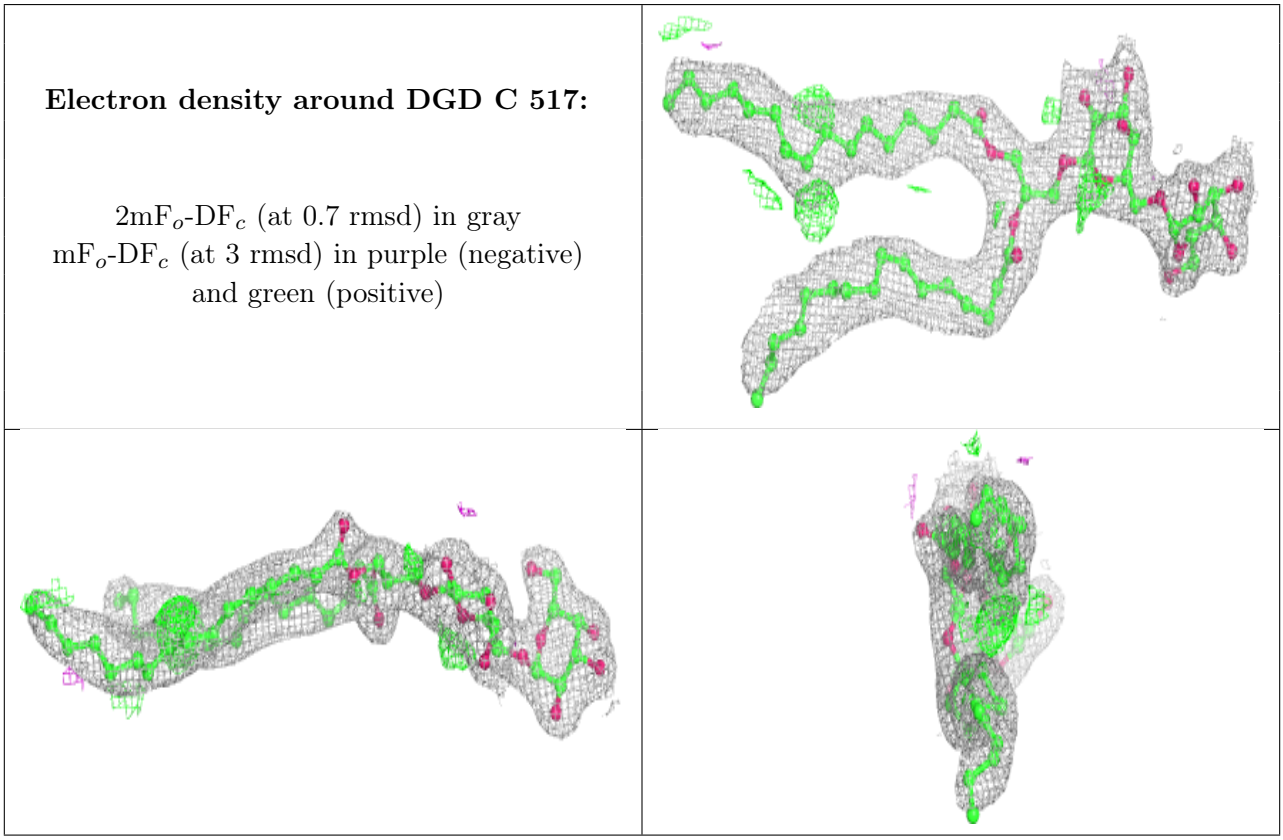
Electron density around DGD C 516:

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



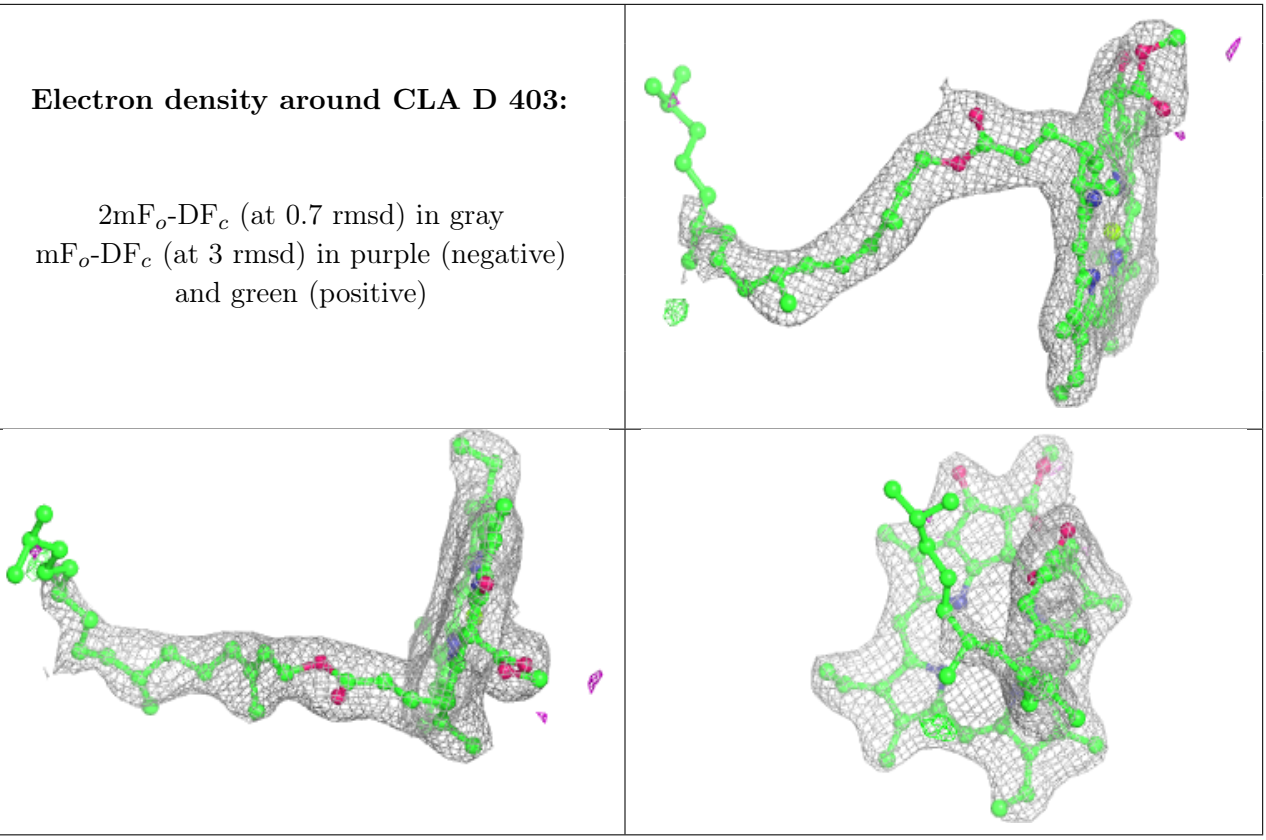
Electron density around DGD C 517:

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



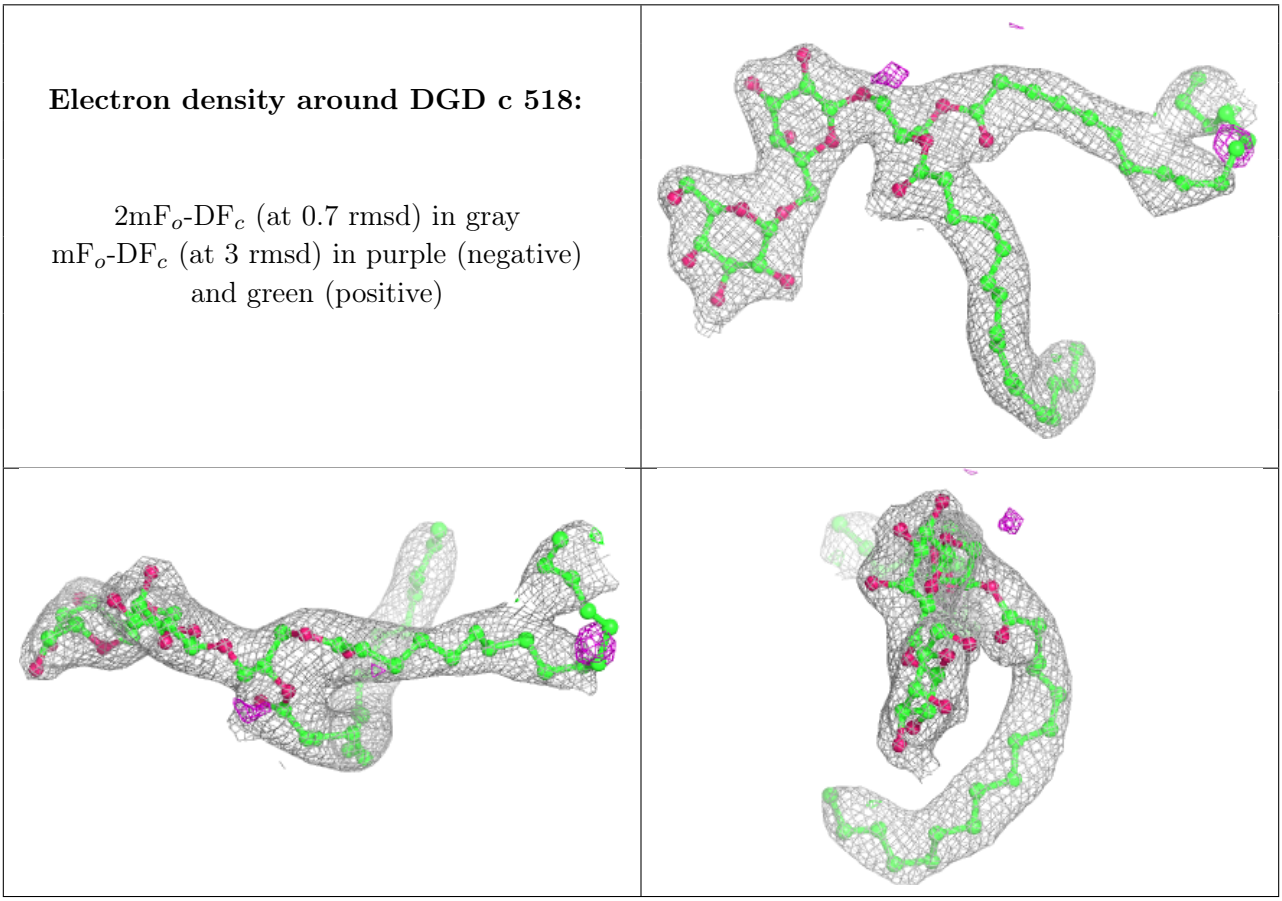
Electron density around CLA D 403:

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



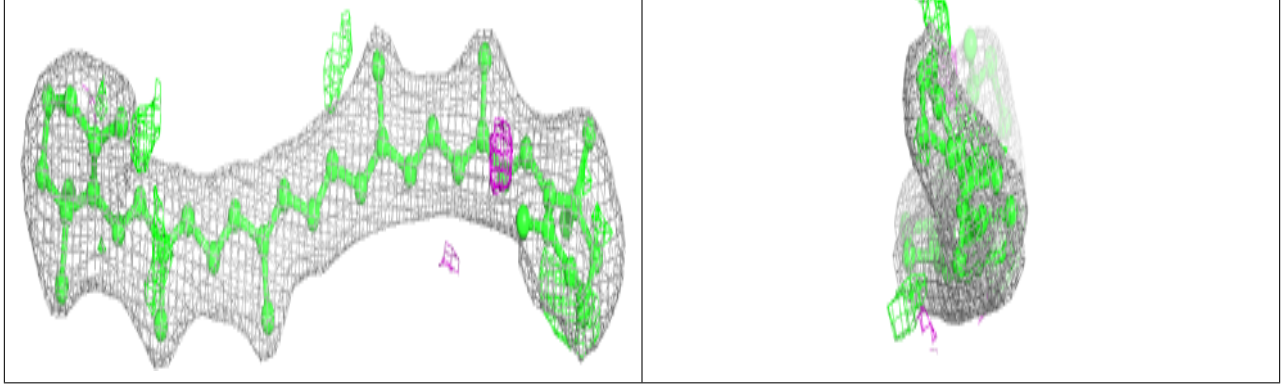
Electron density around DGD c 518:

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



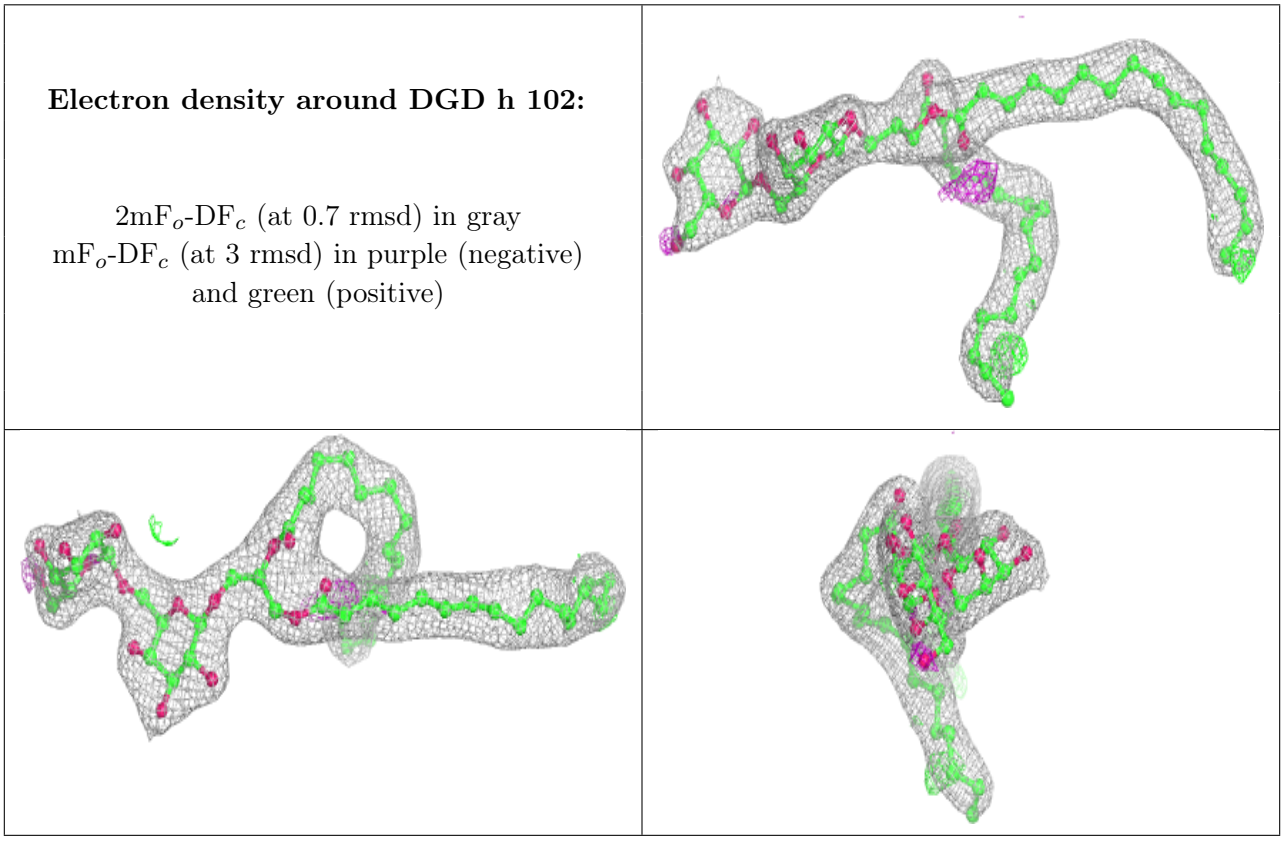
Electron density around BCR D 404:

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



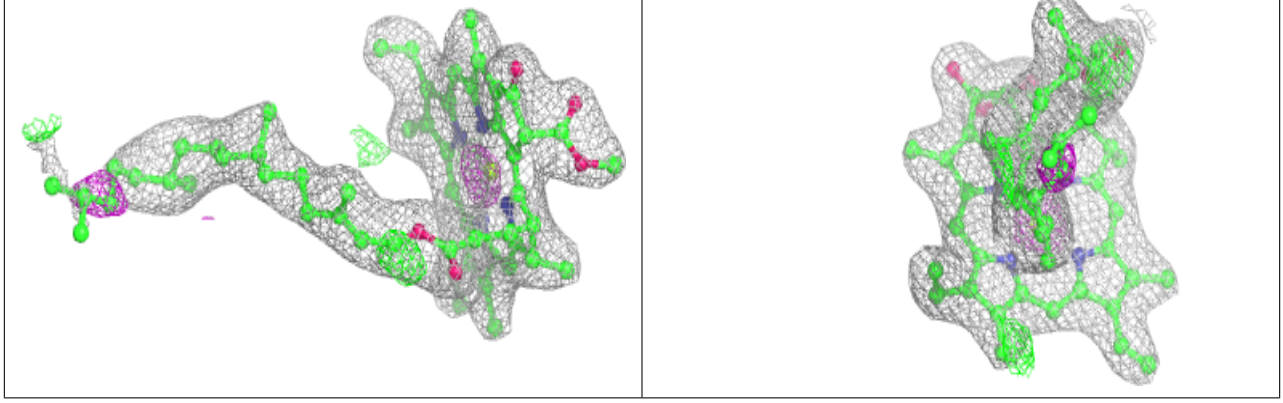
Electron density around DGD h 102:

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



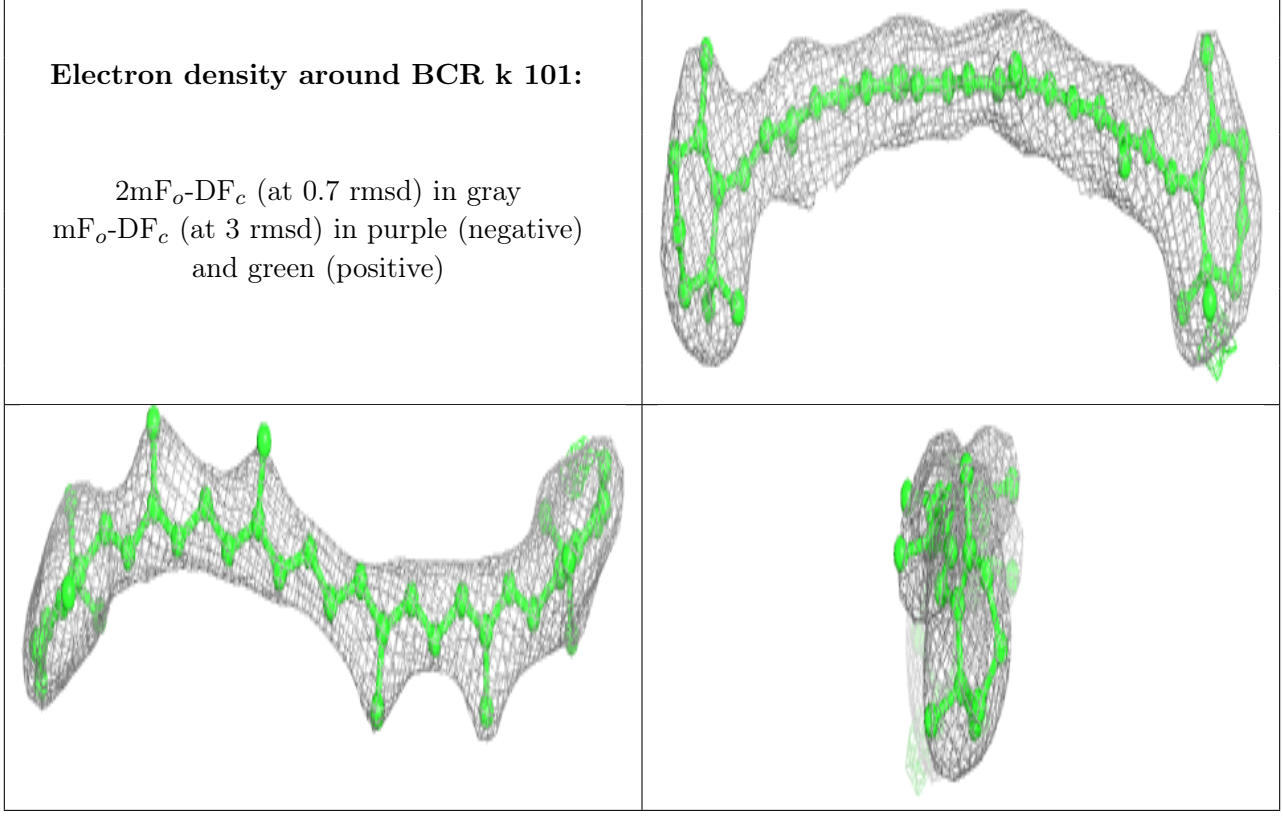
Electron density around CLA C 508:

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



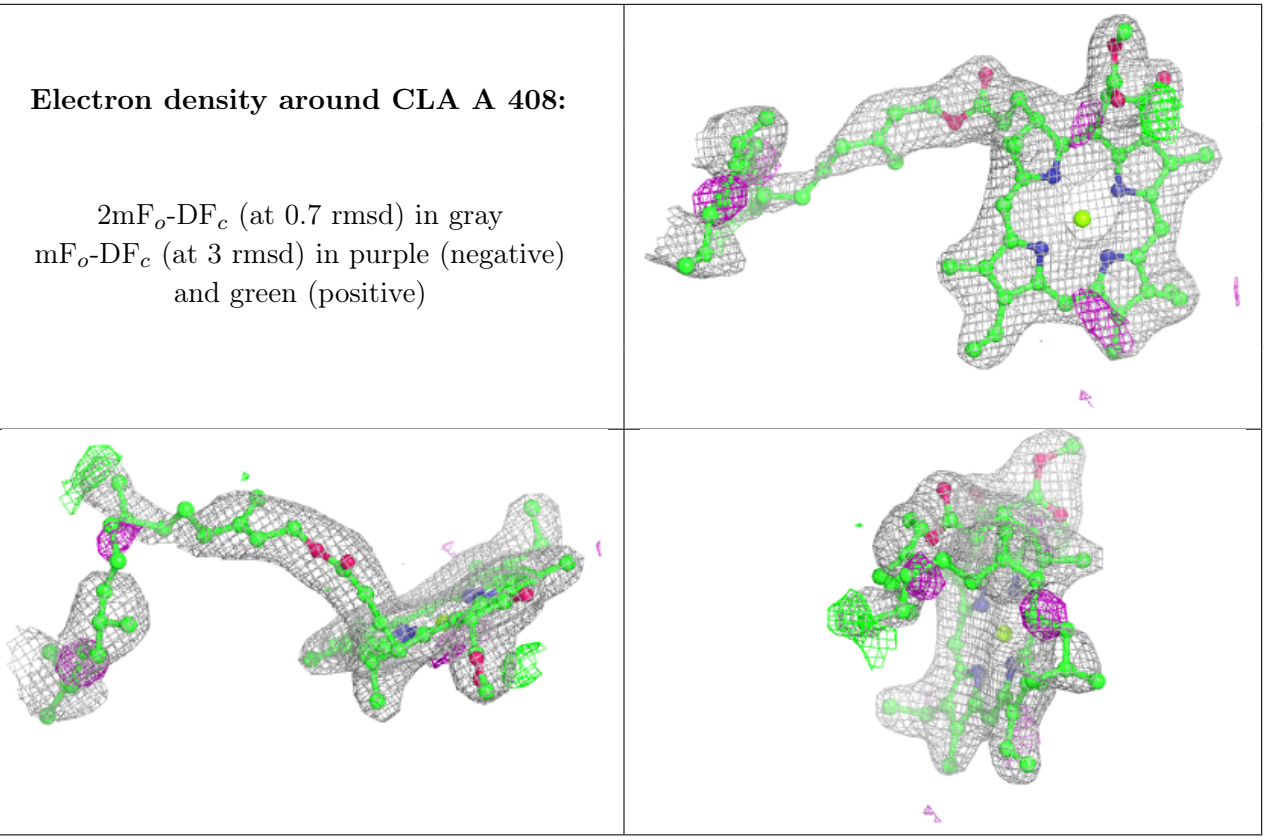
Electron density around BCR k 101:

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



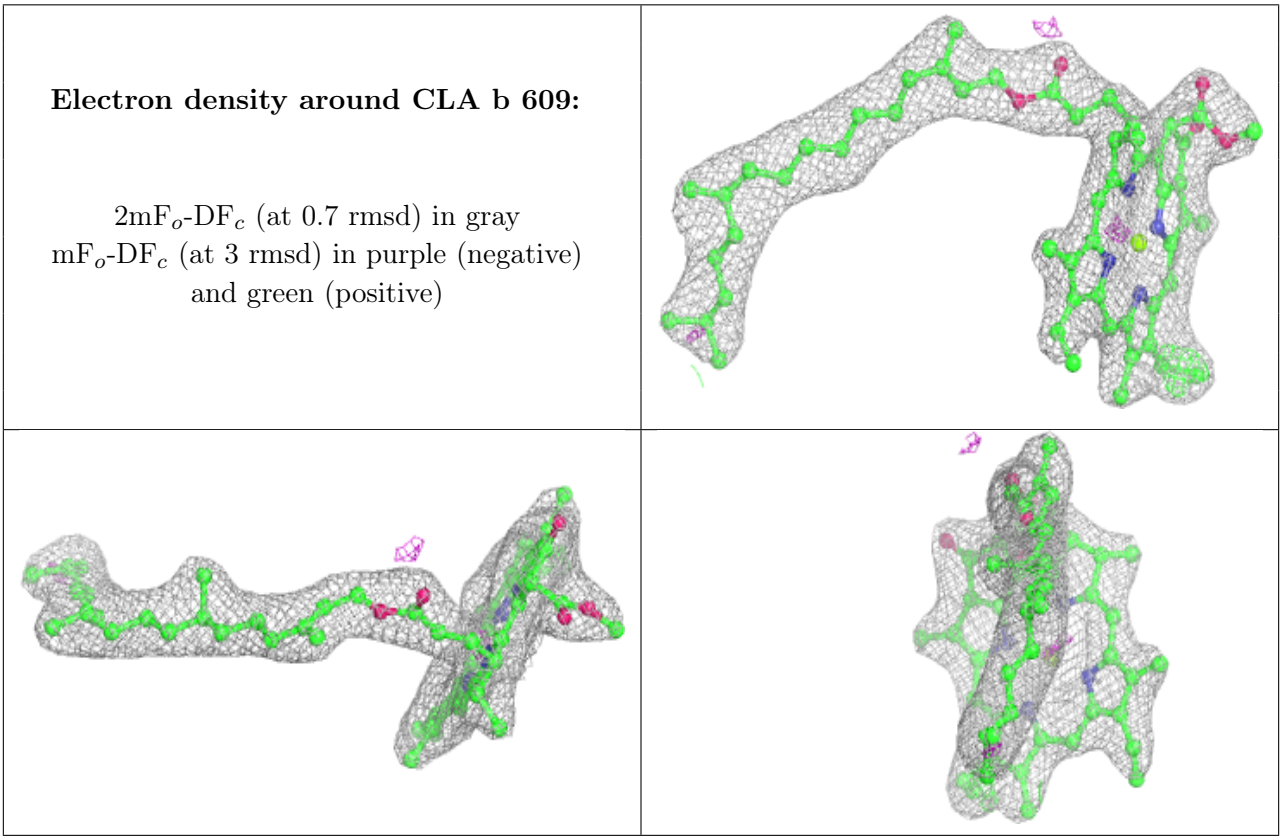
Electron density around CLA A 408:

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



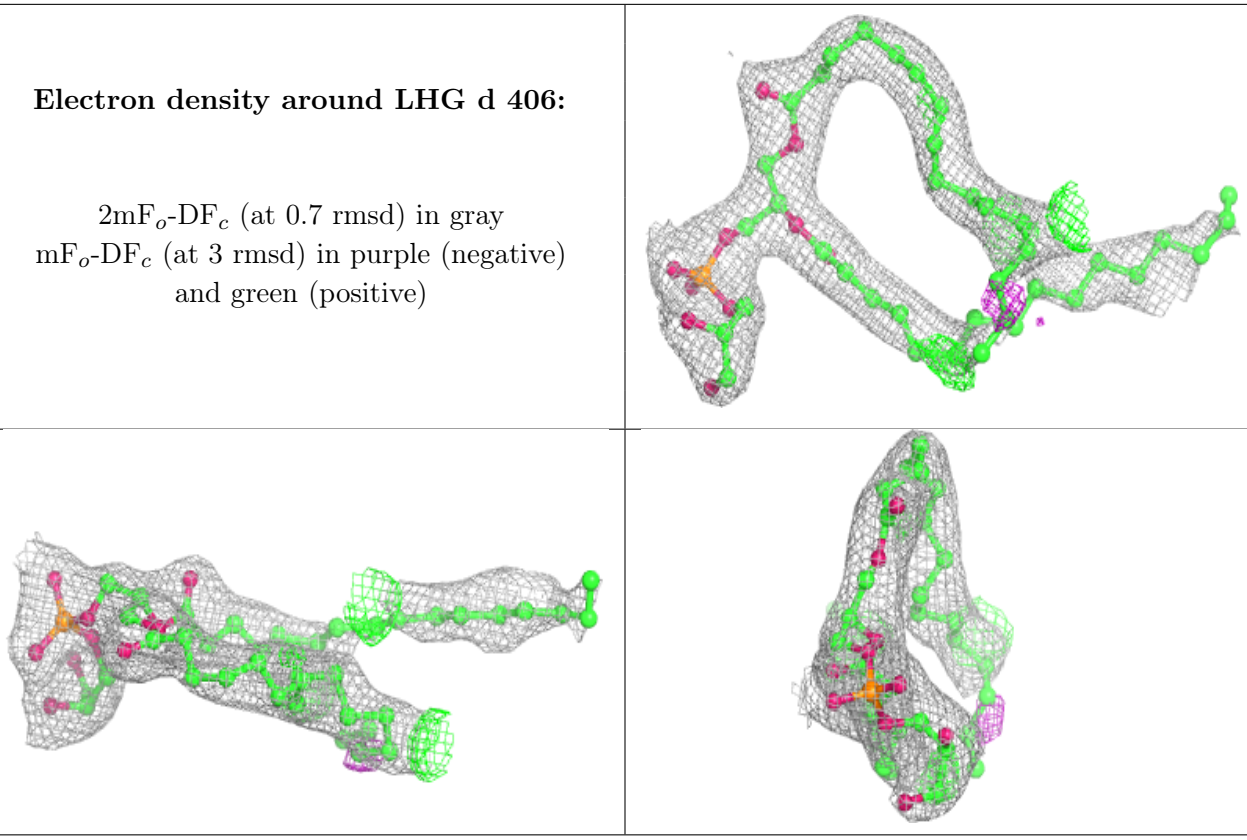
Electron density around CLA b 609:

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



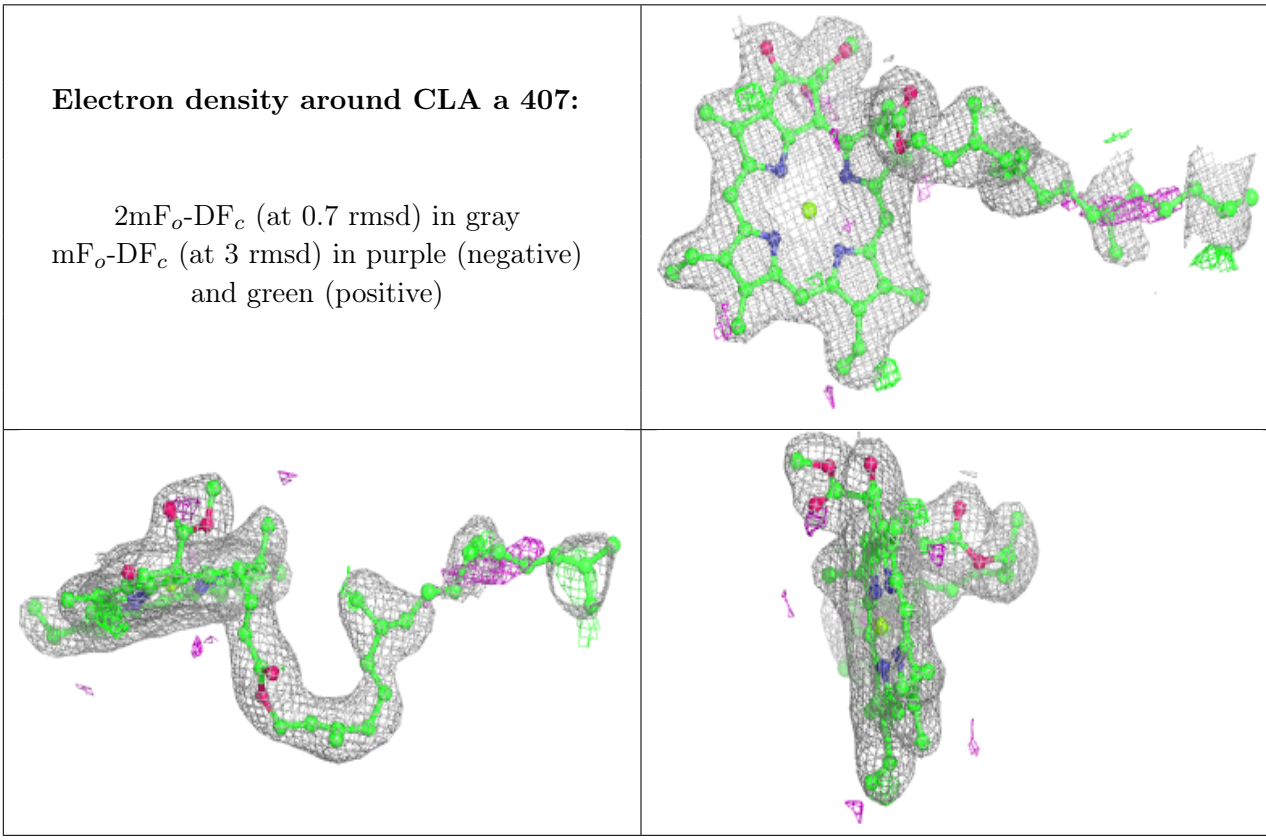
Electron density around LHG d 406:

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



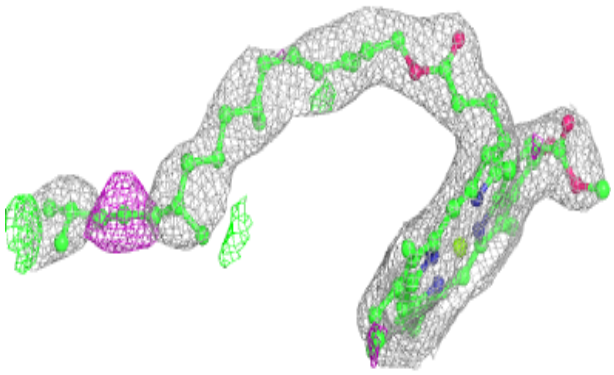
Electron density around CLA a 407:

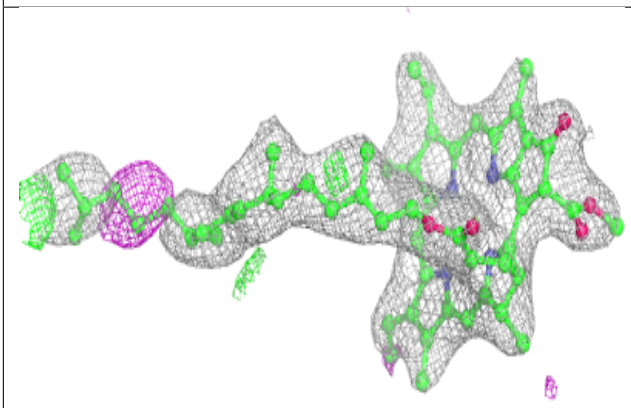
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

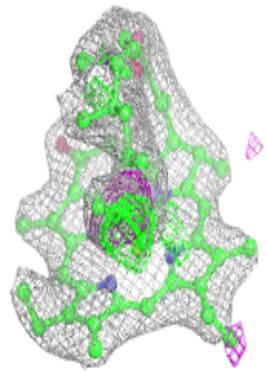


Electron density around CLA c 505:

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

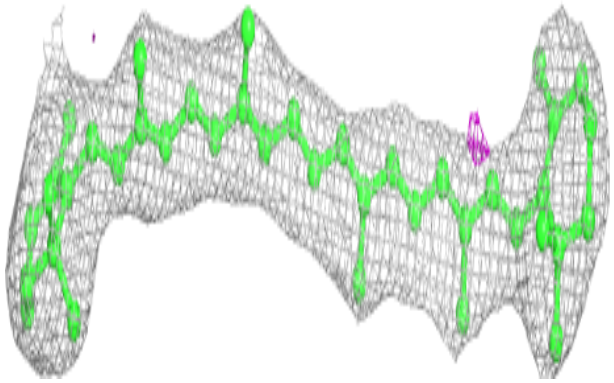


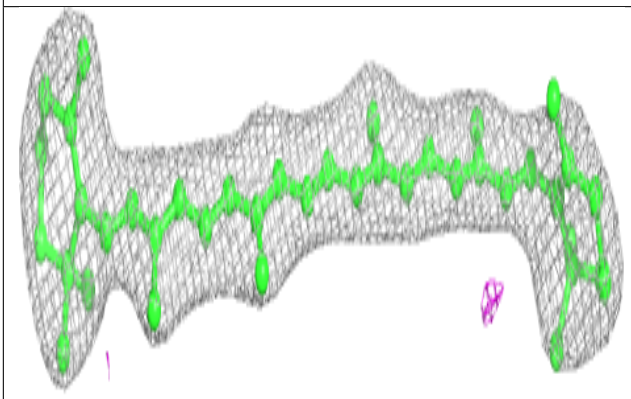


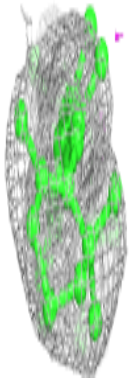


Electron density around BCR c 515:

