wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2023 – 03:59 AM JST

PDB ID	:	8GN2
Title	:	Crystal structure of PPBQ-bound photosystem II complex
Authors	:	Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on	:	2022-08-22
Resolution	:	1.95 Å(reported)

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

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

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

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

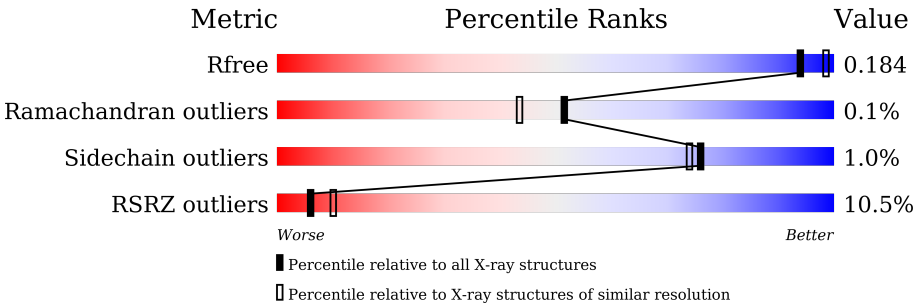
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



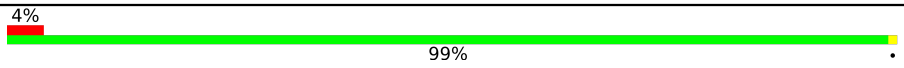
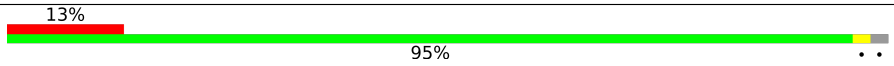
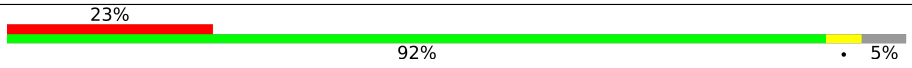
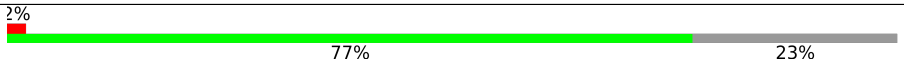
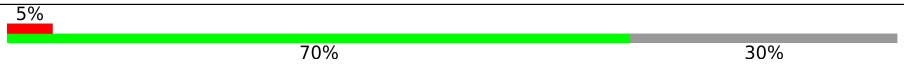
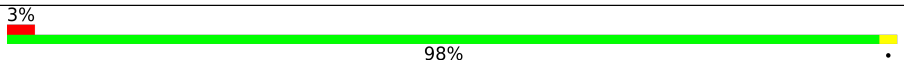
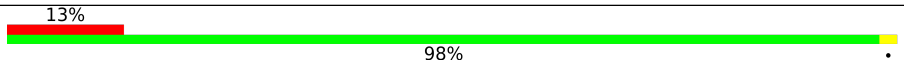
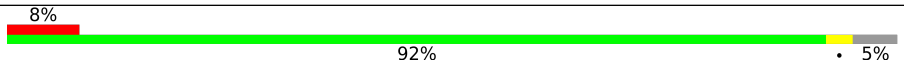
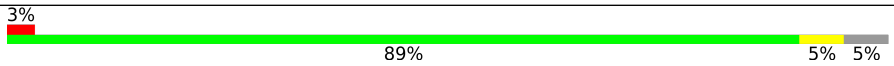
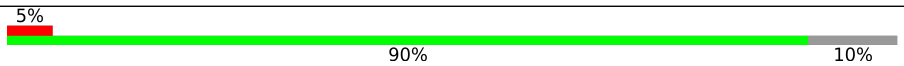
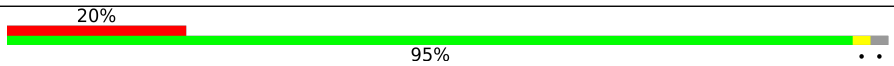
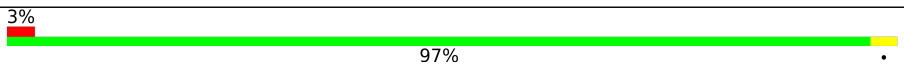
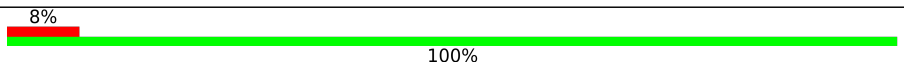
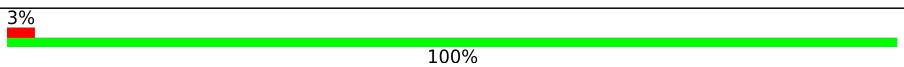
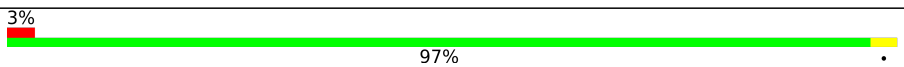
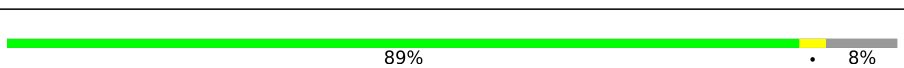
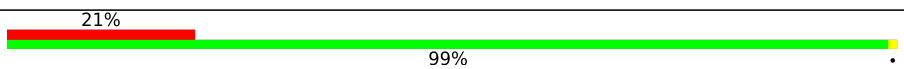
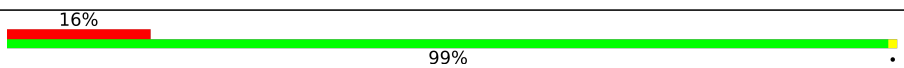
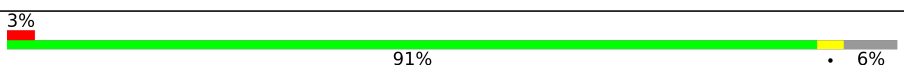
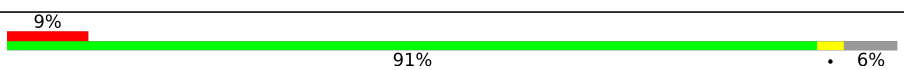
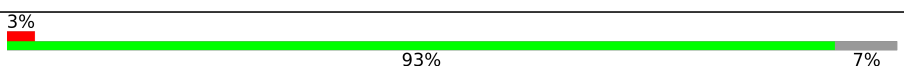
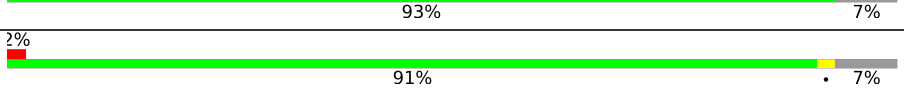
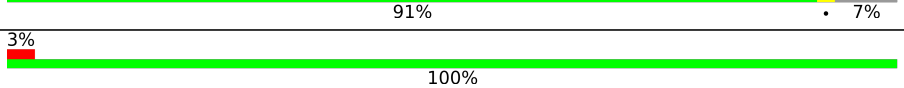
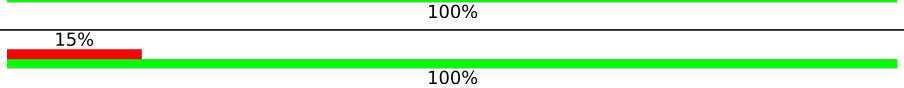
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	344	4% 97%
1	a	344	10% 97%
2	B	505	8% 99%
2	b	505	11% 99%
3	C	455	7% 98%
3	c	455	8% 99%
4	D	342	3% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	Y	30	33% 90% 7%
17	y	30	37% 90% 7%
18	X	40	15% 95% 5%
18	x	40	10% 92% 8%
19	Z	62	39% 97%
19	z	62	58% 92% 5%
20	R	41	83% 80% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	513	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	404	X	-	-	-
29	LMT	C	521	-	-	-	X
29	LMT	c	523	-	-	-	X
31	UNL	A	418	-	-	-	X
31	UNL	B	639	-	-	-	X
31	UNL	E	103	-	-	-	X
31	UNL	a	419	-	-	-	X
31	UNL	b	635	-	-	-	X
31	UNL	h	1201	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	UNL	h	1207	-	-	-	X
31	UNL	i	103	-	-	-	X
33	PL9	A	422[B]	-	-	-	X
33	PL9	a	425[B]	-	-	-	X
36	HTG	D	413	-	-	-	X
36	HTG	c	525	-	-	-	X

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 55061 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
			2624	1720	431	458	15			
1	a	334	Total	C	N	O	S	0	3	0
			2620	1717	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	9	0
			4007	2631	670	693	13			
2	b	503	Total	C	N	O	S	0	10	0
			3989	2621	661	694	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	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	2	0
			3516	2305	587	611	13			

There are 8 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	2	0
			2731	1812	444	463	12			
4	d	342	Total	C	N	O	S	0	3	0
			2738	1815	447	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			657	429	106	122			
5	e	79	Total	C	N	O	0	0	0
			639	419	103	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total 285	C 195	N 42	O 47	S 1	0	0	0
8	i	36	Total 296	C 200	N 46	O 49	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	39	Total 271	C 182	N 40	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 205	N 42	O 46	0	1	0
10	k	37	Total 286	C 198	N 42	O 46	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 305	C 205	N 48	O 51	S 1	0	1	0
11	l	37	Total 309	C 209	N 48	O 51	S 1	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 265	C 178	N 38	O 48	S 1	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	3	0
			281	191	39	50	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	6	0
			1884	1180	313	386	5			
13	o	243	Total	C	N	O	S	0	5	0
			1871	1172	311	382	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			776	493	130	153			
15	u	97	Total	C	N	O	0	1	0
			780	495	130	155			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1063	676	178	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	28	Total	C	N	O	S	0	0	0
			198	130	33	32	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	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
			279	187	45	47			
18	x	37	Total	C	N	O	0	1	0
			273	185	43	45			

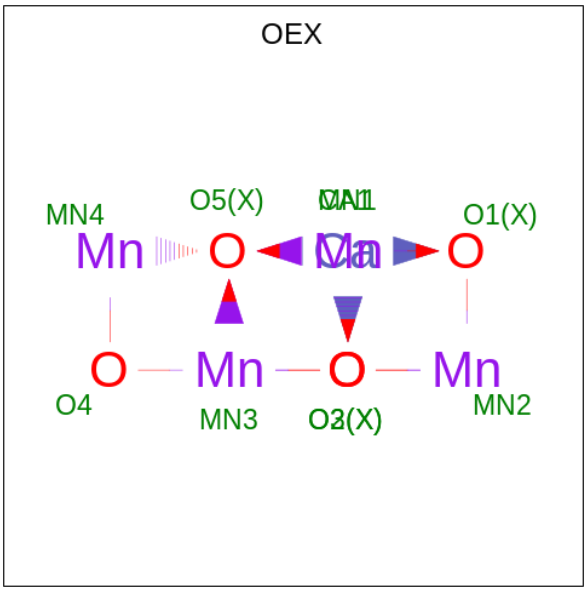
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			461	319	67	73	2			
19	z	60	Total	C	N	O	S	0	0	0
			446	306	69	70	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			240	159	42	39			

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



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

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

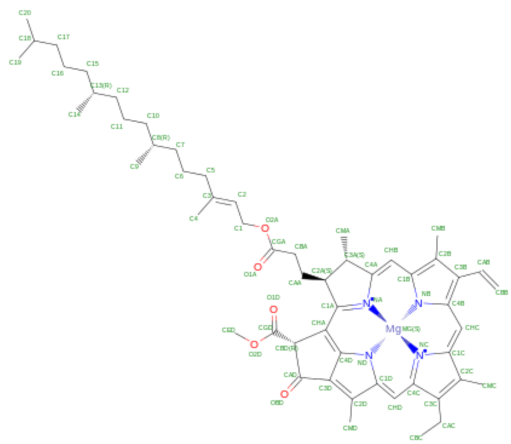
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		
22	a	1	Total	Fe	0	0
			1	1		

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

CLA



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

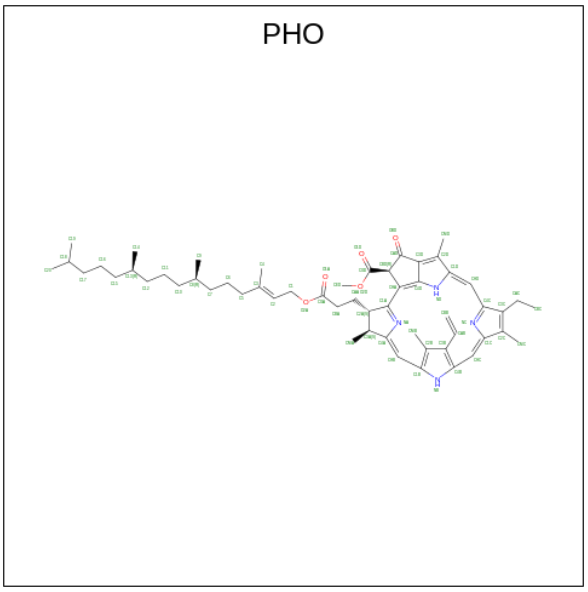
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	a	1	Total C Mg N O 65 55 1 4 5	0	0
24	a	1	Total C Mg N O 65 55 1 4 5	0	0
24	a	1	Total C Mg N O 65 55 1 4 5	0	0
24	a	1	Total C Mg N O 65 55 1 4 5	0	0
24	b	1	Total C Mg N O 65 55 1 4 5	0	0
24	b	1	Total C Mg N O 65 55 1 4 5	0	0
24	b	1	Total C Mg N O 65 55 1 4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

Continued on next page...

Continued from previous page...

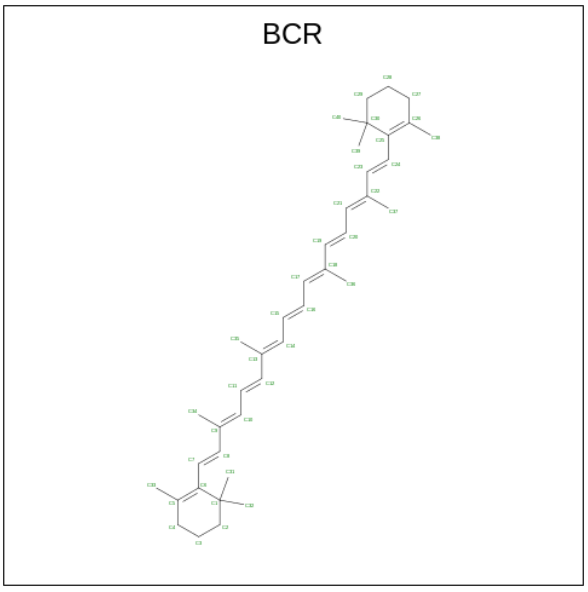
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

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



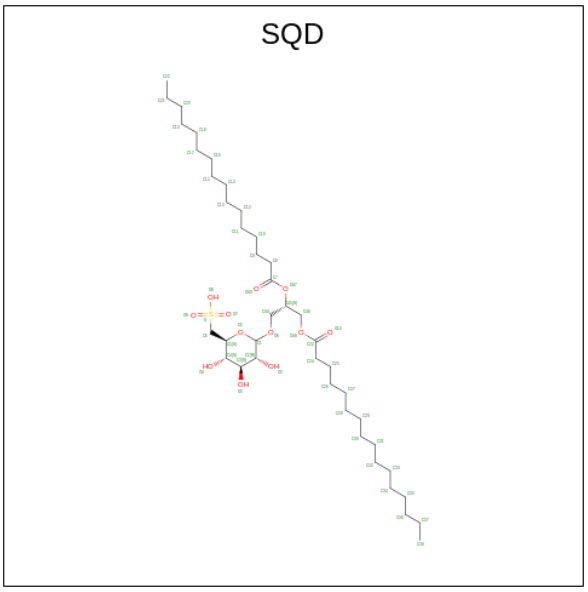
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



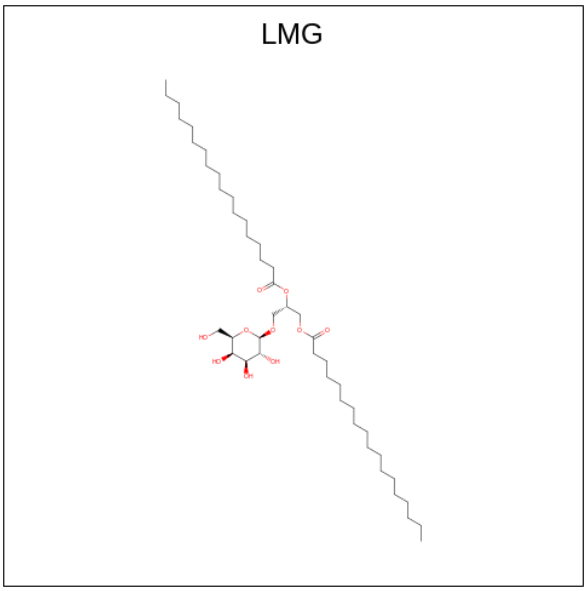
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



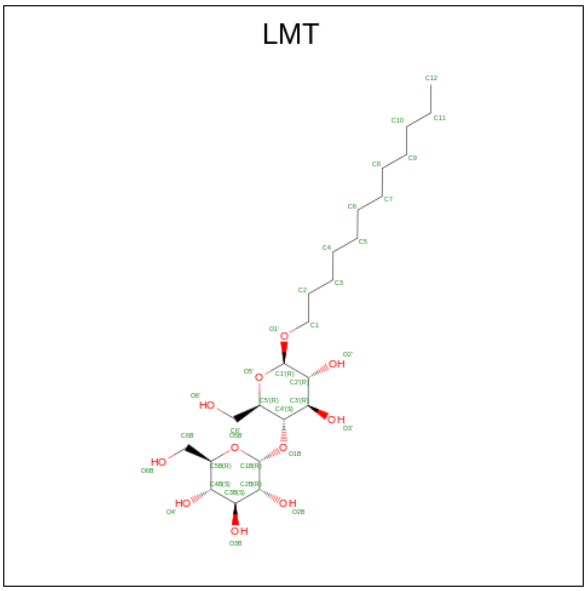
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			45	32	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			33	23	9	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

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



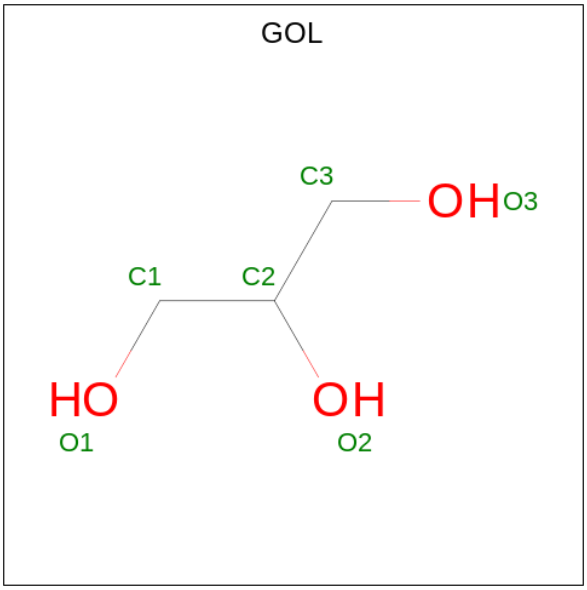
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			24	18	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			24	18	6		
29	J	1	Total	C	O	0	0
			24	18	6		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			24	18	6		
29	Z	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	c	1	Total	C	O	0	0
			35	24	11		
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	z	1	Total C O 32 21 11	0	0

- Molecule 30 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	E	1	Total	C	O	0	0
			6	3	3		
30	L	1	Total	C	O	0	0
			6	3	3		
30	M	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	T	1	Total	C	O	0	0
			6	3	3		
30	T	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	h	1	Total	C	O	0	0
			6	3	3		
30	k	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		

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

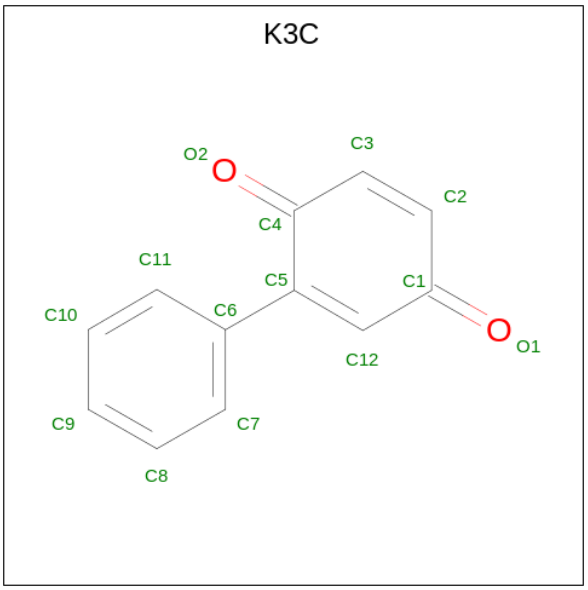
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	4	Total C O 74 69 5	0	0
31	B	7	Total C O 99 95 4	0	0
31	C	3	Total C O 73 66 7	0	0
31	D	3	Total C O 68 63 5	0	0
31	E	2	Total C 30 30	0	0
31	H	1	Total C 8 8	0	0
31	I	3	Total C 47 47	0	0
31	J	2	Total C 31 31	0	0
31	T	1	Total C 9 9	0	0
31	Y	1	Total C 12 12	0	0
31	X	1	Total C 16 16	0	0
31	a	4	Total C O 73 68 5	0	0
31	b	5	Total C 70 70	0	0
31	c	4	Total C O 74 67 7	0	0
31	d	2	Total C O 56 51 5	0	0
31	e	1	Total C 15 15	0	0
31	h	3	Total C 39 39	0	0
31	i	3	Total C O 71 66 5	0	0
31	j	2	Total C O 34 32 2	0	0
31	k	1	Total C 16 16	0	0
31	l	1	Total C O 16 14 2	0	0
31	t	1	Total C 8 8	0	0

Continued on next page...

Continued from previous page...

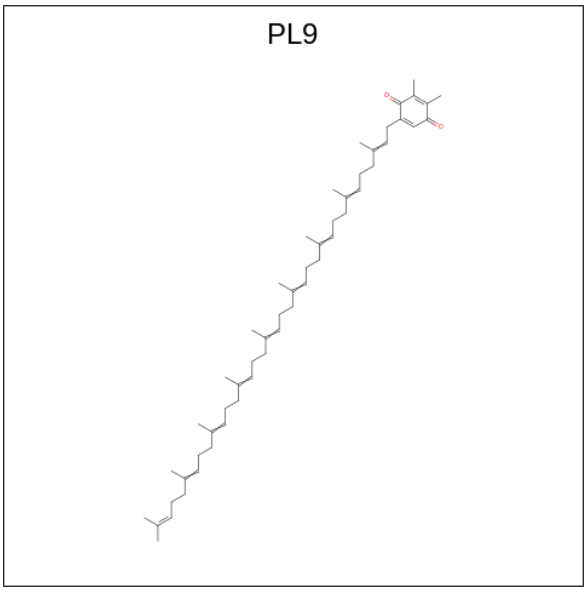
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	x	2	Total C O 30 28 2	0	0

- Molecule 32 is 2-phenylcyclohexa-2,5-diene-1,4-dione (three-letter code: K3C) (formula: $C_{12}H_8O_2$) (labeled as "Ligand of Interest" by depositor).



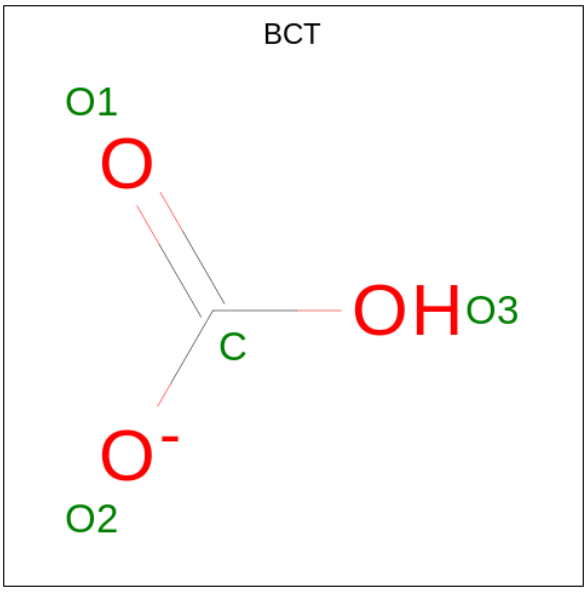
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 14 12 2	0	1
32	a	1	Total C O 14 12 2	0	1

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).

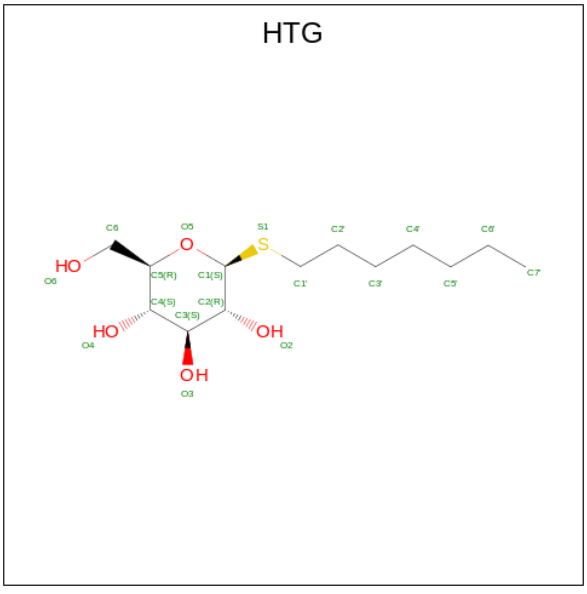


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	1	Total C O 4 1 3	0	0
34	a	1	Total C O 4 1 3	0	0

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

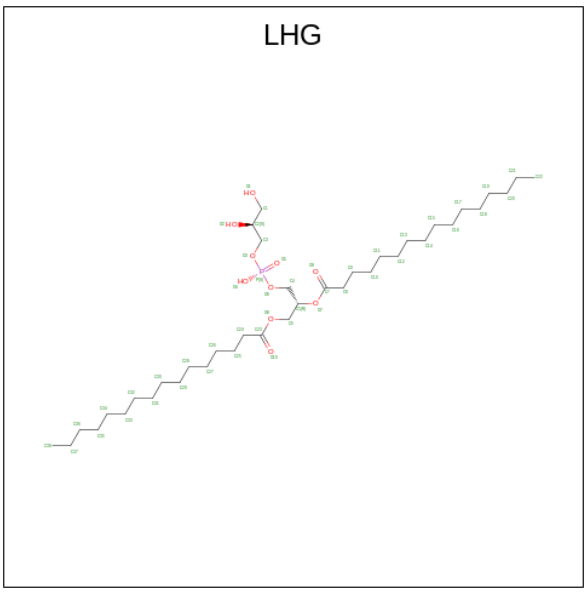
- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 38 26 10 2	0	1
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0
36	C	1	Total C O S 19 13 5 1	0	0
36	D	1	Total C O S 19 13 5 1	0	0
36	I	1	Total C O S 19 13 5 1	0	0
36	O	1	Total C O S 19 13 5 1	0	0
36	U	1	Total C S 9 8 1	0	0
36	V	1	Total C O S 13 7 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	b	1	Total C O S 19 13 5 1	0	0
36	c	1	Total C O S 19 13 5 1	0	0
36	c	1	Total C O S 19 13 5 1	0	0
36	d	1	Total C O S 19 13 5 1	0	0
36	h	1	Total C O S 19 13 5 1	0	0
36	o	1	Total C O S 19 13 5 1	0	0
36	u	1	Total C O S 14 10 3 1	0	0

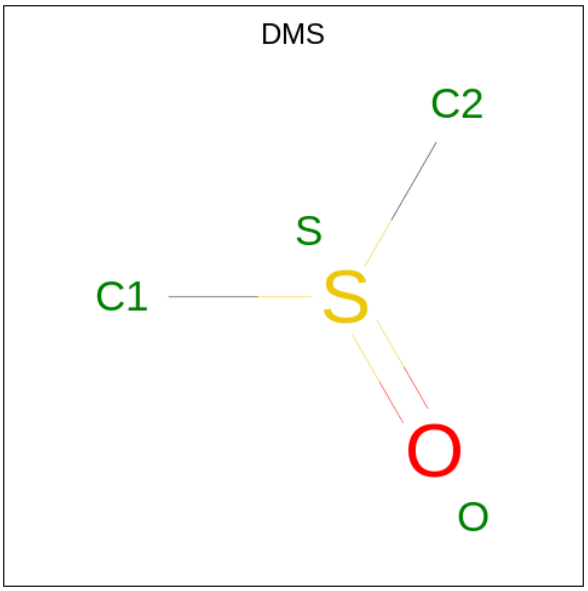
- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	B	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			46	35	10	1		
37	E	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			39	28	10	1		
37	e	1	Total	C	O	P	0	0
			40	29	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



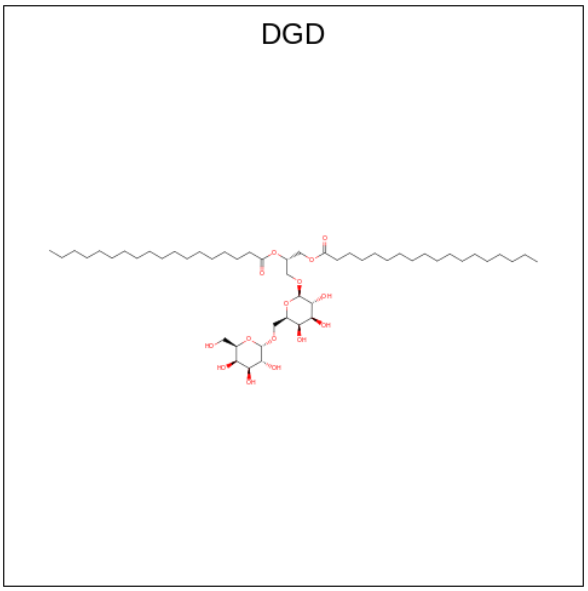
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	B	1	Total	C	O	S	0	0
			4	2	1	1		
38	C	1	Total	C	O	S	0	0
			4	2	1	1		
38	C	1	Total	C	O	S	0	0
			4	2	1	1		
38	D	1	Total	C	O	S	0	0
			4	2	1	1		
38	E	1	Total	C	O	S	0	0
			4	2	1	1		
38	O	1	Total	C	O	S	0	0
			4	2	1	1		
38	V	1	Total	C	O	S	0	0
			4	2	1	1		
38	Y	1	Total	C	O	S	0	0
			4	2	1	1		
38	a	1	Total	C	O	S	0	0
			4	2	1	1		
38	b	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

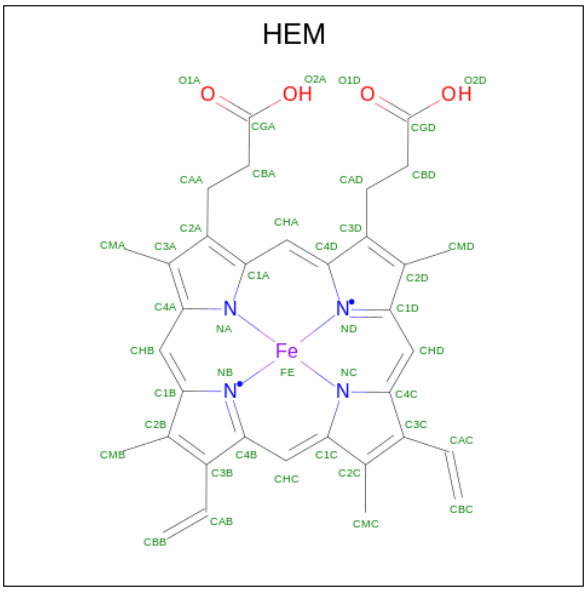
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total	C	O	S	0	0
			4	2	1	1		
38	b	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	c	1	Total	C	O	S	0	0
			4	2	1	1		
38	d	1	Total	C	O	S	0	0
			4	2	1	1		
38	d	1	Total	C	O	S	0	0
			4	2	1	1		
38	i	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	o	1	Total	C	O	S	0	0
			4	2	1	1		
38	v	1	Total	C	O	S	0	0
			4	2	1	1		
38	z	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



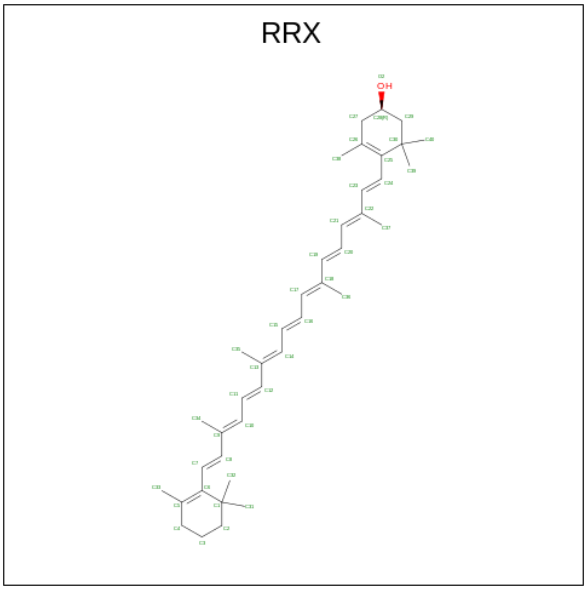
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	C	1	Total C O 62 47 15	0	0
39	C	1	Total C O 62 47 15	0	0
39	C	1	Total C O 62 47 15	0	0
39	D	1	Total C O 53 42 11	0	0
39	H	1	Total C O 62 47 15	0	0
39	c	1	Total C O 62 47 15	0	0
39	c	1	Total C O 62 47 15	0	0
39	c	1	Total C O 62 47 15	0	0
39	h	1	Total C O 62 47 15	0	0

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 41 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

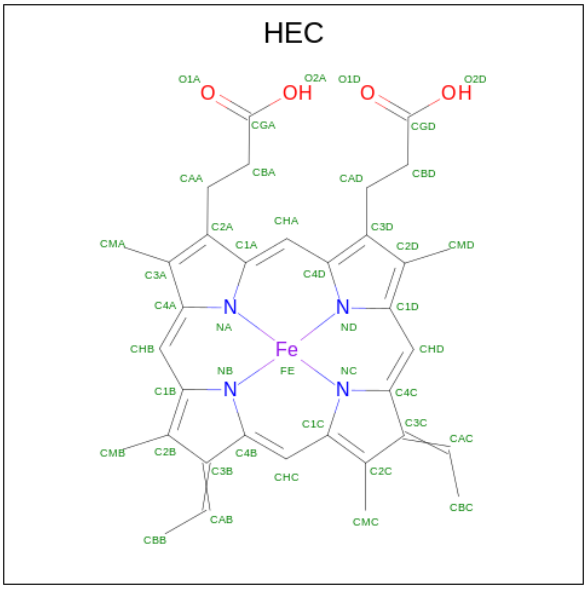


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
41	H	1	Total	C	O	0	0
			41	40	1		
41	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 43 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 44 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	A	176	Total O 176 176	0	0
44	B	363	Total O 364 364	0	1
44	C	284	Total O 284 284	0	0
44	D	166	Total O 166 166	0	0
44	E	47	Total O 47 47	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	F	18	Total O 18 18	0	0
44	H	62	Total O 62 62	0	0
44	I	18	Total O 18 18	0	0
44	J	15	Total O 15 15	0	0
44	K	11	Total O 11 11	0	0
44	L	31	Total O 31 31	0	0
44	M	17	Total O 17 17	0	0
44	O	195	Total O 196 196	0	1
44	T	20	Total O 20 20	0	0
44	U	102	Total O 102 102	0	0
44	V	158	Total O 159 159	0	1
44	Y	9	Total O 9 9	0	0
44	X	16	Total O 16 16	0	0
44	a	164	Total O 164 164	0	0
44	b	323	Total O 325 325	0	2
44	c	273	Total O 275 275	0	2
44	d	157	Total O 157 157	0	0
44	e	29	Total O 29 29	0	0
44	f	11	Total O 11 11	0	0
44	h	45	Total O 45 45	0	0
44	i	10	Total O 10 10	0	0

Continued on next page...

Continued from previous page...

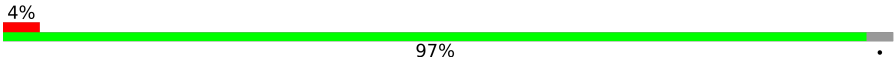
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	j	13	Total O 13 13	0	0
44	k	11	Total O 11 11	0	0
44	l	15	Total O 15 15	0	0
44	m	26	Total O 26 26	0	0
44	o	184	Total O 184 184	0	0
44	t	18	Total O 19 19	0	1
44	u	105	Total O 106 106	0	1
44	v	106	Total O 109 109	0	3
44	y	12	Total O 12 12	0	0
44	x	18	Total O 18 18	0	0
44	z	7	Total O 7 7	0	0
44	R	2	Total O 2 2	0	0

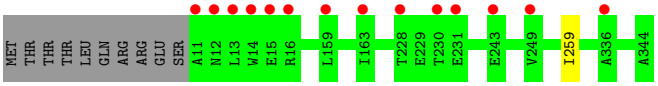
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

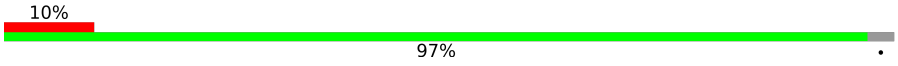
Chain A:

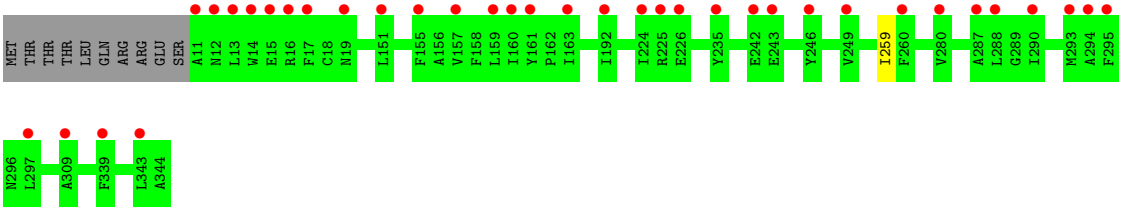




• Molecule 1: Photosystem II protein D1

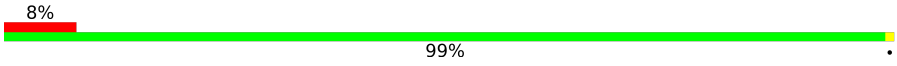
Chain a:

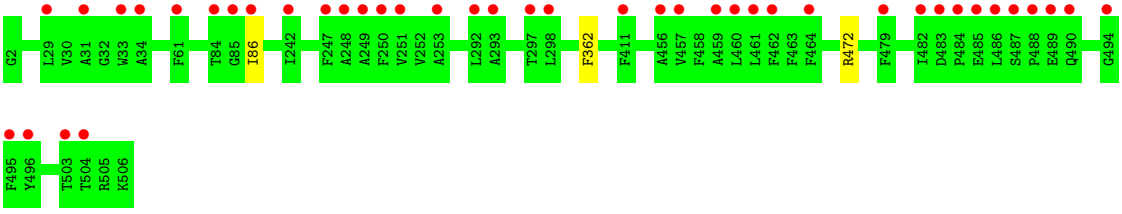




• Molecule 2: Photosystem II CP47 reaction center protein

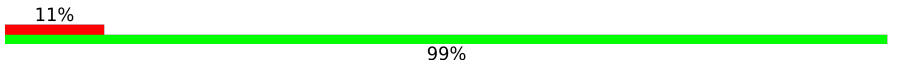
Chain B:

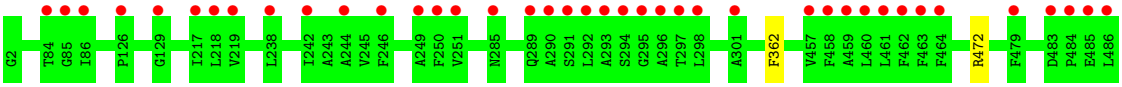


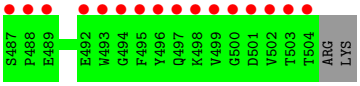


• Molecule 2: Photosystem II CP47 reaction center protein

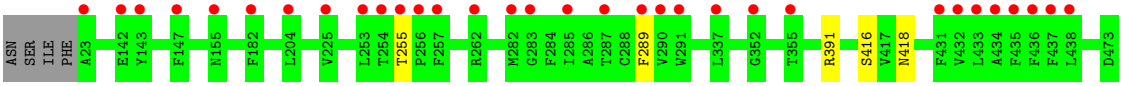
Chain b:



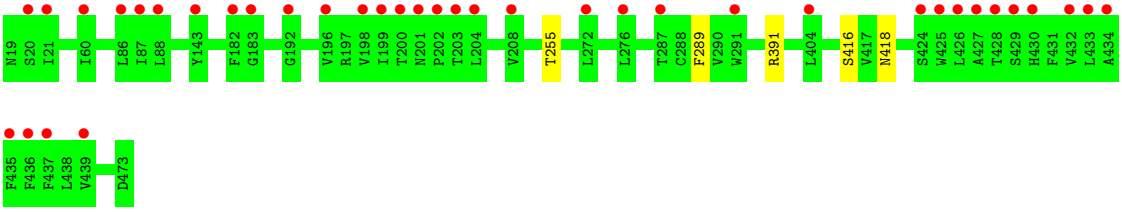




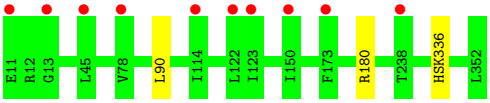
• Molecule 3: Photosystem II CP43 reaction center protein



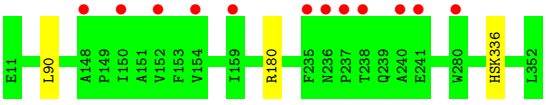
• Molecule 3: Photosystem II CP43 reaction center protein



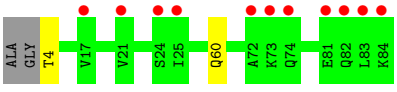
• Molecule 4: Photosystem II D2 protein



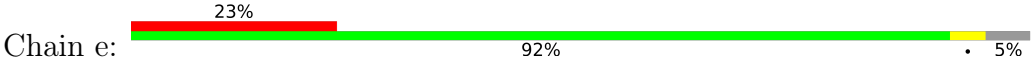
• Molecule 4: Photosystem II D2 protein

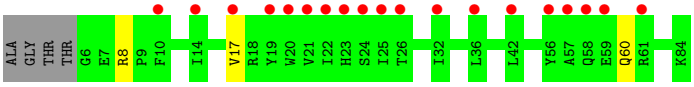


• Molecule 5: Cytochrome b559 subunit alpha

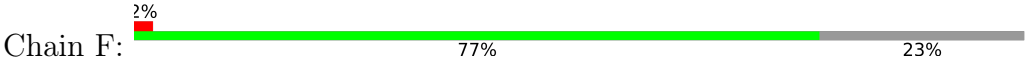


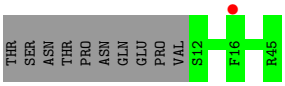
• Molecule 5: Cytochrome b559 subunit alpha



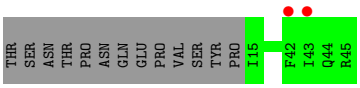


• Molecule 6: Cytochrome b559 subunit beta

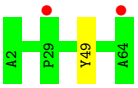




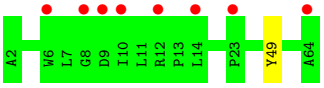
• Molecule 6: Cytochrome b559 subunit beta



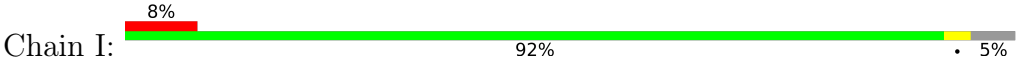
• Molecule 7: Photosystem II reaction center protein H

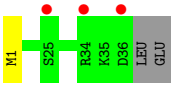


• Molecule 7: Photosystem II reaction center protein H

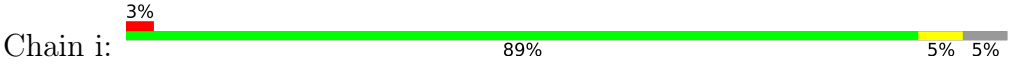


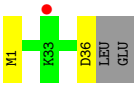
• Molecule 8: Photosystem II reaction center protein I





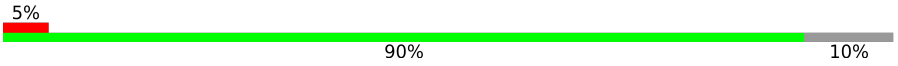
• Molecule 8: Photosystem II reaction center protein I

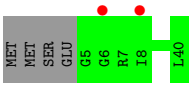




• Molecule 9: Photosystem II reaction center protein J

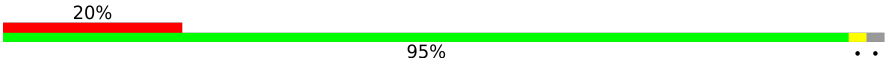
Chain J:

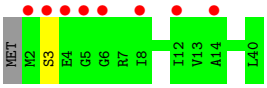




• Molecule 9: Photosystem II reaction center protein J

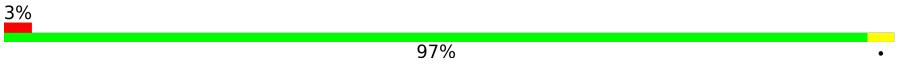
Chain j:

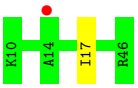




• Molecule 10: Photosystem II reaction center protein K

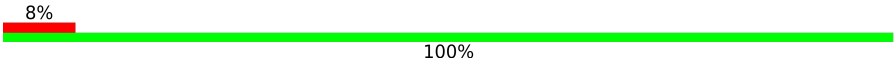
Chain K:

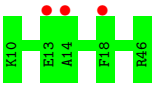




• Molecule 10: Photosystem II reaction center protein K

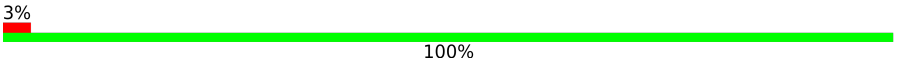
Chain k:





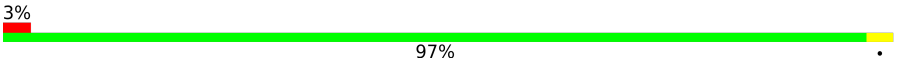
• Molecule 11: Photosystem II reaction center protein L

Chain L:



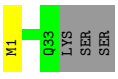
• Molecule 11: Photosystem II reaction center protein L

Chain l:



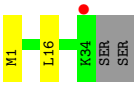
• Molecule 12: Photosystem II reaction center protein M

Chain M:



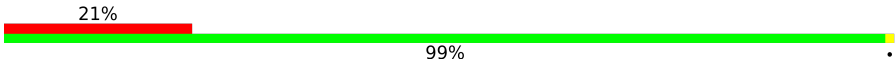
• Molecule 12: Photosystem II reaction center protein M

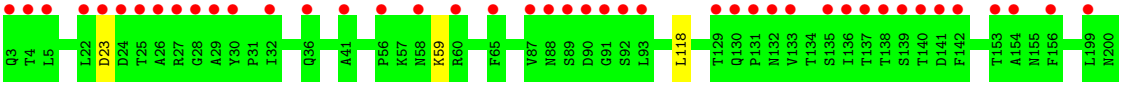
Chain m:

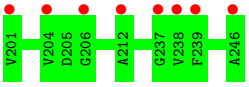


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

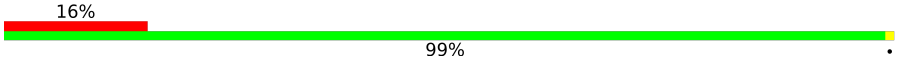


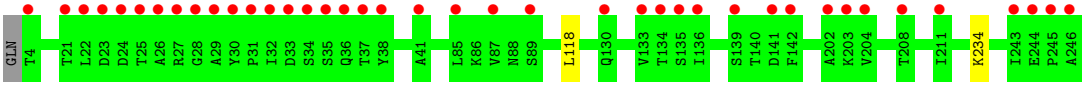




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

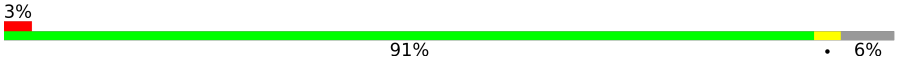
Chain o:





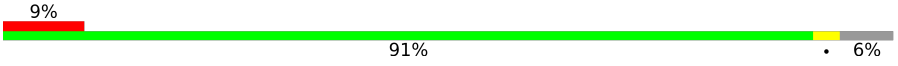
• Molecule 14: Photosystem II reaction center protein T

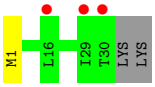
Chain T:



• Molecule 14: Photosystem II reaction center protein T

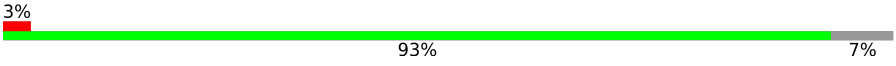
Chain t:

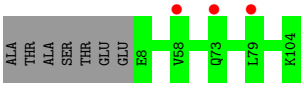




• Molecule 15: Photosystem II 12 kDa extrinsic protein

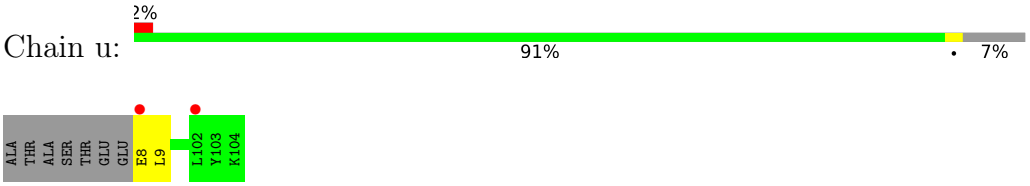
Chain U:





