wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 03:44 PM JST

PDB ID	:	5B66
Title	:	Crystal structure analysis of Photosystem II complex
Authors	:	Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on	:	2016-05-25
Resolution	:	1.85 Å(reported)

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

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

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

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

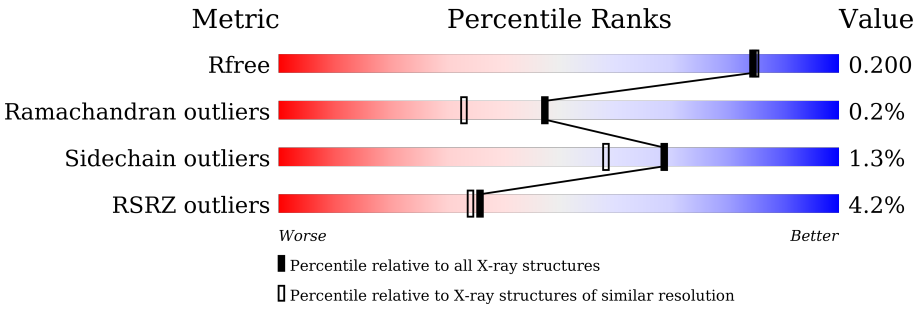
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	95%
1	a	344	95%
2	B	505	97%
2	b	505	95%
3	C	455	96%
3	c	455	97%
4	D	342	98%

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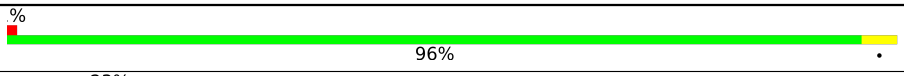
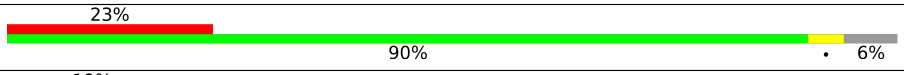
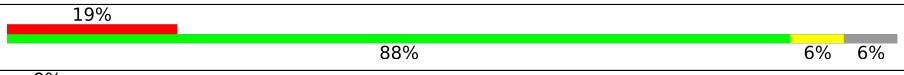
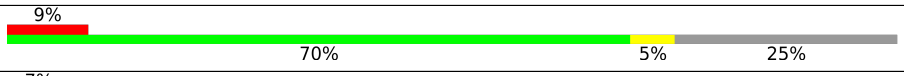
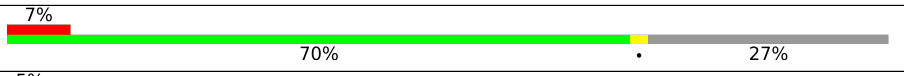
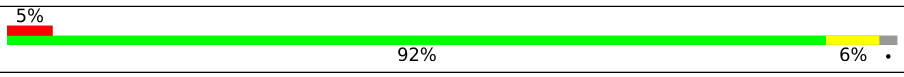
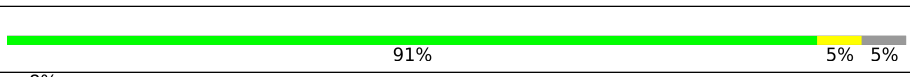
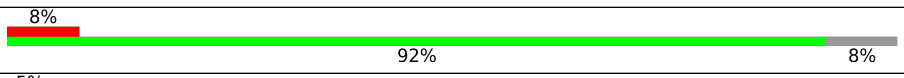
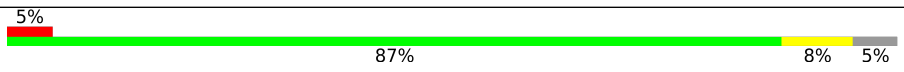
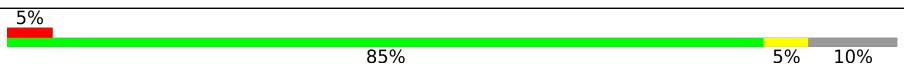
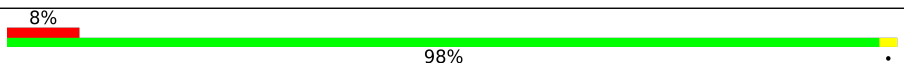
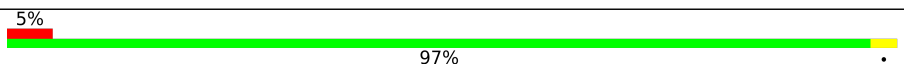
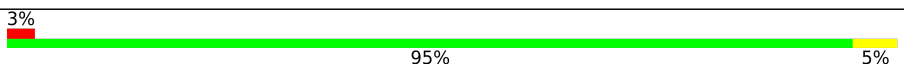
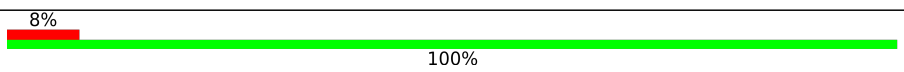
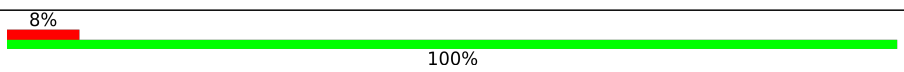
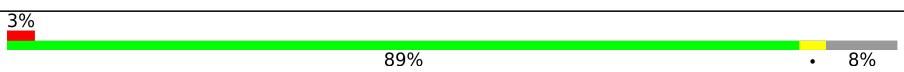
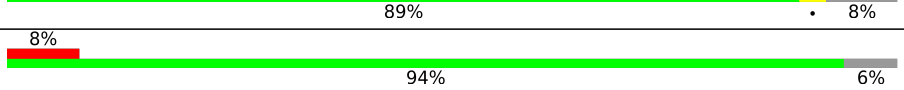
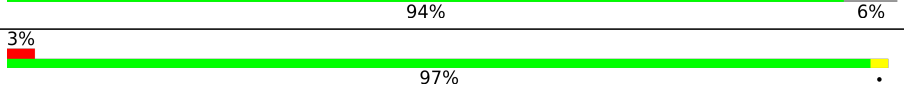
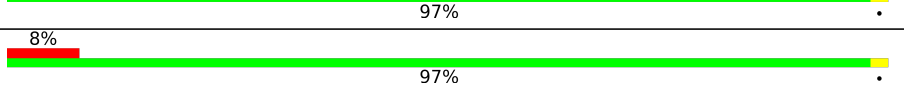
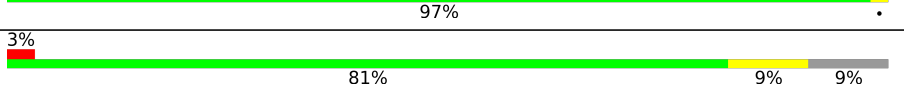
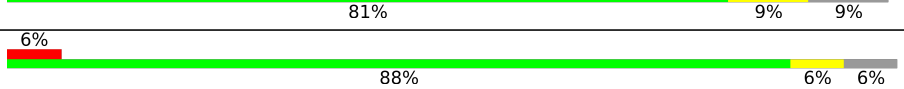
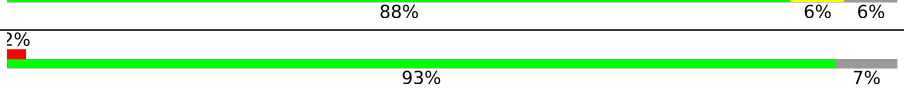
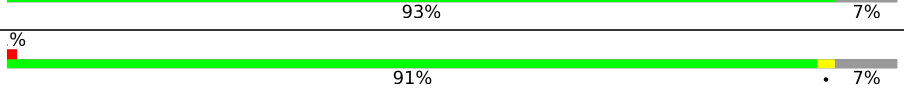
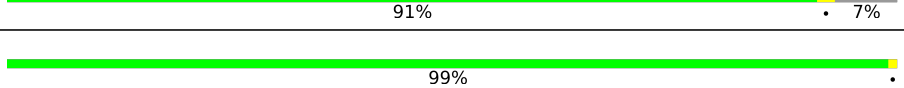
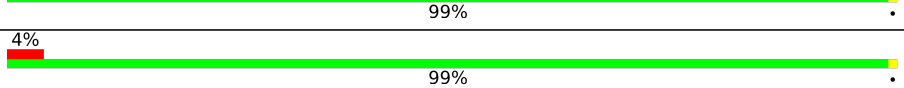
Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	Y	30	20% 90% 7%
17	y	30	13% 97%
18	X	40	12% 95% 5%
18	x	40	5% 88% 12%
19	Z	62	21% 94% 6%
19	z	62	19% 90% 8%

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
20	CLA	A	401	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	D	401	X	-	-	-
20	CLA	D	404	X	-	-	-
20	CLA	a	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	b	603	X	-	-	-
20	CLA	b	604	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	607	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	612	X	-	-	-
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	b	616	X	-	-	-
20	CLA	b	617	X	-	-	-
20	CLA	b	618	X	-	-	-
20	CLA	c	501	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	d	402	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 54996 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	3	0
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	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
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	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
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	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	1	0
			508	339	81	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total 284	C 194	N 45	O 44	S 1	0	0	0
8	i	36	Total 300	C 203	N 49	O 47	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	40	Total 272	C 183	N 41	O 47	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 285	C 199	N 42	O 44	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total 302	C 203	N 48	O 51	0	1	0
11	l	37	Total 296	C 200	N 45	O 51	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 259	C 175	N 37	O 46	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	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	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	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	39	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	97	Total	C	N	O	0	0	0
			766	486	128	152			
15	u	97	Total	C	N	O	0	0	0
			770	489	129	152			

- 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	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

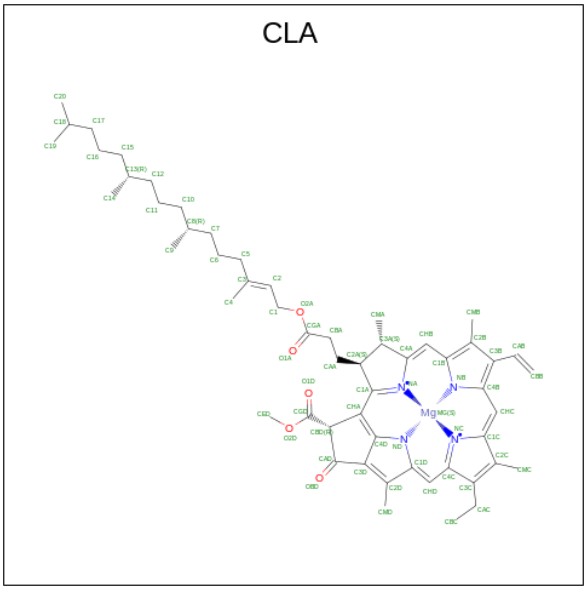
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			274	183	44	47			
18	x	35	Total	C	N	O	0	0	0
			252	171	38	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 59 49 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 60 50 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 55 45 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	a	1	Total C Mg N O 65 55 1 4 5	0	0
20	a	1	Total C Mg N O 60 50 1 4 5	0	0
20	a	1	Total C Mg N O 47 37 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 60 50 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0

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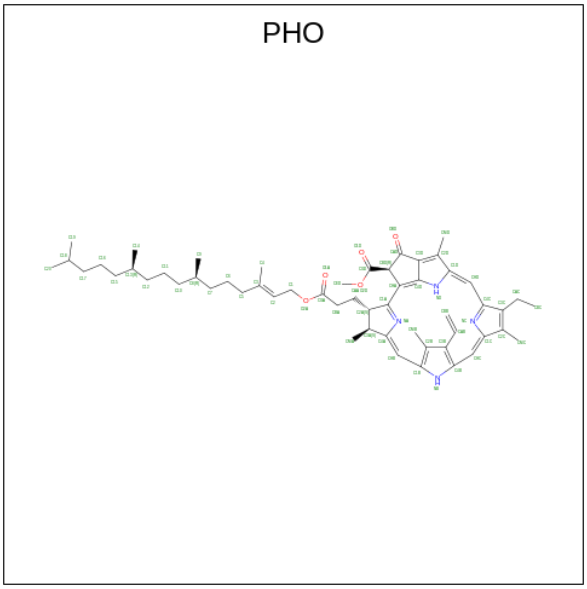
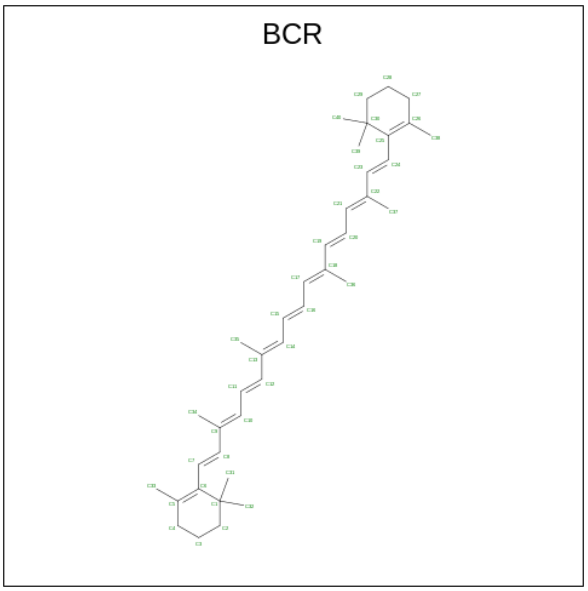
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	D	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	T	1	Total C 40 40	0	0
22	a	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0

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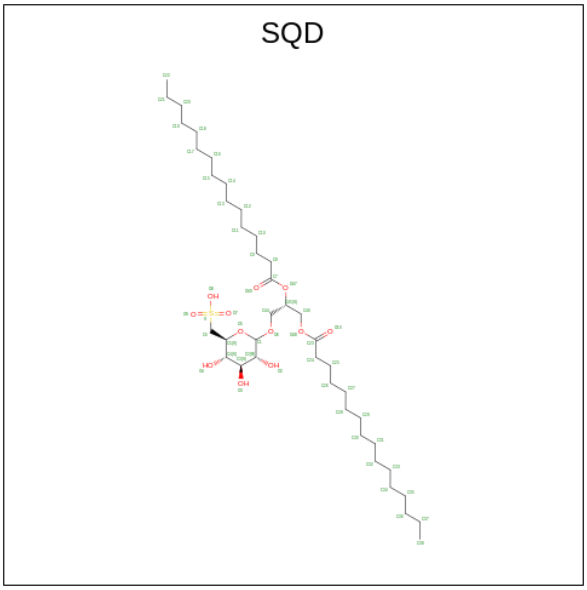
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C 40 40	0	0
22	d	1	Total C 40 40	0	0
22	j	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	t	1	Total C 40 40	0	0

- Molecule 23 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
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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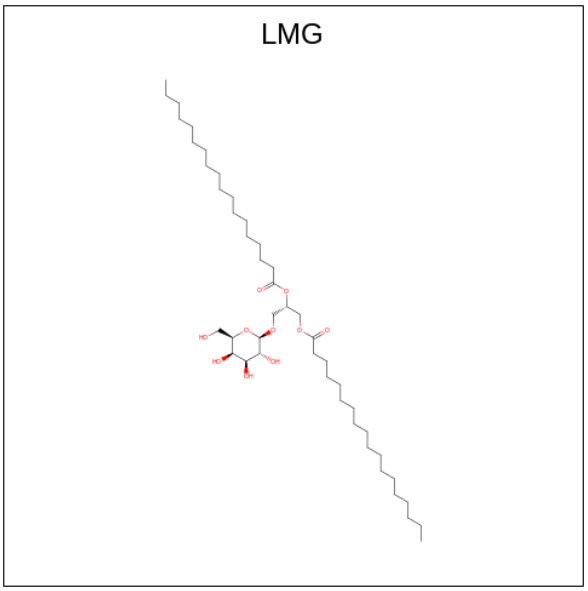
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C O S 54 41 12 1	0	0
23	f	1	Total C O S 40 27 12 1	0	0
23	l	1	Total C O S 54 41 12 1	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C O 51 41 10	0	0
24	B	1	Total C O 51 41 10	0	0
24	C	1	Total C O 51 41 10	0	0
24	C	1	Total C O 45 35 10	0	0
24	J	1	Total C O 45 35 10	0	0
24	a	1	Total C O 51 41 10	0	0
24	b	1	Total C O 49 39 10	0	0
24	c	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C O 51 41 10	0	0
24	j	1	Total C O 45 35 10	0	0

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total C O 40 35 5	0	0
26	B	6	Total C 84 84	0	0
26	C	1	Total C O 34 29 5	0	0
26	D	2	Total C O 53 48 5	0	0
26	E	1	Total C 15 15	0	0
26	H	2	Total C 10 10	0	0
26	I	5	Total C 61 61	0	0
26	J	4	Total C 33 33	0	0
26	L	1	Total C 14 14	0	0
26	M	1	Total C 12 12	0	0
26	T	1	Total C 13 13	0	0
26	U	1	Total C 14 14	0	0
26	X	1	Total C 16 16	0	0

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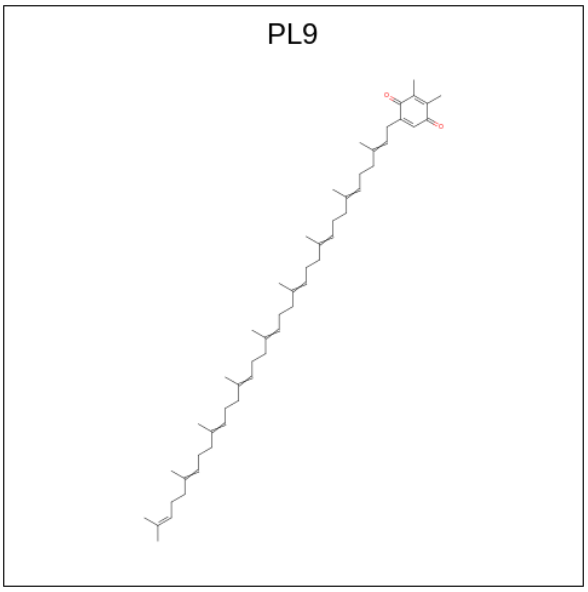
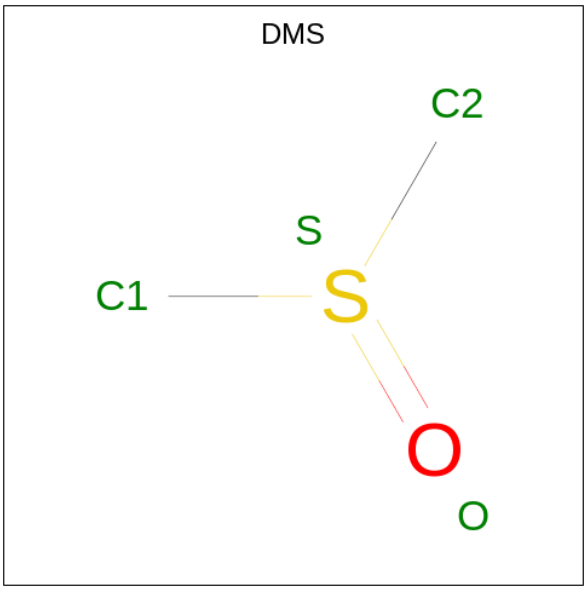
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	b	7	Total C 68 68	0	0
26	c	3	Total C O 48 43 5	0	0
26	d	3	Total C O 68 63 5	0	0
26	e	1	Total C 7 7	0	0
26	h	1	Total C 16 16	0	0
26	i	3	Total C 38 38	0	0
26	j	2	Total C 22 22	0	0
26	t	1	Total C 16 16	0	0
26	x	1	Total C 9 9	0	0
26	z	1	Total C 6 6	0	0

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



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

- Molecule 28 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 8 4 2 2	0	1
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	F	1	Total 4	C 2	O 1	S 1	0	0
28	H	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 8	C 4	O 2	S 2	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	U	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	h	1	Total C O S 4 2 1 1	0	0
28	i	1	Total C O S 4 2 1 1	0	0
28	j	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0

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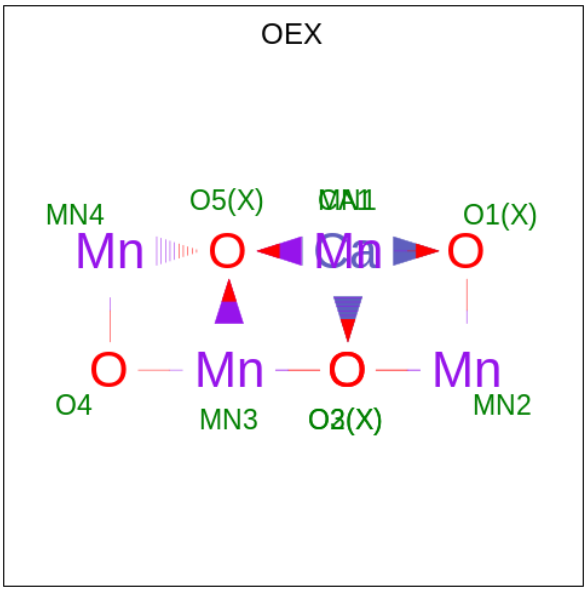
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	u	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

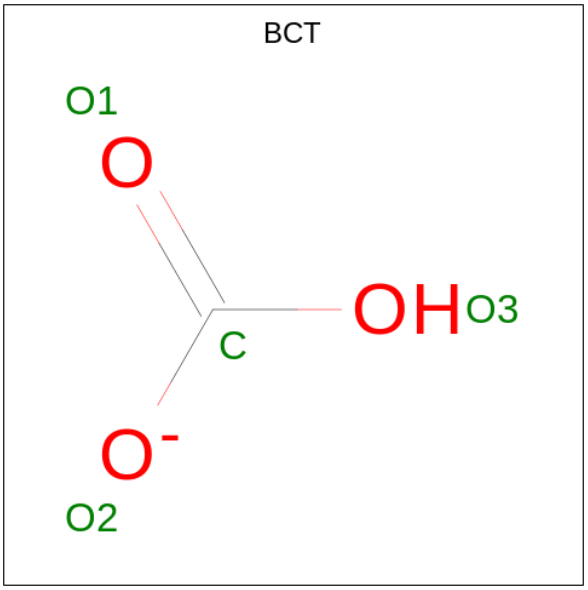
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Fe 1 1	0	0
29	a	1	Total Fe 1 1	0	0

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



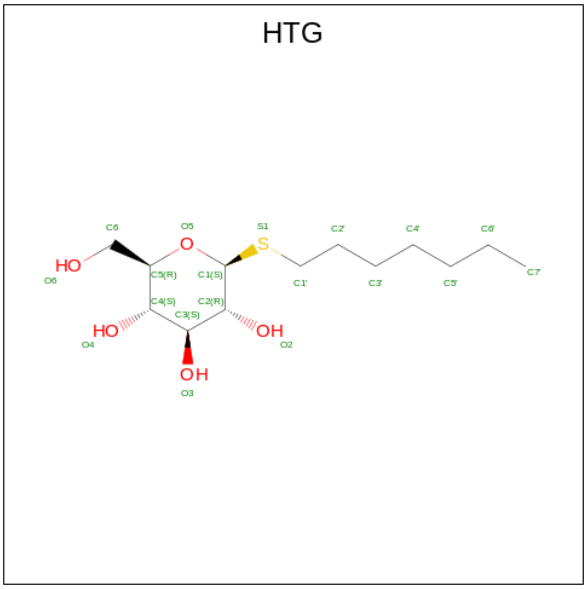
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			19	13	5	1		
32	O	1	Total	C	O	S	0	0
			19	13	5	1		
32	V	1	Total	C	O	S	0	0
			13	7	5	1		

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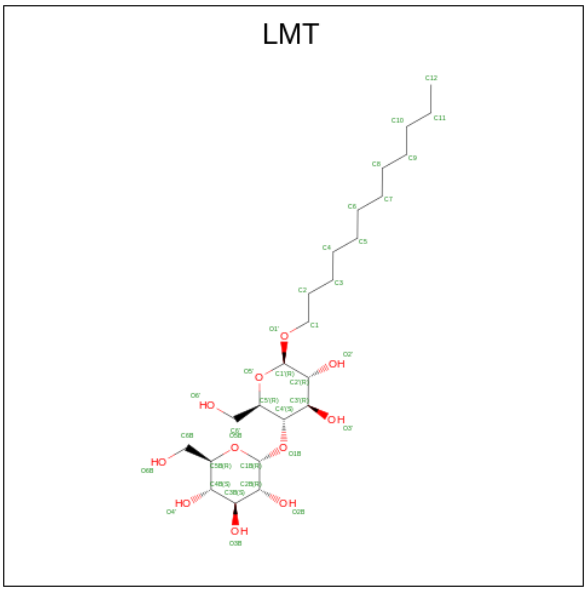
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	d	1	Total C O S 19 13 5 1	0	0
32	u	1	Total C S 8 7 1	0	0
32	v	1	Total C O S 14 8 5 1	0	0

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

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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 24 18 6	0	0
34	B	1	Total C O 24 18 6	0	0
34	B	1	Total C O 16 14 2	0	0
34	E	1	Total C O 24 18 6	0	0
34	I	1	Total C O 35 24 11	0	0
34	J	1	Total C O 24 18 6	0	0
34	M	1	Total C O 35 24 11	0	0
34	T	1	Total C O 24 18 6	0	0
34	Z	1	Total C O 35 24 11	0	0
34	a	1	Total C O 35 24 11	0	0
34	b	1	Total C O 32 21 11	0	0
34	b	1	Total C O 25 19 6	0	0
34	c	1	Total C O 35 24 11	0	0
34	f	1	Total C O 24 18 6	0	0

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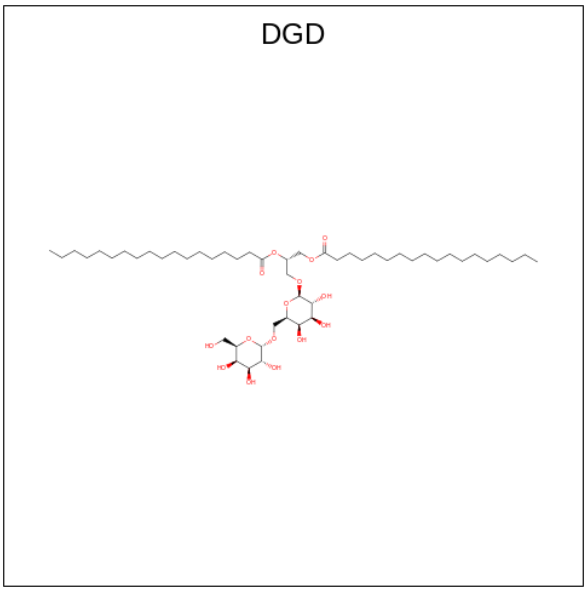
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	m	1	Total C O 35 24 11	0	0
34	m	1	Total C O 35 24 11	0	0
34	z	1	Total C O 35 24 11	0	0

- 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
35	C	1	Total C O 55 40 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	D	1	Total C O 51 41 10	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 57 42 15	0	0
35	c	1	Total C O 62 47 15	0	0

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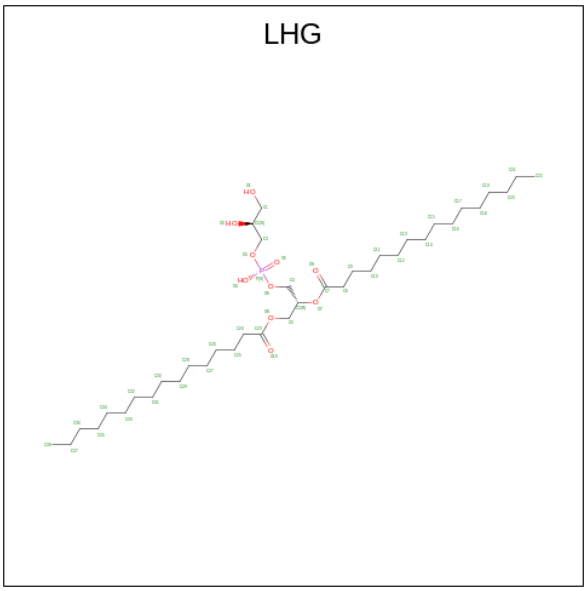
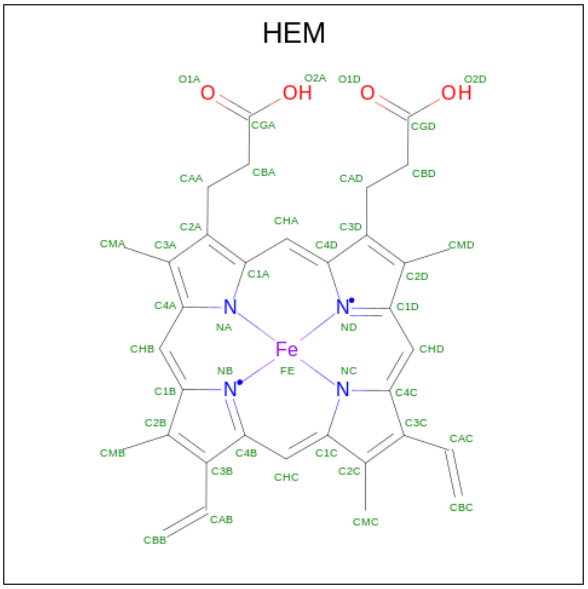
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	d	1	Total C O 51 41 10	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



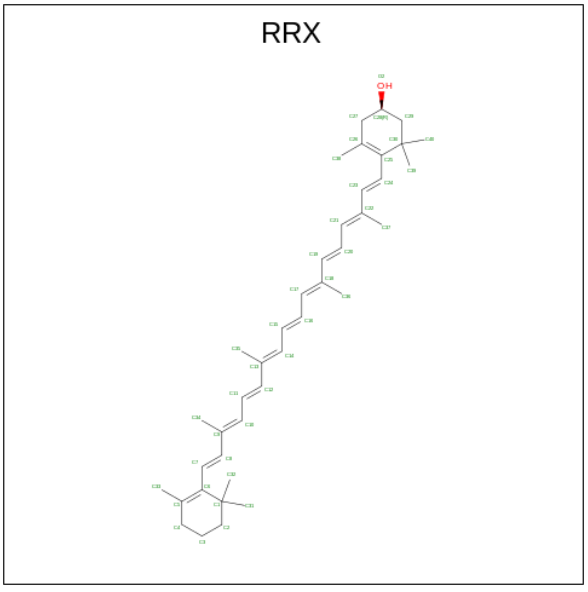
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	E	1	Total C O P 48 37 10 1	0	0
36	L	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	l	1	Total C O P 49 38 10 1	0	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

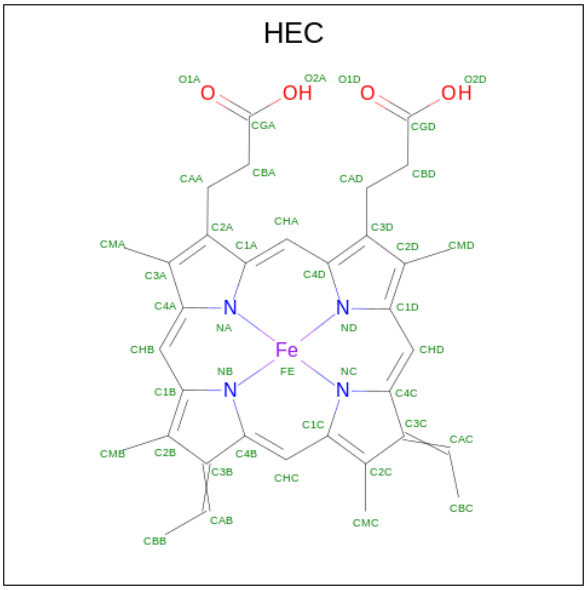


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	H	1	Total C O 41 40 1	0	0
38	x	1	Total C O 41 40 1	0	0

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

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

- 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 43 34 1 4 4	0	0
40	v	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	177	Total O 182 182	0	5

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	B	447	Total O 473 473	0	25
41	C	317	Total O 324 324	0	7
41	D	175	Total O 180 180	0	5
41	E	62	Total O 66 66	0	4
41	F	8	Total O 8 8	0	0
41	H	62	Total O 65 65	0	3
41	I	16	Total O 16 16	0	0
41	J	23	Total O 23 23	0	0
41	K	12	Total O 12 12	0	0
41	L	19	Total O 21 21	0	2
41	M	12	Total O 12 12	0	0
41	O	263	Total O 273 273	0	10
41	T	19	Total O 20 20	0	1
41	U	133	Total O 136 136	0	3
41	V	177	Total O 183 183	0	6
41	Y	7	Total O 7 7	0	0
41	X	22	Total O 22 22	0	0
41	Z	5	Total O 5 5	0	0
41	a	182	Total O 185 185	0	3
41	b	451	Total O 465 465	0	14
41	c	362	Total O 374 374	0	12

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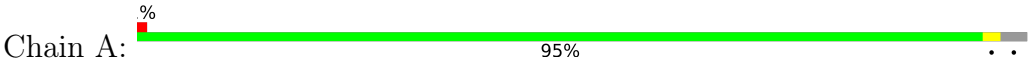
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	d	176	Total O 182 182	0	6
41	e	48	Total O 49 49	0	1
41	f	15	Total O 16 16	0	1
41	h	68	Total O 70 70	0	2
41	i	19	Total O 21 21	0	2
41	j	23	Total O 24 24	0	1
41	k	11	Total O 12 12	0	1
41	l	22	Total O 24 24	0	2
41	m	23	Total O 24 24	0	1
41	o	214	Total O 230 230	0	15
41	t	19	Total O 20 20	0	1
41	u	146	Total O 150 150	0	4
41	v	144	Total O 147 147	0	3
41	y	7	Total O 7 7	0	0
41	x	25	Total O 26 26	0	1
41	z	12	Total O 12 12	0	0

3 Residue-property plots

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.

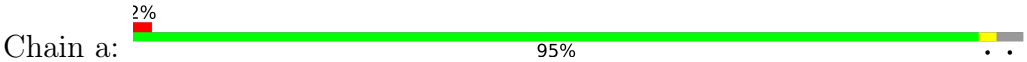
• Molecule 1: Photosystem II protein D1

Chain A:



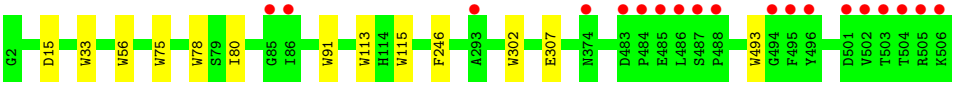
• Molecule 1: Photosystem II protein D1

Chain a:



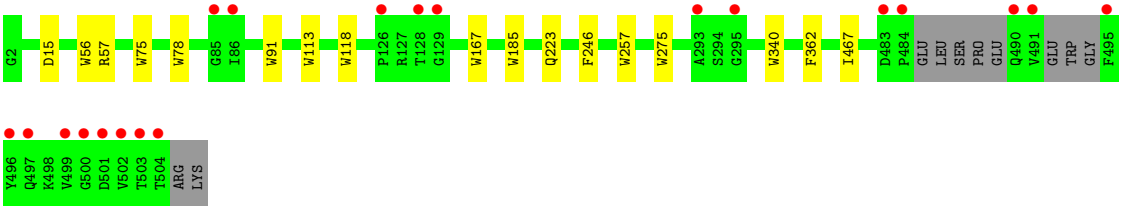
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



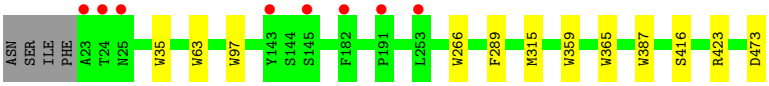
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

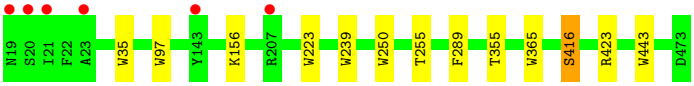


• Molecule 3: Photosystem II CP43 reaction center protein

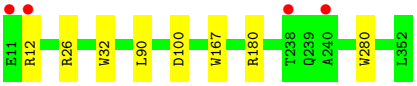
Chain C:



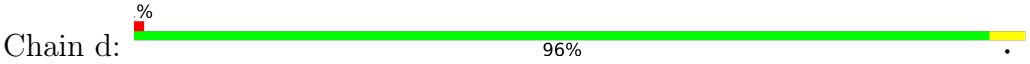
• Molecule 3: Photosystem II CP43 reaction center protein



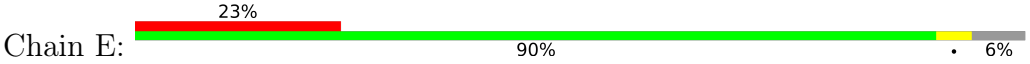
• Molecule 4: Photosystem II D2 protein

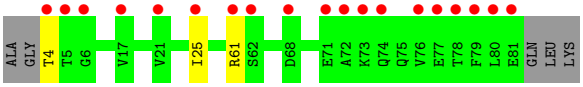


• Molecule 4: Photosystem II D2 protein

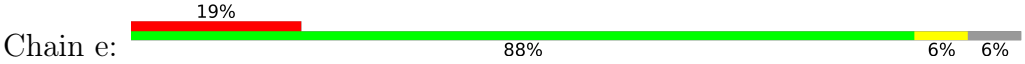


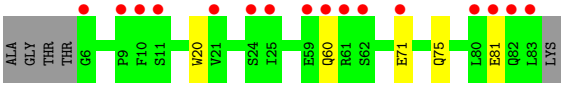
• Molecule 5: Cytochrome b559 subunit alpha



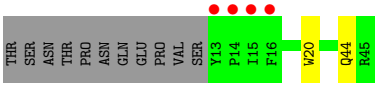


• Molecule 5: Cytochrome b559 subunit alpha



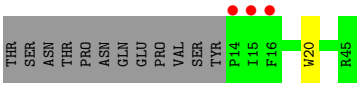


• Molecule 6: Cytochrome b559 subunit beta



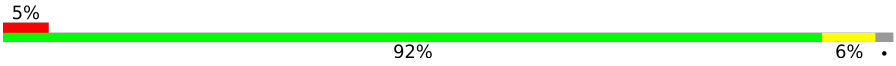
• Molecule 6: Cytochrome b559 subunit beta

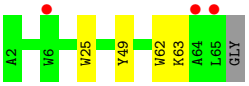
Chain f:



• Molecule 7: Photosystem II reaction center protein H

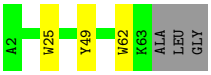
Chain H:





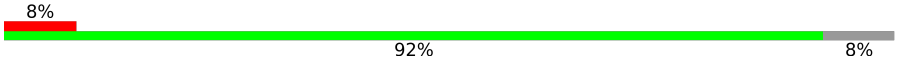
• Molecule 7: Photosystem II reaction center protein H

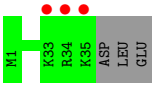
Chain h:



• Molecule 8: Photosystem II reaction center protein I

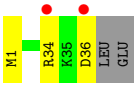
Chain I:





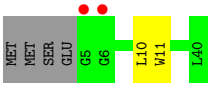
• Molecule 8: Photosystem II reaction center protein I

Chain i:



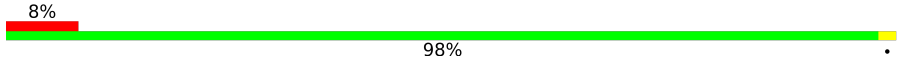
• Molecule 9: Photosystem II reaction center protein J

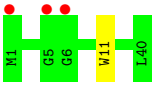
Chain J:



• Molecule 9: Photosystem II reaction center protein J

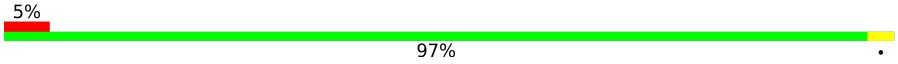
Chain j:

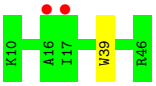




• Molecule 10: Photosystem II reaction center protein K

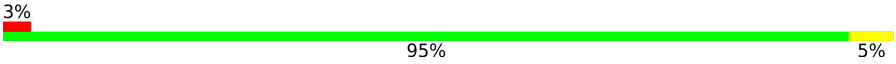
Chain K:

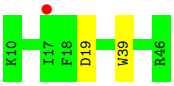




• Molecule 10: Photosystem II reaction center protein K

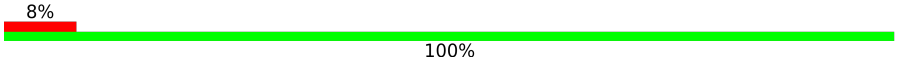
Chain k:





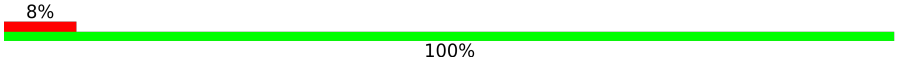
• Molecule 11: Photosystem II reaction center protein L

Chain L:



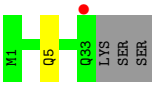
• Molecule 11: Photosystem II reaction center protein L

Chain l:



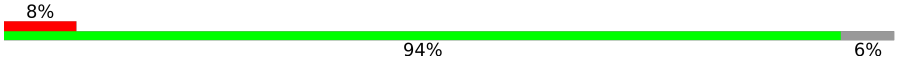
• Molecule 12: Photosystem II reaction center protein M

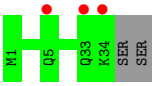
Chain M:



• Molecule 12: Photosystem II reaction center protein M

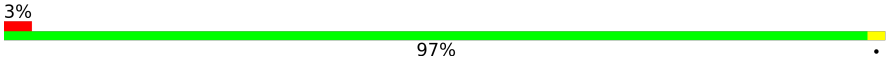
Chain m:

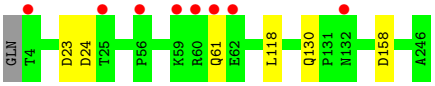




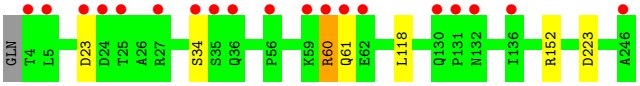
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

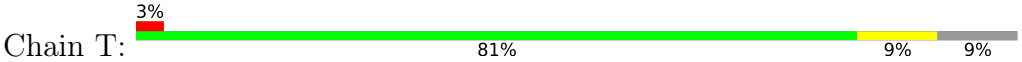


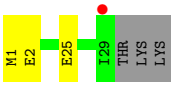


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

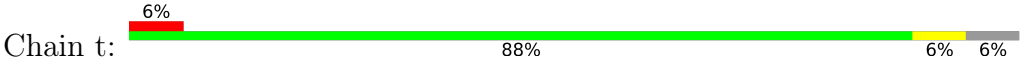


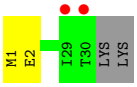
• Molecule 14: Photosystem II reaction center protein T



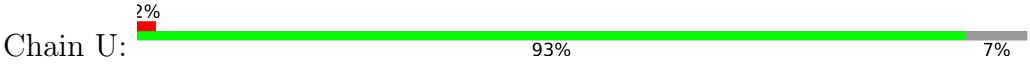


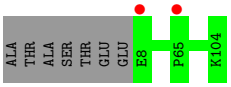
• Molecule 14: Photosystem II reaction center protein T



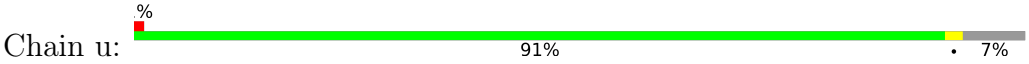


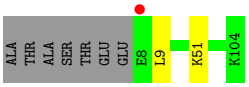
• Molecule 15: Photosystem II 12 kDa extrinsic protein





• Molecule 15: Photosystem II 12 kDa extrinsic protein

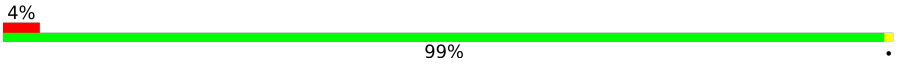


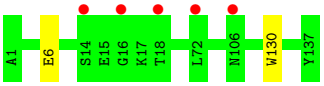


• Molecule 16: Cytochrome c-550

• Molecule 16: Cytochrome c-550

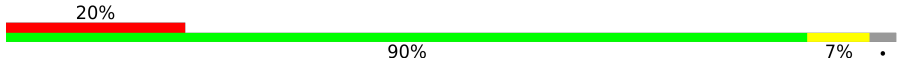
Chain v:

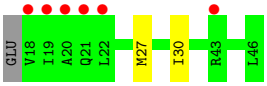




• Molecule 17: Photosystem II reaction center protein Ycf12

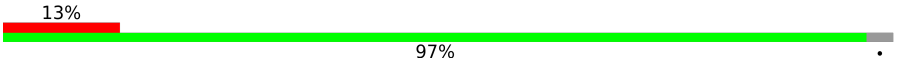
Chain Y:

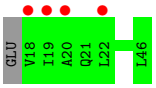




• Molecule 17: Photosystem II reaction center protein Ycf12

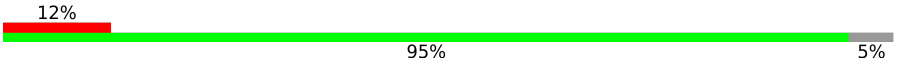
Chain y:

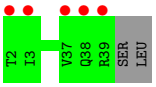




• Molecule 18: Photosystem II reaction center protein X

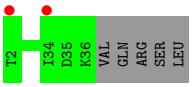
Chain X:





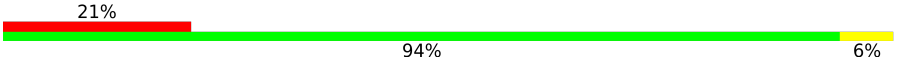
• Molecule 18: Photosystem II reaction center protein X

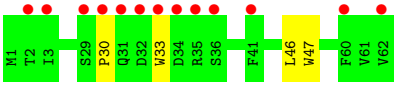
Chain x:



• Molecule 19: Photosystem II reaction center protein Z

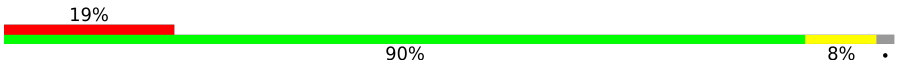
Chain Z:

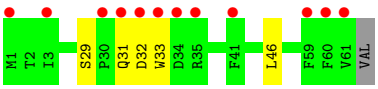




• Molecule 19: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 100.0 (19.99-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	33616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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: FE2, MG, PL9, LHG, FME, SQD, HTG, LMT, LMG, HEM, UNL, DGD, CA, CLA, BCT, CL, DMS, BCR, HEC, RRX, OEX, PHO

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	0.95	5/2717 (0.2%)	0.77	1/3707 (0.0%)
1	a	0.93	4/2718 (0.1%)	0.79	2/3707 (0.1%)
2	B	0.90	9/4181 (0.2%)	0.77	1/5700 (0.0%)
2	b	0.91	11/4029 (0.3%)	0.78	2/5490 (0.0%)
3	C	0.87	7/3599 (0.2%)	0.74	2/4901 (0.0%)
3	c	0.86	8/3640 (0.2%)	0.72	2/4956 (0.0%)
4	D	0.95	3/2826 (0.1%)	0.78	1/3850 (0.0%)
4	d	0.95	8/2817 (0.3%)	0.78	1/3839 (0.0%)
5	E	0.71	0/654	0.68	0/896
5	e	0.69	1/661 (0.2%)	0.72	0/904
6	F	0.79	1/278 (0.4%)	0.60	0/379
6	f	0.81	1/265 (0.4%)	0.62	0/360
7	H	0.84	2/524 (0.4%)	0.75	0/715
7	h	0.86	2/517 (0.4%)	0.71	0/704
8	I	0.63	0/281	0.69	0/380
8	i	0.61	0/300	0.62	0/405
9	J	0.82	1/257 (0.4%)	0.61	0/349
9	j	0.81	1/278 (0.4%)	0.62	0/378
10	K	0.70	1/303 (0.3%)	0.65	0/416
10	k	0.72	1/295 (0.3%)	0.64	0/407
11	L	0.88	0/312	0.76	0/425
11	l	0.91	0/306	0.76	0/418
12	M	0.70	0/265	0.74	0/362
12	m	0.70	0/270	0.76	0/369
13	O	0.72	0/1919	0.80	1/2607 (0.0%)
13	o	0.69	0/1875	0.77	2/2548 (0.1%)
14	T	0.78	0/259	0.77	0/352
14	t	0.79	0/257	0.73	0/349
15	U	0.77	0/777	0.78	0/1055
15	u	0.76	0/781	0.77	0/1059
16	V	0.80	0/1110	0.80	1/1506 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.71	1/1073 (0.1%)	0.75	0/1461
17	Y	0.50	0/213	0.63	0/285
17	y	0.45	0/214	0.60	0/286
18	X	0.54	0/277	0.69	0/375
18	x	0.57	0/255	0.66	0/345
19	Z	0.70	2/461 (0.4%)	0.56	0/632
19	z	0.61	1/444 (0.2%)	0.57	0/611
All	All	0.85	70/42208 (0.2%)	0.75	16/57488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.13	1.50	1.41
1	A	343	LEU	C-N	6.74	1.49	1.34
1	a	131	TRP	CD2-CE2	6.46	1.49	1.41
3	C	266	TRP	CD2-CE2	6.43	1.49	1.41
2	B	33	TRP	CD2-CE2	6.27	1.48	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	342	ASP	CB-CG-OD1	6.34	124.01	118.30
16	V	128	ASP	CB-CG-OD1	6.14	123.82	118.30
3	C	473	ASP	CB-CG-OD2	5.92	123.63	118.30
13	o	152	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	c	423	ARG	NE-CZ-NH2	-5.79	117.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	41	26
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	26
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100	100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100	100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	47	33
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	47	33
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	41	26
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100
6	F	31/44 (70%)	31 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	34	19
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	13	3
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	47	33

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	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	269/279 (96%)	268 (100%)	1 (0%)	91 89
1	a	270/279 (97%)	270 (100%)	0	100 100
2	B	405/403 (100%)	401 (99%)	4 (1%)	76 69
2	b	390/403 (97%)	386 (99%)	4 (1%)	76 69
3	C	351/356 (99%)	349 (99%)	2 (1%)	86 83
3	c	356/356 (100%)	351 (99%)	5 (1%)	67 55
4	D	277/277 (100%)	274 (99%)	3 (1%)	73 65
4	d	276/277 (100%)	272 (99%)	4 (1%)	67 55
5	E	68/72 (94%)	65 (96%)	3 (4%)	28 12
5	e	68/72 (94%)	63 (93%)	5 (7%)	13 3
6	F	27/38 (71%)	26 (96%)	1 (4%)	34 17
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	34 17
7	h	54/54 (100%)	53 (98%)	1 (2%)	57 43
8	I	30/34 (88%)	30 (100%)	0	100 100
8	i	32/34 (94%)	29 (91%)	3 (9%)	8 1
9	J	23/28 (82%)	22 (96%)	1 (4%)	29 12
9	j	24/28 (86%)	24 (100%)	0	100 100
10	K	30/30 (100%)	30 (100%)	0	100 100
10	k	28/30 (93%)	27 (96%)	1 (4%)	35 18
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	33/35 (94%)	33 (100%)	0	100 100
12	M	30/33 (91%)	29 (97%)	1 (3%)	38 21
12	m	30/33 (91%)	30 (100%)	0	100 100
13	O	207/207 (100%)	202 (98%)	5 (2%)	49 33
13	o	199/207 (96%)	197 (99%)	2 (1%)	76 69
14	T	26/28 (93%)	23 (88%)	3 (12%)	5 1
14	t	26/28 (93%)	25 (96%)	1 (4%)	33 16
15	U	82/89 (92%)	82 (100%)	0	100 100
15	u	83/89 (93%)	81 (98%)	2 (2%)	49 33
16	V	120/117 (103%)	119 (99%)	1 (1%)	81 76
16	v	114/117 (97%)	113 (99%)	1 (1%)	78 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	21/23 (91%)	19 (90%)	2 (10%)	8 1
17	y	21/23 (91%)	21 (100%)	0	100 100
18	X	29/33 (88%)	29 (100%)	0	100 100
18	x	27/33 (82%)	27 (100%)	0	100 100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	50 34
19	z	39/52 (75%)	37 (95%)	2 (5%)	24 9
All	All	4223/4376 (96%)	4162 (99%)	61 (1%)	69 55

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Y	30	ILE
14	t	2	GLU
3	c	255	THR
13	o	118	LEU
19	z	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	332	GLN
15	u	73	GLN
16	v	118	HIS
16	v	34	GLN
7	H	59	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)

4 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	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.52	0	7,9,11	1.68	1 (14%)
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	1.11	0
14	FME	T	1	14	8,9,10	0.43	0	7,9,11	1.79	2 (28%)
14	FME	t	1	14	8,9,10	0.49	0	7,9,11	1.86	4 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	2.88	114.93	109.73
14	T	1	FME	CE-SD-CG	2.70	109.68	100.40
14	T	1	FME	O-C-CA	-2.46	118.34	124.78
14	t	1	FME	CG-CB-CA	2.44	119.72	112.95
14	t	1	FME	CE-SD-CG	2.32	108.38	100.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

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 349 ligands modelled in this entry, 14 are monoatomic and 55 are unknown - leaving 280 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	$\#\|Z\| > 2$
34	LMT	c	523	-	36,36,36	0.81	1 (2%)	47,47,47	1.60	6 (12%)
28	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.83	0
20	CLA	b	614	-	65,73,73	1.91	16 (24%)	76,113,113	2.31	24 (31%)
35	DGD	H	102	-	63,63,67	1.04	3 (4%)	77,77,81	1.27	8 (10%)
34	LMT	b	628	-	25,25,36	0.55	0	30,30,47	1.20	2 (6%)
20	CLA	B	602	41	65,73,73	2.65	20 (30%)	76,113,113	2.55	25 (32%)
20	CLA	d	402	-	65,73,73	1.89	16 (24%)	76,113,113	1.95	21 (27%)
28	DMS	v	207	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
28	DMS	b	632	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
20	CLA	A	404	-	65,73,73	2.05	20 (30%)	76,113,113	2.53	25 (32%)
20	CLA	c	505	-	65,73,73	2.12	18 (27%)	76,113,113	2.07	21 (27%)
28	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.74	0
22	BCR	b	619	-	41,41,41	0.95	0	56,56,56	1.77	11 (19%)
22	BCR	k	102	-	41,41,41	0.79	0	56,56,56	1.29	9 (16%)
24	LMG	A	407	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	3 (5%)
28	DMS	B	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.63	0
20	CLA	D	404	-	65,73,73	2.13	20 (30%)	76,113,113	2.26	28 (36%)
28	DMS	B	642	-	3,3,3	2.79	1 (33%)	3,3,3	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	HTG	d	401	-	19,19,19	1.08	1 (5%)	23,24,24	2.36	4 (17%)
20	CLA	a	407	-	47,55,73	2.39	14 (29%)	54,91,113	2.55	24 (44%)
34	LMT	I	101	-	36,36,36	0.65	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	B	613	-	65,73,73	2.10	13 (20%)	76,113,113	2.30	23 (30%)
28	DMS	O	306	-	3,3,3	2.53	1 (33%)	3,3,3	0.64	0
28	DMS	b	633	-	3,3,3	2.55	1 (33%)	3,3,3	1.05	0
36	LHG	D	407	-	48,48,48	0.86	1 (2%)	51,54,54	1.26	5 (9%)
20	CLA	B	608	41	65,73,73	1.93	14 (21%)	76,113,113	2.11	20 (26%)
20	CLA	d	403	41	65,73,73	2.08	15 (23%)	76,113,113	2.22	21 (27%)
23	SQD	b	622	-	53,54,54	1.10	3 (5%)	62,65,65	1.55	11 (17%)
32	HTG	b	625	-	19,19,19	1.21	2 (10%)	23,24,24	1.34	4 (17%)
34	LMT	b	627	-	33,33,36	0.88	1 (3%)	44,44,47	1.80	10 (22%)
28	DMS	V	209	-	3,3,3	2.61	1 (33%)	3,3,3	0.64	0
20	CLA	B	601	-	65,73,73	2.06	17 (26%)	76,113,113	2.11	24 (31%)
23	SQD	A	406	-	53,54,54	1.00	3 (5%)	62,65,65	1.75	14 (22%)
20	CLA	b	604	-	65,73,73	2.09	18 (27%)	76,113,113	2.28	28 (36%)
28	DMS	j	105	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
32	HTG	B	621	-	19,19,19	1.45	3 (15%)	23,24,24	1.79	6 (26%)
28	DMS	h	102	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
37	HEM	E	104	6,5	41,50,50	1.88	7 (17%)	45,82,82	2.01	13 (28%)
22	BCR	a	408	-	41,41,41	1.21	2 (4%)	56,56,56	1.44	7 (12%)
28	DMS	c	535	-	3,3,3	2.78	1 (33%)	3,3,3	0.79	0
32	HTG	C	522	-	19,19,19	1.06	2 (10%)	23,24,24	1.56	1 (4%)
22	BCR	K	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.48	13 (23%)
28	DMS	C	528	-	3,3,3	2.31	1 (33%)	3,3,3	0.59	0
28	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
28	DMS	o	307	-	3,3,3	2.65	1 (33%)	3,3,3	0.85	0
20	CLA	B	605	-	65,73,73	2.10	15 (23%)	76,113,113	2.03	22 (28%)
20	CLA	C	513	-	65,73,73	2.57	18 (27%)	76,113,113	2.11	19 (25%)
20	CLA	c	504	41	65,73,73	2.13	17 (26%)	76,113,113	2.65	23 (30%)
32	HTG	v	210	-	14,14,19	0.62	0	18,19,24	2.19	4 (22%)
21	PHO	a	406	-	51,69,69	1.58	8 (15%)	47,99,99	1.80	9 (19%)
34	LMT	J	103	-	24,24,36	0.65	1 (4%)	29,29,47	1.12	1 (3%)
36	LHG	D	408	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	1 (1%)
24	LMG	c	518	-	51,51,55	1.11	3 (5%)	59,59,63	1.31	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	C	510	-	65,73,73	2.17	18 (27%)	76,113,113	2.16	21 (27%)
20	CLA	c	502	-	65,73,73	2.20	17 (26%)	76,113,113	2.38	25 (32%)
38	RRX	H	101	-	42,42,42	0.77	1 (2%)	57,58,58	1.49	8 (14%)
28	DMS	D	414	-	3,3,3	2.53	1 (33%)	3,3,3	0.25	0
20	CLA	b	615	-	65,73,73	1.87	15 (23%)	76,113,113	2.37	24 (31%)
24	LMG	C	519	-	51,51,55	1.03	2 (3%)	59,59,63	1.23	8 (13%)
20	CLA	b	605	-	65,73,73	2.08	15 (23%)	76,113,113	2.27	28 (36%)
24	LMG	j	101	39	45,45,55	1.00	3 (6%)	53,53,63	1.02	6 (11%)
38	RRX	x	101	-	42,42,42	0.82	0	57,58,58	1.22	6 (10%)
32	HTG	c	521	-	19,19,19	0.96	1 (5%)	23,24,24	2.03	3 (13%)
31	BCT	a	413	29	2,3,3	0.65	0	2,3,3	1.47	0
28	DMS	D	416	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
20	CLA	c	507	41	65,73,73	2.29	16 (24%)	76,113,113	2.34	21 (27%)
22	BCR	C	514	-	41,41,41	0.85	0	56,56,56	1.31	7 (12%)
22	BCR	A	405	-	41,41,41	0.95	3 (7%)	56,56,56	1.27	7 (12%)
32	HTG	C	521	-	19,19,19	0.98	2 (10%)	23,24,24	1.97	4 (17%)
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.84	11 (19%)
32	HTG	V	202	-	12,13,19	0.76	1 (8%)	16,18,24	2.50	6 (37%)
32	HTG	c	520	-	19,19,19	0.89	2 (10%)	23,24,24	1.32	2 (8%)
23	SQD	f	101	-	39,40,54	1.37	3 (7%)	48,51,65	3.70	12 (25%)
36	LHG	l	102	-	48,48,48	0.78	2 (4%)	51,54,54	1.00	2 (3%)
27	PL9	d	412	-	55,55,55	1.09	3 (5%)	68,69,69	1.59	16 (23%)
20	CLA	C	507	41	65,73,73	2.48	19 (29%)	76,113,113	2.31	22 (28%)
23	SQD	a	409	-	53,54,54	1.01	4 (7%)	62,65,65	2.11	11 (17%)
35	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	3 (3%)
20	CLA	a	403	-	65,73,73	1.86	13 (20%)	76,113,113	2.16	23 (30%)
28	DMS	V	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
22	BCR	B	617	-	41,41,41	0.98	0	56,56,56	1.62	11 (19%)
28	DMS	c	530	-	3,3,3	2.80	1 (33%)	3,3,3	1.01	0
28	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.81	0
28	DMS	v	203	-	3,3,3	2.59	1 (33%)	3,3,3	0.85	0
20	CLA	b	618	-	65,73,73	2.18	19 (29%)	76,113,113	2.29	26 (34%)
34	LMT	a	418	-	36,36,36	0.68	2 (5%)	47,47,47	1.54	6 (12%)
28	DMS	C	530	-	3,3,3	2.61	1 (33%)	3,3,3	1.00	0
35	DGD	C	517	-	56,56,67	0.98	2 (3%)	70,70,81	0.93	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	C	506	-	65,73,73	2.39	18 (27%)	76,113,113	2.30	21 (27%)
20	CLA	c	503	-	65,73,73	2.53	20 (30%)	76,113,113	2.29	21 (27%)
21	PHO	a	405	-	51,69,69	1.57	7 (13%)	47,99,99	1.38	5 (10%)
20	CLA	B	615	-	65,73,73	2.01	16 (24%)	76,113,113	2.52	27 (35%)
23	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.71	10 (16%)
28	DMS	B	645	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
28	DMS	o	302	-	3,3,3	2.75	1 (33%)	3,3,3	0.90	0
32	HTG	b	601	-	19,19,19	1.04	2 (10%)	23,24,24	1.27	2 (8%)
35	DGD	h	101	-	63,63,67	0.98	3 (4%)	77,77,81	1.04	4 (5%)
20	CLA	C	503	-	65,73,73	2.35	17 (26%)	76,113,113	1.98	22 (28%)
28	DMS	v	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.66	0
22	BCR	B	618	-	41,41,41	1.05	0	56,56,56	1.26	7 (12%)
28	DMS	A	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
28	DMS	B	641	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
23	SQD	l	101	-	53,54,54	1.08	4 (7%)	62,65,65	1.68	8 (12%)
28	DMS	c	536	-	3,3,3	2.84	1 (33%)	3,3,3	1.23	0
28	DMS	H	103	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
20	CLA	C	505	-	65,73,73	2.15	18 (27%)	76,113,113	2.04	21 (27%)
20	CLA	b	606	-	65,73,73	1.96	14 (21%)	76,113,113	2.37	25 (32%)
20	CLA	C	509	-	65,73,73	2.18	14 (21%)	76,113,113	2.28	23 (30%)
22	BCR	C	515	-	41,41,41	0.97	0	56,56,56	1.19	6 (10%)
22	BCR	k	101	-	41,41,41	0.94	0	56,56,56	1.12	6 (10%)
24	LMG	B	620	-	51,51,55	1.02	2 (3%)	59,59,63	1.31	5 (8%)
34	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.93	2 (4%)
32	HTG	D	417	-	19,19,19	1.05	1 (5%)	23,24,24	1.49	3 (13%)
28	DMS	B	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.82	0
28	DMS	o	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.77	0
20	CLA	c	509	-	65,73,73	2.31	18 (27%)	76,113,113	2.39	26 (34%)
20	CLA	A	402	41	59,67,73	1.73	14 (23%)	68,105,113	2.75	24 (35%)
20	CLA	c	510	-	65,73,73	1.95	18 (27%)	76,113,113	2.22	27 (35%)
35	DGD	c	517	-	63,63,67	1.04	4 (6%)	77,77,81	1.19	8 (10%)
20	CLA	B	603	-	65,73,73	2.21	18 (27%)	76,113,113	2.21	24 (31%)
20	CLA	A	401	-	65,73,73	1.90	17 (26%)	76,113,113	1.99	22 (28%)
28	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.76	0
20	CLA	b	608	-	65,73,73	2.43	18 (27%)	76,113,113	2.15	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	b	634	-	3,3,3	2.67	1 (33%)	3,3,3	0.68	0
27	PL9	A	411	-	55,55,55	0.83	3 (5%)	68,69,69	1.69	18 (26%)
28	DMS	U	902	-	3,3,3	2.66	1 (33%)	3,3,3	1.63	1 (33%)
28	DMS	A	414	-	3,3,3	1.97	1 (33%)	3,3,3	0.54	0
28	DMS	C	532	-	3,3,3	3.28	1 (33%)	3,3,3	1.29	1 (33%)
20	CLA	b	603	41	65,73,73	2.65	19 (29%)	76,113,113	2.29	24 (31%)
28	DMS	C	525[A]	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
28	DMS	U	903[A]	-	3,3,3	2.56	1 (33%)	3,3,3	0.75	0
28	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
20	CLA	D	402	41	65,73,73	1.90	16 (24%)	76,113,113	2.23	21 (27%)
28	DMS	O	303	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
28	DMS	O	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.42	0
28	DMS	O	310	-	3,3,3	2.70	1 (33%)	3,3,3	0.70	0
20	CLA	a	404	41	60,68,73	1.90	16 (26%)	70,107,113	2.32	24 (34%)
35	DGD	d	416	-	51,51,67	1.11	3 (5%)	59,59,81	1.20	6 (10%)
28	DMS	B	644	-	3,3,3	2.87	1 (33%)	3,3,3	1.26	0
34	LMT	B	627	-	15,15,36	0.48	0	14,14,47	0.67	0
20	CLA	c	511	3	65,73,73	2.52	19 (29%)	76,113,113	2.25	20 (26%)
34	LMT	m	101	-	36,36,36	0.61	1 (2%)	47,47,47	0.96	1 (2%)
36	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	5 (9%)
28	DMS	C	526	-	3,3,3	2.56	1 (33%)	3,3,3	0.81	0
24	LMG	a	410	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	2 (3%)
28	DMS	c	528	-	3,3,3	2.57	1 (33%)	3,3,3	0.44	0
27	PL9	a	415	-	55,55,55	0.83	3 (5%)	68,69,69	1.67	16 (23%)
20	CLA	c	501	-	65,73,73	2.17	16 (24%)	76,113,113	2.75	23 (30%)
32	HTG	B	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.56	2 (8%)
28	DMS	v	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
32	HTG	u	201	-	7,7,19	0.43	0	6,6,24	0.70	0
36	LHG	L	101	-	48,48,48	0.90	3 (6%)	51,54,54	0.90	1 (1%)
22	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.23	5 (8%)
28	DMS	u	202	-	3,3,3	2.65	1 (33%)	3,3,3	1.29	0
32	HTG	O	302	-	19,19,19	1.29	2 (10%)	23,24,24	1.18	2 (8%)
20	CLA	c	512	-	65,73,73	2.30	18 (27%)	76,113,113	2.28	21 (27%)
32	HTG	B	622	-	19,19,19	1.34	3 (15%)	23,24,24	1.93	6 (26%)
28	DMS	C	529	-	3,3,3	2.69	1 (33%)	3,3,3	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	SQD	F	101	-	34,35,54	1.01	2 (5%)	42,45,65	1.59	7 (16%)
30	OEX	A	420	1,41,3	0,15,15	-	-	-		
20	CLA	b	609	41	65,73,73	2.05	17 (26%)	76,113,113	2.01	26 (34%)
28	DMS	C	531	-	3,3,3	2.66	1 (33%)	3,3,3	0.97	0
20	CLA	C	512	-	55,63,73	2.72	20 (36%)	64,101,113	2.39	23 (35%)
20	CLA	C	502	-	65,73,73	2.23	16 (24%)	76,113,113	2.29	24 (31%)
37	HEM	e	102	6,5	41,50,50	1.96	10 (24%)	45,82,82	1.94	10 (22%)
36	LHG	d	407	-	48,48,48	0.73	2 (4%)	51,54,54	0.99	4 (7%)
24	LMG	J	101	39	45,45,55	1.01	2 (4%)	53,53,63	0.98	3 (5%)
34	LMT	E	101	-	24,24,36	0.62	1 (4%)	29,29,47	1.01	3 (10%)
40	HEC	V	201	16	32,50,50	1.86	8 (25%)	24,82,82	1.89	5 (20%)
22	BCR	D	405	-	41,41,41	1.03	3 (7%)	56,56,56	1.73	13 (23%)
22	BCR	j	102	-	41,41,41	0.85	0	56,56,56	1.38	9 (16%)
27	PL9	D	412	-	55,55,55	1.06	3 (5%)	68,69,69	1.51	12 (17%)
28	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
28	DMS	c	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
28	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.73	0
28	DMS	v	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
34	LMT	z	102	-	36,36,36	0.76	1 (2%)	47,47,47	1.49	8 (17%)
28	DMS	b	638	-	3,3,3	2.78	1 (33%)	3,3,3	0.94	0
20	CLA	b	611	-	65,73,73	2.57	17 (26%)	76,113,113	1.82	20 (26%)
28	DMS	O	311	-	3,3,3	2.87	1 (33%)	3,3,3	0.92	0
34	LMT	f	102	-	24,24,36	0.79	1 (4%)	29,29,47	0.96	2 (6%)
32	HTG	b	602	-	19,19,19	1.00	2 (10%)	23,24,24	1.15	1 (4%)
28	DMS	b	635	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
20	CLA	C	508	-	60,68,73	2.50	17 (28%)	70,107,113	2.38	24 (34%)
20	CLA	d	404	-	65,73,73	1.99	17 (26%)	76,113,113	2.35	25 (32%)
20	CLA	B	610	-	65,73,73	2.13	16 (24%)	76,113,113	2.17	24 (31%)
28	DMS	D	413	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0
28	DMS	b	639	-	3,3,3	2.81	1 (33%)	3,3,3	0.57	0
34	LMT	B	625	-	24,24,36	0.53	0	29,29,47	1.26	4 (13%)
28	DMS	d	413	-	3,3,3	2.57	1 (33%)	3,3,3	0.91	0
28	DMS	D	415	-	3,3,3	2.92	1 (33%)	3,3,3	0.73	0
35	DGD	c	515	-	63,63,67	0.85	3 (4%)	77,77,81	1.19	8 (10%)
28	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMT	Z	101	-	36,36,36	0.68	1 (2%)	47,47,47	0.98	3 (6%)
28	DMS	i	104	-	3,3,3	2.62	1 (33%)	3,3,3	0.33	0
20	CLA	b	607	-	65,73,73	1.88	14 (21%)	76,113,113	2.34	21 (27%)
20	CLA	b	617	-	65,73,73	2.23	16 (24%)	76,113,113	2.26	24 (31%)
24	LMG	b	623	-	49,49,55	0.96	2 (4%)	57,57,63	1.31	6 (10%)
35	DGD	c	516	-	58,58,67	0.86	2 (3%)	72,72,81	1.13	6 (8%)
22	BCR	T	101	-	41,41,41	0.81	0	56,56,56	1.50	11 (19%)
20	CLA	C	511	3	65,73,73	2.34	19 (29%)	76,113,113	2.40	24 (31%)
30	OEX	a	419	1,41,3	0,15,15	-	-	-		
32	HTG	B	632	-	19,19,19	1.02	1 (5%)	23,24,24	1.26	2 (8%)
20	CLA	B	611	41	65,73,73	2.26	17 (26%)	76,113,113	2.35	23 (30%)
24	LMG	C	524	-	45,45,55	1.10	3 (6%)	53,53,63	1.36	5 (9%)
28	DMS	c	527	-	3,3,3	2.31	1 (33%)	3,3,3	0.49	0
35	DGD	C	516	-	63,63,67	0.89	2 (3%)	77,77,81	1.20	7 (9%)
28	DMS	B	635	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
20	CLA	c	513	-	65,73,73	2.55	18 (27%)	76,113,113	2.22	23 (30%)
22	BCR	t	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.74	19 (33%)
28	DMS	A	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.78	0
28	DMS	B	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.73	0
28	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.49	0
28	DMS	u	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
28	DMS	B	634	-	3,3,3	1.94	1 (33%)	3,3,3	0.29	0
28	DMS	b	640	-	3,3,3	2.76	1 (33%)	3,3,3	1.38	1 (33%)
28	DMS	o	304	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
32	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	1 (4%)
24	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.17	7 (11%)
28	DMS	c	532	-	3,3,3	2.60	1 (33%)	3,3,3	0.47	0
28	DMS	o	306	-	3,3,3	2.79	1 (33%)	3,3,3	1.03	0
34	LMT	m	102	-	36,36,36	0.58	0	47,47,47	1.14	4 (8%)
28	DMS	b	637	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
28	DMS	v	208	-	3,3,3	2.63	1 (33%)	3,3,3	0.66	0
22	BCR	c	514	-	41,41,41	0.85	1 (2%)	56,56,56	1.49	7 (12%)
35	DGD	D	406	-	51,51,67	1.11	2 (3%)	59,59,81	1.21	5 (8%)
20	CLA	B	606	-	65,73,73	1.88	13 (20%)	76,113,113	2.33	26 (34%)
20	CLA	B	607	-	65,73,73	2.40	19 (29%)	76,113,113	2.31	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	PHO	A	403	-	51,69,69	1.34	6 (11%)	47,99,99	1.59	8 (17%)
28	DMS	v	202	-	3,3,3	2.50	1 (33%)	3,3,3	0.58	0
40	HEC	v	201	16	32,50,50	2.09	8 (25%)	24,82,82	2.08	6 (25%)
36	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
34	LMT	T	102	-	24,24,36	0.45	0	29,29,47	1.15	2 (6%)
28	DMS	O	304	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
23	SQD	a	401	-	53,54,54	1.12	3 (5%)	62,65,65	1.40	7 (11%)
32	HTG	B	631	-	19,19,19	0.94	2 (10%)	23,24,24	2.09	6 (26%)
28	DMS	C	525[B]	-	3,3,3	2.59	1 (33%)	3,3,3	0.79	0
32	HTG	C	534	-	19,19,19	1.08	1 (5%)	23,24,24	1.47	5 (21%)
28	DMS	U	903[B]	-	3,3,3	2.44	1 (33%)	3,3,3	0.17	0
28	DMS	B	640	-	3,3,3	2.55	1 (33%)	3,3,3	0.97	0
36	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	5 (9%)
28	DMS	b	636	-	3,3,3	2.71	1 (33%)	3,3,3	0.75	0
32	HTG	b	624	-	19,19,19	1.15	2 (10%)	23,24,24	1.60	2 (8%)
28	DMS	F	102	-	3,3,3	2.63	1 (33%)	3,3,3	0.61	0
28	DMS	V	207	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
20	CLA	C	501	-	65,73,73	1.98	16 (24%)	76,113,113	2.20	18 (23%)
22	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
20	CLA	C	504	41	65,73,73	2.24	14 (21%)	76,113,113	2.24	22 (28%)
20	CLA	D	401	-	65,73,73	1.88	15 (23%)	76,113,113	2.34	26 (34%)
28	DMS	A	415	-	3,3,3	2.75	1 (33%)	3,3,3	1.01	0
28	DMS	V	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.67	0
31	BCT	A	421	29	2,3,3	0.47	0	2,3,3	1.14	0
20	CLA	c	508	-	60,68,73	2.42	19 (31%)	70,107,113	2.24	23 (32%)
28	DMS	O	305	-	3,3,3	2.63	1 (33%)	3,3,3	0.79	0
28	DMS	b	641	-	3,3,3	2.79	1 (33%)	3,3,3	1.11	0
34	LMT	B	626	-	24,24,36	0.54	0	29,29,47	1.14	3 (10%)
22	BCR	b	621	-	41,41,41	0.80	1 (2%)	56,56,56	1.47	8 (14%)
28	DMS	b	631	-	3,3,3	2.88	1 (33%)	3,3,3	1.24	0
20	CLA	B	612	-	65,73,73	1.90	16 (24%)	76,113,113	2.26	24 (31%)
28	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.74	0
28	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
28	DMS	V	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
20	CLA	b	610	-	65,73,73	2.04	15 (23%)	76,113,113	2.19	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	O	309	-	3,3,3	2.67	1 (33%)	3,3,3	1.16	0
20	CLA	B	604	-	65,73,73	1.96	17 (26%)	76,113,113	2.43	25 (32%)
20	CLA	B	616	-	65,73,73	2.15	16 (24%)	76,113,113	2.15	22 (28%)
28	DMS	U	904	-	3,3,3	2.85	1 (33%)	3,3,3	0.70	0
36	LHG	E	103	-	46,46,48	1.03	2 (4%)	49,50,54	1.14	5 (10%)
28	DMS	d	414	-	3,3,3	2.50	1 (33%)	3,3,3	0.24	0
20	CLA	B	614	-	65,73,73	1.94	17 (26%)	76,113,113	2.19	22 (28%)
20	CLA	b	613	-	65,73,73	2.03	11 (16%)	76,113,113	2.23	26 (34%)
20	CLA	B	609	-	65,73,73	1.98	18 (27%)	76,113,113	2.39	25 (32%)
20	CLA	b	612	41	65,73,73	2.05	17 (26%)	76,113,113	2.10	22 (28%)
21	PHO	D	403	-	51,69,69	1.70	7 (13%)	47,99,99	1.60	10 (21%)
28	DMS	B	636	-	3,3,3	2.76	1 (33%)	3,3,3	0.78	0
28	DMS	o	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.81	0
22	BCR	K	102	-	41,41,41	0.92	1 (2%)	56,56,56	1.48	6 (10%)
28	DMS	u	203	-	3,3,3	2.57	1 (33%)	3,3,3	0.78	0
20	CLA	c	506	-	65,73,73	2.27	18 (27%)	76,113,113	2.22	24 (31%)
20	CLA	b	616	-	65,73,73	2.06	15 (23%)	76,113,113	2.47	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
34	LMT	c	523	-	-	8/21/61/61	0/2/2/2
20	CLA	b	614	-	1/1/15/20	4/37/115/115	-
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
34	LMT	b	628	-	-	9/17/37/61	0/1/1/2
20	CLA	B	602	41	1/1/15/20	21/37/115/115	-
20	CLA	d	402	-	1/1/15/20	3/37/115/115	-
20	CLA	A	404	-	-	10/37/115/115	-
20	CLA	c	505	-	1/1/15/20	1/37/115/115	-
22	BCR	b	619	-	-	2/29/63/63	0/2/2/2
22	BCR	k	102	-	-	1/29/63/63	0/2/2/2
24	LMG	A	407	-	-	28/46/66/70	0/1/1/1
20	CLA	D	404	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	d	401	-	-	9/10/30/30	0/1/1/1
20	CLA	a	407	-	-	0/16/94/115	-
34	LMT	I	101	-	-	8/21/61/61	0/2/2/2
20	CLA	B	613	-	1/1/15/20	0/37/115/115	-
36	LHG	D	407	-	-	9/53/53/53	-
20	CLA	B	608	41	1/1/15/20	1/37/115/115	-
20	CLA	d	403	41	-	5/37/115/115	-
23	SQD	b	622	-	-	23/49/69/69	0/1/1/1
32	HTG	b	625	-	-	4/10/30/30	0/1/1/1
34	LMT	b	627	-	-	10/18/58/61	0/2/2/2
20	CLA	B	601	-	1/1/15/20	18/37/115/115	-
23	SQD	A	406	-	-	21/49/69/69	0/1/1/1
20	CLA	b	604	-	1/1/15/20	7/37/115/115	-
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
37	HEM	E	104	6,5	-	5/12/54/54	-
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
22	BCR	K	101	-	-	4/29/63/63	0/2/2/2
34	LMT	J	103	-	-	7/15/35/61	0/1/1/2
36	LHG	D	408	-	-	10/53/53/53	-
20	CLA	B	605	-	1/1/15/20	8/37/115/115	-
20	CLA	C	513	-	-	10/37/115/115	-
20	CLA	c	504	41	1/1/15/20	5/37/115/115	-
32	HTG	v	210	-	-	3/5/25/30	0/1/1/1
21	PHO	a	406	-	-	2/37/103/103	0/5/6/6
24	LMG	c	518	-	-	8/46/66/70	0/1/1/1
20	CLA	C	510	-	1/1/15/20	2/37/115/115	-
20	CLA	c	502	-	-	6/37/115/115	-
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
20	CLA	b	615	-	1/1/15/20	6/37/115/115	-
24	LMG	C	519	-	-	19/46/66/70	0/1/1/1
20	CLA	b	605	-	1/1/15/20	1/37/115/115	-
24	LMG	j	101	39	-	15/40/60/70	0/1/1/1
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
32	HTG	c	521	-	-	5/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	V	202	-	-	1/4/24/30	0/1/1/1
20	CLA	c	507	41	1/1/15/20	6/37/115/115	-
22	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
32	HTG	C	521	-	-	6/10/30/30	0/1/1/1
22	BCR	d	405	-	-	4/29/63/63	0/2/2/2
32	HTG	c	520	-	-	5/10/30/30	0/1/1/1
23	SQD	f	101	-	-	16/34/54/69	0/1/1/1
36	LHG	l	102	-	-	19/53/53/53	-
27	PL9	d	412	-	-	3/53/73/73	0/1/1/1
20	CLA	C	507	41	1/1/15/20	11/37/115/115	-
23	SQD	a	409	-	-	20/49/69/69	0/1/1/1
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
20	CLA	a	403	-	1/1/15/20	4/37/115/115	-
22	BCR	B	617	-	-	2/29/63/63	0/2/2/2
20	CLA	b	618	-	1/1/15/20	17/37/115/115	-
34	LMT	a	418	-	-	11/21/61/61	0/2/2/2
35	DGD	C	517	-	-	14/44/84/95	0/2/2/2
20	CLA	C	506	-	1/1/15/20	12/37/115/115	-
20	CLA	c	503	-	-	3/37/115/115	-
21	PHO	a	405	-	-	4/37/103/103	0/5/6/6
20	CLA	B	615	-	1/1/15/20	10/37/115/115	-
23	SQD	A	412	-	-	24/49/69/69	0/1/1/1
35	DGD	h	101	-	-	15/51/91/95	0/2/2/2
32	HTG	b	601	-	-	2/10/30/30	0/1/1/1
20	CLA	C	503	-	-	4/37/115/115	-
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	SQD	l	101	-	-	28/49/69/69	0/1/1/1
20	CLA	C	505	-	1/1/15/20	1/37/115/115	-
20	CLA	b	606	-	1/1/15/20	3/37/115/115	-
20	CLA	C	509	-	1/1/15/20	8/37/115/115	-
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
22	BCR	k	101	-	-	4/29/63/63	0/2/2/2
24	LMG	B	620	-	-	19/46/66/70	0/1/1/1
34	LMT	M	101	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	D	417	-	-	5/10/30/30	0/1/1/1
20	CLA	c	509	-	1/1/15/20	10/37/115/115	-
20	CLA	A	402	41	-	3/30/108/115	-
20	CLA	c	510	-	1/1/15/20	3/37/115/115	-
35	DGD	c	517	-	-	14/51/91/95	0/2/2/2
20	CLA	B	603	-	1/1/15/20	3/37/115/115	-
20	CLA	A	401	-	1/1/15/20	4/37/115/115	-
20	CLA	b	608	-	1/1/15/20	9/37/115/115	-
27	PL9	A	411	-	-	10/53/73/73	0/1/1/1
20	CLA	b	603	41	1/1/15/20	18/37/115/115	-
20	CLA	D	402	41	-	5/37/115/115	-
35	DGD	d	416	-	-	30/46/66/95	0/1/1/2
20	CLA	a	404	41	-	6/31/109/115	-
34	LMT	B	627	-	-	7/13/13/61	-
20	CLA	c	511	3	1/1/15/20	0/37/115/115	-
34	LMT	m	101	-	-	15/21/61/61	0/2/2/2
36	LHG	d	406	-	-	11/53/53/53	-
24	LMG	a	410	-	-	18/46/66/70	0/1/1/1
27	PL9	a	415	-	-	11/53/73/73	0/1/1/1
20	CLA	c	501	-	1/1/15/20	3/37/115/115	-
32	HTG	B	623	-	-	6/10/30/30	0/1/1/1
32	HTG	u	201	-	-	1/5/5/30	-
36	LHG	L	101	-	-	17/53/53/53	-
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
32	HTG	O	302	-	-	5/10/30/30	0/1/1/1
20	CLA	c	512	-	1/1/15/20	7/37/115/115	-
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
23	SQD	F	101	-	-	17/28/48/69	0/1/1/1
20	CLA	b	609	41	1/1/15/20	2/37/115/115	-
20	CLA	C	512	-	1/1/13/20	6/25/103/115	-
20	CLA	C	502	-	-	5/37/115/115	-
37	HEM	e	102	6,5	-	4/12/54/54	-
36	LHG	d	407	-	-	11/53/53/53	-
24	LMG	J	101	39	-	9/40/60/70	0/1/1/1
34	LMT	E	101	-	-	8/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	201	16	-	2/10/54/54	-
22	BCR	D	405	-	-	4/29/63/63	0/2/2/2
22	BCR	j	102	-	-	2/29/63/63	0/2/2/2
27	PL9	D	412	-	-	3/53/73/73	0/1/1/1
34	LMT	z	102	-	-	13/21/61/61	0/2/2/2
20	CLA	b	611	-	-	0/37/115/115	-
34	LMT	f	102	-	-	8/15/35/61	0/1/1/2
20	CLA	C	508	-	1/1/14/20	6/31/109/115	-
20	CLA	d	404	-	-	8/37/115/115	-
20	CLA	B	610	-	1/1/15/20	1/37/115/115	-
34	LMT	B	625	-	-	4/15/35/61	0/1/1/2
35	DGD	c	515	-	-	18/51/91/95	0/2/2/2
34	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
20	CLA	b	607	-	1/1/15/20	4/37/115/115	-
20	CLA	b	617	-	1/1/15/20	8/37/115/115	-
24	LMG	b	623	-	-	14/44/64/70	0/1/1/1
35	DGD	c	516	-	-	13/46/86/95	0/2/2/2
22	BCR	T	101	-	-	1/29/63/63	0/2/2/2
20	CLA	C	511	3	-	0/37/115/115	-
32	HTG	B	632	-	-	2/10/30/30	0/1/1/1
20	CLA	B	611	41	1/1/15/20	4/37/115/115	-
24	LMG	C	524	-	-	22/40/60/70	0/1/1/1
35	DGD	C	516	-	-	18/51/91/95	0/2/2/2
20	CLA	c	513	-	-	14/37/115/115	-
22	BCR	t	101	-	-	3/29/63/63	0/2/2/2
32	HTG	C	520	-	-	4/10/30/30	0/1/1/1
24	LMG	c	519	-	-	26/46/66/70	0/1/1/1
34	LMT	m	102	-	-	3/21/61/61	0/2/2/2
35	DGD	D	406	-	-	26/46/66/95	0/1/1/2
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
40	HEC	v	201	16	-	2/10/54/54	-
20	CLA	B	606	-	1/1/15/20	4/37/115/115	-
20	CLA	B	607	-	1/1/15/20	11/37/115/115	-
21	PHO	A	403	-	-	2/37/103/103	0/5/6/6
36	LHG	D	409	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	T	102	-	-	11/15/35/61	0/1/1/2
23	SQD	a	401	-	-	20/49/69/69	0/1/1/1
32	HTG	B	631	-	-	5/10/30/30	0/1/1/1
32	HTG	C	534	-	-	6/10/30/30	0/1/1/1
36	LHG	d	408	-	-	14/53/53/53	-
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
20	CLA	C	501	-	1/1/15/20	3/37/115/115	-
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2
20	CLA	D	401	-	1/1/15/20	7/37/115/115	-
20	CLA	C	504	41	-	11/37/115/115	-
20	CLA	c	508	-	-	2/31/109/115	-
34	LMT	B	626	-	-	7/15/35/61	0/1/1/2
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
20	CLA	B	612	-	1/1/15/20	3/37/115/115	-
20	CLA	b	610	-	-	1/37/115/115	-
20	CLA	B	604	-	1/1/15/20	3/37/115/115	-
20	CLA	B	616	-	1/1/15/20	5/37/115/115	-
36	LHG	E	103	-	-	27/45/45/53	-
20	CLA	B	614	-	1/1/15/20	6/37/115/115	-
20	CLA	b	613	-	-	7/37/115/115	-
20	CLA	b	612	41	1/1/15/20	5/37/115/115	-
20	CLA	B	609	-	-	1/37/115/115	-
21	PHO	D	403	-	-	4/37/103/103	0/5/6/6
32	HTG	b	602	-	-	3/10/30/30	0/1/1/1
22	BCR	K	102	-	-	1/29/63/63	0/2/2/2
20	CLA	c	506	-	1/1/15/20	10/37/115/115	-
20	CLA	b	616	-	1/1/15/20	18/37/115/115	-

The worst 5 of 1490 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	MG-NA	12.91	2.36	2.06
20	c	513	CLA	MG-NA	12.66	2.36	2.06
20	B	602	CLA	MG-NA	11.66	2.34	2.06
20	c	507	CLA	MG-NA	10.98	2.32	2.06
20	c	511	CLA	MG-NC	10.70	2.31	2.06

The worst 5 of 2315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	f	101	SQD	O9-S-C6	-14.05	90.24	106.94
20	c	504	CLA	C4A-NA-C1A	12.19	112.19	106.71
20	C	511	CLA	C4A-NA-C1A	11.76	111.99	106.71
20	c	501	CLA	C4A-NA-C1A	11.42	111.84	106.71
20	c	509	CLA	C4A-NA-C1A	10.78	111.55	106.71

5 of 50 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	401	CLA	ND
20	B	601	CLA	ND
20	B	602	CLA	ND
20	B	603	CLA	ND
20	B	604	CLA	ND

5 of 1393 torsion outliers are listed below:

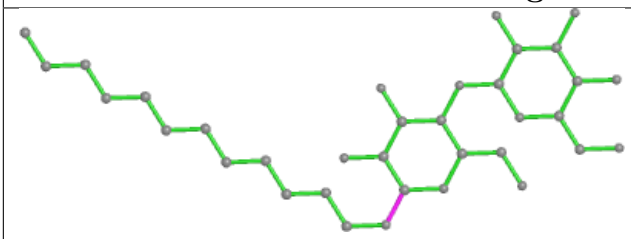
Mol	Chain	Res	Type	Atoms
20	B	601	CLA	C11-C10-C8-C9
20	B	602	CLA	CBA-CGA-O2A-C1
20	B	602	CLA	O1A-CGA-O2A-C1
20	B	602	CLA	CHA-CBD-CGD-O1D
20	B	602	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

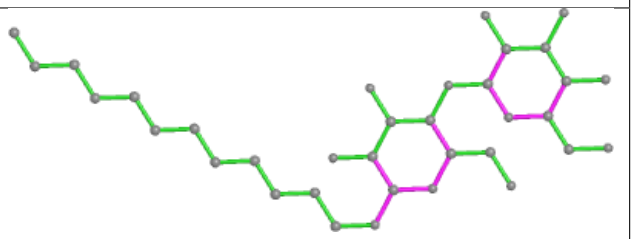
No monomer is involved in short contacts.

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

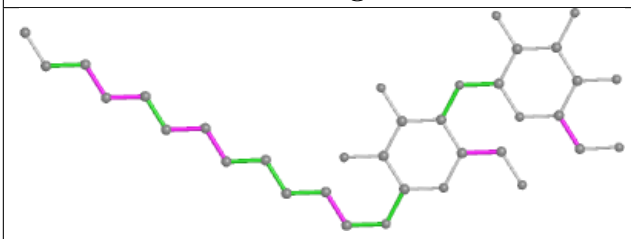
Ligand LMT c 523



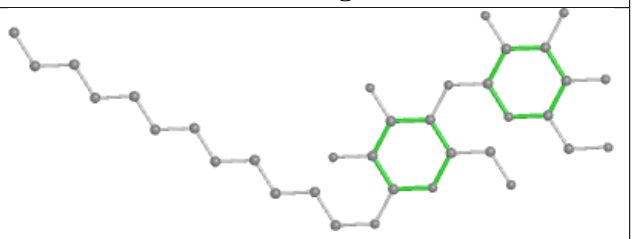
Bond lengths



Bond angles

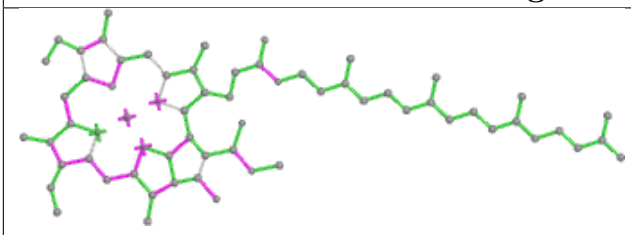


Torsions

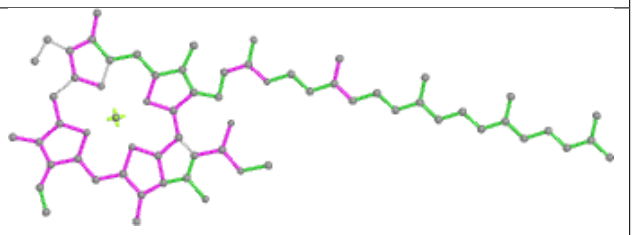


Rings

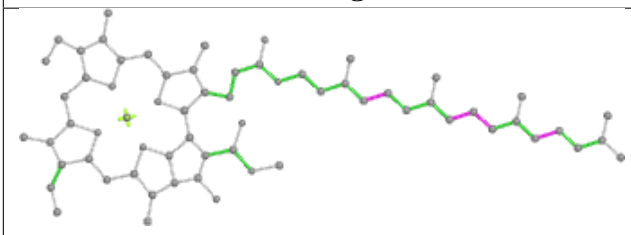
Ligand CLA b 614



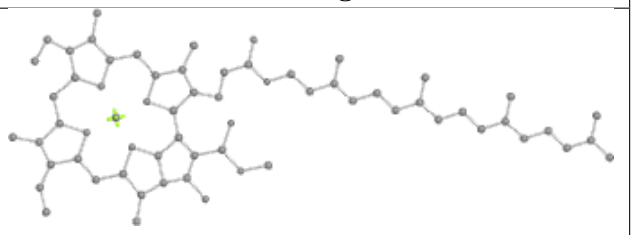
Bond lengths



Bond angles

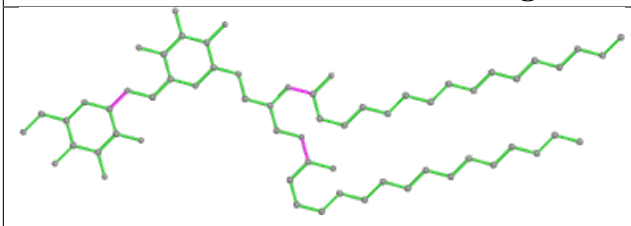


Torsions

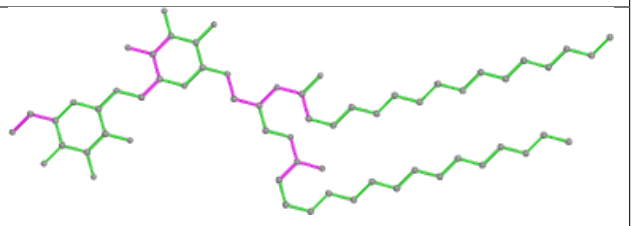


Rings

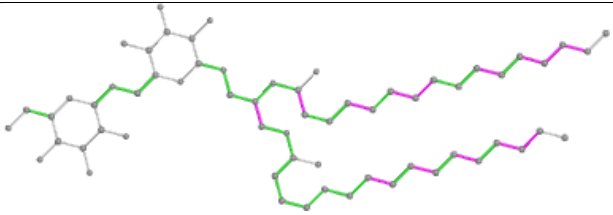
Ligand DGD H 102



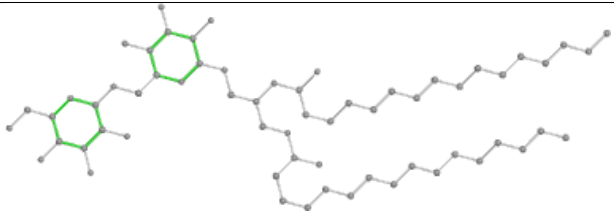
Bond lengths



Bond angles

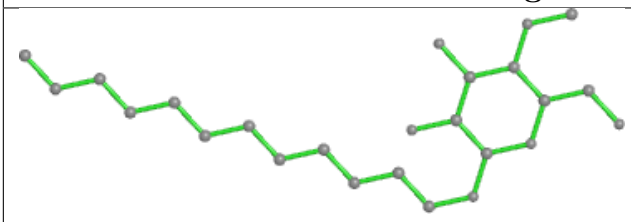


Torsions

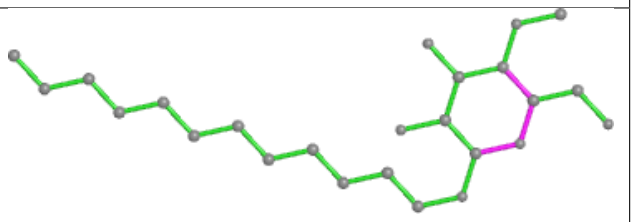


Rings

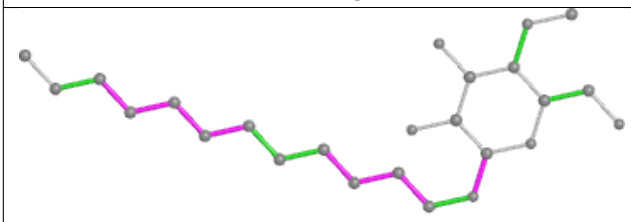
Ligand LMT b 628



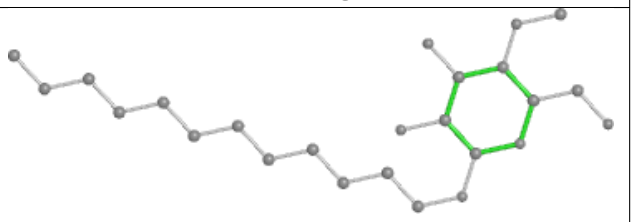
Bond lengths



Bond angles

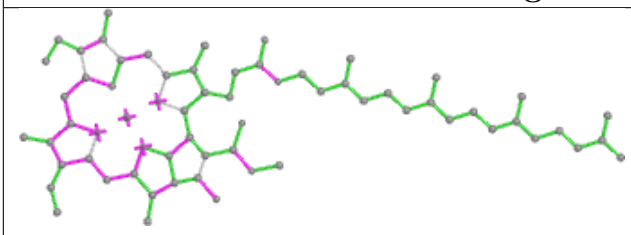


Torsions

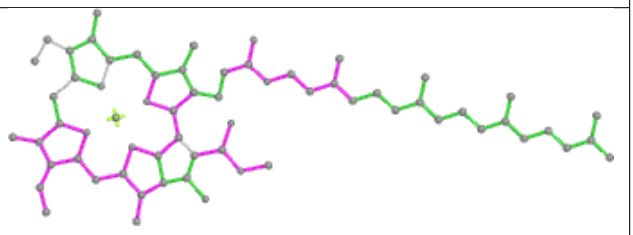


Rings

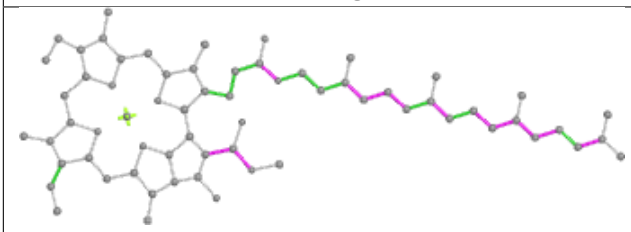
Ligand CLA B 602



Bond lengths



Bond angles



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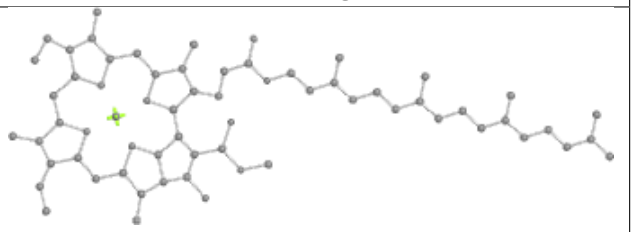
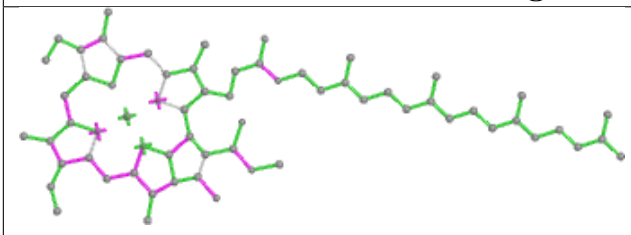
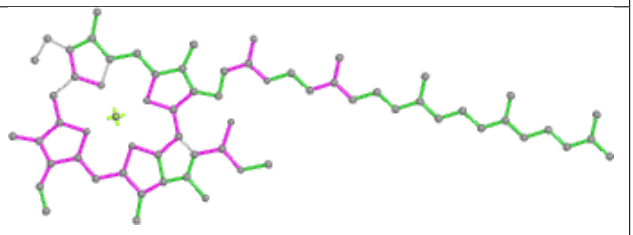


Rings

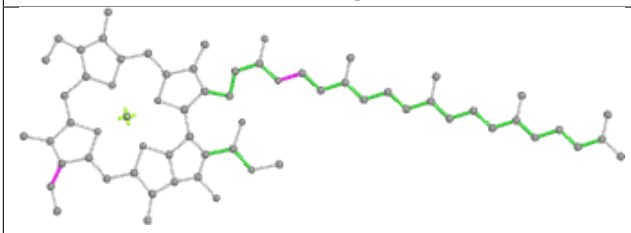
Ligand CLA d 402



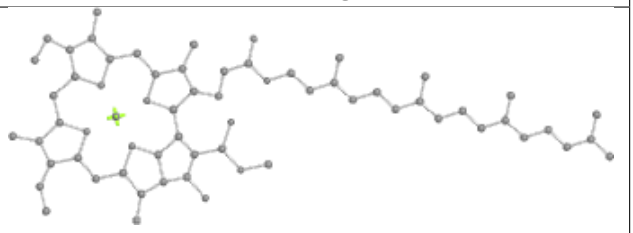
Bond lengths



Bond angles

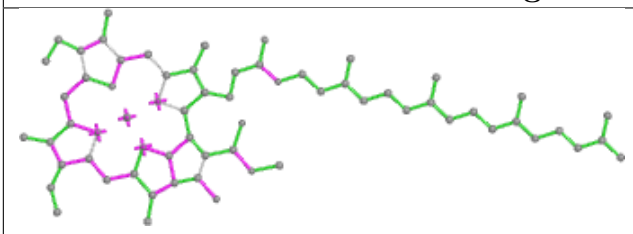


Torsions

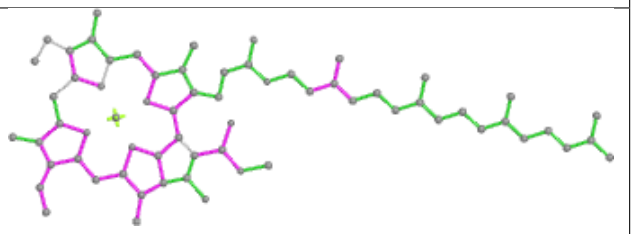


Rings

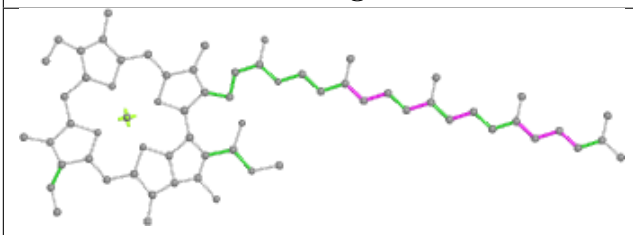
Ligand CLA A 404



Bond lengths



Bond angles



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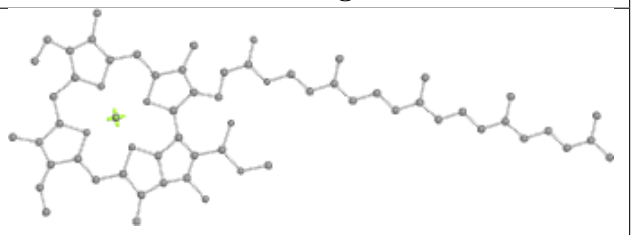
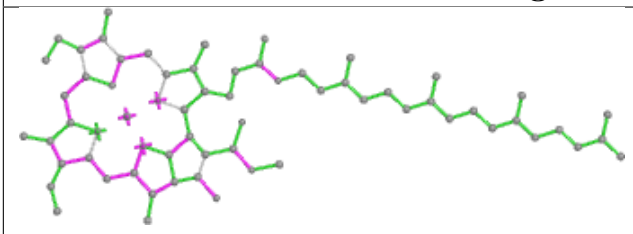
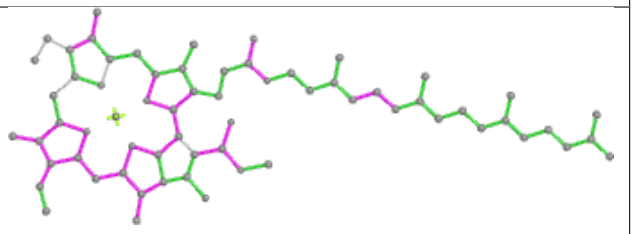


Rings

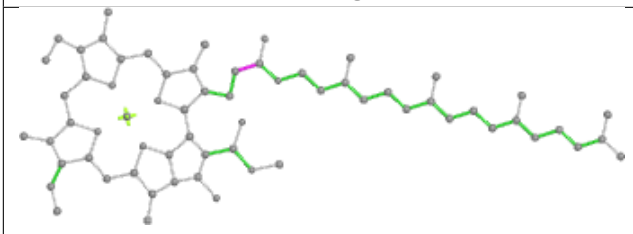
Ligand CLA c 505



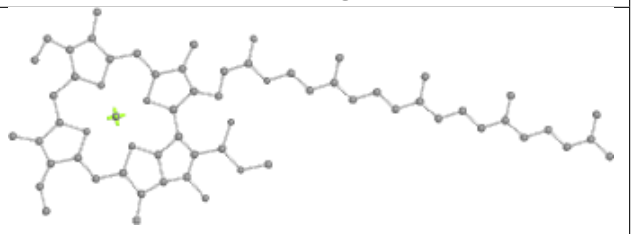
Bond lengths



Bond angles

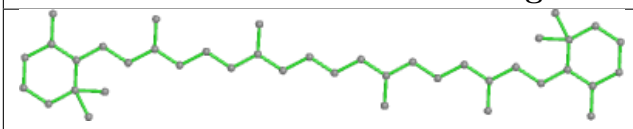


Torsions

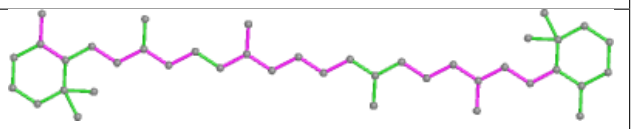


Rings

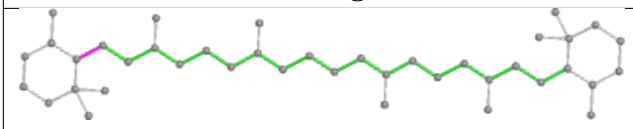
Ligand BCR b 619



Bond lengths



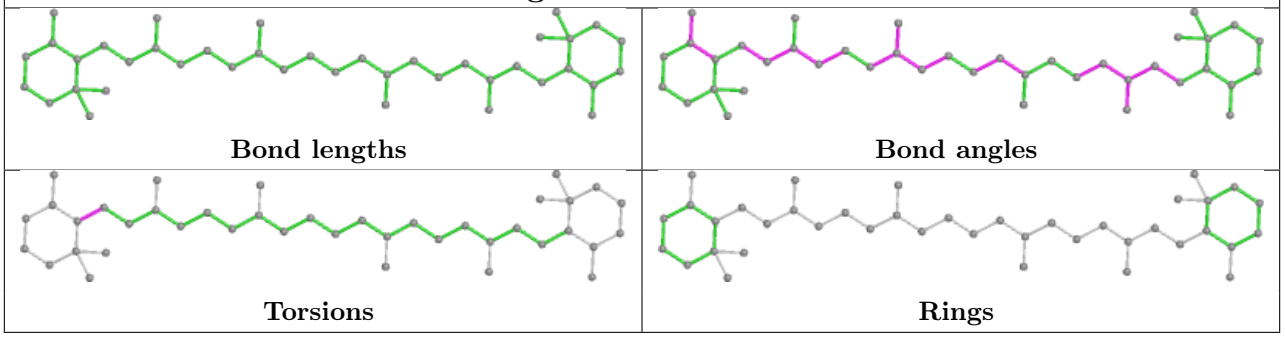
Bond angles



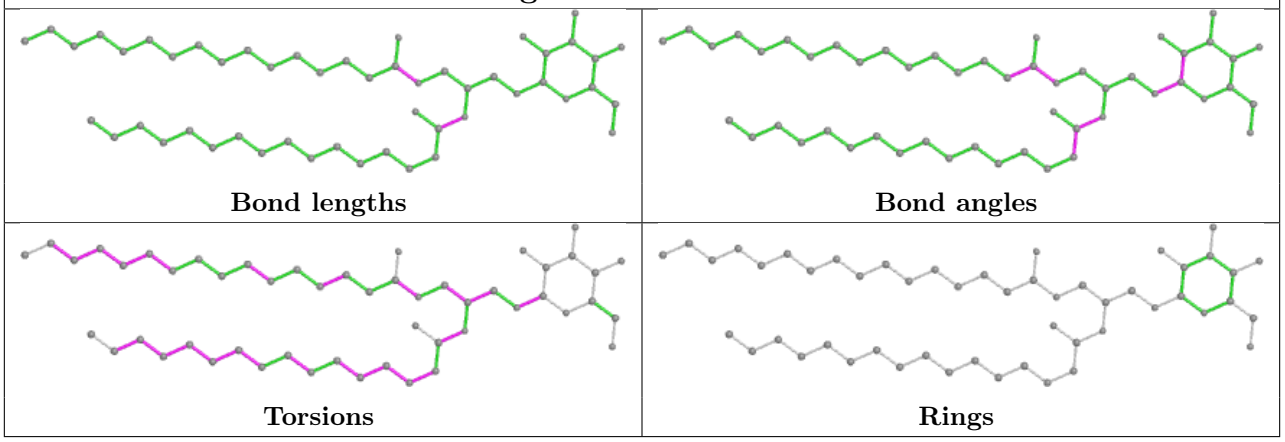
Torsions

Rings

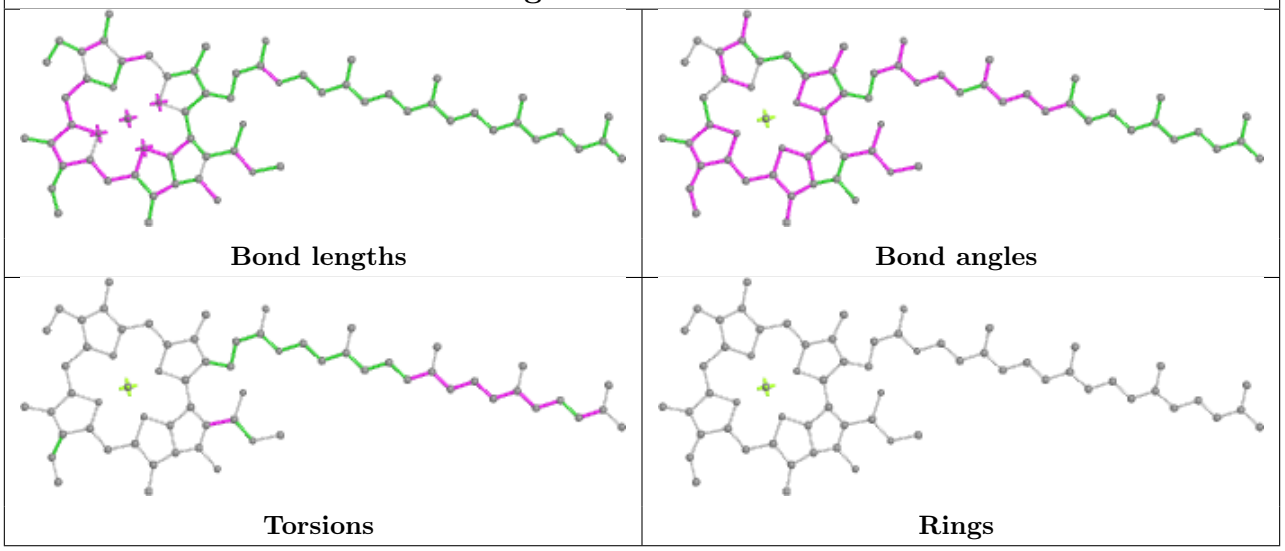
Ligand BCR k 102



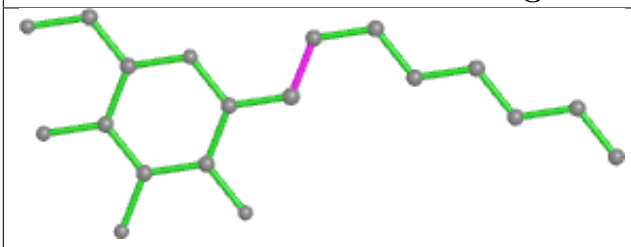
Ligand LMG A 407



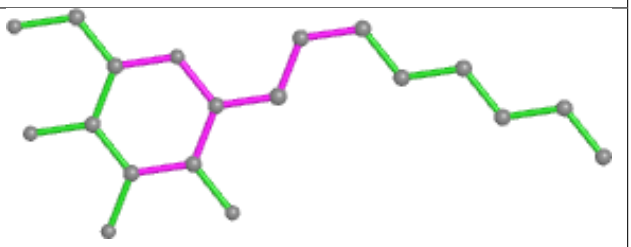
Ligand CLA D 404



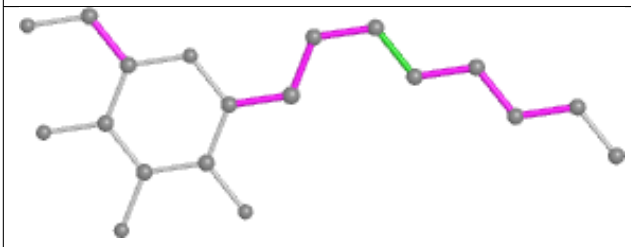
Ligand HTG d 401



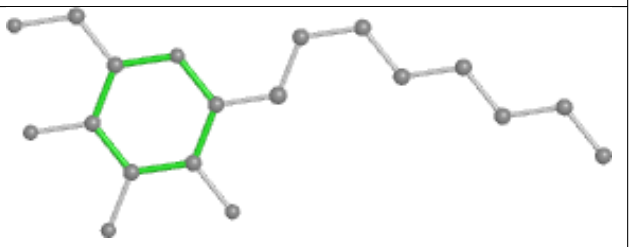
Bond lengths



Bond angles

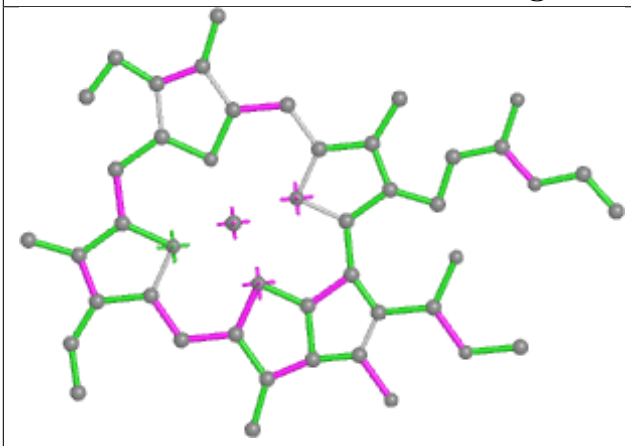


Torsions



Rings

Ligand CLA a 407



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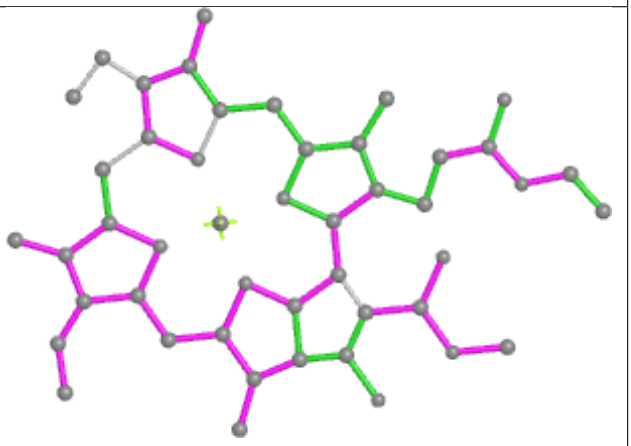
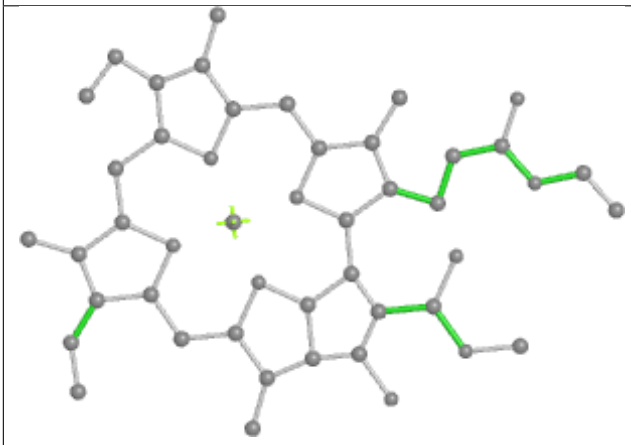


Bond angles



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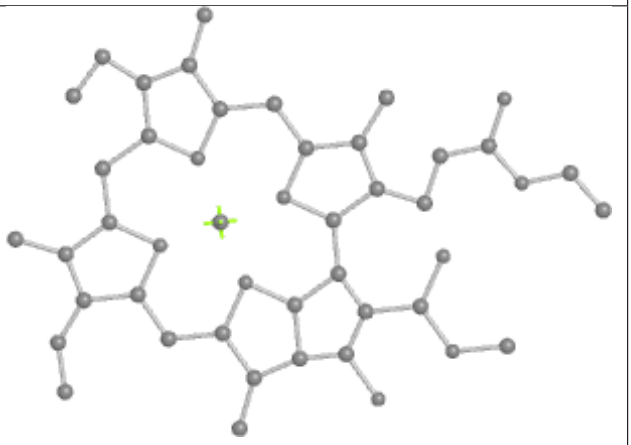
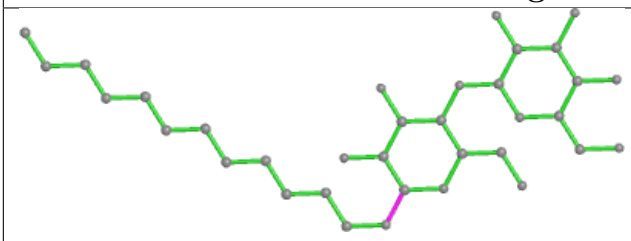


Rings

Ligand LMT I 101



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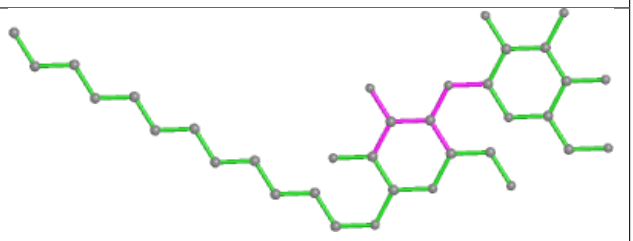
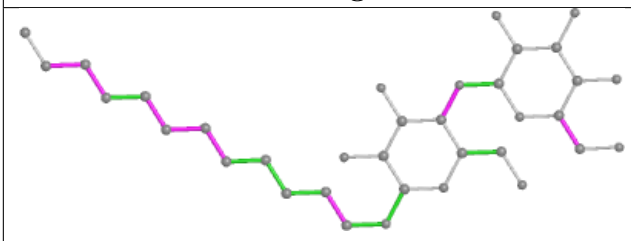


Bond angles



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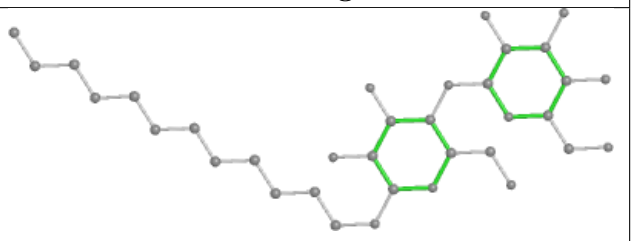
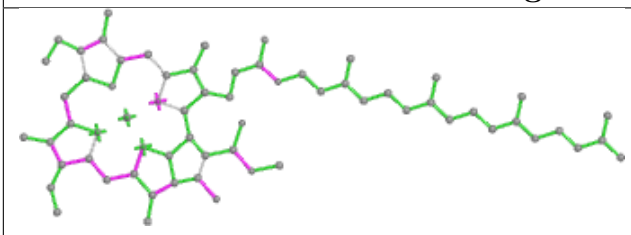


Rings

Ligand CLA B 613



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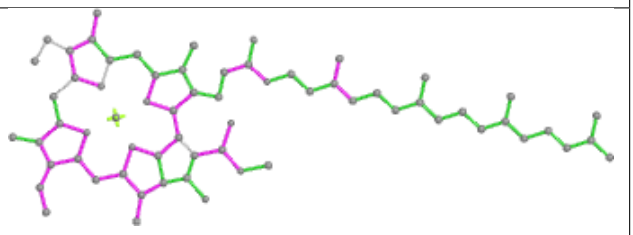
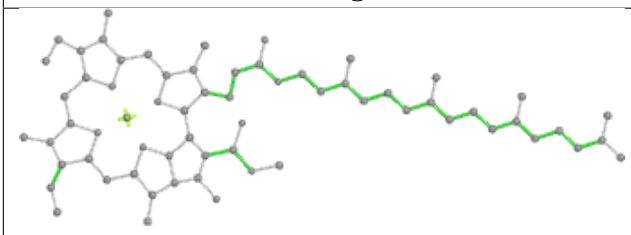


Bond angles



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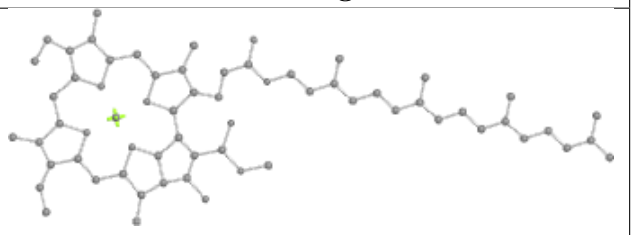
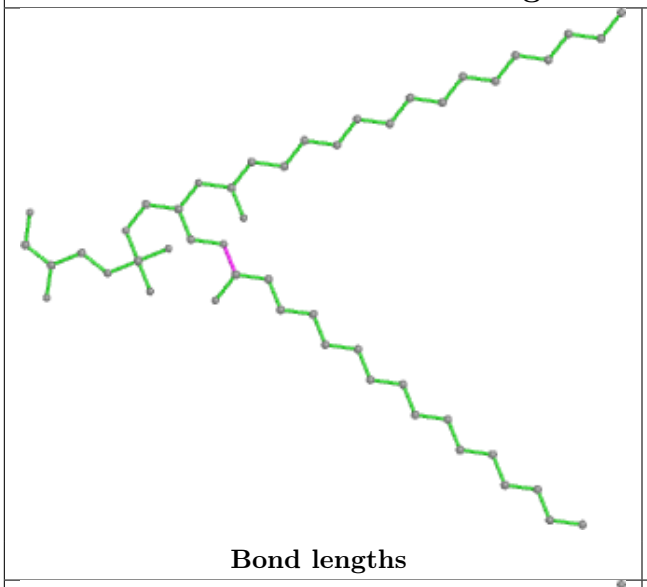


Rings

Ligand LHG D 407



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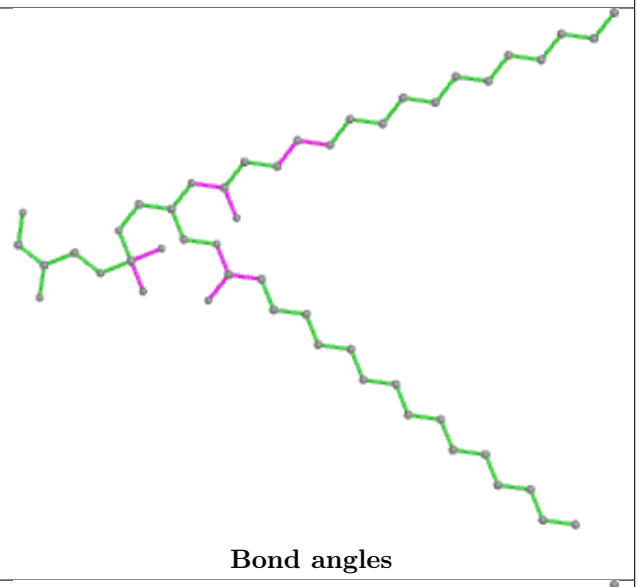
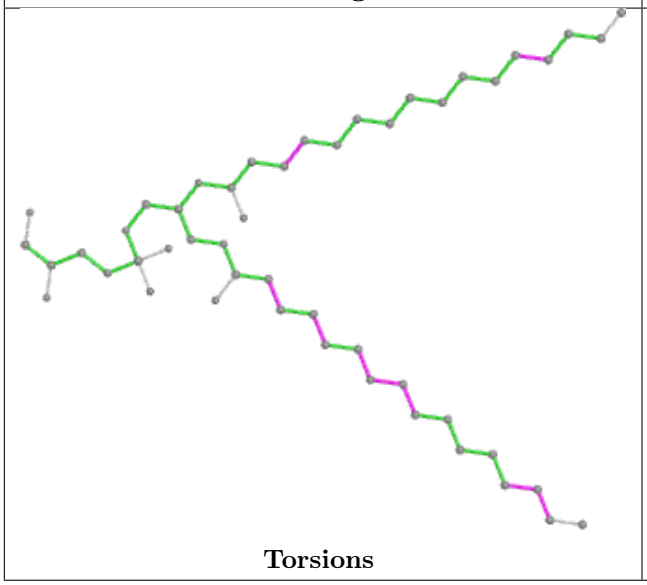


Bond angles



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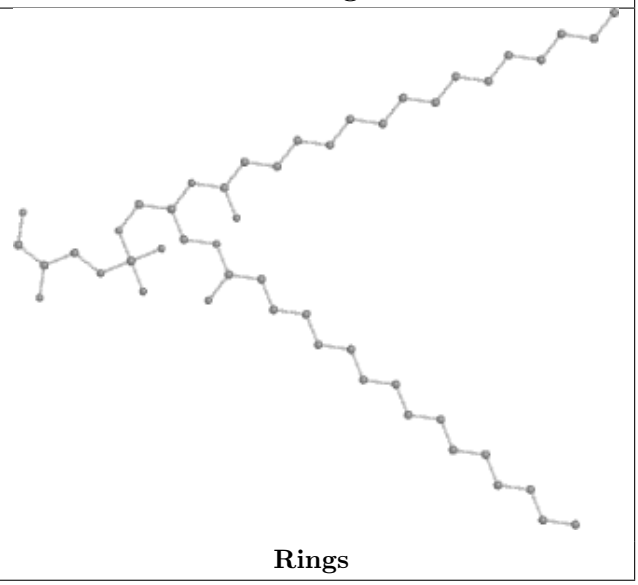
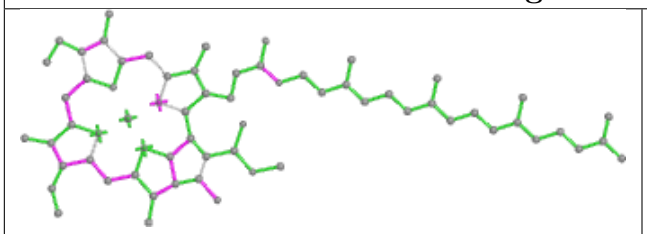
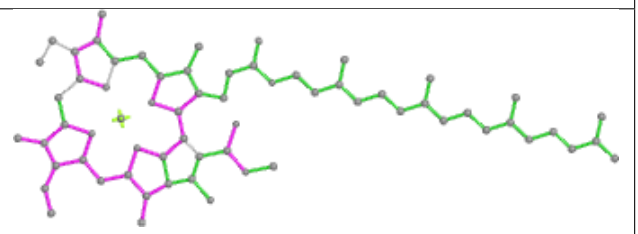


Rings

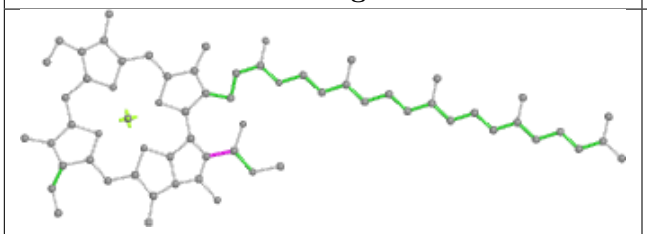
Ligand CLA B 608



Bond lengths



Bond angles



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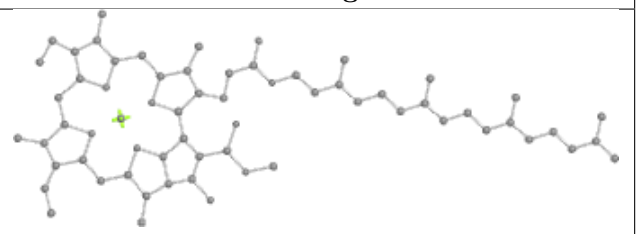
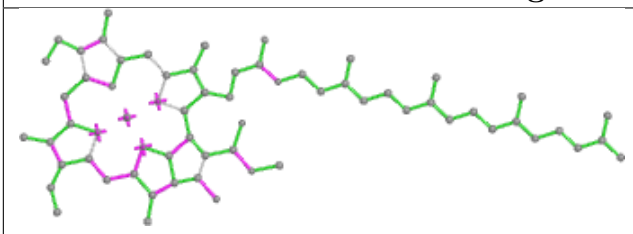
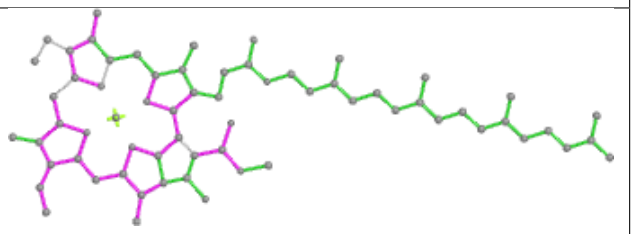


Rings

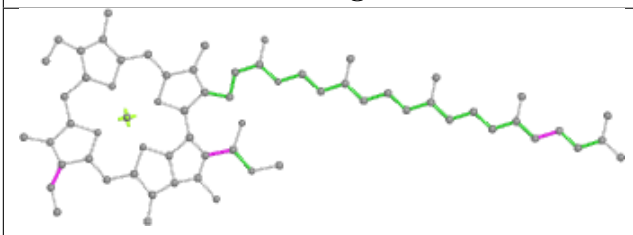
Ligand CLA d 403



Bond lengths



Bond angles



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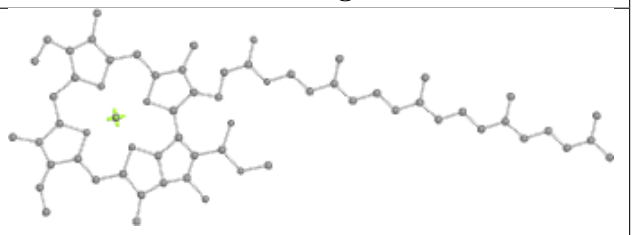
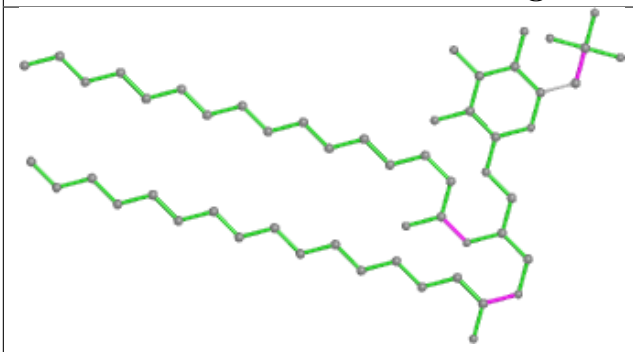


Rings

Ligand SQD b 622



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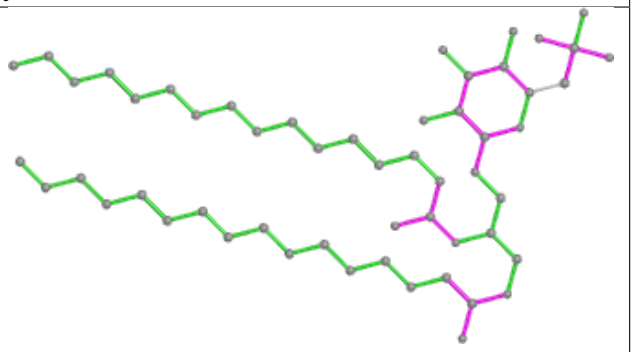
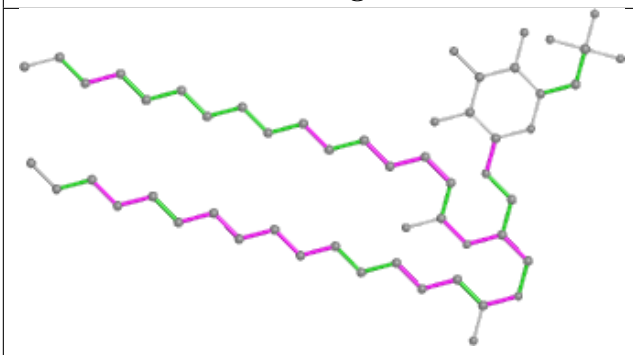


Bond angles



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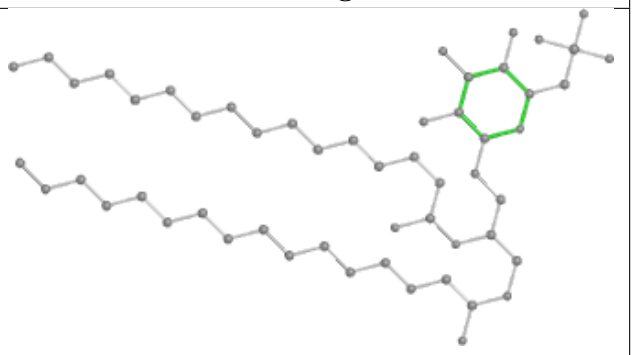
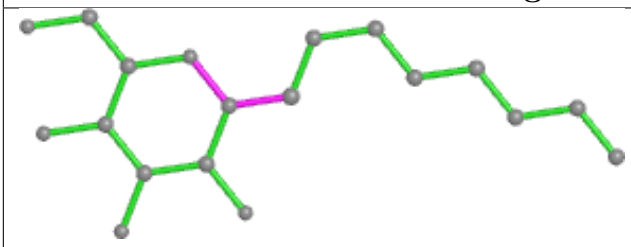