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

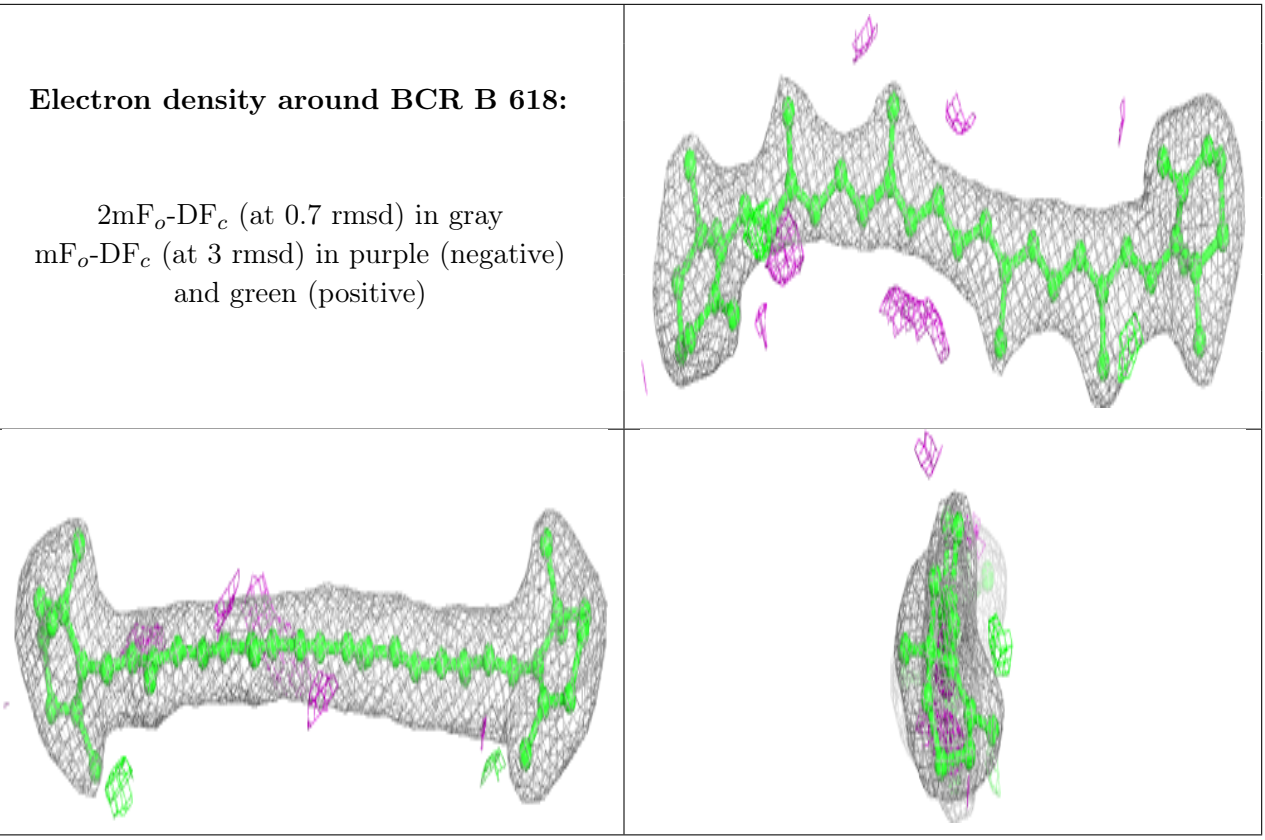






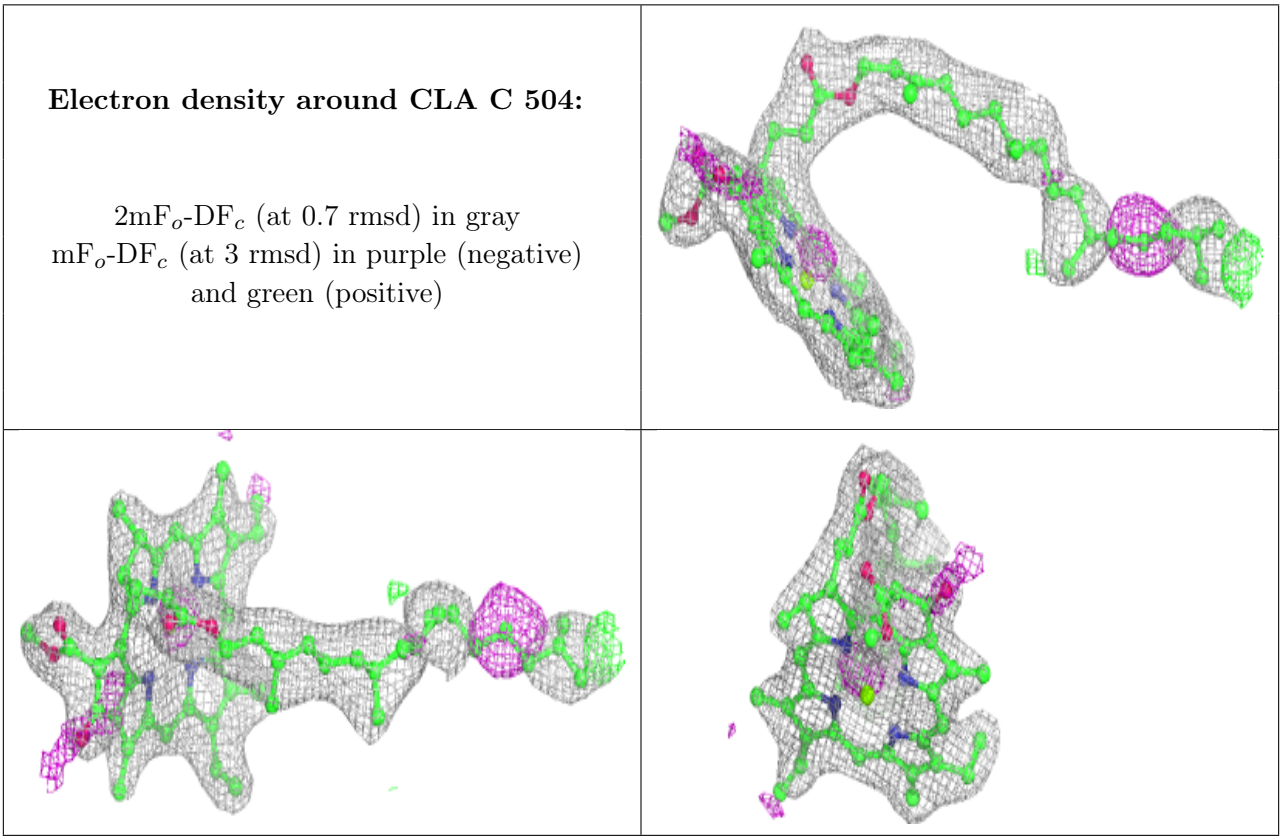
Electron density around BCR B 618:

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



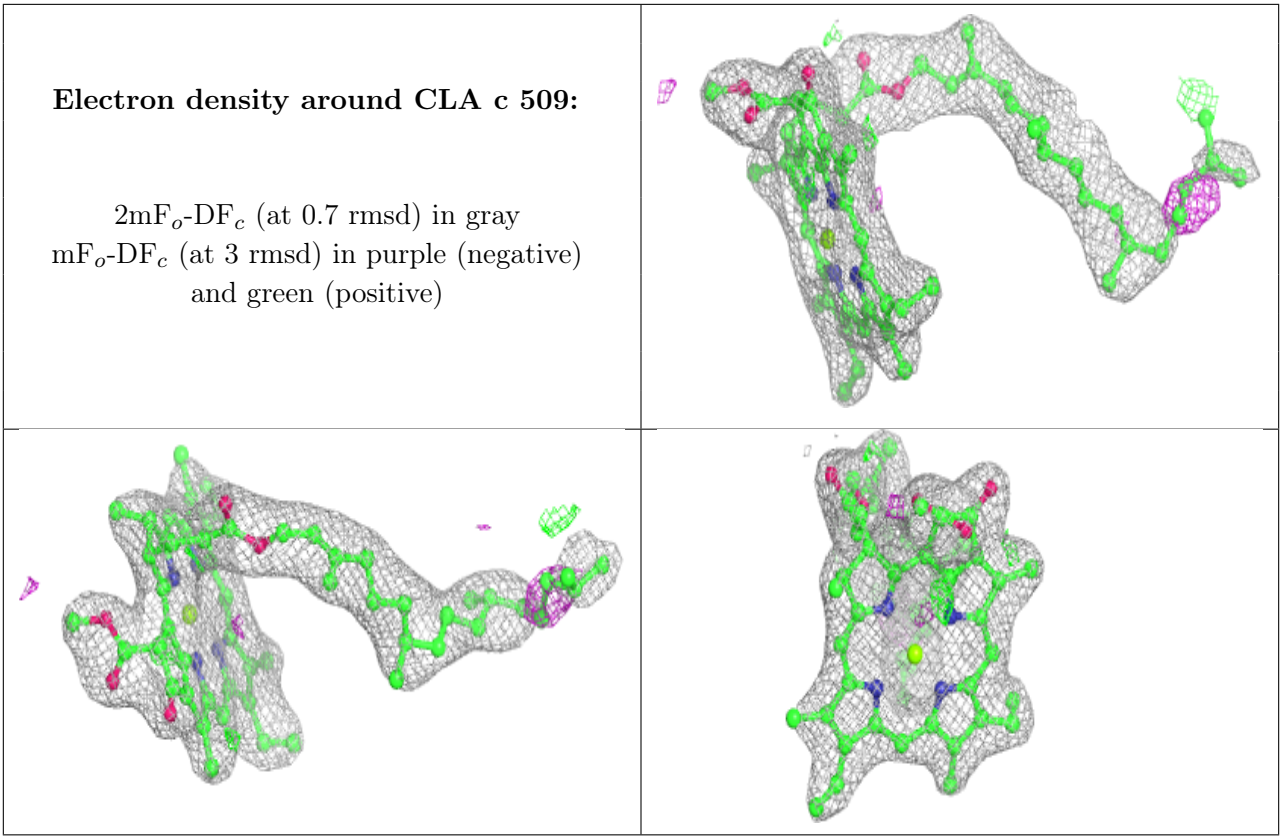
Electron density around CLA C 504:

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



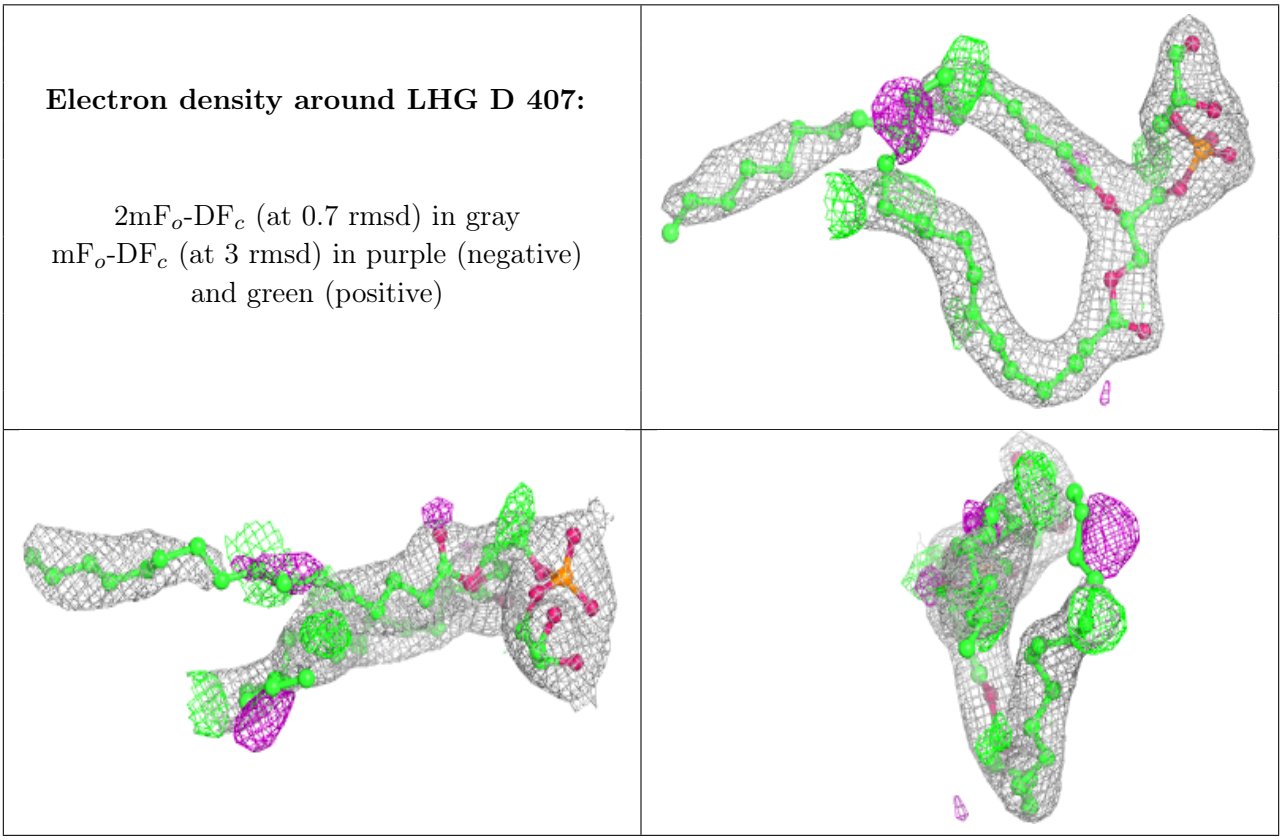
Electron density around CLA c 509:

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



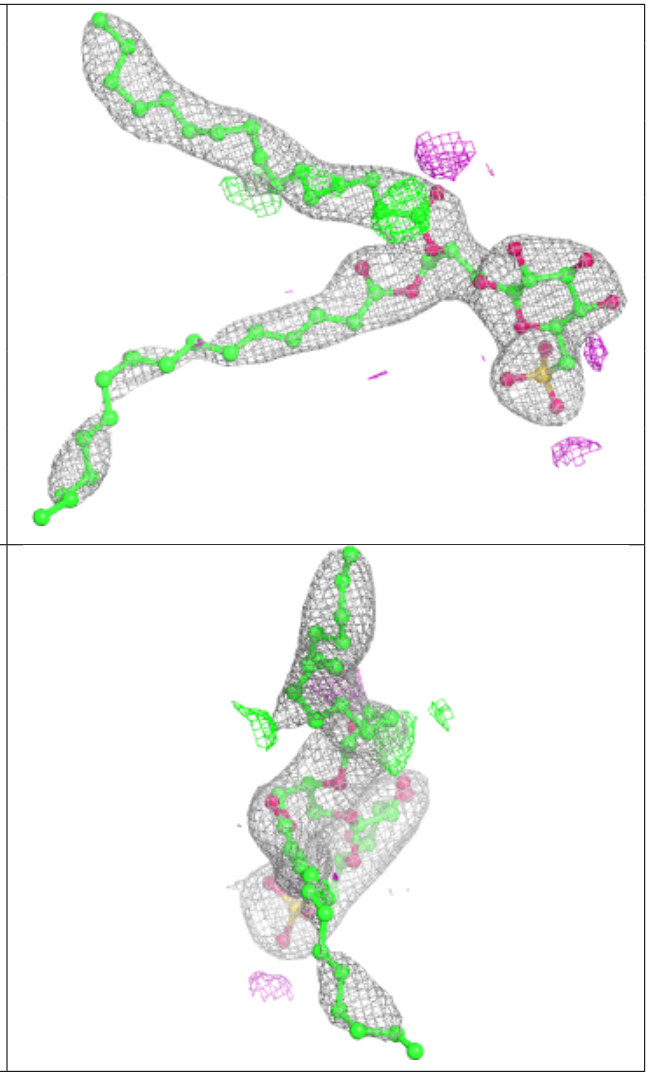
Electron density around LHG D 407:

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



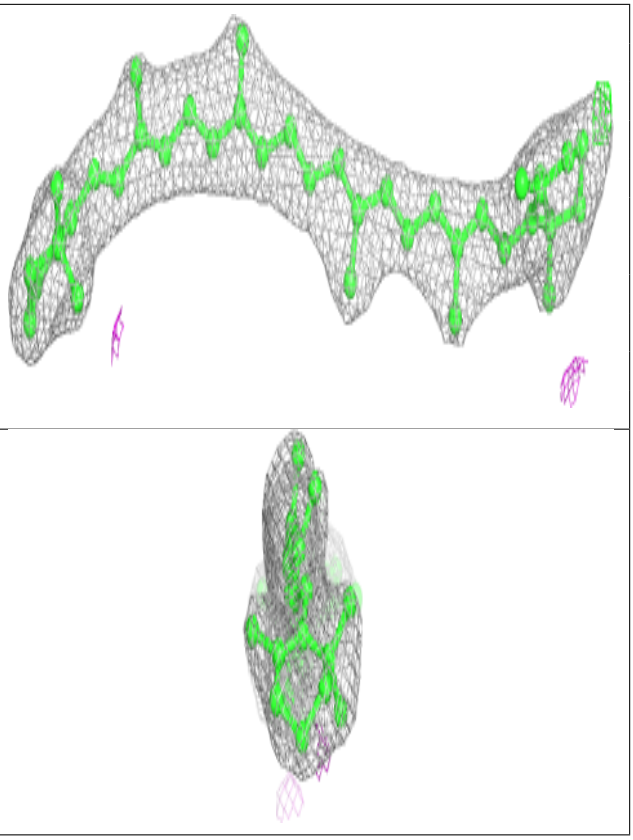
Electron density around SQD A 410:

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



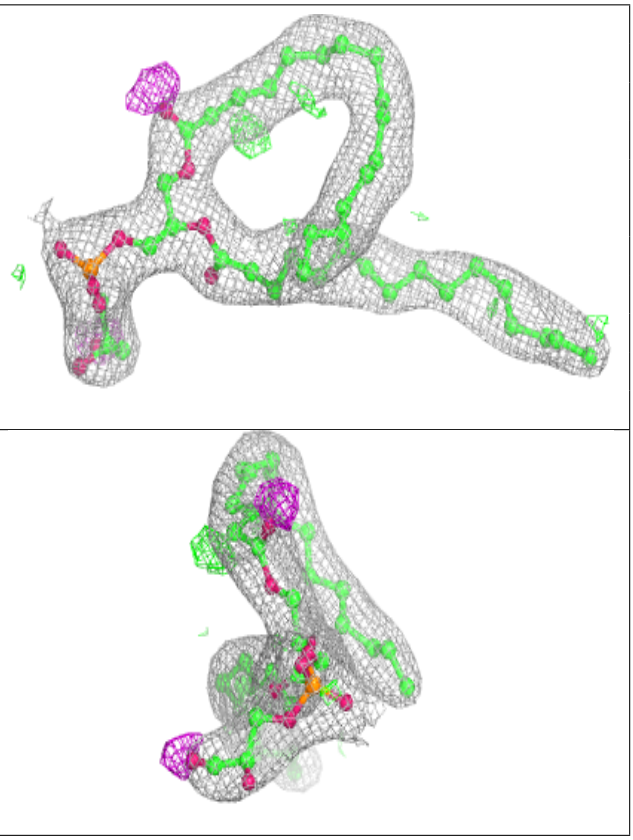
Electron density around BCR H 101:

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



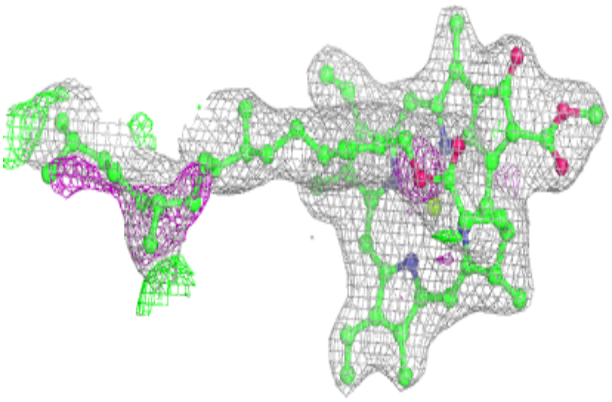
Electron density around LHG A 420:

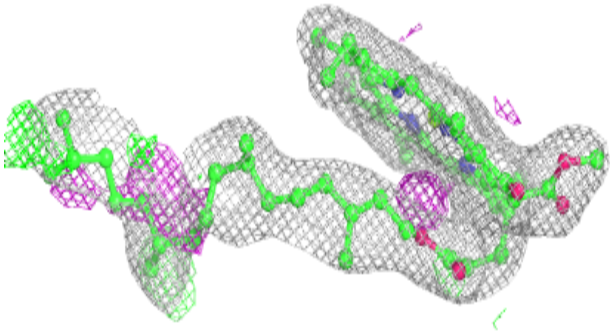
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

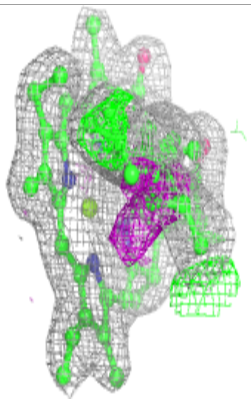


Electron density around CLA B 614:

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

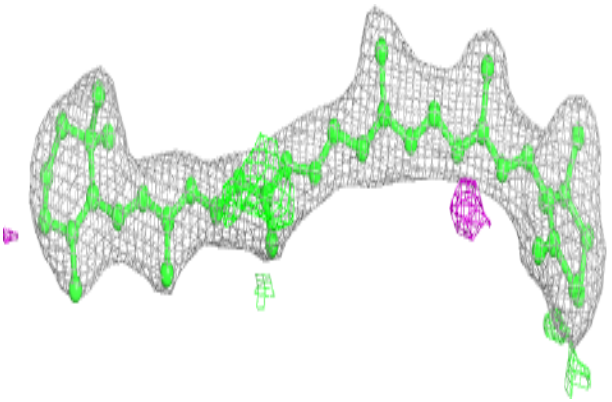


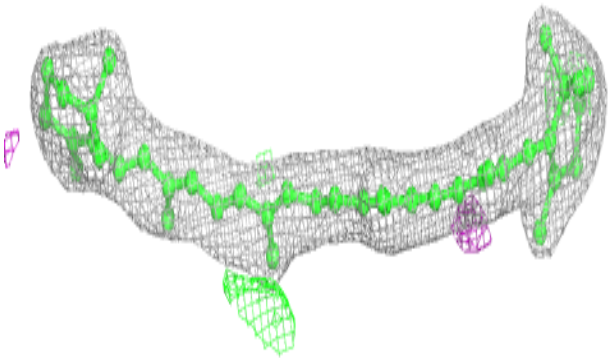


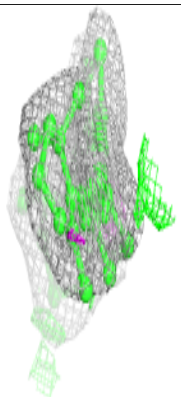


Electron density around BCR t 102:

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

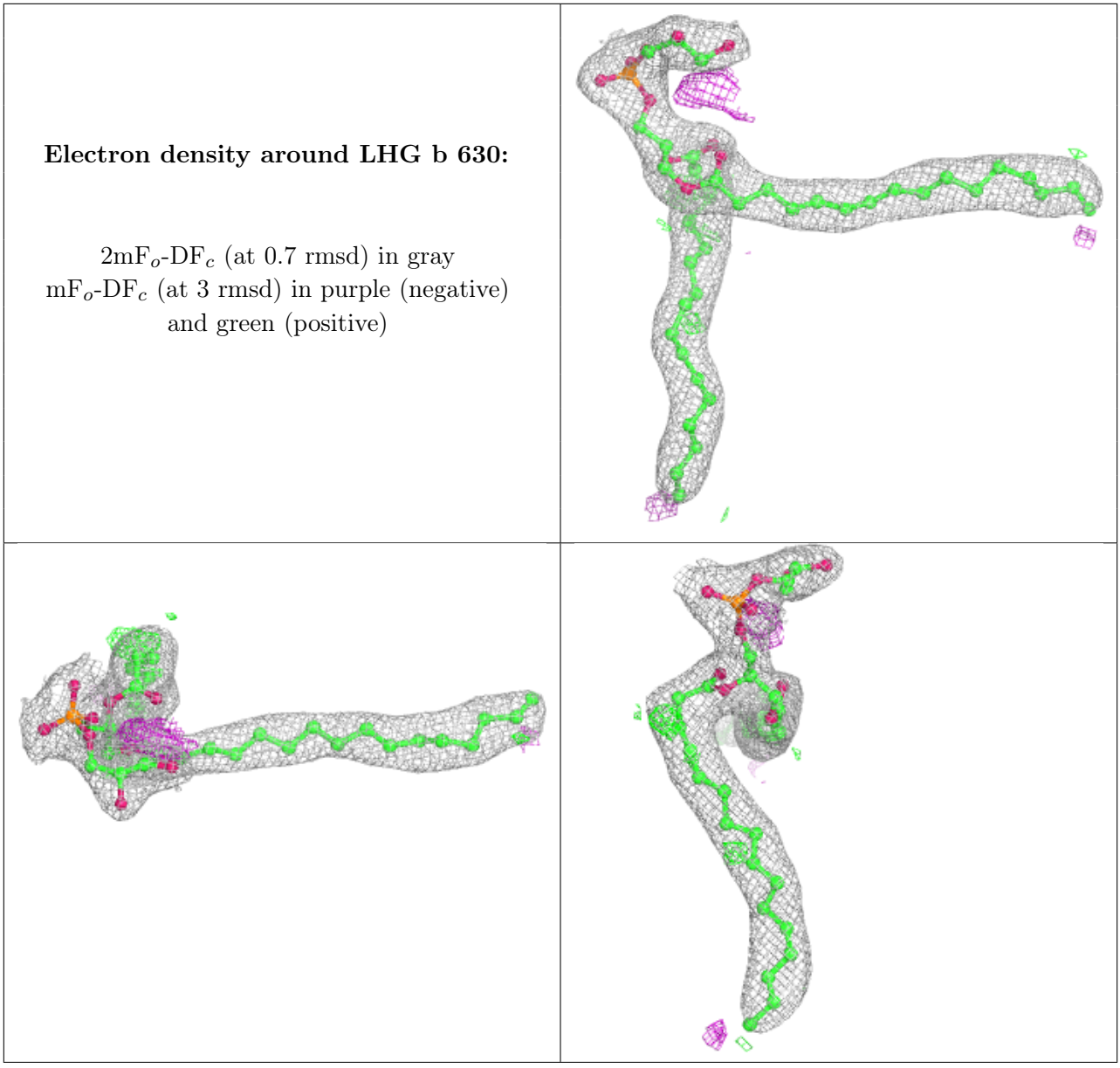






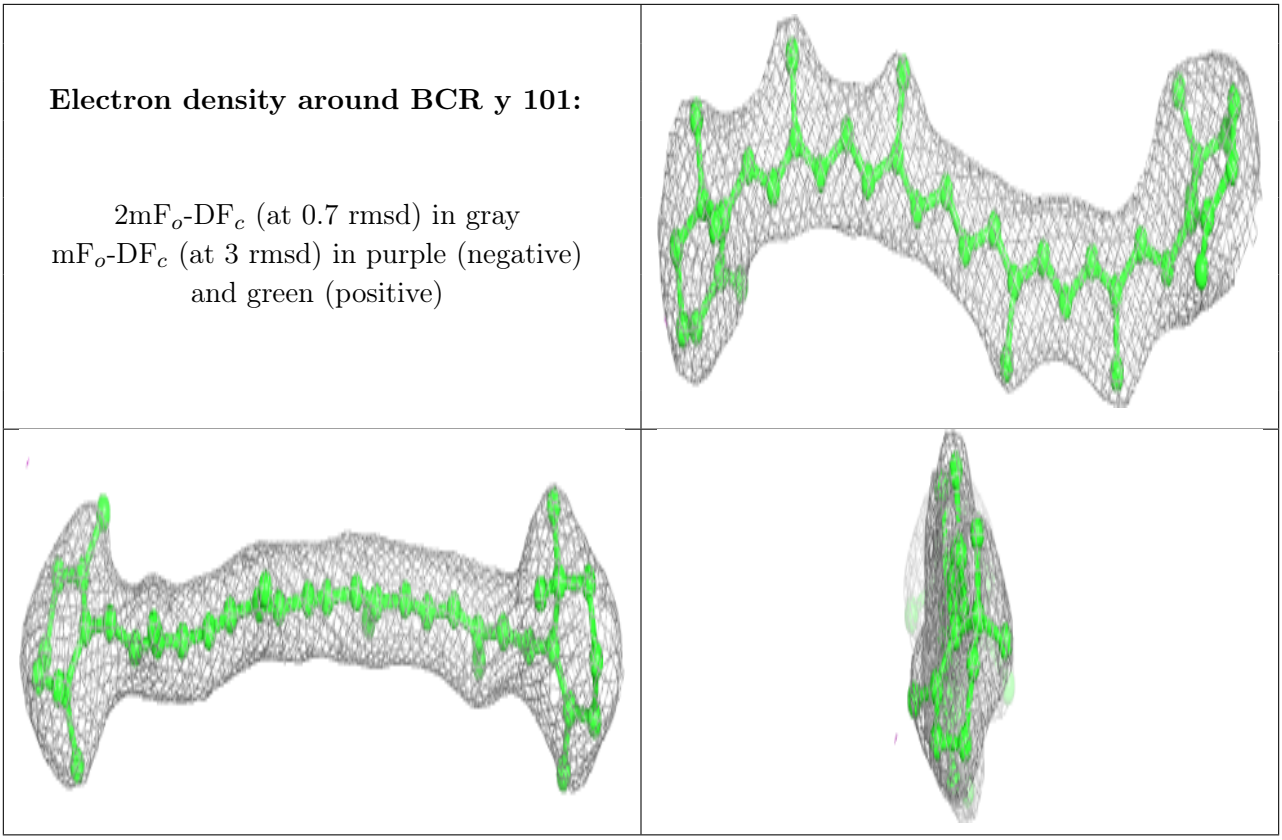
Electron density around LHG b 630:

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



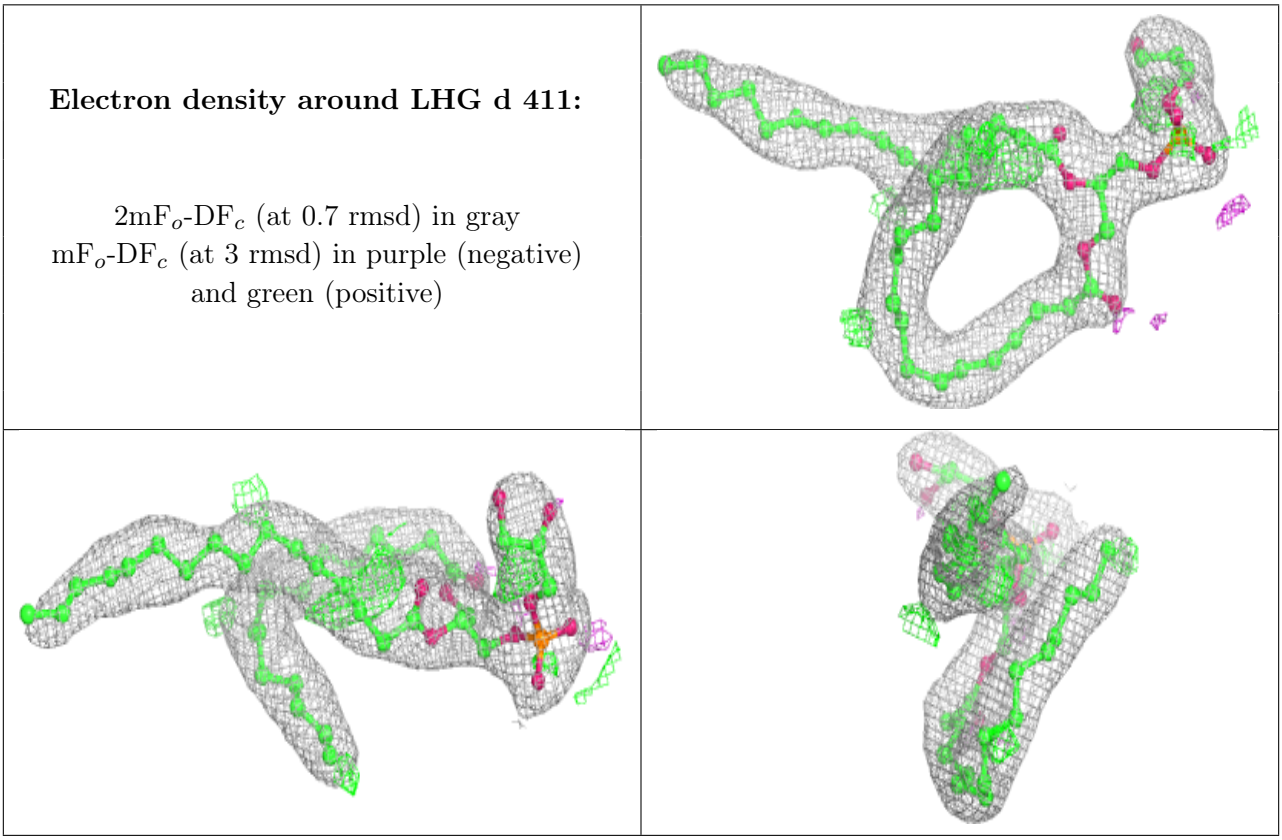
Electron density around BCR y 101:

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



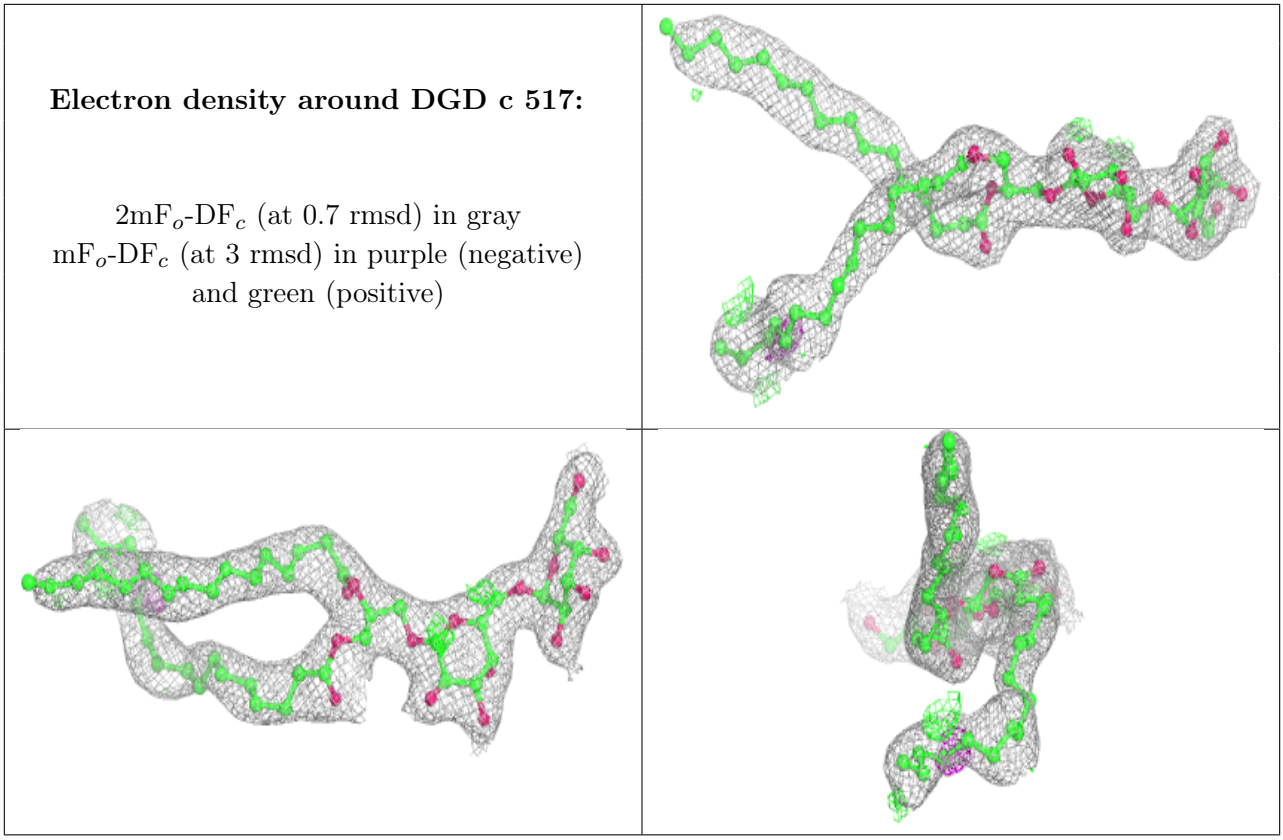
Electron density around LHG d 411:

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



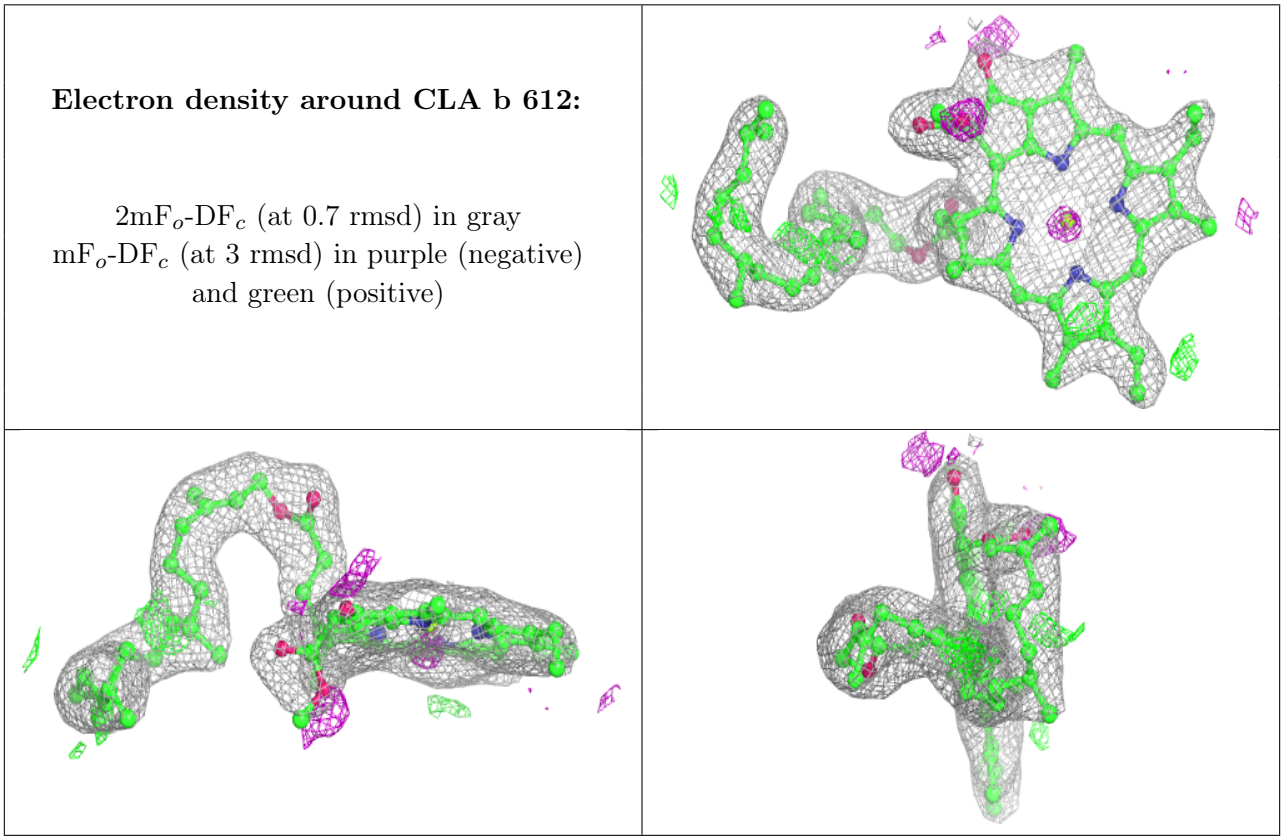
Electron density around DGD c 517:

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



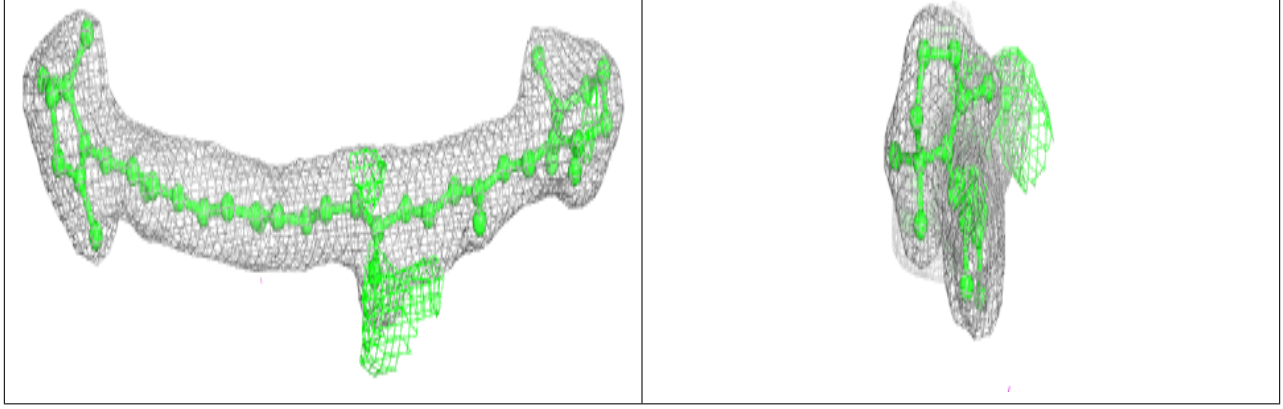
Electron density around CLA b 612:

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



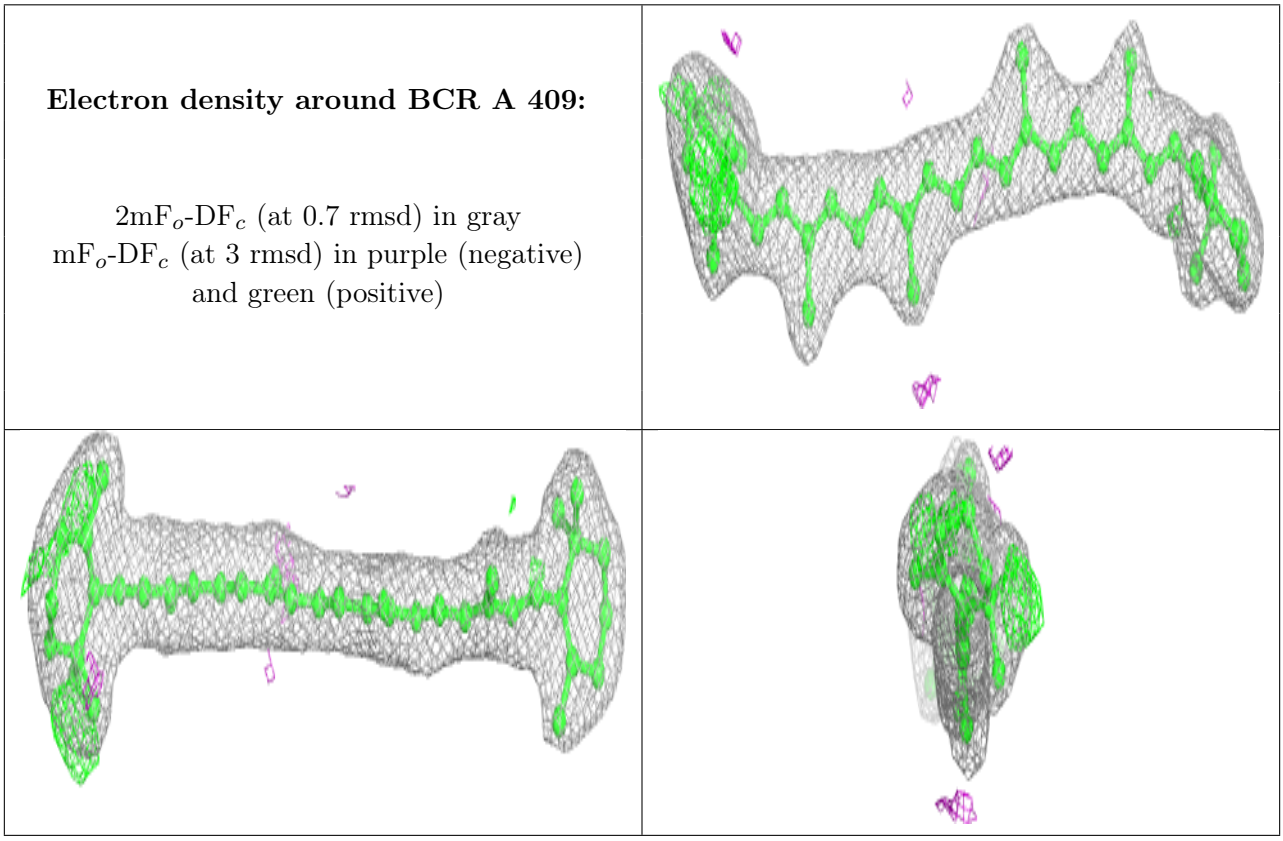
Electron density around BCR T 102:

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



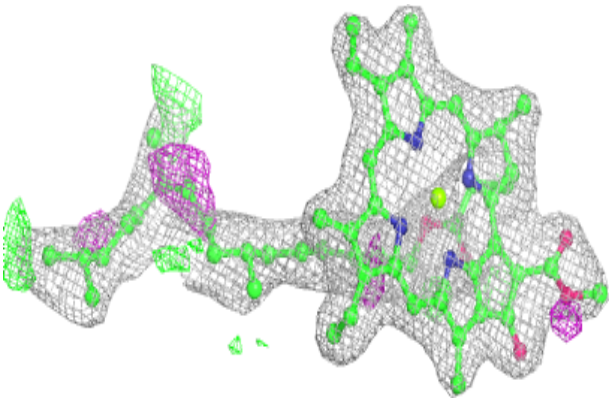
Electron density around BCR A 409:

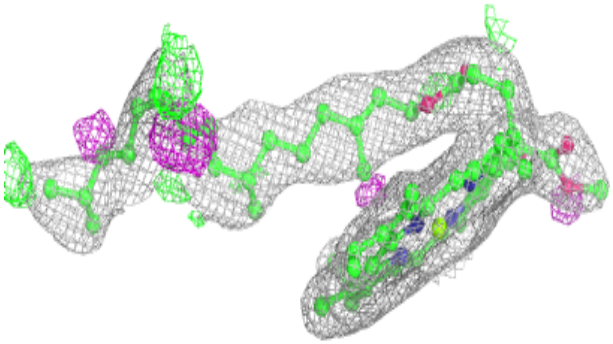
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

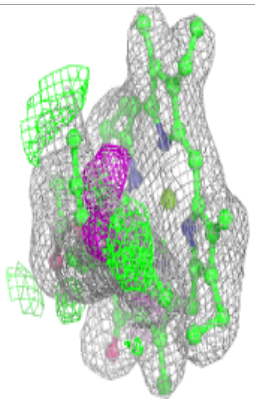


Electron density around CLA b 614:

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

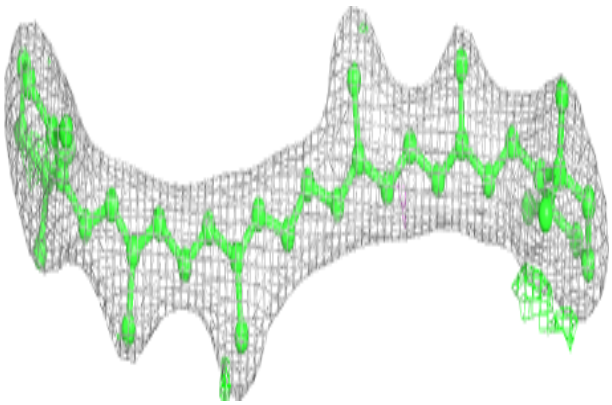


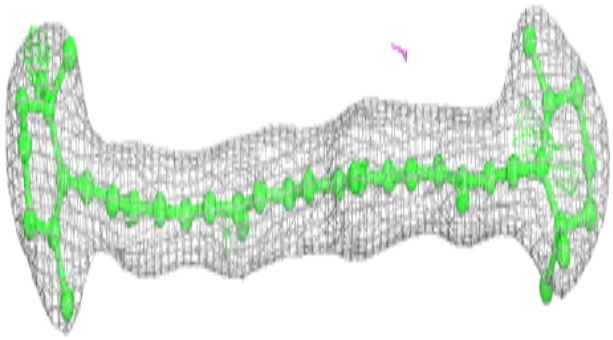


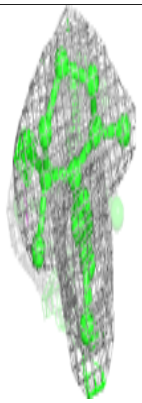


Electron density around BCR C 514:

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

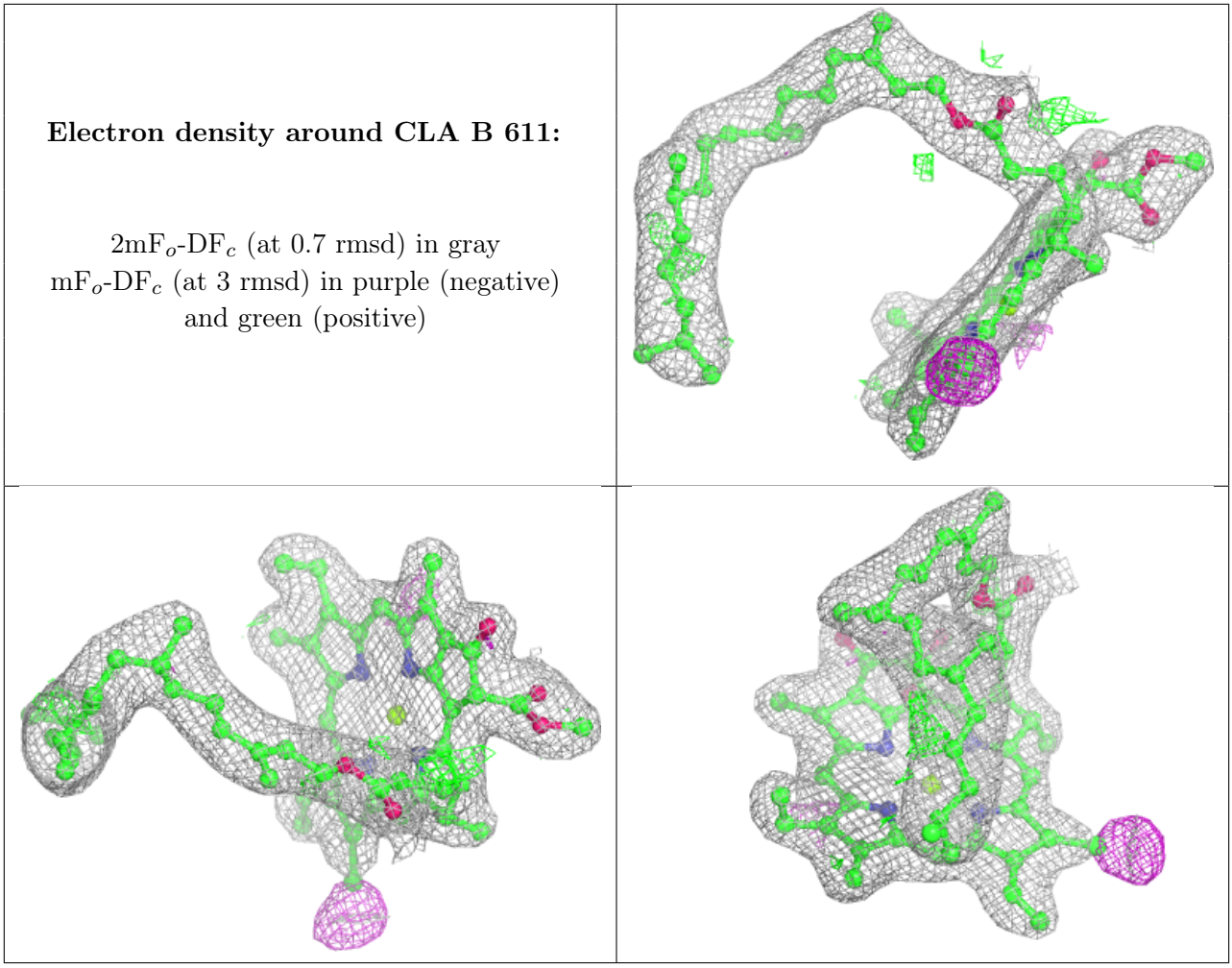






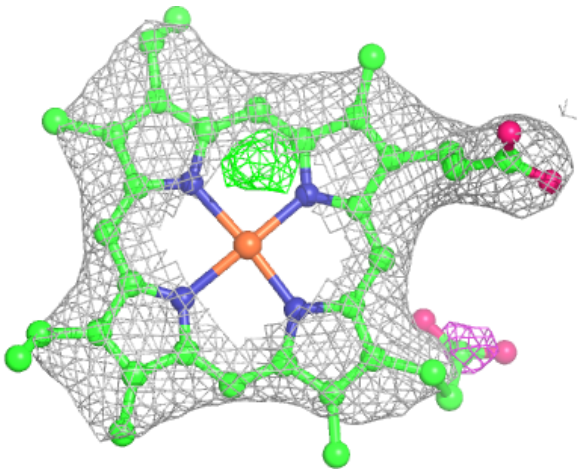
Electron density around CLA B 611:

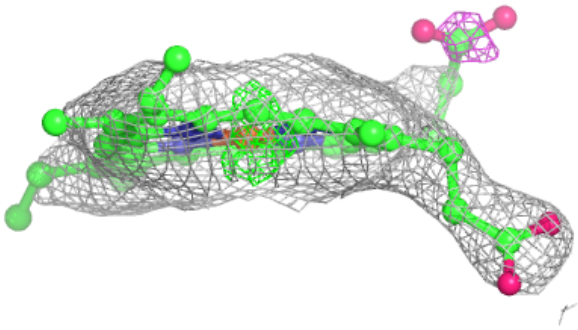
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

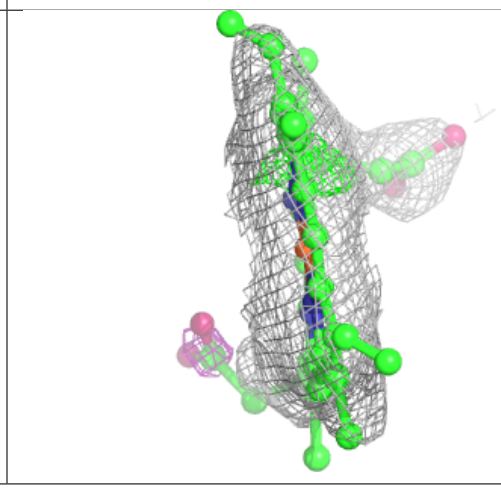


Electron density around HEM f 101:

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

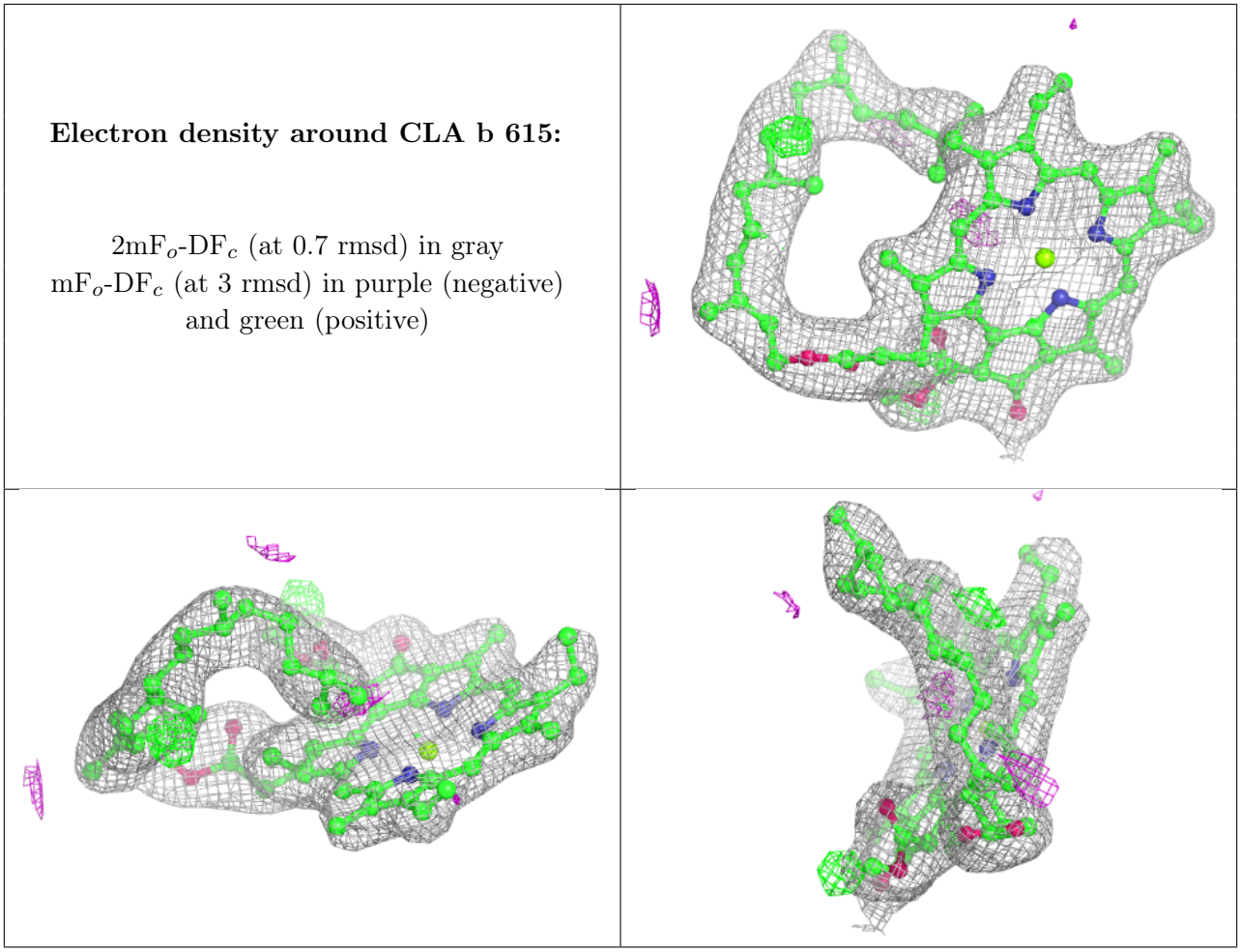






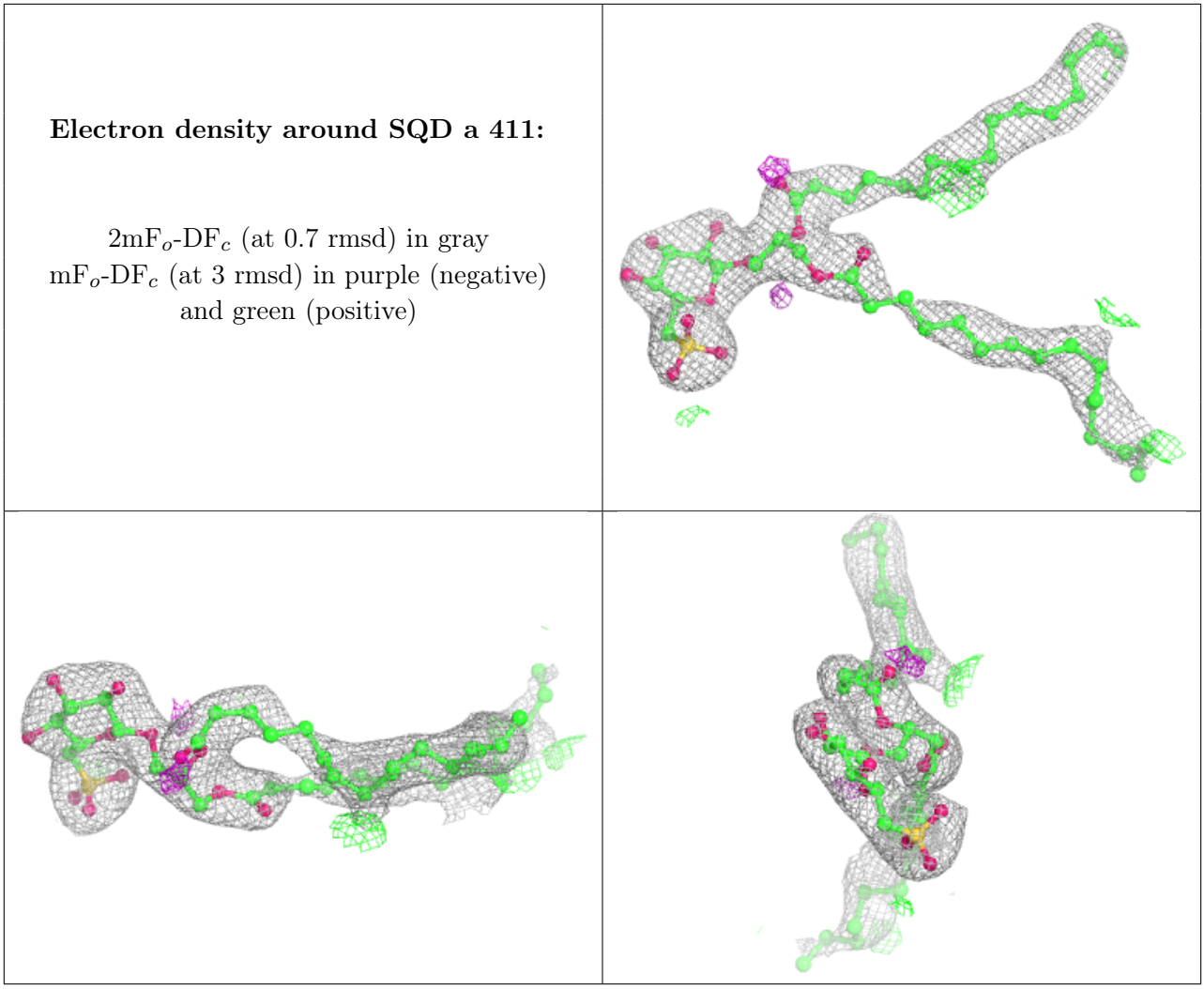
Electron density around CLA b 615:

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



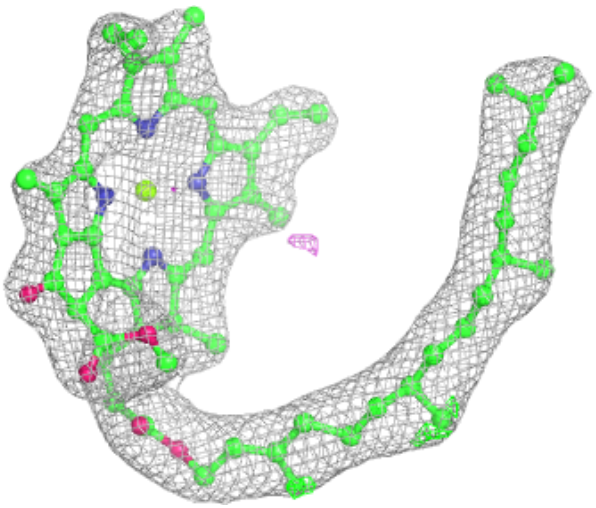
Electron density around SQD a 411:

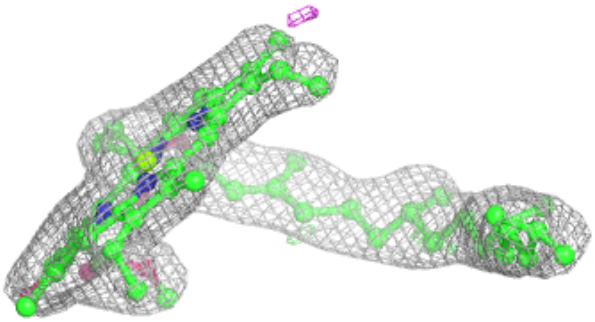
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

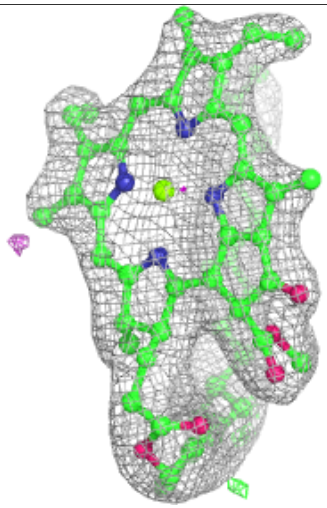


Electron density around CLA C 507:

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

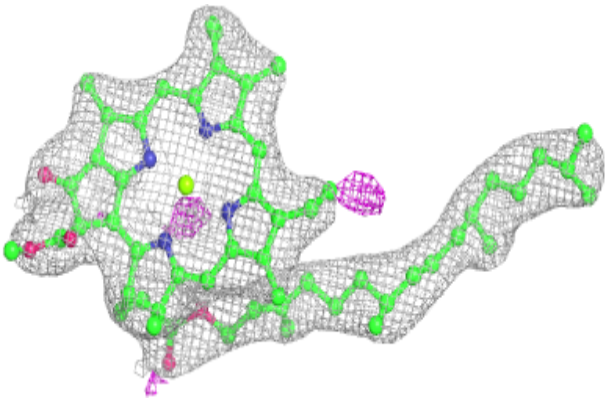


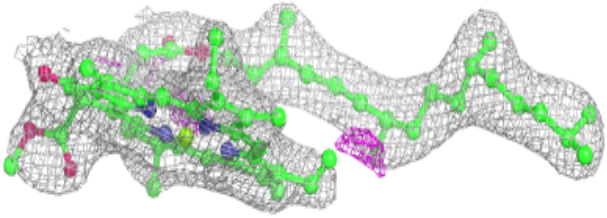


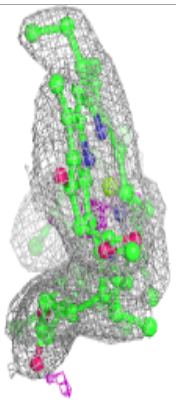


Electron density around CLA c 502:

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

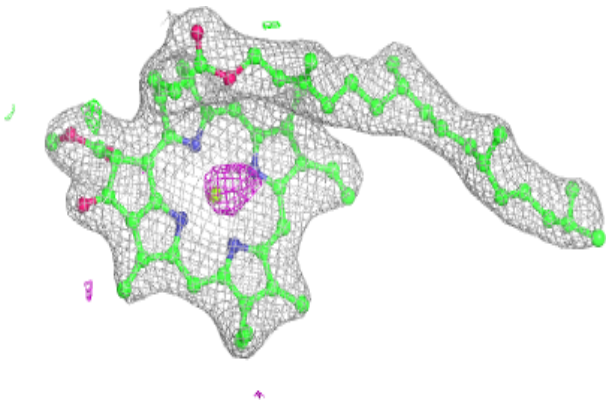


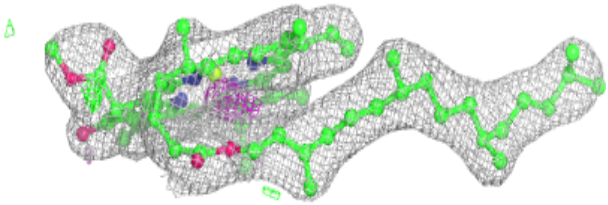


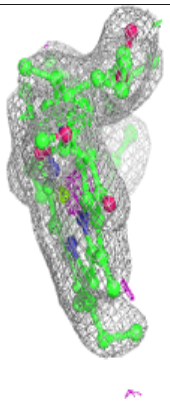


Electron density around CLA C 501:

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

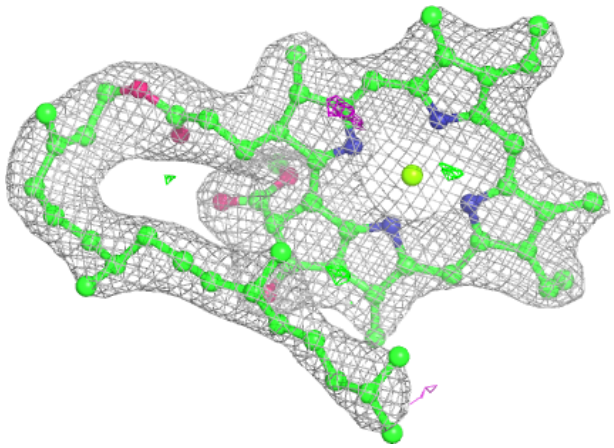


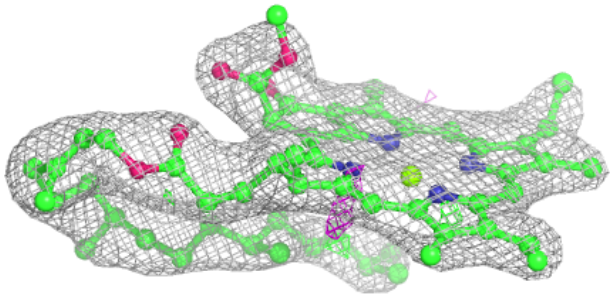


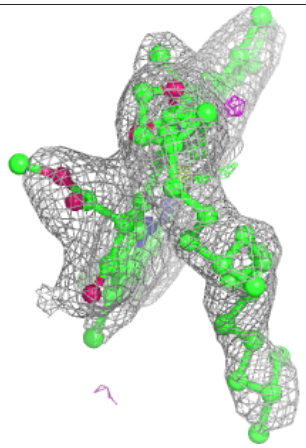


Electron density around CLA C 509:

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

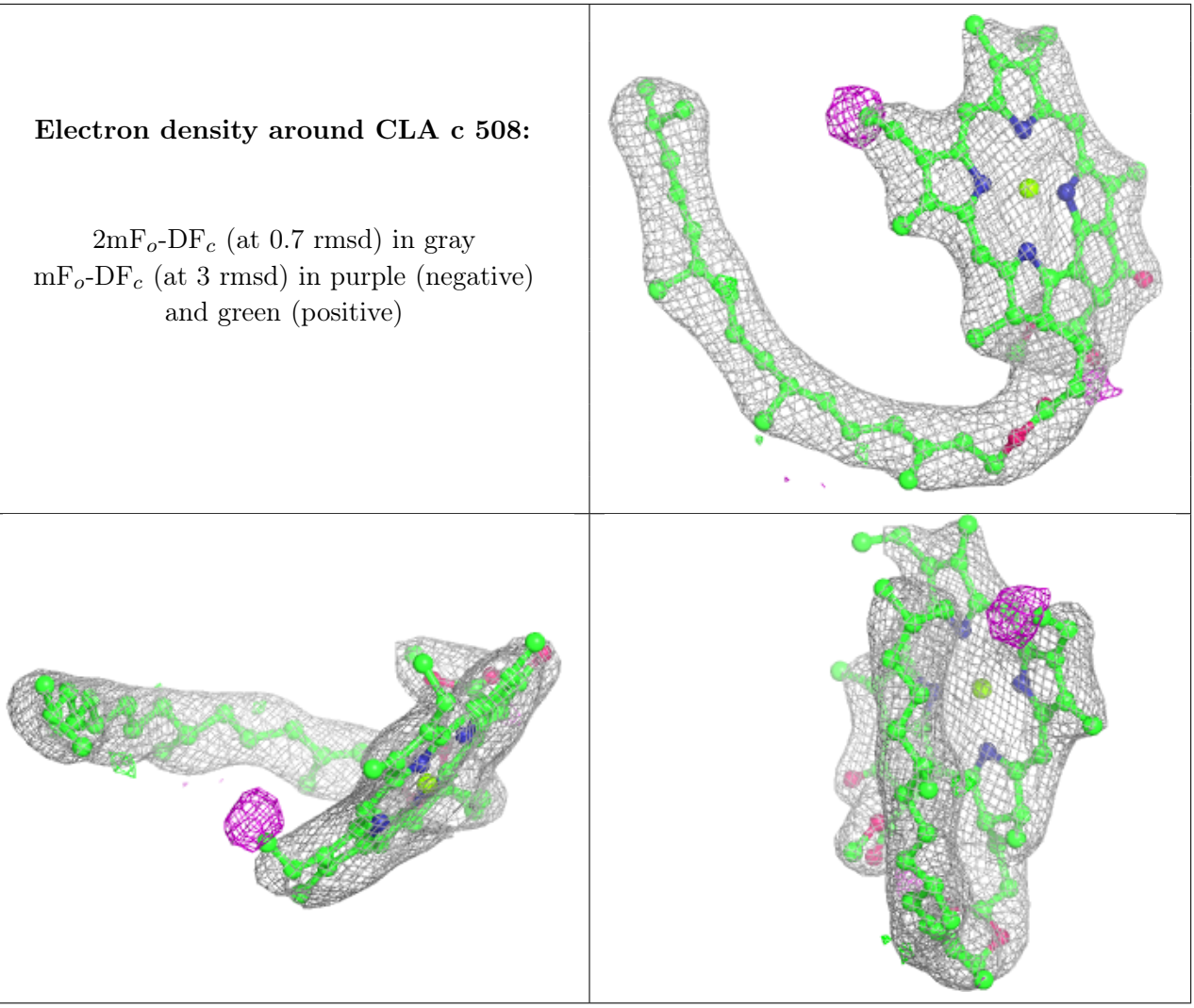






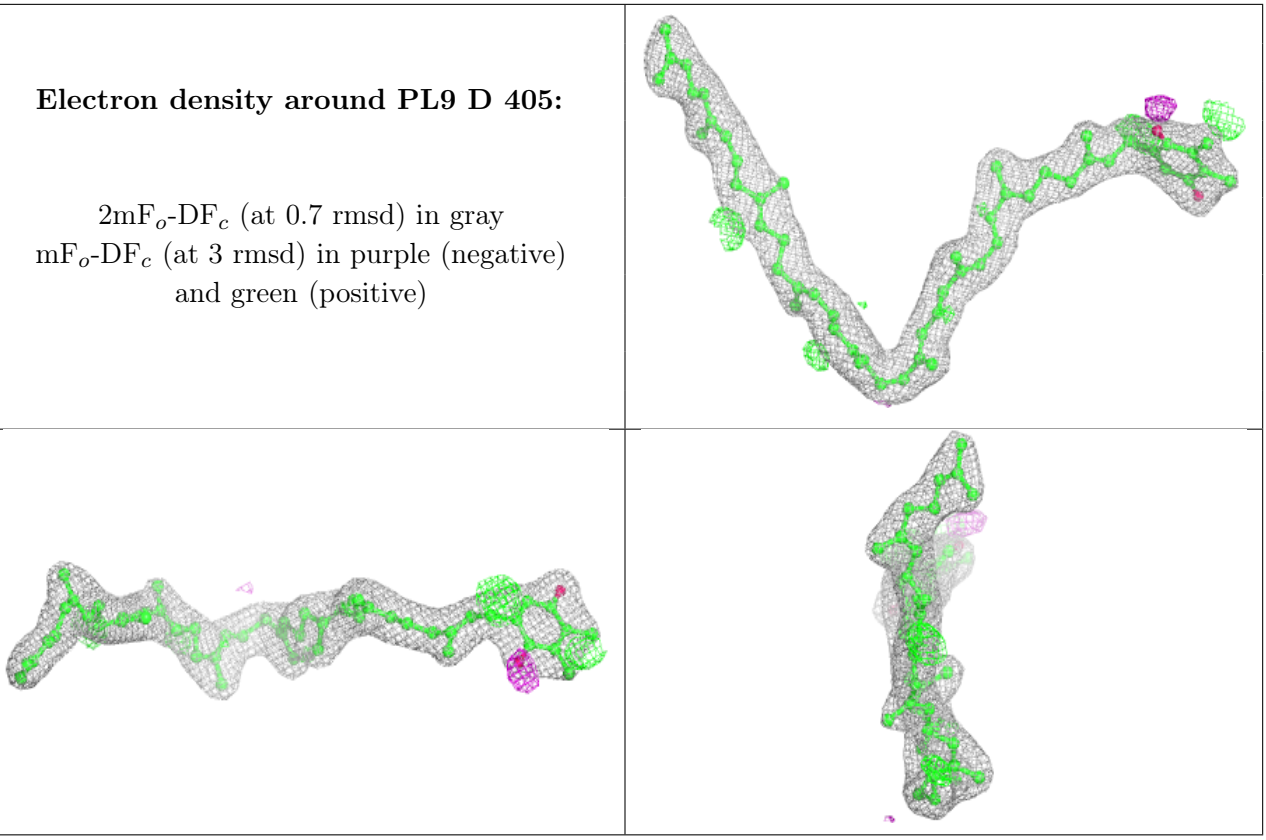
Electron density around CLA c 508:

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



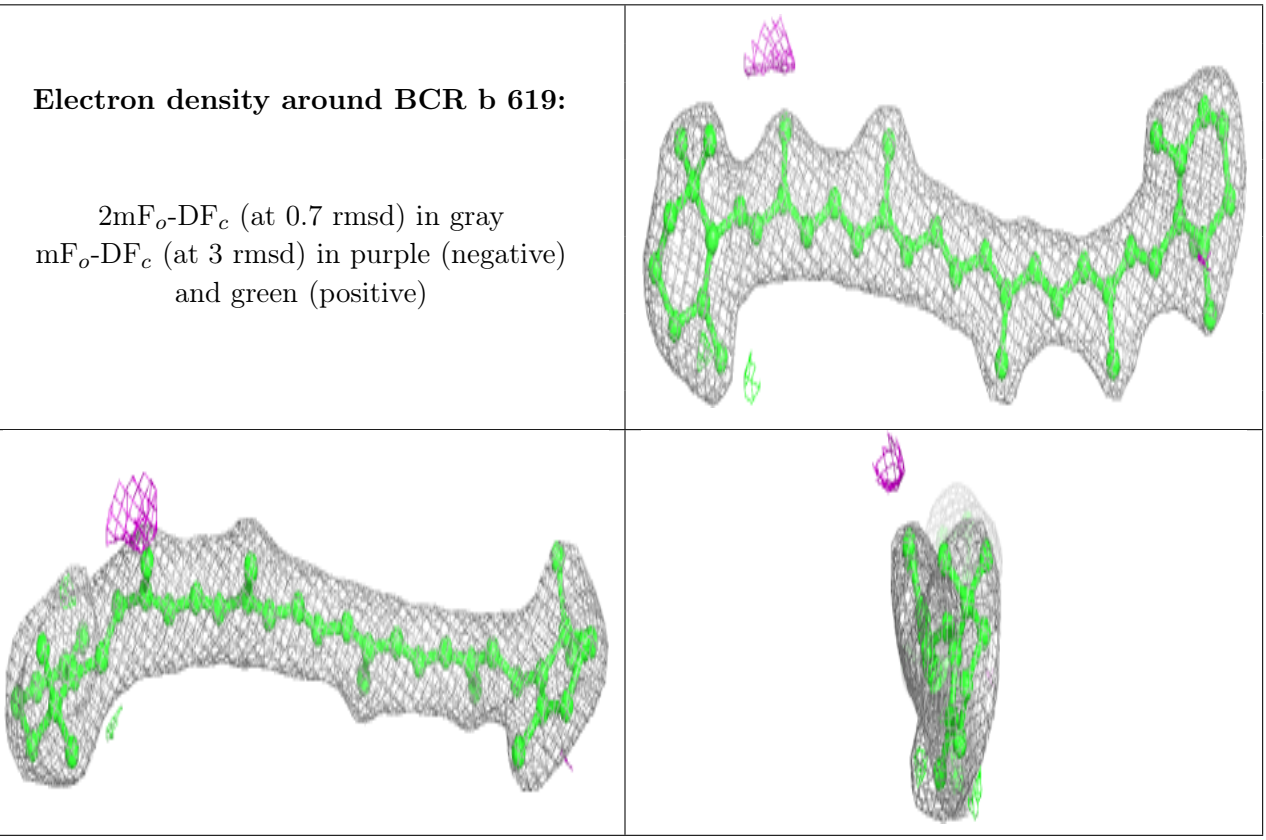
Electron density around PL9 D 405:

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



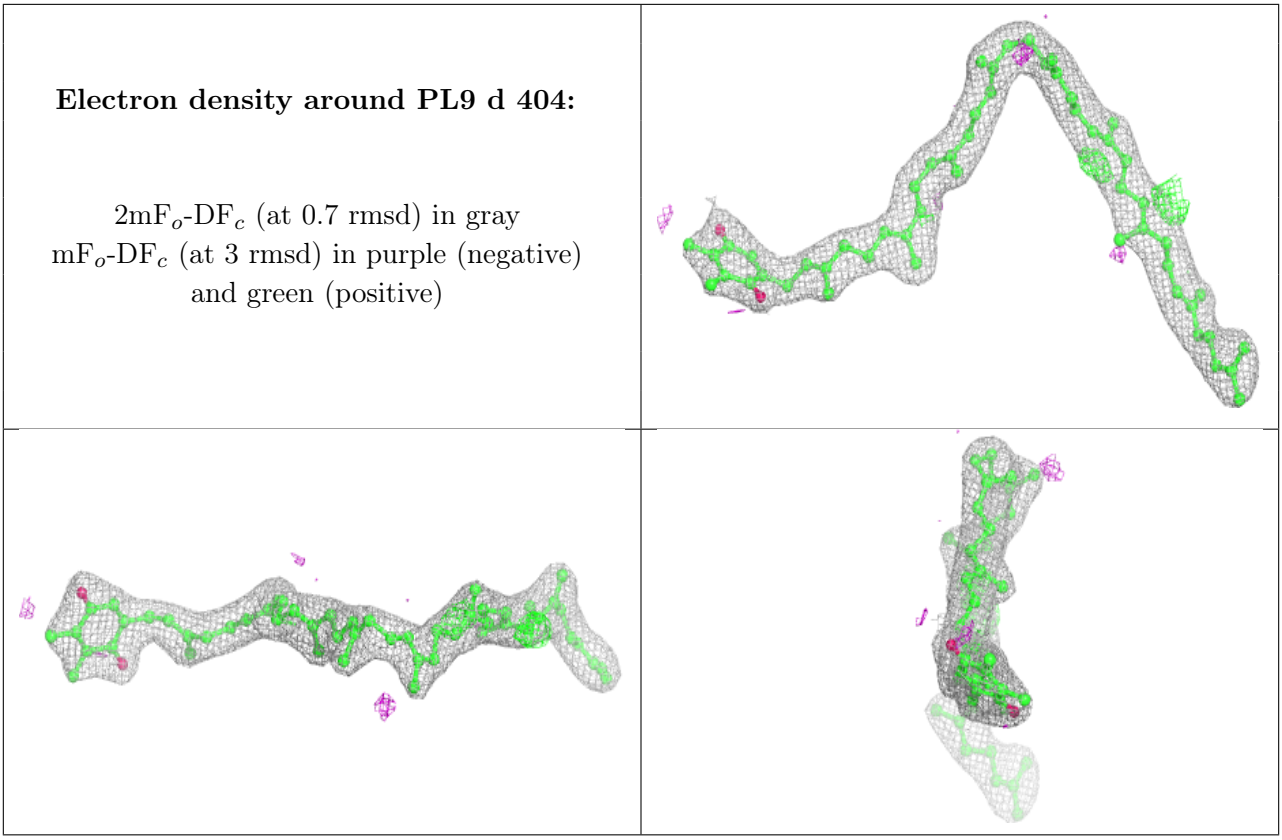
Electron density around BCR b 619:

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



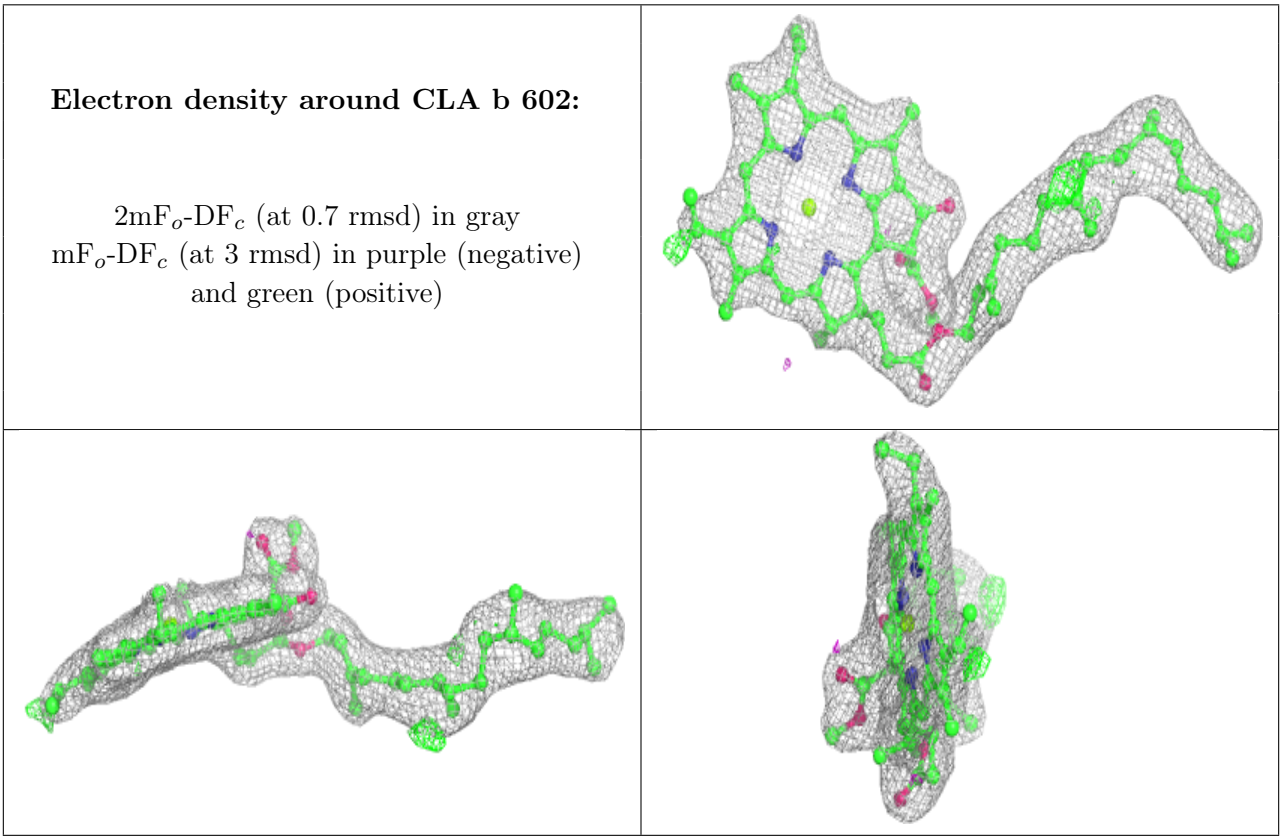
Electron density around PL9 d 404:

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



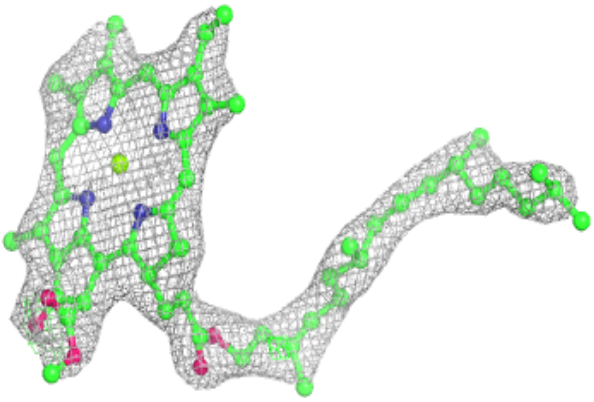
Electron density around CLA b 602:

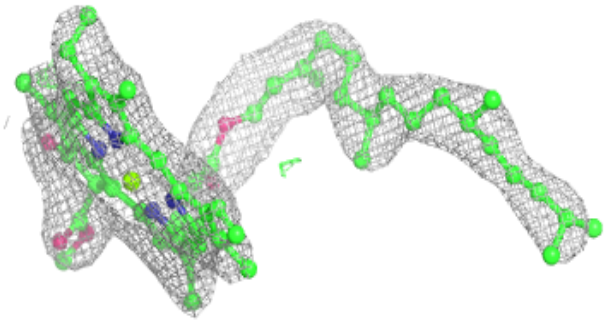
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

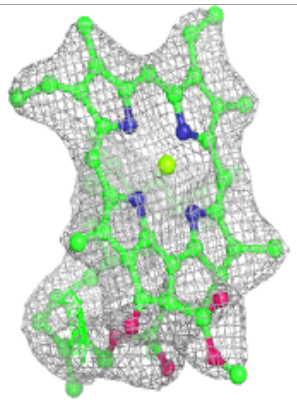


Electron density around CLA c 512:

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

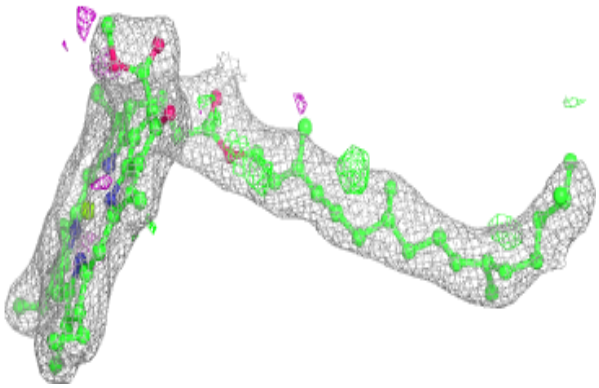


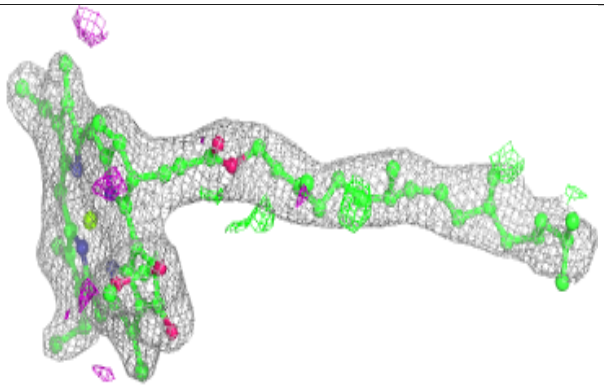


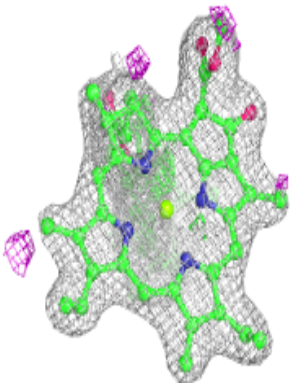


Electron density around CLA b 604:

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

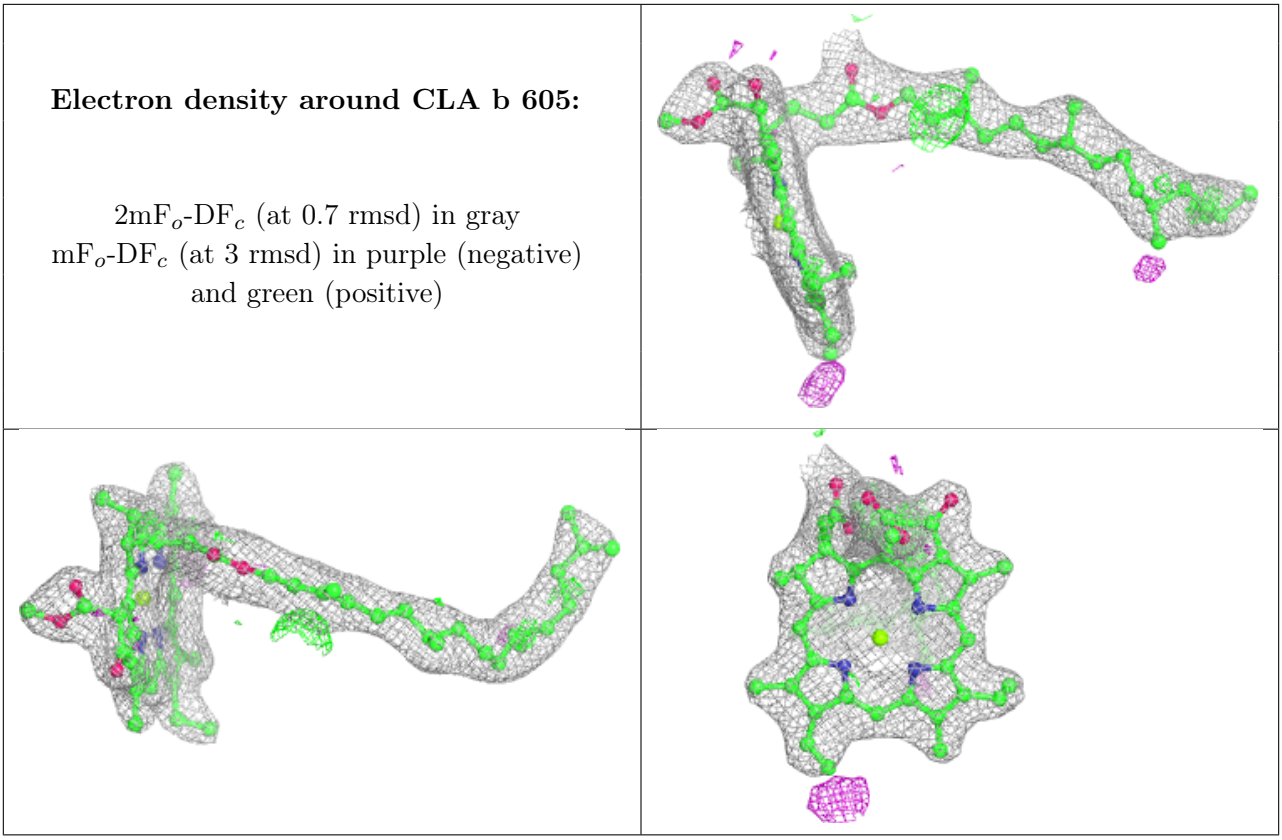






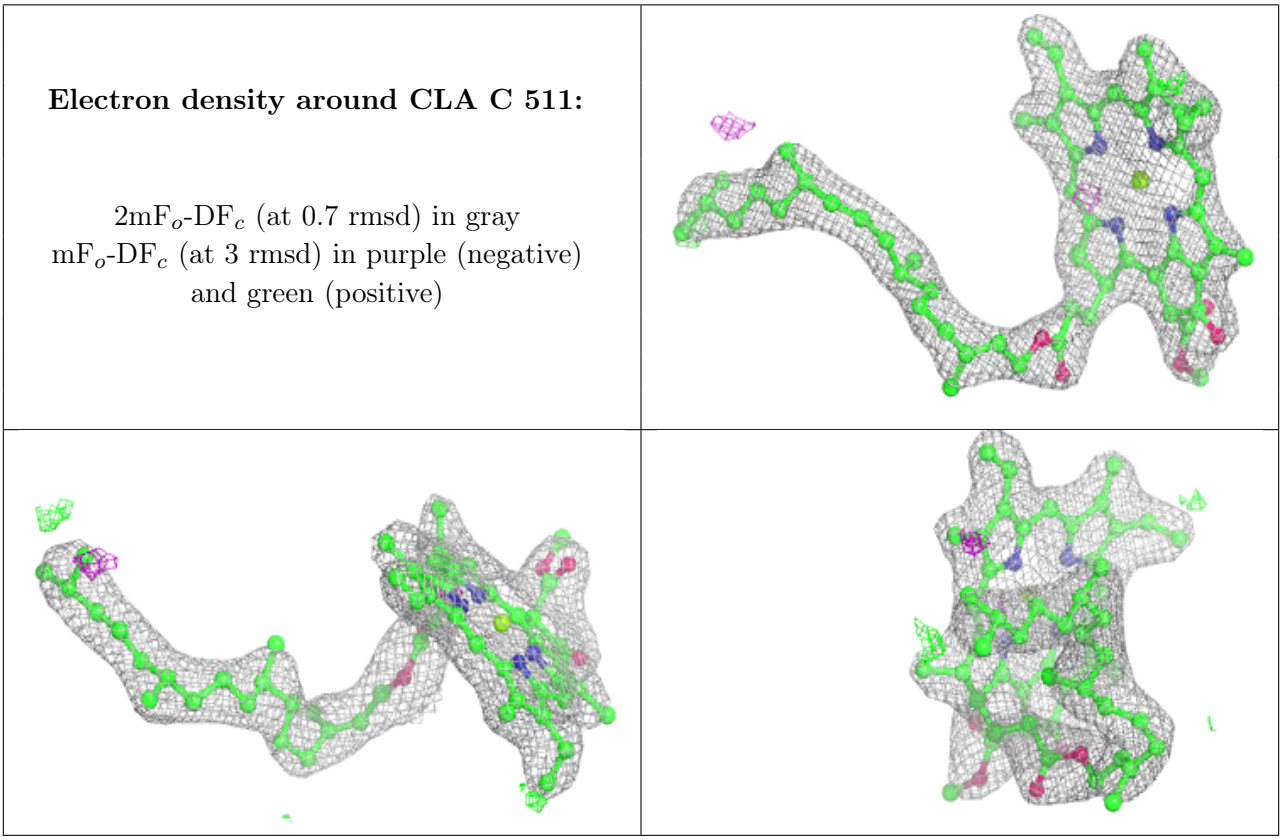
Electron density around CLA b 605:

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



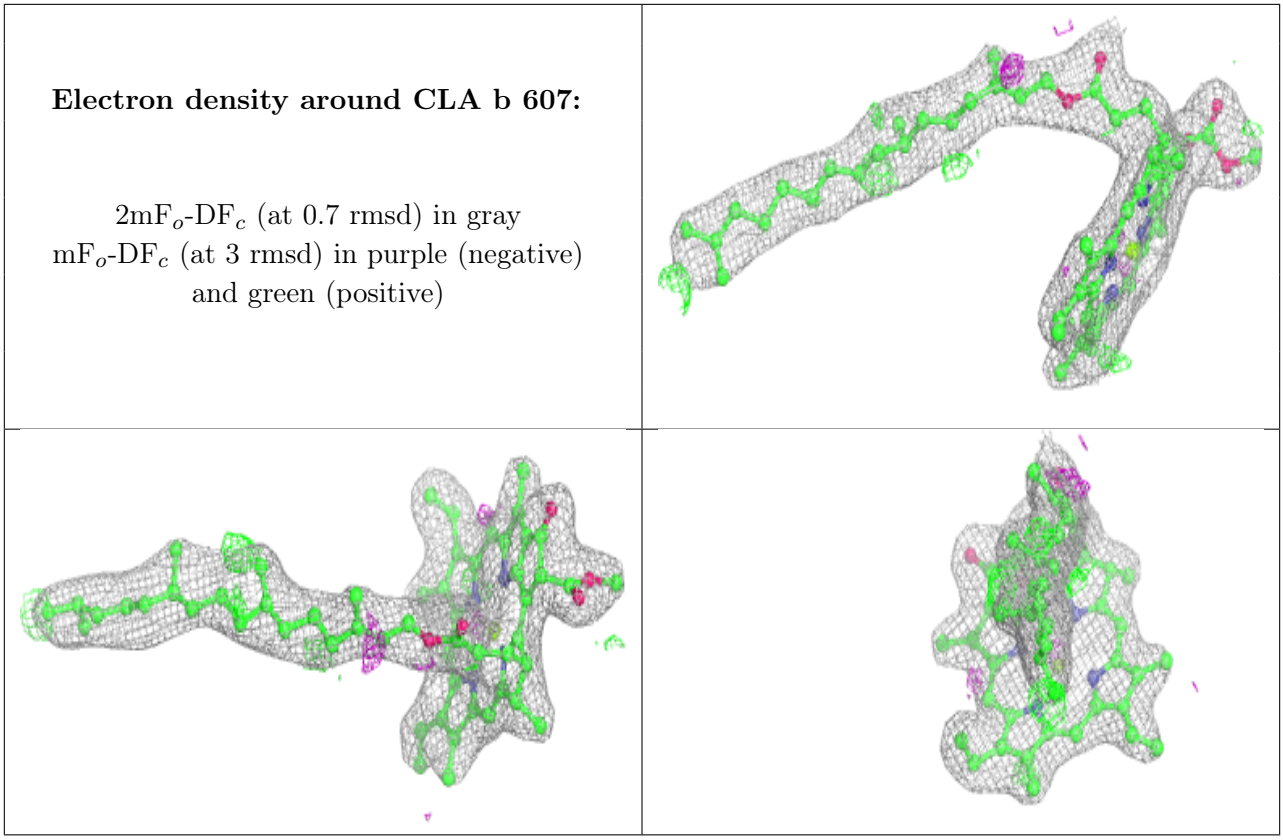
Electron density around CLA C 511:

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



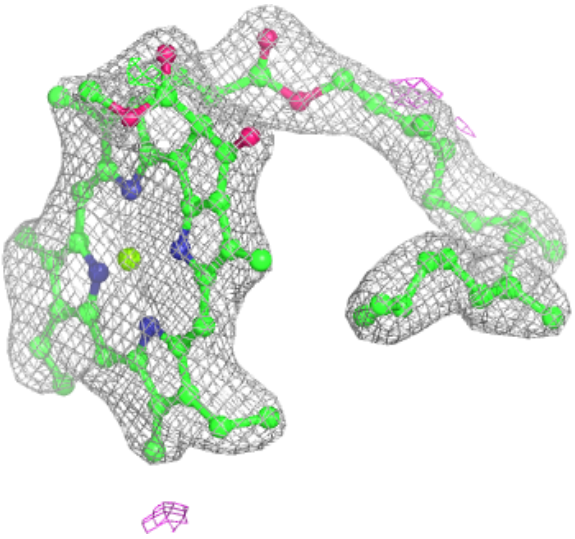
Electron density around CLA b 607:

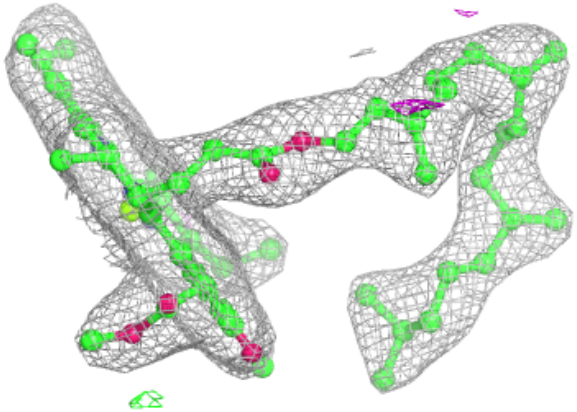
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

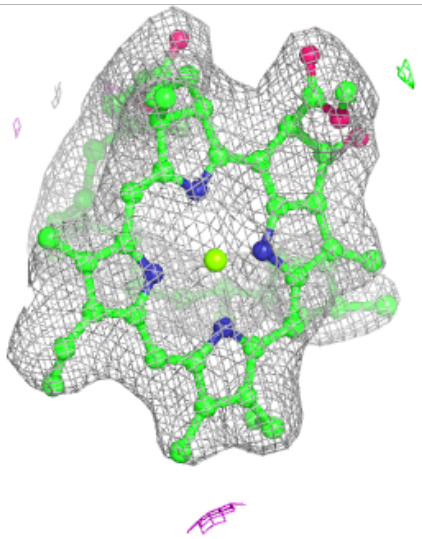


Electron density around CLA C 503:

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

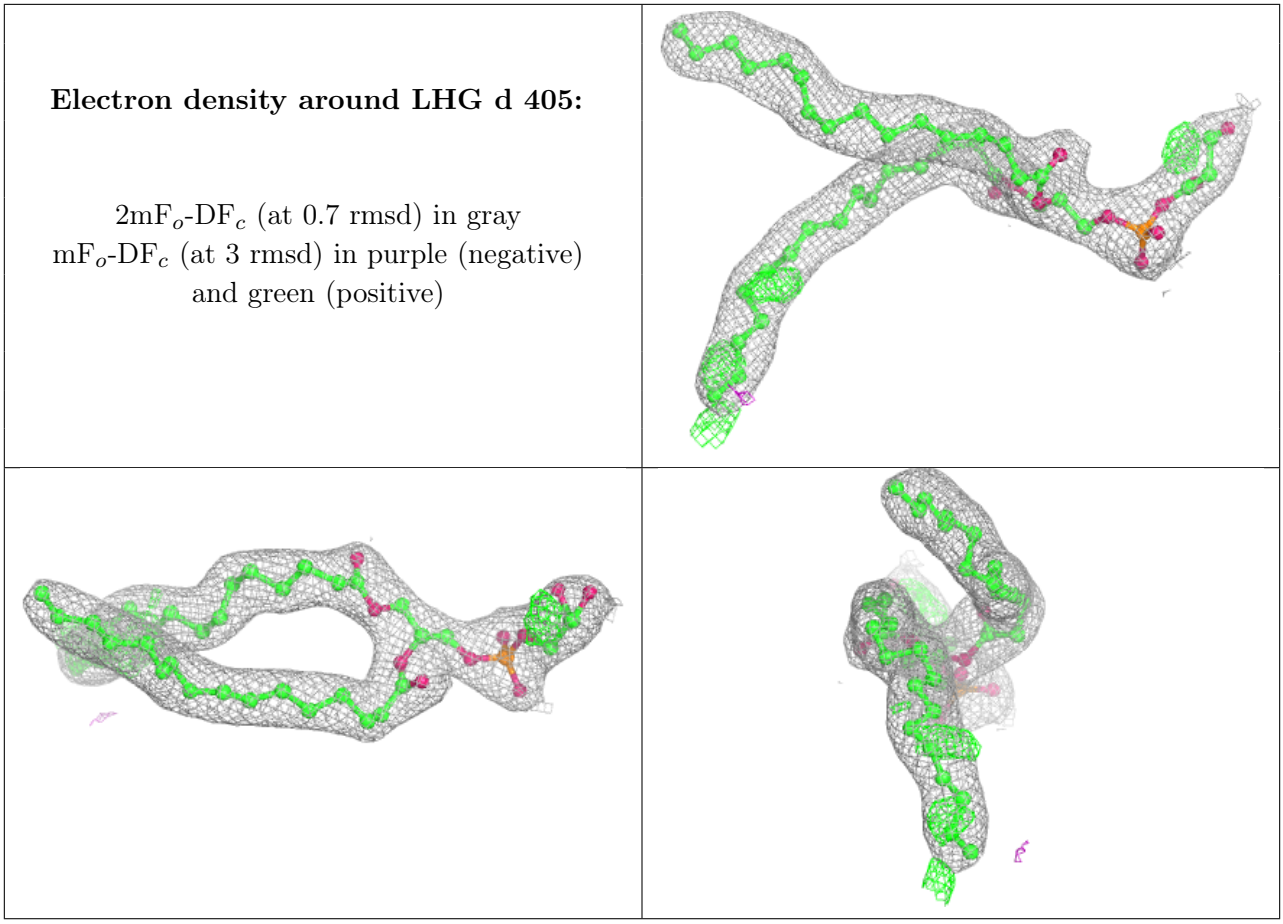






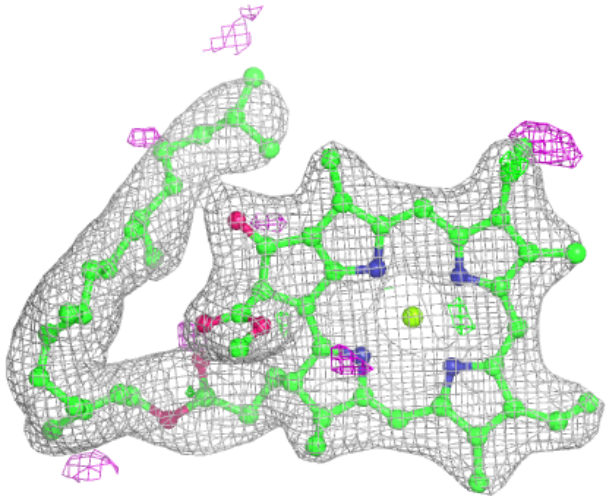
Electron density around LHG d 405:

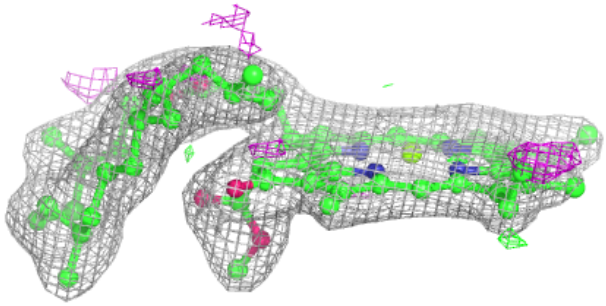
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

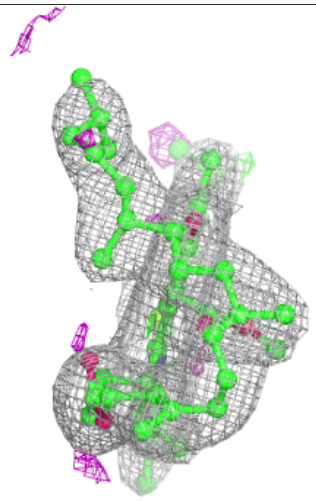


Electron density around CLA B 610:

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

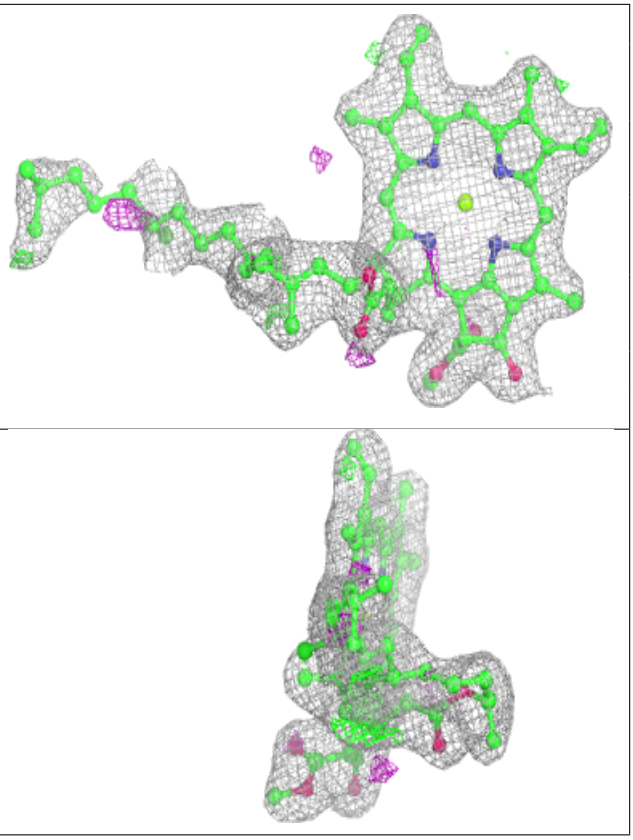






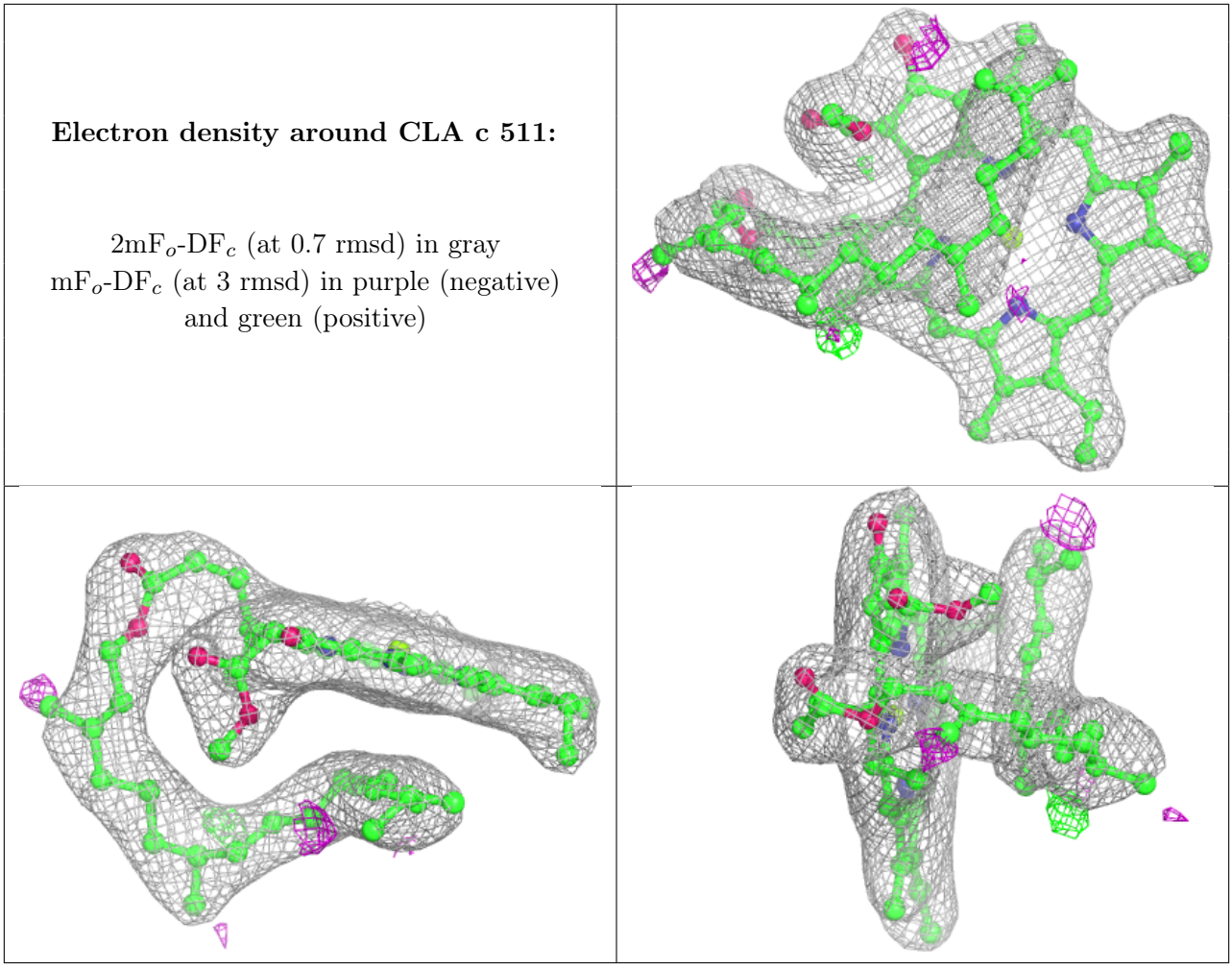
Electron density around CLA A 406:

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



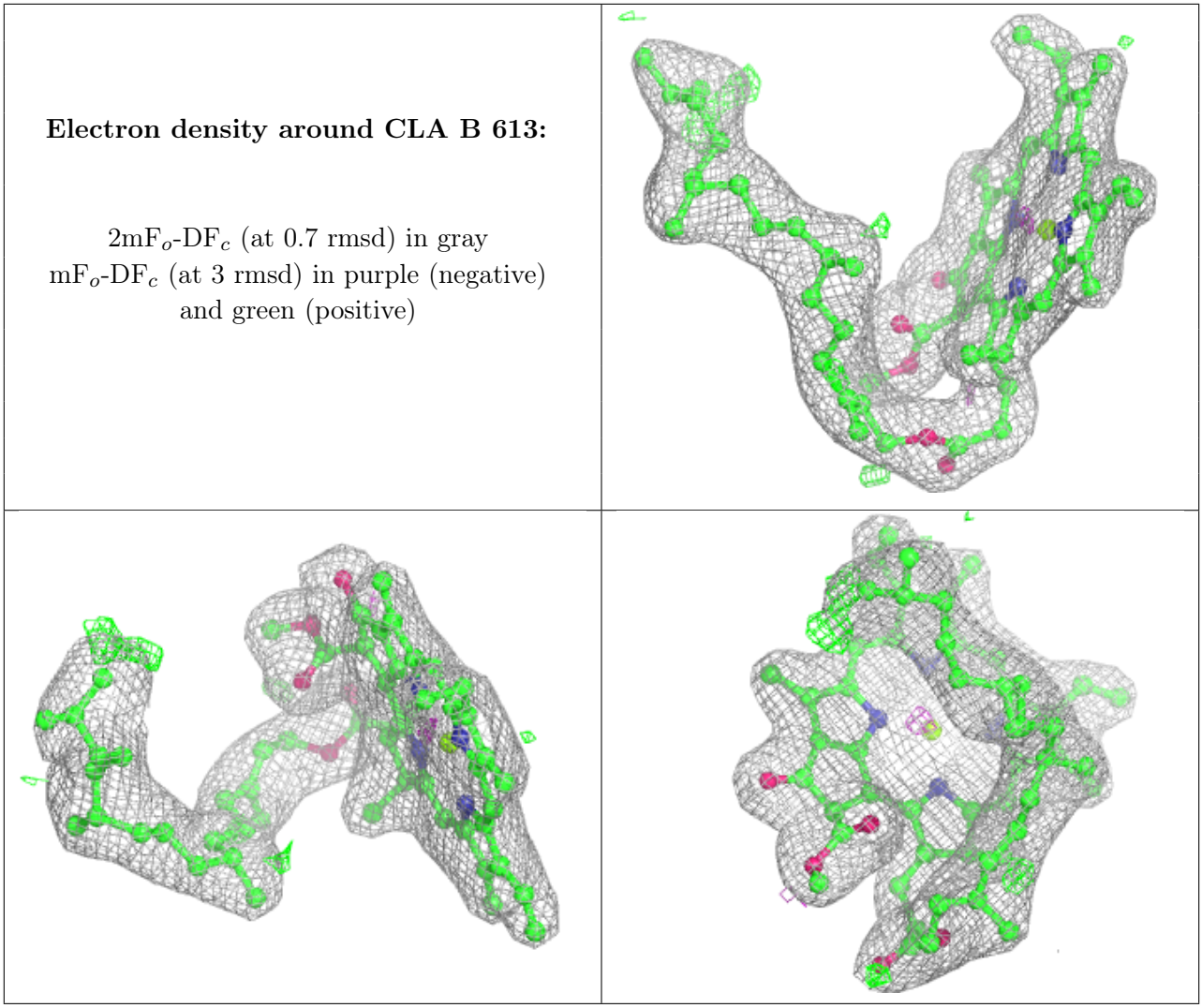
Electron density around CLA c 511:

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



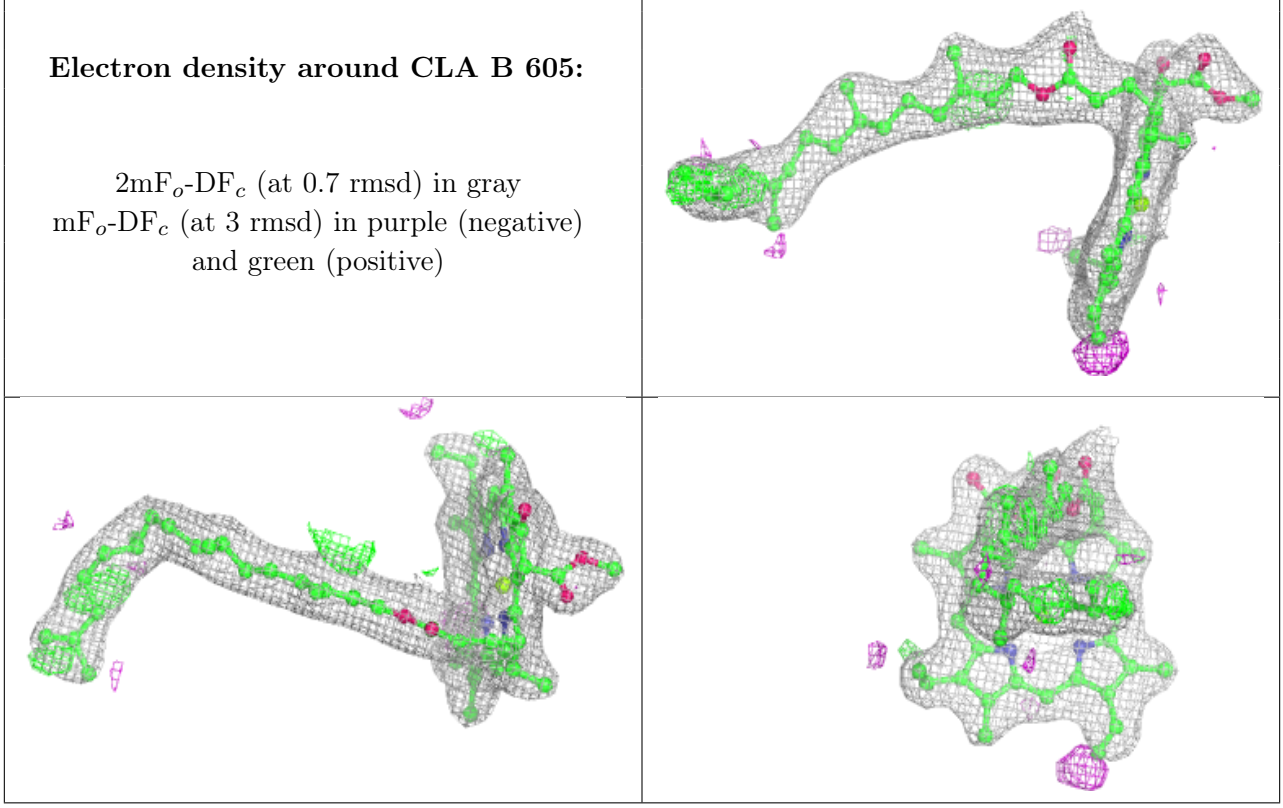
Electron density around CLA B 613:

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



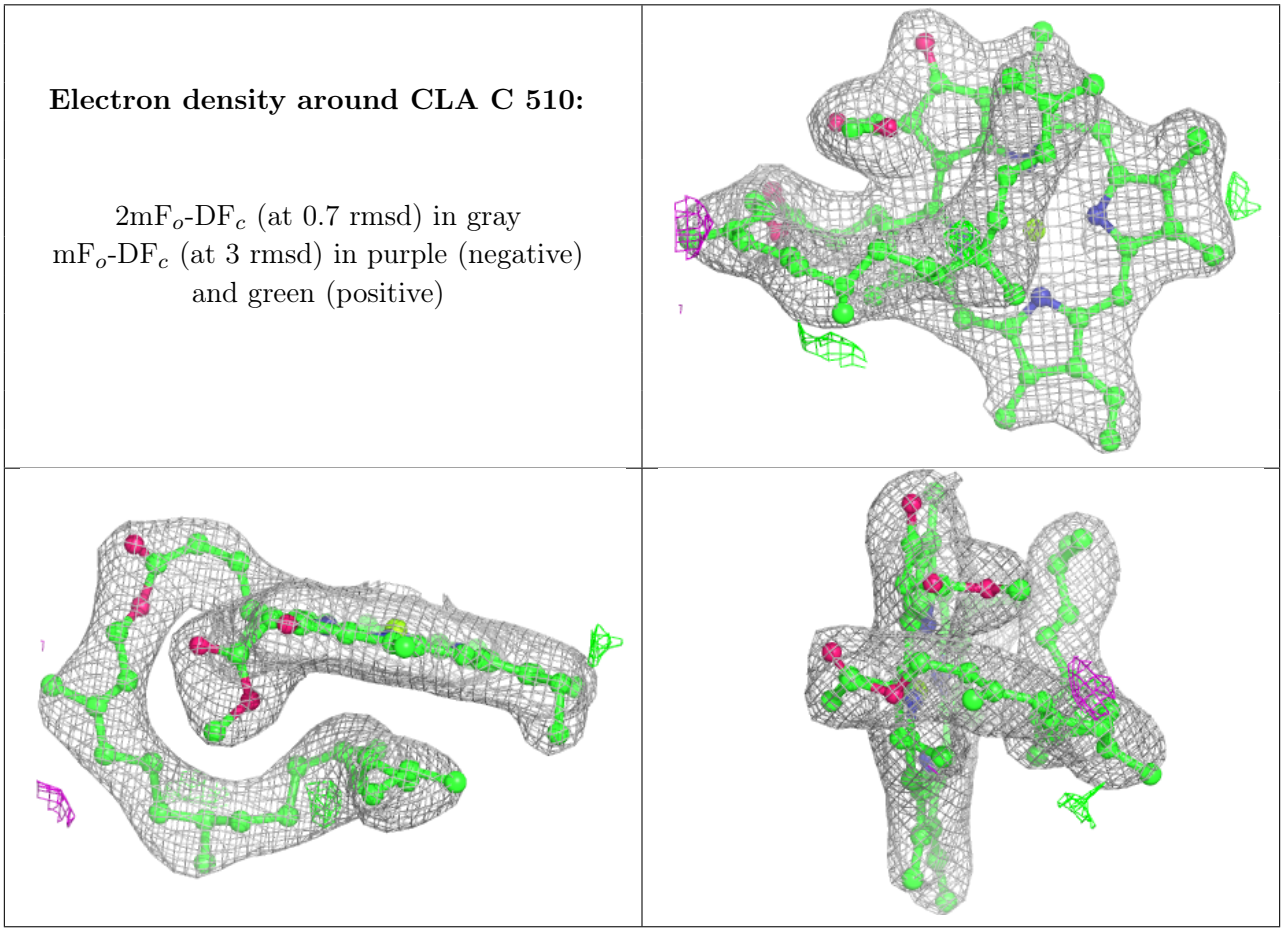
Electron density around CLA B 605:

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



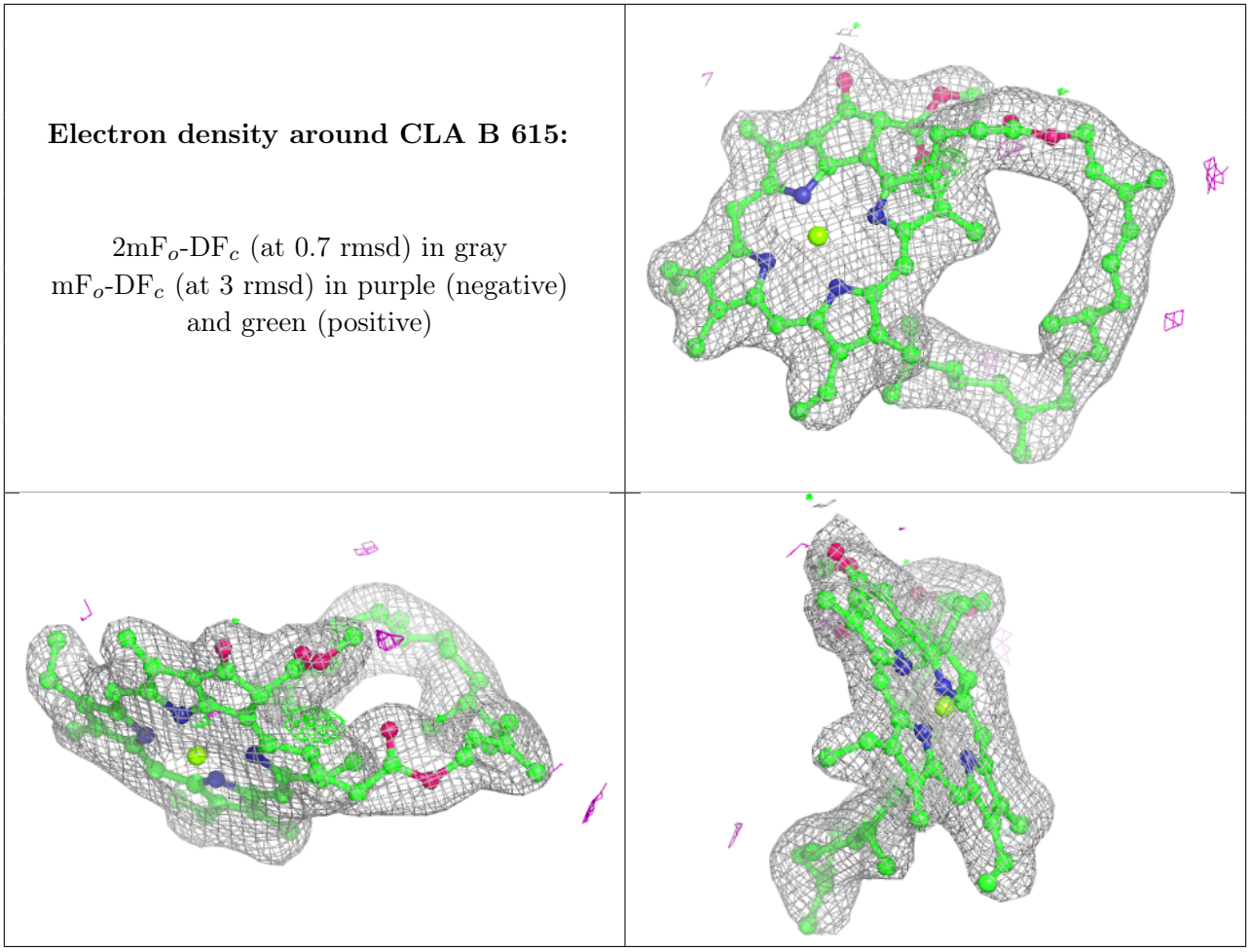
Electron density around CLA C 510:

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



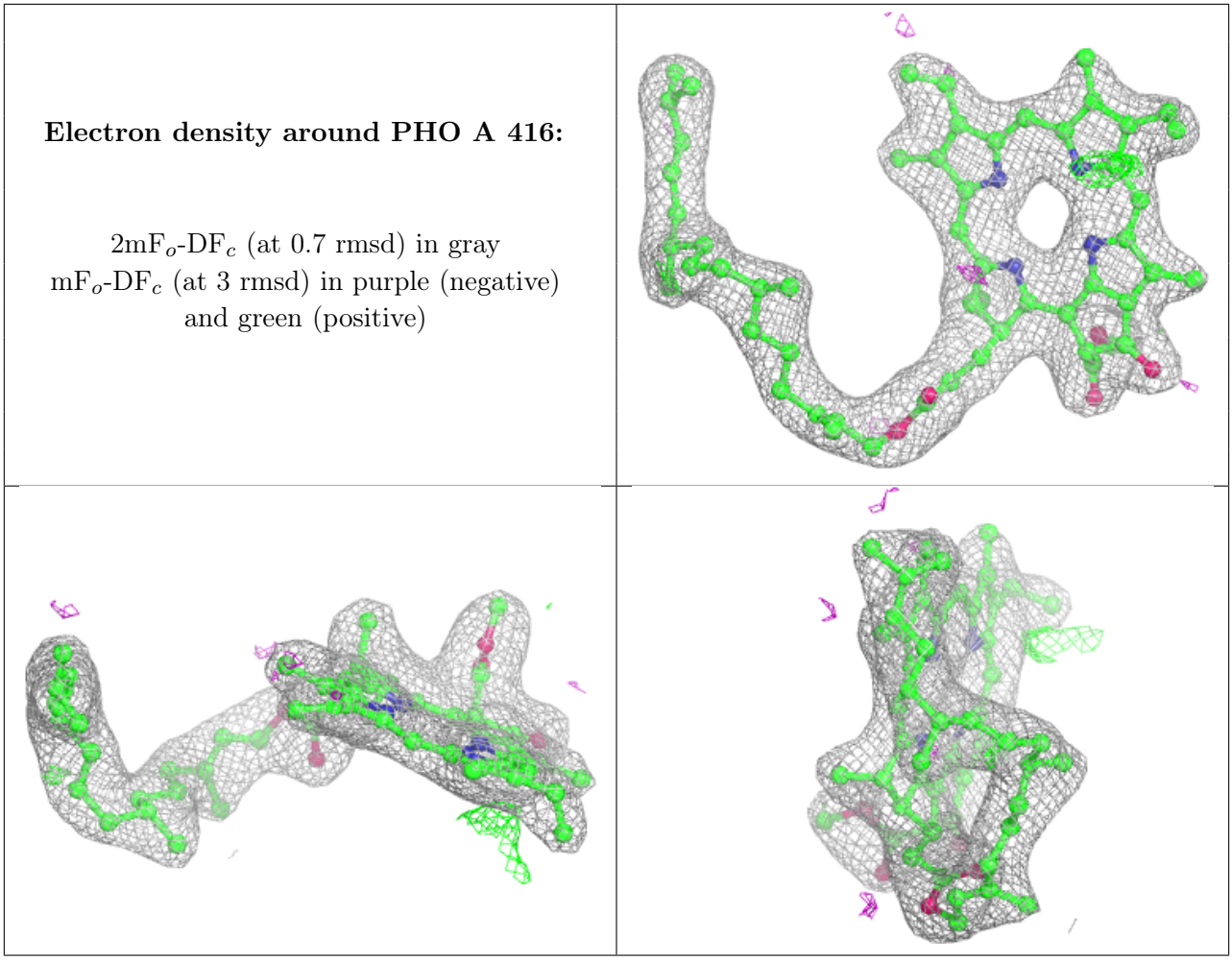
Electron density around CLA B 615:

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



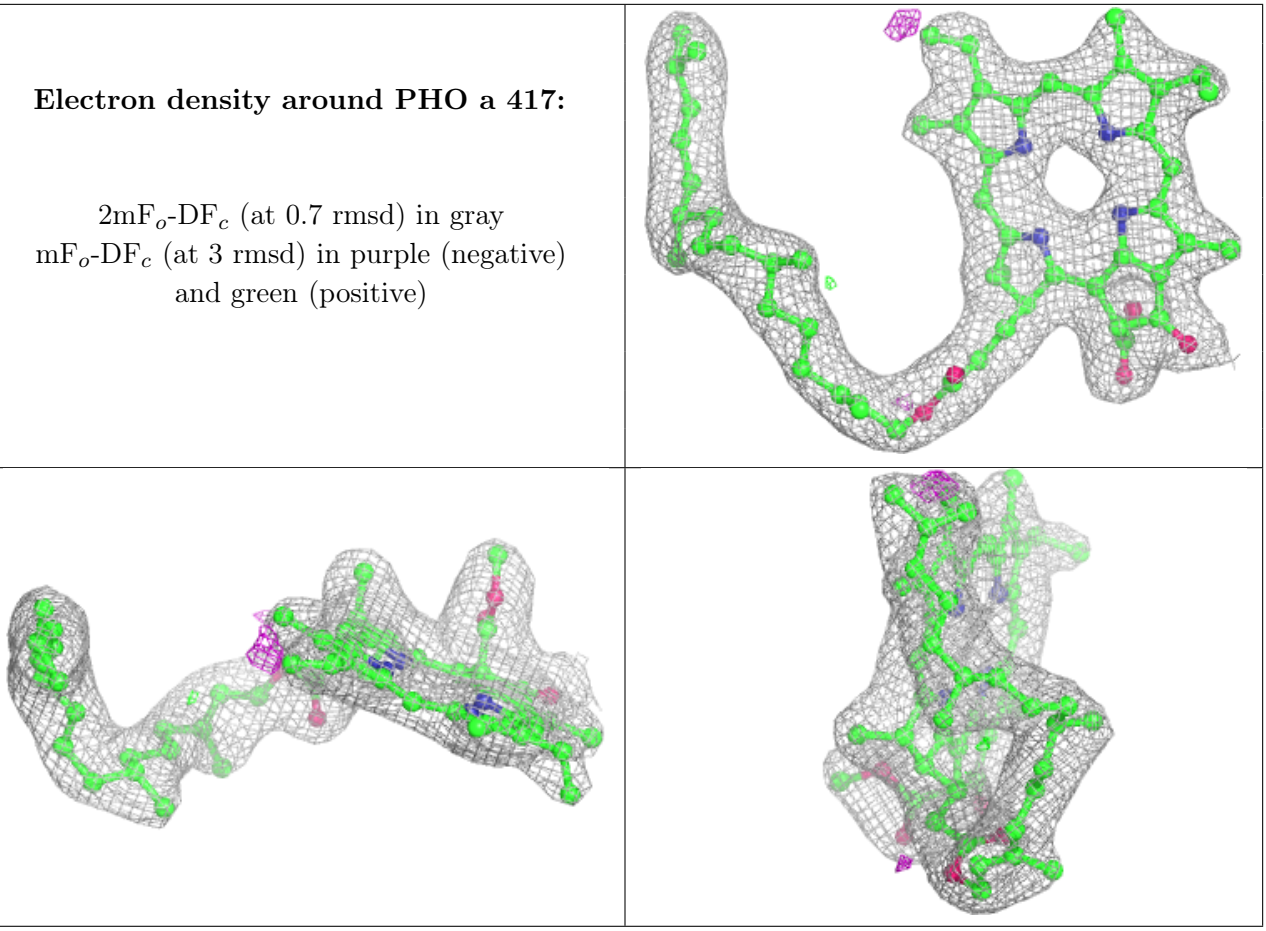
Electron density around PHO A 416:

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



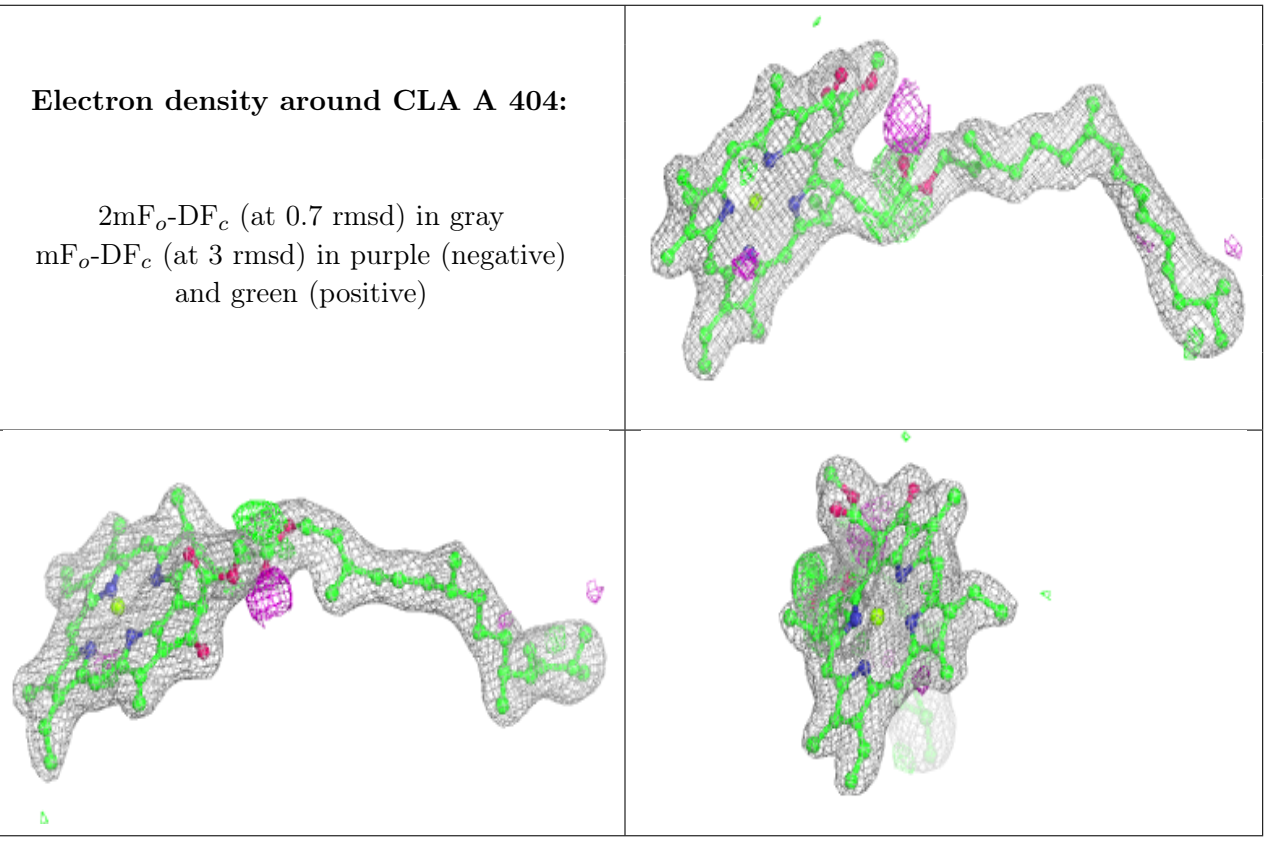
Electron density around PHO a 417:

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



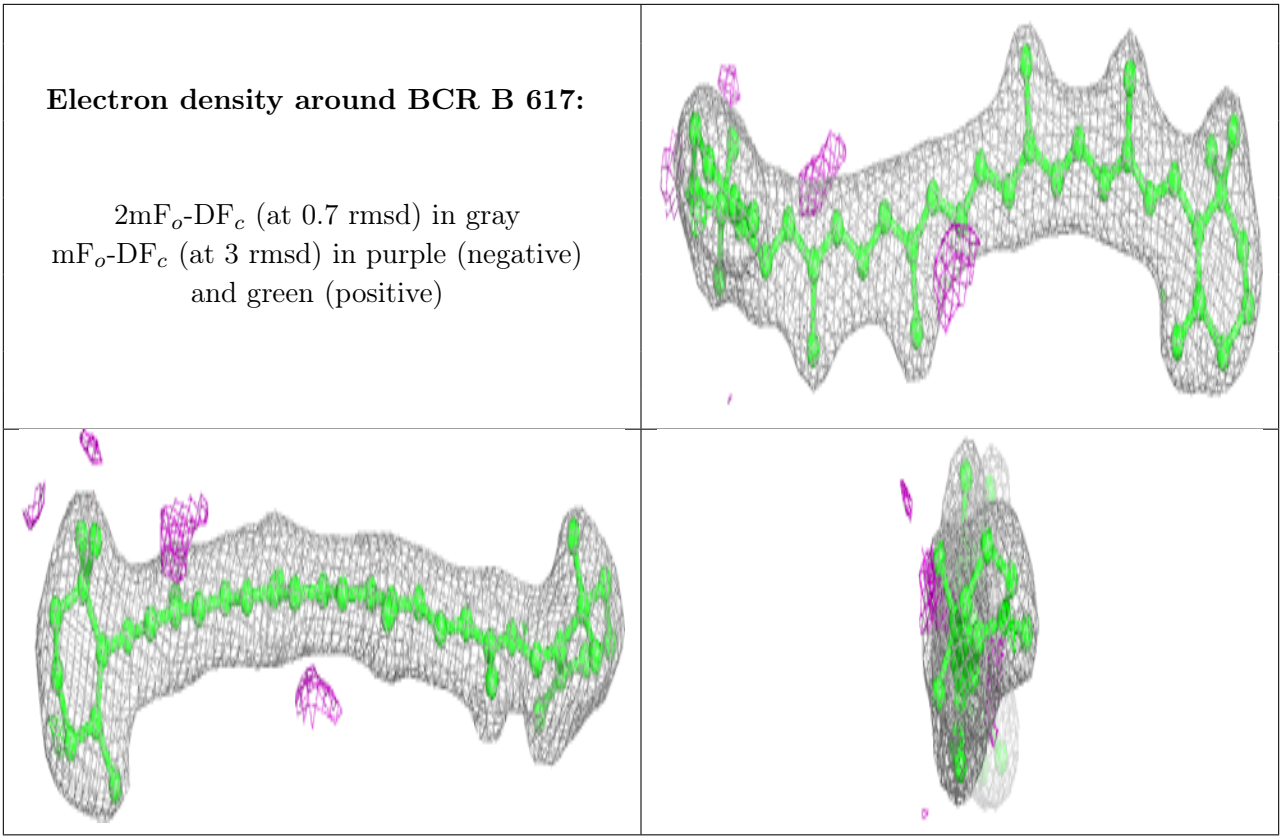
Electron density around CLA A 404:

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



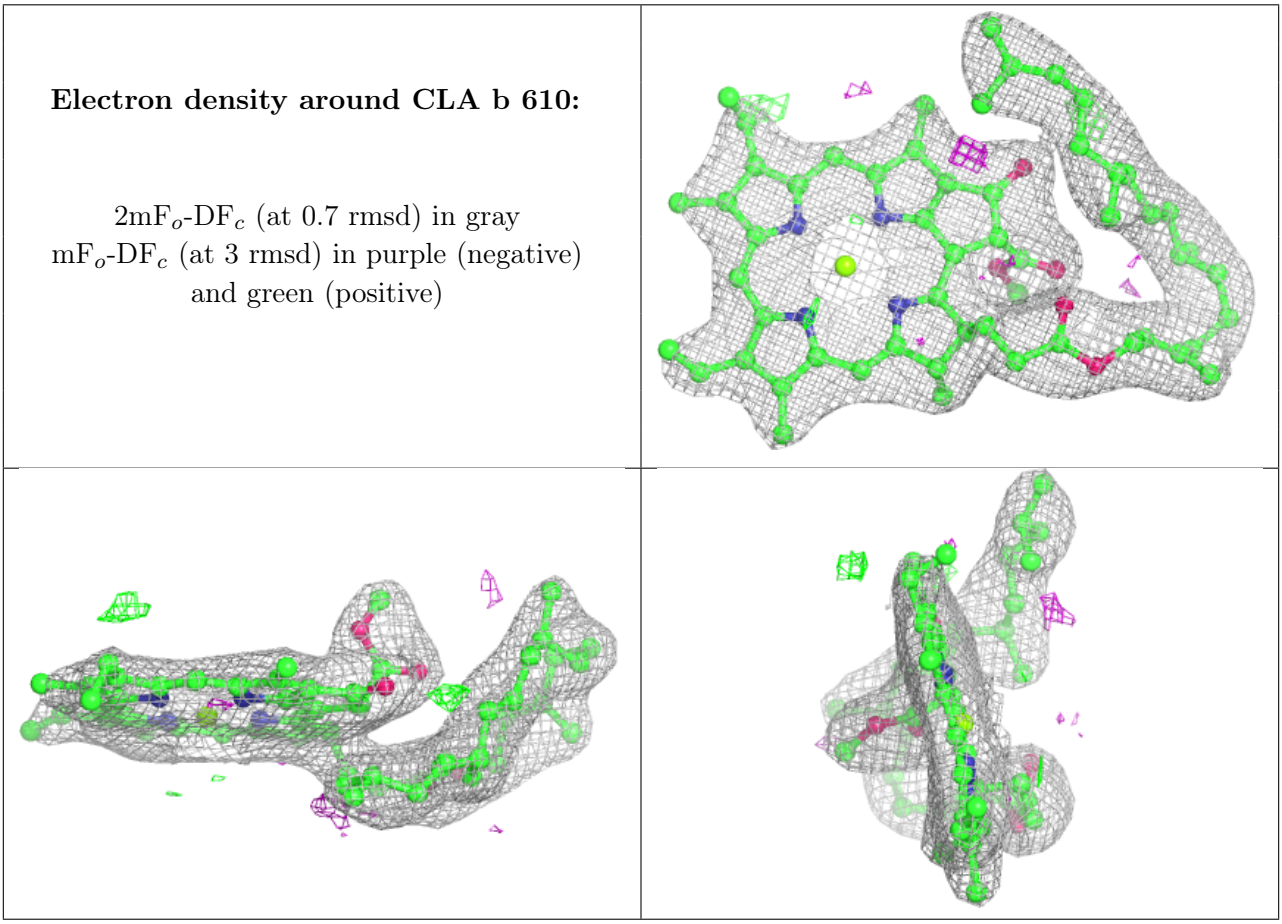
Electron density around BCR B 617:

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



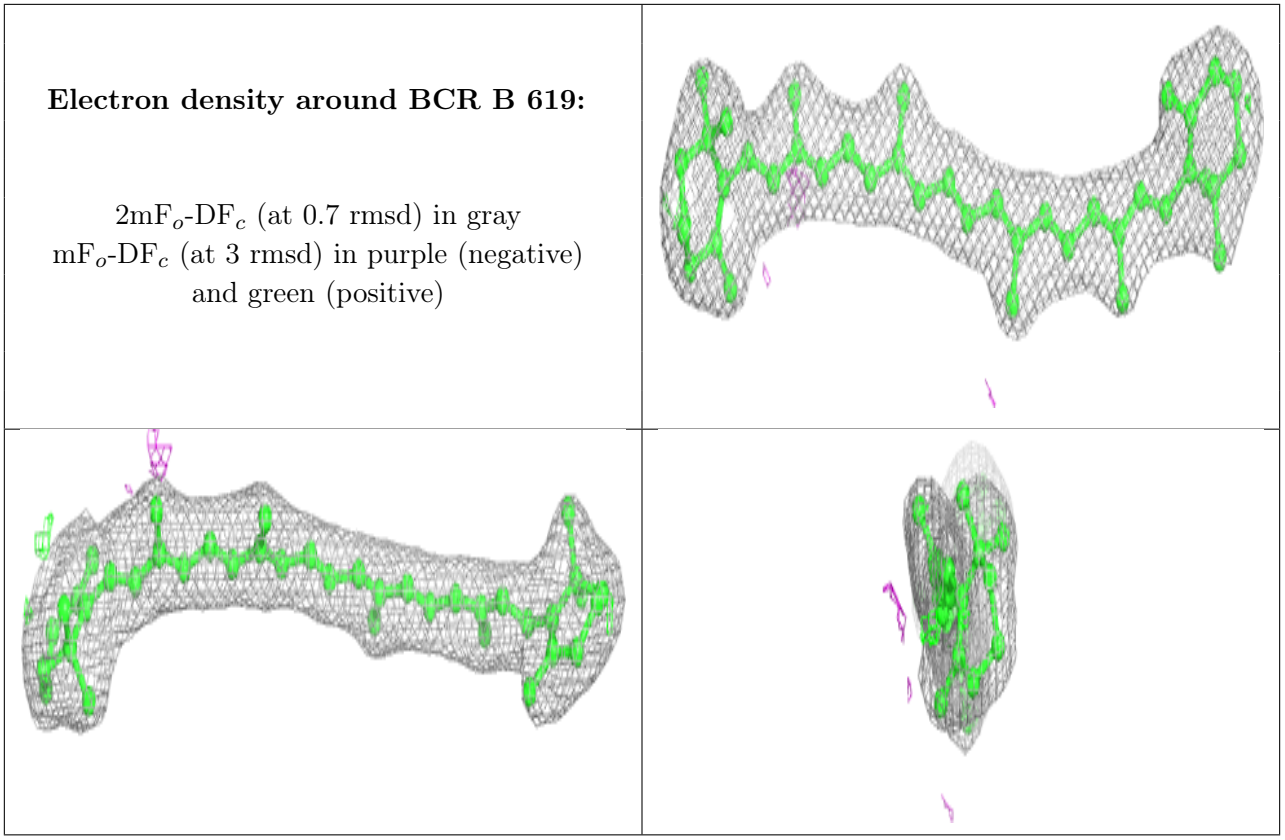
Electron density around CLA b 610:

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



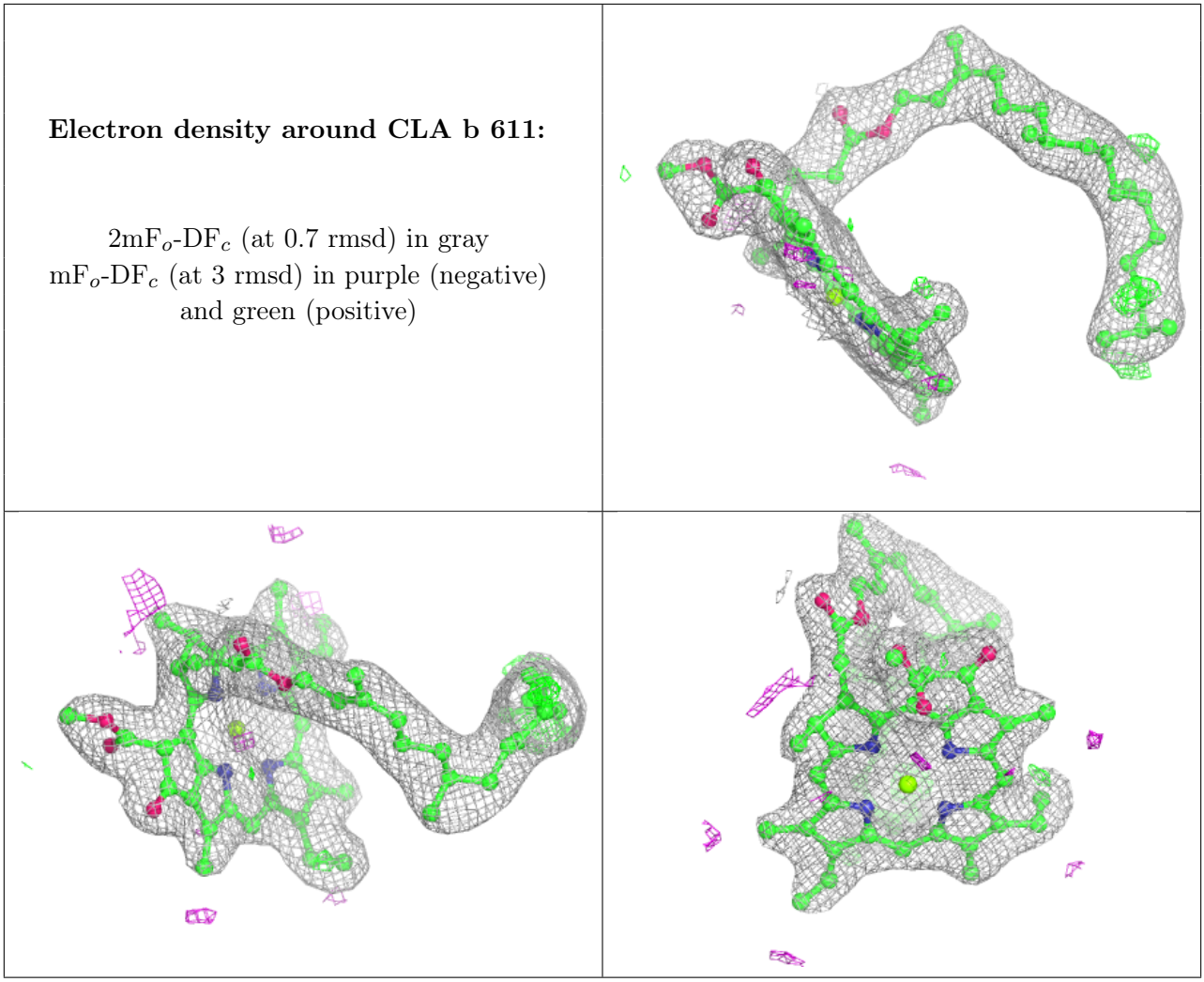
Electron density around BCR B 619:

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



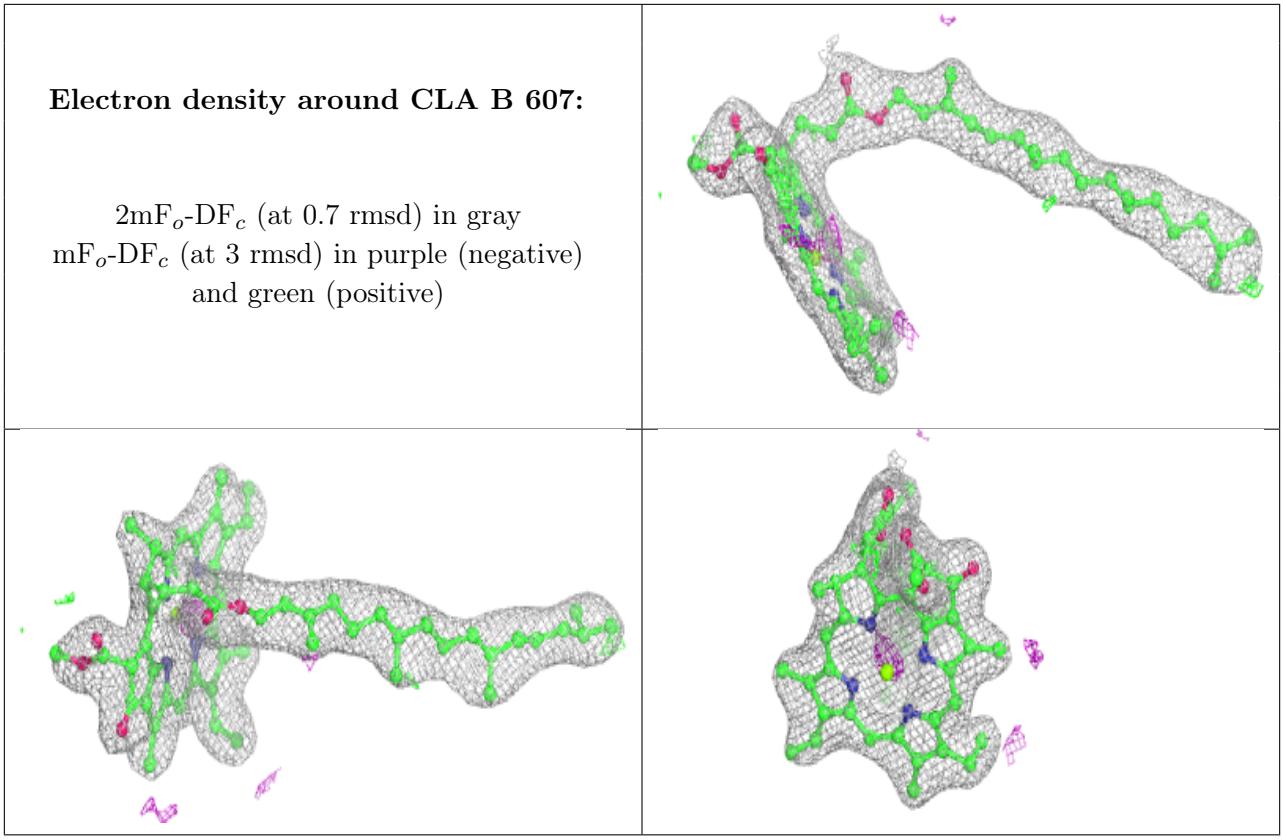
Electron density around CLA b 611:

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



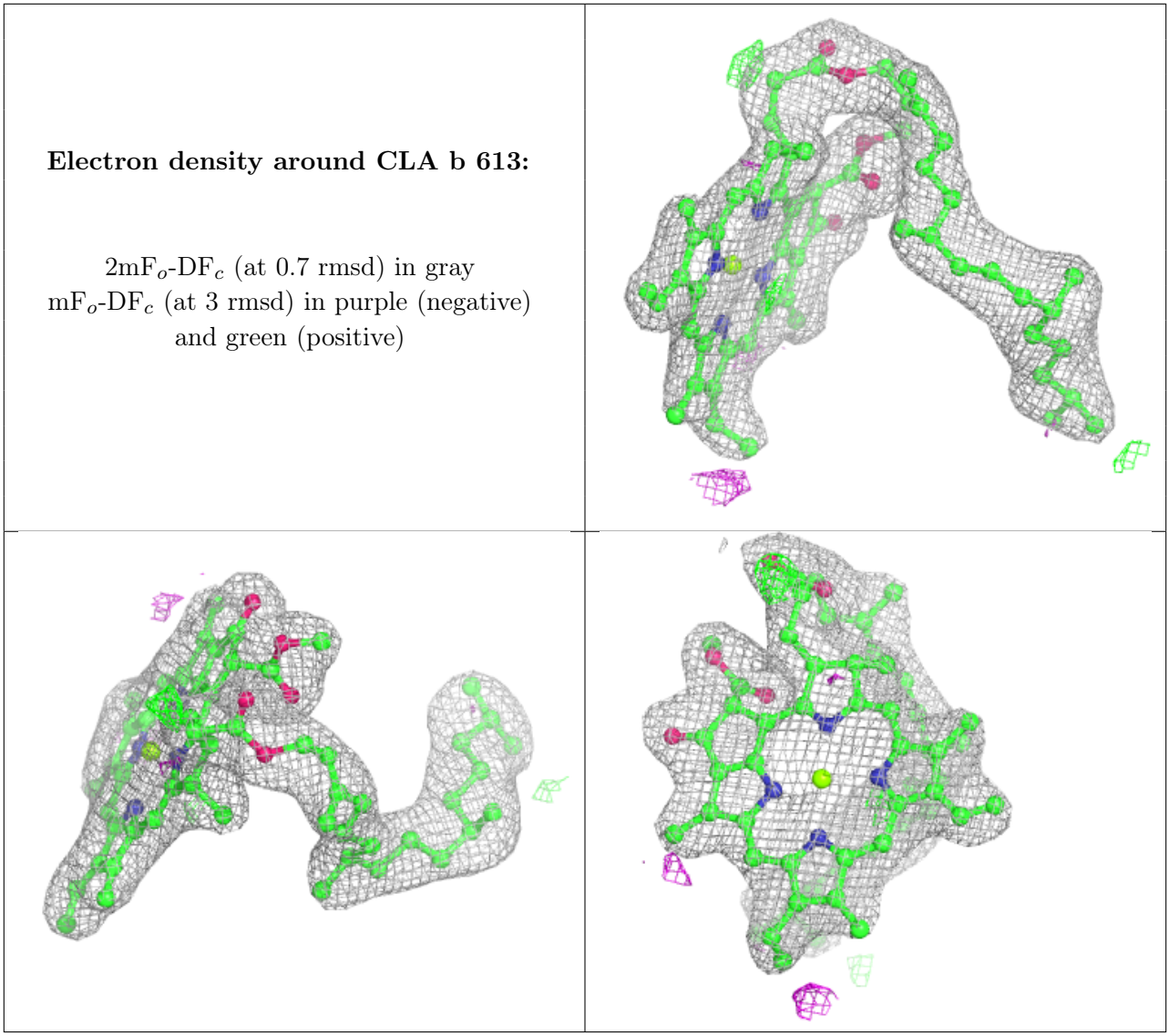
Electron density around CLA B 607:

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



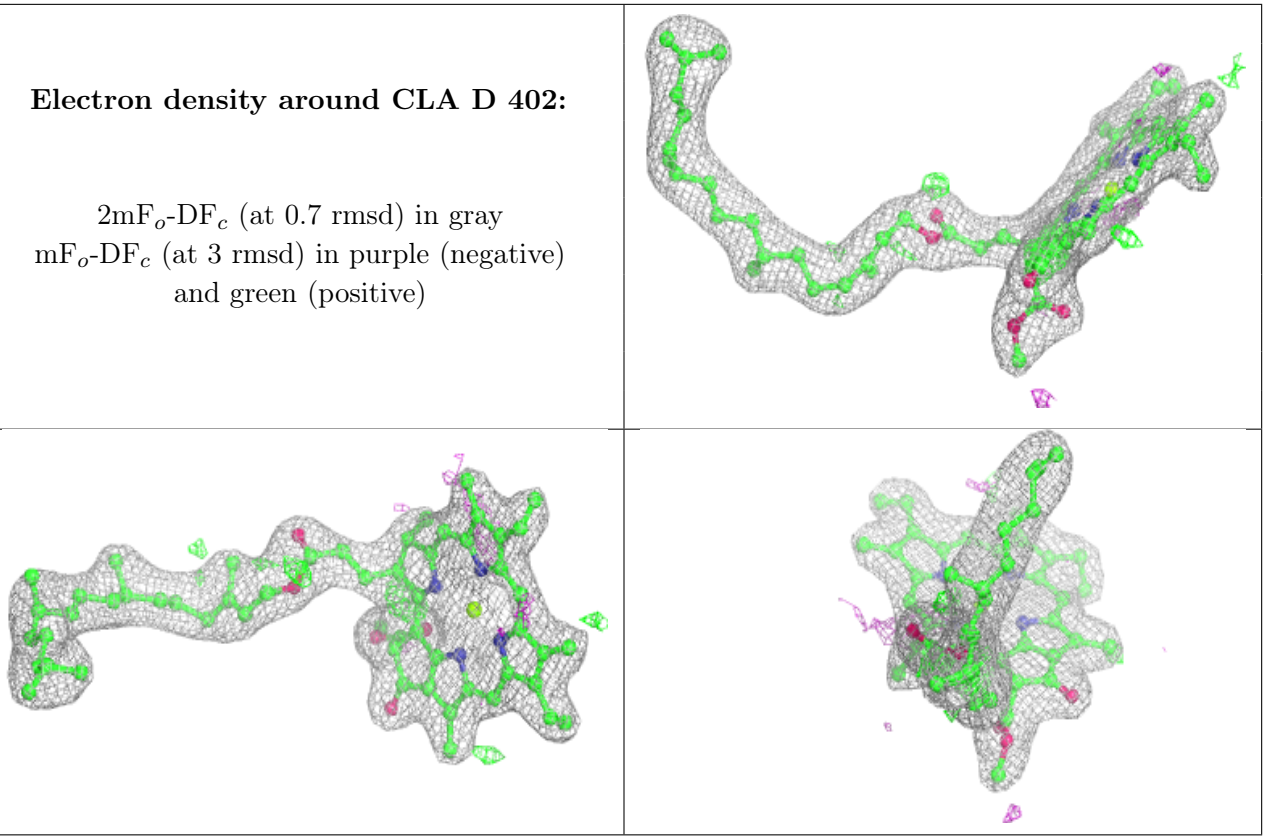
Electron density around CLA b 613:

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



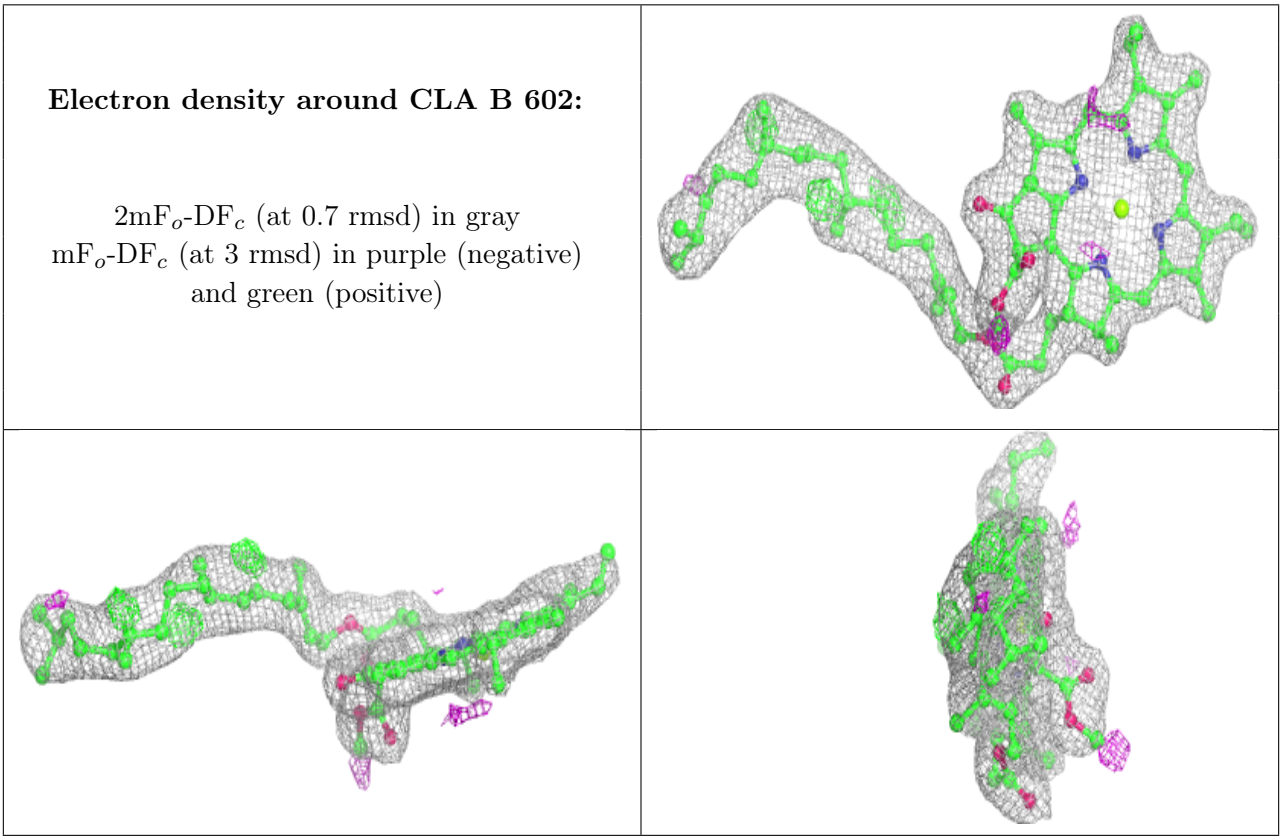
Electron density around CLA D 402:

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



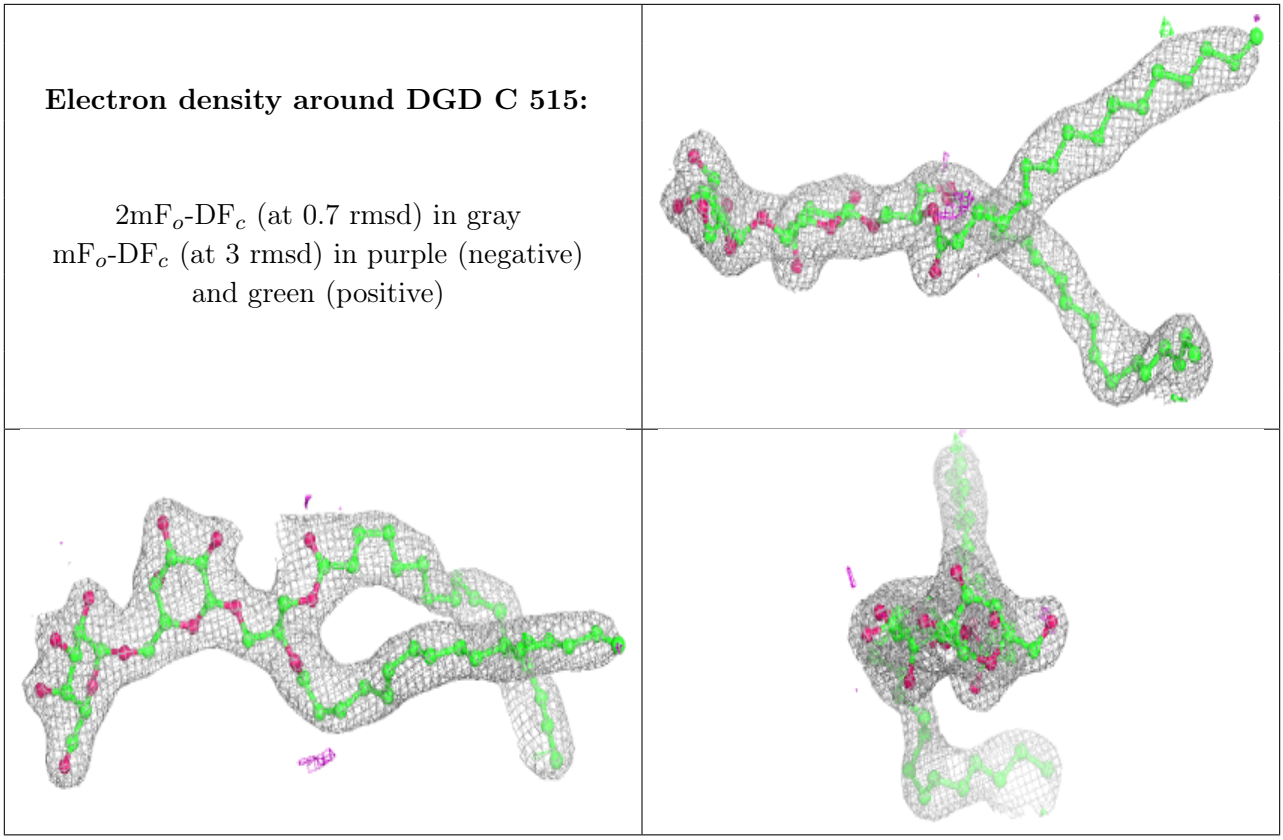
Electron density around CLA B 602:

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



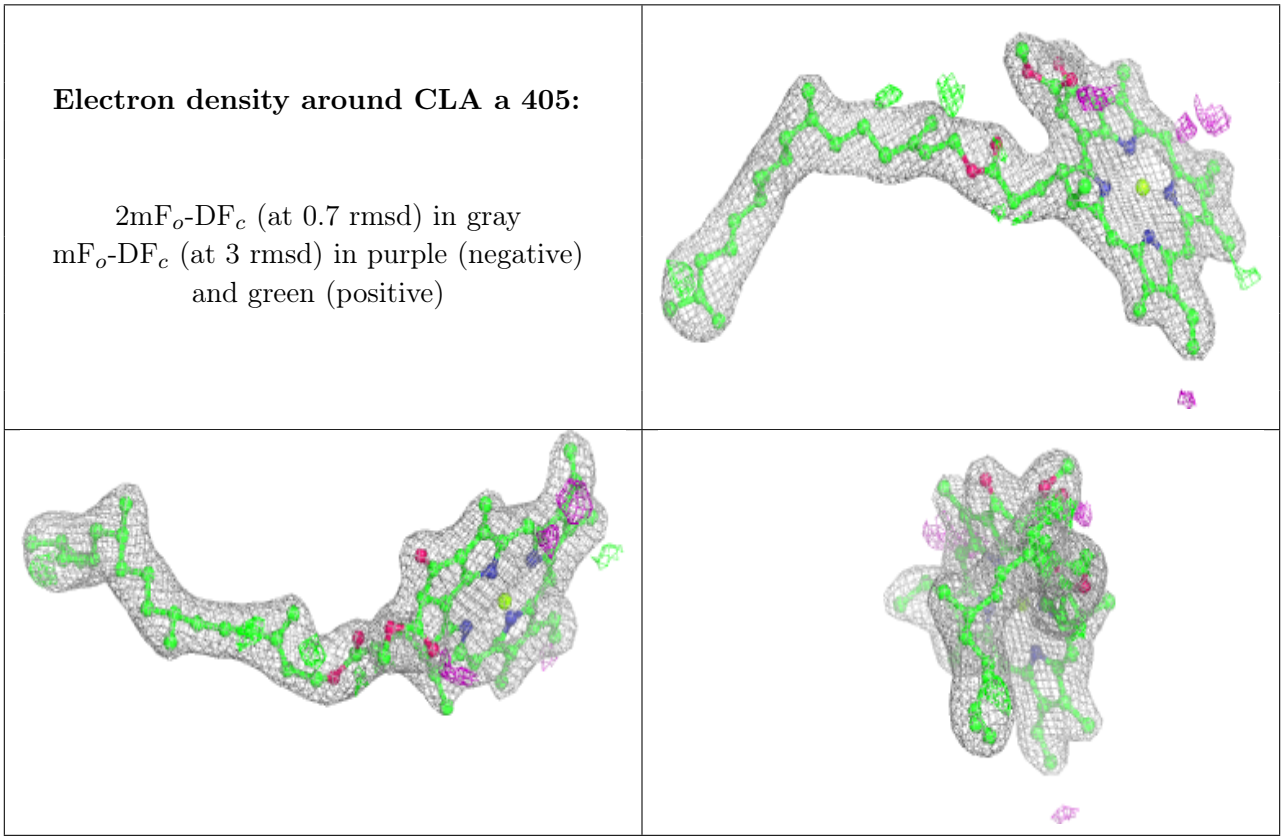
Electron density around DGD C 515:

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



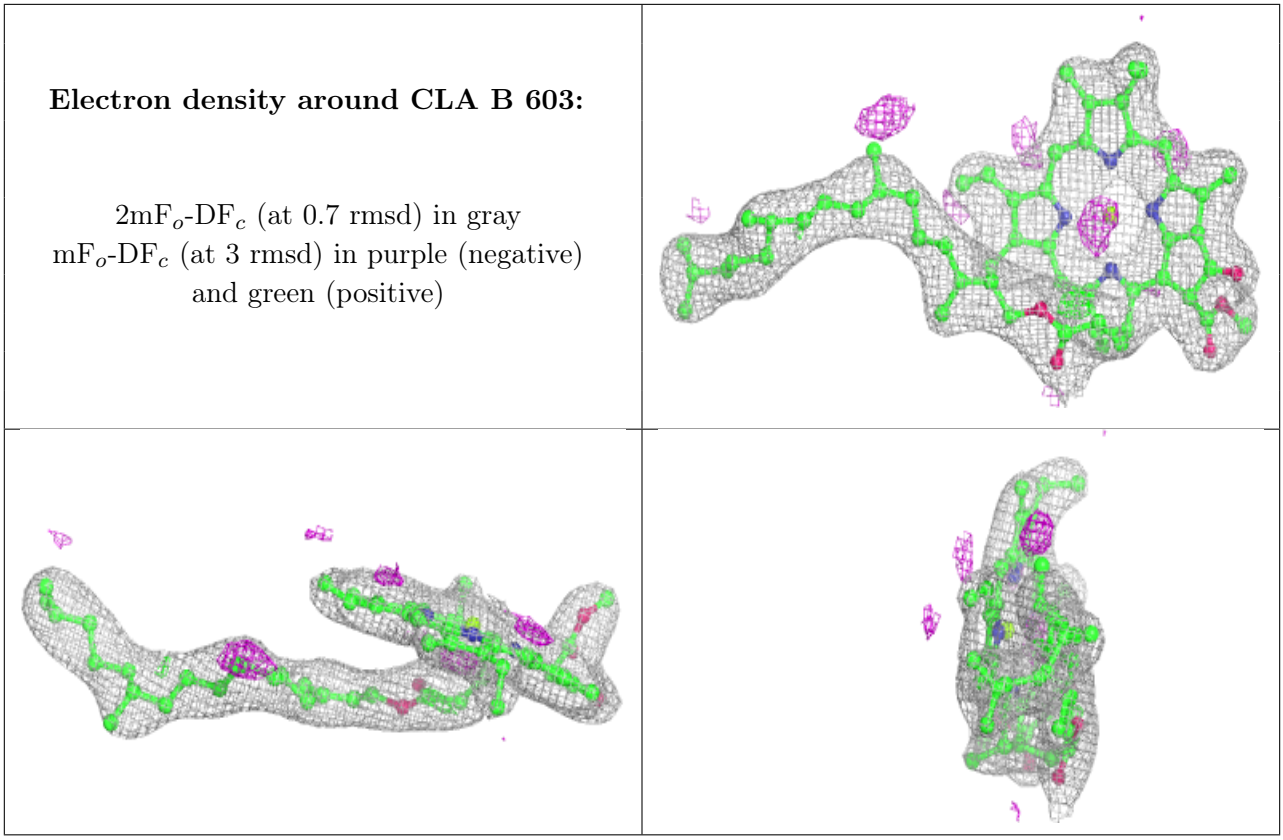
Electron density around CLA a 405:

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



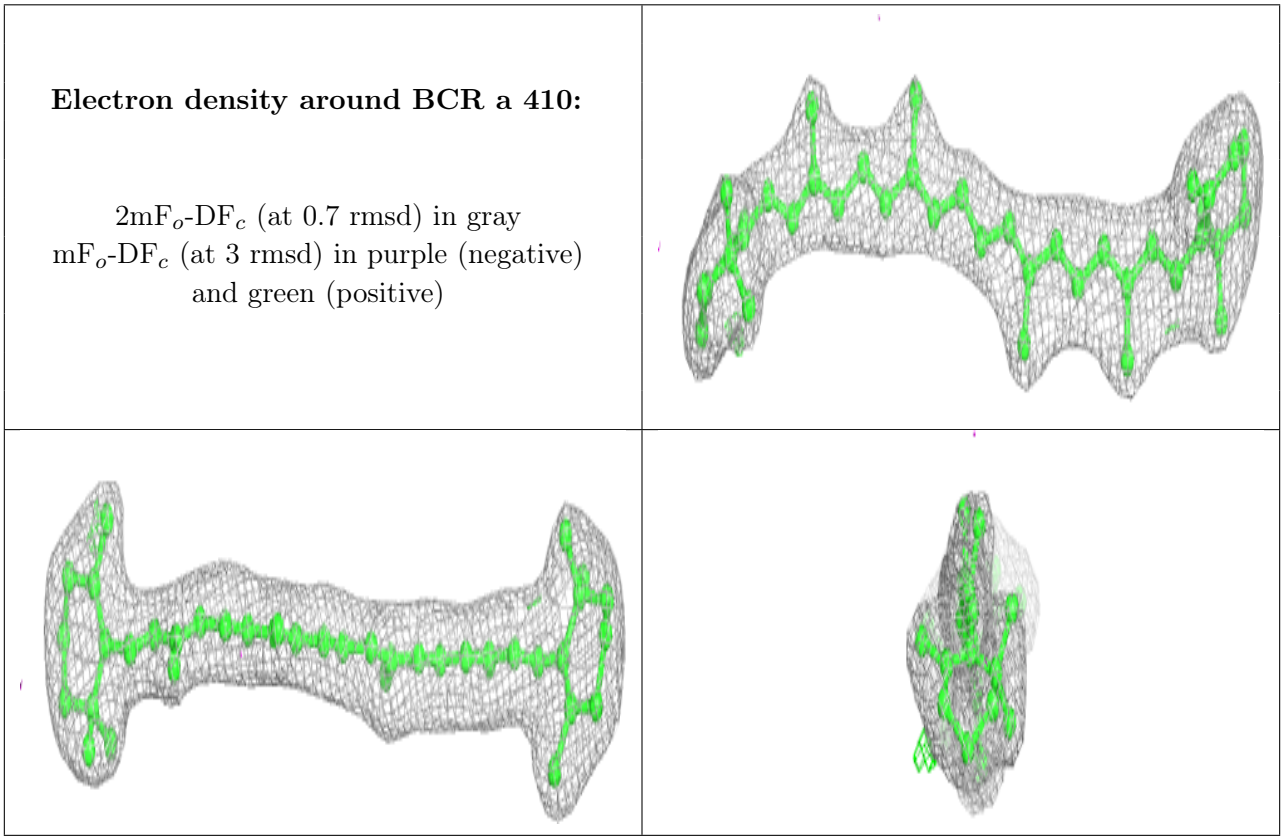
Electron density around CLA B 603:

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



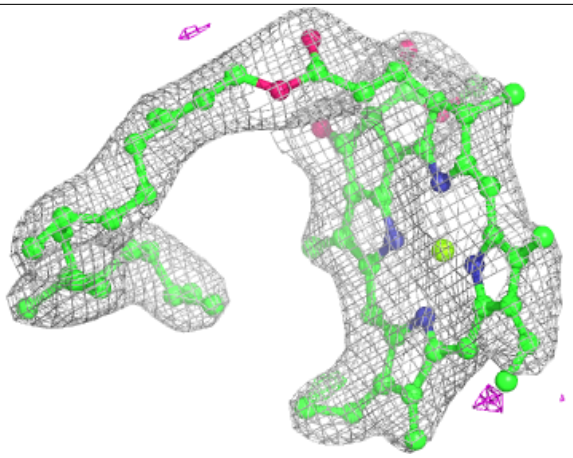
Electron density around BCR a 410:

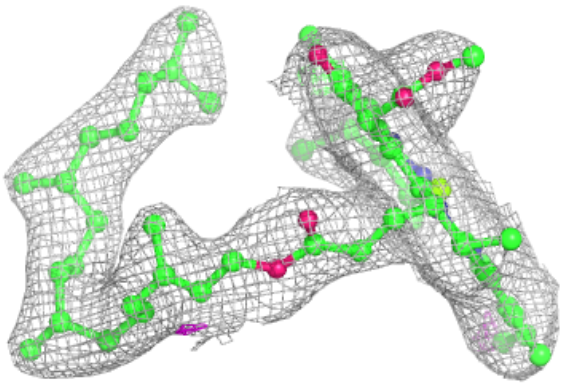
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

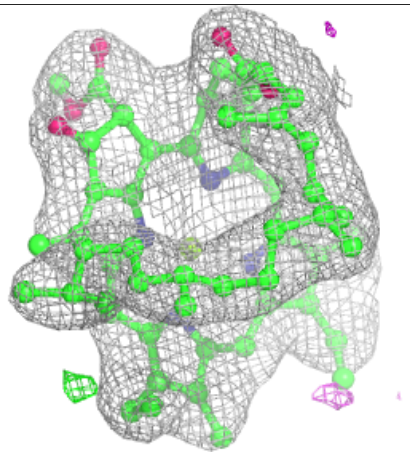


Electron density around CLA c 504:

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

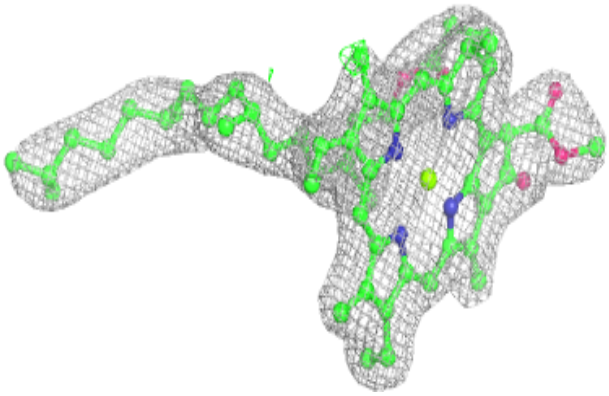


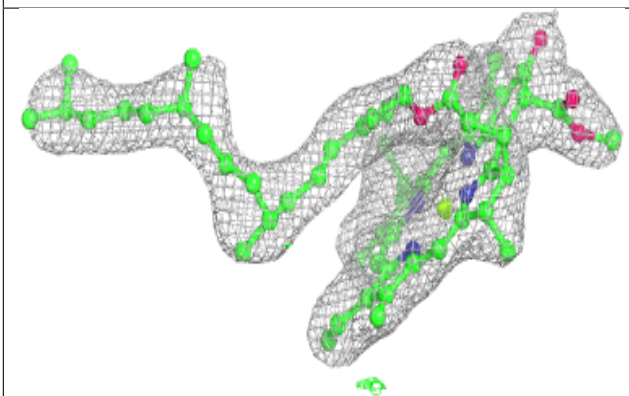


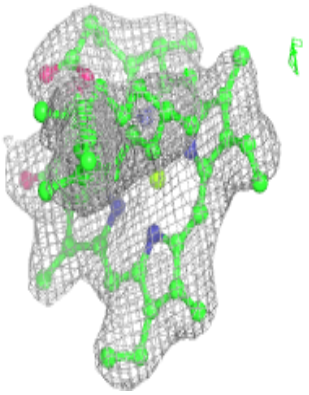


Electron density around CLA C 505:

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

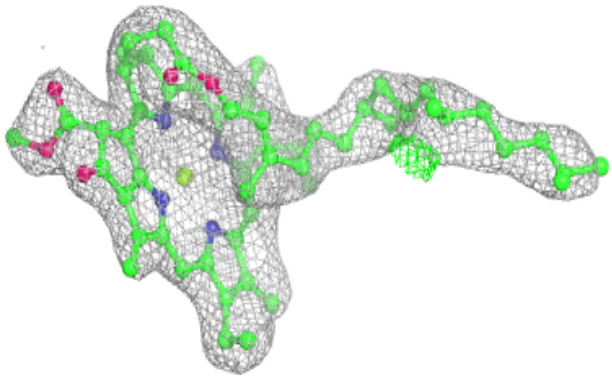


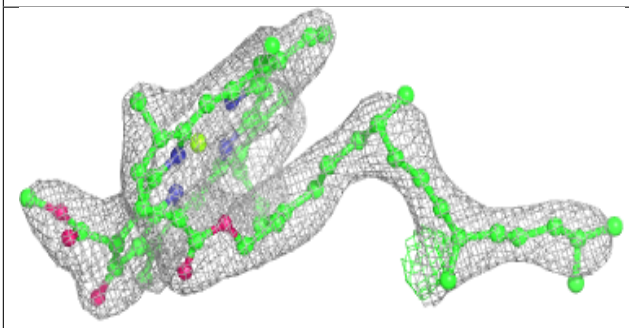


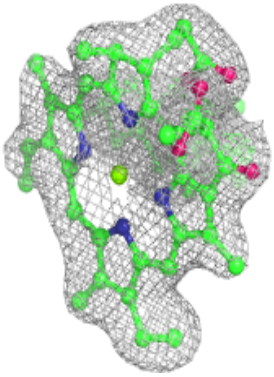


Electron density around CLA c 506:

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

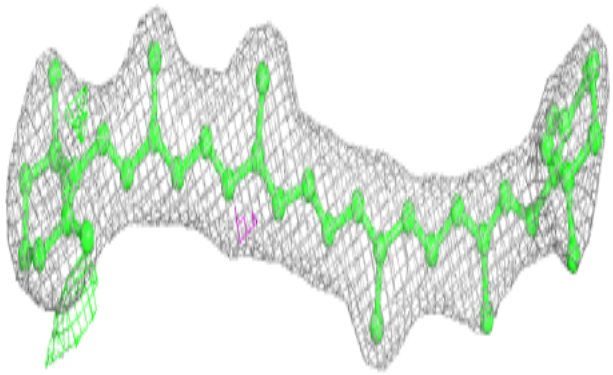


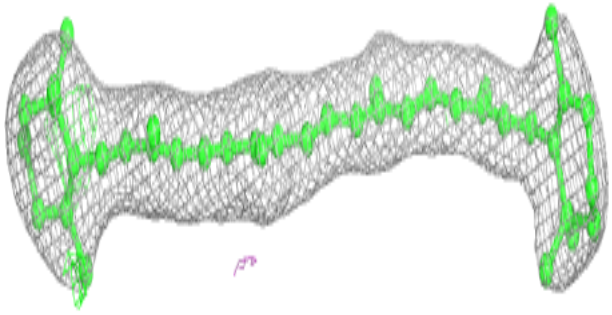


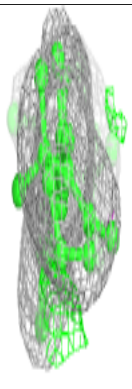


Electron density around BCR c 516:

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

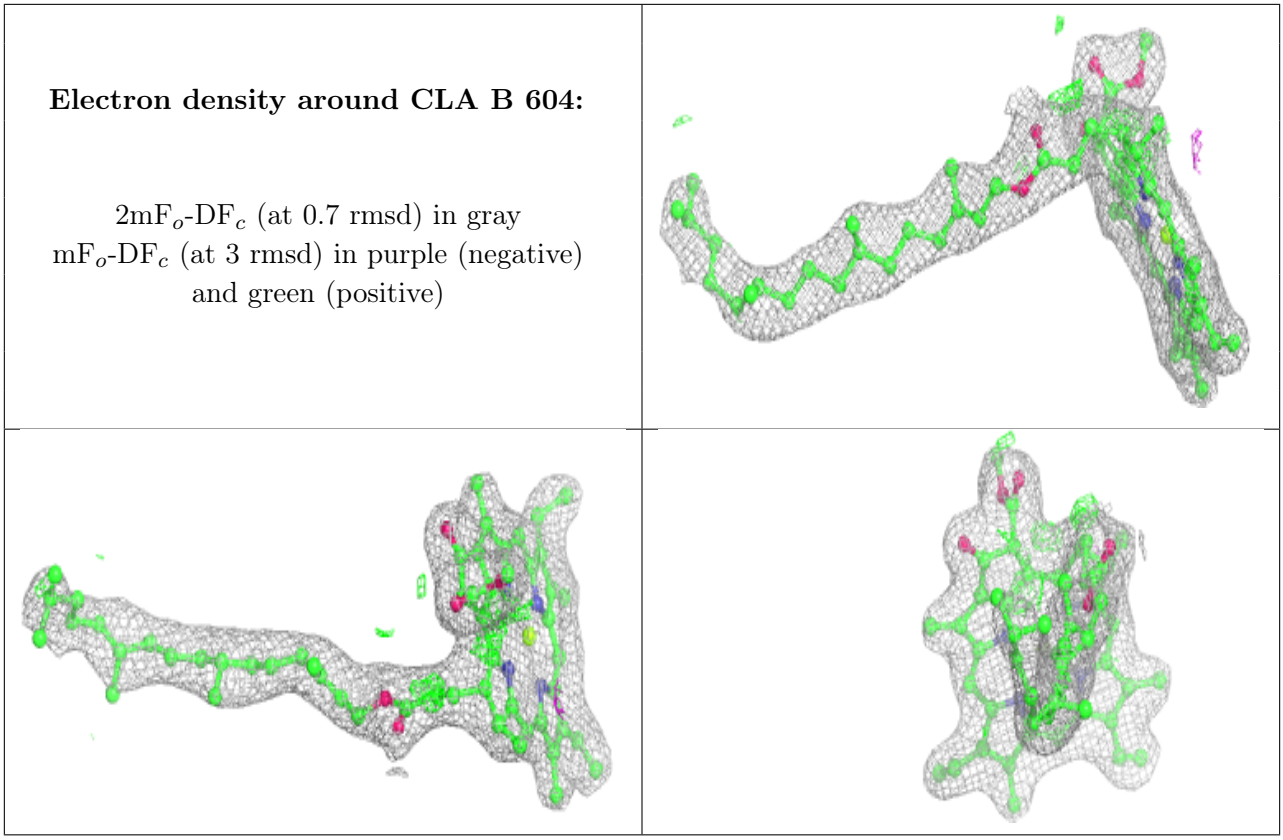






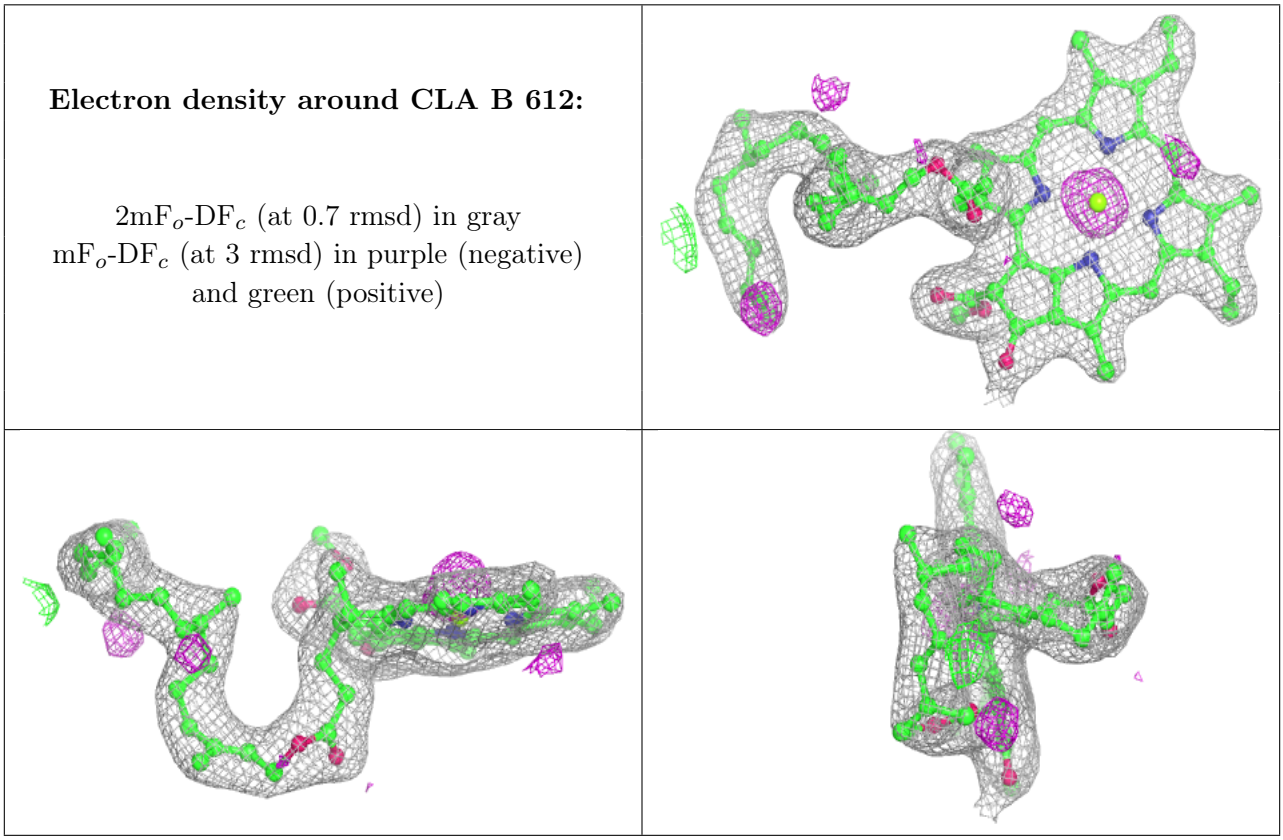
Electron density around CLA B 604:

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



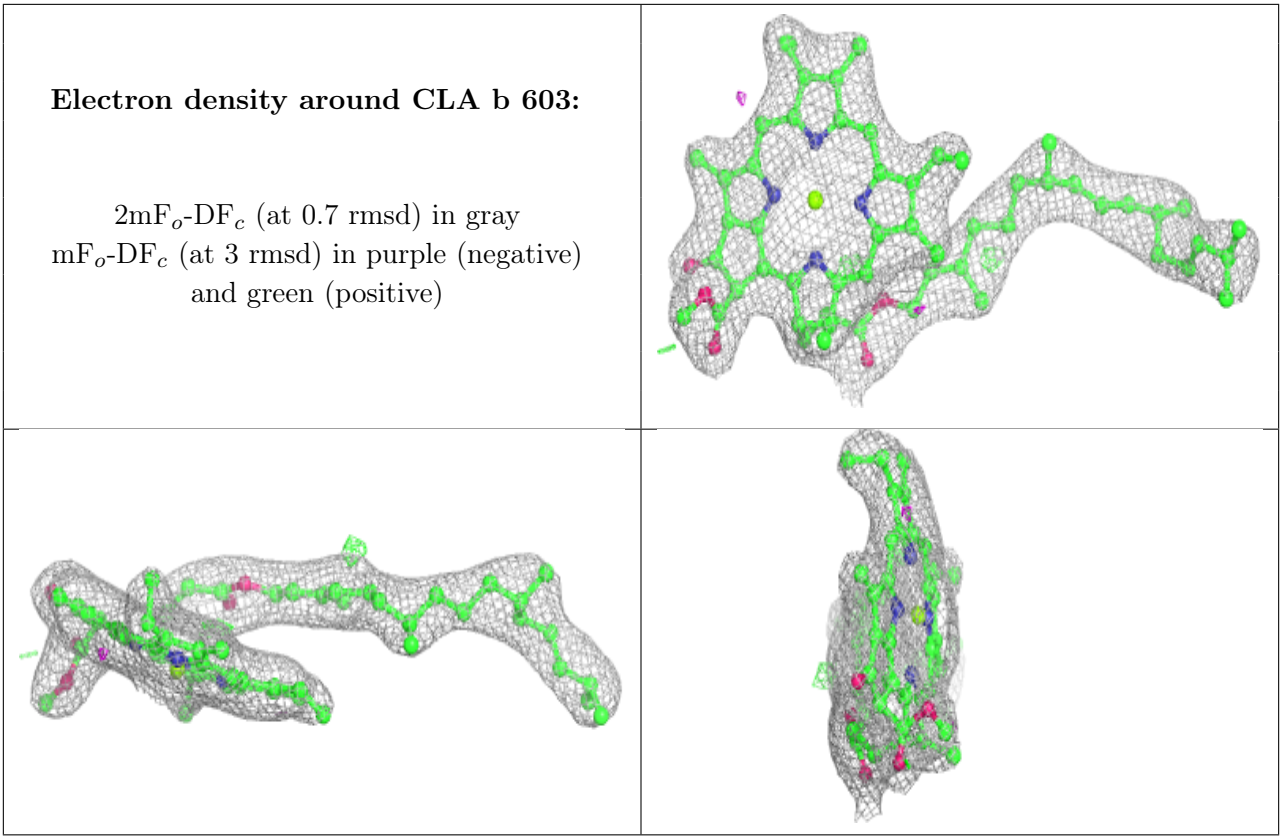
Electron density around CLA B 612:

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



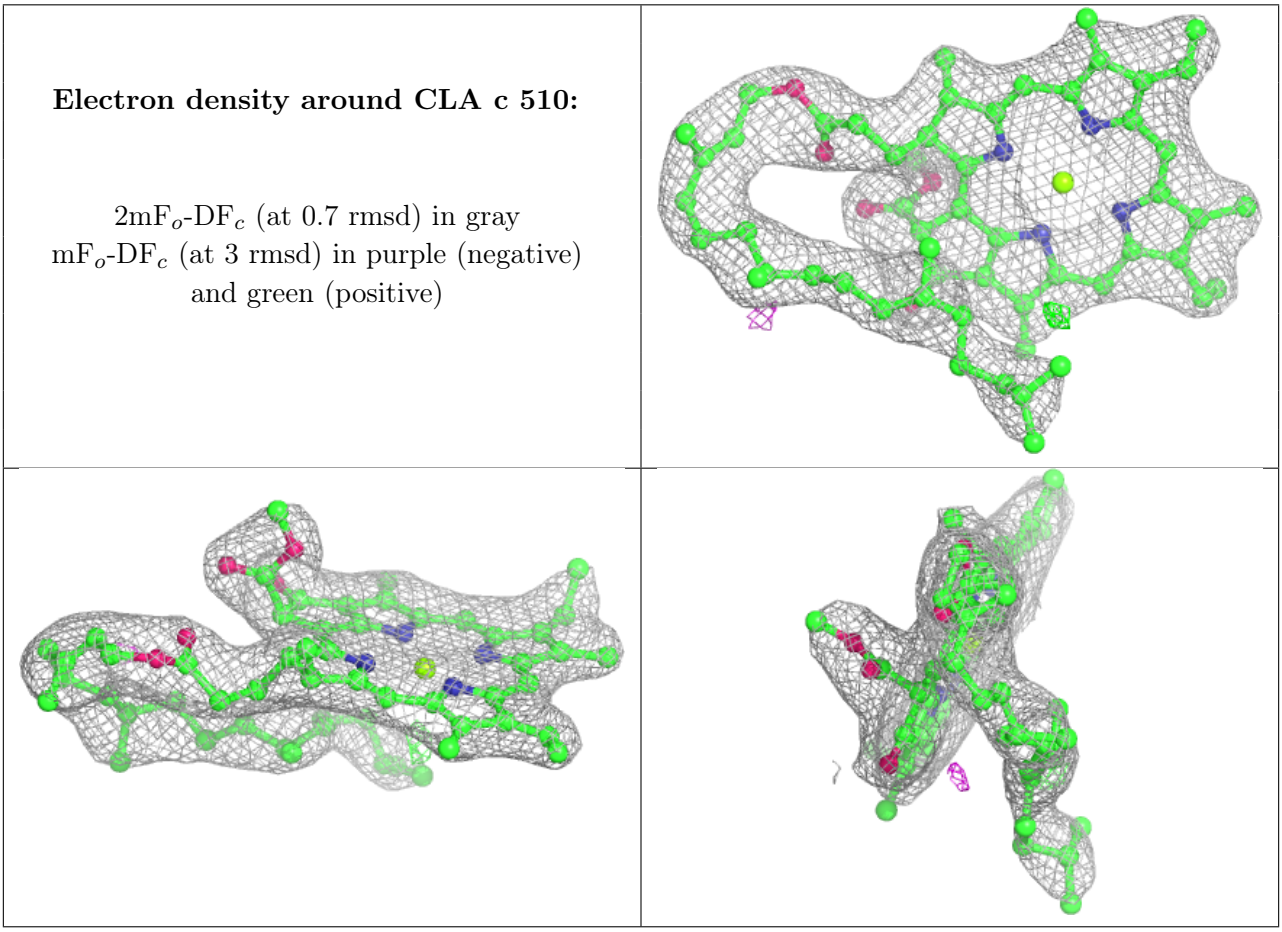
Electron density around CLA b 603:

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



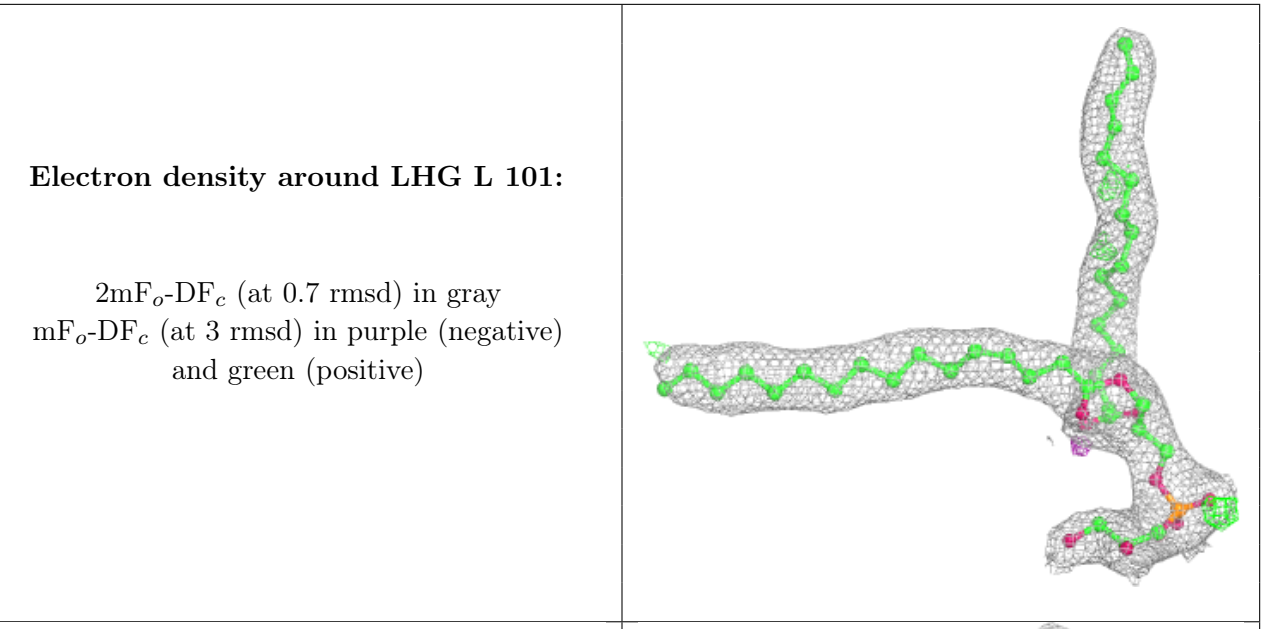
Electron density around CLA c 510:

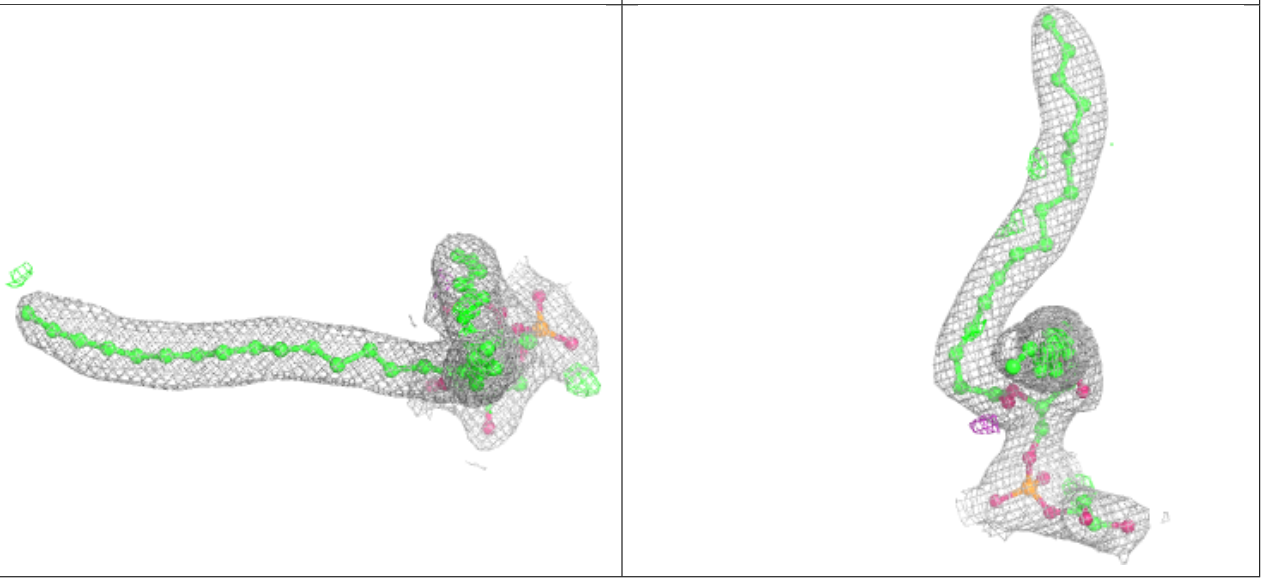
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG L 101:

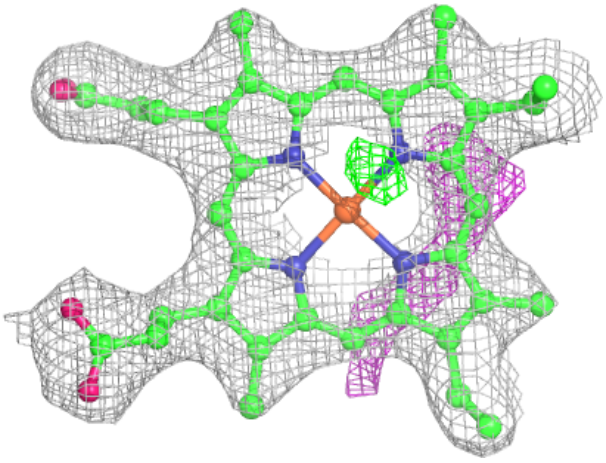
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

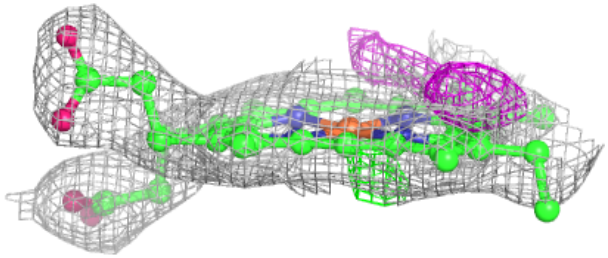


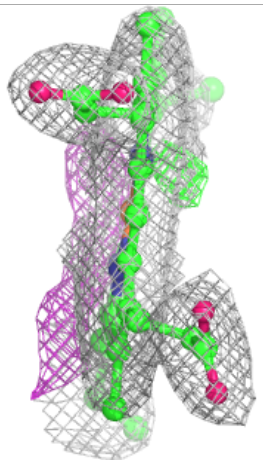


Electron density around HEC v 201:

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

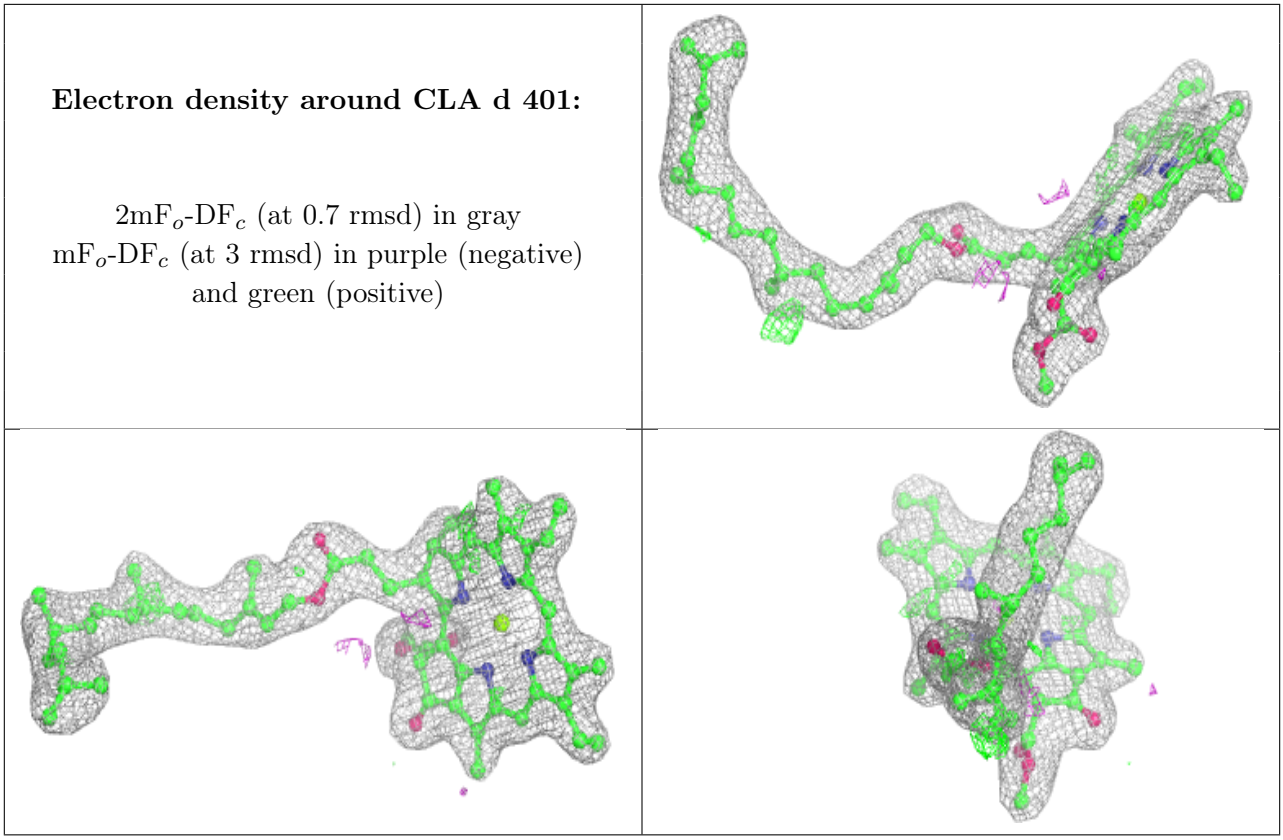






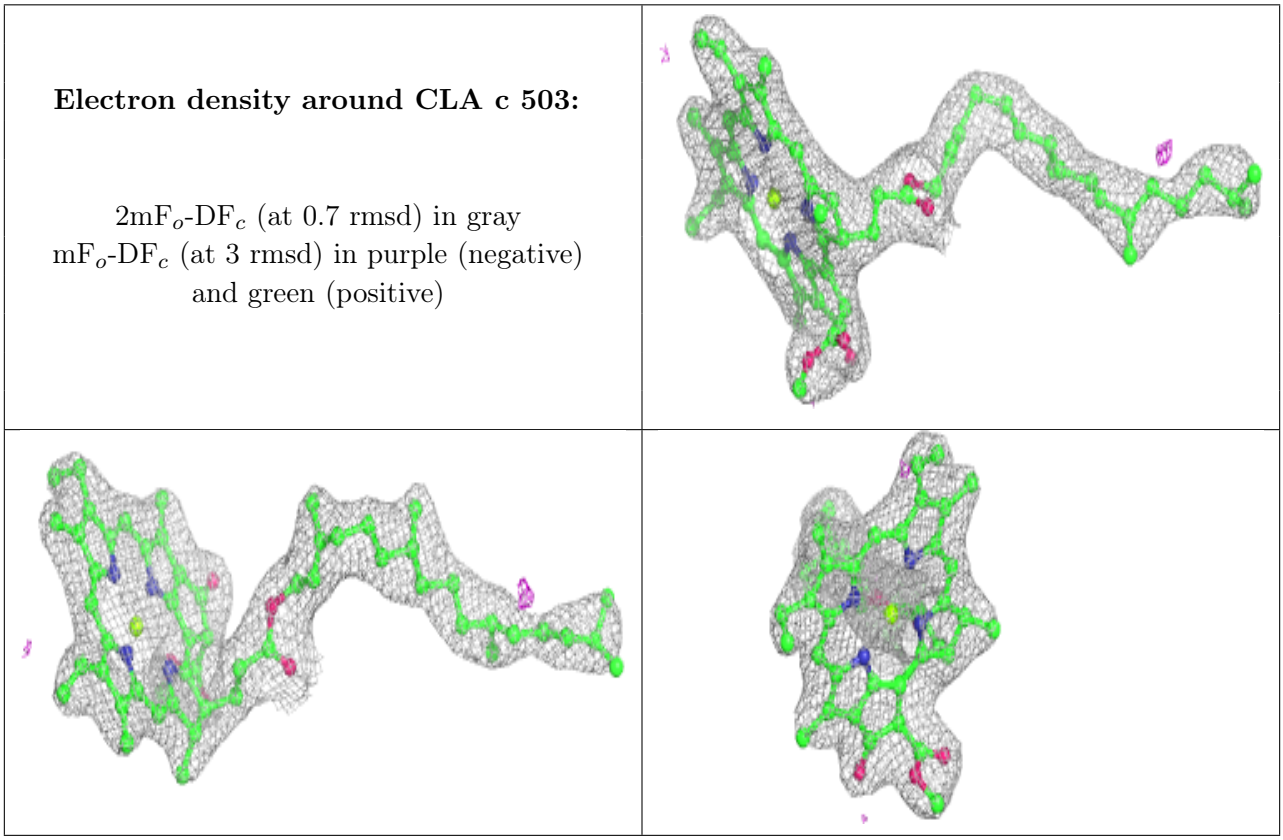
Electron density around CLA d 401:

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



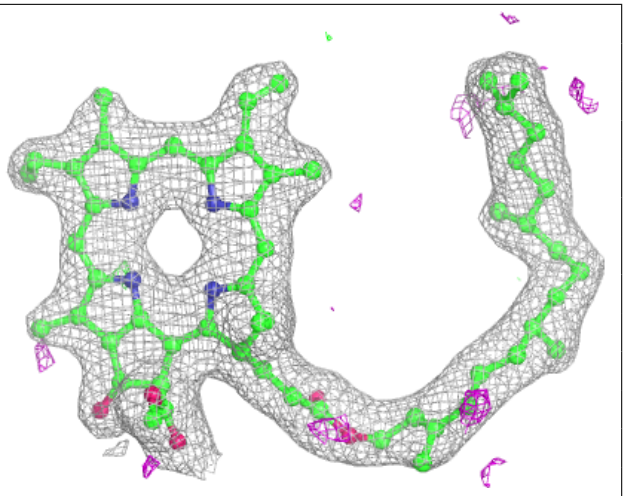
Electron density around CLA c 503:

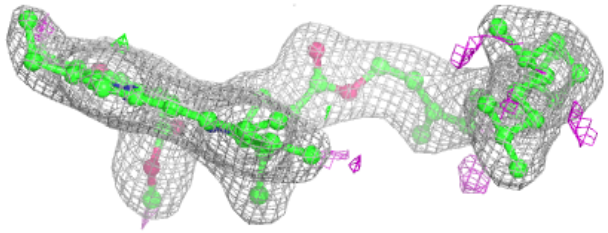
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

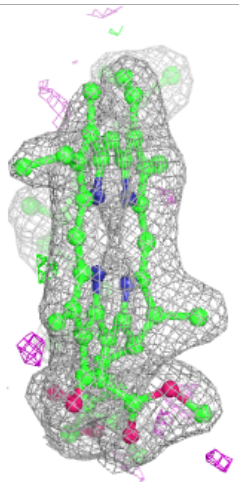


Electron density around PHO A 407:

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

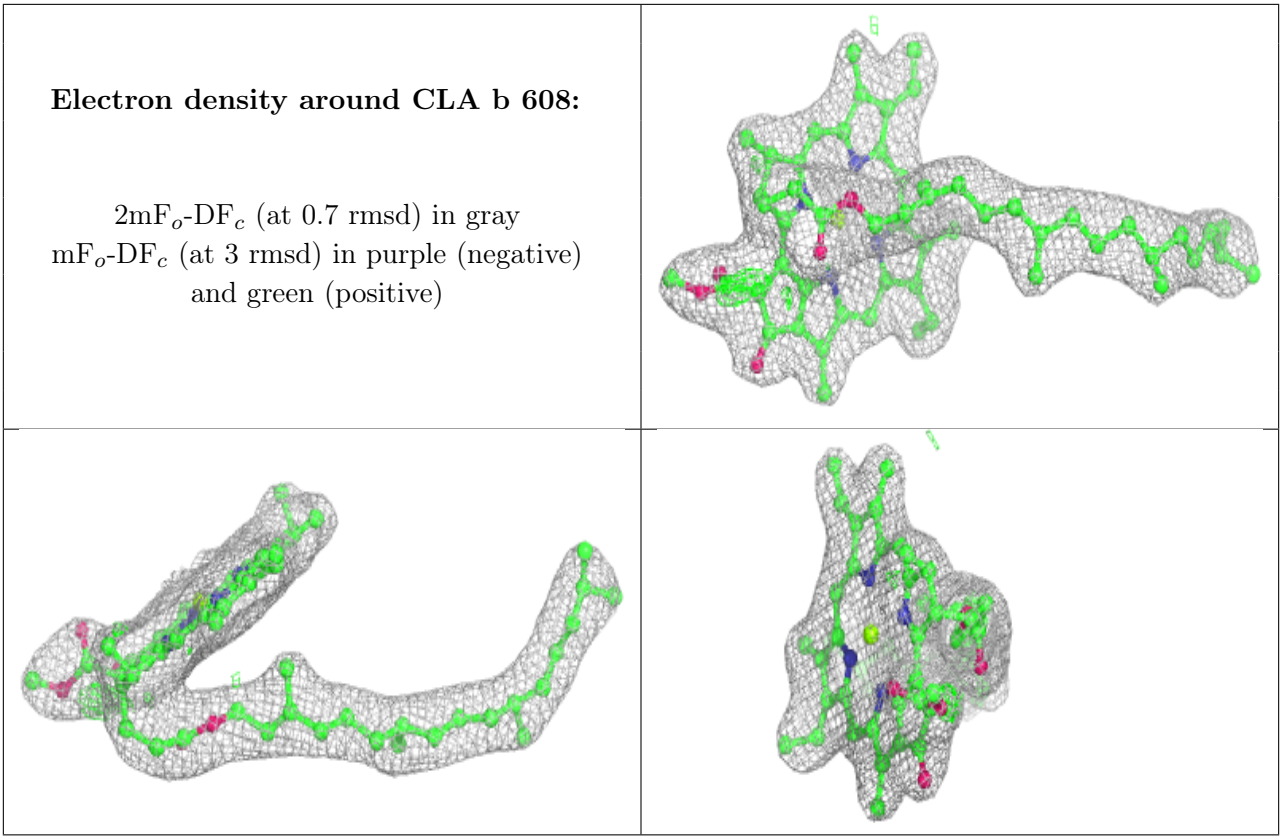






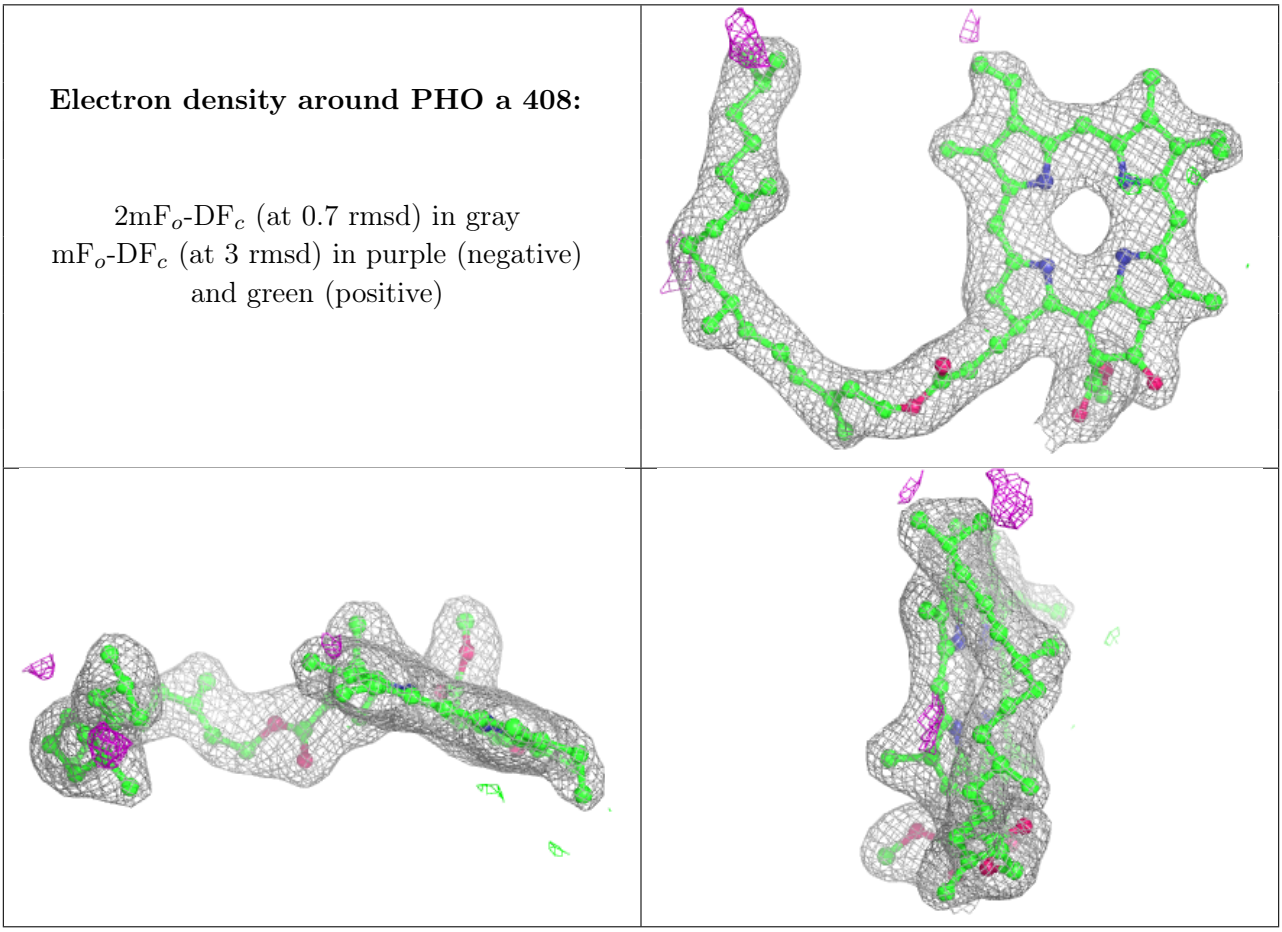
Electron density around CLA b 608:

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



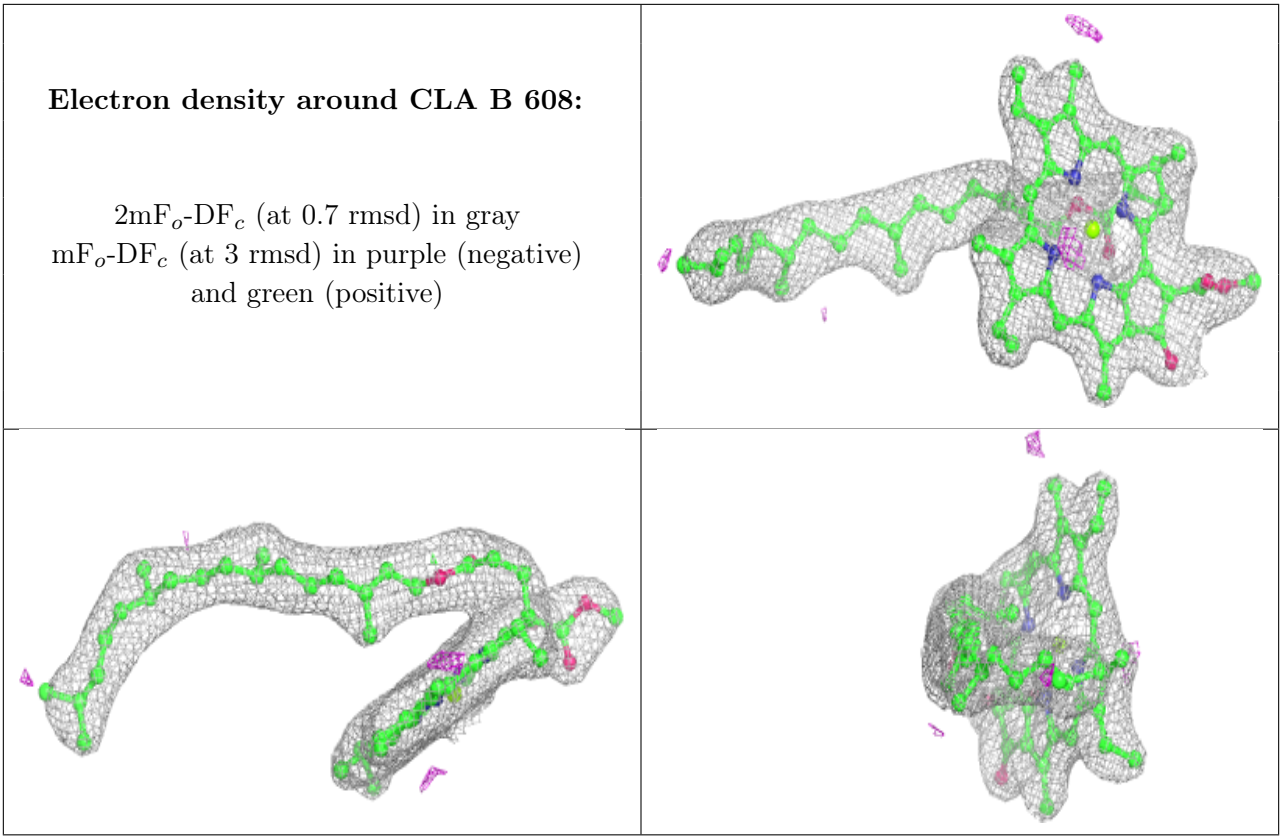
Electron density around PHO a 408:

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



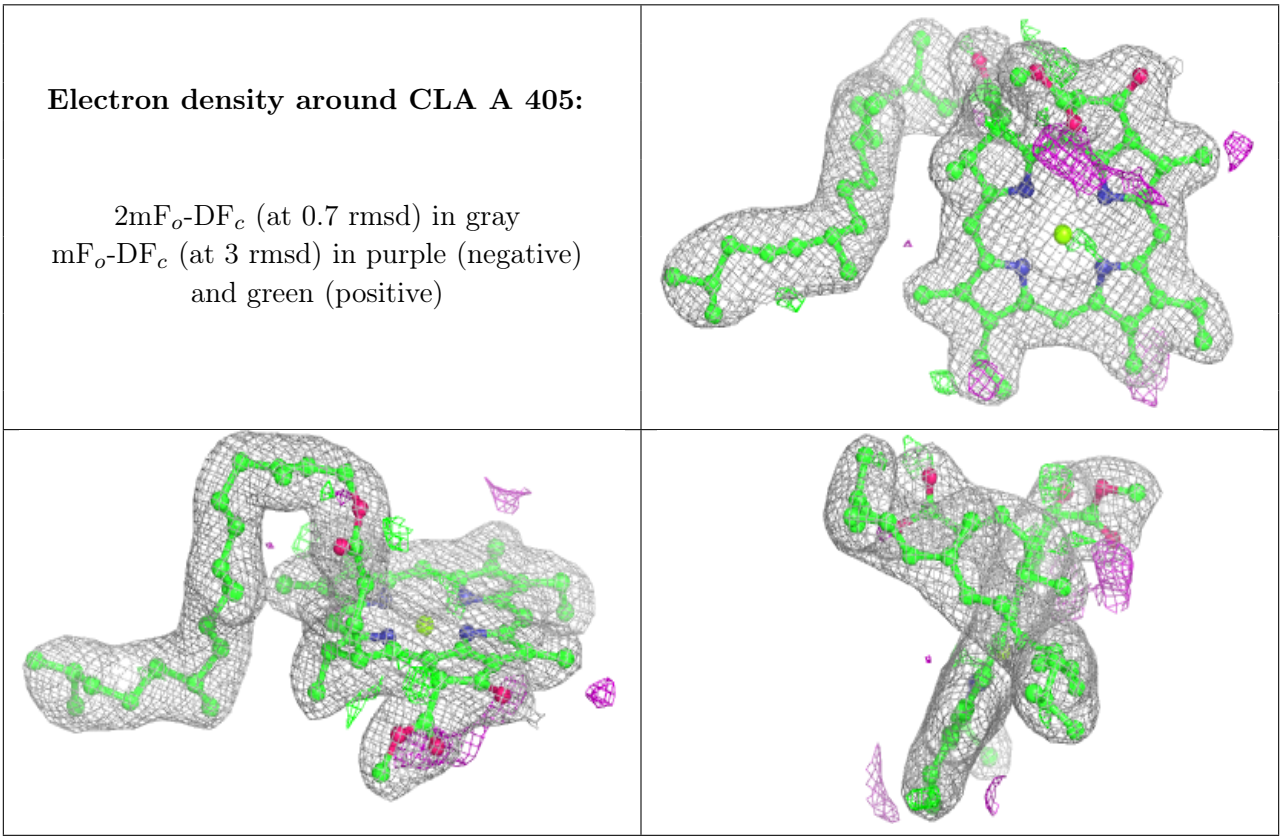
Electron density around CLA B 608:

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



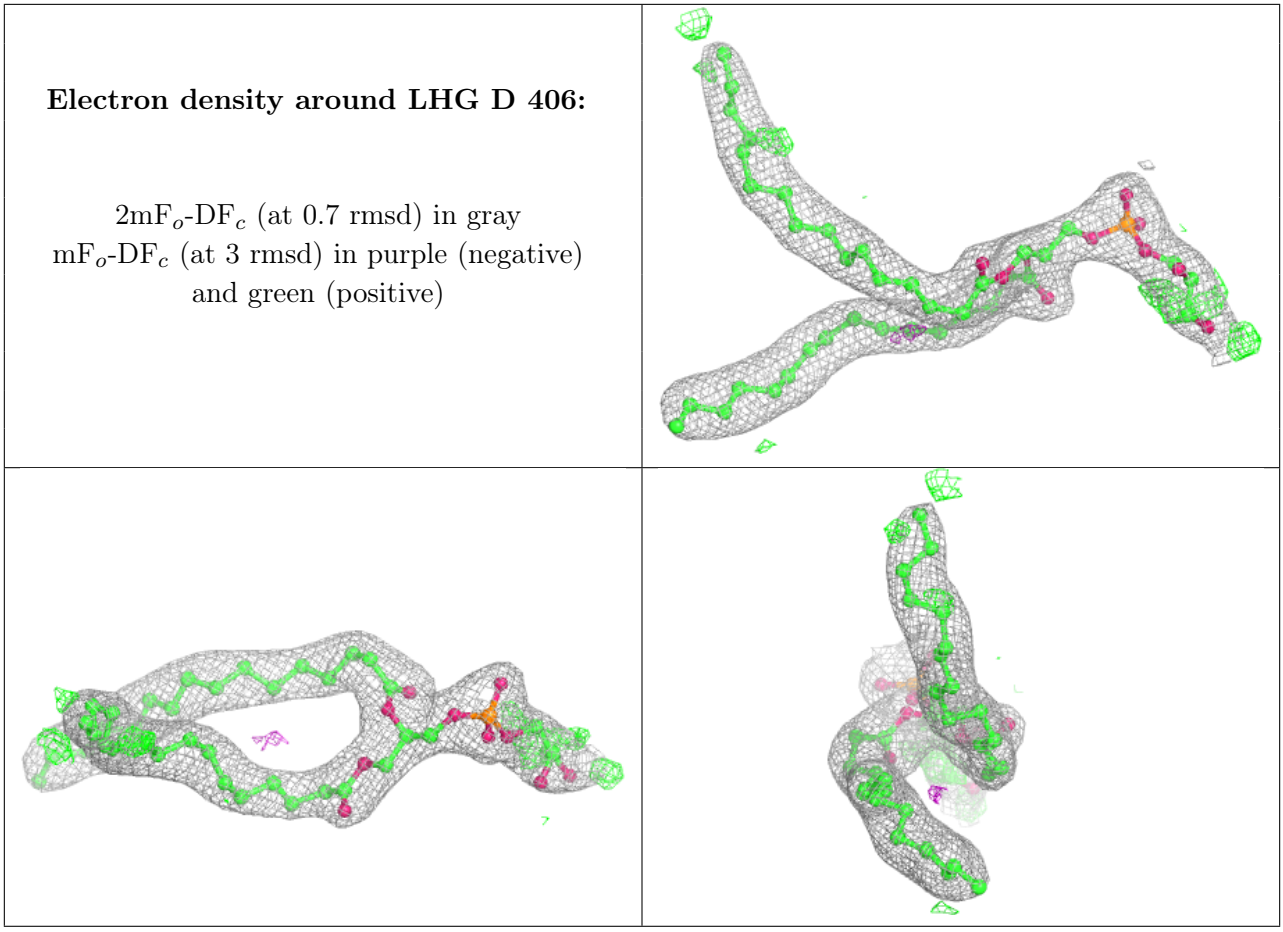
Electron density around CLA A 405:

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



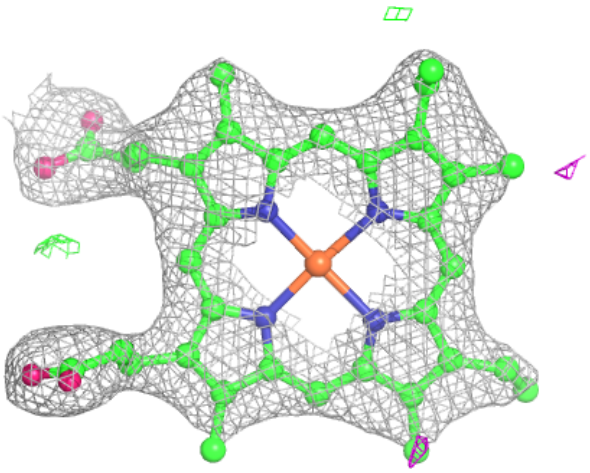
Electron density around LHG D 406:

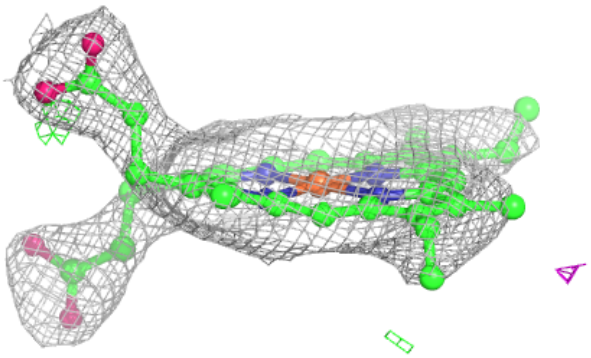
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

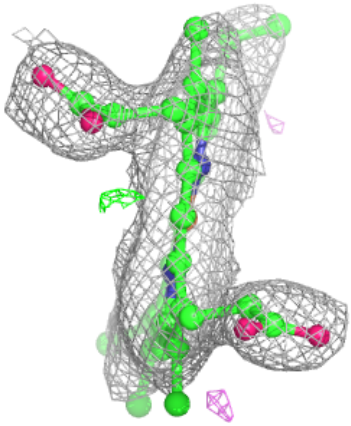


Electron density around HEM F 102:

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

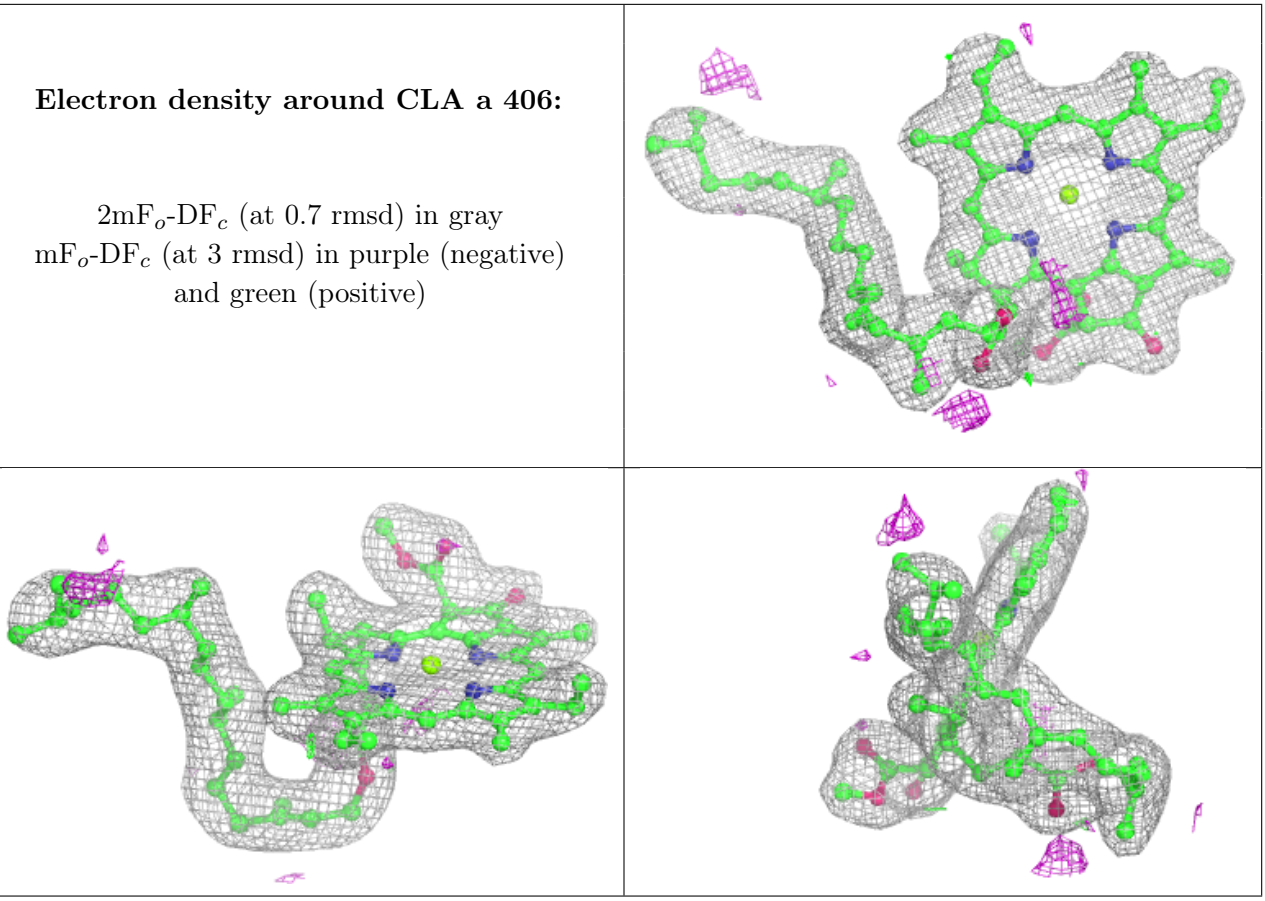






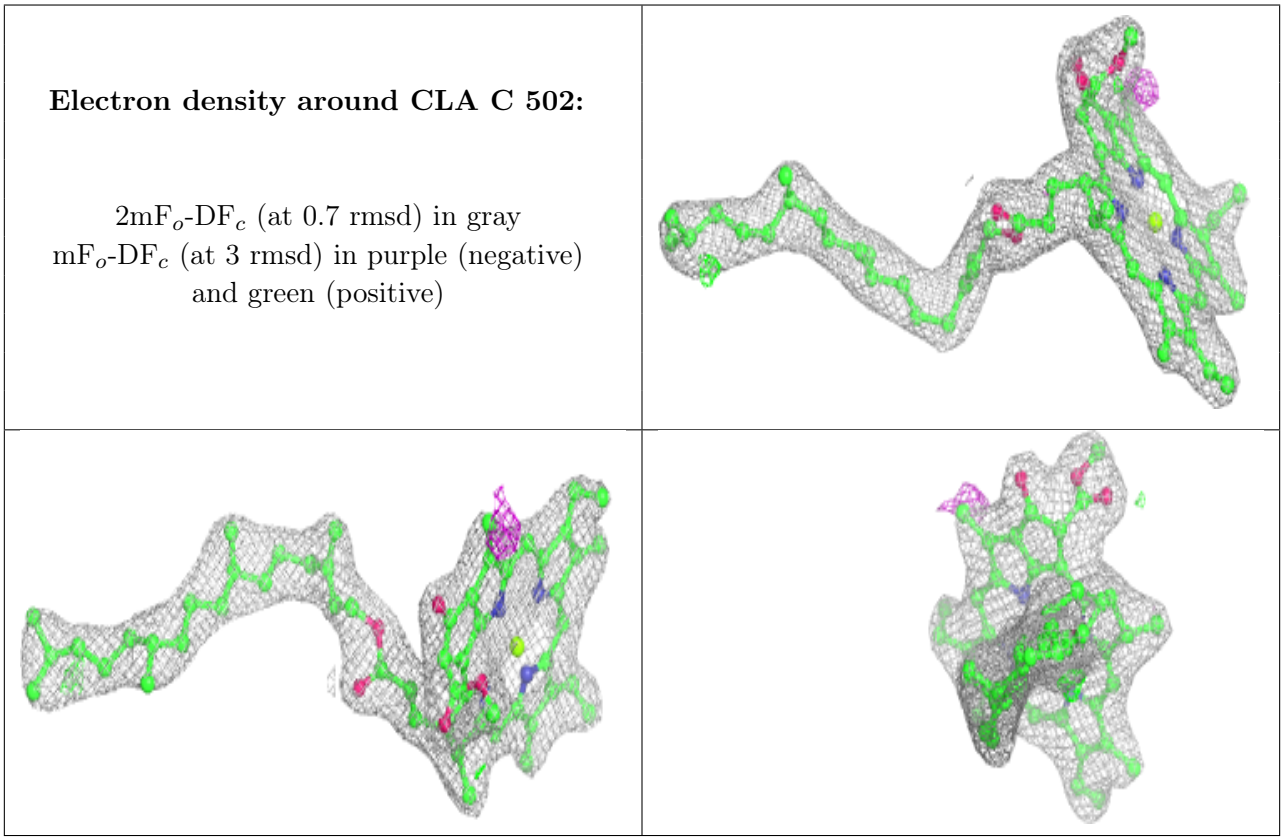
Electron density around CLA a 406:

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



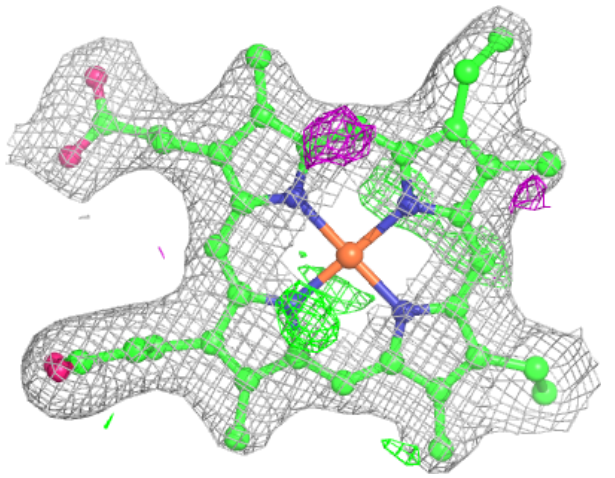
Electron density around CLA C 502:

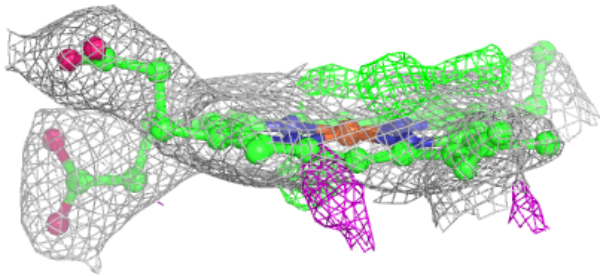
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

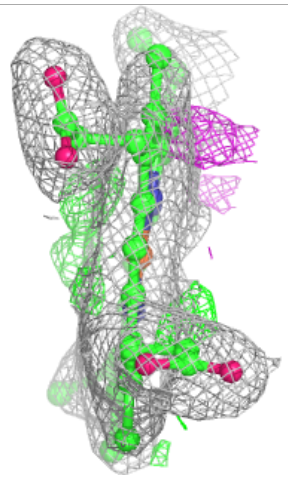


Electron density around HEC V 201:

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

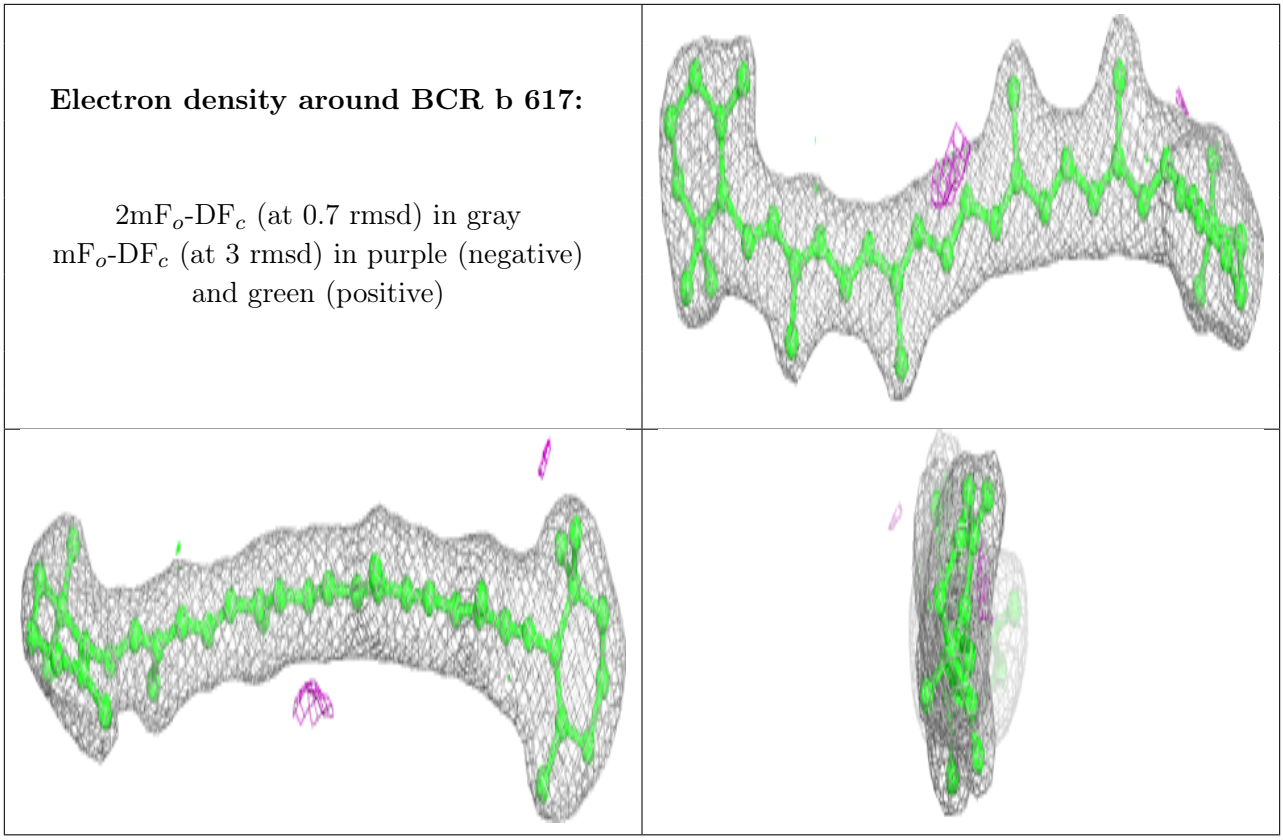






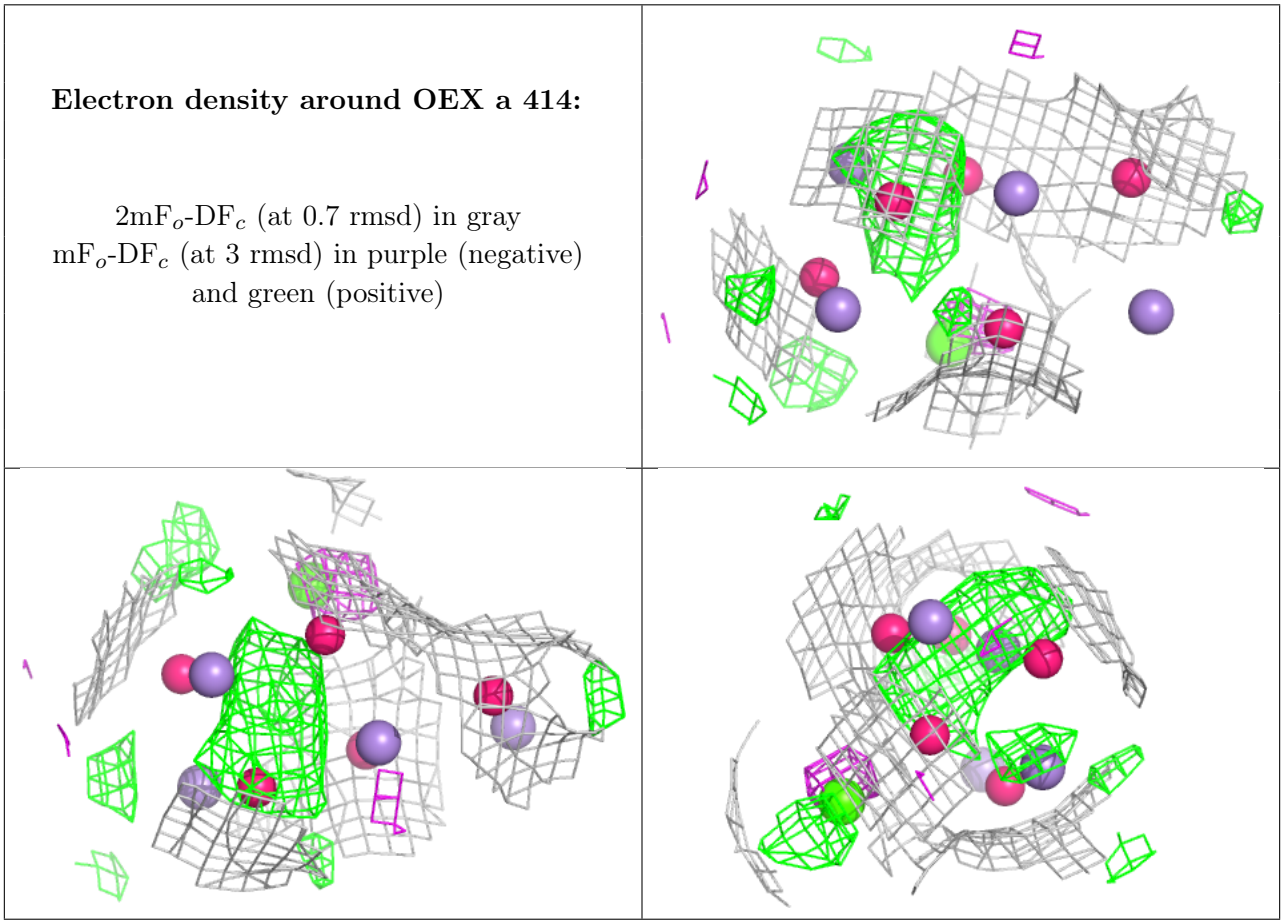
Electron density around BCR b 617:

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



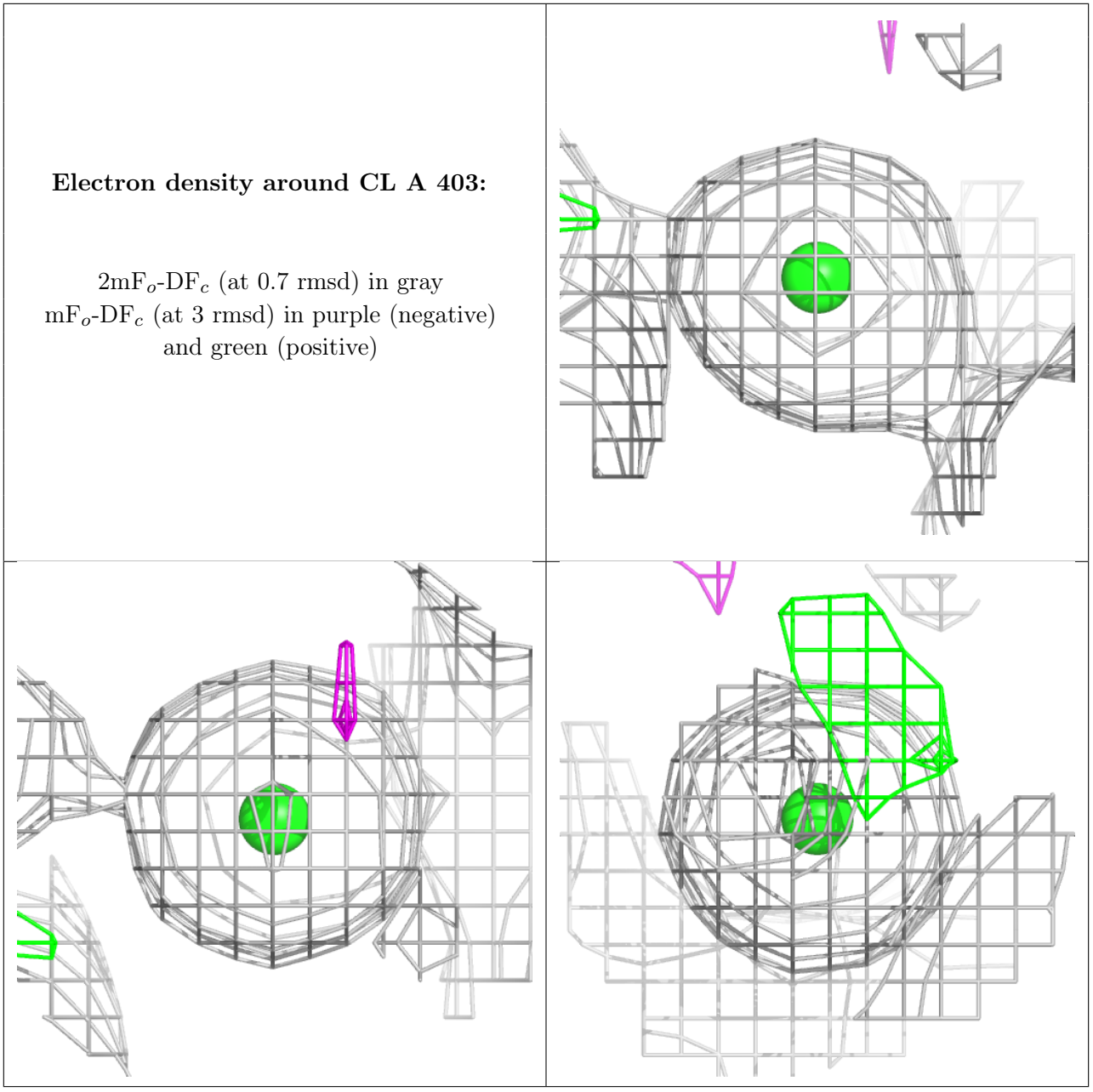
Electron density around OEX a 414:

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



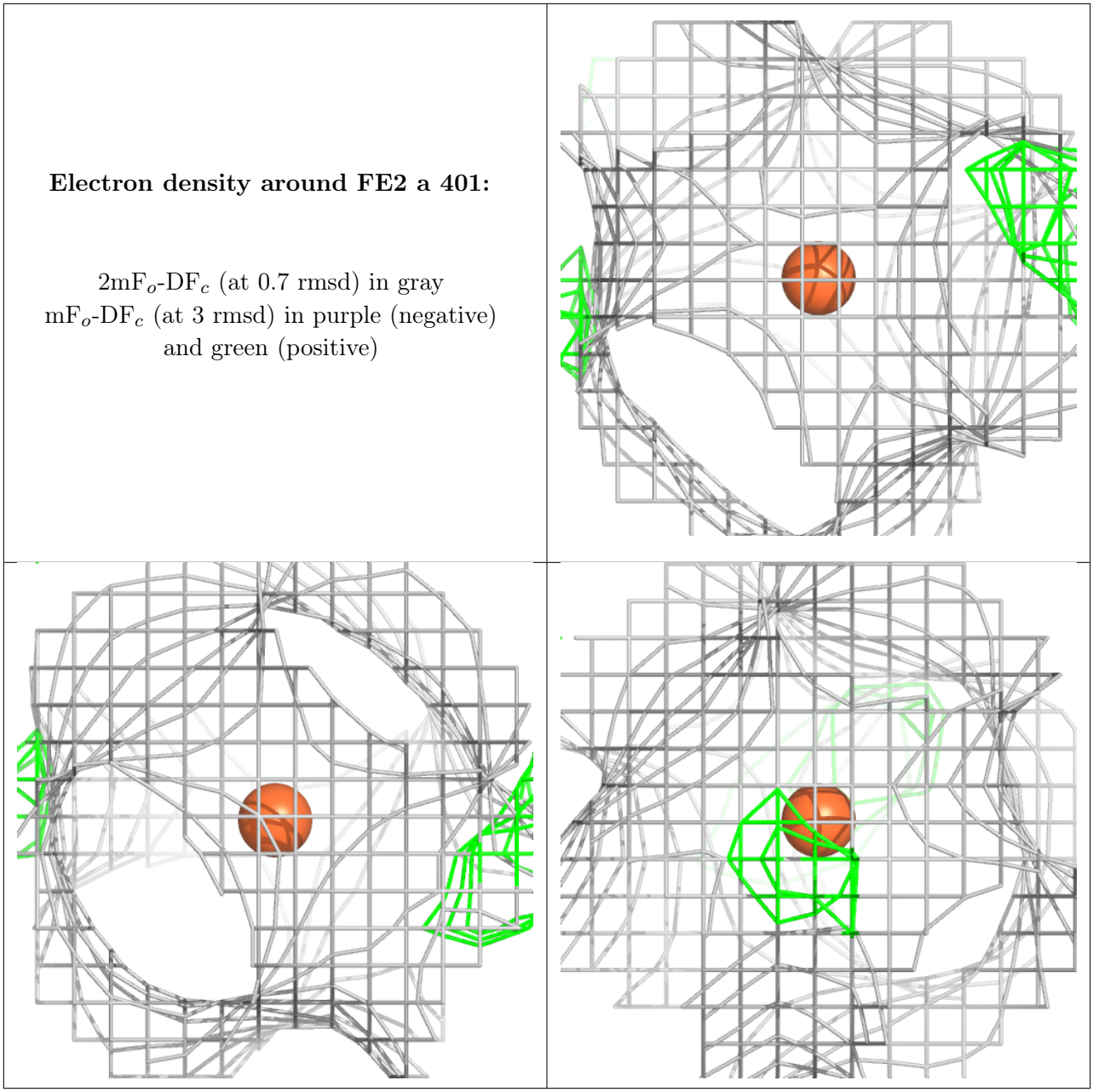
Electron density around CL A 403:

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



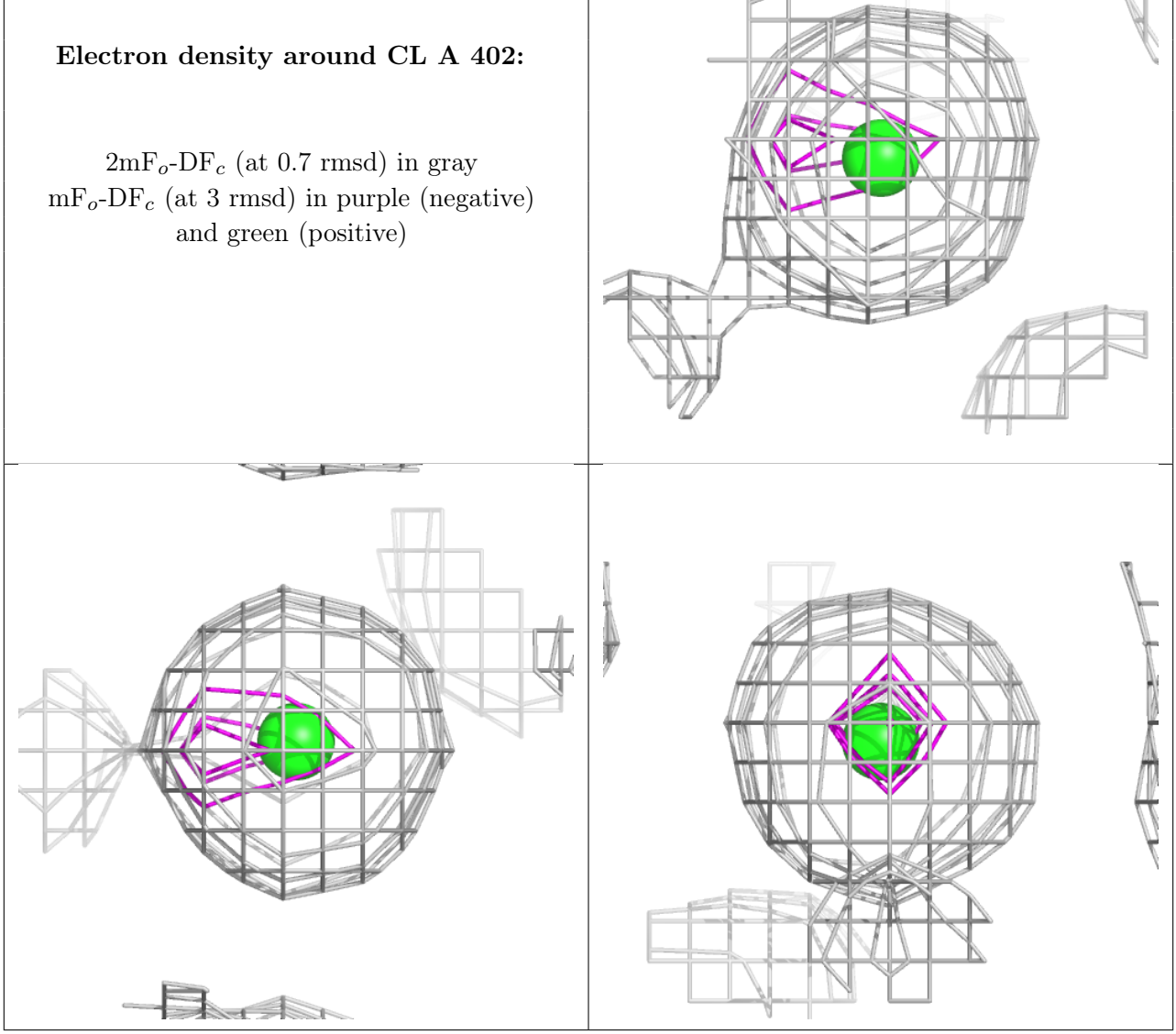
Electron density around FE2 a 401:

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



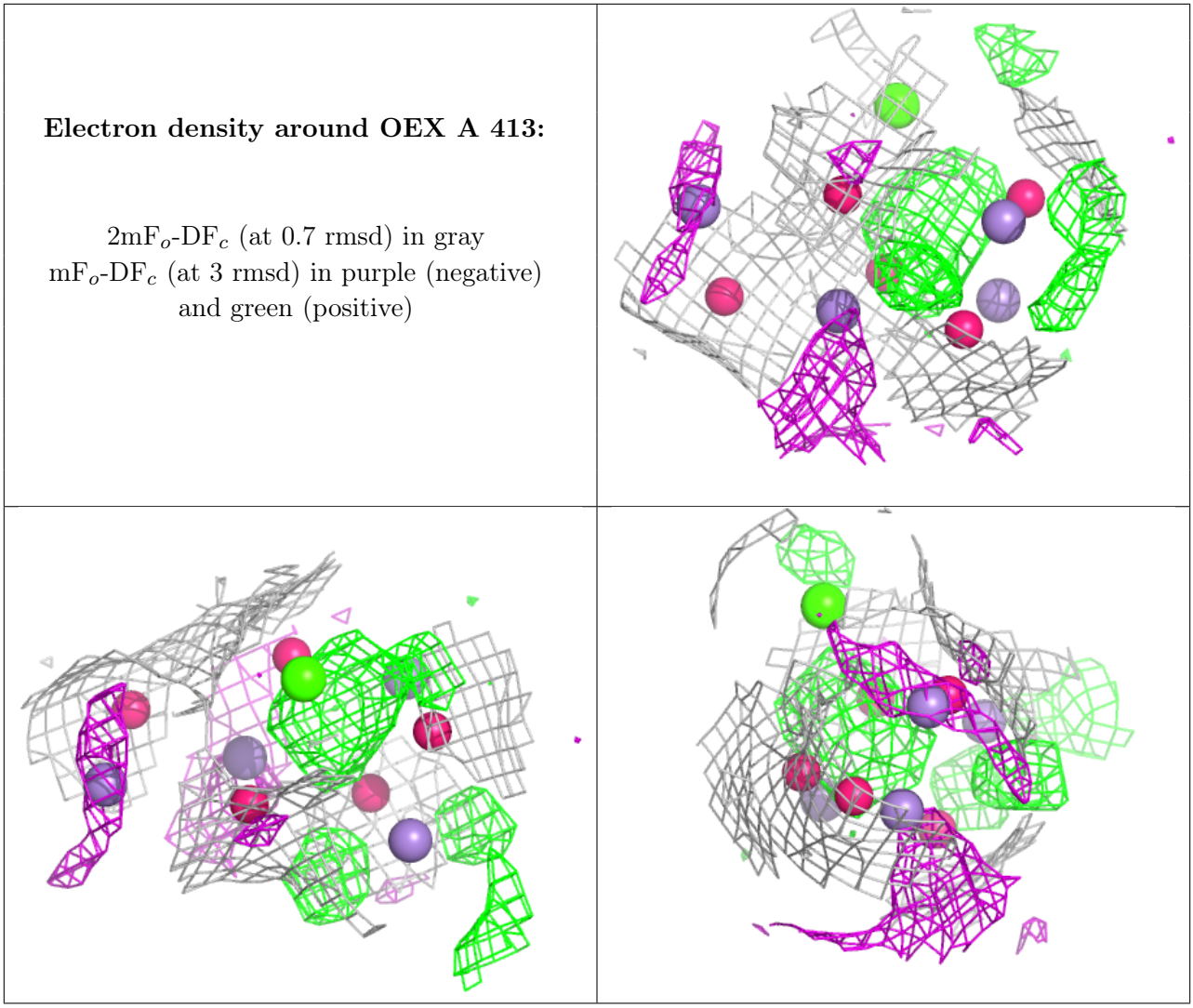
Electron density around CL A 402:

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



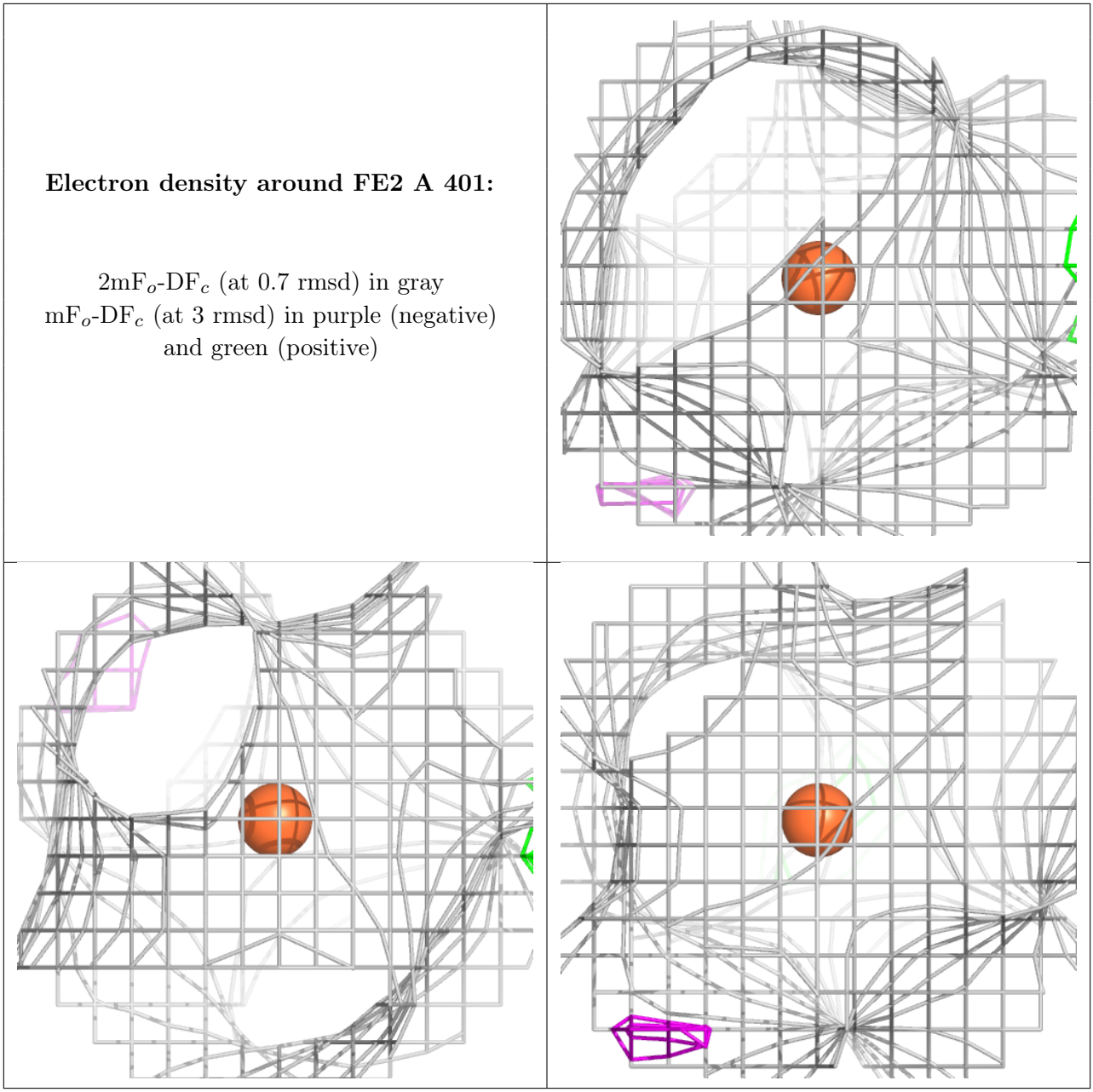
Electron density around OEX A 413:

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



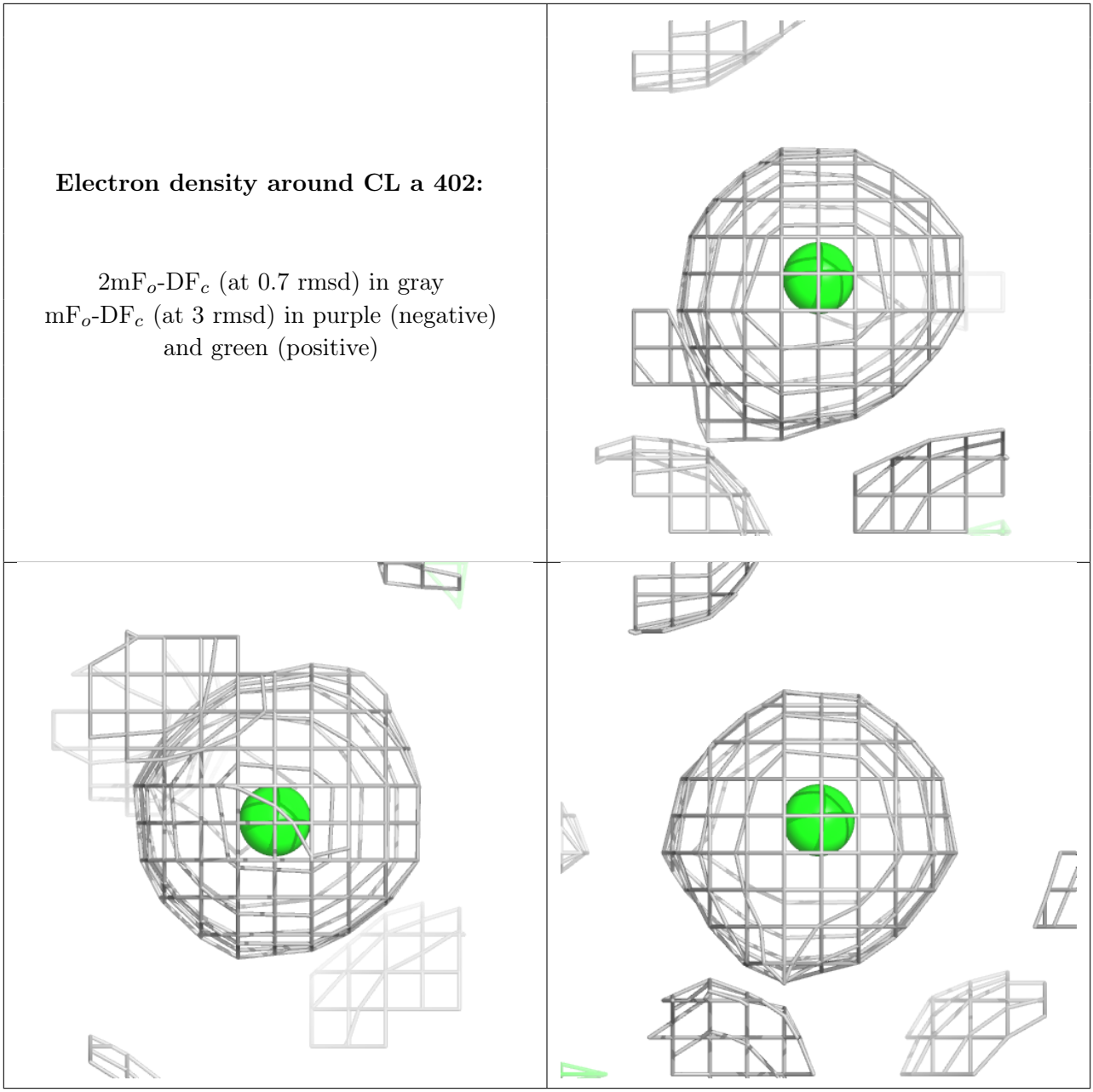
Electron density around FE2 A 401:

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



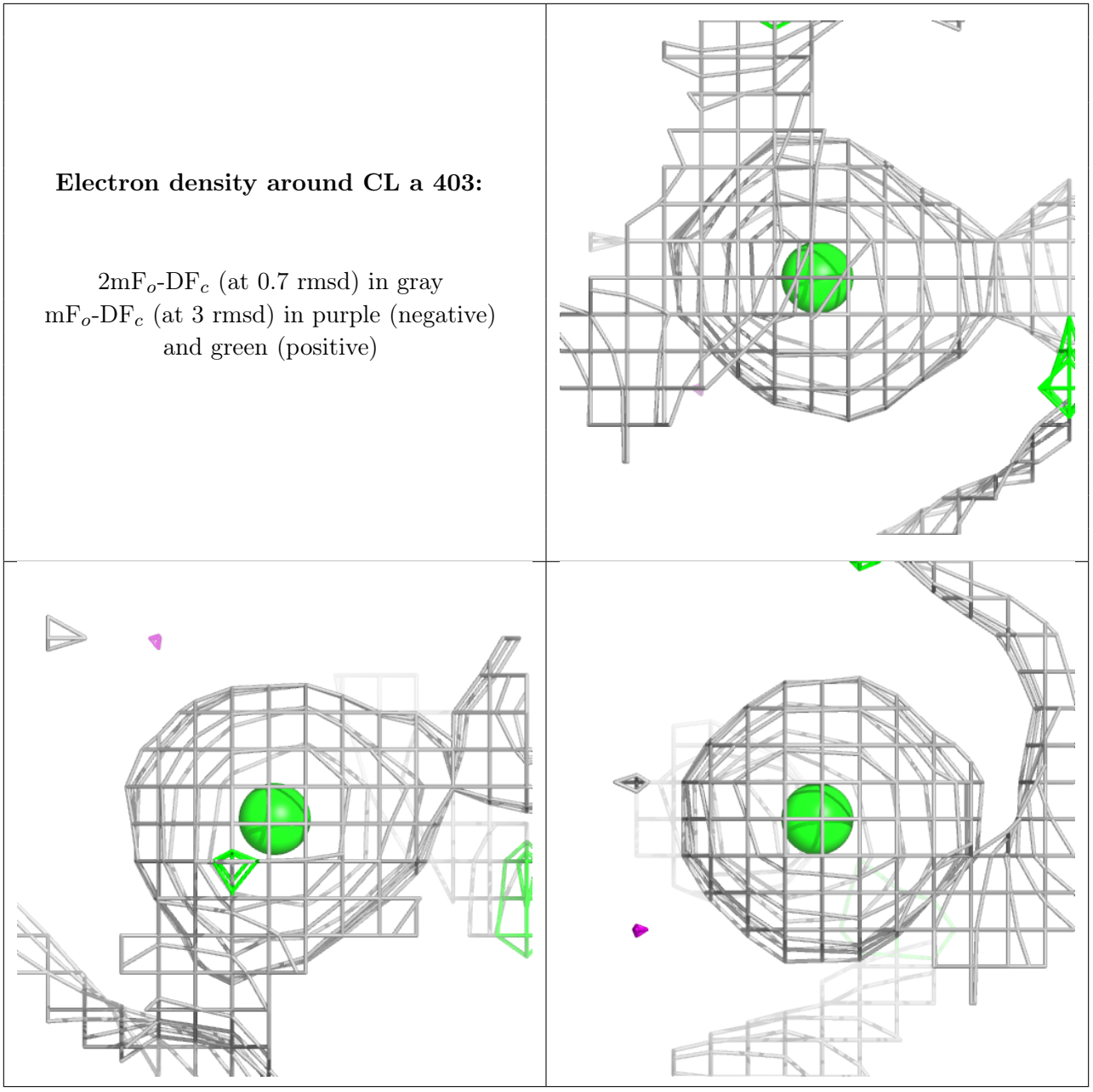
Electron density around CL a 402:

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



Electron density around CL a 403:

$2mF_o$-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.