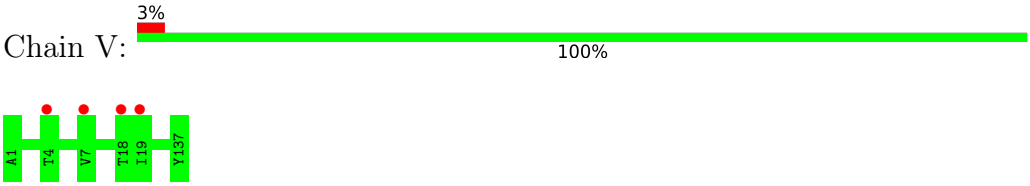
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



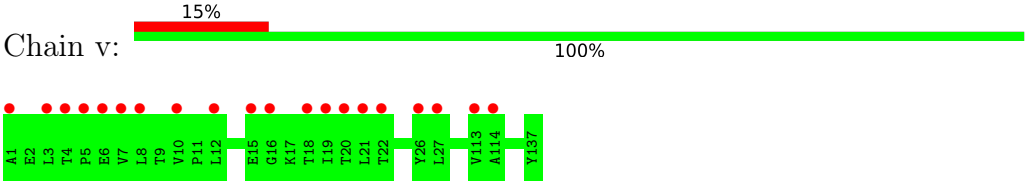
• Molecule 16: Cytochrome c-550

Chain V:



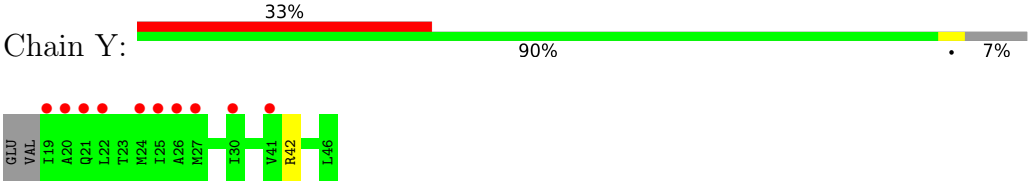
• Molecule 16: Cytochrome c-550

Chain v:



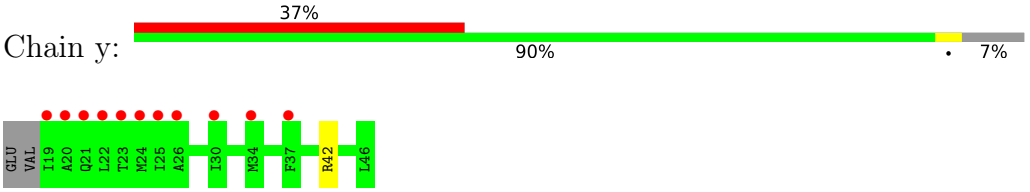
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



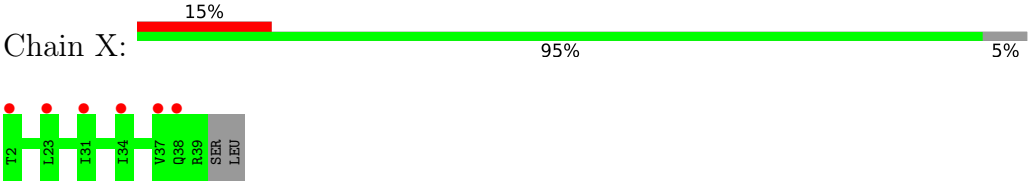
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



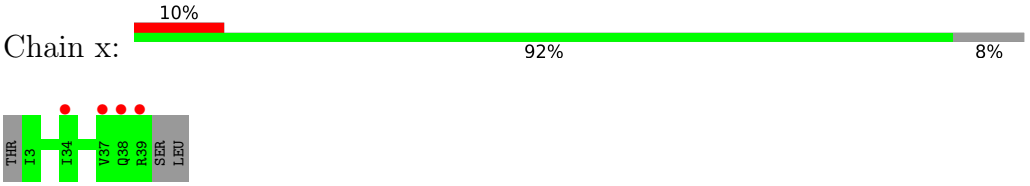
• Molecule 18: Photosystem II reaction center protein X

Chain X:



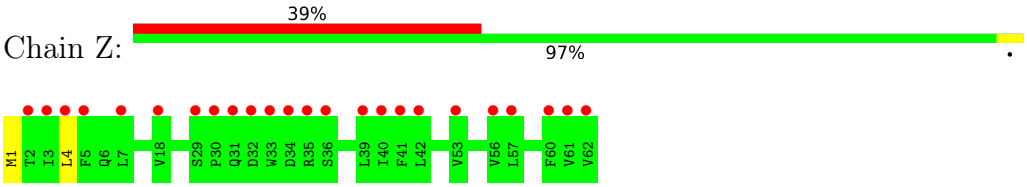
• Molecule 18: Photosystem II reaction center protein X

Chain x:



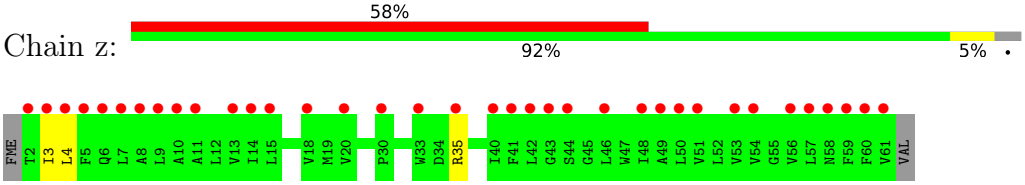
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



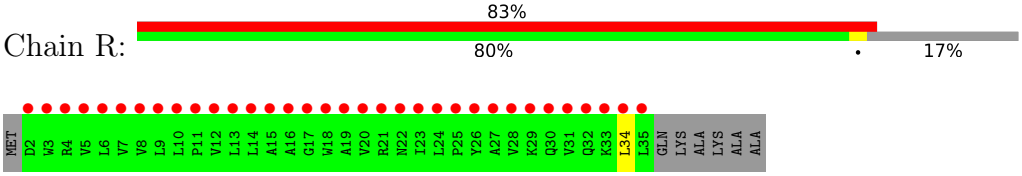
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.02Å 229.58Å 287.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 1.95 49.22 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.22-1.95) 88.5 (49.22-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.153 , 0.181 0.157 , 0.184	Depositor DCC
R_{free} test set	29246 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 73.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55061	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: LMT, RRX, SQD, HEC, HSK, CL, PL9, DGD, FME, LHG, DMS, HEM, LMG, MG, UNL, PHO, FE2, CA, K3C, BCR, BCT, HTG, OEX, CLA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/2718	0.54	0/3707
1	a	0.42	0/2713	0.53	0/3700
2	B	0.40	0/4174	0.51	0/5687
2	b	0.38	0/4158	0.52	0/5667
3	C	0.37	0/3613	0.49	0/4919
3	c	0.36	0/3636	0.50	0/4952
4	D	0.44	0/2809	0.54	0/3827
4	d	0.42	0/2819	0.52	0/3840
5	E	0.34	0/676	0.49	0/924
5	e	0.30	0/658	0.45	0/899
6	F	0.35	0/283	0.47	0/386
6	f	0.34	0/257	0.43	0/349
7	H	0.35	0/511	0.50	0/697
7	h	0.31	0/511	0.49	0/697
8	I	0.31	0/282	0.44	0/383
8	i	0.32	0/293	0.48	0/396
9	J	0.33	0/257	0.46	0/349
9	j	0.30	0/277	0.46	0/376
10	K	0.33	0/306	0.46	0/422
10	k	0.32	0/296	0.46	0/408
11	L	0.40	0/315	0.50	0/428
11	l	0.42	0/322	0.50	0/438
12	M	0.38	0/261	0.59	0/357
12	m	0.39	0/283	0.49	0/386
13	O	0.37	0/1933	0.58	0/2623
13	o	0.34	0/1917	0.57	0/2601
14	T	0.44	0/255	0.48	0/346
14	t	0.46	0/255	0.48	0/346
15	U	0.37	0/790	0.54	0/1071
15	u	0.38	0/794	0.53	0/1076
16	V	0.38	0/1090	0.53	0/1481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.34	0/1084	0.51	0/1475
17	Y	0.30	0/199	0.44	0/266
17	y	0.27	0/197	0.45	0/264
18	X	0.31	0/282	0.40	0/381
18	x	0.27	0/279	0.39	0/377
19	Z	0.29	0/462	0.42	0/635
19	z	0.29	0/457	0.44	0/626
20	R	0.26	0/246	0.36	0/341
All	All	0.38	0/42668	0.51	0/58103

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	30
1	a	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	41	30
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	511/505 (101%)	505 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	443 (98%)	7 (2%)	1 (0%)	47	38
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	47	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	77/83 (93%)	77 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	35/36 (97%)	35 (100%)	0	0	100	100
13	O	248/244 (102%)	244 (98%)	4 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	135 (98%)	2 (2%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
17	y	26/30 (87%)	26 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	z	58/62 (94%)	56 (97%)	1 (2%)	1 (2%)	9 2
20	R	32/41 (78%)	32 (100%)	0	0	100 100
All	All	5258/5387 (98%)	5169 (98%)	84 (2%)	5 (0%)	51 43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	z	3	ILE
3	C	416	SER
3	c	416	SER
1	a	259	ILE
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/279 (97%)	270 (100%)	0	100 100
1	a	270/279 (97%)	270 (100%)	0	100 100
2	B	406/403 (101%)	403 (99%)	3 (1%)	84 82
2	b	405/403 (100%)	403 (100%)	2 (0%)	88 88
3	C	354/356 (99%)	350 (99%)	4 (1%)	73 71
3	c	353/356 (99%)	348 (99%)	5 (1%)	67 62
4	D	275/276 (100%)	273 (99%)	2 (1%)	84 82
4	d	277/276 (100%)	275 (99%)	2 (1%)	84 82
5	E	71/72 (99%)	69 (97%)	2 (3%)	43 33
5	e	68/72 (94%)	65 (96%)	3 (4%)	28 15
6	F	27/38 (71%)	27 (100%)	0	100 100
6	f	25/38 (66%)	25 (100%)	0	100 100
7	H	53/53 (100%)	52 (98%)	1 (2%)	57 50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	h	53/53 (100%)	52 (98%)	1 (2%)	57 50
8	I	29/34 (85%)	29 (100%)	0	100 100
8	i	32/34 (94%)	31 (97%)	1 (3%)	40 28
9	J	23/28 (82%)	23 (100%)	0	100 100
9	j	25/28 (89%)	24 (96%)	1 (4%)	31 19
10	K	30/30 (100%)	29 (97%)	1 (3%)	38 26
10	k	28/30 (93%)	28 (100%)	0	100 100
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	36/35 (103%)	35 (97%)	1 (3%)	43 33
12	M	30/32 (94%)	30 (100%)	0	100 100
12	m	32/32 (100%)	30 (94%)	2 (6%)	18 7
13	O	209/207 (101%)	206 (99%)	3 (1%)	67 62
13	o	207/207 (100%)	205 (99%)	2 (1%)	76 74
14	T	25/28 (89%)	25 (100%)	0	100 100
14	t	25/28 (89%)	25 (100%)	0	100 100
15	U	84/89 (94%)	84 (100%)	0	100 100
15	u	85/89 (96%)	83 (98%)	2 (2%)	49 40
16	V	115/117 (98%)	115 (100%)	0	100 100
16	v	115/117 (98%)	115 (100%)	0	100 100
17	Y	18/23 (78%)	17 (94%)	1 (6%)	21 9
17	y	18/23 (78%)	17 (94%)	1 (6%)	21 9
18	X	30/33 (91%)	30 (100%)	0	100 100
18	x	29/33 (88%)	29 (100%)	0	100 100
19	Z	46/51 (90%)	45 (98%)	1 (2%)	52 44
19	z	44/51 (86%)	42 (96%)	2 (4%)	27 15
20	R	19/33 (58%)	18 (95%)	1 (5%)	22 10
All	All	4276/4401 (97%)	4232 (99%)	44 (1%)	76 74

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	17	VAL
12	m	16[B]	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	60	GLN
9	j	3	SER
13	o	234	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	l	8	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	0.60	0	7,9,11	1.57	2 (28%)
4	HSK	d	336[B]	-	7,11,12	1.29	1 (14%)	3,14,16	1.40	1 (33%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.86	4 (57%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.50	1 (14%)
14	FME	t	1	14	8,9,10	0.60	0	7,9,11	1.50	2 (28%)
4	HSK	D	336[B]	-	7,11,12	1.26	1 (14%)	3,14,16	1.45	1 (33%)
4	HSK	D	336[A]	-	7,10,12	0.87	0	3,12,16	1.15	0
4	HSK	d	336[A]	-	7,10,12	1.06	1 (14%)	3,12,16	1.05	0
14	FME	T	1	14	8,9,10	0.56	0	7,9,11	1.84	3 (42%)
19	FME	Z	1	19	8,9,10	0.64	0	7,9,11	1.63	2 (28%)
12	FME	m	1	12	8,9,10	0.64	0	7,9,11	1.72	1 (14%)

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	-	0/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[A]	-	-	2/5/6/8	0/1/1/1
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	2/7/9/11	-
19	FME	Z	1	19	-	3/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[B]	HSK	CE1-ND1	-3.02	1.33	1.36
4	D	336[B]	HSK	CE1-ND1	-2.86	1.33	1.36
4	d	336[A]	HSK	CE1-ND1	-2.27	1.34	1.36

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	1	FME	CE-SD-CG	3.48	112.35	100.40
8	I	1	FME	CA-N-CN	-3.41	117.57	122.82
14	T	1	FME	O-C-CA	-2.80	117.43	124.78
12	M	1	FME	CE-SD-CG	2.55	109.15	100.40
14	T	1	FME	CA-N-CN	-2.52	118.95	122.82

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
19	Z	1	FME	O1-CN-N-CA
14	t	1	FME	CB-CG-SD-CE
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 337 ligands modelled in this entry, 15 are monoatomic and 57 are unknown - leaving 265 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	c	507	-	65,73,73	2.64	20 (30%)	76,113,113	2.38	23 (30%)
36	HTG	b	602	-	19,19,19	1.09	2 (10%)	23,24,24	1.25	1 (4%)
24	CLA	A	405	-	65,73,73	2.49	19 (29%)	76,113,113	2.31	25 (32%)
24	CLA	b	613	44	65,73,73	2.52	20 (30%)	76,113,113	2.36	25 (32%)
30	GOL	B	629	-	5,5,5	1.04	0	5,5,5	0.75	0
30	GOL	V	201	35	5,5,5	0.78	0	5,5,5	1.02	0
36	HTG	d	414	-	19,19,19	1.03	2 (10%)	23,24,24	1.80	4 (17%)
24	CLA	C	504	-	65,73,73	2.50	19 (29%)	76,113,113	2.31	22 (28%)
24	CLA	D	404	-	65,73,73	2.48	18 (27%)	76,113,113	2.41	26 (34%)
29	LMT	C	521	-	36,36,36	0.46	0	47,47,47	1.19	4 (8%)
36	HTG	I	102	-	19,19,19	1.11	2 (10%)	23,24,24	1.89	4 (17%)
28	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	0.99	4 (6%)
34	BCT	a	407	22	2,3,3	0.64	0	2,3,3	0.68	0
28	LMG	a	415	-	51,51,55	0.94	2 (3%)	59,59,63	1.27	7 (11%)
36	HTG	o	301	-	19,19,19	1.15	1 (5%)	23,24,24	1.19	1 (4%)
32	K3C	A	421[A]	-	15,15,15	0.95	1 (6%)	19,20,20	0.88	1 (5%)
25	PHO	a	411	-	51,69,69	1.79	7 (13%)	47,99,99	1.68	7 (14%)
36	HTG	V	203	-	12,13,19	0.48	0	16,18,24	2.08	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	606	-	65,73,73	2.50	21 (32%)	76,113,113	2.49	25 (32%)
24	CLA	b	617	-	65,73,73	2.35	20 (30%)	76,113,113	2.58	26 (34%)
26	BCR	B	620	-	41,41,41	0.71	0	56,56,56	1.24	4 (7%)
28	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.24	5 (8%)
28	LMG	C	532	-	51,51,55	0.98	2 (3%)	59,59,63	1.30	4 (6%)
41	RRX	h	1204	-	42,42,42	0.73	0	57,58,58	1.33	7 (12%)
30	GOL	v	1601	-	5,5,5	0.94	0	5,5,5	0.92	0
43	HEC	v	1603	16	32,50,50	2.35	5 (15%)	24,82,82	1.85	4 (16%)
24	CLA	C	509	-	65,73,73	2.48	19 (29%)	76,113,113	2.36	24 (31%)
37	LHG	d	410	-	38,38,48	1.07	2 (5%)	41,44,54	1.08	3 (7%)
24	CLA	B	609	-	65,73,73	2.60	18 (27%)	76,113,113	2.40	26 (34%)
30	GOL	T	101	-	5,5,5	0.96	0	5,5,5	0.81	0
39	DGD	c	518	-	63,63,67	0.80	2 (3%)	77,77,81	1.11	7 (9%)
24	CLA	d	405	-	65,73,73	2.43	21 (32%)	76,113,113	2.42	28 (36%)
24	CLA	c	505	-	65,73,73	2.66	19 (29%)	76,113,113	2.24	24 (31%)
38	DMS	B	643	-	3,3,3	2.67	1 (33%)	3,3,3	0.47	0
30	GOL	V	204	-	5,5,5	1.12	0	5,5,5	0.90	0
38	DMS	C	533	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
33	PL9	a	425[B]	-	55,55,55	0.60	2 (3%)	68,69,69	1.86	21 (30%)
38	DMS	o	304	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
38	DMS	B	646	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
37	LHG	d	409	-	48,48,48	0.86	2 (4%)	51,54,54	0.97	3 (5%)
26	BCR	c	516	-	41,41,41	0.78	0	56,56,56	1.42	5 (8%)
38	DMS	c	536	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
38	DMS	o	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
39	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	8 (10%)
30	GOL	b	630	-	5,5,5	1.21	0	5,5,5	0.97	0
38	DMS	a	426	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
24	CLA	c	513	3	65,73,73	2.52	16 (24%)	76,113,113	2.46	31 (40%)
38	DMS	c	533	-	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
26	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.34	7 (12%)
24	CLA	b	605	-	65,73,73	2.51	20 (30%)	76,113,113	2.37	24 (31%)
26	BCR	D	405	-	41,41,41	0.83	1 (2%)	56,56,56	1.75	10 (17%)
26	BCR	B	619	-	41,41,41	0.83	0	56,56,56	1.20	4 (7%)
29	LMT	A	414	-	36,36,36	0.40	0	47,47,47	0.96	2 (4%)
30	GOL	V	205	-	5,5,5	0.86	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	GOL	k	304	-	5,5,5	0.87	0	5,5,5	0.91	0
38	DMS	b	637	-	3,3,3	2.69	1 (33%)	3,3,3	0.65	0
24	CLA	c	511	-	65,73,73	2.61	19 (29%)	76,113,113	2.44	27 (35%)
36	HTG	O	302	-	19,19,19	1.09	1 (5%)	23,24,24	0.98	1 (4%)
36	HTG	b	601	-	19,19,19	1.10	2 (10%)	23,24,24	1.52	2 (8%)
36	HTG	C	522	-	19,19,19	0.96	2 (10%)	23,24,24	1.16	1 (4%)
36	HTG	B	623[A]	-	19,19,19	1.02	1 (5%)	23,24,24	1.33	2 (8%)
41	RRX	H	101	-	42,42,42	0.74	0	57,58,58	1.29	6 (10%)
24	CLA	B	611	44	65,73,73	2.54	20 (30%)	76,113,113	2.39	23 (30%)
25	PHO	d	401	-	51,69,69	1.83	9 (17%)	47,99,99	1.83	10 (21%)
24	CLA	c	508	-	65,73,73	2.65	20 (30%)	76,113,113	2.40	30 (39%)
24	CLA	b	619	-	65,73,73	2.47	19 (29%)	76,113,113	2.48	26 (34%)
30	GOL	L	103	-	5,5,5	1.03	0	5,5,5	0.88	0
24	CLA	c	510	-	65,73,73	2.55	20 (30%)	76,113,113	2.49	26 (34%)
39	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.08	4 (5%)
24	CLA	b	604	44	65,73,73	2.52	20 (30%)	76,113,113	2.28	23 (30%)
29	LMT	b	624	-	25,25,36	0.45	0	30,30,47	0.77	0
26	BCR	a	413	-	41,41,41	0.77	0	56,56,56	1.22	4 (7%)
27	SQD	a	414	-	53,54,54	0.94	3 (5%)	62,65,65	1.69	10 (16%)
34	BCT	A	423	22	2,3,3	0.61	0	2,3,3	0.79	0
38	DMS	d	416	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
24	CLA	b	607	-	65,73,73	2.64	20 (30%)	76,113,113	2.44	27 (35%)
24	CLA	C	507	-	65,73,73	2.53	20 (30%)	76,113,113	2.52	26 (34%)
24	CLA	a	412	-	65,73,73	2.22	18 (27%)	76,113,113	2.52	29 (38%)
38	DMS	D	416	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
43	HEC	V	202	16	32,50,50	2.24	6 (18%)	24,82,82	1.91	7 (29%)
24	CLA	a	409	44	65,73,73	2.42	18 (27%)	76,113,113	2.67	27 (35%)
30	GOL	C	530	-	5,5,5	1.20	0	5,5,5	1.14	1 (20%)
30	GOL	a	416	-	5,5,5	1.00	0	5,5,5	1.12	1 (20%)
29	LMT	z	101	-	32,32,36	0.55	1 (3%)	42,42,47	1.46	4 (9%)
24	CLA	B	612	-	65,73,73	2.40	19 (29%)	76,113,113	2.56	28 (36%)
26	BCR	K	101	-	41,41,41	0.75	0	56,56,56	1.51	11 (19%)
26	BCR	b	622	-	41,41,41	0.70	0	56,56,56	1.36	10 (17%)
38	DMS	o	309	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
24	CLA	B	603	-	65,73,73	2.53	19 (29%)	76,113,113	2.47	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	a	408	-	65,73,73	2.38	19 (29%)	76,113,113	2.49	26 (34%)
38	DMS	Y	303	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
26	BCR	c	517	-	41,41,41	0.76	0	56,56,56	1.40	7 (12%)
30	GOL	d	413	-	5,5,5	0.87	0	5,5,5	0.99	0
39	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.92	5 (6%)
24	CLA	b	608	-	65,73,73	2.26	19 (29%)	76,113,113	2.56	26 (34%)
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	0.85	0
28	LMG	A	412	-	51,51,55	0.93	2 (3%)	59,59,63	1.16	6 (10%)
24	CLA	C	508	44	65,73,73	2.74	21 (32%)	76,113,113	2.39	24 (31%)
30	GOL	V	206	-	5,5,5	0.98	0	5,5,5	0.96	0
30	GOL	O	303	-	5,5,5	0.83	0	5,5,5	1.05	0
40	HEM	F	101	6,5	41,50,50	1.92	5 (12%)	45,82,82	1.83	10 (22%)
24	CLA	B	606	-	65,73,73	2.38	20 (30%)	76,113,113	2.32	20 (26%)
24	CLA	B	614	-	65,73,73	2.42	18 (27%)	76,113,113	2.47	27 (35%)
24	CLA	B	617	-	65,73,73	2.31	18 (27%)	76,113,113	2.51	25 (32%)
24	CLA	d	404	-	65,73,73	2.31	20 (30%)	76,113,113	2.57	27 (35%)
24	CLA	B	616	-	65,73,73	2.44	19 (29%)	76,113,113	2.57	29 (38%)
30	GOL	b	629	-	5,5,5	0.97	0	5,5,5	0.98	0
38	DMS	B	647	-	3,3,3	2.64	1 (33%)	3,3,3	0.41	0
28	LMG	b	623	-	51,51,55	0.90	2 (3%)	59,59,63	1.06	3 (5%)
24	CLA	C	506	-	65,73,73	2.55	20 (30%)	76,113,113	2.28	21 (27%)
39	DGD	D	407	-	53,53,67	1.01	3 (5%)	60,61,81	1.41	6 (10%)
24	CLA	c	503	-	65,73,73	2.55	20 (30%)	76,113,113	2.67	24 (31%)
30	GOL	A	415	-	5,5,5	0.82	0	5,5,5	1.06	1 (20%)
37	LHG	e	101	-	39,39,48	1.03	2 (5%)	42,45,54	1.06	3 (7%)
25	PHO	D	401	-	51,69,69	1.84	7 (13%)	47,99,99	1.86	8 (17%)
33	PL9	D	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.54	14 (20%)
37	LHG	d	408	-	48,48,48	0.84	2 (4%)	51,54,54	1.07	4 (7%)
40	HEM	f	101	6,5	41,50,50	1.94	7 (17%)	45,82,82	1.71	6 (13%)
39	DGD	h	1205	-	63,63,67	0.92	3 (4%)	77,77,81	0.99	4 (5%)
26	BCR	k	302	-	41,41,41	0.77	1 (2%)	56,56,56	1.56	12 (21%)
27	SQD	A	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.71	12 (19%)
38	DMS	i	104	-	3,3,3	2.65	1 (33%)	3,3,3	0.60	0
24	CLA	C	502	-	65,73,73	2.36	20 (30%)	76,113,113	2.37	21 (27%)
24	CLA	C	505	44	65,73,73	2.38	19 (29%)	76,113,113	2.48	25 (32%)
24	CLA	b	614	-	65,73,73	2.55	20 (30%)	76,113,113	2.38	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	GOL	h	1206	-	5,5,5	0.95	0	5,5,5	0.90	0
24	CLA	A	406	44	65,73,73	2.26	20 (30%)	76,113,113	2.63	27 (35%)
24	CLA	b	611	-	65,73,73	2.60	20 (30%)	76,113,113	2.35	24 (31%)
39	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	5 (6%)
39	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.97	4 (5%)
30	GOL	b	627	-	5,5,5	0.96	0	5,5,5	0.84	0
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.63	11 (17%)
21	OEX	A	401	1,44,3	0,15,15	-	-	-		
30	GOL	T	103	-	5,5,5	0.83	0	5,5,5	1.07	0
30	GOL	o	305	-	5,5,5	1.09	0	5,5,5	0.79	0
38	DMS	z	102	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
24	CLA	b	610	44	65,73,73	2.46	19 (29%)	76,113,113	2.38	27 (35%)
38	DMS	O	304	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
37	LHG	D	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.90	3 (5%)
24	CLA	a	410	44	65,73,73	2.38	20 (30%)	76,113,113	2.49	24 (31%)
26	BCR	b	620	-	41,41,41	0.80	0	56,56,56	1.39	6 (10%)
39	DGD	c	520	-	63,63,67	0.85	3 (4%)	77,77,81	0.96	5 (6%)
26	BCR	A	410	-	41,41,41	0.76	0	56,56,56	1.30	6 (10%)
24	CLA	b	618	-	65,73,73	2.43	20 (30%)	76,113,113	2.34	25 (32%)
30	GOL	c	526	-	5,5,5	1.06	0	5,5,5	0.83	0
30	GOL	B	631	-	5,5,5	1.06	0	5,5,5	0.97	0
30	GOL	v	1605	-	5,5,5	1.09	0	5,5,5	0.81	0
29	LMT	J	102	-	24,24,36	0.50	0	29,29,47	1.19	3 (10%)
36	HTG	B	625	-	19,19,19	1.03	2 (10%)	23,24,24	1.36	1 (4%)
26	BCR	b	621	-	41,41,41	0.77	0	56,56,56	1.17	6 (10%)
38	DMS	b	636	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
27	SQD	f	102	-	31,32,54	1.97	4 (12%)	34,36,65	1.44	3 (8%)
24	CLA	C	503	-	65,73,73	2.57	20 (30%)	76,113,113	2.37	24 (31%)
38	DMS	V	207	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
38	DMS	c	537	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	b	615	-	65,73,73	2.38	19 (29%)	76,113,113	2.54	23 (30%)
26	BCR	B	641	-	41,41,41	0.68	0	56,56,56	1.60	14 (25%)
38	DMS	b	638	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
38	DMS	B	645	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
36	HTG	b	625	-	19,19,19	0.80	1 (5%)	23,24,24	1.15	2 (8%)
24	CLA	b	609	-	65,73,73	2.59	19 (29%)	76,113,113	2.34	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	k	303	-	41,41,41	0.71	0	56,56,56	1.39	6 (10%)
30	GOL	B	630	-	5,5,5	0.58	0	5,5,5	1.04	0
24	CLA	A	407	44	65,73,73	2.34	19 (29%)	76,113,113	2.51	25 (32%)
24	CLA	B	613	-	65,73,73	2.38	18 (27%)	76,113,113	2.59	25 (32%)
30	GOL	b	628	-	5,5,5	0.85	0	5,5,5	0.94	0
24	CLA	c	514	-	65,73,73	2.59	19 (29%)	76,113,113	2.58	28 (36%)
30	GOL	A	416	-	5,5,5	1.00	0	5,5,5	0.90	0
30	GOL	C	527	-	5,5,5	0.83	0	5,5,5	1.06	0
36	HTG	U	201	-	8,8,19	0.37	0	7,7,24	1.01	1 (14%)
29	LMT	B	642	-	24,24,36	0.56	1 (4%)	29,29,47	0.72	0
24	CLA	c	504	-	65,73,73	2.33	19 (29%)	76,113,113	2.48	22 (28%)
26	BCR	B	618	-	41,41,41	0.76	0	56,56,56	1.31	6 (10%)
24	CLA	c	509	44	65,73,73	2.50	19 (29%)	76,113,113	2.53	27 (35%)
26	BCR	C	515	-	41,41,41	0.69	0	56,56,56	1.47	7 (12%)
28	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.05	3 (5%)
38	DMS	v	1608	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
26	BCR	T	102	-	41,41,41	0.72	0	56,56,56	1.55	15 (26%)
30	GOL	C	529	-	5,5,5	0.98	0	5,5,5	0.79	0
24	CLA	C	512	3	65,73,73	2.60	19 (29%)	76,113,113	2.39	25 (32%)
24	CLA	c	506	44	65,73,73	2.27	20 (30%)	76,113,113	2.59	27 (35%)
28	LMG	D	412	42	51,51,55	0.84	2 (3%)	59,59,63	0.89	3 (5%)
30	GOL	a	421	-	5,5,5	0.99	0	5,5,5	0.94	0
30	GOL	v	1604	-	5,5,5	0.93	0	5,5,5	0.97	0
30	GOL	C	528	-	5,5,5	0.74	0	5,5,5	1.12	1 (20%)
38	DMS	o	308	-	3,3,3	2.69	1 (33%)	3,3,3	0.48	0
24	CLA	B	602	44	65,73,73	2.55	22 (33%)	76,113,113	2.38	23 (30%)
27	SQD	A	413	-	53,54,54	1.02	3 (5%)	62,65,65	1.30	10 (16%)
38	DMS	c	534	-	3,3,3	2.67	1 (33%)	3,3,3	0.44	0
30	GOL	c	527	-	5,5,5	1.03	0	5,5,5	0.88	0
33	PL9	A	422[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.72	16 (23%)
30	GOL	C	524	-	5,5,5	0.86	0	5,5,5	1.14	1 (20%)
29	LMT	f	104	-	36,36,36	0.44	0	47,47,47	0.77	0
29	LMT	E	104	-	24,24,36	0.48	0	29,29,47	0.71	0
26	BCR	d	406	-	41,41,41	0.80	0	56,56,56	1.82	13 (23%)
33	PL9	d	407	-	55,55,55	0.68	1 (1%)	68,69,69	1.50	13 (19%)
37	LHG	l	302	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	1 (1%)
29	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	GOL	v	1607	-	5,5,5	0.83	0	5,5,5	0.95	0
36	HTG	h	1202	-	19,19,19	1.07	2 (10%)	23,24,24	1.81	1 (4%)
37	LHG	B	640	-	48,48,48	0.93	3 (6%)	51,54,54	1.00	3 (5%)
29	LMT	B	622	-	36,36,36	0.40	0	47,47,47	1.17	4 (8%)
21	OEX	a	403	1,44,3	0,15,15	-	-	-		
30	GOL	B	633	-	5,5,5	0.87	0	5,5,5	0.98	0
27	SQD	a	401	-	53,54,54	1.04	3 (5%)	62,65,65	1.26	7 (11%)
30	GOL	c	528	-	5,5,5	0.95	0	5,5,5	0.95	0
36	HTG	B	624	-	19,19,19	1.08	2 (10%)	23,24,24	1.75	2 (8%)
38	DMS	E	106	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
24	CLA	A	409	-	65,73,73	2.28	19 (29%)	76,113,113	2.58	27 (35%)
36	HTG	b	626	-	19,19,19	1.06	1 (5%)	23,24,24	1.66	1 (4%)
30	GOL	B	627	-	5,5,5	1.00	0	5,5,5	0.87	0
36	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.69	4 (17%)
38	DMS	d	415	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
38	DMS	C	525	-	3,3,3	2.67	1 (33%)	3,3,3	0.54	0
30	GOL	v	1606	-	5,5,5	0.76	0	5,5,5	1.08	0
38	DMS	o	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
24	CLA	B	604	-	65,73,73	2.42	19 (29%)	76,113,113	2.65	24 (31%)
26	BCR	Y	302	-	41,41,41	0.78	0	56,56,56	1.61	10 (17%)
24	CLA	C	514	-	65,73,73	2.53	19 (29%)	76,113,113	2.45	23 (30%)
30	GOL	o	302	-	5,5,5	1.06	0	5,5,5	0.79	0
30	GOL	u	202	-	5,5,5	0.97	0	5,5,5	0.94	0
36	HTG	u	201	-	10,13,19	1.12	1 (10%)	13,14,24	1.72	1 (7%)
29	LMT	Z	101	-	36,36,36	0.44	0	47,47,47	0.83	1 (2%)
27	SQD	D	408	-	44,45,54	1.10	3 (6%)	53,56,65	1.73	11 (20%)
30	GOL	a	417	-	5,5,5	1.05	0	5,5,5	0.92	0
36	HTG	c	525	-	19,19,19	1.03	2 (10%)	23,24,24	1.48	3 (13%)
25	PHO	A	408	-	51,69,69	1.82	8 (15%)	47,99,99	1.58	9 (19%)
24	CLA	b	616	-	65,73,73	2.58	20 (30%)	76,113,113	2.51	23 (30%)
36	HTG	B	623[B]	-	19,19,19	0.93	1 (5%)	23,24,24	1.47	2 (8%)
38	DMS	c	535	-	3,3,3	2.71	1 (33%)	3,3,3	0.64	0
29	LMT	m	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	0
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.90	0
37	LHG	E	101	-	48,48,48	0.97	2 (4%)	51,54,54	1.13	3 (5%)
30	GOL	a	418	-	5,5,5	0.91	0	5,5,5	0.94	0
24	CLA	D	403	-	65,73,73	2.20	20 (30%)	76,113,113	2.73	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	GOL	c	532	-	5,5,5	0.82	0	5,5,5	1.04	0
24	CLA	B	615	-	65,73,73	2.29	16 (24%)	76,113,113	2.63	27 (35%)
30	GOL	d	402	-	5,5,5	0.91	0	5,5,5	0.96	0
28	LMG	d	411	42	51,51,55	0.91	2 (3%)	59,59,63	0.92	2 (3%)
24	CLA	C	513	-	65,73,73	2.64	18 (27%)	76,113,113	2.48	25 (32%)
24	CLA	c	512	-	65,73,73	2.57	20 (30%)	76,113,113	2.45	25 (32%)
38	DMS	B	644	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
32	K3C	a	424[A]	-	15,15,15	0.94	1 (6%)	19,20,20	0.88	1 (5%)
24	CLA	B	608	44	65,73,73	2.27	20 (30%)	76,113,113	2.53	22 (28%)
29	LMT	a	402	-	36,36,36	0.43	0	47,47,47	0.88	1 (2%)
37	LHG	D	409	-	48,48,48	0.86	3 (6%)	51,54,54	1.17	5 (9%)
24	CLA	C	511	-	65,73,73	2.51	21 (32%)	76,113,113	2.47	27 (35%)
30	GOL	B	628	-	5,5,5	1.01	0	5,5,5	0.89	0
30	GOL	M	102	-	5,5,5	0.59	0	5,5,5	1.17	1 (20%)
24	CLA	c	515	-	65,73,73	2.40	20 (30%)	76,113,113	2.32	23 (30%)
28	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)
30	GOL	E	105	-	5,5,5	0.89	0	5,5,5	1.01	0
24	CLA	B	607	-	65,73,73	2.40	18 (27%)	76,113,113	2.53	24 (31%)
36	HTG	D	413	-	19,19,19	1.11	2 (10%)	23,24,24	1.09	2 (8%)
36	HTG	c	524	-	19,19,19	0.99	2 (10%)	23,24,24	1.39	1 (4%)
24	CLA	B	610	-	65,73,73	2.58	19 (29%)	76,113,113	2.38	27 (35%)
29	LMT	c	523	-	36,36,36	0.49	1 (2%)	47,47,47	1.06	4 (8%)
36	HTG	B	626	-	19,19,19	1.02	2 (10%)	23,24,24	1.83	5 (21%)
24	CLA	B	605	-	65,73,73	2.63	19 (29%)	76,113,113	2.52	24 (31%)
24	CLA	b	612	-	65,73,73	2.52	19 (29%)	76,113,113	2.35	23 (30%)
30	GOL	v	1602	35	5,5,5	0.88	0	5,5,5	0.93	0
24	CLA	C	510	-	65,73,73	2.43	20 (30%)	76,113,113	2.38	25 (32%)
29	LMT	T	104	-	24,24,36	0.46	0	29,29,47	1.05	3 (10%)
37	LHG	D	411	-	45,45,48	0.91	2 (4%)	48,51,54	0.99	3 (6%)
27	SQD	L	101	-	53,54,54	1.03	3 (5%)	62,65,65	1.37	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	507	-	1/1/15/20	8/37/115/115	-
36	HTG	b	602	-	-	1/10/30/30	0/1/1/1
24	CLA	A	405	-	1/1/15/20	2/37/115/115	-
24	CLA	b	613	44	1/1/15/20	7/37/115/115	-
30	GOL	B	629	-	-	2/4/4/4	-
30	GOL	V	201	35	-	0/4/4/4	-
36	HTG	d	414	-	-	1/10/30/30	0/1/1/1
24	CLA	D	404	-	1/1/15/20	5/37/115/115	-
24	CLA	C	504	-	-	4/37/115/115	-
29	LMT	C	521	-	-	12/21/61/61	0/2/2/2
36	HTG	I	102	-	-	5/10/30/30	0/1/1/1
28	LMG	c	521	-	-	16/46/66/70	0/1/1/1
28	LMG	a	415	-	-	14/46/66/70	0/1/1/1
36	HTG	o	301	-	-	0/10/30/30	0/1/1/1
32	K3C	A	421[A]	-	-	4/4/17/17	0/2/2/2
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
36	HTG	V	203	-	-	1/4/24/30	0/1/1/1
24	CLA	b	606	-	1/1/15/20	5/37/115/115	-
24	CLA	b	617	-	1/1/15/20	9/37/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	LMG	c	522	-	-	6/46/66/70	0/1/1/1
28	LMG	C	532	-	-	10/46/66/70	0/1/1/1
41	RRX	h	1204	-	-	2/29/65/65	0/2/2/2
30	GOL	v	1601	-	-	0/4/4/4	-
43	HEC	v	1603	16	-	2/10/54/54	-
24	CLA	C	509	-	1/1/15/20	5/37/115/115	-
37	LHG	d	410	-	-	8/43/43/53	-
24	CLA	B	609	-	-	2/37/115/115	-
30	GOL	T	101	-	-	4/4/4/4	-
39	DGD	c	518	-	-	15/51/91/95	0/2/2/2
24	CLA	d	405	-	-	5/37/115/115	-
24	CLA	c	505	-	1/1/15/20	4/37/115/115	-
30	GOL	V	204	-	-	2/4/4/4	-
33	PL9	a	425[B]	-	-	10/53/73/73	0/1/1/1
39	DGD	C	517	-	-	13/51/91/95	0/2/2/2
37	LHG	d	409	-	-	12/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
30	GOL	b	630	-	-	2/4/4/4	-
24	CLA	c	513	3	1/1/15/20	0/37/115/115	-
26	BCR	C	516	-	-	1/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/15/20	2/37/115/115	-
26	BCR	D	405	-	-	8/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMT	A	414	-	-	5/21/61/61	0/2/2/2
30	GOL	V	205	-	-	0/4/4/4	-
30	GOL	k	304	-	-	4/4/4/4	-
24	CLA	c	511	-	1/1/15/20	11/37/115/115	-
36	HTG	O	302	-	-	2/10/30/30	0/1/1/1
36	HTG	b	601	-	-	1/10/30/30	0/1/1/1
36	HTG	C	522	-	-	1/10/30/30	0/1/1/1
36	HTG	B	623[A]	-	-	1/10/30/30	0/1/1/1
41	RRX	H	101	-	-	3/29/65/65	0/2/2/2
24	CLA	B	611	44	1/1/15/20	8/37/115/115	-
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6
24	CLA	c	508	-	1/1/15/20	7/37/115/115	-
24	CLA	b	619	-	1/1/15/20	9/37/115/115	-
30	GOL	L	103	-	-	0/4/4/4	-
24	CLA	c	510	-	1/1/15/20	3/37/115/115	-
39	DGD	C	519	-	-	11/51/91/95	0/2/2/2
24	CLA	b	604	44	1/1/15/20	14/37/115/115	-
29	LMT	b	624	-	-	4/17/37/61	0/1/1/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
27	SQD	a	414	-	-	12/49/69/69	0/1/1/1
24	CLA	b	607	-	1/1/15/20	4/37/115/115	-
24	CLA	C	507	-	1/1/15/20	14/37/115/115	-
24	CLA	a	412	-	1/1/15/20	10/37/115/115	-
43	HEC	V	202	16	-	2/10/54/54	-
24	CLA	a	409	44	1/1/15/20	4/37/115/115	-
30	GOL	C	530	-	-	0/4/4/4	-
30	GOL	a	416	-	-	2/4/4/4	-
29	LMT	z	101	-	-	5/15/55/61	0/2/2/2
24	CLA	B	612	-	1/1/15/20	2/37/115/115	-
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/15/20	4/37/115/115	-
24	CLA	a	408	-	1/1/15/20	4/37/115/115	-
26	BCR	c	517	-	-	2/29/63/63	0/2/2/2
30	GOL	d	413	-	-	2/4/4/4	-
39	DGD	H	102	-	-	9/51/91/95	0/2/2/2
24	CLA	b	608	-	1/1/15/20	3/37/115/115	-
29	LMT	m	102	-	-	1/21/61/61	0/2/2/2
28	LMG	A	412	-	-	21/46/66/70	0/1/1/1
24	CLA	C	508	44	1/1/15/20	11/37/115/115	-
30	GOL	V	206	-	-	0/4/4/4	-
30	GOL	O	303	-	-	0/4/4/4	-
40	HEM	F	101	6,5	-	2/12/54/54	-
24	CLA	B	606	-	1/1/15/20	4/37/115/115	-
24	CLA	B	614	-	1/1/15/20	3/37/115/115	-
24	CLA	B	617	-	1/1/15/20	11/37/115/115	-
24	CLA	d	404	-	1/1/15/20	1/37/115/115	-
24	CLA	B	616	-	1/1/15/20	6/37/115/115	-
30	GOL	b	629	-	-	1/4/4/4	-
28	LMG	b	623	-	-	19/46/66/70	0/1/1/1
24	CLA	C	506	-	1/1/15/20	2/37/115/115	-
39	DGD	D	407	-	-	17/47/68/95	0/1/1/2
24	CLA	c	503	-	1/1/15/20	4/37/115/115	-
30	GOL	A	415	-	-	0/4/4/4	-
37	LHG	e	101	-	-	23/44/44/53	-
25	PHO	D	401	-	-	1/37/103/103	0/5/6/6
33	PL9	D	406	-	-	5/53/73/73	0/1/1/1
37	LHG	d	408	-	-	6/53/53/53	-
40	HEM	f	101	6,5	-	2/12/54/54	-
39	DGD	h	1205	-	-	8/51/91/95	0/2/2/2
26	BCR	k	302	-	-	6/29/63/63	0/2/2/2
27	SQD	A	411	-	-	9/49/69/69	0/1/1/1
24	CLA	C	502	-	1/1/15/20	3/37/115/115	-
24	CLA	C	505	44	1/1/15/20	7/37/115/115	-
24	CLA	b	614	-	1/1/15/20	5/37/115/115	-
30	GOL	h	1206	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	406	44	-	3/37/115/115	-
24	CLA	b	611	-	-	3/37/115/115	-
39	DGD	C	518	-	-	19/51/91/95	0/2/2/2
39	DGD	c	519	-	-	16/51/91/95	0/2/2/2
30	GOL	b	627	-	-	0/4/4/4	-
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
30	GOL	T	103	-	-	0/4/4/4	-
30	GOL	o	305	-	-	2/4/4/4	-
24	CLA	b	610	44	1/1/15/20	3/37/115/115	-
37	LHG	D	410	-	-	8/53/53/53	-
24	CLA	a	410	44	-	5/37/115/115	-
26	BCR	b	620	-	-	2/29/63/63	0/2/2/2
39	DGD	c	520	-	-	14/51/91/95	0/2/2/2
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
24	CLA	b	618	-	1/1/15/20	9/37/115/115	-
30	GOL	c	526	-	-	4/4/4/4	-
30	GOL	B	631	-	-	0/4/4/4	-
30	GOL	v	1605	-	-	2/4/4/4	-
29	LMT	J	102	-	-	2/15/35/61	0/1/1/2
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	SQD	f	102	-	-	10/33/33/69	-
24	CLA	C	503	-	-	7/37/115/115	-
24	CLA	b	615	-	1/1/15/20	0/37/115/115	-
26	BCR	B	641	-	-	1/29/63/63	0/2/2/2
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
24	CLA	b	609	-	1/1/15/20	10/37/115/115	-
26	BCR	k	303	-	-	1/29/63/63	0/2/2/2
30	GOL	B	630	-	-	0/4/4/4	-
24	CLA	A	407	44	-	4/37/115/115	-
24	CLA	B	613	-	1/1/15/20	3/37/115/115	-
30	GOL	b	628	-	-	0/4/4/4	-
24	CLA	c	514	-	1/1/15/20	8/37/115/115	-
30	GOL	A	416	-	-	1/4/4/4	-
30	GOL	C	527	-	-	1/4/4/4	-
36	HTG	U	201	-	-	3/6/6/30	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	B	642	-	-	7/15/35/61	0/1/1/2
24	CLA	c	504	-	1/1/15/20	7/37/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	c	509	44	1/1/15/20	6/37/115/115	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
28	LMG	B	621	-	-	9/46/66/70	0/1/1/1
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
30	GOL	C	529	-	-	0/4/4/4	-
24	CLA	C	512	3	1/1/15/20	3/37/115/115	-
24	CLA	c	506	44	1/1/15/20	5/37/115/115	-
28	LMG	D	412	42	-	10/46/66/70	0/1/1/1
30	GOL	a	421	-	-	4/4/4/4	-
30	GOL	v	1604	-	-	0/4/4/4	-
30	GOL	C	528	-	-	0/4/4/4	-
24	CLA	B	602	44	1/1/15/20	15/37/115/115	-
27	SQD	A	413	-	-	11/49/69/69	0/1/1/1
30	GOL	c	527	-	-	0/4/4/4	-
33	PL9	A	422[B]	-	-	13/53/73/73	0/1/1/1
30	GOL	C	524	-	-	0/4/4/4	-
29	LMT	f	104	-	-	7/21/61/61	0/2/2/2
29	LMT	E	104	-	-	6/15/35/61	0/1/1/2
26	BCR	d	406	-	-	8/29/63/63	0/2/2/2
33	PL9	d	407	-	-	6/53/73/73	0/1/1/1
37	LHG	l	302	-	-	13/53/53/53	-
29	LMT	m	103	-	-	2/21/61/61	0/2/2/2
30	GOL	v	1607	-	-	4/4/4/4	-
36	HTG	h	1202	-	-	4/10/30/30	0/1/1/1
37	LHG	B	640	-	-	12/53/53/53	-
29	LMT	B	622	-	-	8/21/61/61	0/2/2/2
30	GOL	B	633	-	-	0/4/4/4	-
27	SQD	a	401	-	-	12/49/69/69	0/1/1/1
30	GOL	c	528	-	-	0/4/4/4	-
36	HTG	B	624	-	-	3/10/30/30	0/1/1/1
24	CLA	A	409	-	-	7/37/115/115	-
36	HTG	b	626	-	-	3/10/30/30	0/1/1/1
30	GOL	B	627	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	C	523	-	-	4/10/30/30	0/1/1/1
30	GOL	v	1606	-	-	2/4/4/4	-
24	CLA	B	604	-	1/1/15/20	2/37/115/115	-
26	BCR	Y	302	-	-	6/29/63/63	0/2/2/2
24	CLA	C	514	-	-	4/37/115/115	-
30	GOL	o	302	-	-	4/4/4/4	-
30	GOL	u	202	-	-	2/4/4/4	-
36	HTG	u	201	-	-	2/12/14/30	-
29	LMT	Z	101	-	-	12/21/61/61	0/2/2/2
27	SQD	D	408	-	-	15/40/60/69	0/1/1/1
30	GOL	a	417	-	-	3/4/4/4	-
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
24	CLA	b	616	-	1/1/15/20	2/37/115/115	-
36	HTG	B	623[B]	-	-	1/10/30/30	0/1/1/1
29	LMT	m	101	-	-	4/21/61/61	0/2/2/2
29	LMT	M	101	-	-	1/21/61/61	0/2/2/2
37	LHG	E	101	-	-	26/53/53/53	-
30	GOL	a	418	-	-	2/4/4/4	-
24	CLA	D	403	-	1/1/15/20	1/37/115/115	-
30	GOL	c	532	-	-	0/4/4/4	-
24	CLA	B	615	-	1/1/15/20	10/37/115/115	-
30	GOL	d	402	-	-	1/4/4/4	-
28	LMG	d	411	42	-	11/46/66/70	0/1/1/1
24	CLA	C	513	-	1/1/15/20	6/37/115/115	-
24	CLA	c	512	-	1/1/15/20	5/37/115/115	-
32	K3C	a	424[A]	-	-	4/4/17/17	0/2/2/2
24	CLA	B	608	44	1/1/15/20	4/37/115/115	-
29	LMT	a	402	-	-	8/21/61/61	0/2/2/2
37	LHG	D	409	-	-	10/53/53/53	-
24	CLA	C	511	-	1/1/15/20	4/37/115/115	-
30	GOL	B	628	-	-	0/4/4/4	-
30	GOL	M	102	-	-	0/4/4/4	-
24	CLA	c	515	-	-	10/37/115/115	-
28	LMG	C	520	-	-	18/46/66/70	0/1/1/1
30	GOL	E	105	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607	-	1/1/15/20	5/37/115/115	-
36	HTG	D	413	-	-	1/10/30/30	0/1/1/1
36	HTG	c	524	-	-	1/10/30/30	0/1/1/1
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
29	LMT	c	523	-	-	6/21/61/61	0/2/2/2
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
24	CLA	B	605	-	1/1/15/20	5/37/115/115	-
24	CLA	b	612	-	1/1/15/20	3/37/115/115	-
30	GOL	v	1602	35	-	2/4/4/4	-
24	CLA	C	510	-	1/1/15/20	4/37/115/115	-
29	LMT	T	104	-	-	8/15/35/61	0/1/1/2
37	LHG	D	411	-	-	11/50/50/53	-
27	SQD	L	101	-	-	24/49/69/69	0/1/1/1

The worst 5 of 1576 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	11.28	2.33	2.06
24	c	513	CLA	MG-NA	10.92	2.32	2.06
24	C	508	CLA	MG-NA	10.63	2.31	2.06
24	B	605	CLA	MG-ND	-10.09	1.85	2.05
24	c	505	CLA	MG-NA	9.46	2.28	2.06

The worst 5 of 2346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C1D-ND-C4D	-10.69	98.74	106.33
24	D	403	CLA	C1D-ND-C4D	-10.62	98.79	106.33
24	c	503	CLA	C1D-ND-C4D	-10.50	98.88	106.33
24	a	409	CLA	C1D-ND-C4D	-10.11	99.15	106.33
24	B	605	CLA	C1D-ND-C4D	-9.99	99.24	106.33

5 of 59 chirality outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	B	605	CLA	ND

5 of 1191 torsion outliers are listed below:

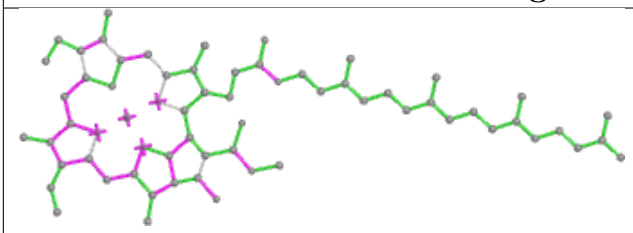
Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	C2-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

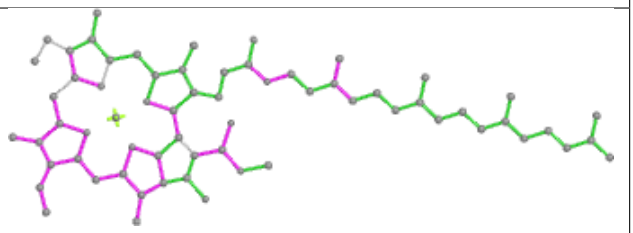
No monomer is involved in short contacts.