Rings

Ligand HTG b 625



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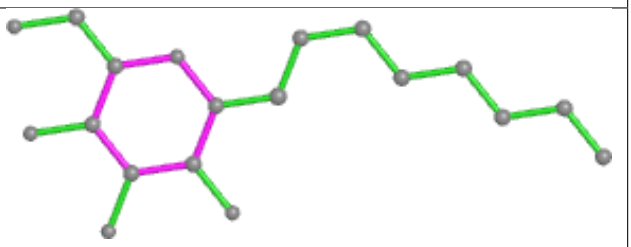
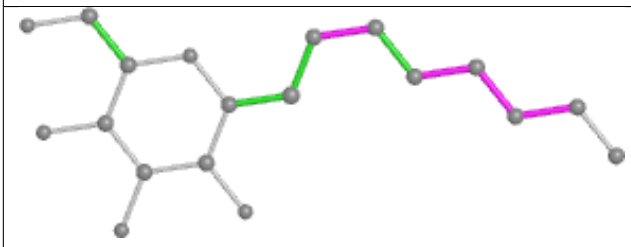


Bond angles



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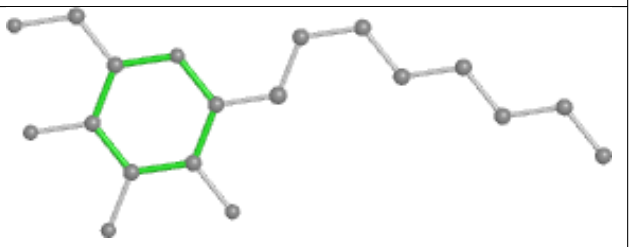
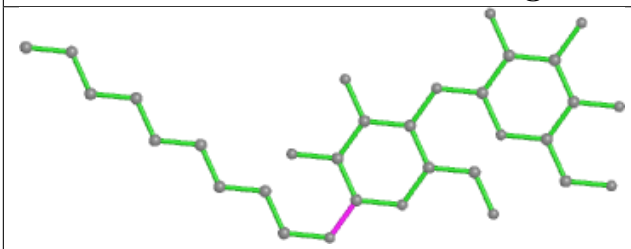
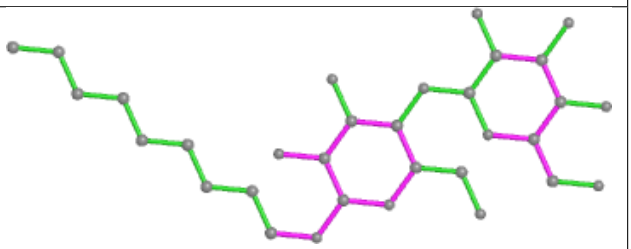


Rings

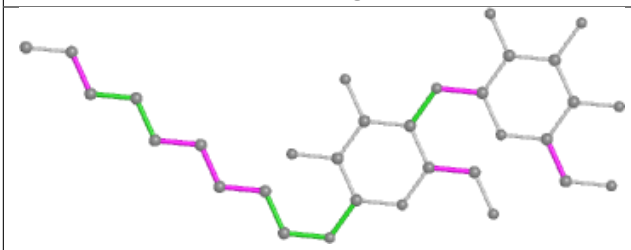
Ligand LMT b 627



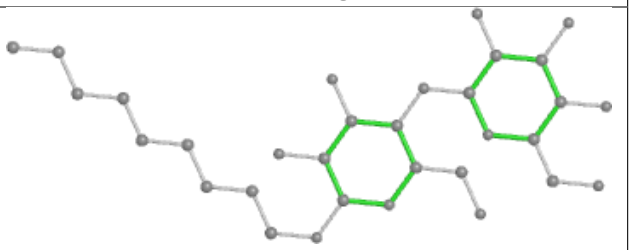
Bond lengths



Bond angles

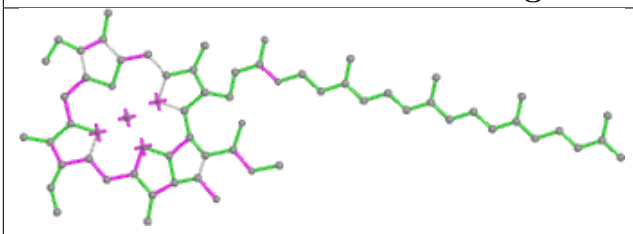


Torsions



Rings

Ligand CLA B 601



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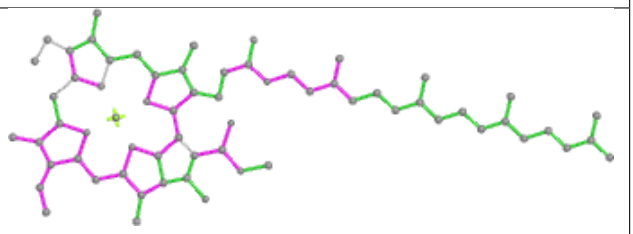
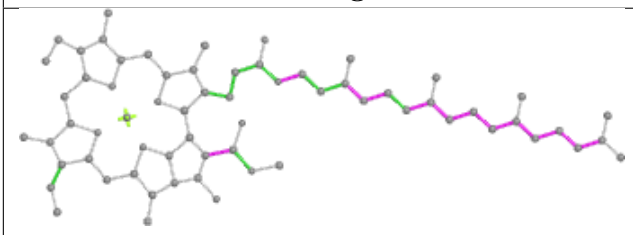


Bond angles



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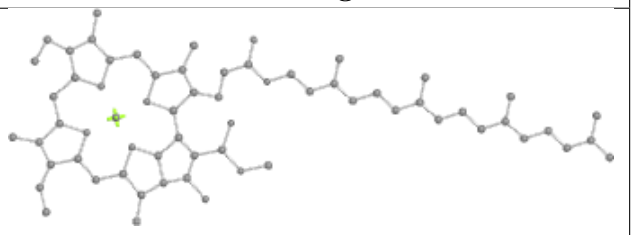
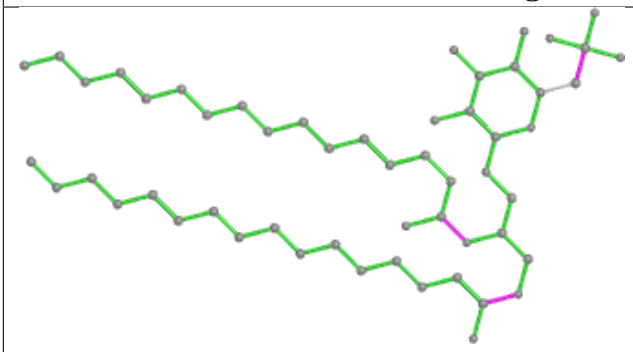
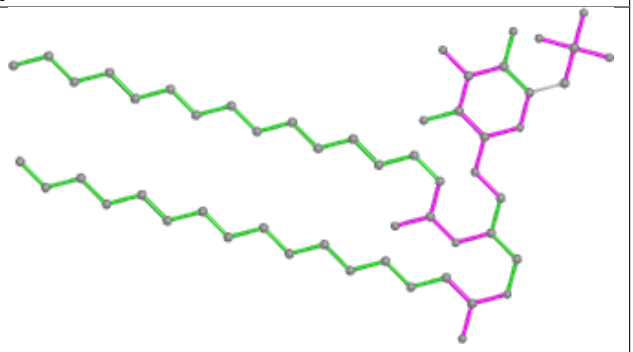


Rings

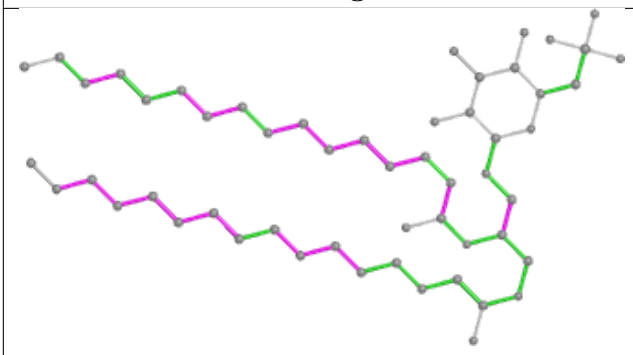
Ligand SQD A 406



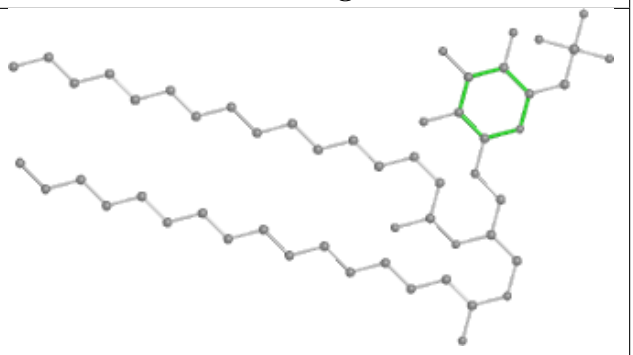
Bond lengths



Bond angles

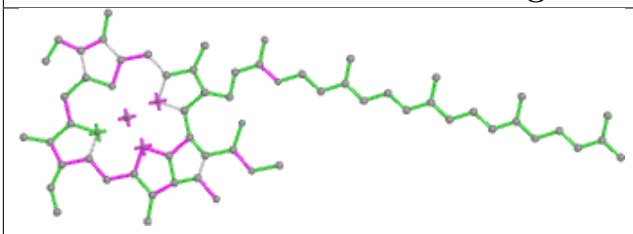


Torsions

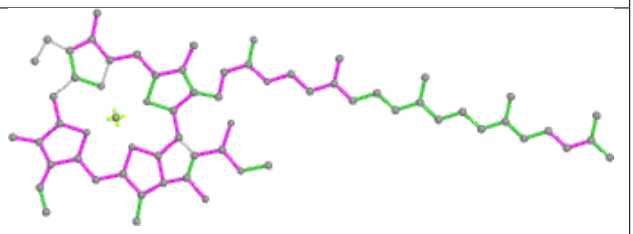


Rings

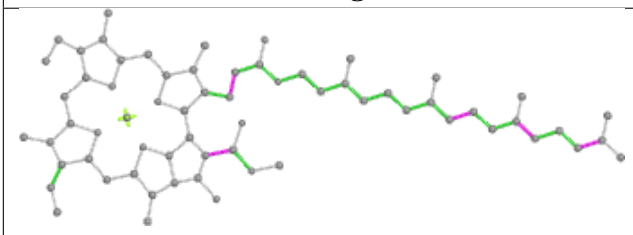
Ligand CLA b 604



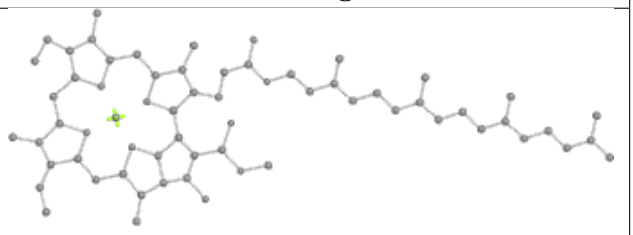
Bond lengths



Bond angles

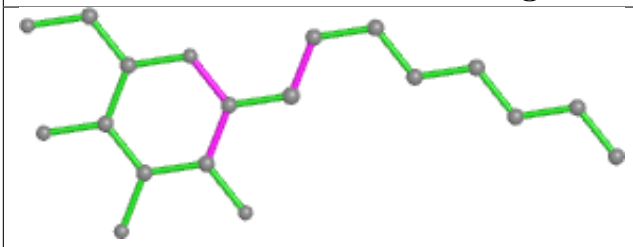


Torsions

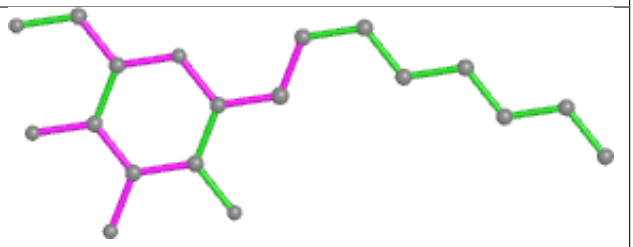


Rings

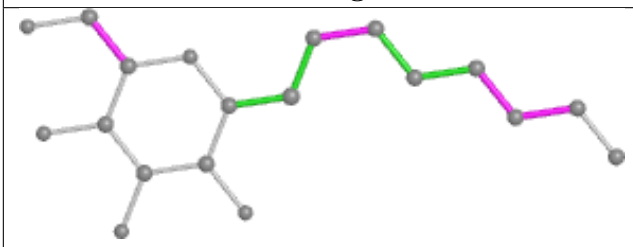
Ligand HTG B 621



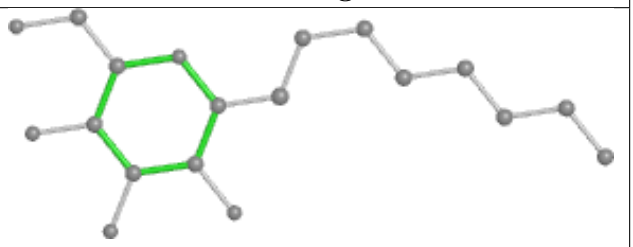
Bond lengths



Bond angles

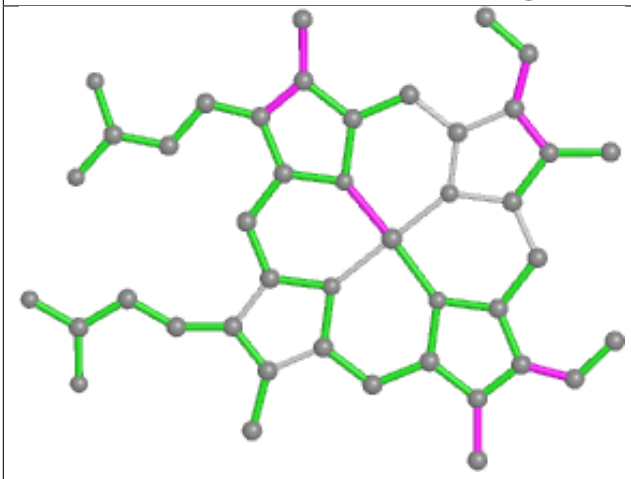


Torsions

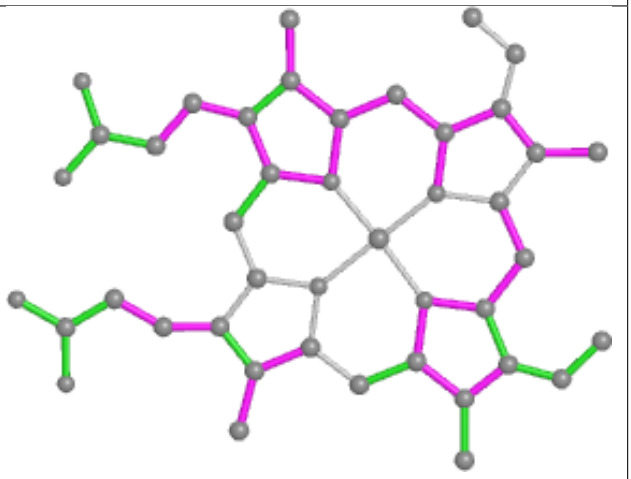


Rings

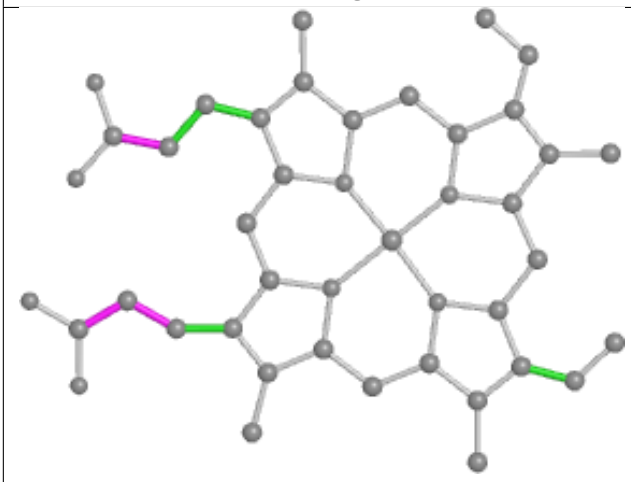
Ligand HEM E 104



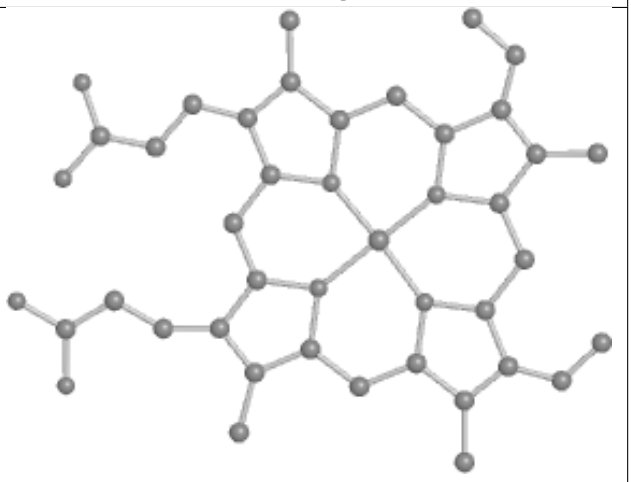
Bond lengths



Bond angles

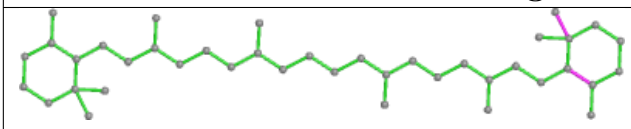


Torsions



Rings

Ligand BCR a 408



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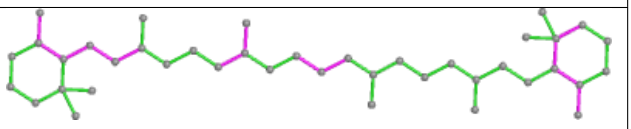
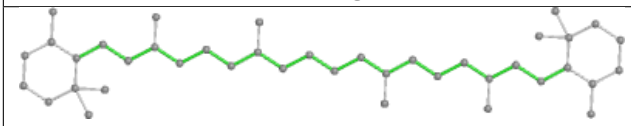


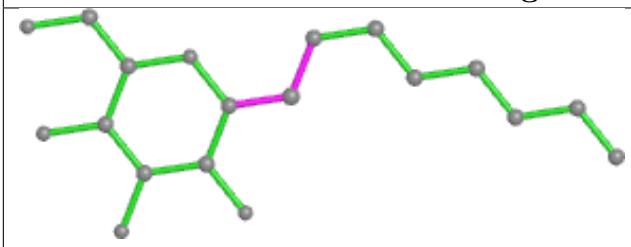
Bond angles



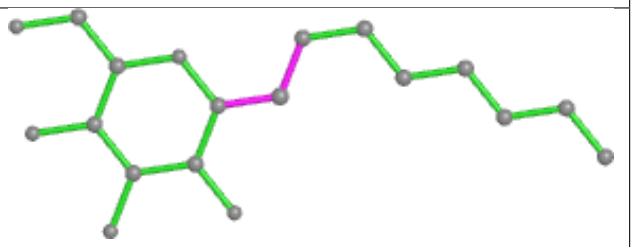
Torsions

Rings

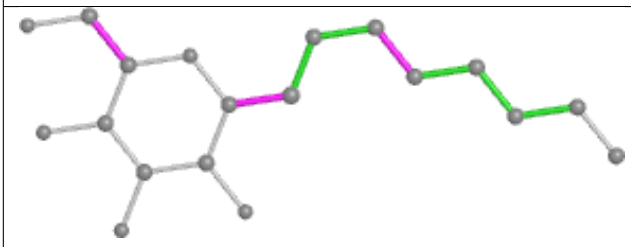
Ligand HTG C 522



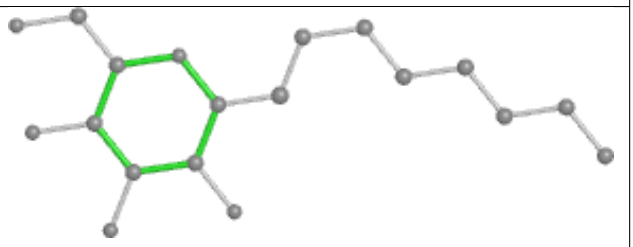
Bond lengths



Bond angles

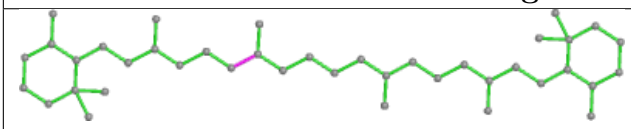


Torsions

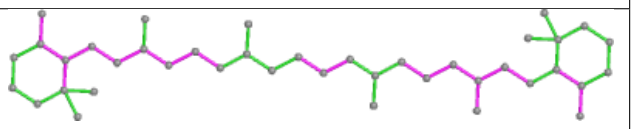


Rings

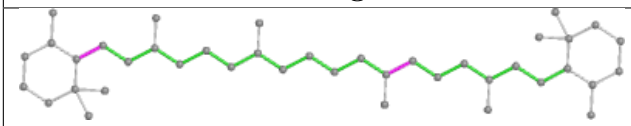
Ligand BCR K 101



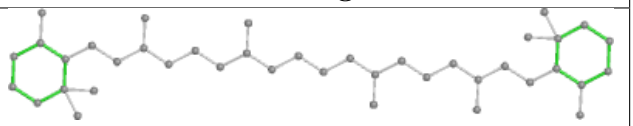
Bond lengths



Bond angles

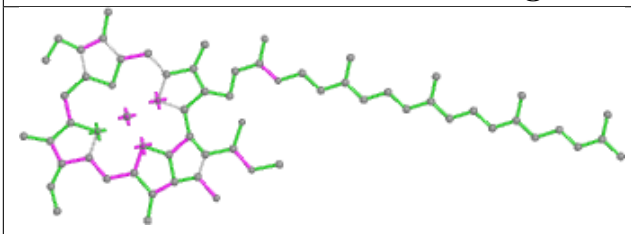


Torsions

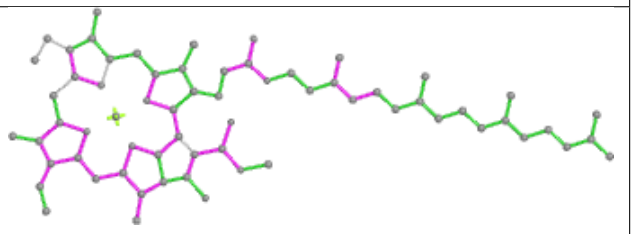


Rings

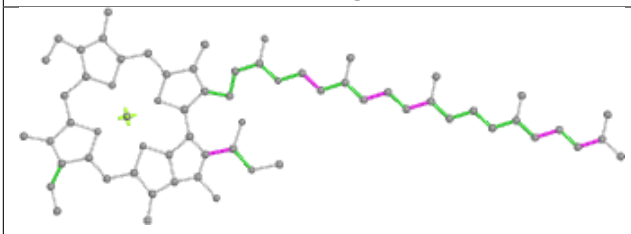
Ligand CLA B 605



Bond lengths



Bond angles



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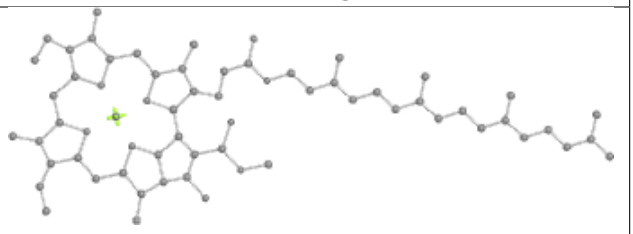
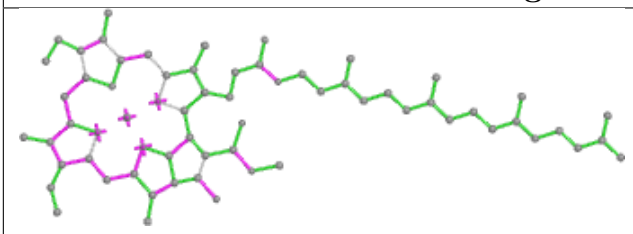


Rings

Ligand CLA C 513



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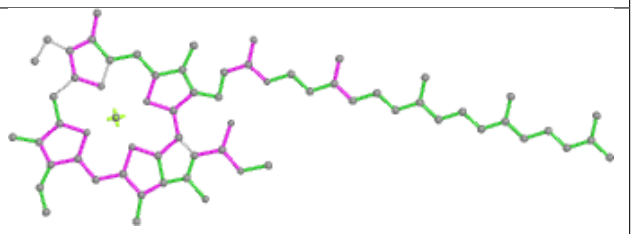
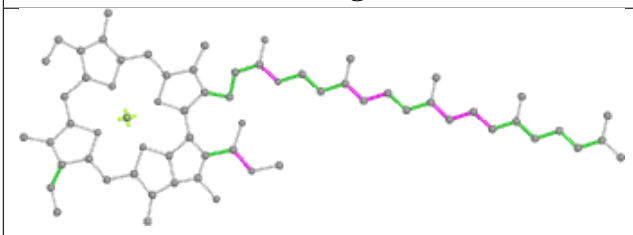


Bond angles



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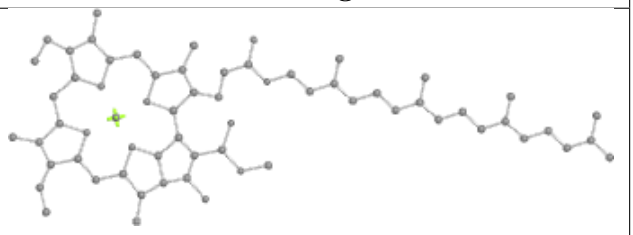
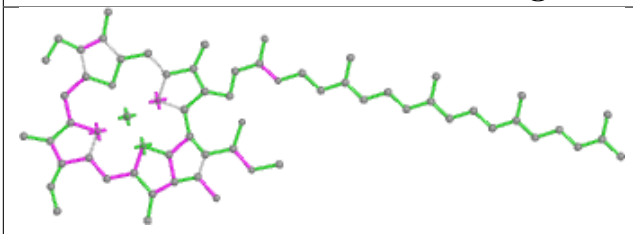


Rings

Ligand CLA c 504



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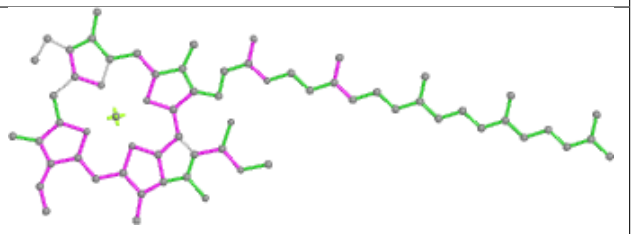
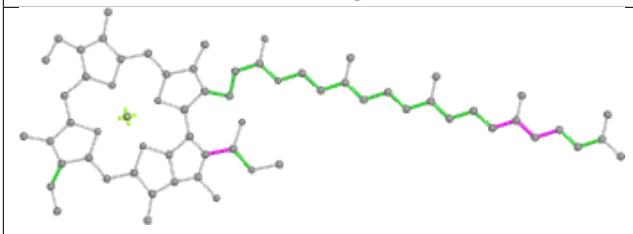


Bond angles



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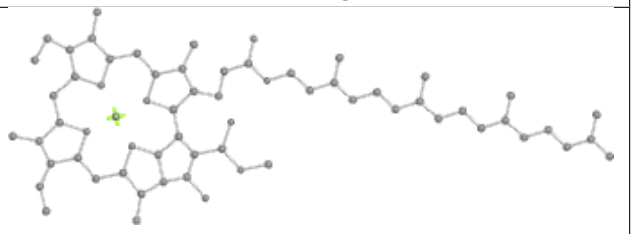
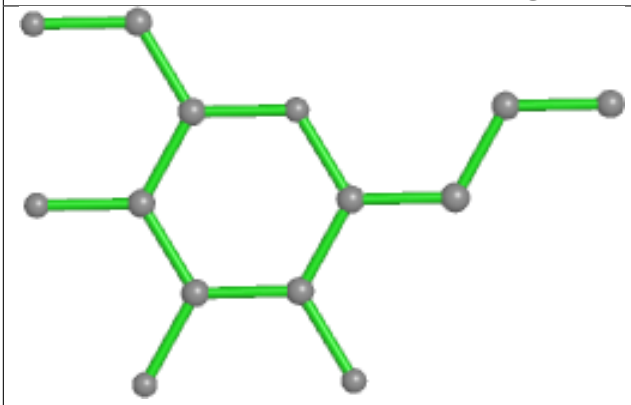


Rings

Ligand HTG v 210



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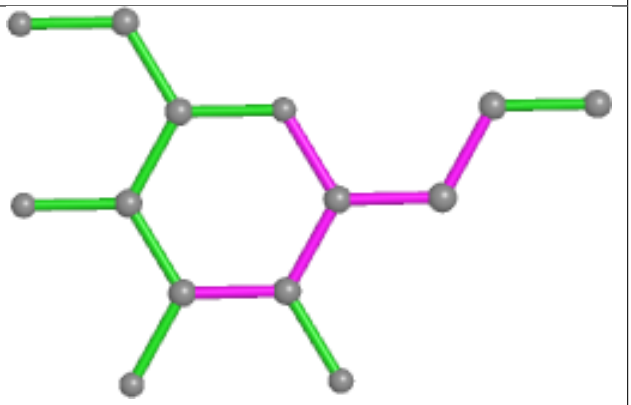
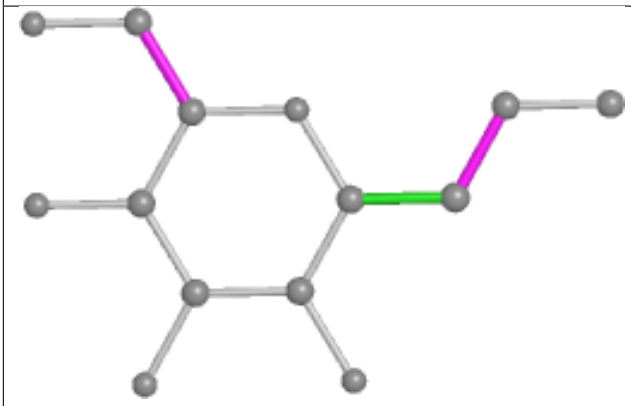


Bond angles



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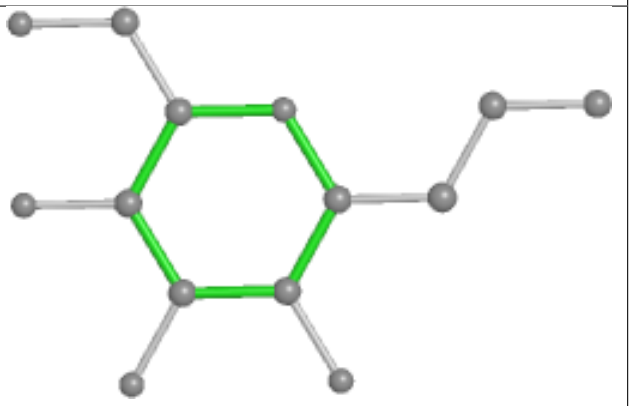
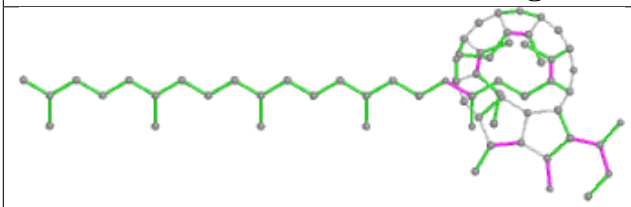
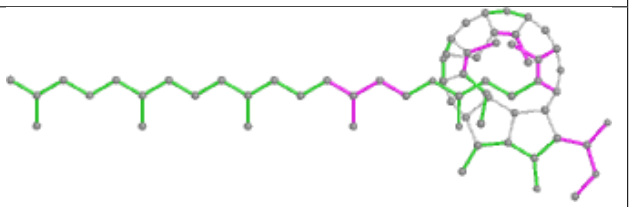


Rings

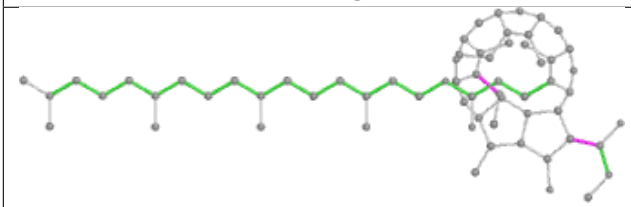
Ligand PHO a 406



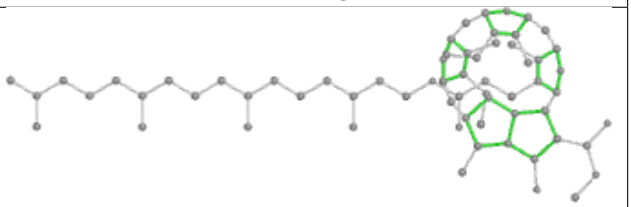
Bond lengths



Bond angles

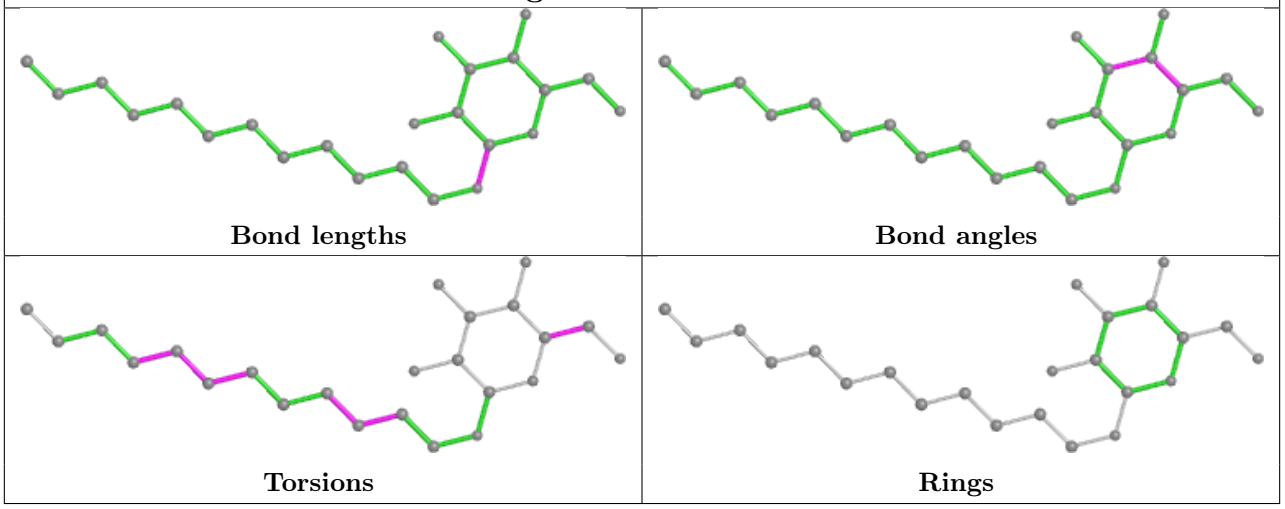


Torsions

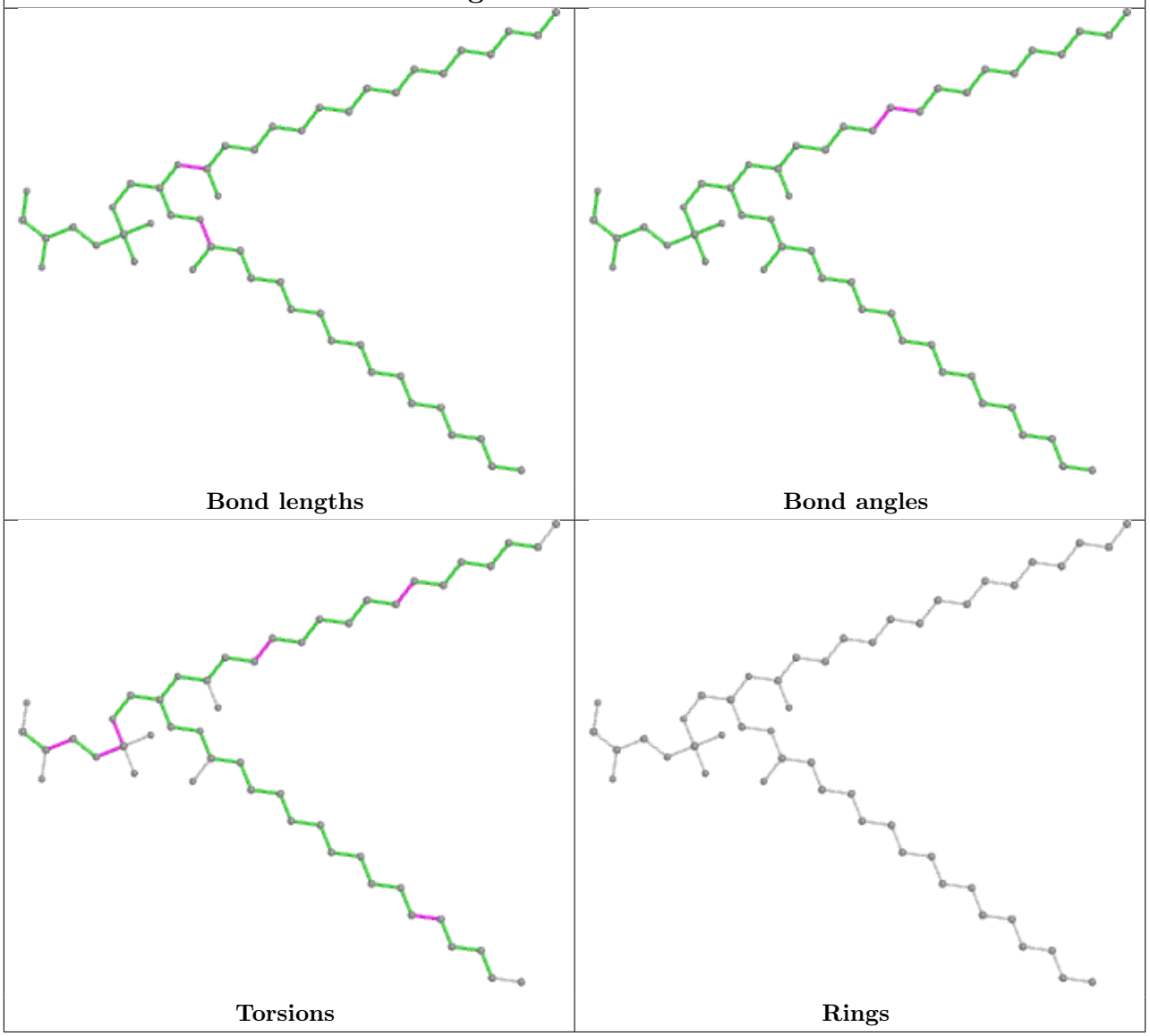


Rings

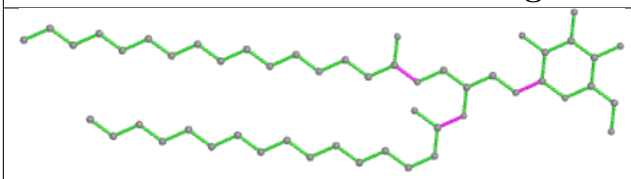
Ligand LMT J 103



Ligand LHG D 408



Ligand LMG c 518



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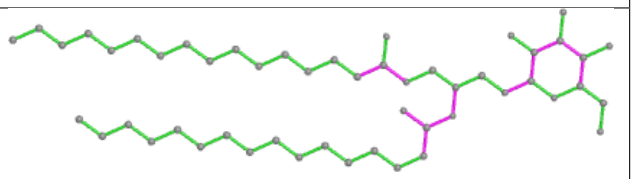
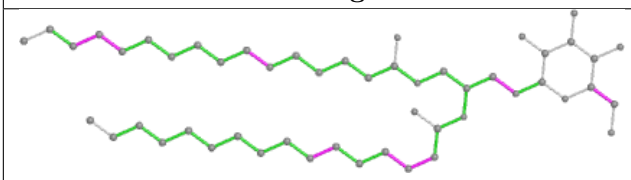
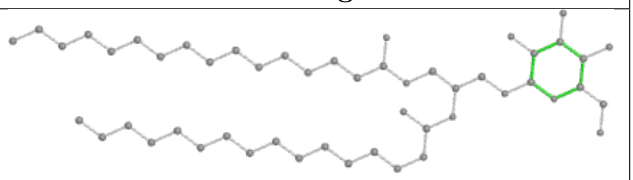


Bond angles

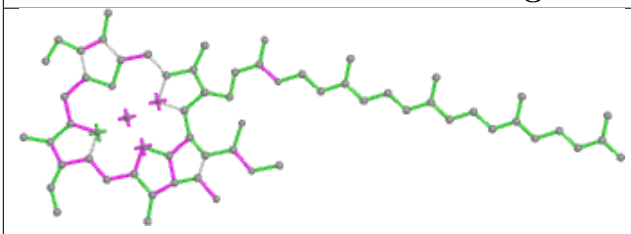


Torsions



Rings

Ligand CLA C 510



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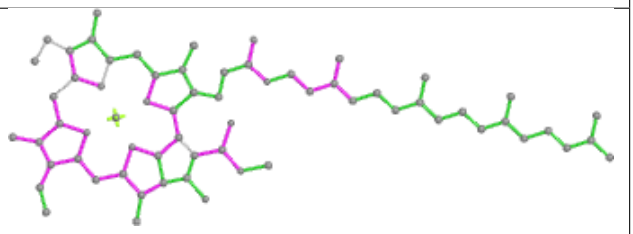
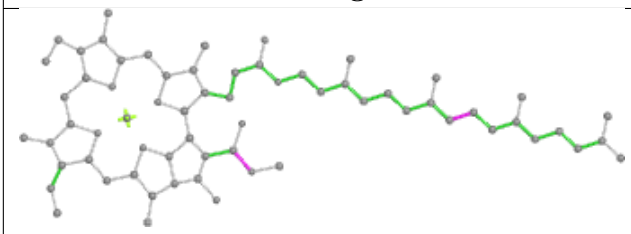
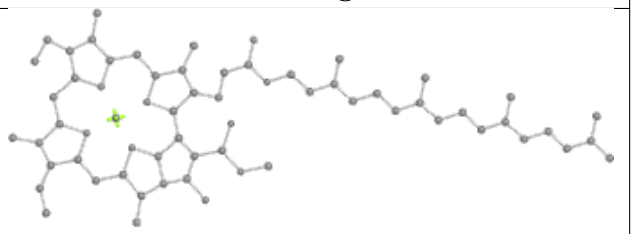


Bond angles

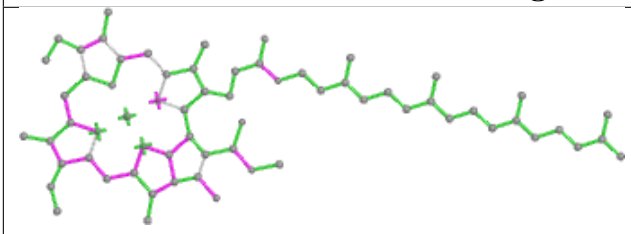


Torsions

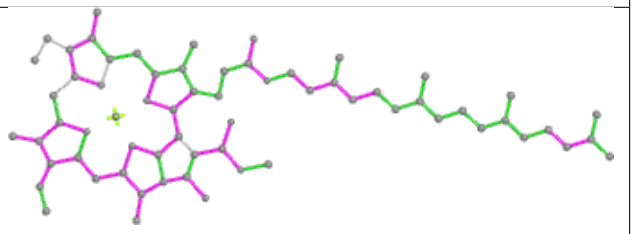


Rings

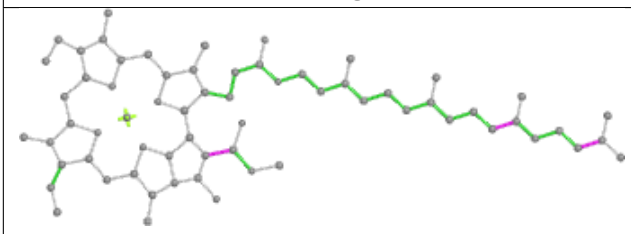
Ligand CLA c 502



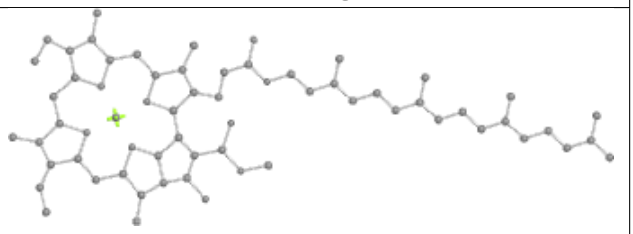
Bond lengths



Bond angles

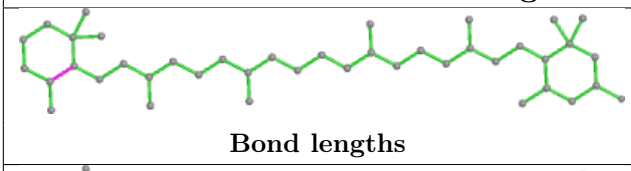


Torsions

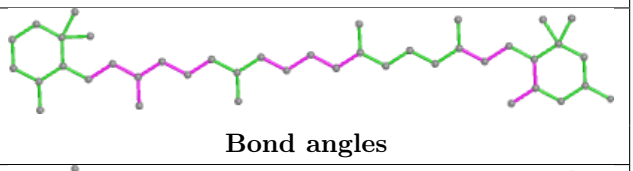


Rings

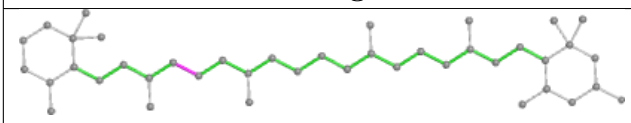
Ligand RRX H 101



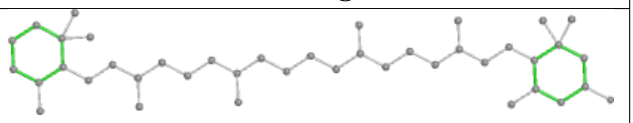
Bond lengths



Bond angles

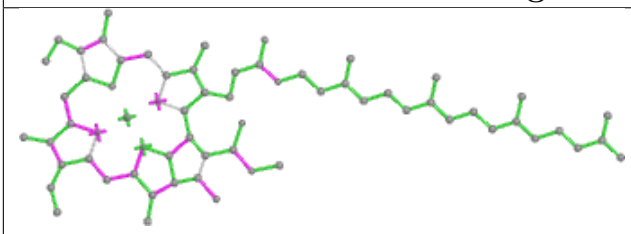


Torsions

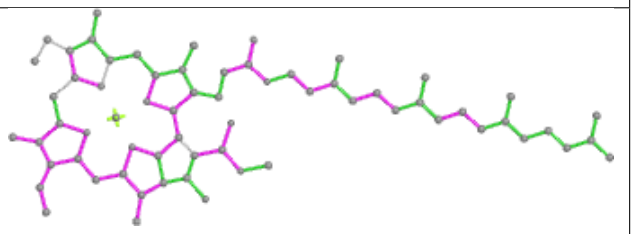


Rings

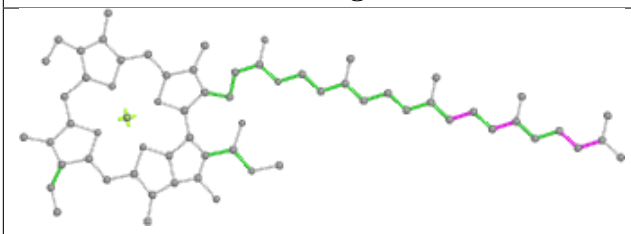
Ligand CLA b 615



Bond lengths



Bond angles



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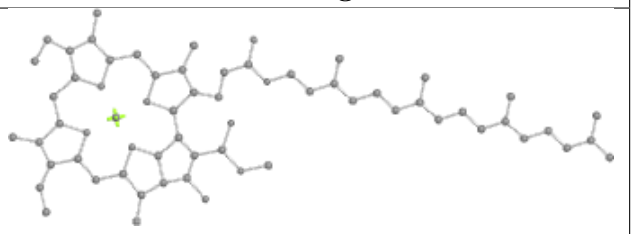
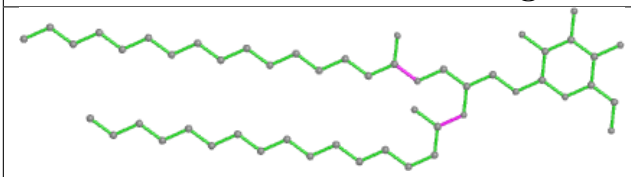
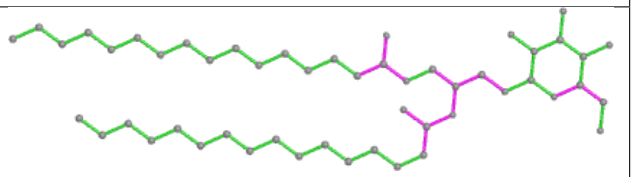


Rings

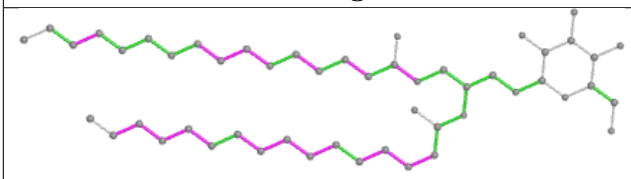
Ligand LMG C 519



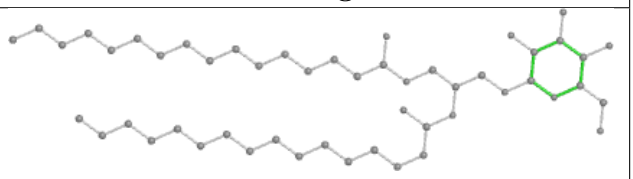
Bond lengths



Bond angles

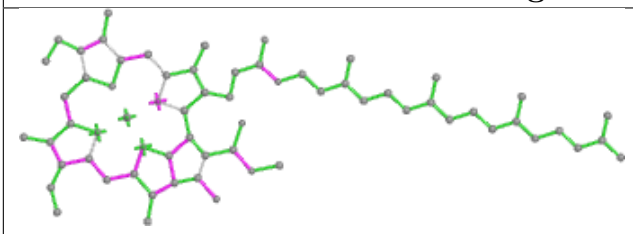


Torsions



Rings

Ligand CLA b 605



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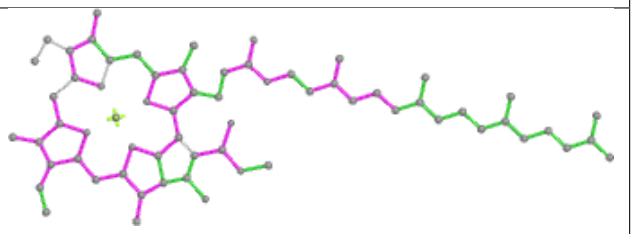
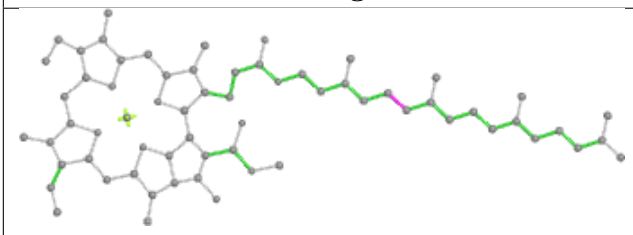


Bond angles



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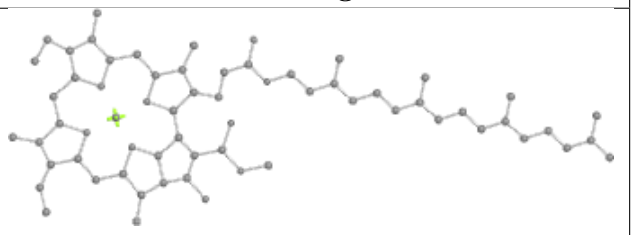
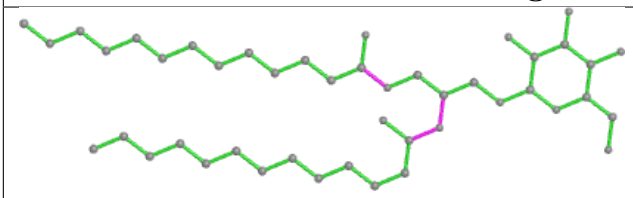


Rings

Ligand LMG j 101



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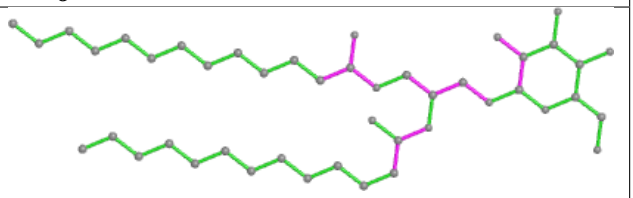
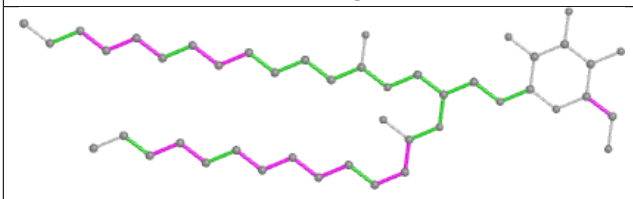


Bond angles



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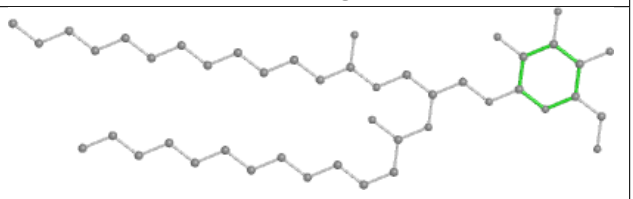
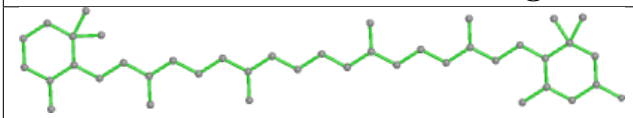


Rings

Ligand RRX x 101



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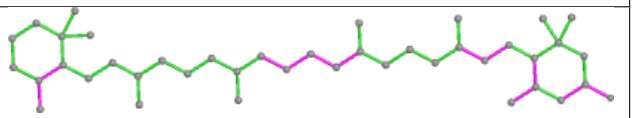
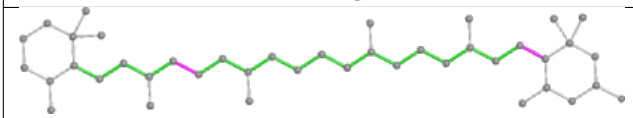
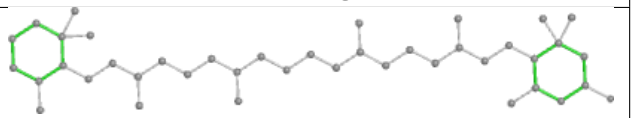


Bond angles

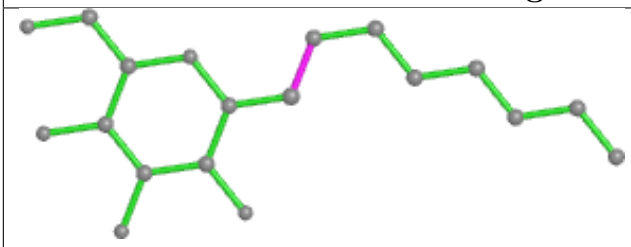


Torsions



Rings

Ligand HTG c 521



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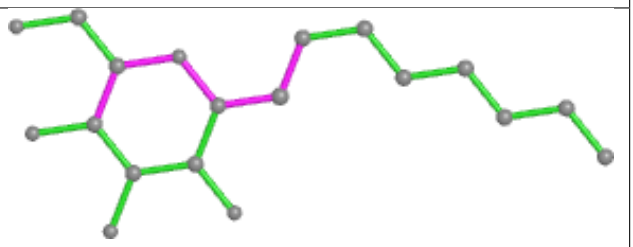
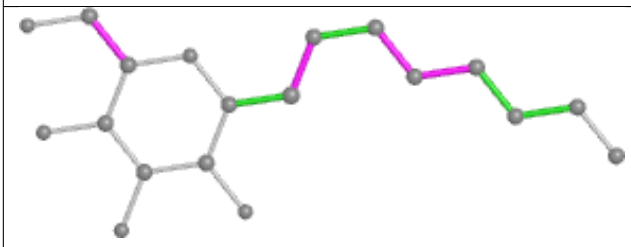


Bond angles



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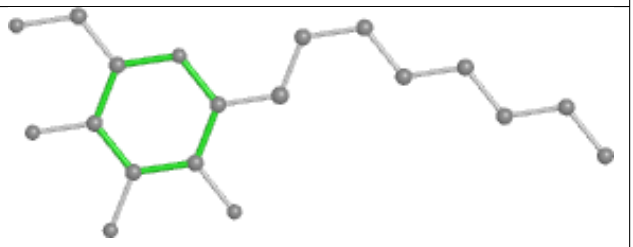
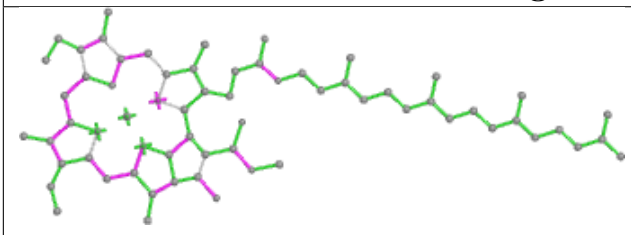


Rings

Ligand CLA c 507



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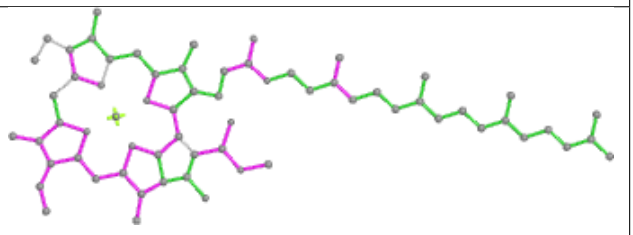
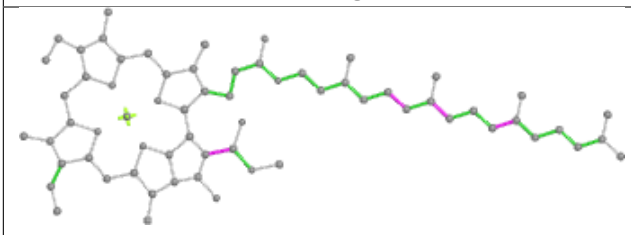


Bond angles



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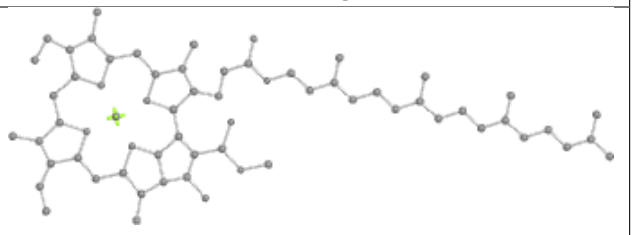
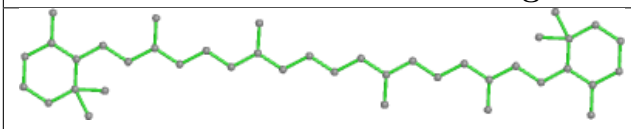


Rings

Ligand BCR C 514



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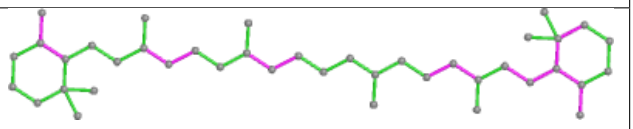
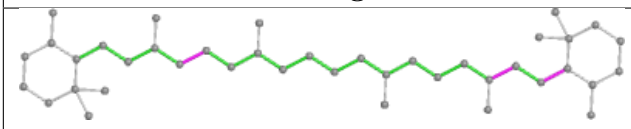


Bond angles



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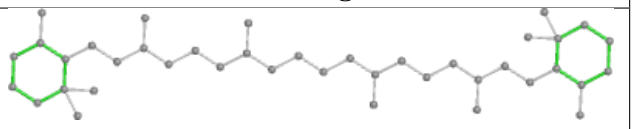
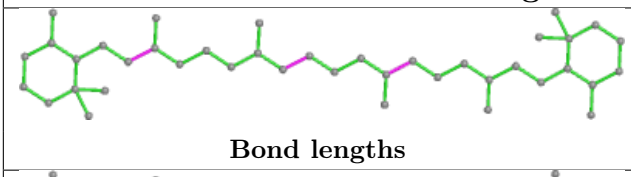


Rings

Ligand BCR A 405



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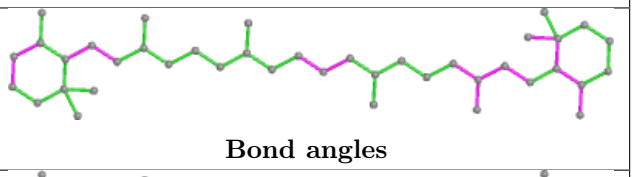
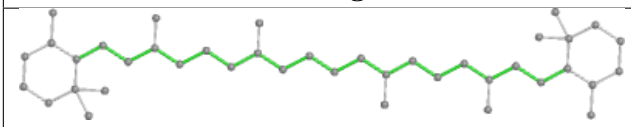


Bond angles



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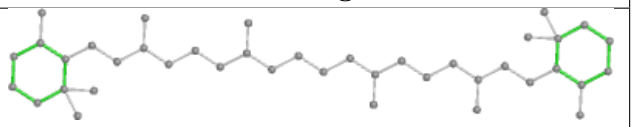
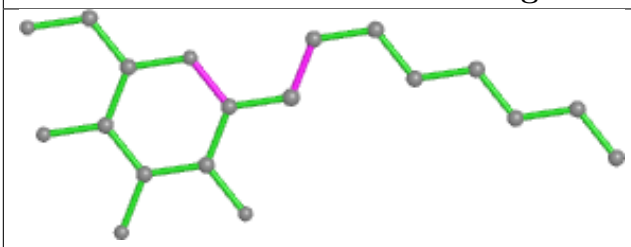


Rings

Ligand HTG C 521



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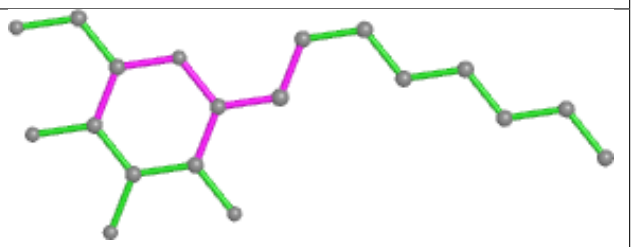
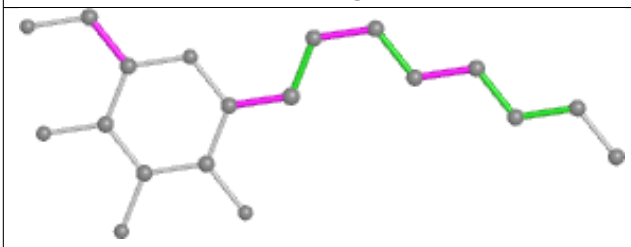


Bond angles



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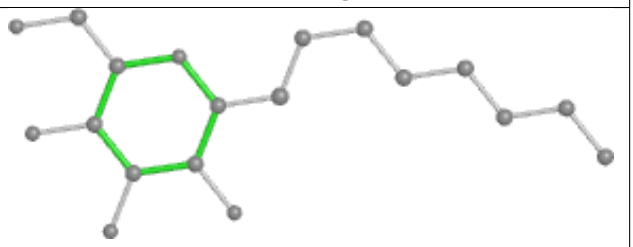
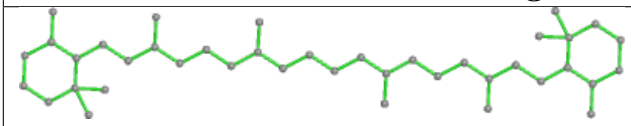
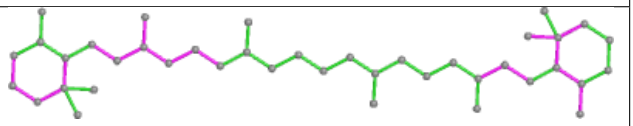


Rings

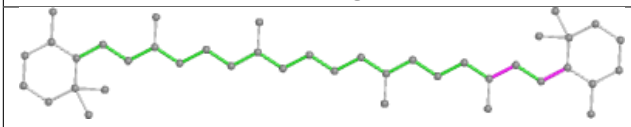
Ligand BCR d 405



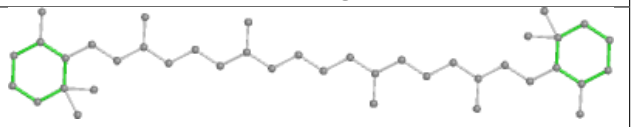
Bond lengths



Bond angles

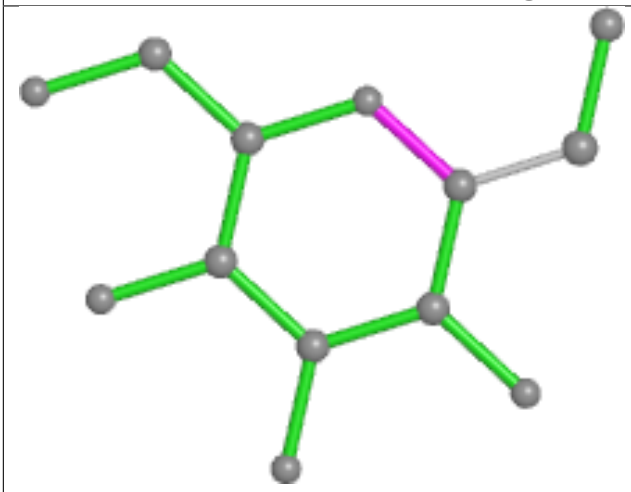


Torsions



Rings

Ligand HTG V 202



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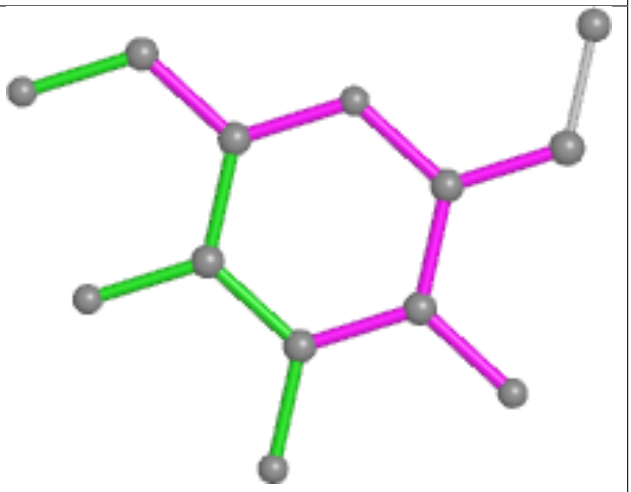
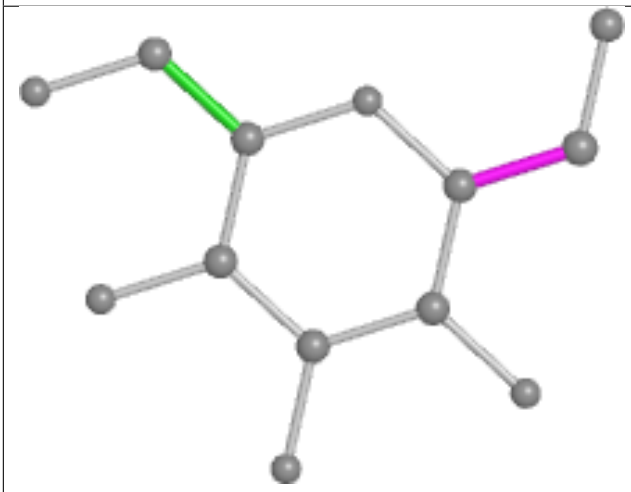


Bond angles



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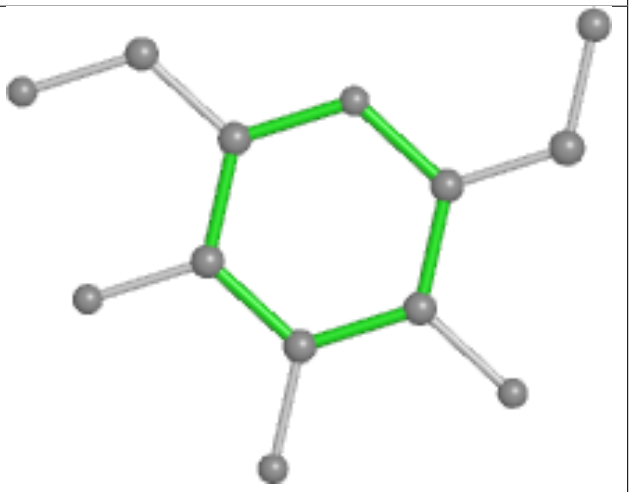
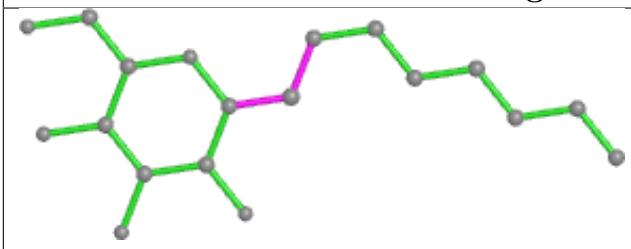


Rings

Ligand HTG c 520



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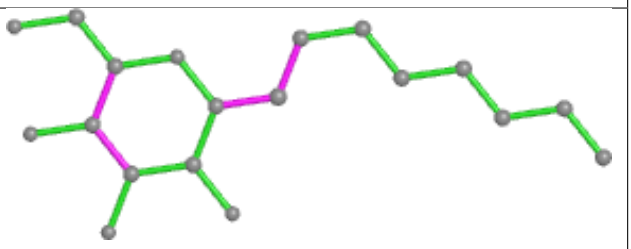
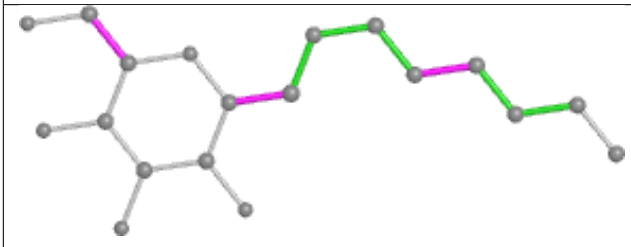


Bond angles



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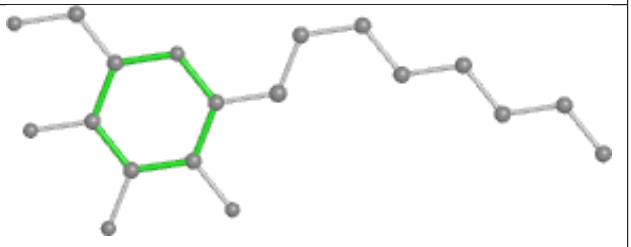
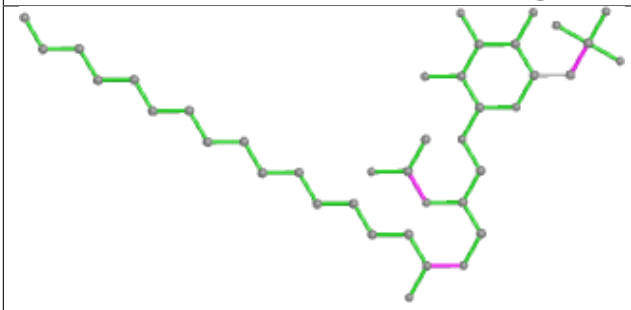


Rings

Ligand SQD f 101



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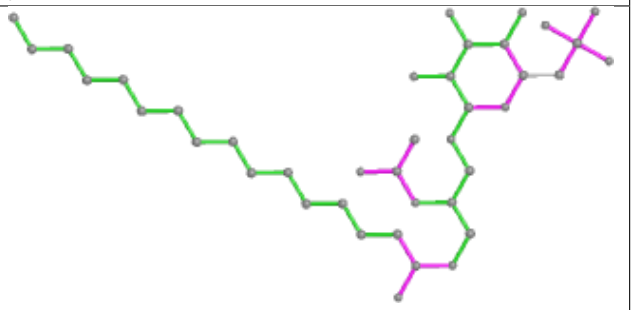
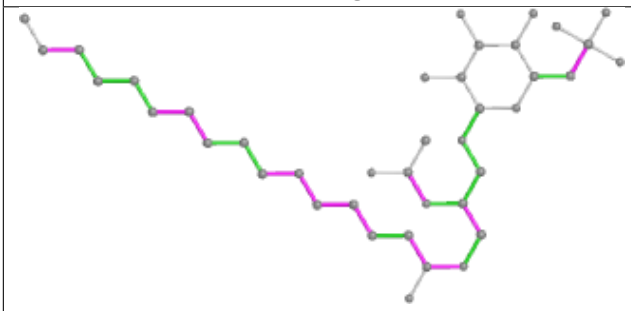
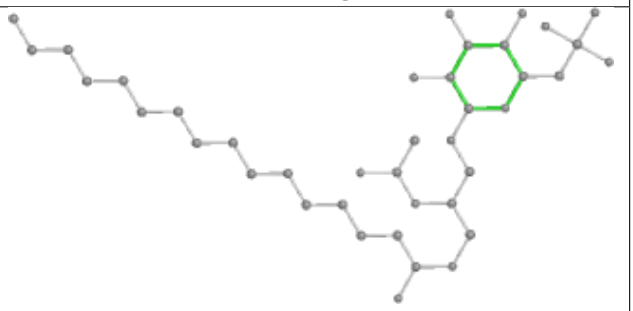


Bond angles

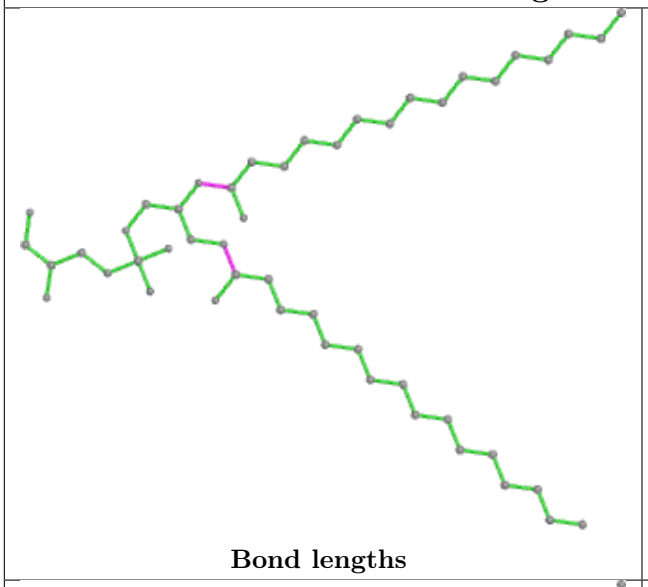


Torsions

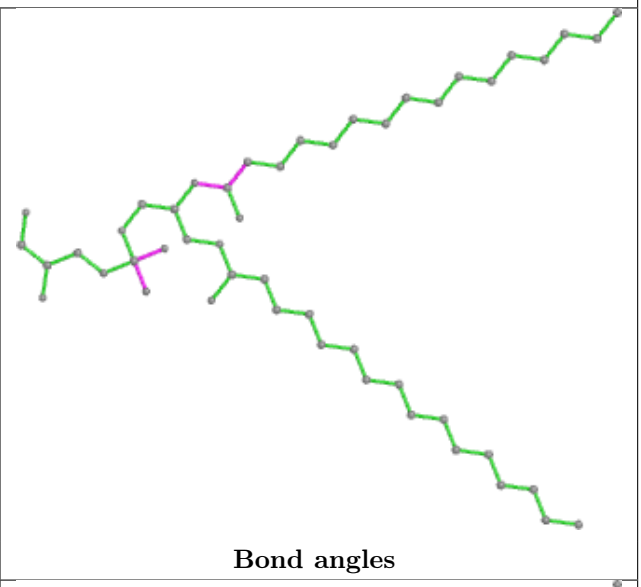


Rings

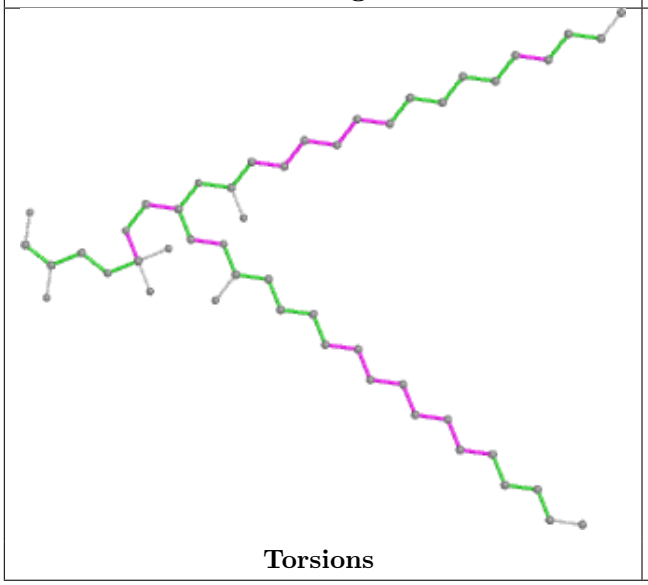
Ligand LHG l 102



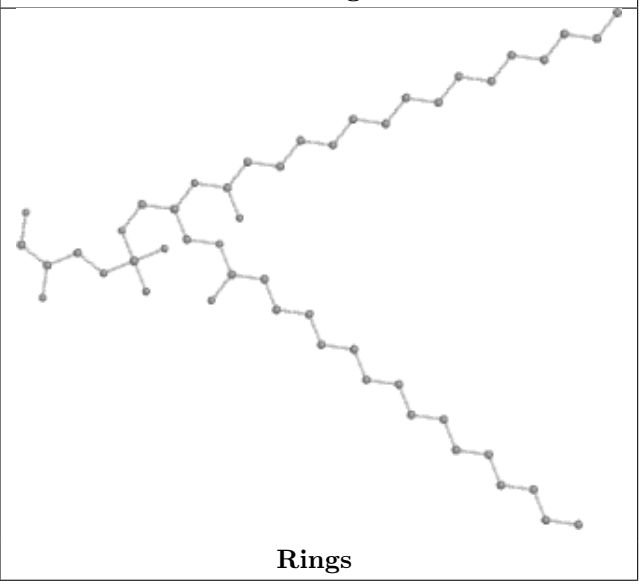
Bond lengths



Bond angles

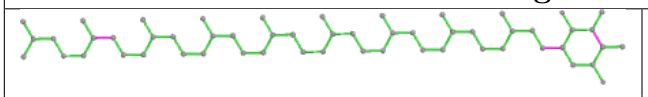


Torsions

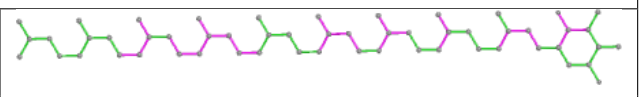


Rings

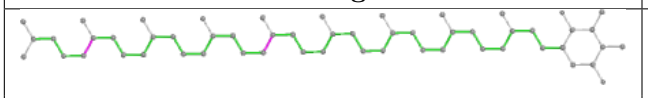
Ligand PL9 d 412



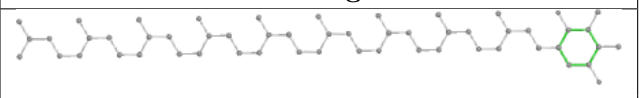
Bond lengths



Bond angles

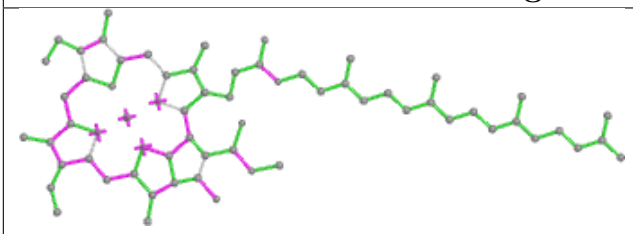


Torsions

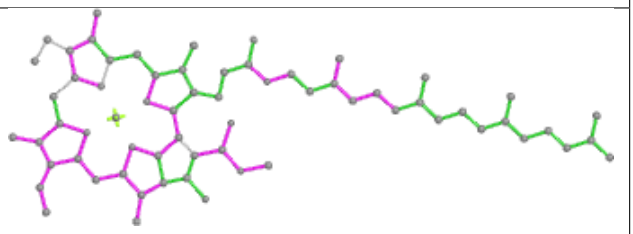


Rings

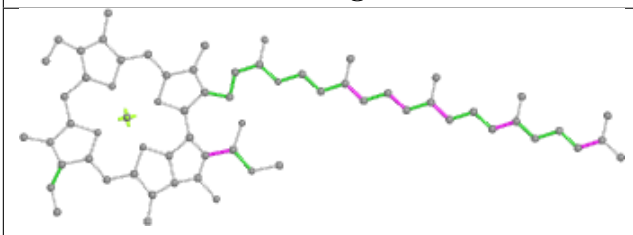
Ligand CLA C 507



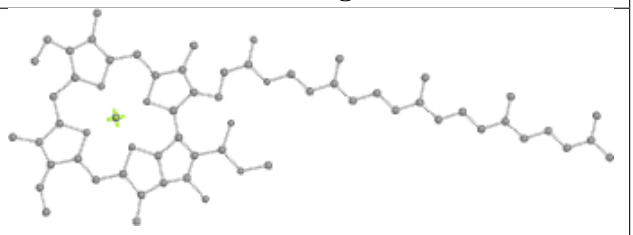
Bond lengths



Bond angles

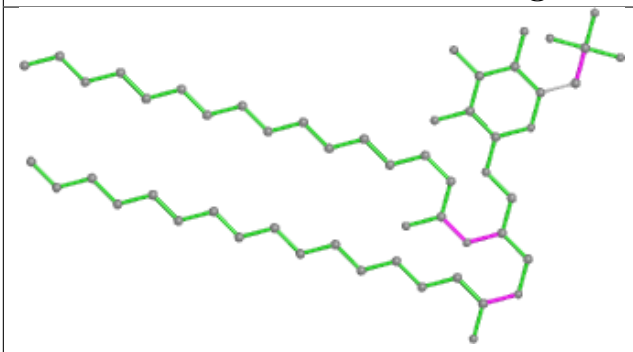


Torsions

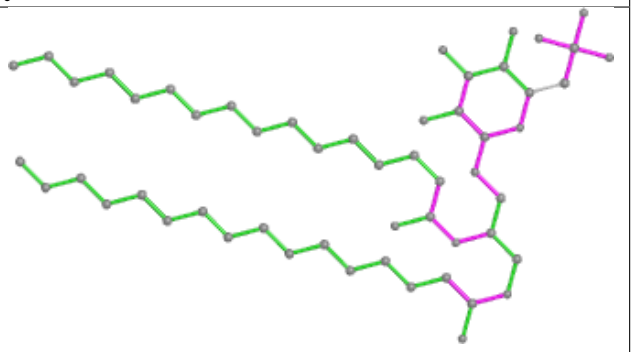


Rings

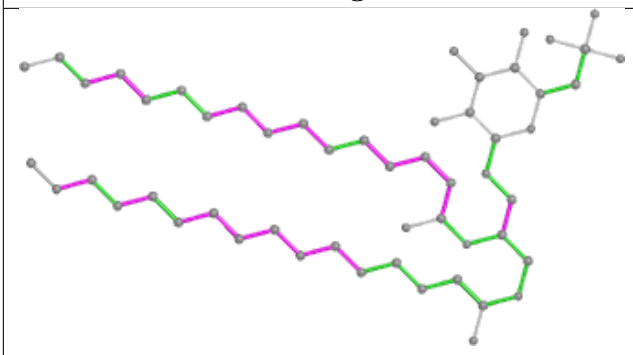
Ligand SQD a 409



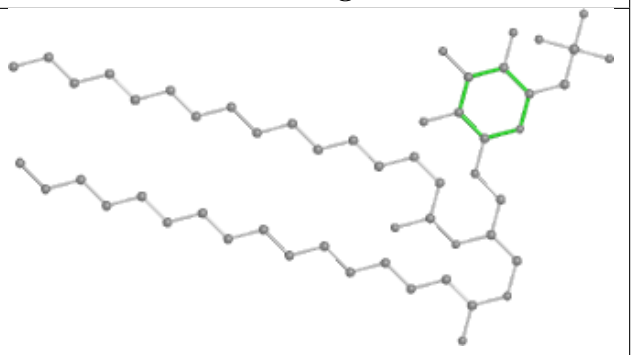
Bond lengths



Bond angles

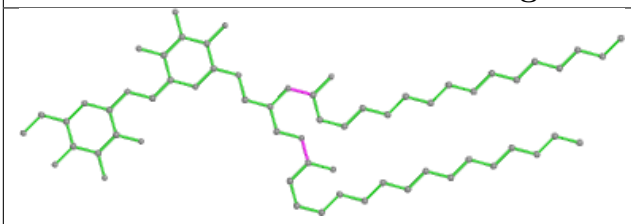


Torsions

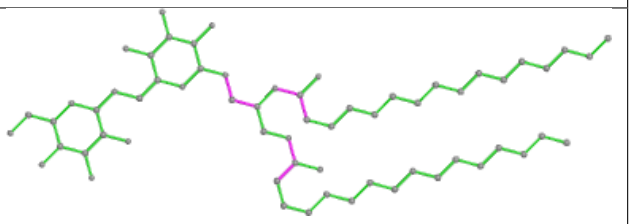


Rings

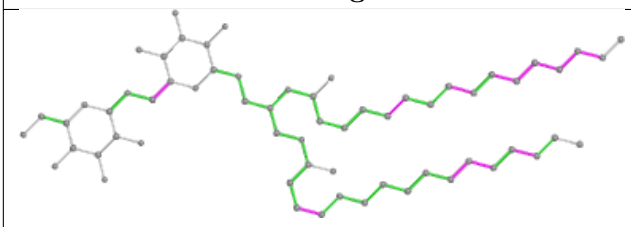
Ligand DGD C 518



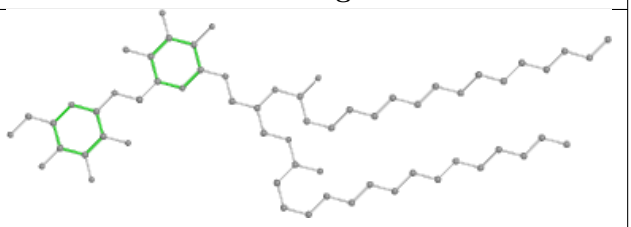
Bond lengths



Bond angles

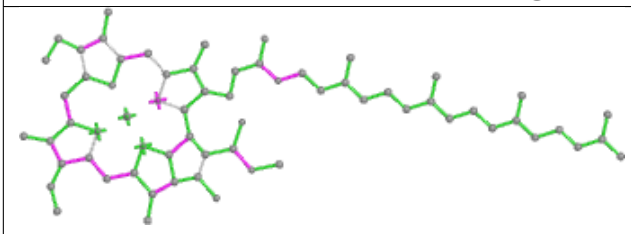


Torsions

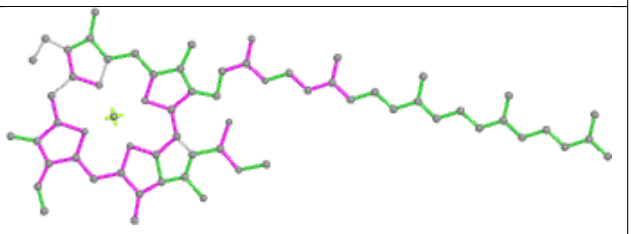


Rings

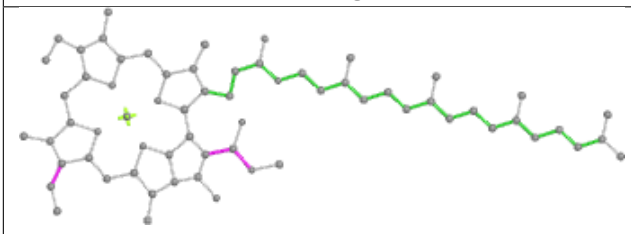
Ligand CLA a 403



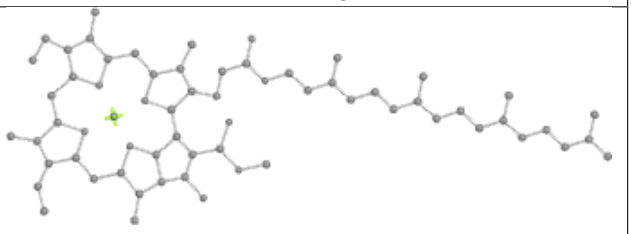
Bond lengths



Bond angles

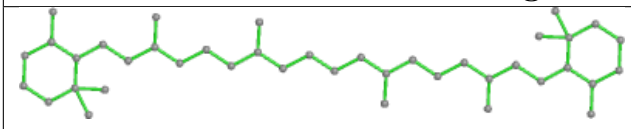


Torsions

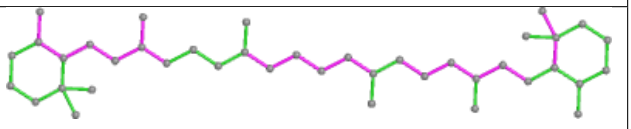


Rings

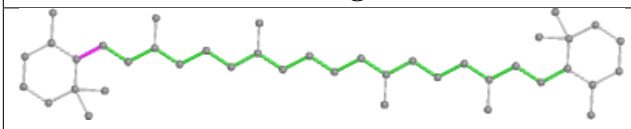
Ligand BCR B 617



Bond lengths



Bond angles



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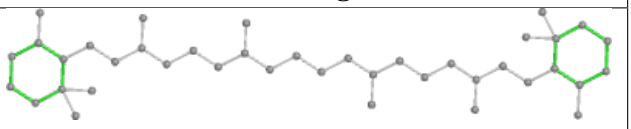
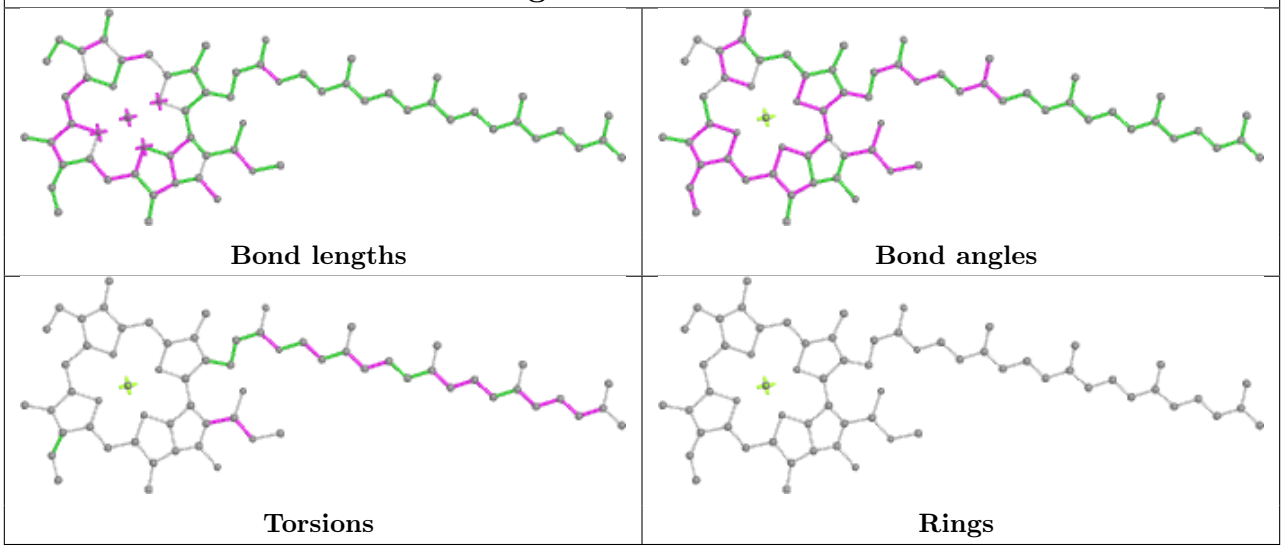
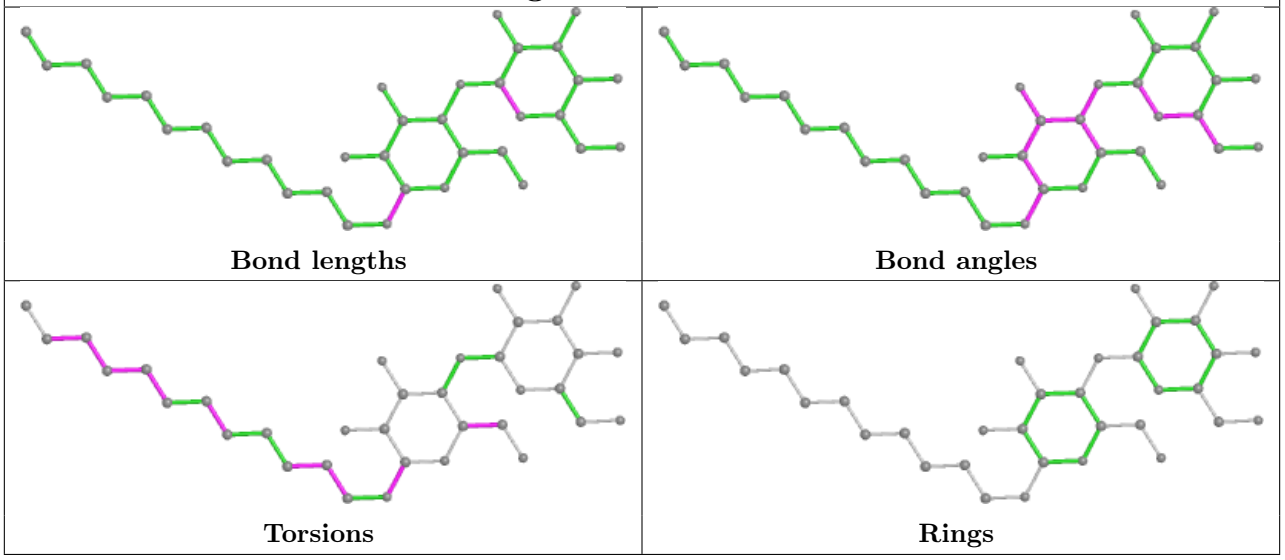


Rings

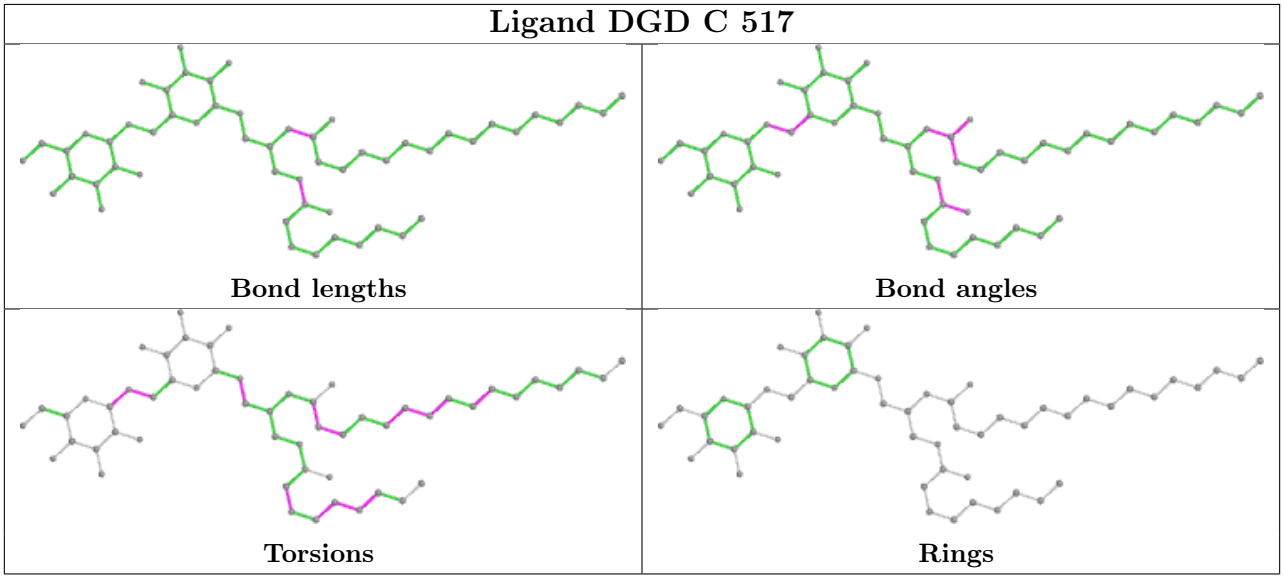
Ligand CLA b 618



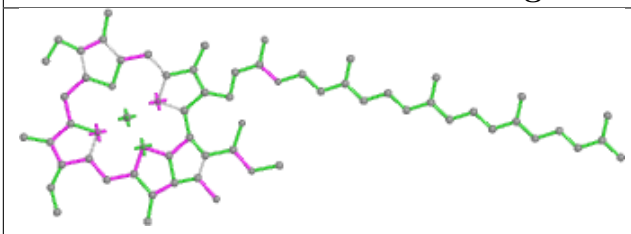
Ligand LMT a 418



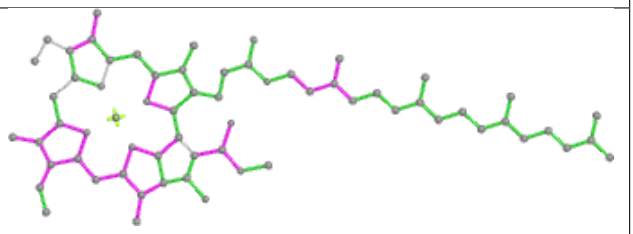
Ligand DGD C 517



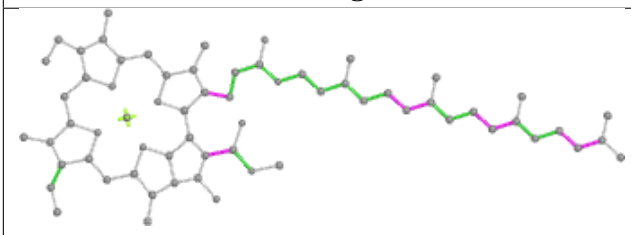
Ligand CLA C 506



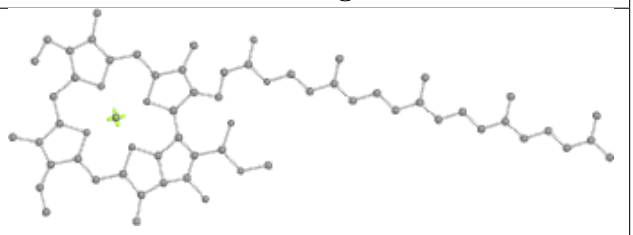
Bond lengths



Bond angles

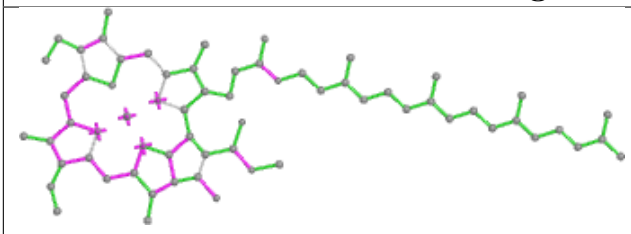


Torsions

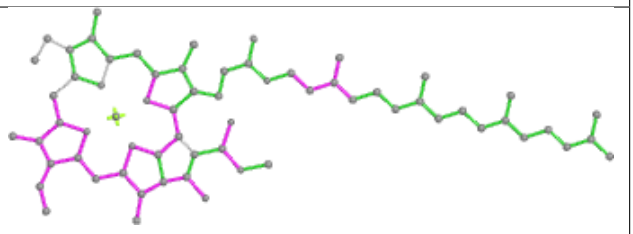


Rings

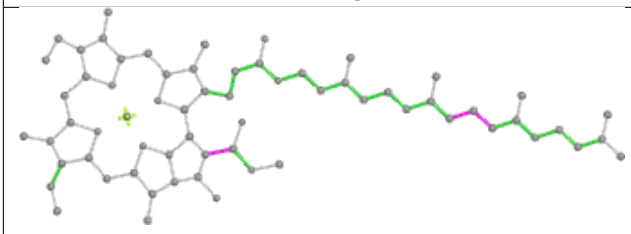
Ligand CLA c 503



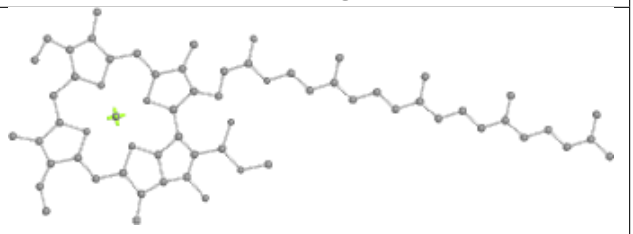
Bond lengths



Bond angles

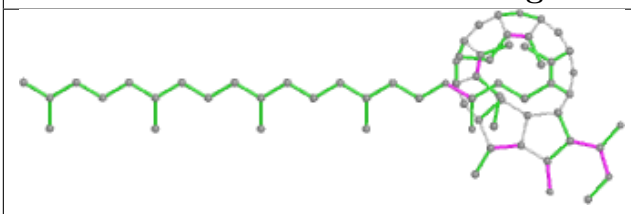


Torsions

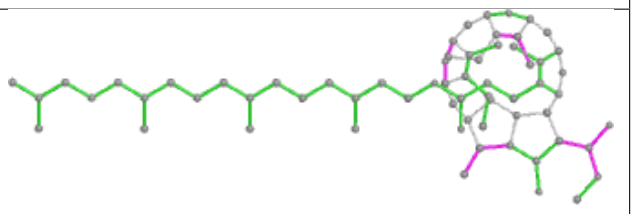


Rings

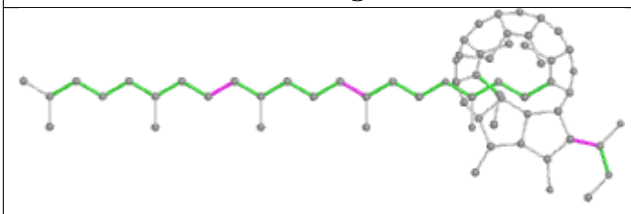
Ligand PHO a 405



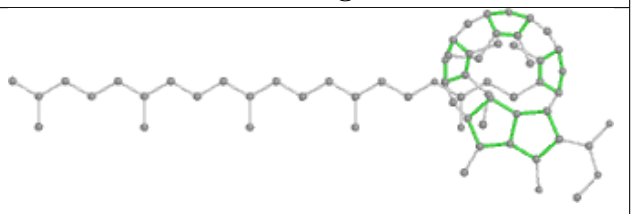
Bond lengths



Bond angles

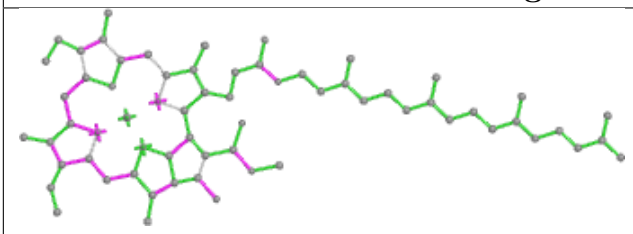


Torsions

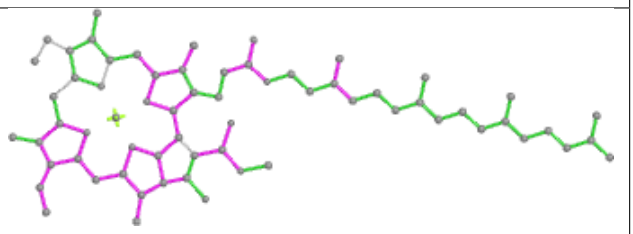


Rings

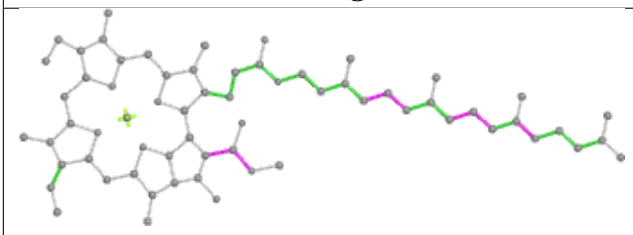
Ligand CLA B 615



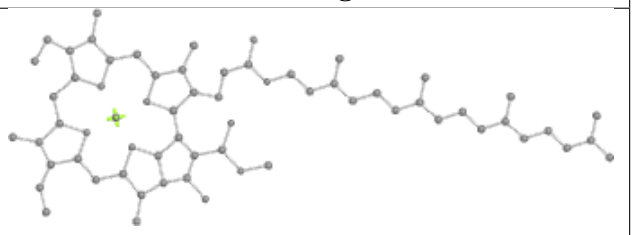
Bond lengths



Bond angles

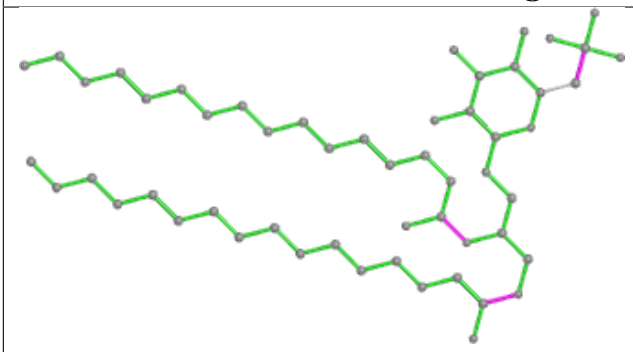


Torsions

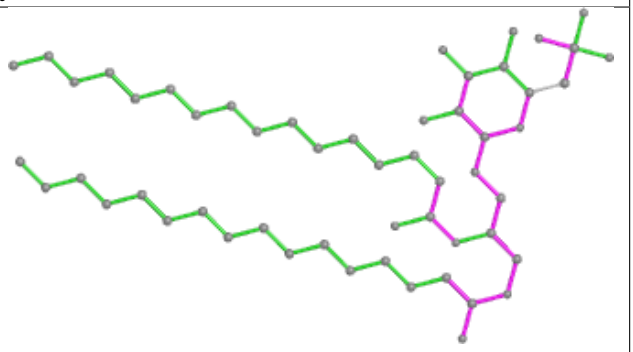


Rings

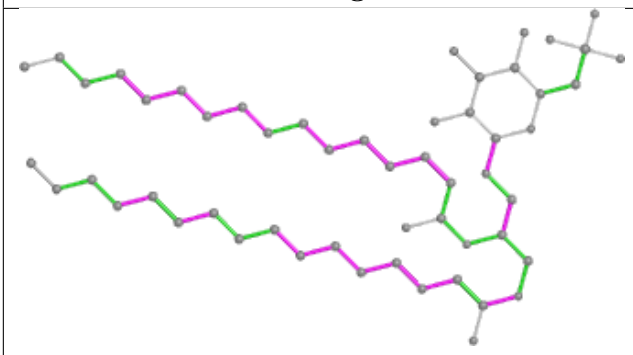
Ligand SQD A 412



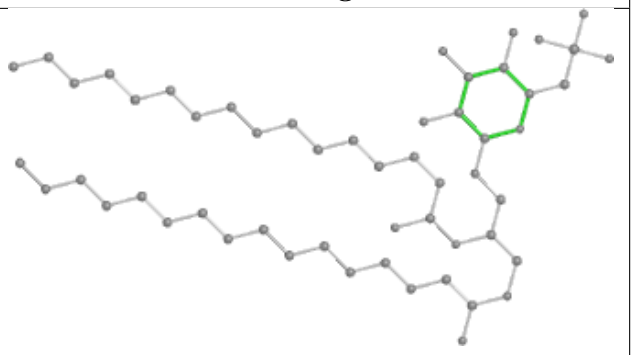
Bond lengths



Bond angles

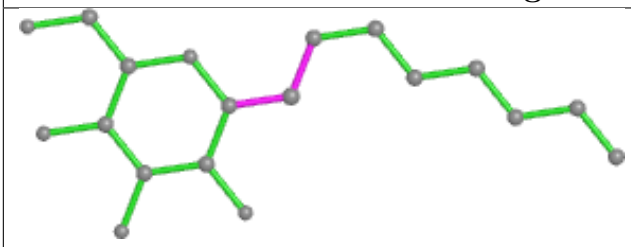


Torsions

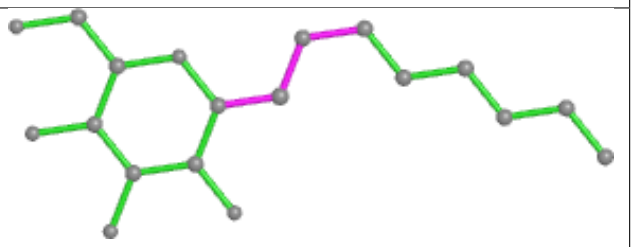


Rings

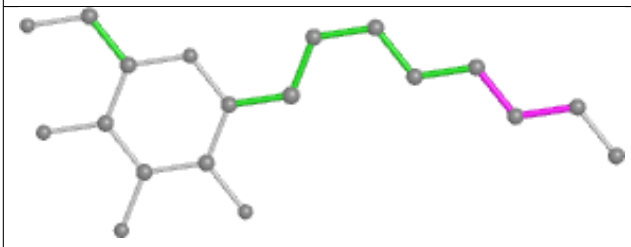
Ligand HTG b 601



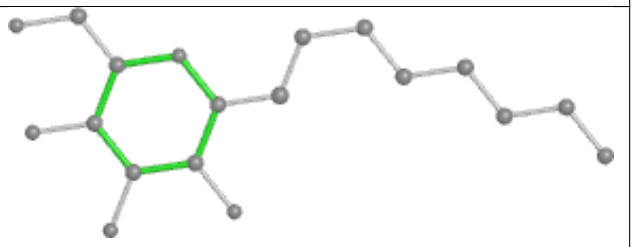
Bond lengths



Bond angles

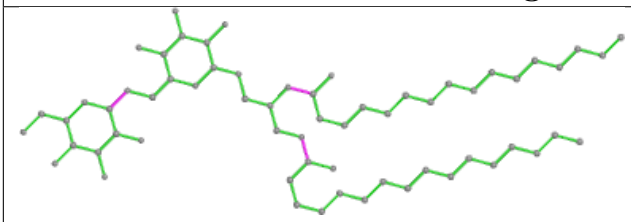


Torsions

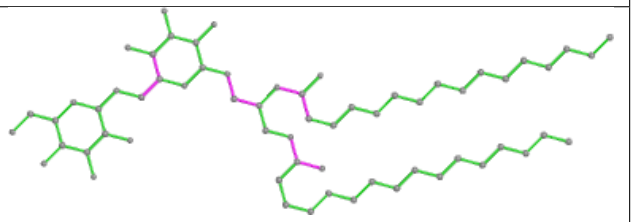


Rings

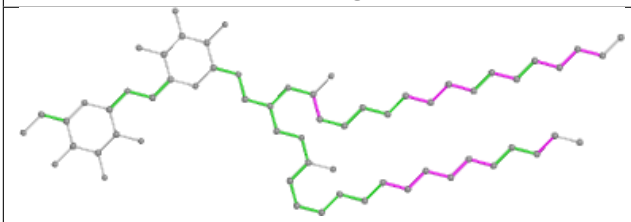
Ligand DGD h 101



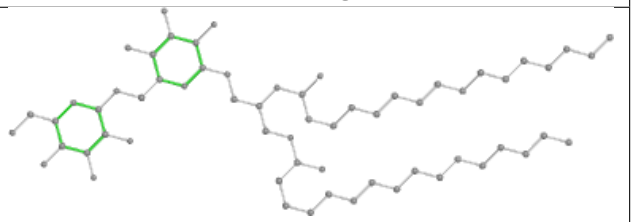
Bond lengths



Bond angles

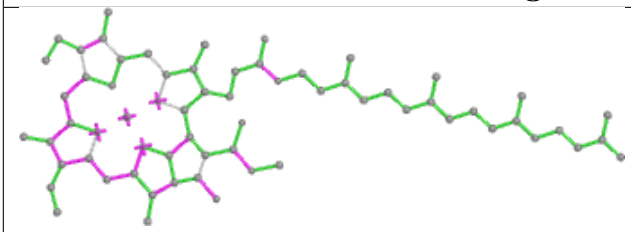


Torsions

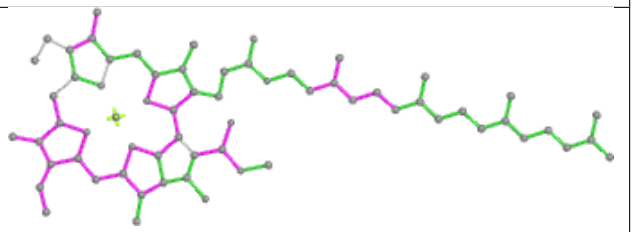


Rings

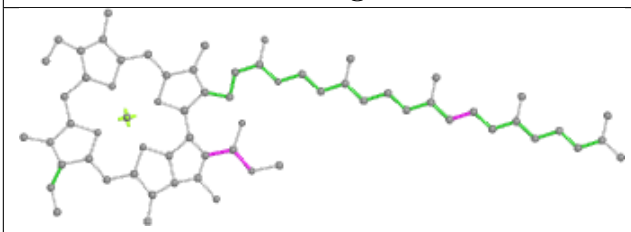
Ligand CLA C 503



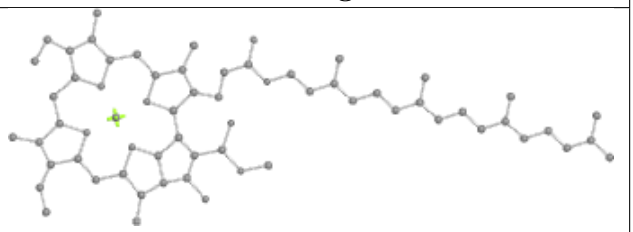
Bond lengths



Bond angles

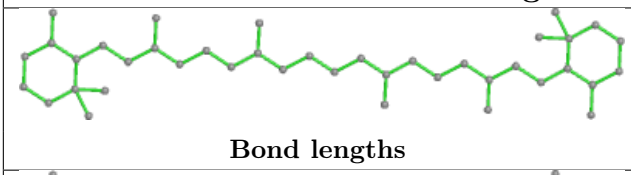


Torsions

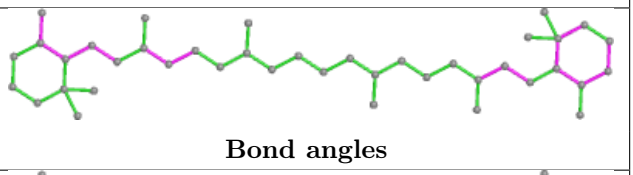


Rings

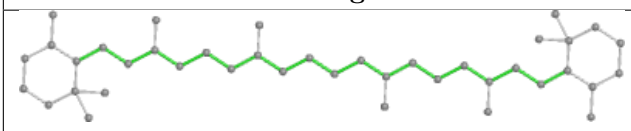
Ligand BCR B 618



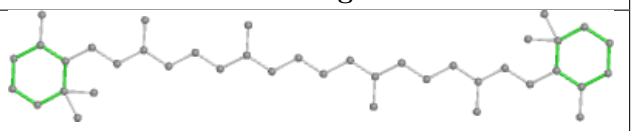
Bond lengths



Bond angles

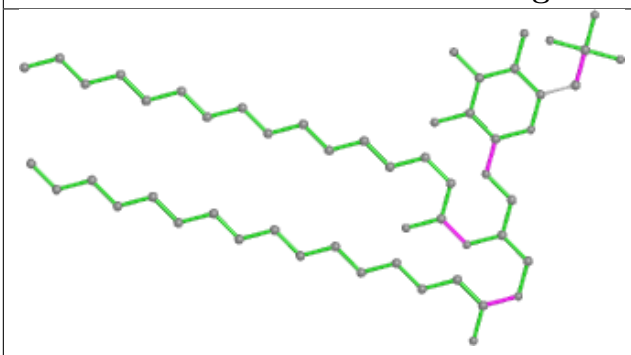


Torsions

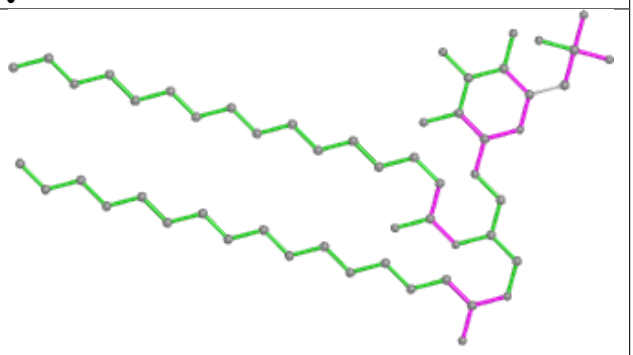


Rings

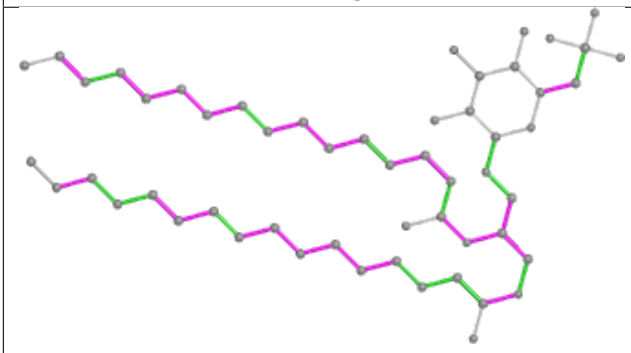
Ligand SQD l 101



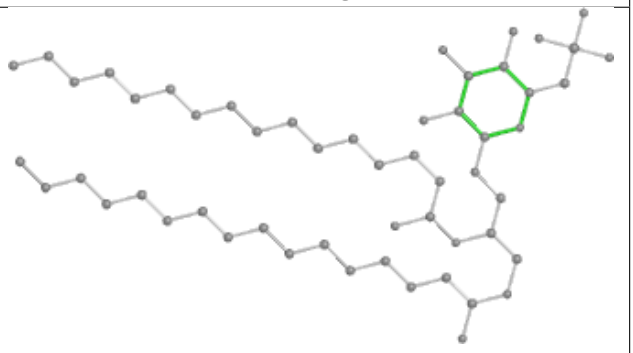
Bond lengths



Bond angles

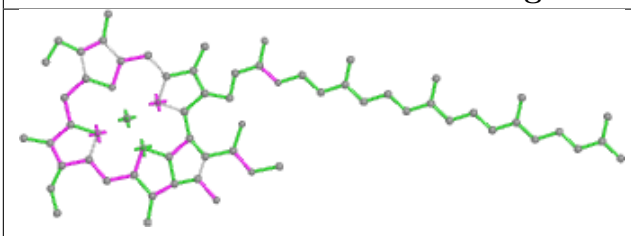


Torsions

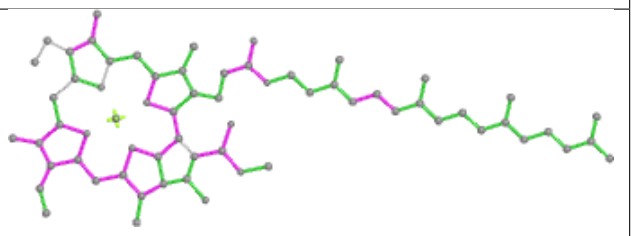


Rings

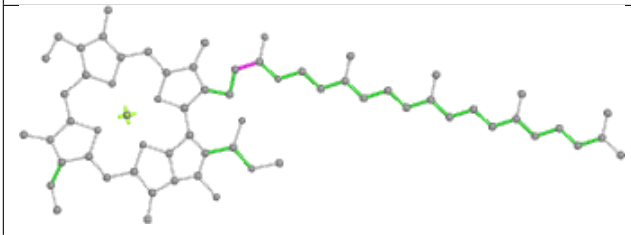
Ligand CLA C 505



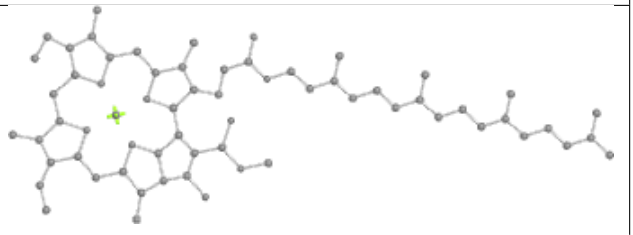
Bond lengths



Bond angles

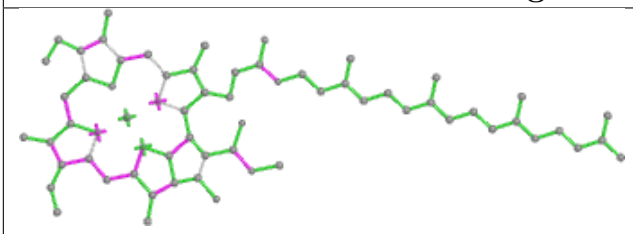


Torsions

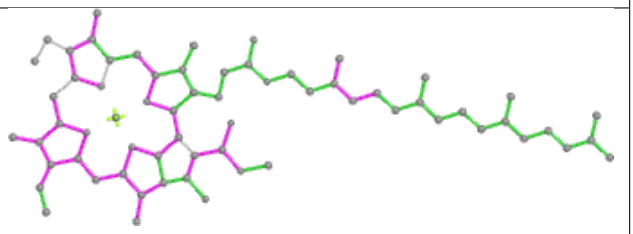


Rings

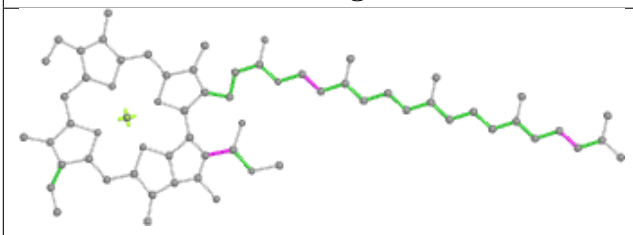
Ligand CLA b 606



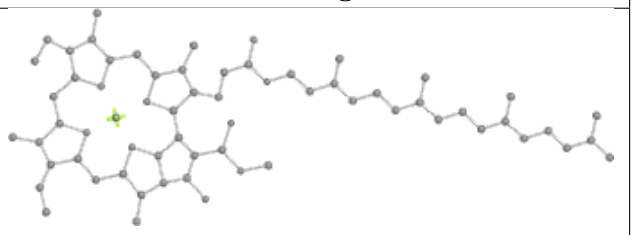
Bond lengths



Bond angles

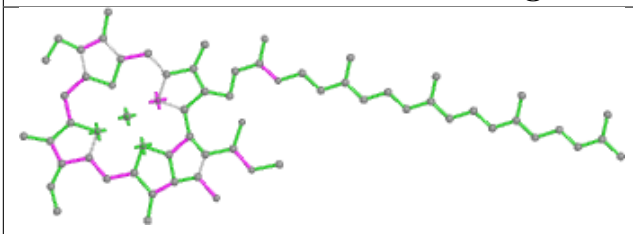


Torsions

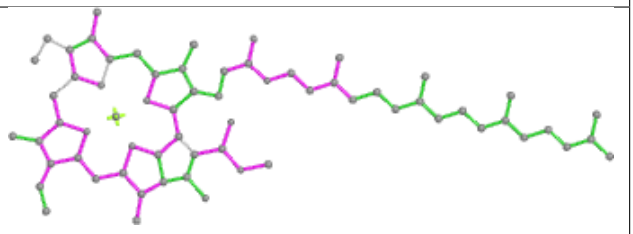


Rings

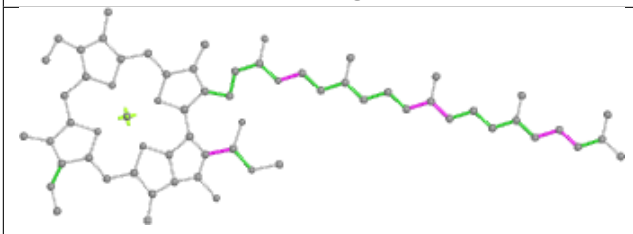
Ligand CLA C 509



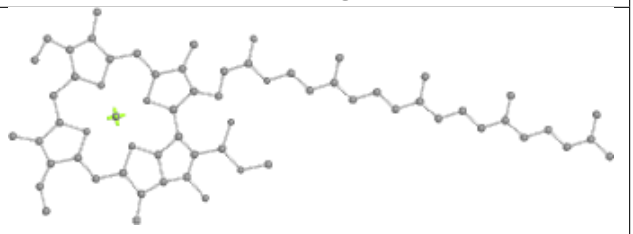
Bond lengths



Bond angles

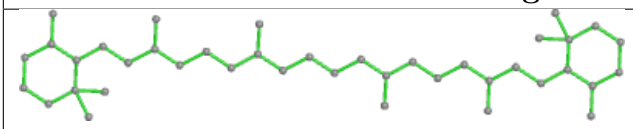


Torsions



Rings

Ligand BCR C 515



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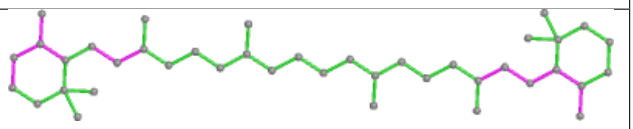
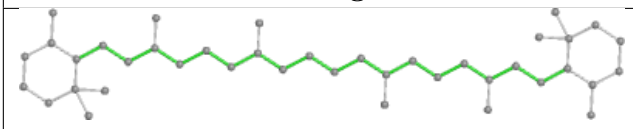


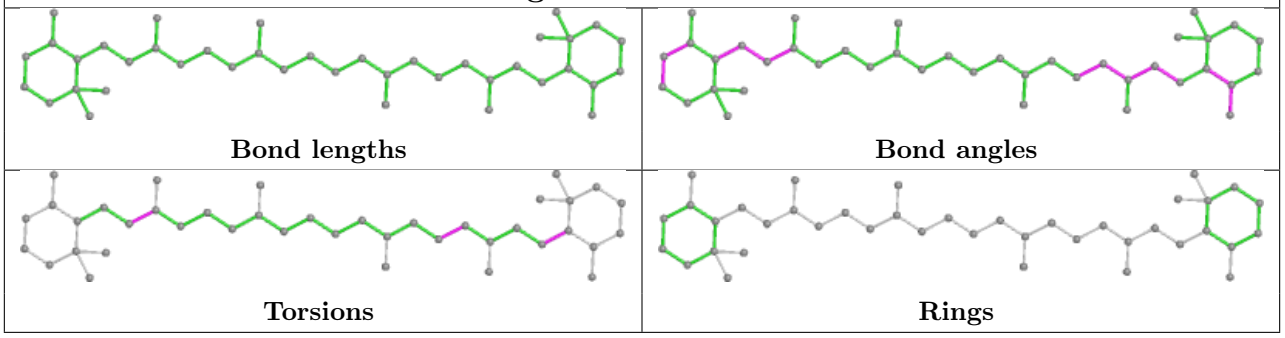
Bond angles



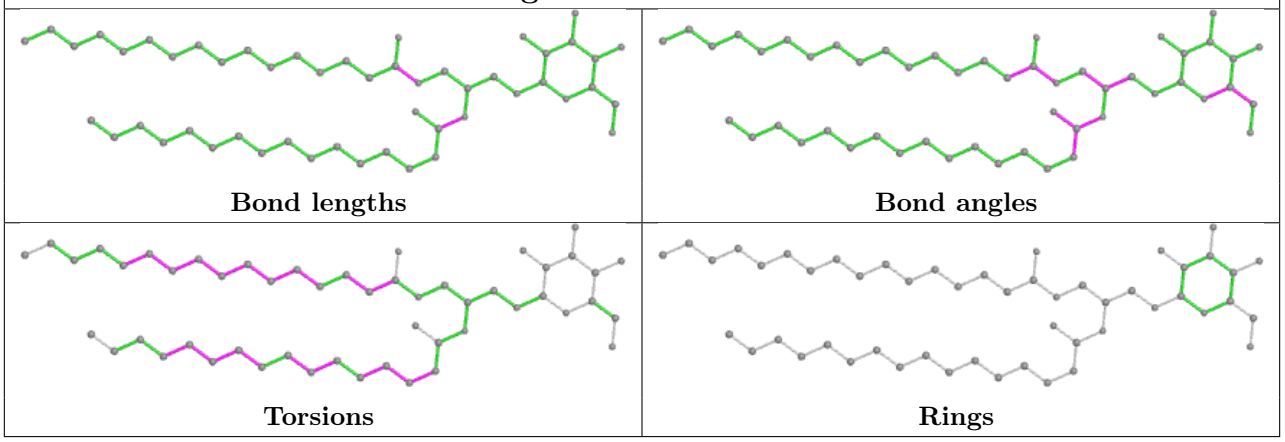
Torsions

Rings

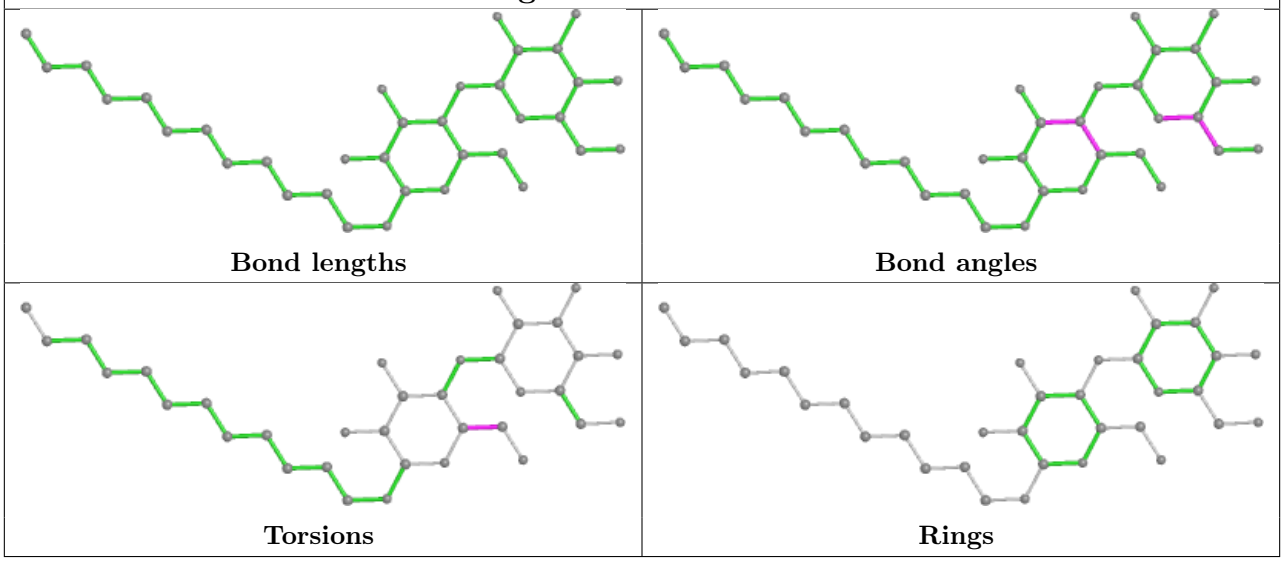
Ligand BCR k 101



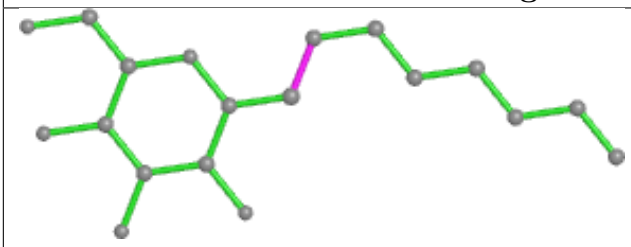
Ligand LMG B 620



Ligand LMT M 101



Ligand HTG D 417



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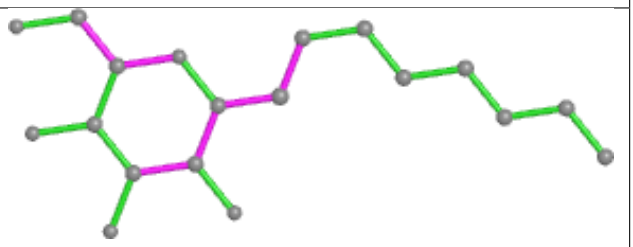
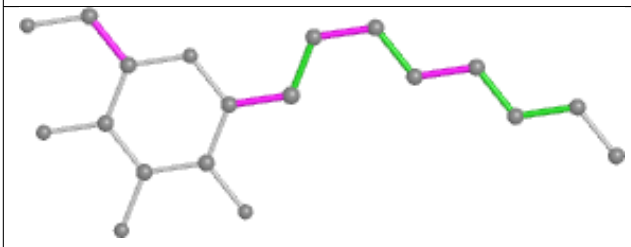
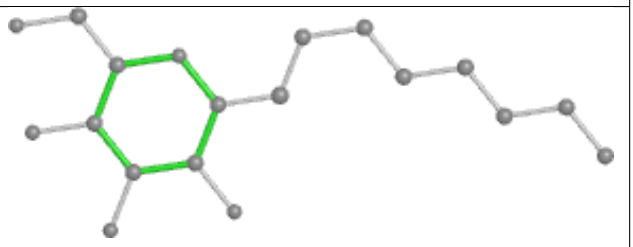


Bond angles

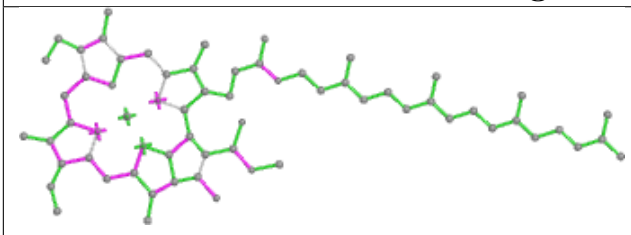


Torsions



Rings

Ligand CLA c 509



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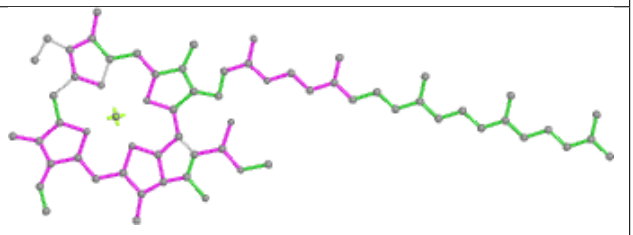
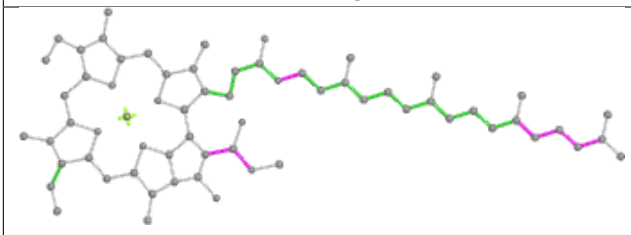


Bond angles



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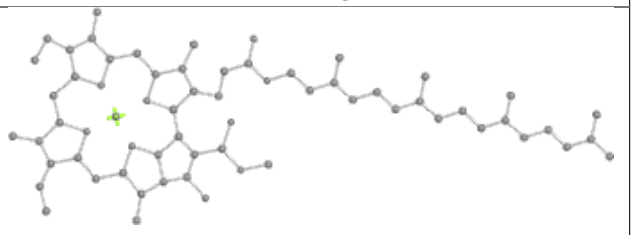
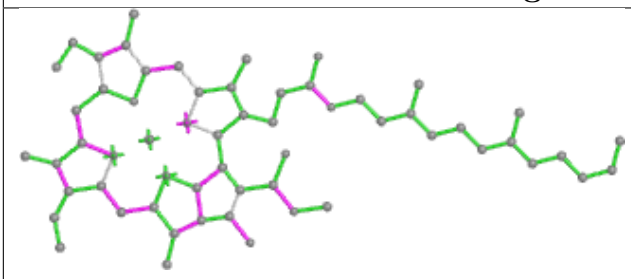
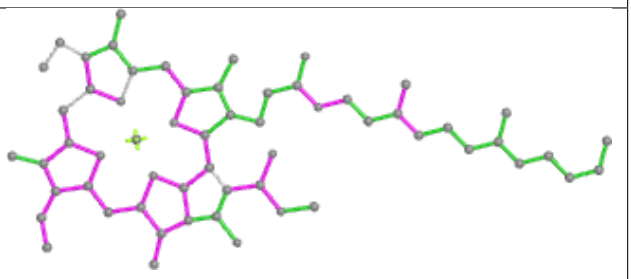


Rings

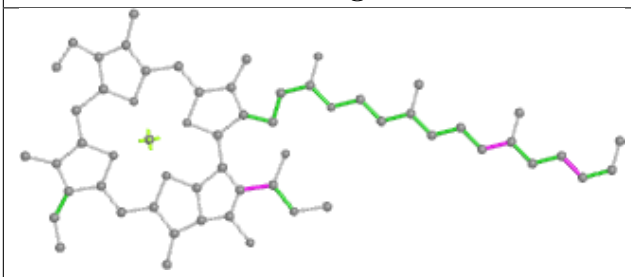
Ligand CLA A 402



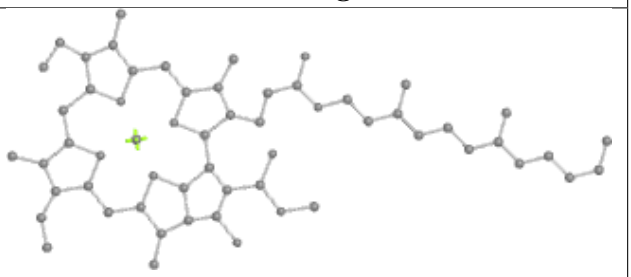
Bond lengths



Bond angles

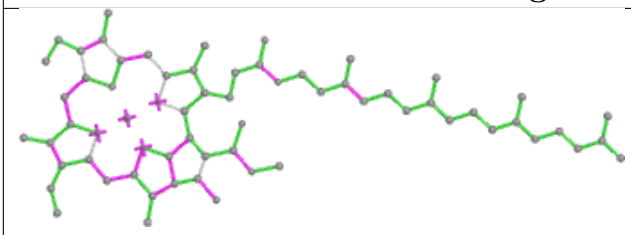


Torsions



Rings

Ligand CLA c 510



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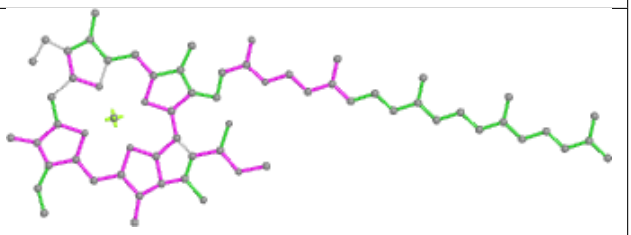
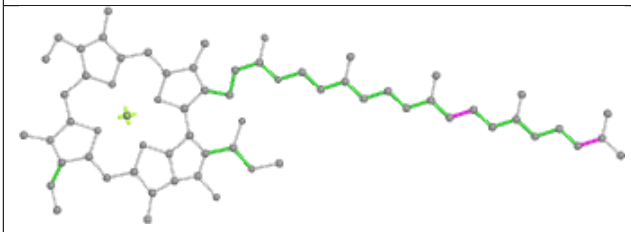
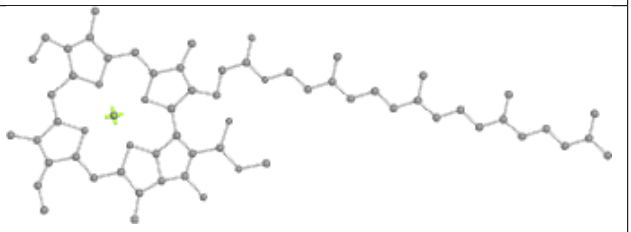


Bond angles

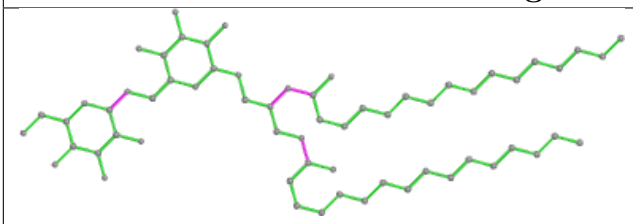


Torsions



Rings

Ligand DGD c 517



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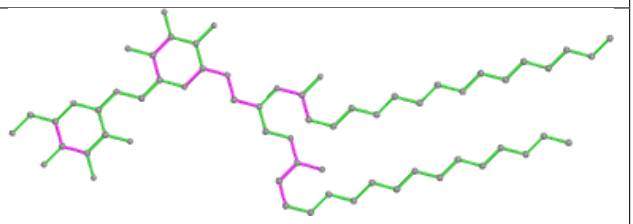
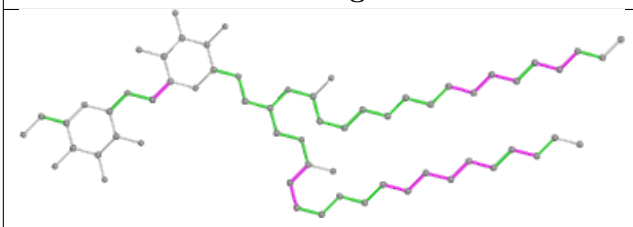


Bond angles



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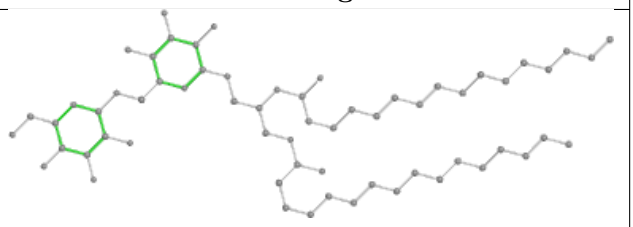
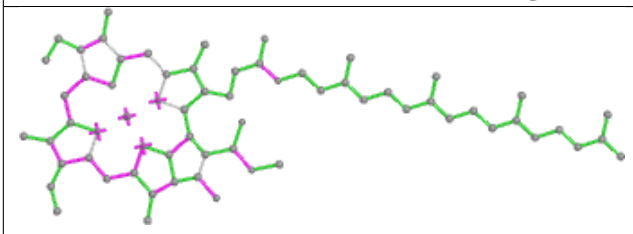


Rings

Ligand CLA B 603



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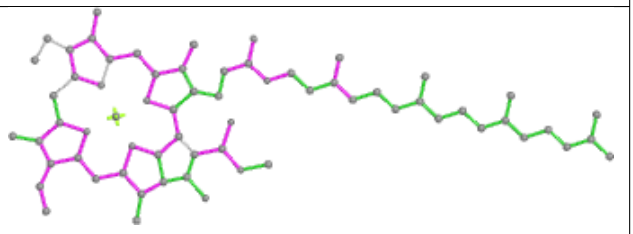
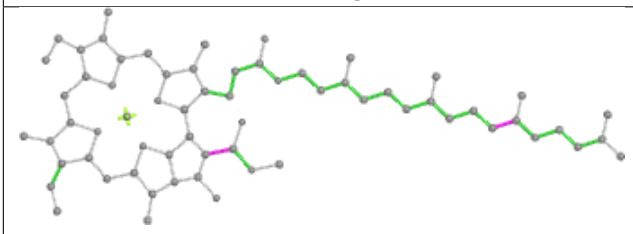


Bond angles



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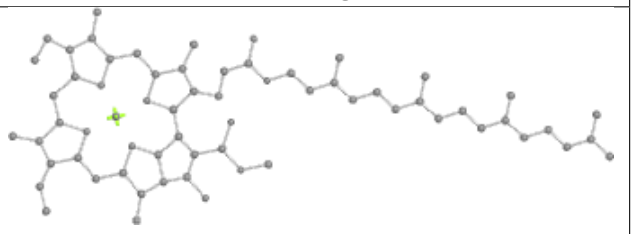
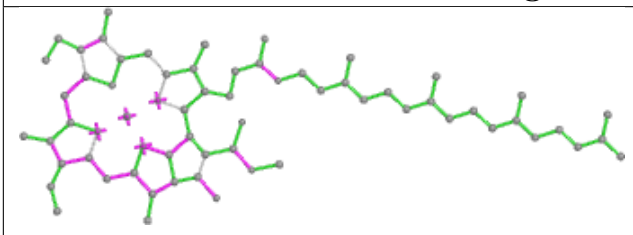
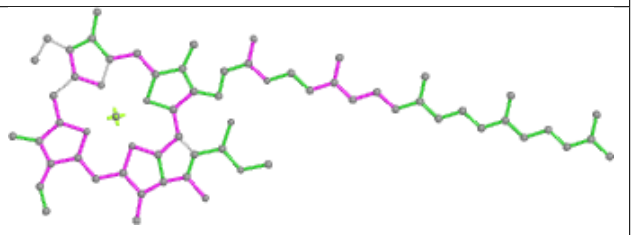


Rings

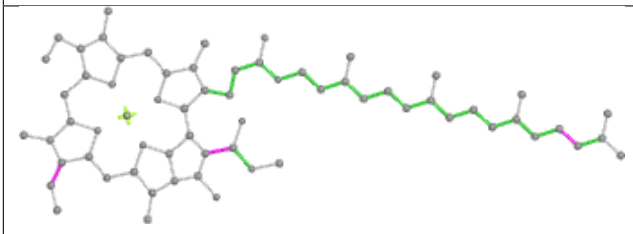
Ligand CLA A 401



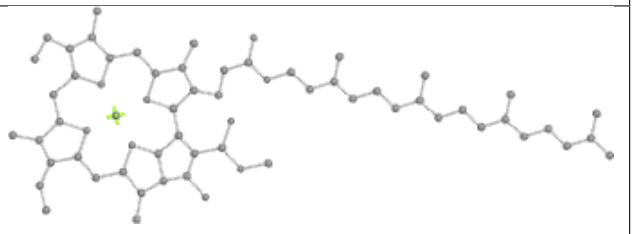
Bond lengths



Bond angles

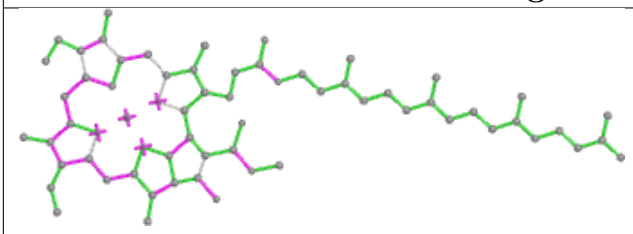


Torsions

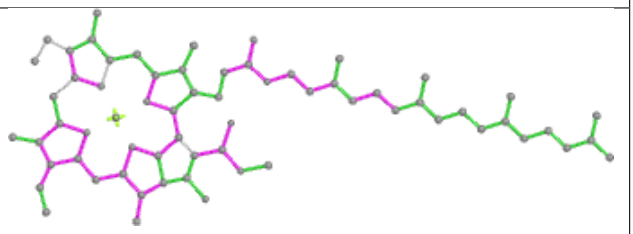


Rings

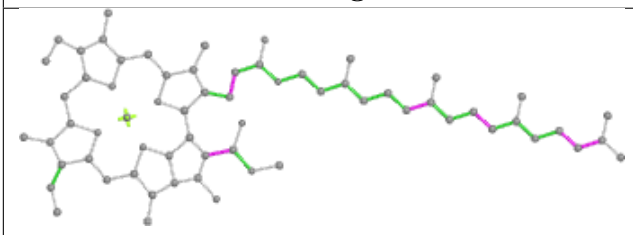
Ligand CLA b 608



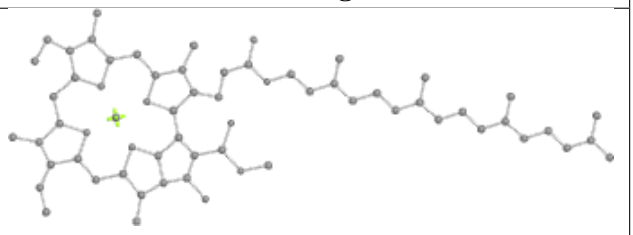
Bond lengths



Bond angles

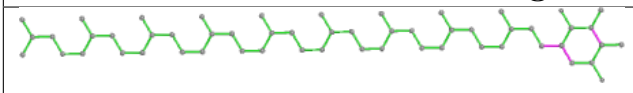


Torsions

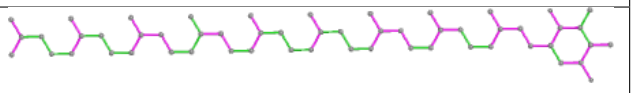


Rings

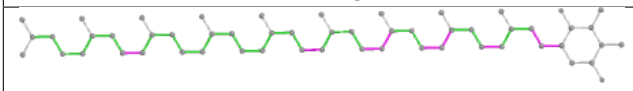
Ligand PL9 A 411



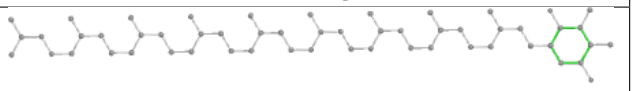
Bond lengths



Bond angles

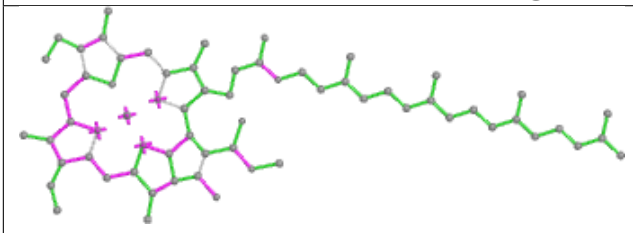


Torsions

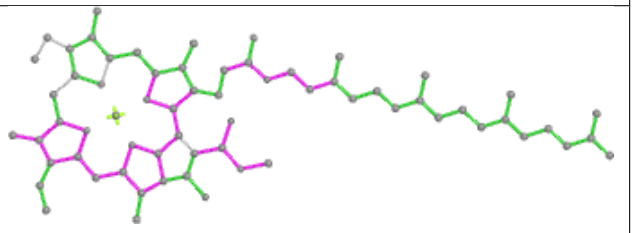


Rings

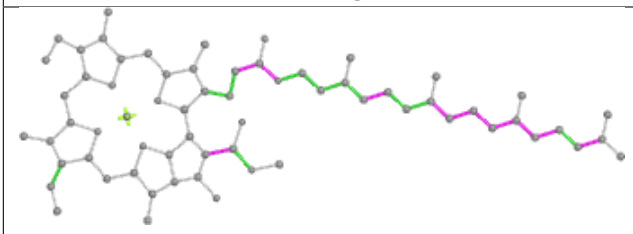
Ligand CLA b 603



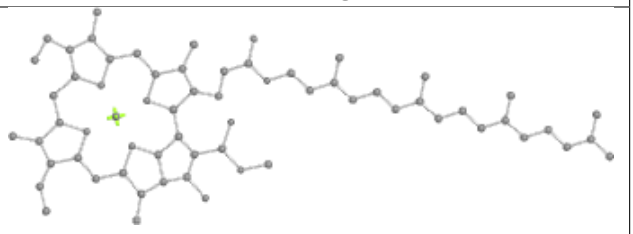
Bond lengths



Bond angles

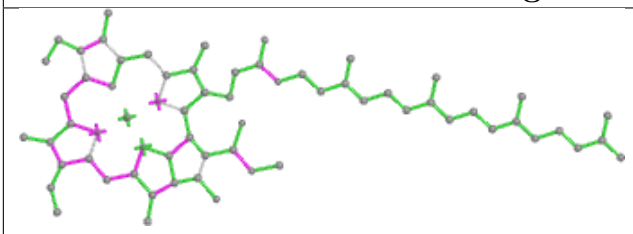


Torsions

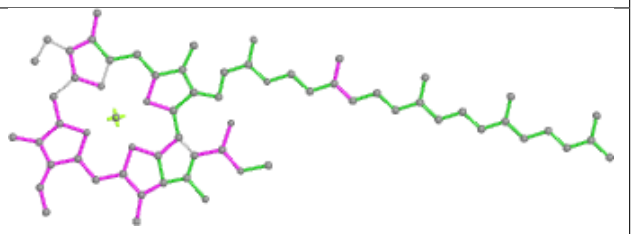


Rings

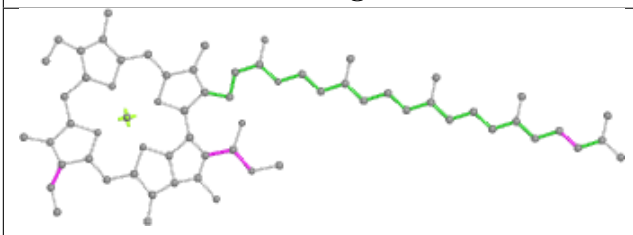
Ligand CLA D 402



Bond lengths



Bond angles



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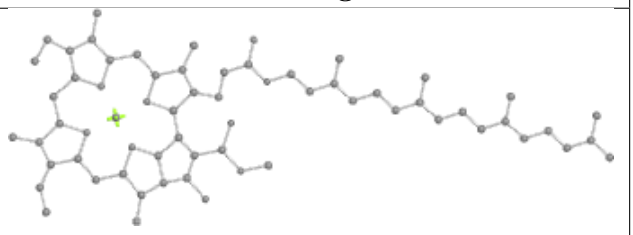
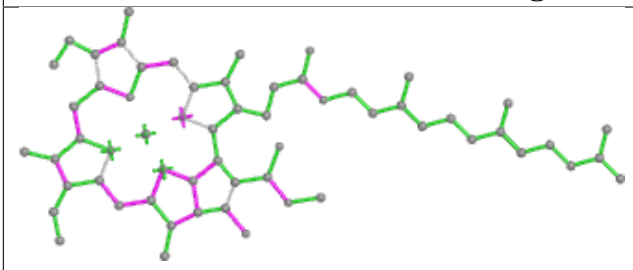


Rings

Ligand CLA a 404



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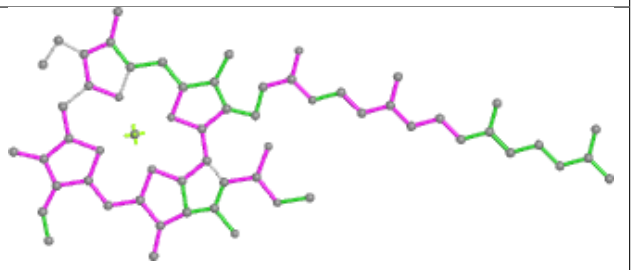
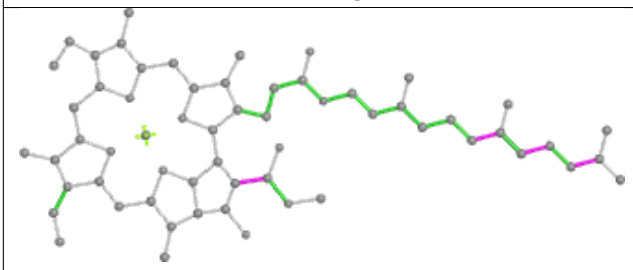
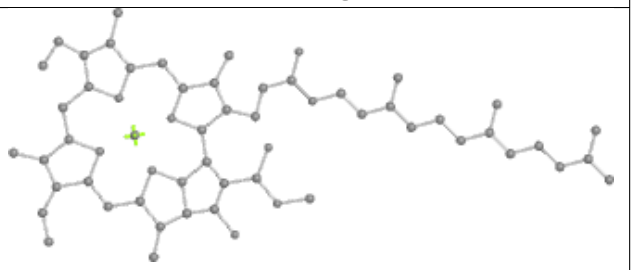


Bond angles

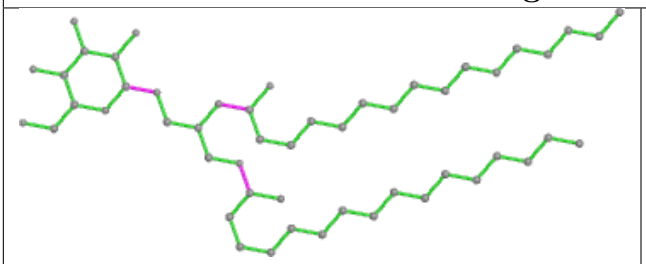


Torsions

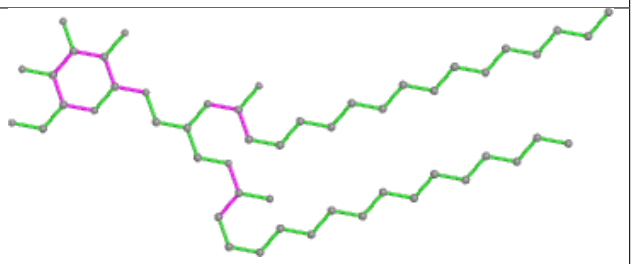


Rings

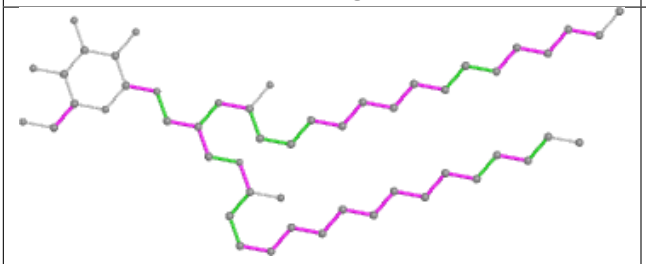
Ligand DGD d 416



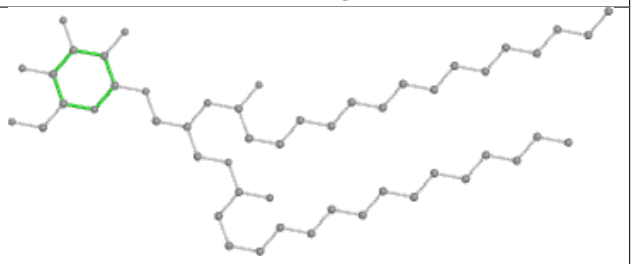
Bond lengths



Bond angles

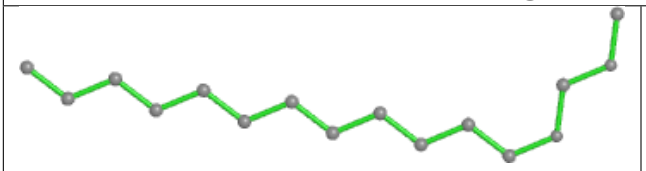


Torsions

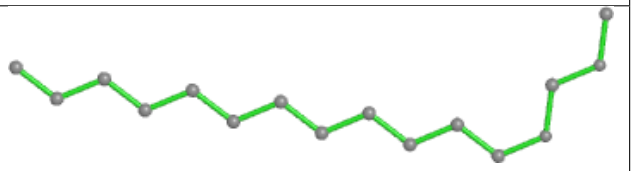


Rings

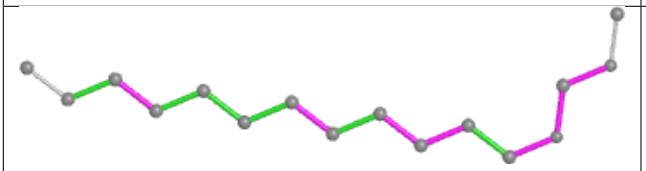
Ligand LMT B 627



Bond lengths



Bond angles



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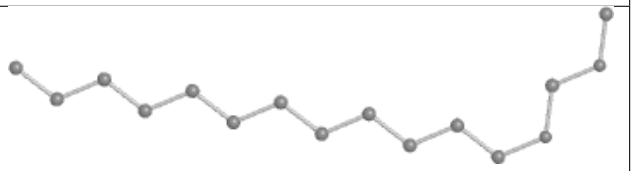
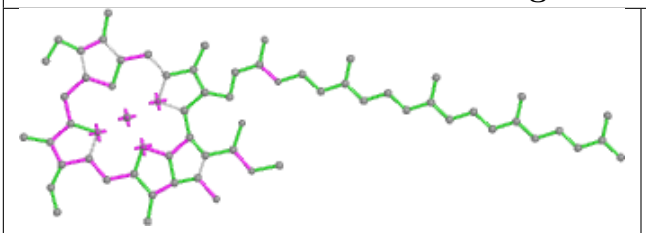
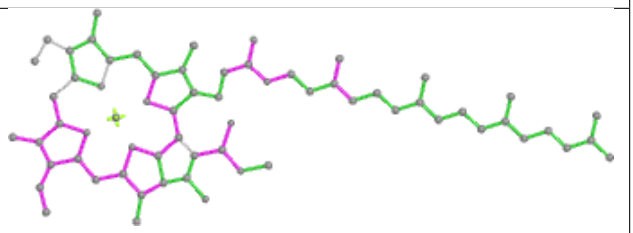


Rings

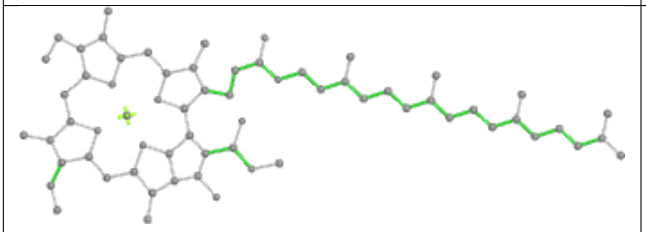
Ligand CLA c 511



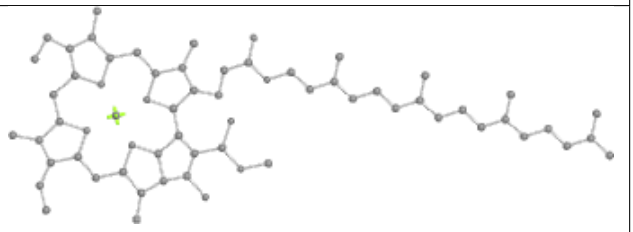
Bond lengths



Bond angles

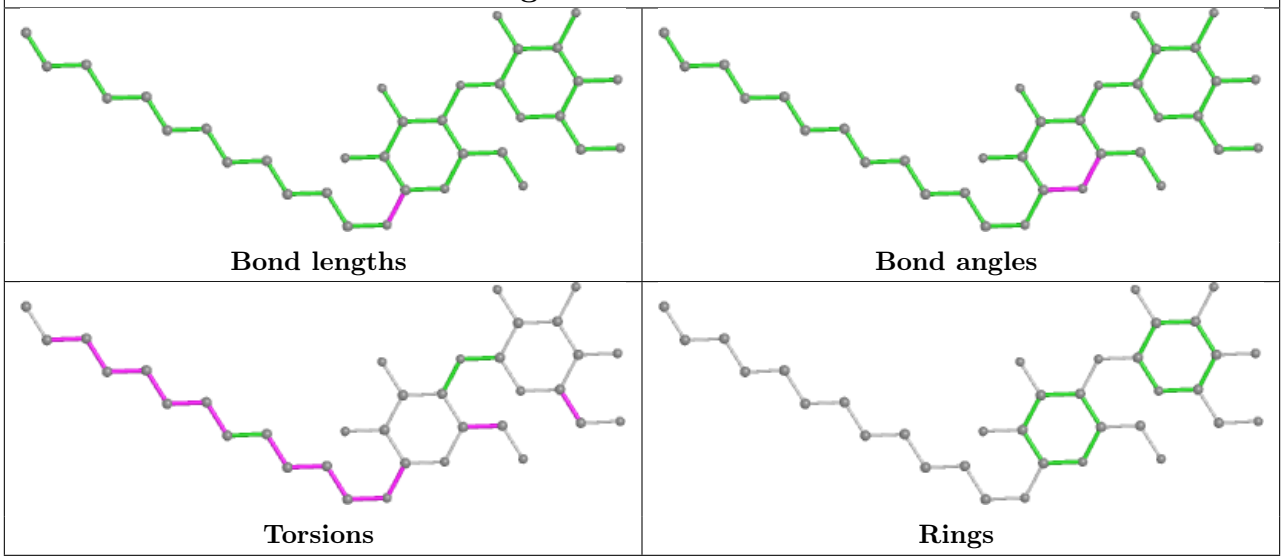


Torsions

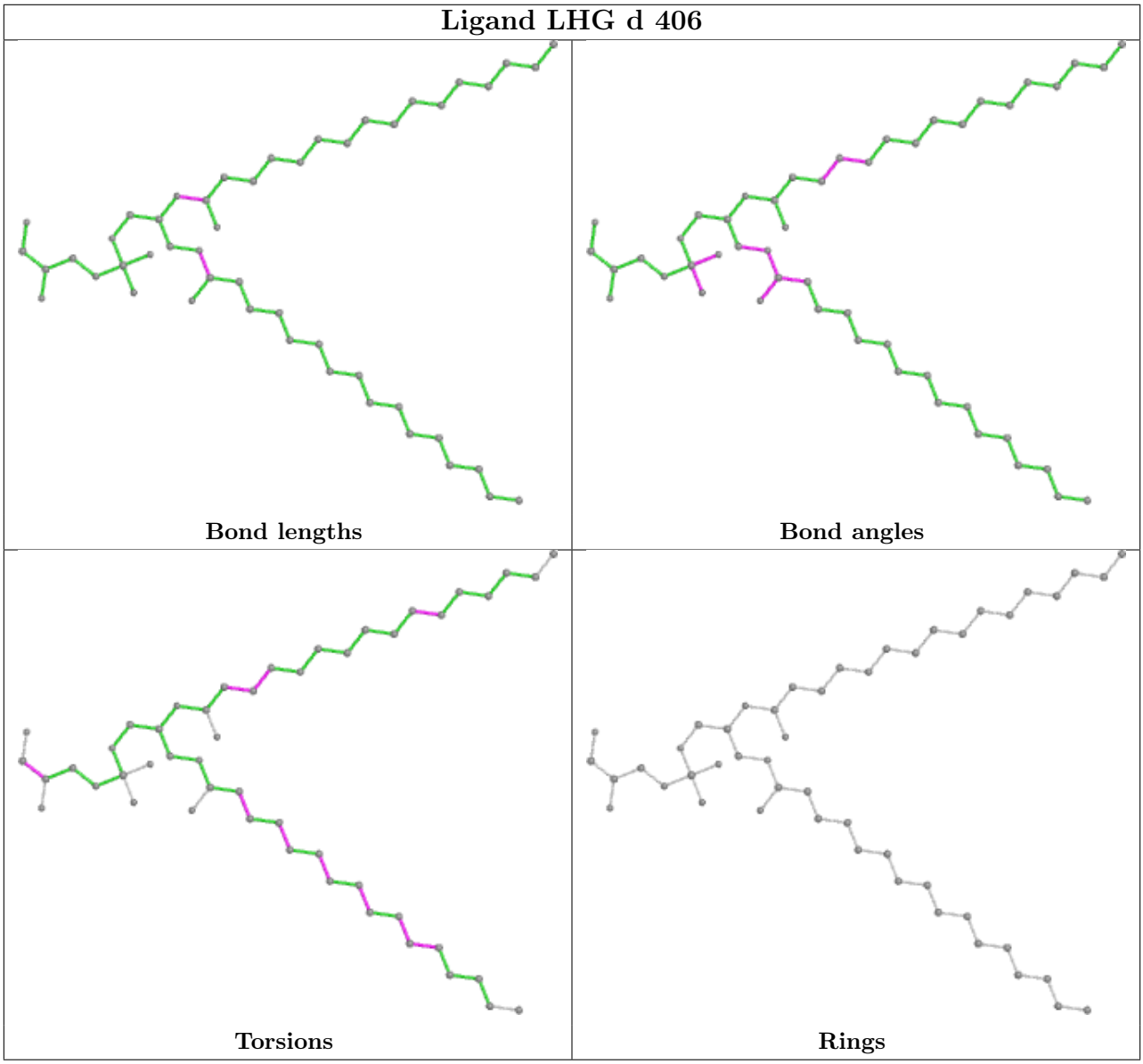


Rings

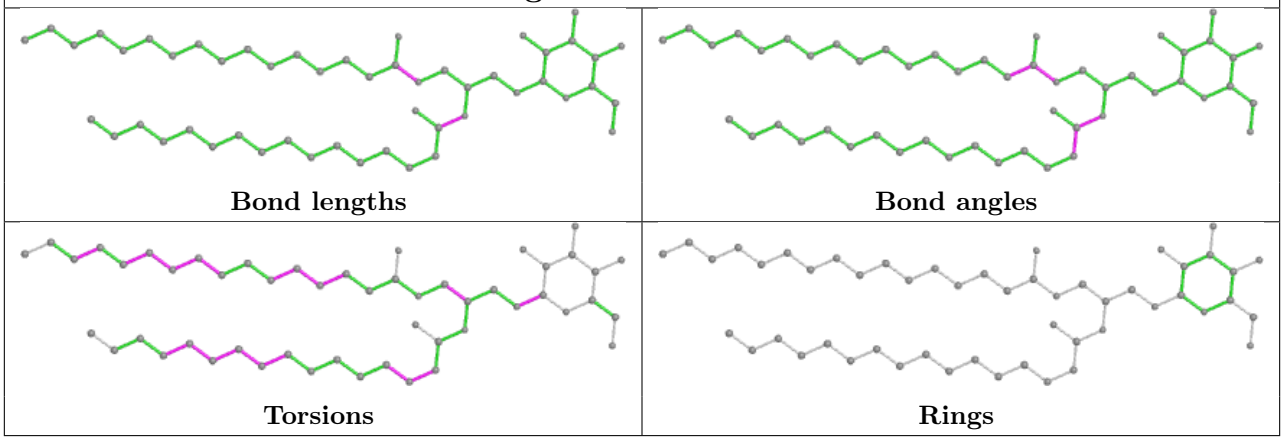
Ligand LMT m 101



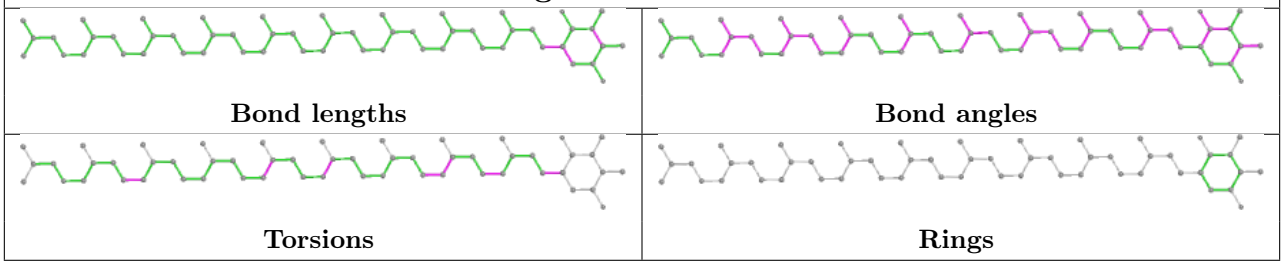
Ligand LHG d 406



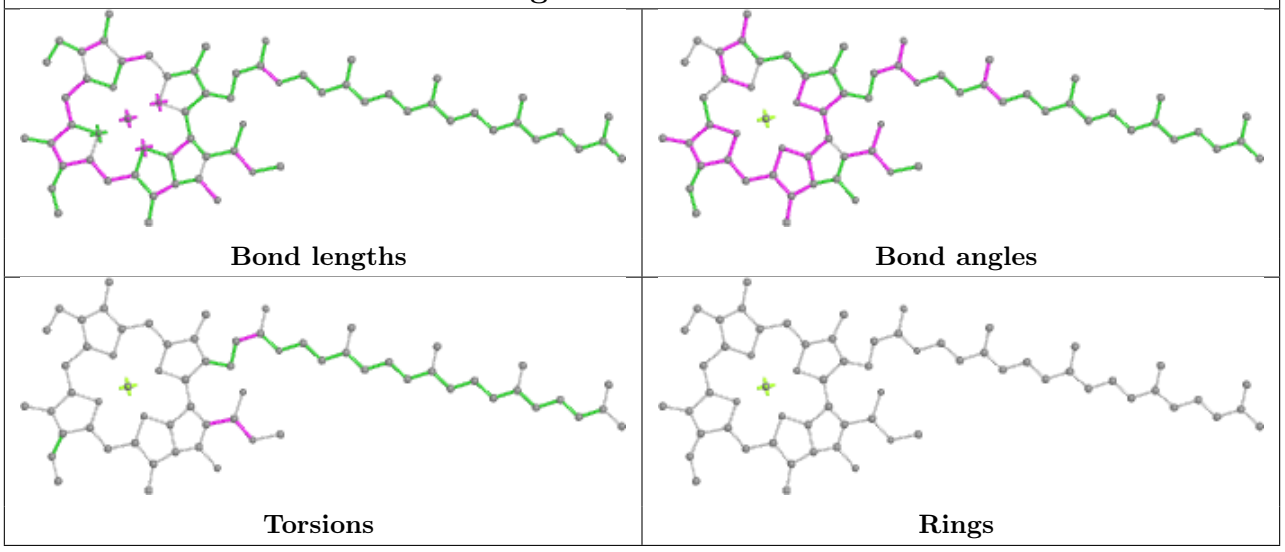
Ligand LMG a 410



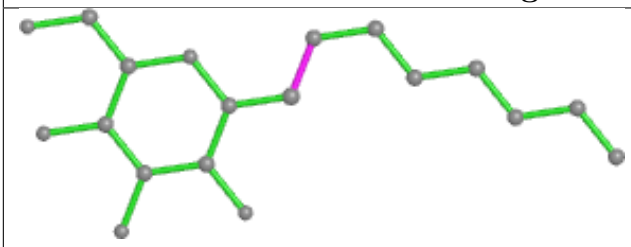
Ligand PL9 a 415



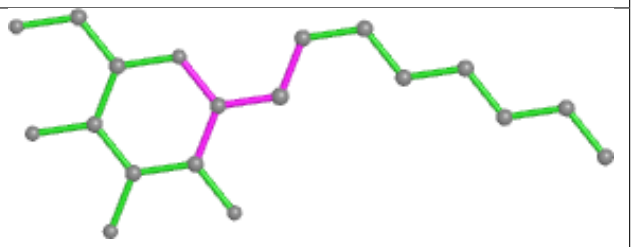
Ligand CLA c 501



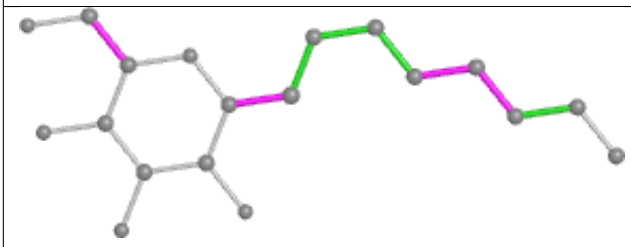
Ligand HTG B 623



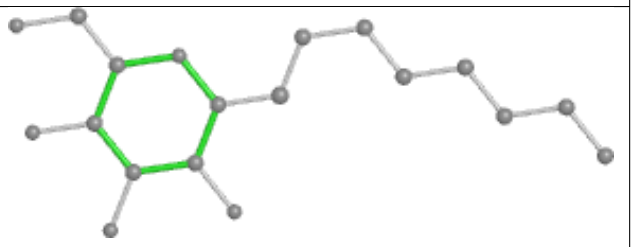
Bond lengths



Bond angles

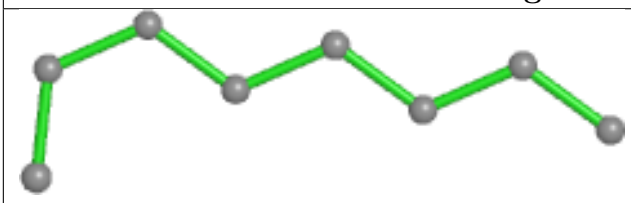


Torsions

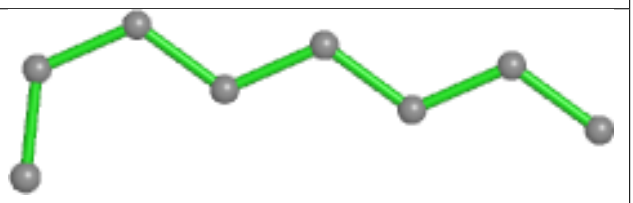


Rings

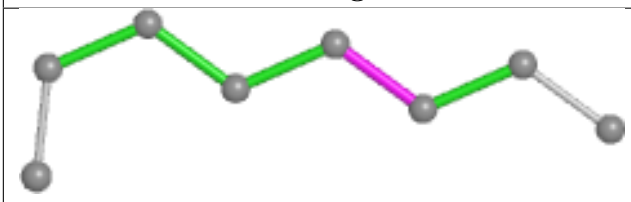
Ligand HTG u 201



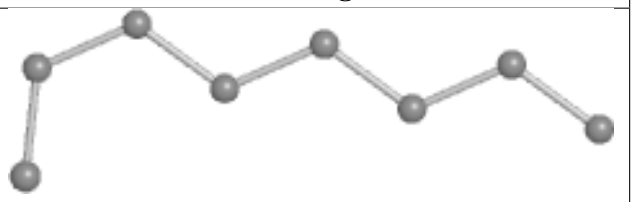
Bond lengths



Bond angles

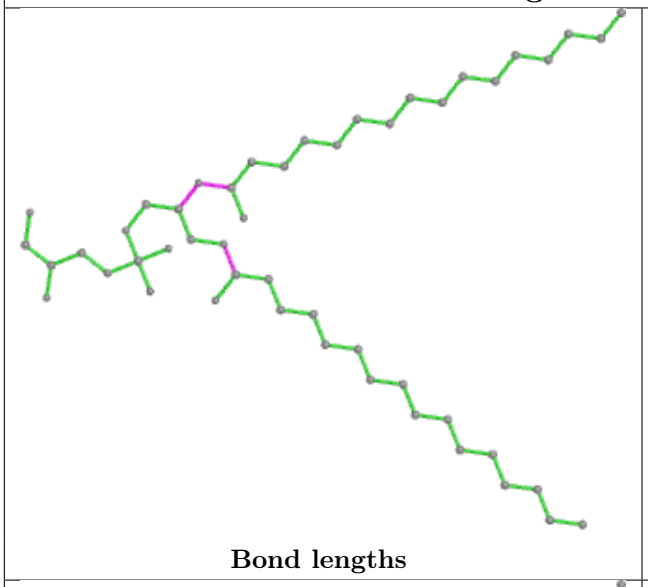


Torsions

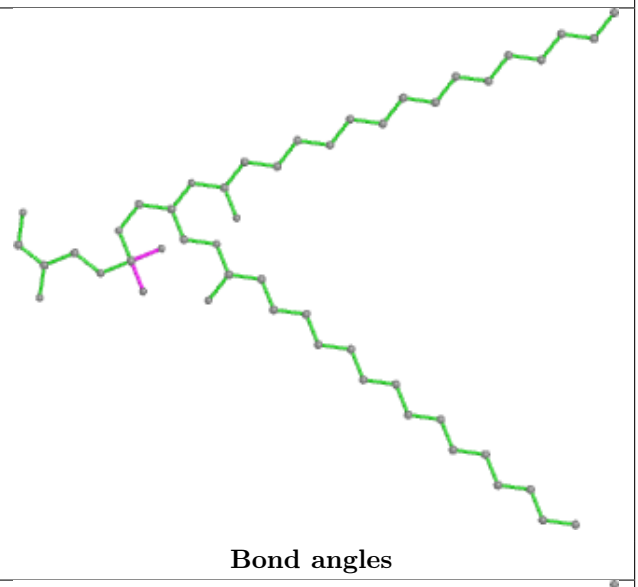


Rings

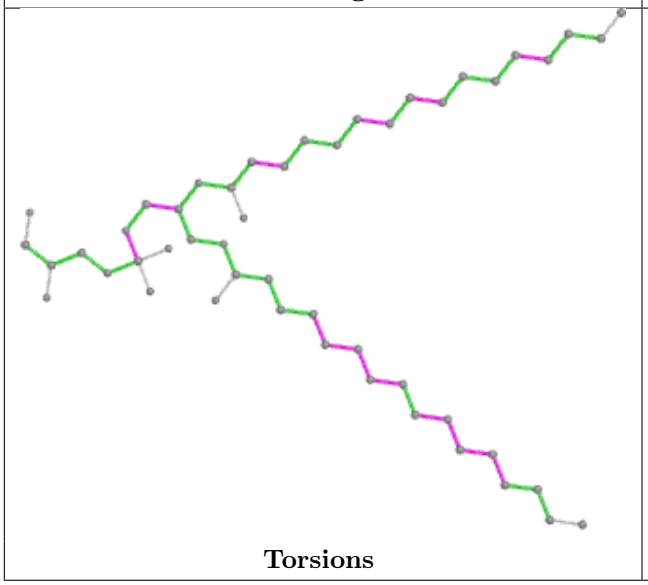
Ligand LHG L 101



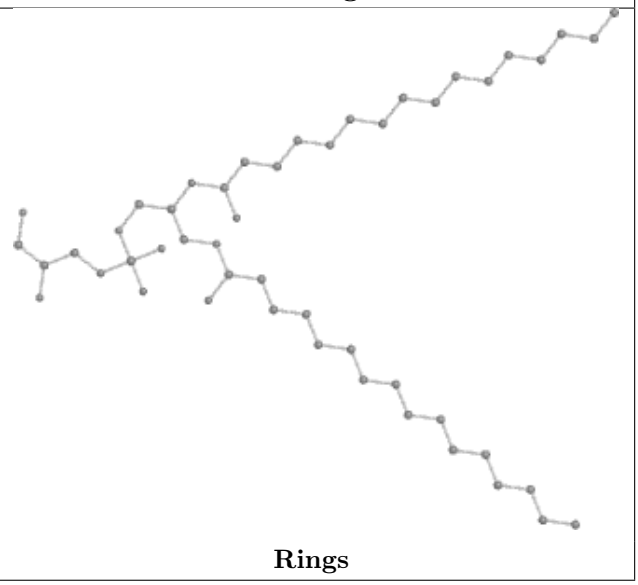
Bond lengths



Bond angles

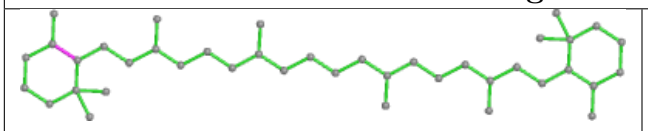


Torsions

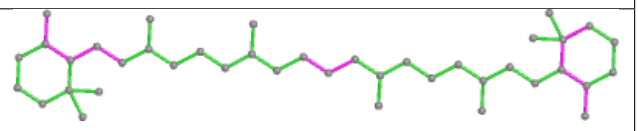


Rings

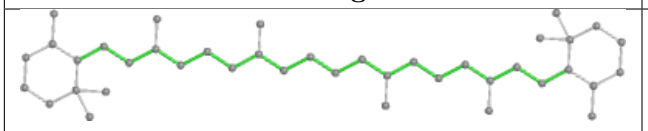
Ligand BCR b 620



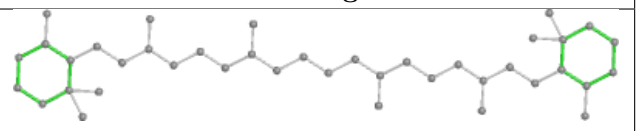
Bond lengths



Bond angles

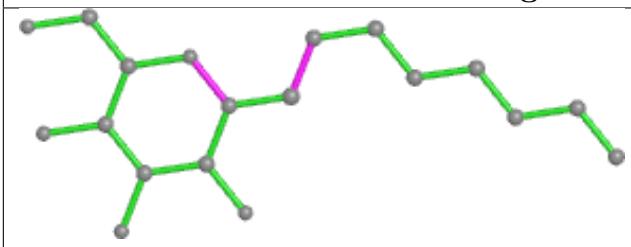


Torsions

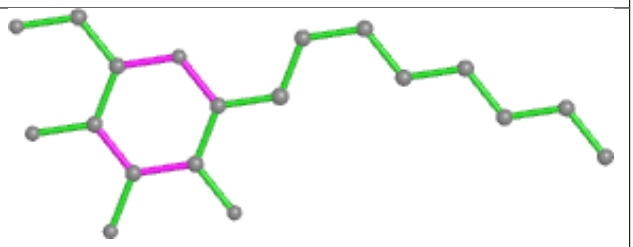


Rings

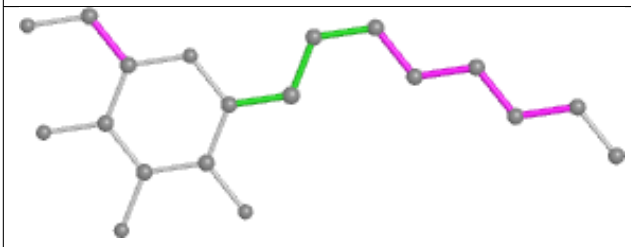
Ligand HTG O 302



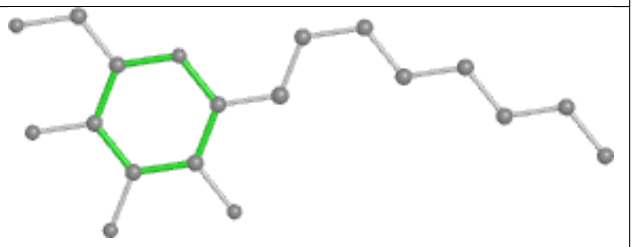
Bond lengths



Bond angles

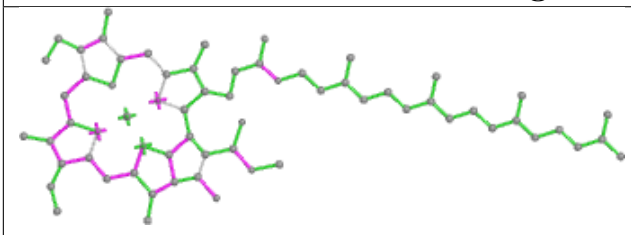


Torsions

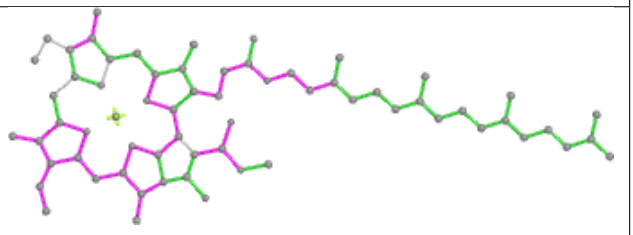


Rings

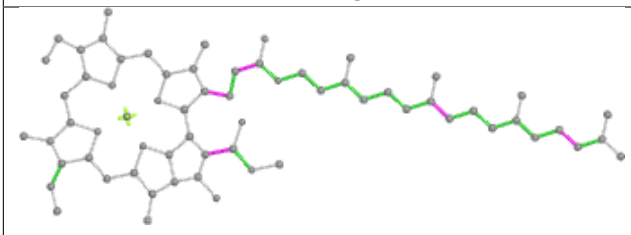
Ligand CLA c 512



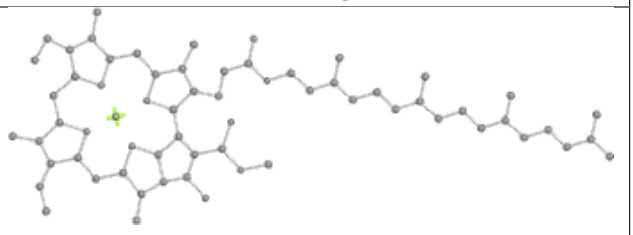
Bond lengths



Bond angles

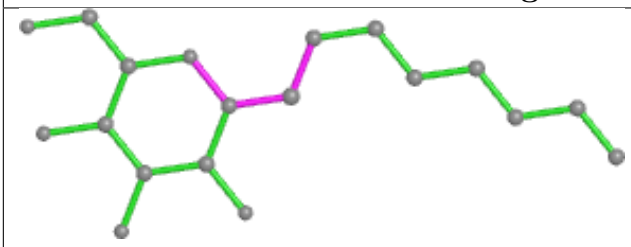


Torsions

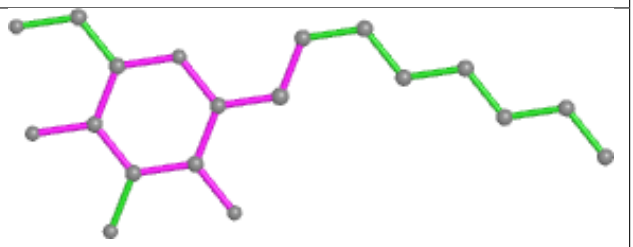


Rings

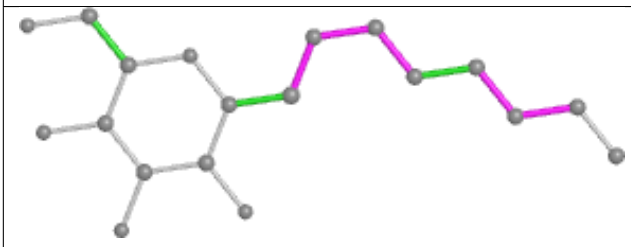
Ligand HTG B 622



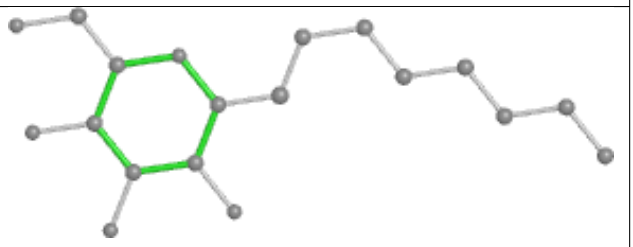
Bond lengths



Bond angles

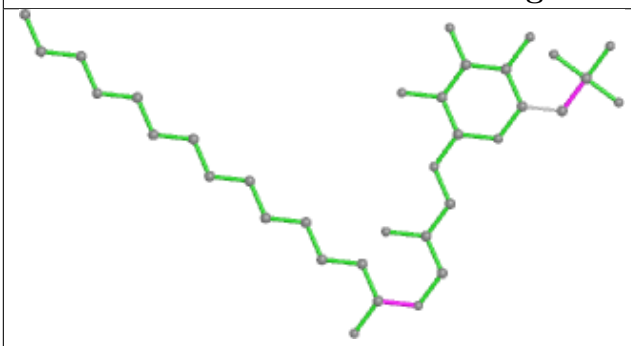


Torsions

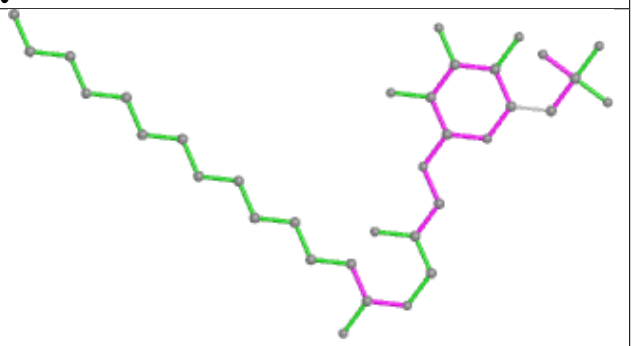


Rings

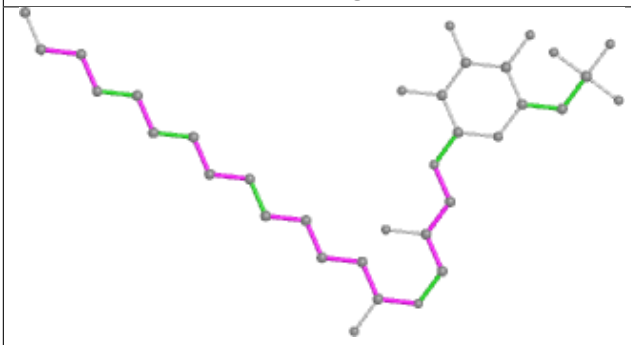
Ligand SQD F 101



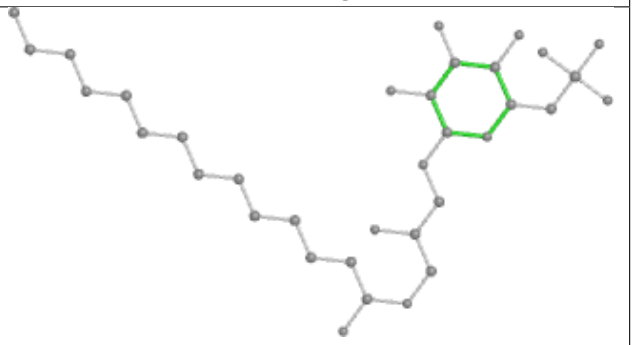
Bond lengths



Bond angles

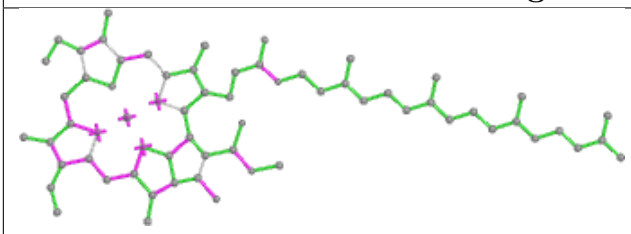


Torsions



Rings

Ligand CLA b 609



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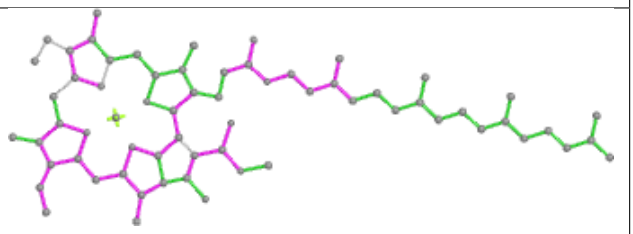

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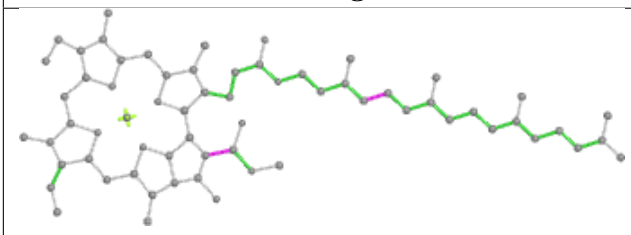

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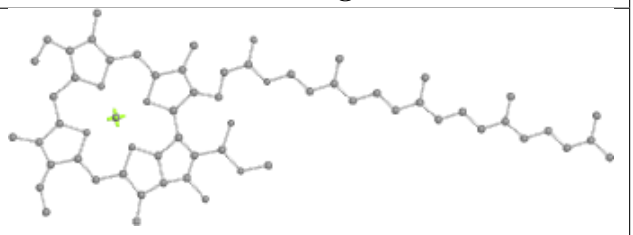
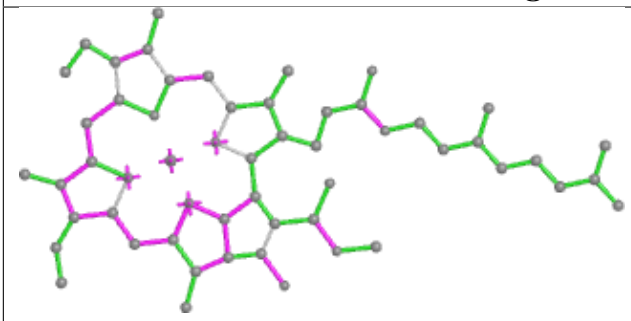


Rings

Ligand CLA C 512



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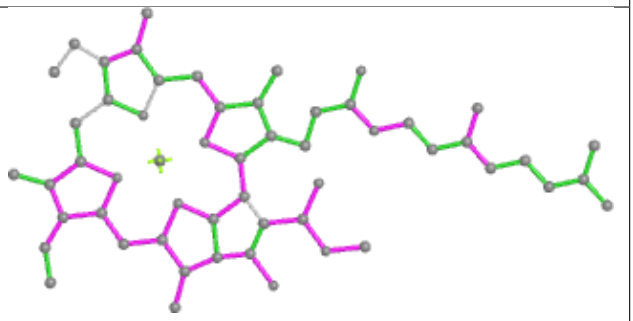

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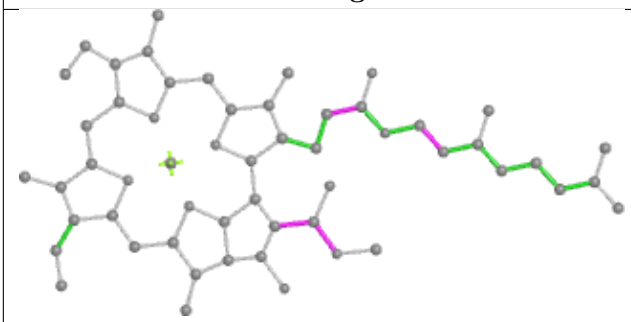

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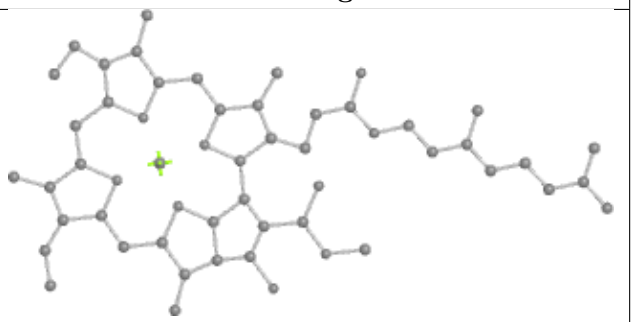
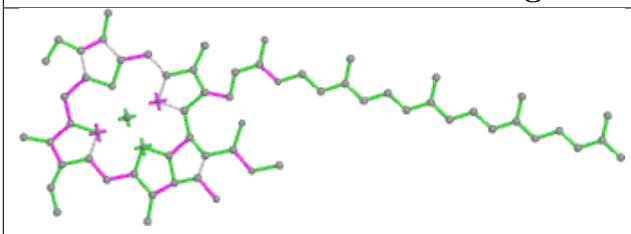


Rings

Ligand CLA C 502



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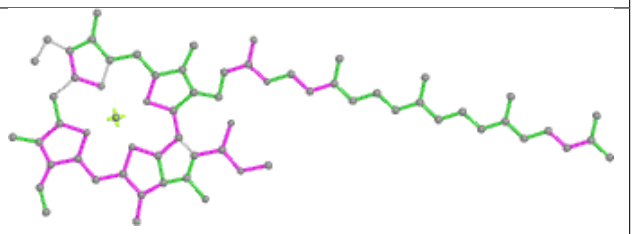

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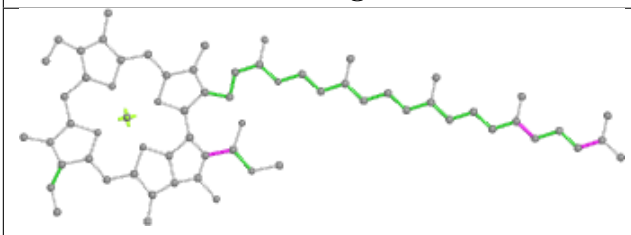

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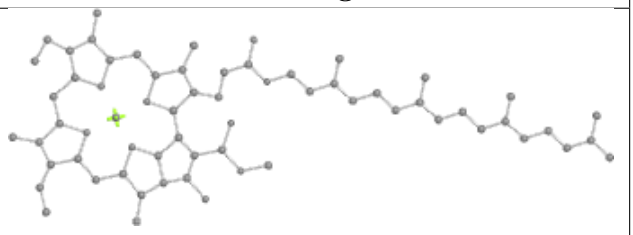
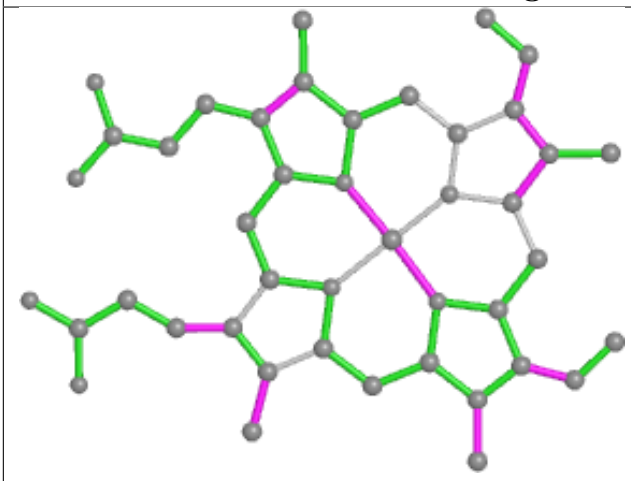


Rings

Ligand HEM e 102



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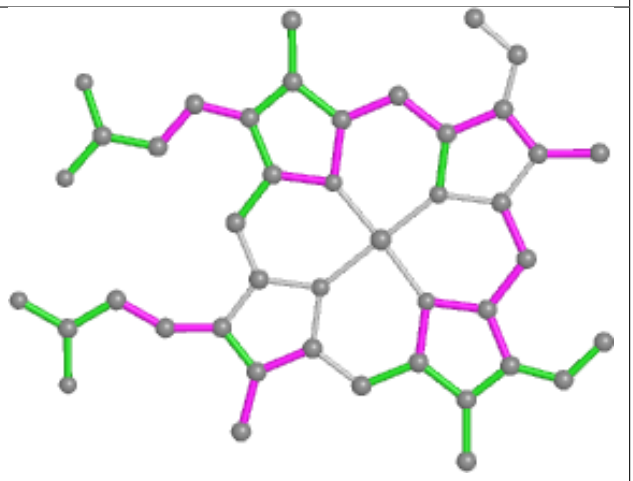

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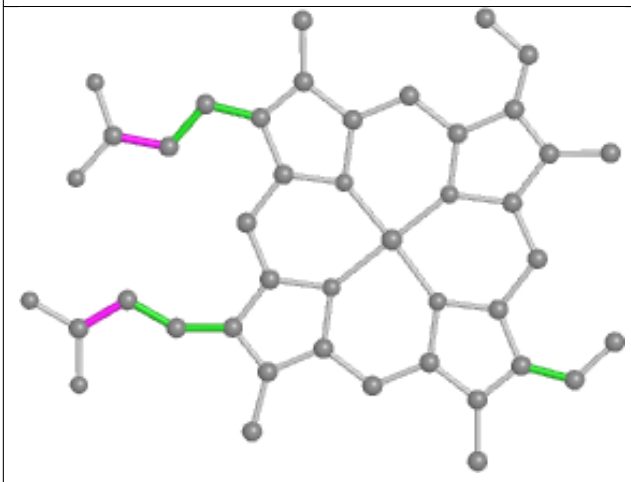

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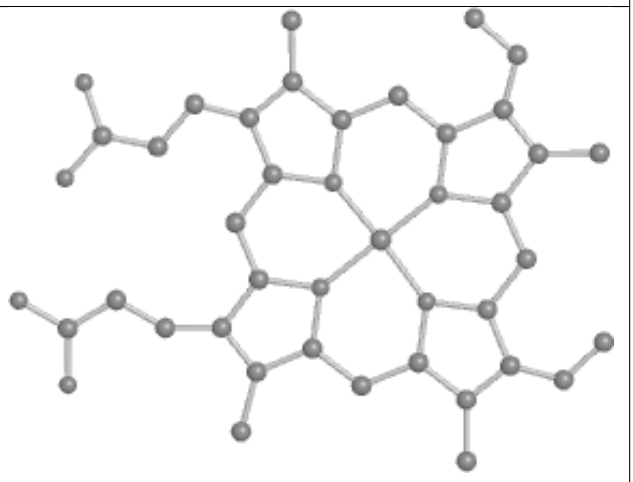
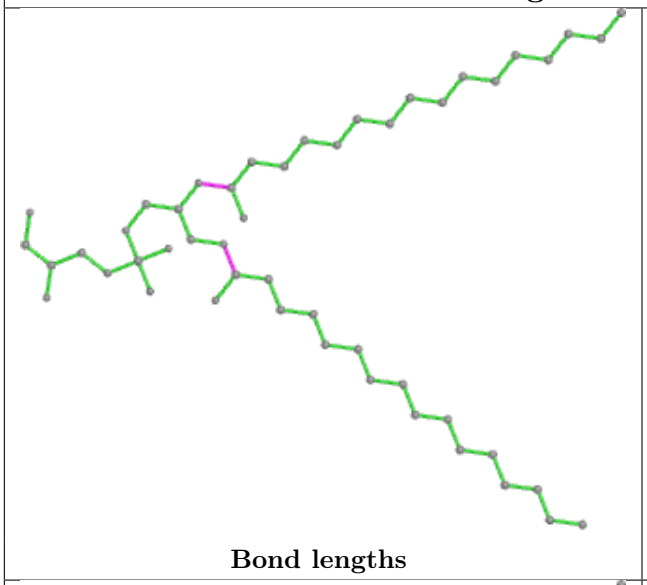


Rings

Ligand LHG d 407



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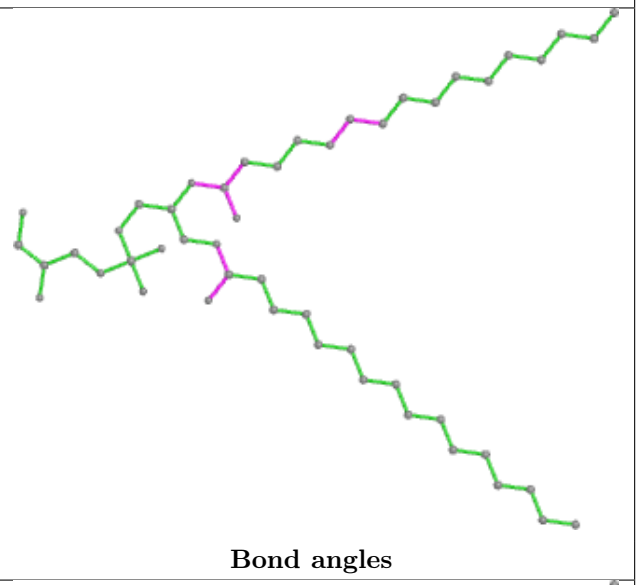
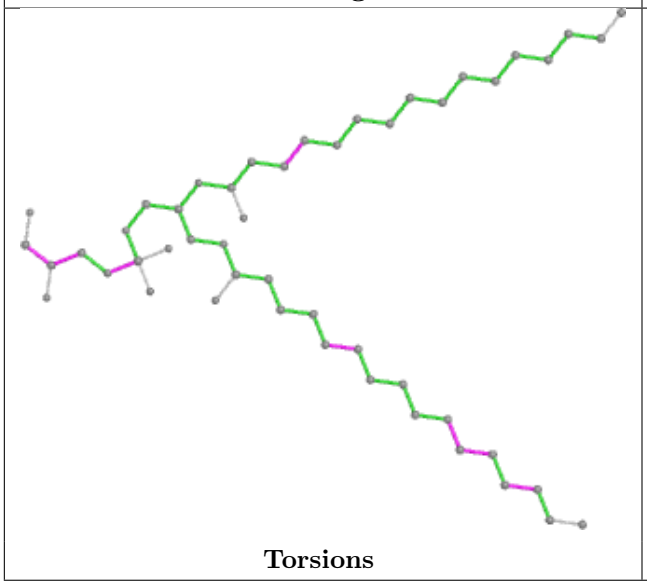


Bond angles



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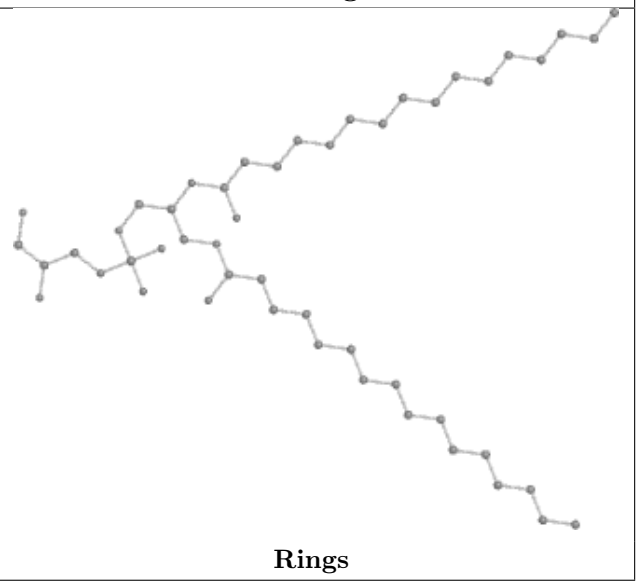
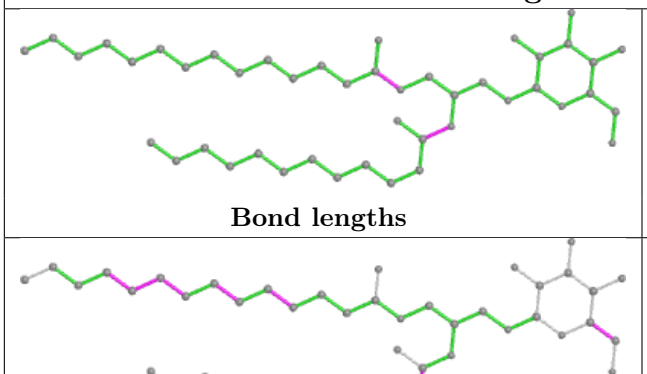


Rings

Ligand LMG J 101



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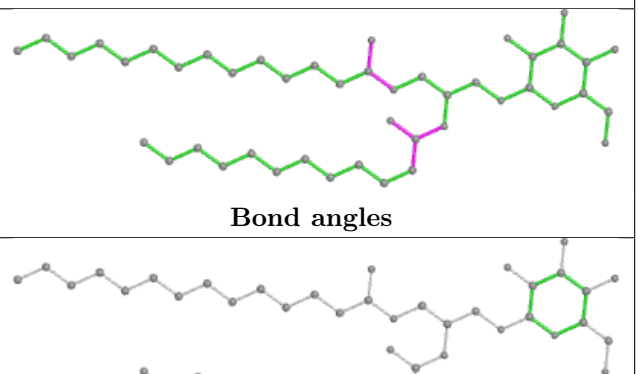
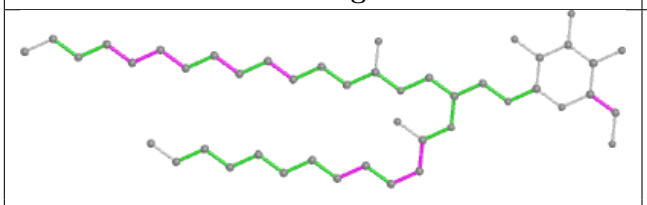


Bond angles



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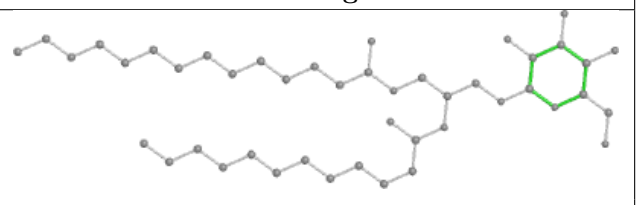
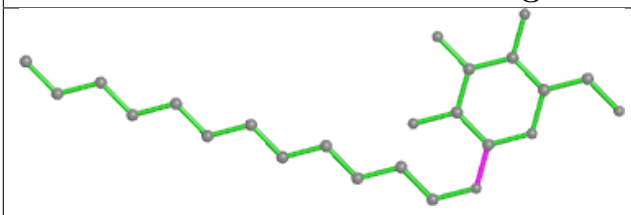


Rings

Ligand LMT E 101



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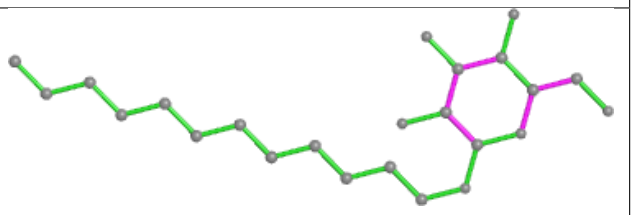
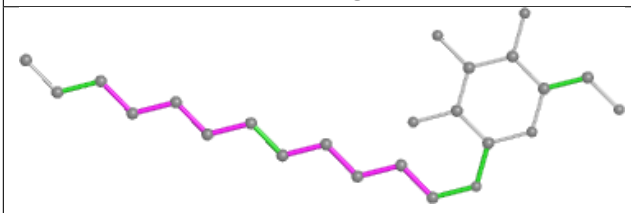


Bond angles



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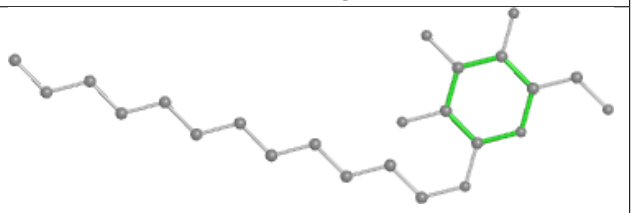
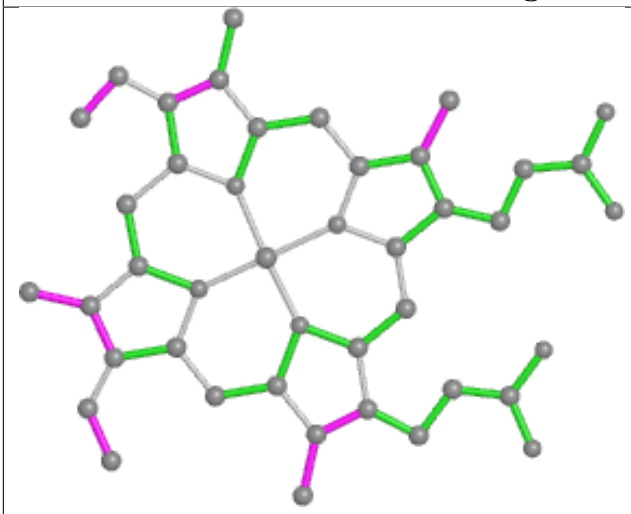
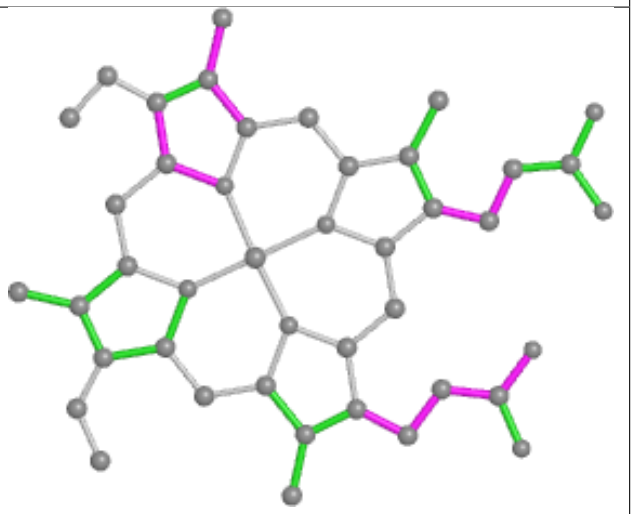


Rings

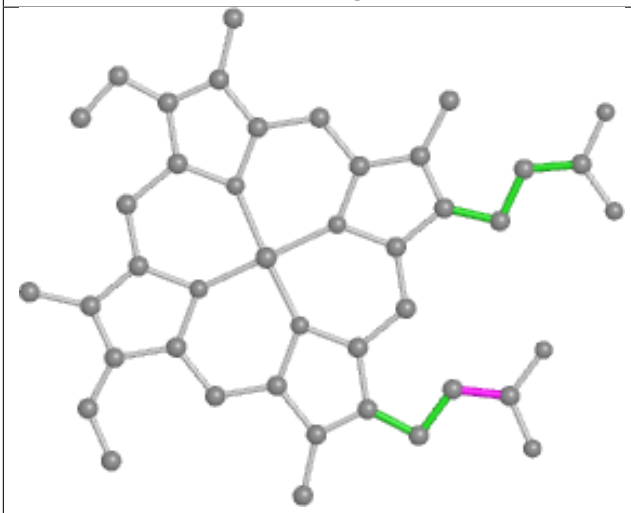
Ligand HEC V 201



Bond lengths



Bond angles



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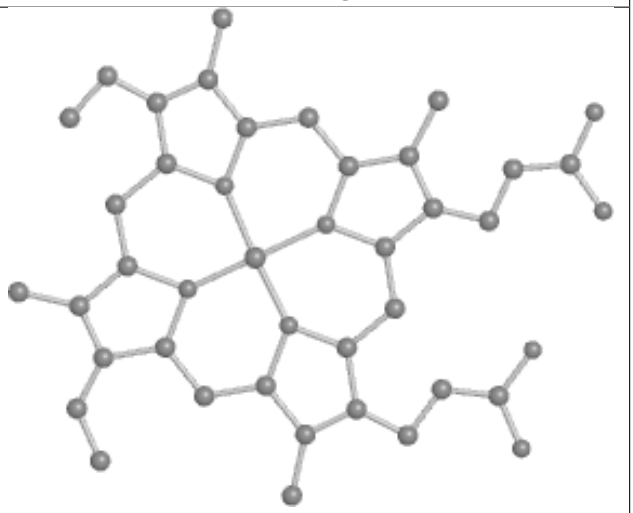
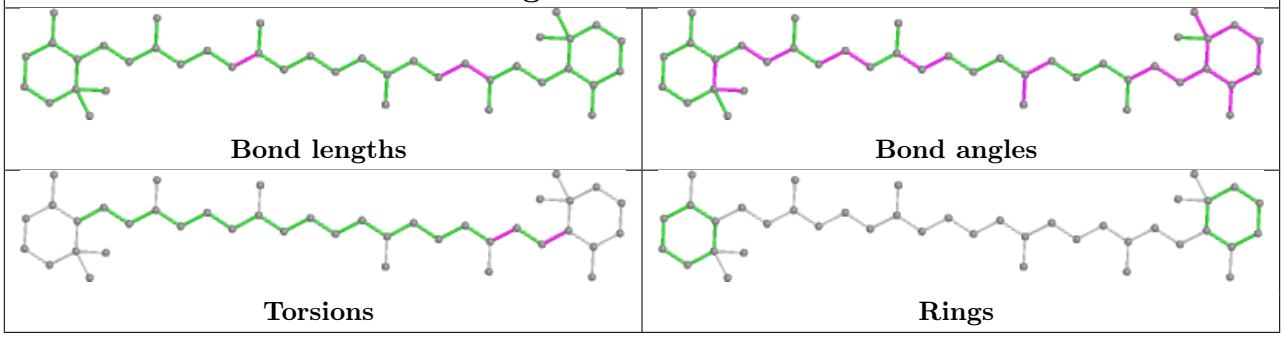
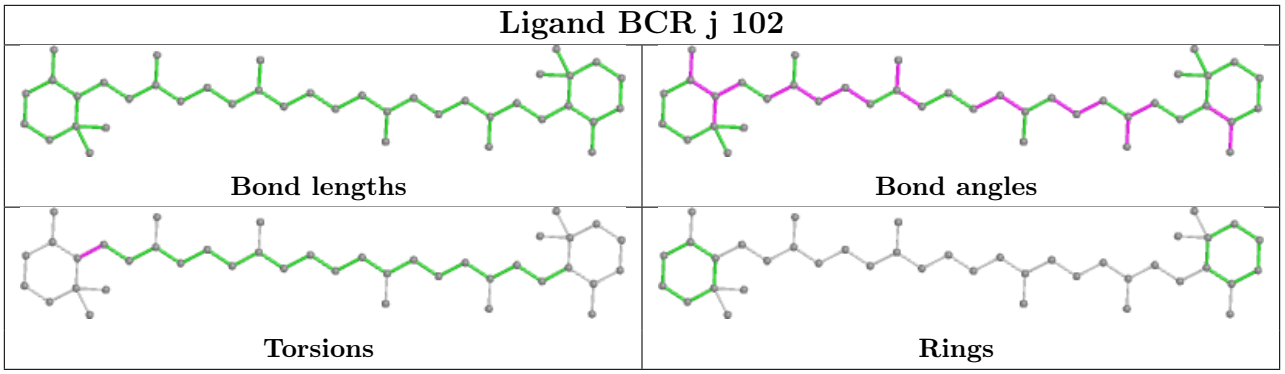


Rings

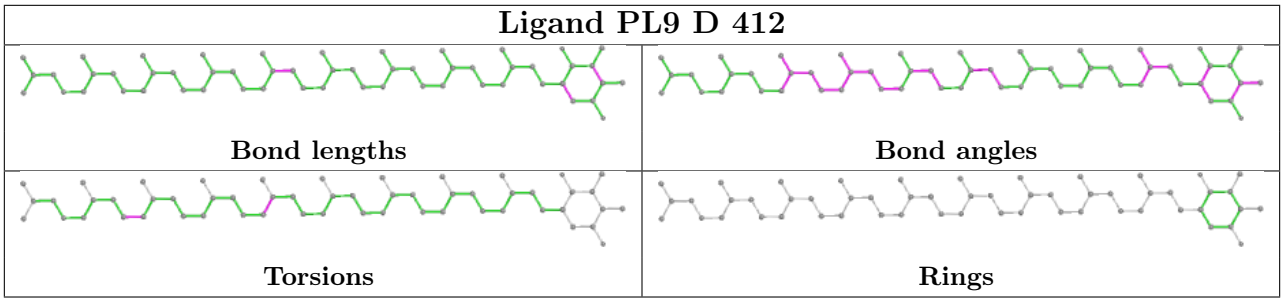
Ligand BCR D 405



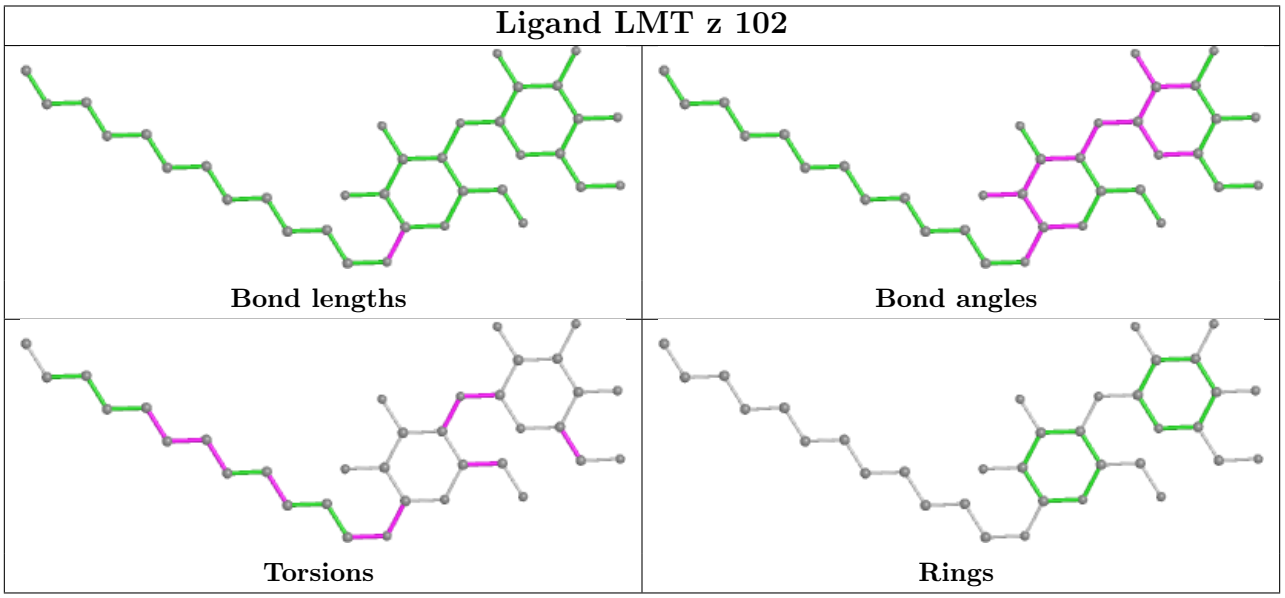
Ligand BCR j 102



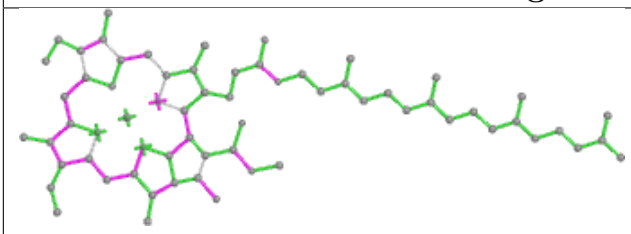
Ligand PL9 D 412



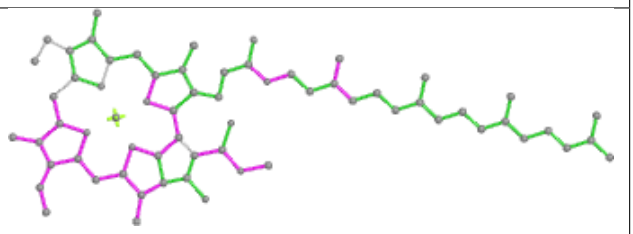
Ligand LMT z 102



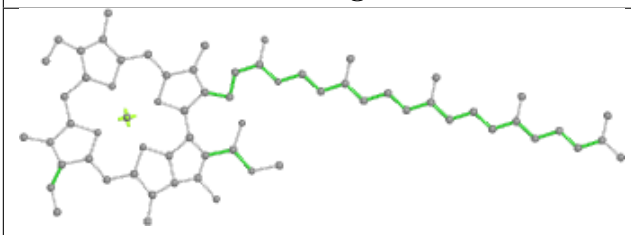
Ligand CLA b 611



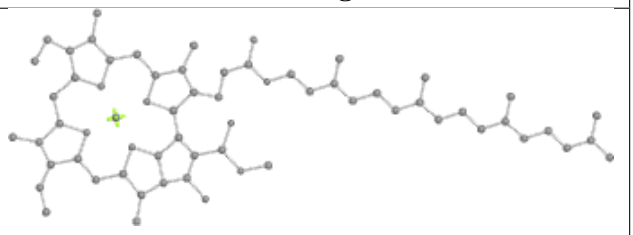
Bond lengths



Bond angles

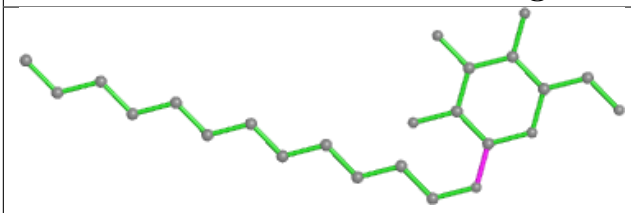


Torsions



Rings

Ligand LMT f 102



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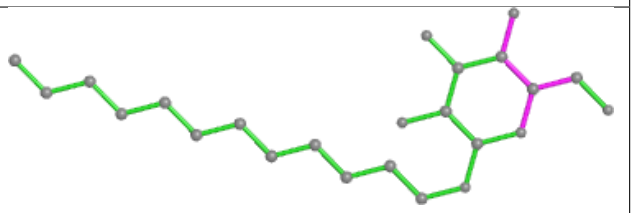
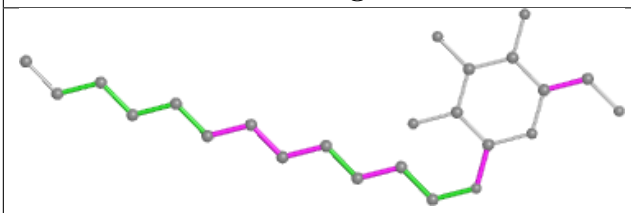


Bond angles



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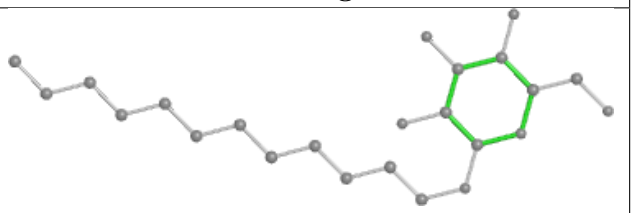
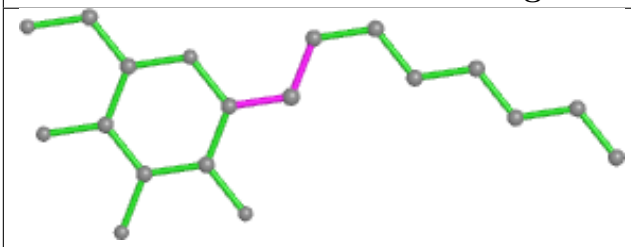
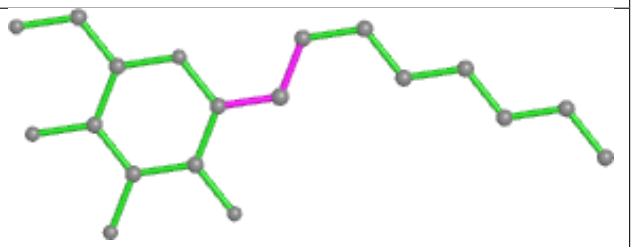


Rings

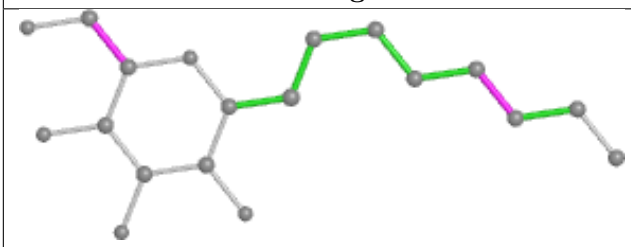
Ligand HTG b 602



Bond lengths



Bond angles



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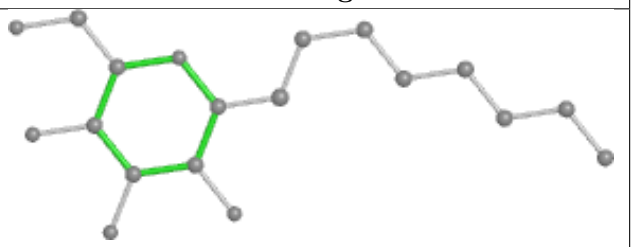
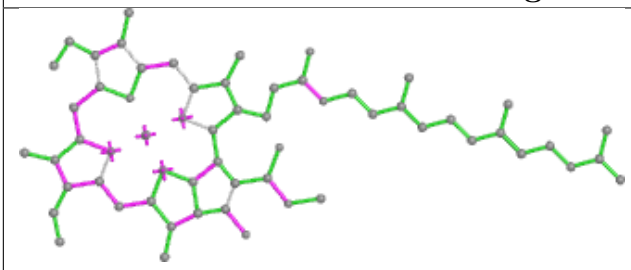
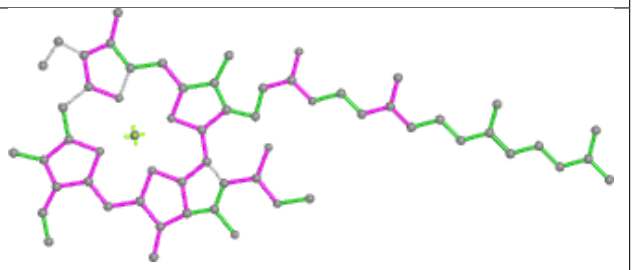


Rings

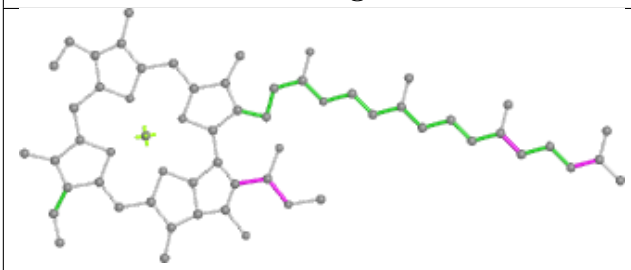
Ligand CLA C 508



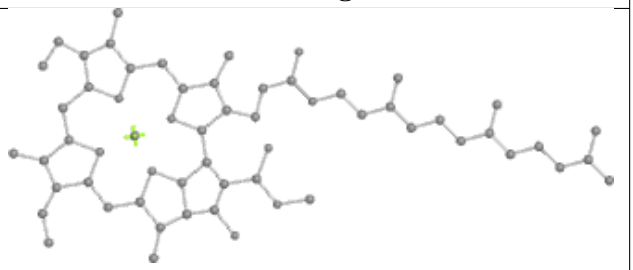
Bond lengths



Bond angles

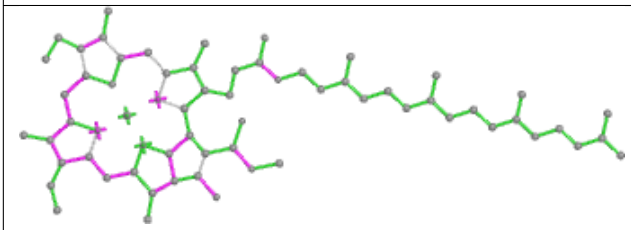


Torsions

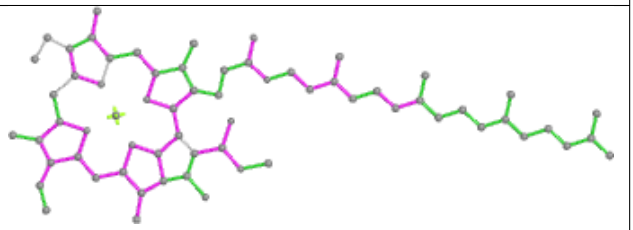


Rings

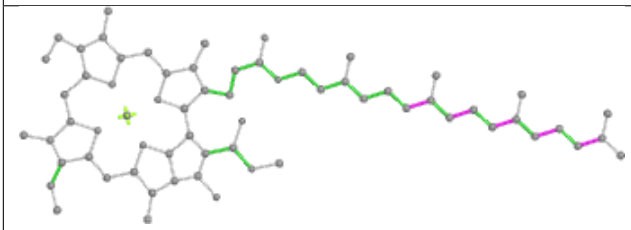
Ligand CLA d 404



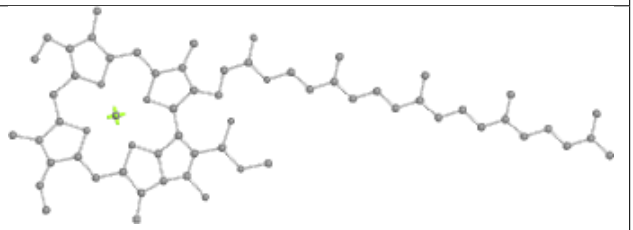
Bond lengths



Bond angles

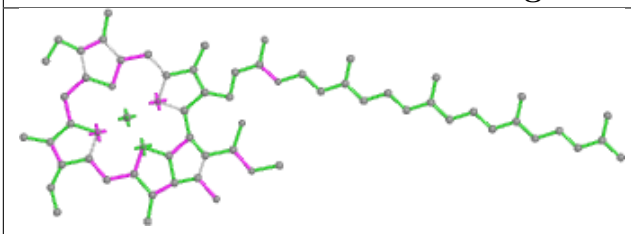


Torsions



Rings

Ligand CLA B 610



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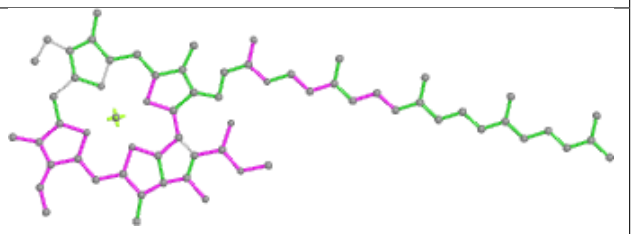
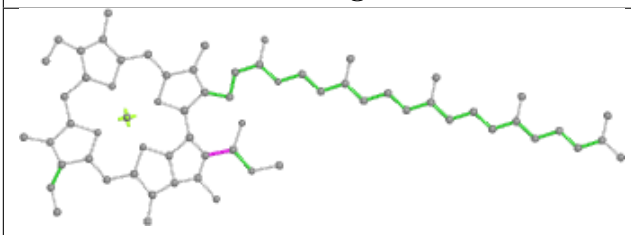
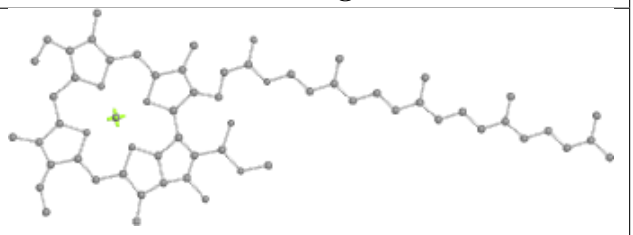


Bond angles

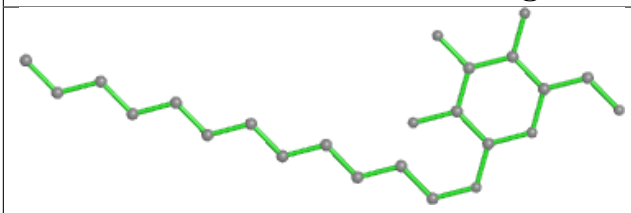


Torsions



Rings

Ligand LMT B 625



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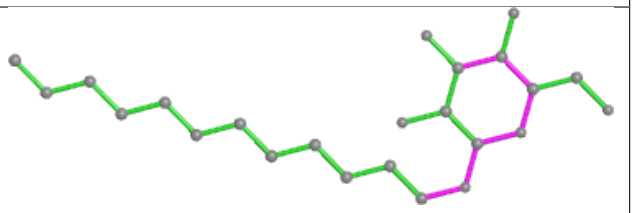
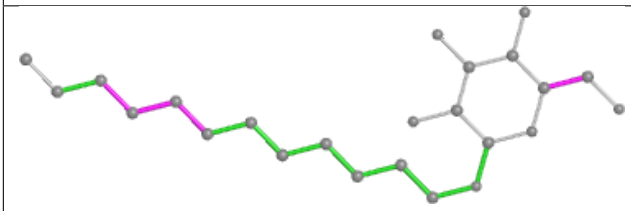


Bond angles



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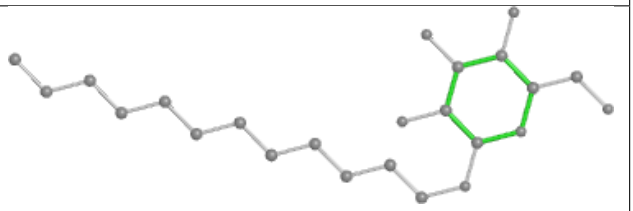
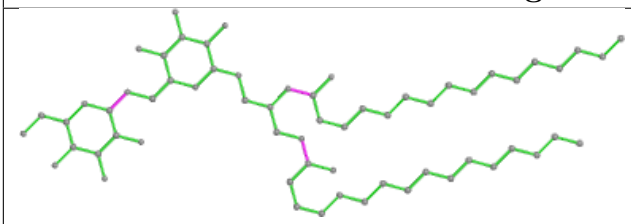


Rings

Ligand DGD c 515



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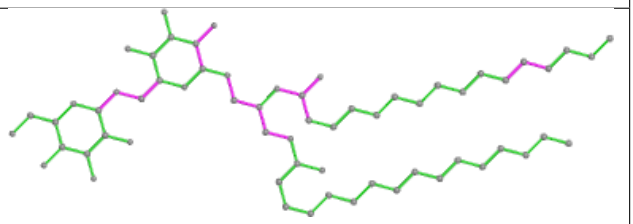
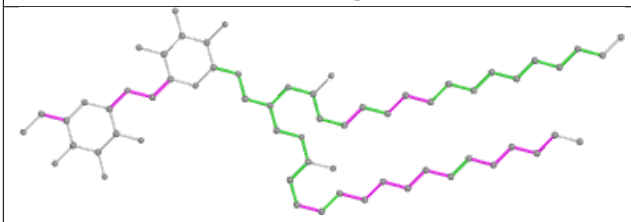


Bond angles



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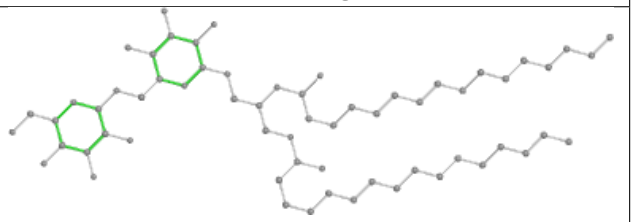
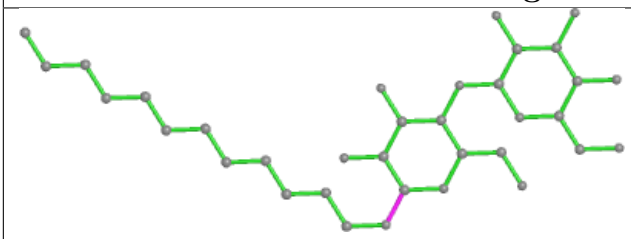


Rings

Ligand LMT Z 101



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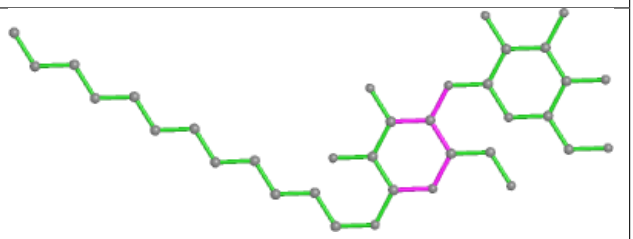
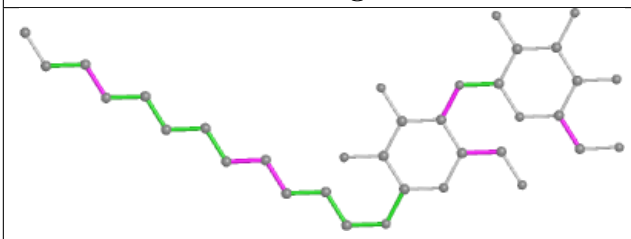


Bond angles



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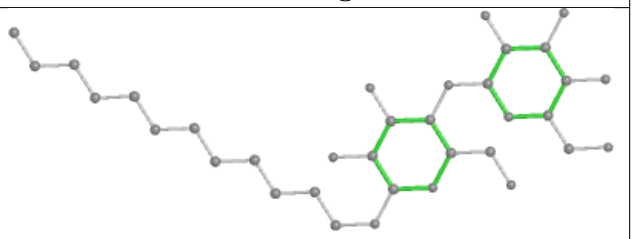
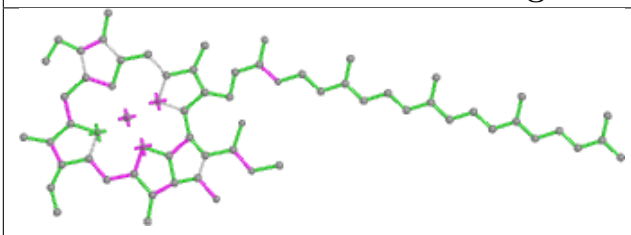


Rings

Ligand CLA b 607



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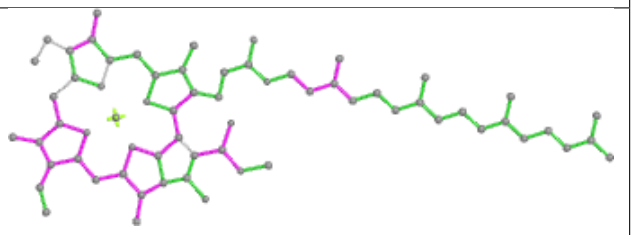
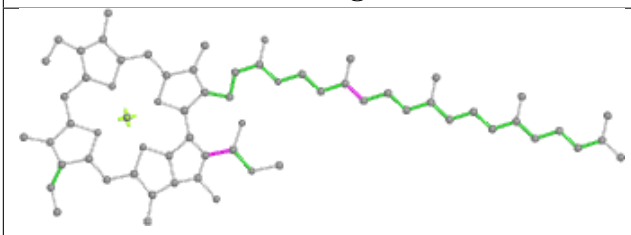


Bond angles



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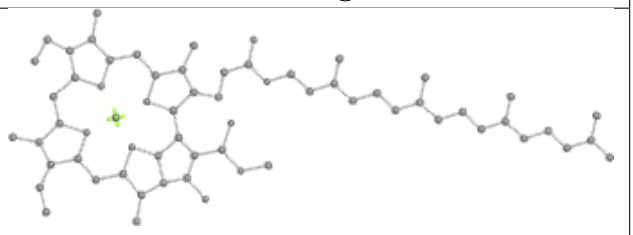
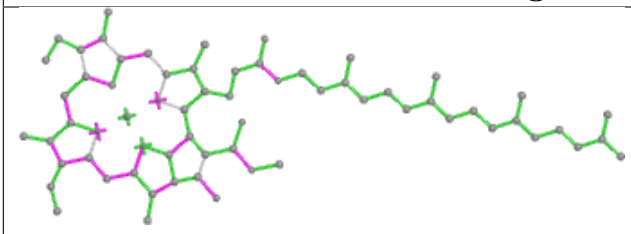


Rings

Ligand CLA b 617



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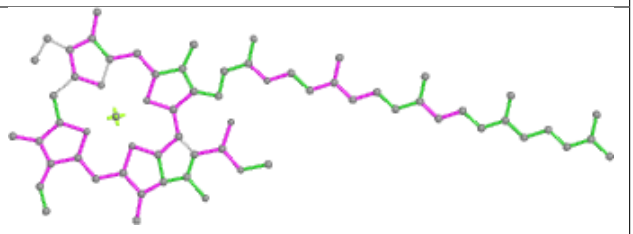
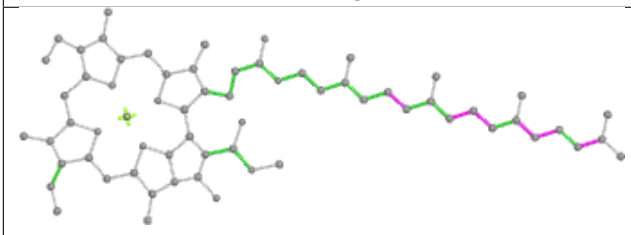


Bond angles



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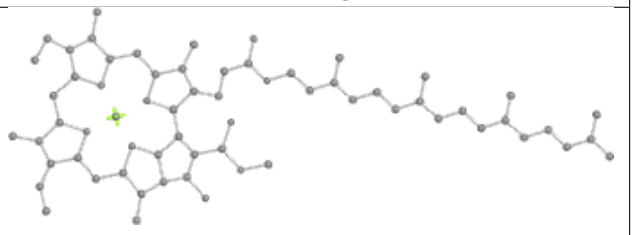
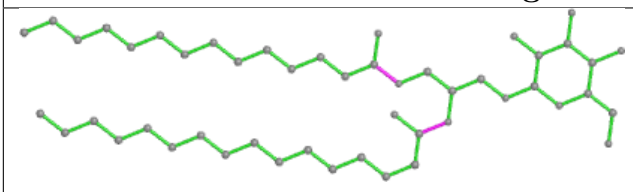


Rings

Ligand LMG b 623



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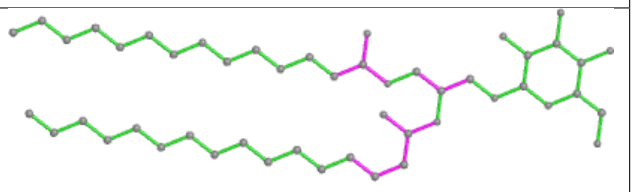
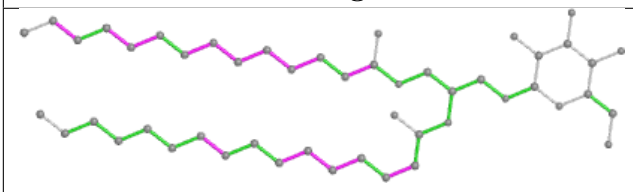
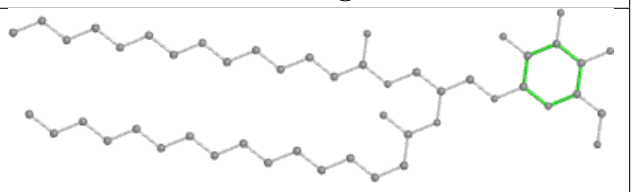


Bond angles

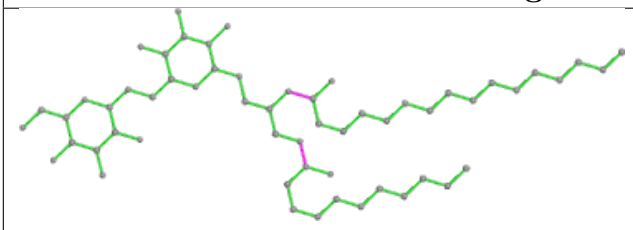


Torsions

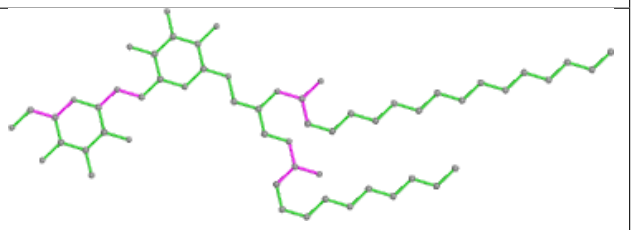


Rings

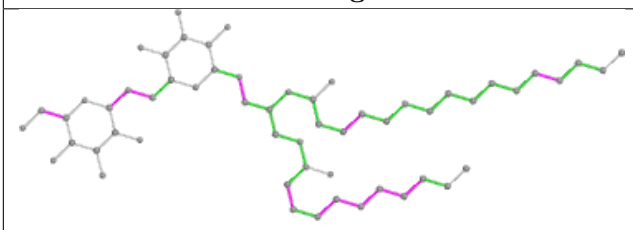
Ligand DGD c 516



Bond lengths



Bond angles



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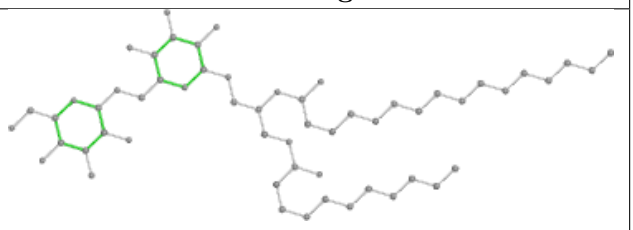
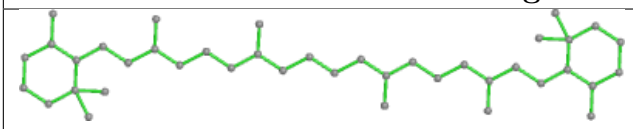


Rings

Ligand BCR T 101



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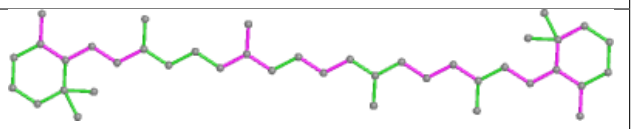
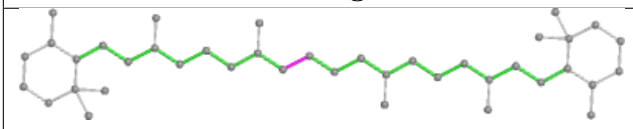


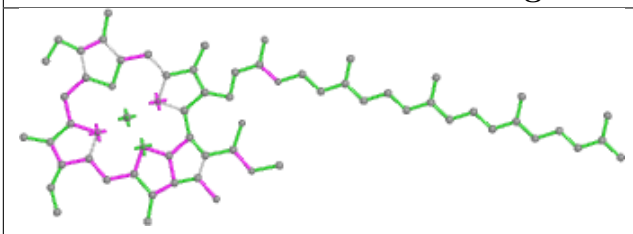
Bond angles



Torsions

Rings

Ligand CLA C 511



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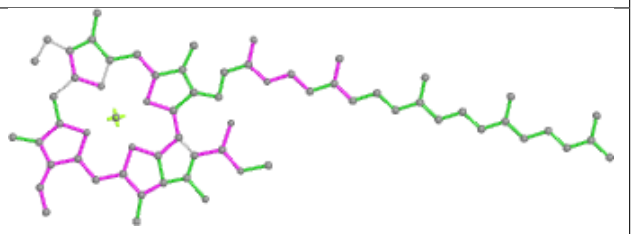
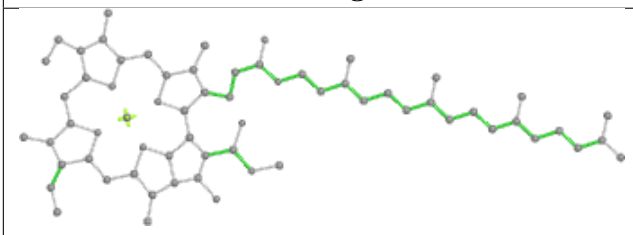
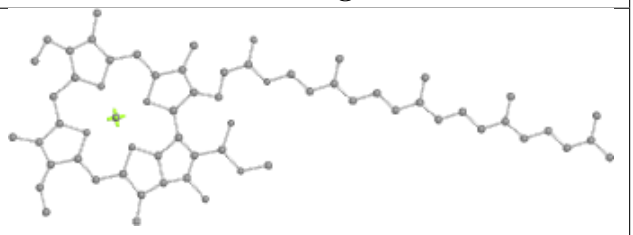


Bond angles

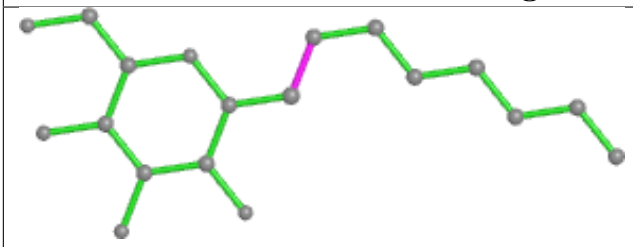


Torsions



Rings

Ligand HTG B 632



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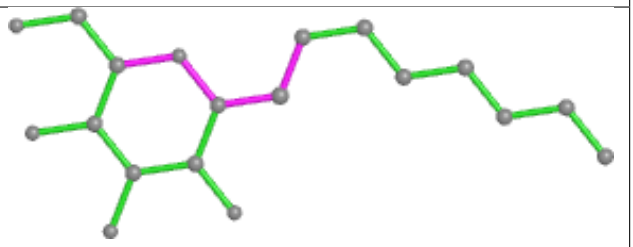
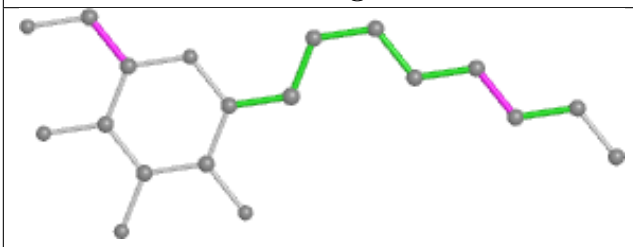


Bond angles



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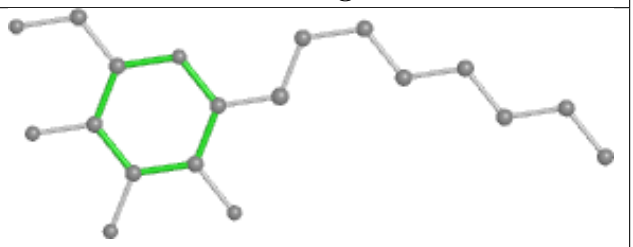
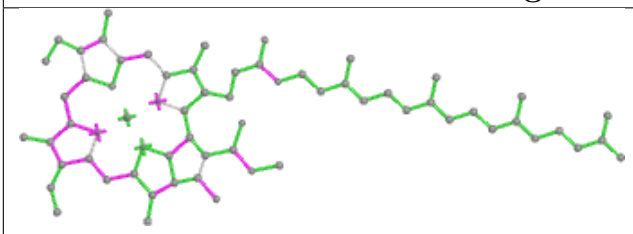
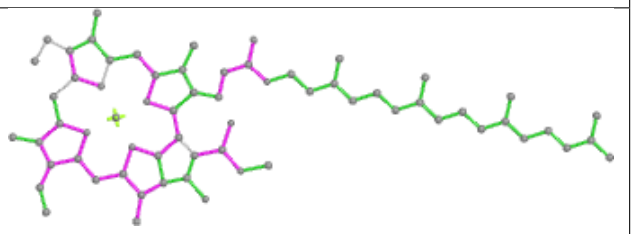


Rings

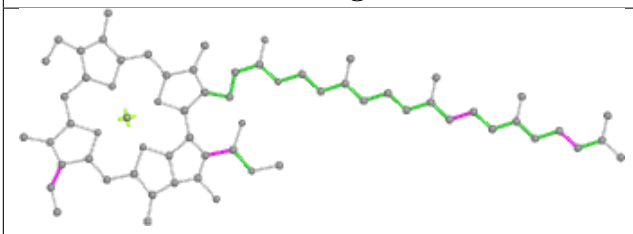
Ligand CLA B 611



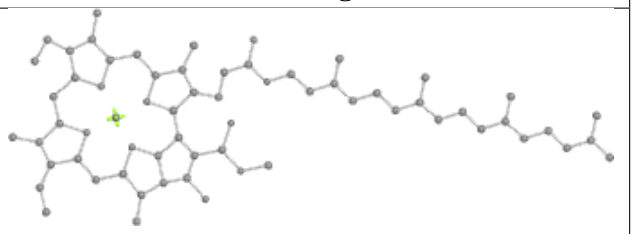
Bond lengths



Bond angles

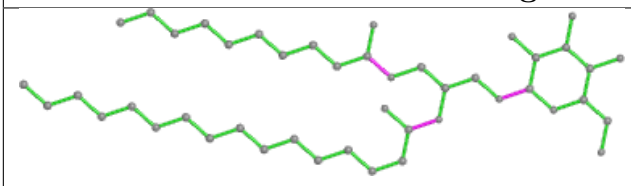


Torsions

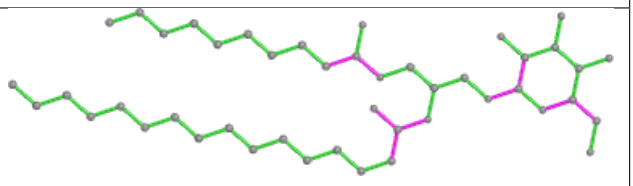


Rings

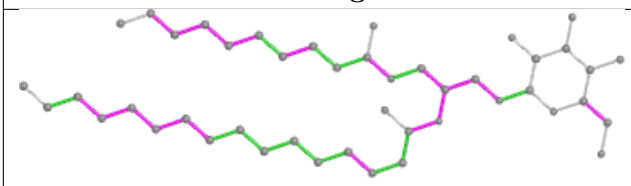
Ligand LMG C 524



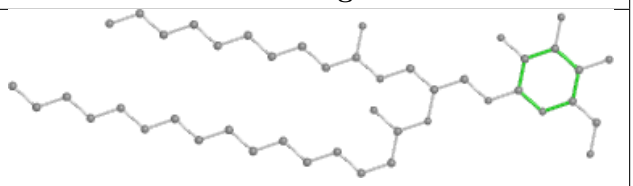
Bond lengths



Bond angles

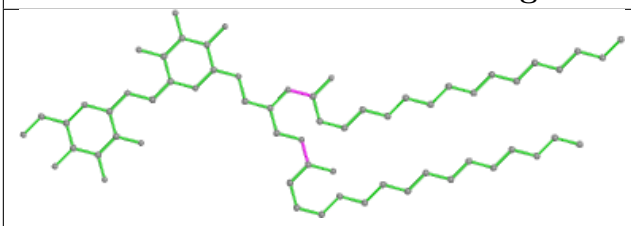


Torsions

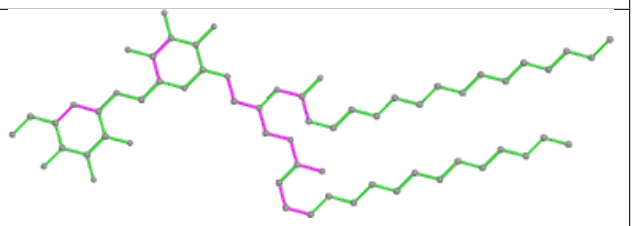


Rings

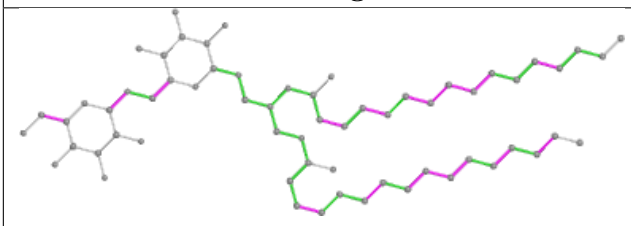
Ligand DGD C 516



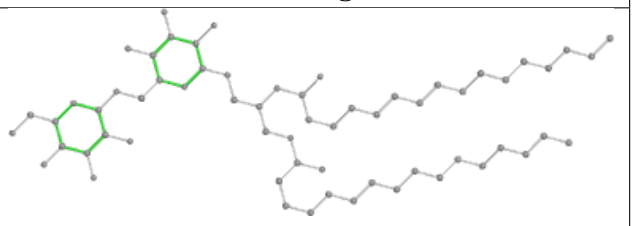
Bond lengths



Bond angles

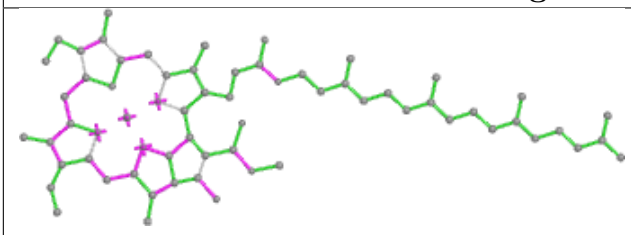


Torsions

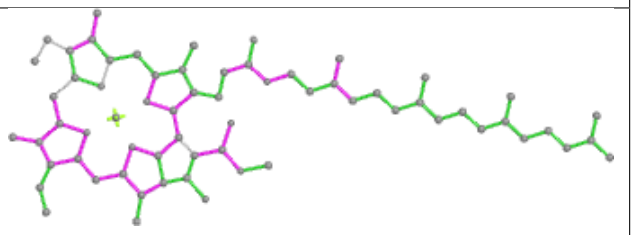


Rings

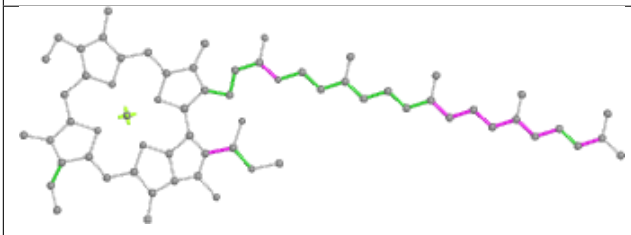
Ligand CLA c 513



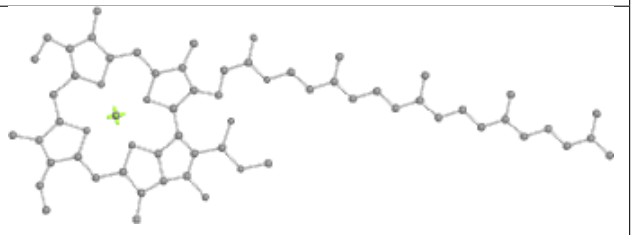
Bond lengths



Bond angles

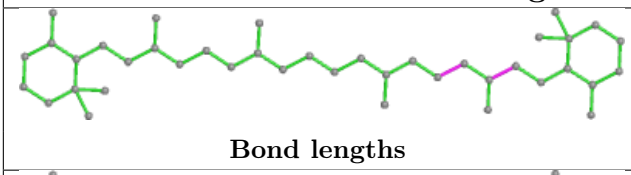


Torsions



Rings

Ligand BCR t 101



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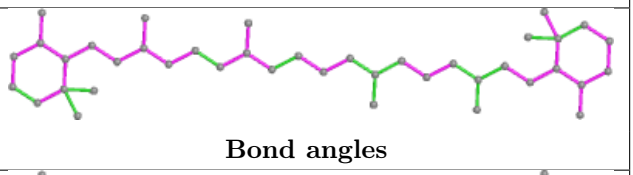

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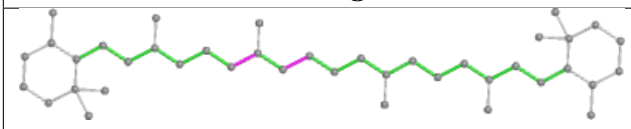

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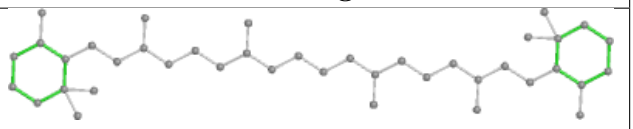
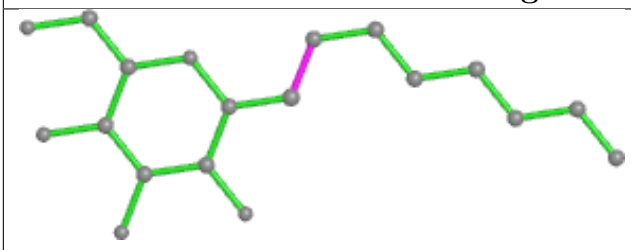


Rings

Ligand HTG C 520



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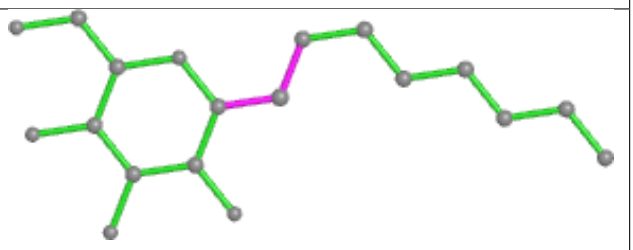
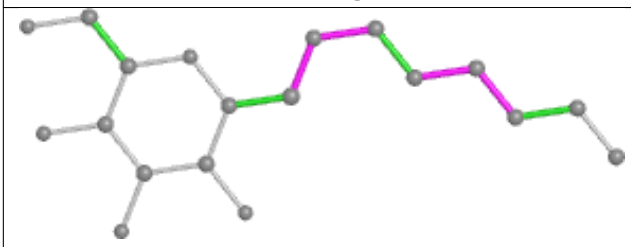


Bond angles



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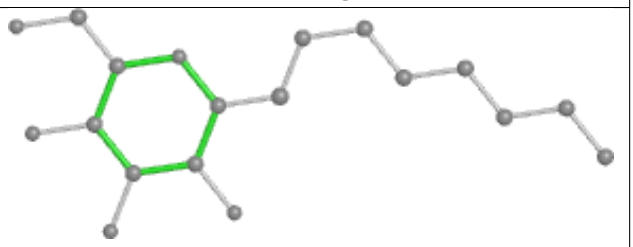
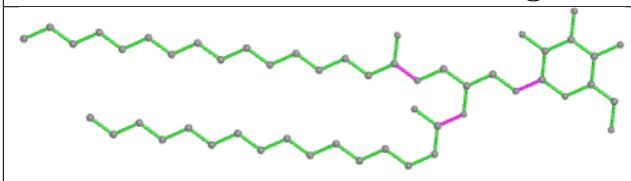


Rings

Ligand LMG c 519



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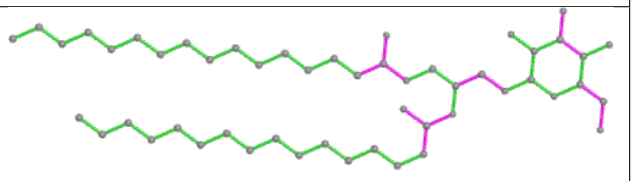
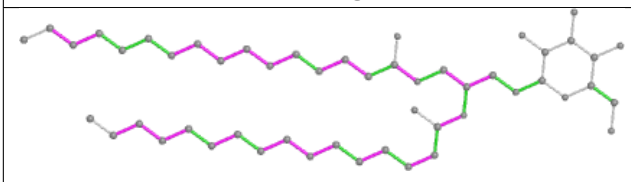


Bond angles



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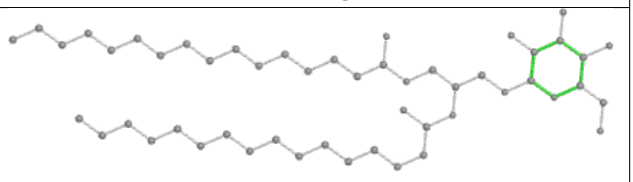
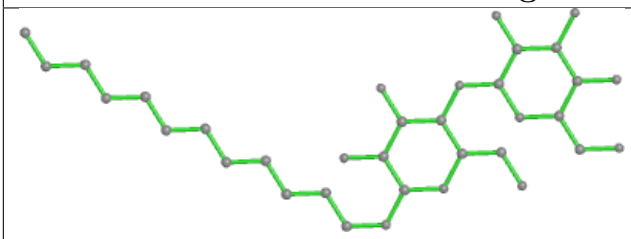


Rings

Ligand LMT m 102



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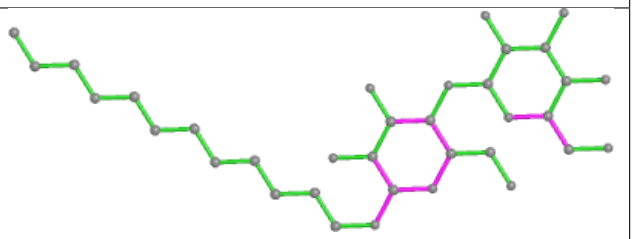
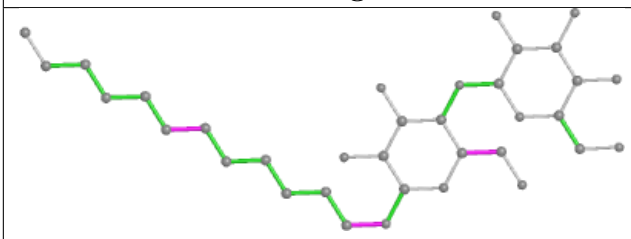