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.

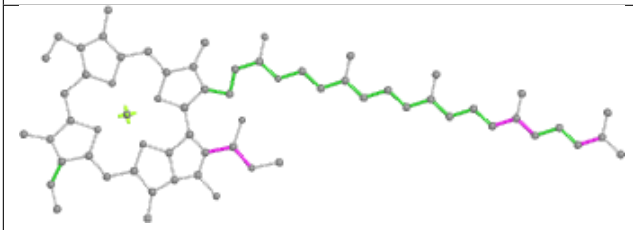
Ligand CLA c 507



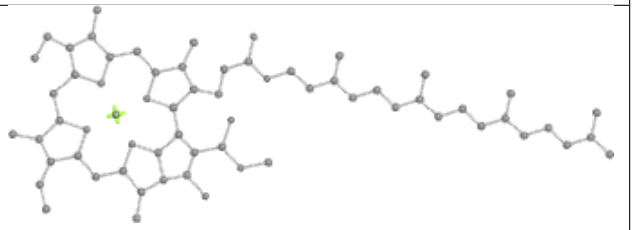
Bond lengths



Bond angles

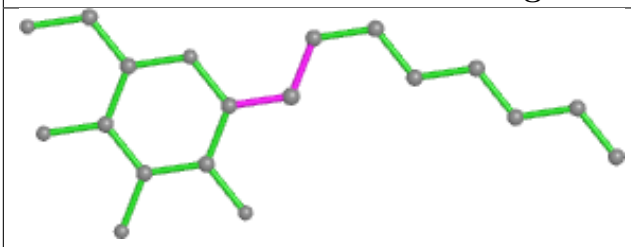


Torsions

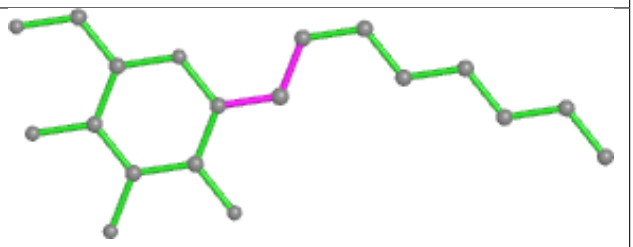


Rings

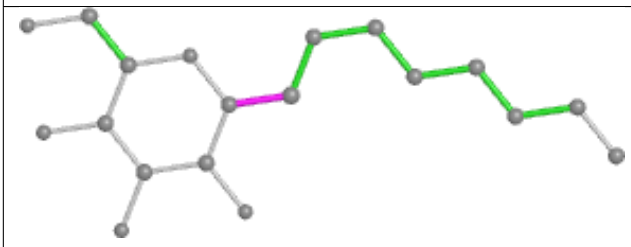
Ligand HTG b 602



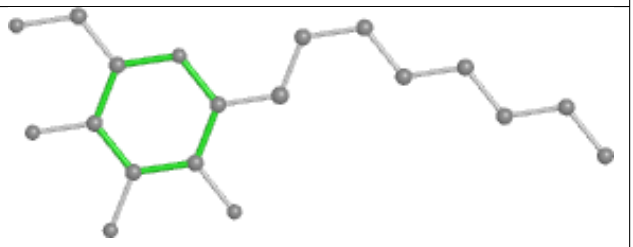
Bond lengths



Bond angles

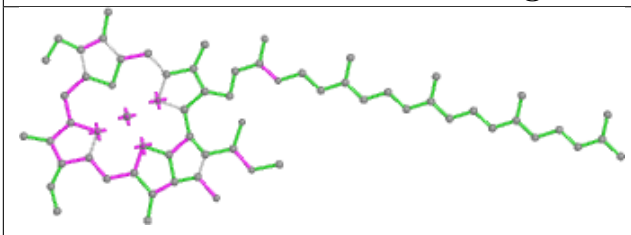


Torsions

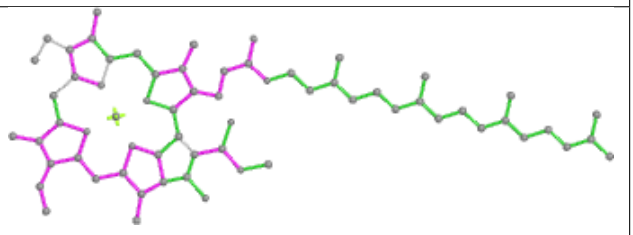


Rings

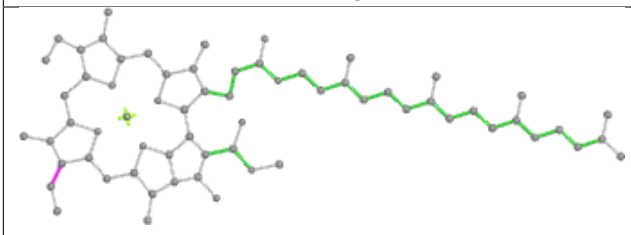
Ligand CLA A 405



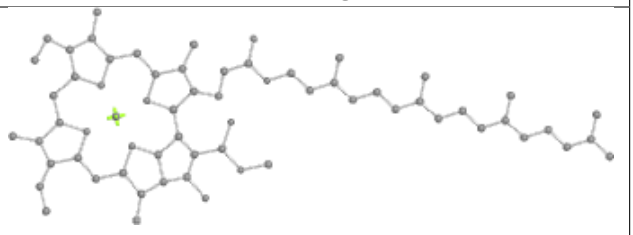
Bond lengths



Bond angles

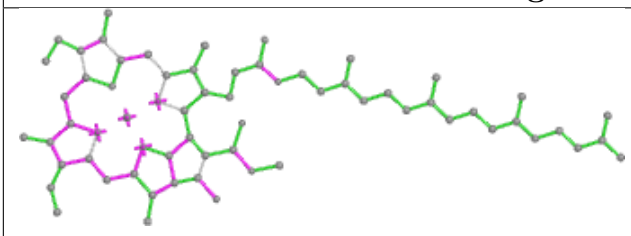


Torsions

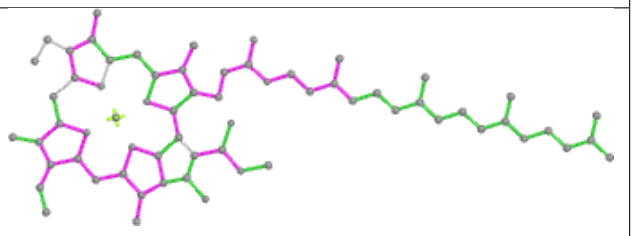


Rings

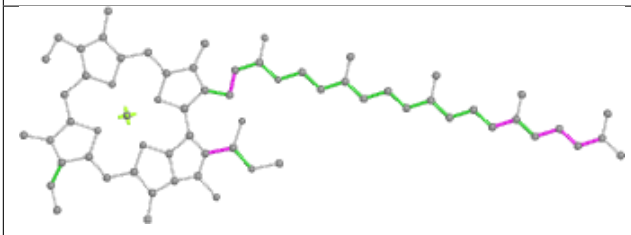
Ligand CLA b 613



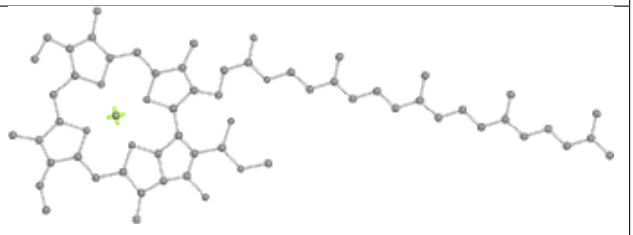
Bond lengths



Bond angles

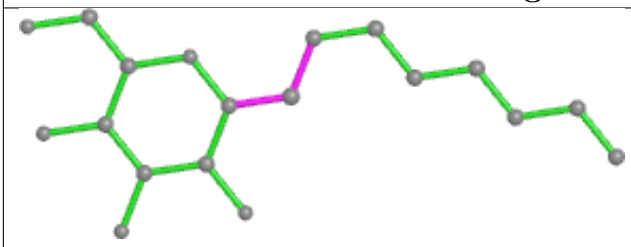


Torsions

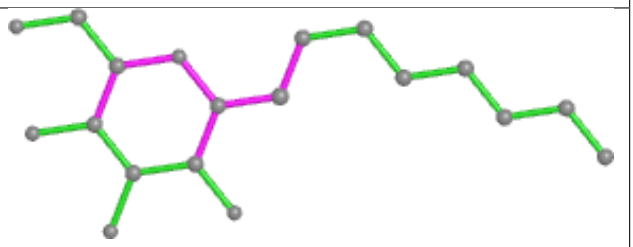


Rings

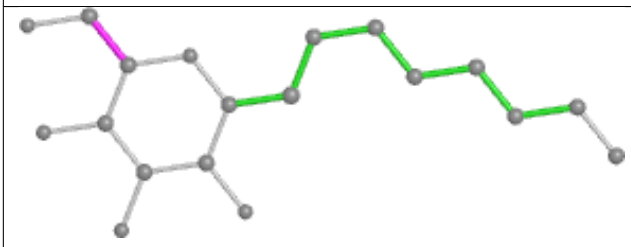
Ligand HTG d 414



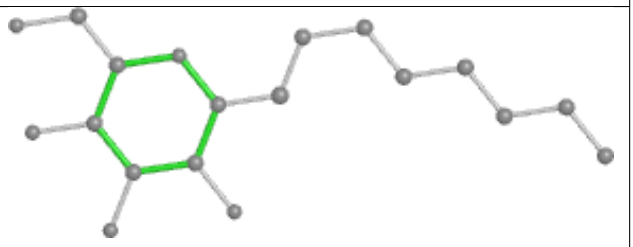
Bond lengths



Bond angles

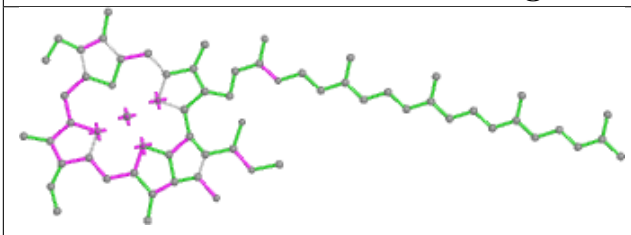


Torsions

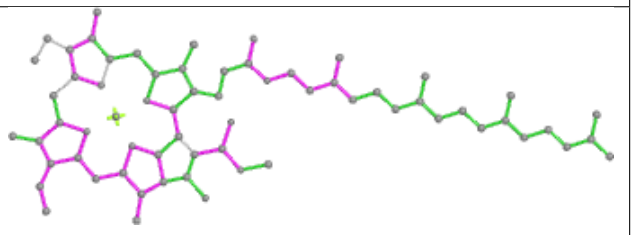


Rings

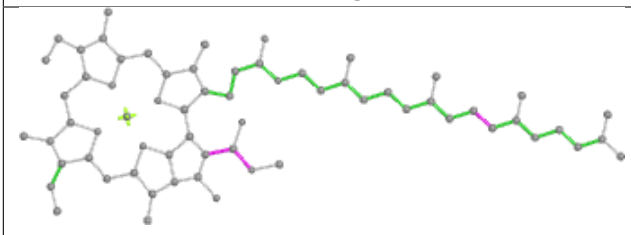
Ligand CLA C 504



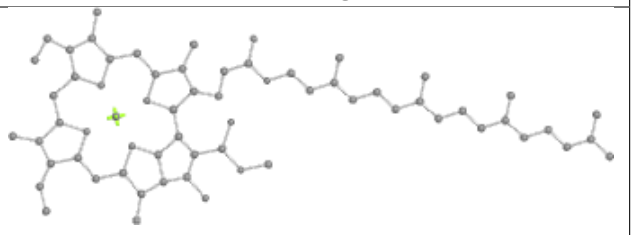
Bond lengths



Bond angles

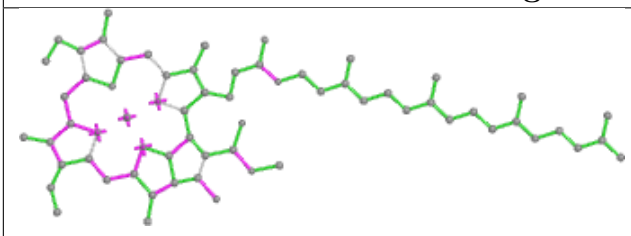


Torsions

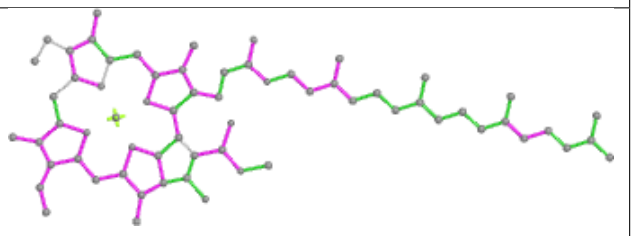


Rings

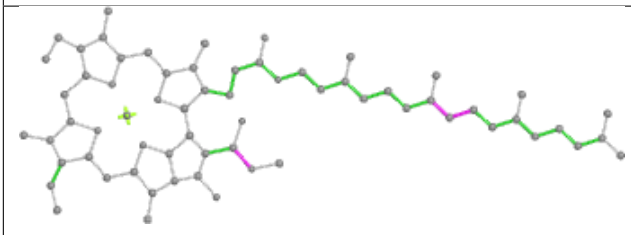
Ligand CLA D 404



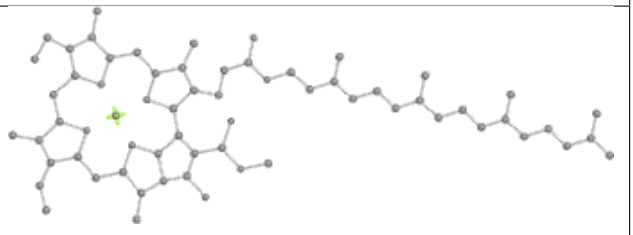
Bond lengths



Bond angles

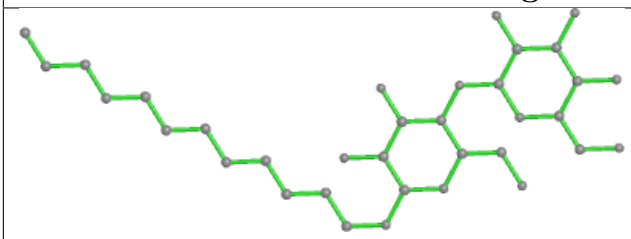


Torsions

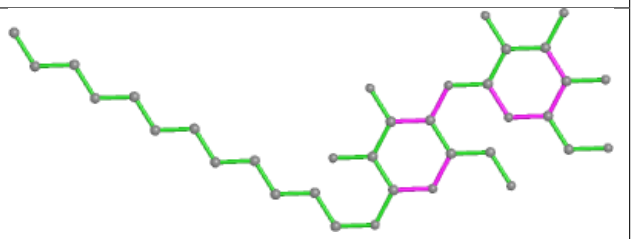


Rings

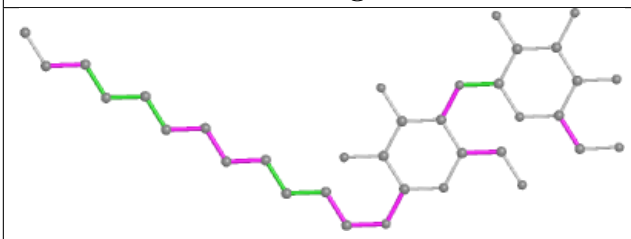
Ligand LMT C 521



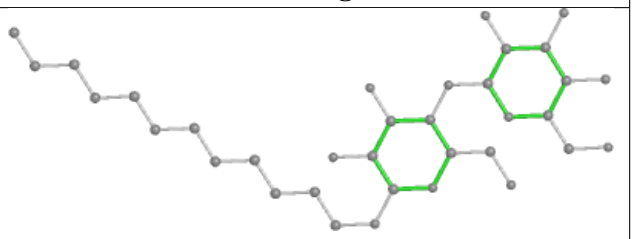
Bond lengths



Bond angles

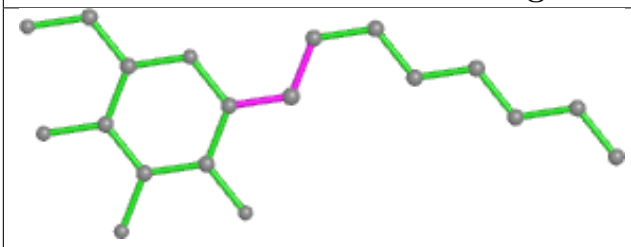


Torsions

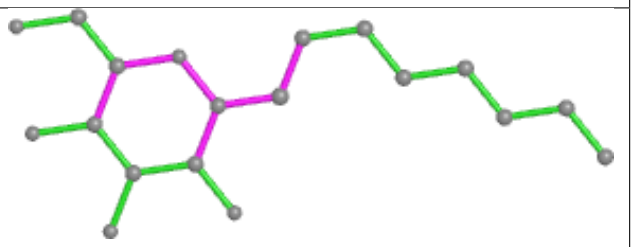


Rings

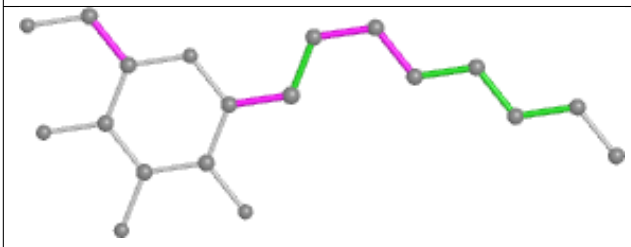
Ligand HTG I 102



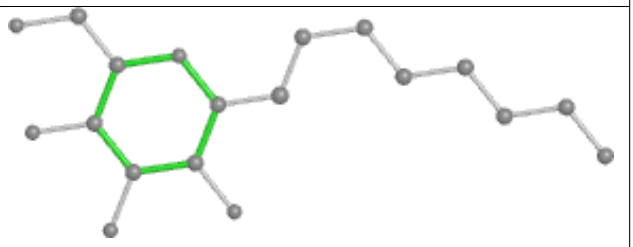
Bond lengths



Bond angles

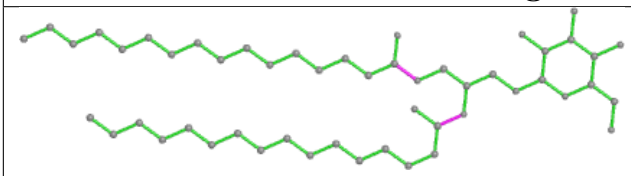


Torsions

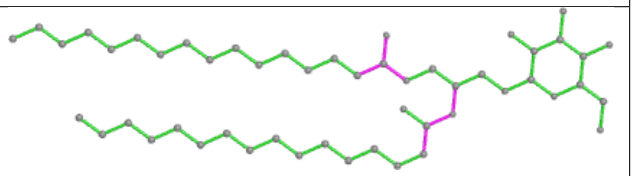


Rings

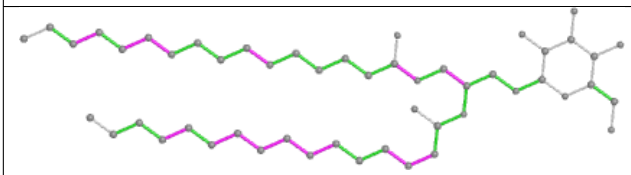
Ligand LMG c 521



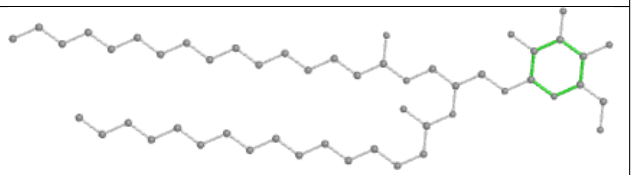
Bond lengths



Bond angles

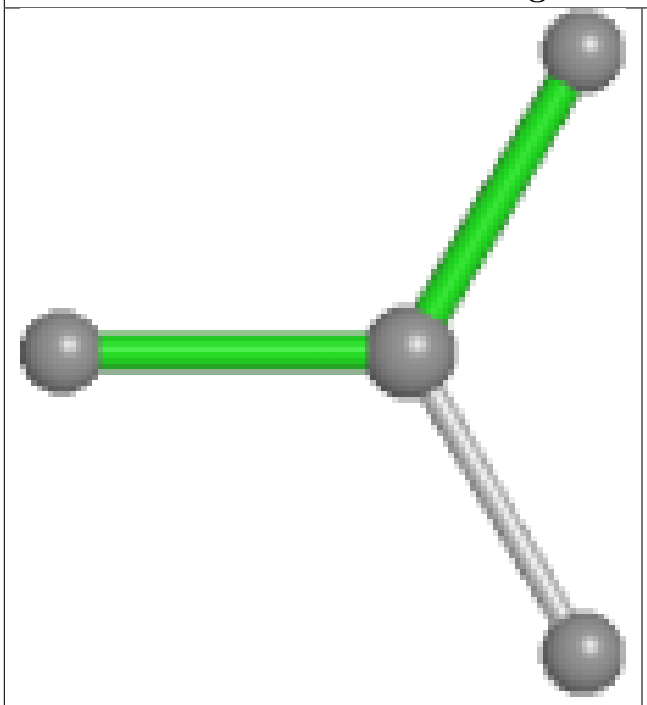


Torsions

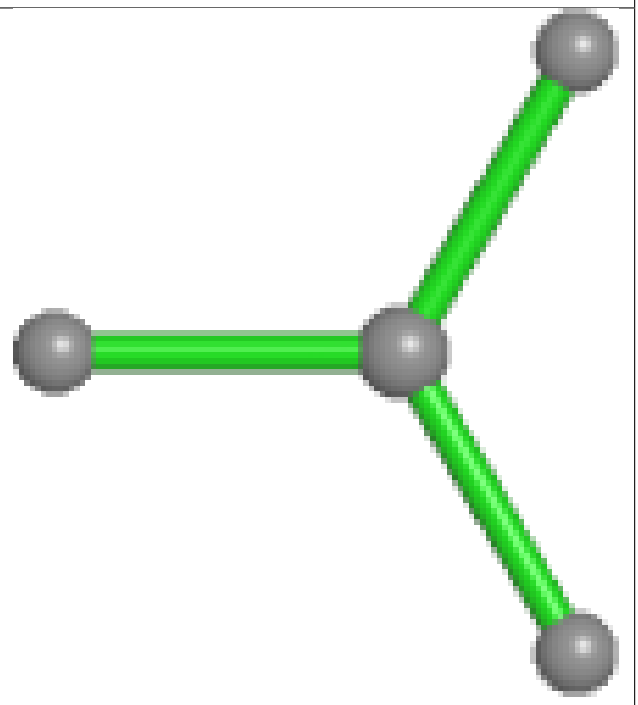


Rings

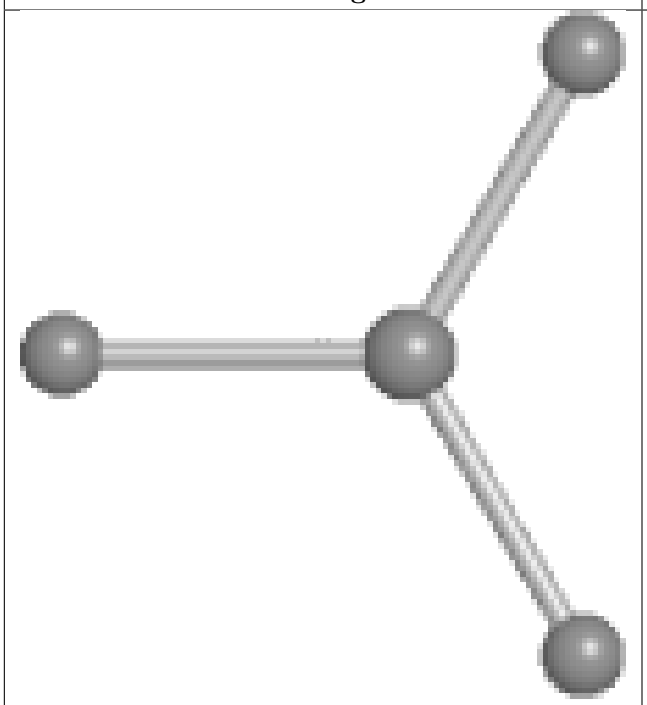
Ligand BCT a 407



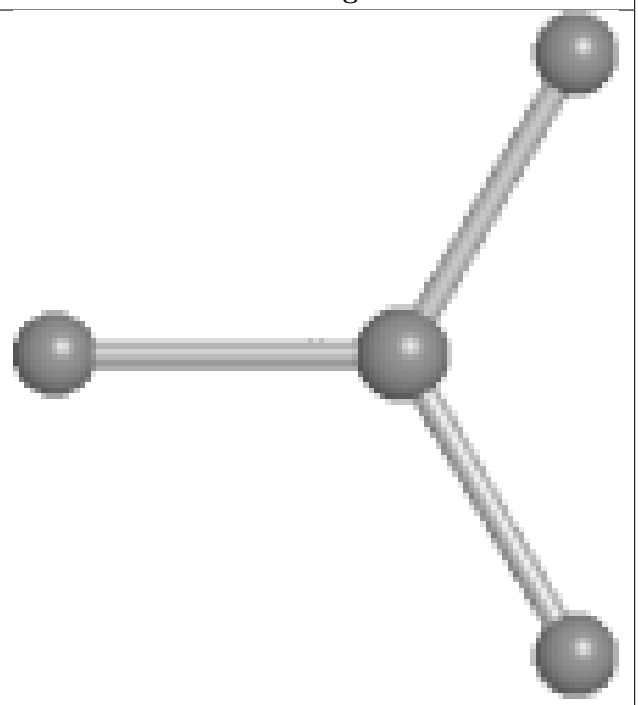
Bond lengths



Bond angles

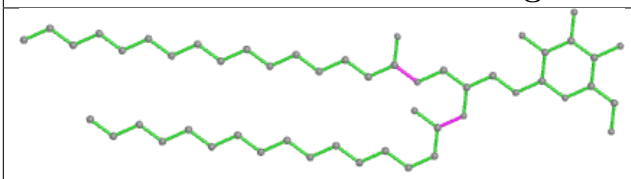


Torsions

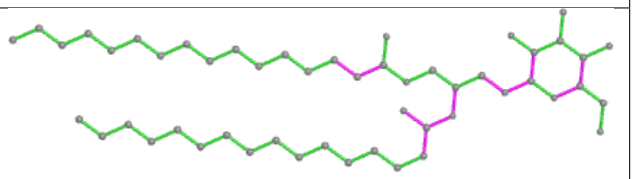


Rings

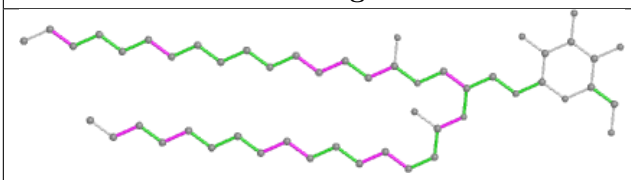
Ligand LMG a 415



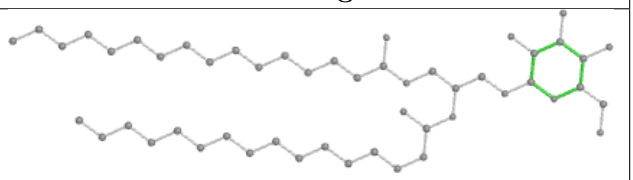
Bond lengths



Bond angles

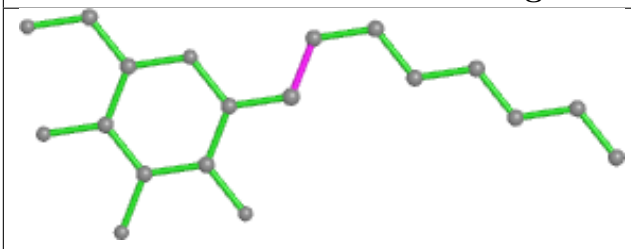


Torsions

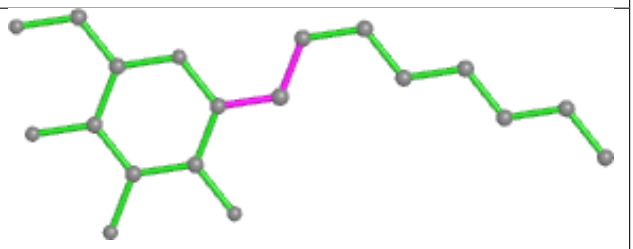


Rings

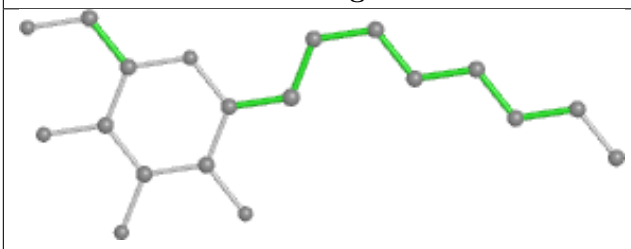
Ligand HTG o 301



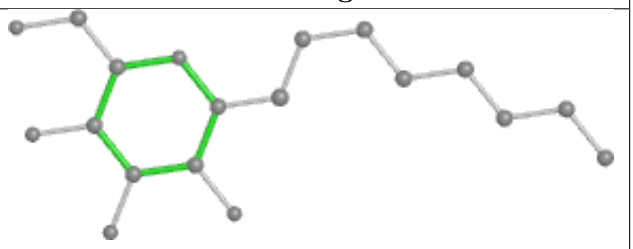
Bond lengths



Bond angles

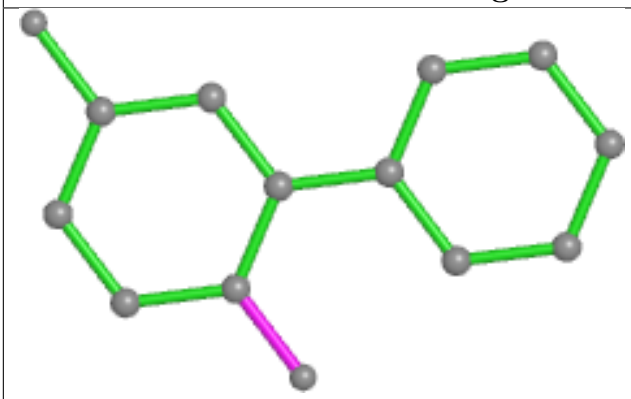


Torsions

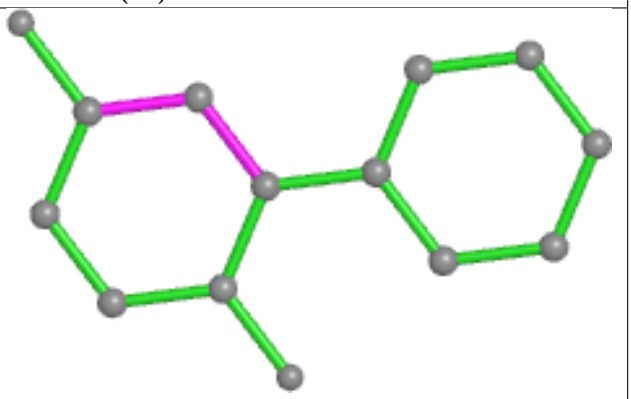


Rings

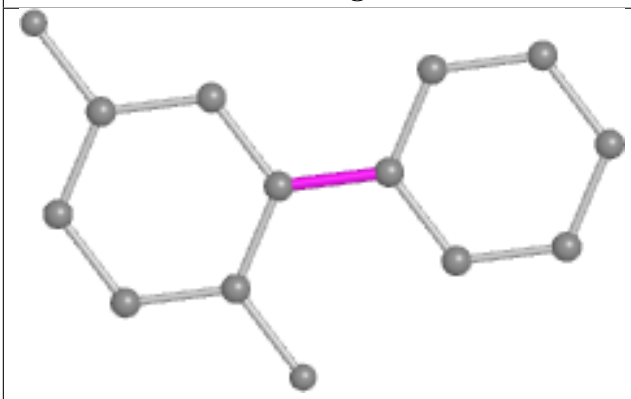
Ligand K3C A 421 (A)