Bond angles



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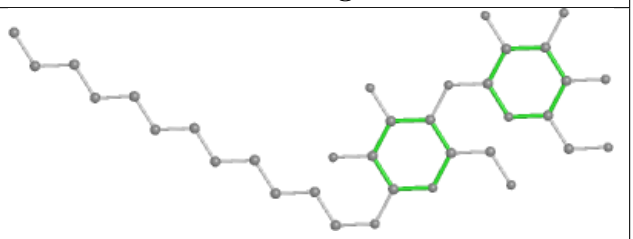
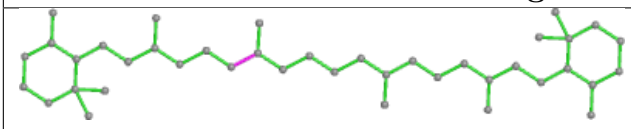


Rings

Ligand BCR c 514



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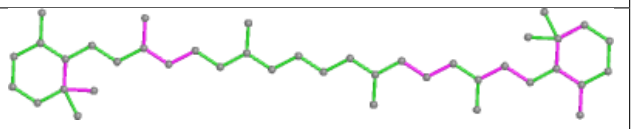
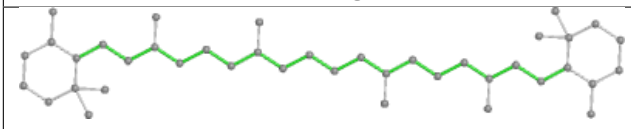


Bond angles



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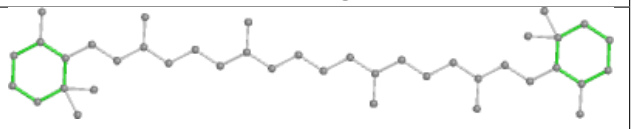
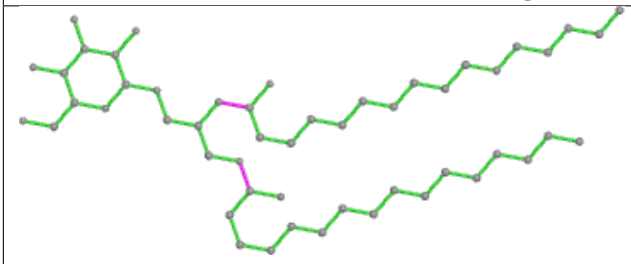


Rings

Ligand DGD D 406



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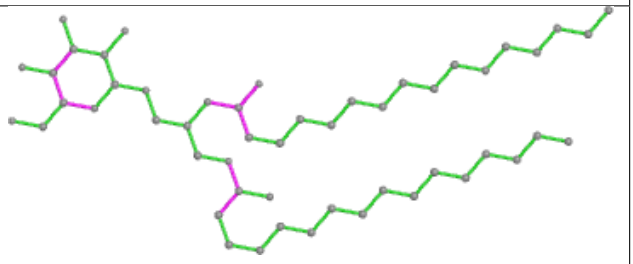
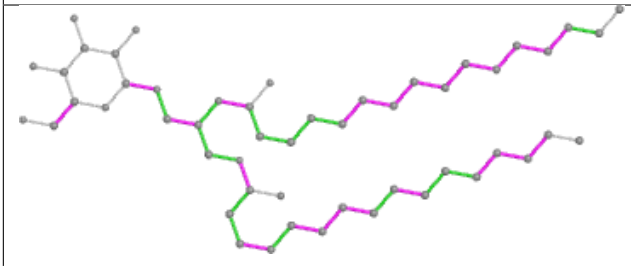


Bond angles



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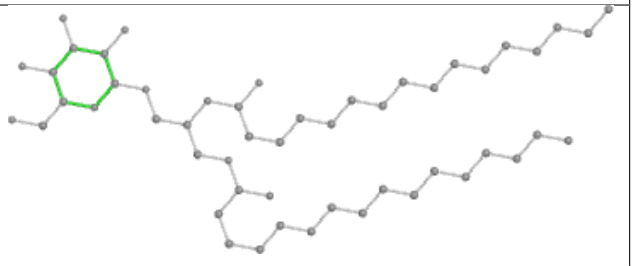
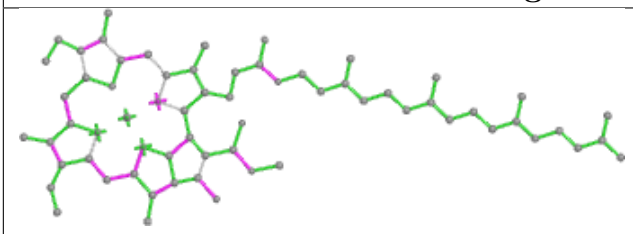


Rings

Ligand CLA B 606



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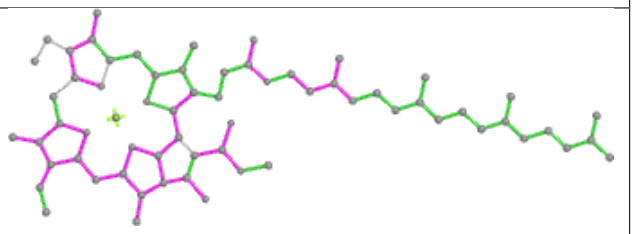
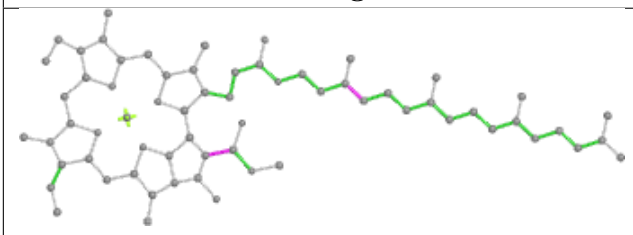


Bond angles



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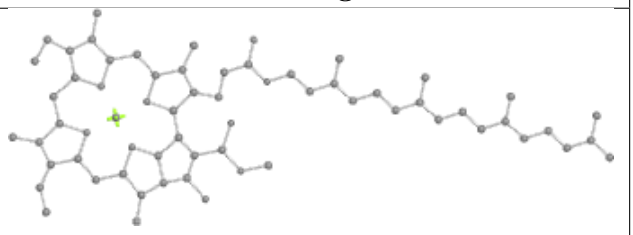
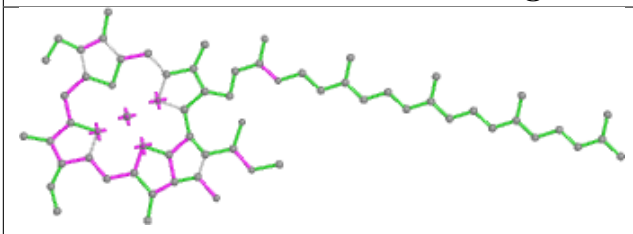
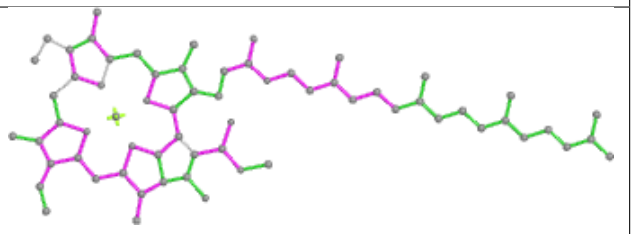


Rings

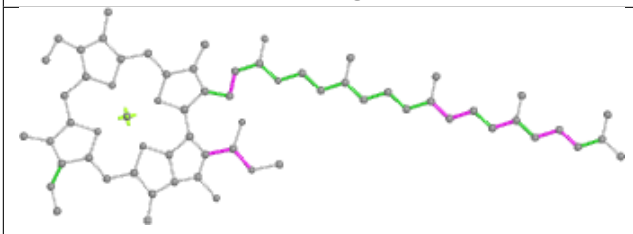
Ligand CLA B 607



Bond lengths



Bond angles



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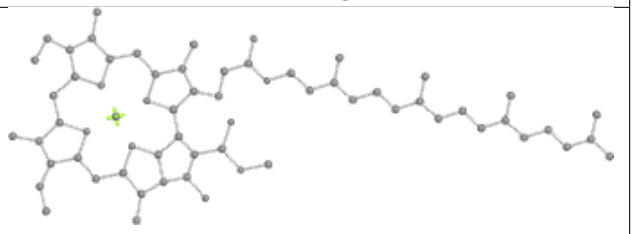
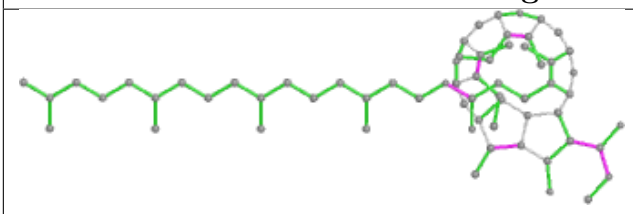


Rings

Ligand PHO A 403



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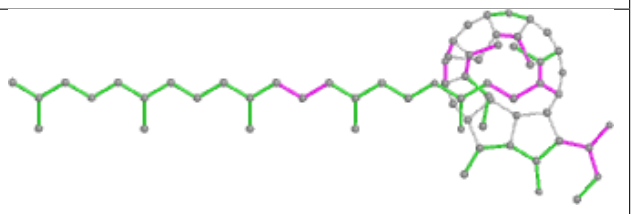
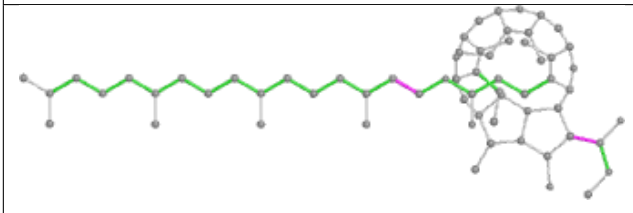


Bond angles



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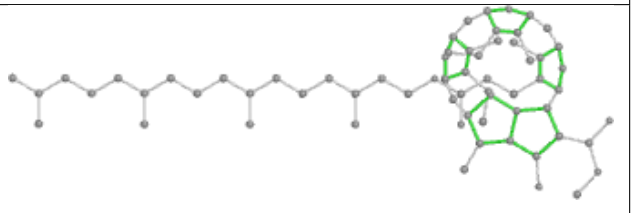
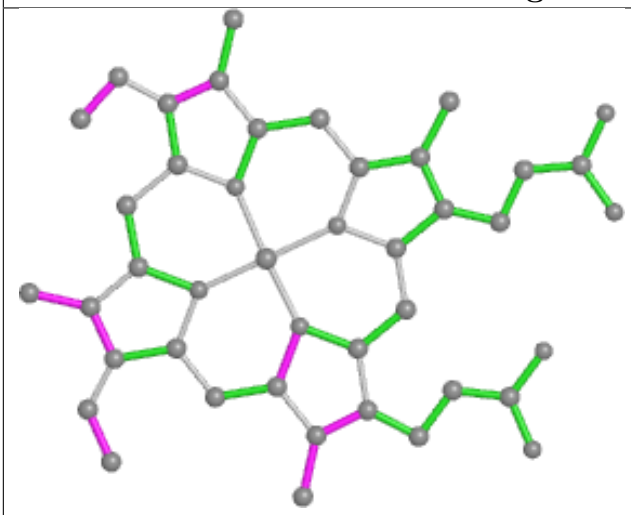


Rings

Ligand HEC v 201



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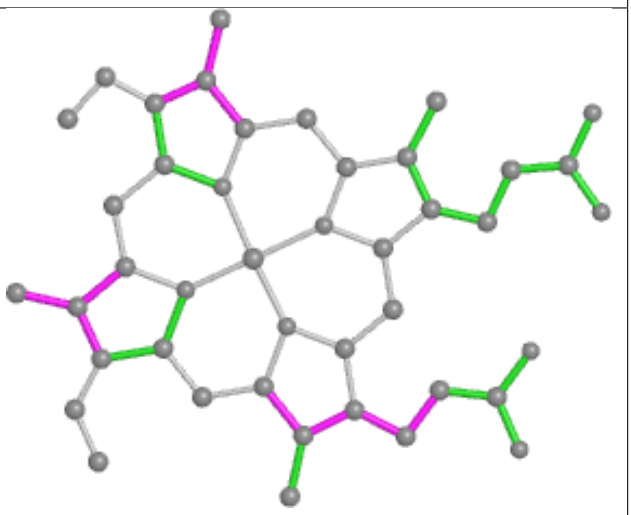
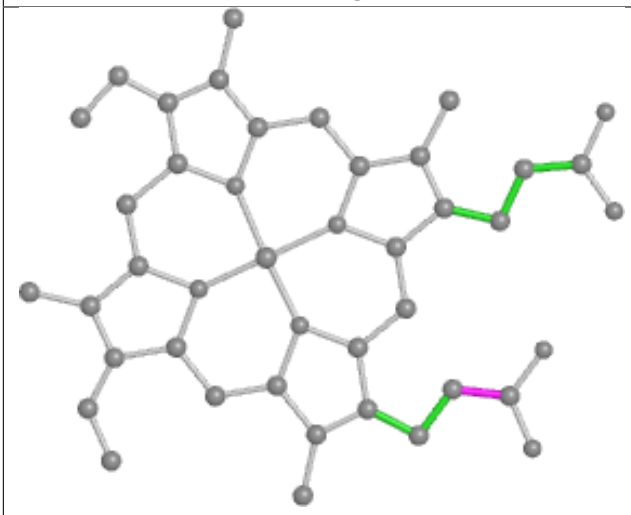


Bond angles



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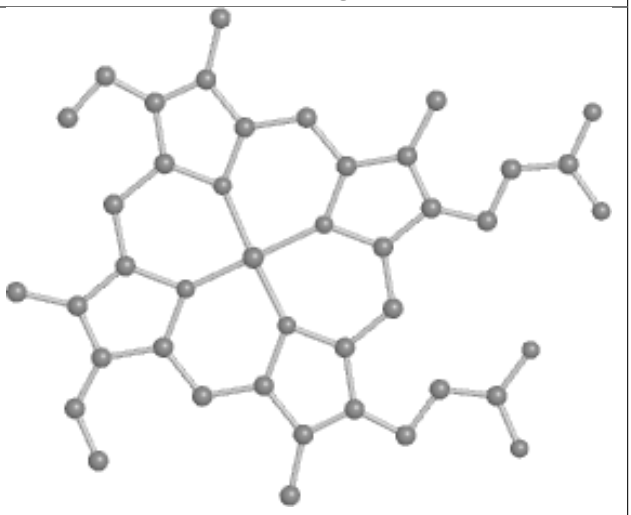
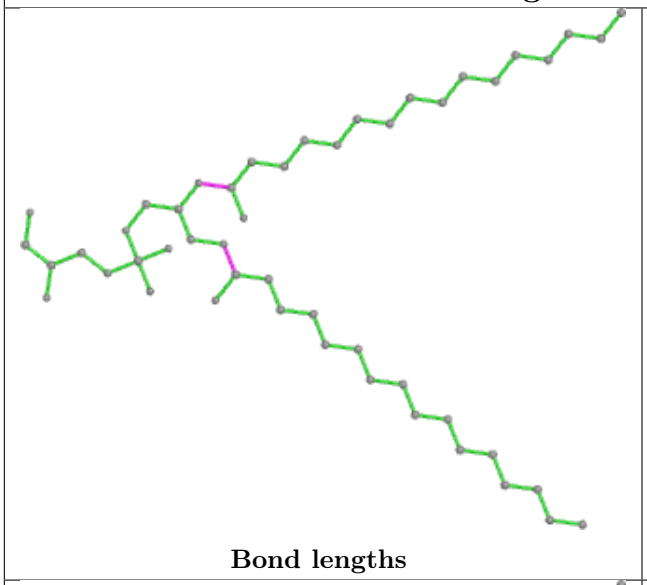


Rings

Ligand LHG D 409



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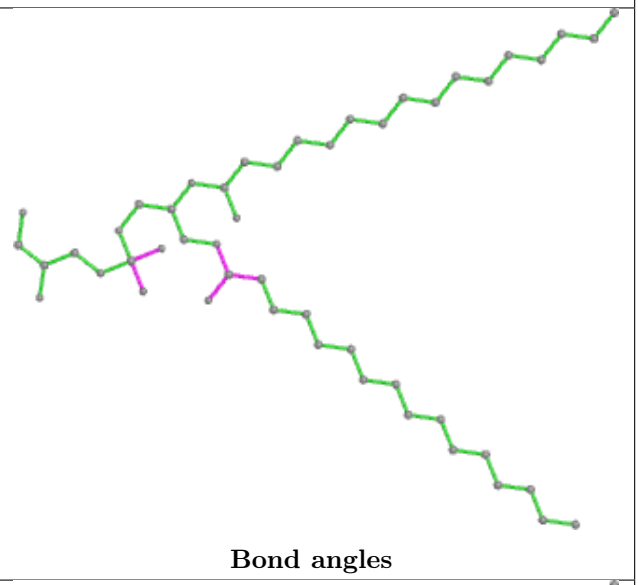
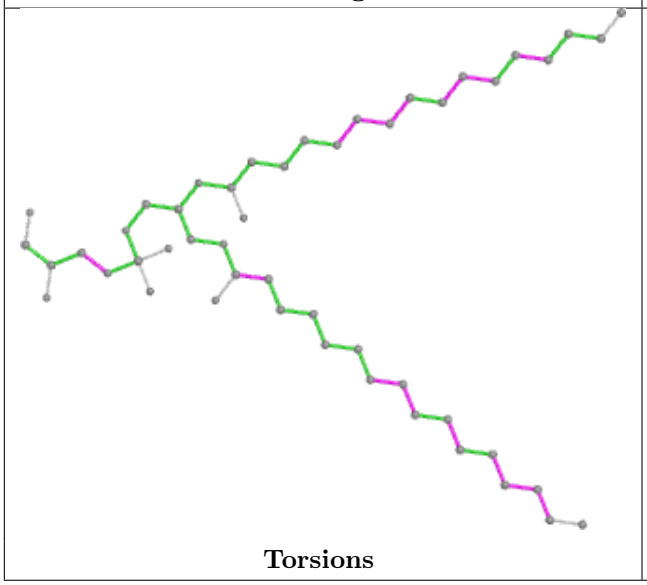


Bond angles



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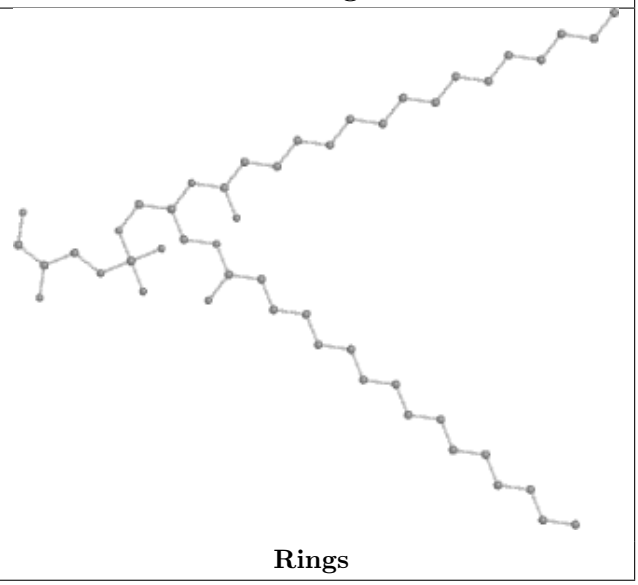
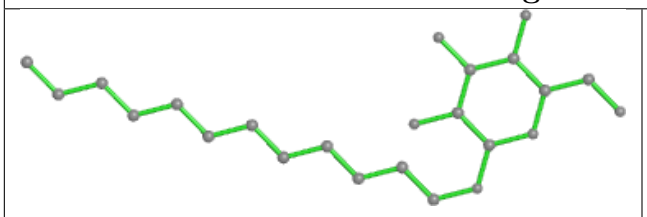


Rings

Ligand LMT T 102



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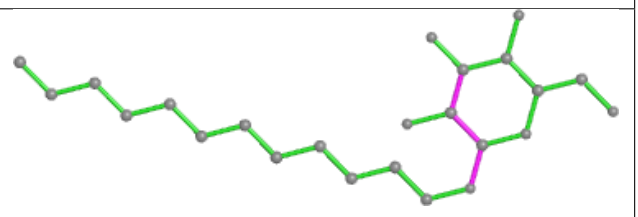
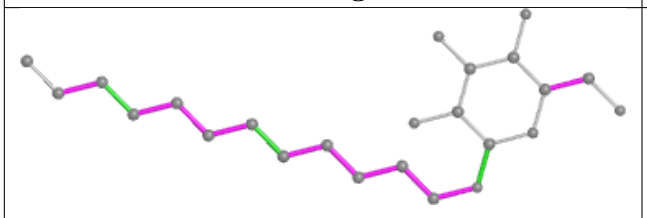


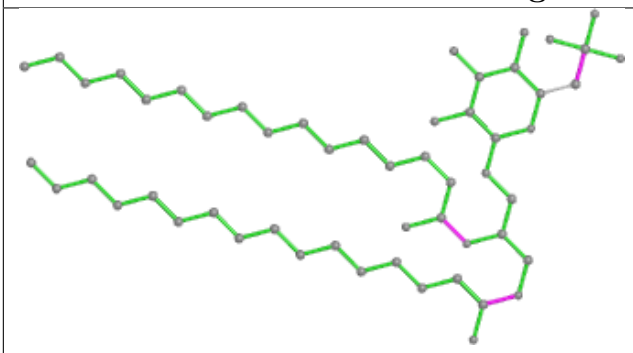
Bond angles



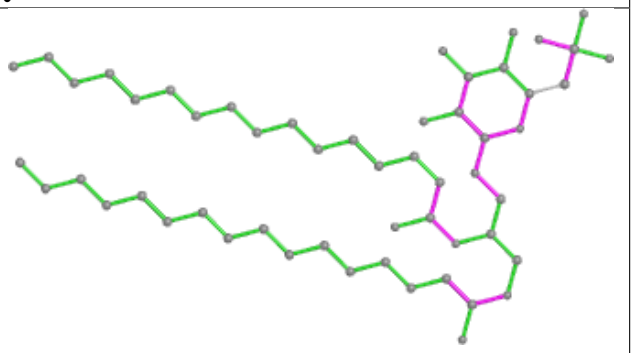
Torsions

Rings

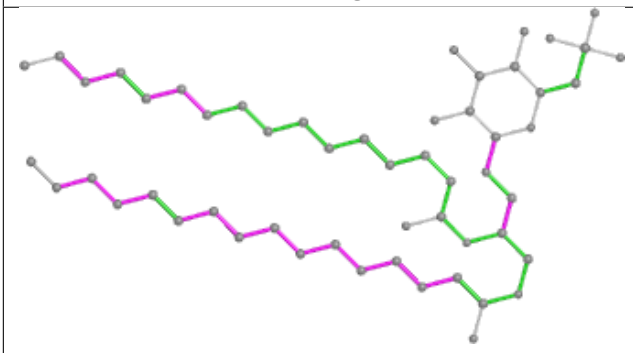
Ligand SQD a 401



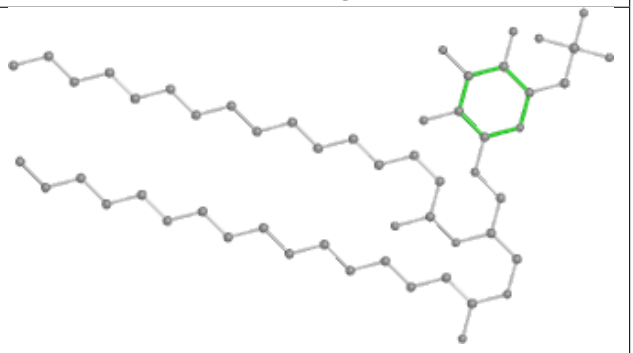
Bond lengths



Bond angles

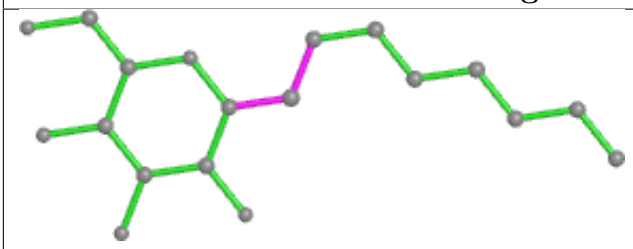


Torsions

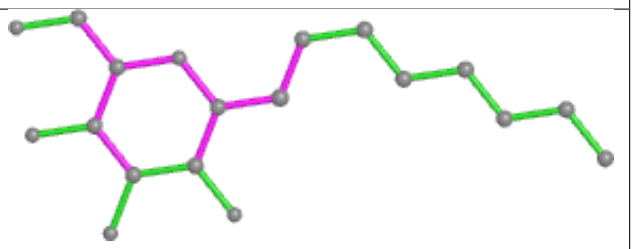


Rings

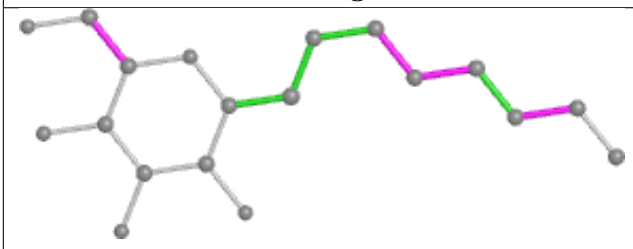
Ligand HTG B 631



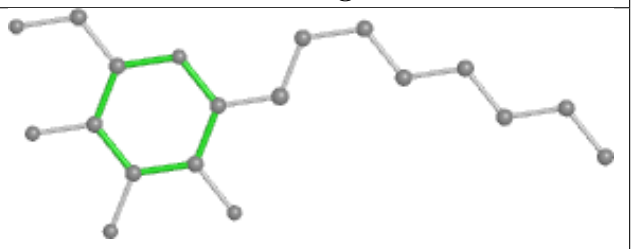
Bond lengths



Bond angles

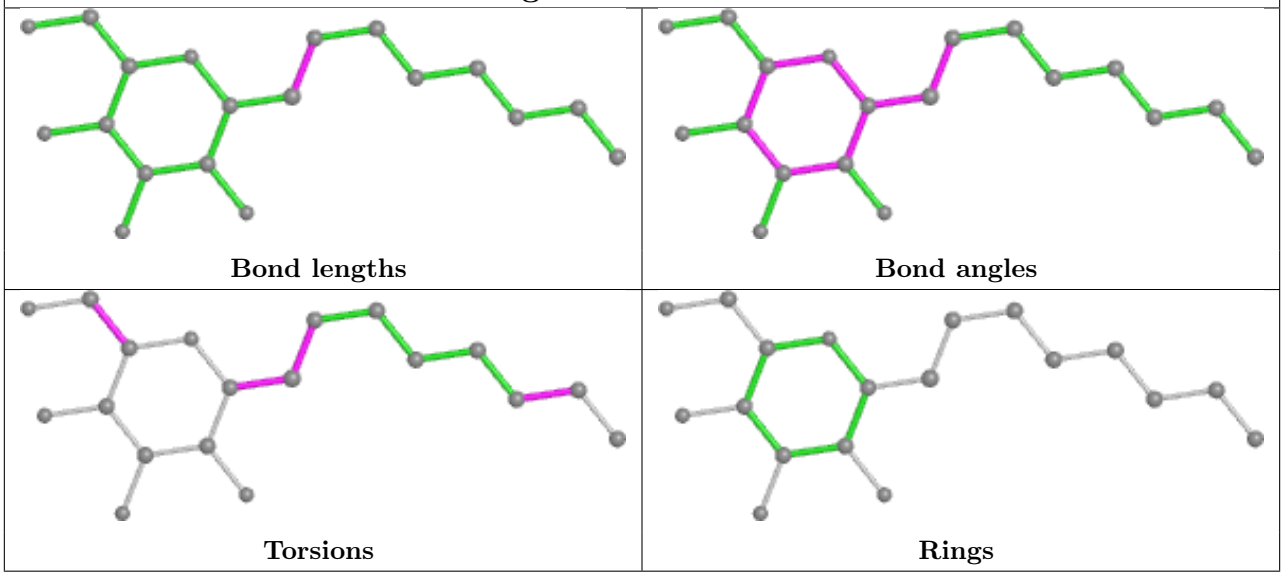


Torsions

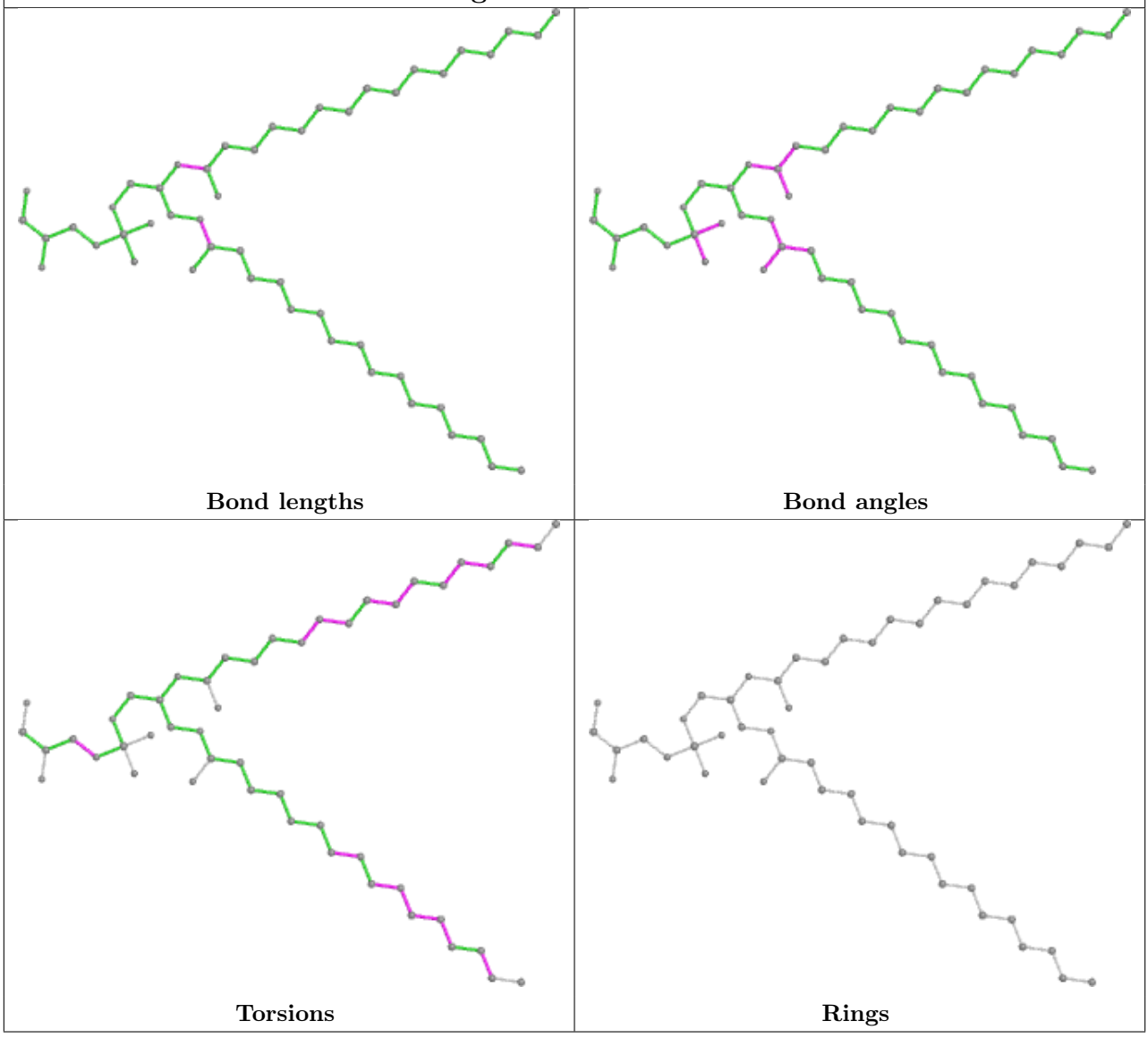


Rings

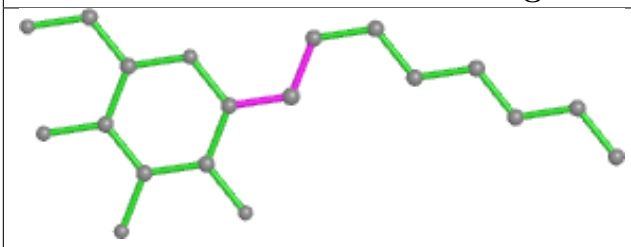
Ligand HTG C 534

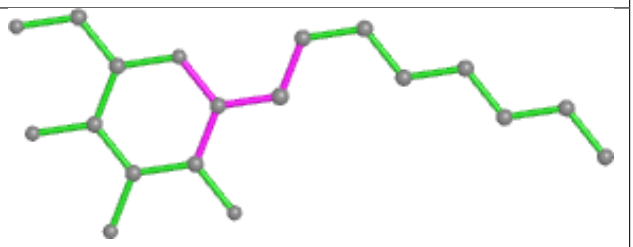


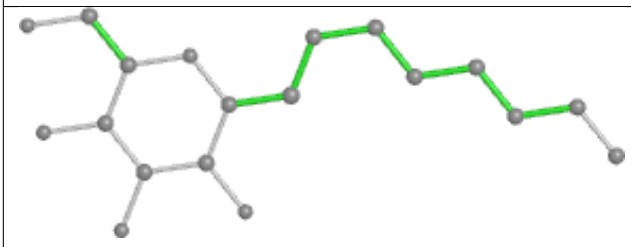
Ligand LHG d 408

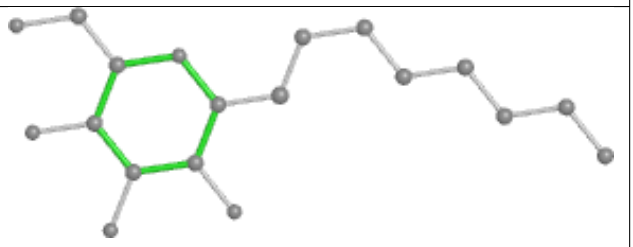


Ligand HTG b 624

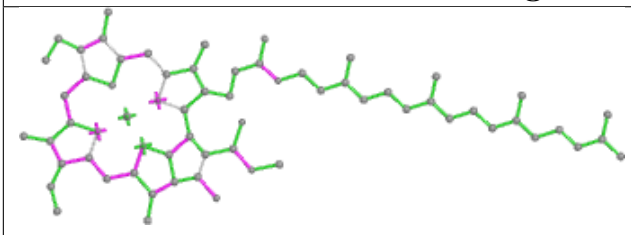

Bond lengths

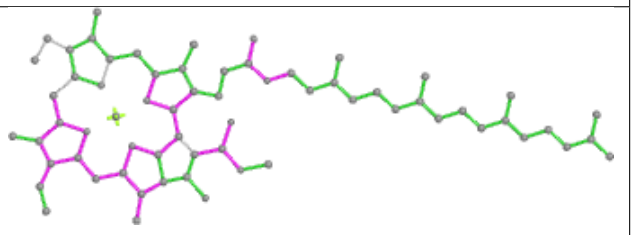

Bond angles

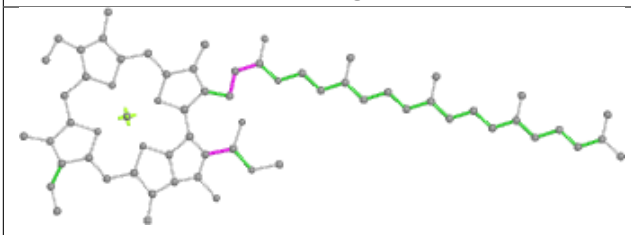

Torsions

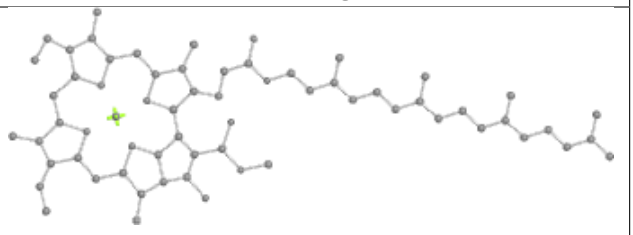

Rings

Ligand CLA C 501

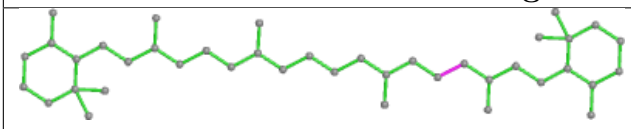

Bond lengths

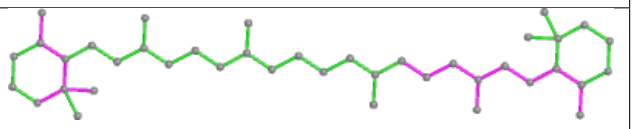

Bond angles

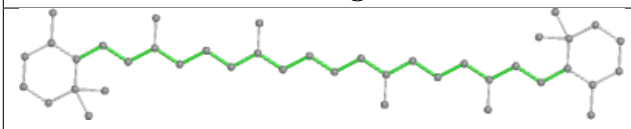

Torsions

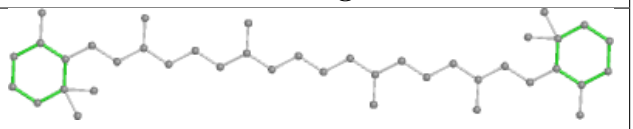

Rings

Ligand BCR B 619

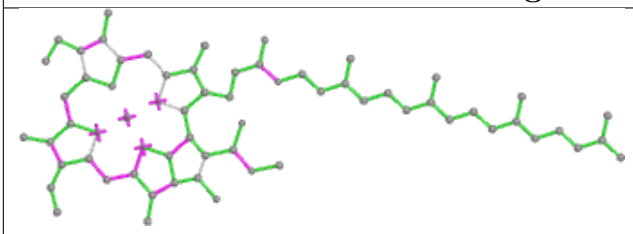

Bond lengths


Bond angles

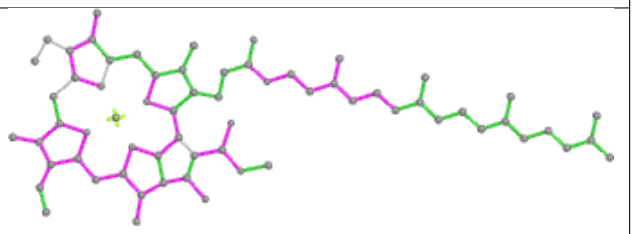

Torsions


Rings

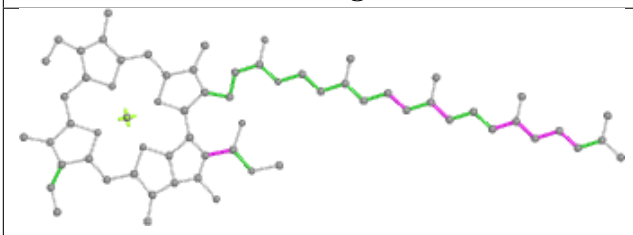
Ligand CLA C 504



Bond lengths



Bond angles



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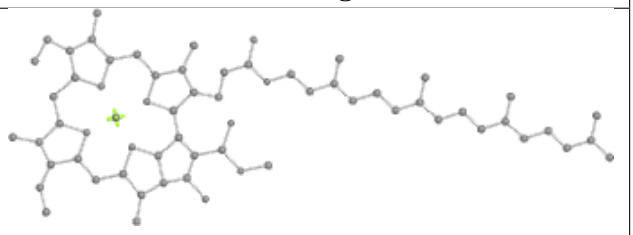
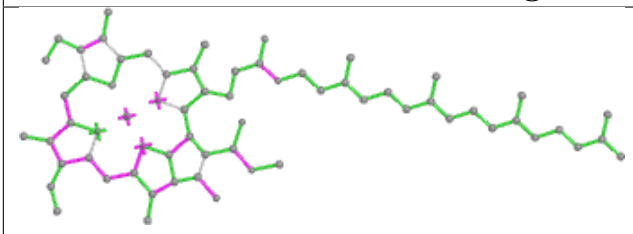
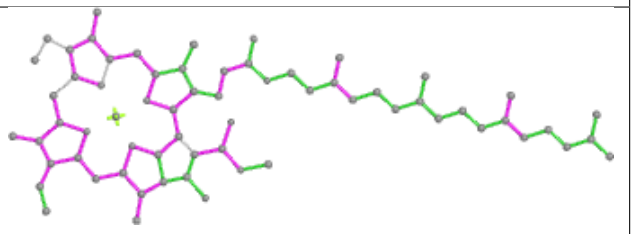


Rings

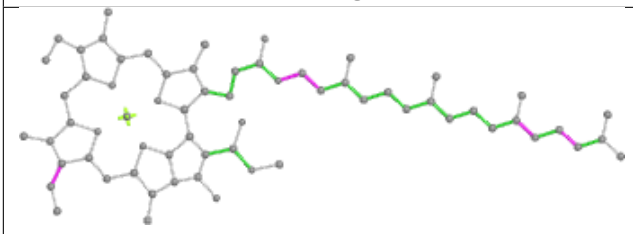
Ligand CLA D 401



Bond lengths



Bond angles



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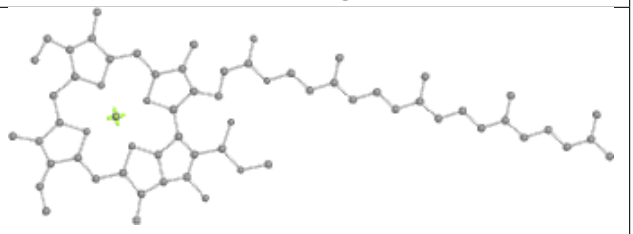
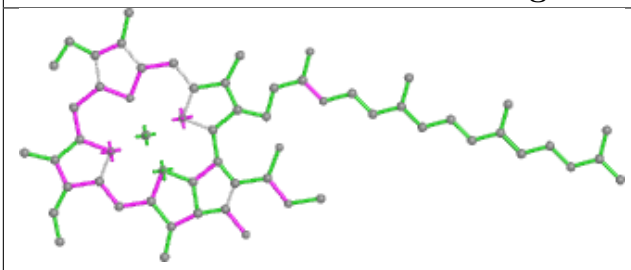
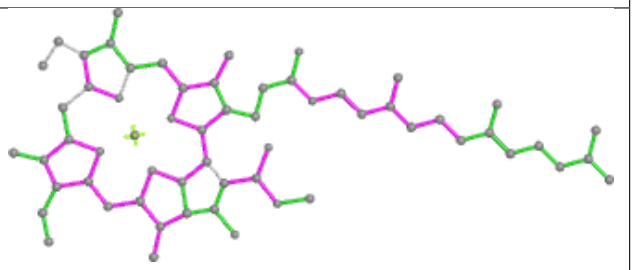


Rings

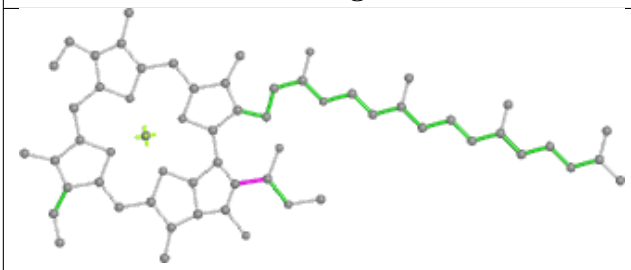
Ligand CLA c 508



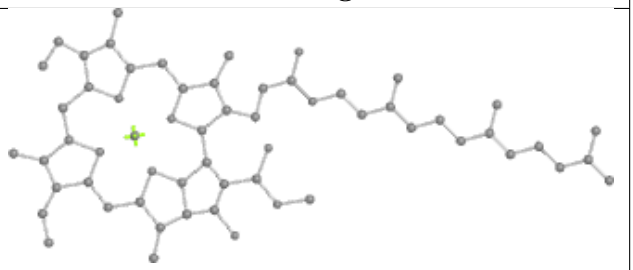
Bond lengths



Bond angles

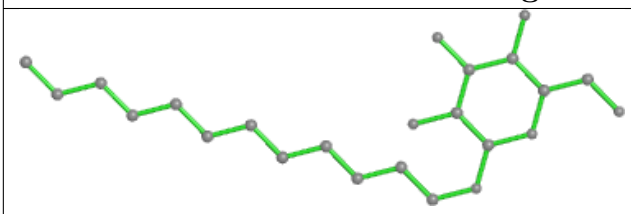


Torsions

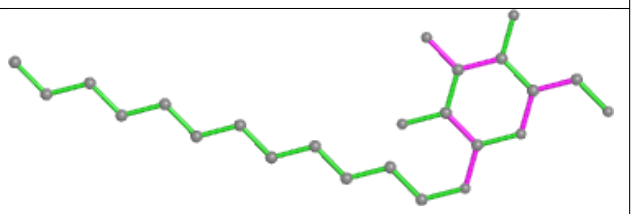


Rings

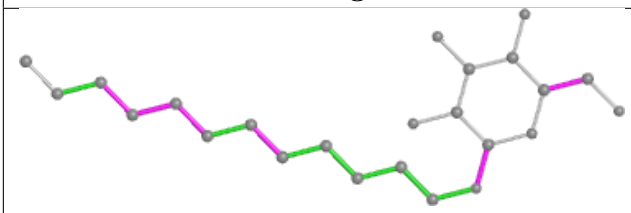
Ligand LMT B 626



Bond lengths



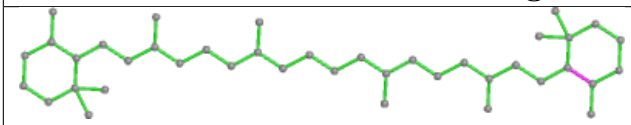
Bond angles



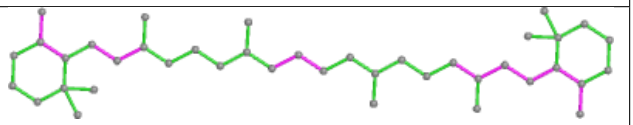
Torsions

Rings

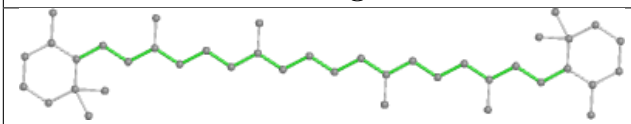
Ligand BCR b 621



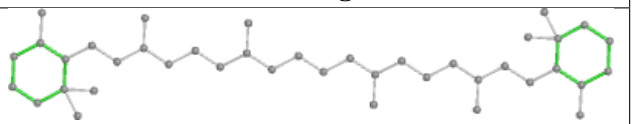
Bond lengths



Bond angles

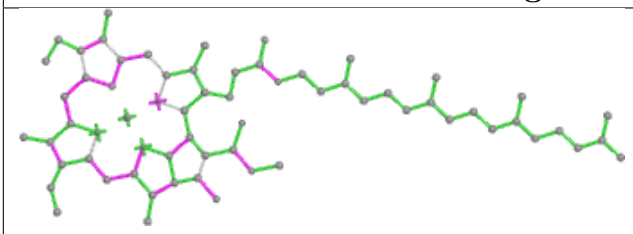


Torsions



Rings

Ligand CLA B 612



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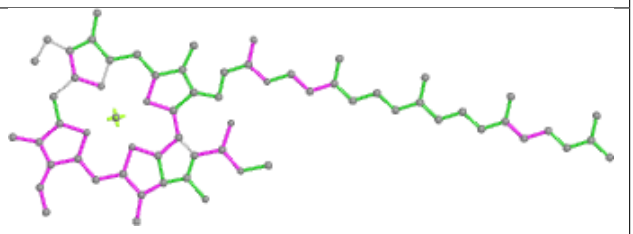
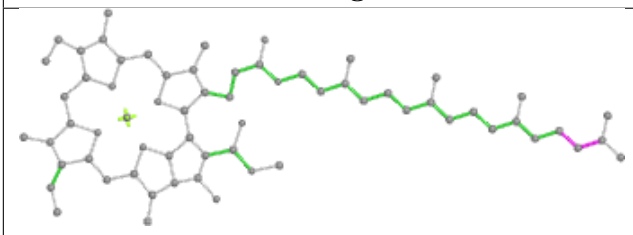
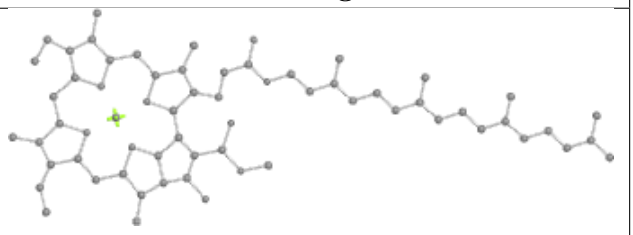


Bond angles

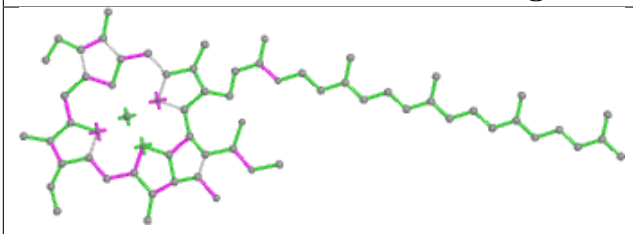


Torsions



Rings

Ligand CLA b 610



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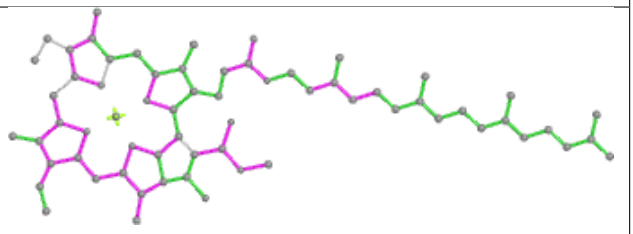
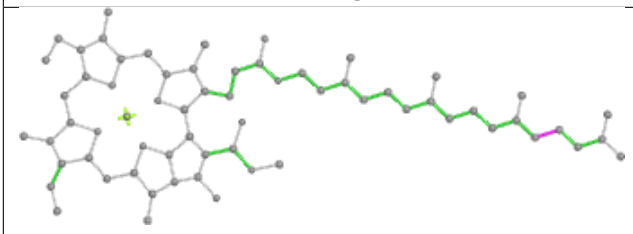


Bond angles



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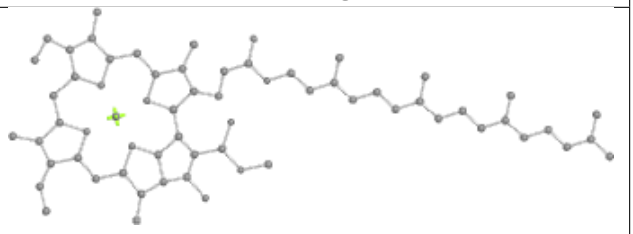
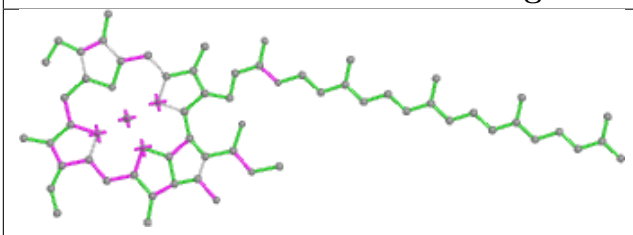
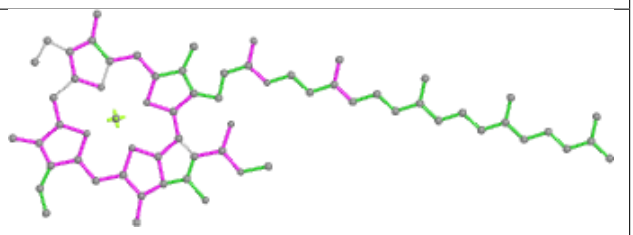


Rings

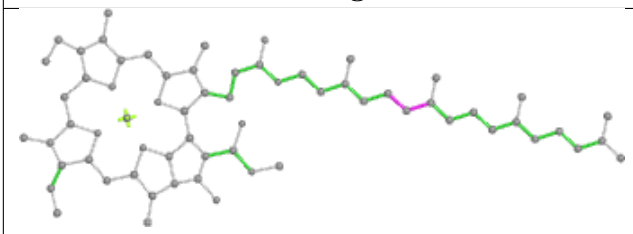
Ligand CLA B 604



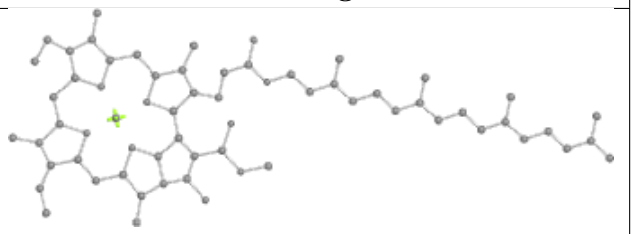
Bond lengths



Bond angles

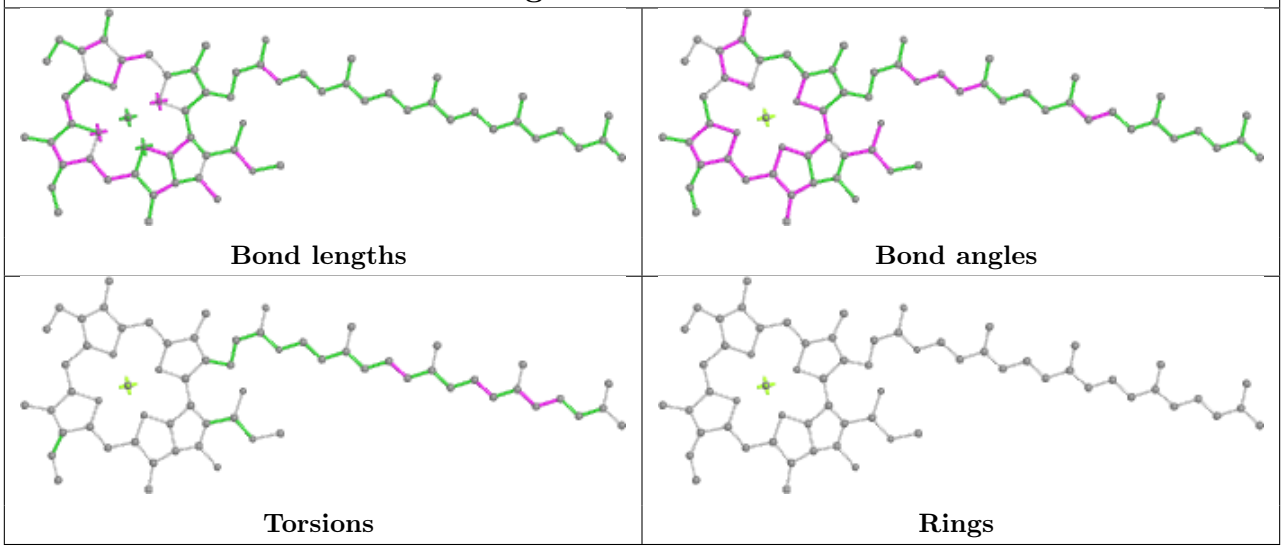


Torsions

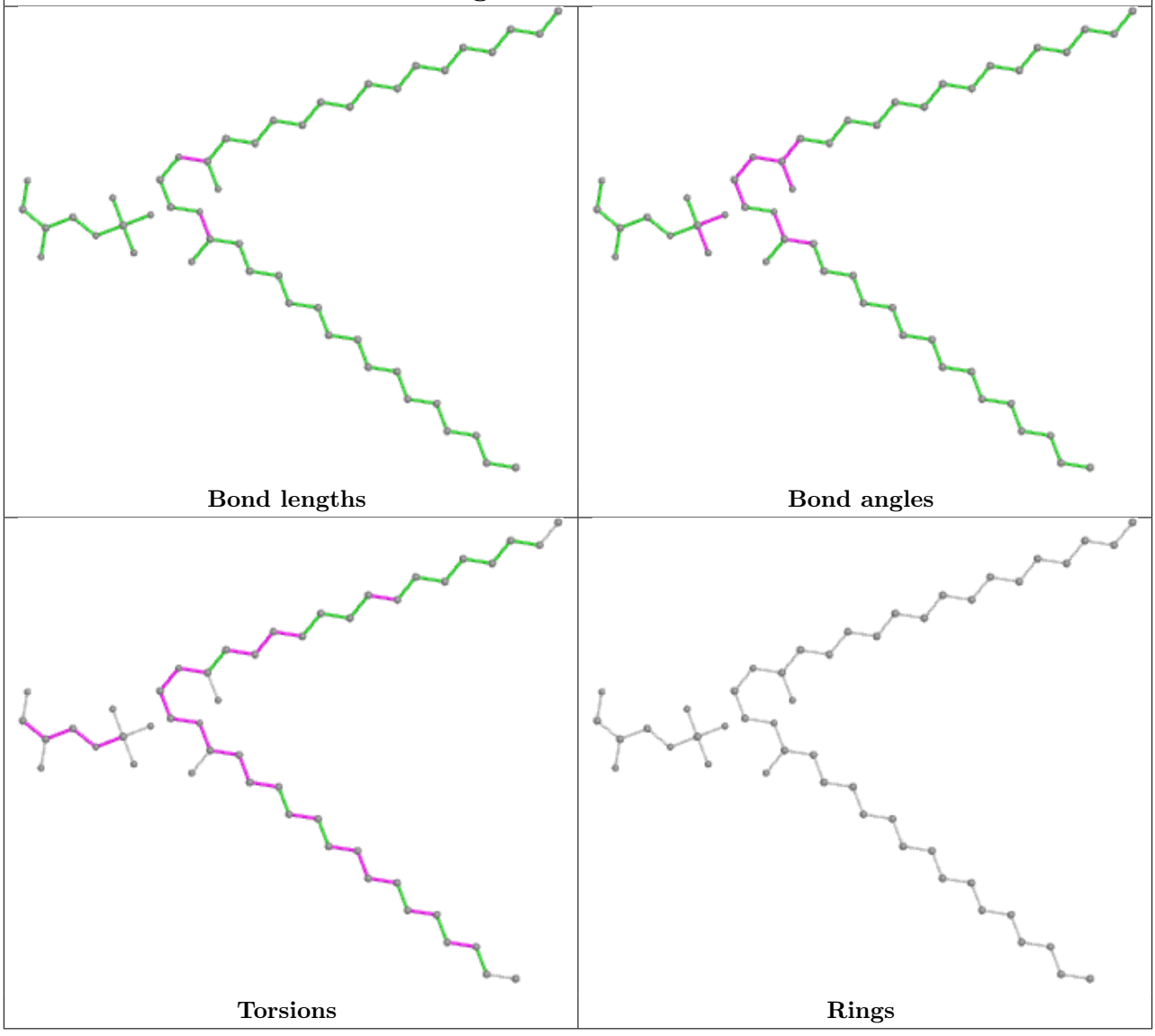


Rings

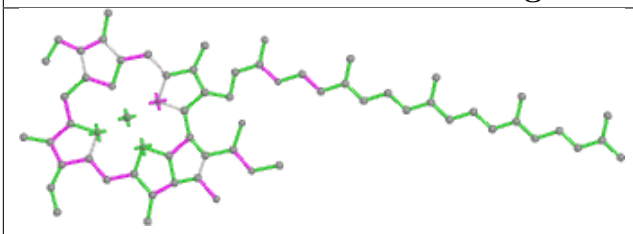
Ligand CLA B 616



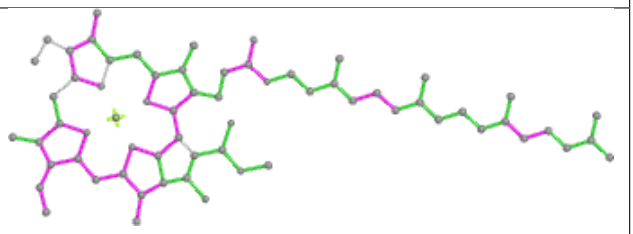
Ligand LHG E 103



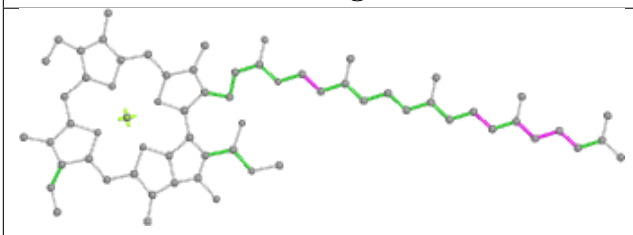
Ligand CLA B 614



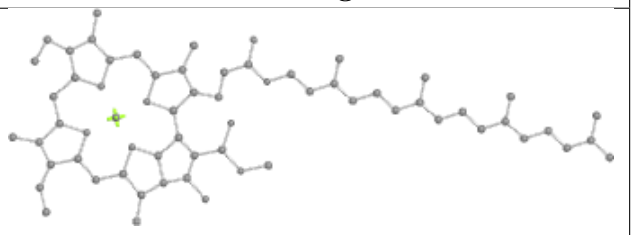
Bond lengths



Bond angles

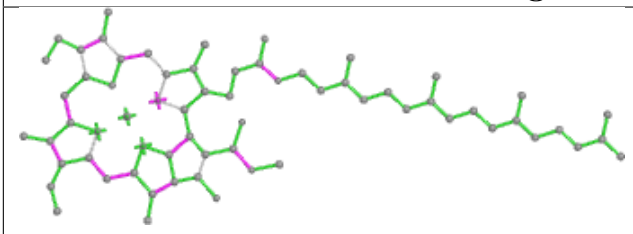


Torsions

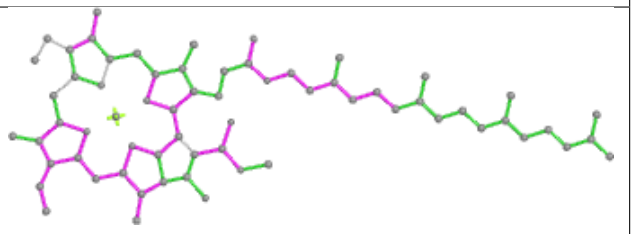


Rings

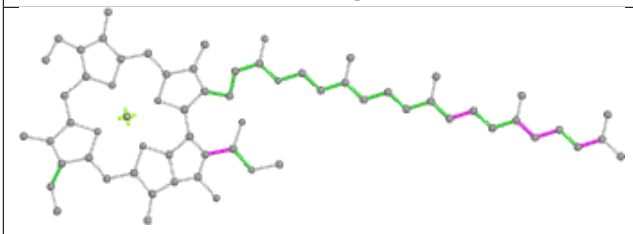
Ligand CLA b 613



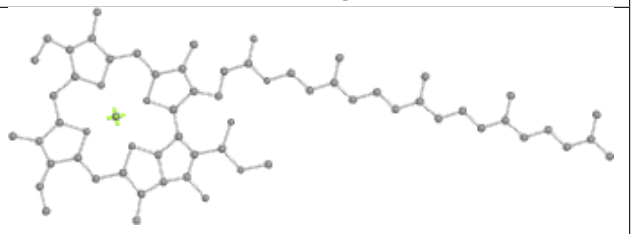
Bond lengths



Bond angles

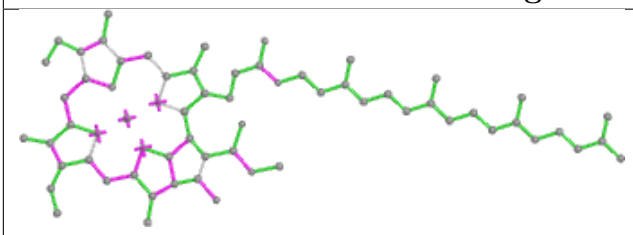


Torsions

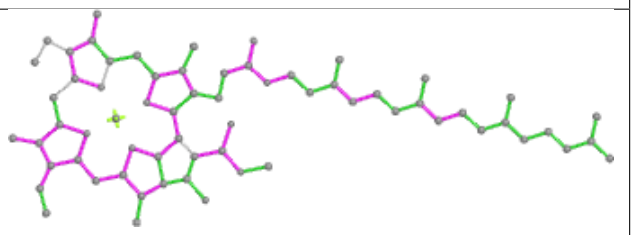


Rings

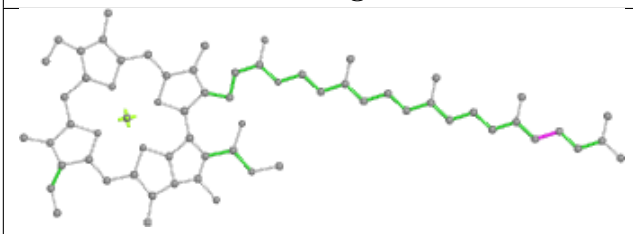
Ligand CLA B 609



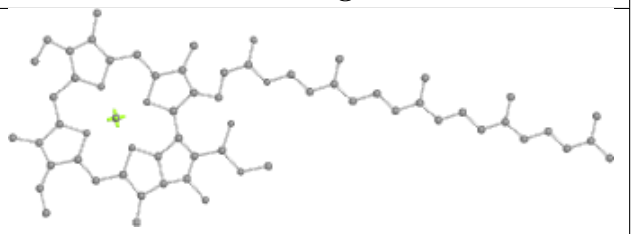
Bond lengths



Bond angles

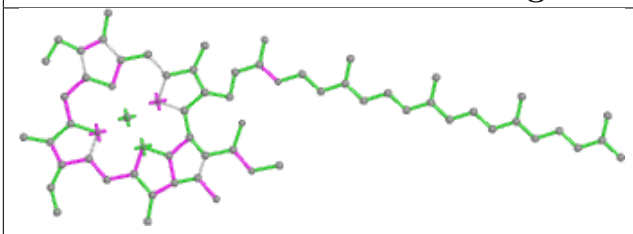


Torsions

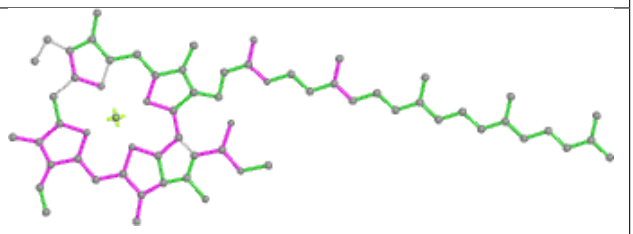


Rings

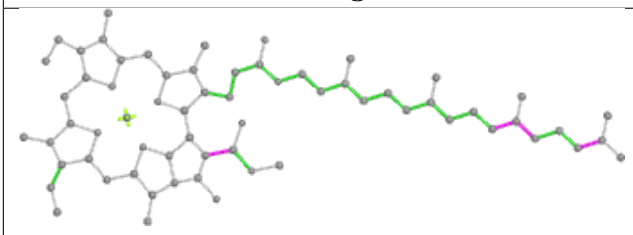
Ligand CLA b 612



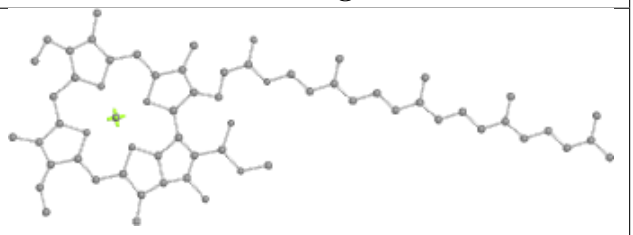
Bond lengths



Bond angles

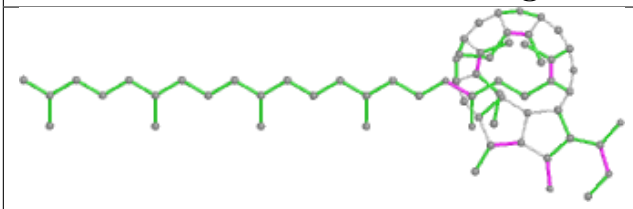


Torsions

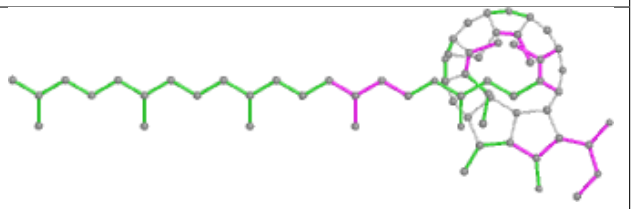


Rings

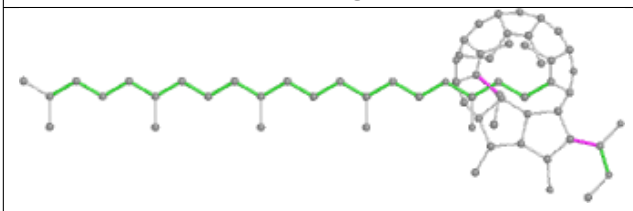
Ligand PHO D 403



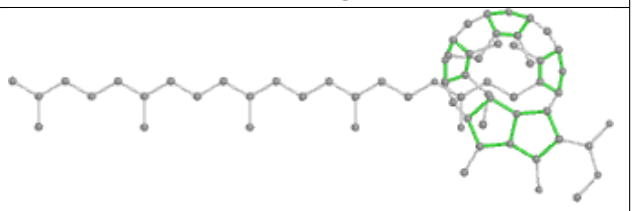
Bond lengths



Bond angles

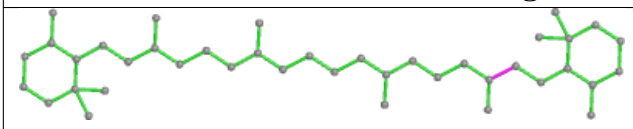


Torsions

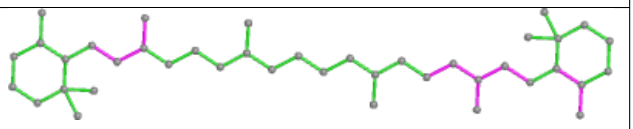


Rings

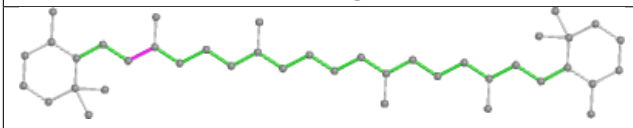
Ligand BCR K 102



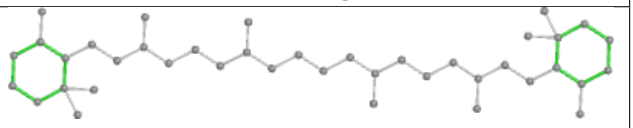
Bond lengths



Bond angles

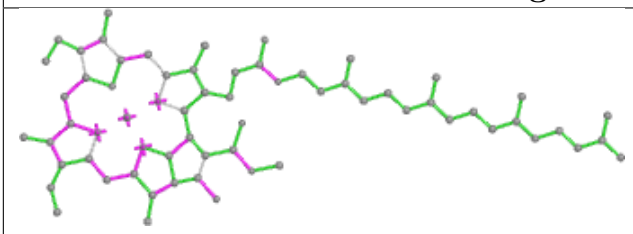


Torsions

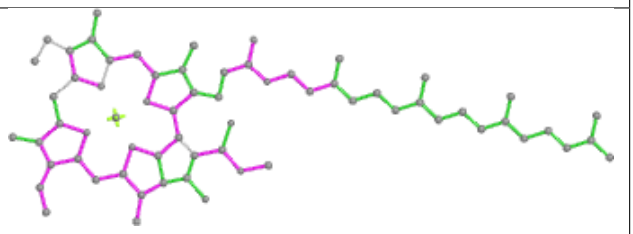


Rings

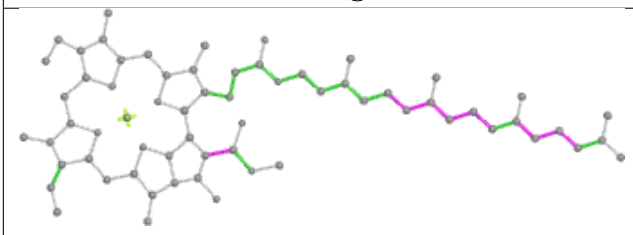
Ligand CLA c 506



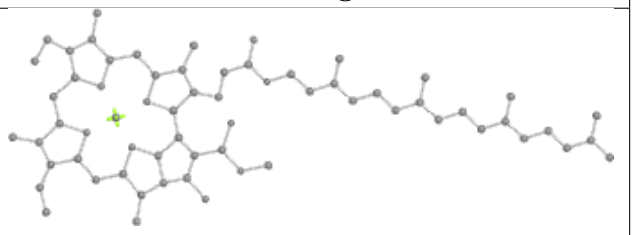
Bond lengths



Bond angles

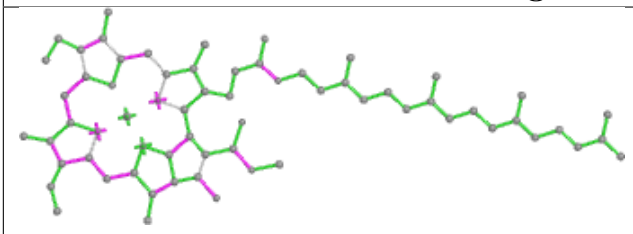


Torsions

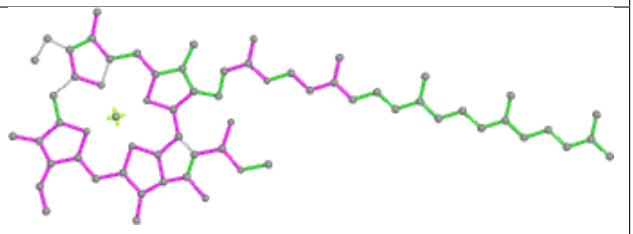


Rings

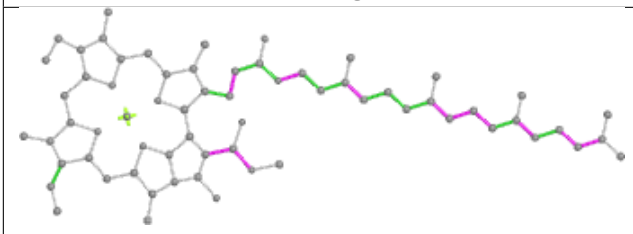
Ligand CLA b 616



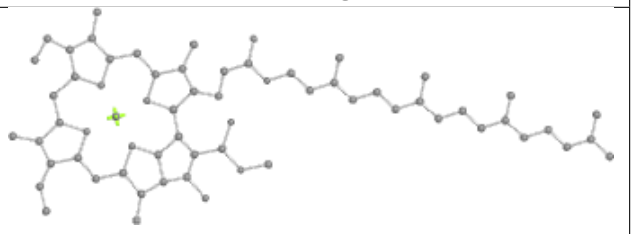
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.70	3 (0%) 84 84	16, 23, 46, 68	0
1	a	334/344 (97%)	-0.63	7 (2%) 63 63	18, 23, 48, 78	0
2	B	505/505 (100%)	-0.47	19 (3%) 40 38	19, 28, 54, 85	0
2	b	495/505 (98%)	-0.40	20 (4%) 38 36	19, 28, 53, 95	0
3	C	451/455 (99%)	-0.45	8 (1%) 68 68	21, 33, 49, 83	0
3	c	455/455 (100%)	-0.47	6 (1%) 77 78	22, 33, 46, 79	0
4	D	342/342 (100%)	-0.67	4 (1%) 79 79	17, 24, 44, 90	0
4	d	342/342 (100%)	-0.73	5 (1%) 73 74	18, 25, 42, 86	0
5	E	78/83 (93%)	0.76	19 (24%) 0 0	28, 47, 75, 87	0
5	e	78/83 (93%)	0.64	16 (20%) 1 1	29, 44, 67, 81	0
6	F	33/44 (75%)	-0.09	4 (12%) 4 4	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.04	3 (9%) 8 8	28, 34, 72, 90	0
7	H	64/65 (98%)	0.08	3 (4%) 31 30	26, 37, 50, 78	0
7	h	62/65 (95%)	-0.24	0 100 100	25, 36, 48, 58	0
8	I	34/38 (89%)	-0.11	3 (8%) 10 9	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.15	2 (5%) 23 23	29, 34, 52, 85	0
9	J	36/40 (90%)	-0.04	2 (5%) 24 23	26, 41, 74, 90	0
9	j	40/40 (100%)	-0.03	3 (7%) 14 14	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.27	2 (5%) 25 24	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.22	1 (2%) 54 53	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.36	3 (8%) 12 12	18, 22, 65, 81	0
11	l	37/37 (100%)	-0.22	3 (8%) 12 12	18, 22, 76, 91	0
12	M	33/36 (91%)	-0.65	1 (3%) 50 48	21, 25, 39, 57	0
12	m	34/36 (94%)	-0.55	3 (8%) 10 9	20, 26, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.23	8 (3%) 46 44	18, 32, 56, 85	0
13	o	243/244 (99%)	-0.09	19 (7%) 13 13	19, 35, 67, 89	0
14	T	28/32 (87%)	-0.69	1 (3%) 42 40	19, 24, 37, 54	0
14	t	29/32 (90%)	-0.36	2 (6%) 16 16	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.34	2 (2%) 63 63	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.36	1 (1%) 82 82	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.62	0 100 100	22, 28, 43, 60	0
16	v	137/137 (100%)	-0.25	5 (3%) 42 40	25, 36, 53, 74	0
17	Y	29/30 (96%)	1.08	6 (20%) 1 0	41, 51, 72, 79	0
17	y	29/30 (96%)	0.76	4 (13%) 2 3	41, 50, 66, 70	0
18	X	38/40 (95%)	0.26	5 (13%) 3 3	32, 42, 68, 72	0
18	x	35/40 (87%)	-0.09	2 (5%) 23 23	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.66	13 (20%) 1 0	38, 48, 86, 98	0
19	z	61/62 (98%)	0.71	12 (19%) 1 1	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.37	220 (4%) 36 34	16, 30, 57, 98	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	9.7
2	b	495	PHE	9.2
2	b	503	THR	8.4
13	o	246	ALA	8.3
2	b	502	VAL	7.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.97	0.07	23,29,48,51	0
14	FME	t	1	10/11	0.97	0.06	23,27,49,50	0
8	FME	i	1	10/11	0.98	0.09	30,31,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.98	0.07	26,32,36,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	HTG	C	534	19/19	0.39	0.39	68,110,128,130	0
26	UNL	Z	102	4/-	0.52	0.17	59,61,62,63	0
24	LMG	C	524	45/55	0.52	0.32	22,46,51,56	45
32	HTG	D	417	19/19	0.53	0.31	67,105,119,120	0
28	DMS	U	904	4/4	0.55	0.22	58,66,66,83	0
32	HTG	c	521	19/19	0.56	0.35	57,85,102,105	0
26	UNL	b	642	13/-	0.57	0.22	71,80,87,90	0
26	UNL	b	645	6/-	0.58	0.24	57,65,76,76	0
32	HTG	d	401	19/19	0.58	0.29	58,99,111,120	0
32	HTG	B	623	19/19	0.59	0.35	53,88,93,94	0
34	LMT	f	102	24/35	0.59	0.26	62,77,94,98	0
35	DGD	D	406	51/66	0.59	0.30	57,74,100,108	0
26	UNL	J	104	14/-	0.60	0.24	67,77,80,81	0
34	LMT	J	103	24/35	0.60	0.23	53,61,81,85	0
28	DMS	H	103	4/4	0.61	0.40	84,101,109,112	0
28	DMS	B	636	4/4	0.61	0.40	77,86,90,96	0
34	LMT	m	101	35/35	0.63	0.25	48,94,110,114	0
34	LMT	b	628	25/35	0.64	0.22	54,79,95,96	0
26	UNL	A	410	36/-	0.64	0.25	57,78,84,91	0
35	DGD	d	416	51/66	0.64	0.27	56,75,96,103	0
32	HTG	B	632	19/19	0.65	0.23	51,97,108,114	0
36	LHG	E	103	48/49	0.66	0.29	44,99,108,119	0
32	HTG	C	521	19/19	0.67	0.26	46,78,89,90	0
26	UNL	a	414	28/-	0.67	0.23	59,68,84,87	0
28	DMS	v	207	4/4	0.67	0.20	53,66,72,87	0
26	UNL	E	102	15/-	0.68	0.28	55,62,76,77	0
26	UNL	b	643	9/-	0.68	0.18	67,67,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	UNL	B	646	16/-	0.68	0.24	85,89,93,94	0
26	UNL	T	103	13/-	0.69	0.17	64,68,72,72	0
28	DMS	j	105	4/4	0.69	0.19	70,74,75,88	0
32	HTG	v	210	14/19	0.69	0.27	60,80,92,100	0
26	UNL	a	402	6/-	0.69	0.17	50,57,62,63	0
28	DMS	O	305	4/4	0.69	0.30	64,66,77,86	0
26	UNL	B	630	14/-	0.70	0.20	67,74,83,84	0
32	HTG	b	602	19/19	0.70	0.20	51,103,117,118	0
34	LMT	Z	101	35/35	0.70	0.23	44,90,107,109	0
34	LMT	b	627	32/35	0.71	0.24	42,67,84,87	0
26	UNL	B	629	10/-	0.72	0.27	54,69,74,74	0
24	LMG	c	518	51/55	0.72	0.21	37,72,84,87	0
26	UNL	c	524	30/-	0.72	0.19	59,74,86,87	0
34	LMT	a	418	35/35	0.73	0.21	45,69,78,81	0
26	UNL	J	107	3/-	0.73	0.21	61,61,63,64	0
26	UNL	U	901	14/-	0.74	0.27	40,49,59,59	0
34	LMT	m	102	35/35	0.74	0.20	34,53,58,59	0
34	LMT	B	626	24/35	0.74	0.20	37,54,86,95	0
26	UNL	h	103	16/-	0.74	0.29	61,69,73,76	0
32	HTG	u	201	8/19	0.74	0.21	45,52,69,89	0
26	UNL	a	416	11/-	0.75	0.16	66,68,76,78	0
28	DMS	b	638	4/4	0.75	0.28	67,75,77,86	0
23	SQD	l	101	54/54	0.75	0.20	47,68,101,106	0
26	UNL	C	523	34/-	0.75	0.22	59,80,92,101	0
34	LMT	M	101	35/35	0.75	0.20	34,53,63,64	0
26	UNL	I	106	11/-	0.76	0.19	61,73,81,81	0
28	DMS	b	640	4/4	0.76	0.27	49,58,71,73	0
34	LMT	B	625	24/35	0.76	0.16	48,67,86,89	0
26	UNL	B	647	13/-	0.76	0.24	71,81,90,91	0
28	DMS	O	308	4/4	0.77	0.24	66,74,76,87	0
28	DMS	B	642	4/4	0.77	0.31	43,51,68,71	0
34	LMT	I	101	35/35	0.77	0.24	67,82,91,92	0
27	PL9	a	415	55/55	0.77	0.23	52,67,89,94	0
26	UNL	t	102	16/-	0.77	0.17	61,71,80,80	0
34	LMT	z	102	35/35	0.78	0.19	46,85,99,101	0
26	UNL	H	105	6/-	0.78	0.14	51,55,63,65	0
32	HTG	c	520	19/19	0.78	0.21	77,88,99,100	0
26	UNL	c	526	8/-	0.78	0.15	54,59,64,65	0
27	PL9	A	411	55/55	0.79	0.20	43,67,89,92	0
26	UNL	J	105	12/-	0.79	0.23	63,67,71,71	0
26	UNL	d	409	36/-	0.79	0.18	36,60,91,102	0
23	SQD	b	622	54/54	0.80	0.17	46,63,95,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	HTG	C	522	19/19	0.80	0.27	66,83,104,107	0
26	UNL	B	633	16/-	0.80	0.25	53,61,69,70	0
34	LMT	T	102	24/35	0.80	0.19	36,53,78,85	0
26	UNL	i	102	11/-	0.80	0.16	48,54,64,65	0
34	LMT	c	523	35/35	0.81	0.23	67,77,83,85	0
26	UNL	X	101	16/-	0.81	0.17	37,40,59,59	0
28	DMS	V	205	4/4	0.81	0.25	67,76,77,79	0
26	UNL	b	630	11/-	0.81	0.21	55,60,67,68	0
32	HTG	b	624	19/19	0.81	0.23	49,74,80,85	0
23	SQD	a	401	54/54	0.81	0.16	39,58,82,86	0
34	LMT	E	101	24/35	0.81	0.26	64,78,84,90	0
28	DMS	O	309	4/4	0.81	0.23	58,65,72,73	0
34	LMT	B	627	16/35	0.82	0.18	52,60,78,78	0
28	DMS	O	303	4/4	0.82	0.29	63,72,77,78	0
26	UNL	d	410	16/-	0.82	0.18	33,45,63,63	0
26	UNL	j	106	6/-	0.82	0.19	52,55,58,59	0
26	UNL	e	101	7/-	0.82	0.24	54,58,64,65	0
23	SQD	A	412	54/54	0.82	0.16	41,60,78,81	0
26	UNL	I	104	11/-	0.83	0.18	53,56,59,62	0
26	UNL	J	106	4/-	0.83	0.16	57,60,61,67	0
28	DMS	b	641	4/4	0.83	0.17	63,65,75,80	0
23	SQD	f	101	40/54	0.83	0.25	57,86,102,107	0
28	DMS	o	308	4/4	0.83	0.21	60,61,62,63	0
28	DMS	u	204	4/4	0.83	0.20	71,78,83,86	0
26	UNL	x	102	9/-	0.83	0.28	56,68,72,72	0
26	UNL	D	410	37/-	0.83	0.15	42,57,93,98	0
28	DMS	O	310	4/4	0.84	0.32	76,78,82,94	0
26	UNL	I	105	10/-	0.84	0.15	60,66,71,72	0
32	HTG	B	622	19/19	0.84	0.16	28,46,54,54	0
26	UNL	M	102	12/-	0.84	0.22	49,53,95,98	0
28	DMS	o	306	4/4	0.84	0.25	55,58,65,77	0
26	UNL	c	525	10/-	0.84	0.15	58,65,66,67	0
28	DMS	D	415	4/4	0.85	0.25	57,58,63,65	0
26	UNL	i	101	16/-	0.85	0.18	41,45,65,65	0
26	UNL	L	102	14/-	0.85	0.22	56,60,84,84	0
26	UNL	I	102	16/-	0.85	0.19	38,47,63,64	0
32	HTG	b	625	19/19	0.85	0.20	30,44,66,70	0
28	DMS	c	533	4/4	0.85	0.27	73,75,77,87	0
28	DMS	o	304	4/4	0.86	0.32	68,79,82,83	0
26	UNL	b	646	6/-	0.86	0.14	54,58,60,62	0
32	HTG	C	520	19/19	0.86	0.21	64,70,76,79	0
23	SQD	F	101	35/54	0.86	0.23	51,76,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	UNL	A	413	4/-	0.86	0.19	64,64,64,66	0
28	DMS	B	635	4/4	0.86	0.24	90,94,95,96	0
28	DMS	v	209	4/4	0.86	0.31	71,78,79,79	0
32	HTG	V	202	13/19	0.86	0.21	45,49,70,82	0
26	UNL	B	628	15/-	0.86	0.15	45,50,60,66	0
24	LMG	B	620	51/55	0.87	0.12	33,43,55,58	0
20	CLA	C	513	65/65	0.87	0.14	40,48,72,77	0
28	DMS	B	638	4/4	0.87	0.19	53,61,63,68	0
32	HTG	b	601	19/19	0.87	0.15	45,61,67,80	0
28	DMS	b	637	4/4	0.87	0.17	77,79,84,93	0
24	LMG	A	407	51/55	0.87	0.13	40,55,70,78	0
28	DMS	B	644	4/4	0.87	0.32	52,53,61,69	0
28	DMS	C	532	4/4	0.87	0.19	33,40,41,48	0
33	CA	V	203	1/1	0.88	0.11	63,63,63,63	0
26	UNL	H	104	4/-	0.88	0.20	60,62,65,67	0
32	HTG	B	631	19/19	0.88	0.12	41,57,69,73	0
20	CLA	B	602	65/65	0.88	0.14	29,42,77,81	0
24	LMG	a	410	51/55	0.88	0.15	44,55,65,67	0
26	UNL	I	103	13/-	0.88	0.13	47,53,84,87	0
28	DMS	U	902	4/4	0.88	0.23	35,44,49,58	0
24	LMG	C	519	51/55	0.89	0.15	31,67,83,84	0
24	LMG	c	519	51/55	0.89	0.13	29,59,86,88	0
26	UNL	j	104	16/-	0.89	0.11	49,58,64,66	0
26	UNL	D	411	16/-	0.89	0.16	39,45,58,62	0
28	DMS	O	306	4/4	0.89	0.29	66,73,73,75	0
20	CLA	b	603	65/65	0.89	0.15	30,45,75,82	0
22	BCR	d	405	40/40	0.89	0.12	24,30,56,58	0
28	DMS	C	527	4/4	0.89	0.17	73,76,79,87	0
24	LMG	b	623	49/55	0.89	0.12	33,42,54,61	0
28	DMS	O	311	4/4	0.90	0.26	57,65,69,72	0
22	BCR	D	405	40/40	0.90	0.11	26,30,58,60	0
28	DMS	c	534	4/4	0.90	0.24	70,71,75,81	0
28	DMS	A	418	4/4	0.90	0.31	68,74,80,85	0
26	UNL	b	644	7/-	0.90	0.18	64,65,70,70	0
28	DMS	b	632	4/4	0.90	0.15	55,58,66,70	0
28	DMS	b	636	4/4	0.90	0.14	66,71,72,79	0
26	UNL	z	101	6/-	0.90	0.13	49,55,55,57	0
22	BCR	C	514	40/40	0.90	0.10	36,45,49,50	0
28	DMS	B	639	4/4	0.90	0.24	65,70,71,76	0
28	DMS	d	415	4/4	0.91	0.26	68,71,71,72	0
26	UNL	b	629	16/-	0.91	0.14	41,48,60,60	0
28	DMS	A	416	4/4	0.91	0.23	59,60,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DMS	o	305	4/4	0.91	0.23	73,75,77,87	0
28	DMS	V	204	4/4	0.91	0.32	58,64,64,72	0
20	CLA	b	618	65/65	0.91	0.13	23,33,92,98	0
28	DMS	u	202	4/4	0.91	0.18	40,46,52,54	0
28	DMS	u	203	4/4	0.91	0.29	47,55,56,65	0
28	DMS	V	209	4/4	0.91	0.20	57,73,77,81	0
26	UNL	i	103	11/-	0.91	0.27	58,61,65,66	0
28	DMS	v	208	4/4	0.91	0.26	89,92,92,95	0
28	DMS	b	634	4/4	0.91	0.29	59,67,67,75	0
28	DMS	c	535	4/4	0.91	0.18	58,59,65,68	0
22	BCR	K	101	40/40	0.92	0.10	33,37,42,45	0
28	DMS	c	536	4/4	0.92	0.15	33,33,45,46	0
28	DMS	b	635	4/4	0.92	0.27	58,62,69,73	0
26	UNL	d	411	16/-	0.92	0.12	33,42,55,55	0
28	DMS	o	303	4/4	0.92	0.38	66,69,75,79	0
22	BCR	K	102	40/40	0.92	0.13	31,36,40,41	0
28	DMS	O	304	4/4	0.92	0.28	63,68,72,73	0
20	CLA	c	513	65/65	0.92	0.11	36,46,81,87	0
20	CLA	C	506	65/65	0.92	0.10	32,45,86,87	0
28	DMS	C	529	4/4	0.92	0.19	70,73,74,74	0
20	CLA	c	512	65/65	0.92	0.11	28,41,70,72	0
38	RRX	x	101	41/41	0.92	0.09	26,32,47,58	0
32	HTG	B	621	19/19	0.93	0.12	36,41,48,52	0
28	DMS	D	416	4/4	0.93	0.17	83,87,89,91	0
28	DMS	B	640	4/4	0.93	0.33	45,48,49,50	0
28	DMS	A	417	4/4	0.93	0.17	70,72,77,81	0
20	CLA	C	512	55/65	0.93	0.09	37,44,49,54	0
28	DMS	c	529	4/4	0.93	0.23	79,82,86,87	0
22	BCR	k	102	40/40	0.93	0.09	41,46,51,51	0
23	SQD	A	406	54/54	0.93	0.13	34,59,71,76	0
28	DMS	O	307	4/4	0.93	0.16	69,76,77,88	0
28	DMS	v	203	4/4	0.93	0.16	67,69,76,79	0
28	DMS	v	204	4/4	0.93	0.15	48,54,57,69	0
35	DGD	H	102	62/66	0.93	0.11	25,33,40,43	0
28	DMS	C	531	4/4	0.93	0.24	53,54,58,74	0
35	DGD	h	101	62/66	0.93	0.10	25,34,41,49	0
20	CLA	B	601	65/65	0.93	0.12	23,29,82,86	0
38	RRX	H	101	41/41	0.93	0.10	27,31,41,46	0
20	CLA	c	506	65/65	0.93	0.10	24,39,71,74	0
32	HTG	O	302	19/19	0.94	0.10	34,42,50,53	0
33	CA	o	301	1/1	0.94	0.07	48,48,48,48	0
28	DMS	C	533	4/4	0.94	0.28	72,73,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DMS	B	643	4/4	0.94	0.14	51,53,62,71	0
28	DMS	A	415	4/4	0.94	0.20	55,58,65,71	0
24	LMG	J	101	45/55	0.94	0.10	27,32,64,70	0
23	SQD	a	409	54/54	0.94	0.12	33,56,75,78	0
24	LMG	j	101	45/55	0.94	0.09	27,32,60,64	0
28	DMS	v	206	4/4	0.94	0.20	52,53,61,66	0
28	DMS	c	531	4/4	0.94	0.15	73,78,85,86	0
28	DMS	c	532	4/4	0.94	0.23	65,70,76,77	0
20	CLA	d	404	65/65	0.94	0.10	24,29,78,87	0
33	CA	O	301	1/1	0.94	0.06	47,47,47,47	0
20	CLA	c	511	65/65	0.95	0.09	27,33,40,43	0
20	CLA	B	607	65/65	0.95	0.09	22,29,55,62	0
22	BCR	j	102	40/40	0.95	0.09	30,35,42,45	0
22	BCR	k	101	40/40	0.95	0.09	28,36,41,42	0
20	CLA	D	404	65/65	0.95	0.10	26,29,77,81	0
28	DMS	V	208	4/4	0.95	0.12	75,77,82,85	0
22	BCR	t	101	40/40	0.95	0.07	22,29,41,43	0
28	DMS	B	641	4/4	0.95	0.31	68,69,75,80	0
28	DMS	d	413	4/4	0.95	0.17	47,53,55,57	0
31	BCT	A	421	4/4	0.95	0.10	31,34,40,44	0
28	DMS	d	414	4/4	0.95	0.16	57,62,64,68	0
20	CLA	C	507	65/65	0.95	0.09	28,37,52,57	0
22	BCR	B	619	40/40	0.95	0.07	22,30,42,44	0
35	DGD	C	517	55/66	0.95	0.07	26,34,59,62	0
20	CLA	b	608	65/65	0.95	0.09	24,31,59,63	0
33	CA	b	626	1/1	0.95	0.07	42,42,42,42	0
35	DGD	c	515	62/66	0.95	0.10	23,32,71,75	0
35	DGD	c	517	62/66	0.95	0.09	23,30,56,71	0
22	BCR	C	515	40/40	0.95	0.09	31,37,43,45	0
20	CLA	C	511	65/65	0.95	0.08	30,37,42,45	0
36	LHG	D	409	49/49	0.95	0.12	27,33,81,83	0
28	DMS	b	639	4/4	0.95	0.20	46,49,49,50	0
28	DMS	o	307	4/4	0.95	0.16	53,58,63,65	0
20	CLA	C	503	65/65	0.95	0.08	28,33,37,42	0
28	DMS	V	206	4/4	0.96	0.21	59,61,63,65	0
28	DMS	V	207	4/4	0.96	0.10	62,63,63,70	0
20	CLA	C	508	60/65	0.96	0.07	23,31,47,51	0
20	CLA	c	501	65/65	0.96	0.08	26,30,41,48	0
20	CLA	c	503	65/65	0.96	0.08	25,35,40,43	0
28	DMS	B	645	4/4	0.96	0.11	56,59,64,71	0
28	DMS	v	205	4/4	0.96	0.18	67,70,72,73	0
20	CLA	C	509	65/65	0.96	0.09	29,34,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	c	509	65/65	0.96	0.09	25,30,53,58	0
28	DMS	C	530	4/4	0.96	0.16	44,44,46,50	0
20	CLA	C	510	65/65	0.96	0.08	26,31,38,44	0
20	CLA	C	501	65/65	0.96	0.08	27,33,45,52	0
31	BCT	a	413	4/4	0.96	0.07	32,32,38,42	0
20	CLA	B	603	65/65	0.96	0.08	23,28,35,39	0
28	DMS	D	413	4/4	0.96	0.11	50,56,60,61	0
28	DMS	c	528	4/4	0.96	0.18	58,62,63,65	0
20	CLA	C	504	65/65	0.96	0.08	27,30,59,61	0
22	BCR	B	618	40/40	0.96	0.08	21,28,42,45	0
20	CLA	C	505	65/65	0.96	0.08	28,33,44,48	0
20	CLA	a	404	60/65	0.96	0.09	18,22,66,75	0
27	PL9	d	412	55/55	0.96	0.08	18,23,29,35	0
20	CLA	A	404	65/65	0.96	0.10	20,25,88,90	0
20	CLA	b	604	65/65	0.96	0.08	23,27,33,35	0
35	DGD	C	518	62/66	0.96	0.09	24,30,62,73	0
20	CLA	B	610	65/65	0.96	0.10	26,31,35,38	0
20	CLA	b	611	65/65	0.96	0.09	24,30,34,41	0
22	BCR	T	101	40/40	0.96	0.07	24,32,43,45	0
35	DGD	c	516	57/66	0.96	0.08	27,32,62,68	0
28	DMS	h	102	4/4	0.96	0.17	50,51,53,62	0
22	BCR	a	408	40/40	0.96	0.07	21,25,30,31	0
28	DMS	B	637	4/4	0.96	0.17	53,53,54,60	0
36	LHG	D	407	49/49	0.96	0.09	28,37,44,52	0
22	BCR	b	620	40/40	0.96	0.07	22,27,43,46	0
22	BCR	c	514	40/40	0.96	0.07	28,36,39,39	0
37	HEM	E	104	43/43	0.96	0.10	39,44,52,56	0
20	CLA	b	612	65/65	0.96	0.08	21,27,36,41	0
20	CLA	b	616	65/65	0.96	0.09	20,26,73,80	0
28	DMS	F	102	4/4	0.97	0.11	51,52,56,64	0
20	CLA	A	402	59/65	0.97	0.07	18,22,52,58	0
20	CLA	B	608	65/65	0.97	0.07	18,21,34,39	0
20	CLA	b	613	65/65	0.97	0.07	20,22,38,44	0
27	PL9	D	412	55/55	0.97	0.08	19,23,29,34	0
28	DMS	i	104	4/4	0.97	0.21	63,66,67,71	0
20	CLA	b	614	65/65	0.97	0.07	21,25,31,37	0
20	CLA	B	604	65/65	0.97	0.07	21,24,33,39	0
20	CLA	b	617	65/65	0.97	0.07	23,30,44,50	0
20	CLA	B	611	65/65	0.97	0.08	21,26,34,40	0
22	BCR	b	619	40/40	0.97	0.07	23,26,32,35	0
20	CLA	a	403	65/65	0.97	0.09	17,20,29,38	0
22	BCR	b	621	40/40	0.97	0.07	27,32,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DMS	U	903[A]	4/4	0.97	0.17	32,34,40,41	4
28	DMS	U	903[B]	4/4	0.97	0.17	26,28,29,32	4
20	CLA	c	502	65/65	0.97	0.07	22,26,39,48	0
20	CLA	B	615	65/65	0.97	0.08	20,24,70,79	0
20	CLA	c	504	65/65	0.97	0.07	25,29,55,60	0
20	CLA	c	505	65/65	0.97	0.06	25,30,46,50	0
20	CLA	a	407	47/65	0.97	0.08	19,22,41,48	0
20	CLA	c	507	65/65	0.97	0.08	25,30,49,57	0
20	CLA	c	508	60/65	0.97	0.07	24,28,52,54	0
28	DMS	b	631	4/4	0.97	0.10	23,24,27,35	0
20	CLA	B	616	65/65	0.97	0.07	25,29,48,52	0
28	DMS	b	633	4/4	0.97	0.13	45,48,49,53	0
20	CLA	c	510	65/65	0.97	0.07	23,29,39,42	0
35	DGD	C	516	62/66	0.97	0.09	22,32,74,79	0
20	CLA	B	605	65/65	0.97	0.08	19,23,55,58	0
28	DMS	C	525[A]	4/4	0.97	0.19	48,49,51,57	4
28	DMS	C	525[B]	4/4	0.97	0.19	32,33,35,35	4
28	DMS	C	526	4/4	0.97	0.15	59,60,63,65	0
20	CLA	b	605	65/65	0.97	0.07	21,25,34,37	0
20	CLA	b	606	65/65	0.97	0.07	20,24,54,59	0
20	CLA	C	502	65/65	0.97	0.07	24,29,41,48	0
21	PHO	D	403	64/64	0.97	0.07	18,24,29,35	0
21	PHO	a	405	64/64	0.97	0.07	17,20,22,25	0
28	DMS	c	530	4/4	0.97	0.16	36,43,45,49	0
22	BCR	A	405	40/40	0.97	0.08	21,26,32,35	0
22	BCR	B	617	40/40	0.97	0.07	22,26,32,33	0
36	LHG	L	101	49/49	0.97	0.09	24,31,49,53	0
36	LHG	d	406	49/49	0.97	0.10	29,36,43,48	0
36	LHG	d	407	49/49	0.97	0.12	22,27,46,50	0
36	LHG	d	408	49/49	0.97	0.10	24,31,83,88	0
36	LHG	l	102	49/49	0.97	0.08	22,30,51,54	0
28	DMS	D	414	4/4	0.97	0.14	55,56,57,58	0
37	HEM	e	102	43/43	0.97	0.09	34,41,56,68	0
20	CLA	b	609	65/65	0.97	0.07	19,22,33,37	0
20	CLA	b	610	65/65	0.97	0.07	20,26,31,33	0
39	MG	J	102	1/1	0.97	0.05	33,33,33,33	0
20	CLA	D	401	65/65	0.98	0.08	16,20,35,41	0
21	PHO	a	406	64/64	0.98	0.08	19,24,29,32	0
28	DMS	o	302	4/4	0.98	0.07	20,28,31,36	0
20	CLA	b	615	65/65	0.98	0.06	18,22,53,59	0
20	CLA	D	402	65/65	0.98	0.06	15,19,30,36	0
20	CLA	b	607	65/65	0.98	0.08	20,24,33,35	0

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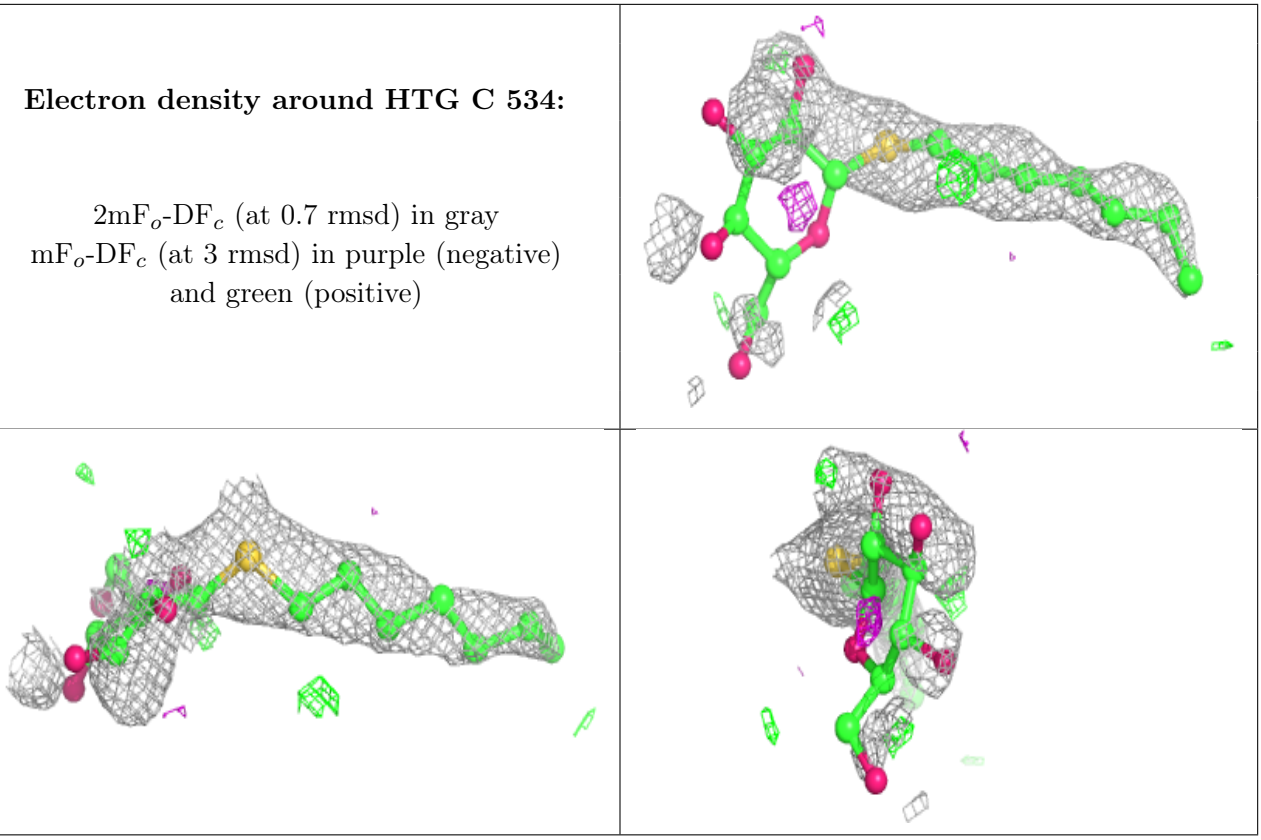
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	LHG	D	408	49/49	0.98	0.09	23,30,44,49	0
28	DMS	B	634	4/4	0.98	0.08	23,24,25,26	0
20	CLA	B	612	65/65	0.98	0.07	19,22,36,42	0
20	CLA	B	613	65/65	0.98	0.07	21,25,30,34	0
20	CLA	B	614	65/65	0.98	0.06	19,22,48,53	0
20	CLA	B	609	65/65	0.98	0.07	22,25,31,33	0
20	CLA	d	402	65/65	0.98	0.08	16,20,35,41	0
33	CA	c	522	1/1	0.98	0.04	41,41,41,41	0
28	DMS	v	202	4/4	0.98	0.15	50,51,53,55	0
20	CLA	d	403	65/65	0.98	0.07	17,19,27,34	0
20	CLA	A	401	65/65	0.98	0.08	16,19,30,36	0
21	PHO	A	403	64/64	0.98	0.07	18,22,24,25	0
20	CLA	B	606	65/65	0.98	0.09	19,24,35,37	0
40	HEC	v	201	43/43	0.98	0.08	25,29,34,37	0
33	CA	B	624	1/1	0.99	0.16	43,43,43,43	0
25	CL	a	412	1/1	0.99	0.06	24,24,24,24	0
25	CL	A	409	1/1	0.99	0.03	22,22,22,22	0
28	DMS	C	528	4/4	0.99	0.09	33,37,39,41	0
29	FE2	A	419	1/1	0.99	0.03	29,29,29,29	0
29	FE2	a	417	1/1	0.99	0.05	27,27,27,27	0
28	DMS	A	414	4/4	0.99	0.07	25,28,28,29	0
40	HEC	V	201	43/43	0.99	0.08	21,23,27,31	0
28	DMS	c	527	4/4	0.99	0.05	33,33,34,38	0
25	CL	a	411	1/1	1.00	0.02	22,22,22,22	0
25	CL	A	408	1/1	1.00	0.05	22,22,22,22	0
39	MG	j	103	1/1	1.00	0.08	31,31,31,31	0
30	OEX	A	420	10/10	1.00	0.04	21,23,24,24	0
30	OEX	a	419	10/10	1.00	0.04	21,24,26,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

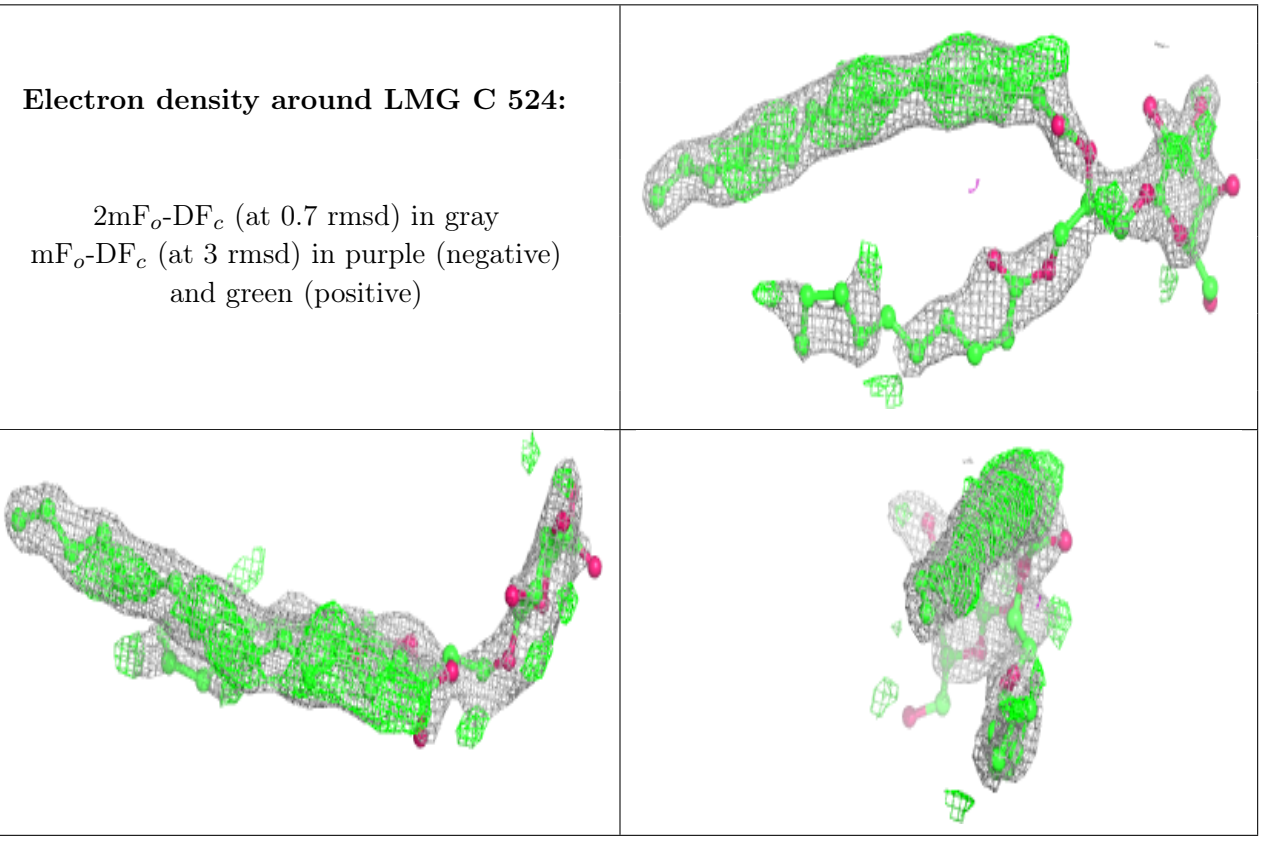
Electron density around HTG C 534:

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



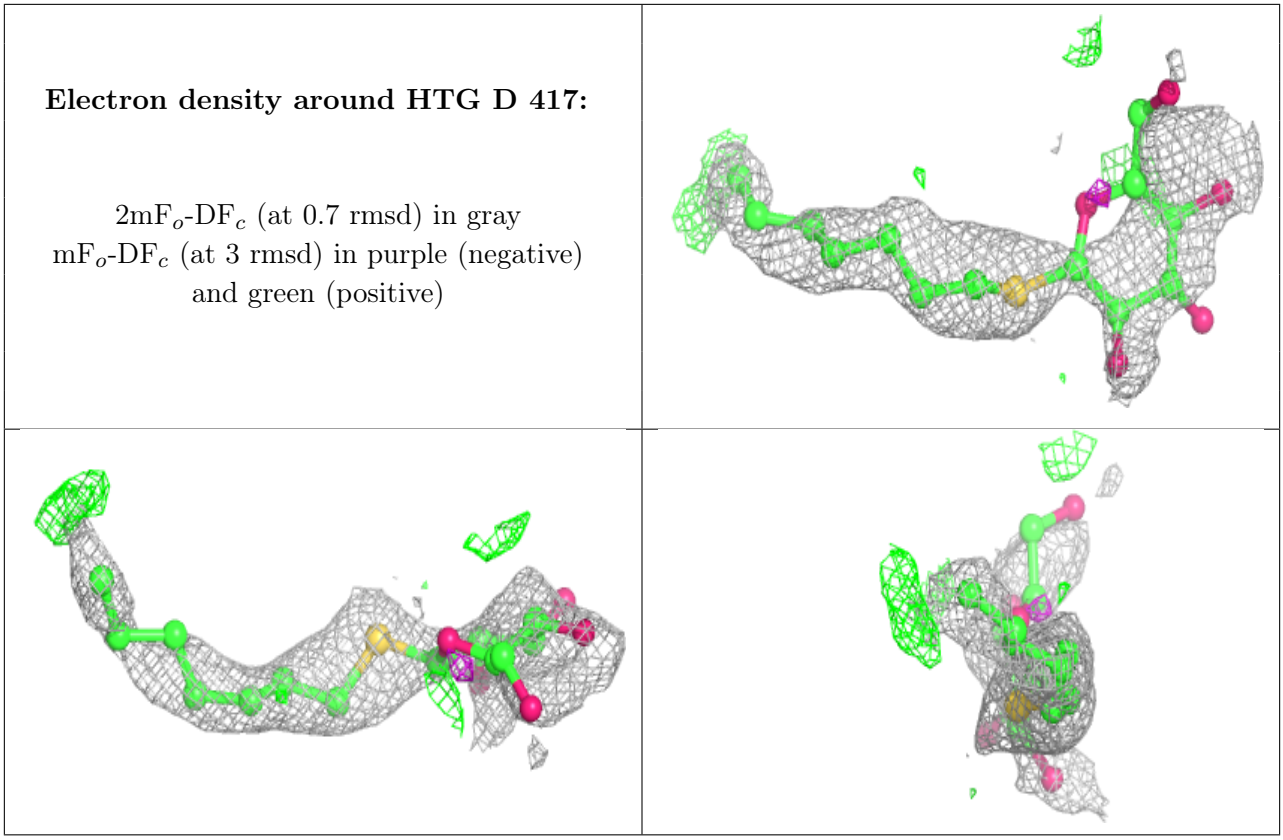
Electron density around LMG C 524:

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



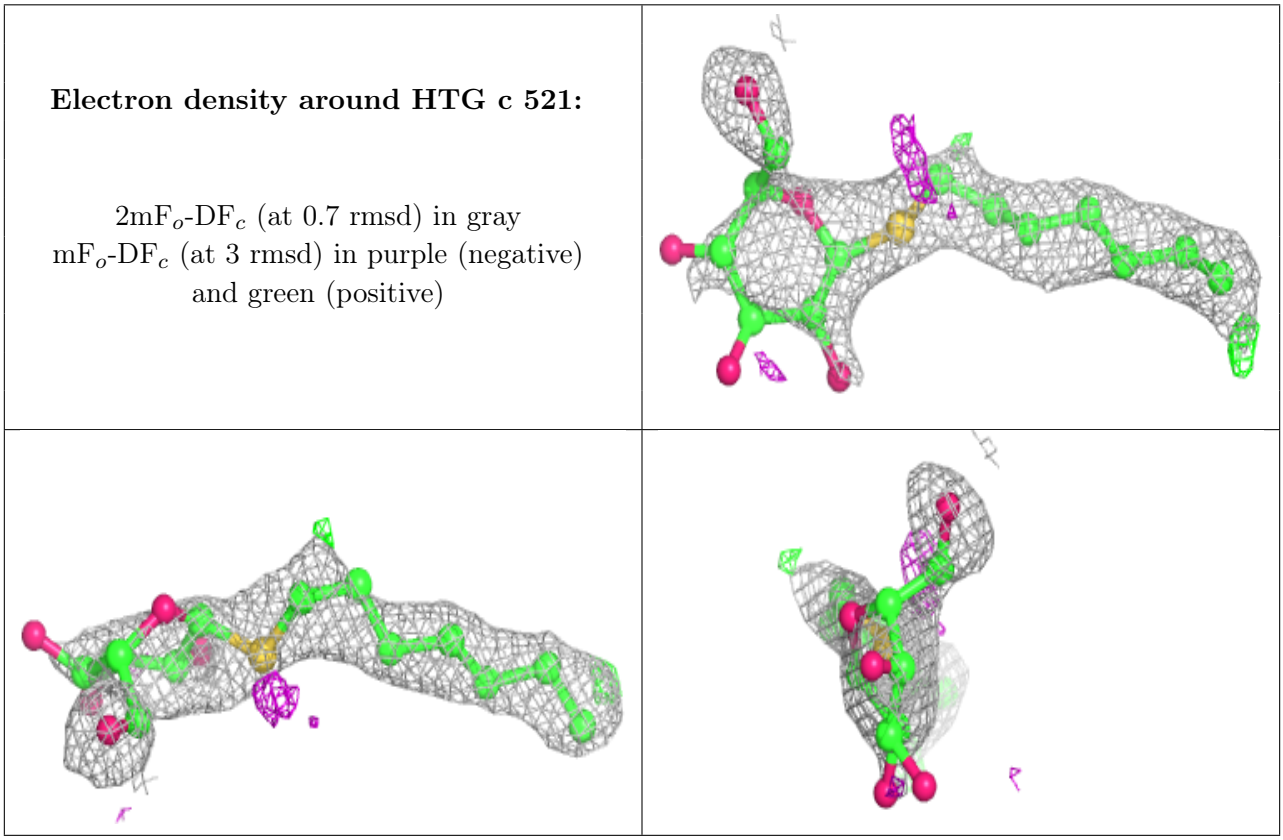
Electron density around HTG D 417:

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



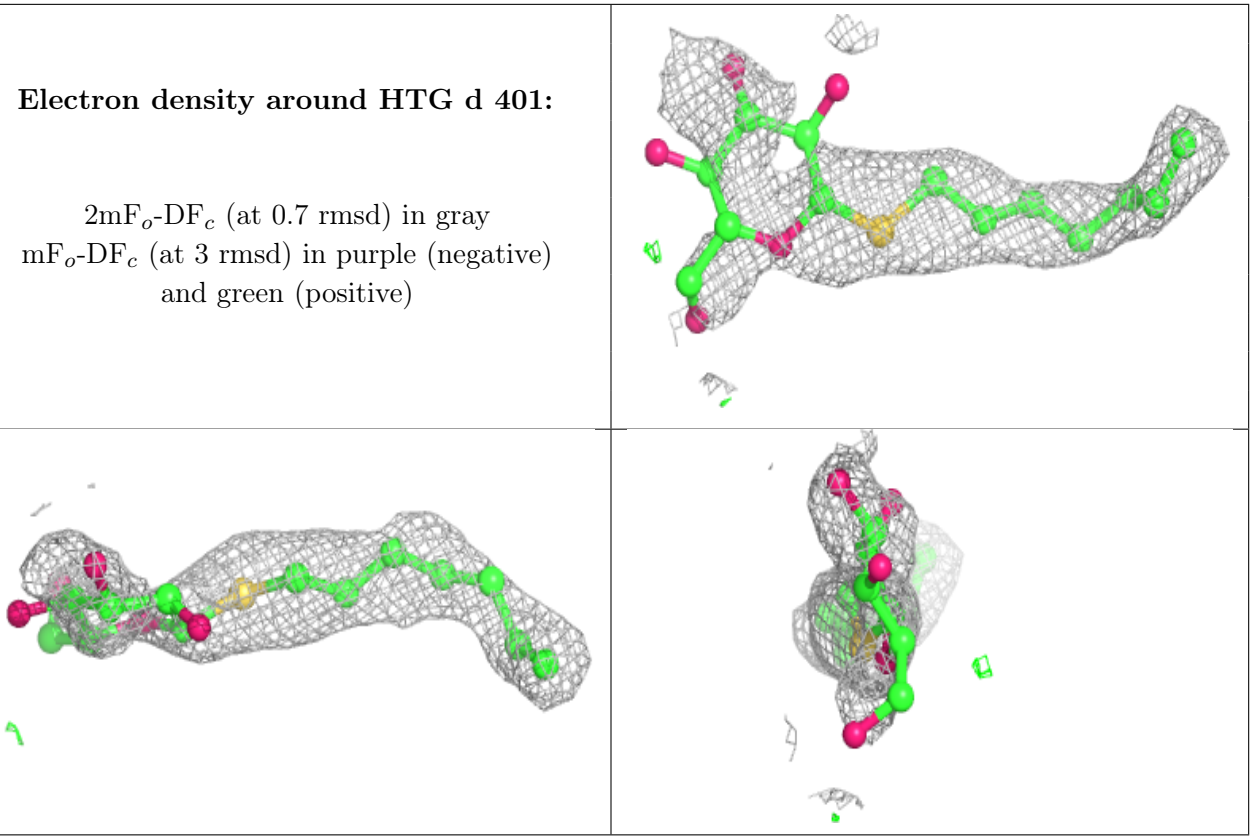
Electron density around HTG c 521:

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



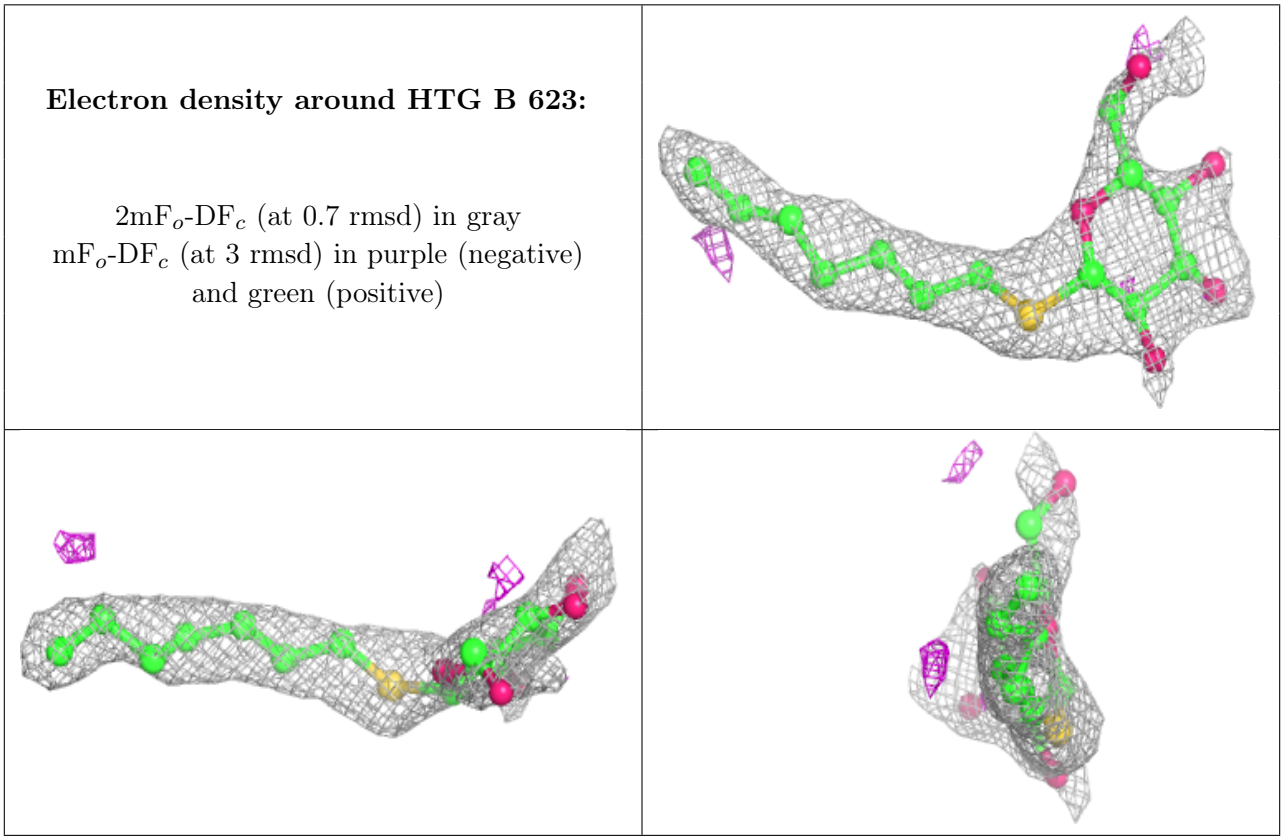
Electron density around HTG d 401:

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



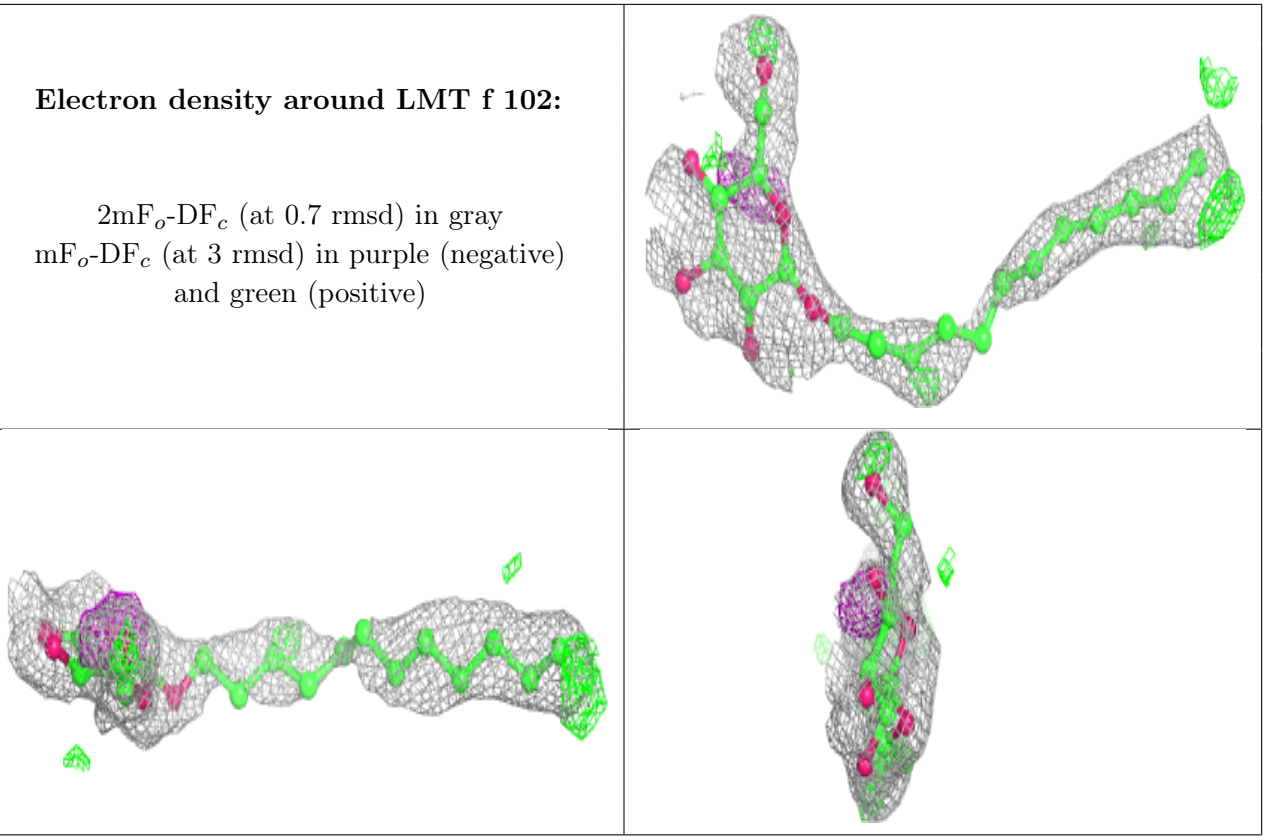
Electron density around HTG B 623:

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



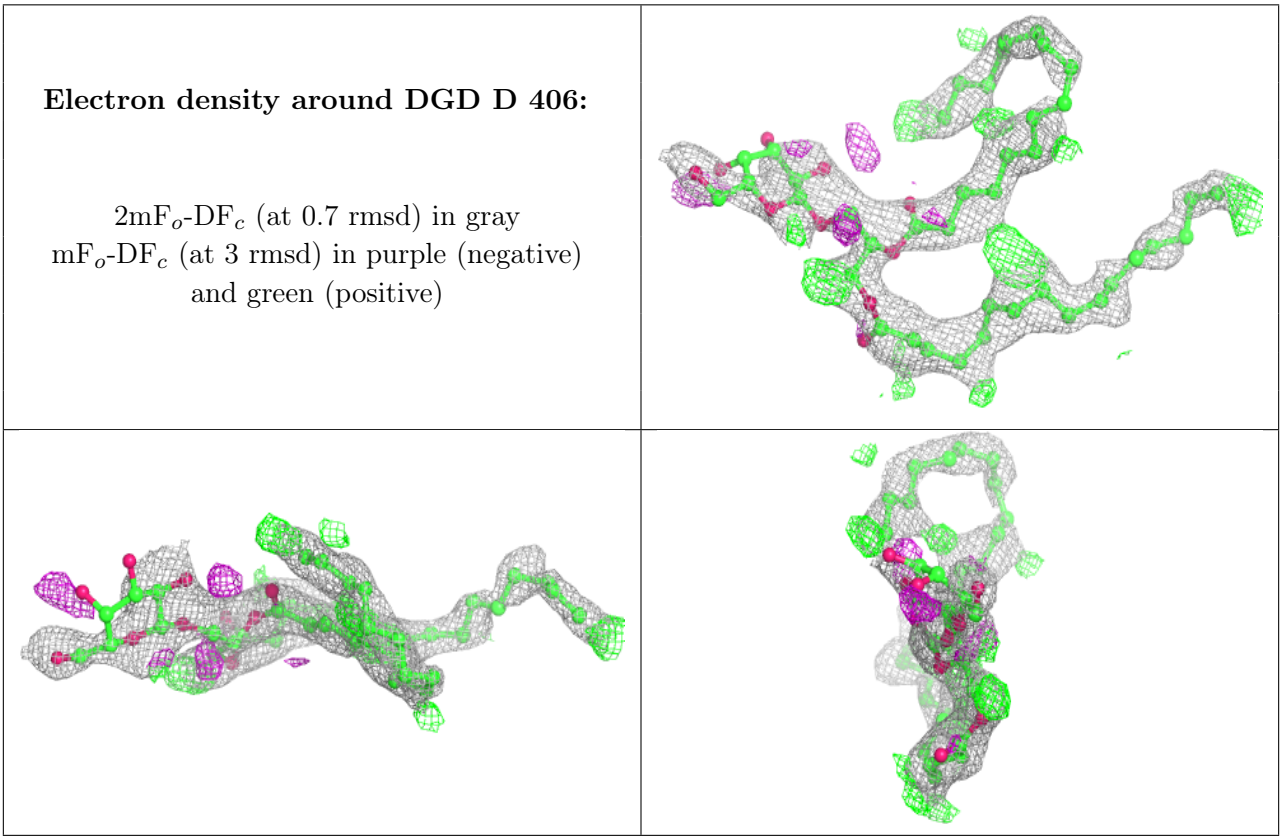
Electron density around LMT f 102:

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



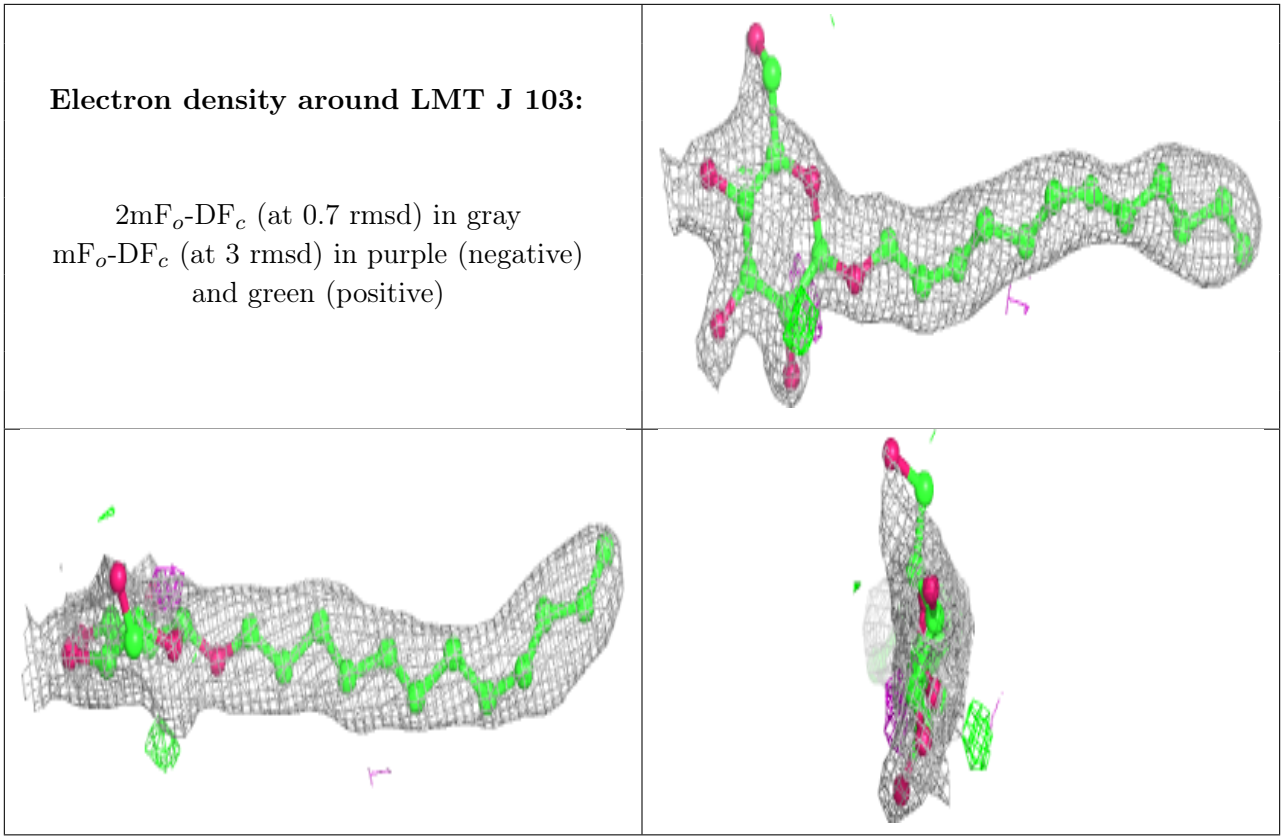
Electron density around DGD D 406:

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



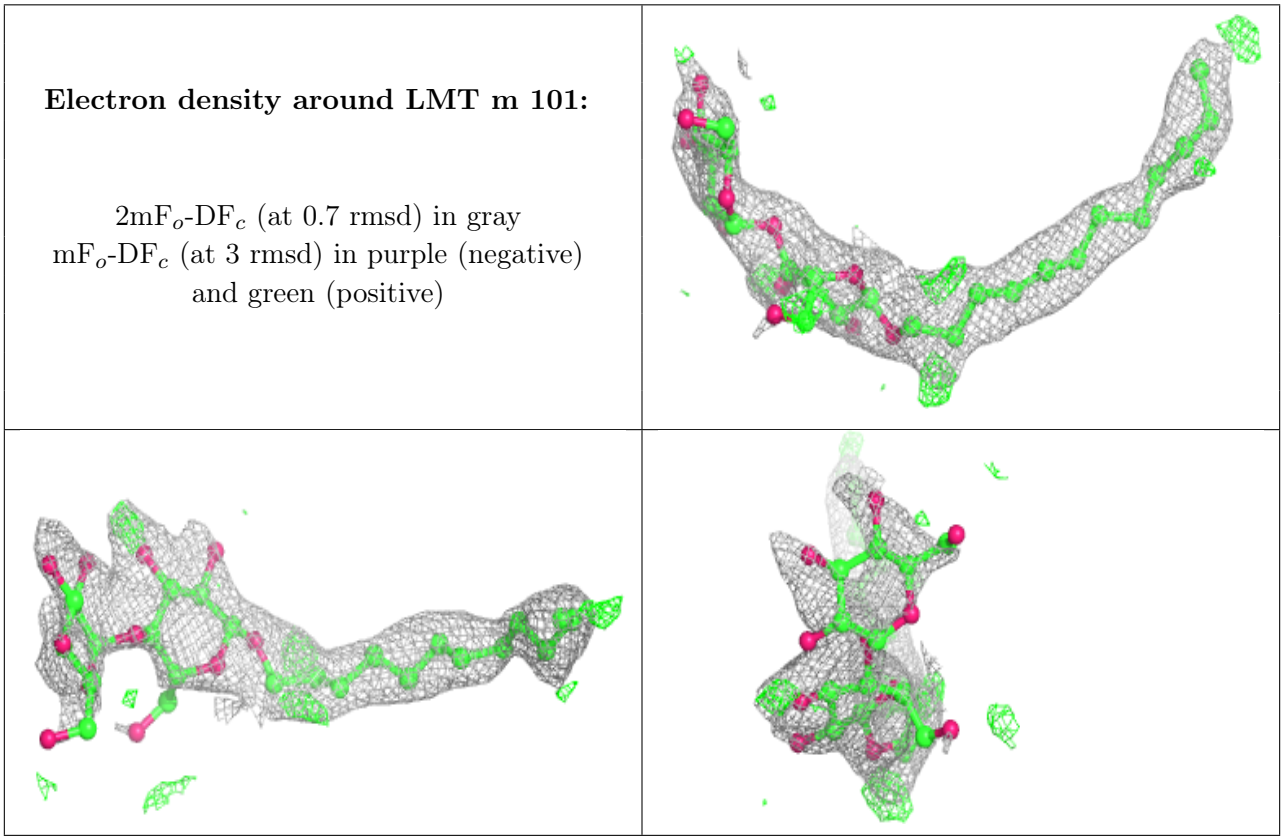
Electron density around LMT J 103:

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



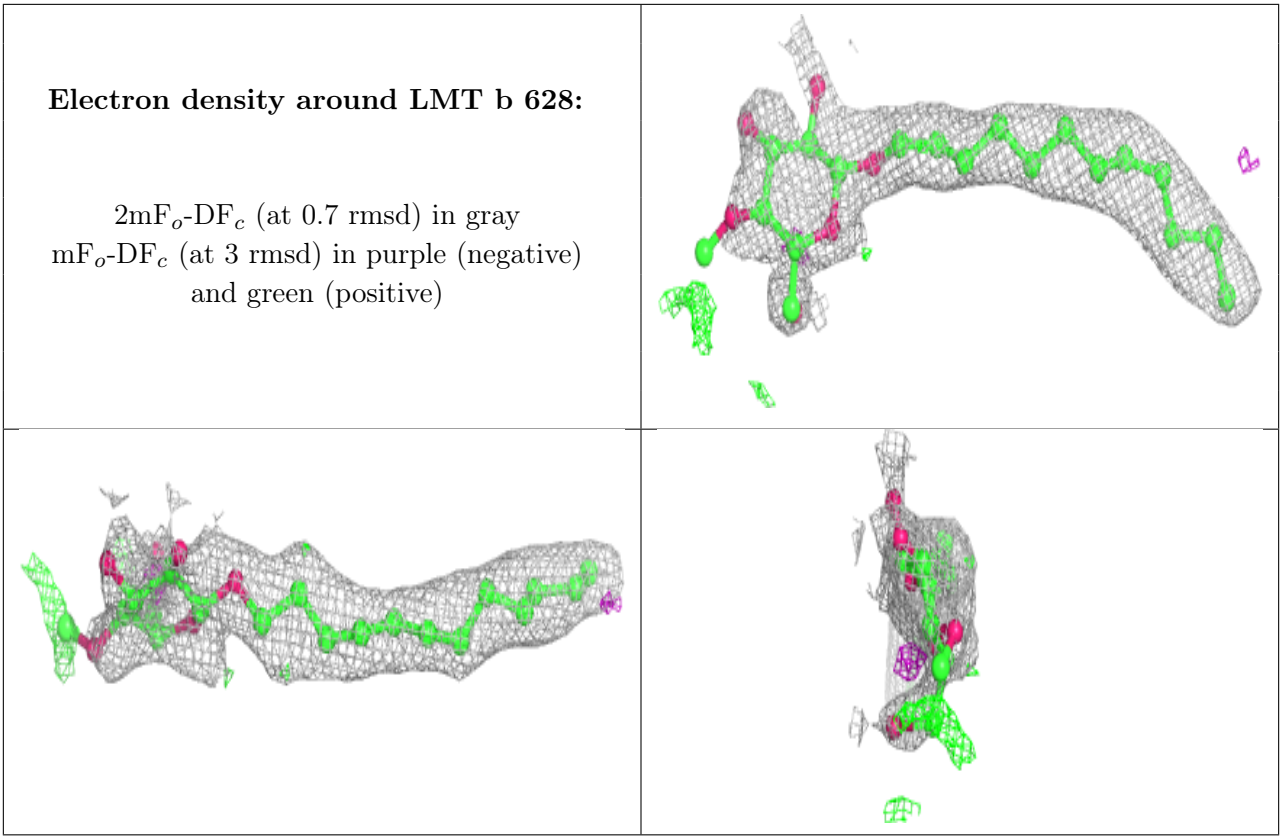
Electron density around LMT m 101:

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



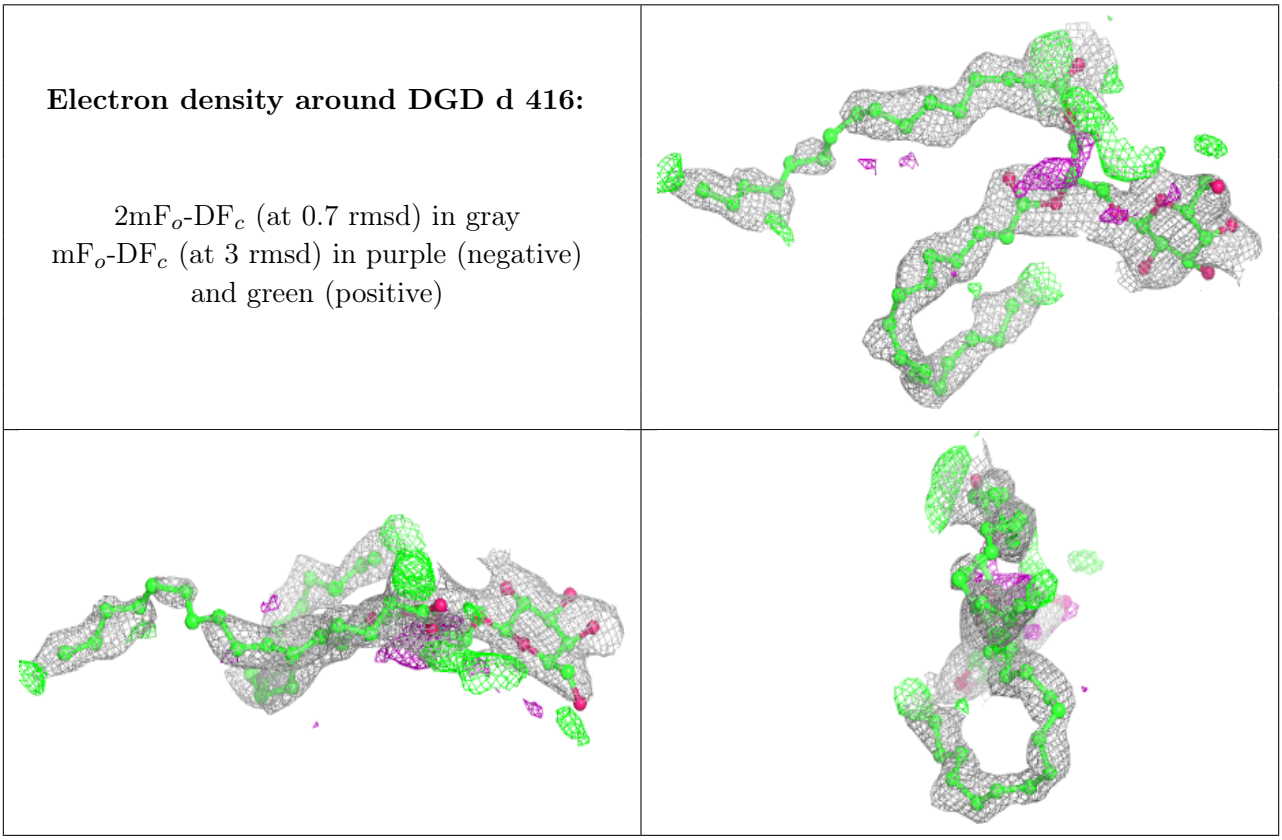
Electron density around LMT b 628:

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



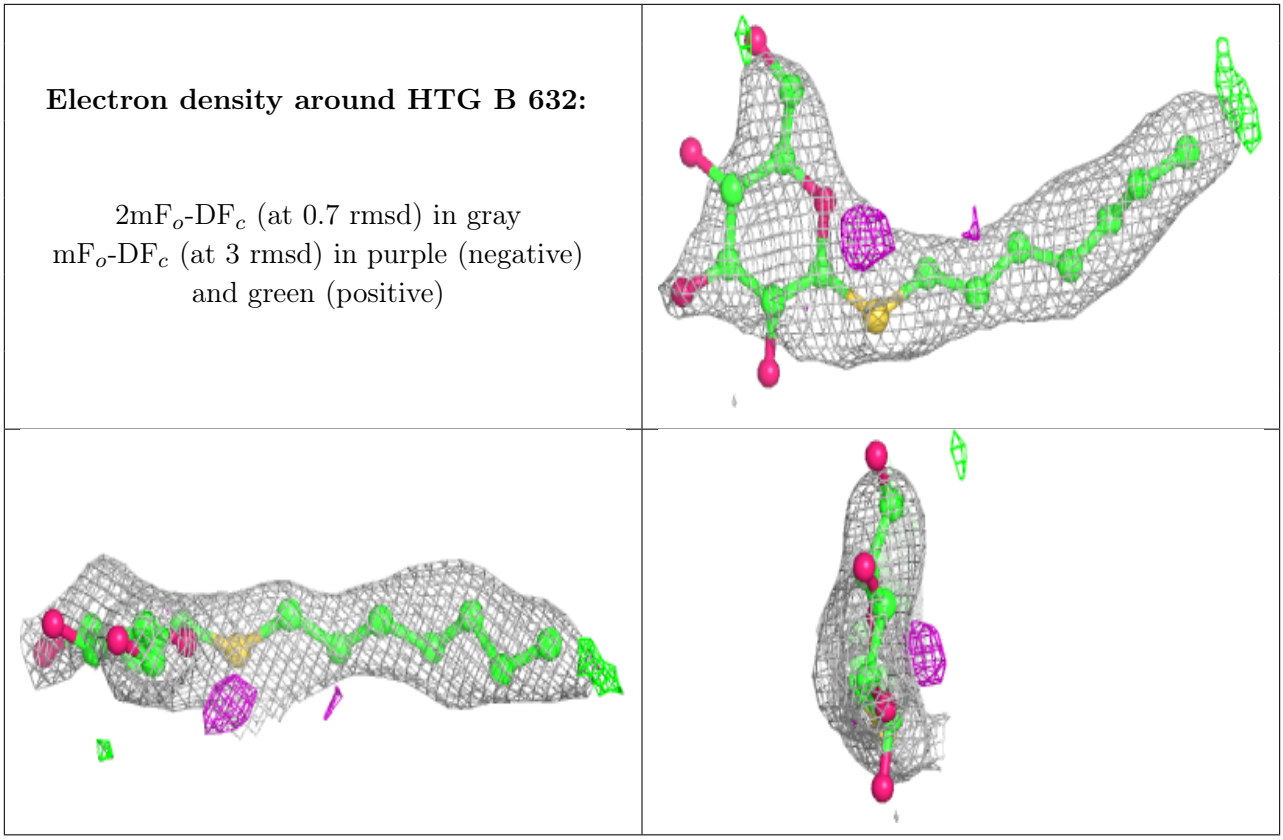
Electron density around DGD d 416:

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



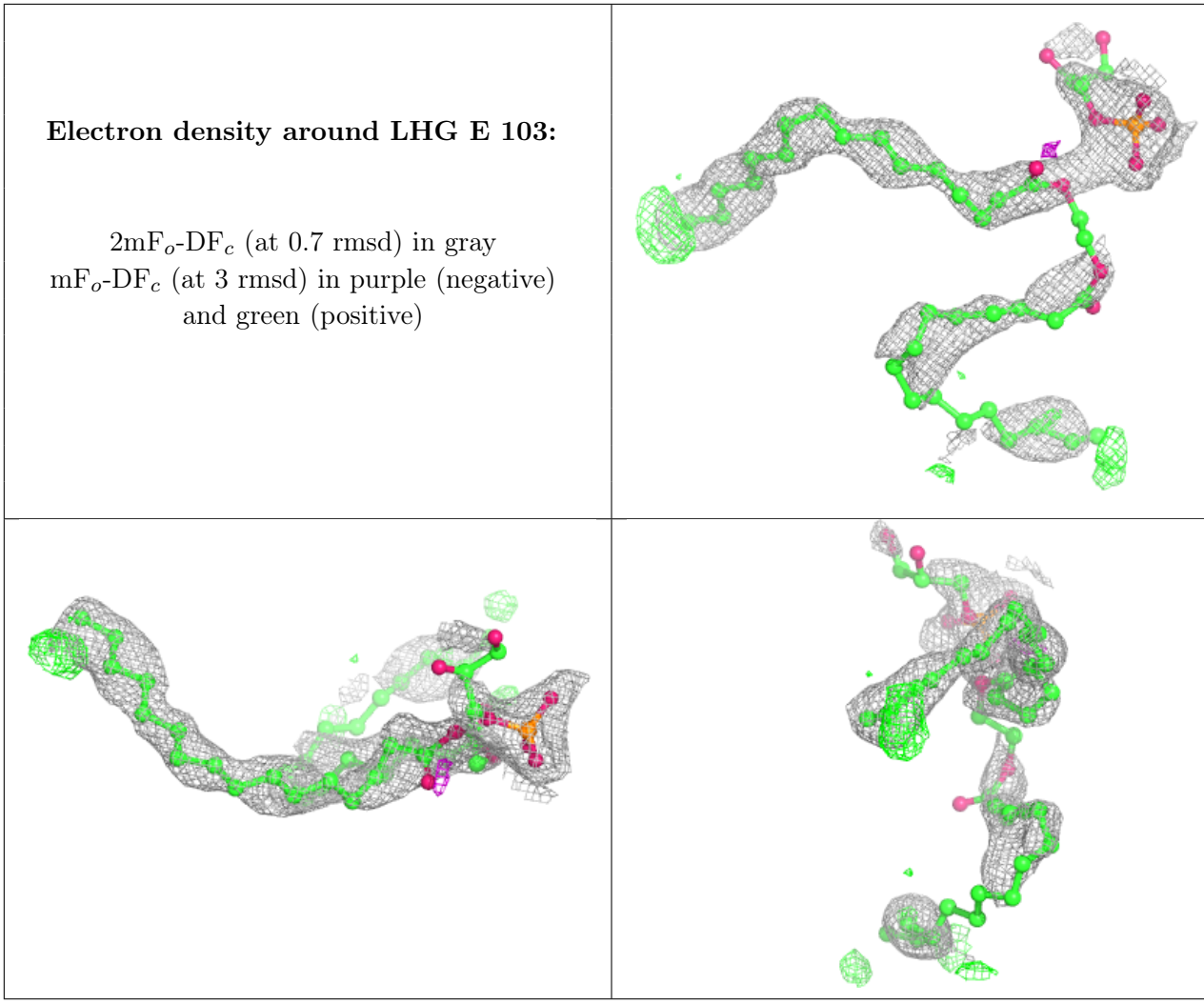
Electron density around HTG B 632:

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



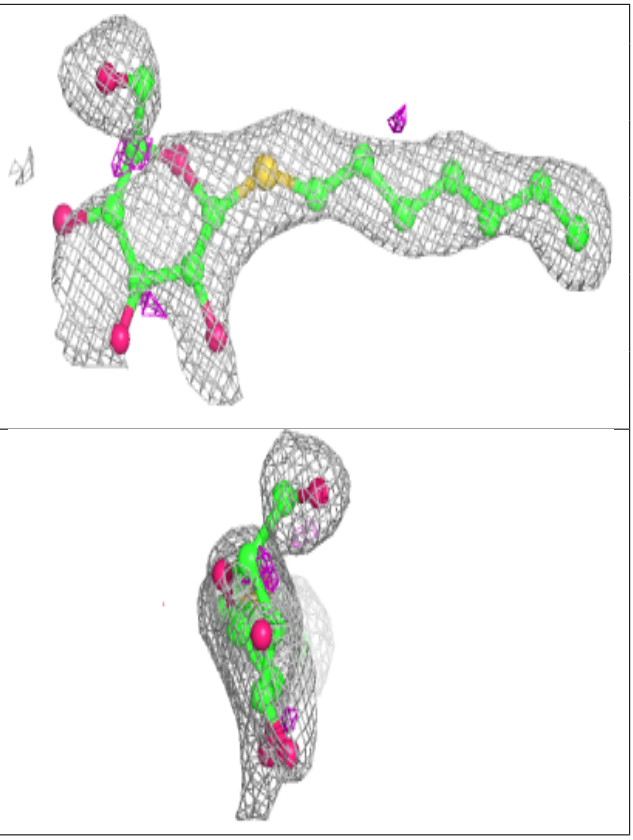
Electron density around LHG E 103:

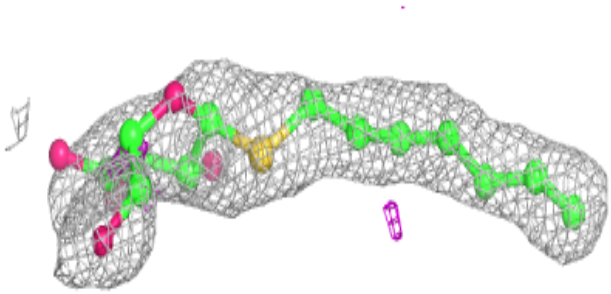
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HTG C 521:

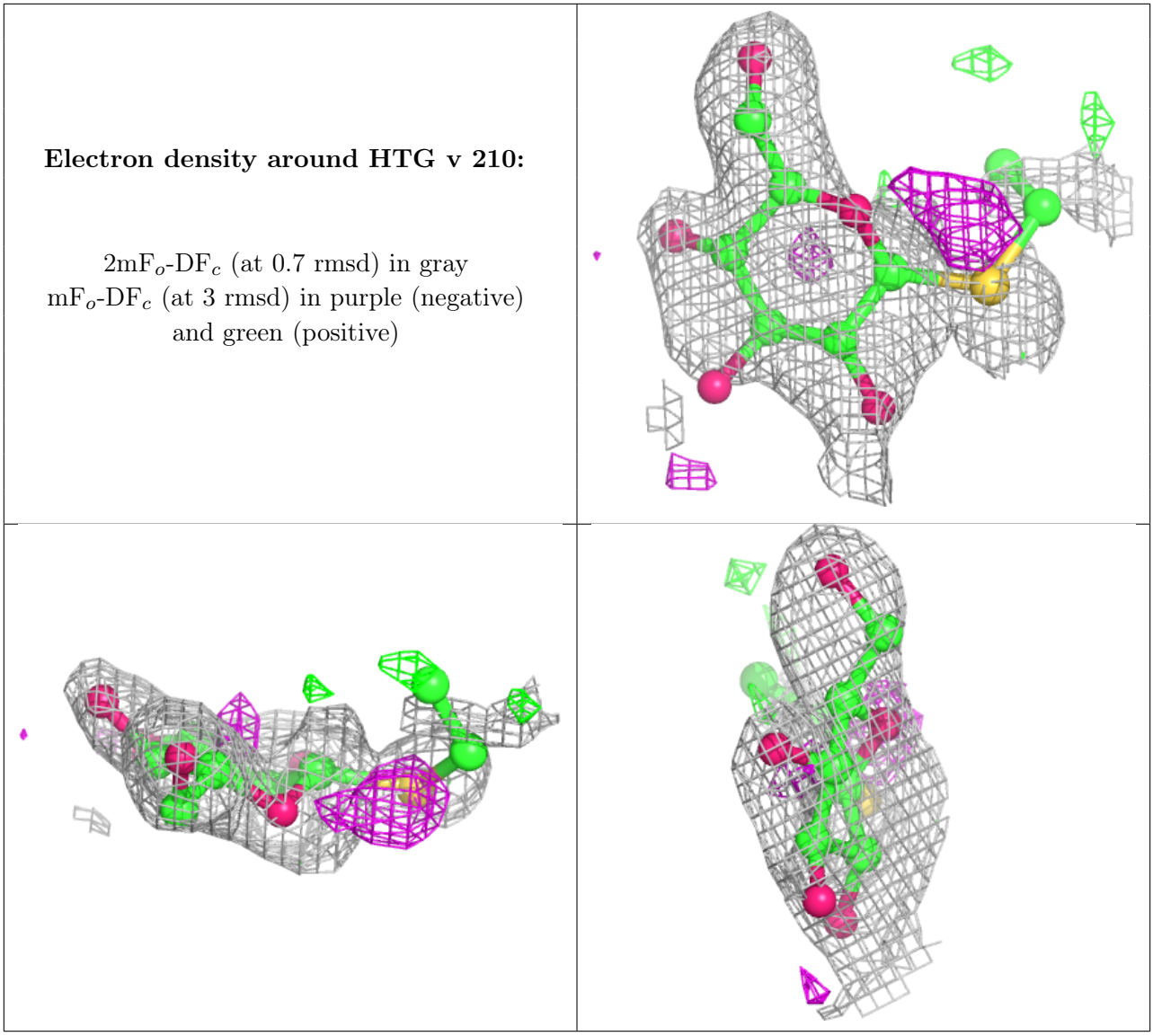
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





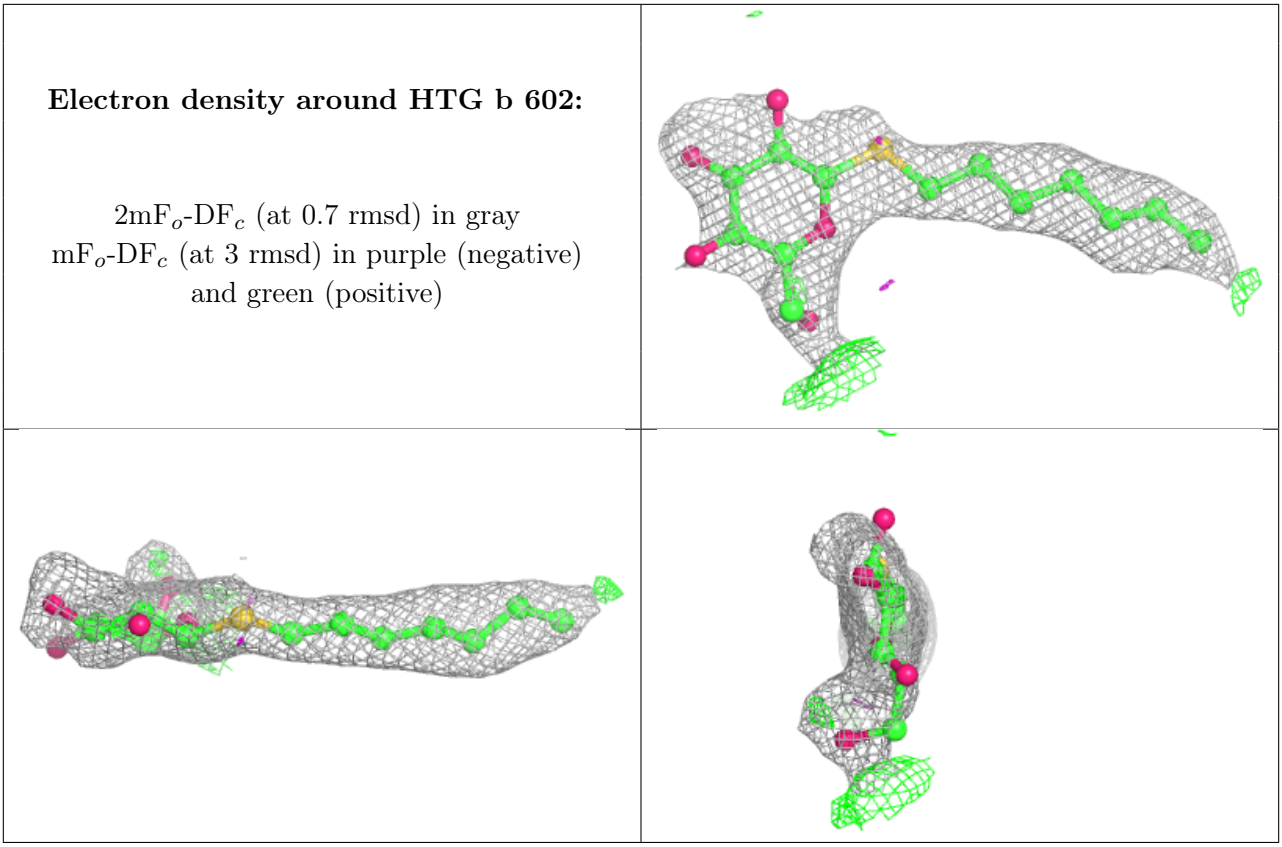
Electron density around HTG v 210:

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



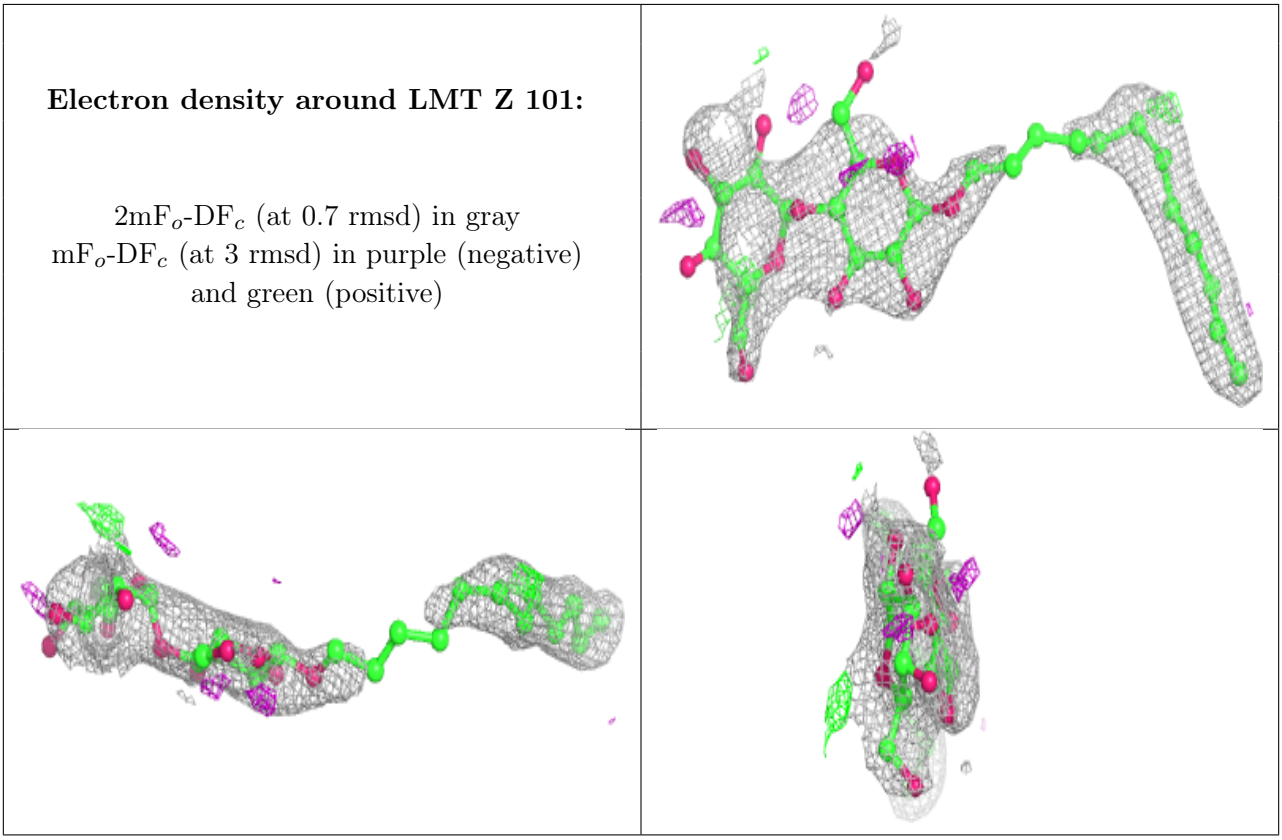
Electron density around HTG b 602:

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



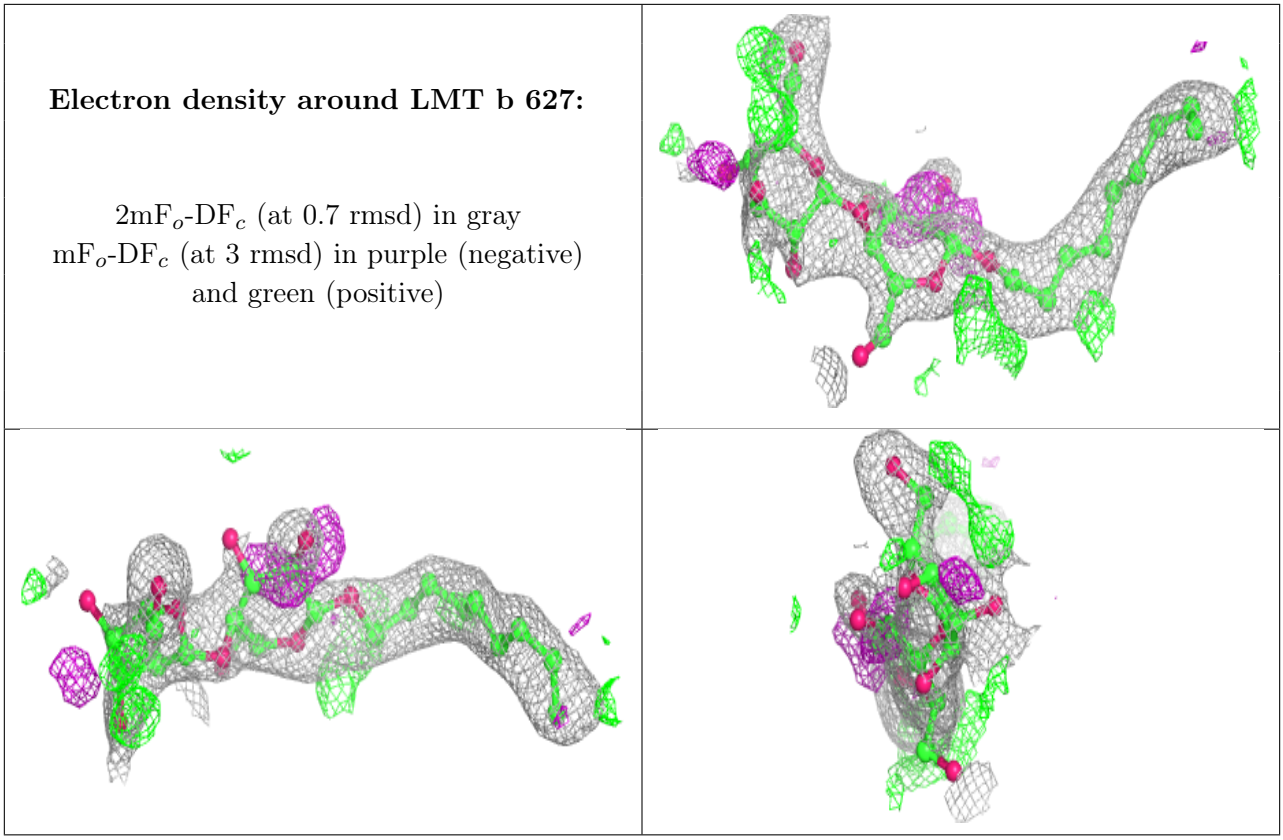
Electron density around LMT Z 101:

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



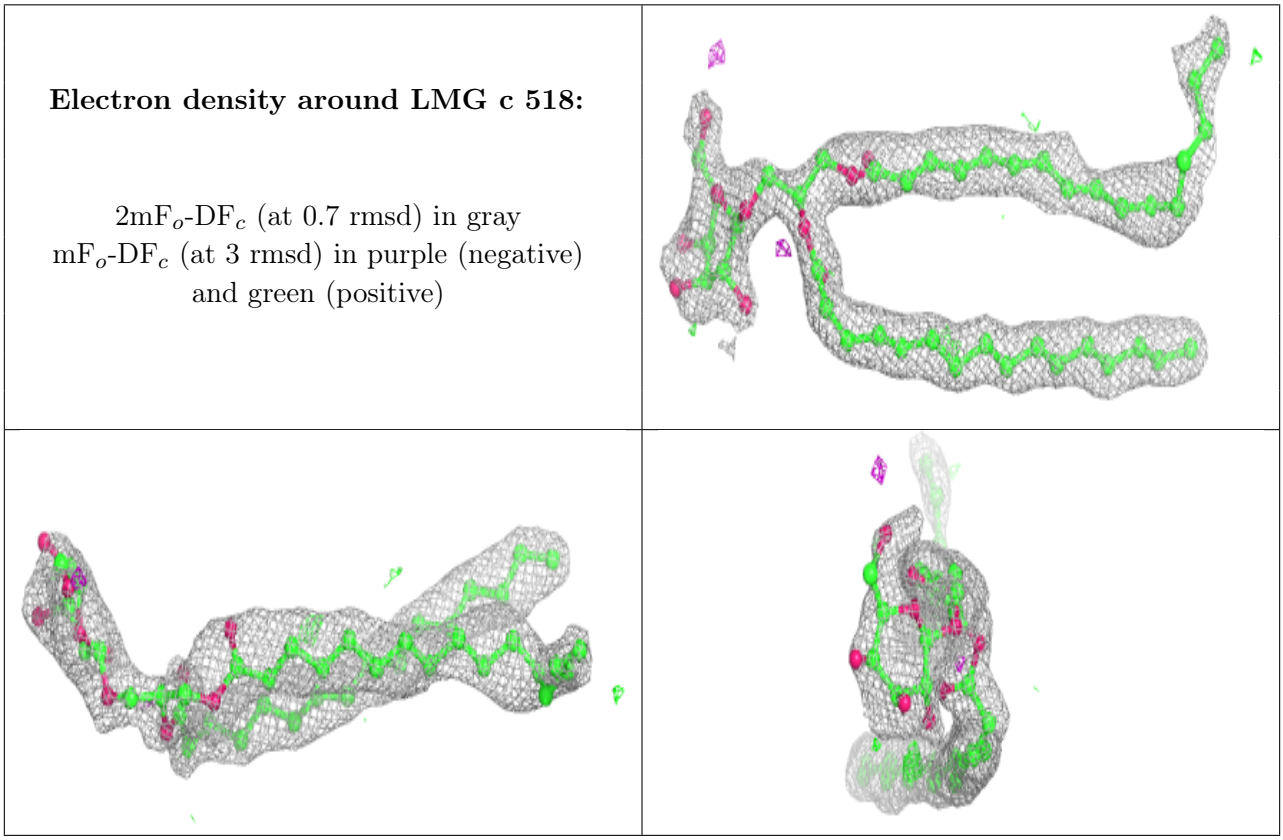
Electron density around LMT b 627:

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



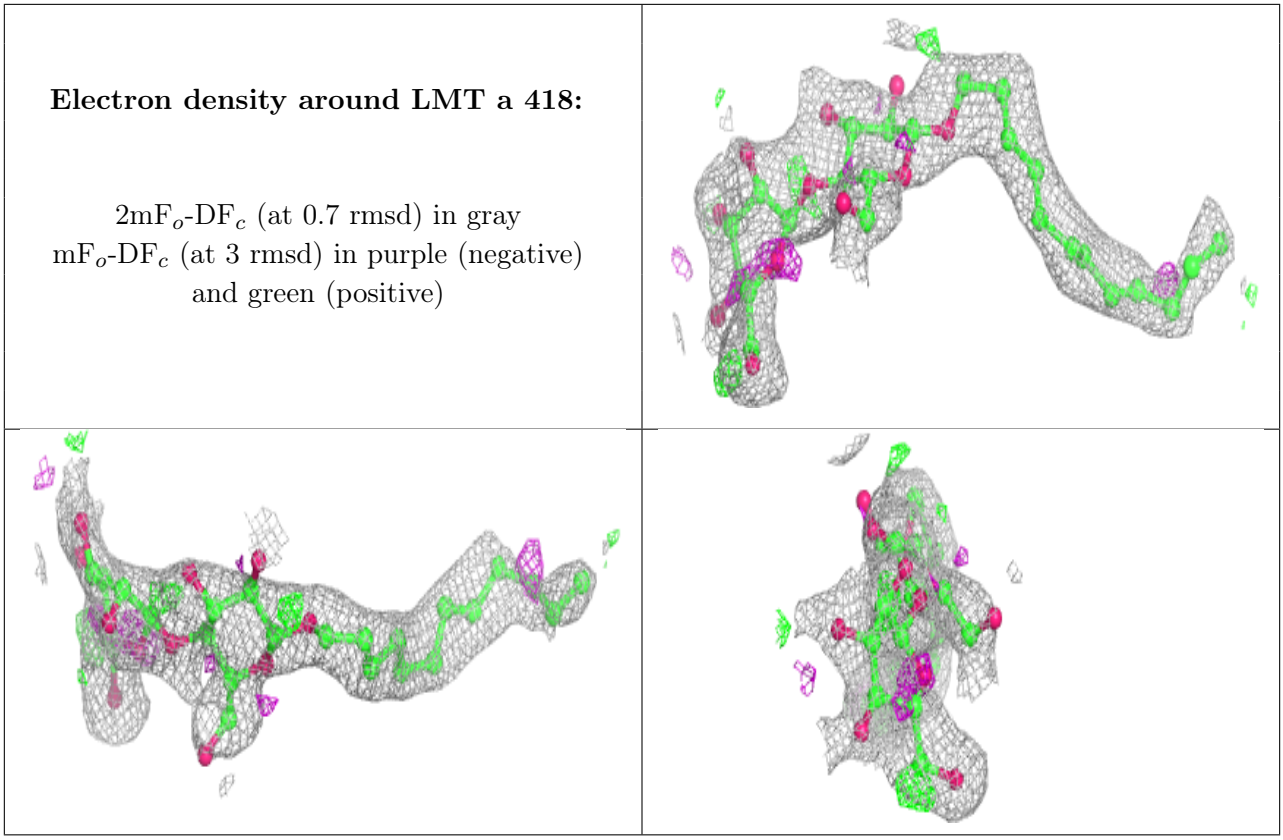
Electron density around LMG c 518:

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



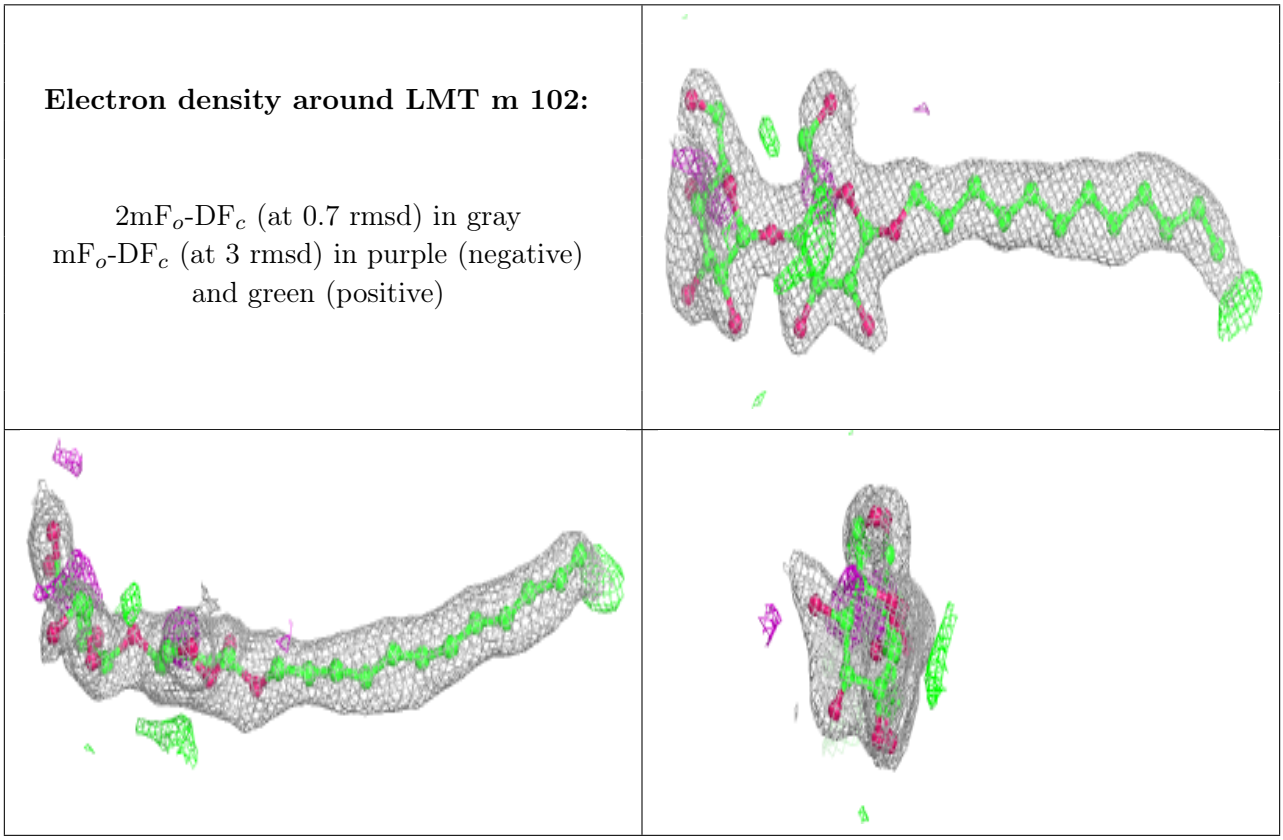
Electron density around LMT a 418:

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



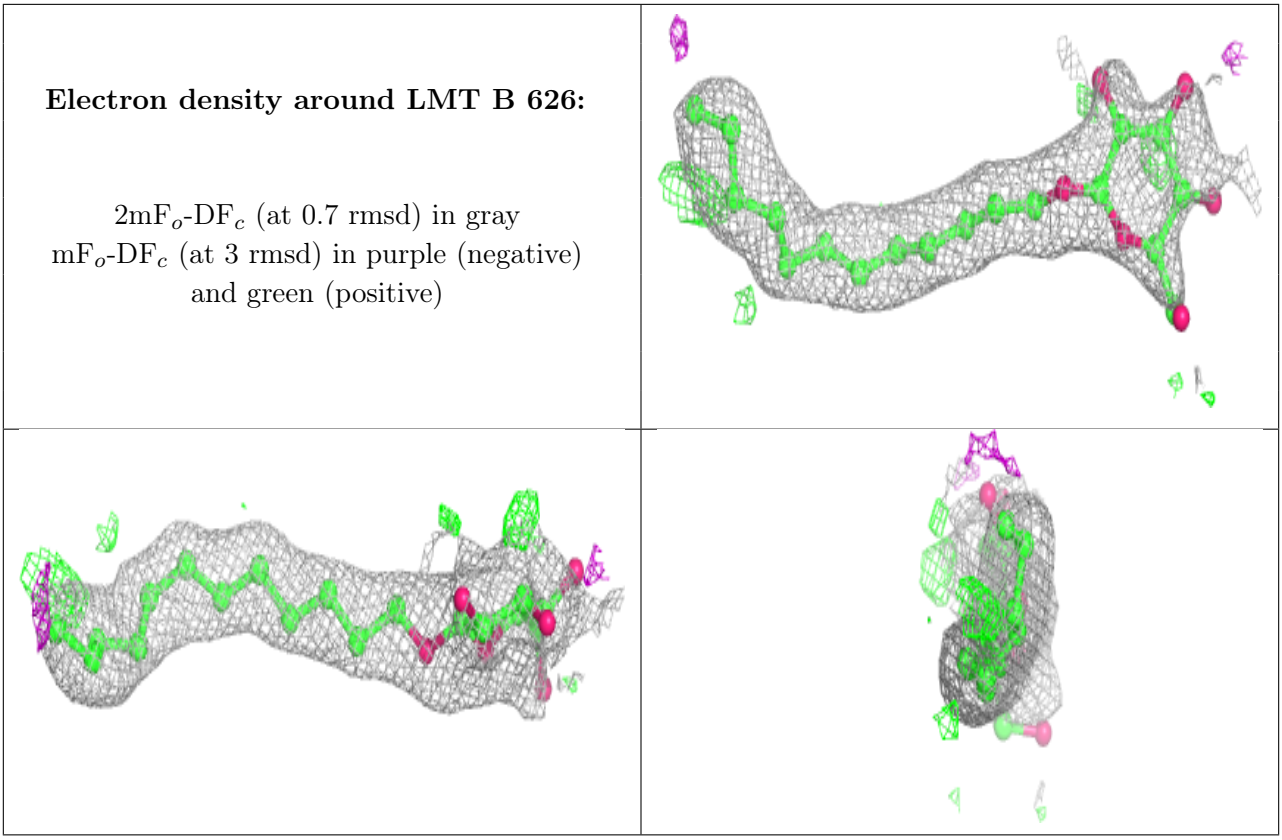
Electron density around LMT m 102:

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



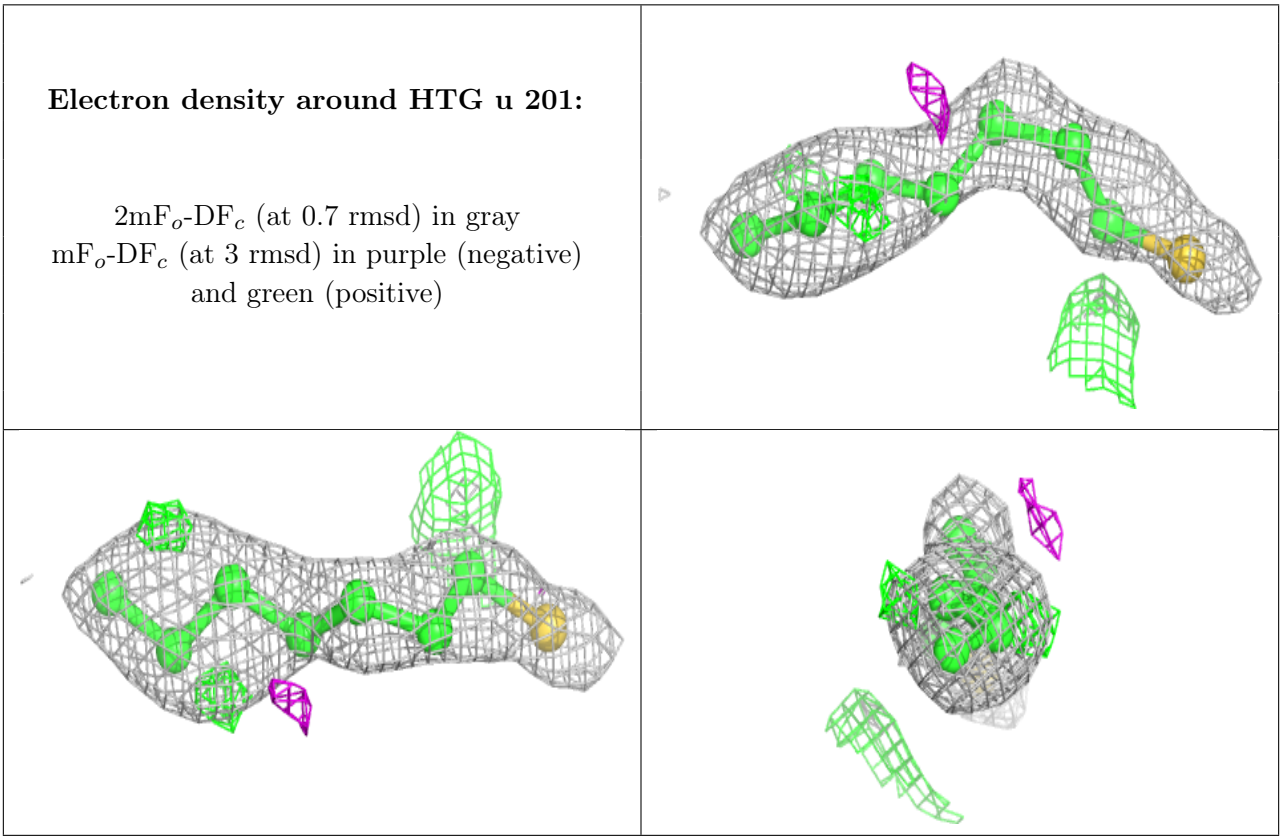
Electron density around LMT B 626:

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



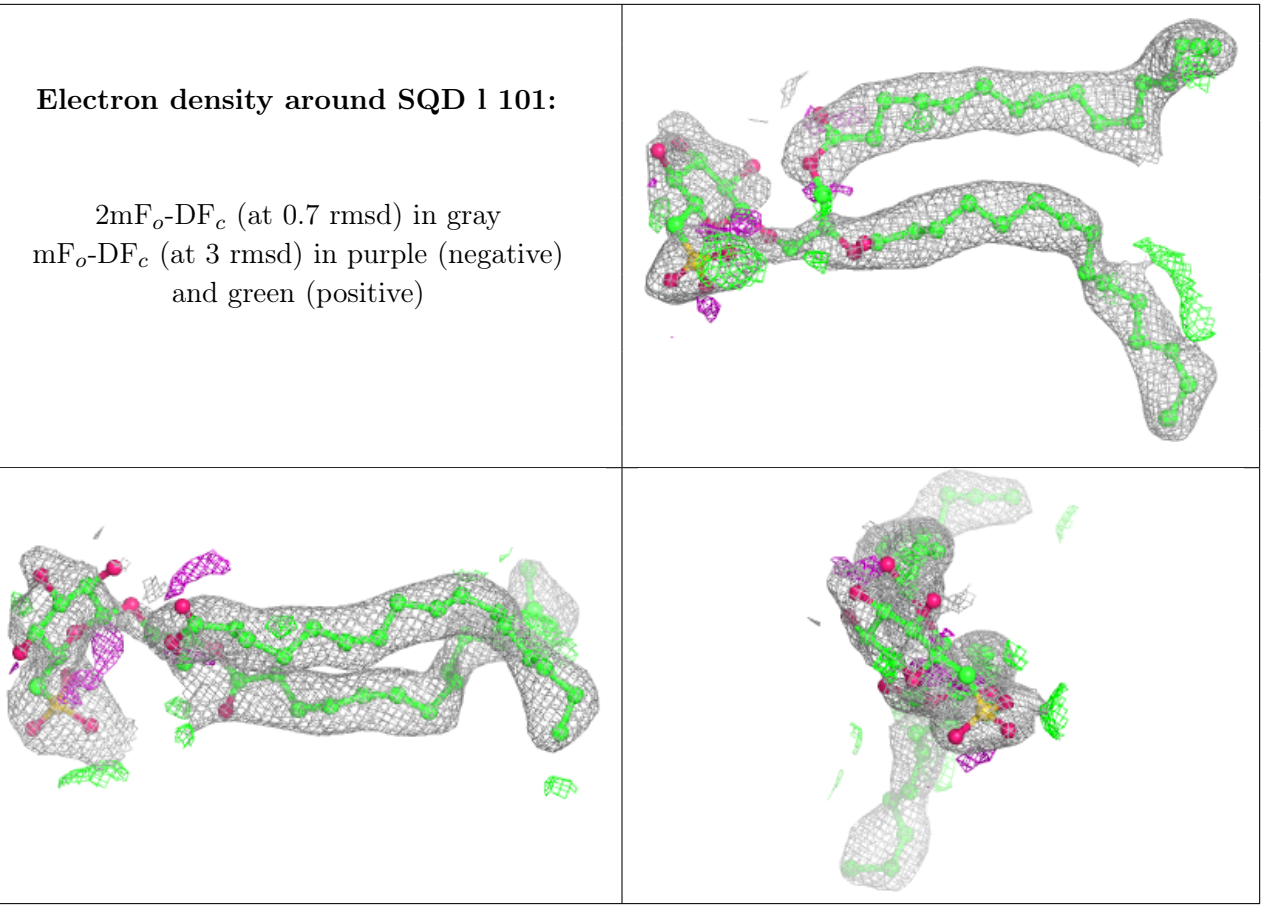
Electron density around HTG u 201:

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



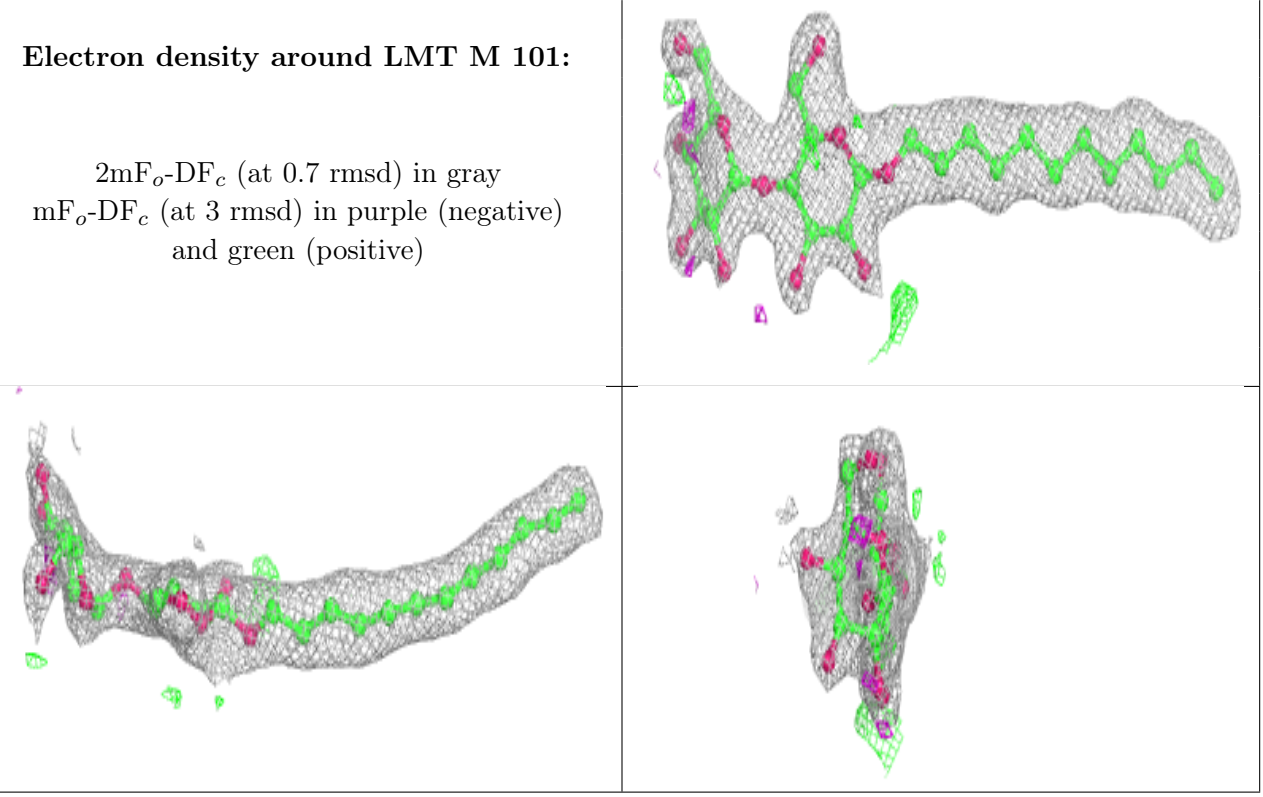
Electron density around SQD l 101:

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



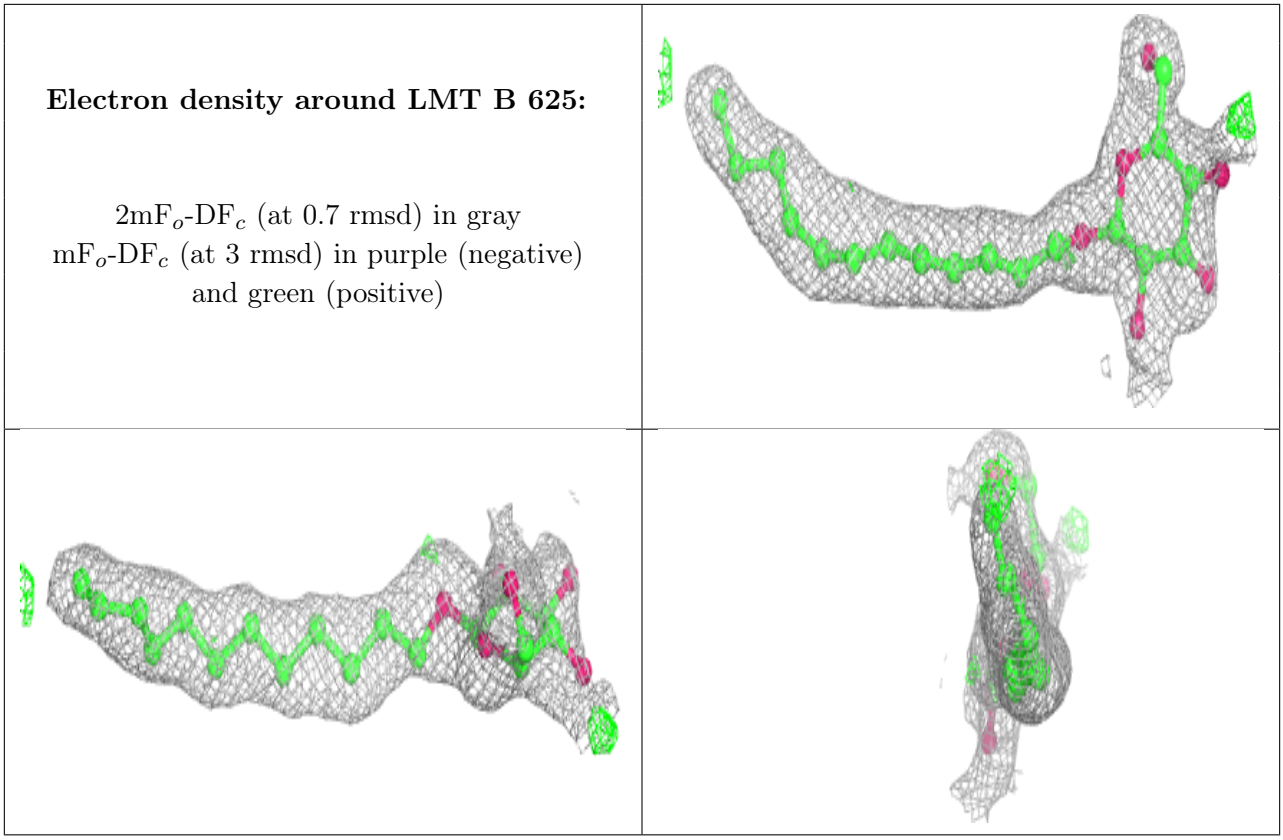
Electron density around LMT M 101:

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



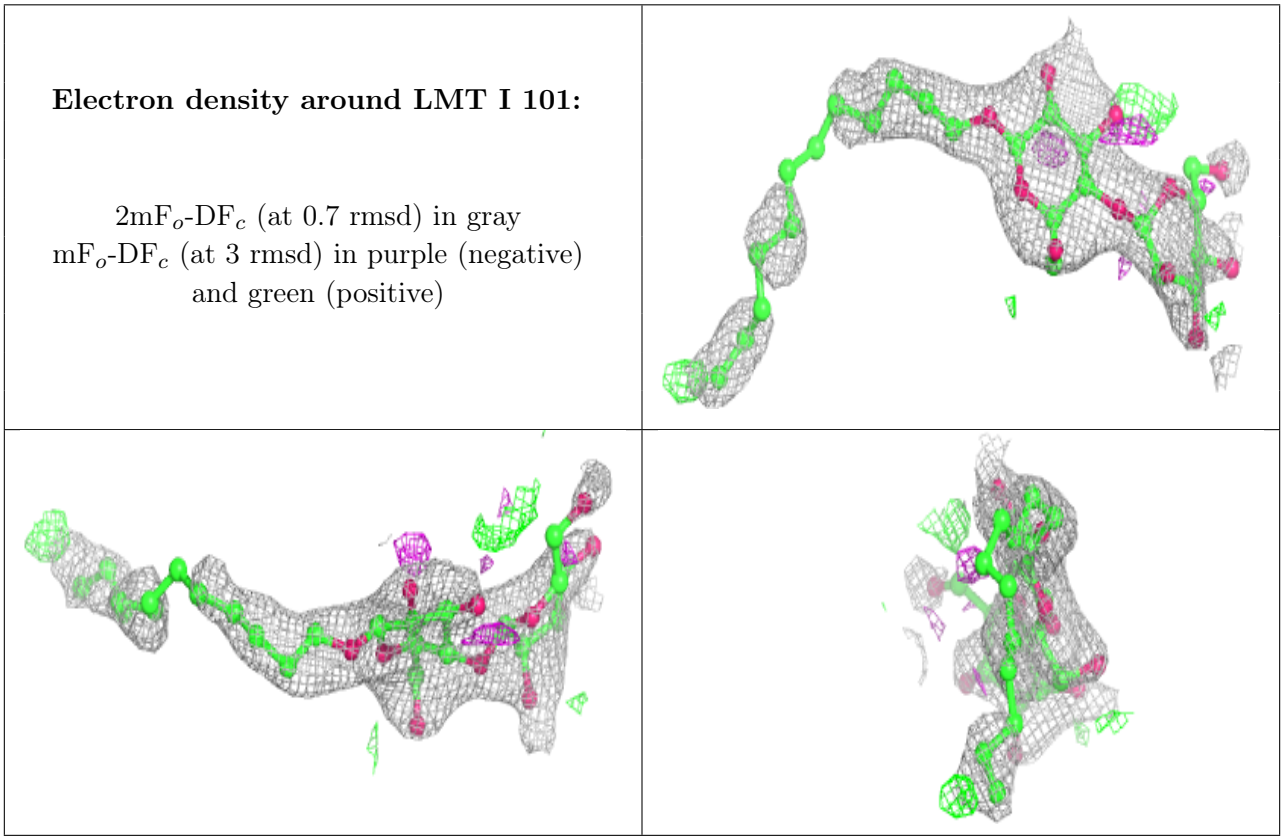
Electron density around LMT B 625:

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



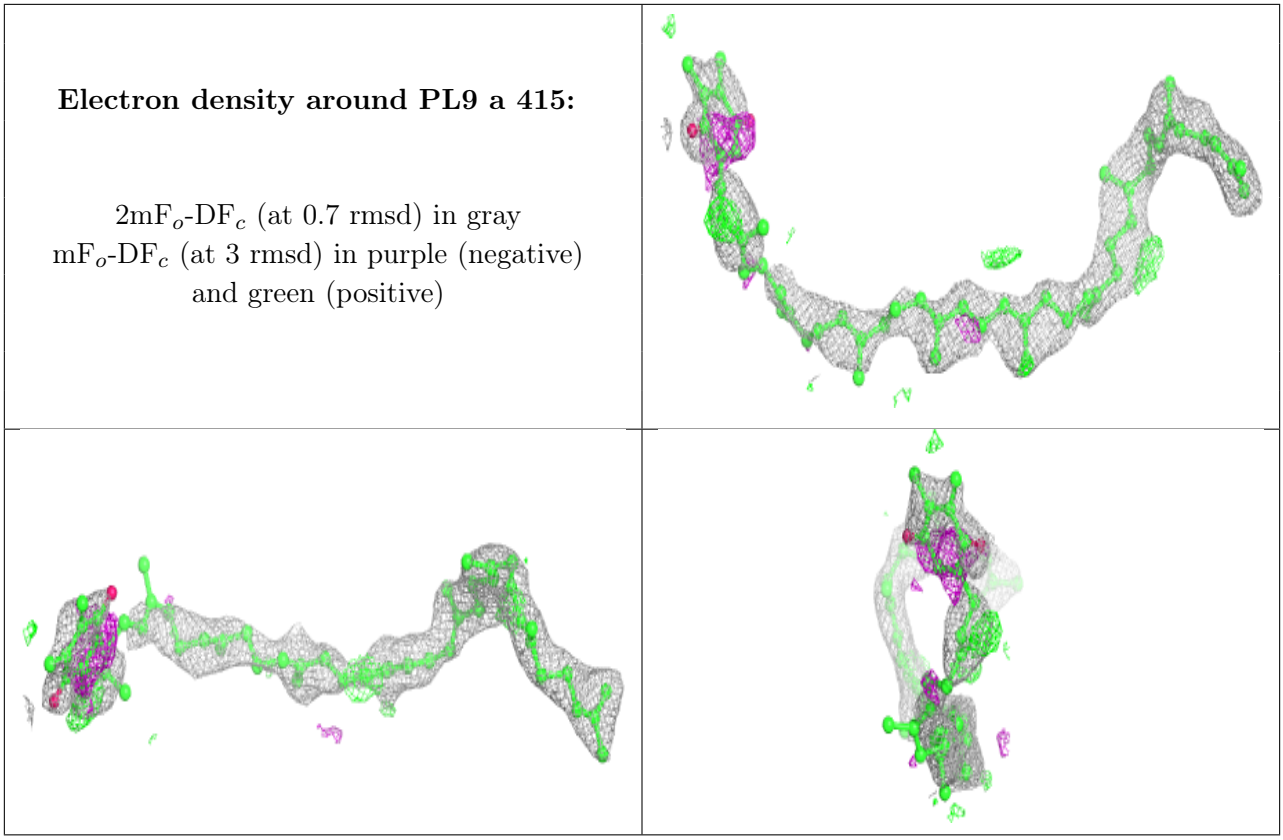
Electron density around LMT I 101:

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



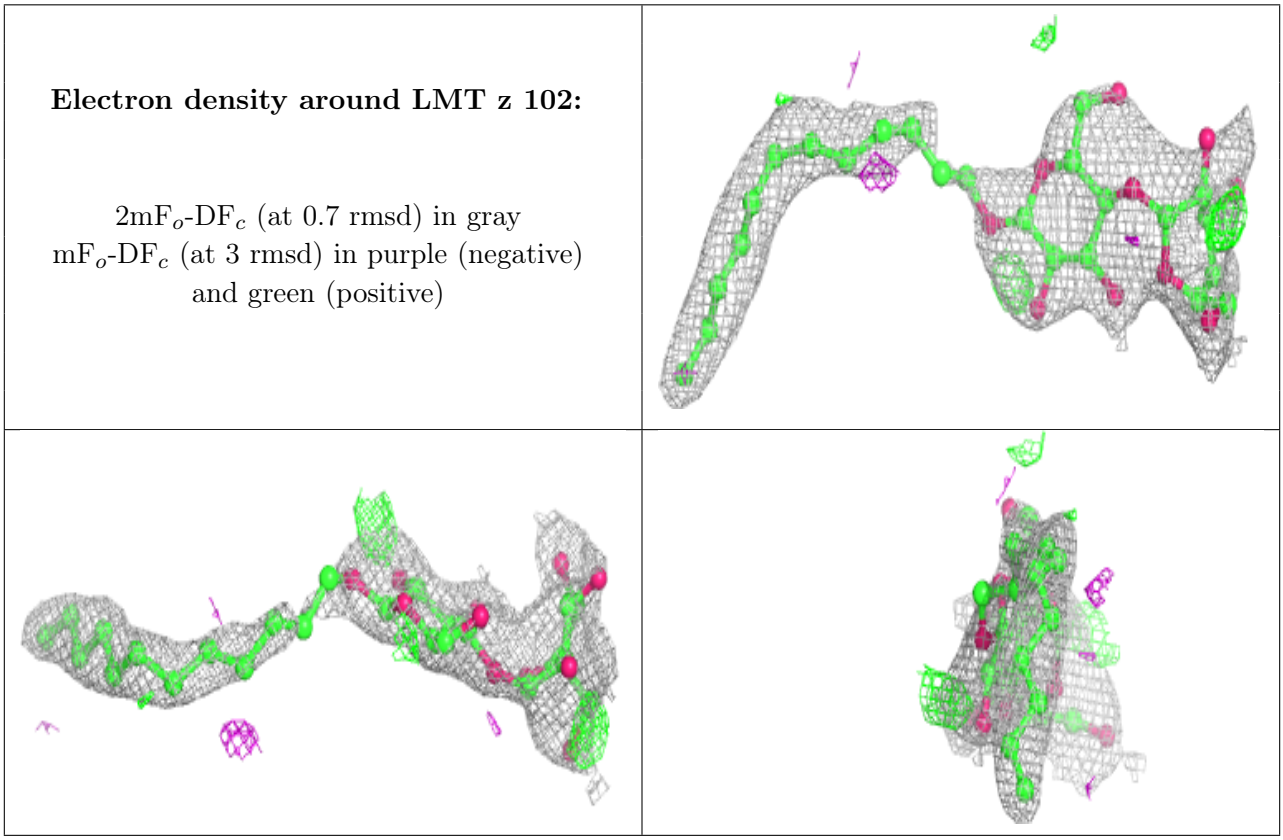
Electron density around PL9 a 415:

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



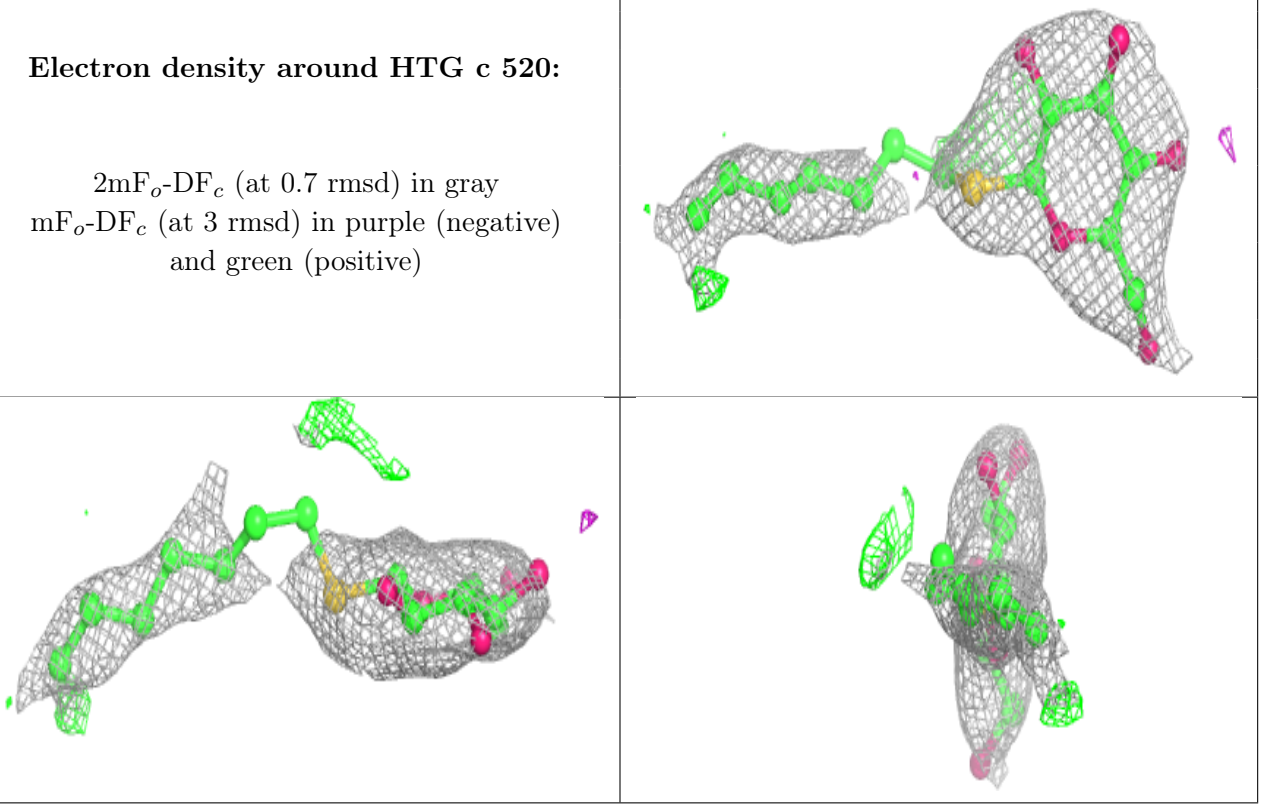
Electron density around LMT z 102:

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



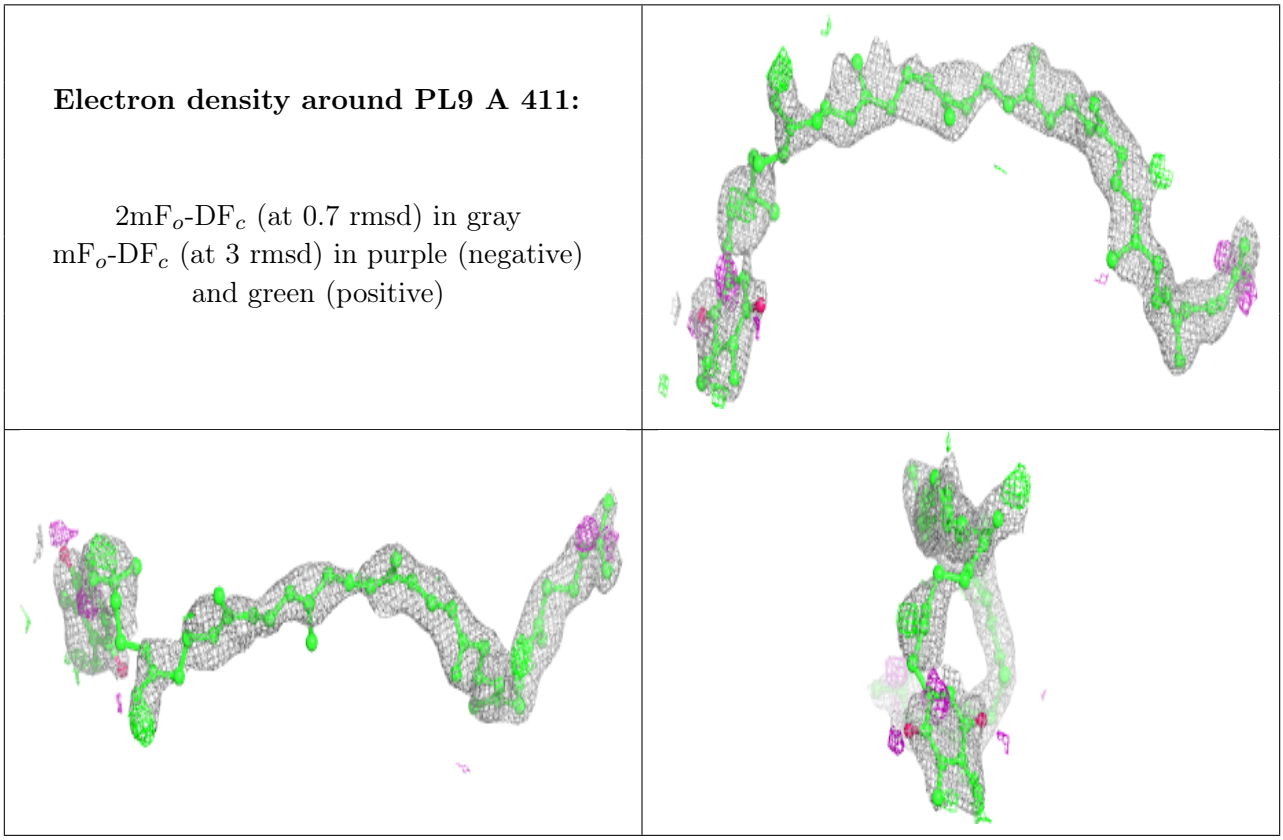
Electron density around HTG c 520:

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



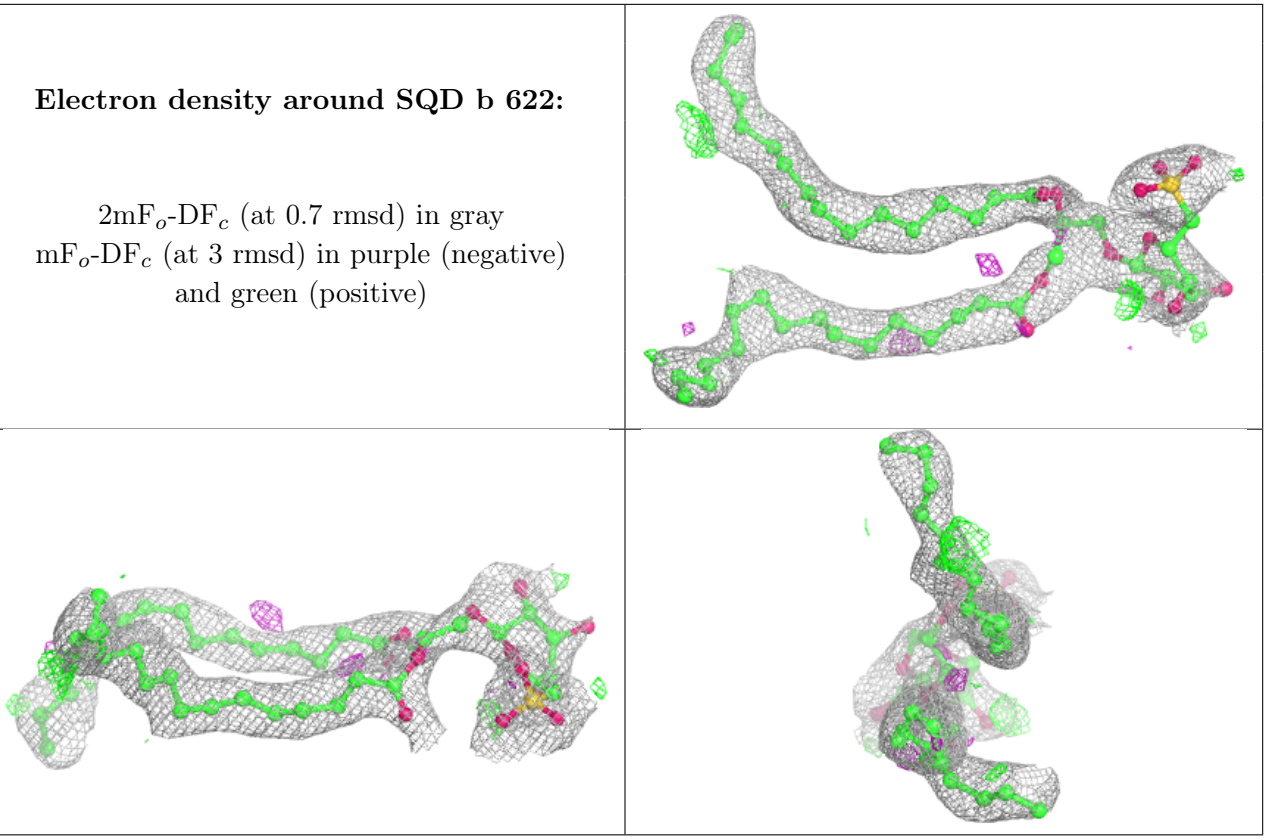
Electron density around PL9 A 411:

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



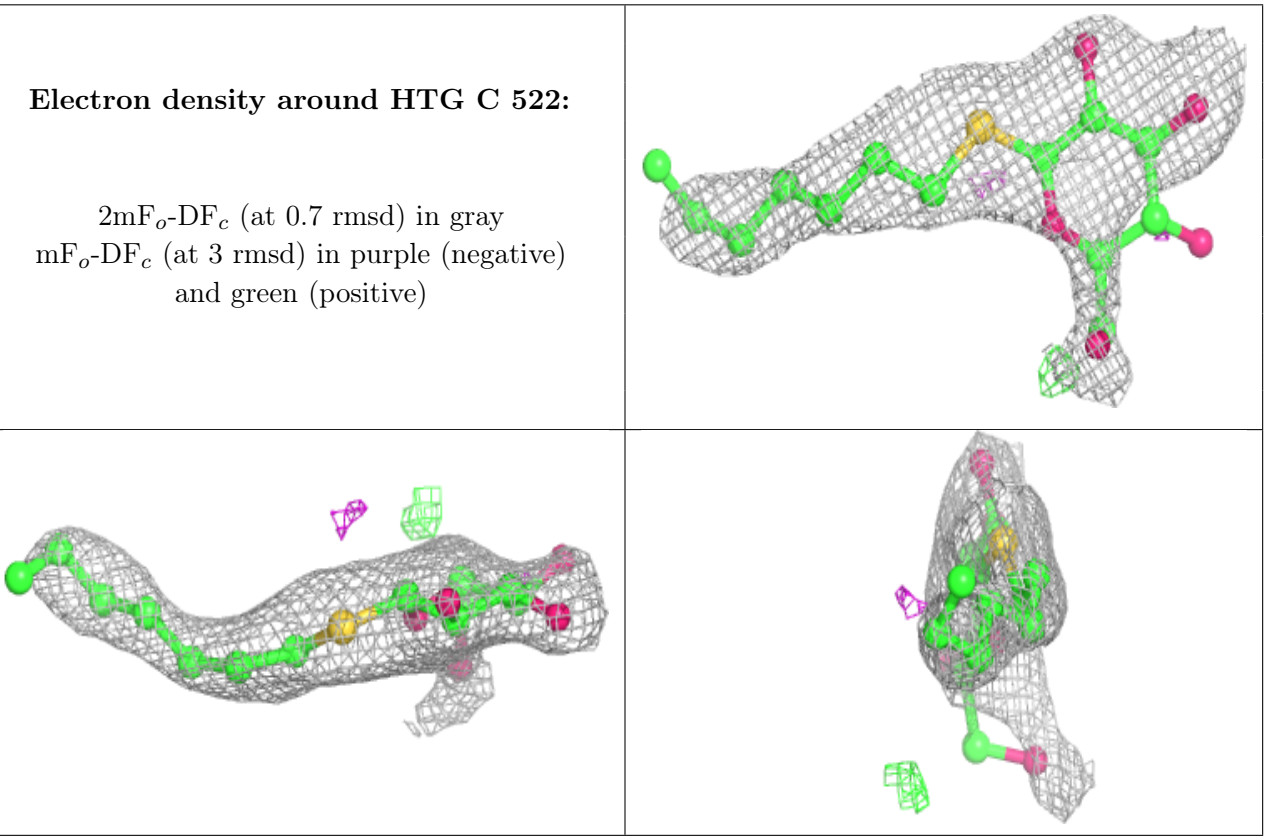
Electron density around SQD b 622:

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



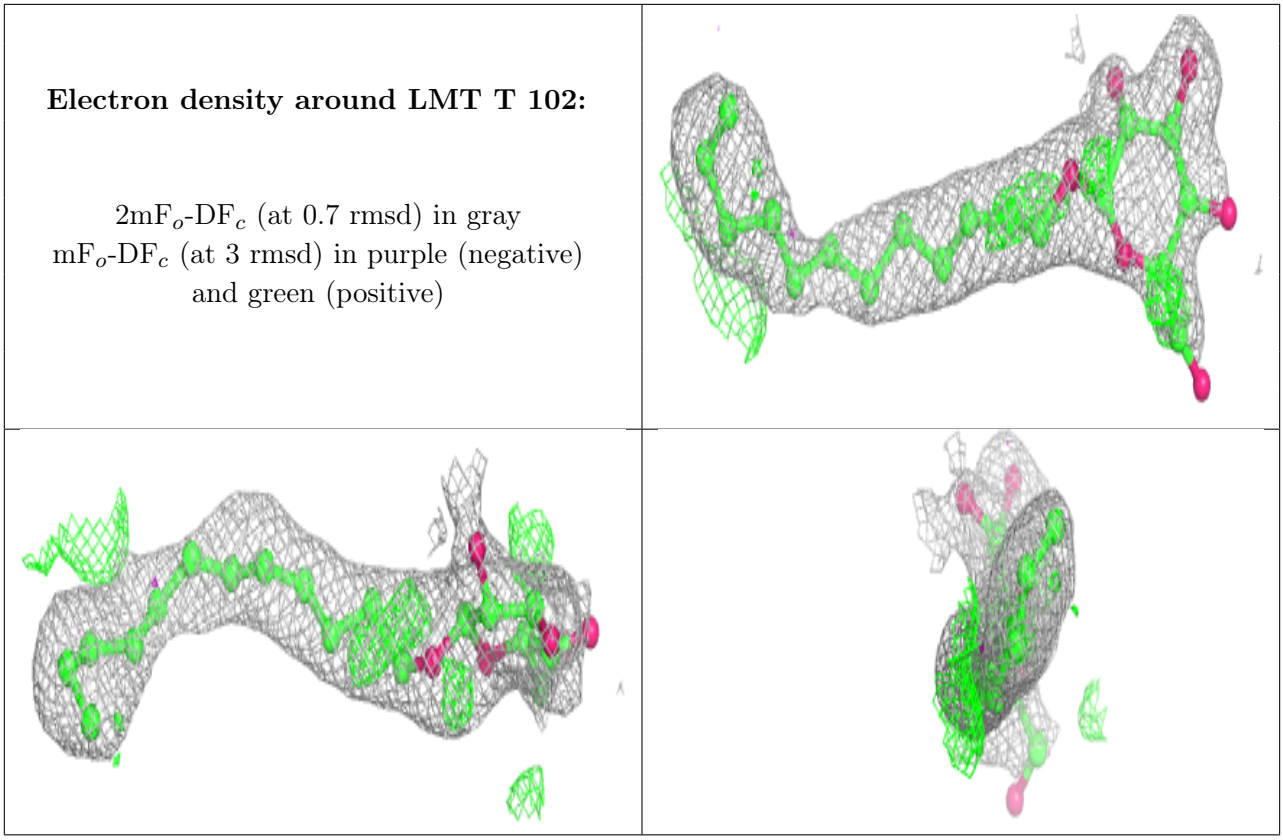
Electron density around HTG C 522:

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



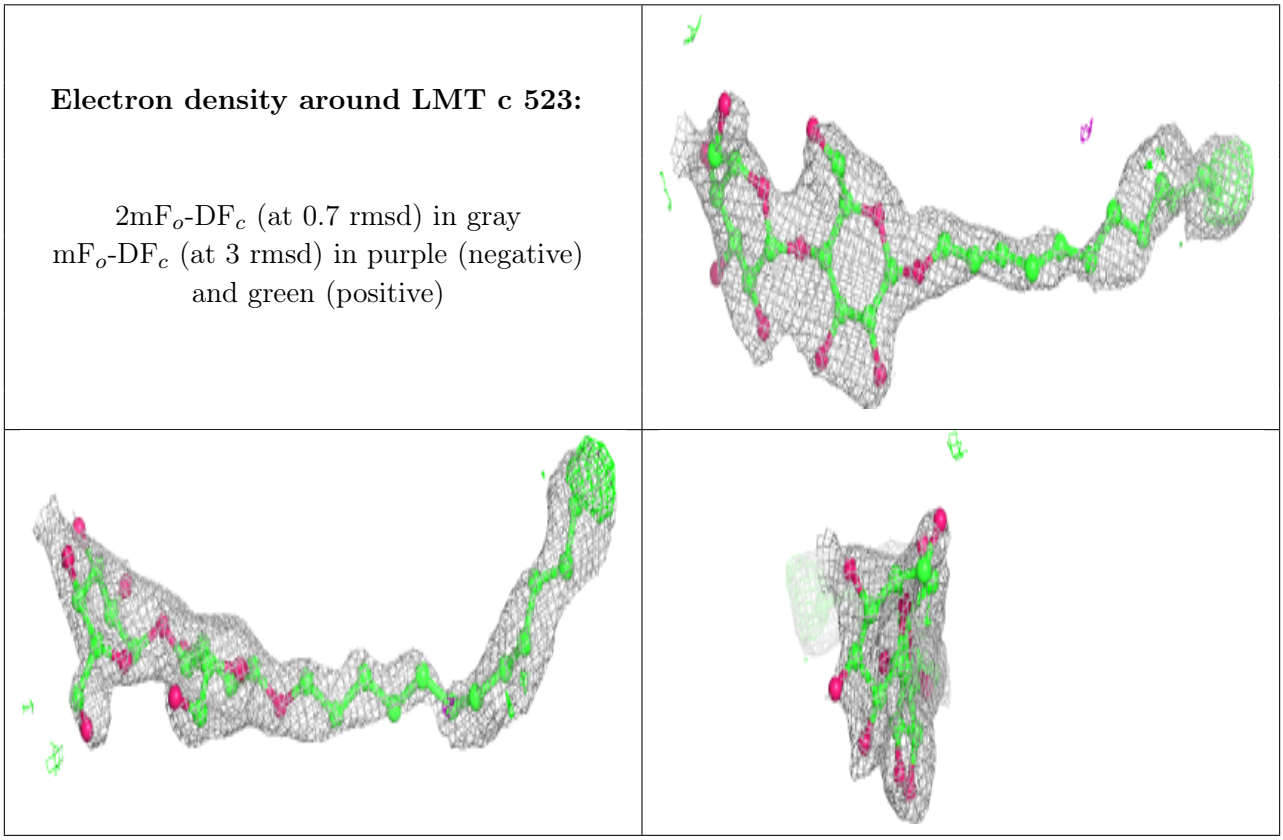
Electron density around LMT T 102:

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



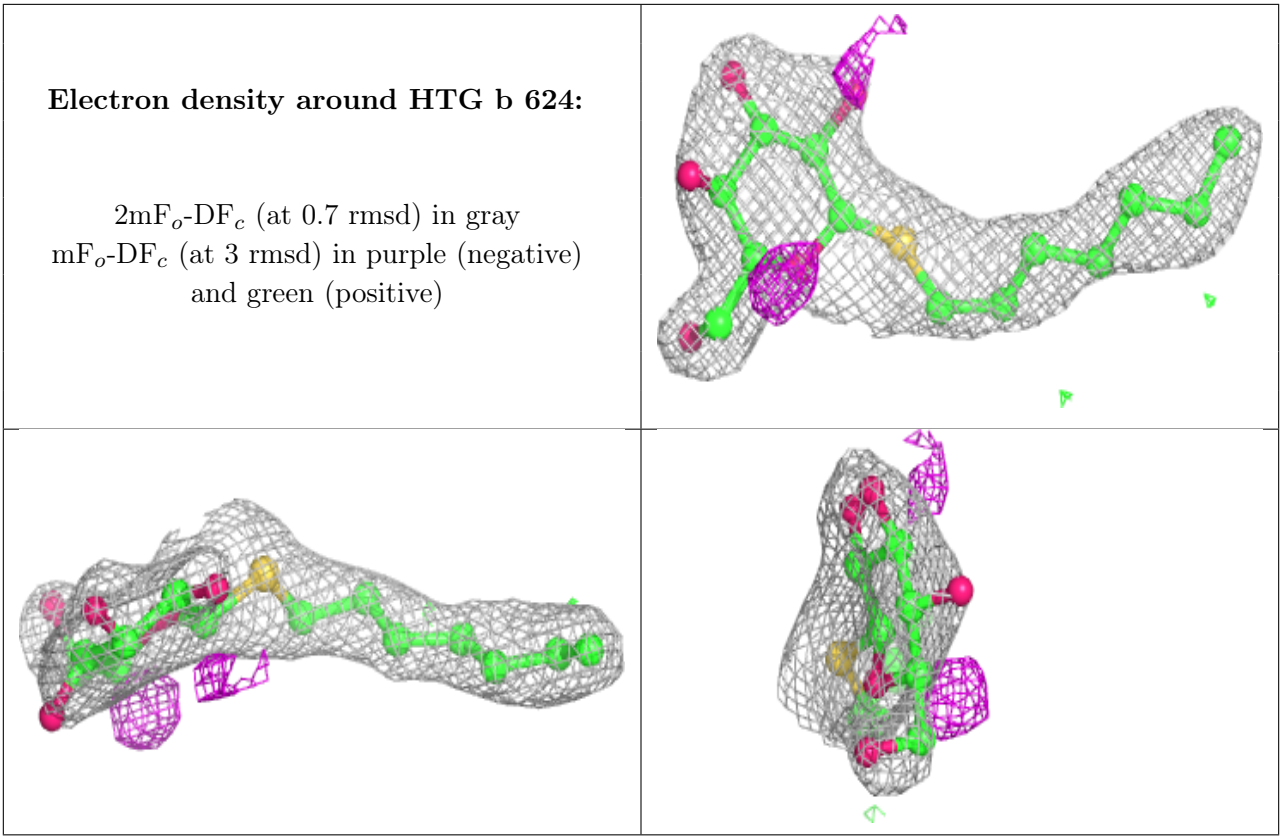
Electron density around LMT c 523:

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



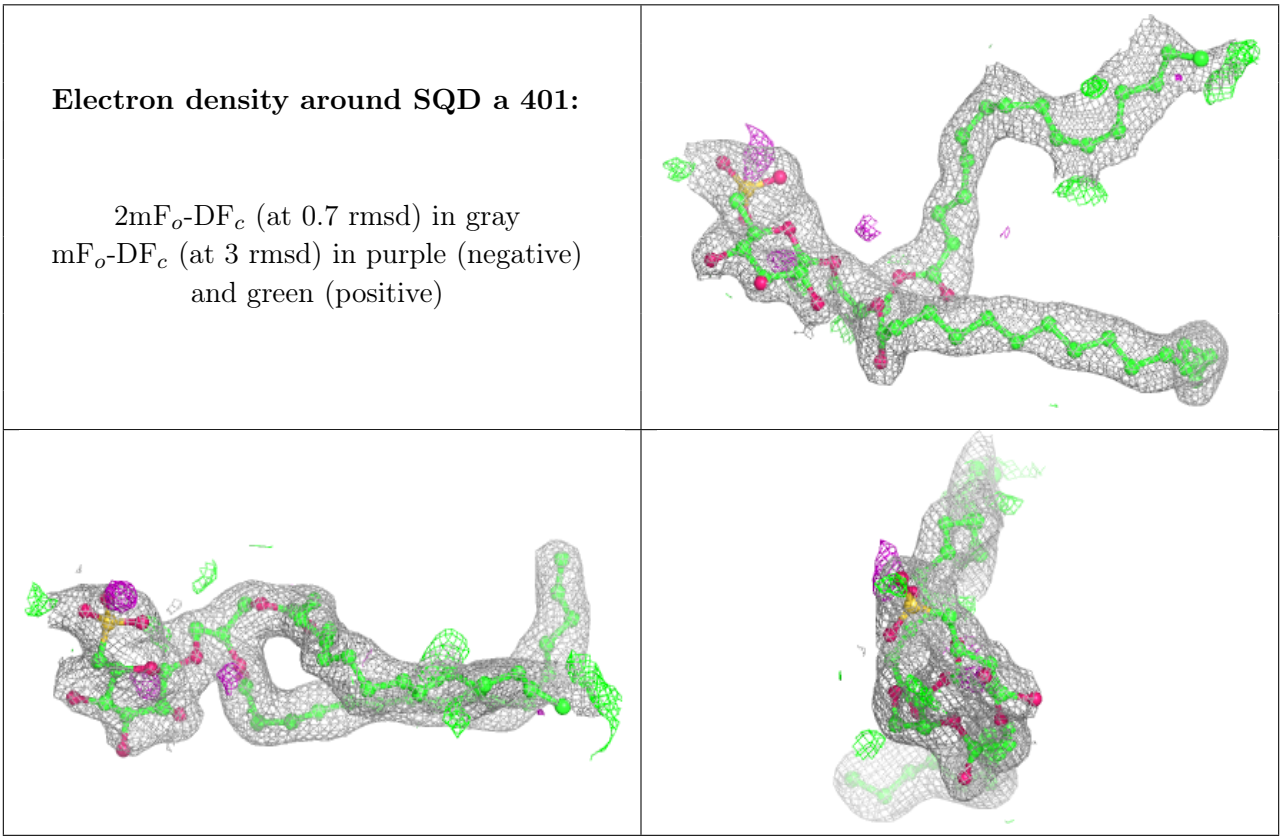
Electron density around HTG b 624:

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



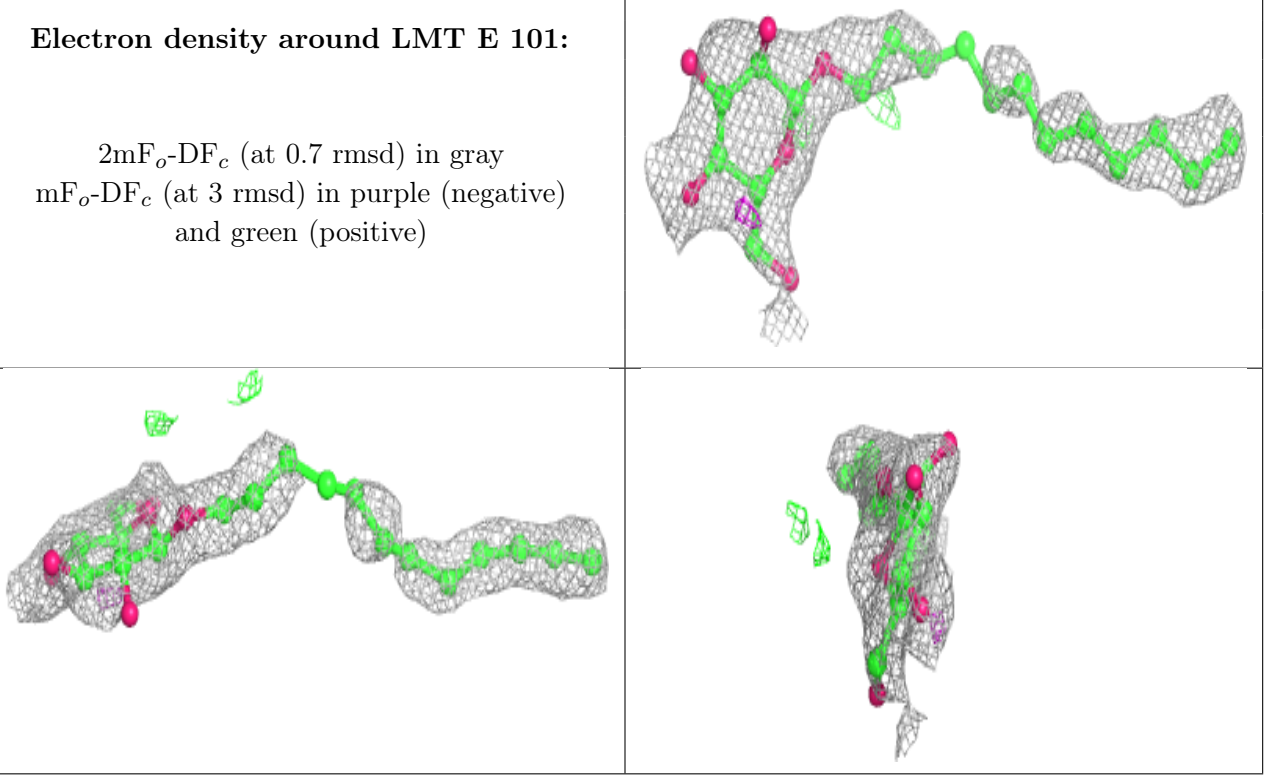
Electron density around SQD a 401:

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



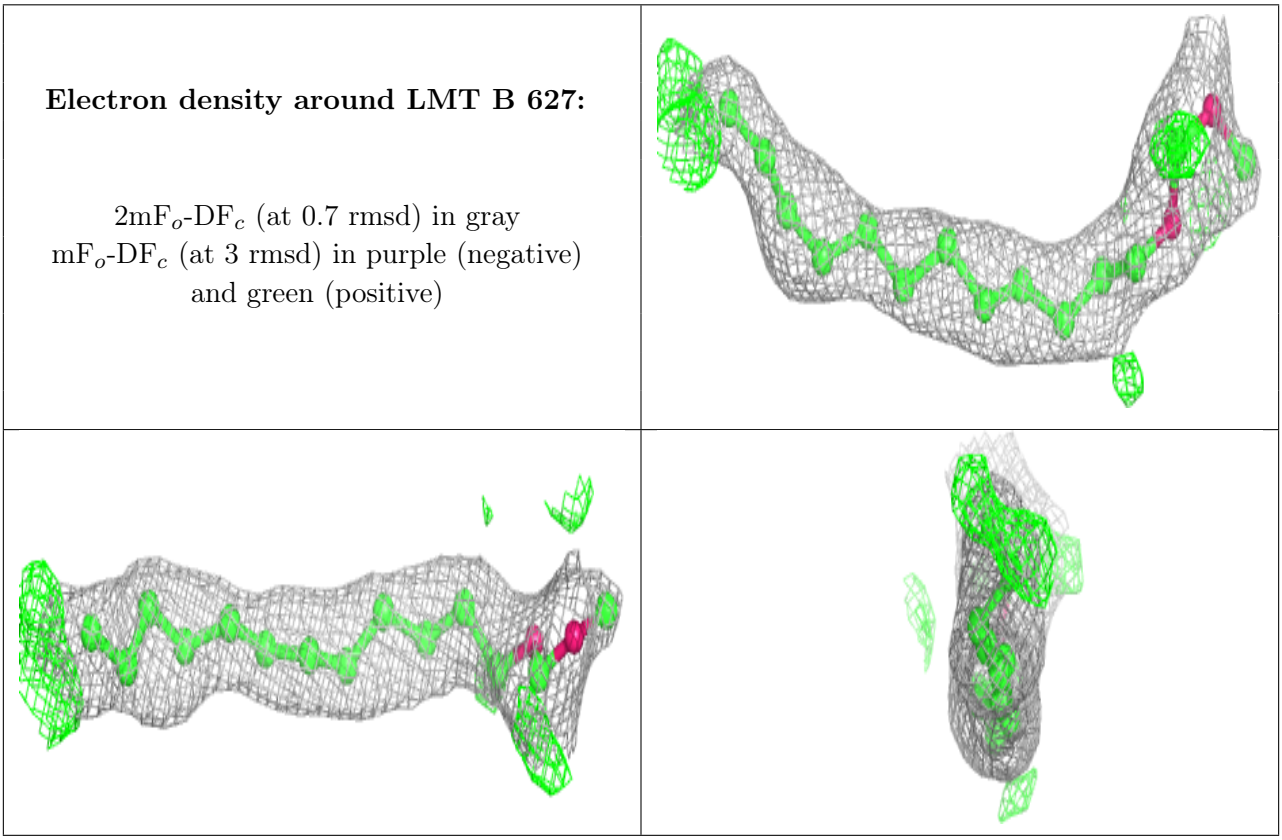
Electron density around LMT E 101:

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



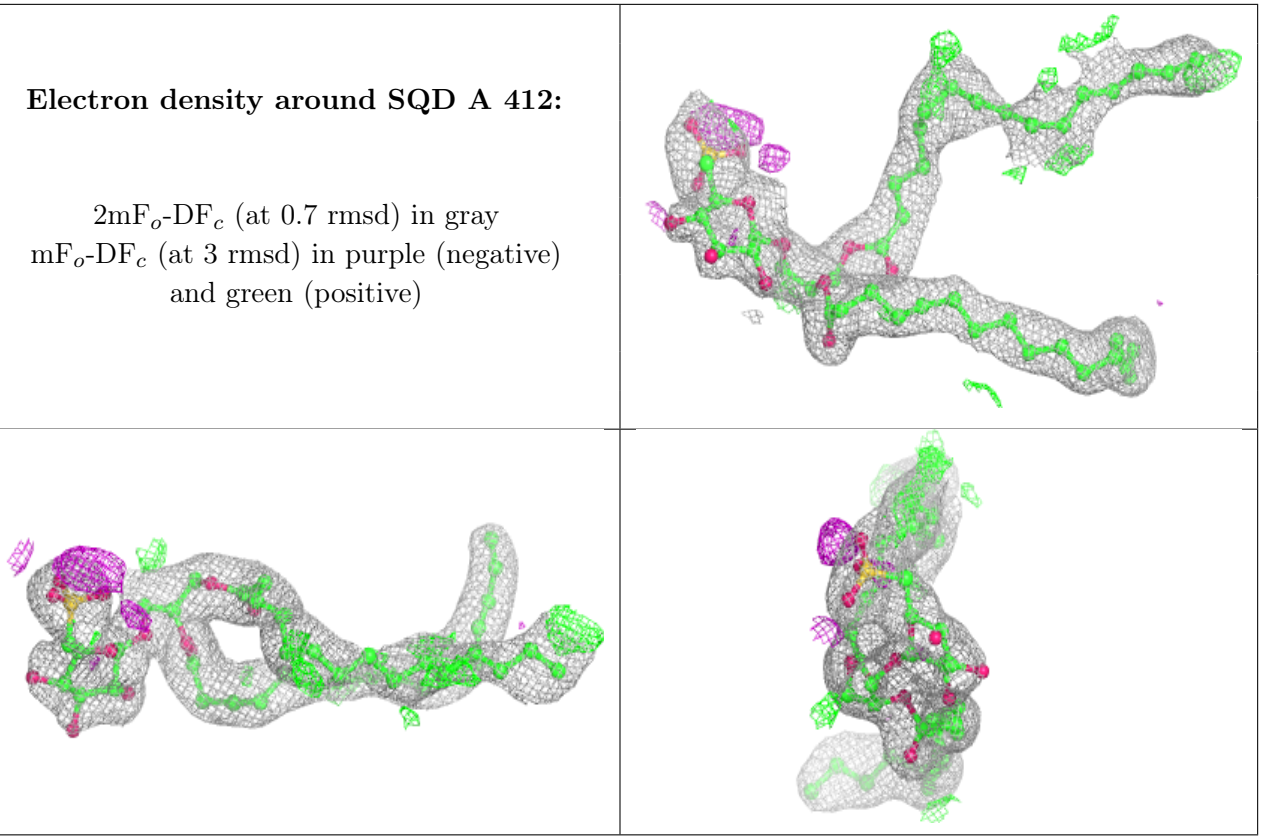
Electron density around LMT B 627:

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



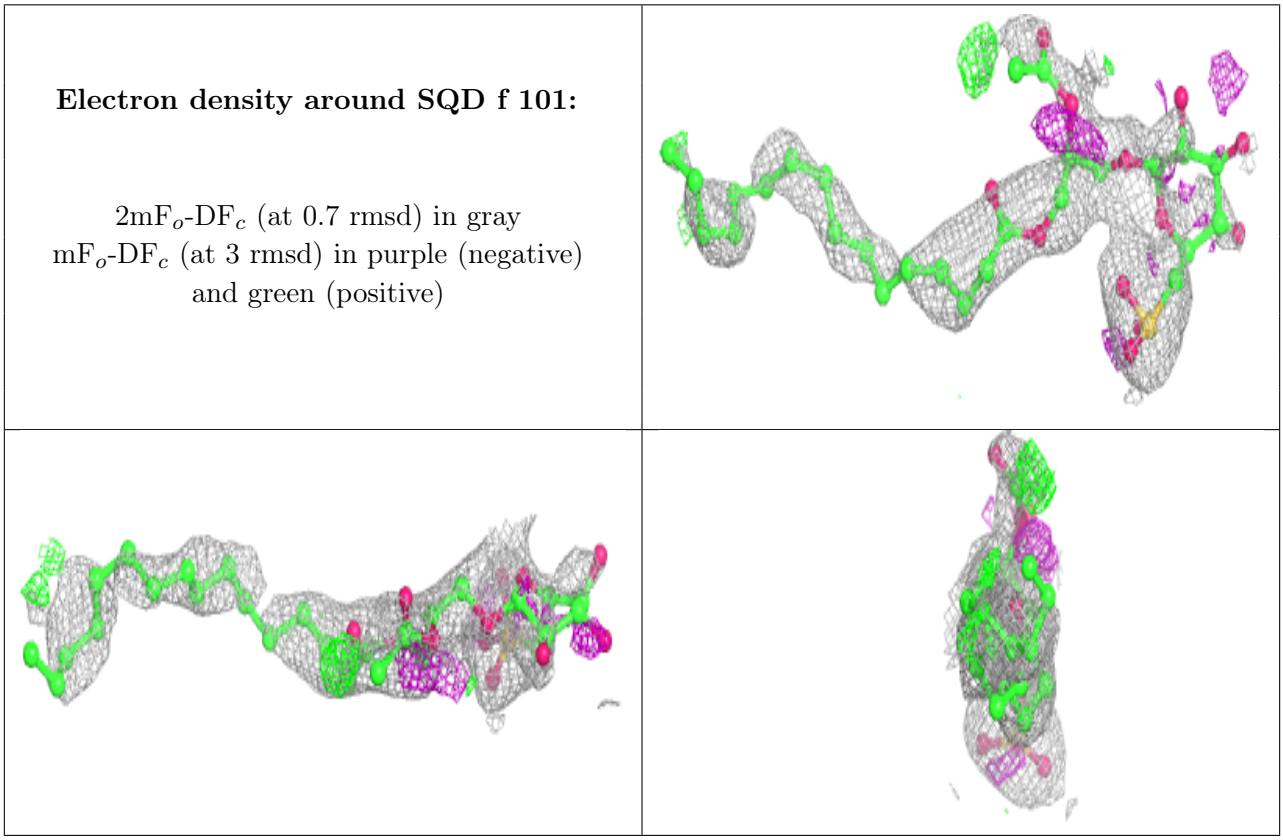
Electron density around SQD A 412:

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



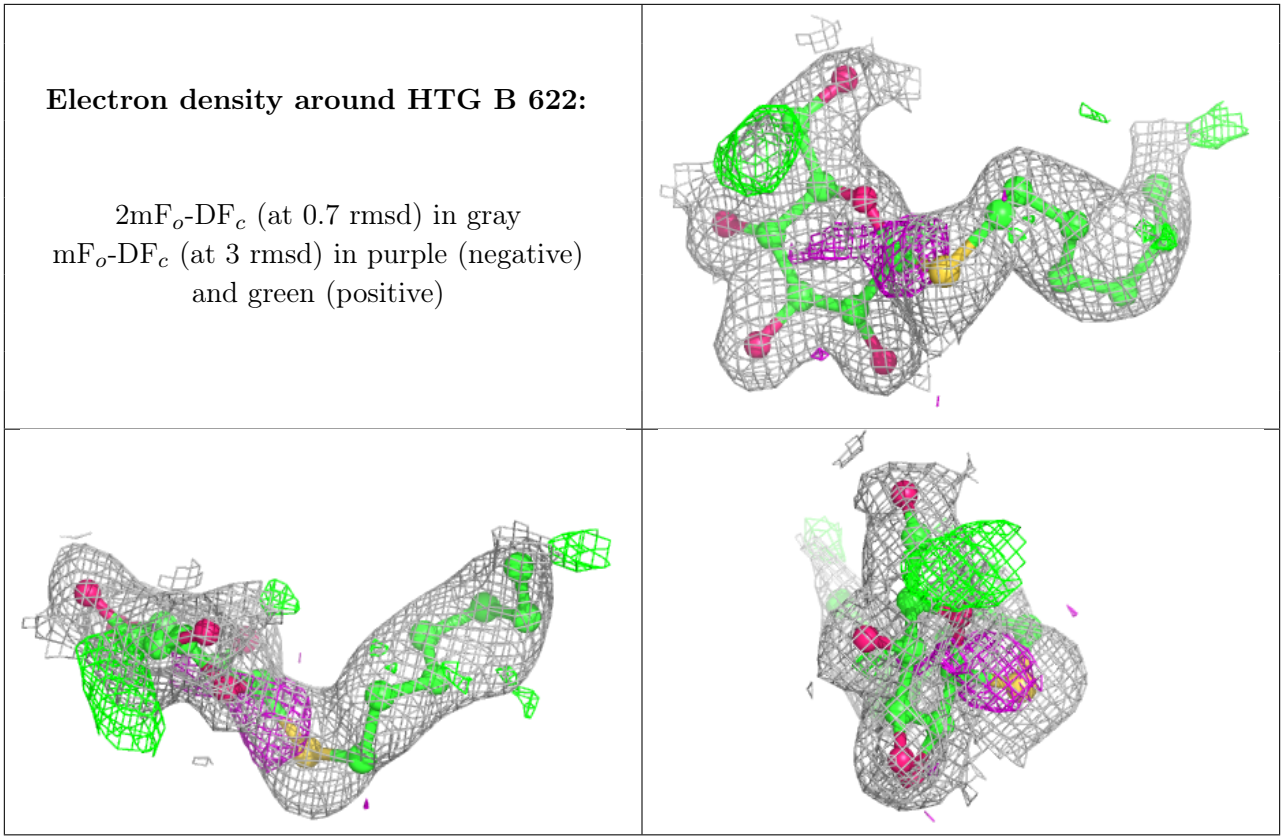
Electron density around SQD f 101:

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



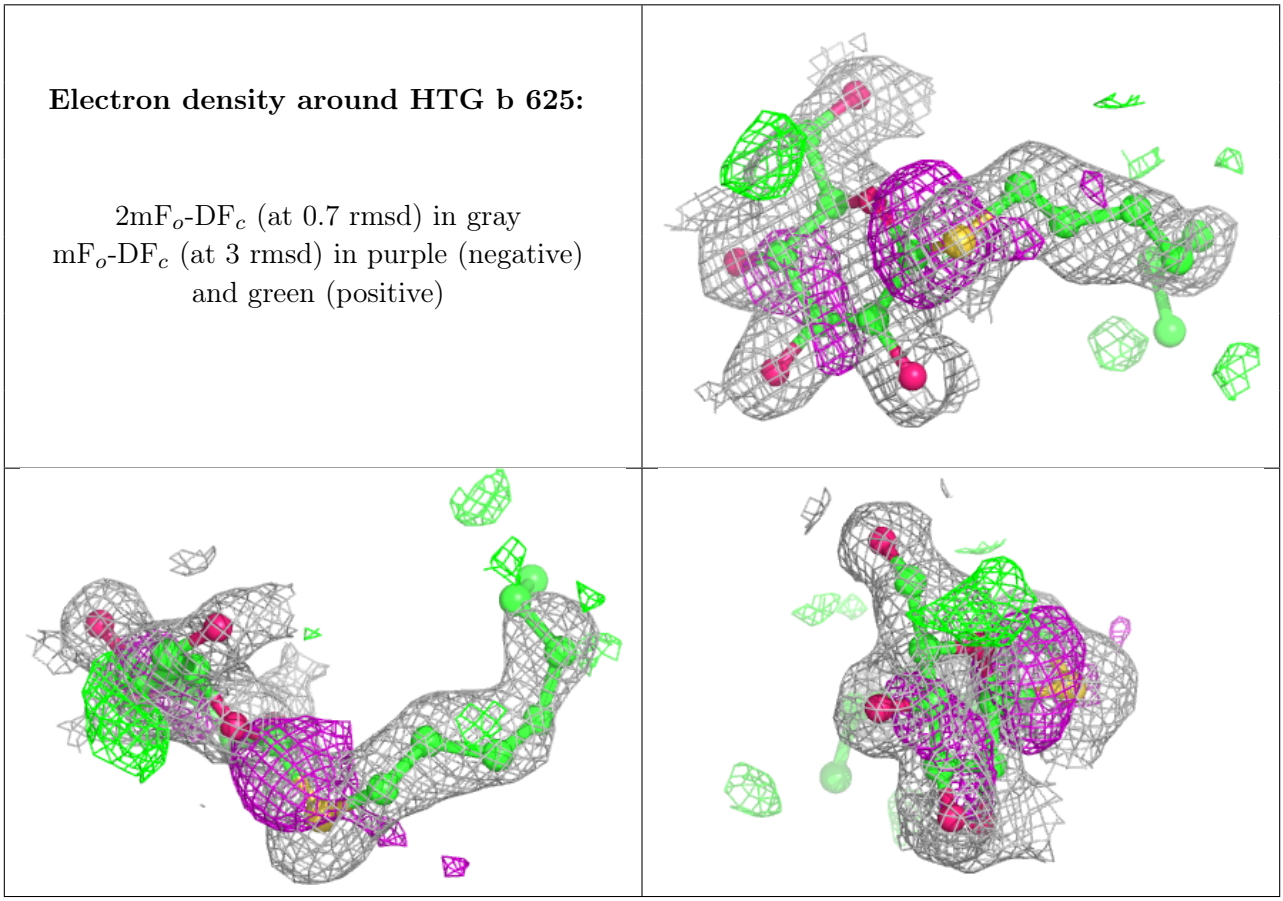
Electron density around HTG B 622:

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



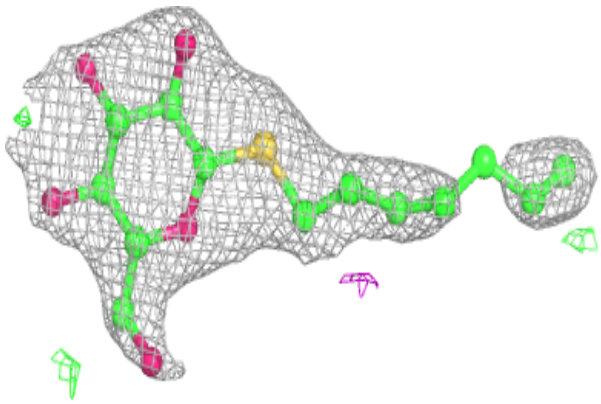
Electron density around HTG b 625:

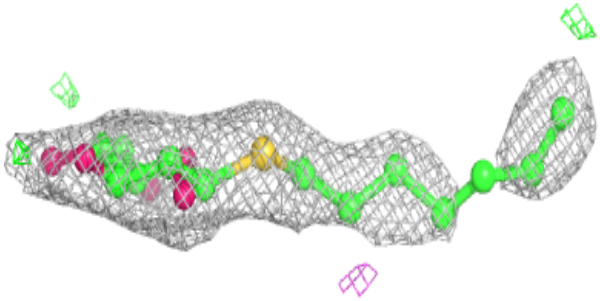
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

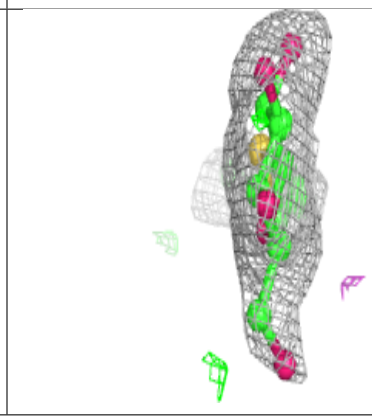


Electron density around HTG C 520:

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

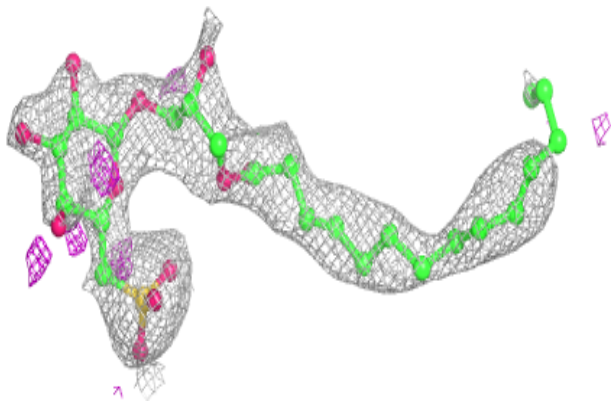


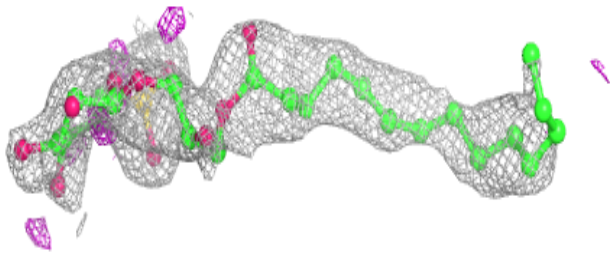


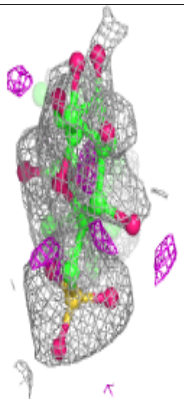


Electron density around SQD F 101:

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

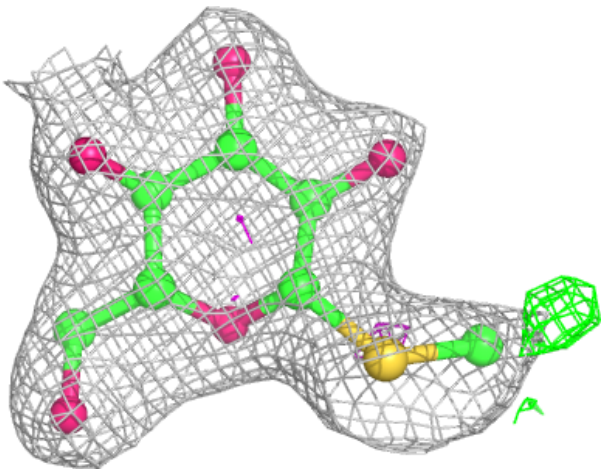


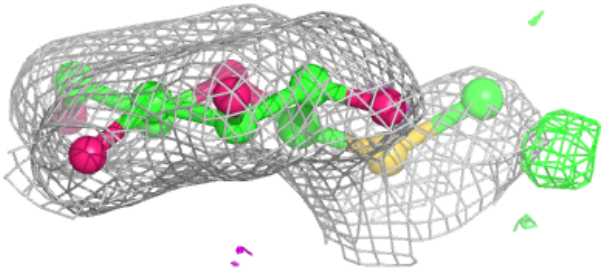


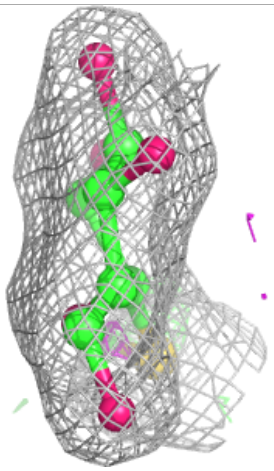


Electron density around HTG V 202:

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

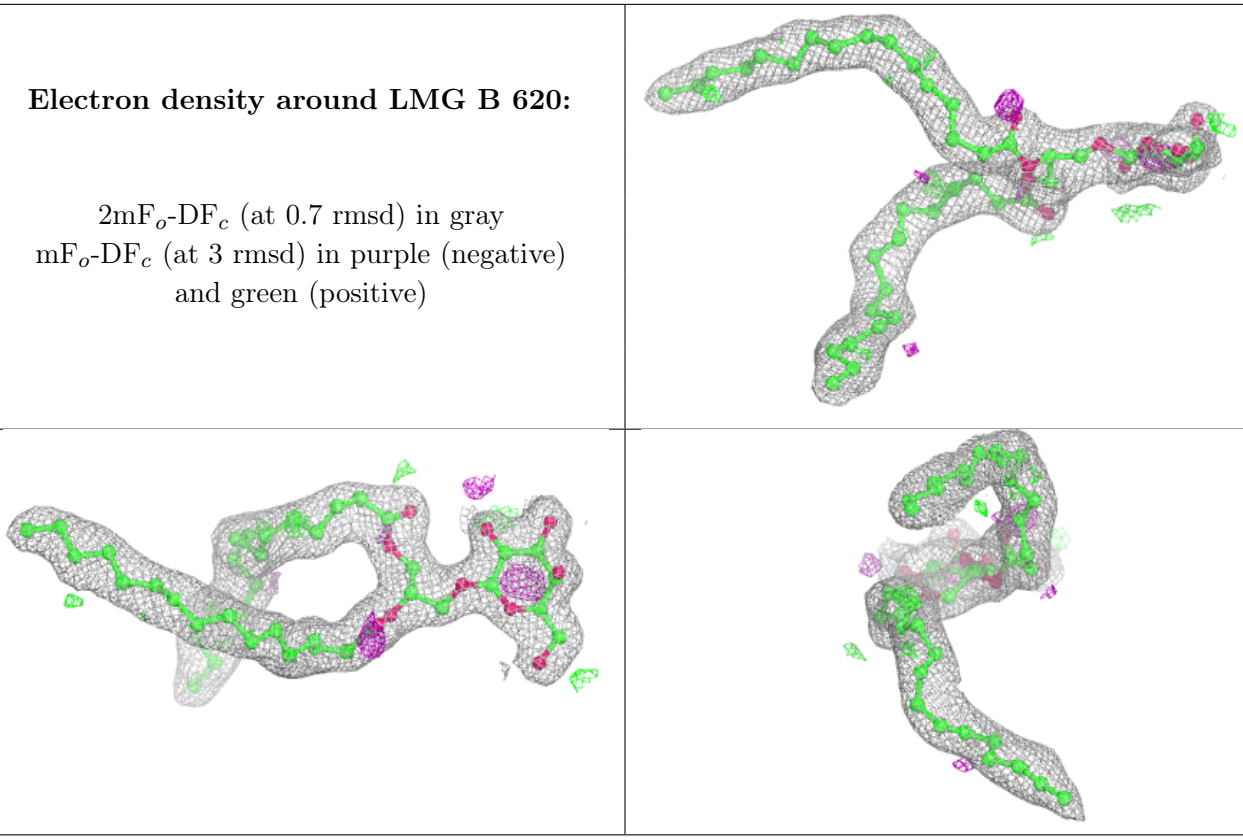






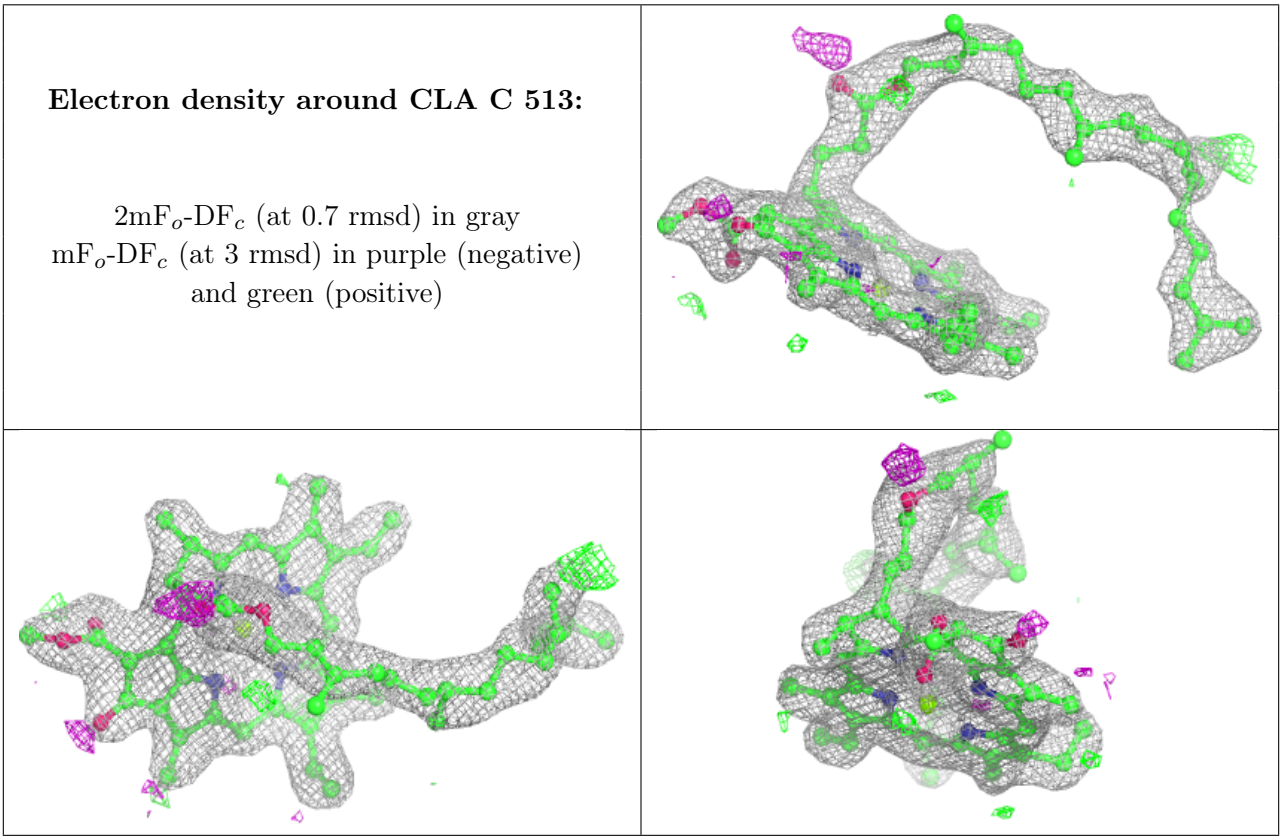
Electron density around LMG B 620:

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



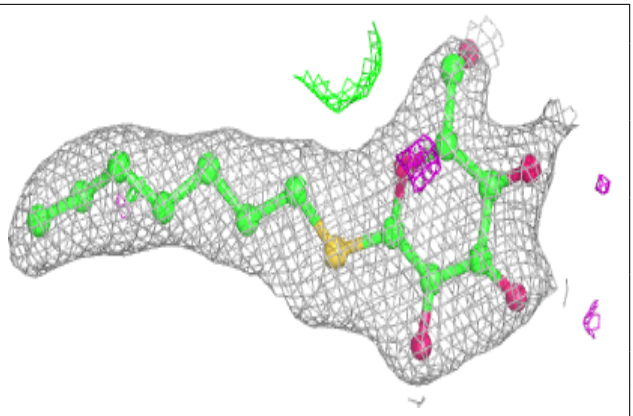
Electron density around CLA C 513:

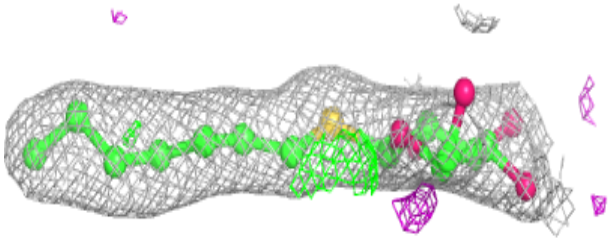
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

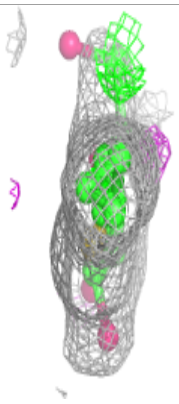


Electron density around HTG b 601:

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

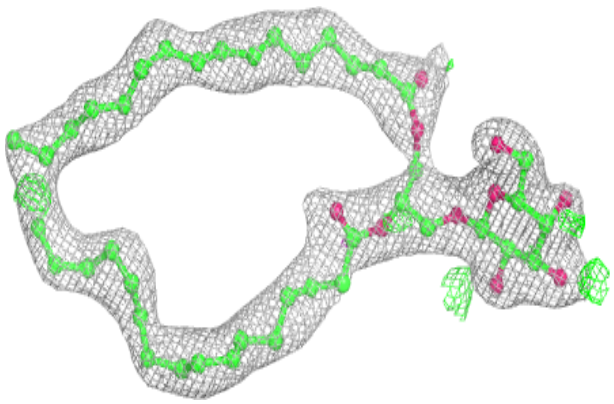


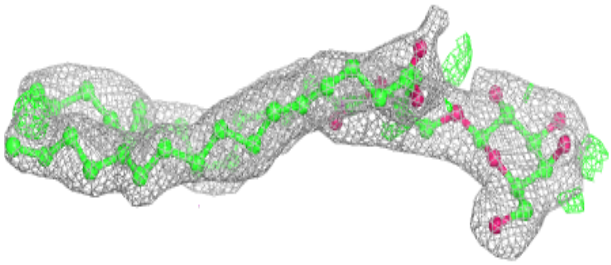


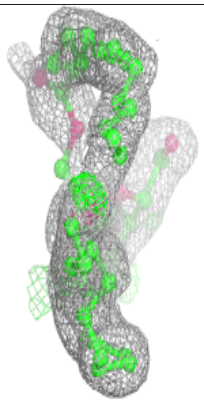


Electron density around LMG A 407:

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

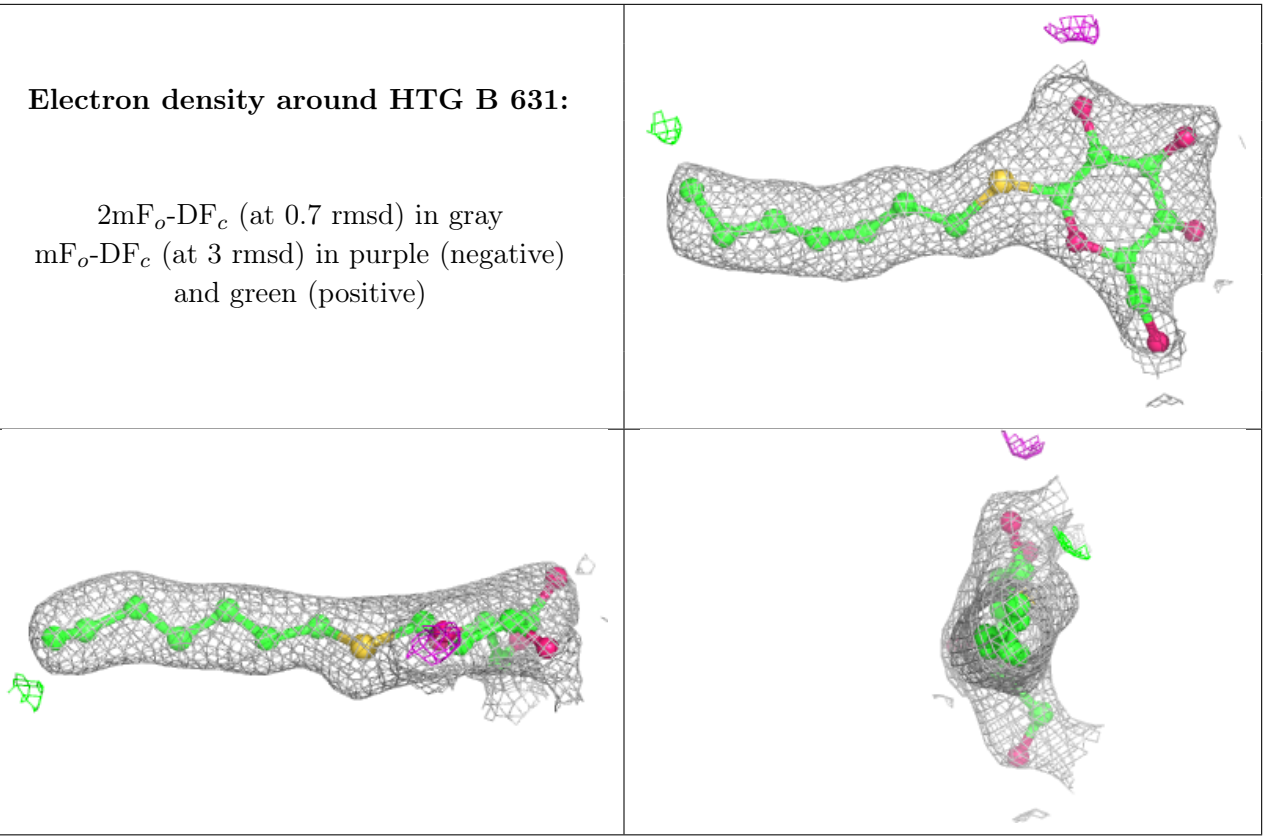






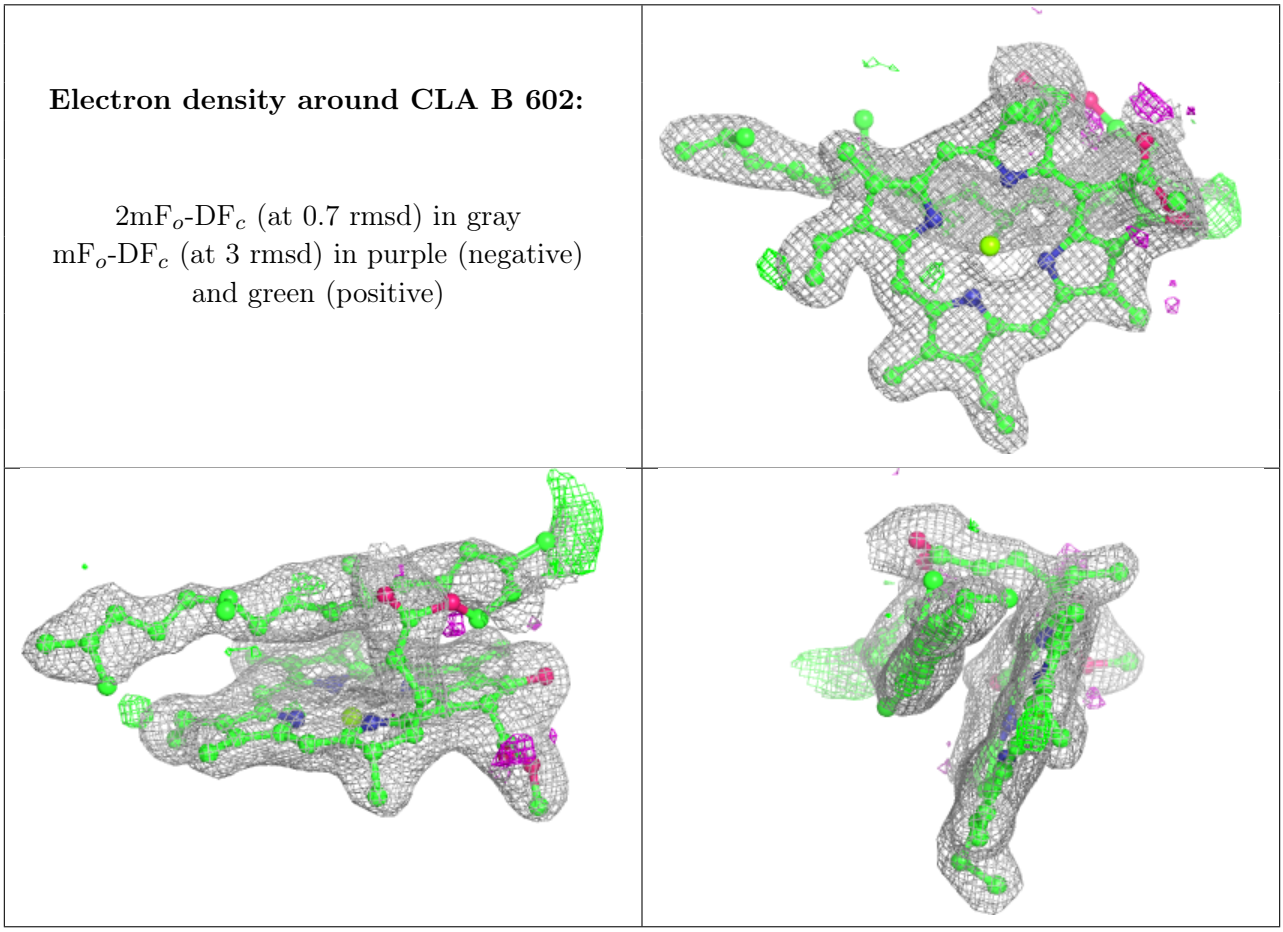
Electron density around HTG B 631:

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



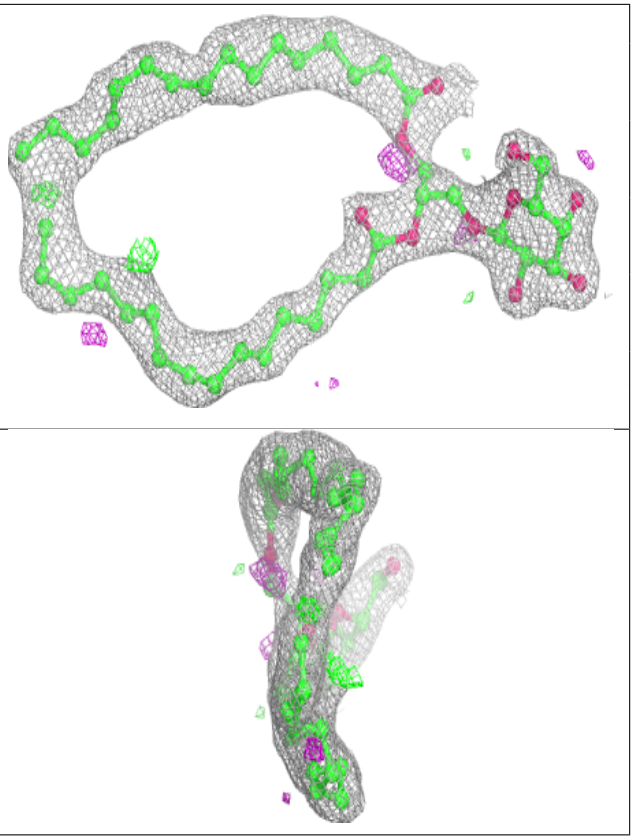
Electron density around CLA B 602:

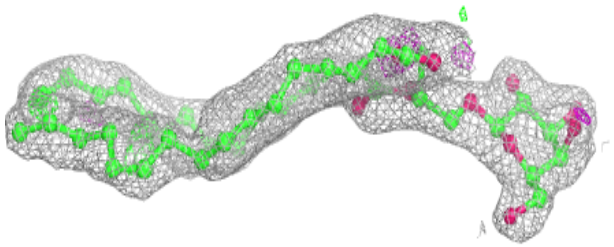
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG a 410:

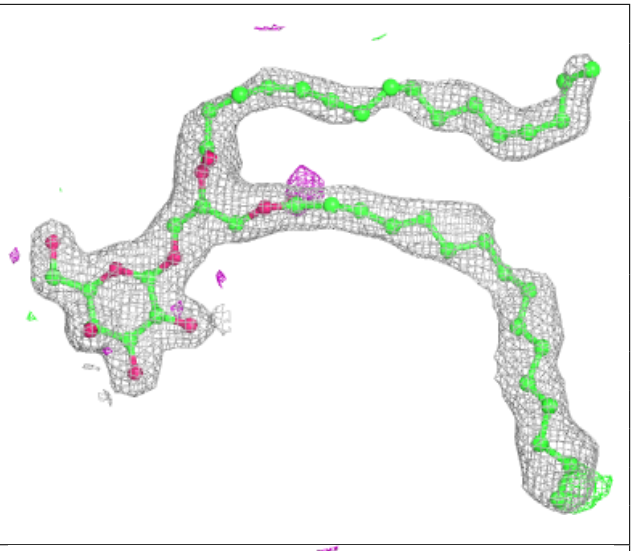
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

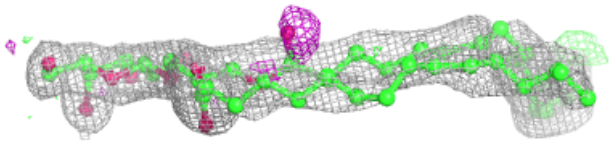


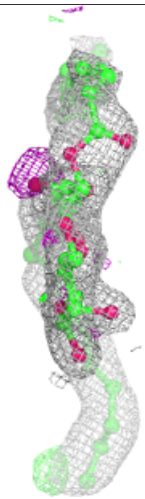


Electron density around LMG C 519:

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

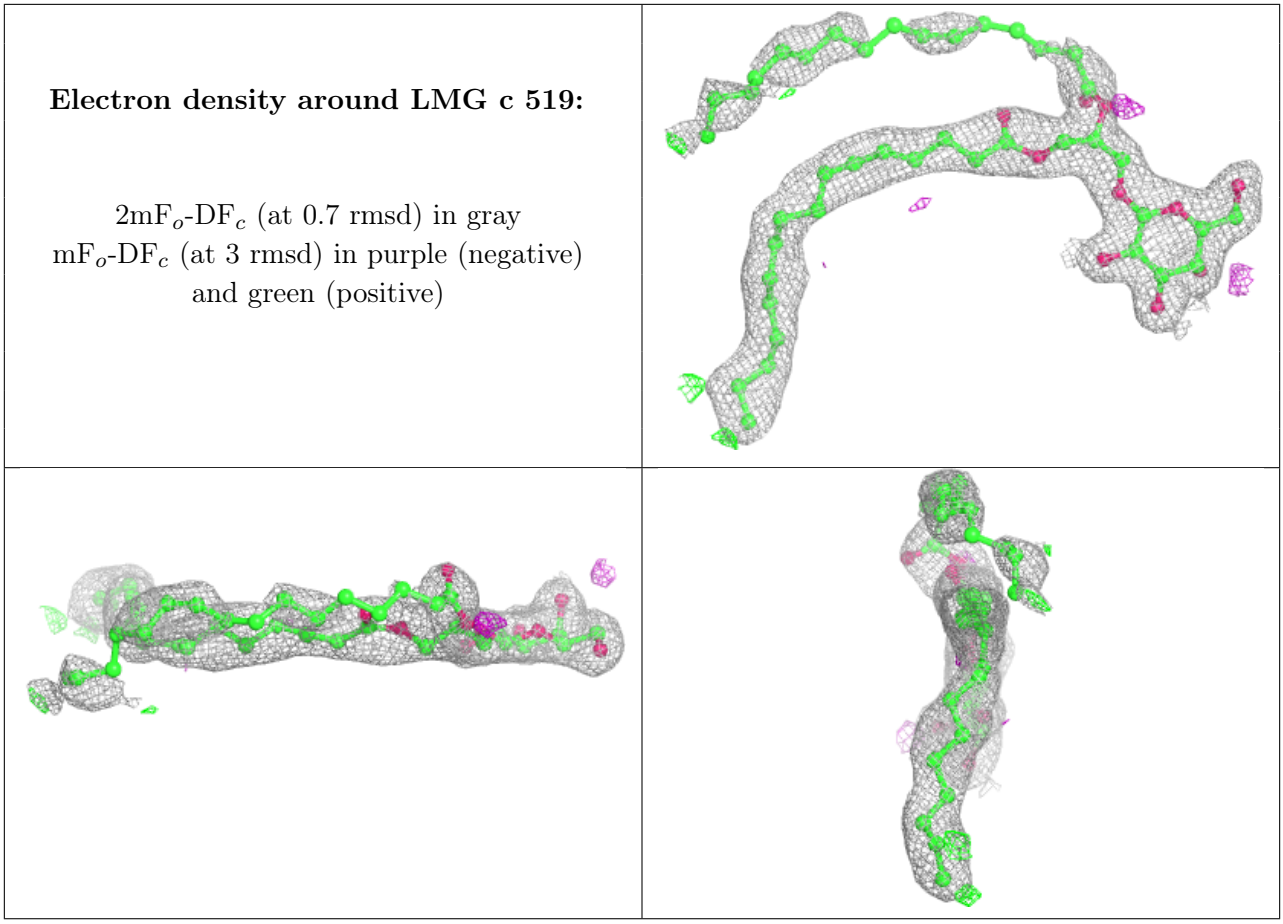






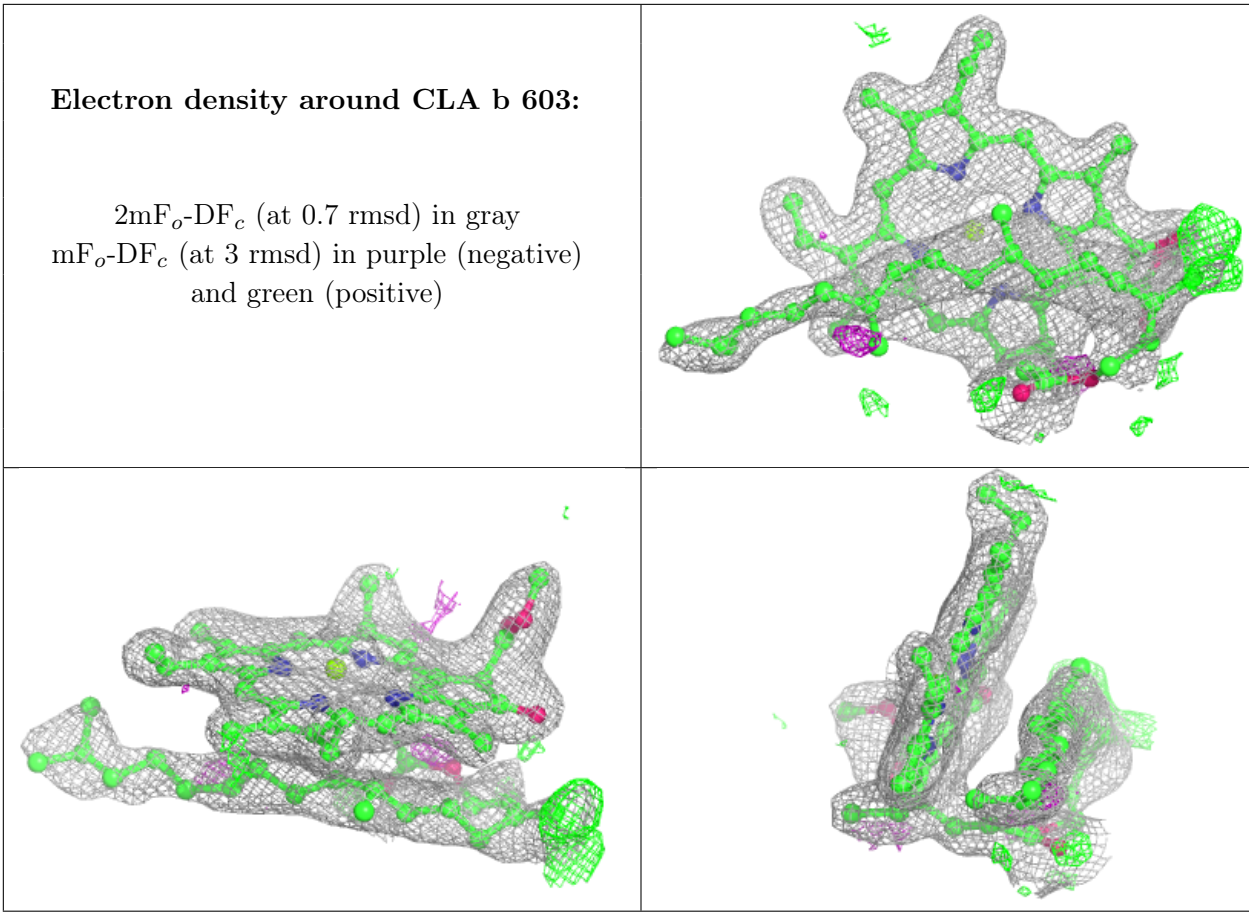
Electron density around LMG c 519:

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



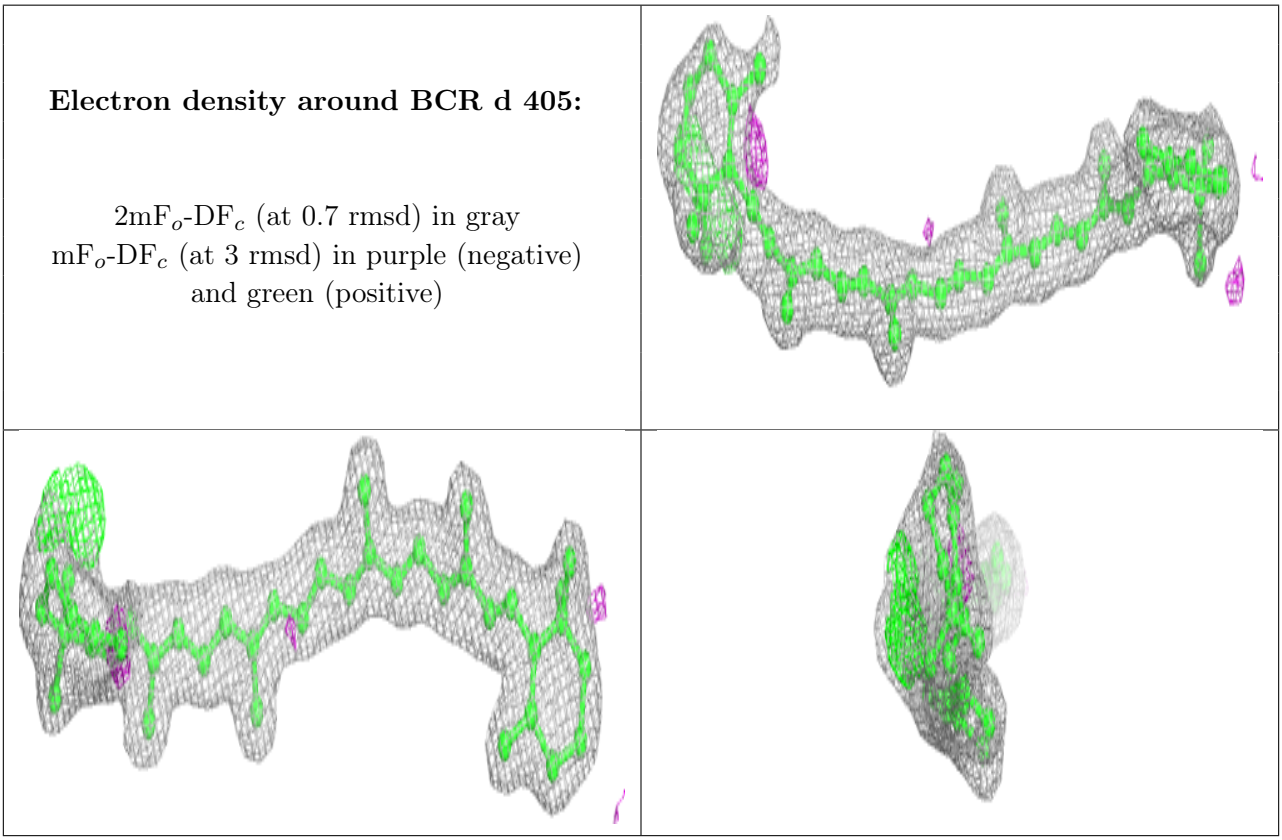
Electron density around CLA b 603:

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



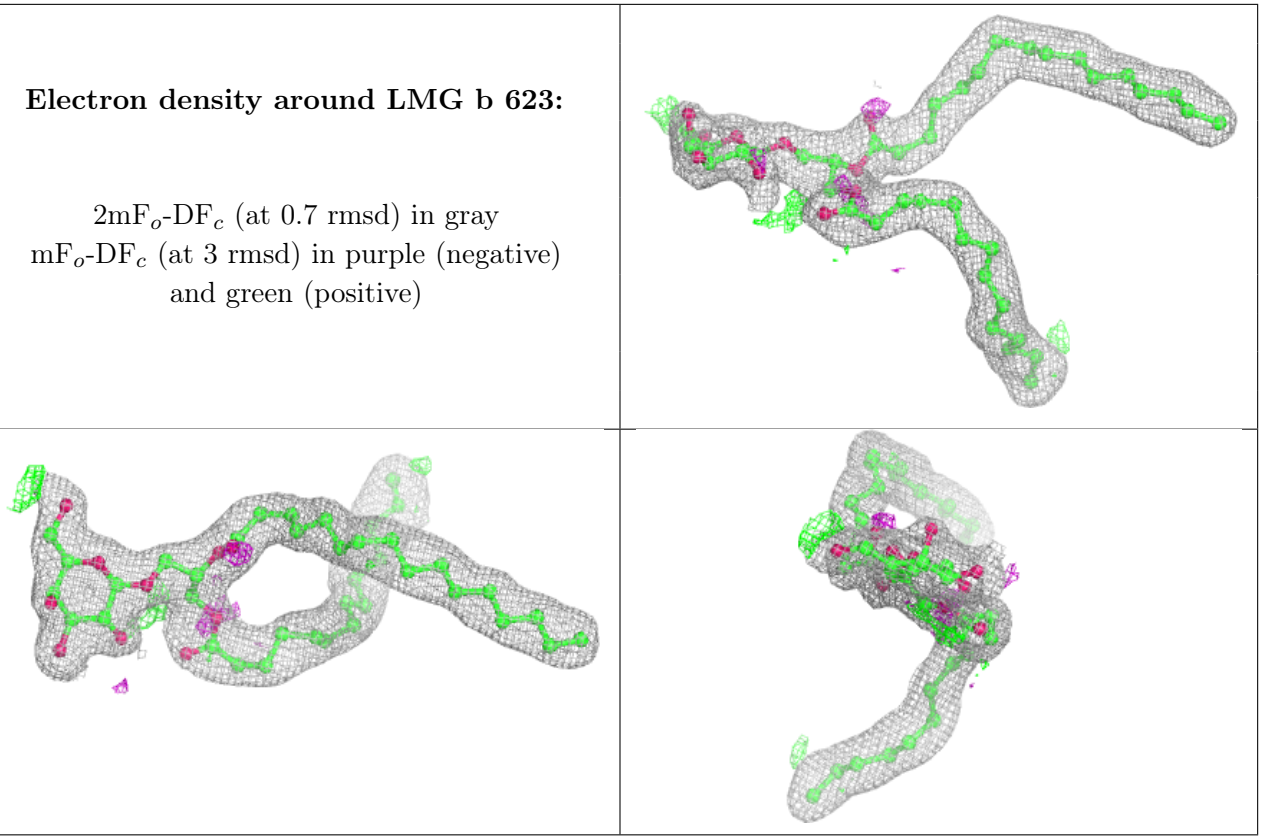
Electron density around BCR d 405:

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



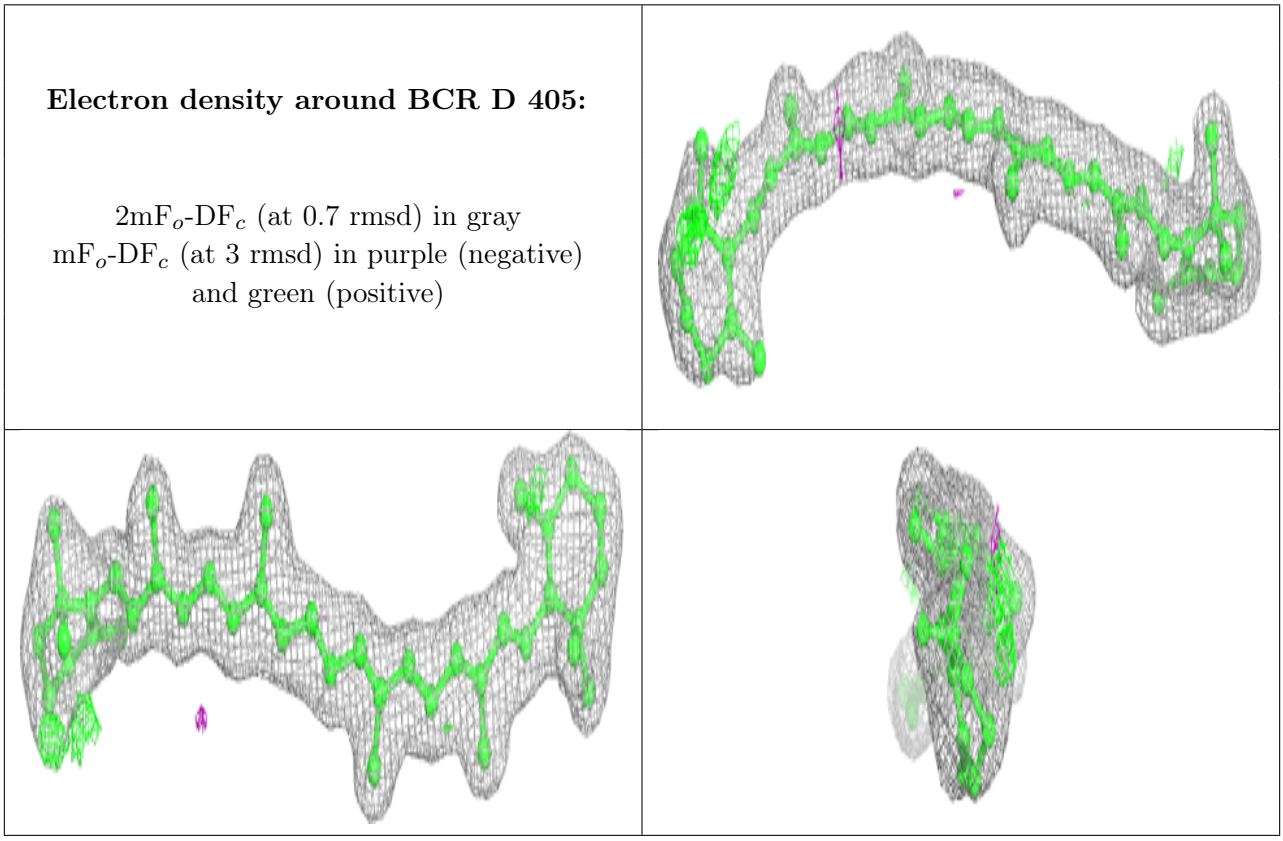
Electron density around LMG b 623:

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



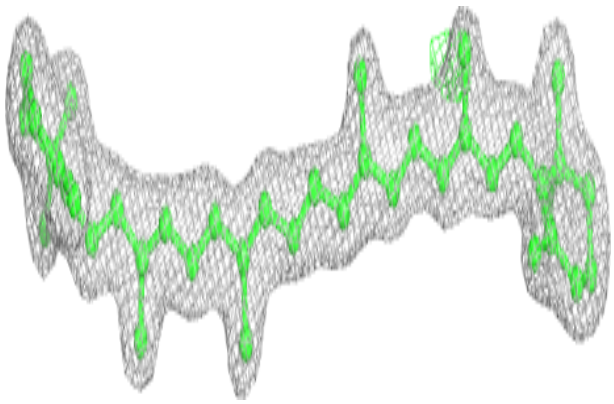
Electron density around BCR D 405:

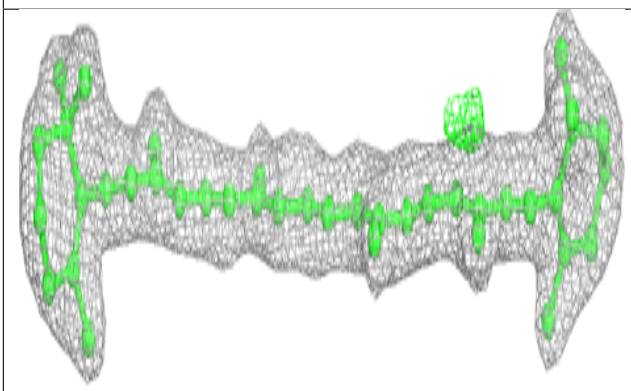
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

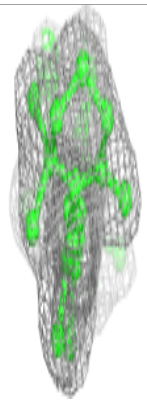


Electron density around BCR C 514:

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

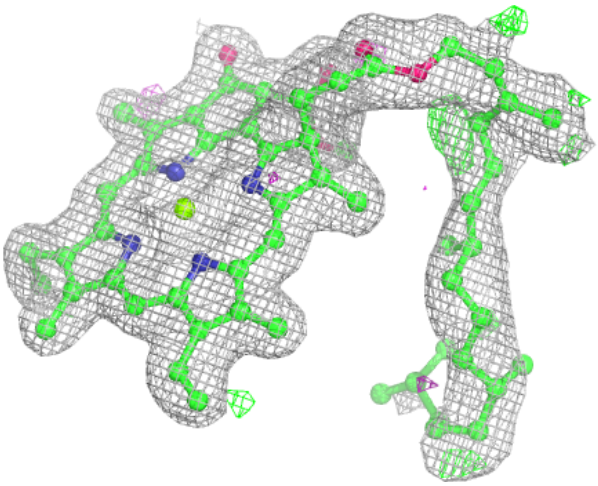


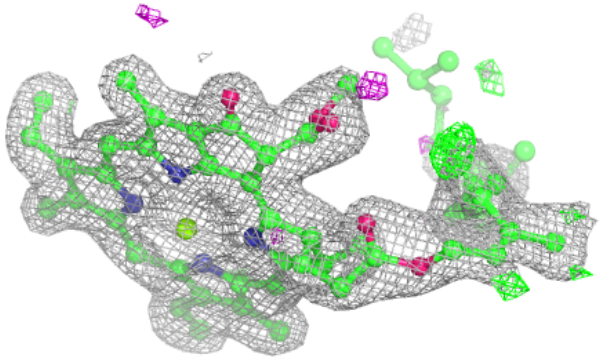


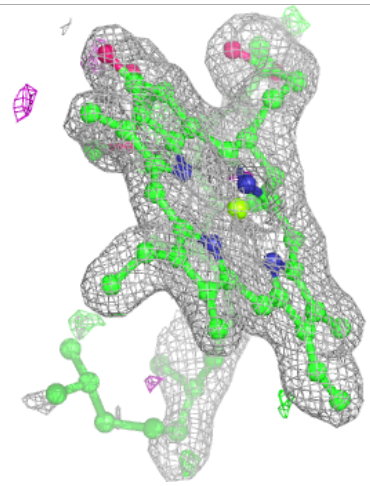


Electron density around CLA b 618:

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

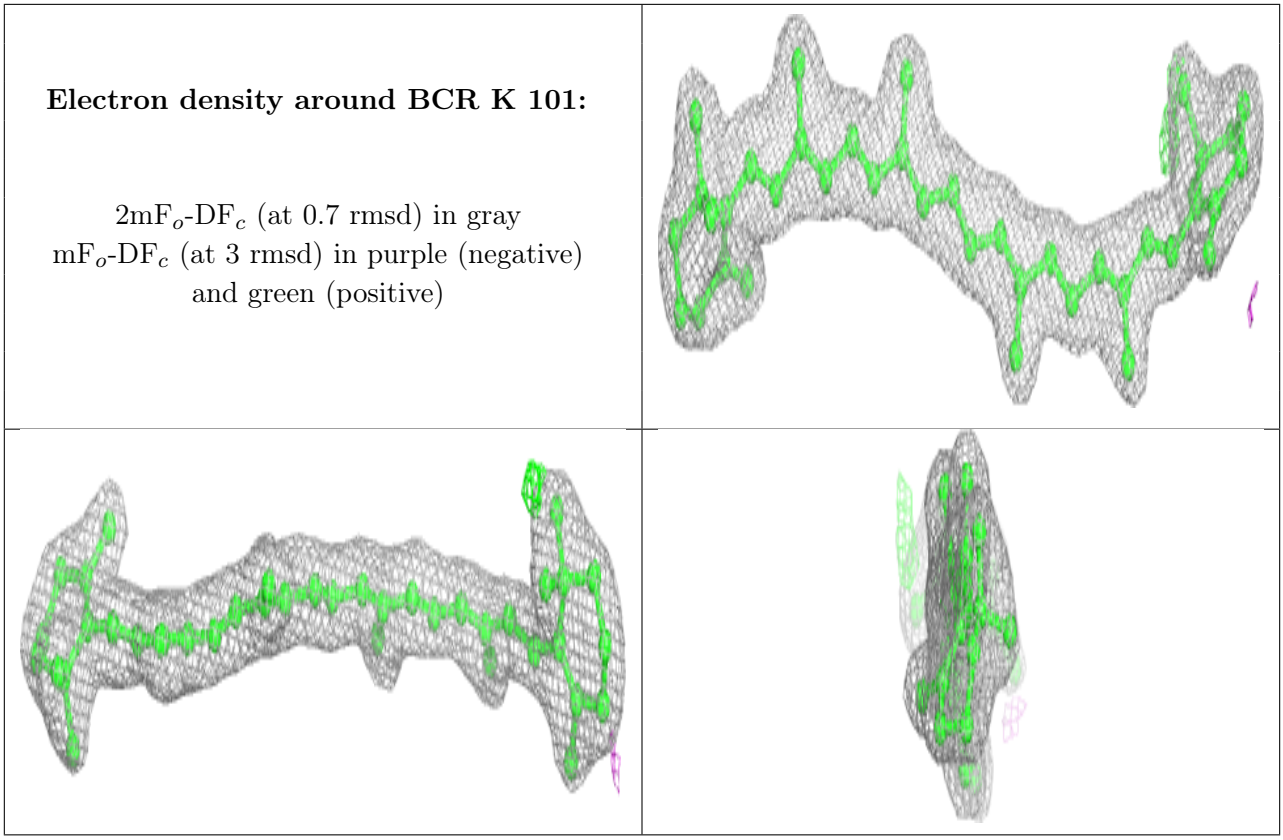






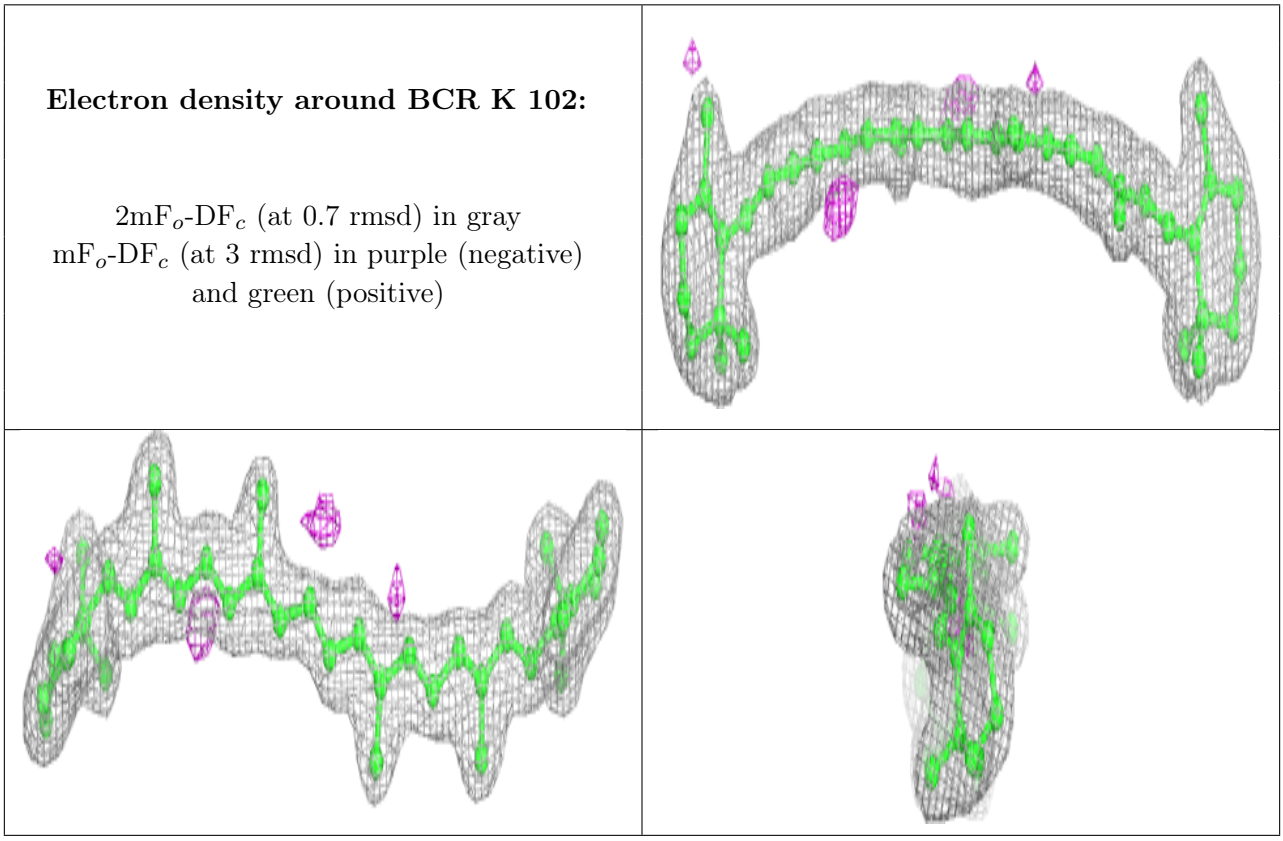
Electron density around BCR K 101:

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



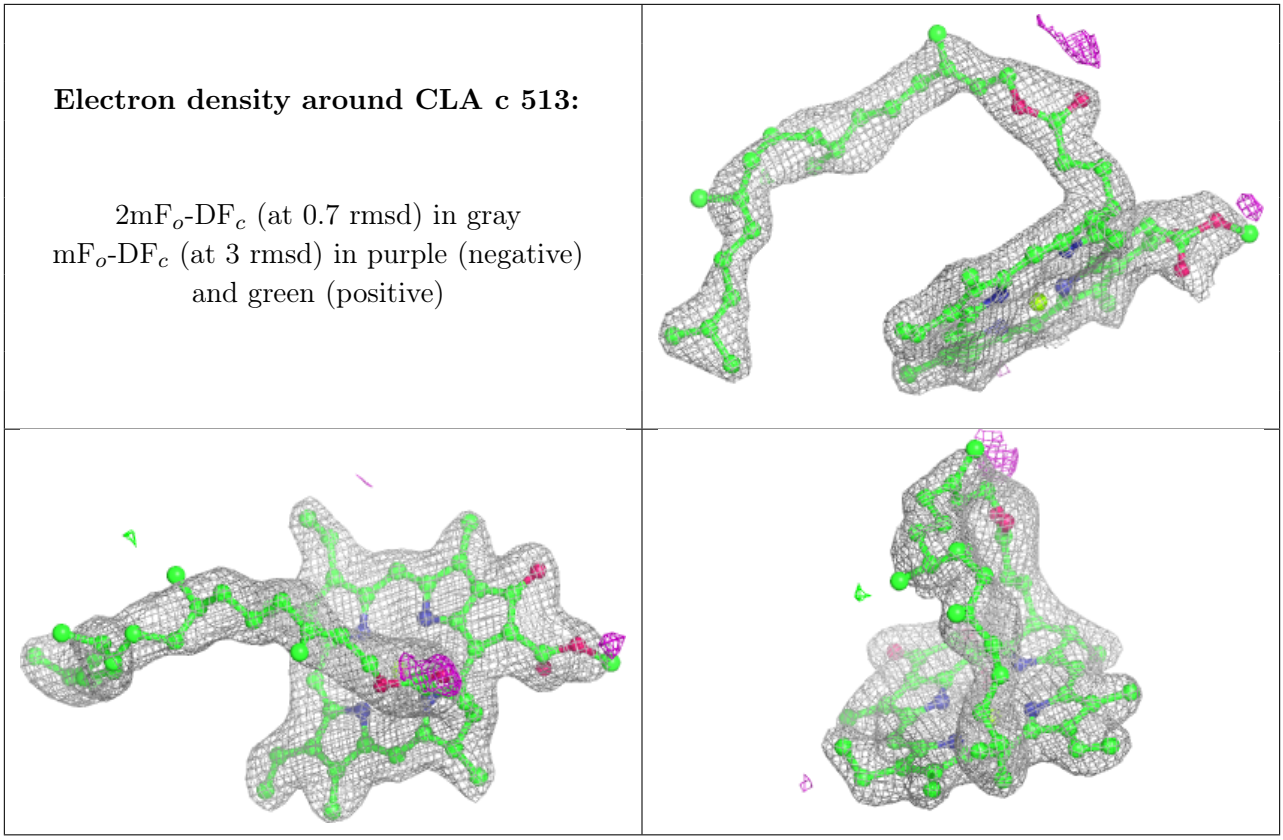
Electron density around BCR K 102:

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



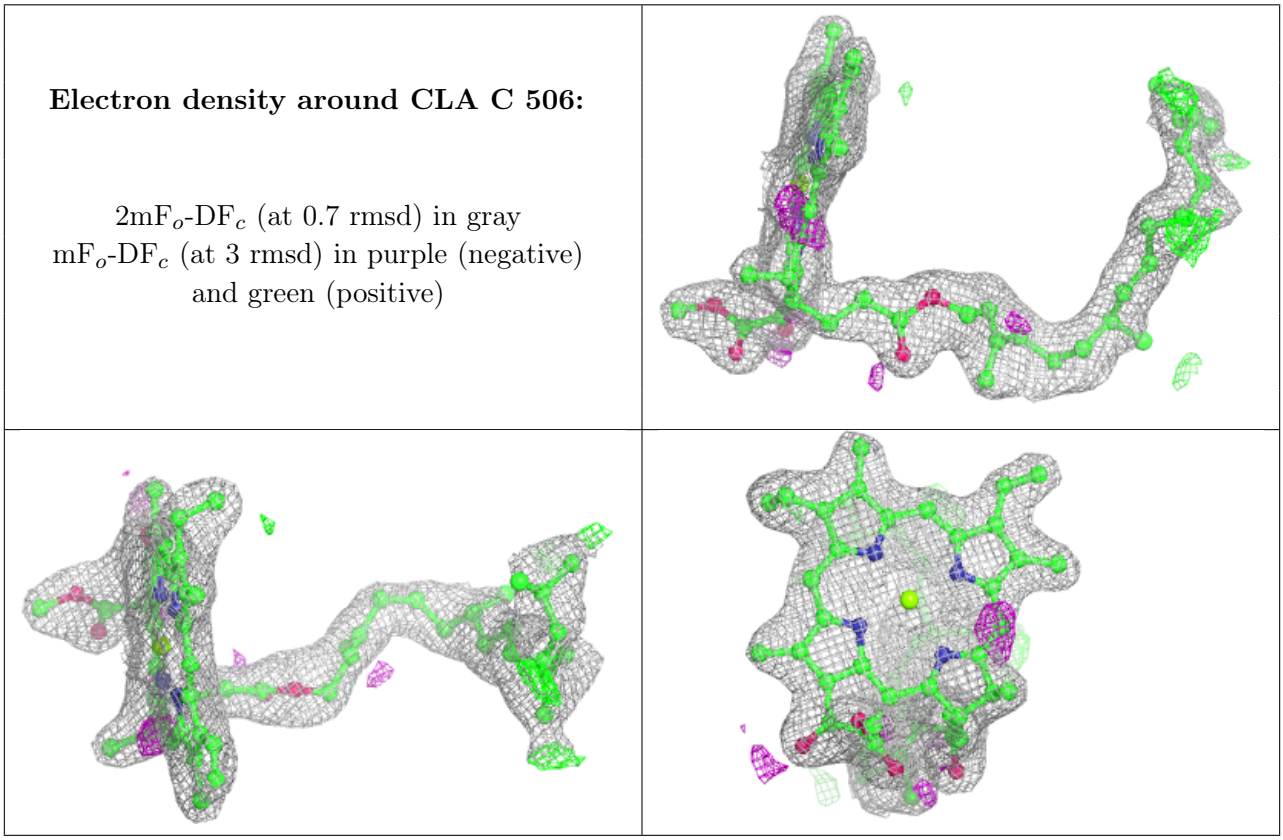
Electron density around CLA c 513:

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



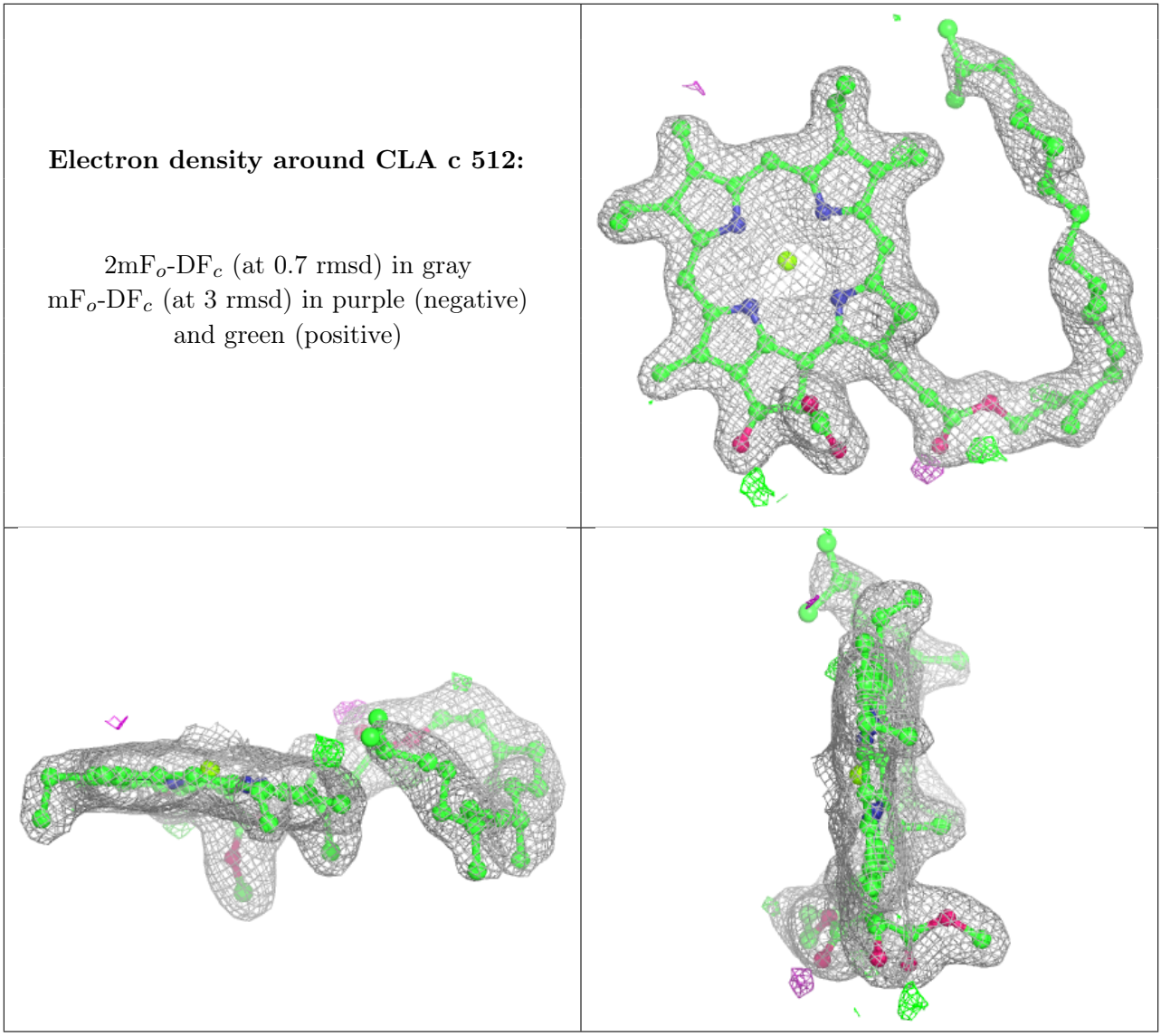
Electron density around CLA C 506:

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



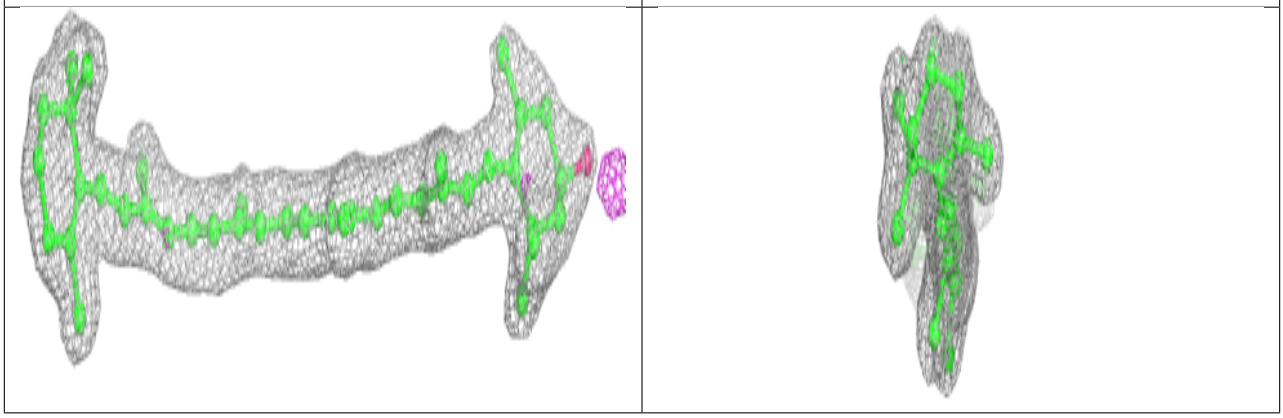
Electron density around CLA c 512:

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



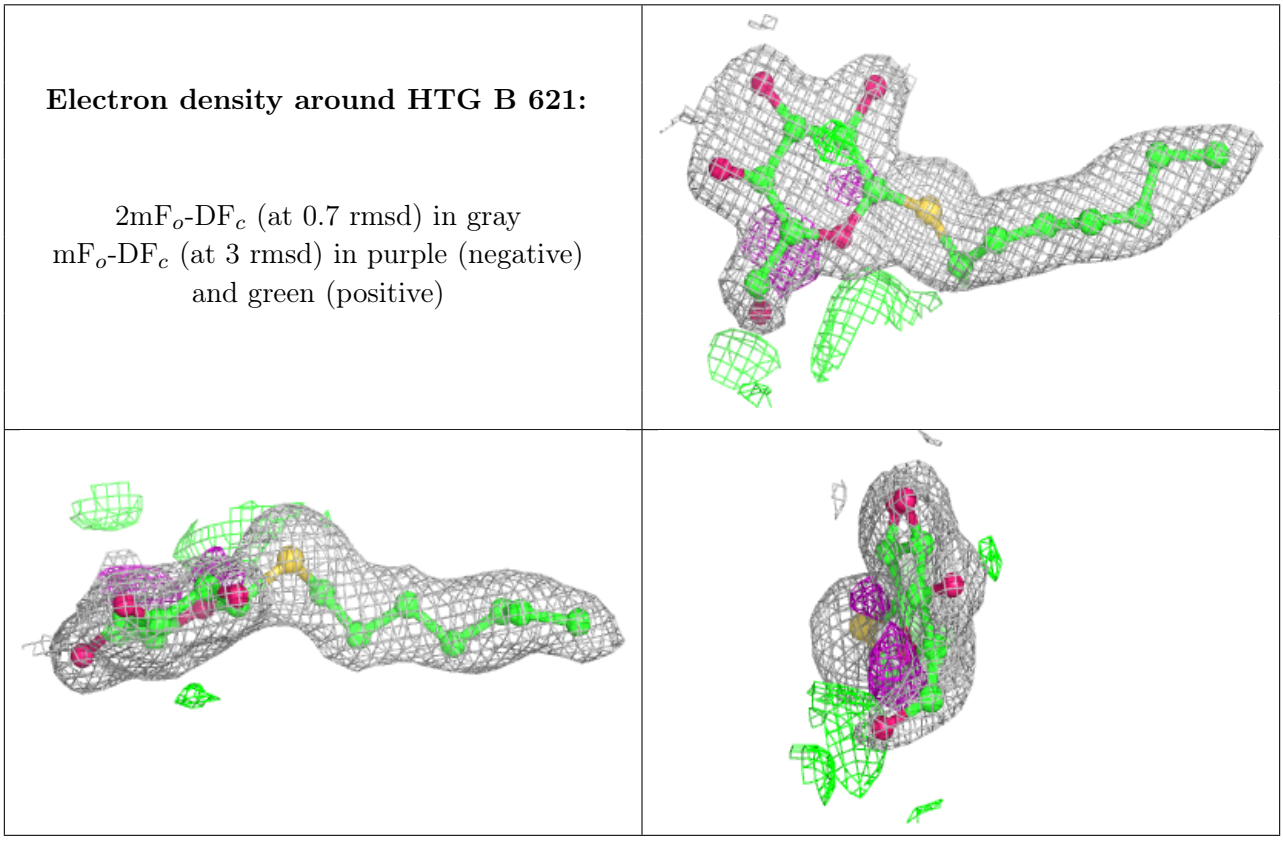
Electron density around RRX x 101:

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



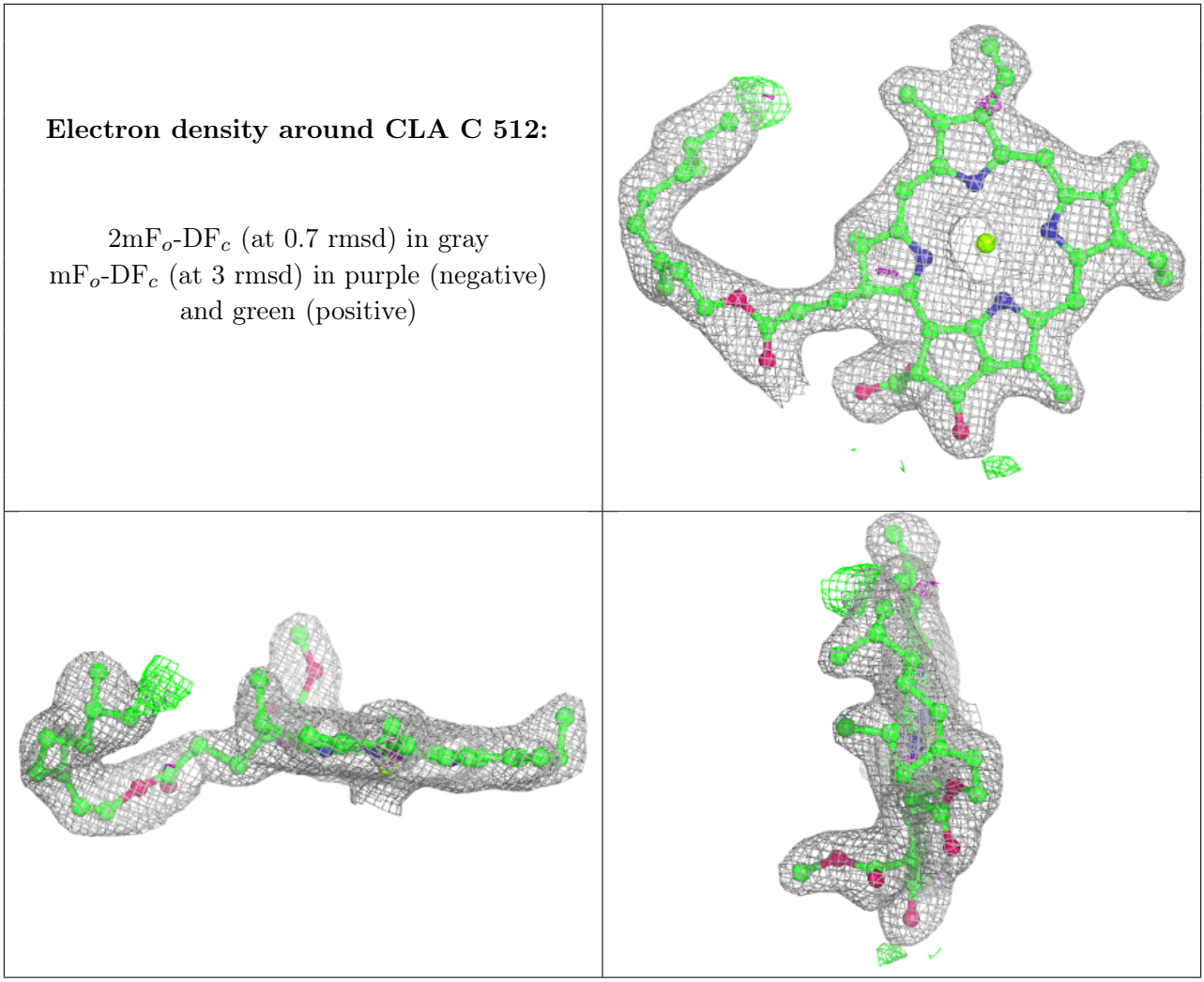
Electron density around HTG B 621:

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



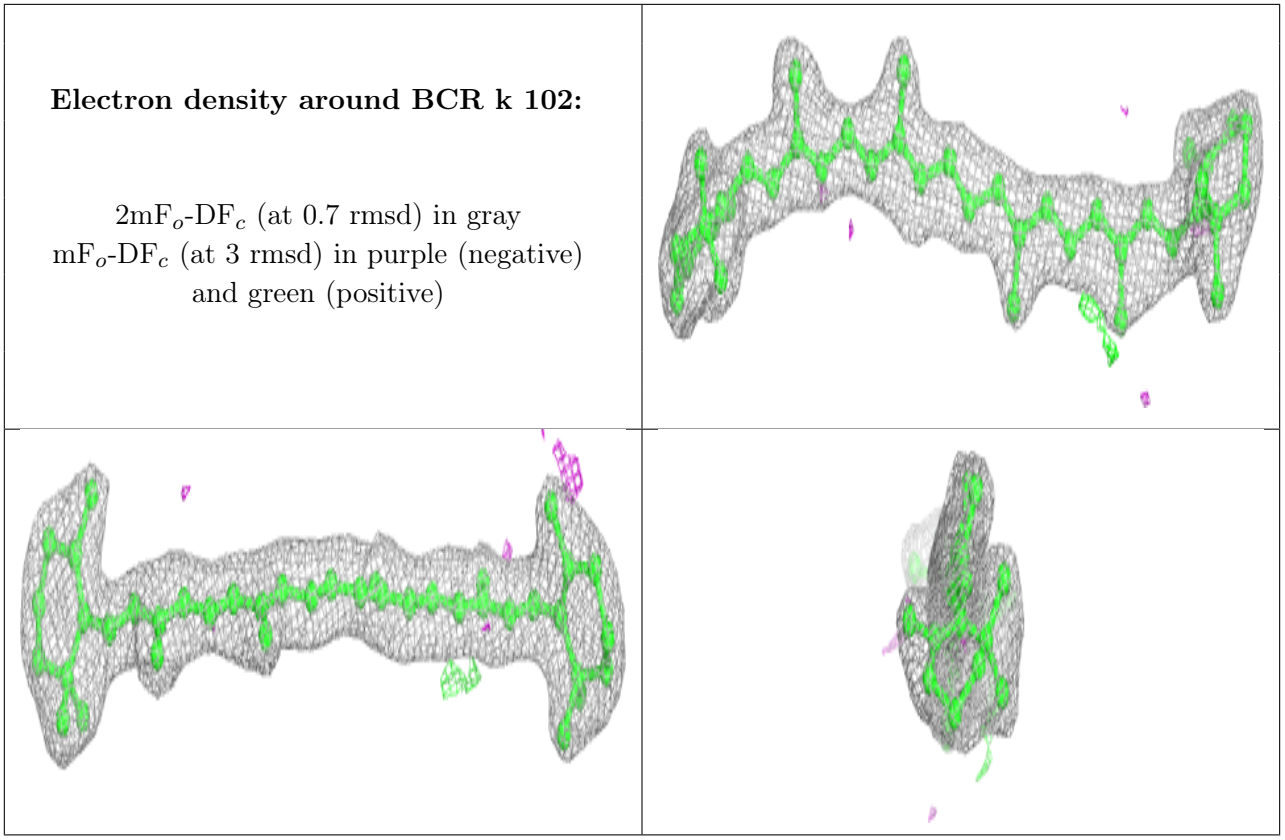
Electron density around CLA C 512:

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



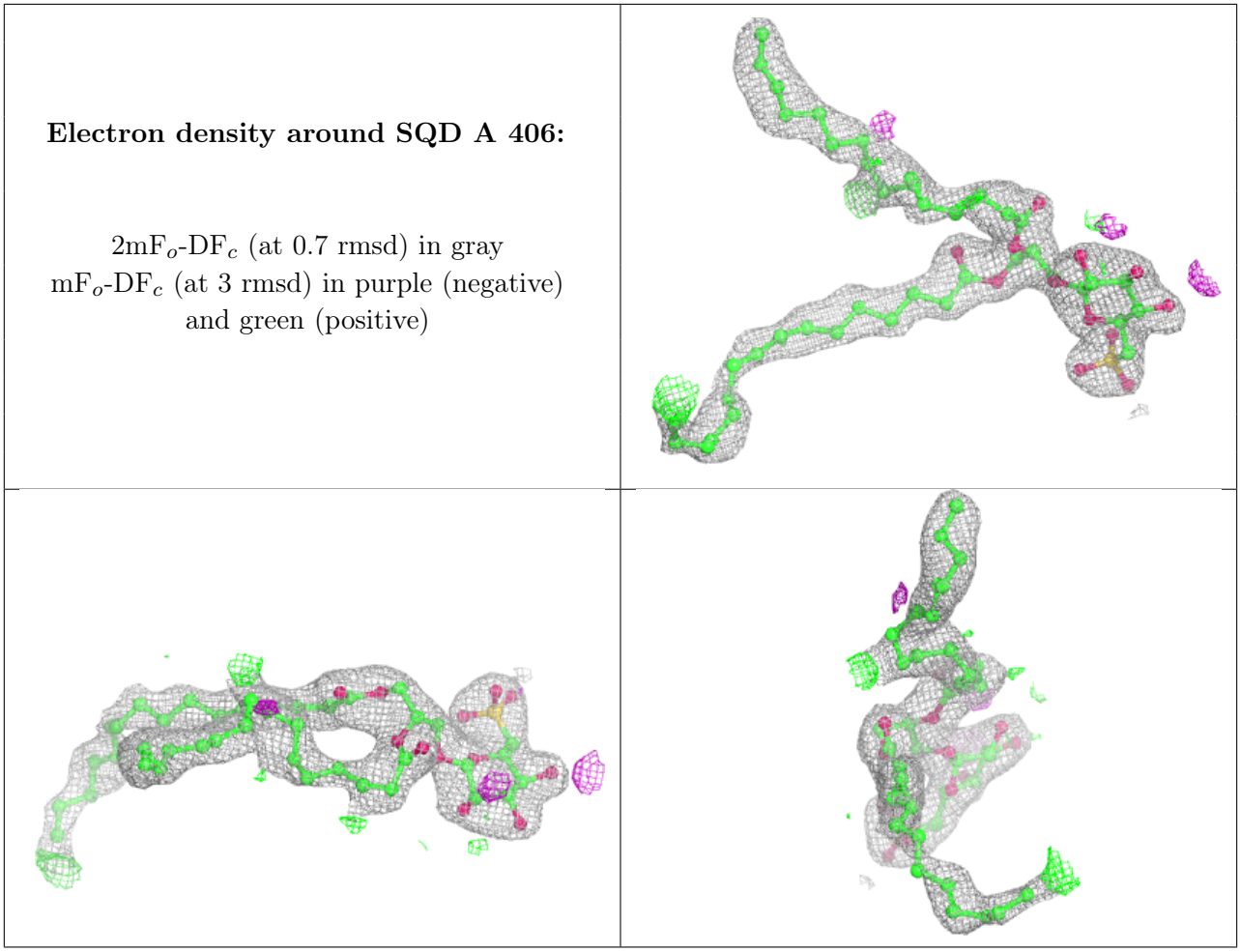
Electron density around BCR k 102:

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



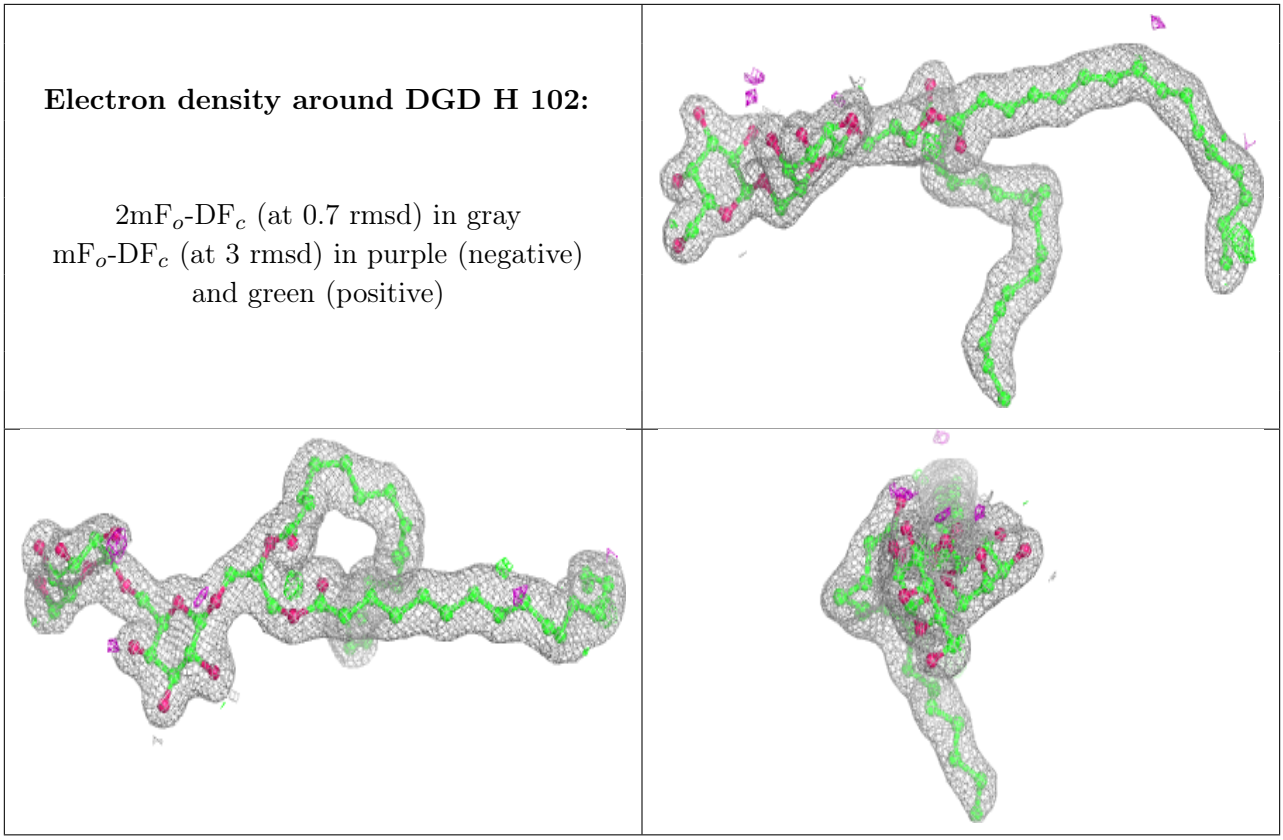
Electron density around SQD A 406:

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



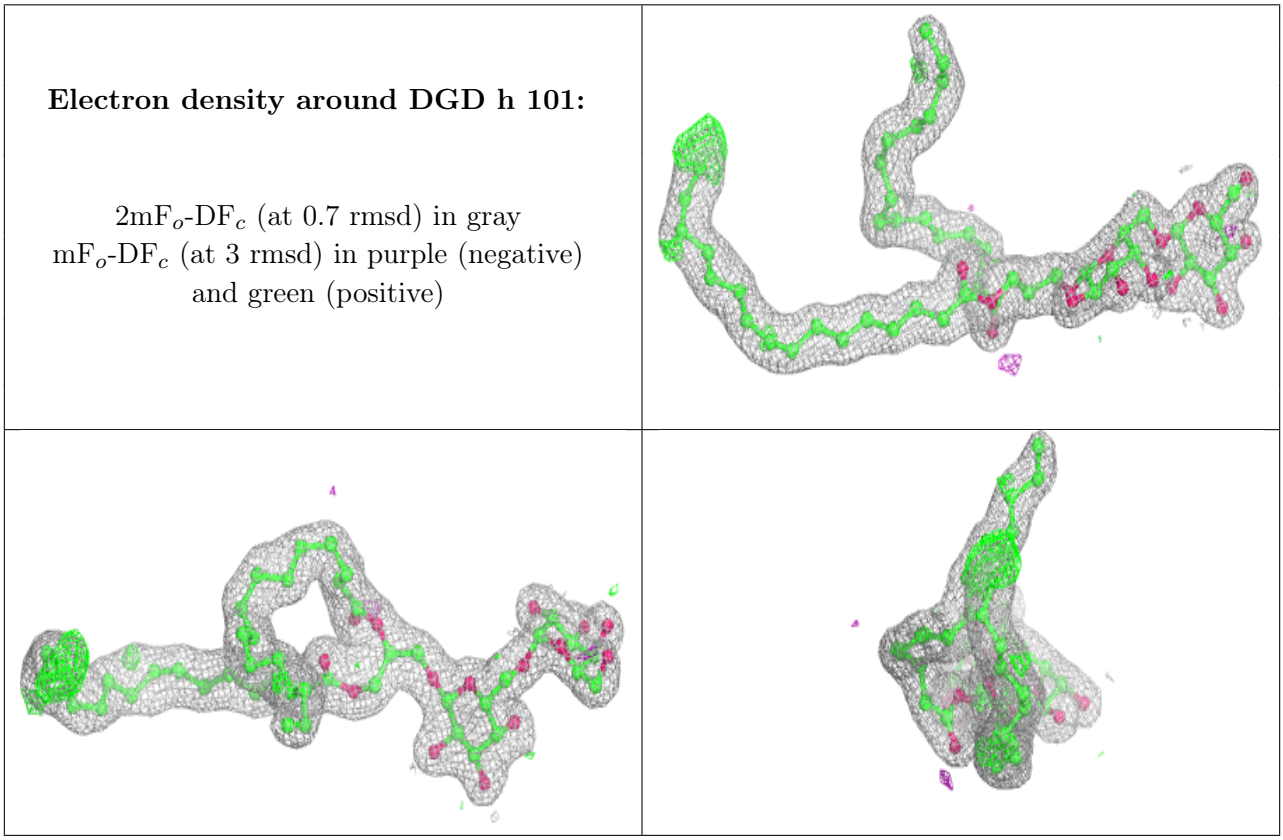
Electron density around DGD H 102:

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



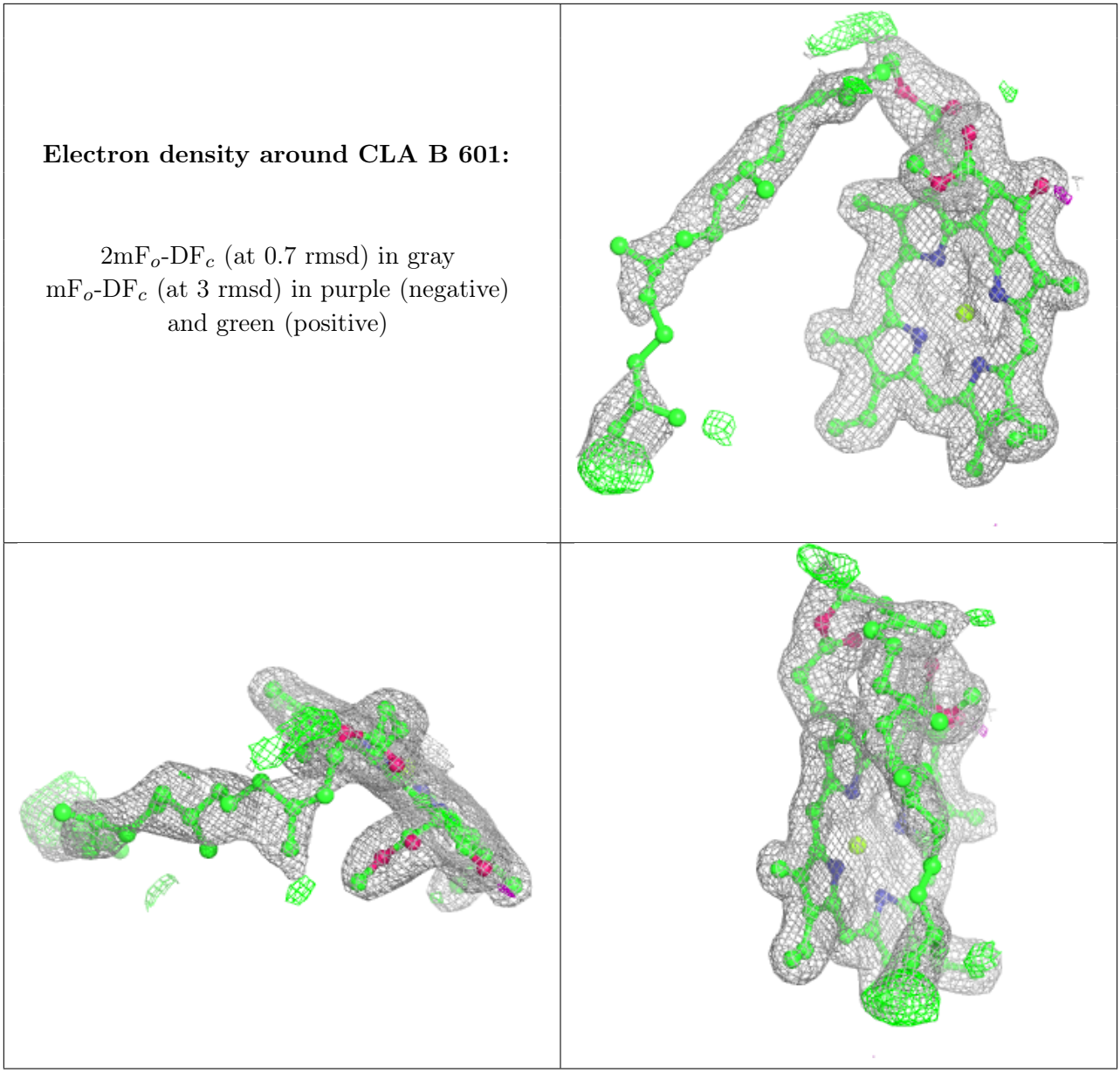
Electron density around DGD h 101:

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



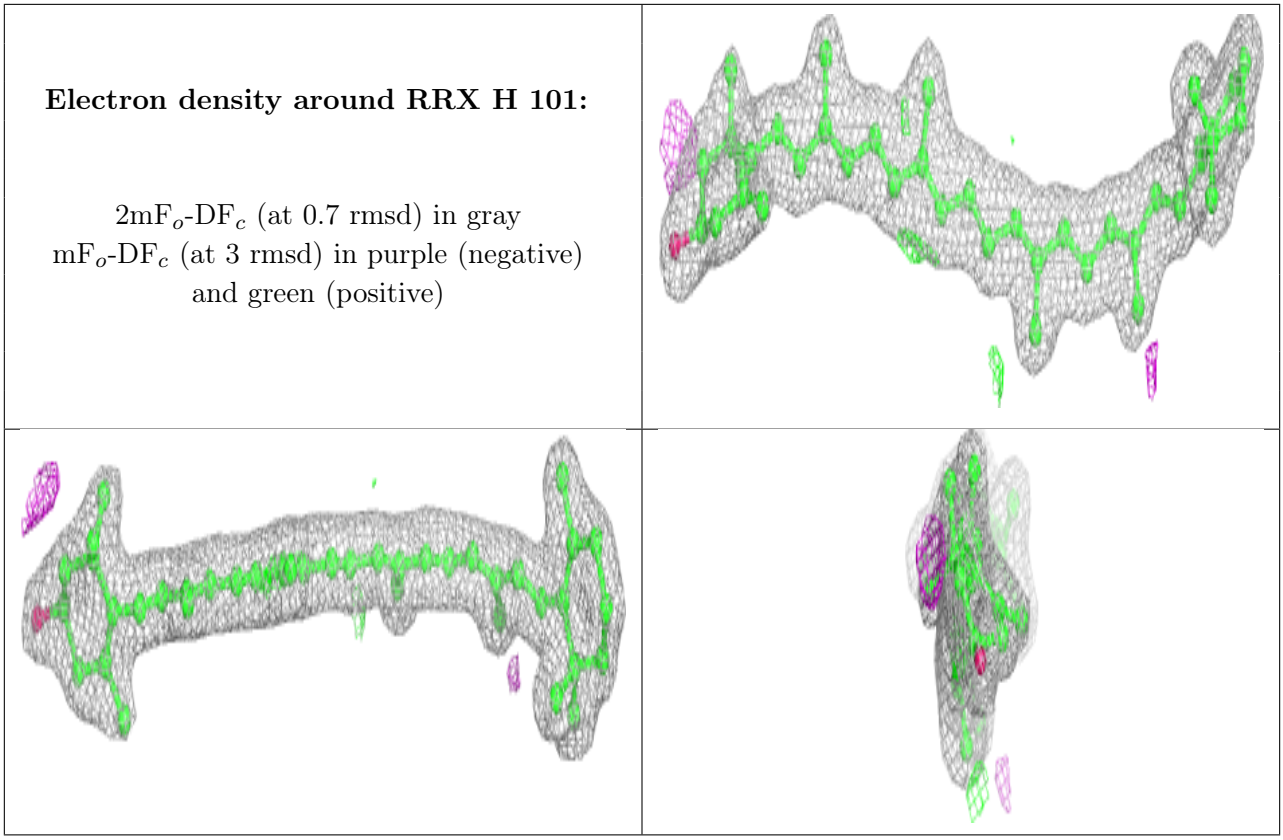
Electron density around CLA B 601:

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



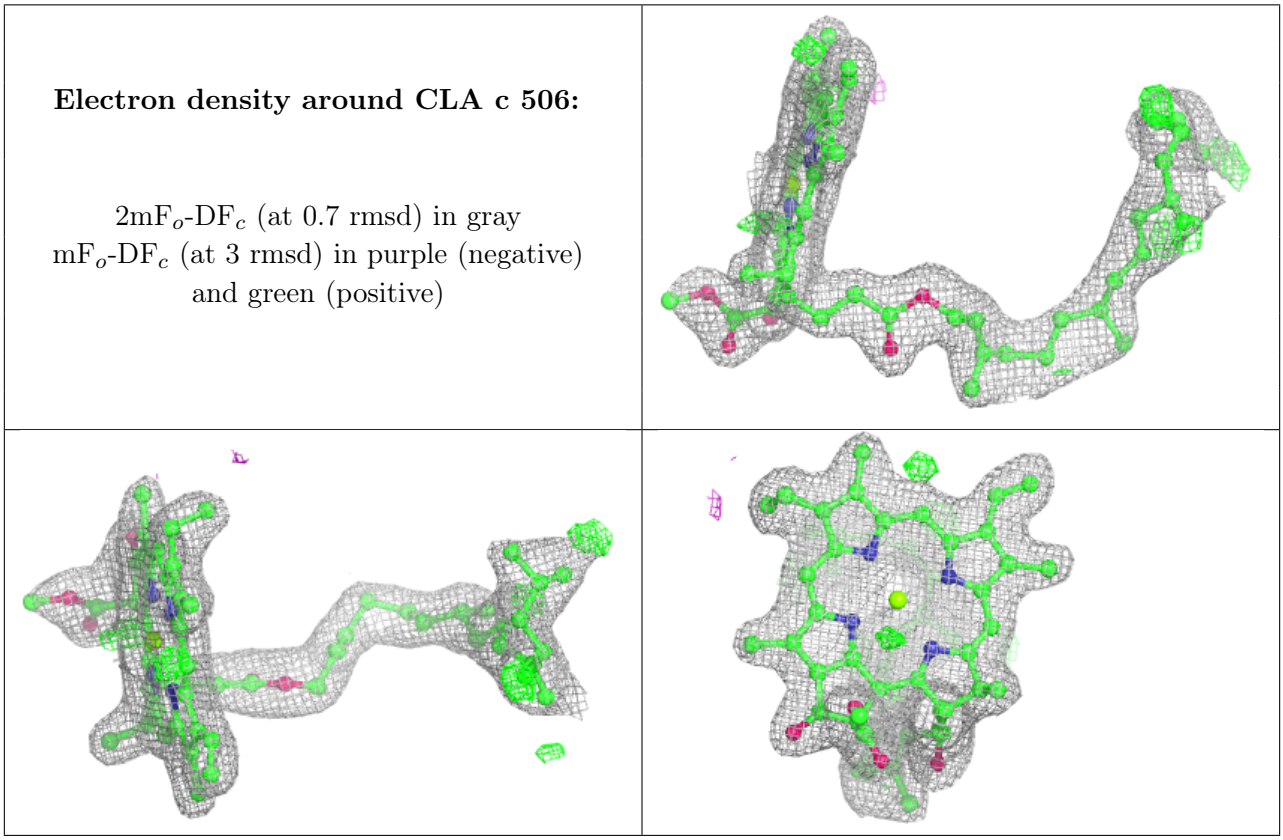
Electron density around RRX H 101:

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



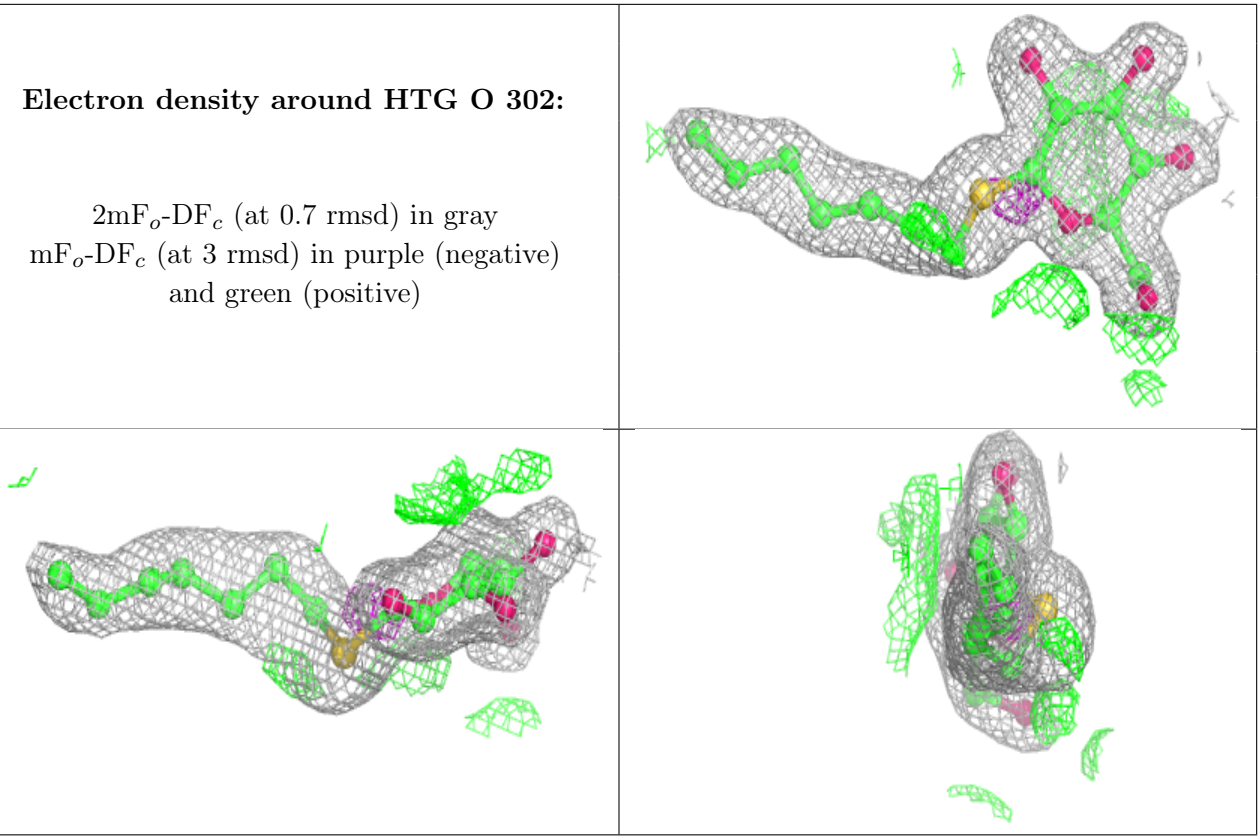
Electron density around CLA c 506:

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



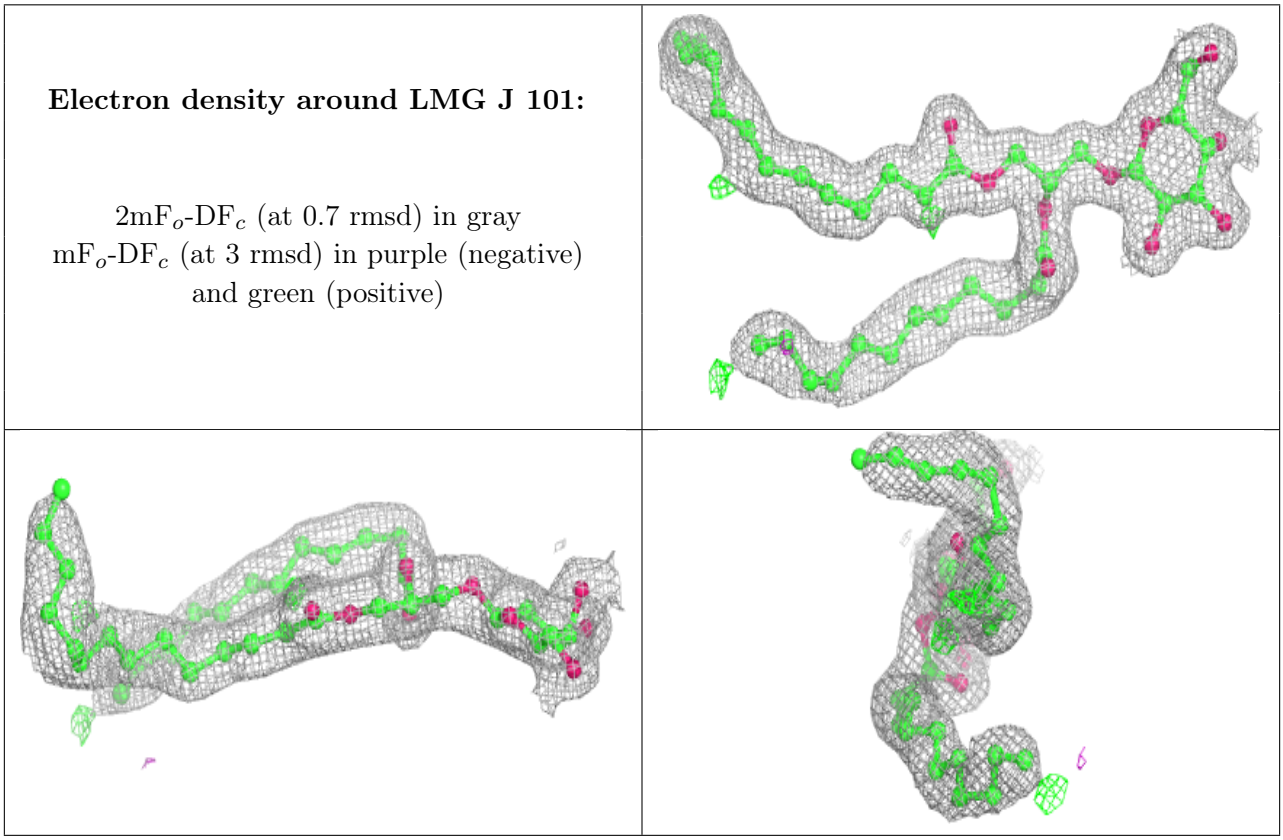
Electron density around HTG O 302:

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



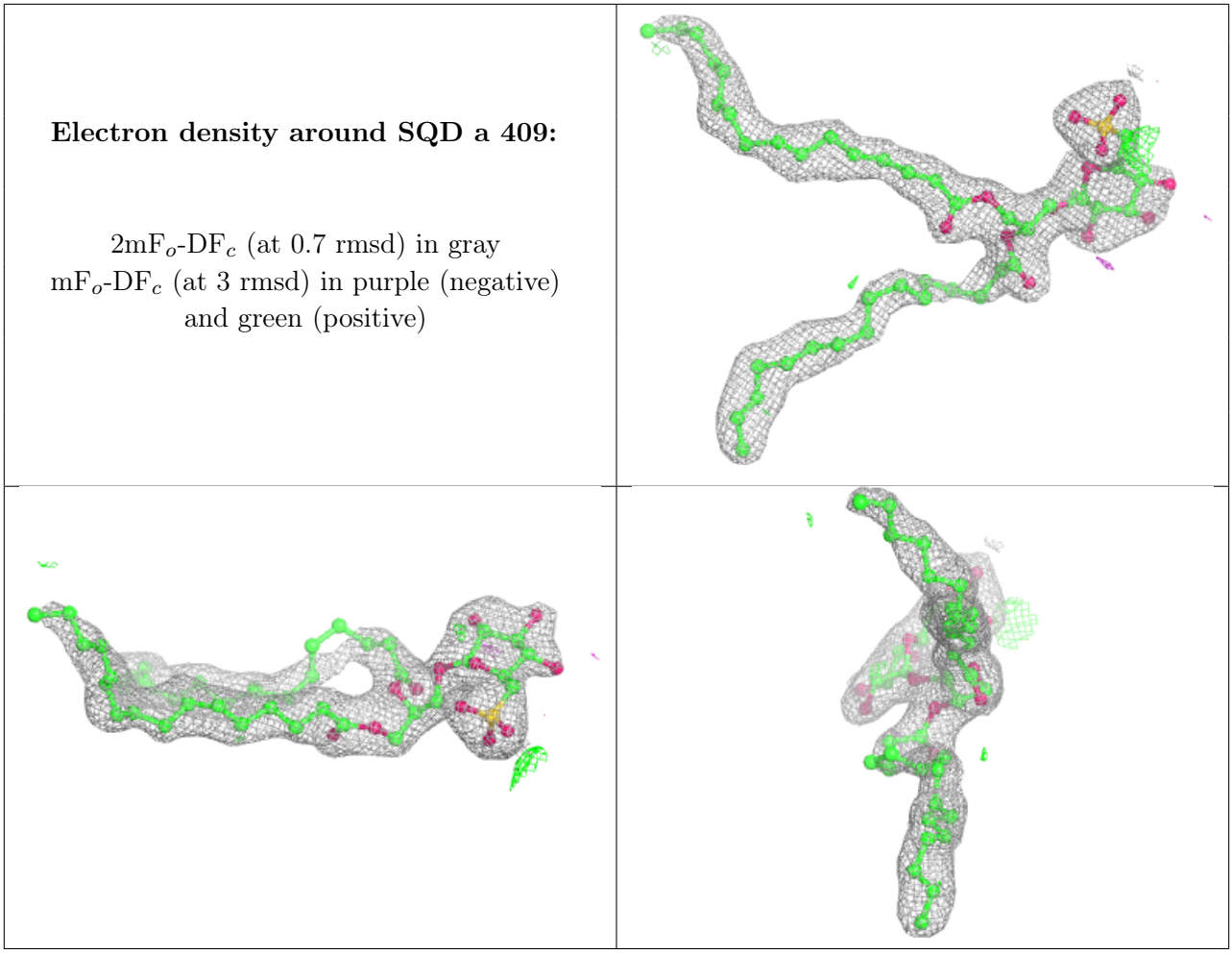
Electron density around LMG J 101:

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



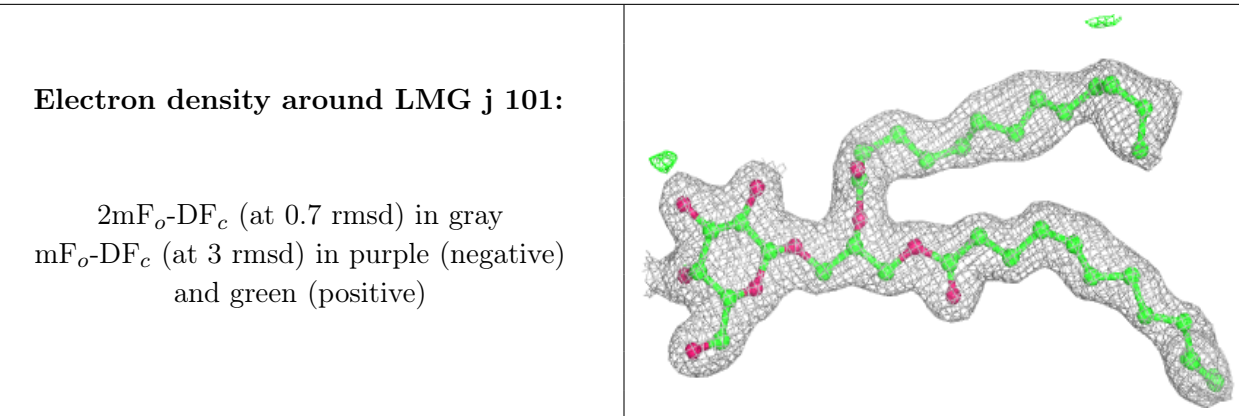
Electron density around SQD a 409:

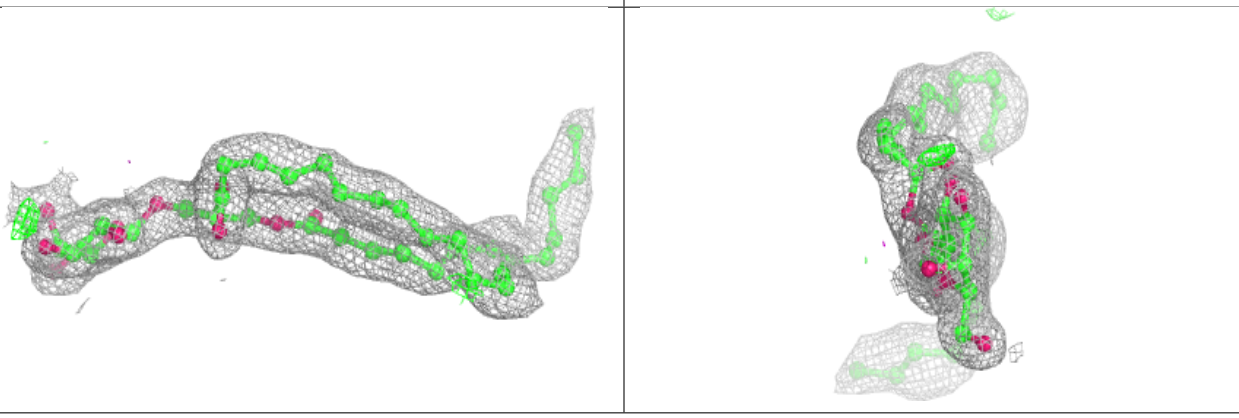
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG j 101:

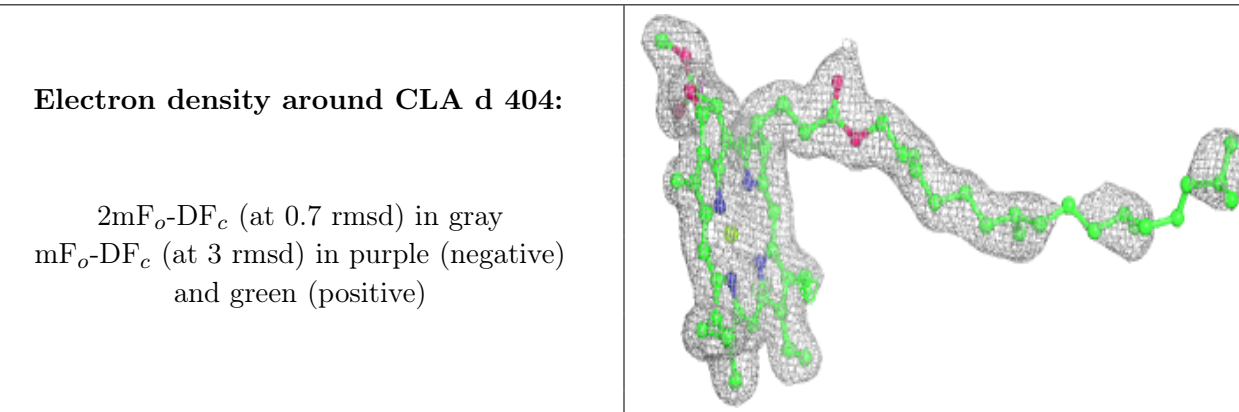
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

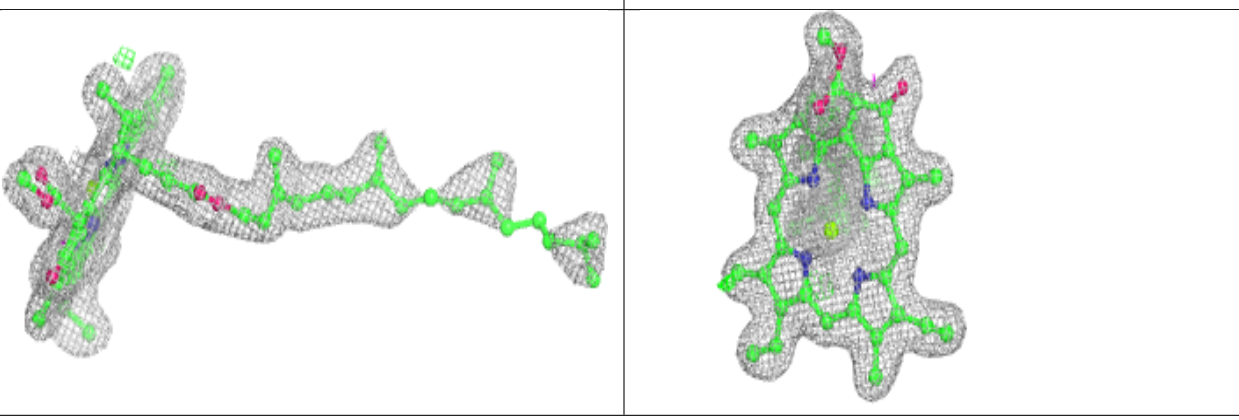




Electron density around CLA d 404:

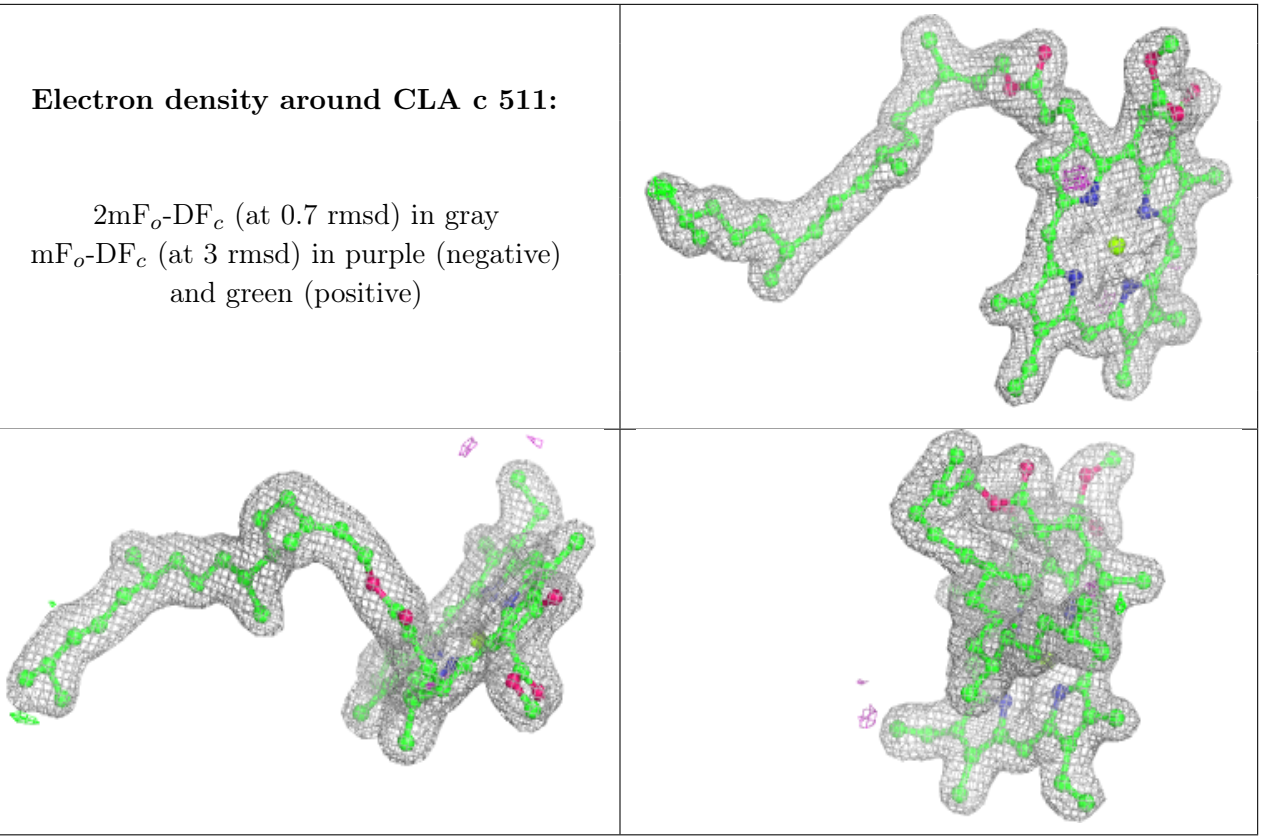
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





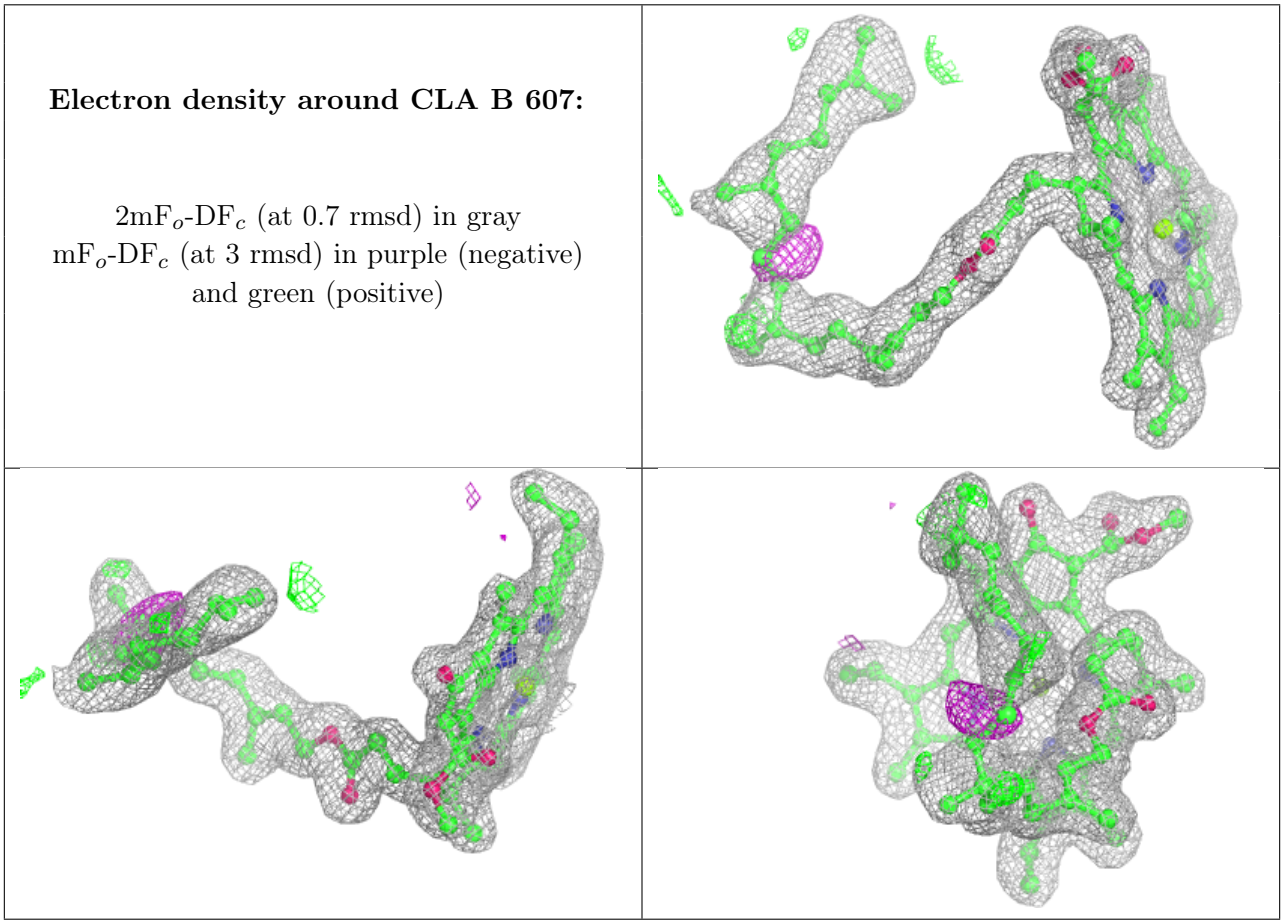
Electron density around CLA c 511:

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



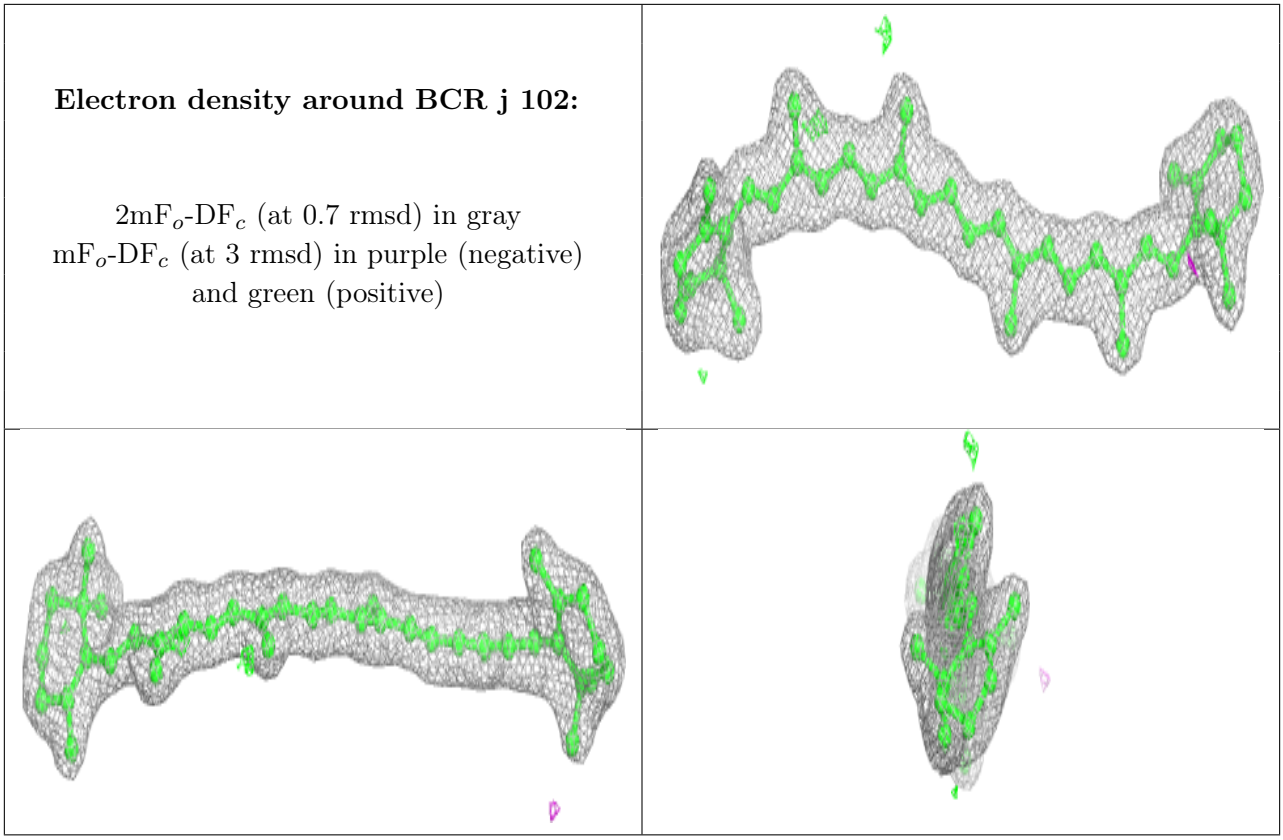
Electron density around CLA B 607:

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



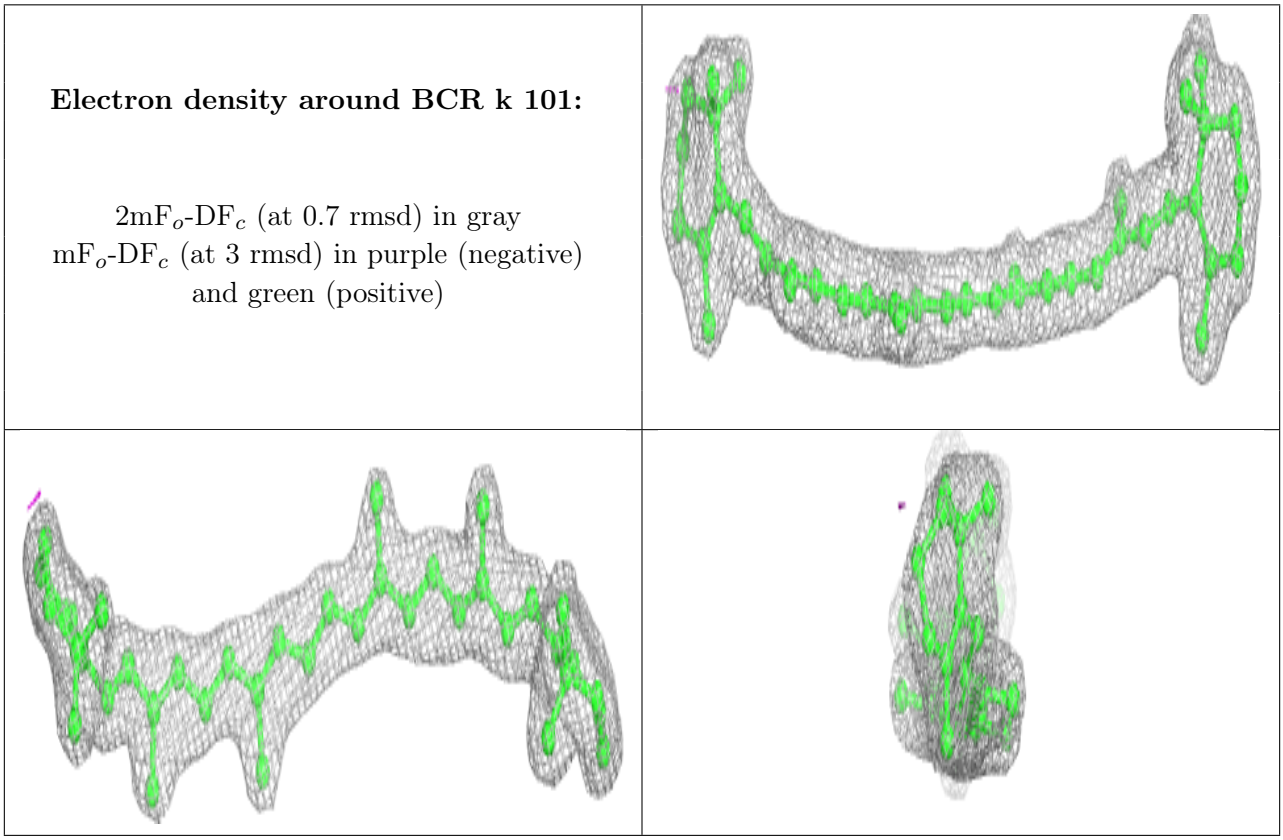
Electron density around BCR j 102:

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



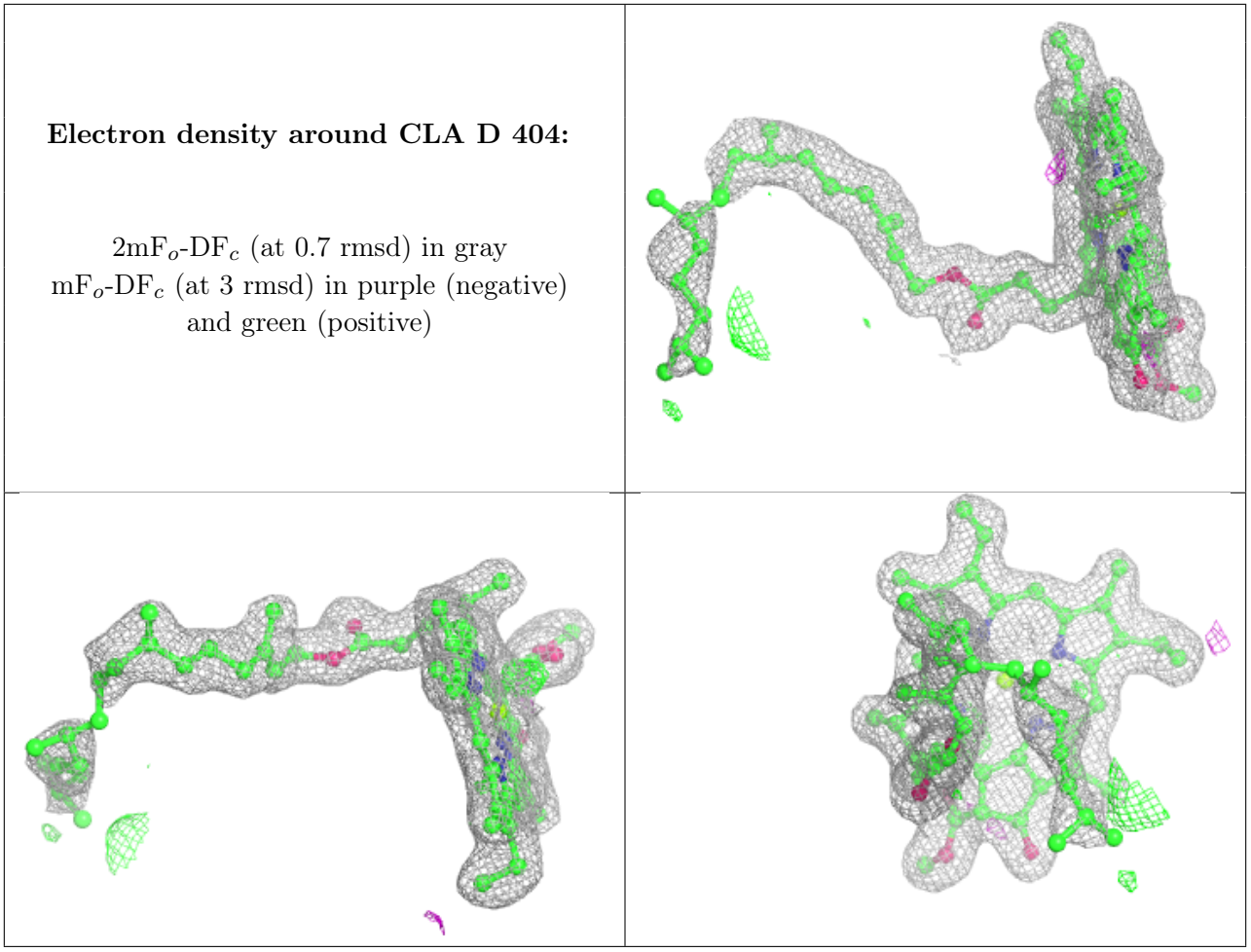
Electron density around BCR k 101:

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



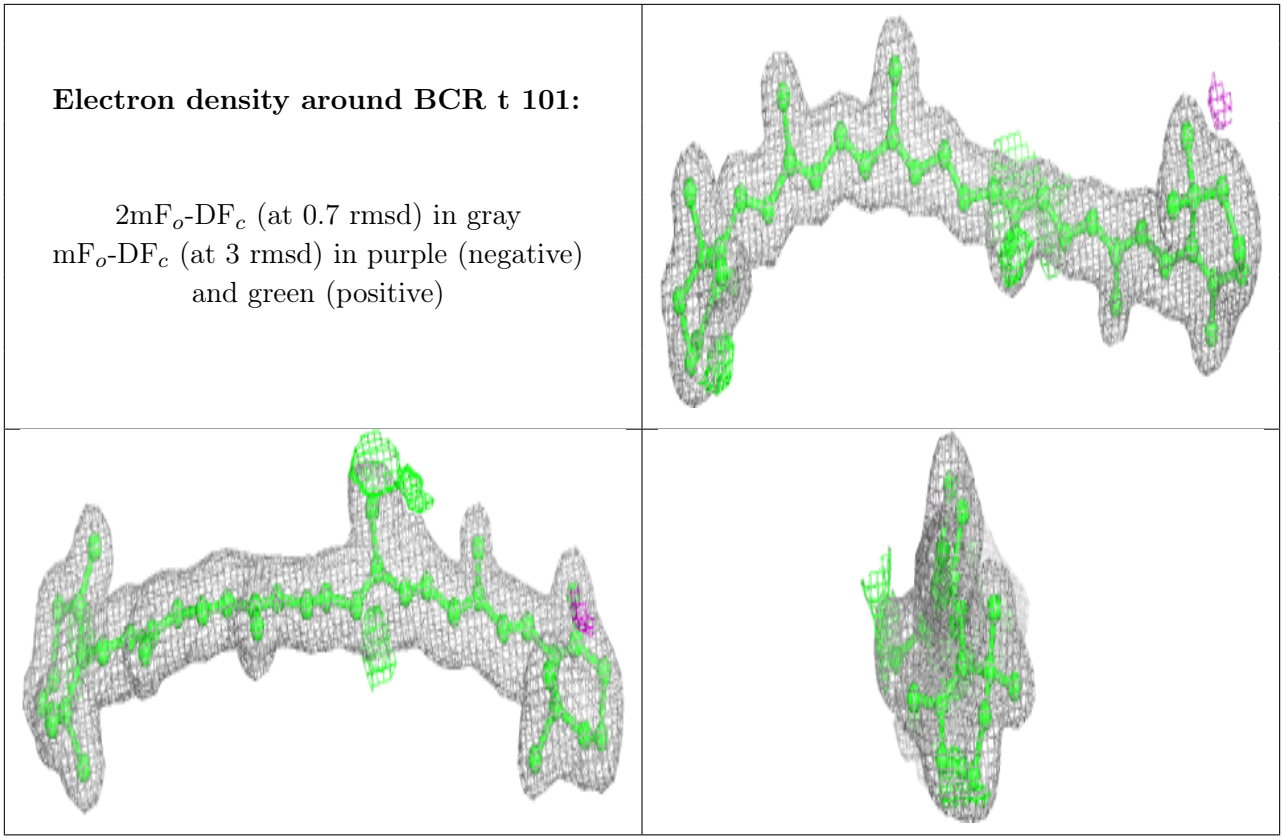
Electron density around CLA D 404:

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



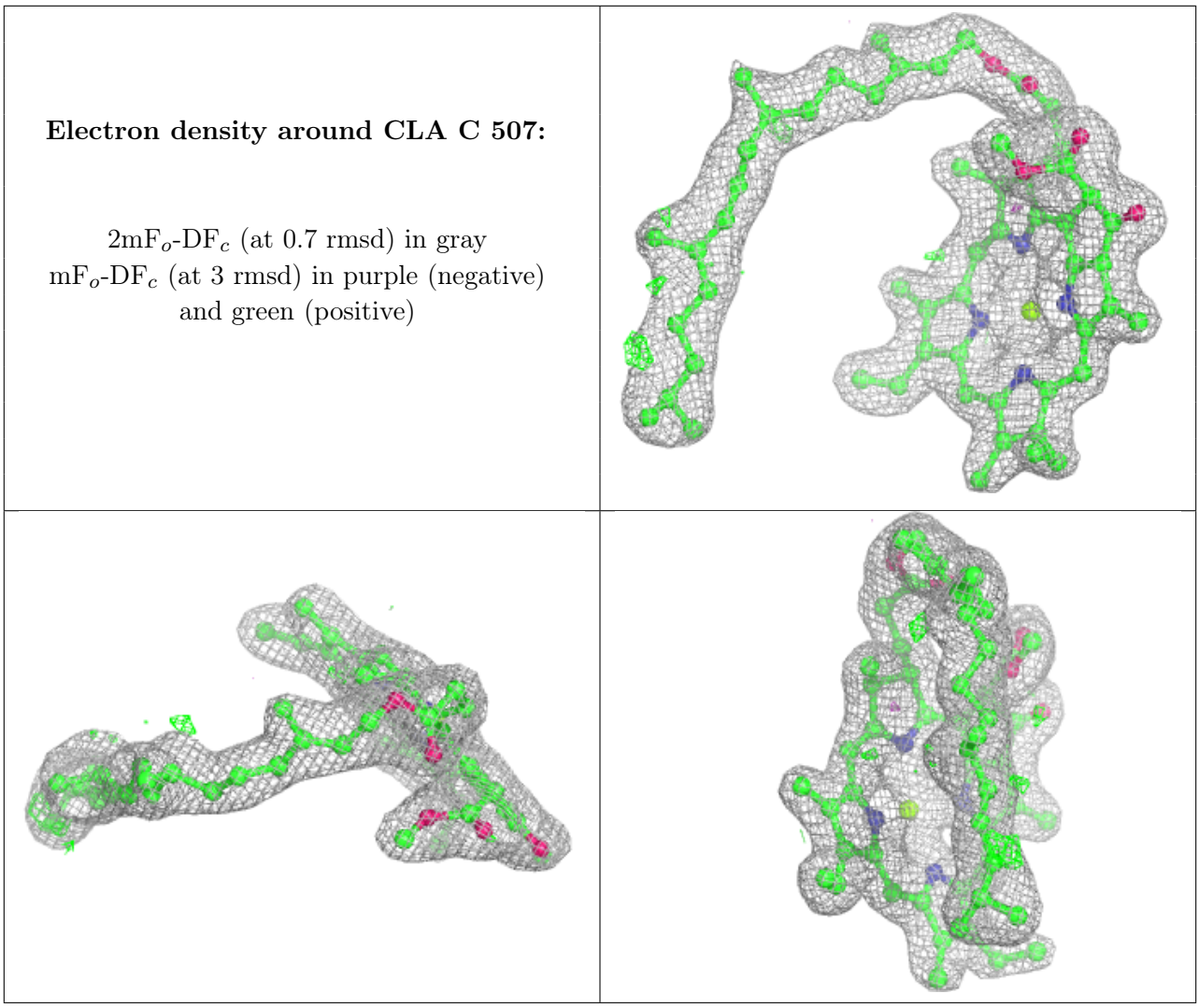
Electron density around BCR t 101:

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



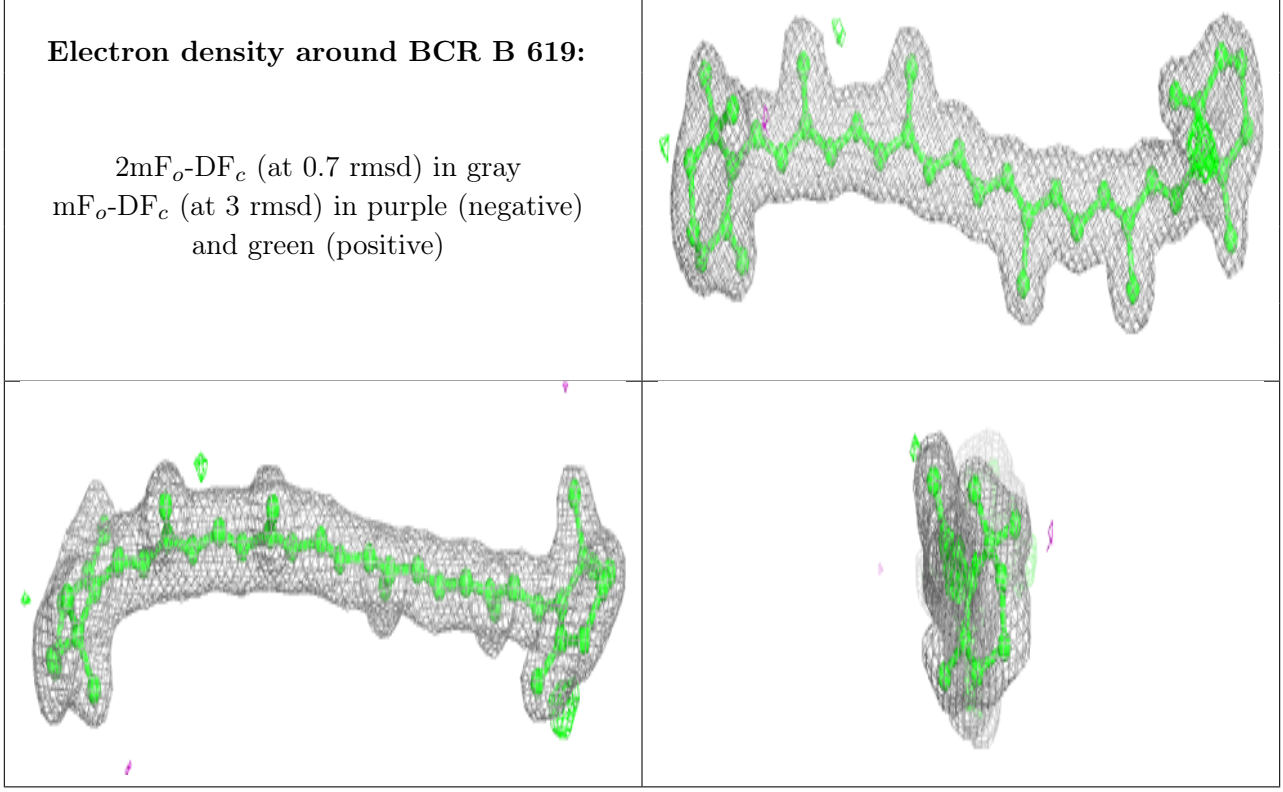
Electron density around CLA C 507:

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



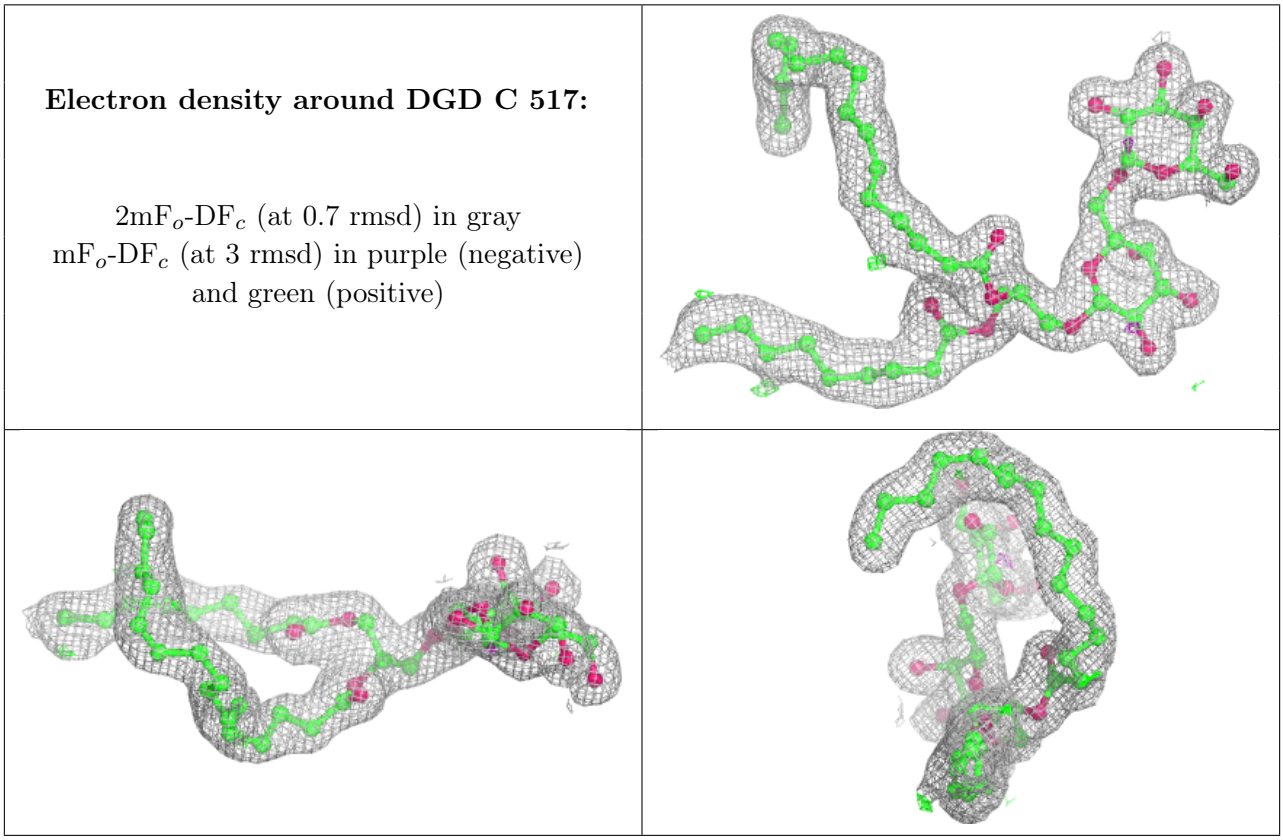
Electron density around BCR B 619:

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



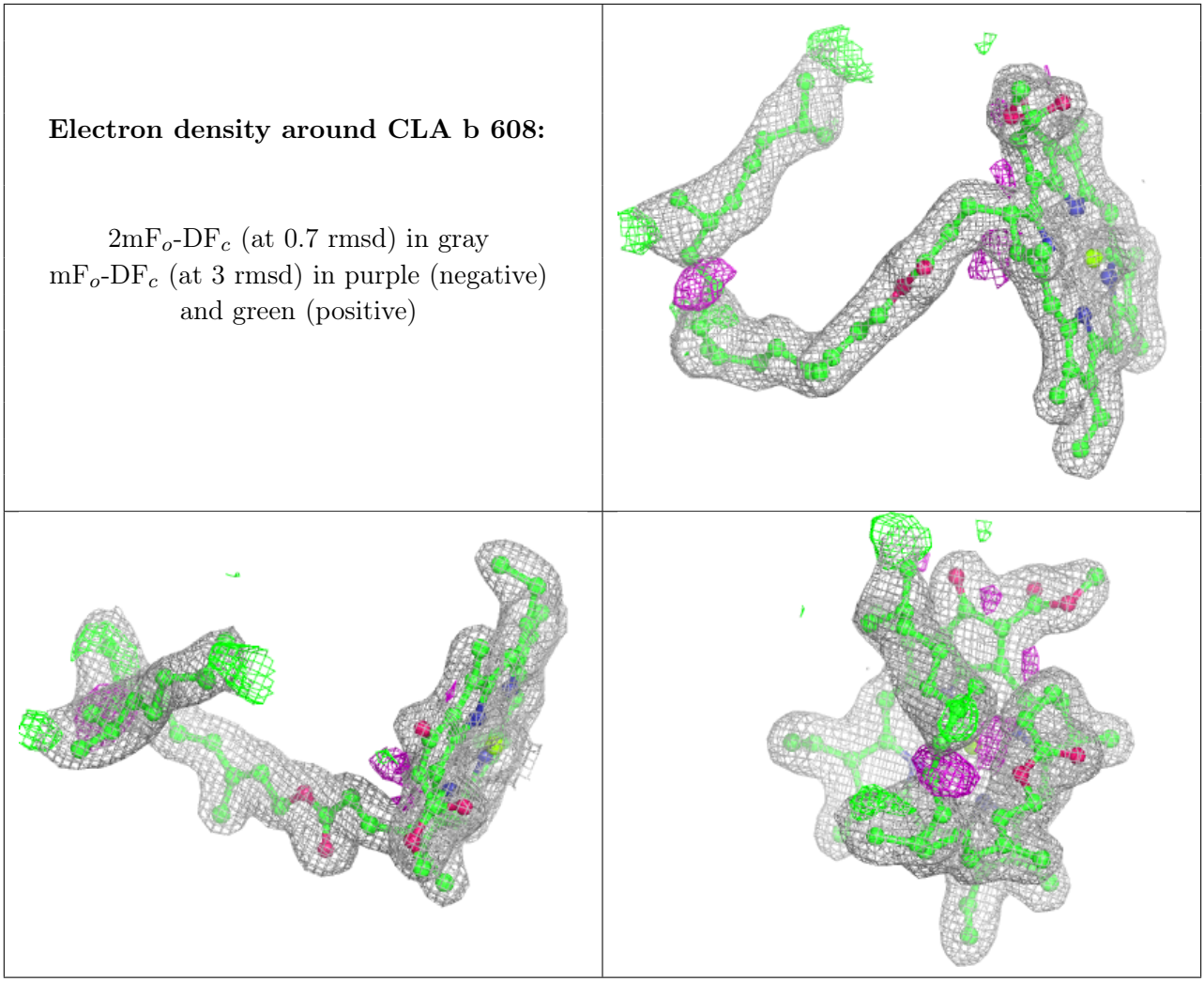
Electron density around DGD C 517:

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



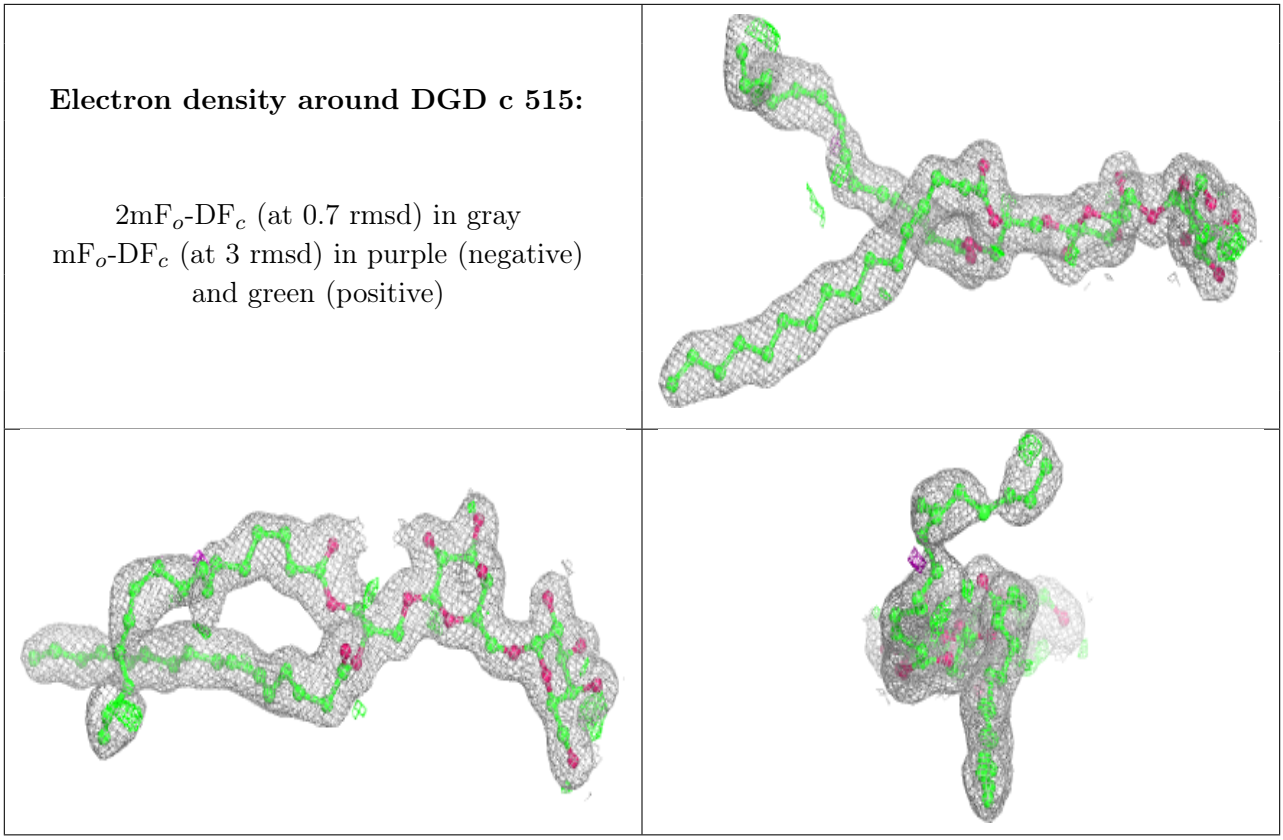
Electron density around CLA b 608:

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



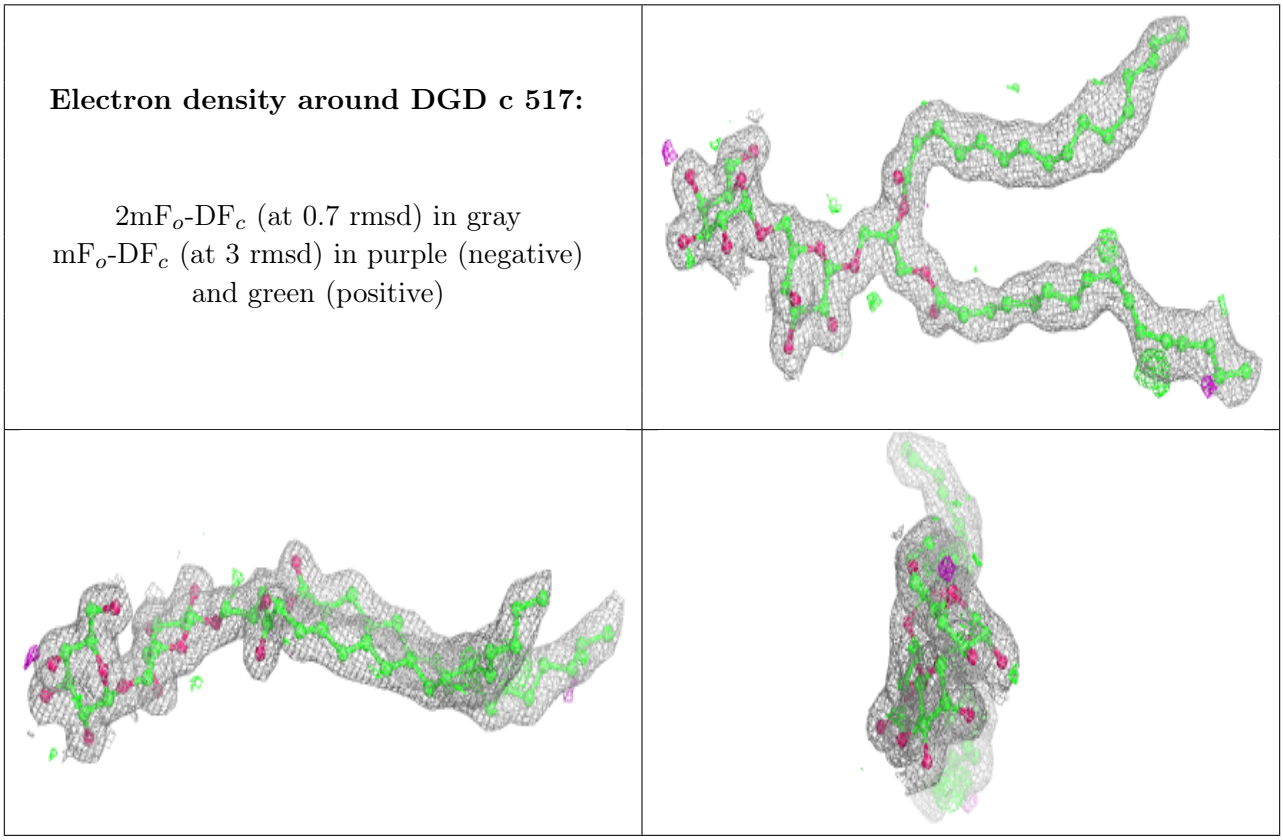
Electron density around DGD c 515:

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



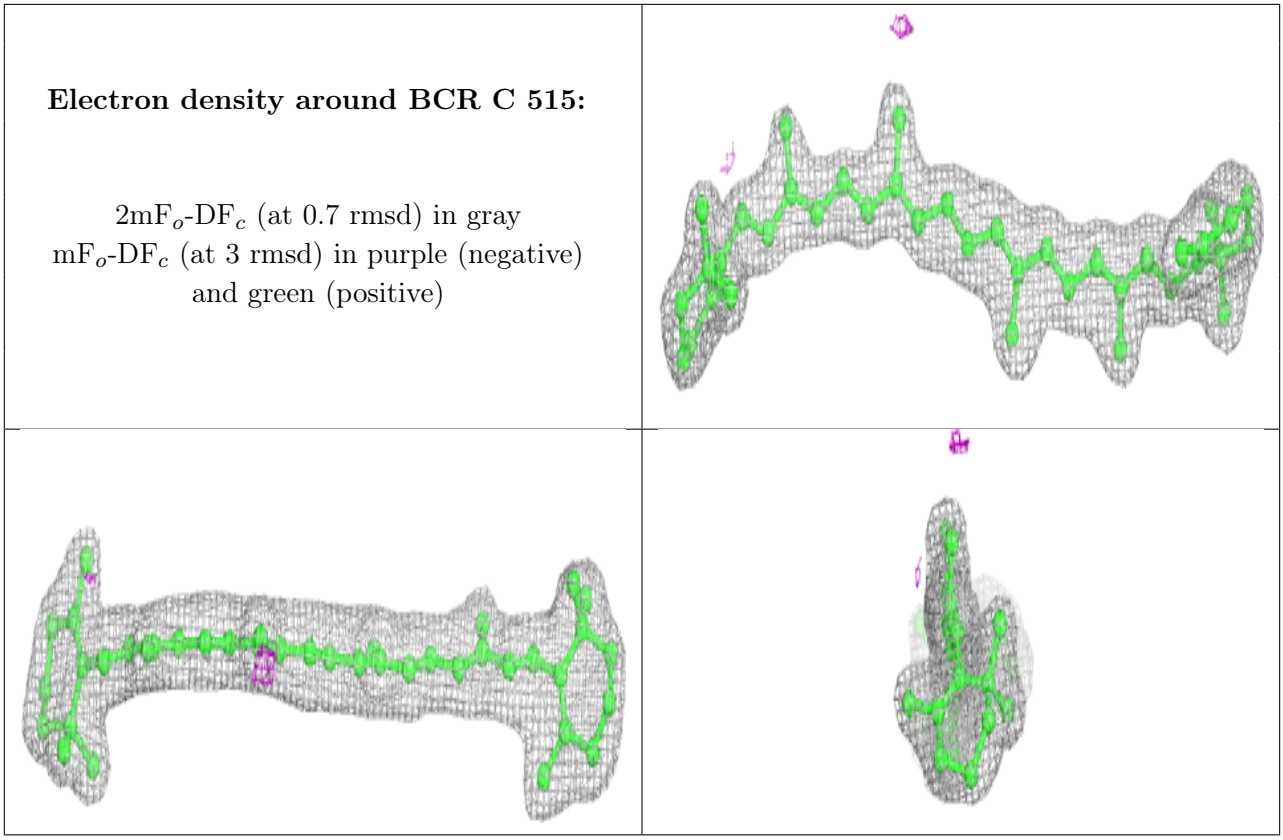
Electron density around DGD c 517:

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



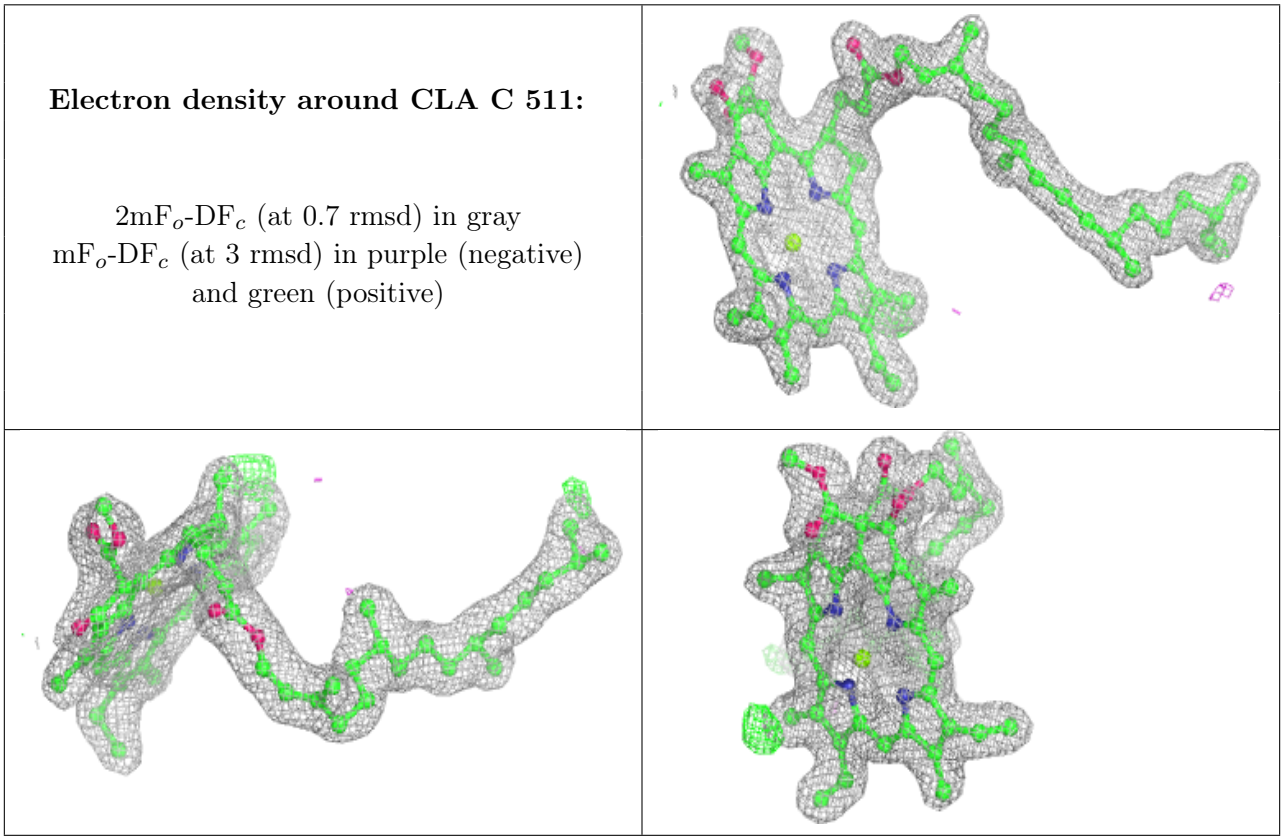
Electron density around BCR C 515:

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



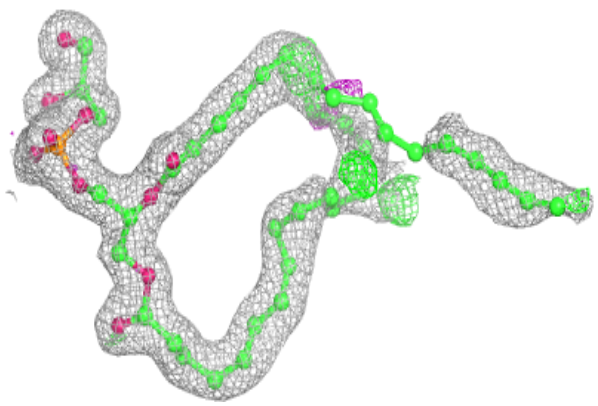
Electron density around CLA C 511:

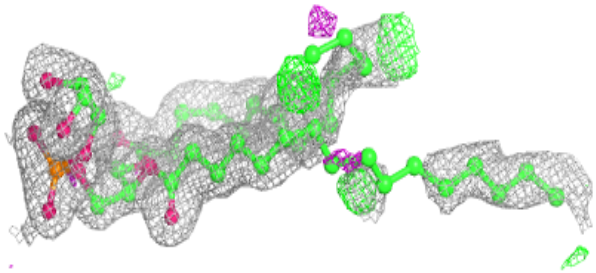
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

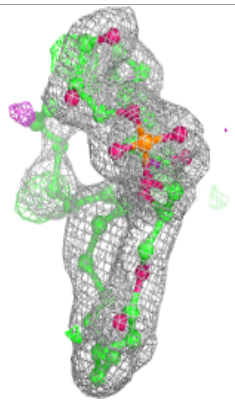


Electron density around LHG D 409:

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

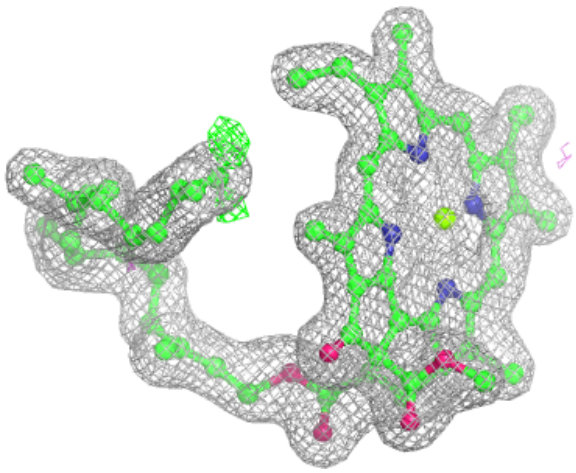


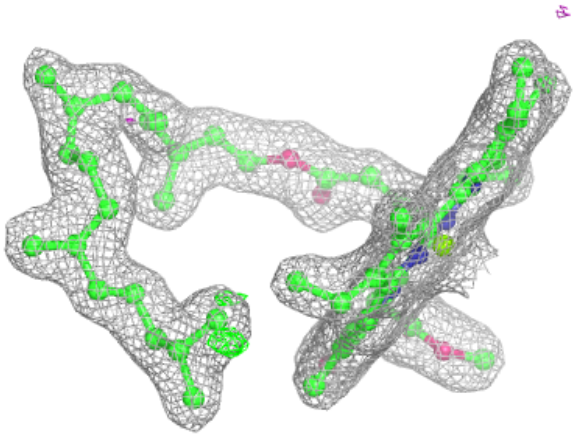


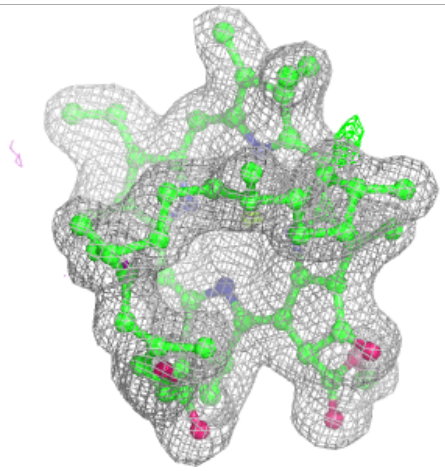


Electron density around CLA C 503:

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

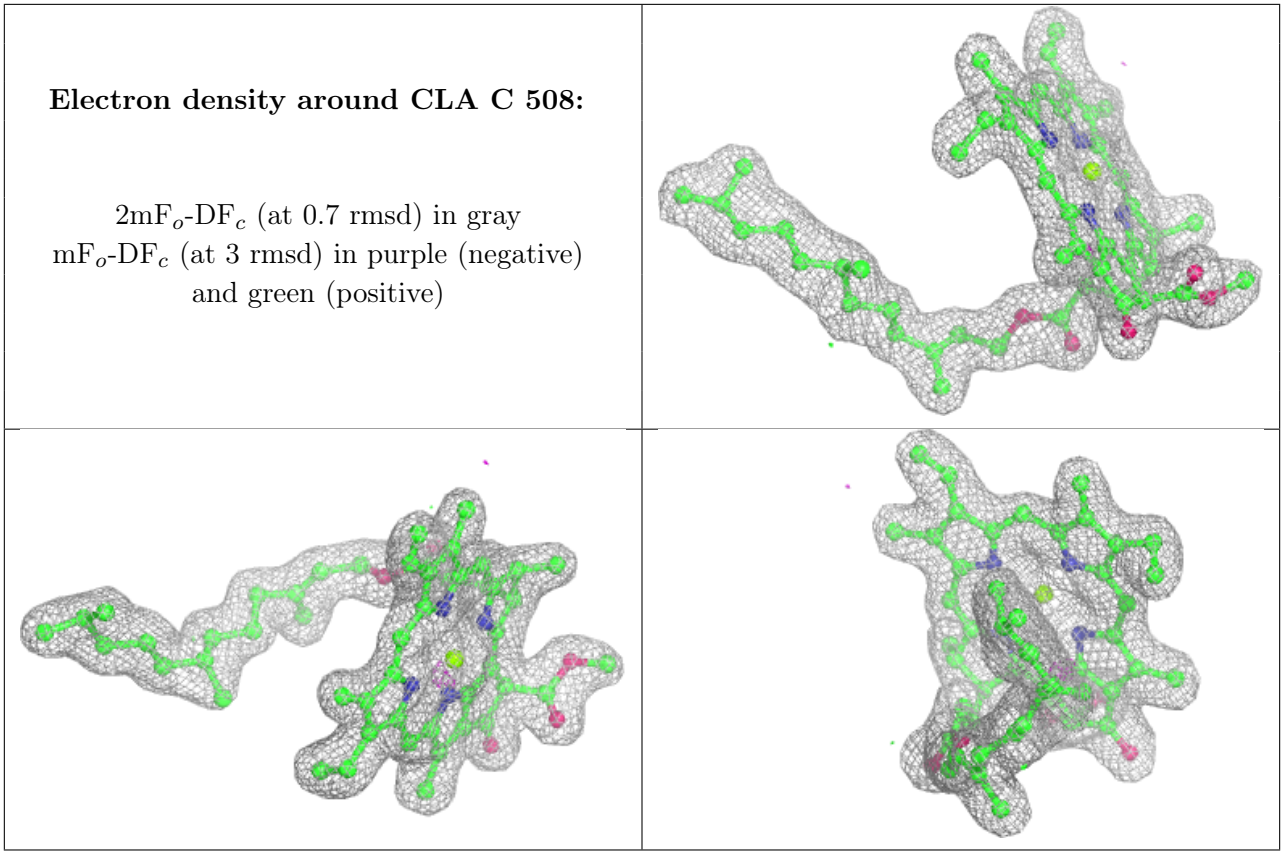






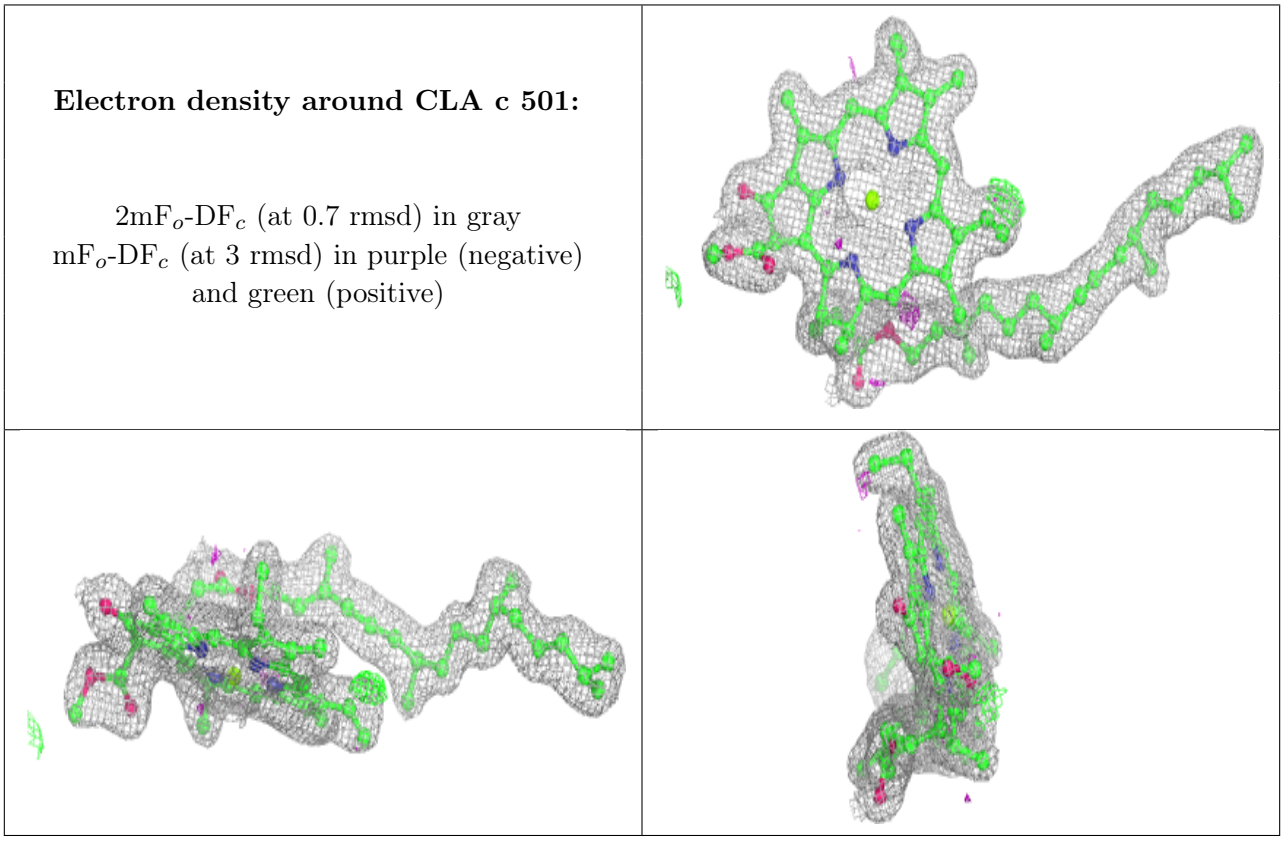
Electron density around CLA C 508:

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



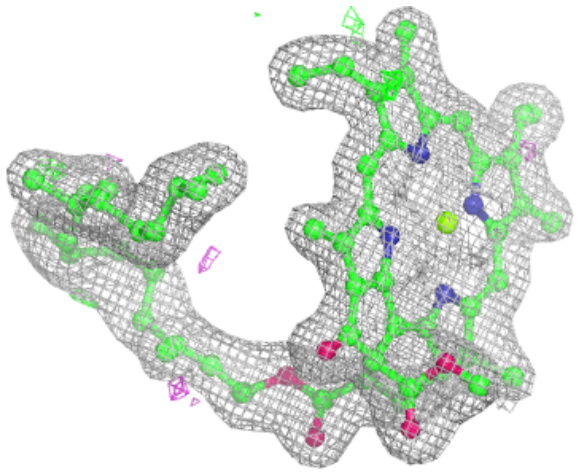
Electron density around CLA c 501:

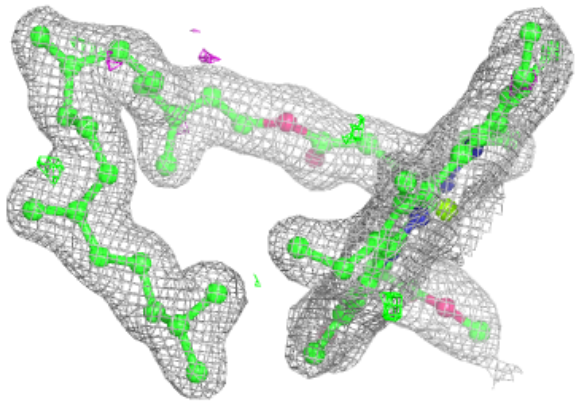
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

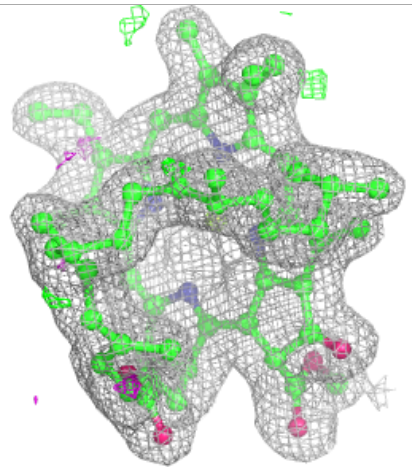


Electron density around CLA c 503:

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

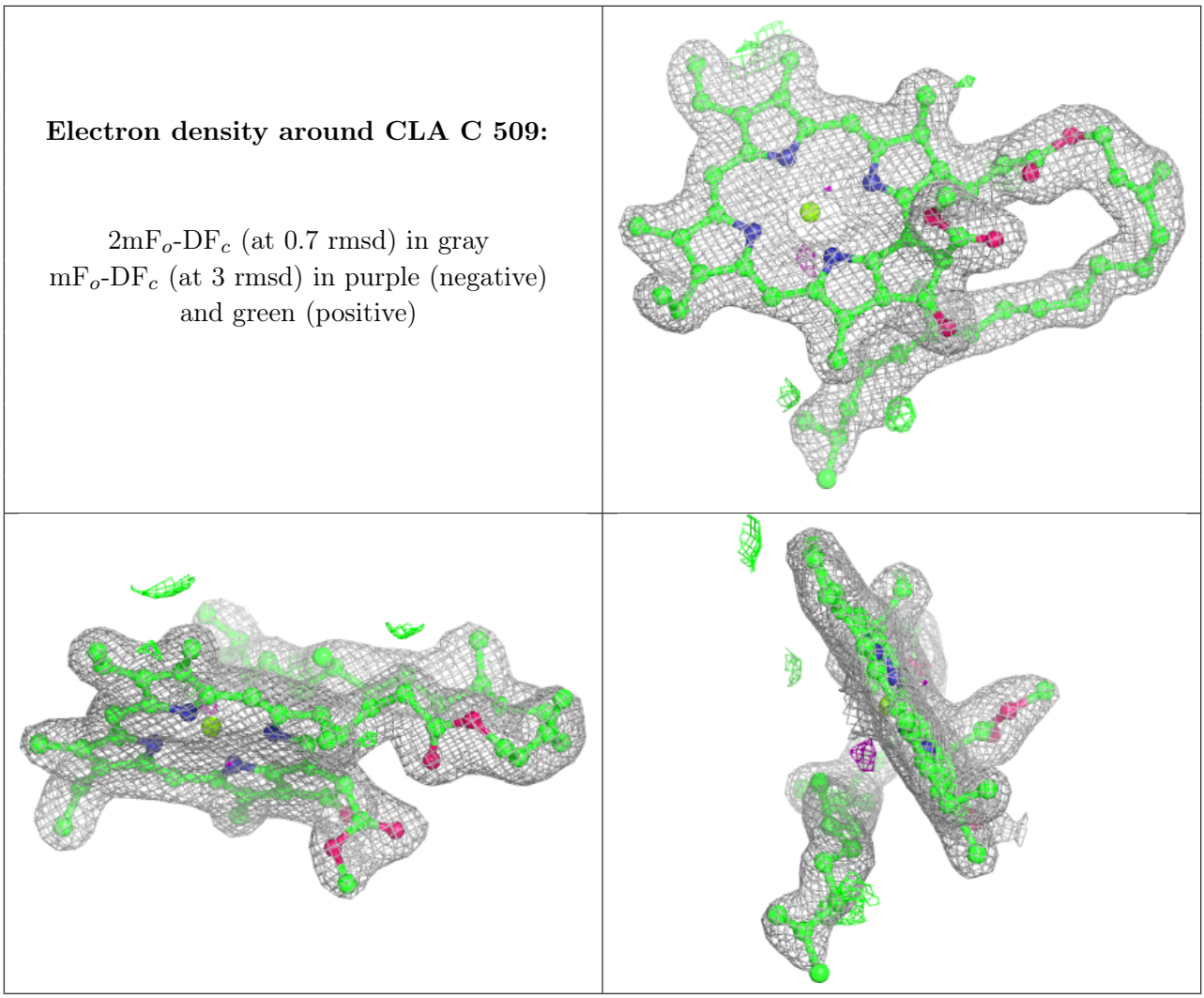






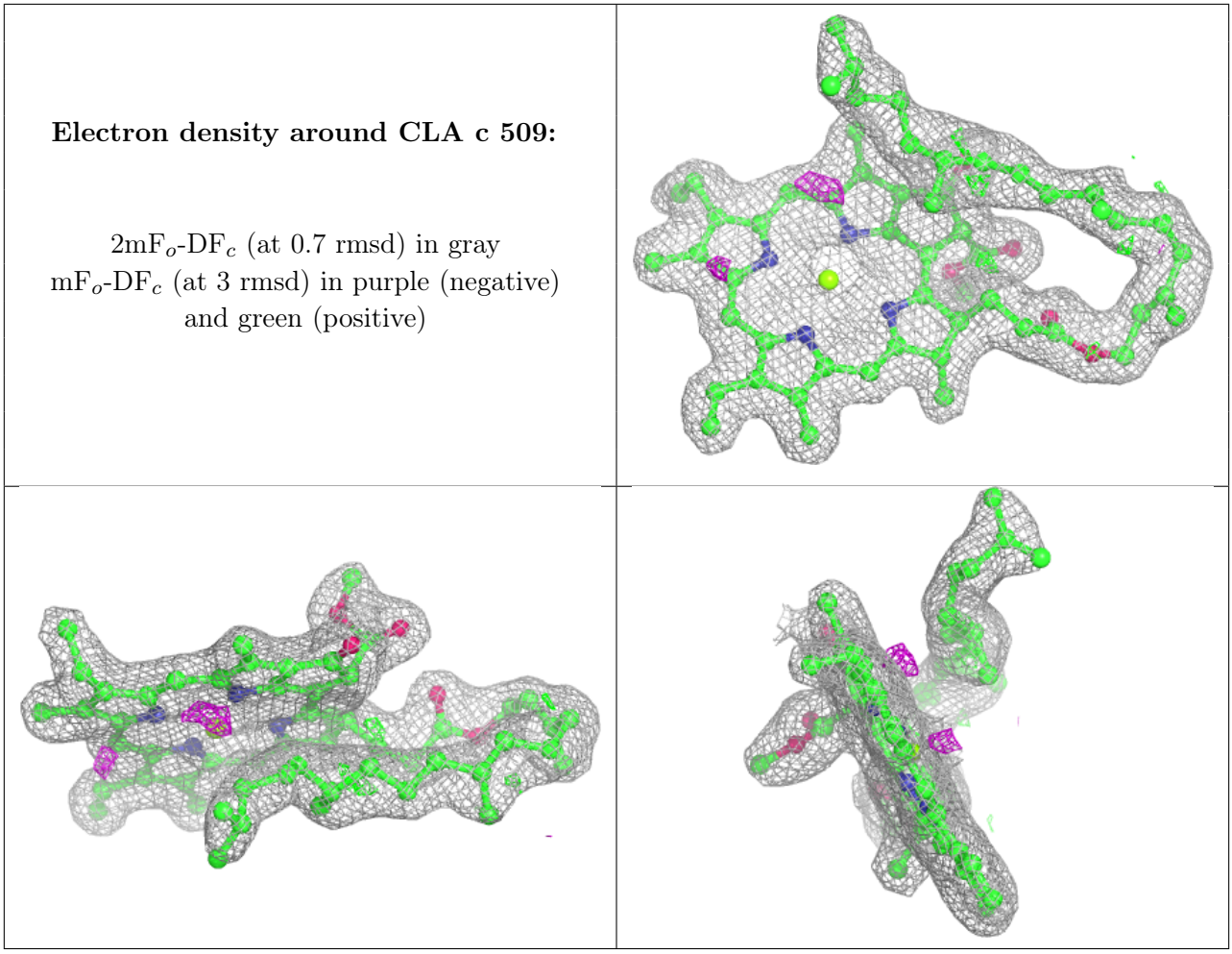
Electron density around CLA C 509:

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



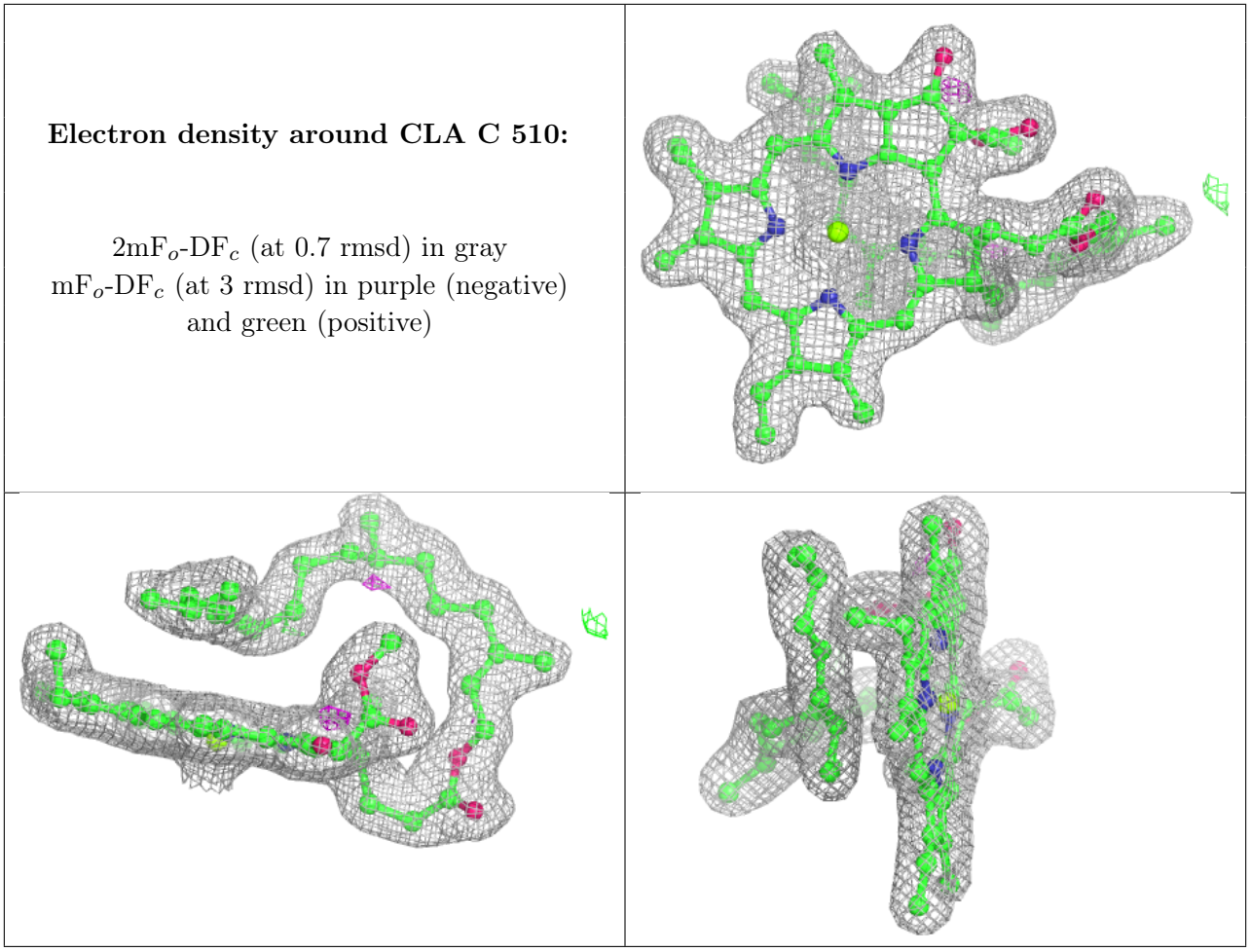
Electron density around CLA c 509:

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



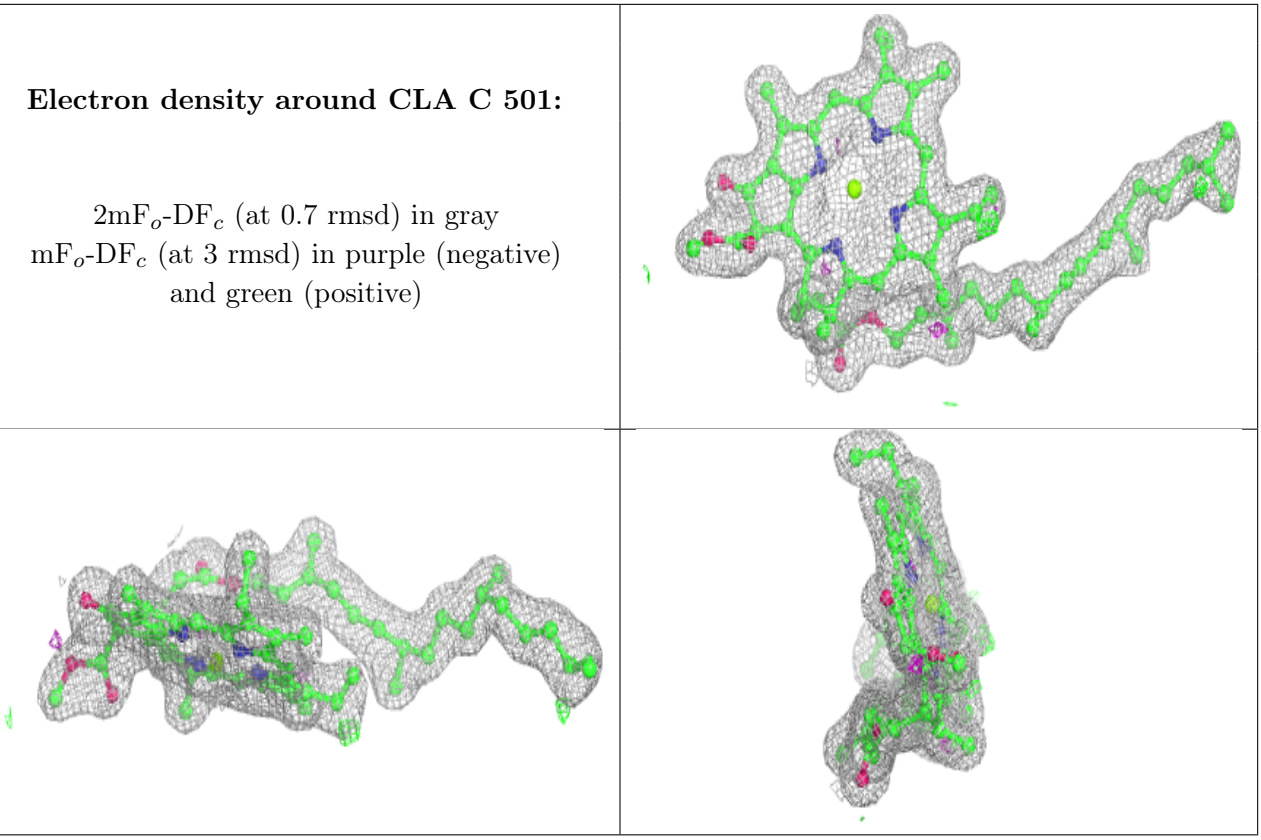
Electron density around CLA C 510:

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



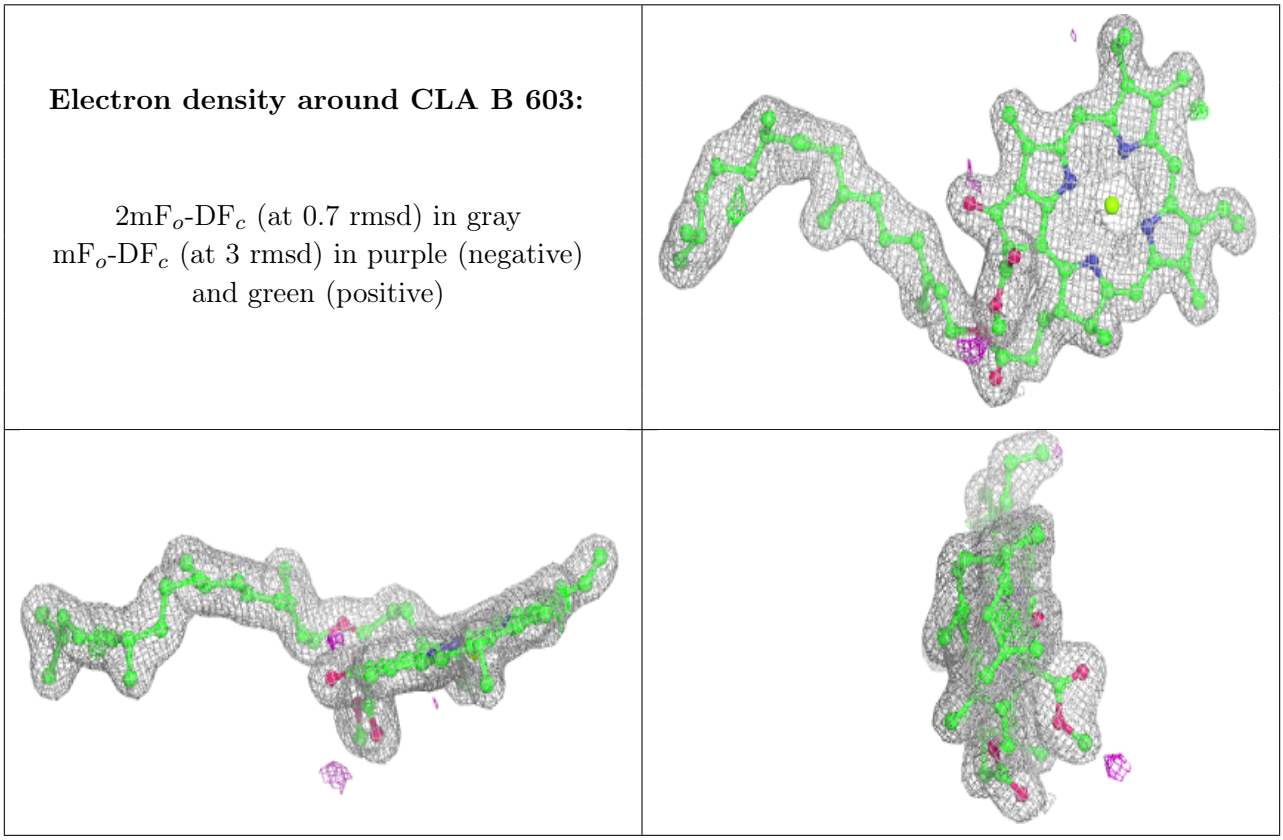
Electron density around CLA C 501:

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



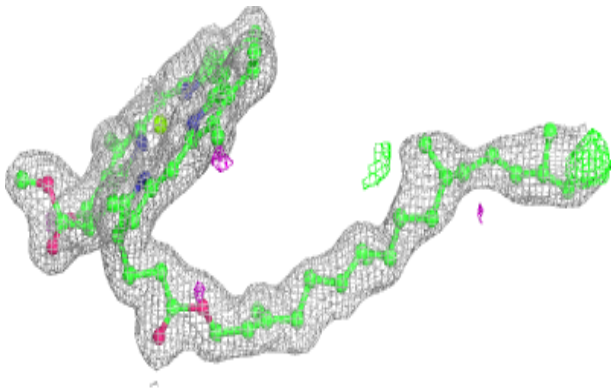
Electron density around CLA B 603:

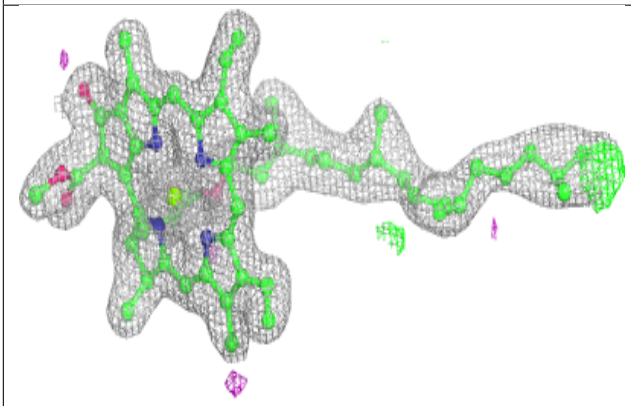
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 504:

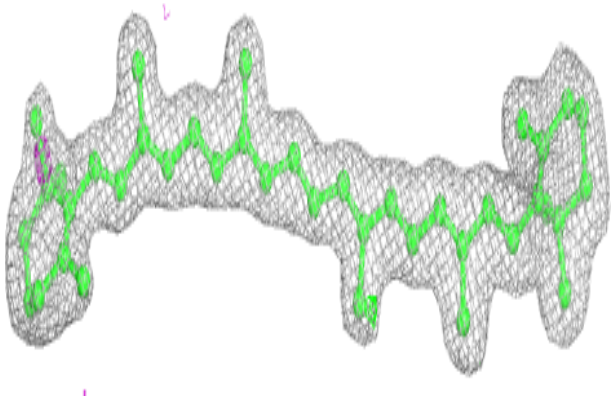
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

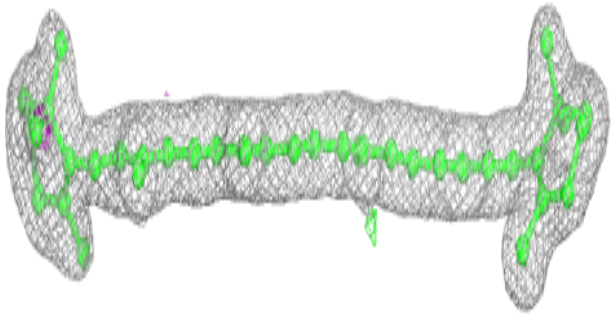


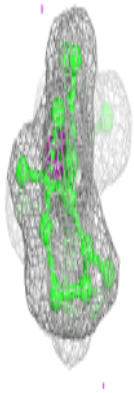


Electron density around BCR B 618:

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

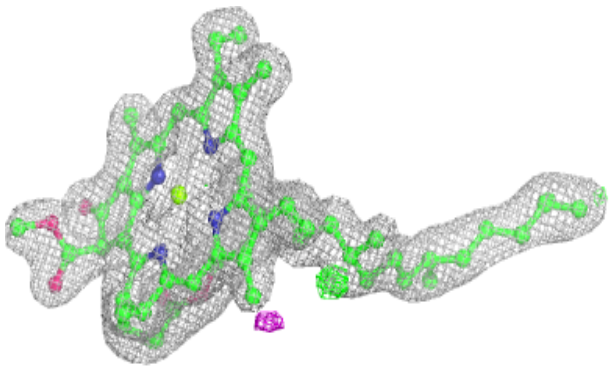


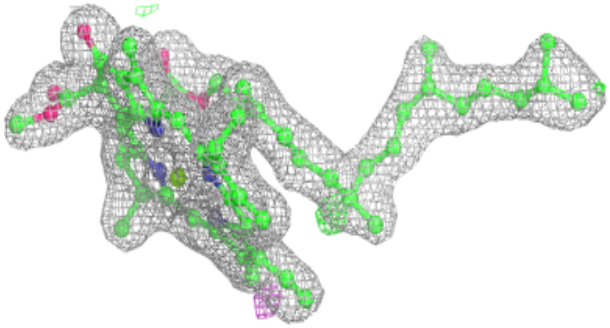


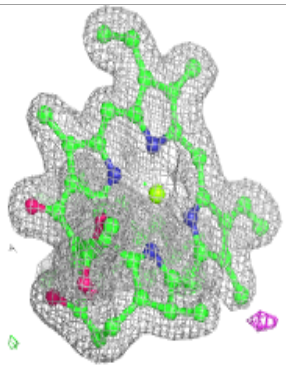


Electron density around CLA C 505:

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

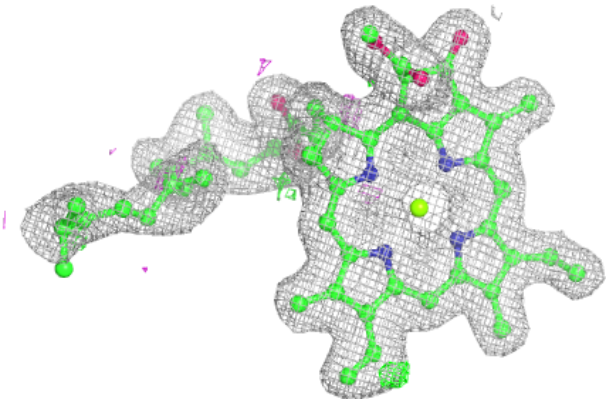


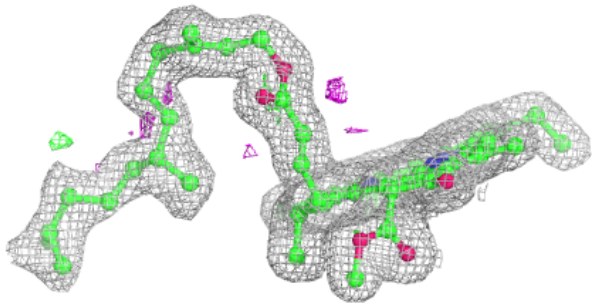


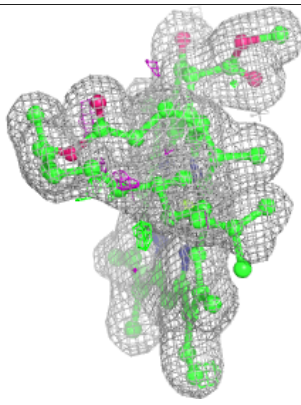


Electron density around CLA a 404:

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

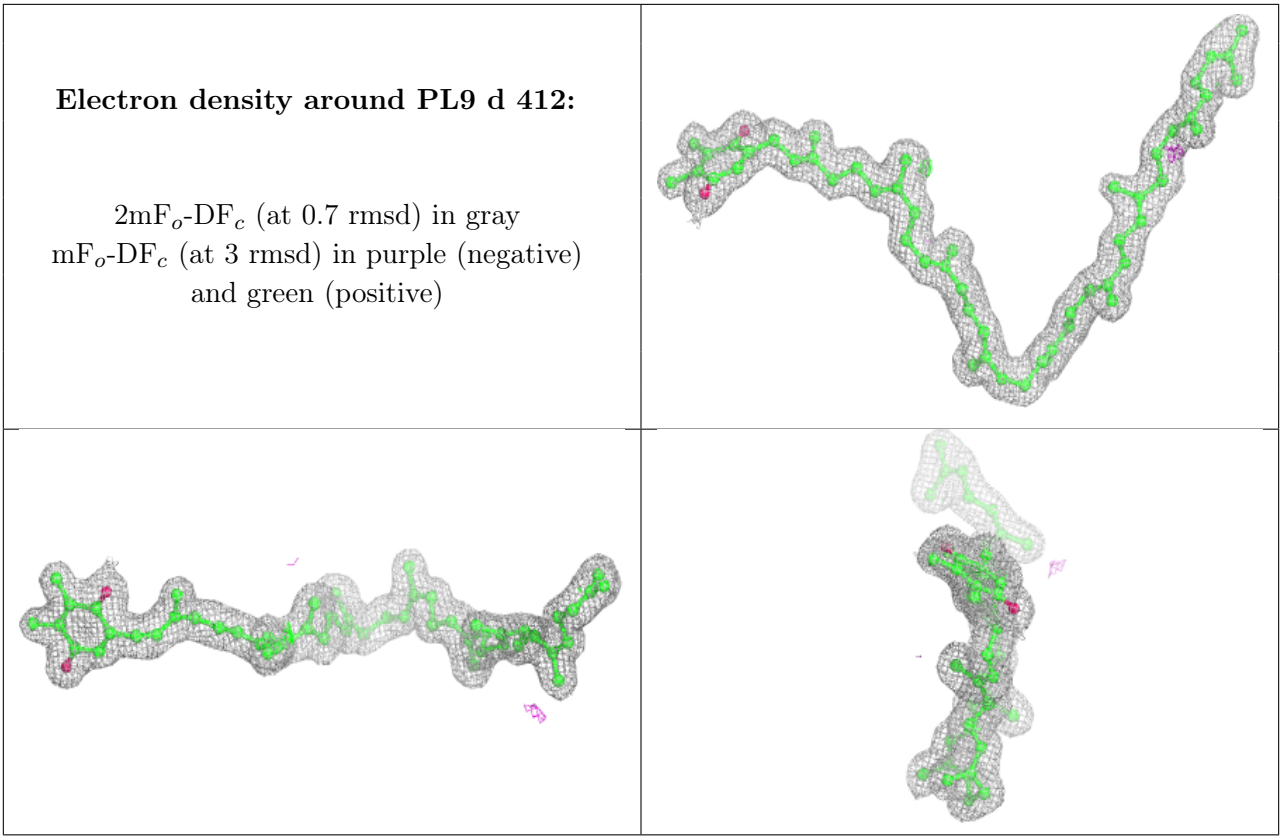






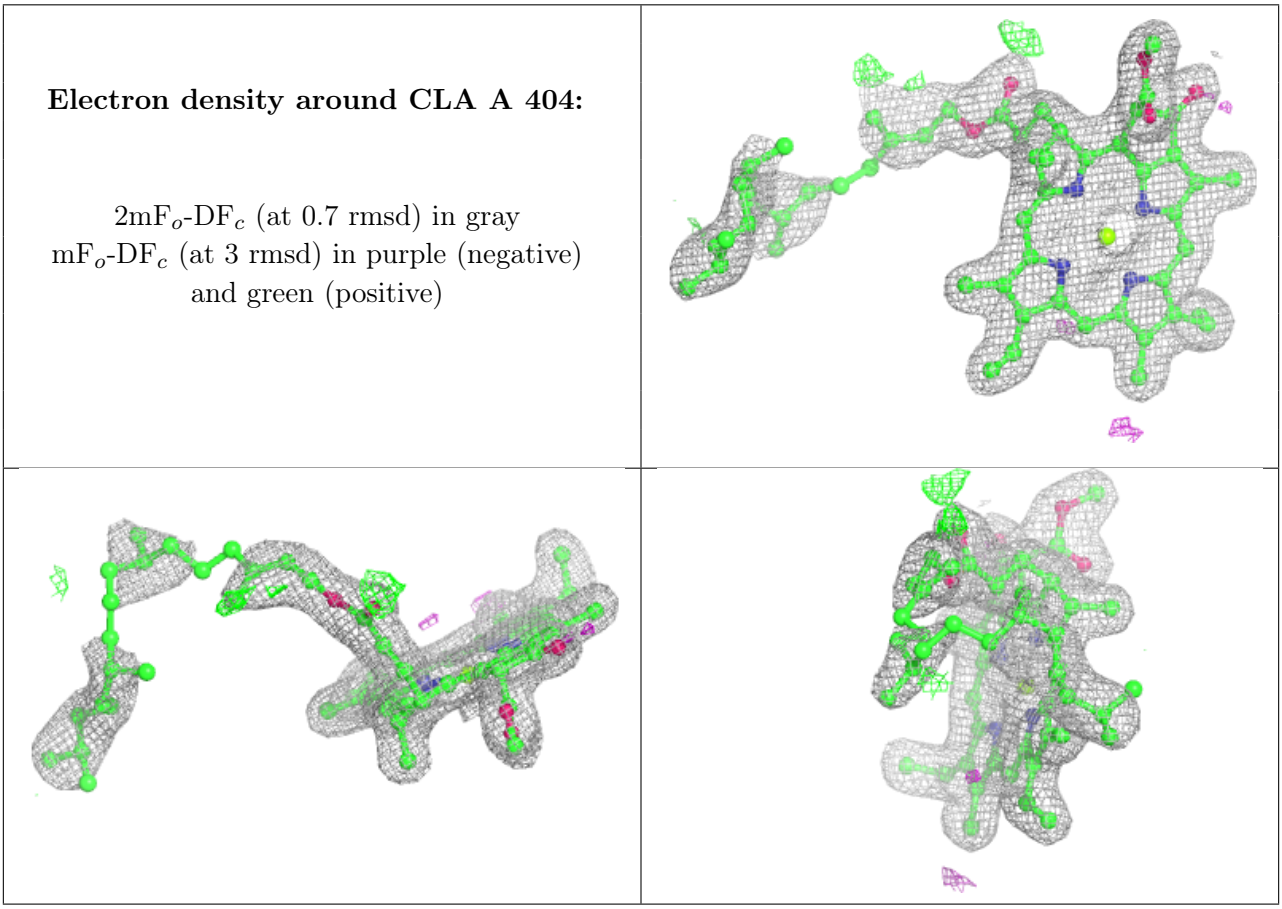
Electron density around PL9 d 412:

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



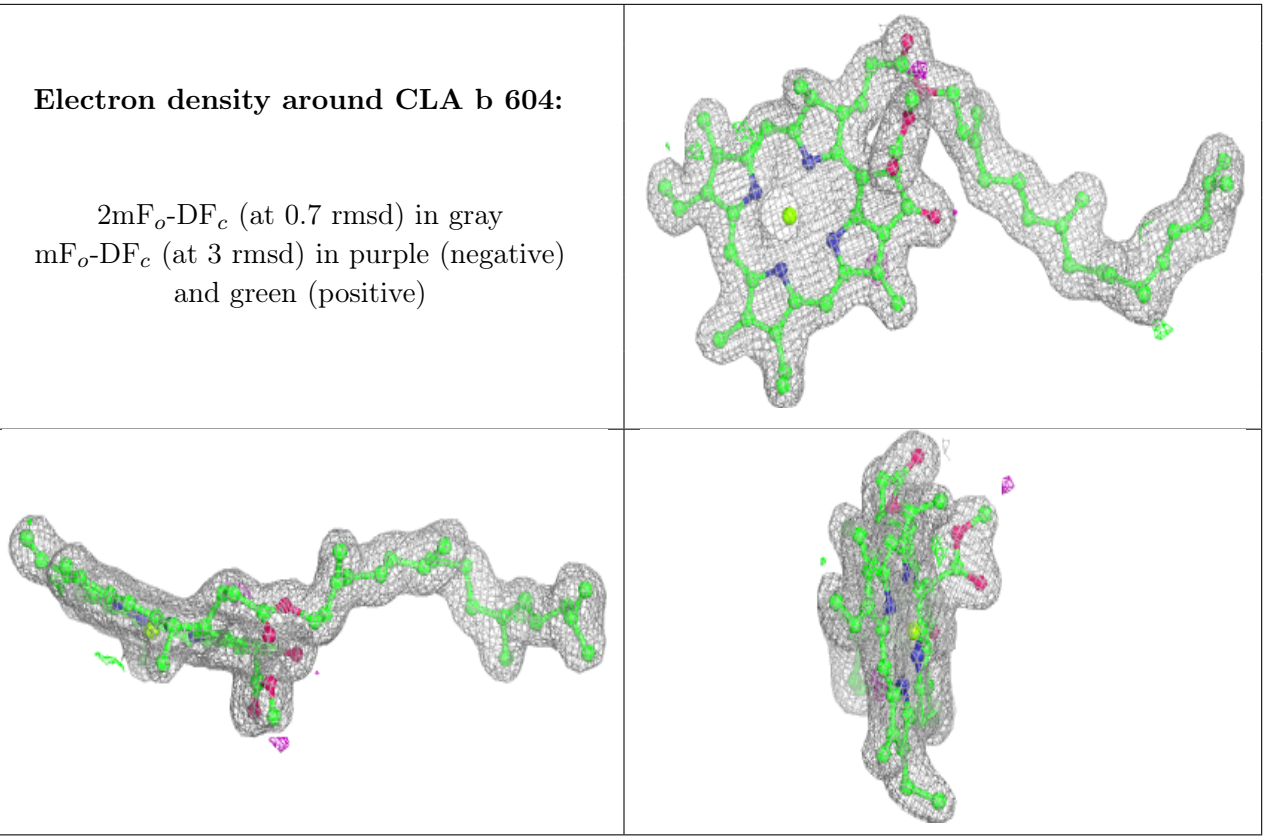
Electron density around CLA A 404:

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



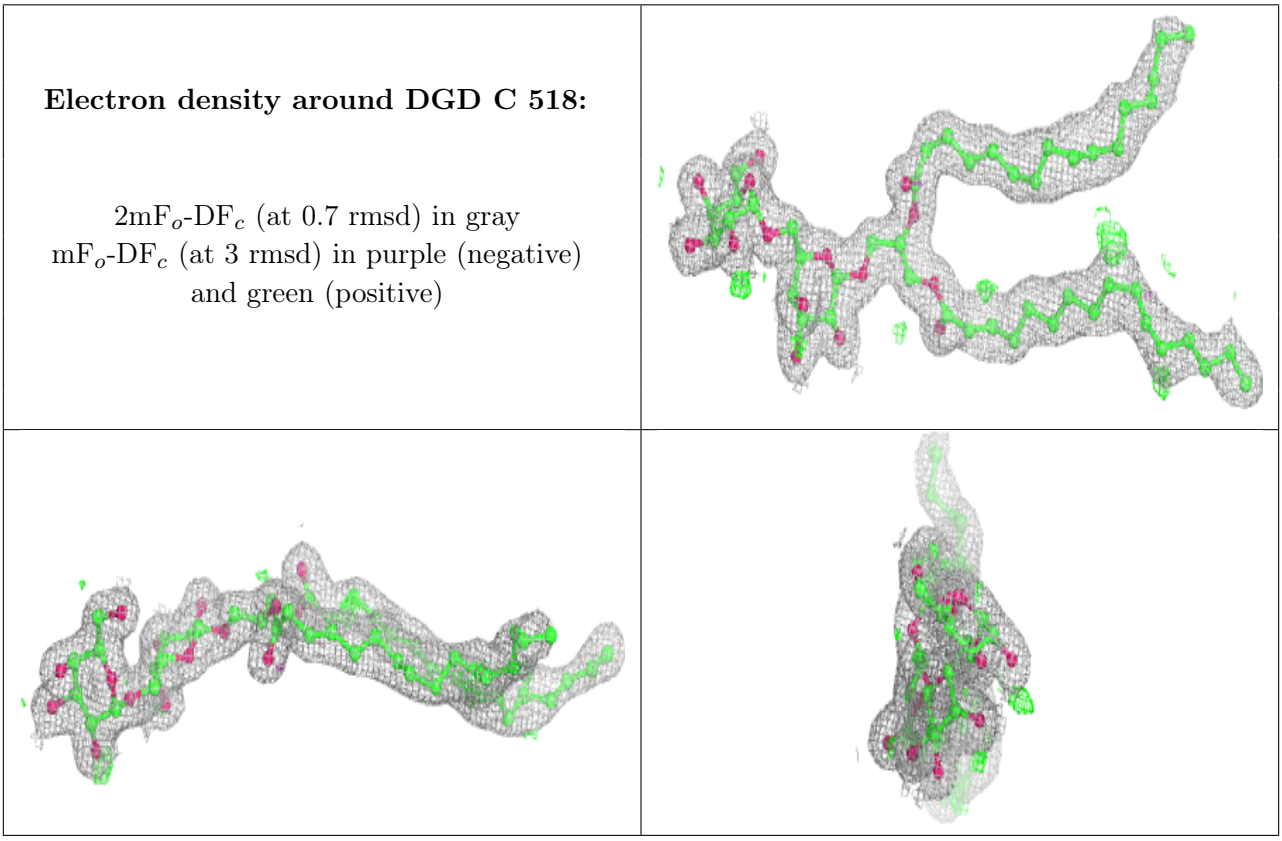
Electron density around CLA b 604:

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



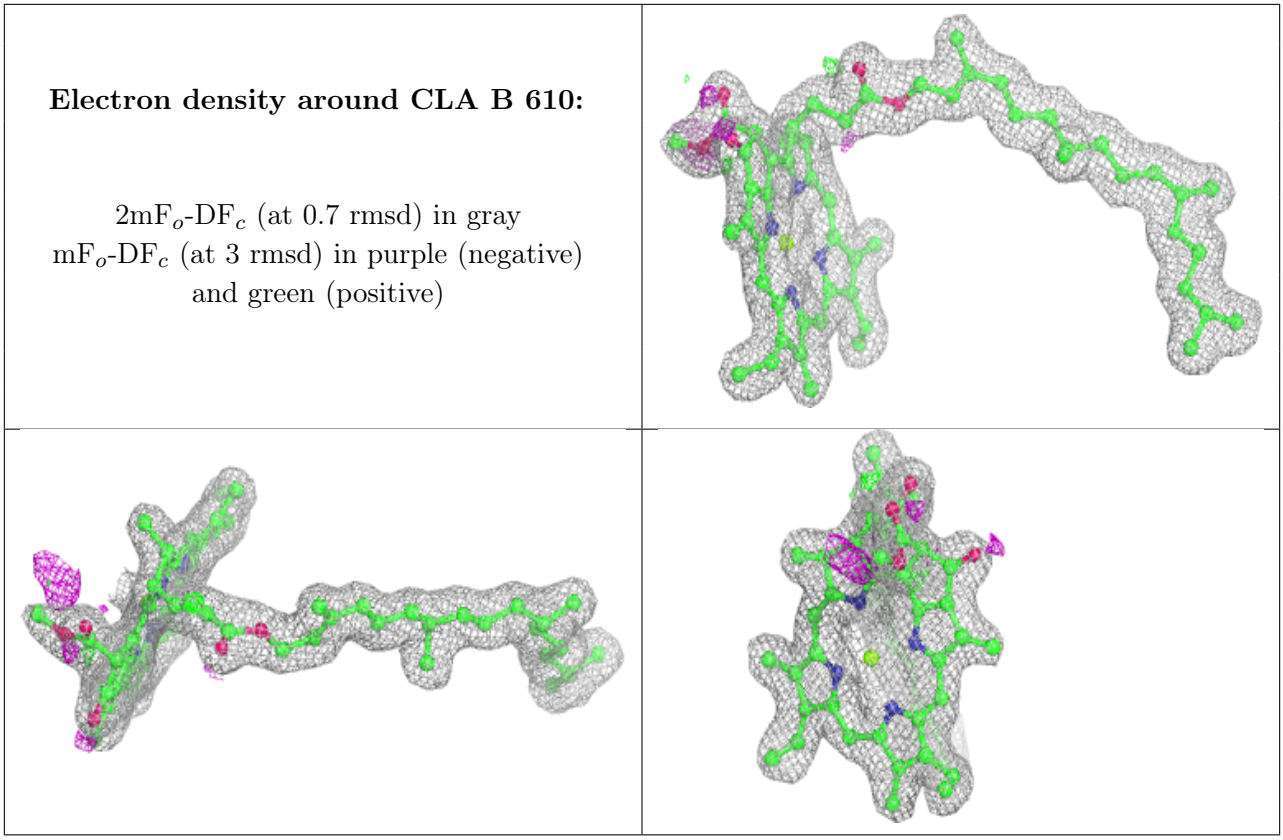
Electron density around DGD C 518:

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



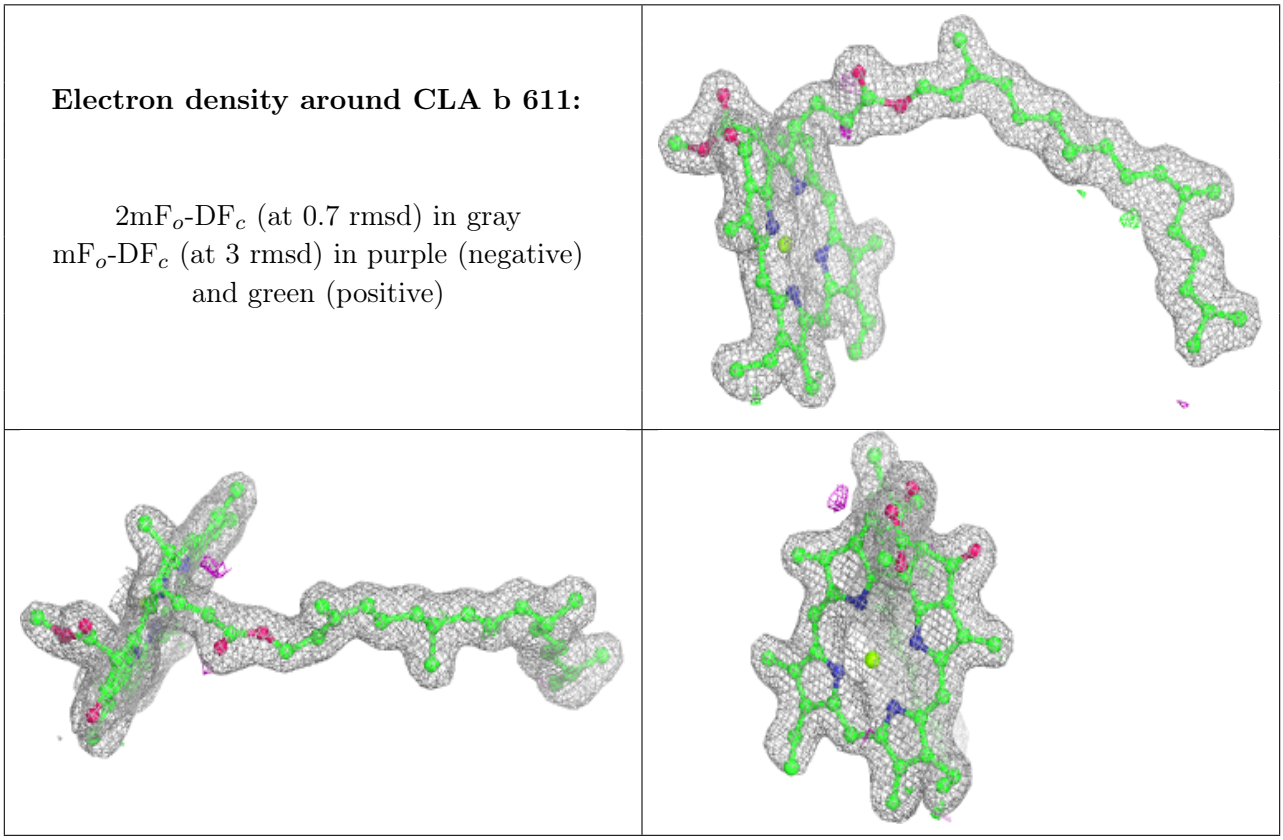
Electron density around CLA B 610:

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



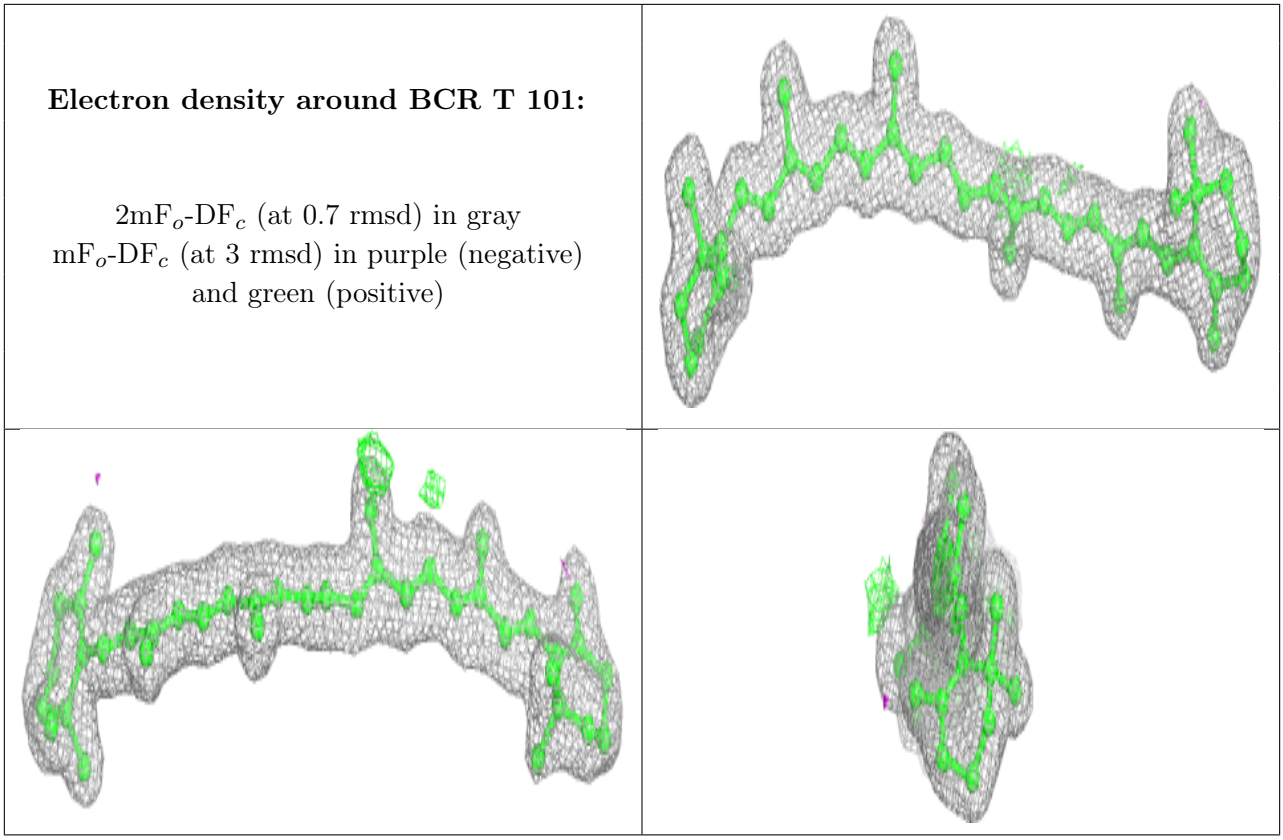
Electron density around CLA b 611:

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



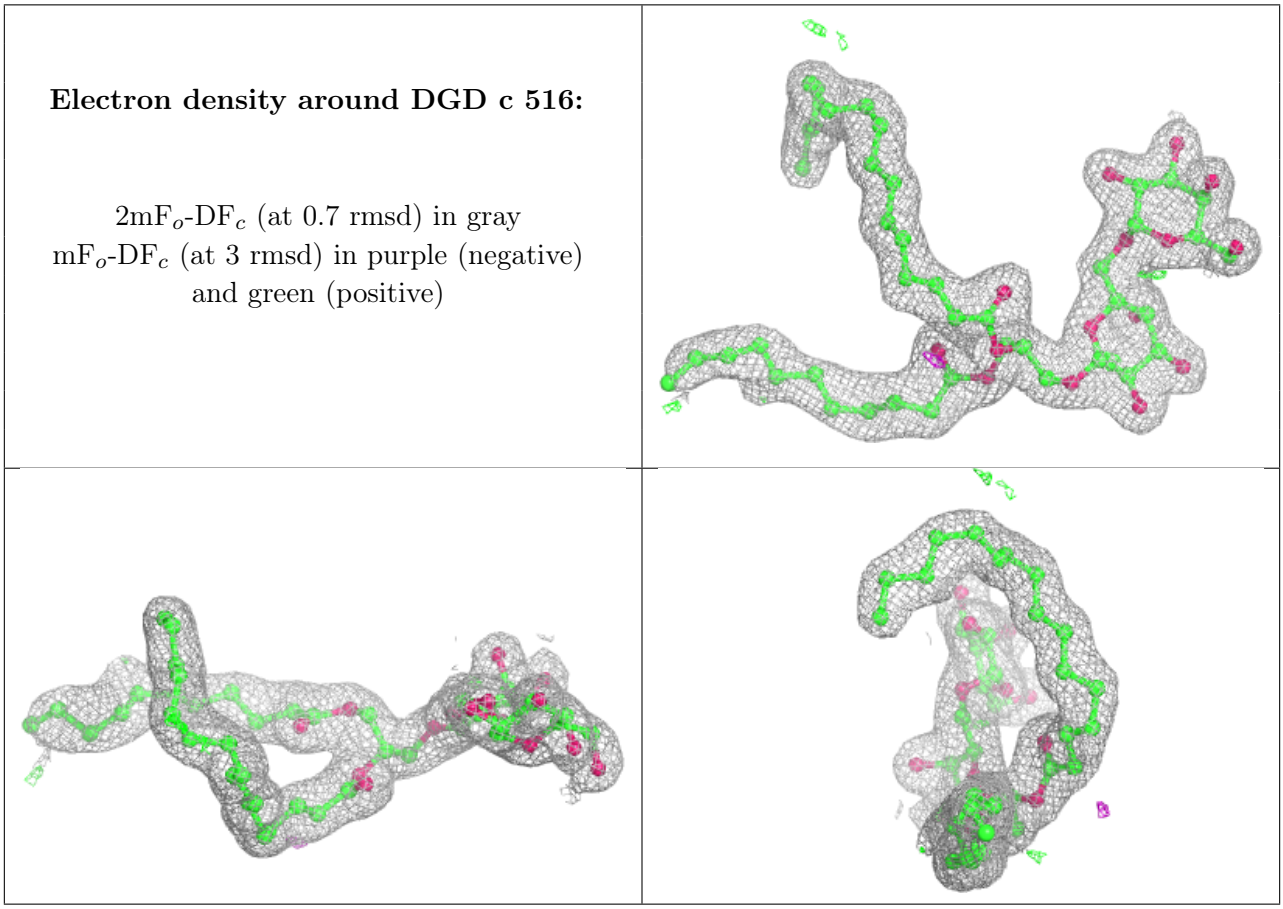
Electron density around BCR T 101:

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



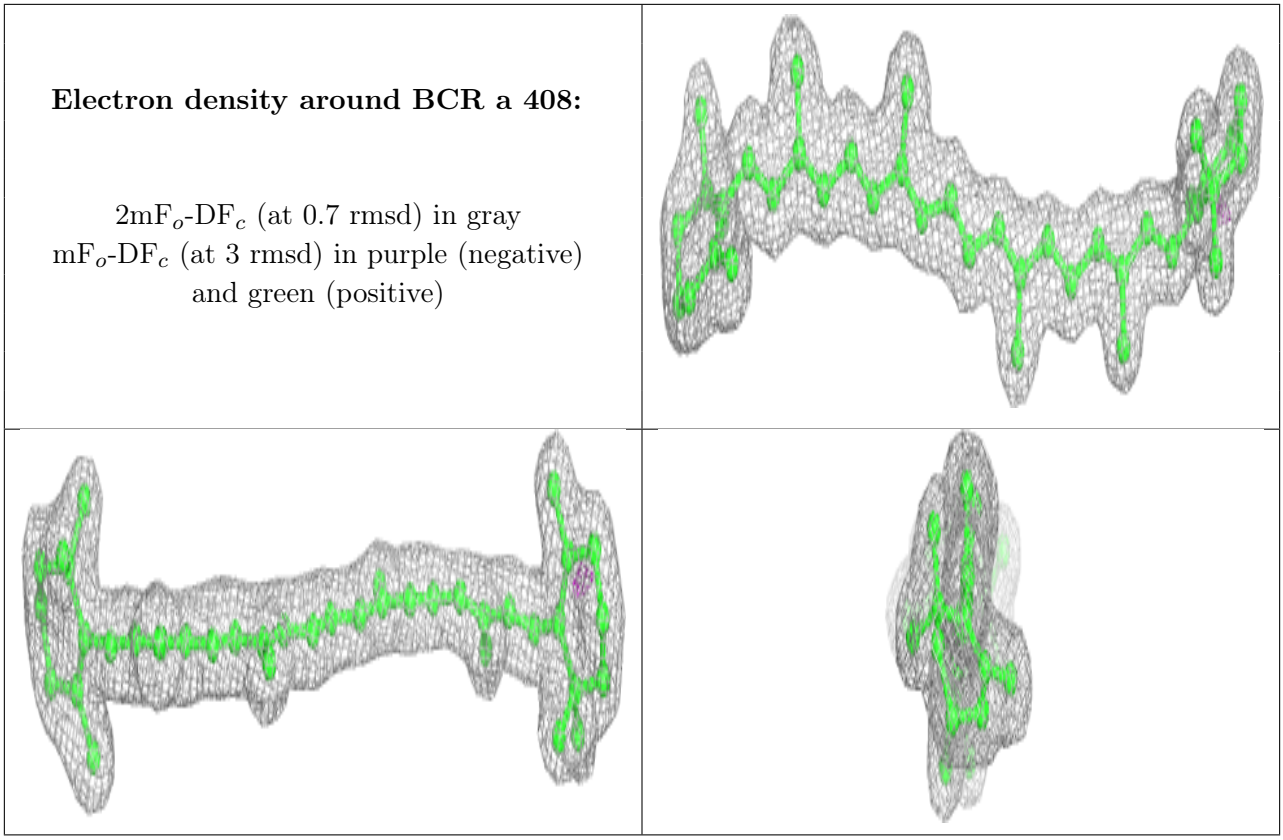
Electron density around DGD c 516:

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



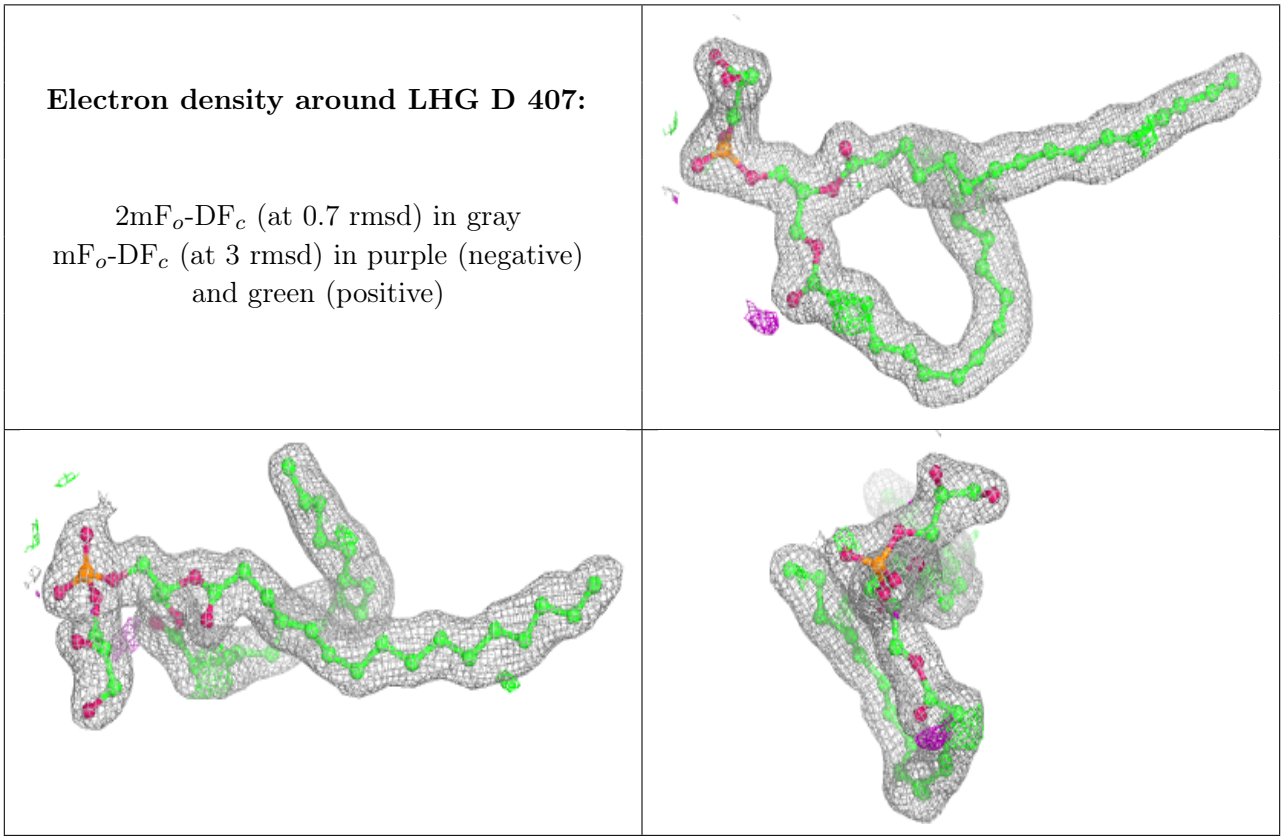
Electron density around BCR a 408:

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



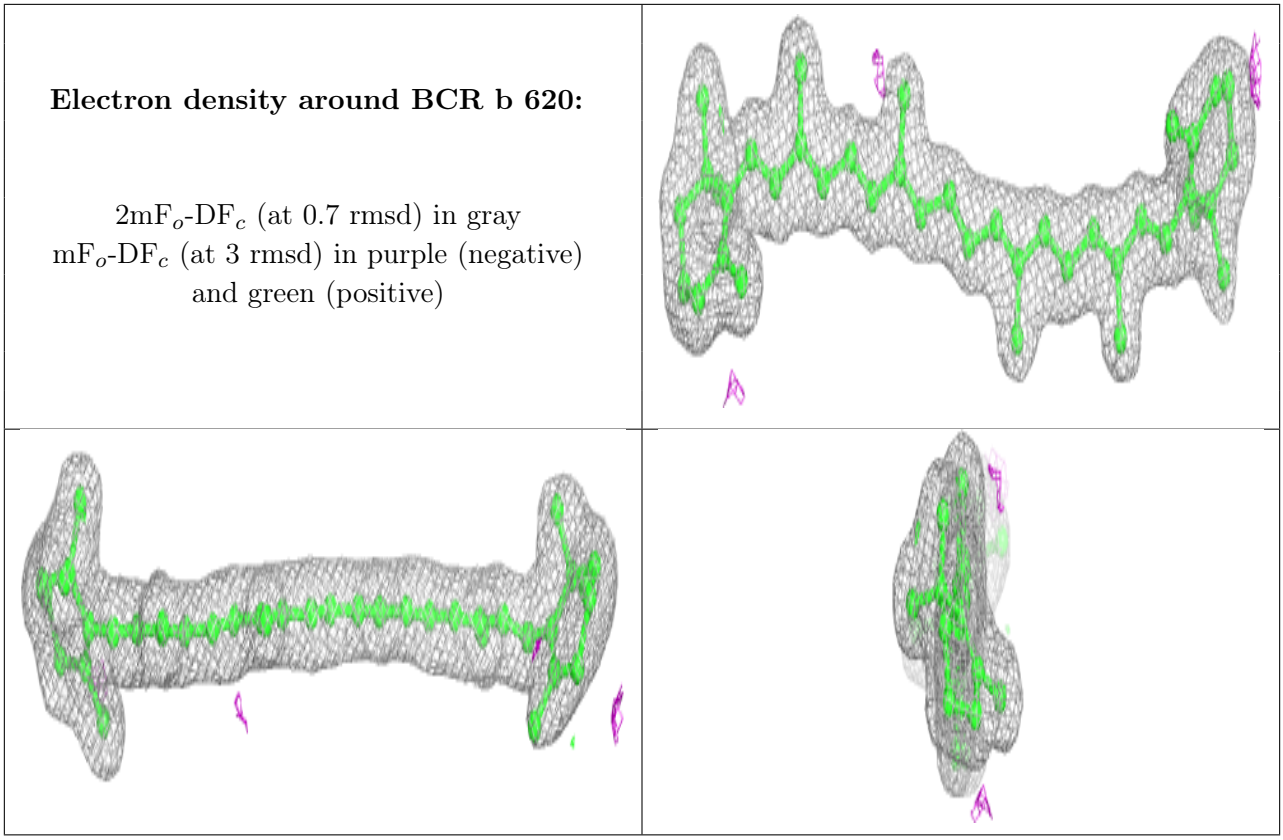
Electron density around LHG D 407:

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



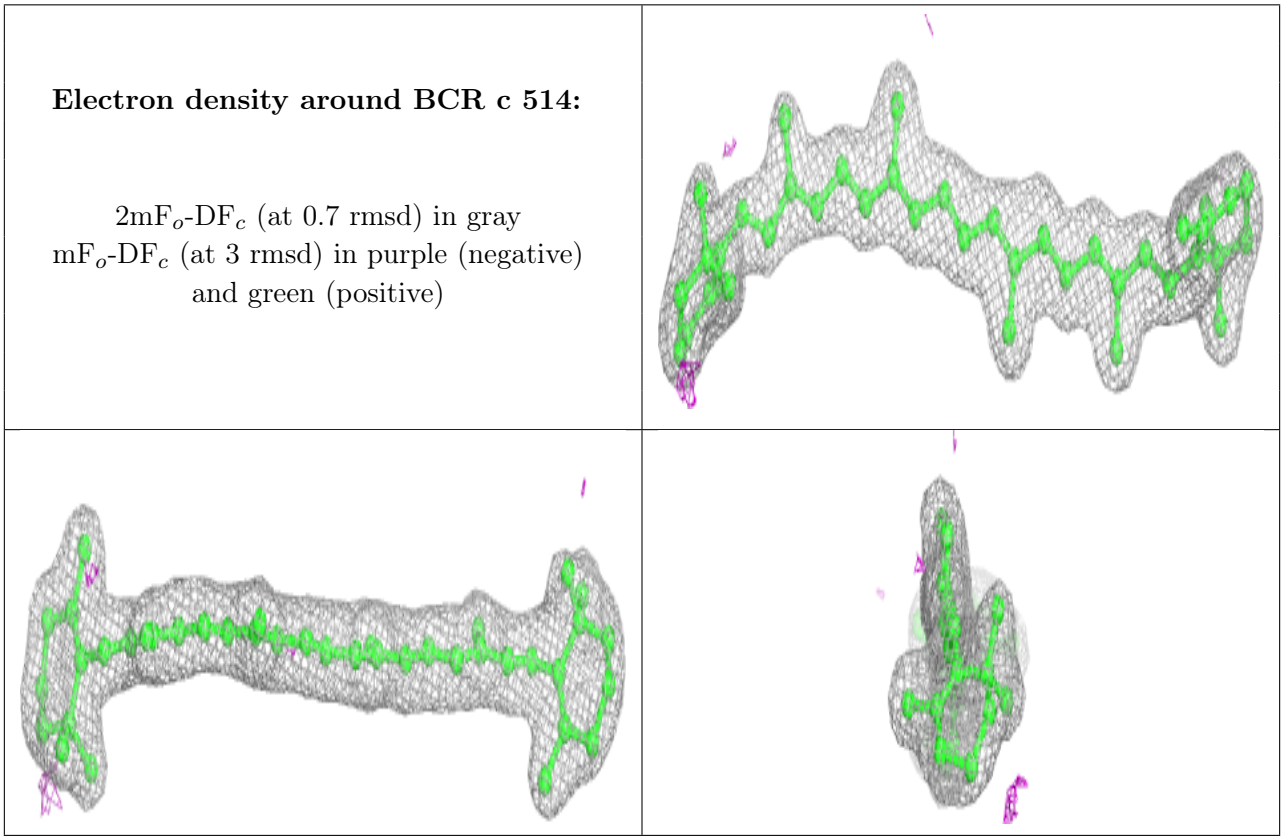
Electron density around BCR b 620:

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



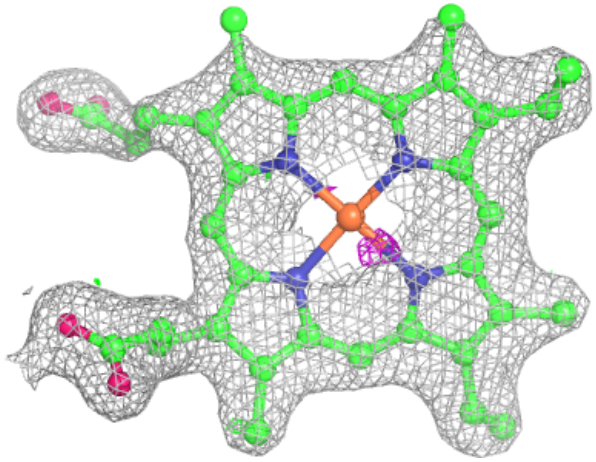
Electron density around BCR c 514:

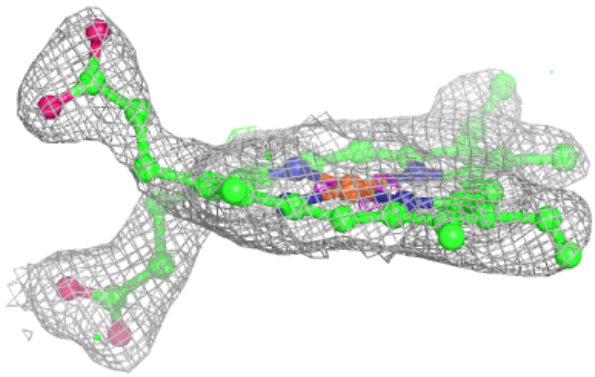
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

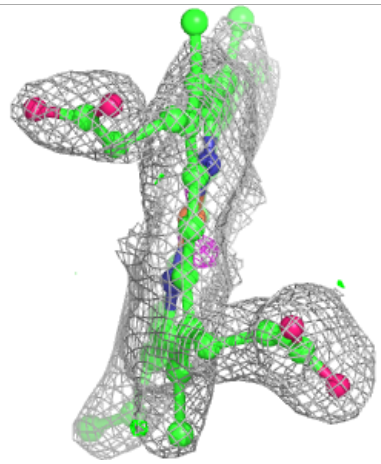


Electron density around HEM E 104:

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

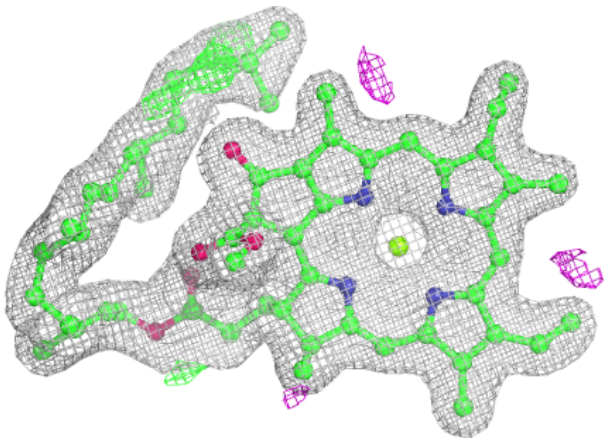


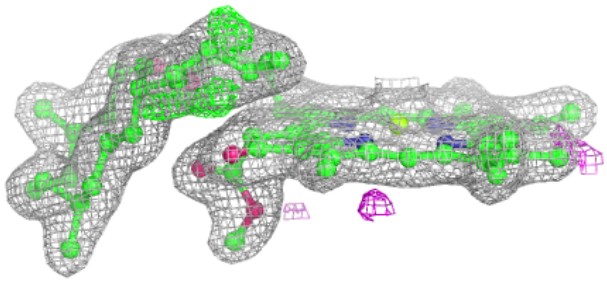


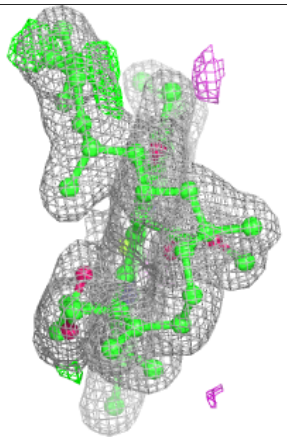


Electron density around CLA b 612:

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

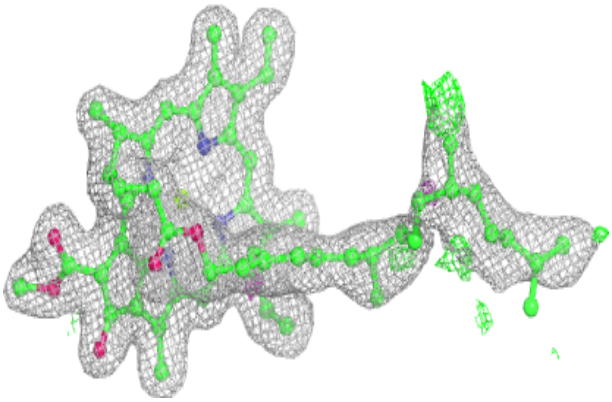


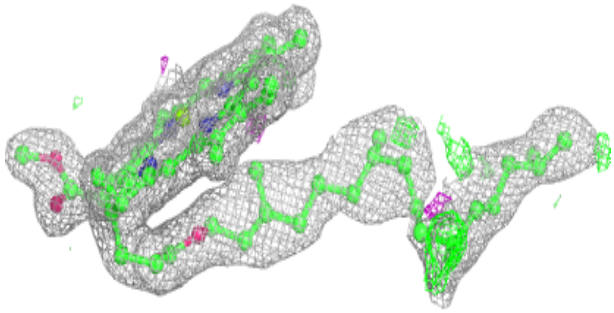


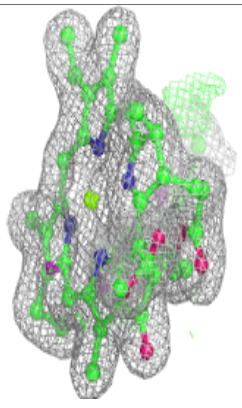


Electron density around CLA b 616:

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

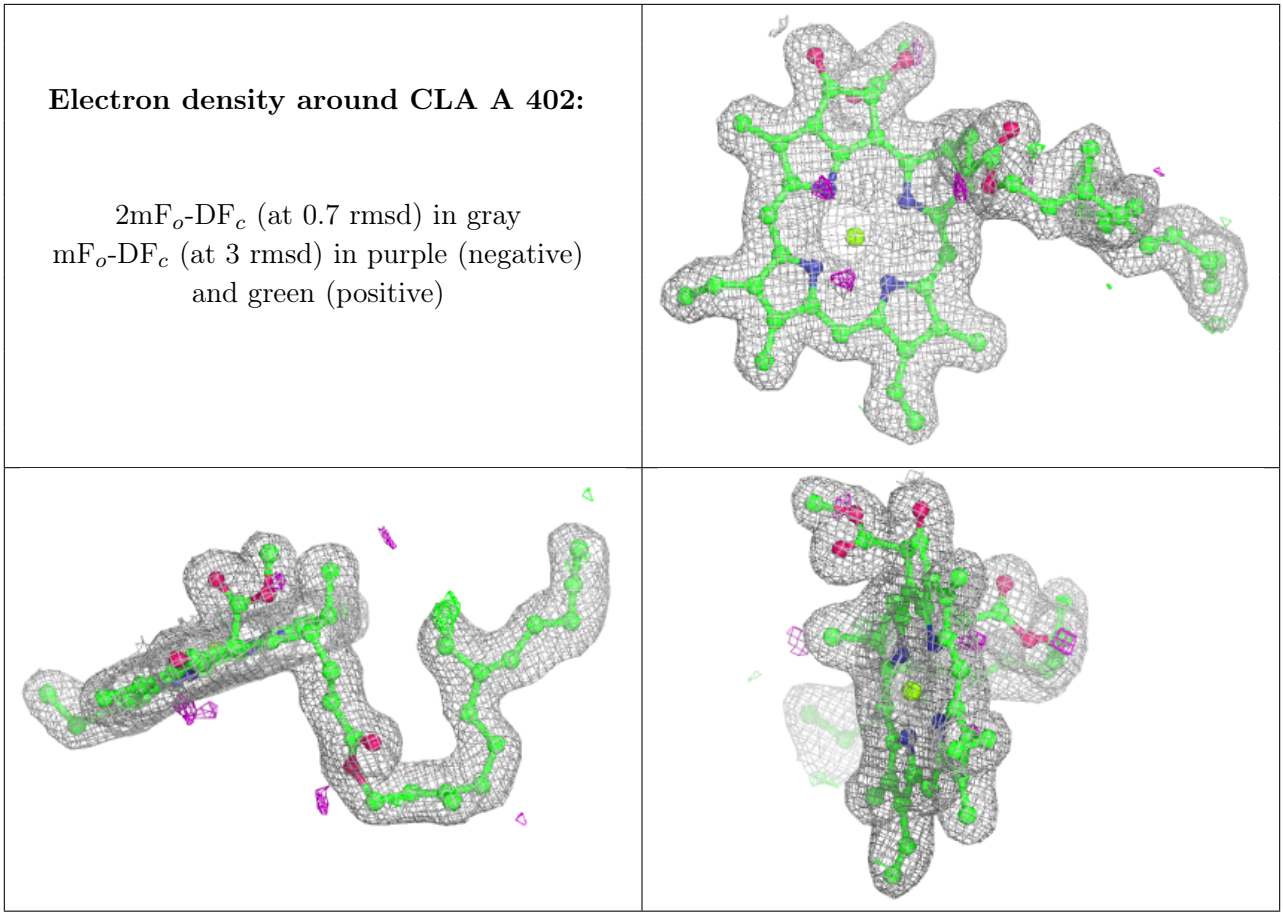






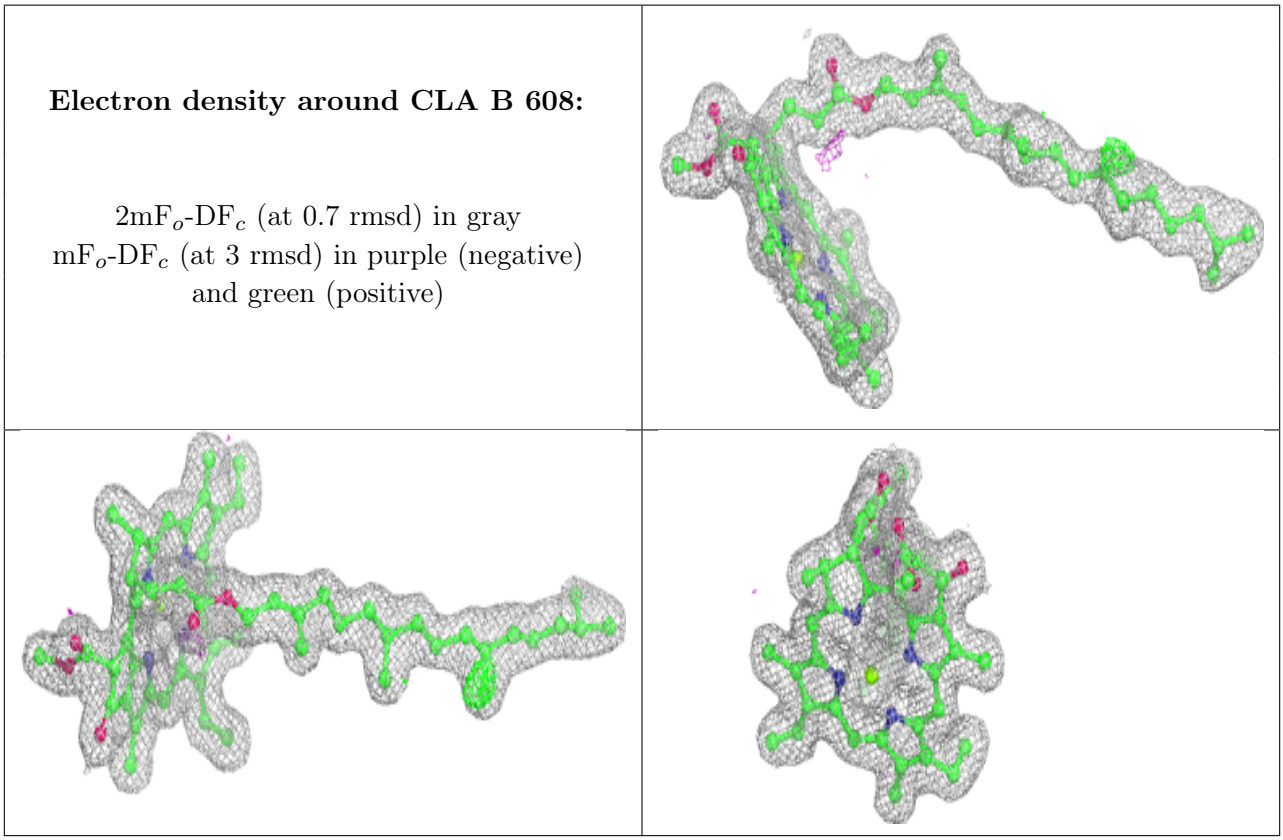
Electron density around CLA A 402:

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



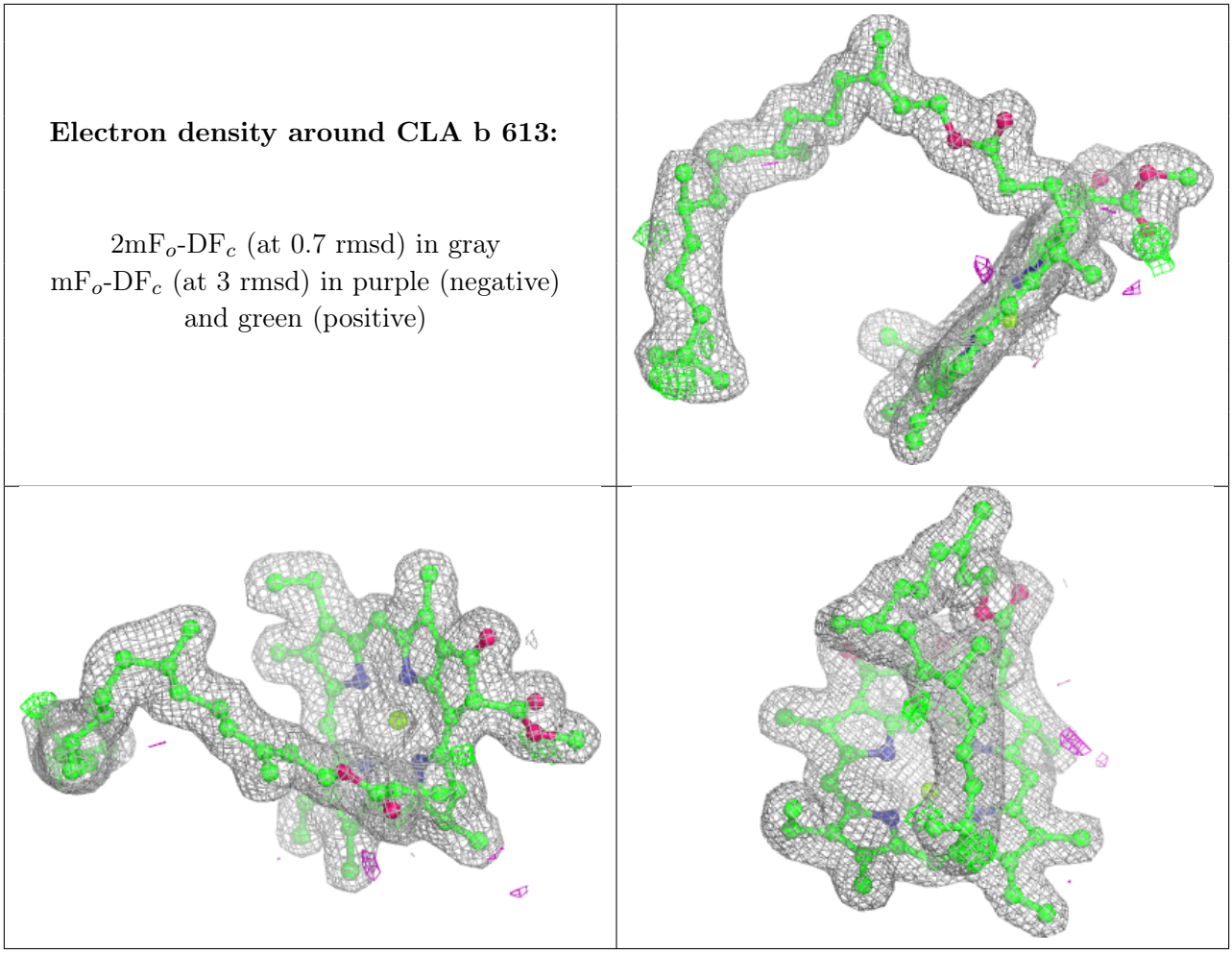
Electron density around CLA B 608:

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



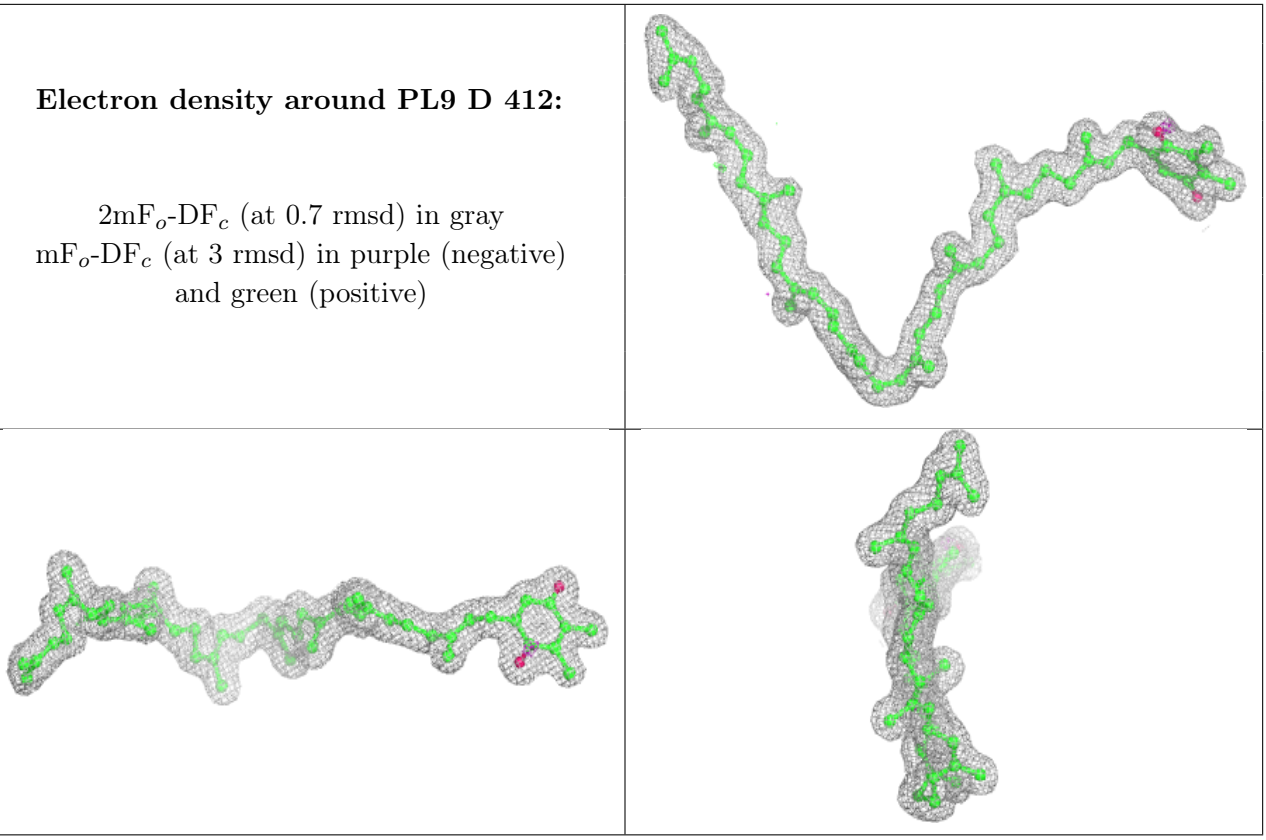
Electron density around CLA b 613:

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



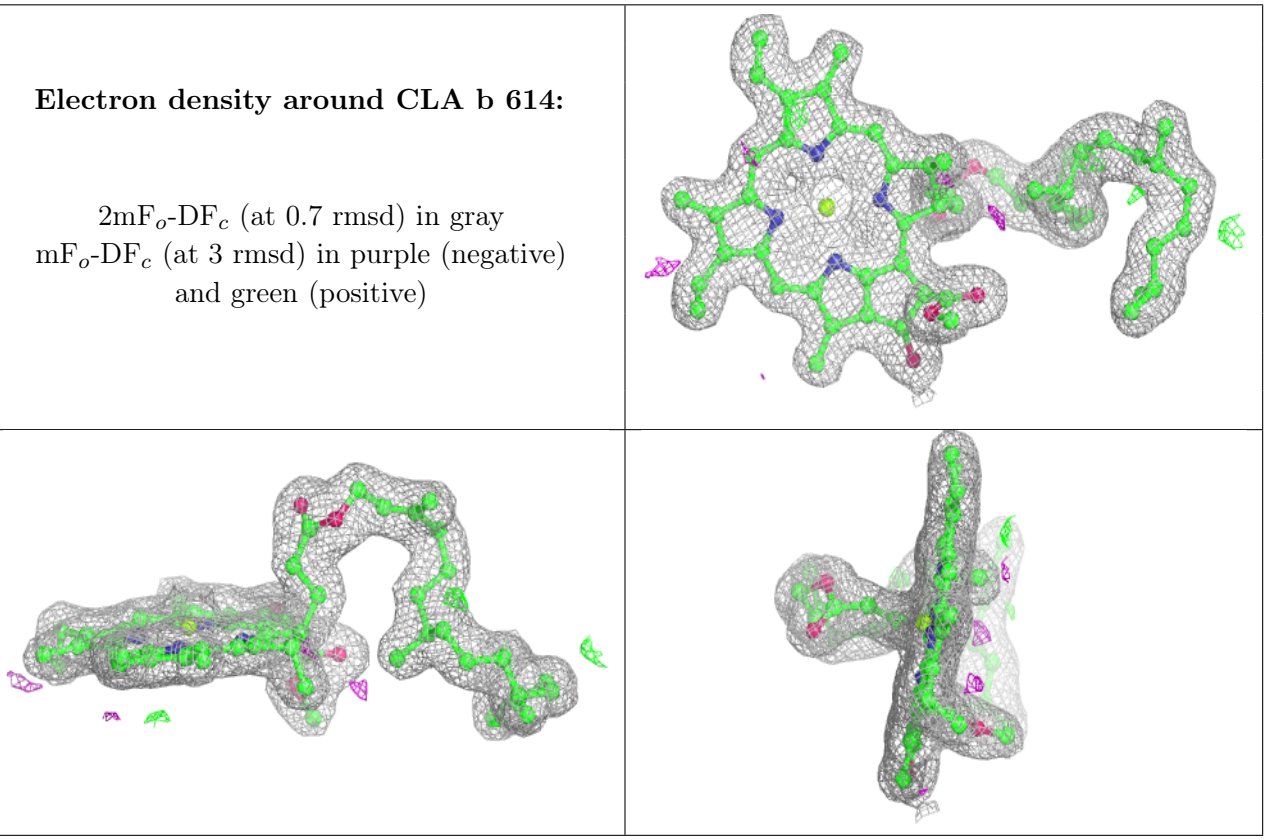
Electron density around PL9 D 412:

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



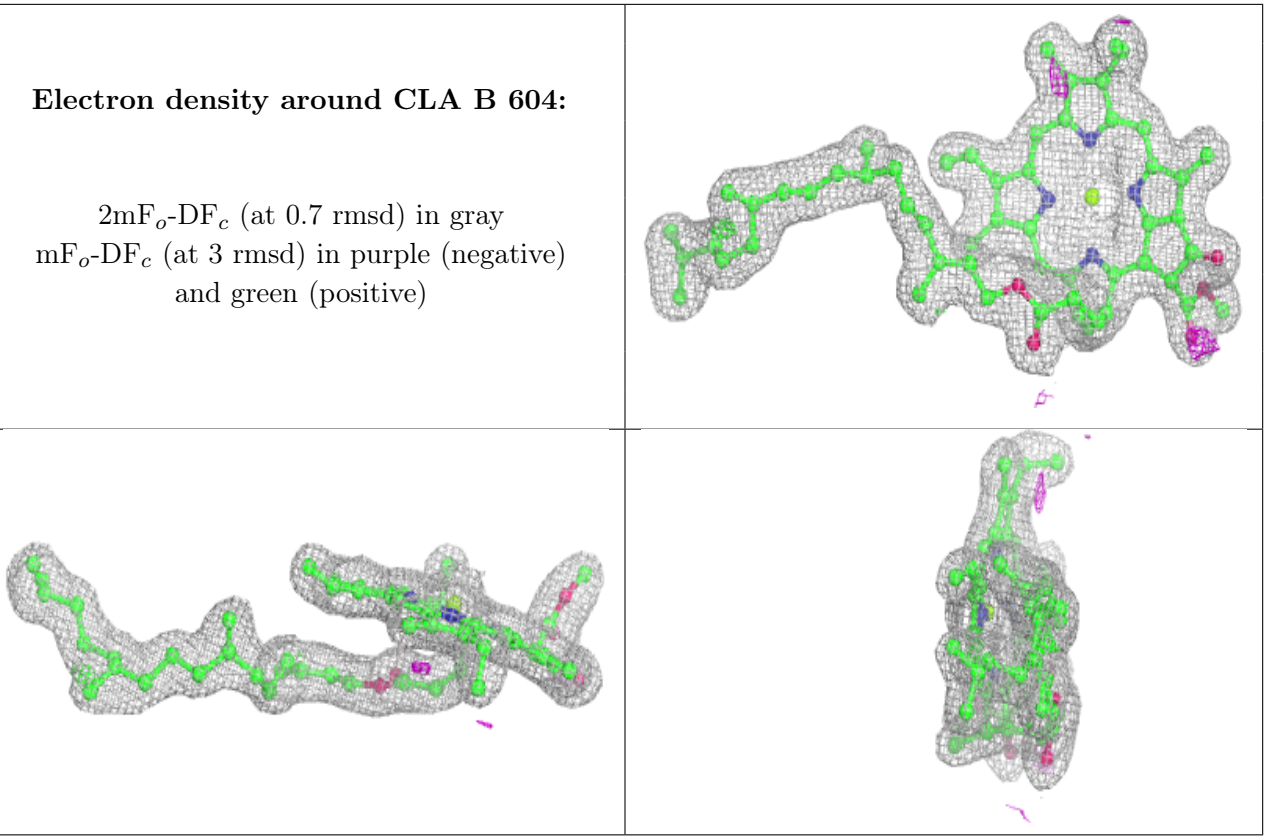
Electron density around CLA b 614:

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



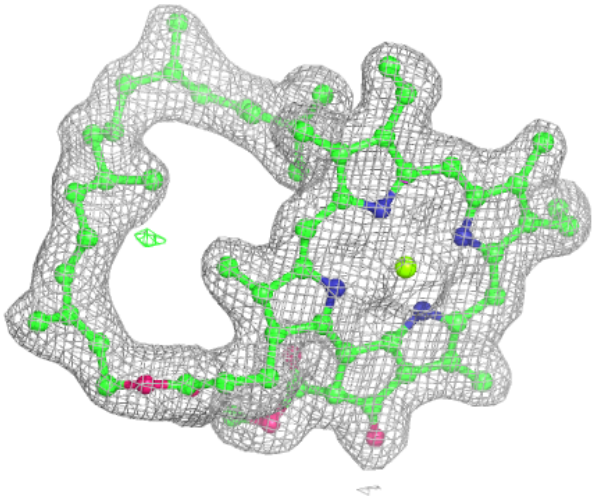
Electron density around CLA B 604:

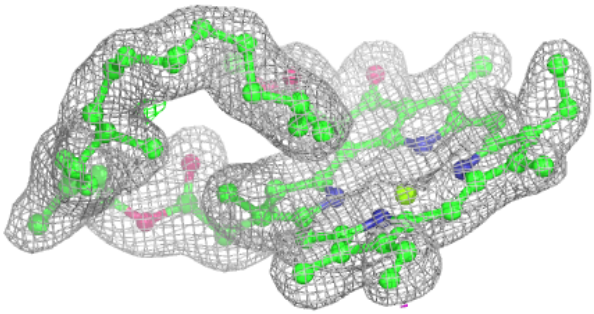
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

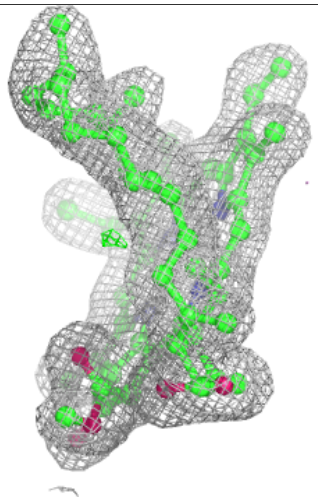


Electron density around CLA b 617:

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

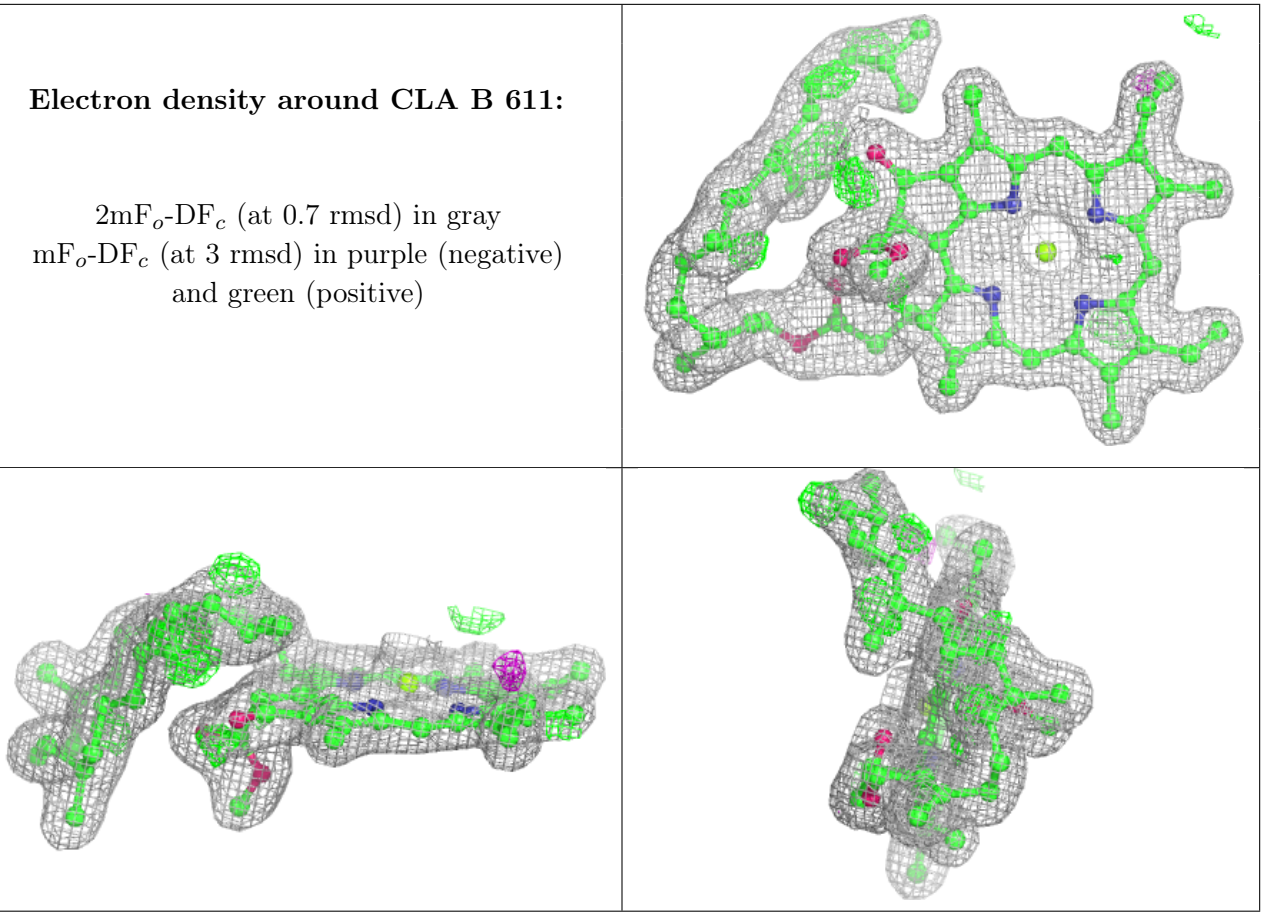






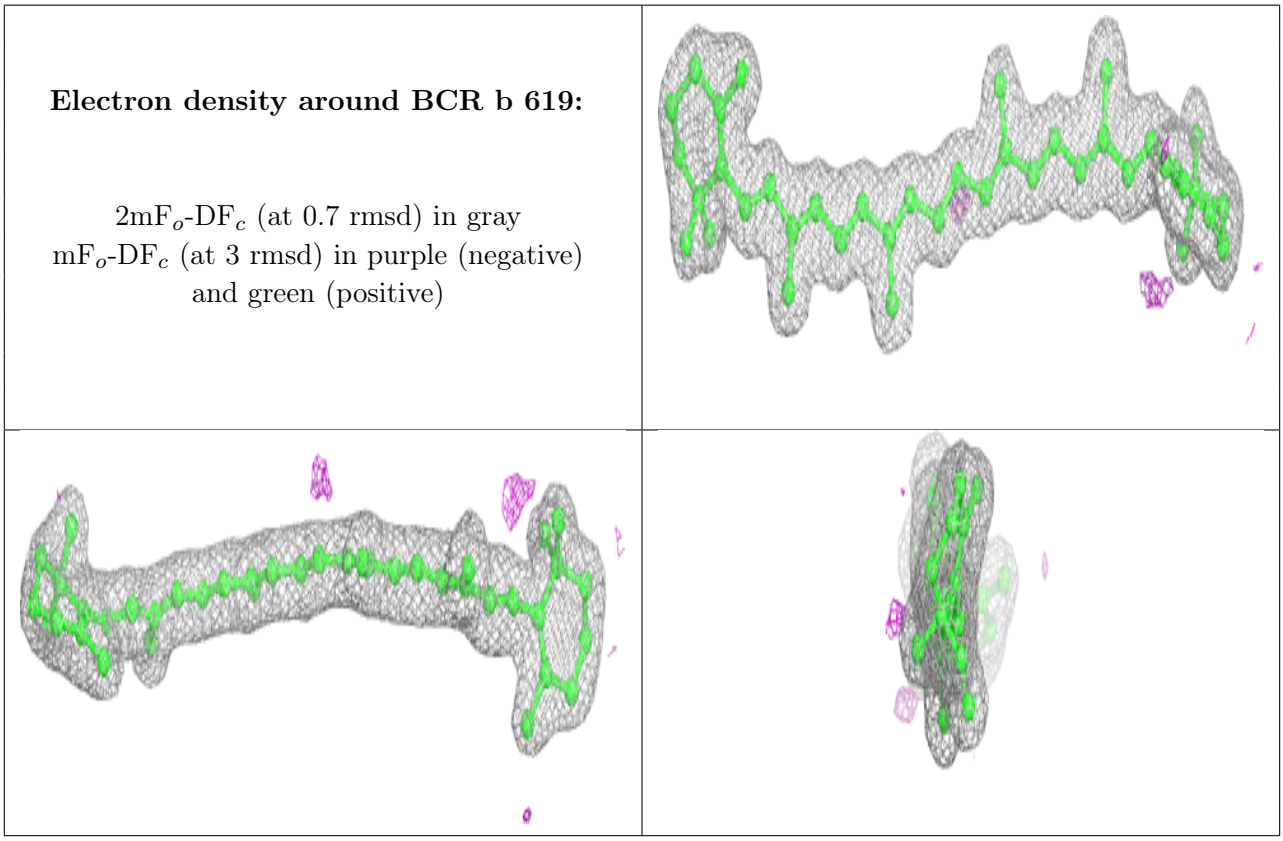
Electron density around CLA B 611:

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



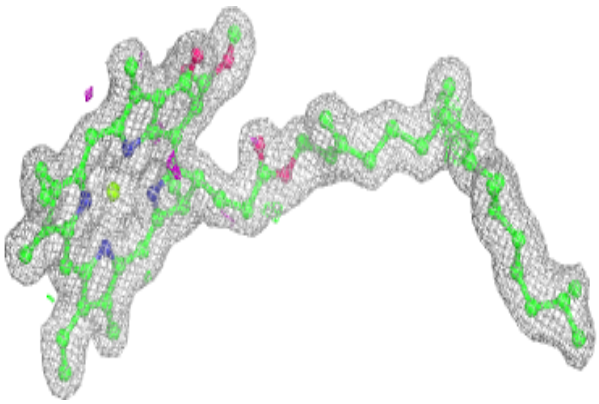
Electron density around BCR b 619:

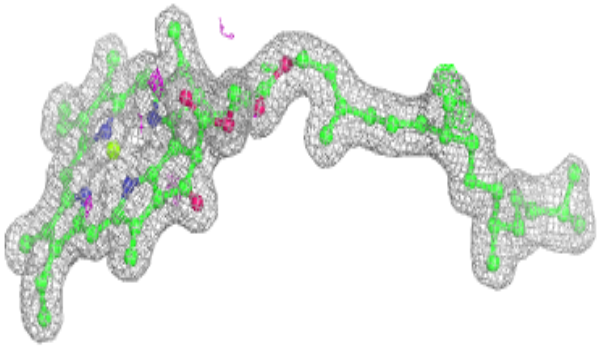
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

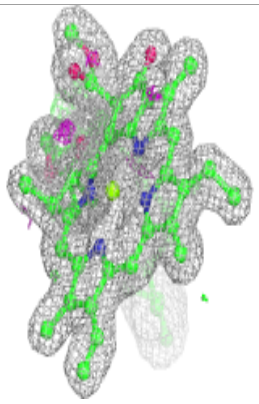


Electron density around CLA a 403:

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

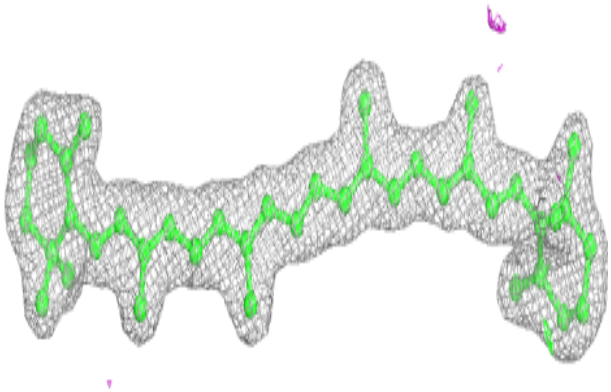


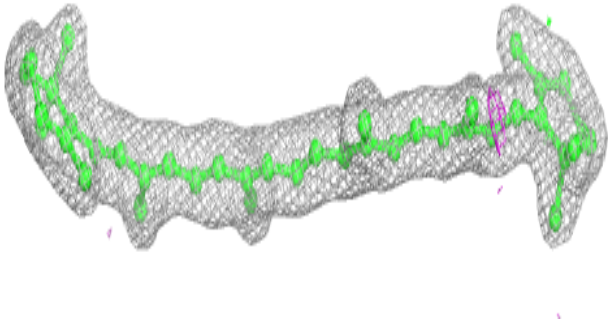


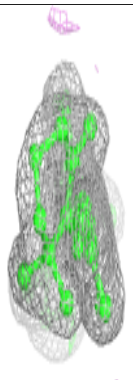


Electron density around BCR b 621:

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

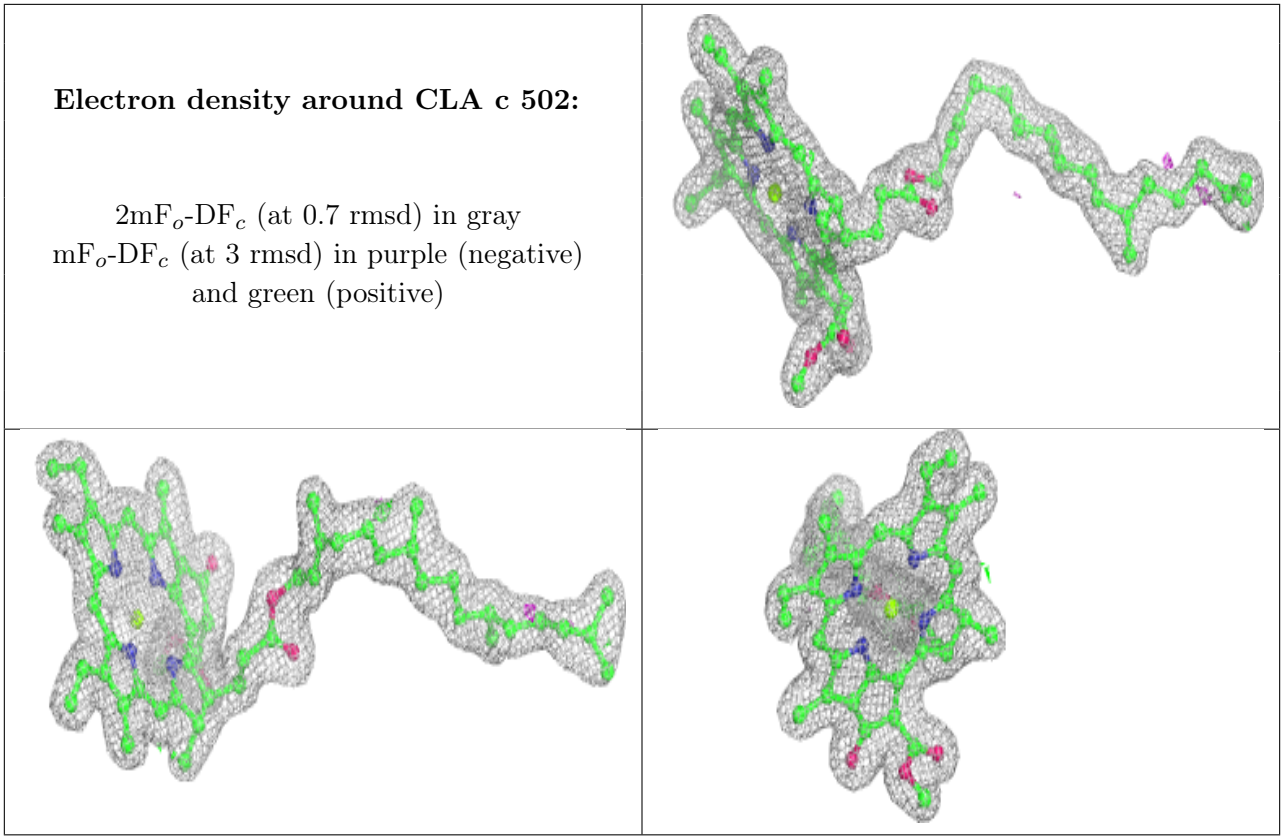






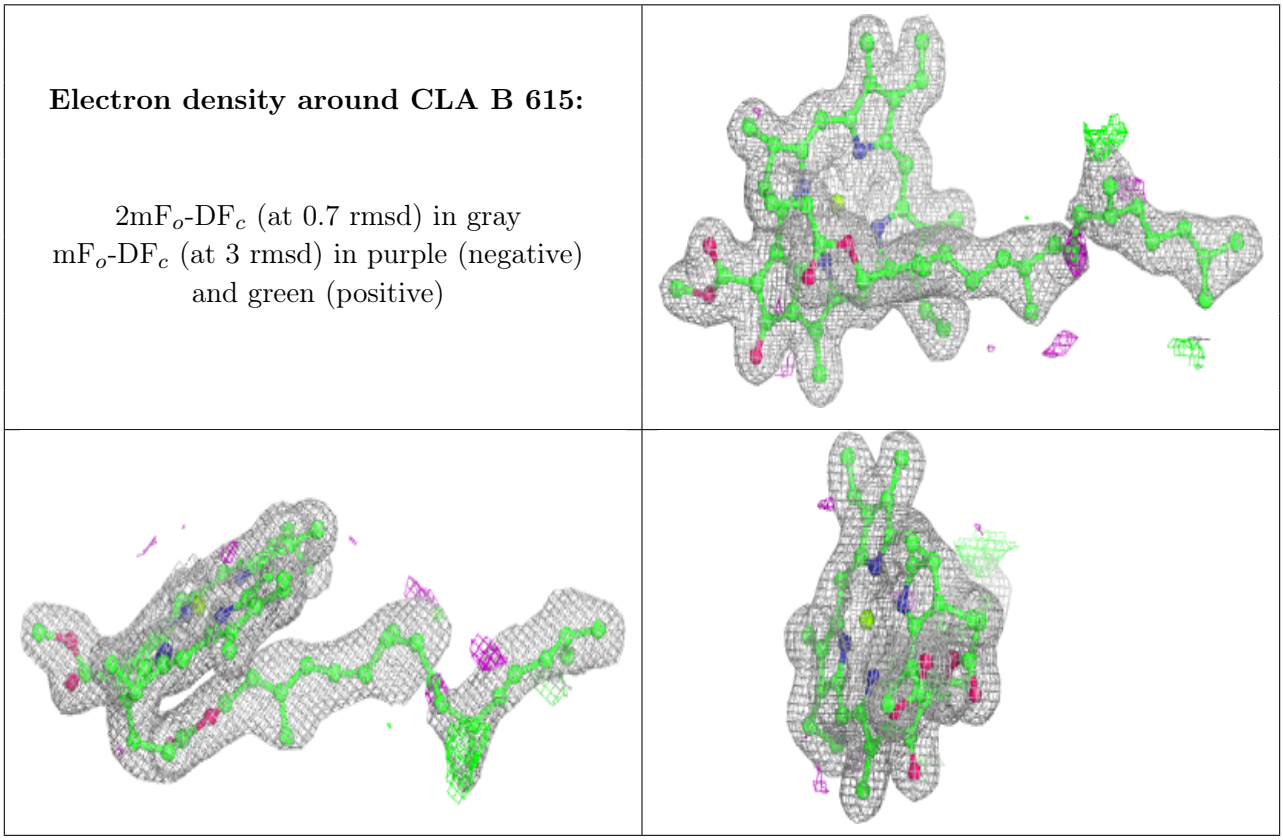
Electron density around CLA c 502:

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



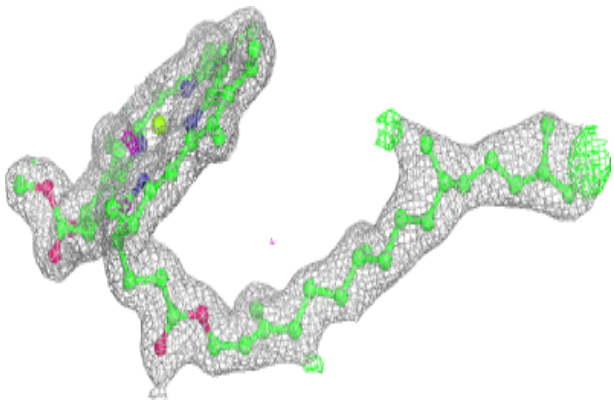
Electron density around CLA B 615:

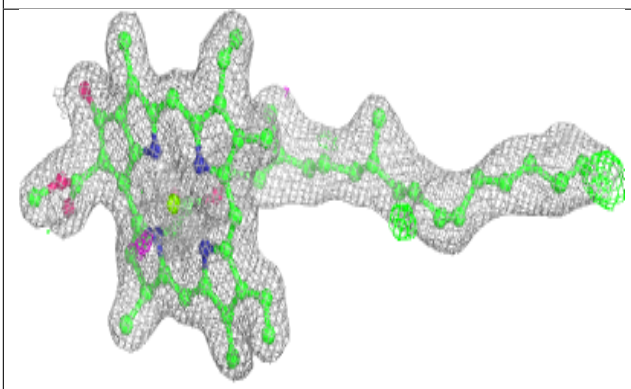
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

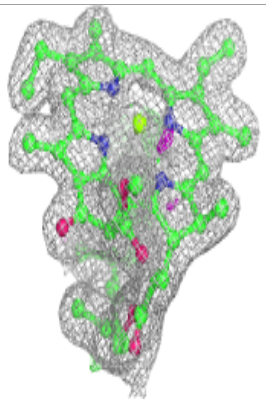


Electron density around CLA c 504:

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

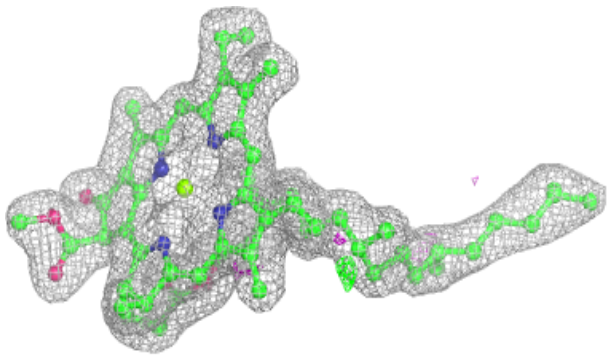


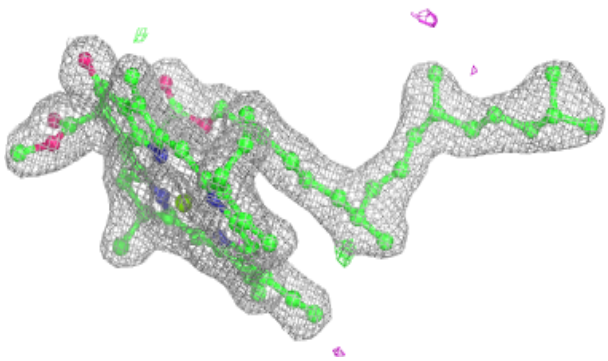


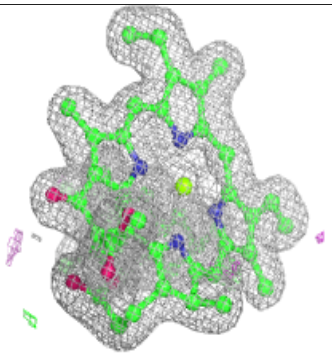


Electron density around CLA c 505:

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

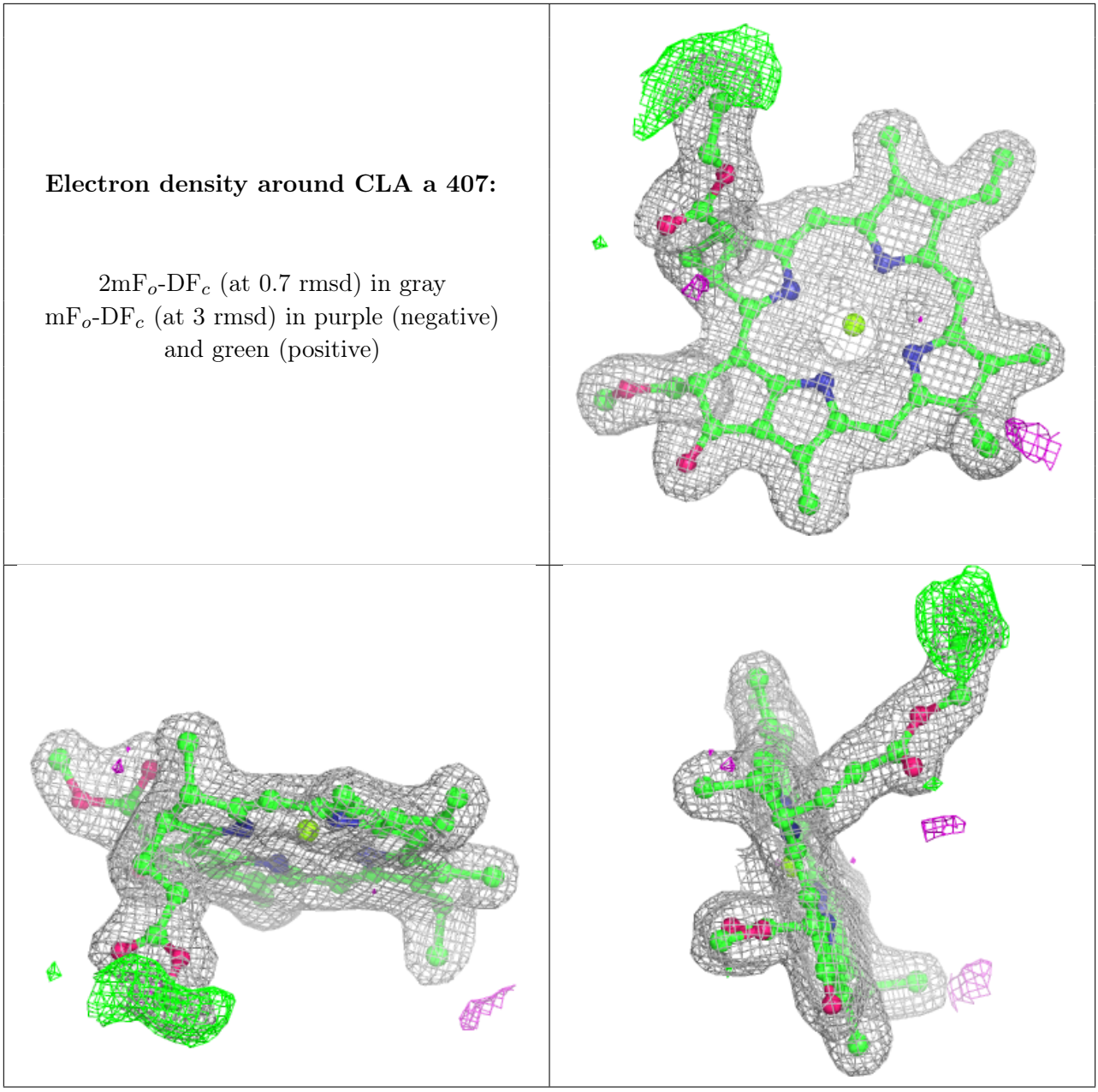






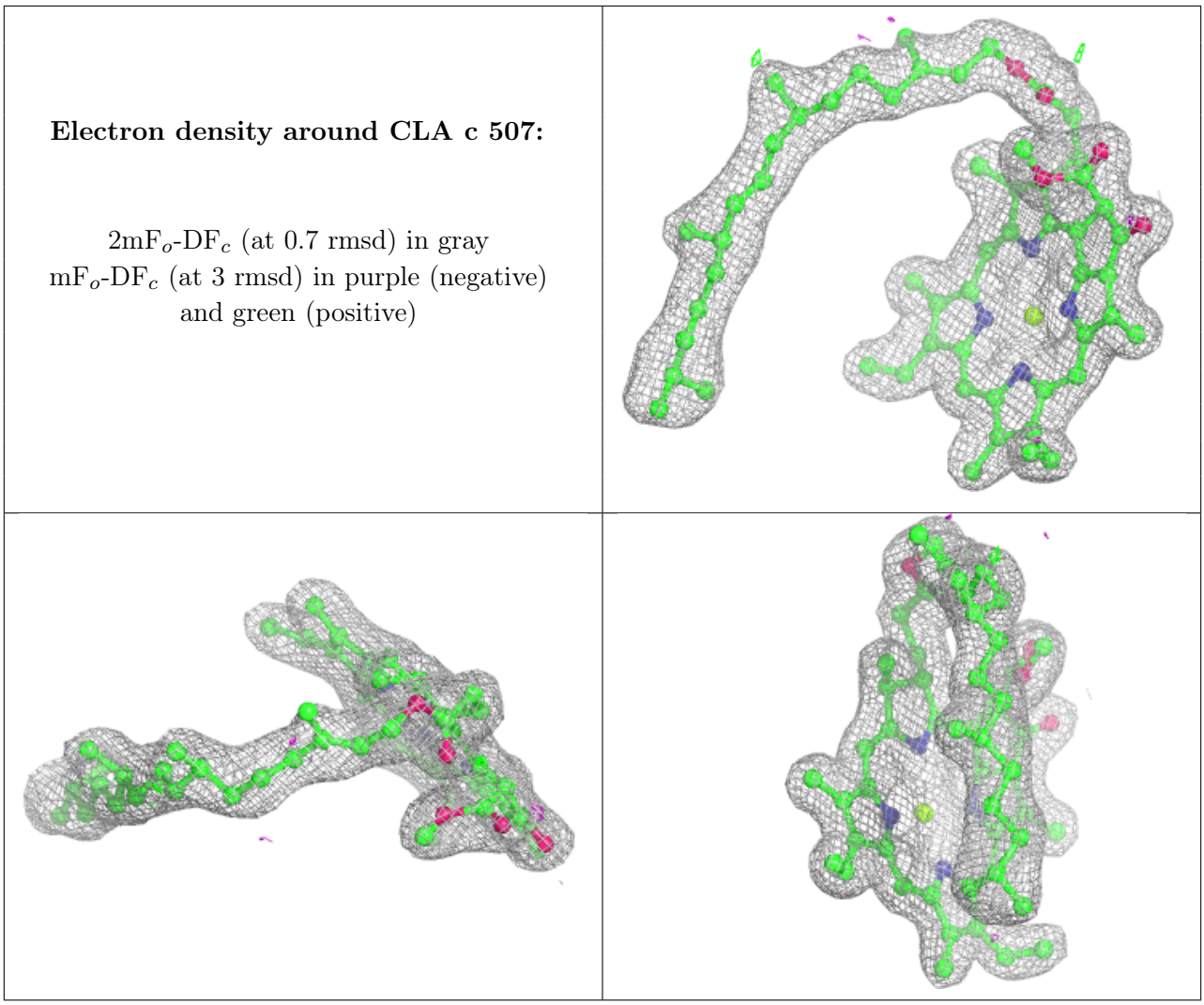
Electron density around CLA a 407:

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



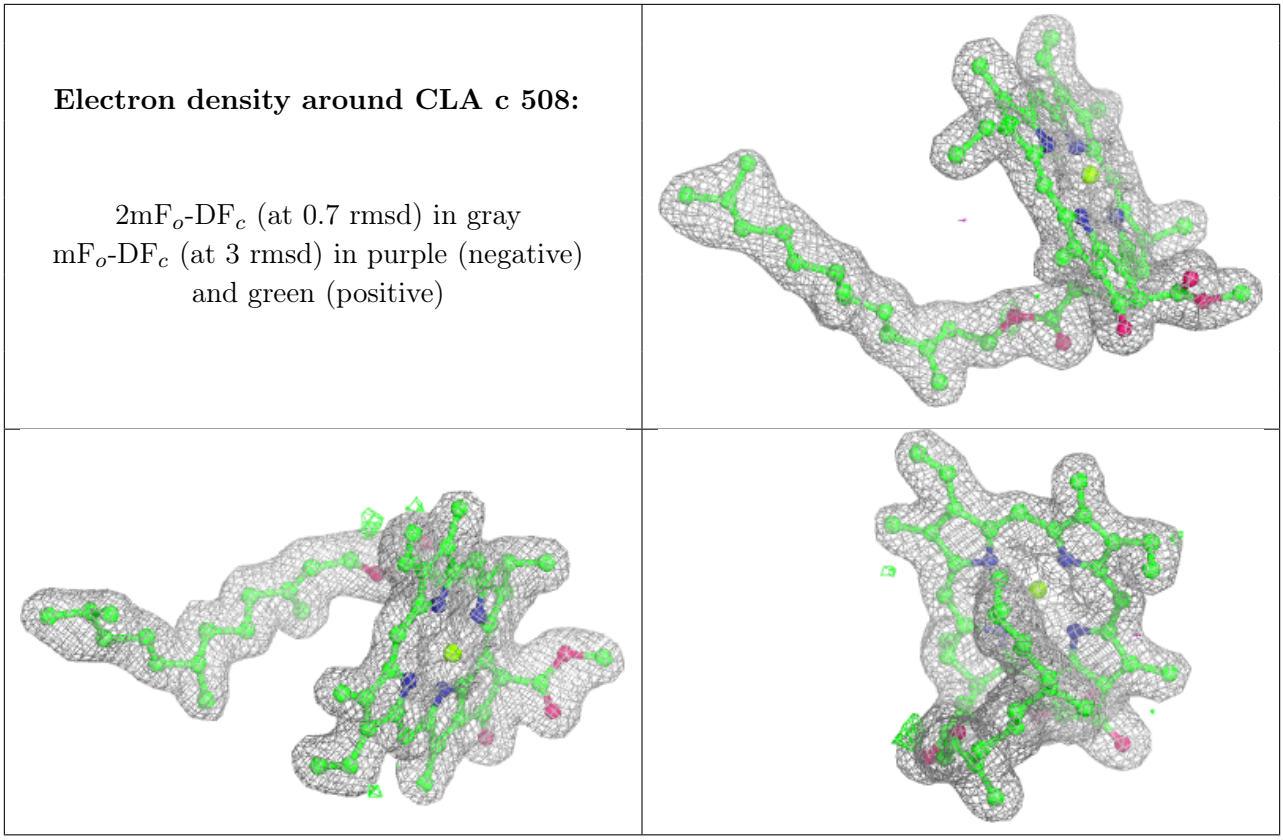
Electron density around CLA c 507:

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



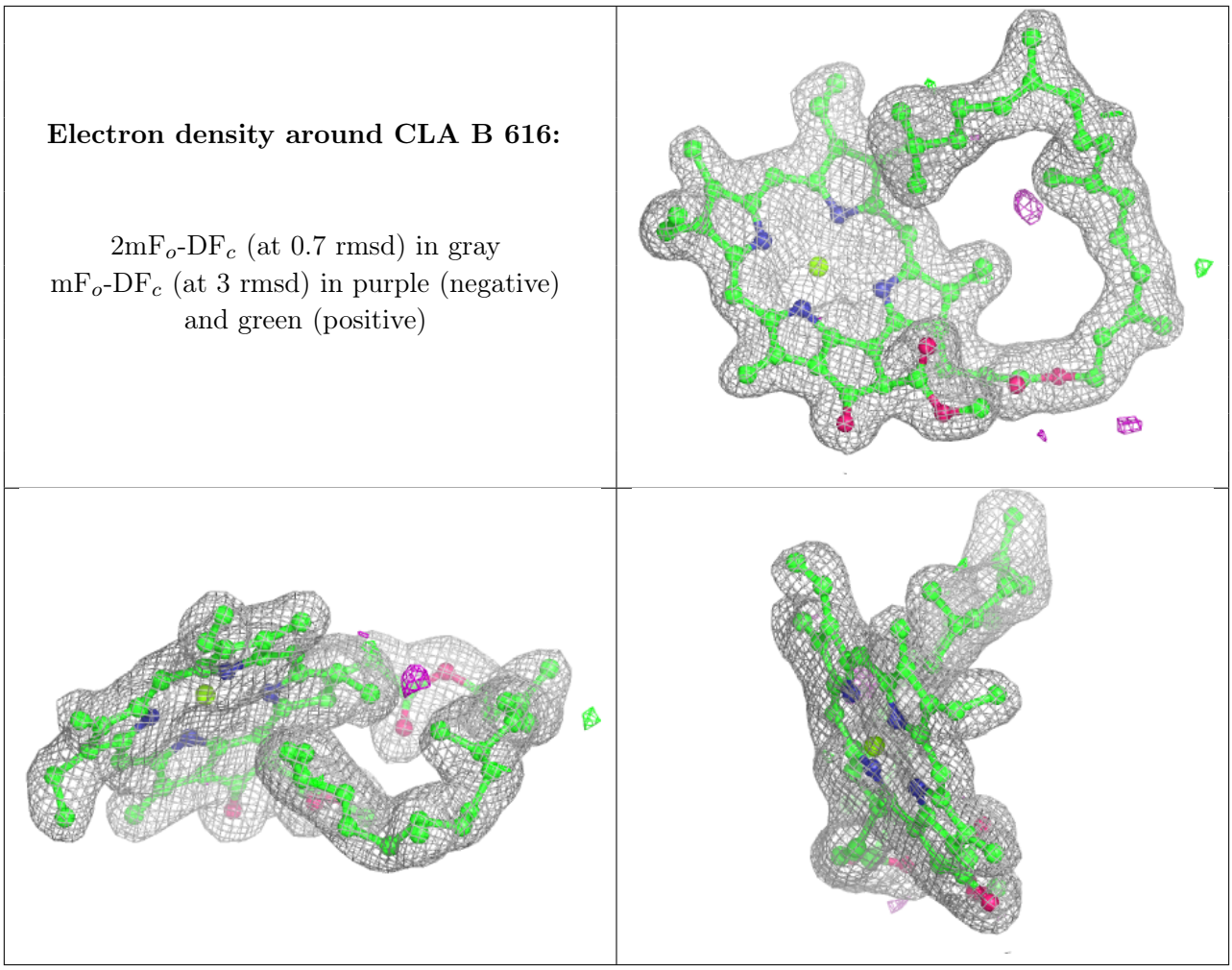
Electron density around CLA c 508:

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



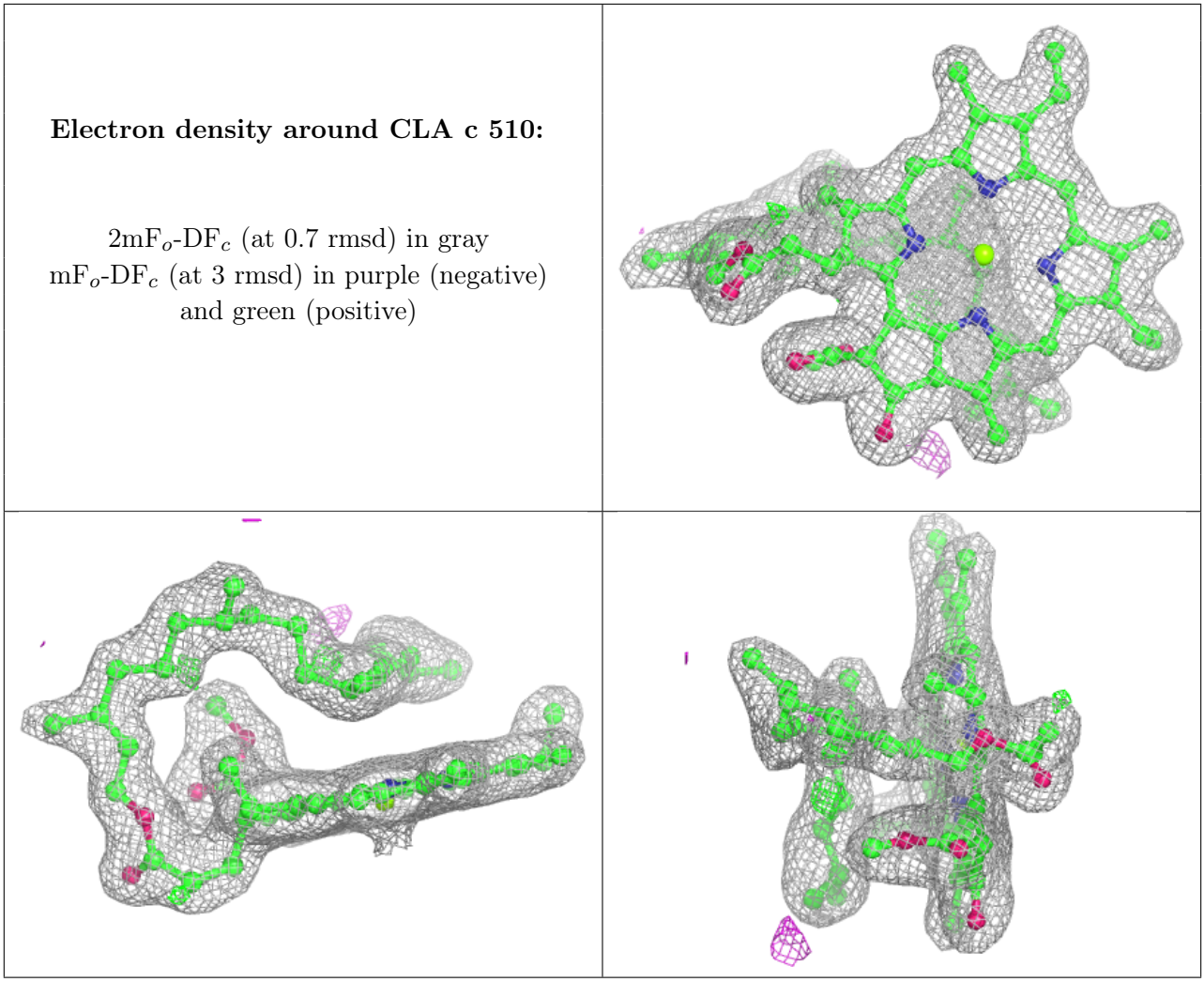
Electron density around CLA B 616:

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



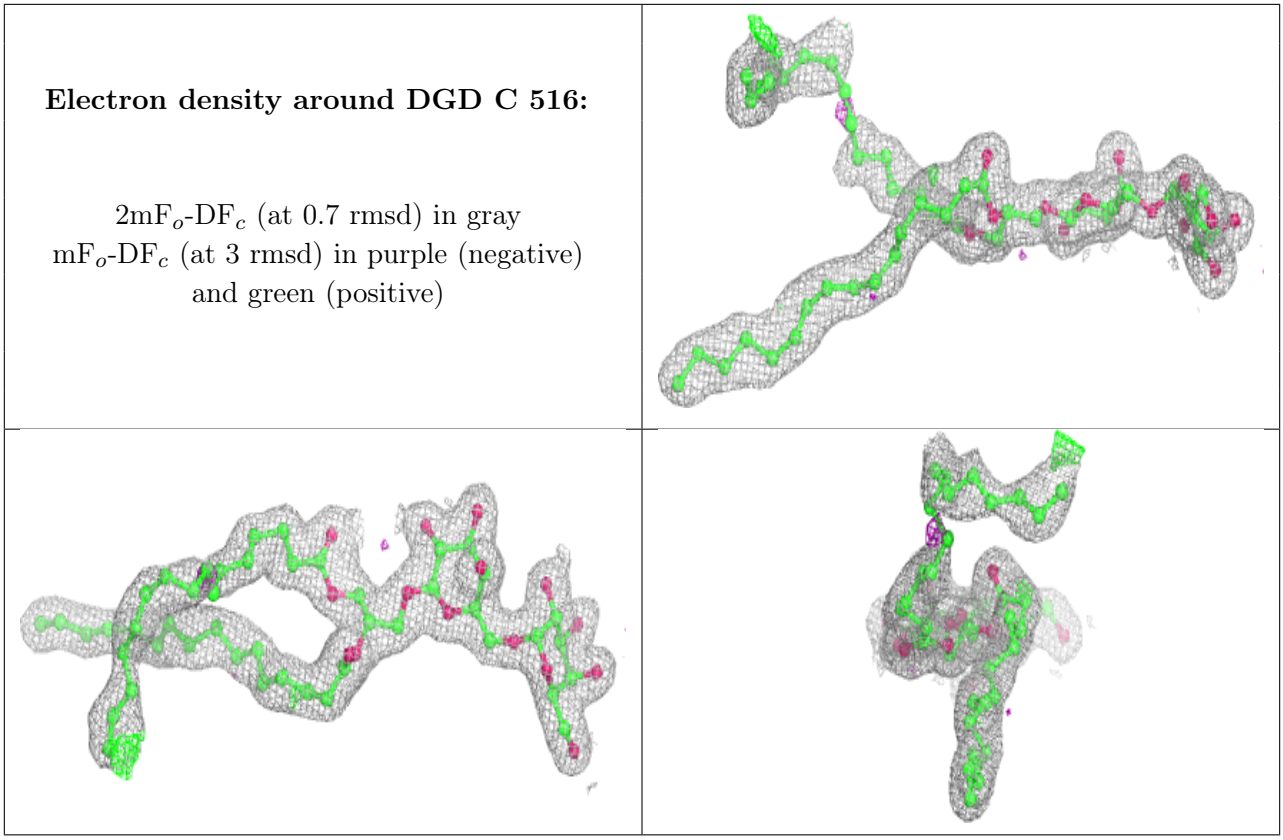
Electron density around CLA c 510:

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



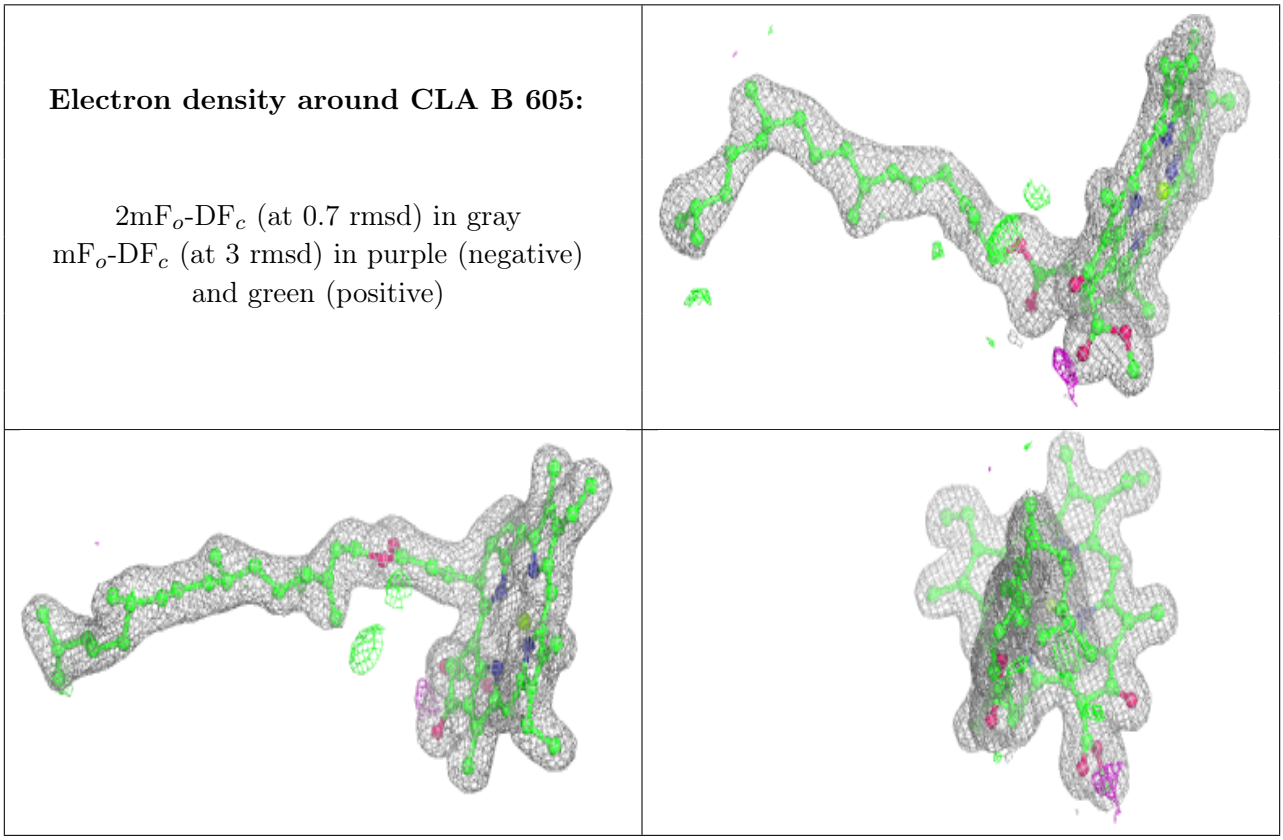
Electron density around DGD C 516:

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



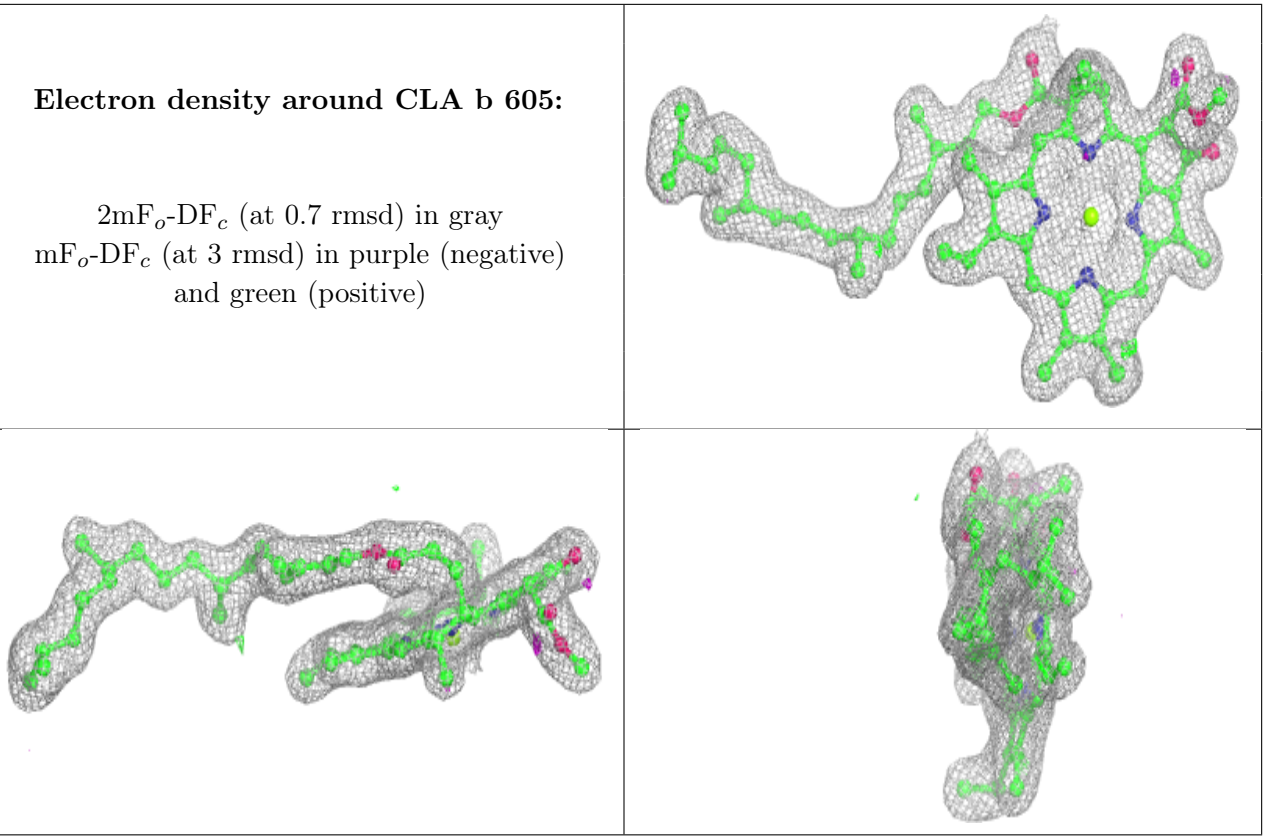
Electron density around CLA B 605:

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



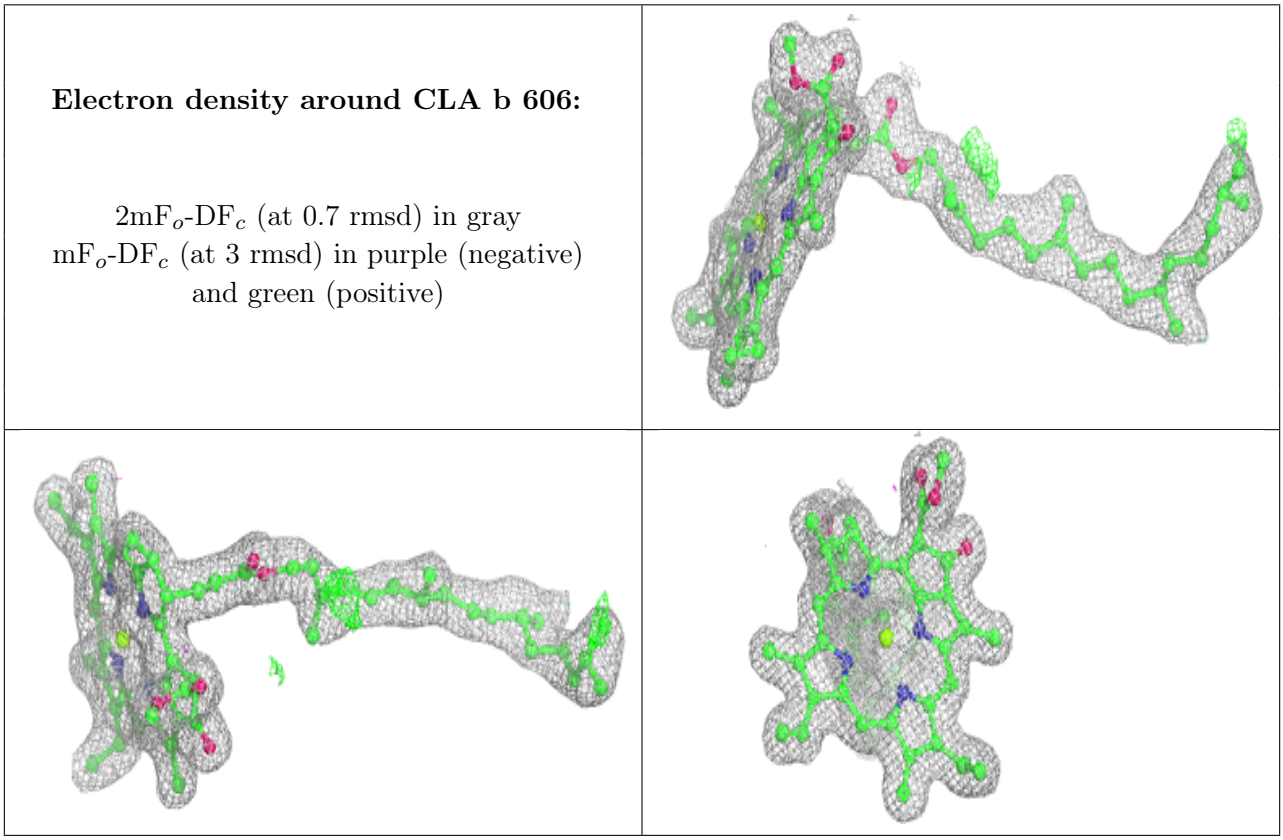
Electron density around CLA b 605:

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



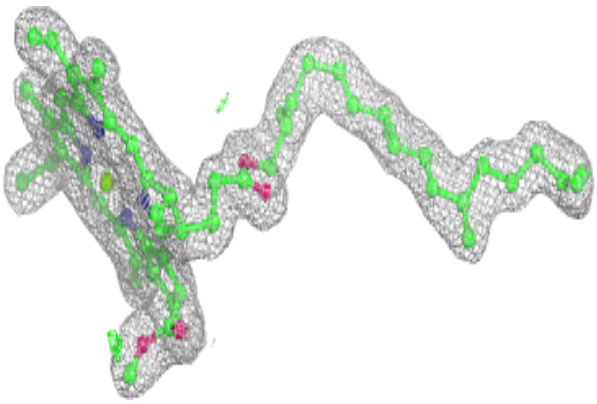
Electron density around CLA b 606:

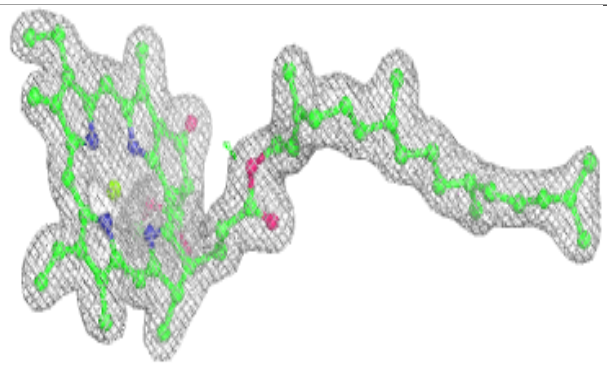
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

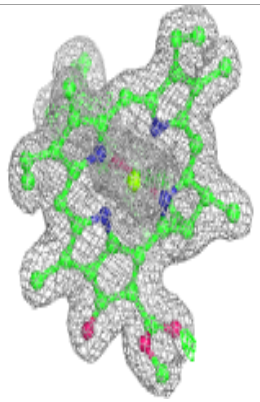


Electron density around CLA C 502:

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

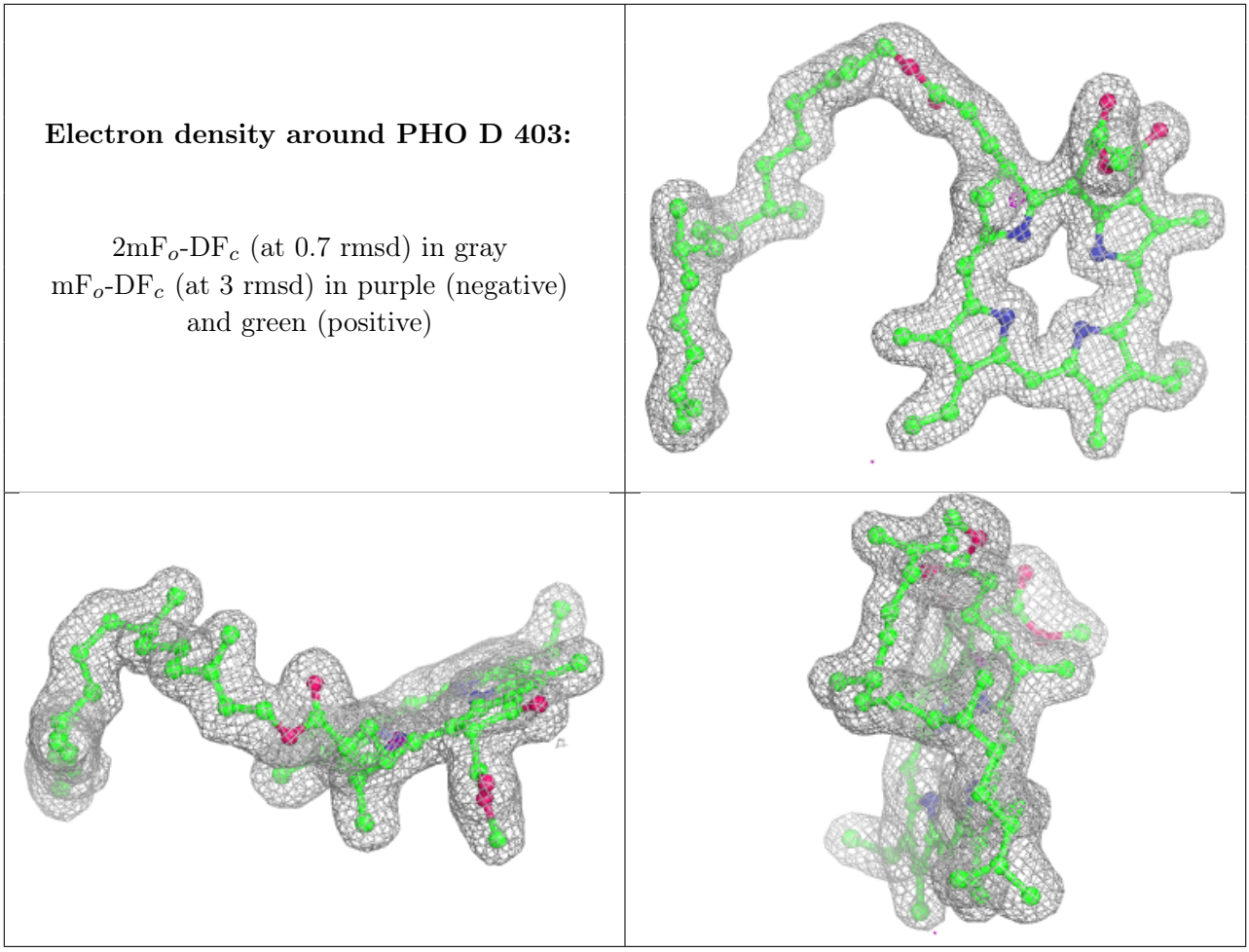






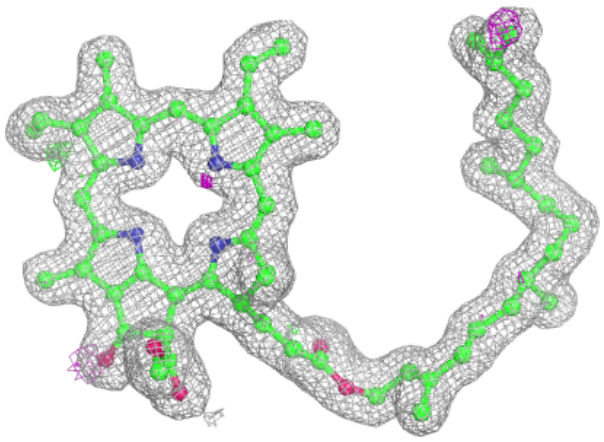
Electron density around PHO D 403:

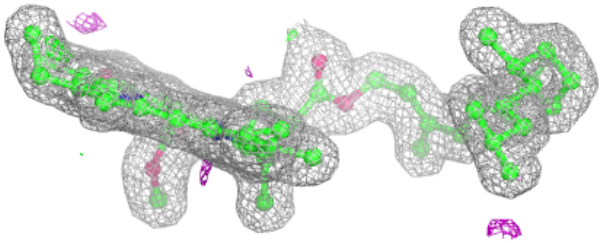
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

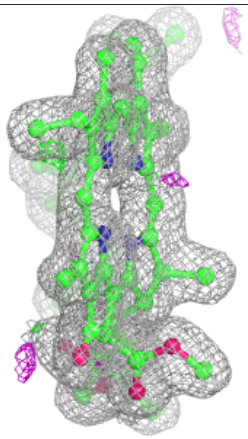


Electron density around PHO a 405:

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

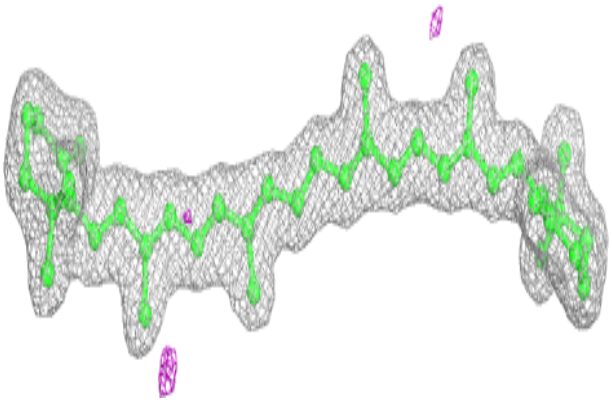


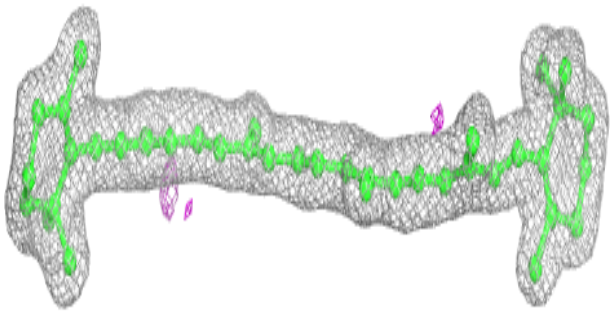


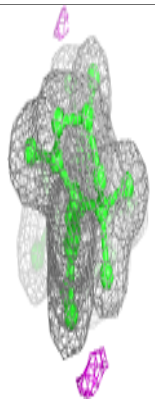


Electron density around BCR A 405:

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

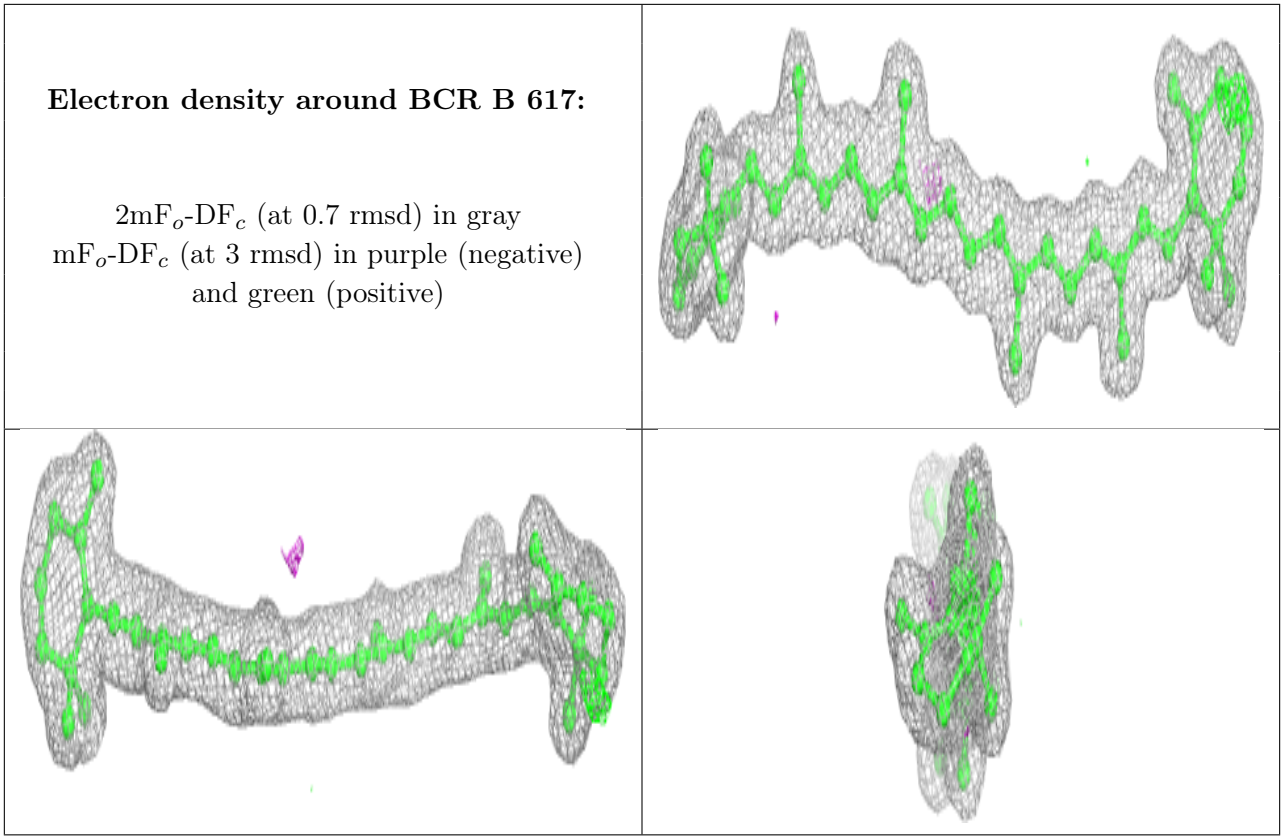






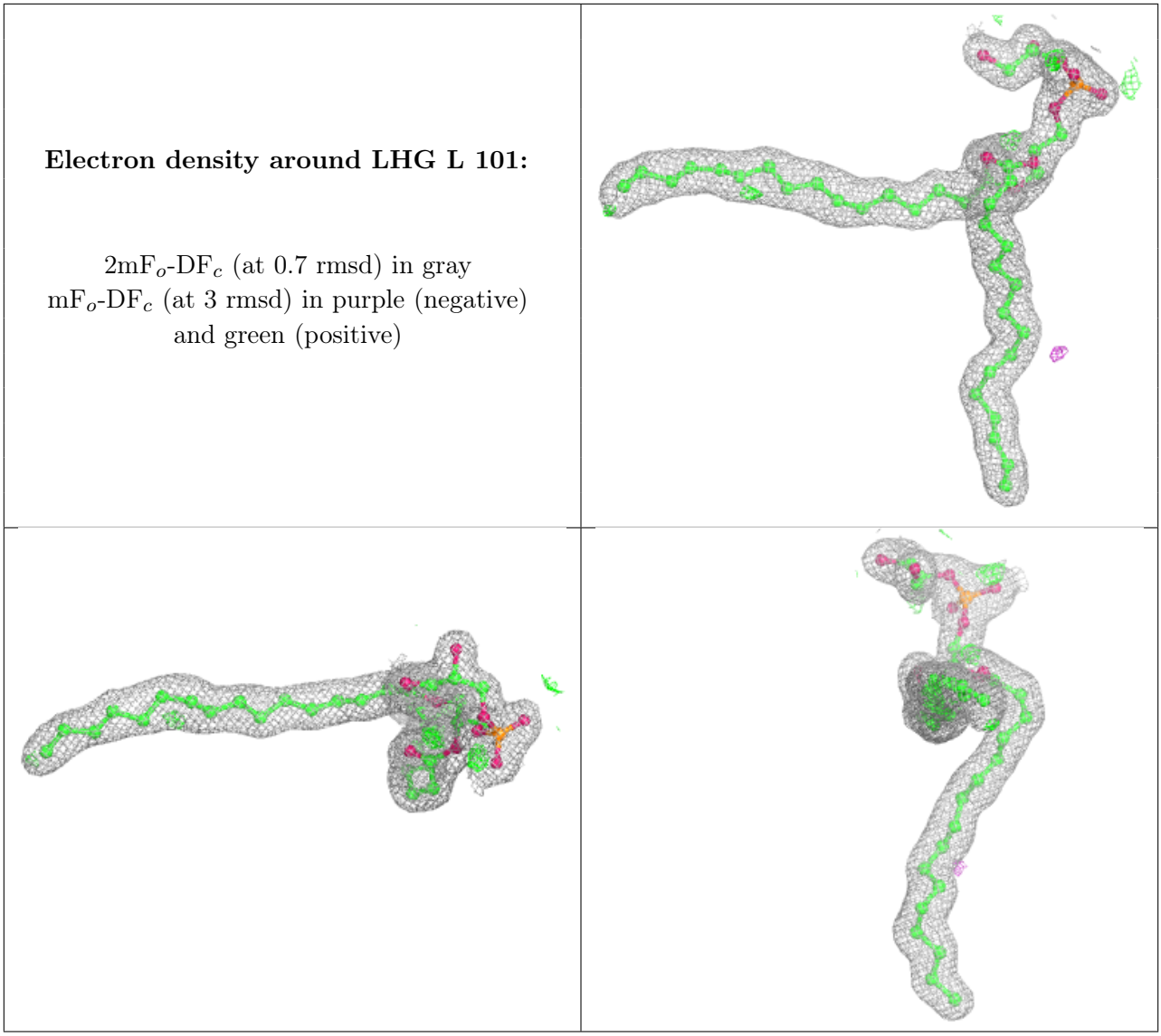
Electron density around BCR B 617:

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



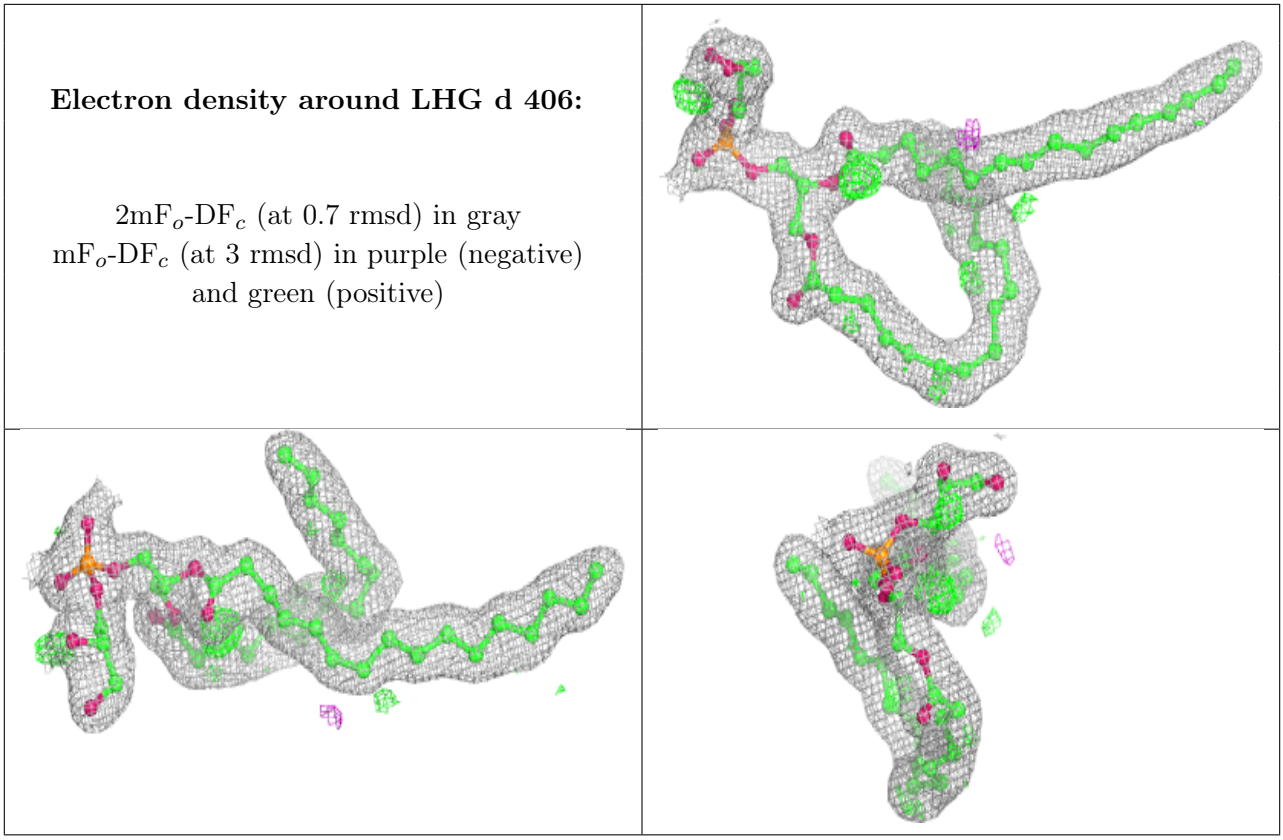
Electron density around LHG L 101:

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



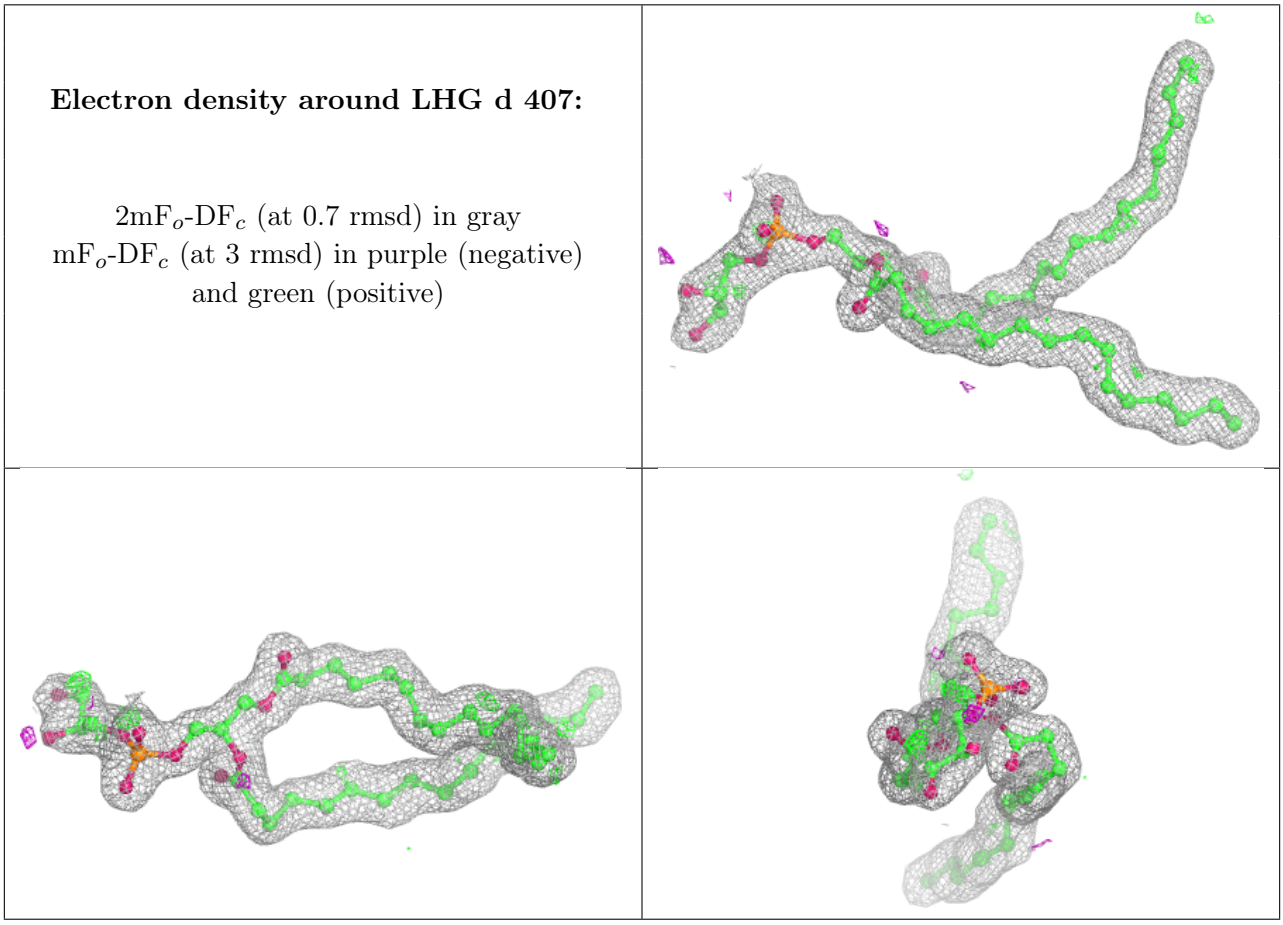
Electron density around LHG d 406:

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



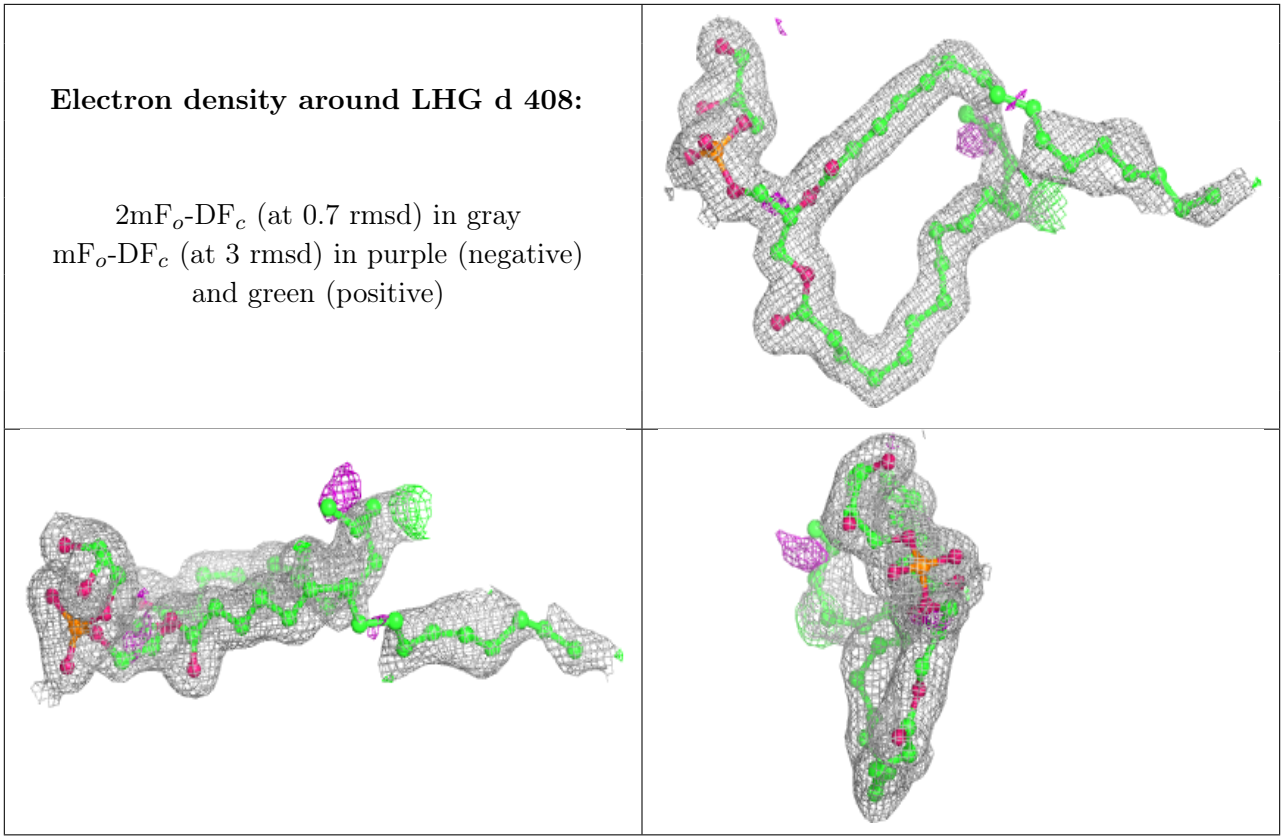
Electron density around LHG d 407:

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



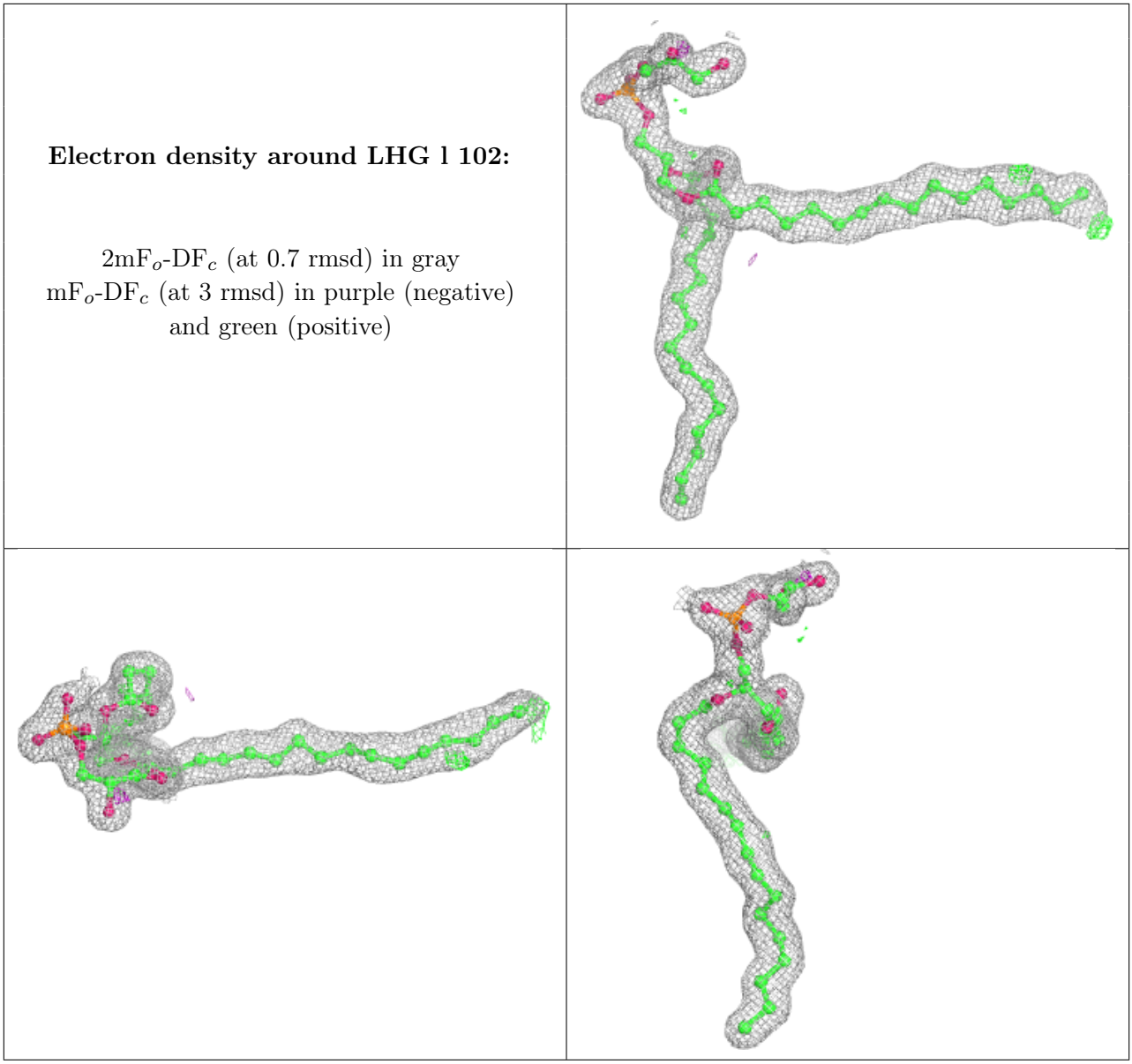
Electron density around LHG d 408:

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



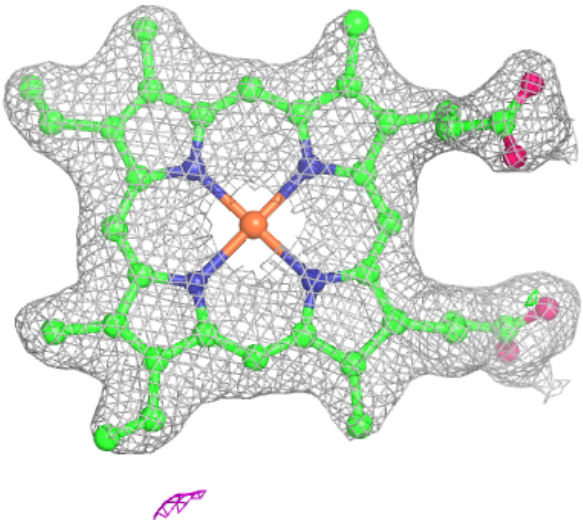
Electron density around LHG l 102:

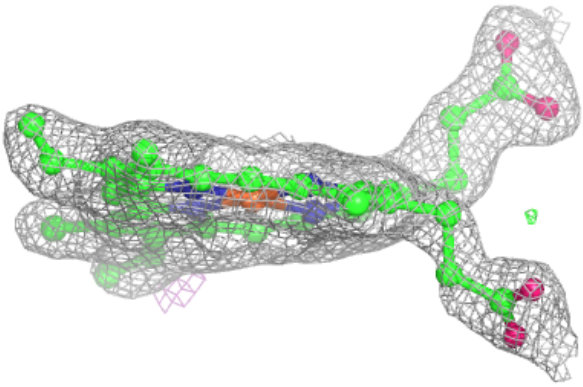
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

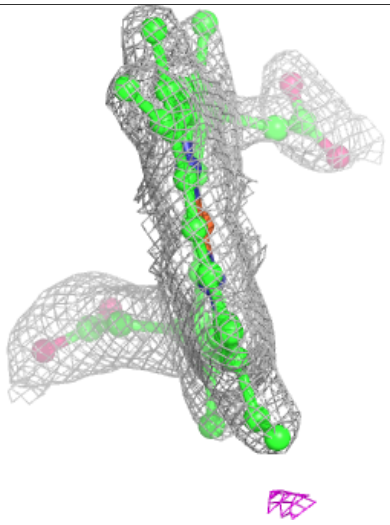


Electron density around HEM e 102:

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

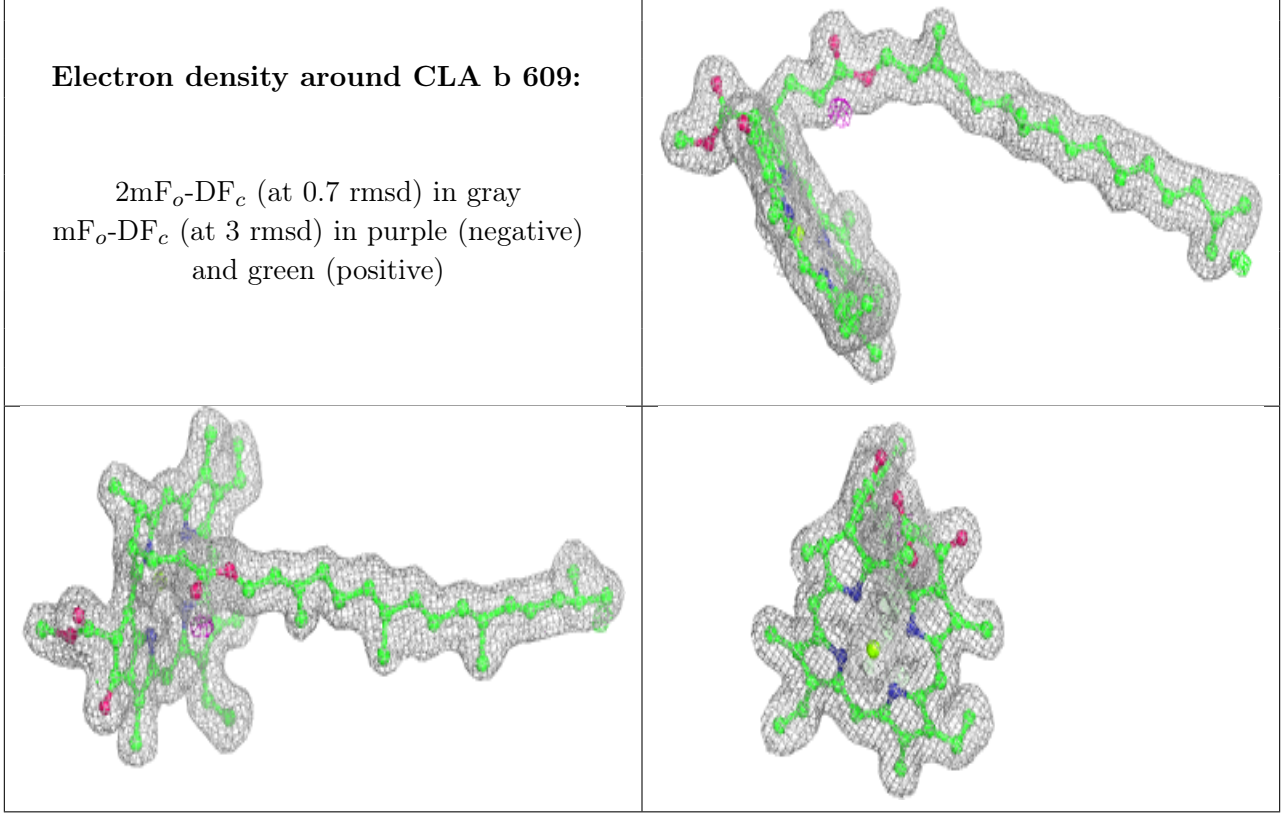






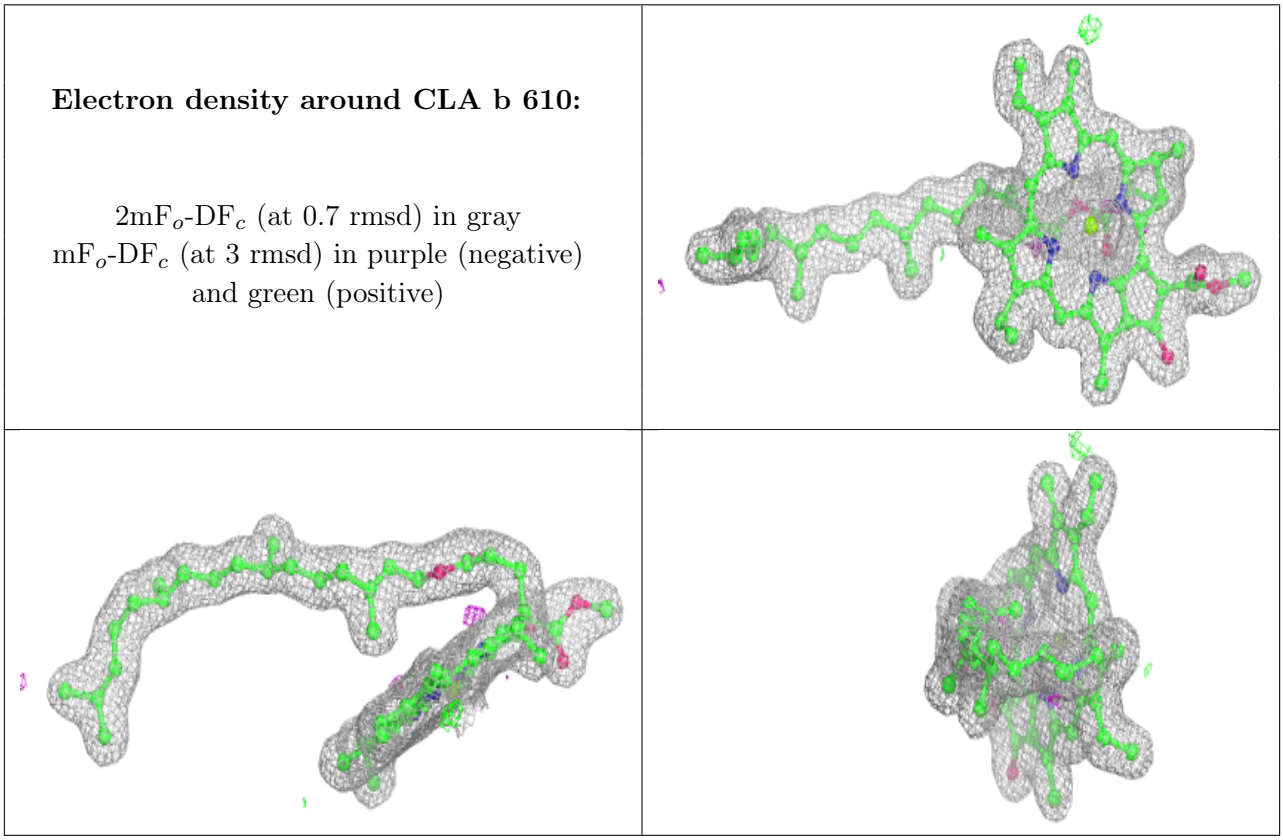
Electron density around CLA b 609:

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



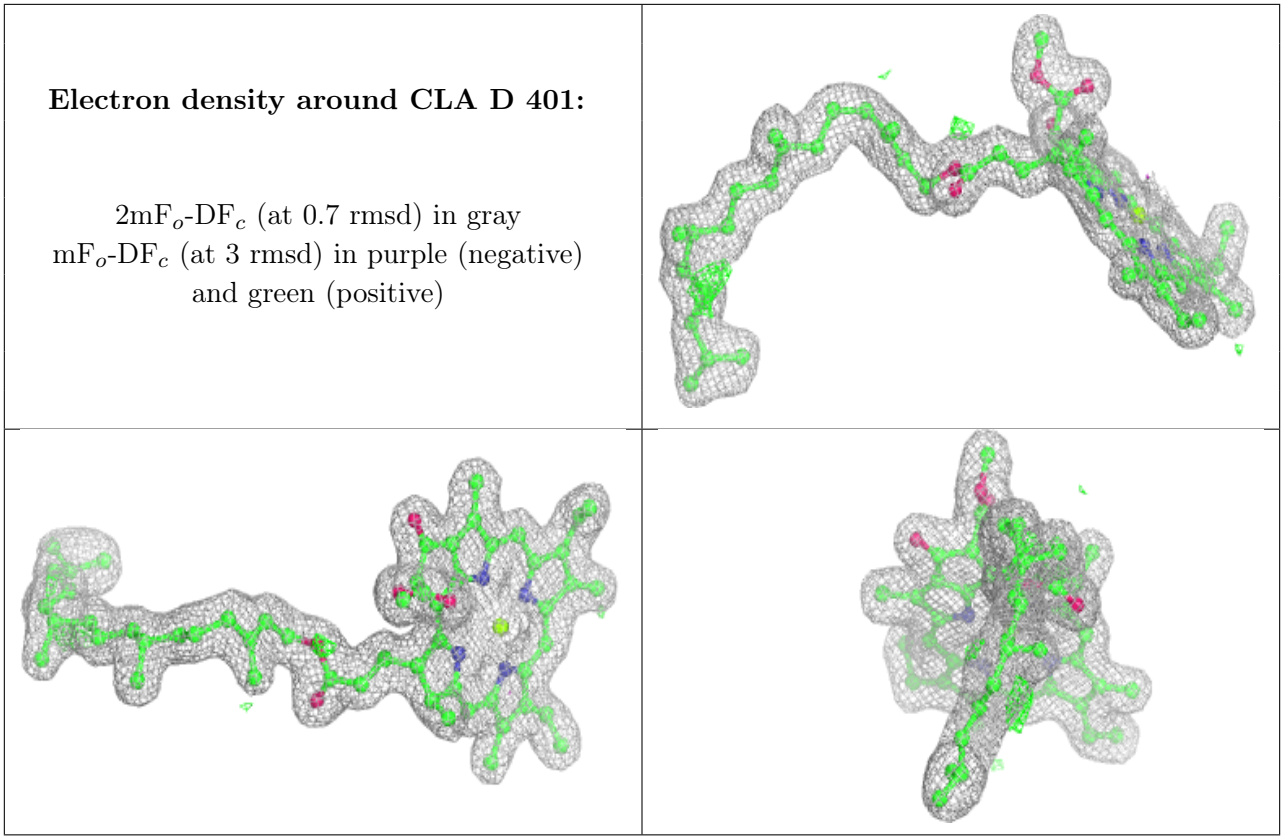
Electron density around CLA b 610:

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



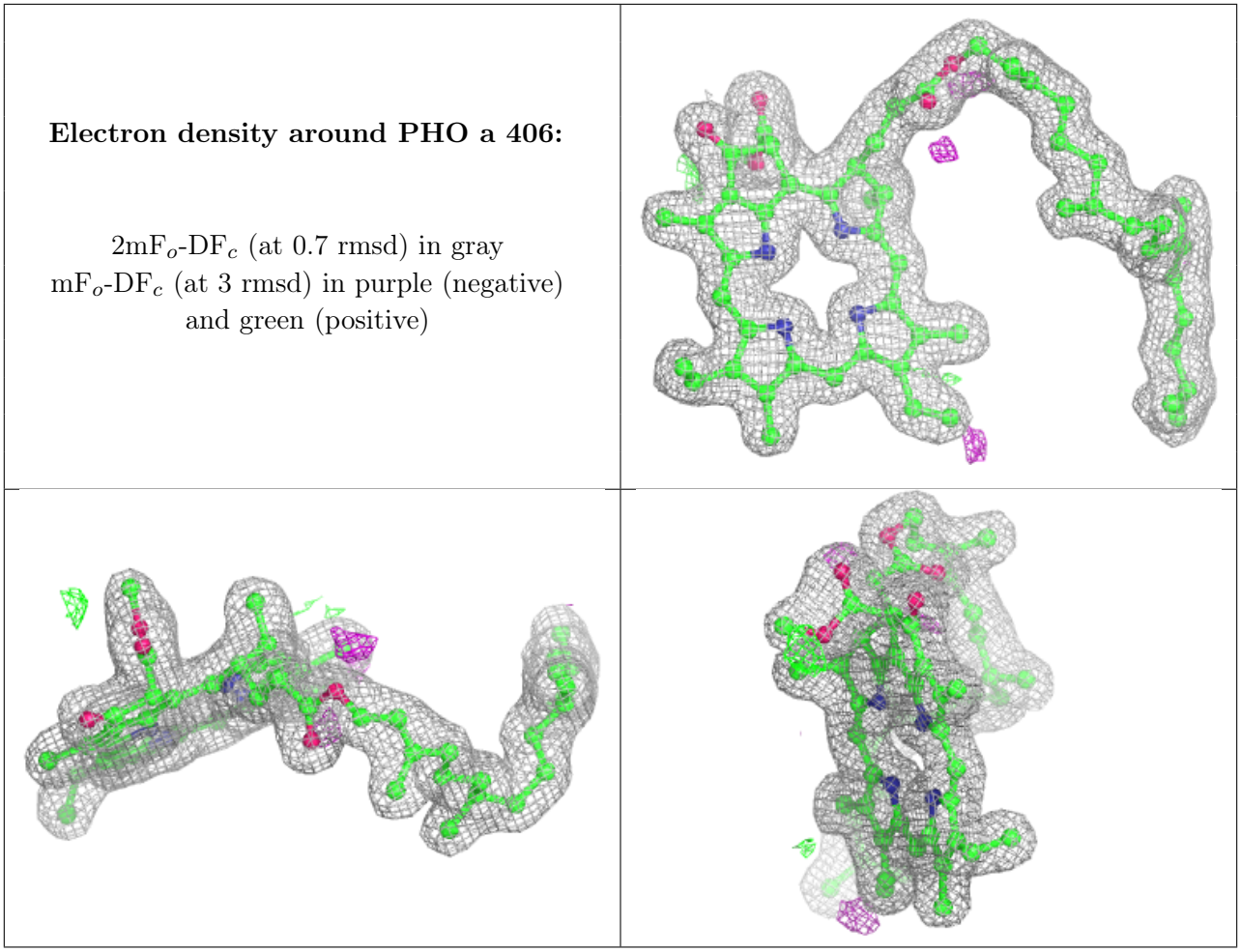
Electron density around CLA D 401:

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



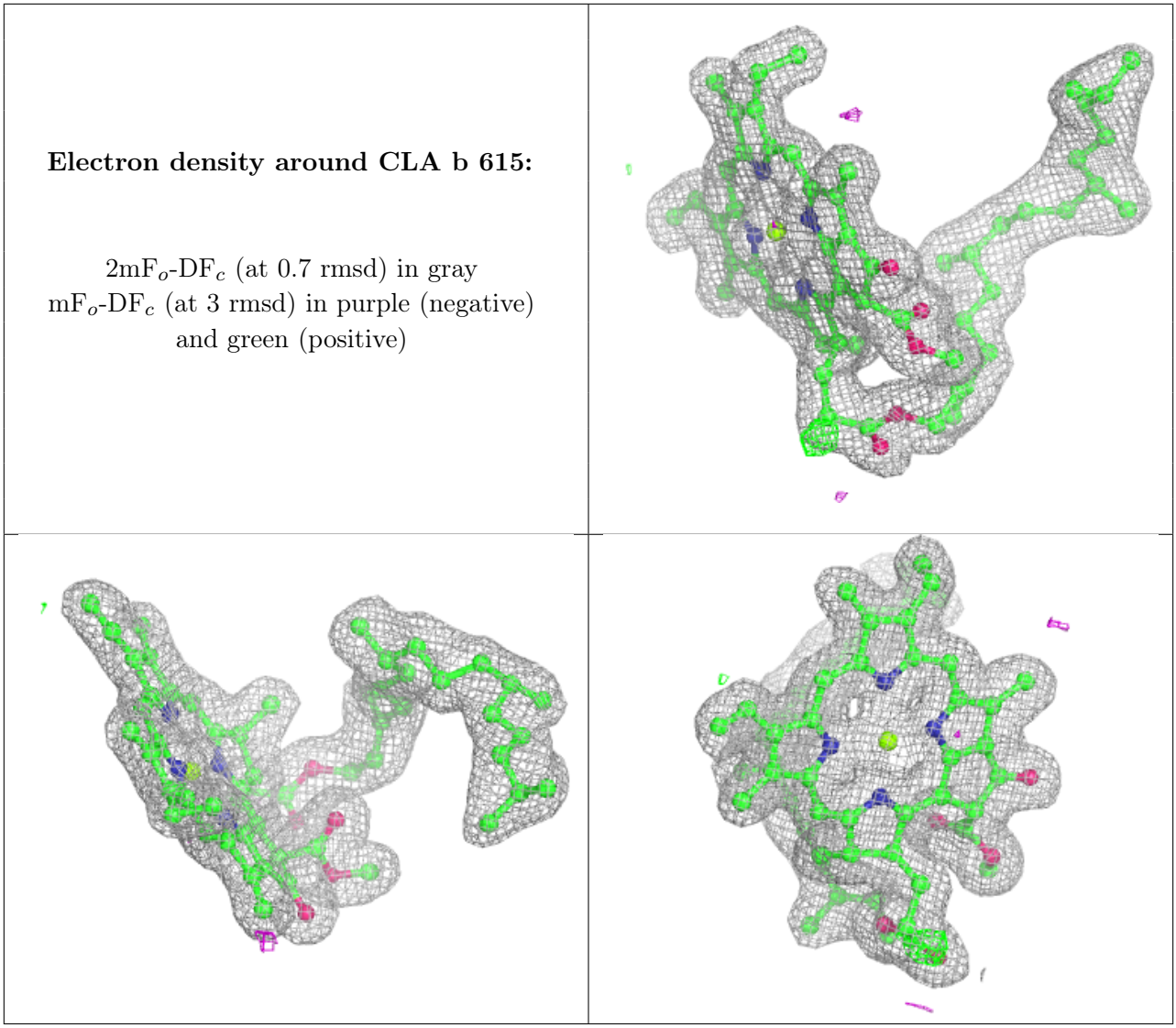
Electron density around PHO a 406:

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



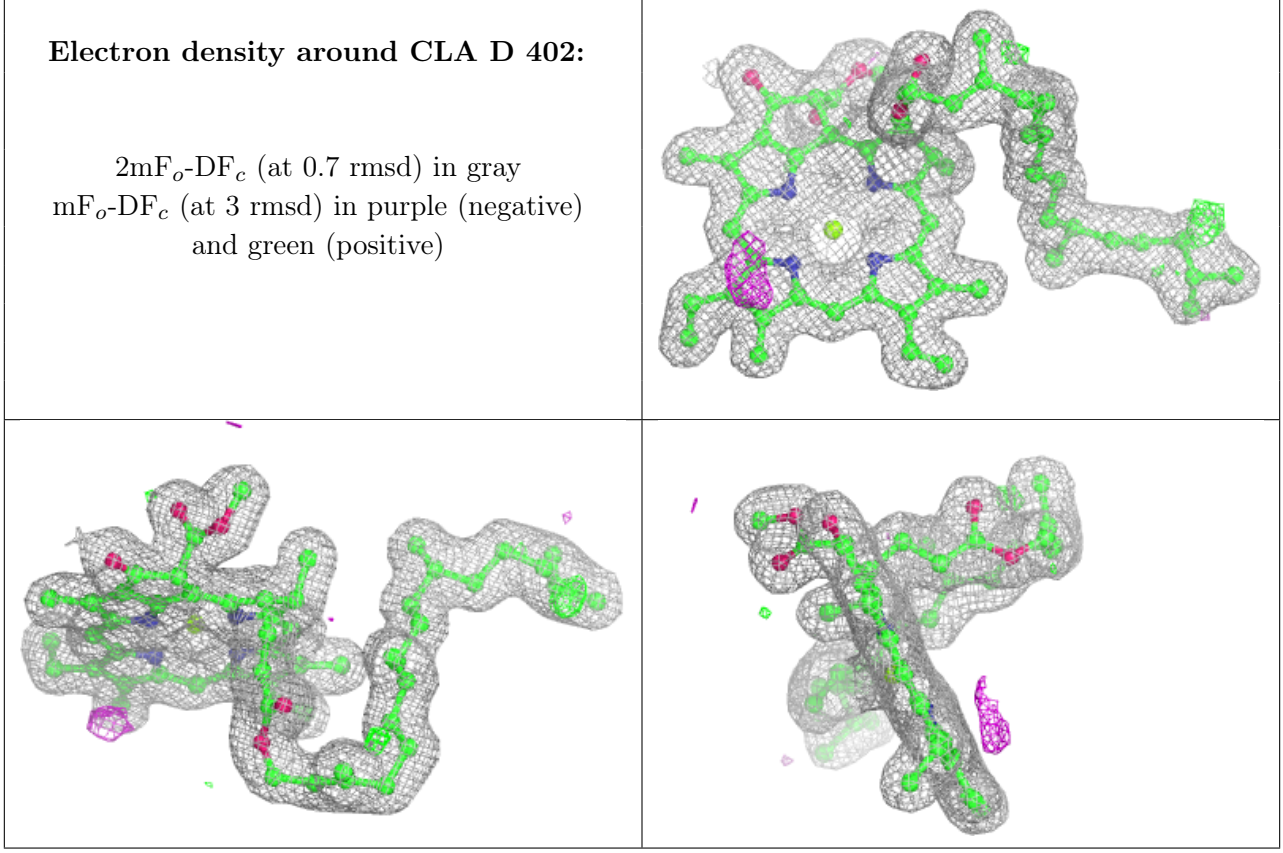
Electron density around CLA b 615:

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



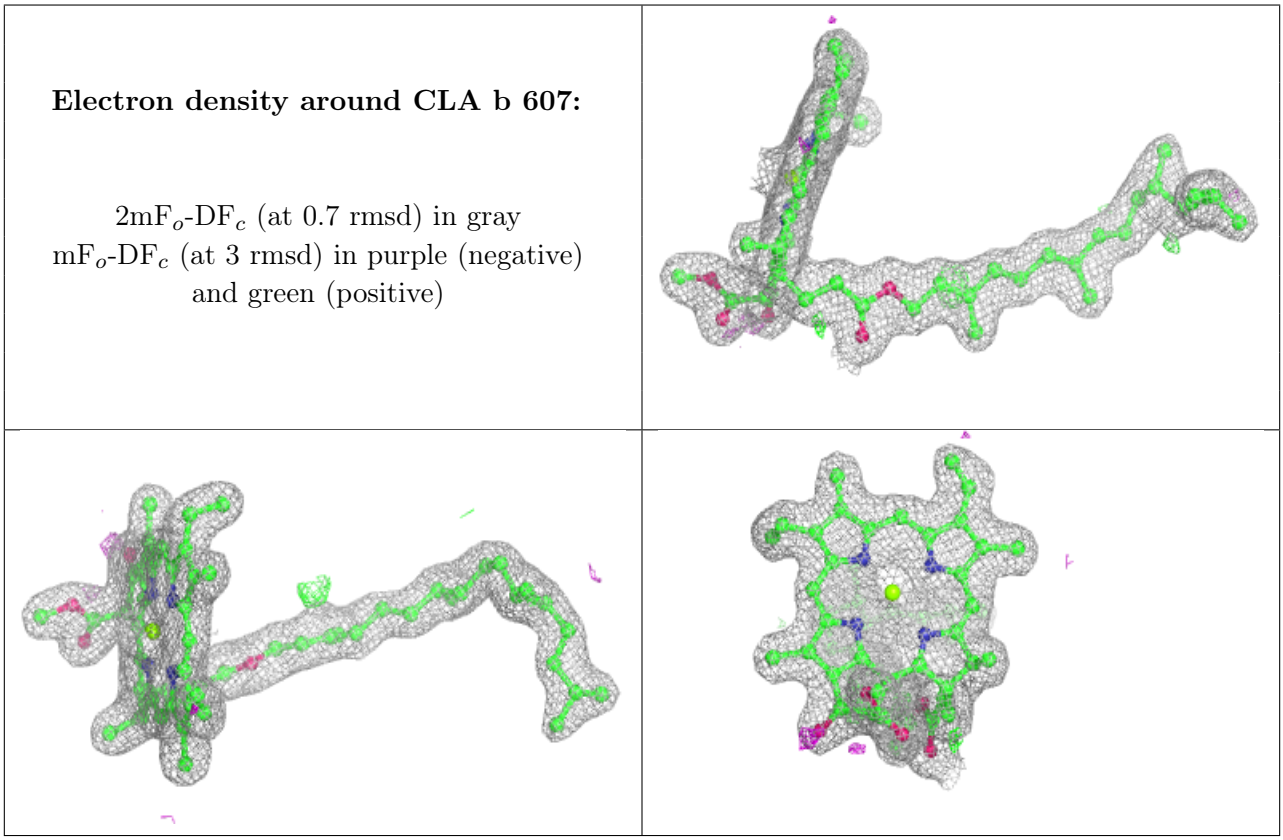
Electron density around CLA D 402:

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



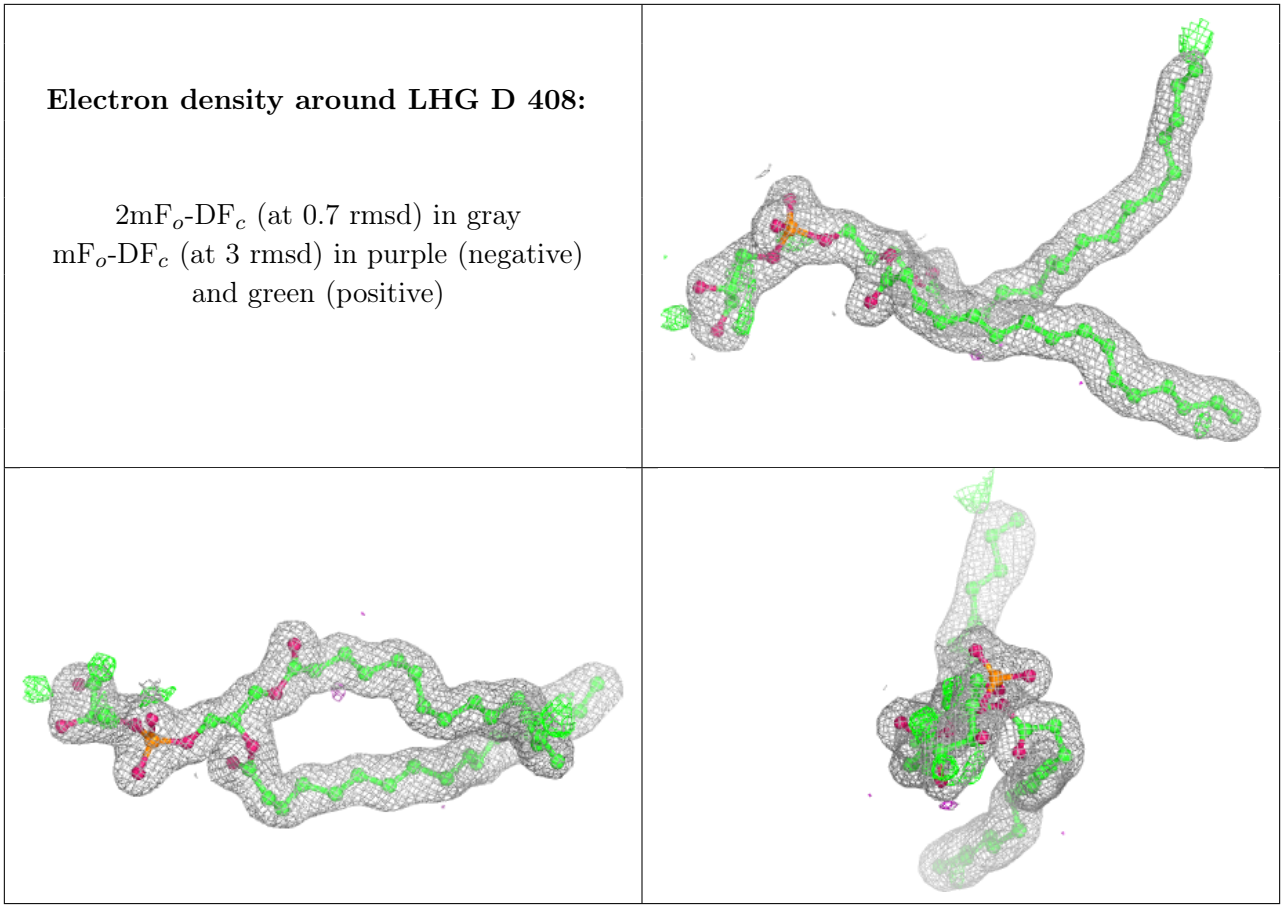
Electron density around CLA b 607:

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



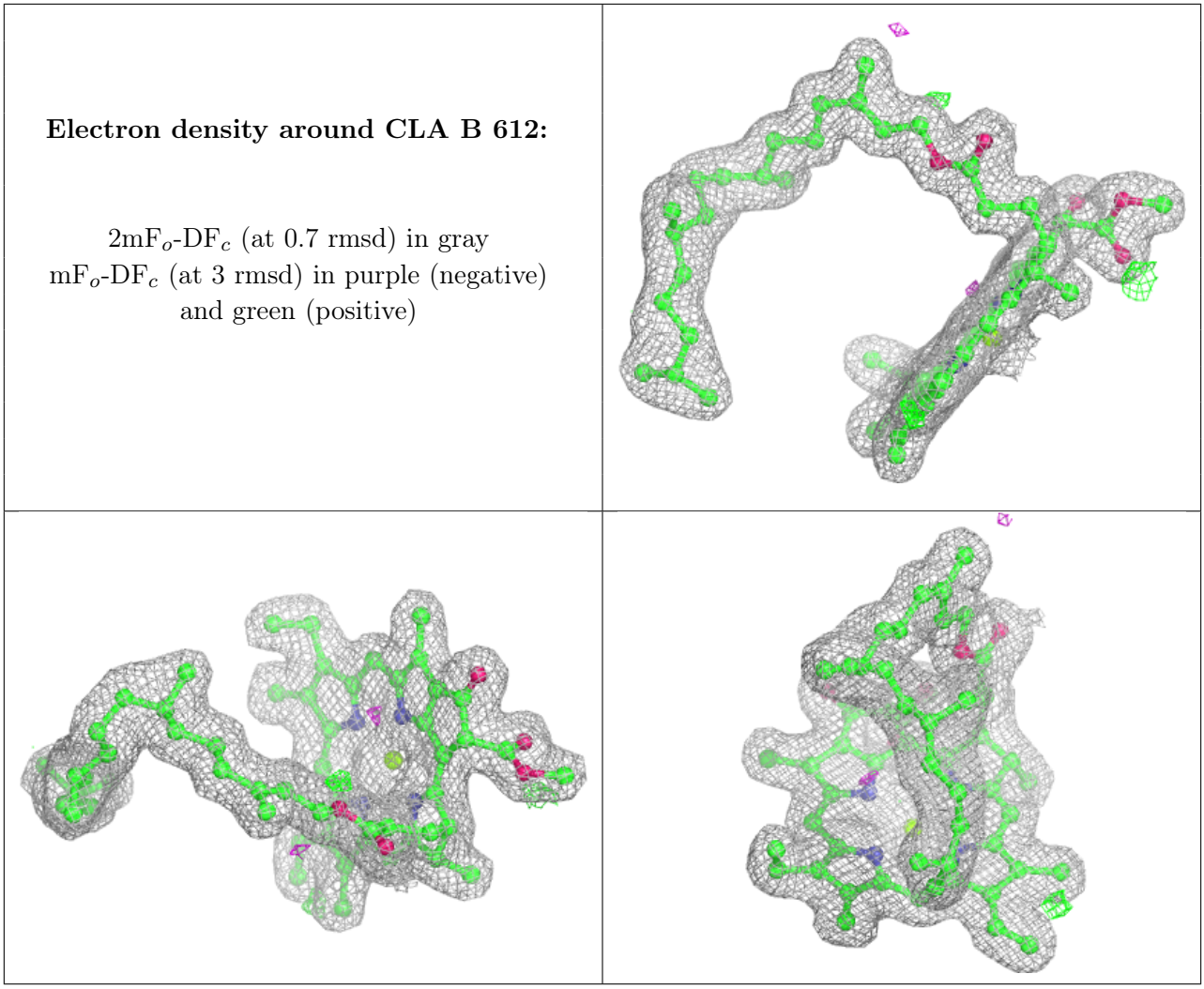
Electron density around LHG D 408:

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



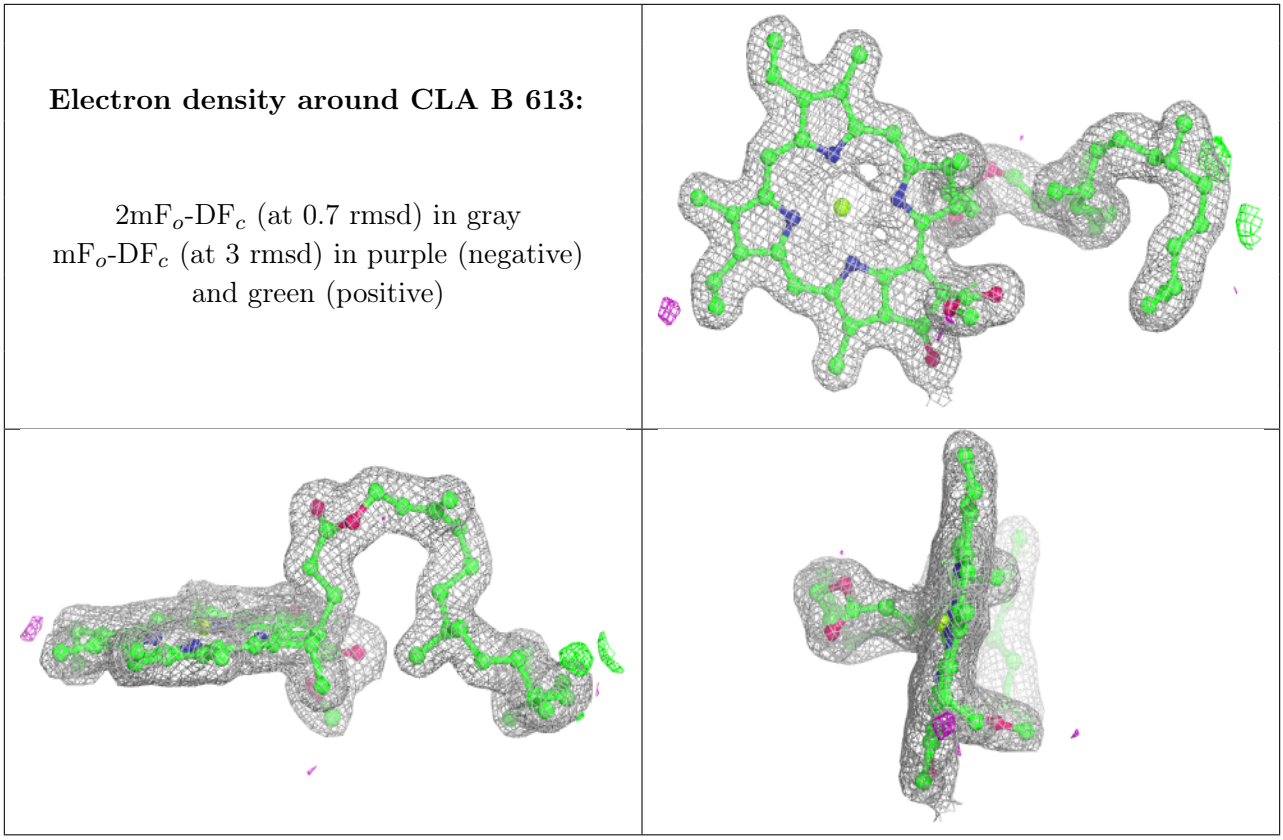
Electron density around CLA B 612:

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



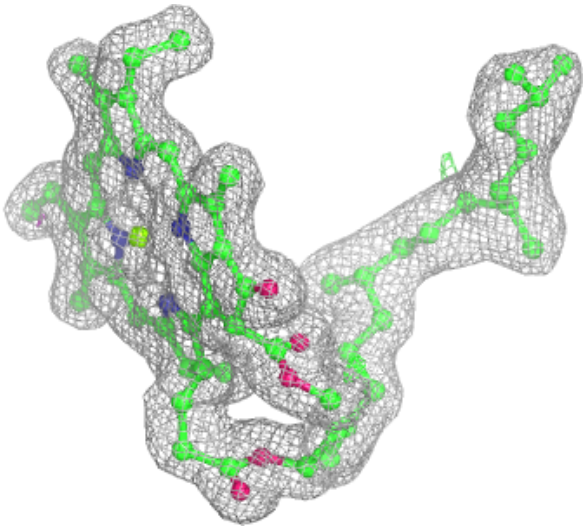
Electron density around CLA B 613:

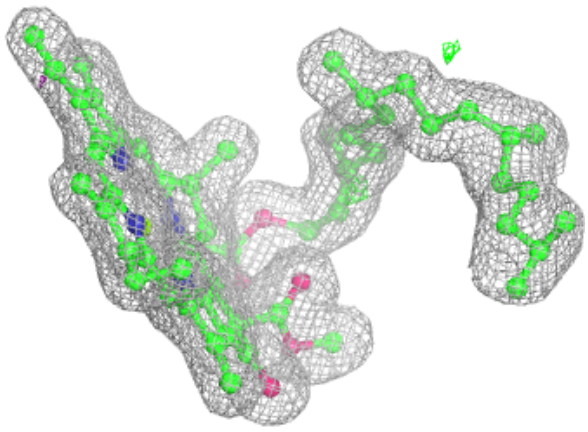
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

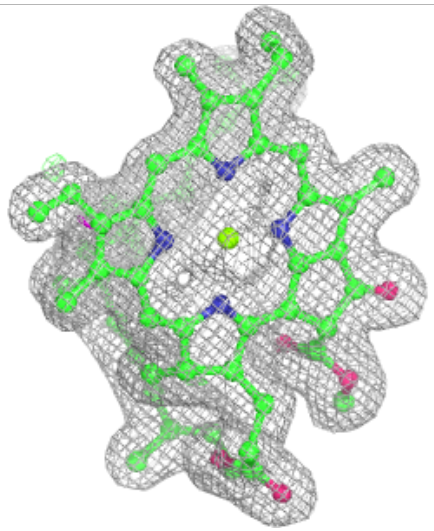


Electron density around CLA B 614:

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

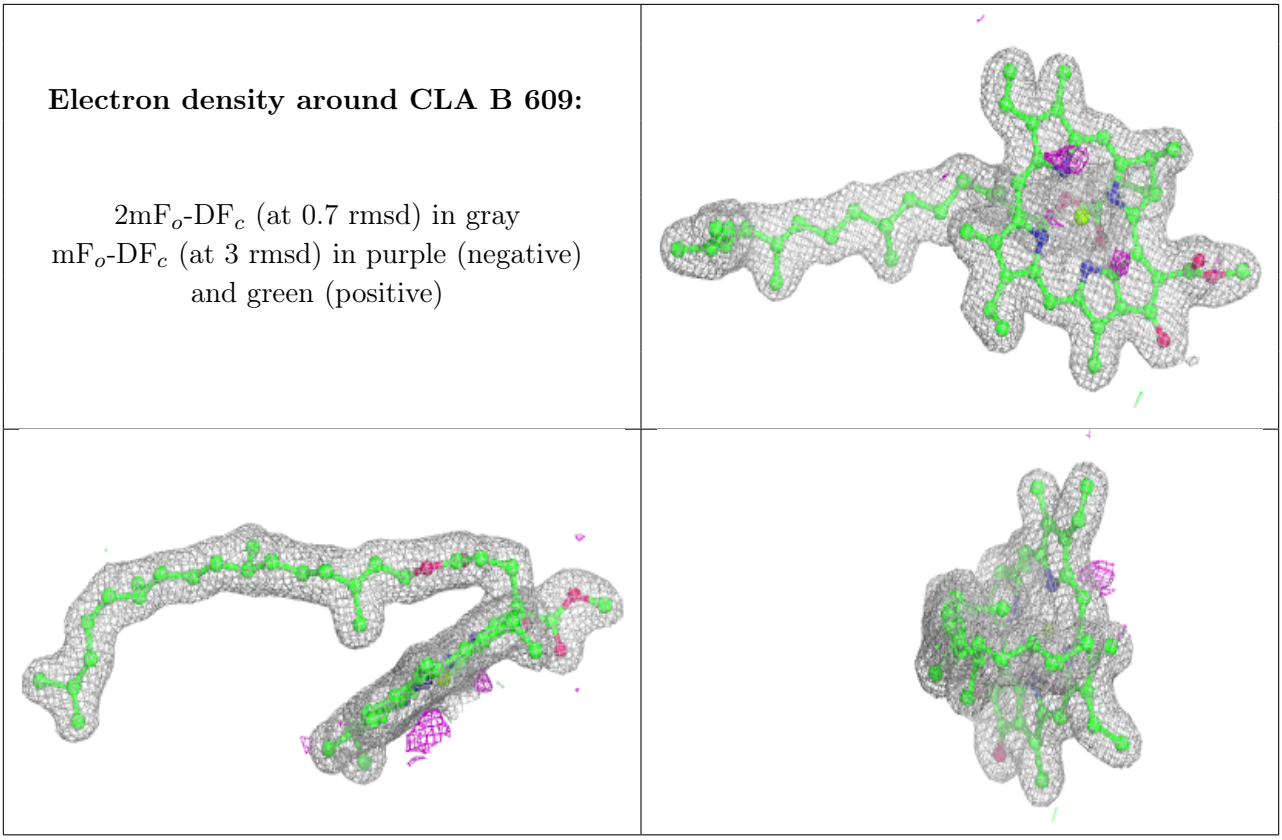






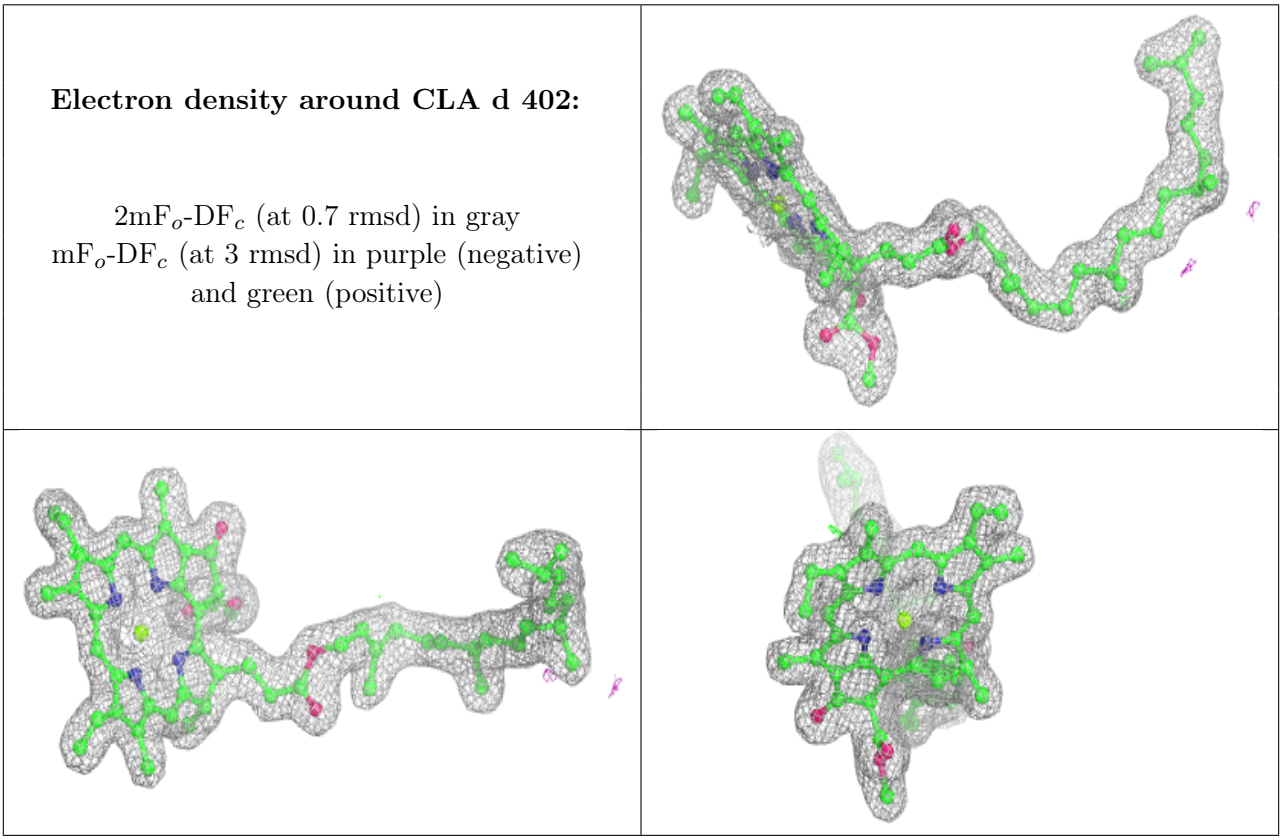
Electron density around CLA B 609:

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



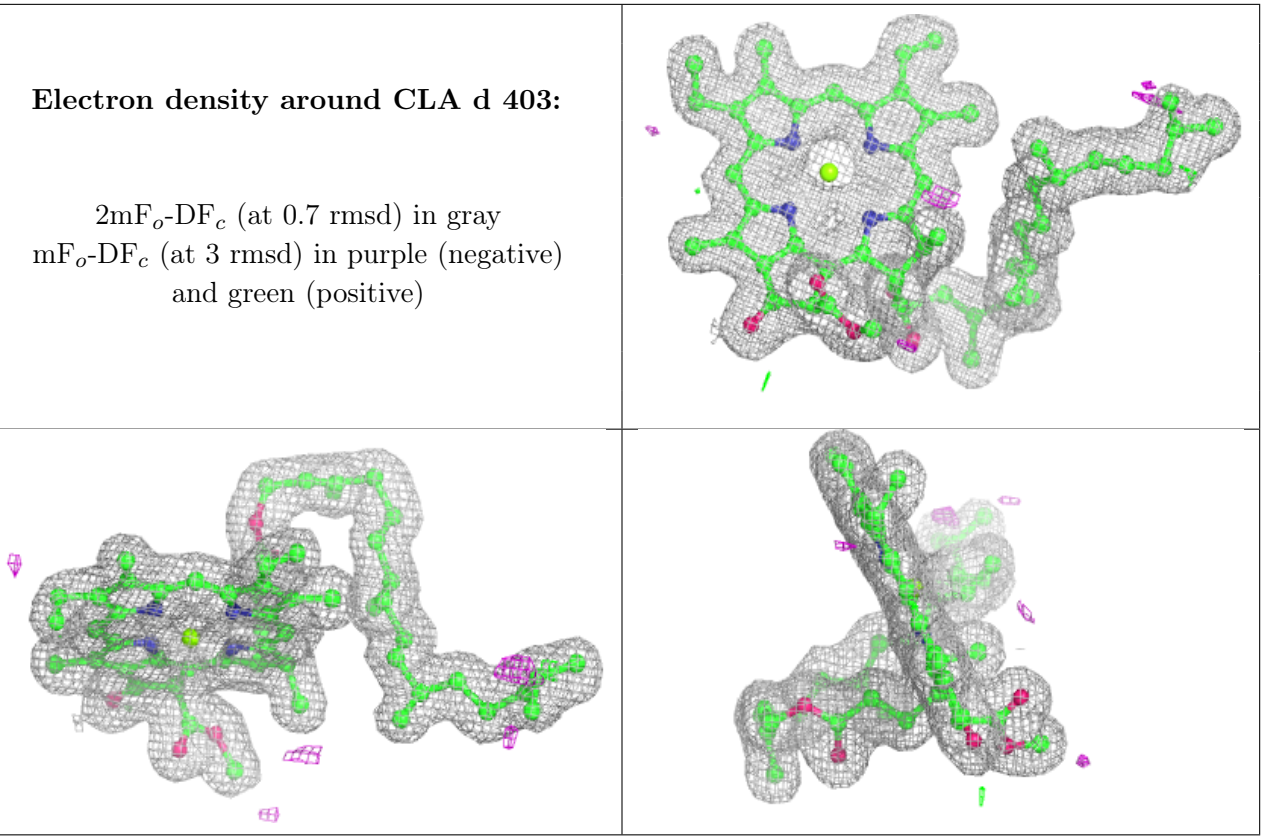
Electron density around CLA d 402:

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



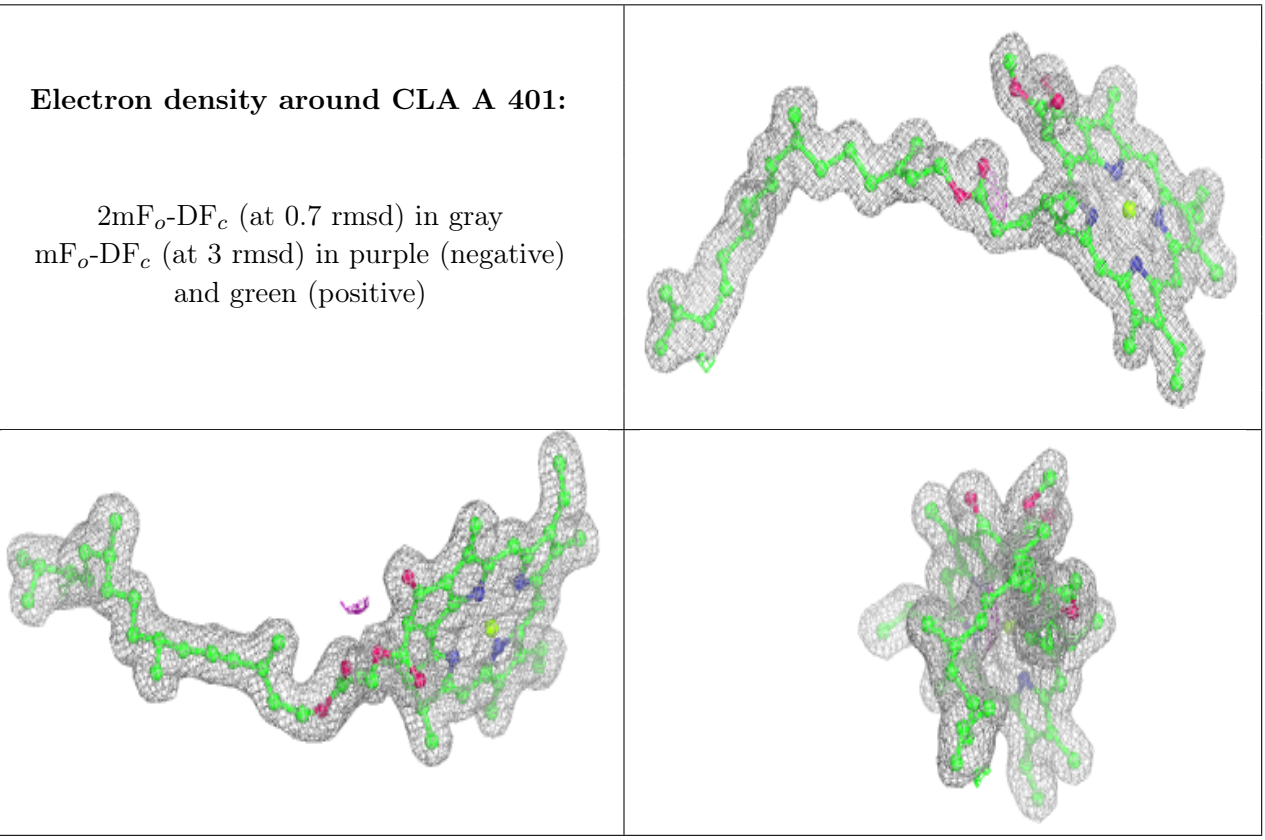
Electron density around CLA d 403:

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



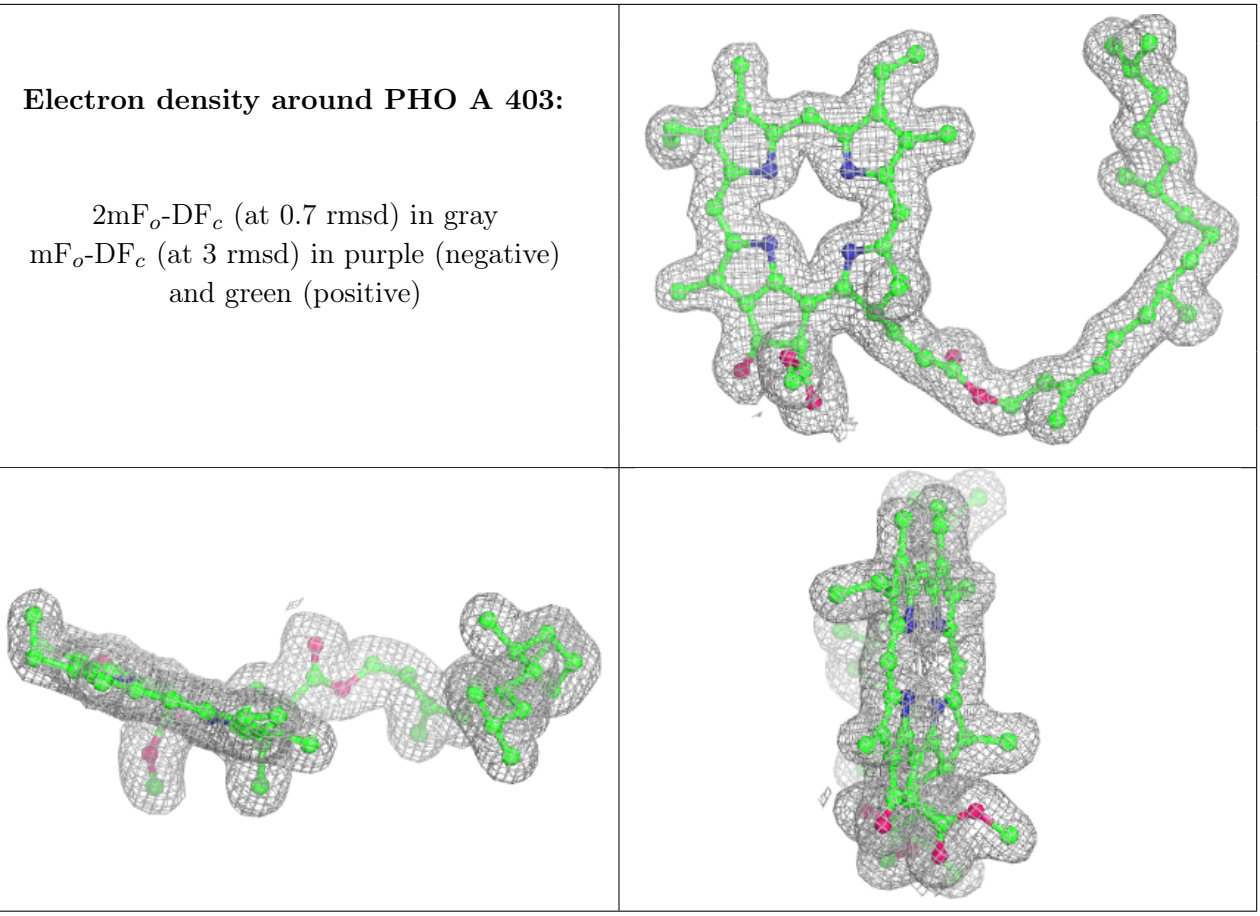
Electron density around CLA A 401:

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



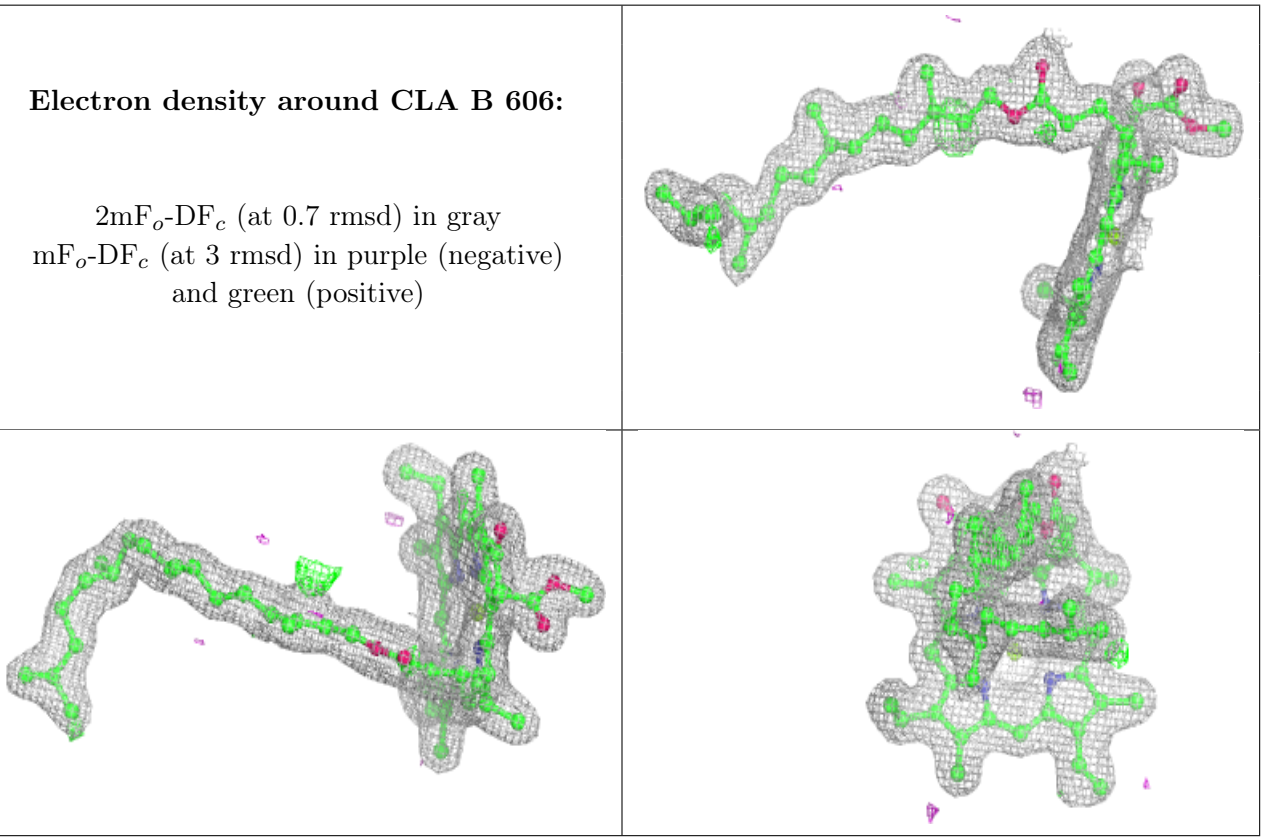
Electron density around PHO A 403:

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



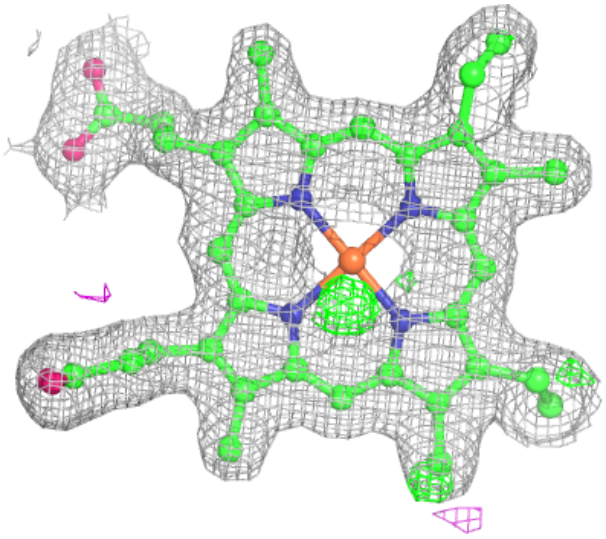
Electron density around CLA B 606:

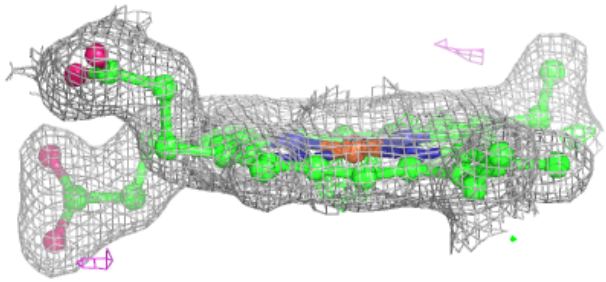
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC v 201:

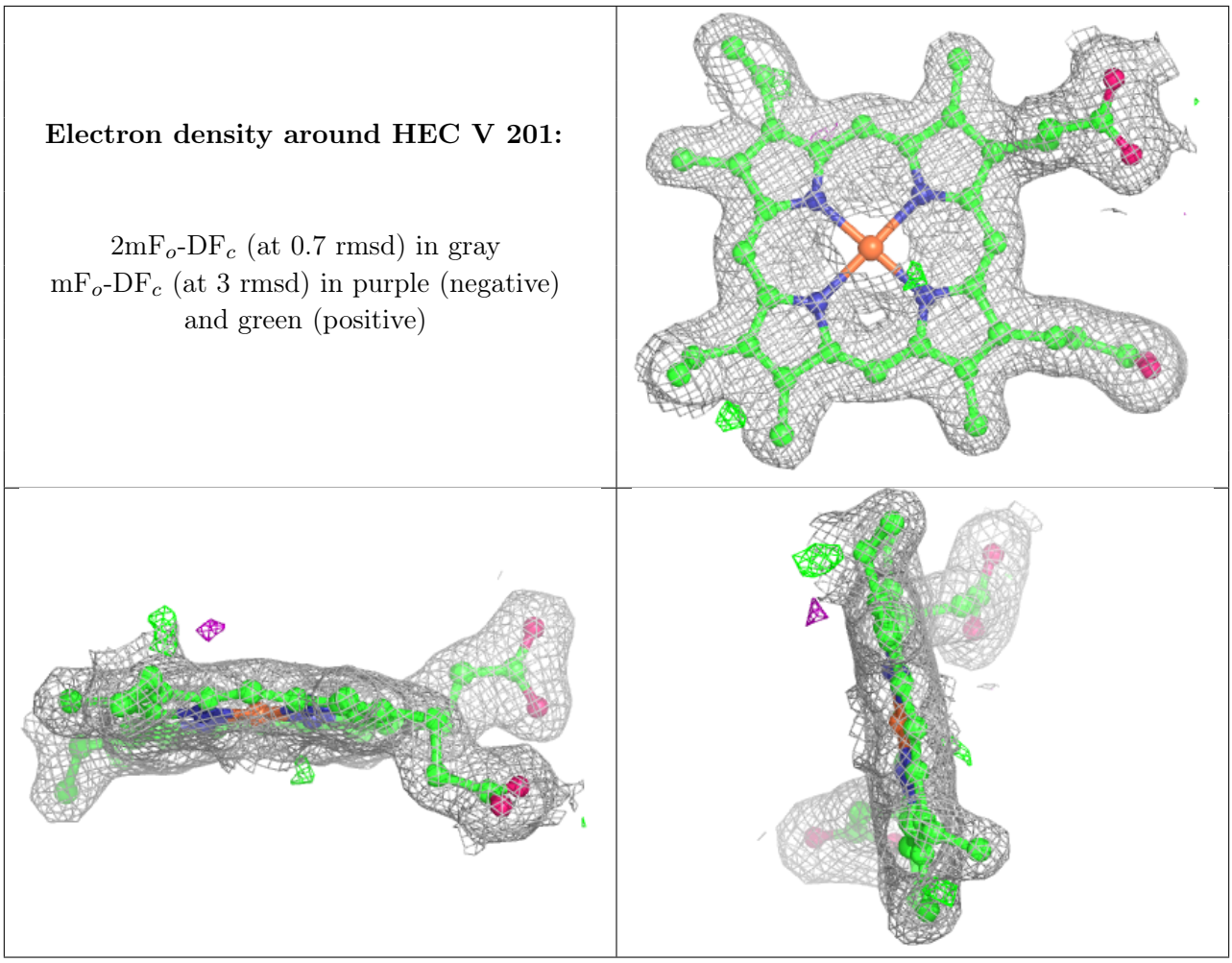
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.