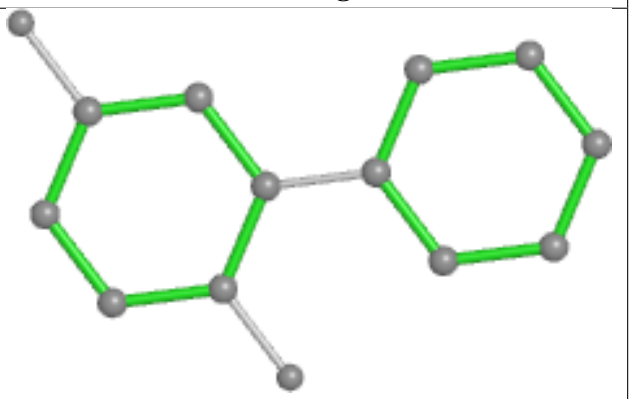
Bond lengths



Bond angles

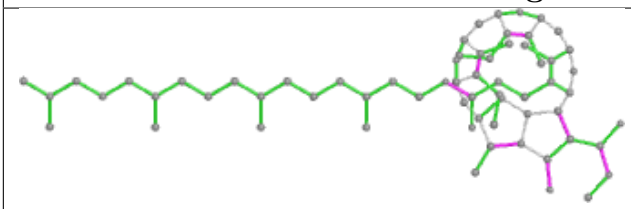


Torsions

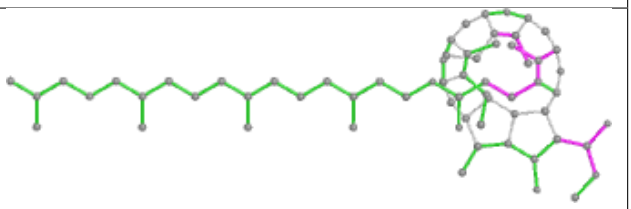


Rings

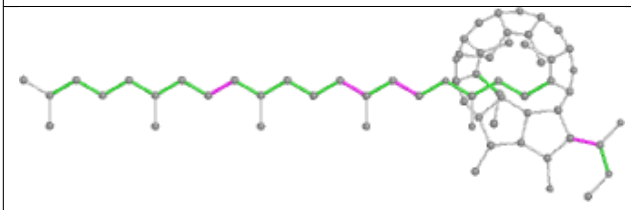
Ligand PHO a 411



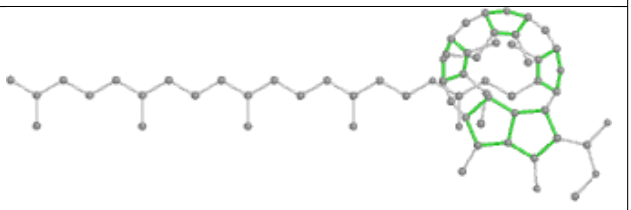
Bond lengths



Bond angles

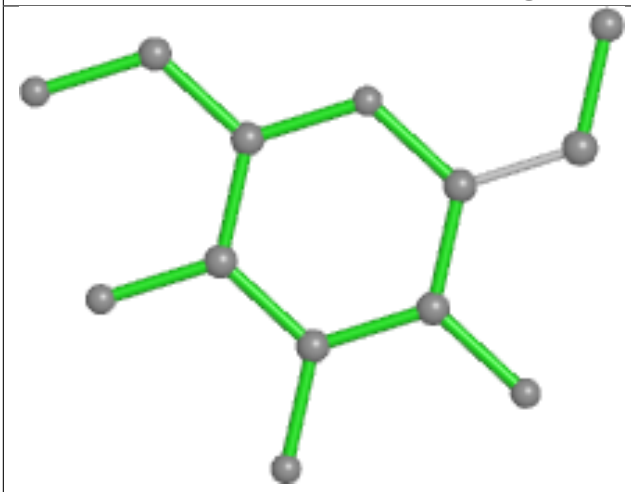


Torsions

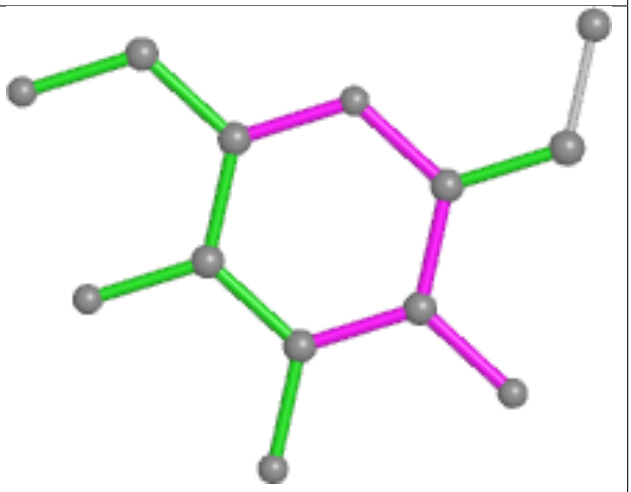


Rings

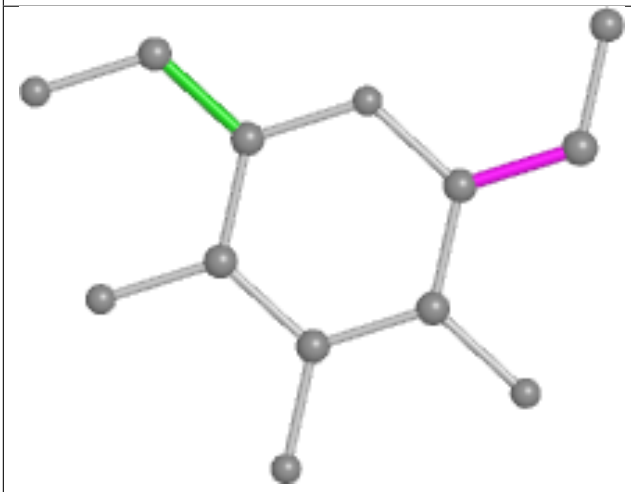
Ligand HTG V 203



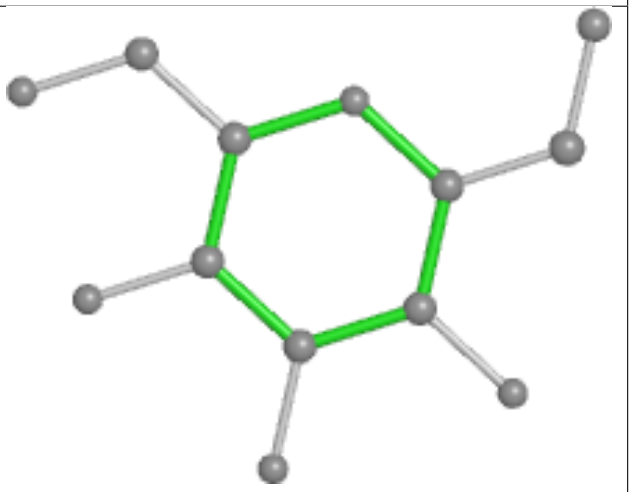
Bond lengths



Bond angles

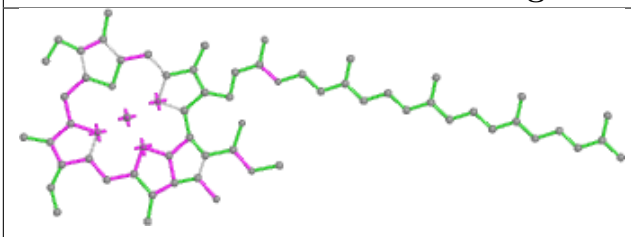


Torsions

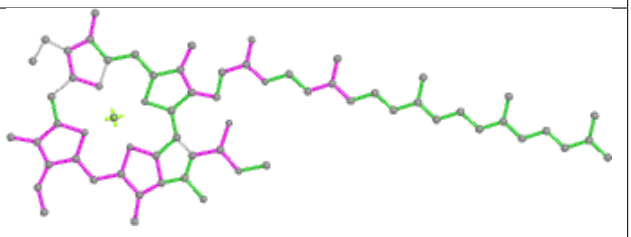


Rings

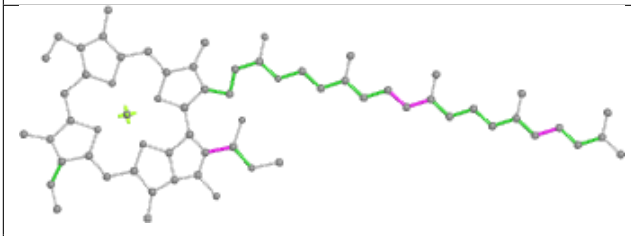
Ligand CLA b 606



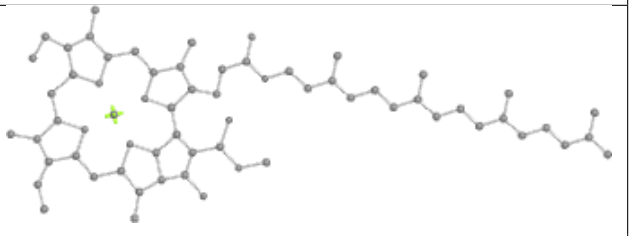
Bond lengths



Bond angles

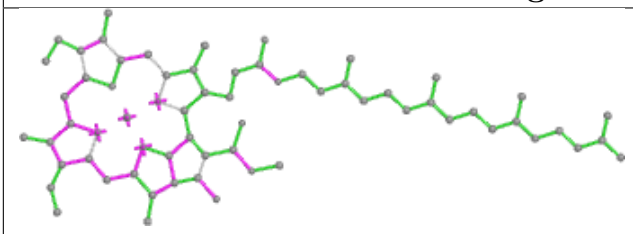


Torsions

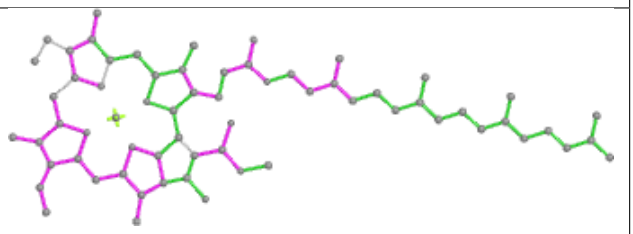


Rings

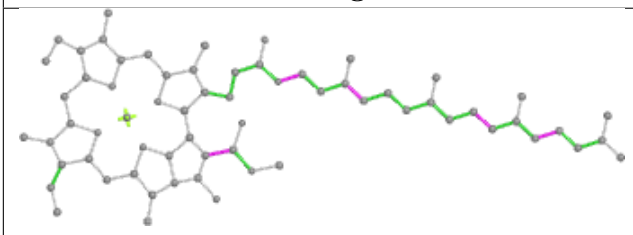
Ligand CLA b 617



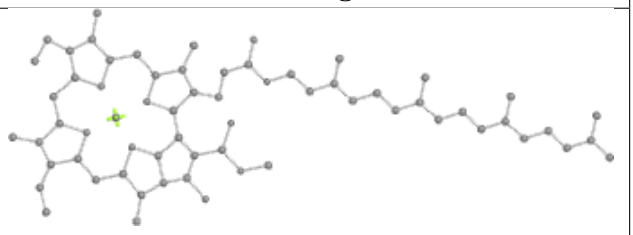
Bond lengths



Bond angles

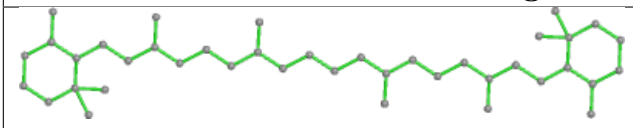


Torsions

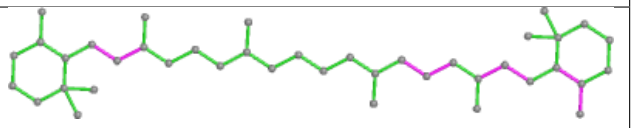


Rings

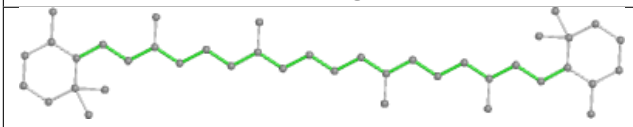
Ligand BCR B 620



Bond lengths



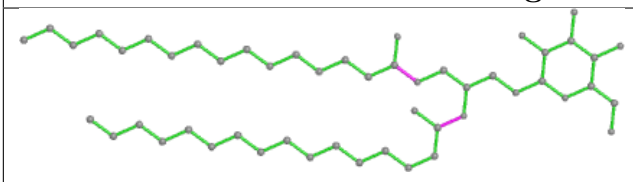
Bond angles



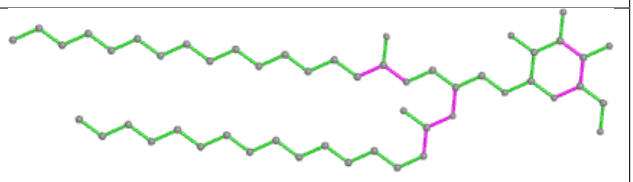
Torsions

Rings

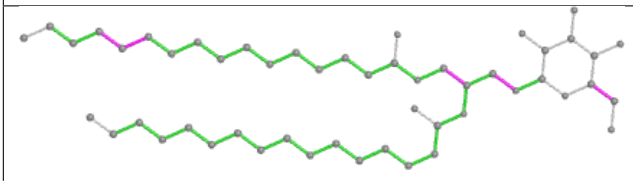
Ligand LMG c 522



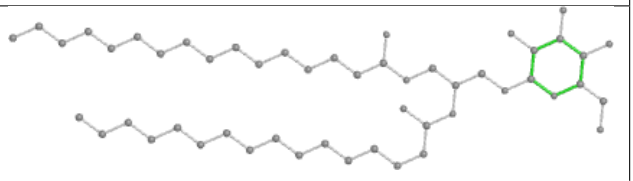
Bond lengths



Bond angles

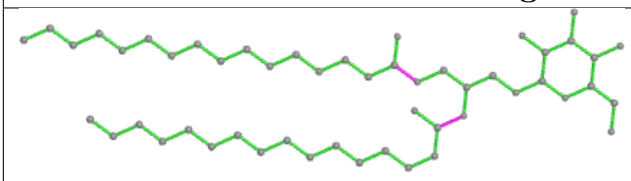


Torsions

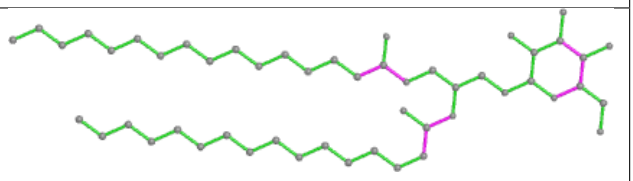


Rings

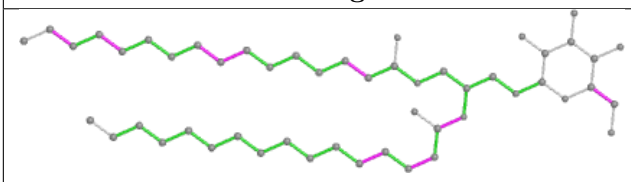
Ligand LMG C 532



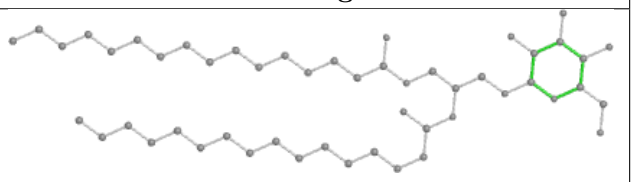
Bond lengths



Bond angles

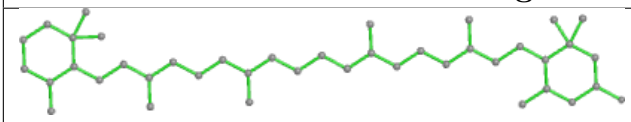


Torsions

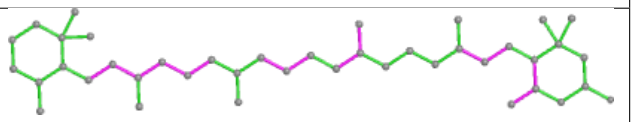


Rings

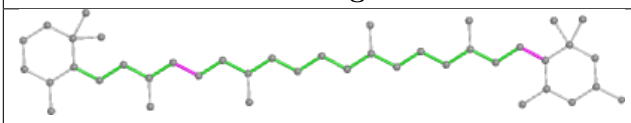
Ligand RRX h 1204



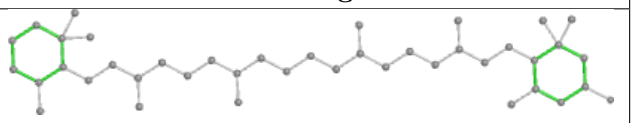
Bond lengths



Bond angles

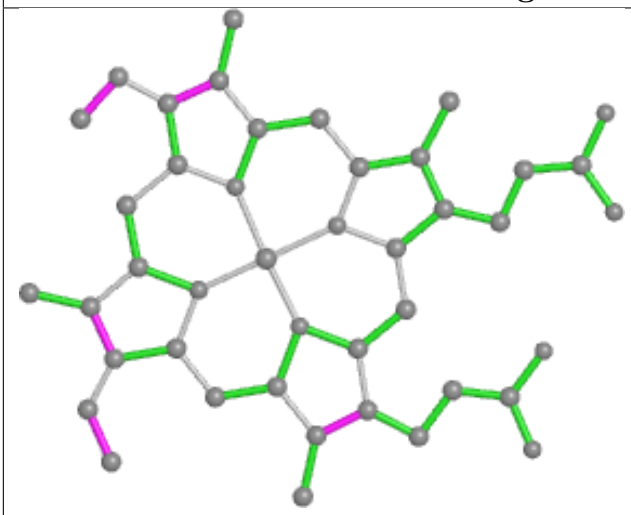


Torsions

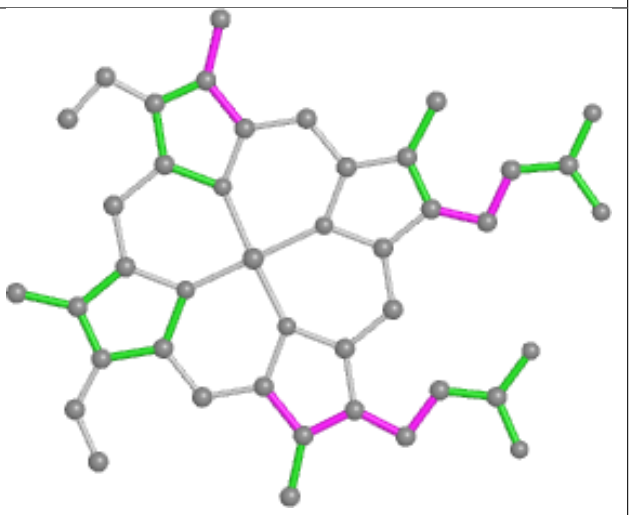


Rings

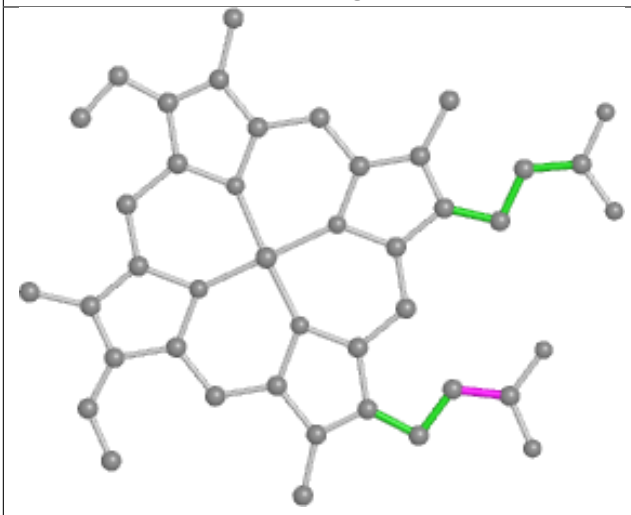
Ligand HEC v 1603



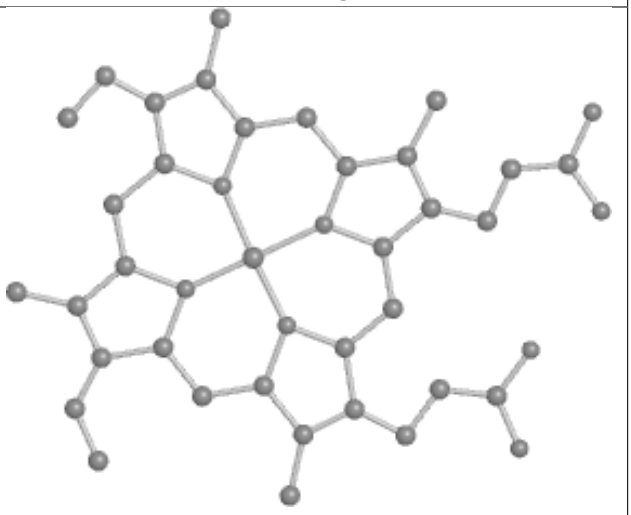
Bond lengths



Bond angles

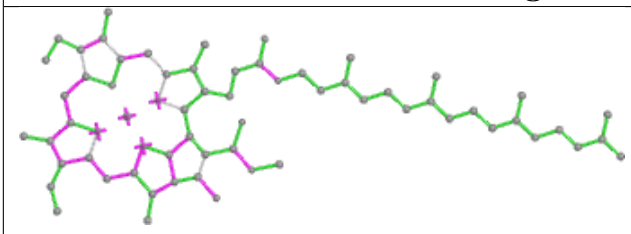


Torsions

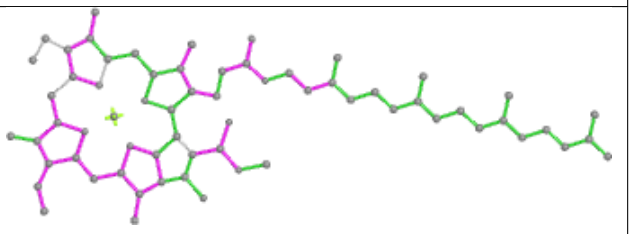


Rings

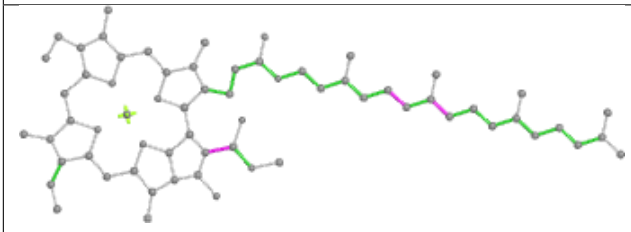
Ligand CLA C 509



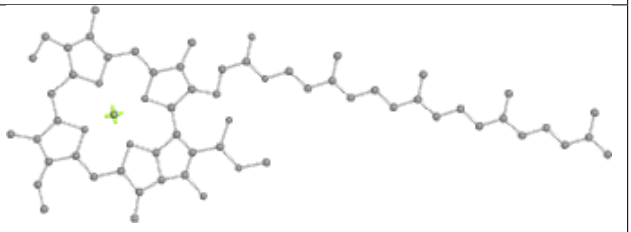
Bond lengths



Bond angles

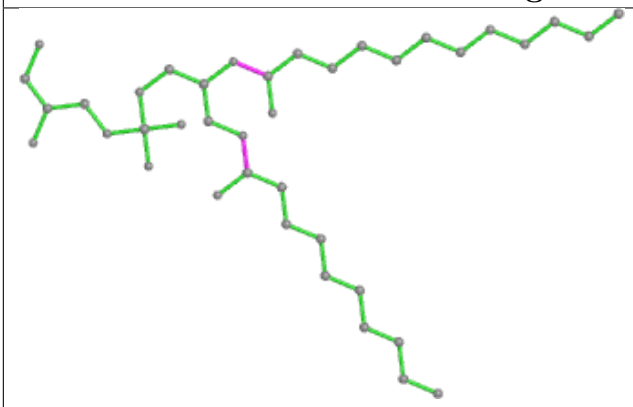


Torsions

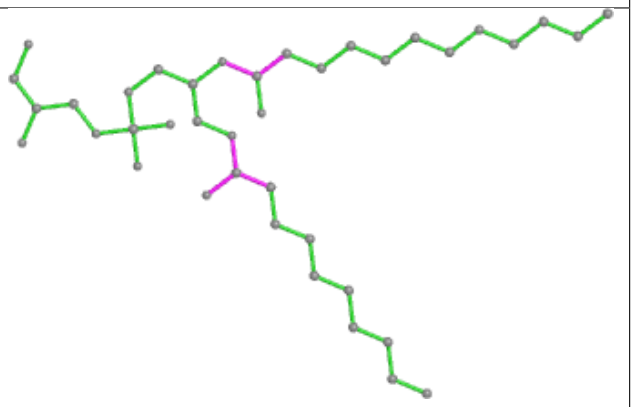


Rings

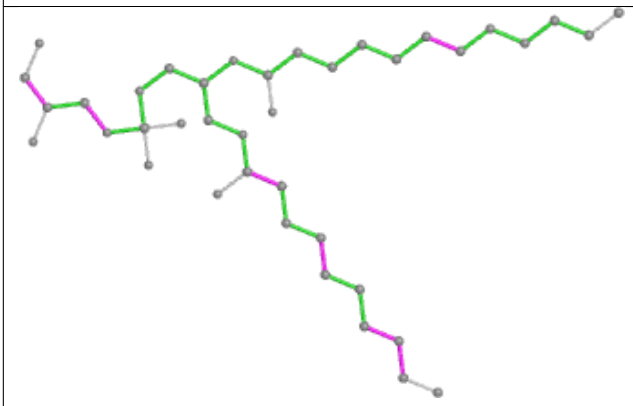
Ligand LHG d 410



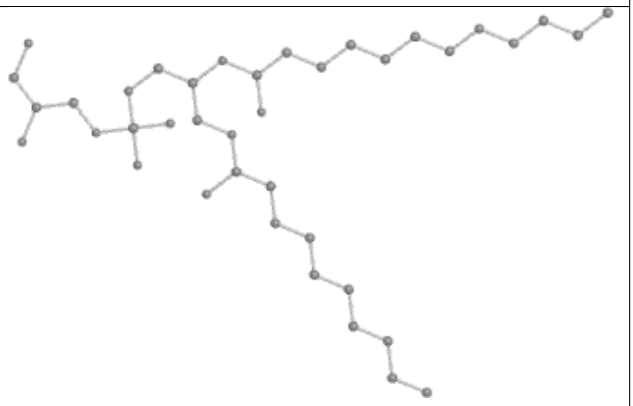
Bond lengths



Bond angles

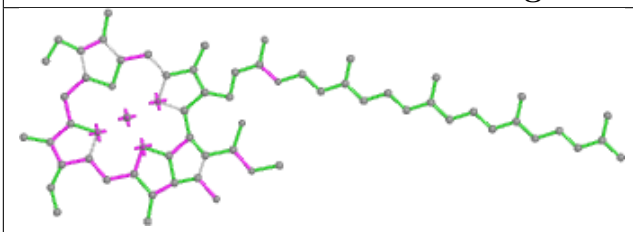


Torsions

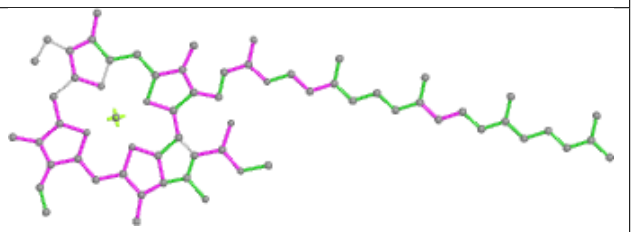


Rings

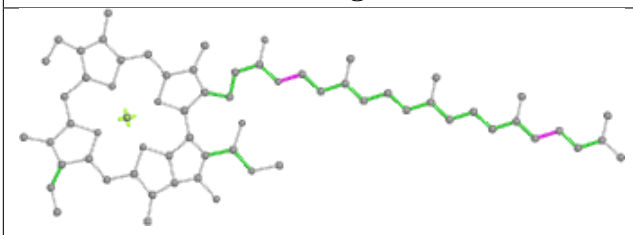
Ligand CLA B 609



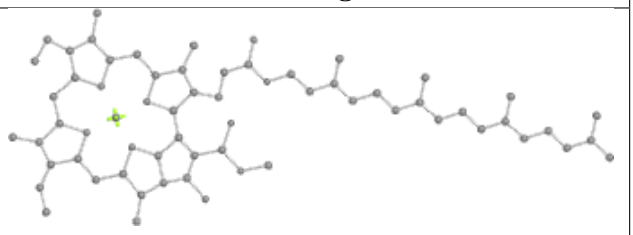
Bond lengths



Bond angles

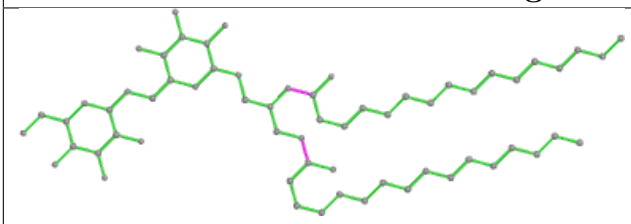


Torsions

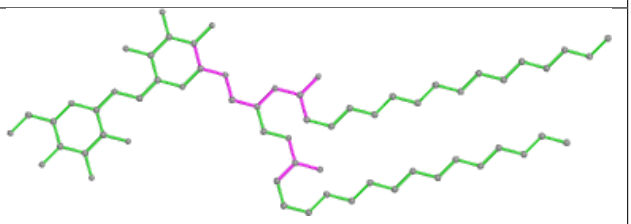


Rings

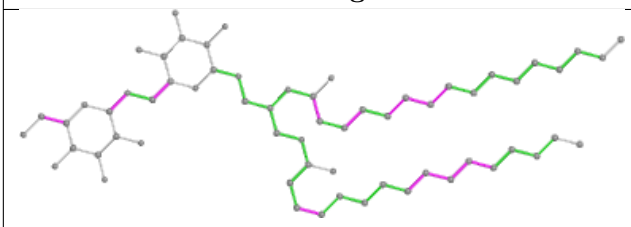
Ligand DGD c 518



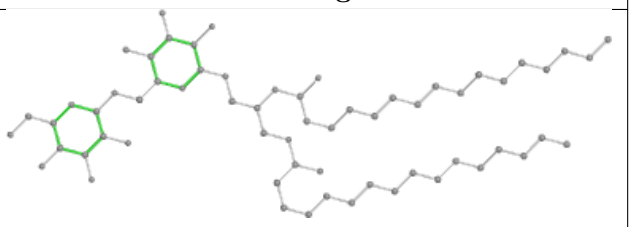
Bond lengths



Bond angles

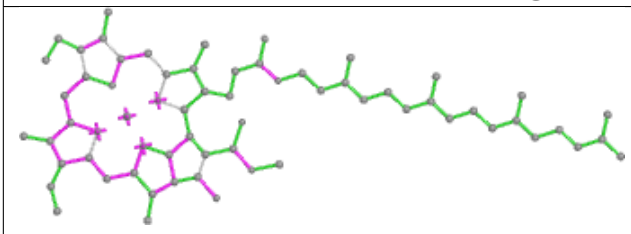


Torsions

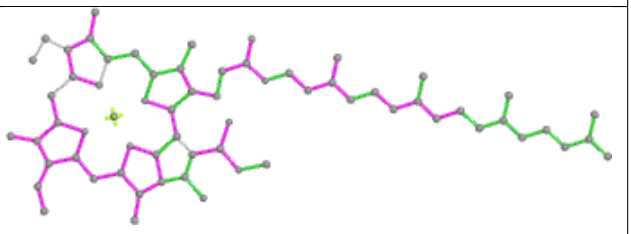


Rings

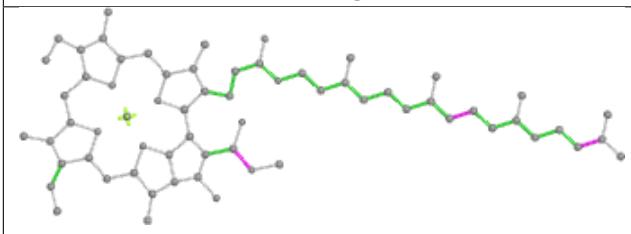
Ligand CLA d 405



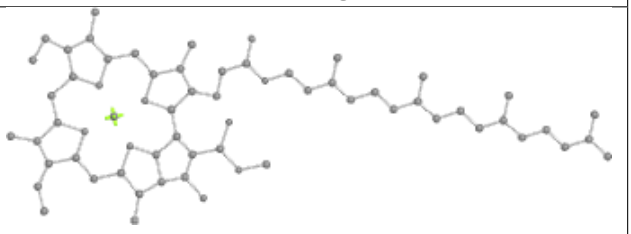
Bond lengths



Bond angles

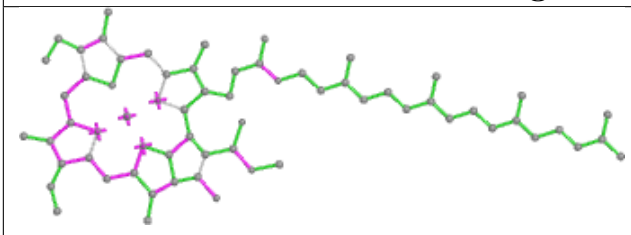


Torsions

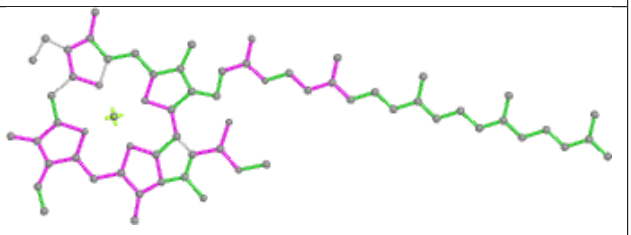


Rings

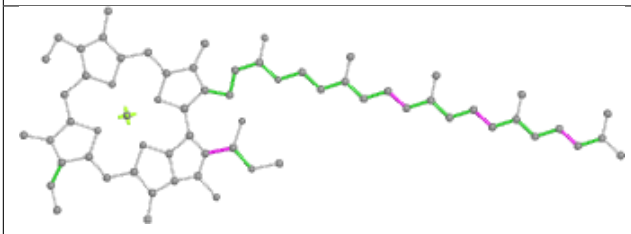
Ligand CLA c 505



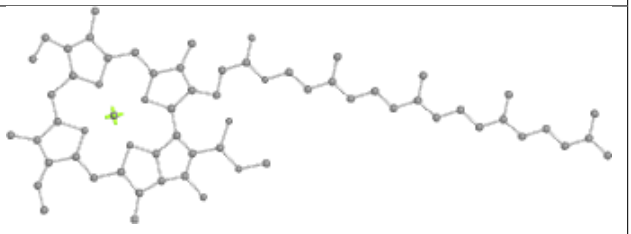
Bond lengths



Bond angles

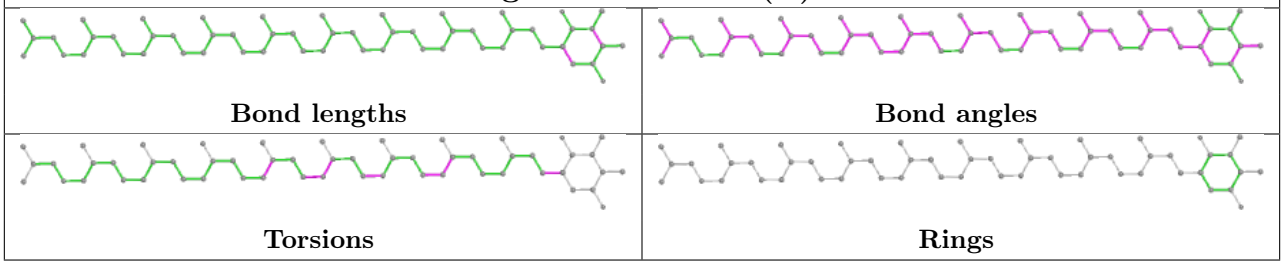


Torsions

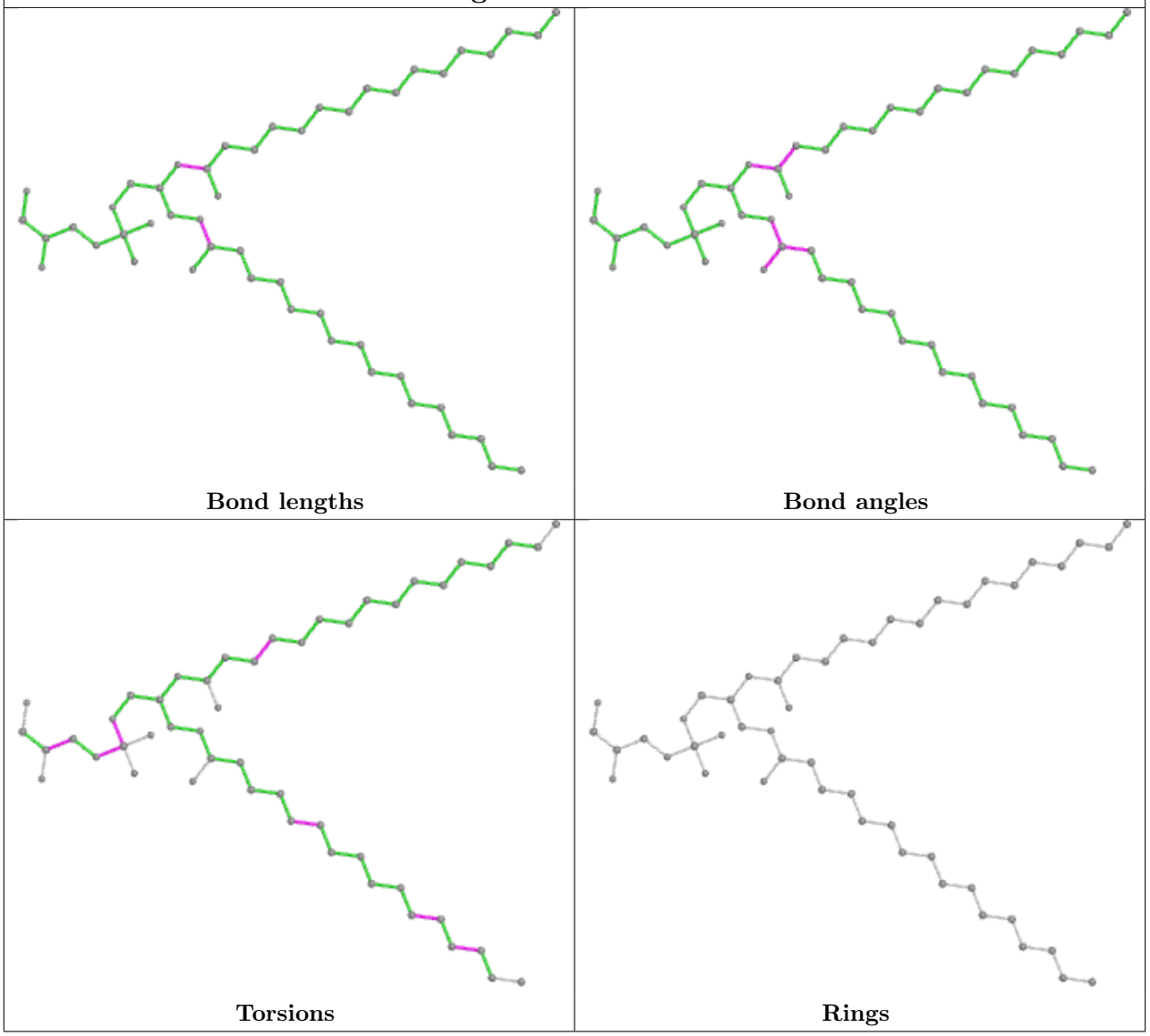


Rings

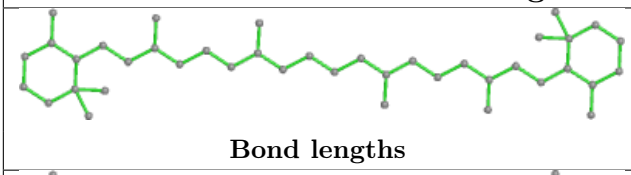
Ligand PL9 a 425 (B)



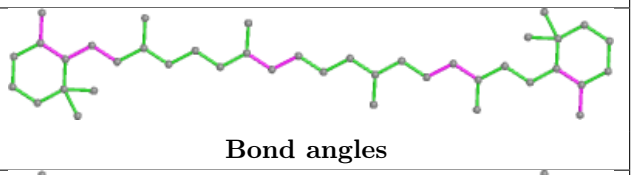
Ligand LHG d 409



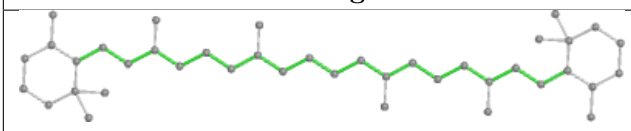
Ligand BCR c 516



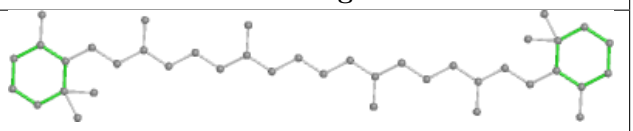
Bond lengths



Bond angles

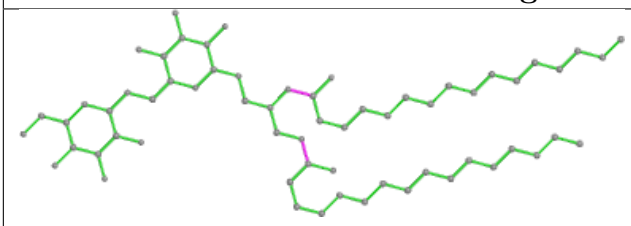


Torsions

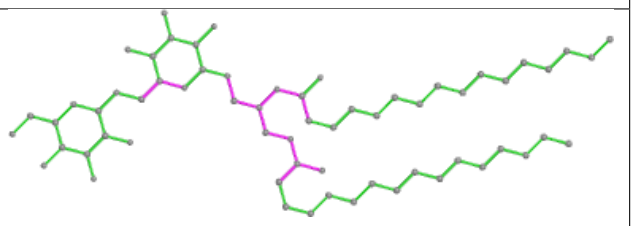


Rings

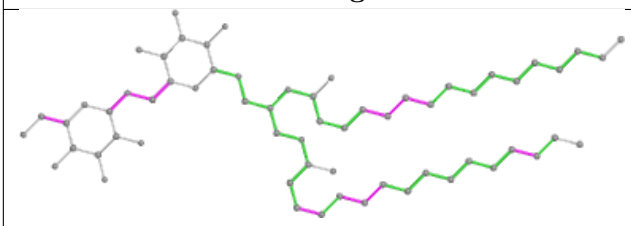
Ligand DGD C 517



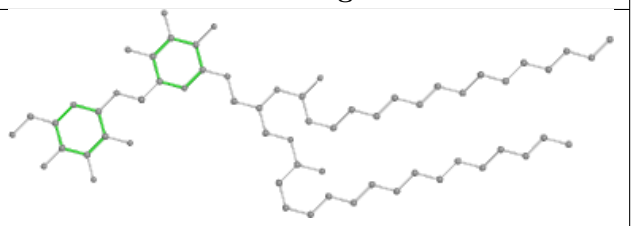
Bond lengths



Bond angles

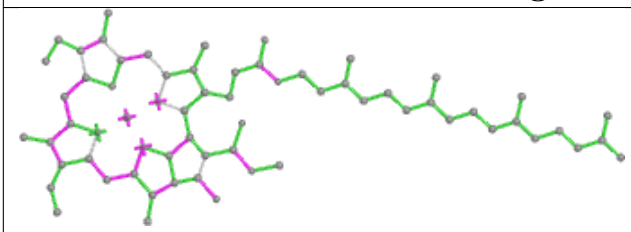


Torsions

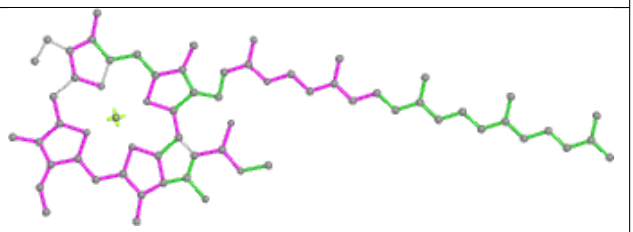


Rings

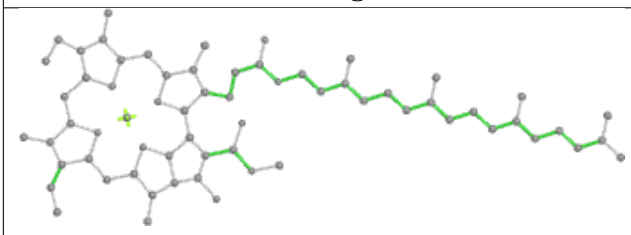
Ligand CLA c 513



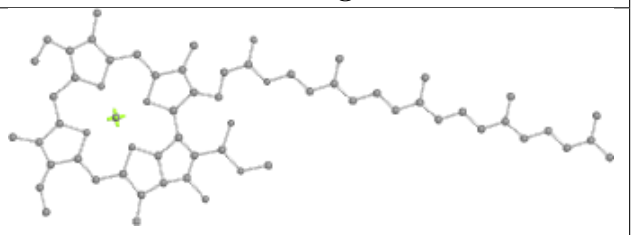
Bond lengths



Bond angles

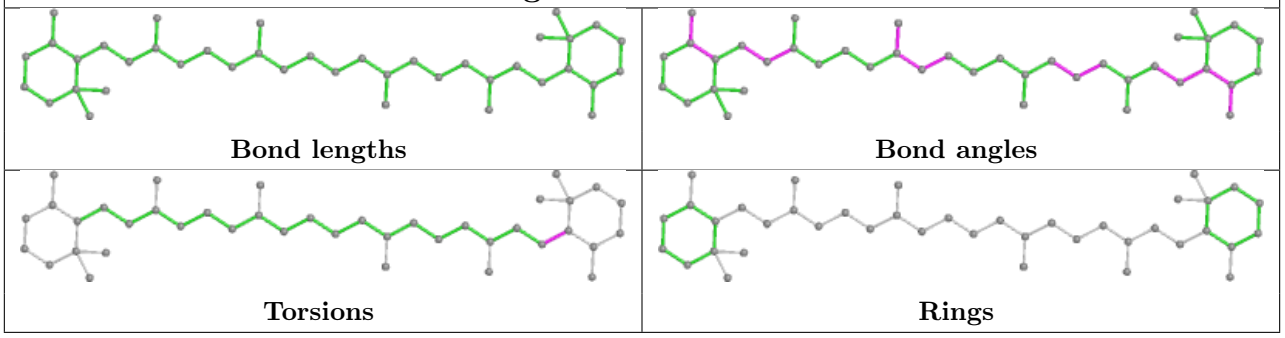


Torsions

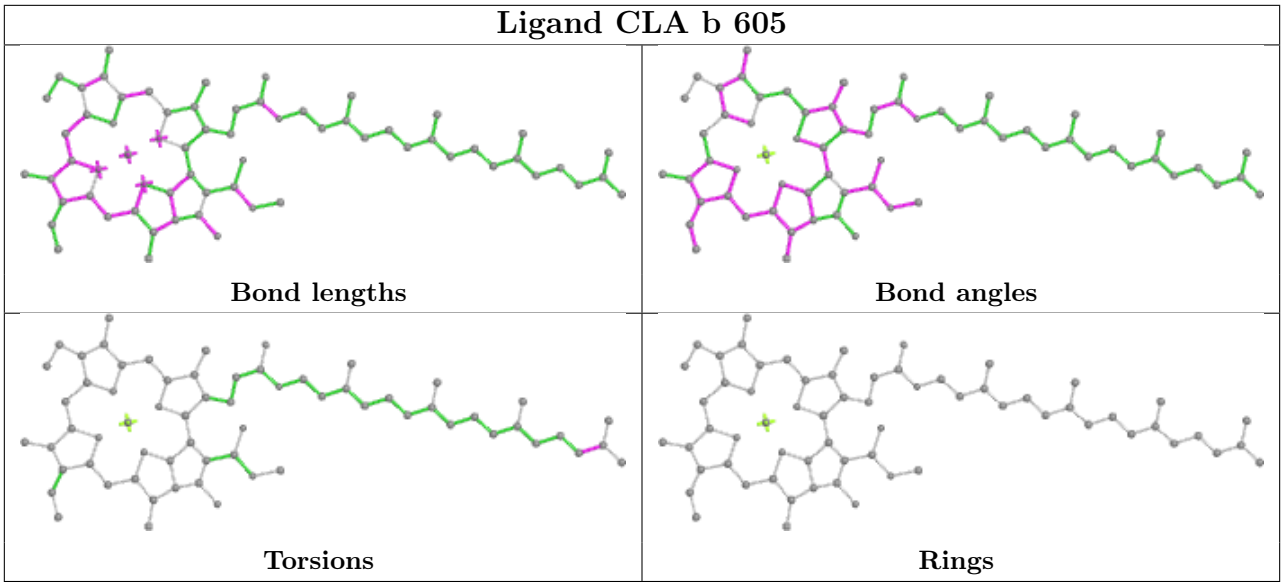


Rings

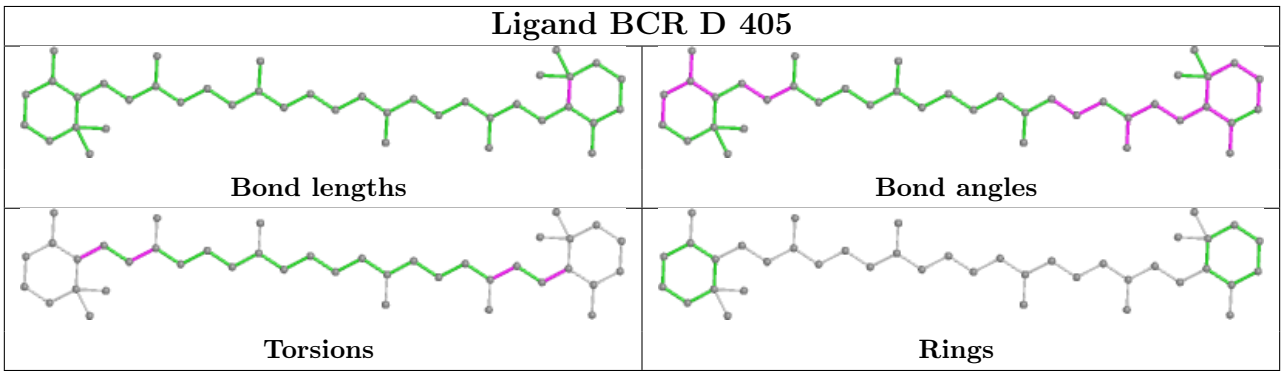
Ligand BCR C 516



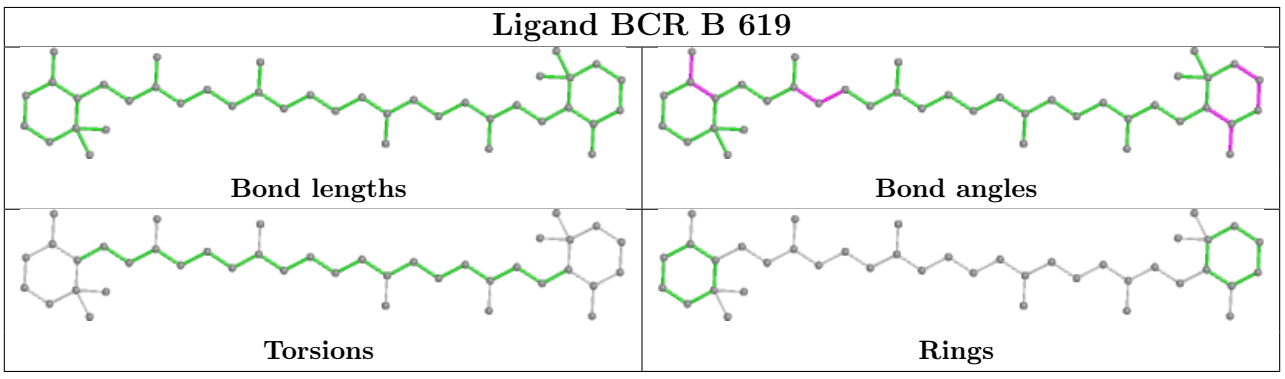
Ligand CLA b 605



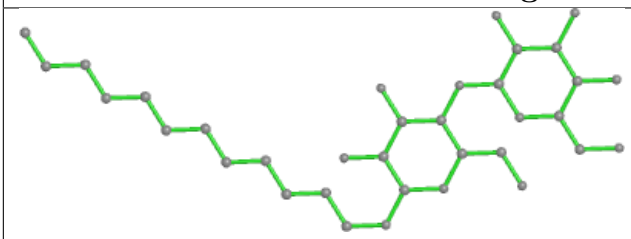
Ligand BCR D 405



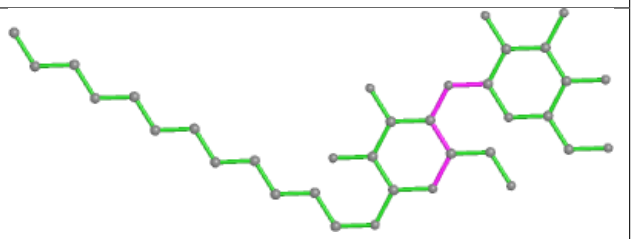
Ligand BCR B 619



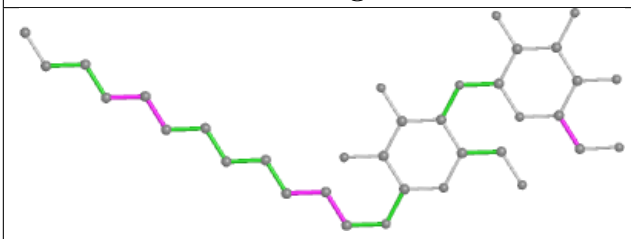
Ligand LMT A 414



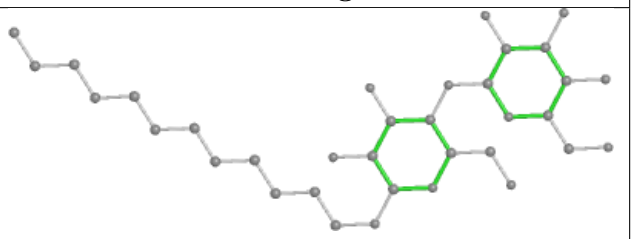
Bond lengths



Bond angles

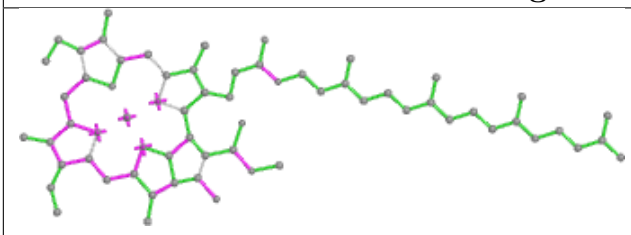


Torsions

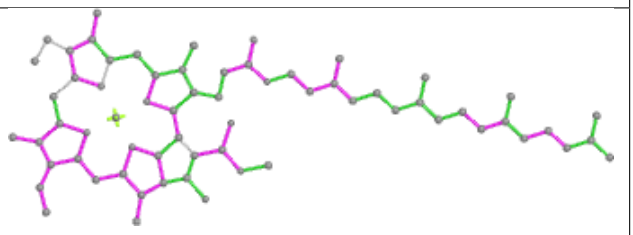


Rings

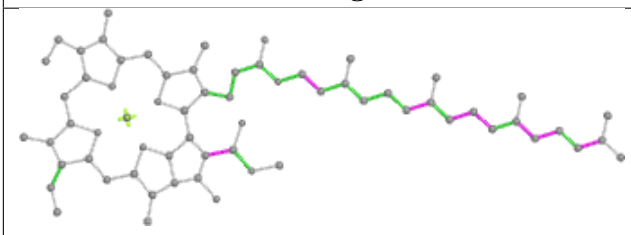
Ligand CLA c 511



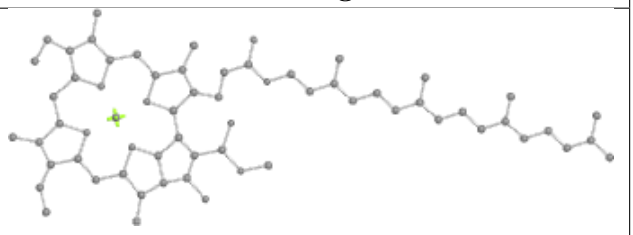
Bond lengths



Bond angles

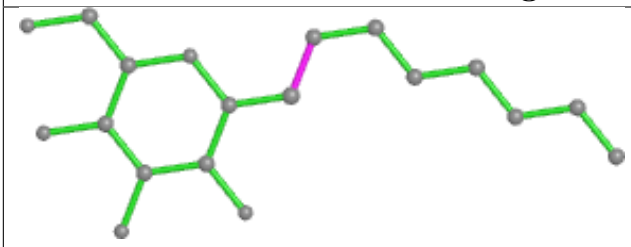


Torsions

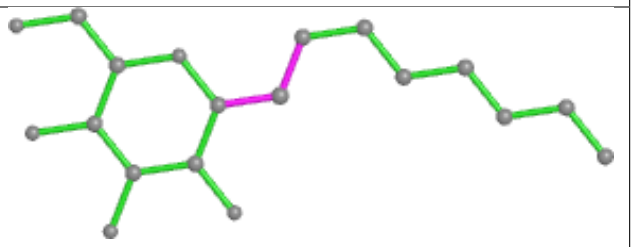


Rings

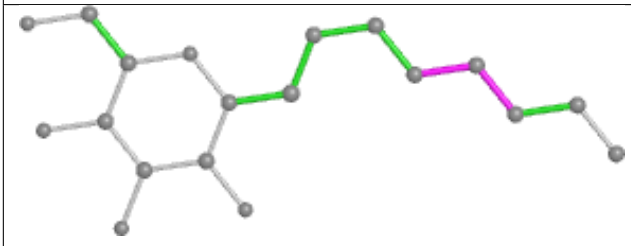
Ligand HTG O 302



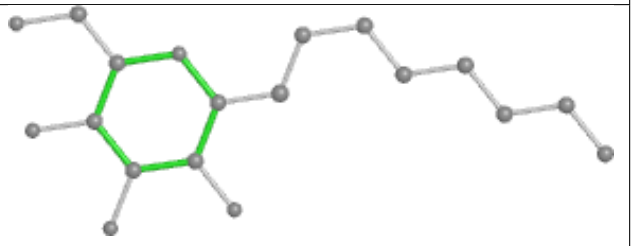
Bond lengths



Bond angles

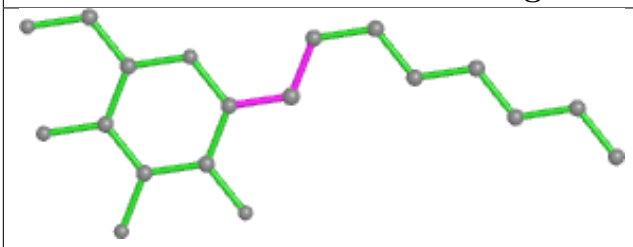


Torsions

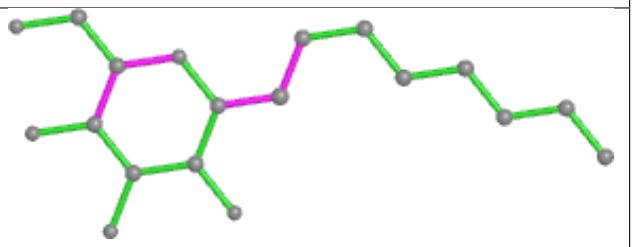


Rings

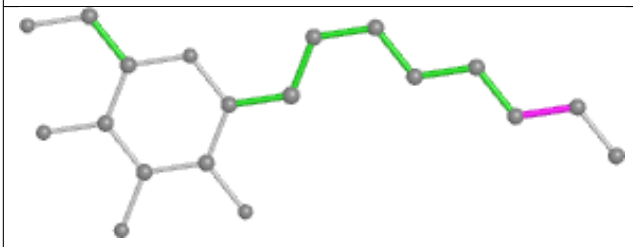
Ligand HTG b 601



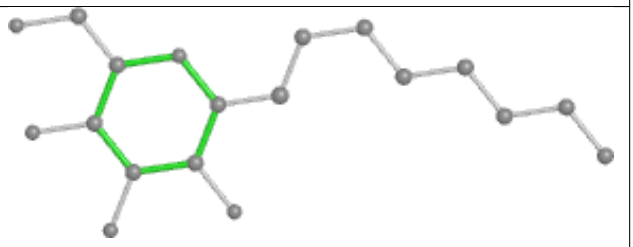
Bond lengths



Bond angles

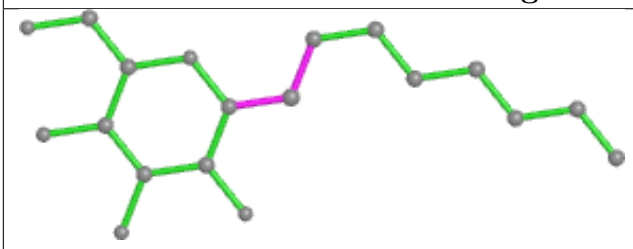


Torsions

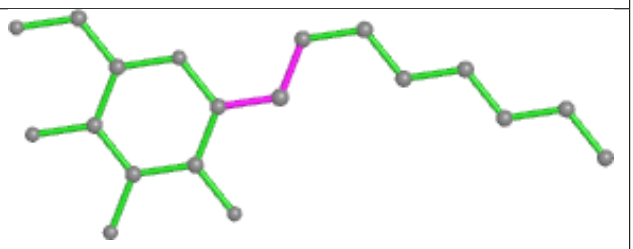


Rings

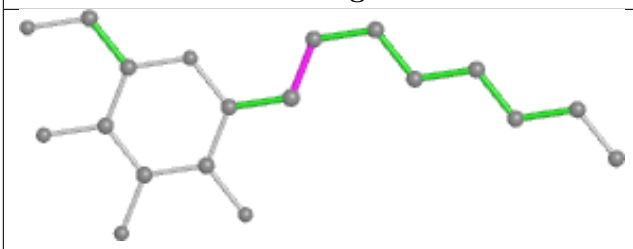
Ligand HTG C 522



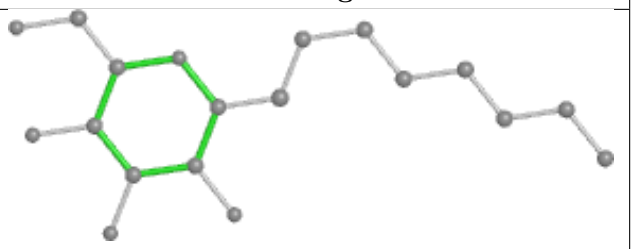
Bond lengths



Bond angles

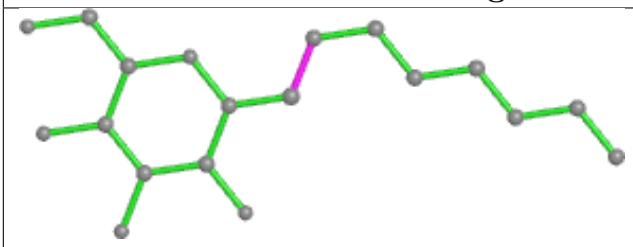


Torsions

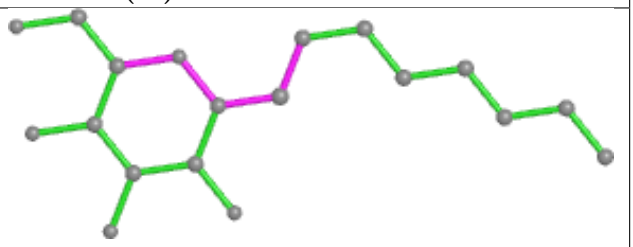


Rings

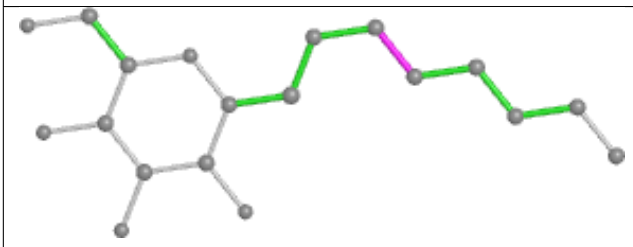
Ligand HTG B 623 (A)



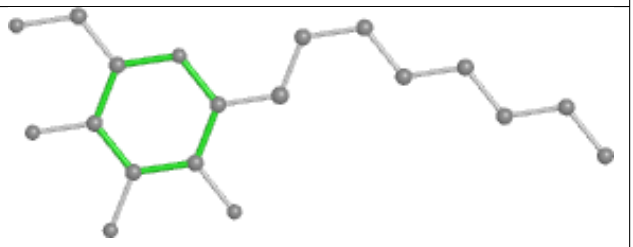
Bond lengths



Bond angles

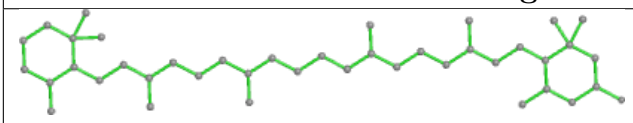


Torsions

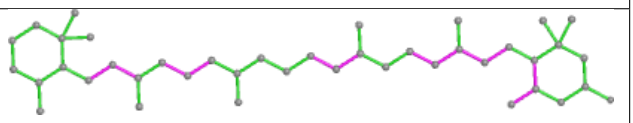


Rings

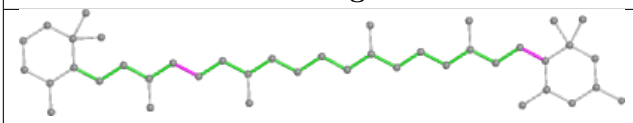
Ligand RRX H 101



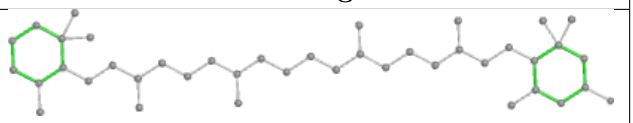
Bond lengths



Bond angles

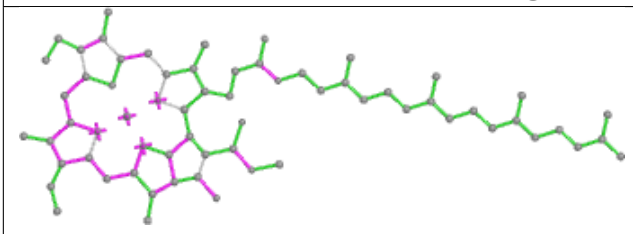


Torsions

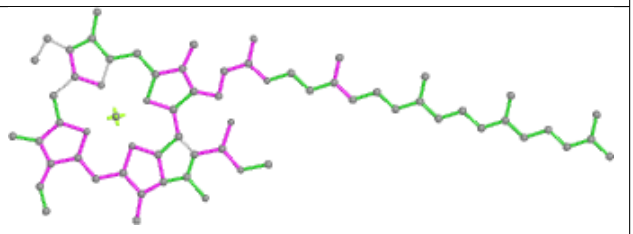


Rings

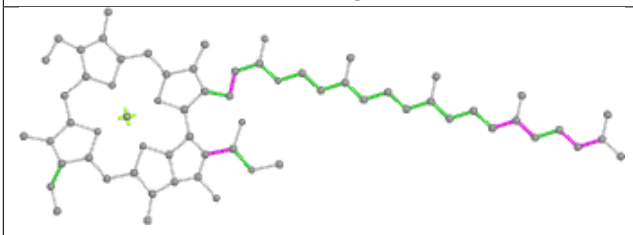
Ligand CLA B 611



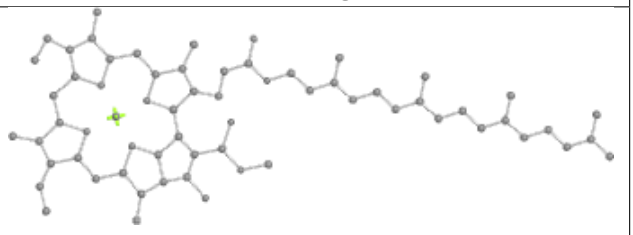
Bond lengths



Bond angles

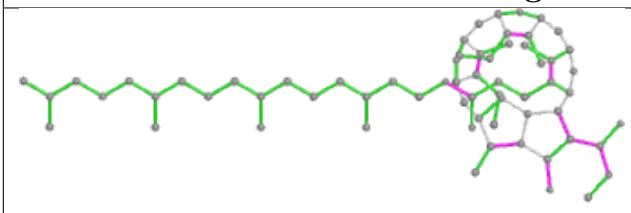


Torsions

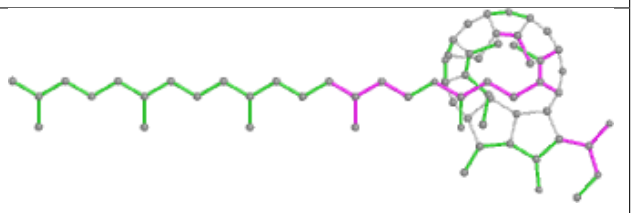


Rings

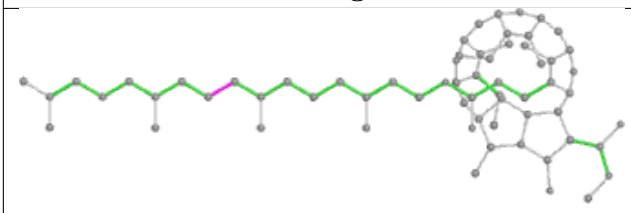
Ligand PHO d 401



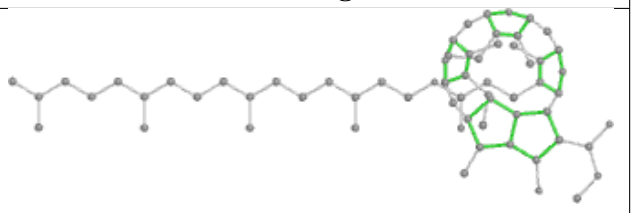
Bond lengths



Bond angles

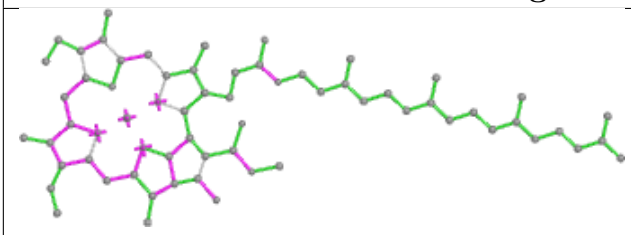


Torsions

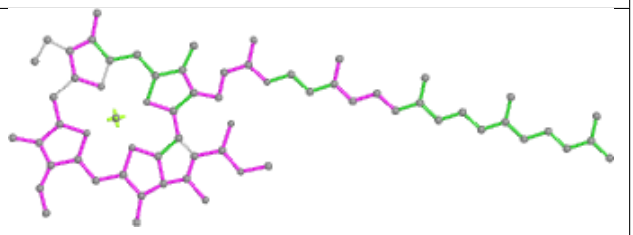


Rings

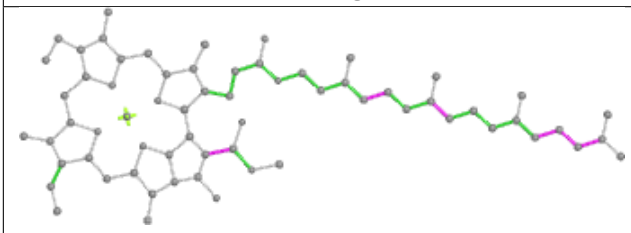
Ligand CLA c 508



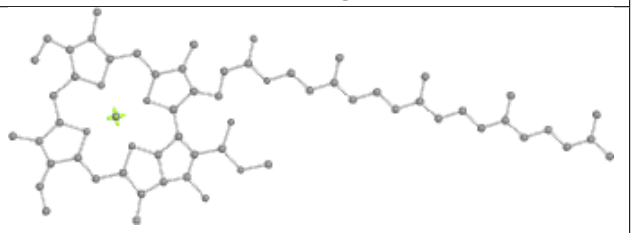
Bond lengths



Bond angles

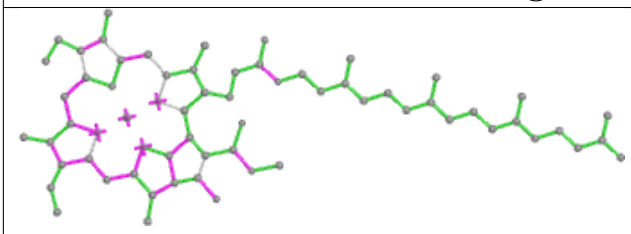


Torsions

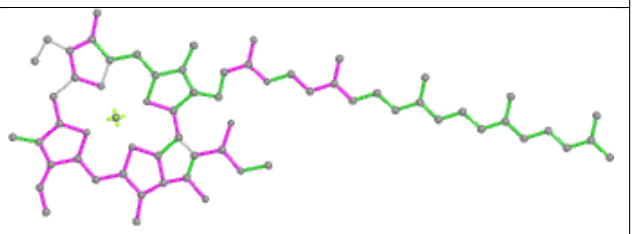


Rings

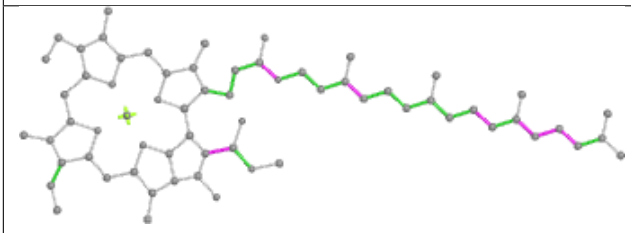
Ligand CLA b 619



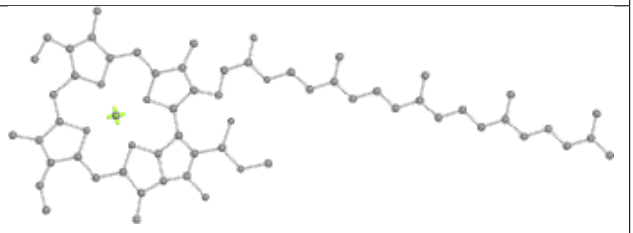
Bond lengths



Bond angles

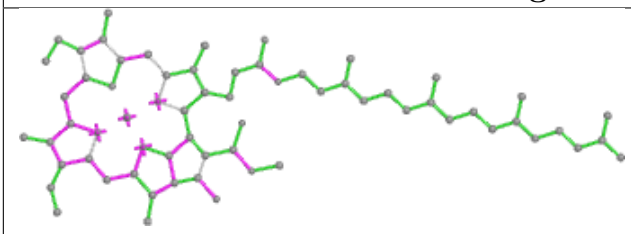


Torsions

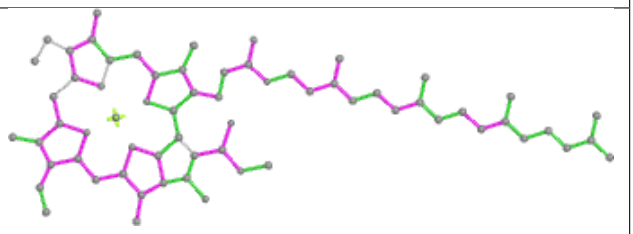


Rings

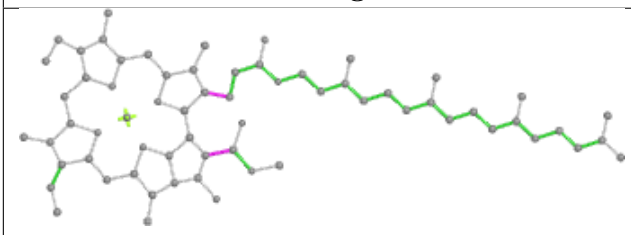
Ligand CLA c 510



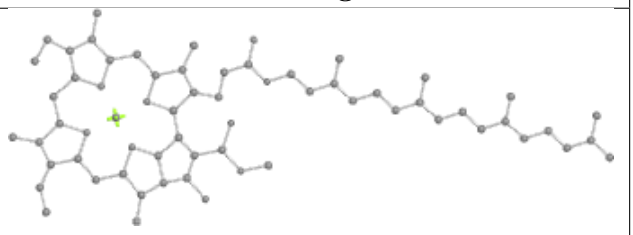
Bond lengths



Bond angles

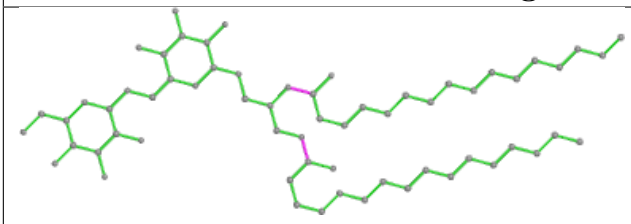


Torsions

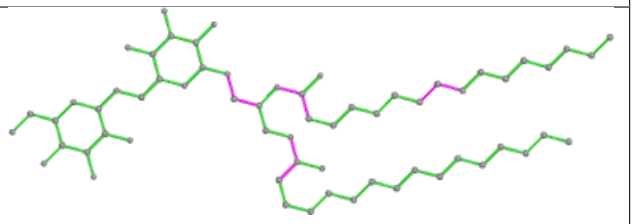


Rings

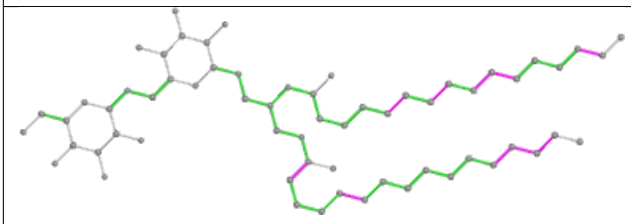
Ligand DGD C 519



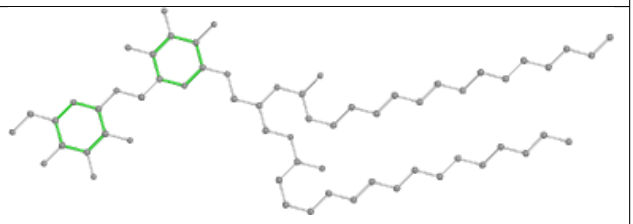
Bond lengths



Bond angles

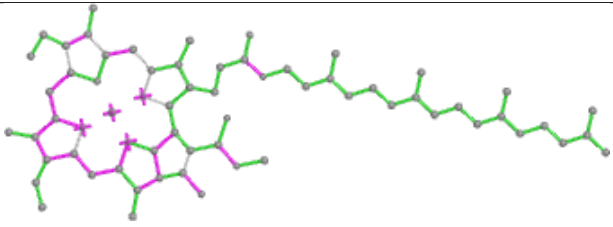


Torsions

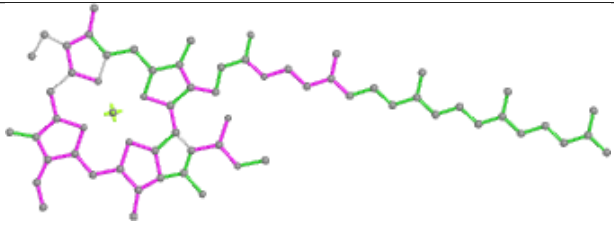


Rings

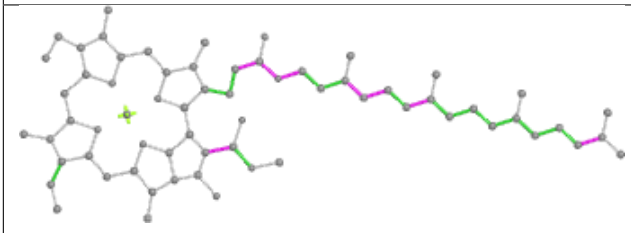
Ligand CLA b 604



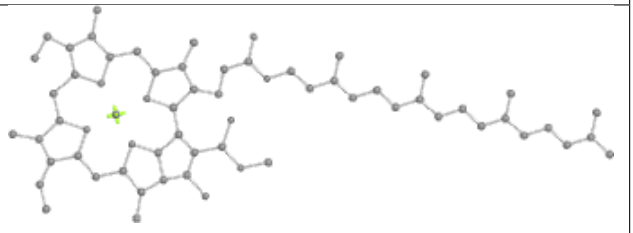
Bond lengths



Bond angles

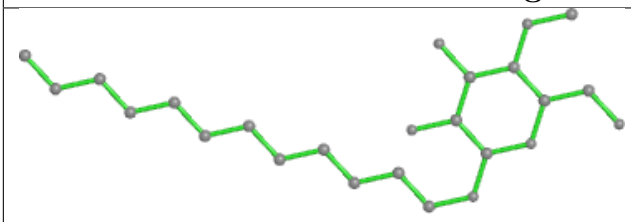


Torsions

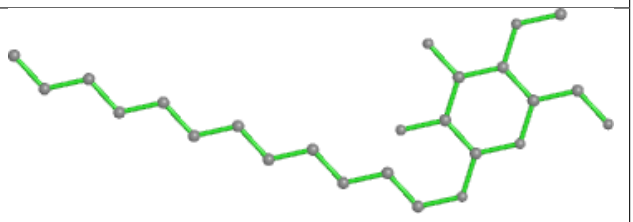


Rings

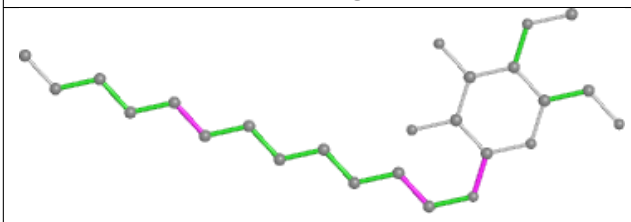
Ligand LMT b 624



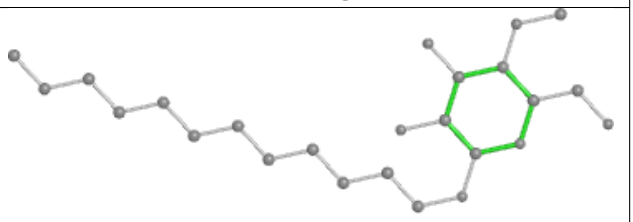
Bond lengths



Bond angles

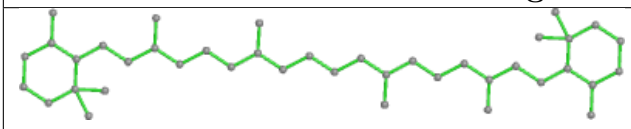


Torsions

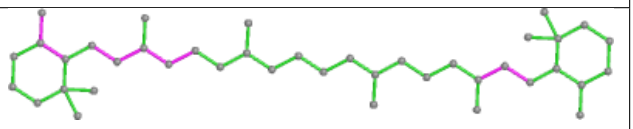


Rings

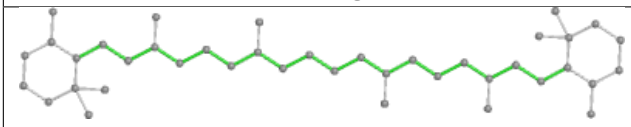
Ligand BCR a 413



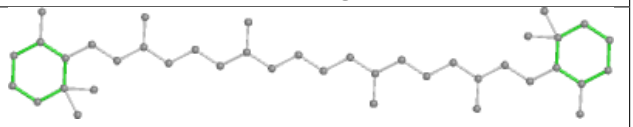
Bond lengths



Bond angles

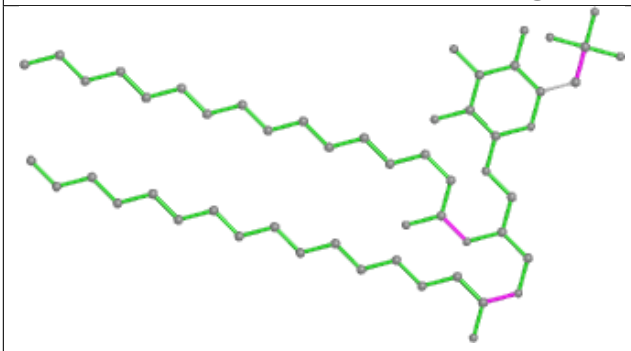


Torsions

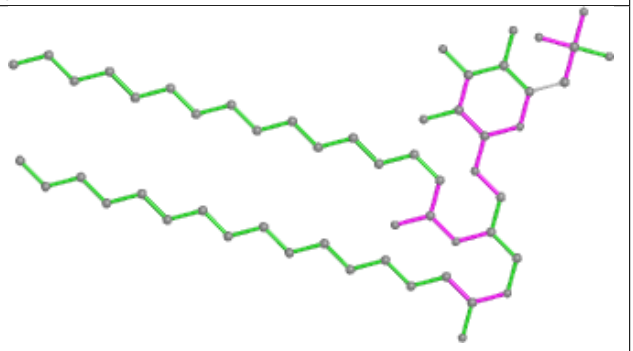


Rings

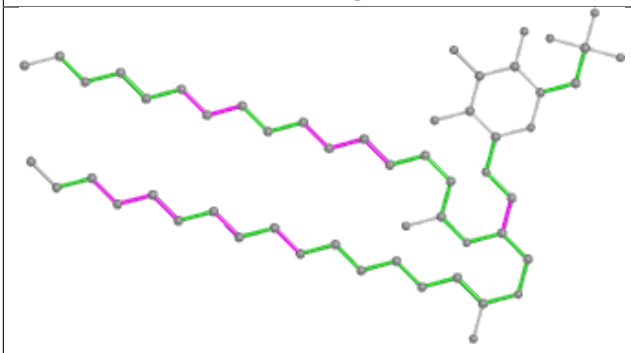
Ligand SQD a 414



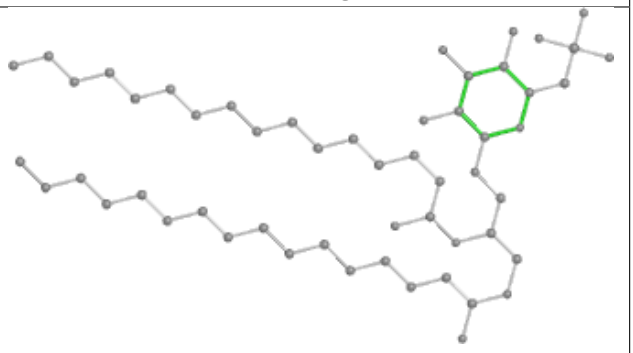
Bond lengths



Bond angles

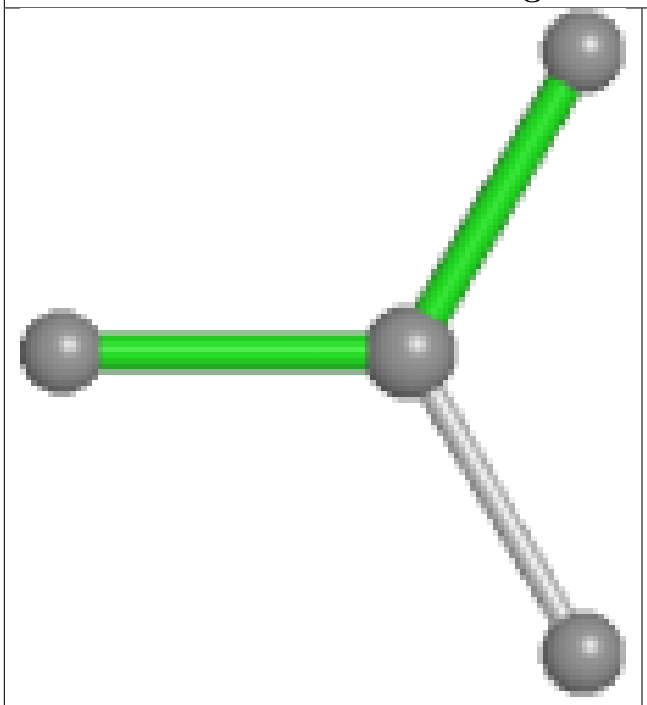


Torsions

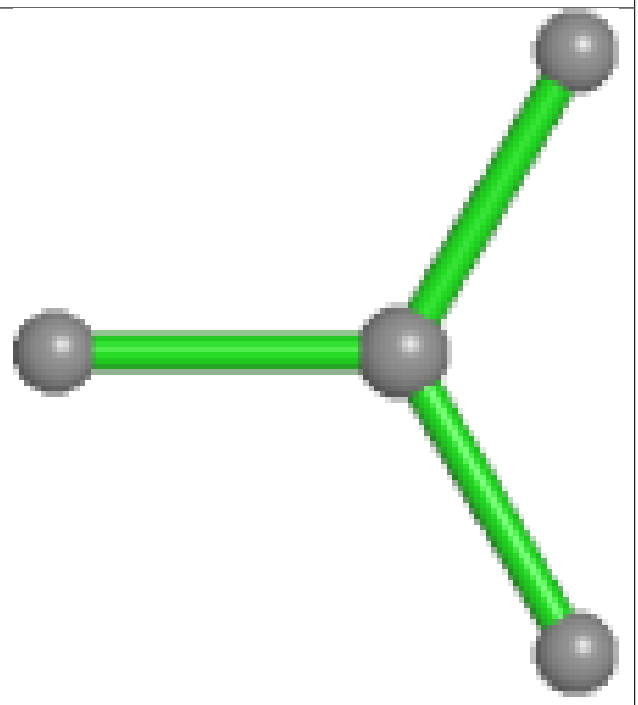


Rings

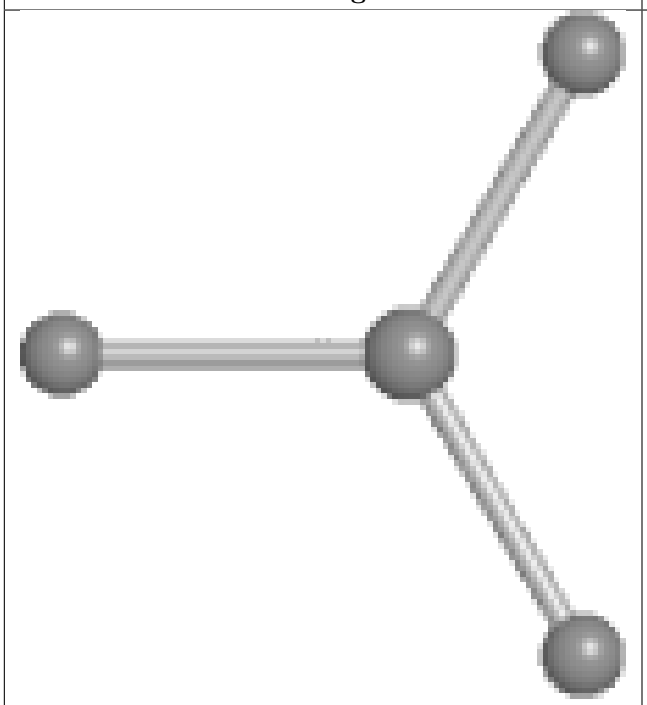
Ligand BCT A 423



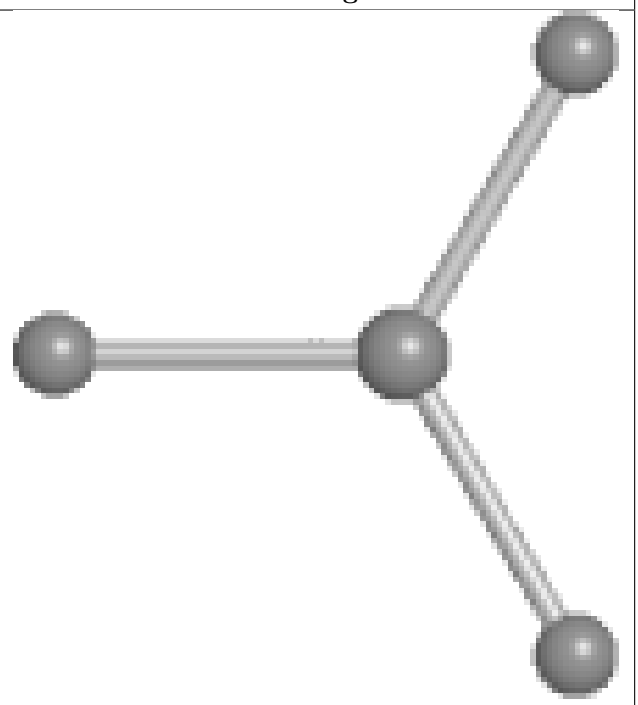
Bond lengths



Bond angles

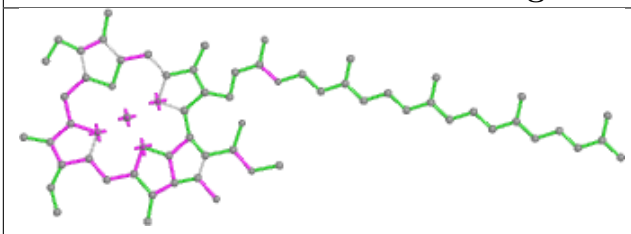


Torsions

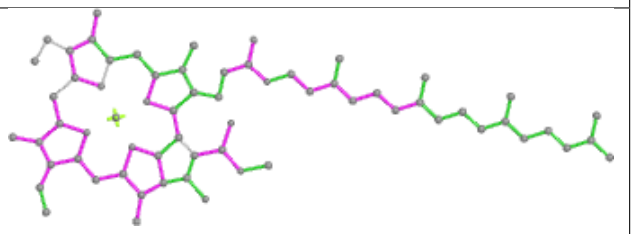


Rings

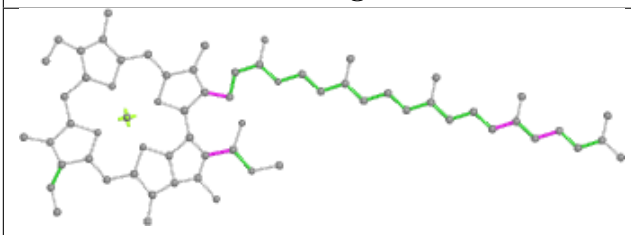
Ligand CLA b 607



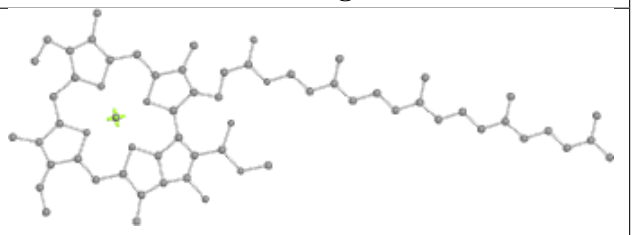
Bond lengths



Bond angles

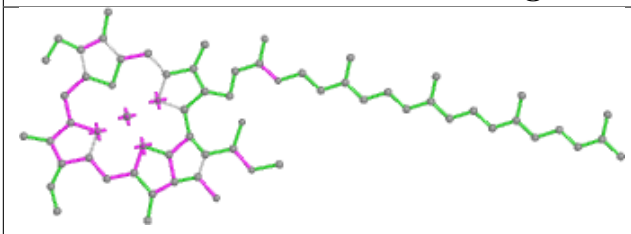


Torsions

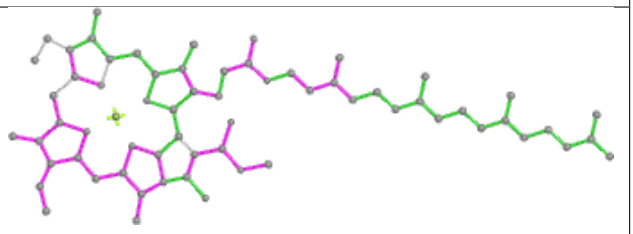


Rings

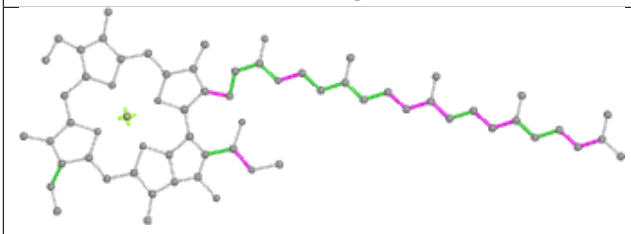
Ligand CLA C 507



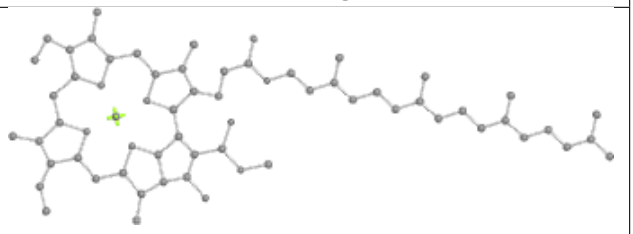
Bond lengths



Bond angles

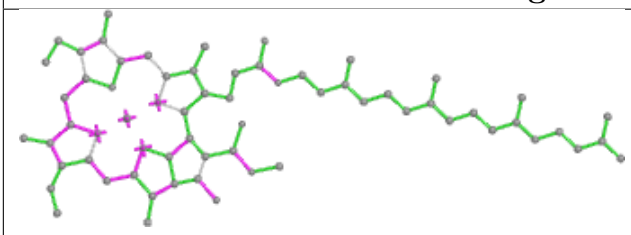


Torsions

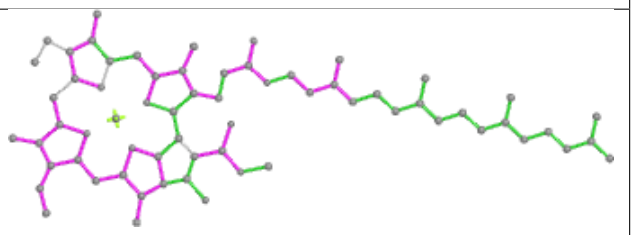


Rings

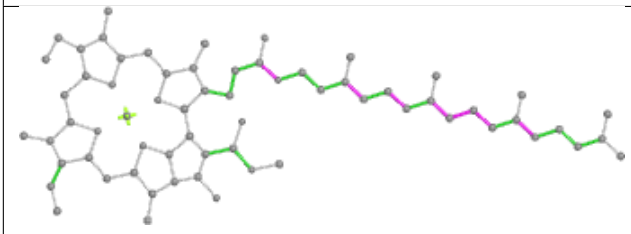
Ligand CLA a 412



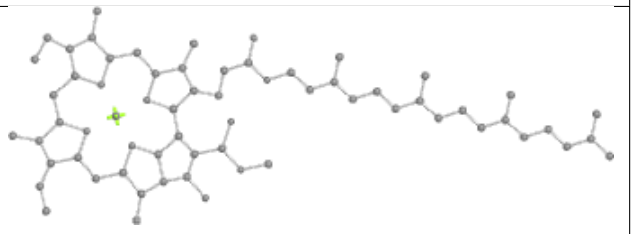
Bond lengths



Bond angles

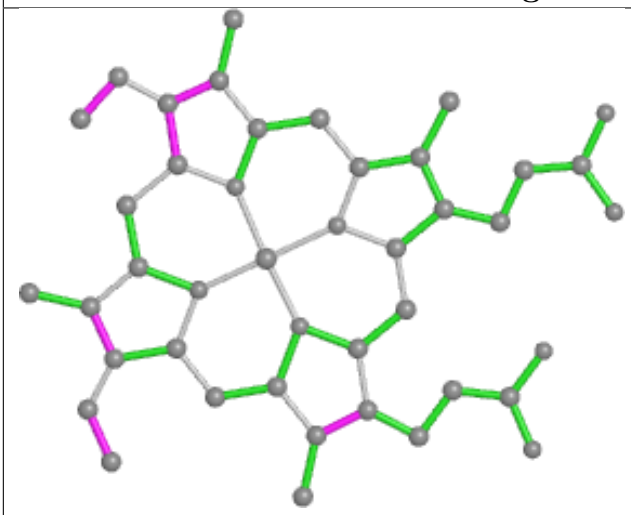


Torsions

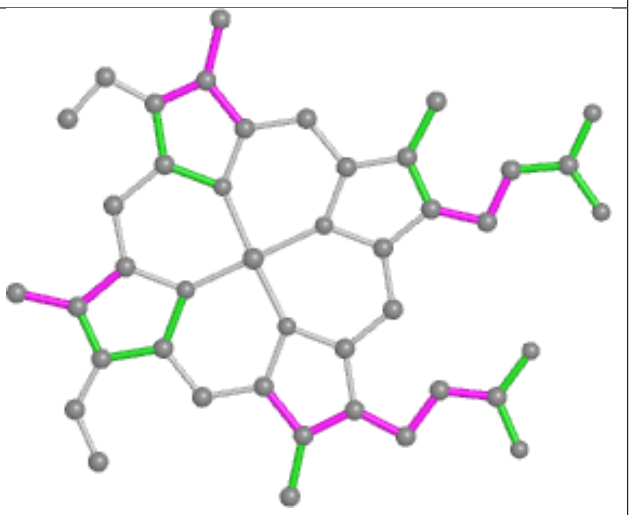


Rings

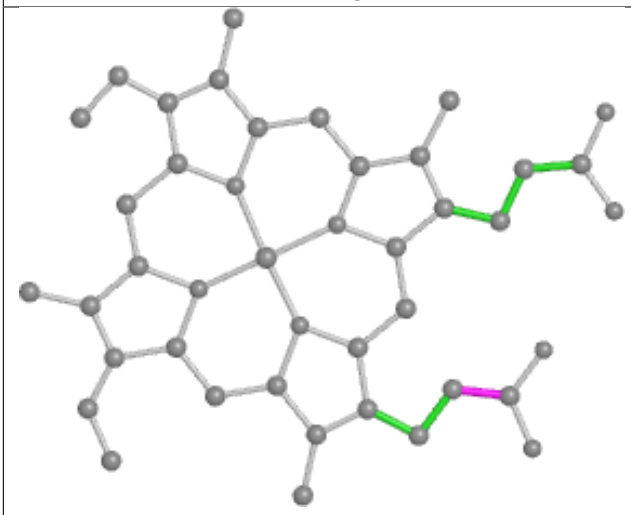
Ligand HEC V 202



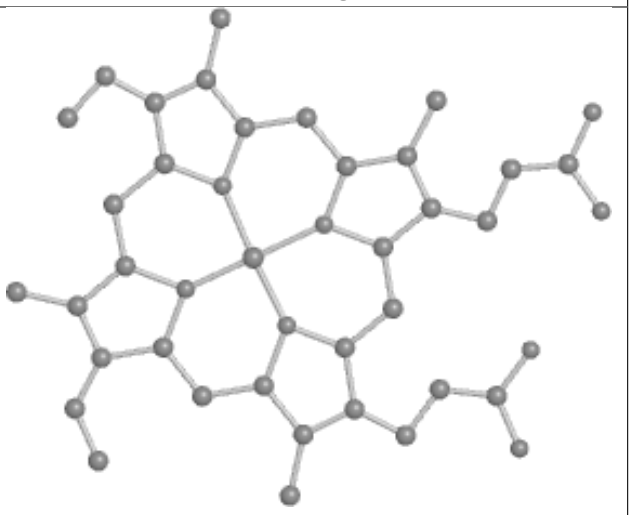
Bond lengths



Bond angles

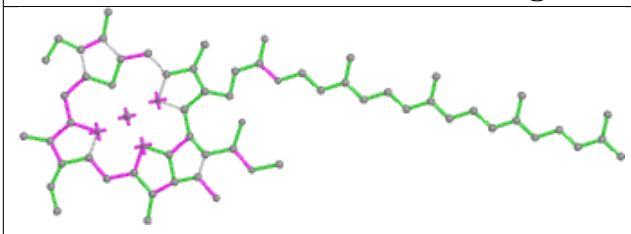


Torsions

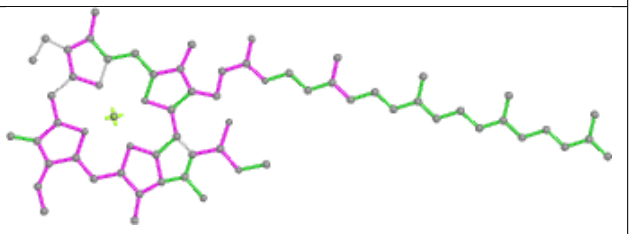


Rings

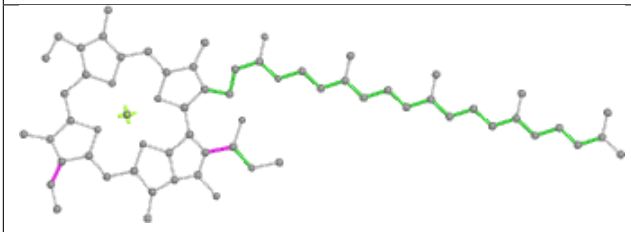
Ligand CLA a 409



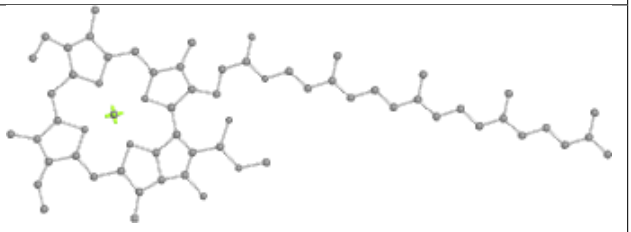
Bond lengths



Bond angles

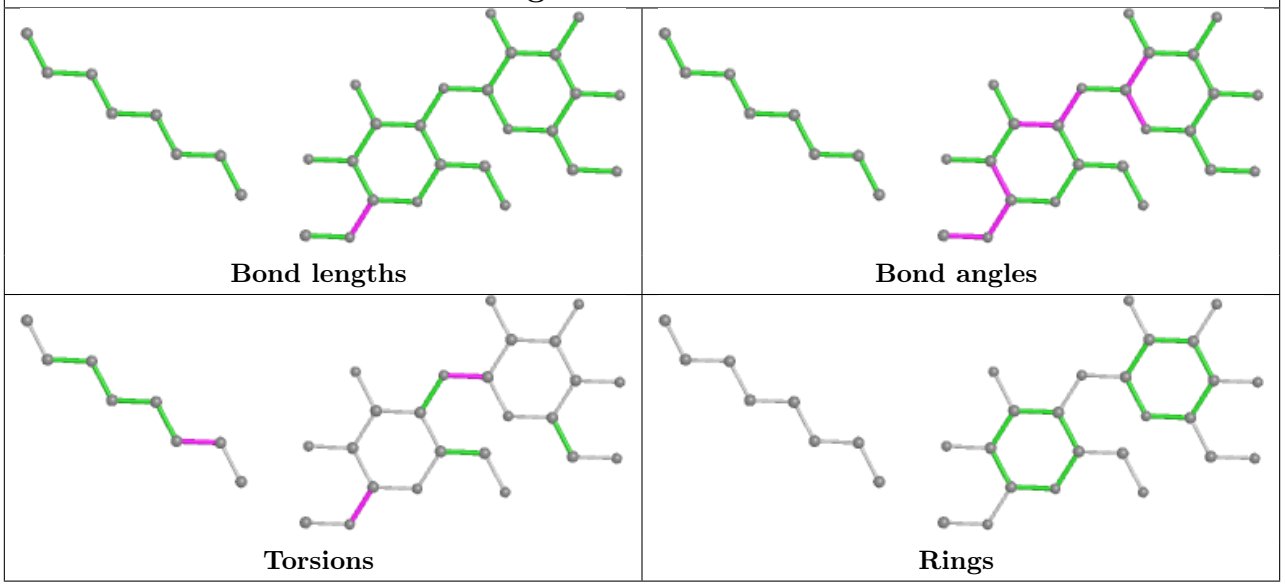


Torsions

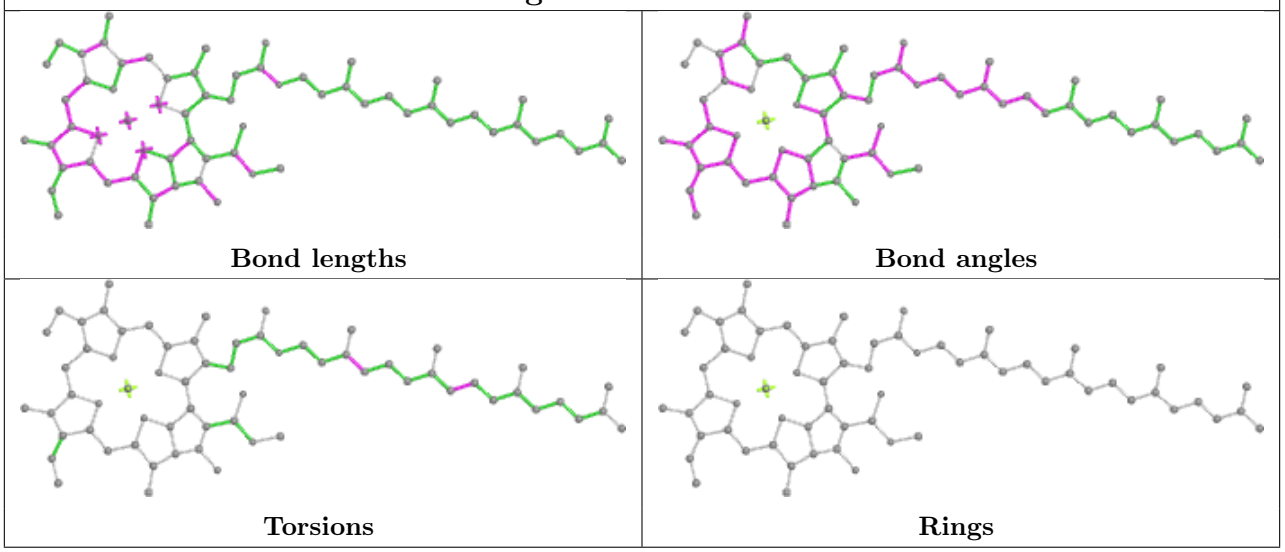


Rings

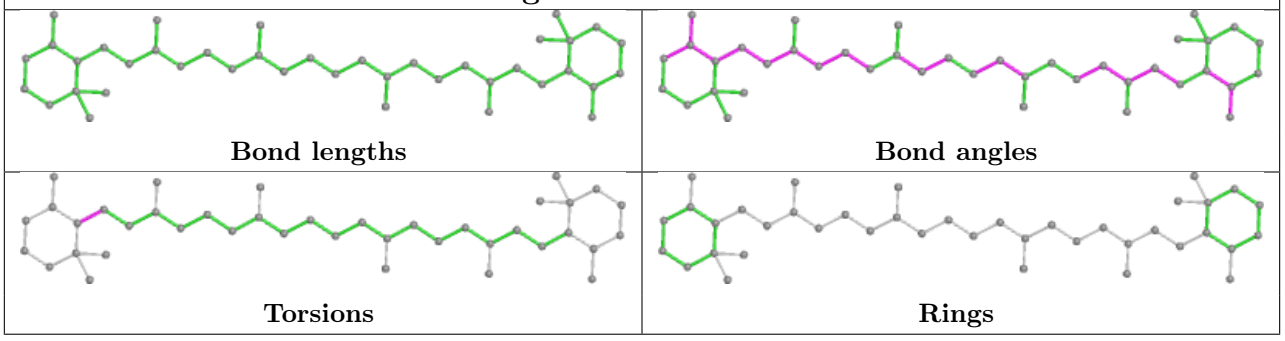
Ligand LMT z 101



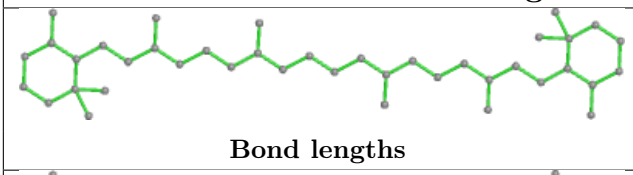
Ligand CLA B 612



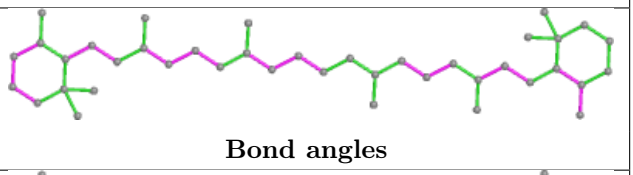
Ligand BCR K 101



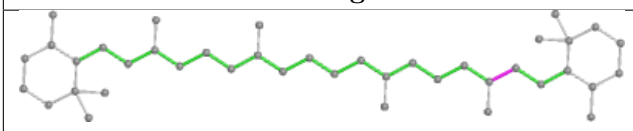
Ligand BCR b 622



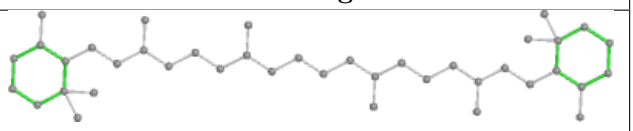
Bond lengths



Bond angles

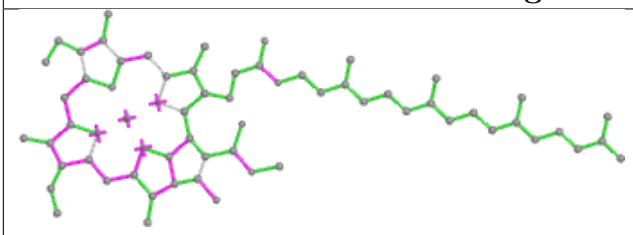


Torsions

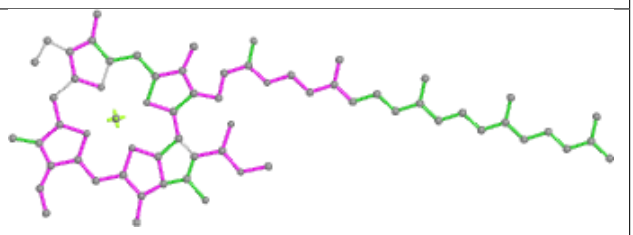


Rings

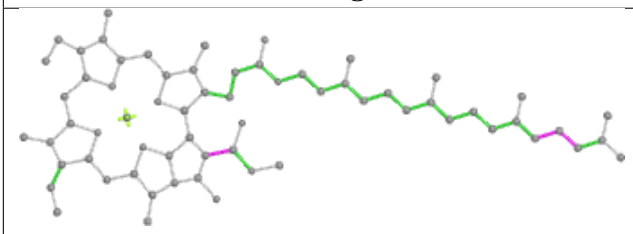
Ligand CLA B 603



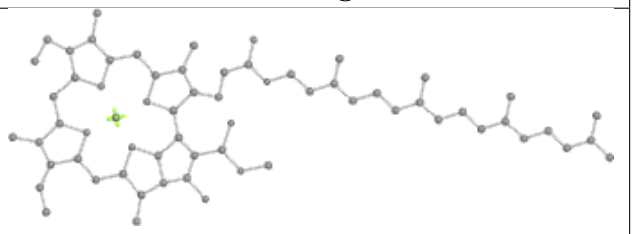
Bond lengths



Bond angles

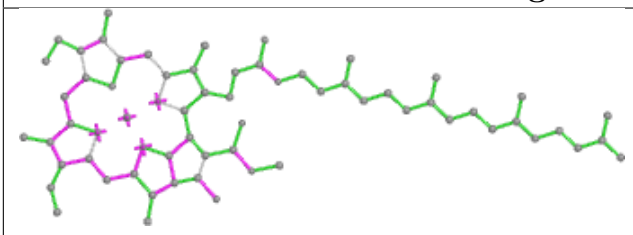


Torsions

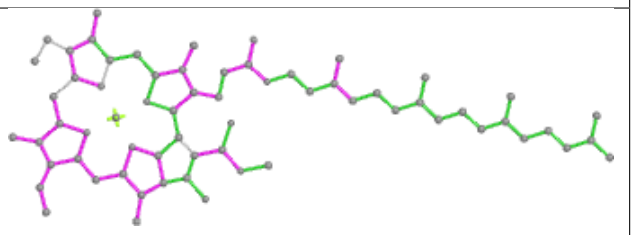


Rings

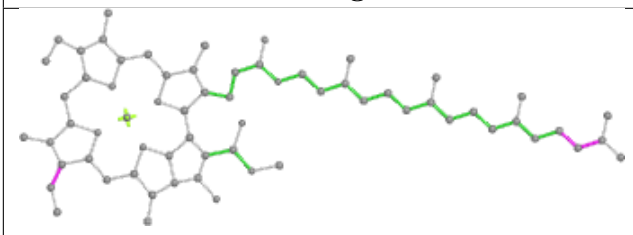
Ligand CLA a 408



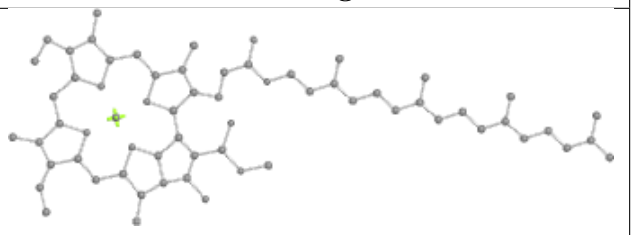
Bond lengths



Bond angles

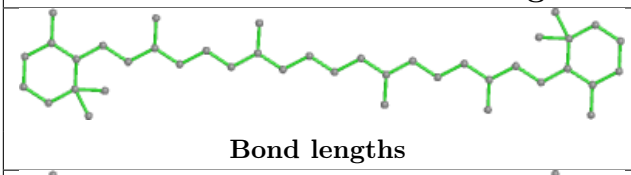


Torsions

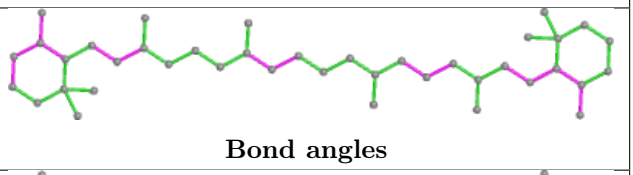


Rings

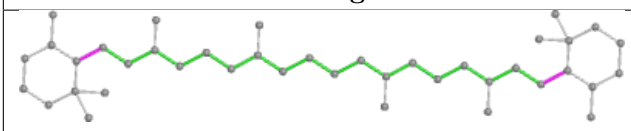
Ligand BCR c 517



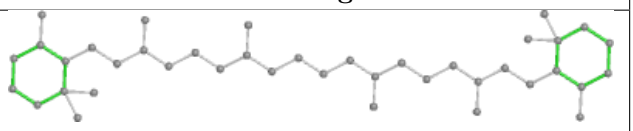
Bond lengths



Bond angles

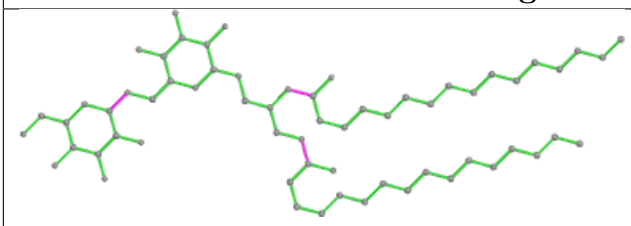


Torsions

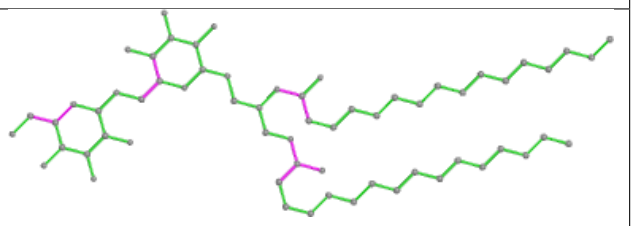


Rings

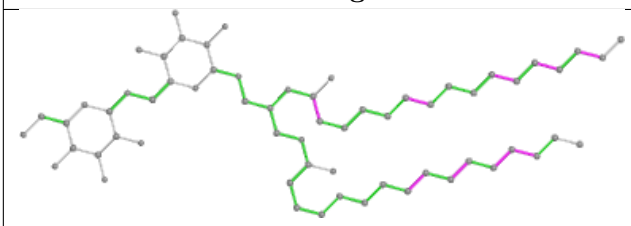
Ligand DGD H 102



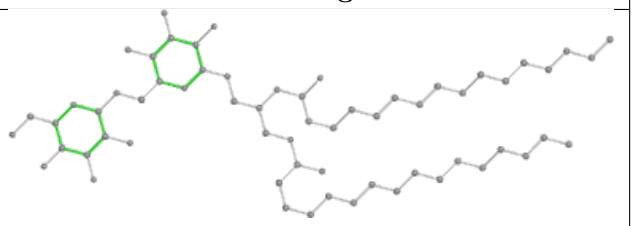
Bond lengths



Bond angles

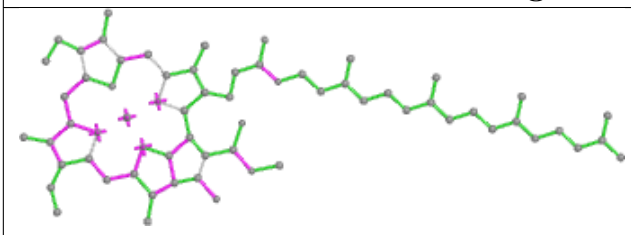


Torsions

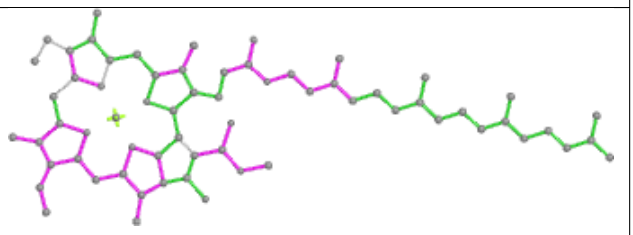


Rings

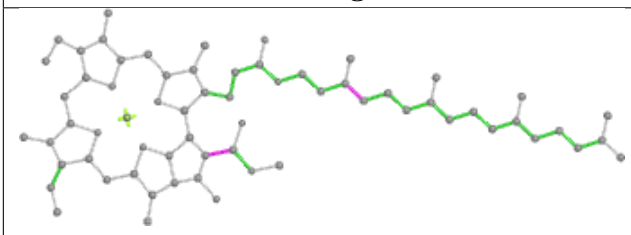
Ligand CLA b 608



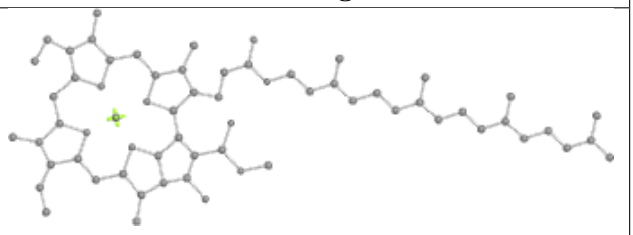
Bond lengths



Bond angles

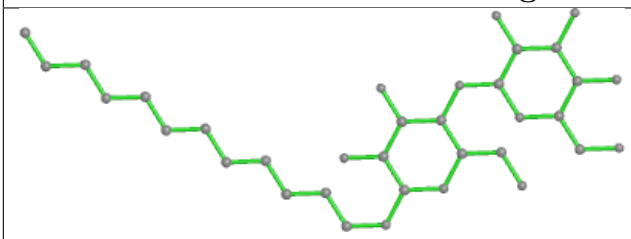


Torsions

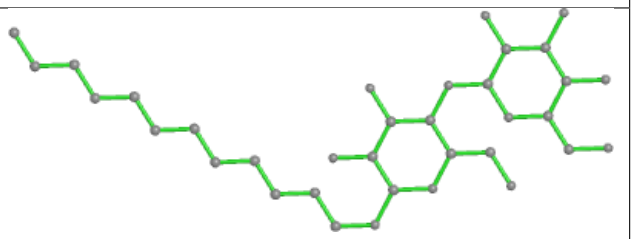


Rings

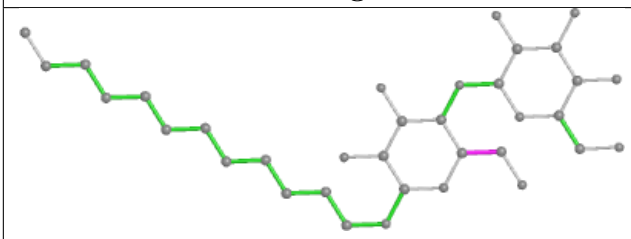
Ligand LMT m 102



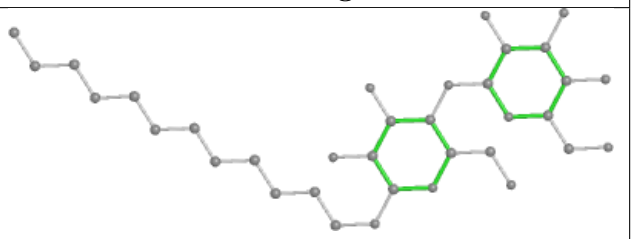
Bond lengths



Bond angles

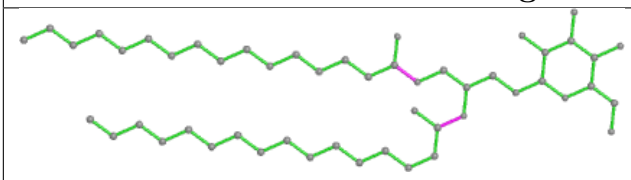


Torsions

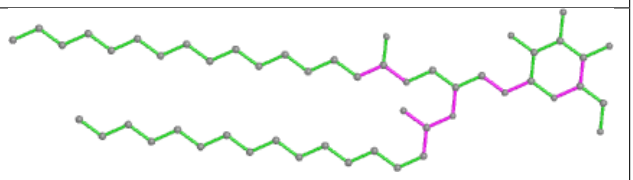


Rings

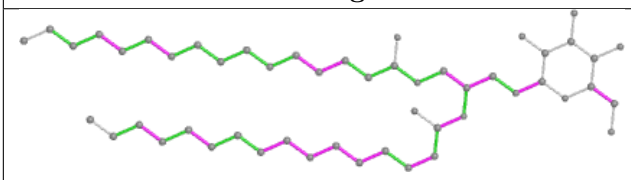
Ligand LMG A 412



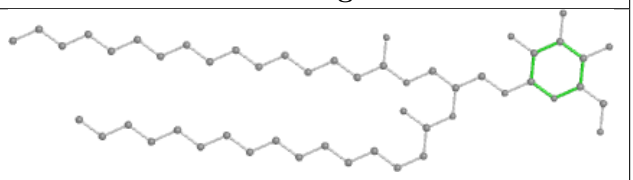
Bond lengths



Bond angles

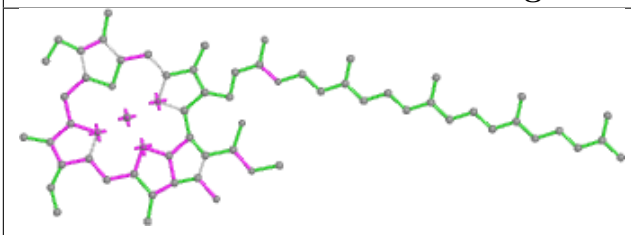


Torsions

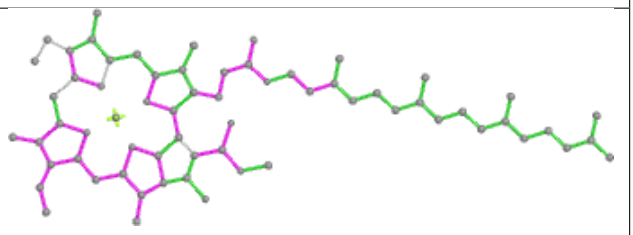


Rings

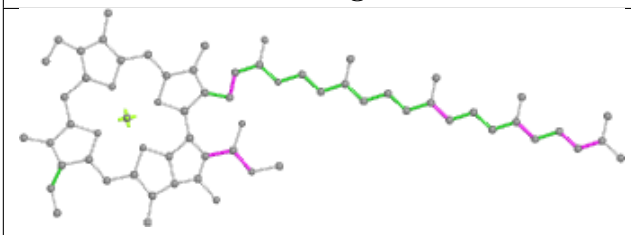
Ligand CLA C 508



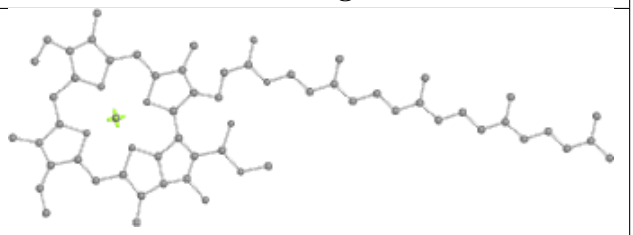
Bond lengths



Bond angles

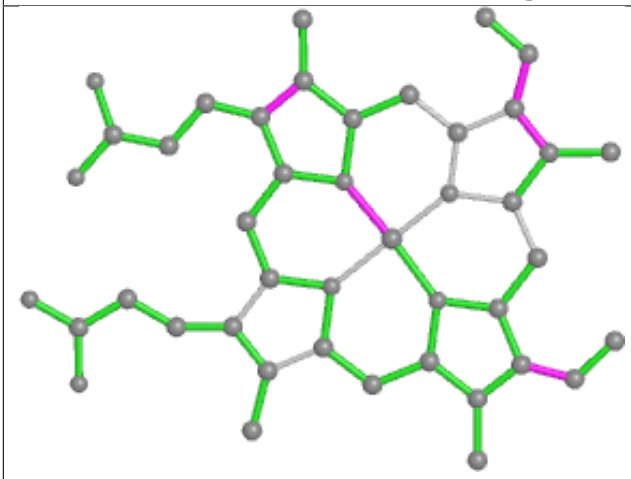


Torsions

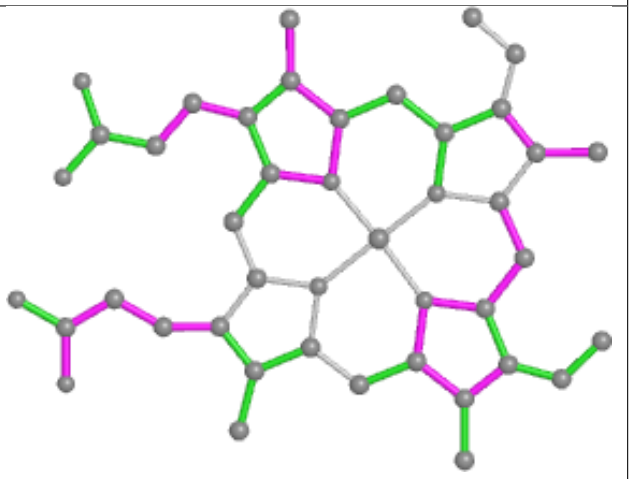


Rings

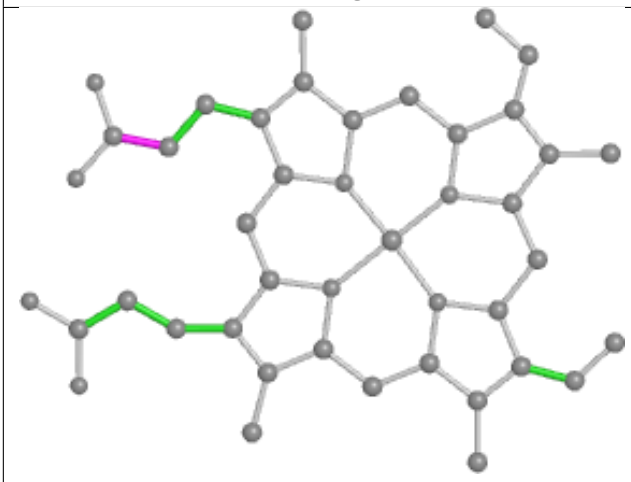
Ligand HEM F 101



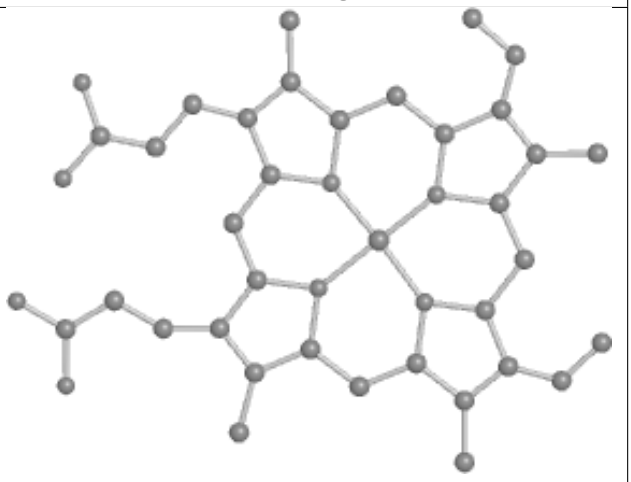
Bond lengths



Bond angles

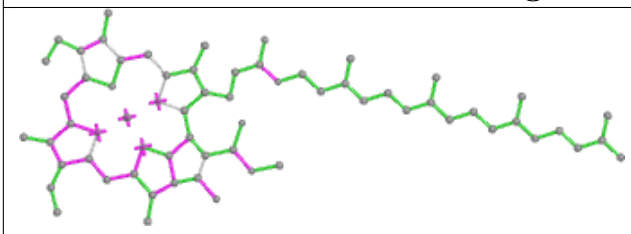


Torsions

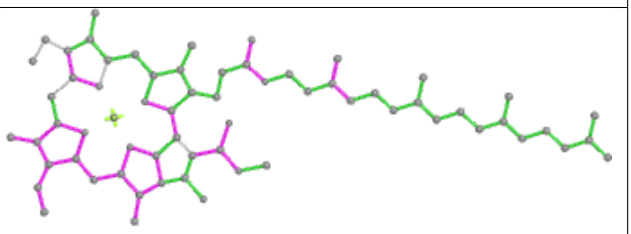


Rings

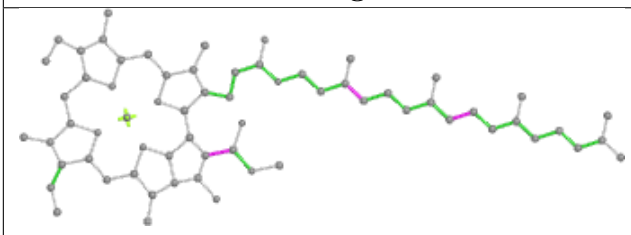
Ligand CLA B 606



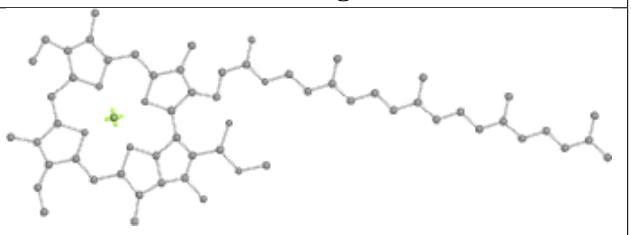
Bond lengths



Bond angles

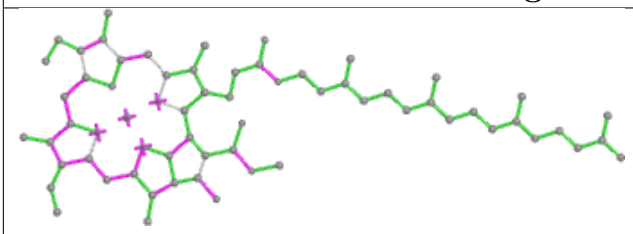


Torsions

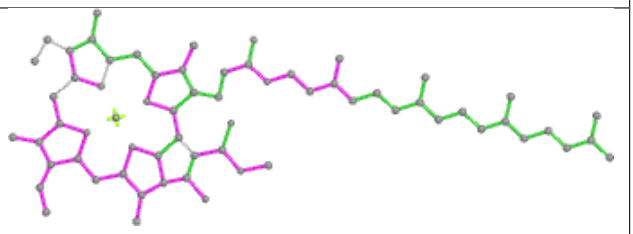


Rings

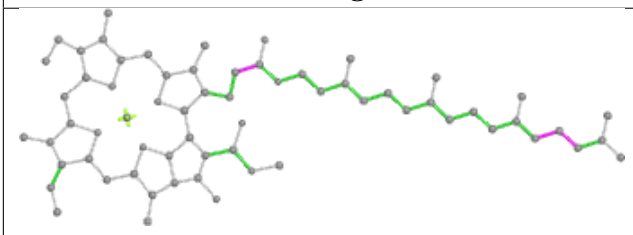
Ligand CLA B 614



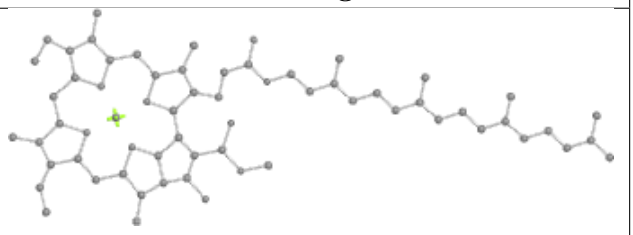
Bond lengths



Bond angles

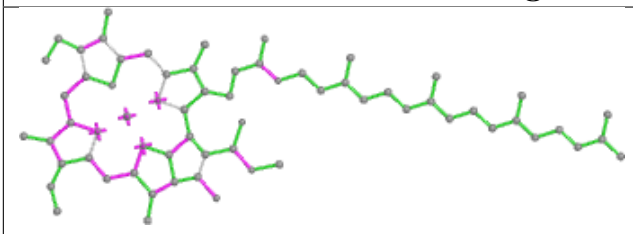


Torsions

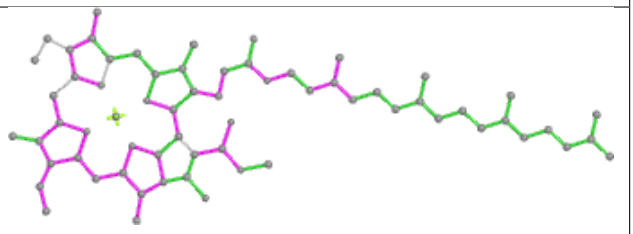


Rings

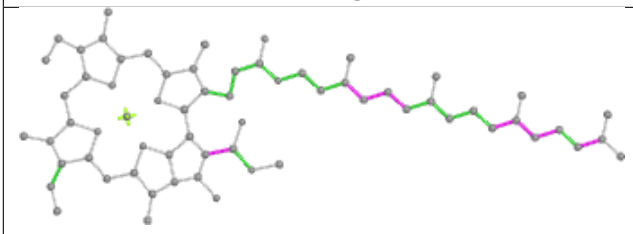
Ligand CLA B 617



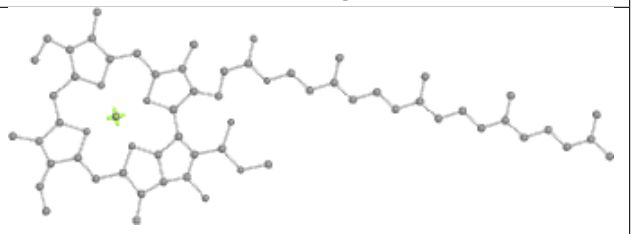
Bond lengths



Bond angles

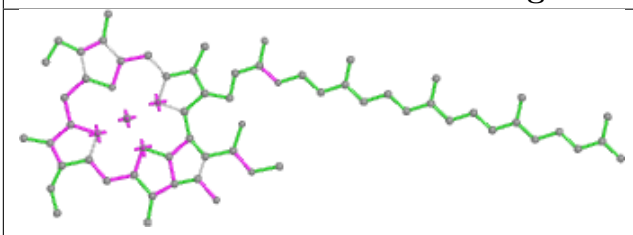


Torsions

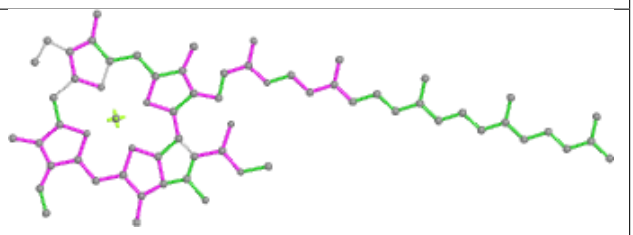


Rings

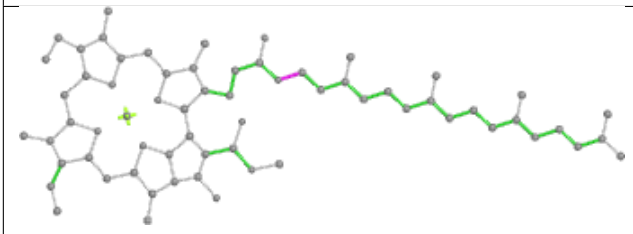
Ligand CLA d 404



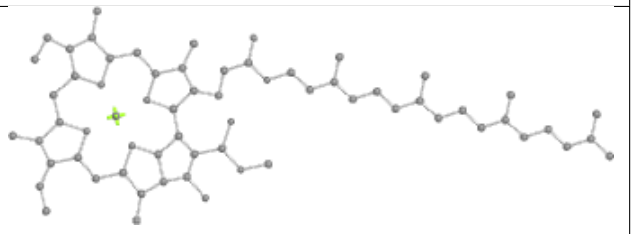
Bond lengths



Bond angles

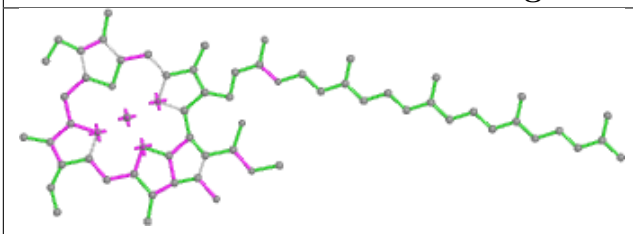


Torsions

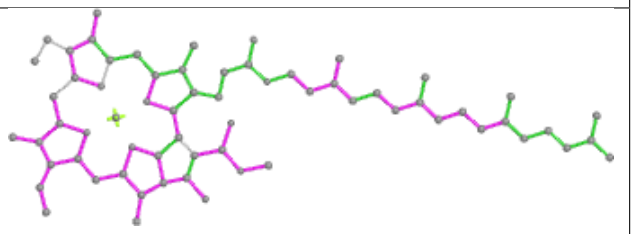


Rings

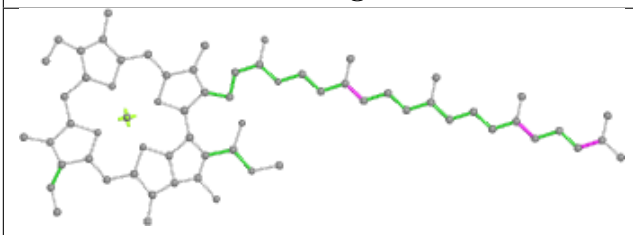
Ligand CLA B 616



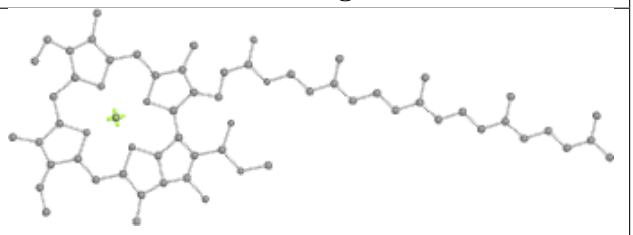
Bond lengths



Bond angles

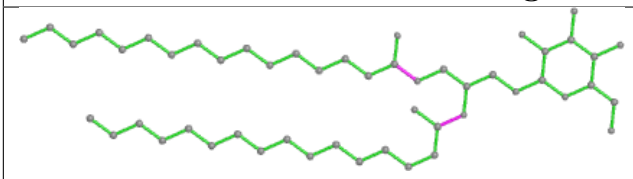


Torsions

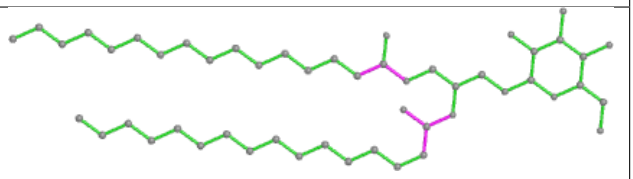


Rings

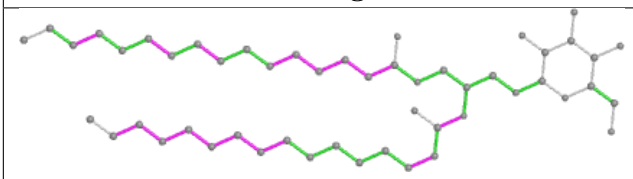
Ligand LMG b 623



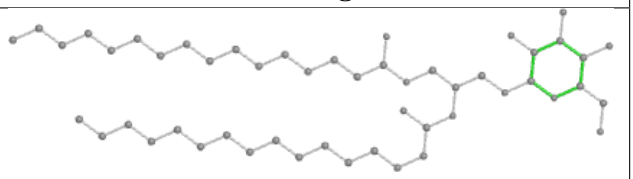
Bond lengths



Bond angles

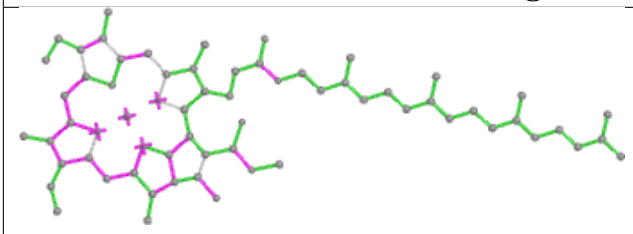


Torsions

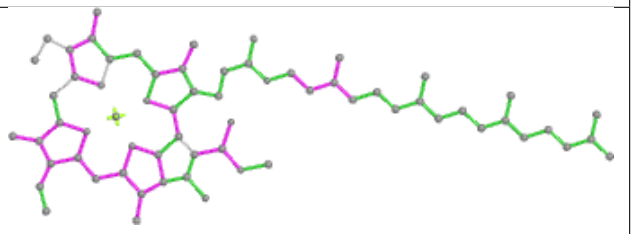


Rings

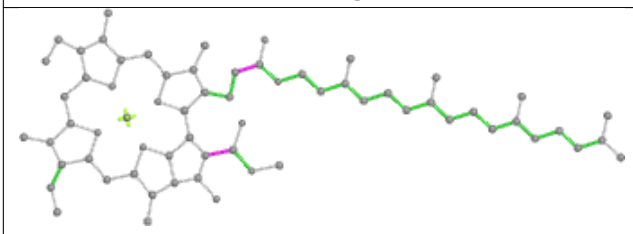
Ligand CLA C 506



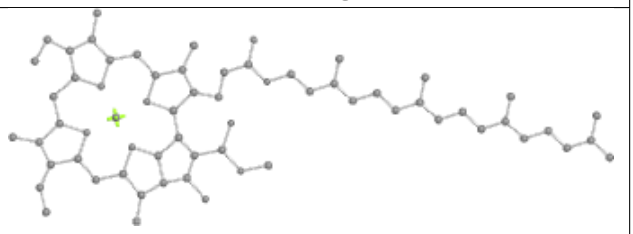
Bond lengths



Bond angles

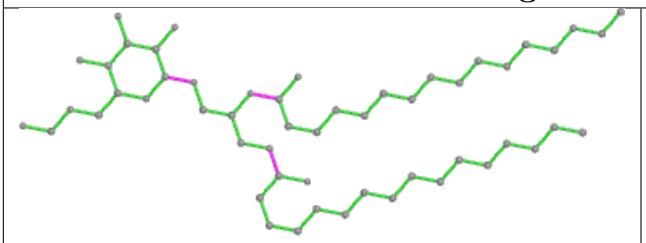


Torsions

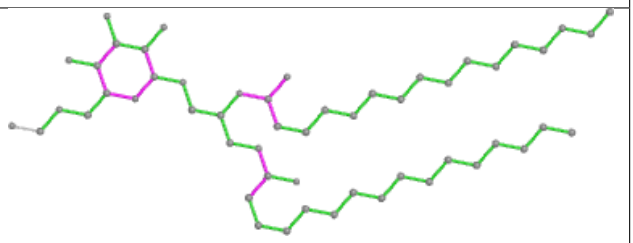


Rings

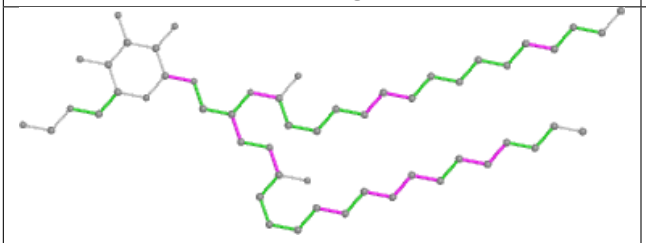
Ligand DGD D 407



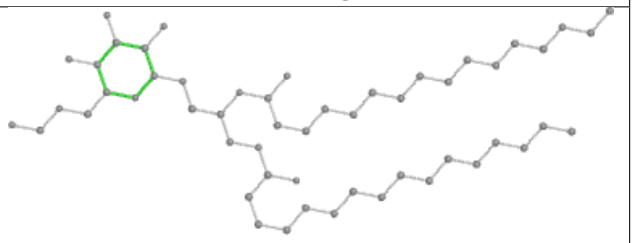
Bond lengths



Bond angles

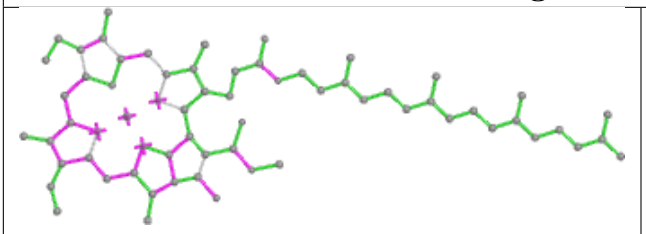


Torsions

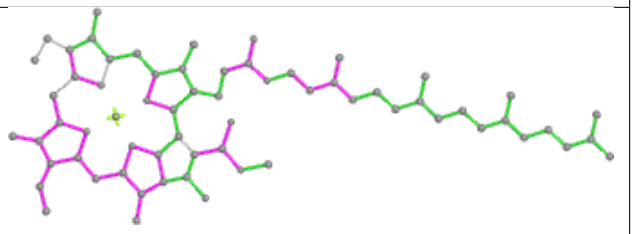


Rings

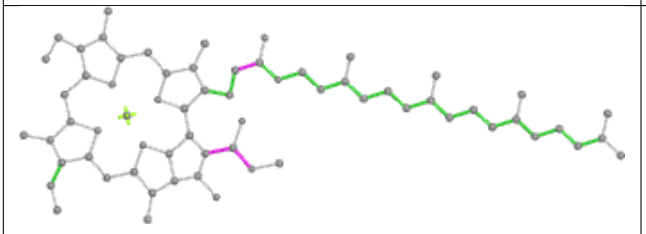
Ligand CLA c 503



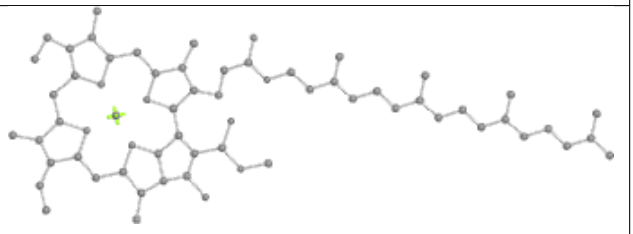
Bond lengths



Bond angles

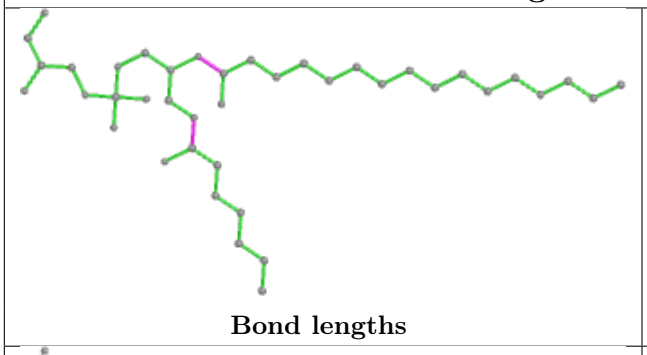


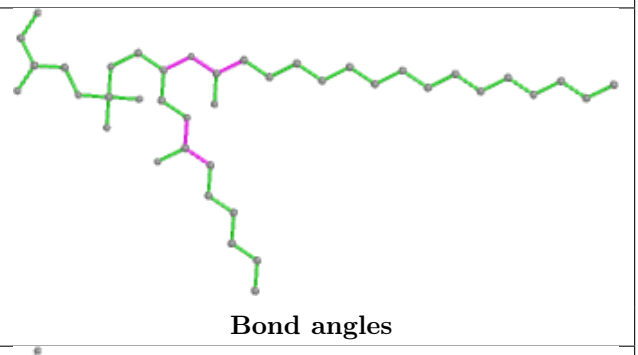
Torsions

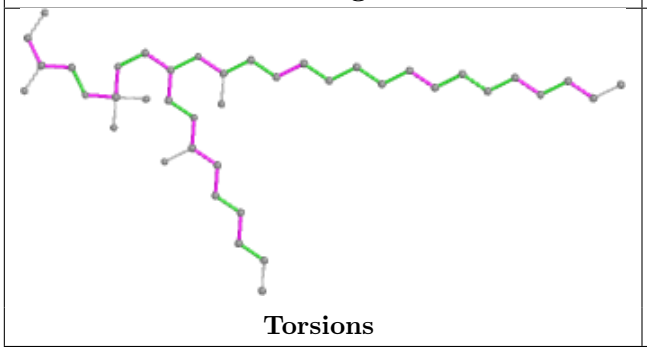


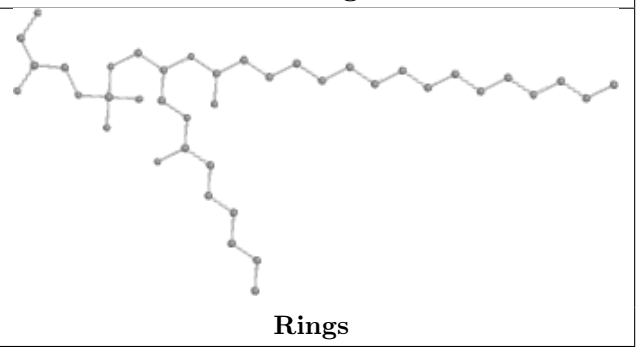
Rings

Ligand LHG e 101

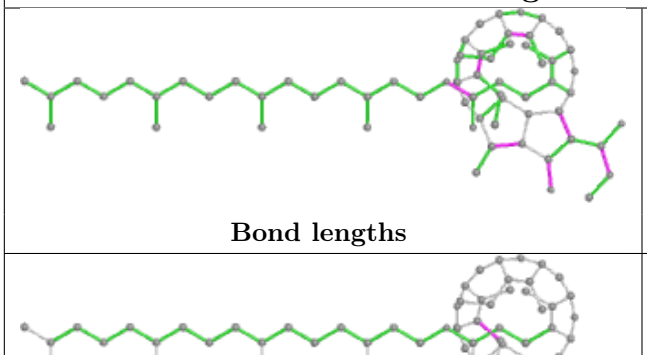

Bond lengths

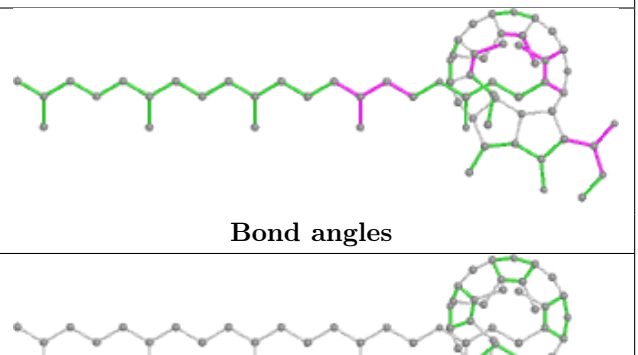

Bond angles

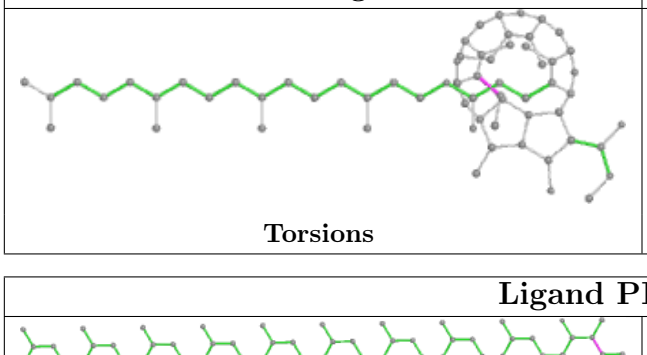

Torsions

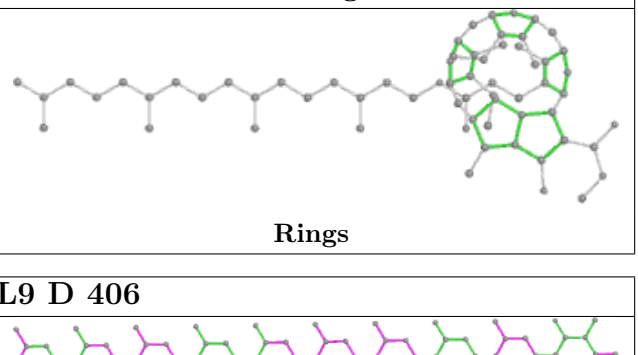

Rings

Ligand PHO D 401

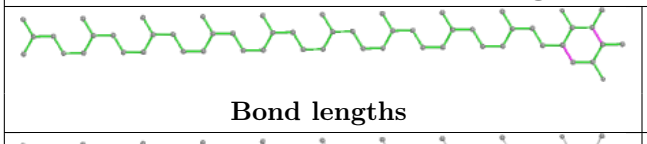

Bond lengths

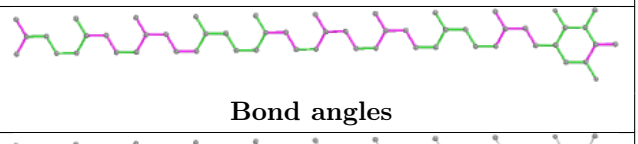

Bond angles

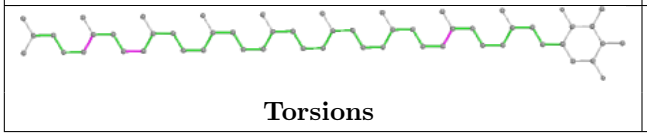

Torsions

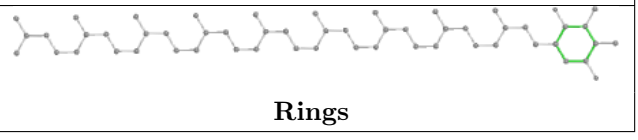

Rings

Ligand PL9 D 406

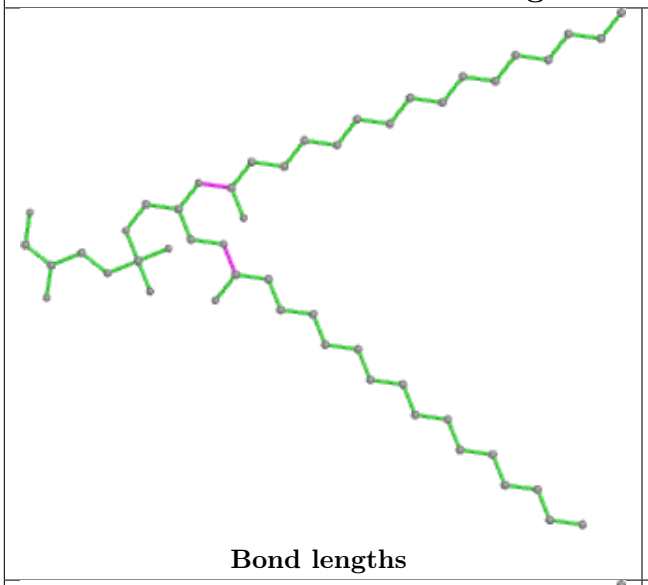

Bond lengths


Bond angles

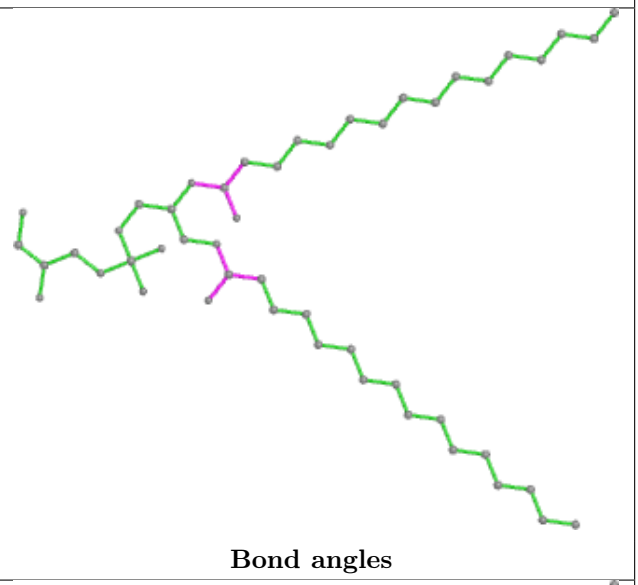

Torsions


Rings

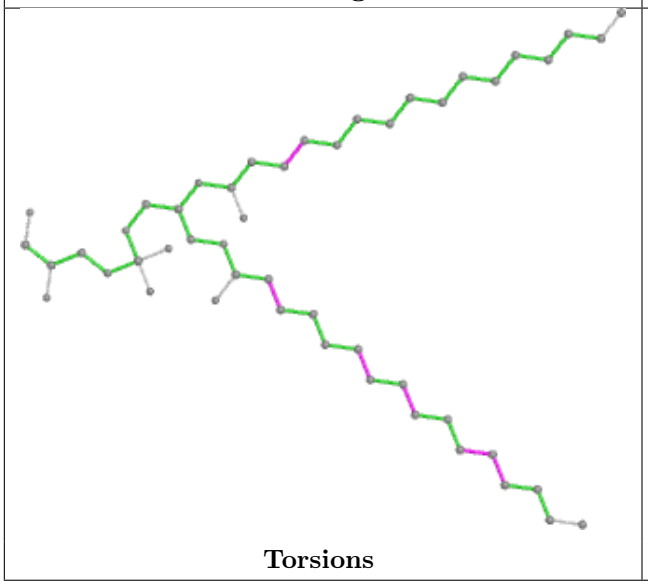
Ligand LHG d 408



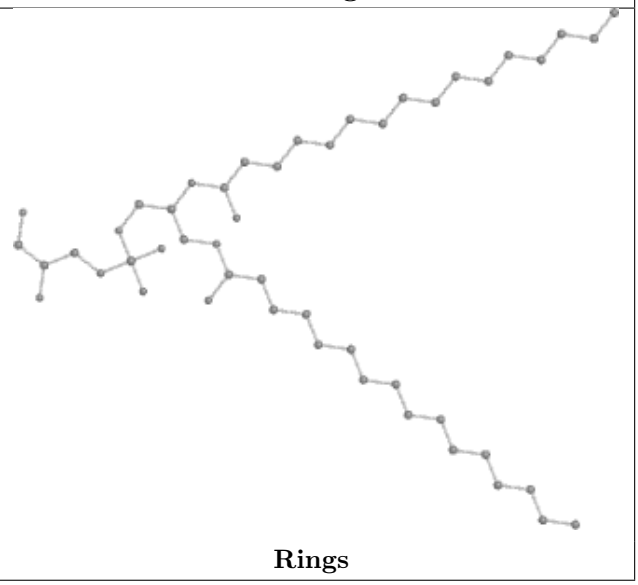
Bond lengths



Bond angles

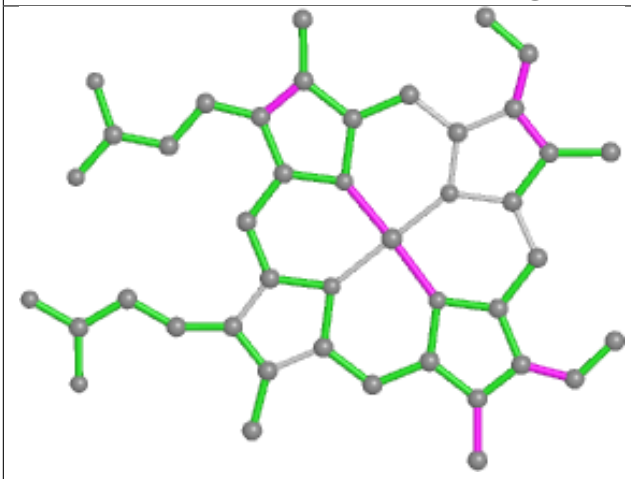


Torsions

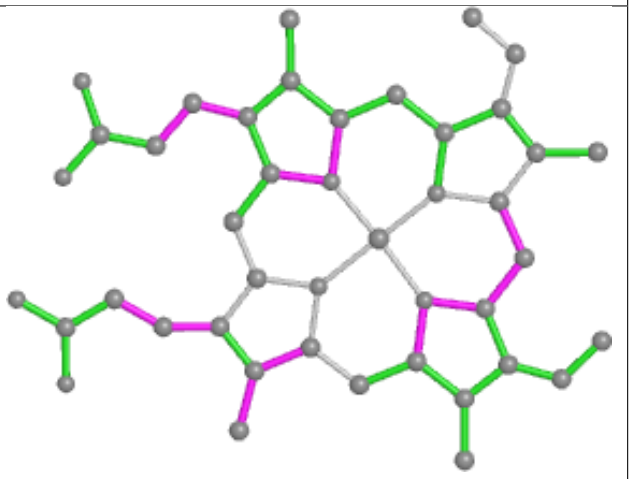


Rings

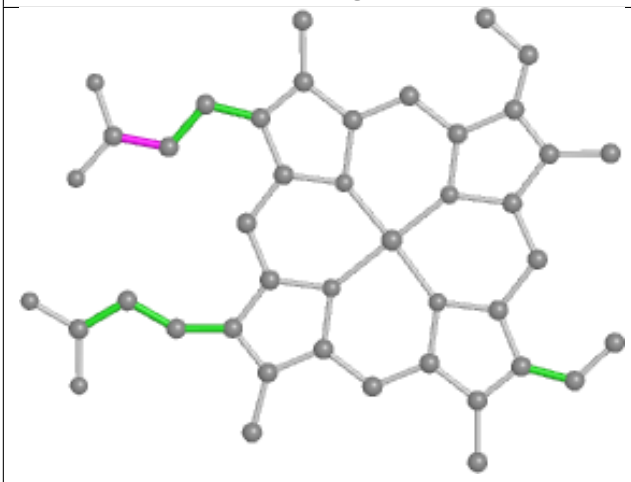
Ligand HEM f 101



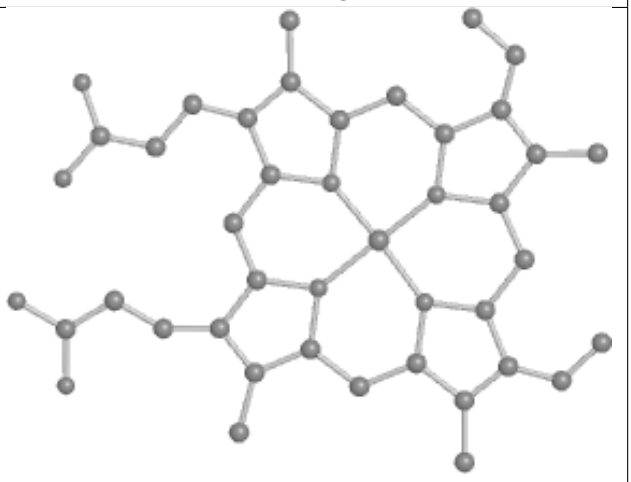
Bond lengths



Bond angles

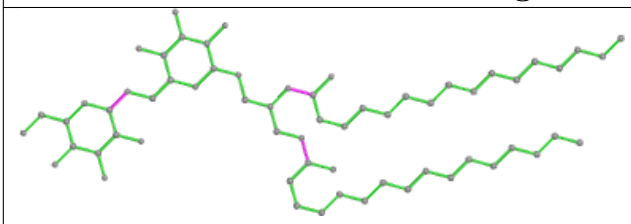


Torsions

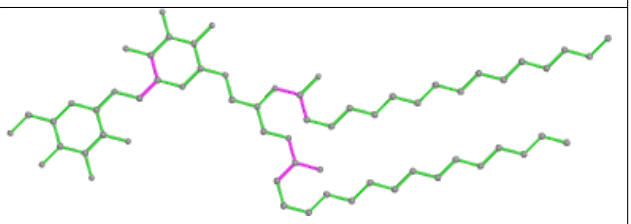


Rings

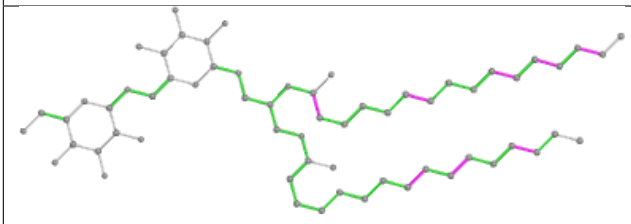
Ligand DGD h 1205



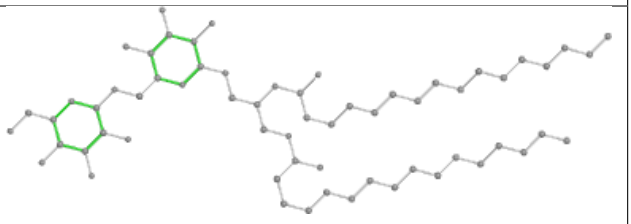
Bond lengths



Bond angles

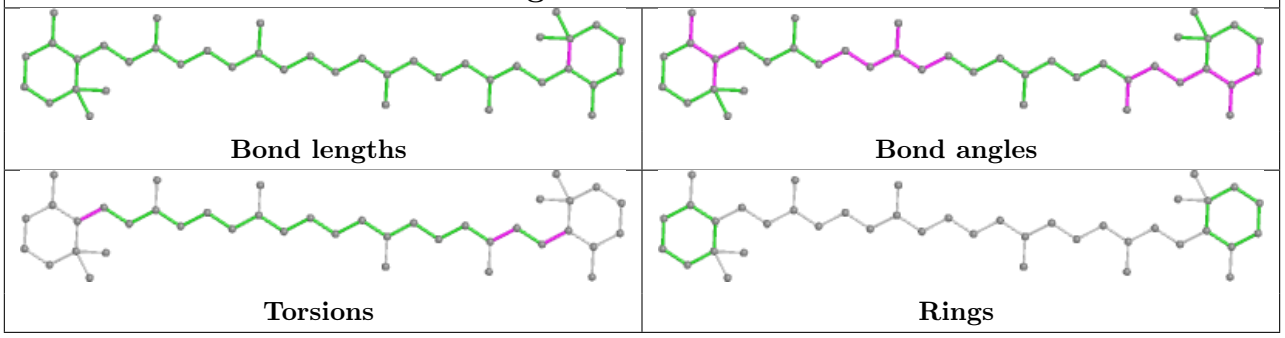


Torsions

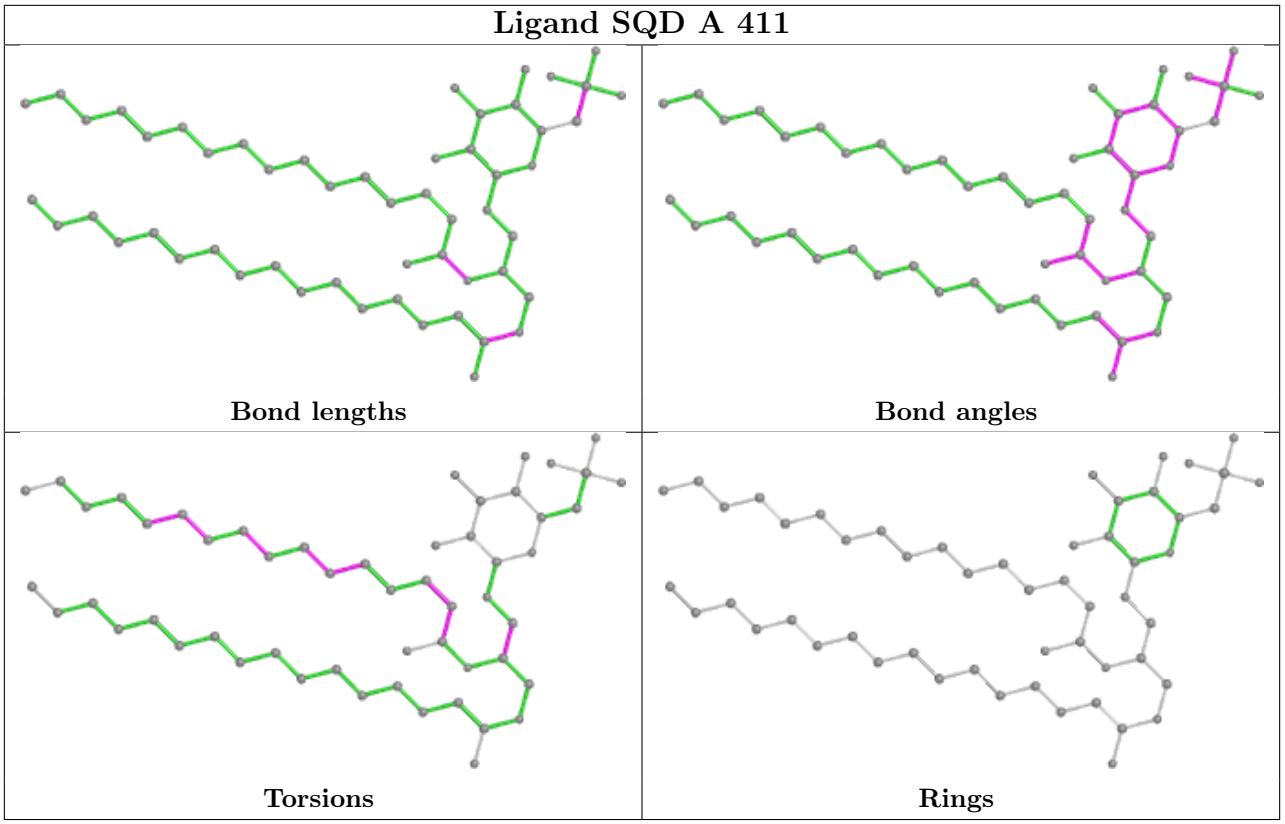


Rings

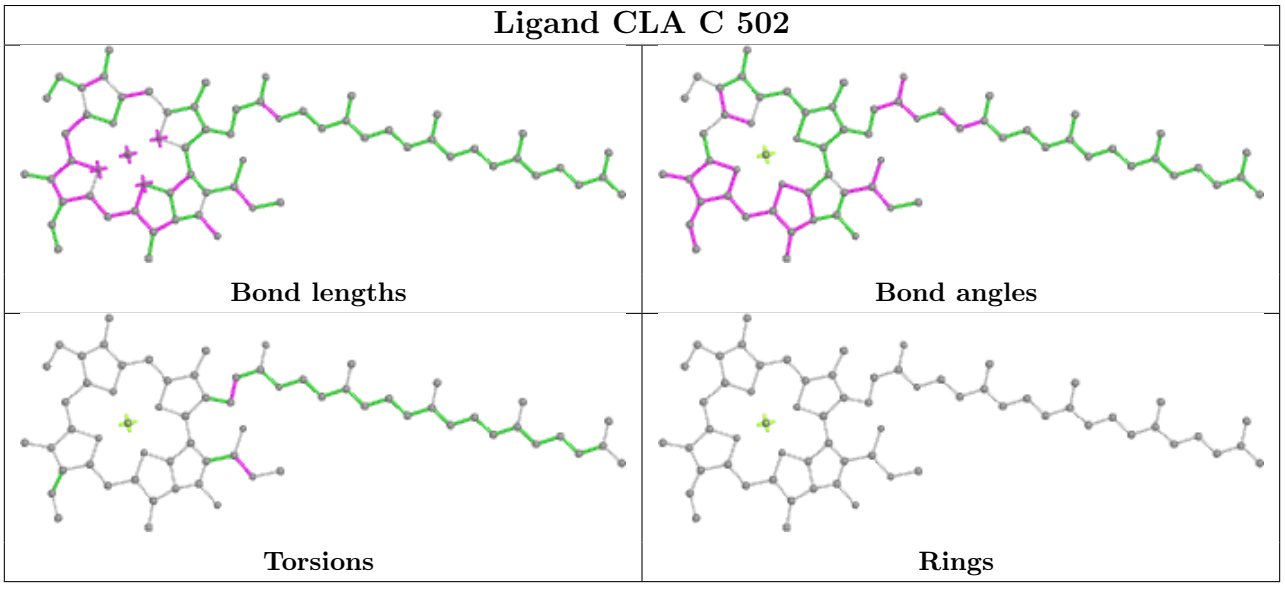
Ligand BCR k 302



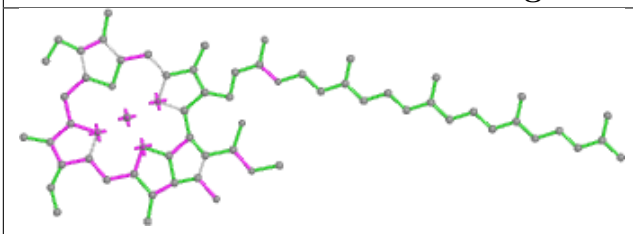
Ligand SQD A 411



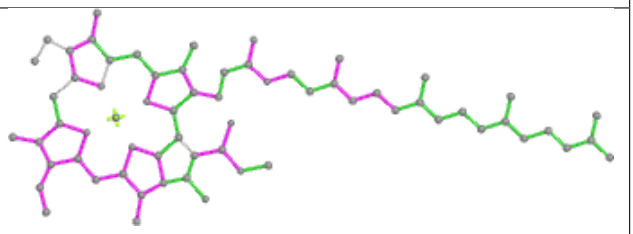
Ligand CLA C 502



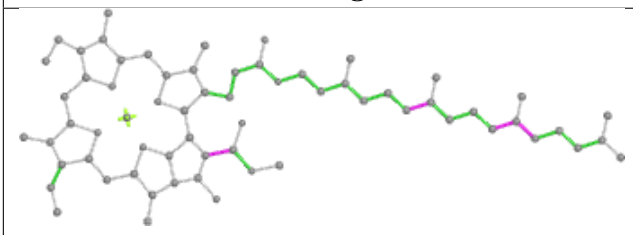
Ligand CLA C 505



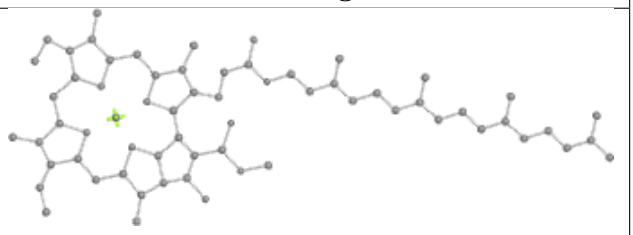
Bond lengths



Bond angles

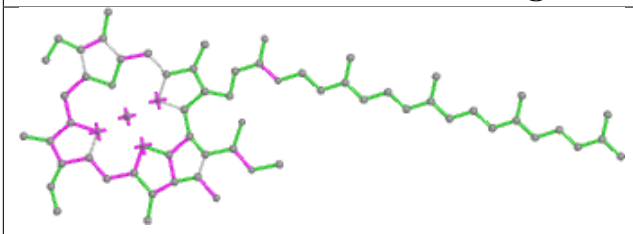


Torsions

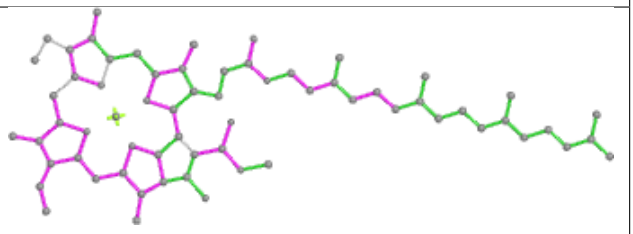


Rings

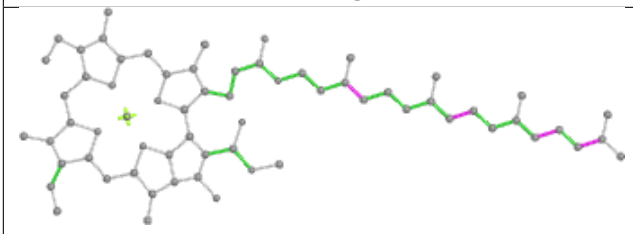
Ligand CLA b 614



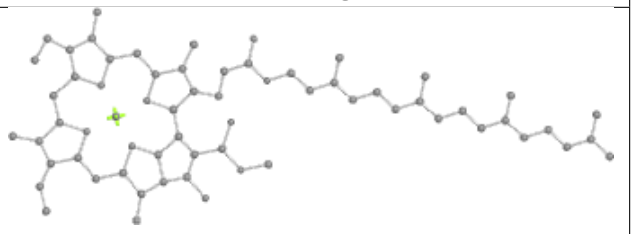
Bond lengths



Bond angles

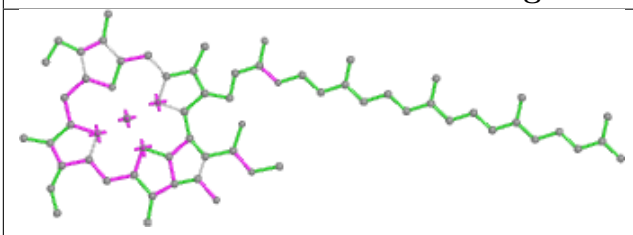


Torsions

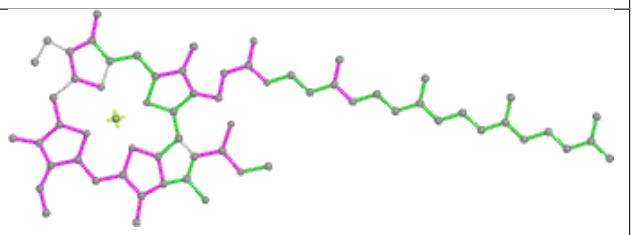


Rings

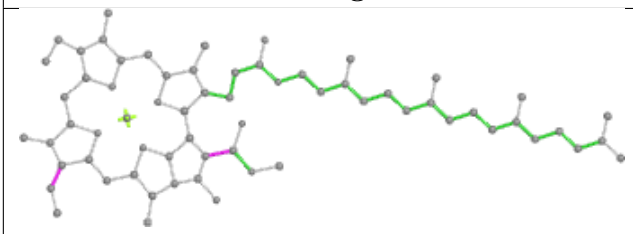
Ligand CLA A 406



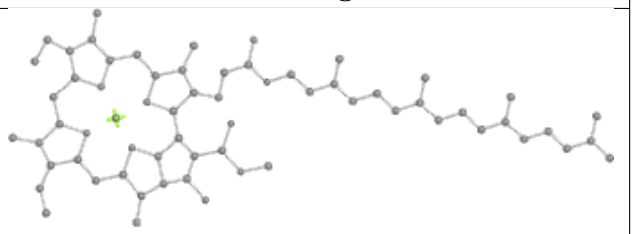
Bond lengths



Bond angles

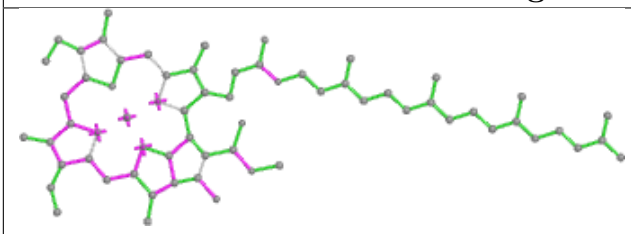


Torsions

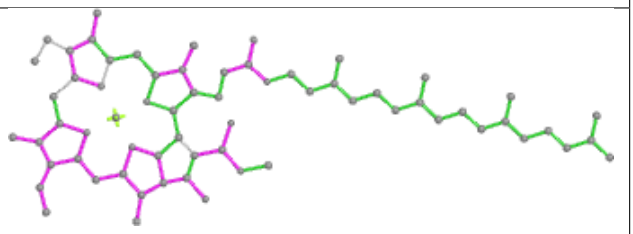


Rings

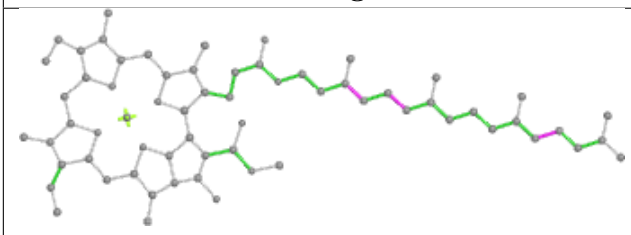
Ligand CLA b 611



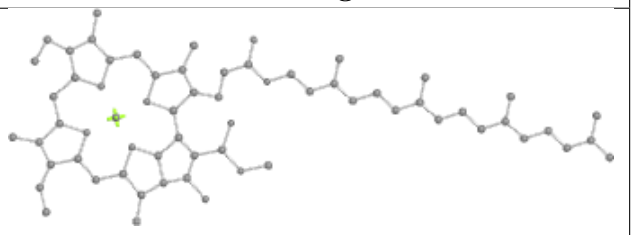
Bond lengths



Bond angles

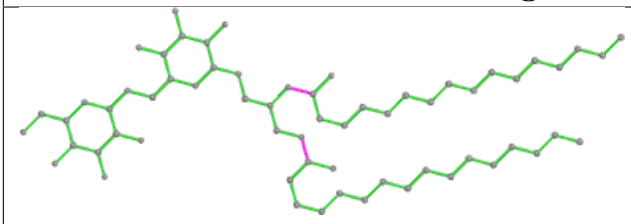


Torsions

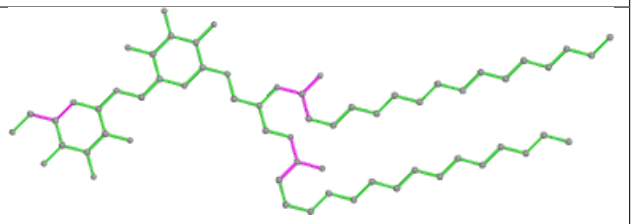


Rings

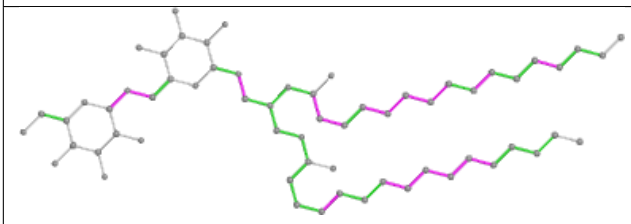
Ligand DGD C 518



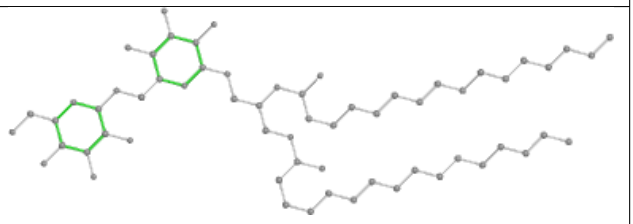
Bond lengths



Bond angles

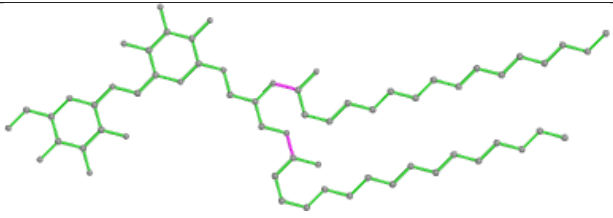


Torsions

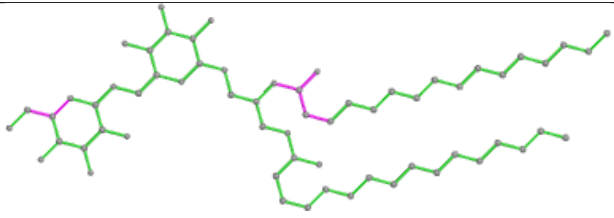


Rings

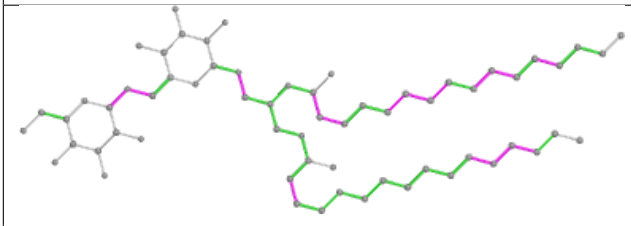
Ligand DGD c 519



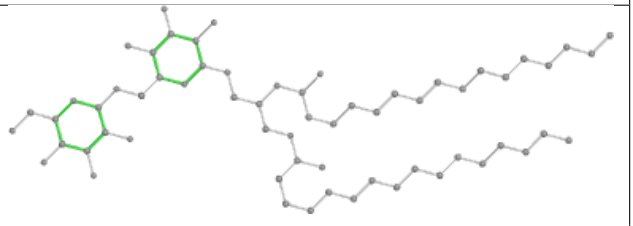
Bond lengths



Bond angles

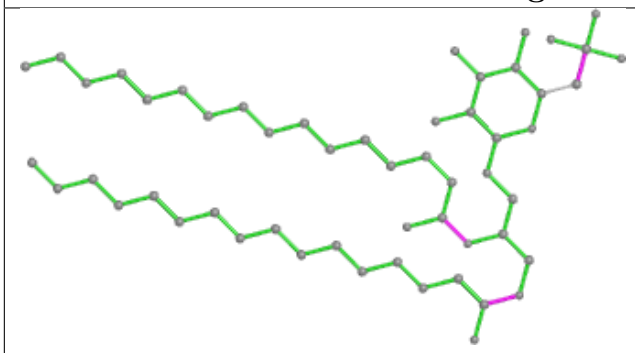


Torsions

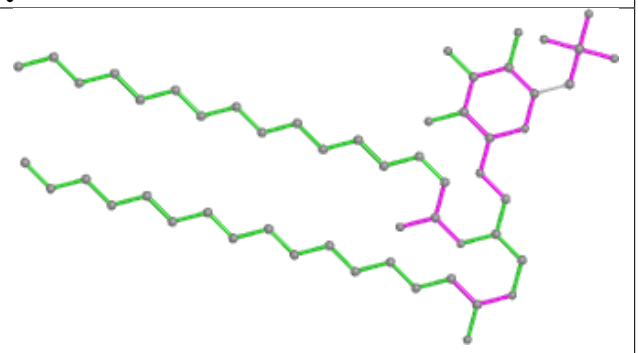


Rings

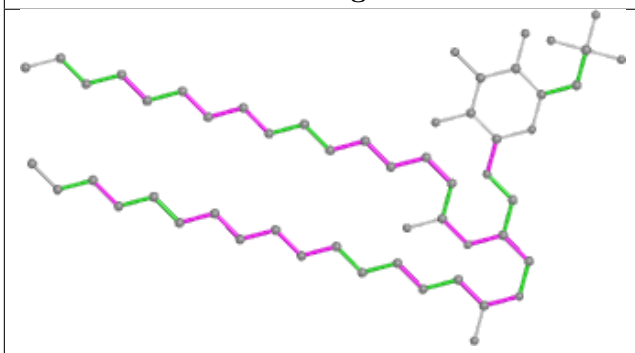
Ligand SQD L 102



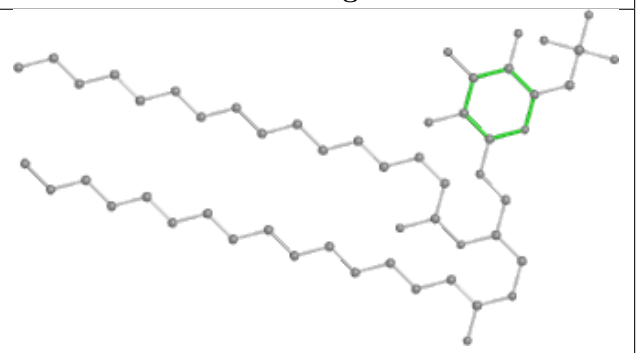
Bond lengths



Bond angles

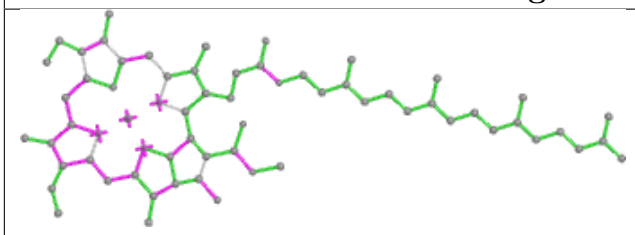


Torsions

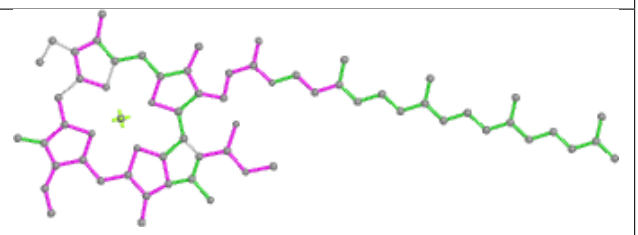


Rings

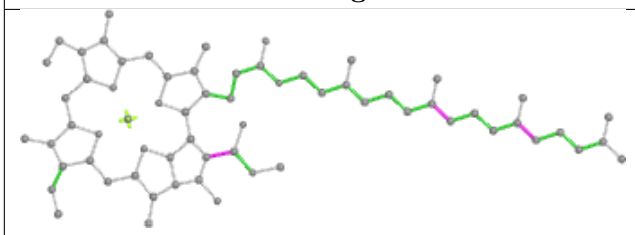
Ligand CLA b 610



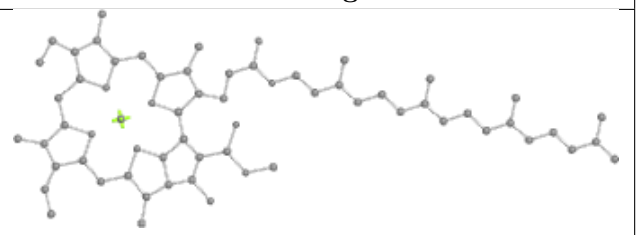
Bond lengths



Bond angles

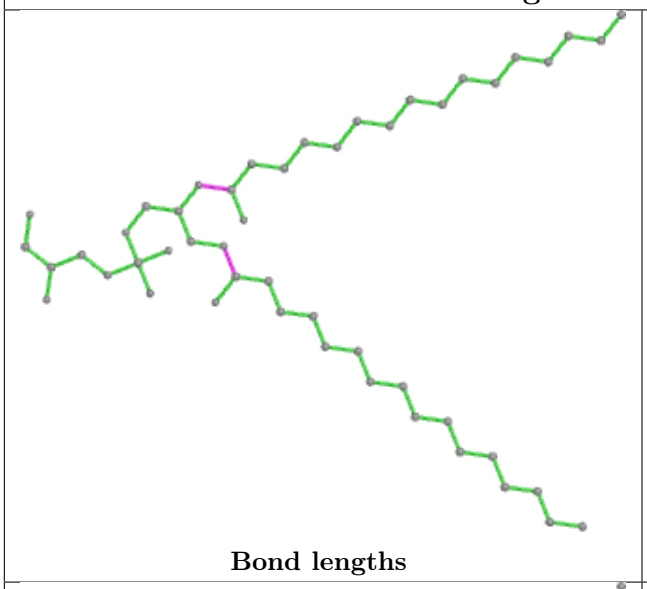


Torsions

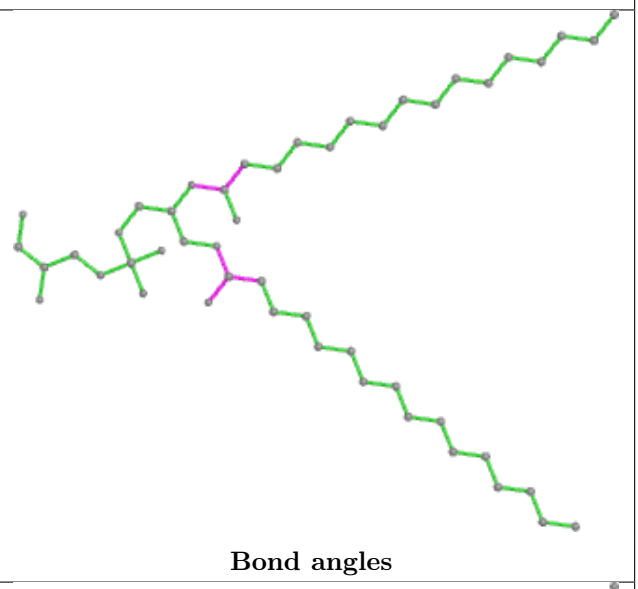


Rings

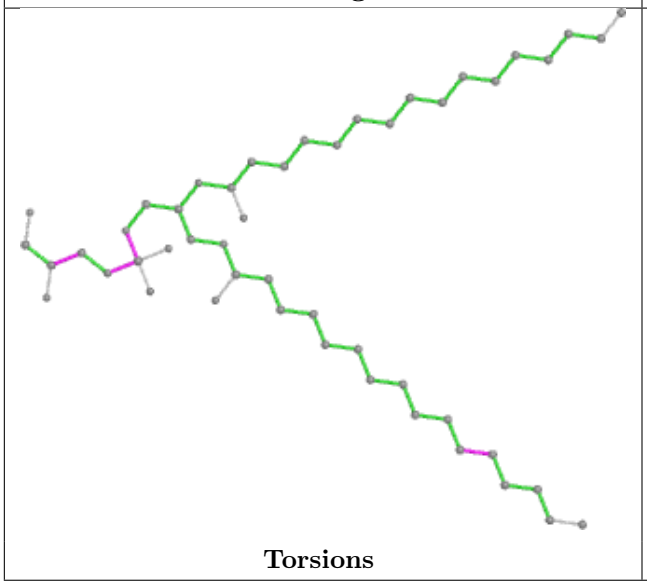
Ligand LHG D 410



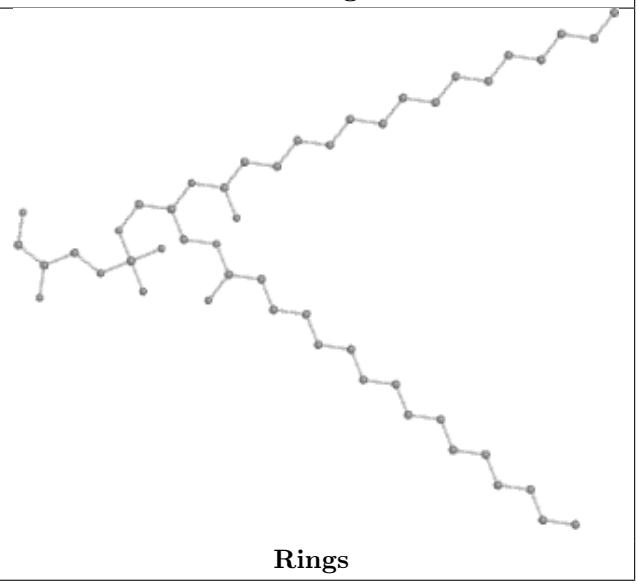
Bond lengths



Bond angles

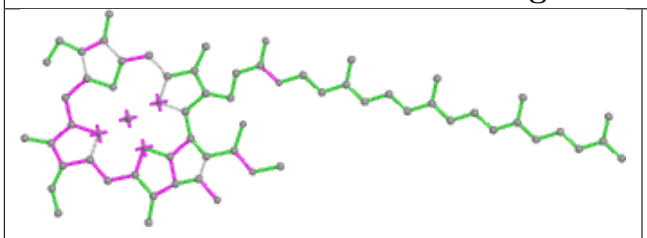


Torsions

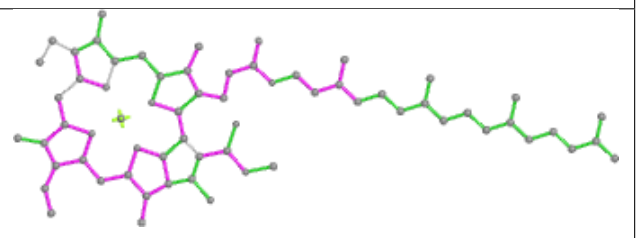


Rings

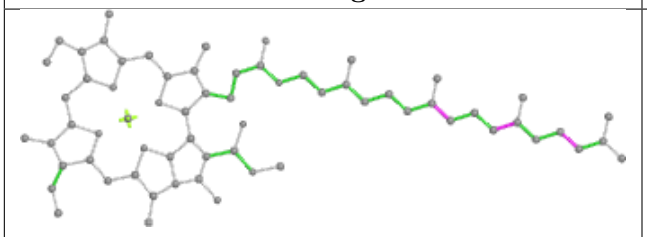
Ligand CLA a 410



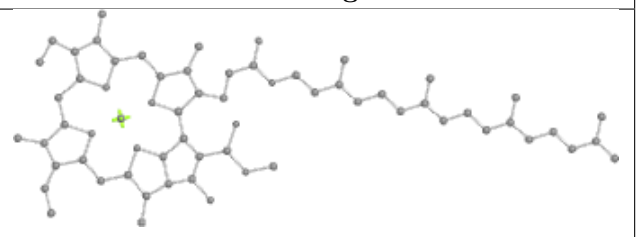
Bond lengths



Bond angles

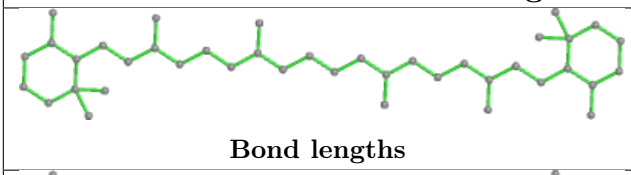


Torsions

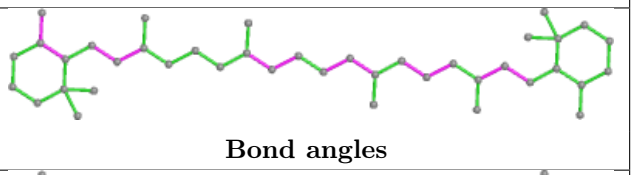


Rings

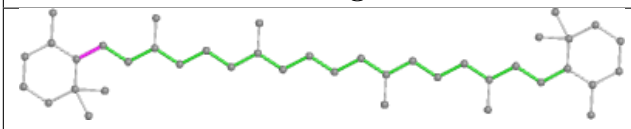
Ligand BCR b 620



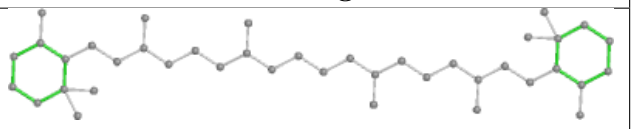
Bond lengths



Bond angles

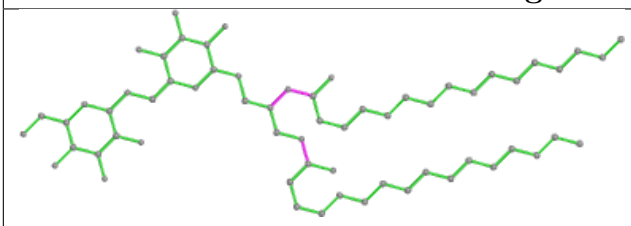


Torsions

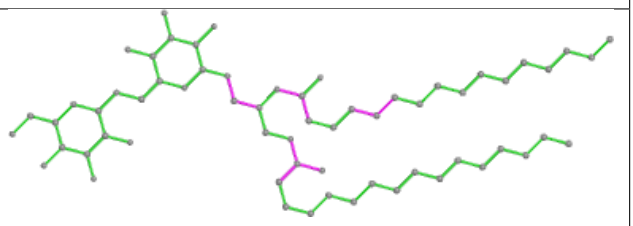


Rings

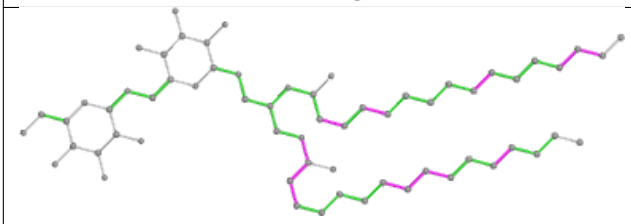
Ligand DGD c 520



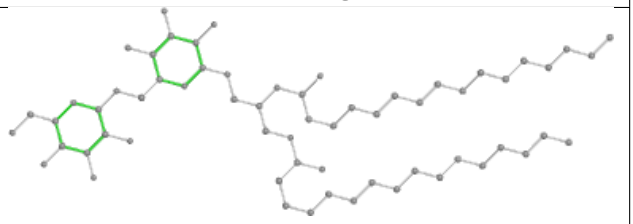
Bond lengths



Bond angles

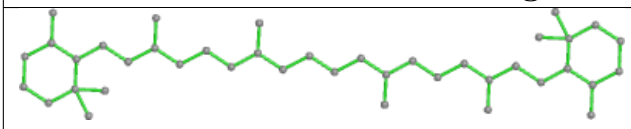


Torsions

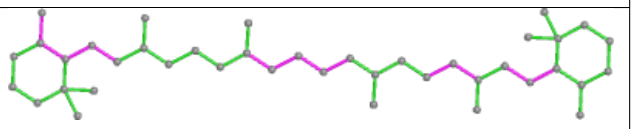


Rings

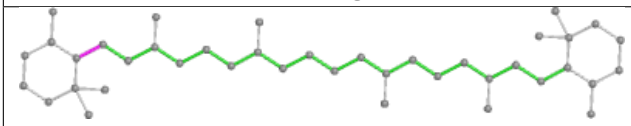
Ligand BCR A 410



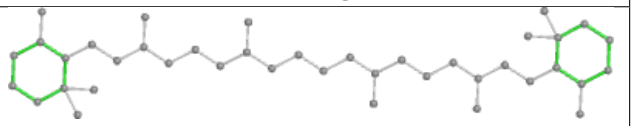
Bond lengths



Bond angles

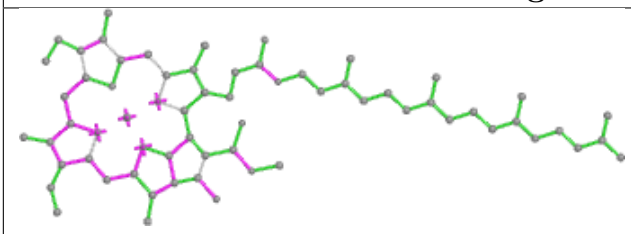


Torsions

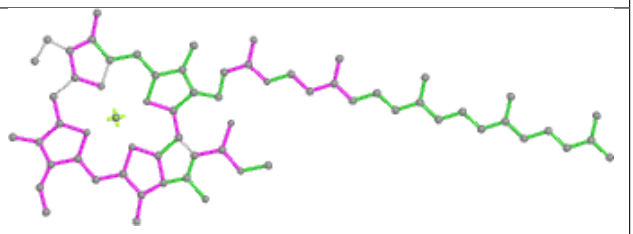


Rings

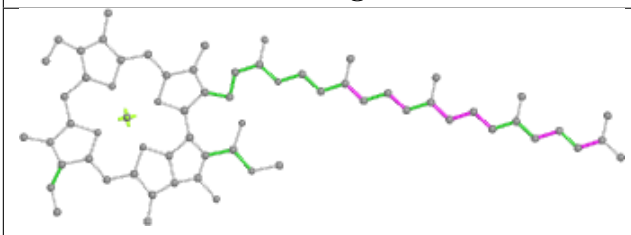
Ligand CLA b 618



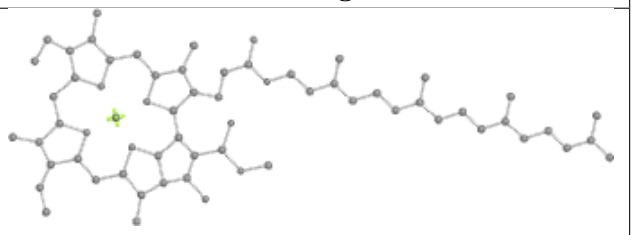
Bond lengths



Bond angles

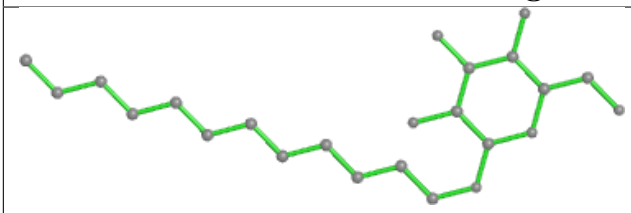


Torsions

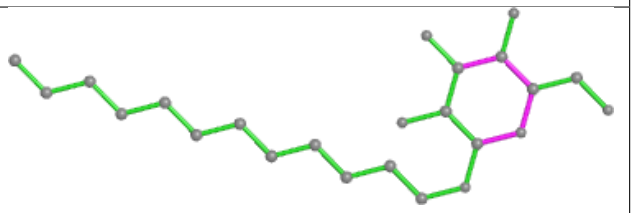


Rings

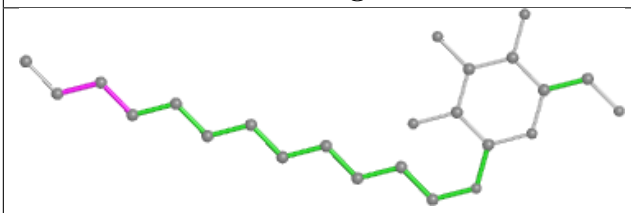
Ligand LMT J 102



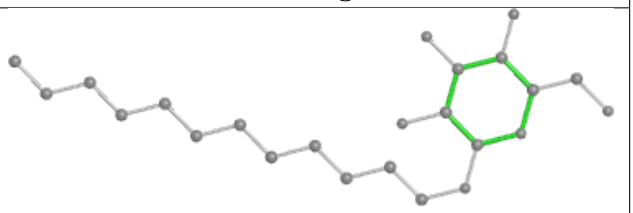
Bond lengths



Bond angles

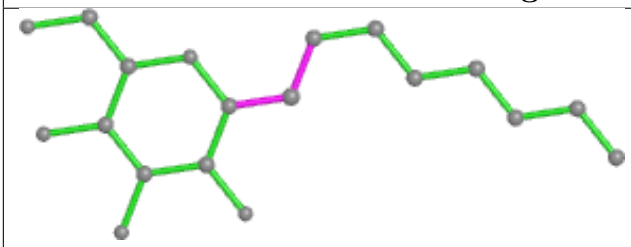


Torsions

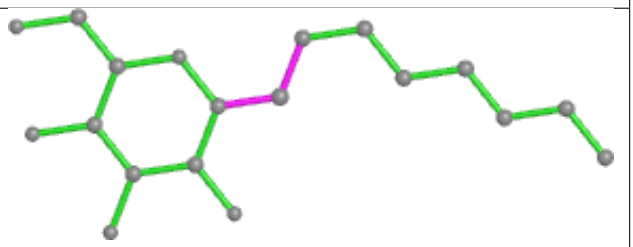


Rings

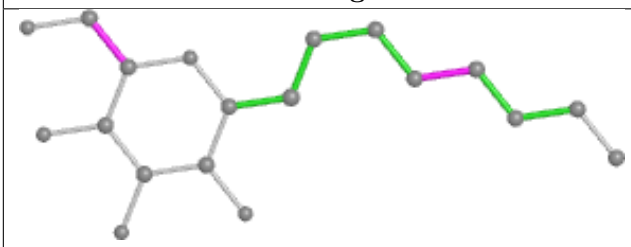
Ligand HTG B 625



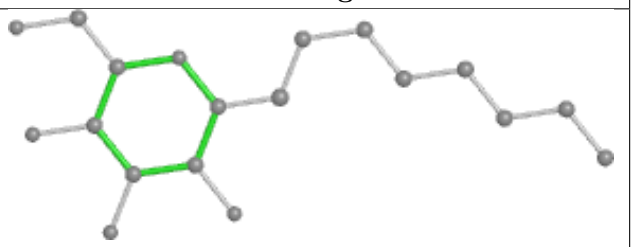
Bond lengths



Bond angles

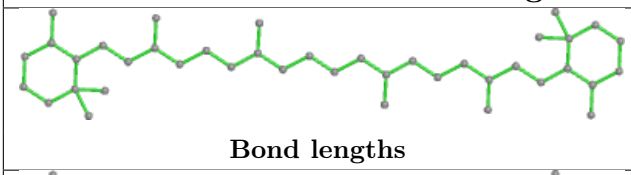


Torsions

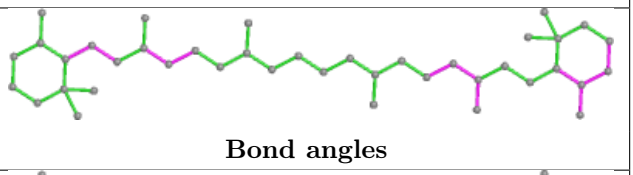


Rings

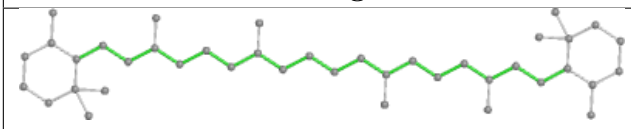
Ligand BCR b 621



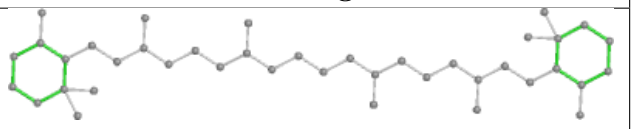
Bond lengths



Bond angles

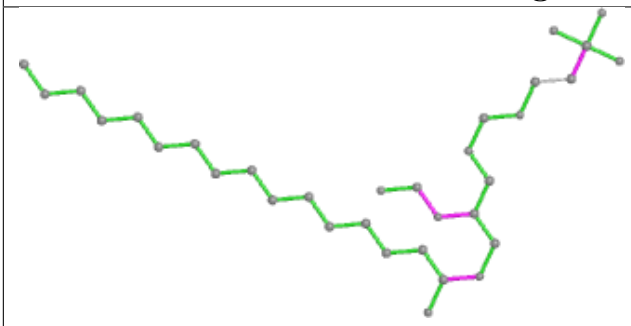


Torsions

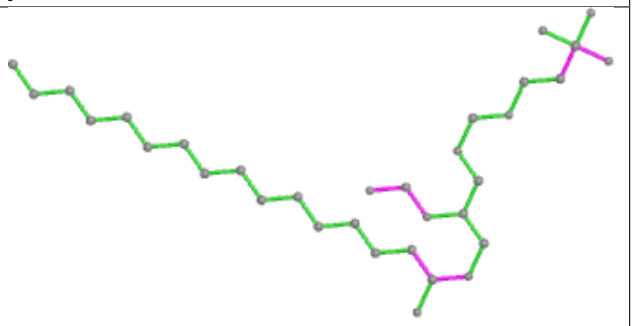


Rings

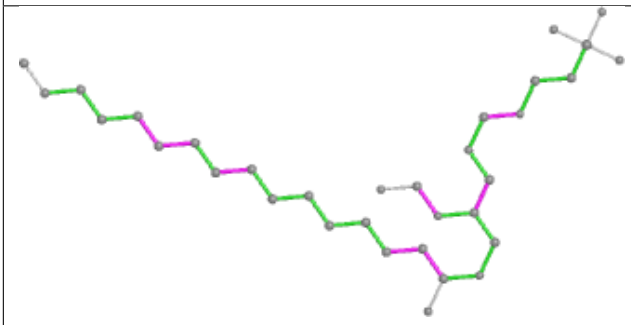
Ligand SQD f 102



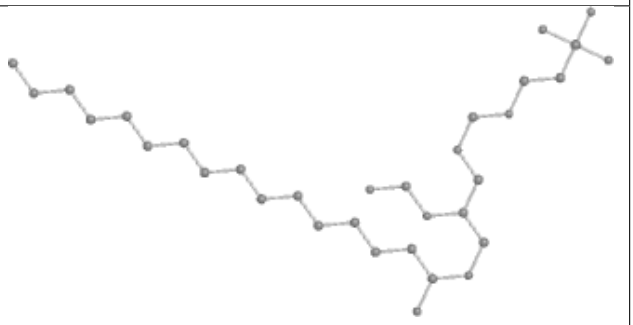
Bond lengths



Bond angles

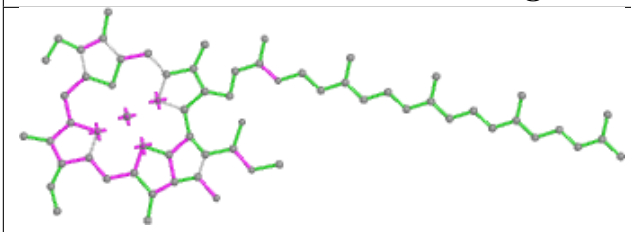


Torsions

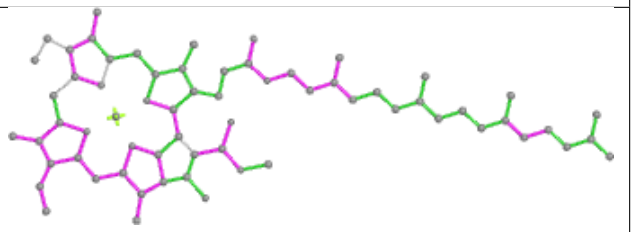


Rings

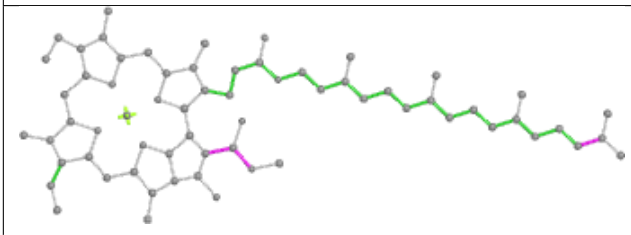
Ligand CLA C 503



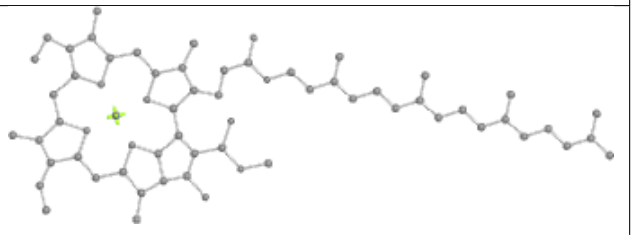
Bond lengths



Bond angles

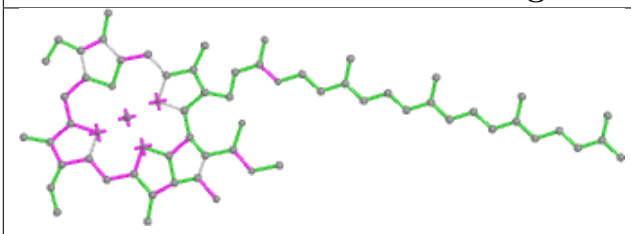


Torsions

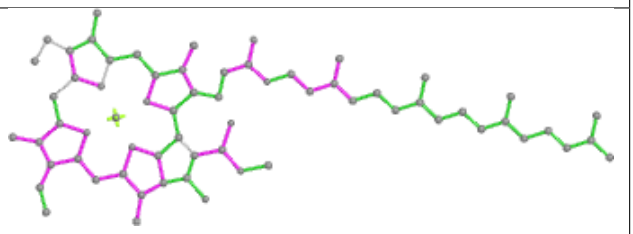


Rings

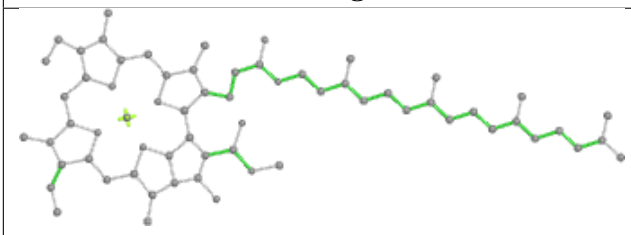
Ligand CLA b 615



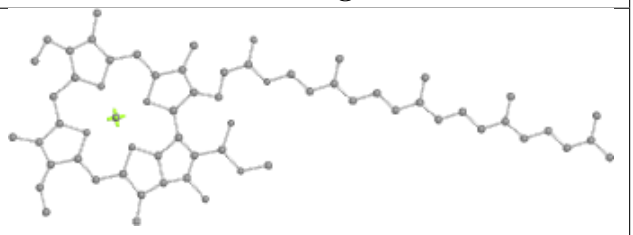
Bond lengths



Bond angles

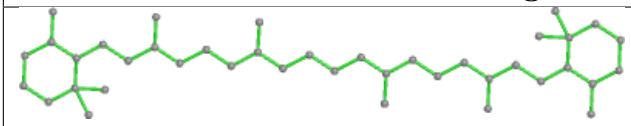


Torsions

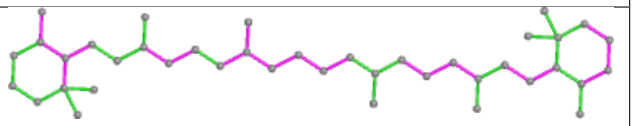


Rings

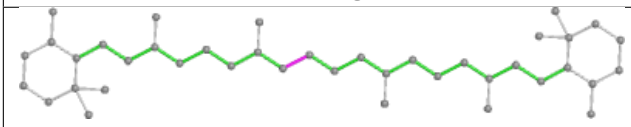
Ligand BCR B 641



Bond lengths



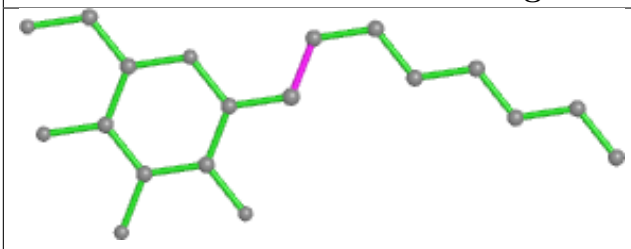
Bond angles



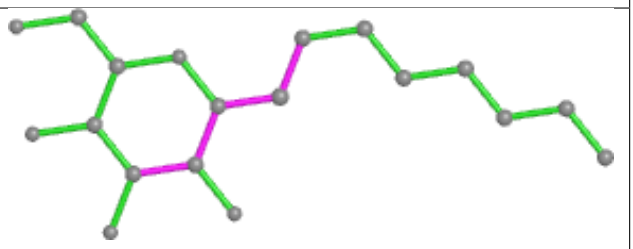
Torsions

Rings

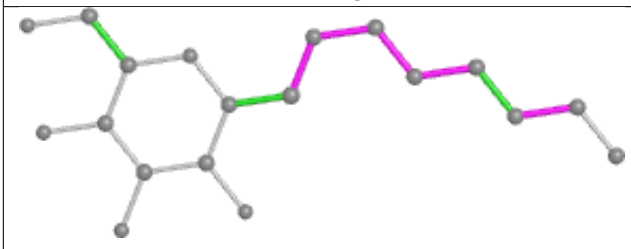
Ligand HTG b 625



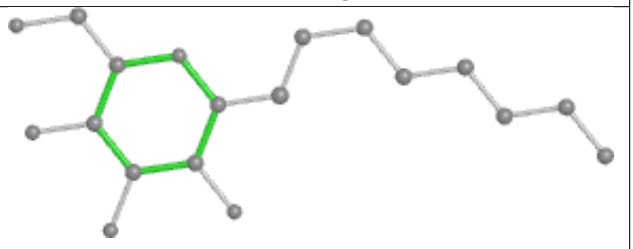
Bond lengths



Bond angles

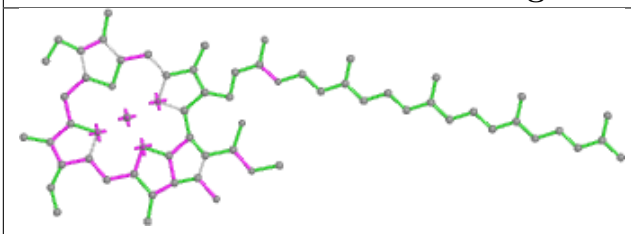


Torsions

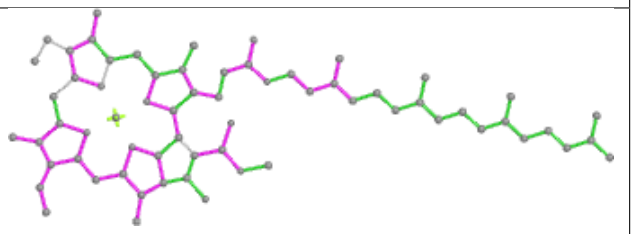


Rings

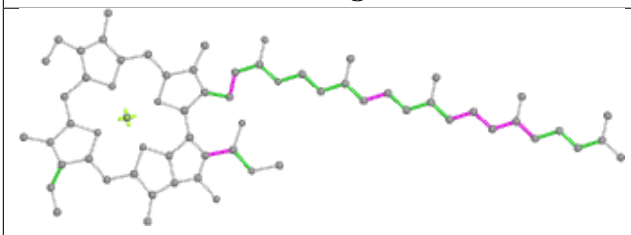
Ligand CLA b 609



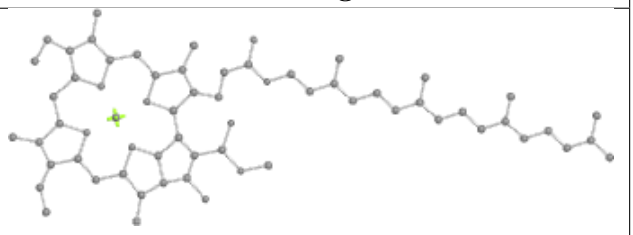
Bond lengths



Bond angles

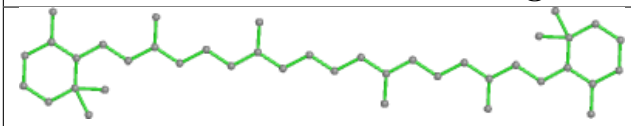


Torsions

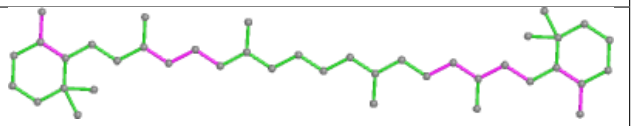


Rings

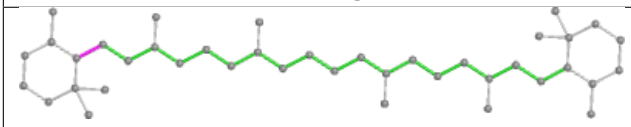
Ligand BCR k 303



Bond lengths



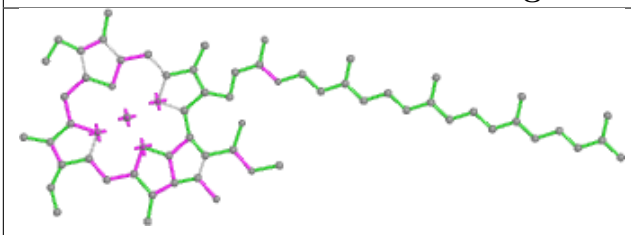
Bond angles



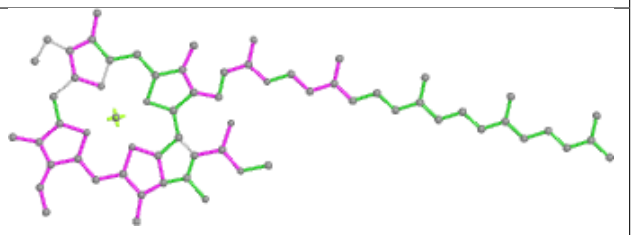
Torsions

Rings

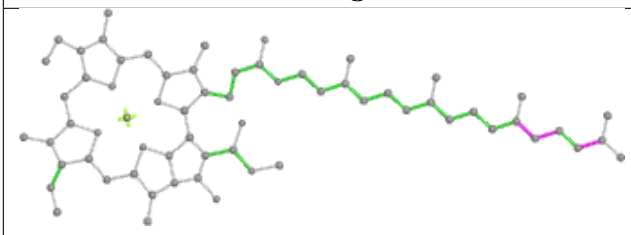
Ligand CLA A 407



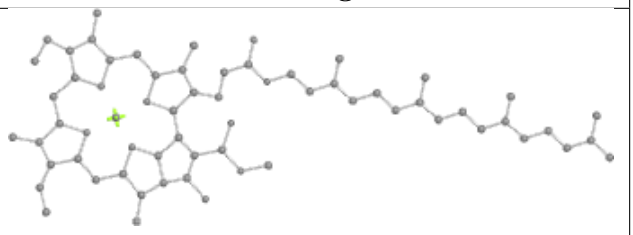
Bond lengths



Bond angles

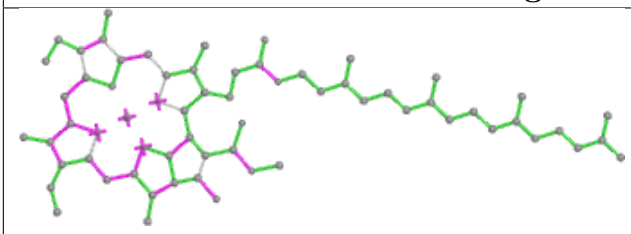


Torsions

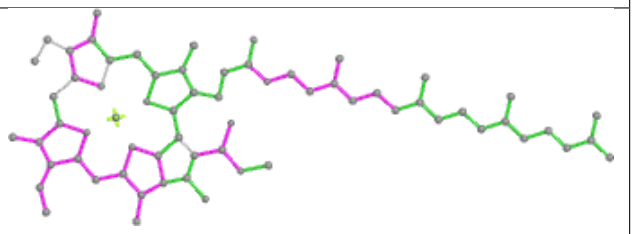


Rings

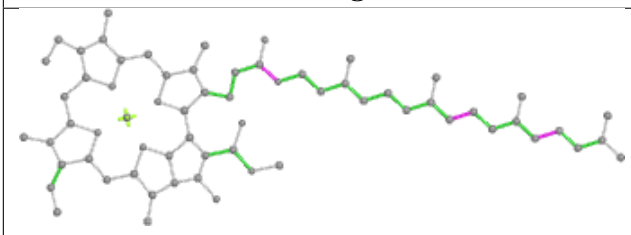
Ligand CLA B 613



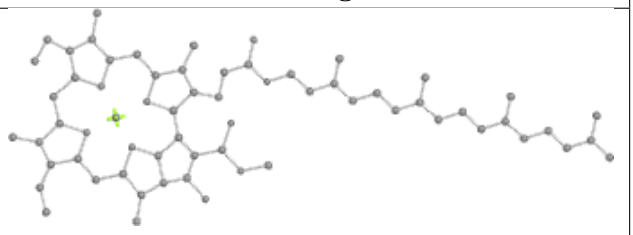
Bond lengths



Bond angles

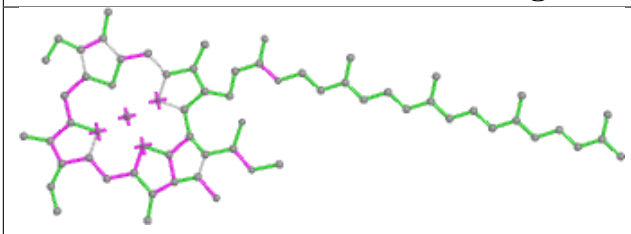


Torsions

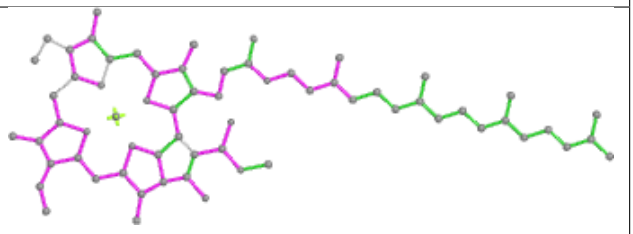


Rings

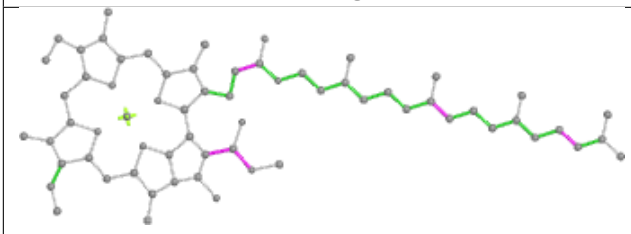
Ligand CLA c 514



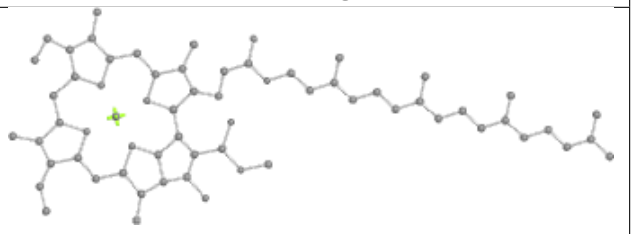
Bond lengths



Bond angles

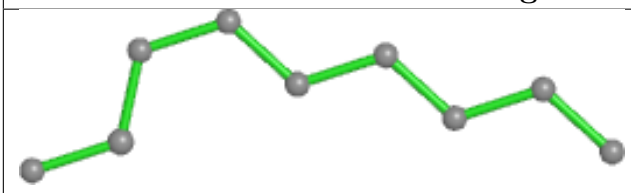


Torsions

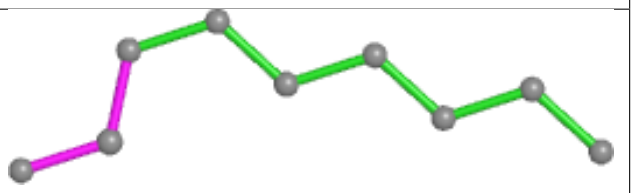


Rings

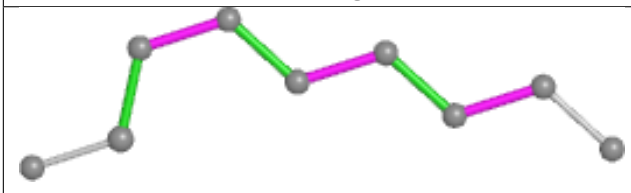
Ligand HTG U 201



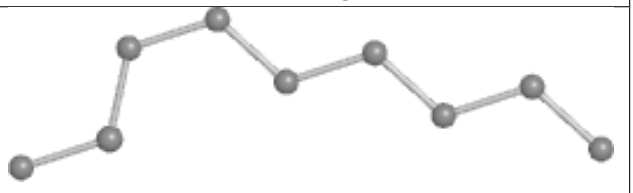
Bond lengths



Bond angles

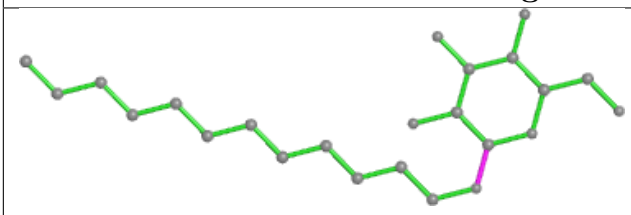


Torsions

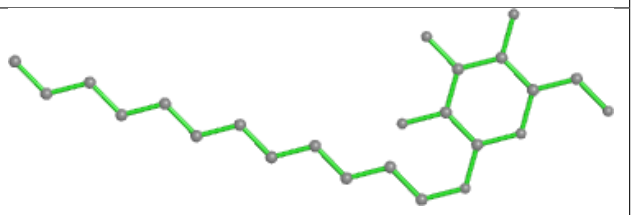


Rings

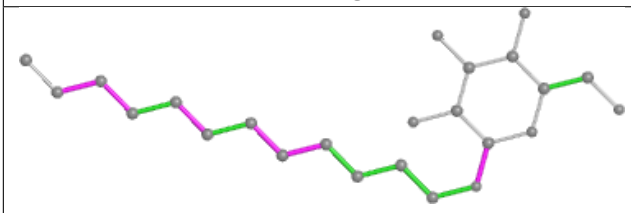
Ligand LMT B 642



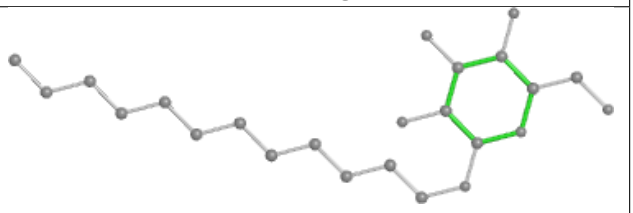
Bond lengths



Bond angles

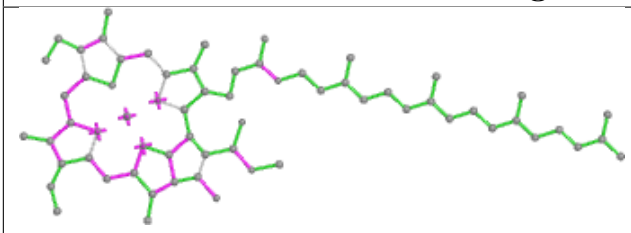


Torsions

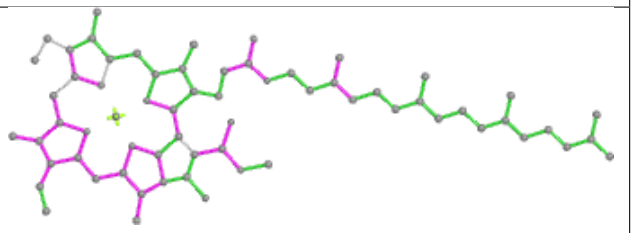


Rings

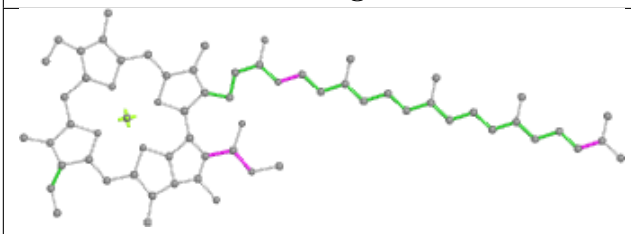
Ligand CLA c 504



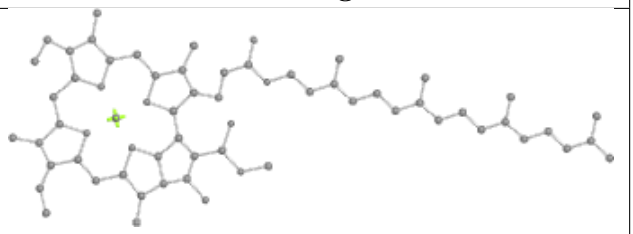
Bond lengths



Bond angles

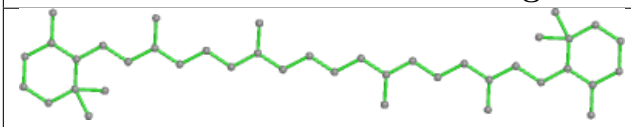


Torsions

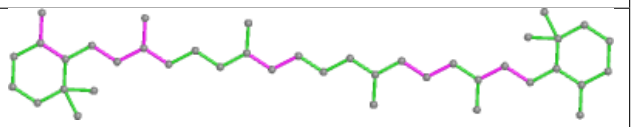


Rings

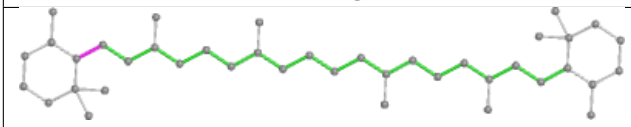
Ligand BCR B 618



Bond lengths



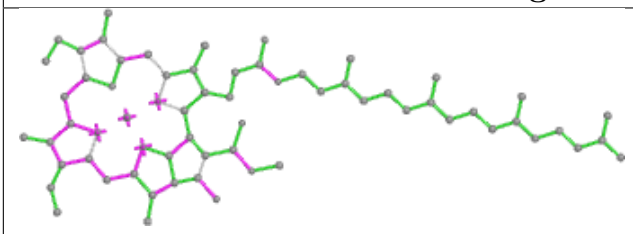
Bond angles



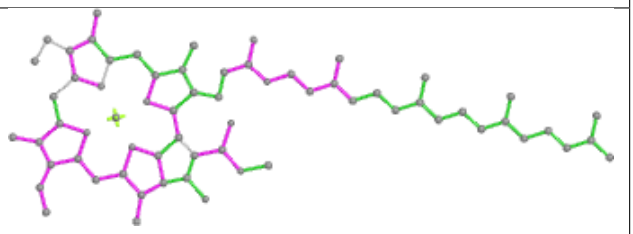
Torsions

Rings

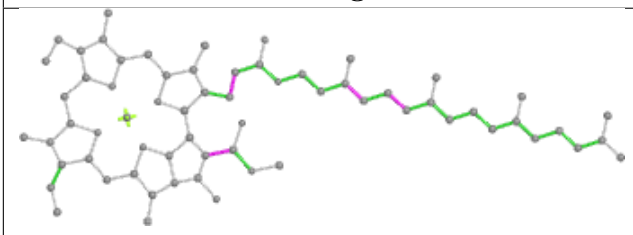
Ligand CLA c 509



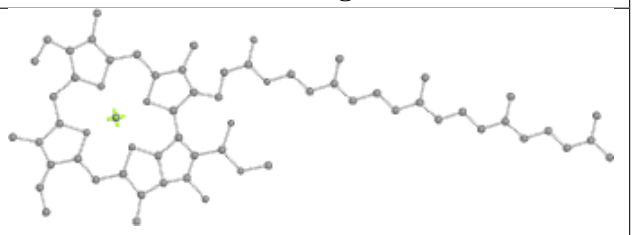
Bond lengths



Bond angles

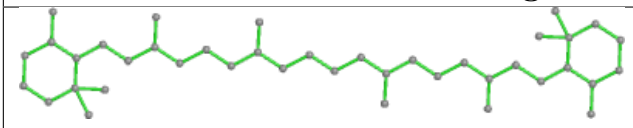


Torsions

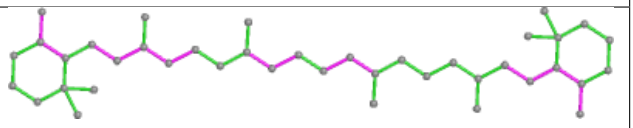


Rings

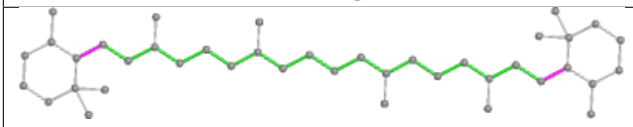
Ligand BCR C 515



Bond lengths



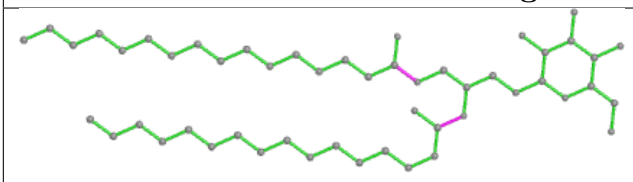
Bond angles



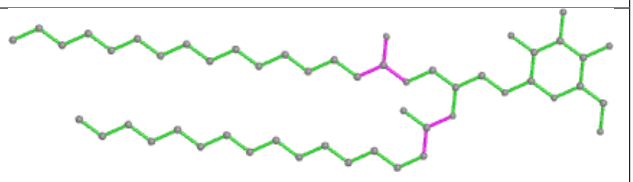
Torsions

Rings

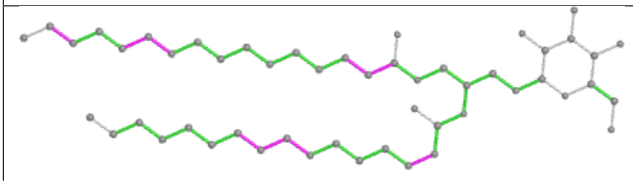
Ligand LMG B 621



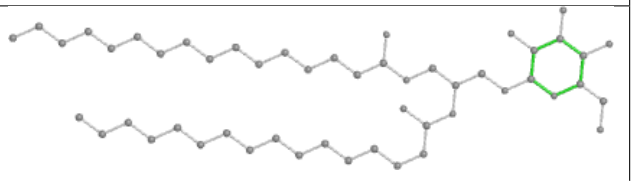
Bond lengths



Bond angles

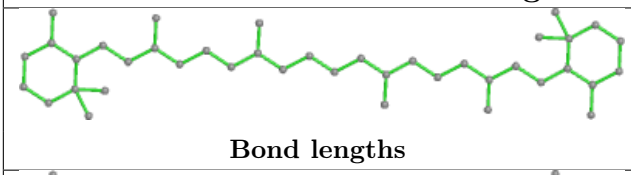


Torsions

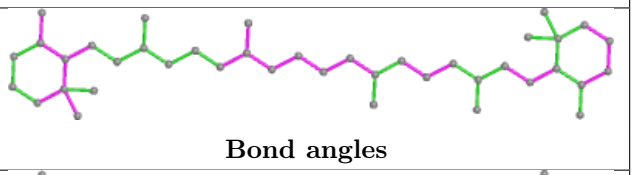


Rings

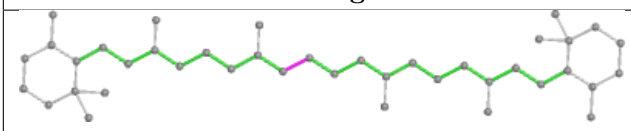
Ligand BCR T 102



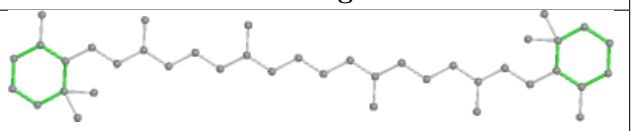
Bond lengths



Bond angles

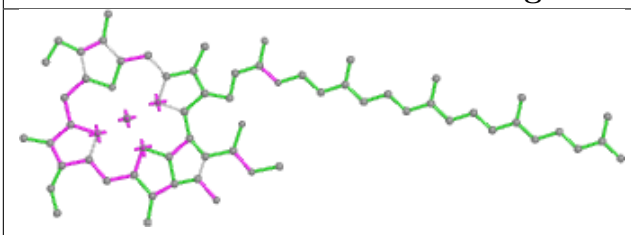


Torsions

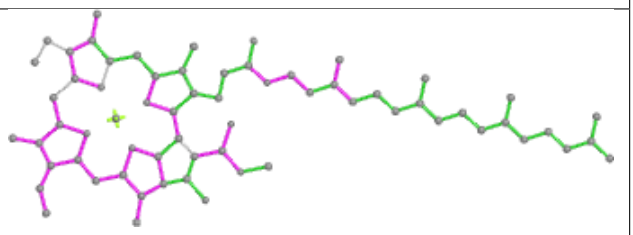


Rings

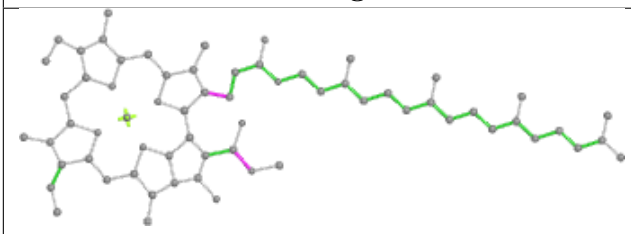
Ligand CLA C 512



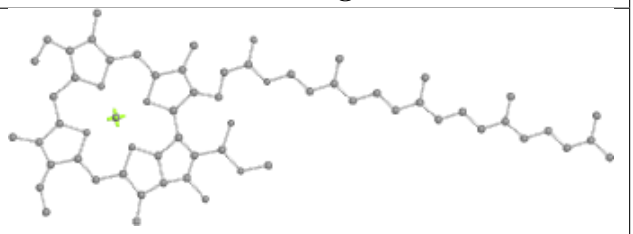
Bond lengths



Bond angles

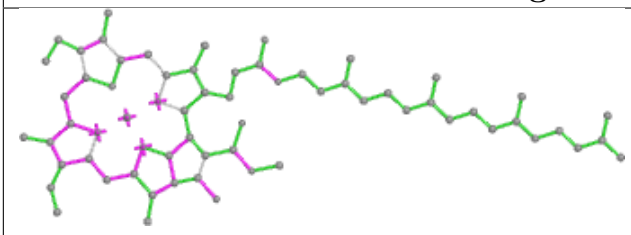


Torsions

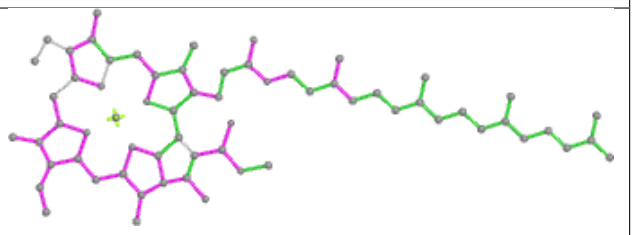


Rings

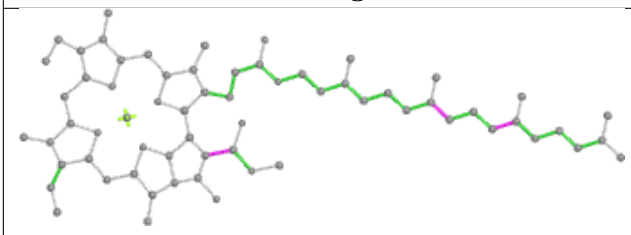
Ligand CLA c 506



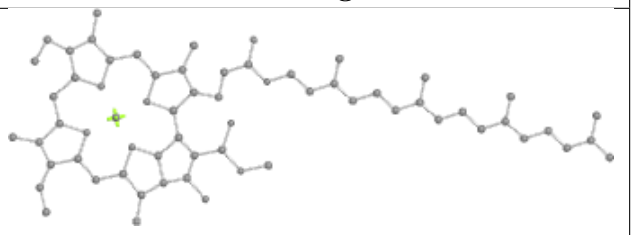
Bond lengths



Bond angles

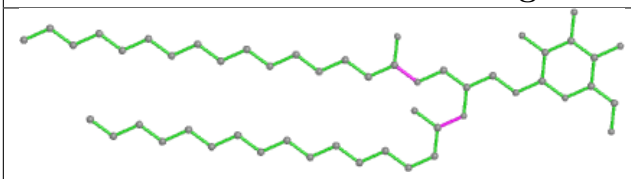


Torsions

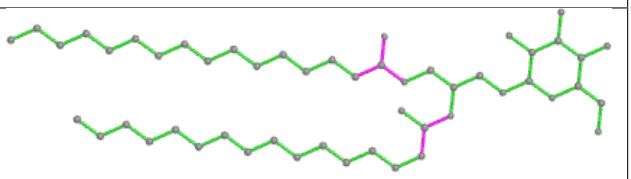


Rings

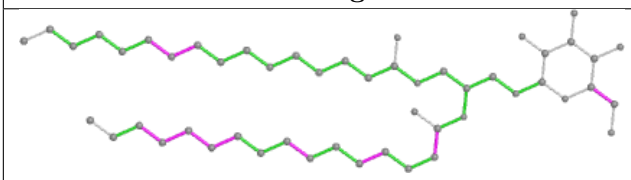
Ligand LMG D 412



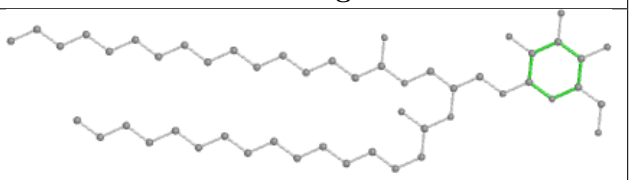
Bond lengths



Bond angles

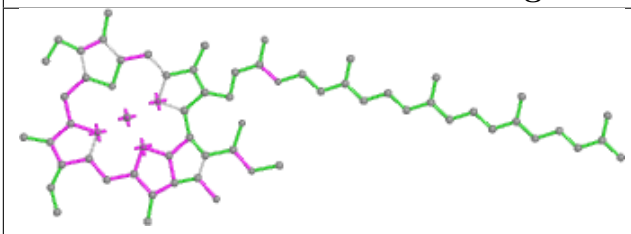


Torsions

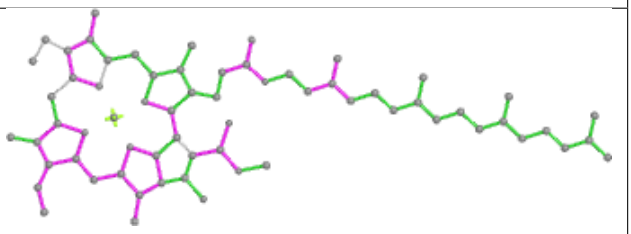


Rings

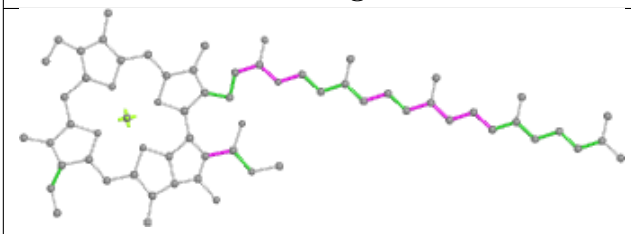
Ligand CLA B 602



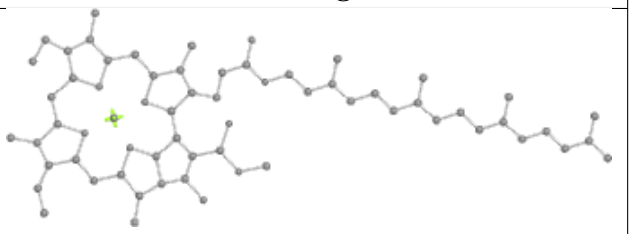
Bond lengths



Bond angles

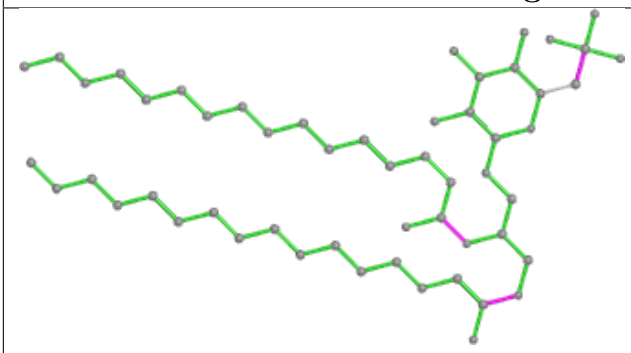


Torsions

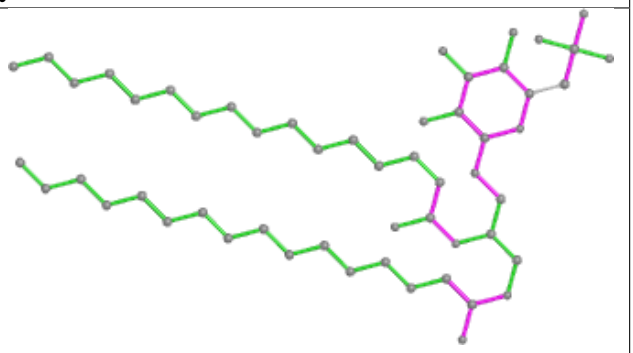


Rings

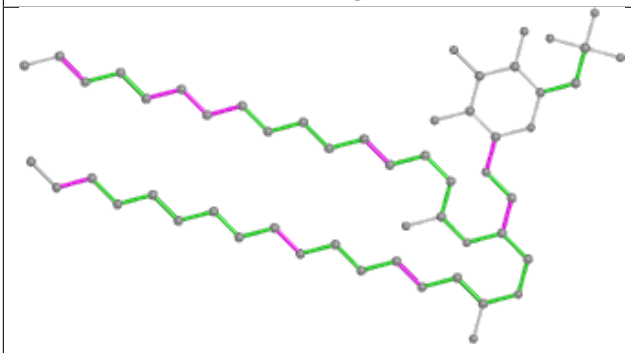
Ligand SQD A 413



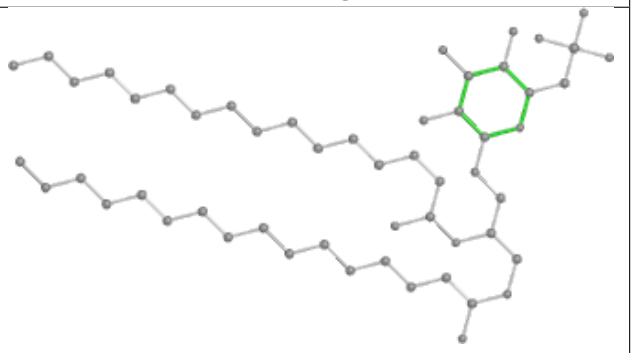
Bond lengths



Bond angles

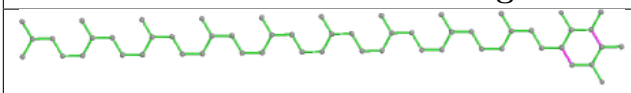


Torsions

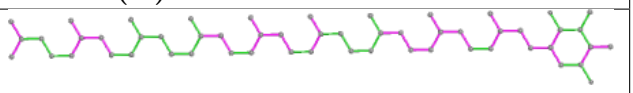


Rings

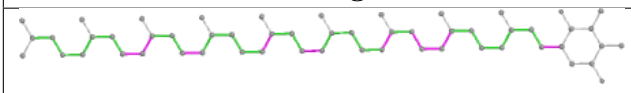
Ligand PL9 A 422 (B)



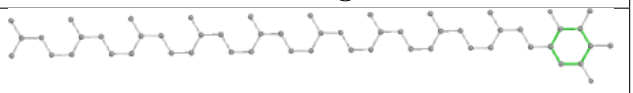
Bond lengths



Bond angles

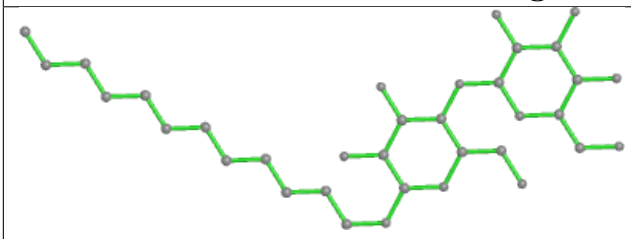


Torsions

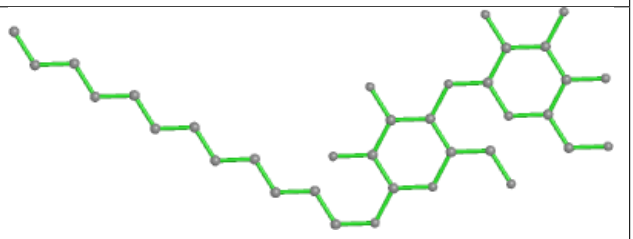


Rings

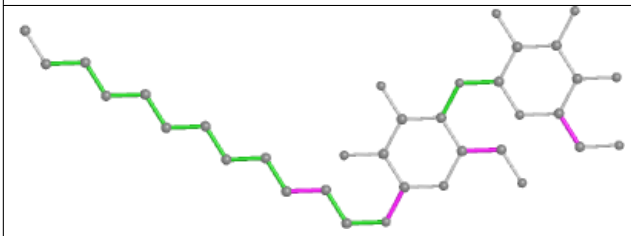
Ligand LMT f 104



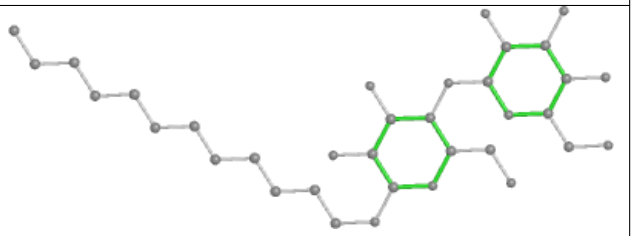
Bond lengths



Bond angles

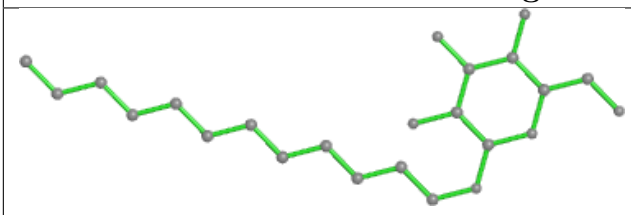


Torsions

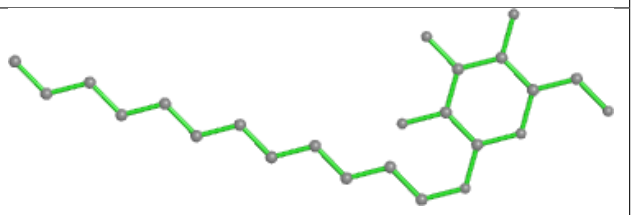


Rings

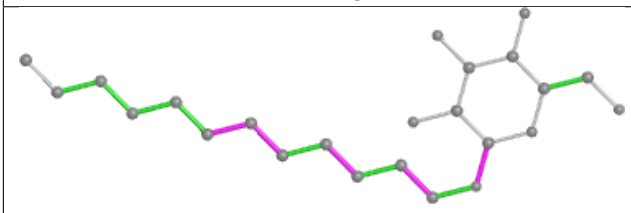
Ligand LMT E 104



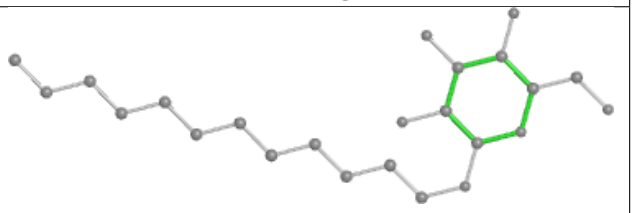
Bond lengths



Bond angles

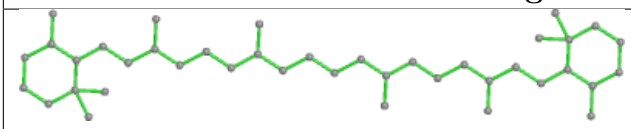


Torsions

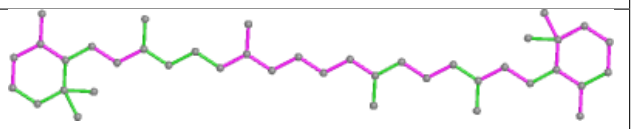


Rings

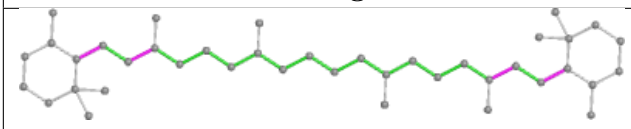
Ligand BCR d 406



Bond lengths



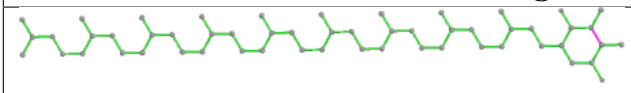
Bond angles



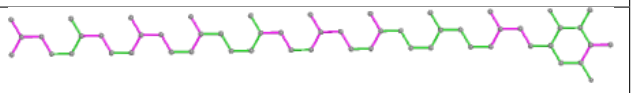
Torsions

Rings

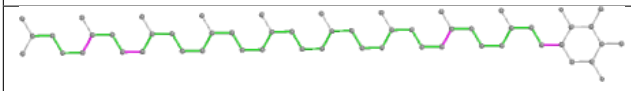
Ligand PL9 d 407



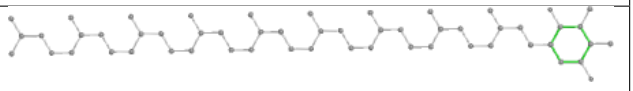
Bond lengths



Bond angles

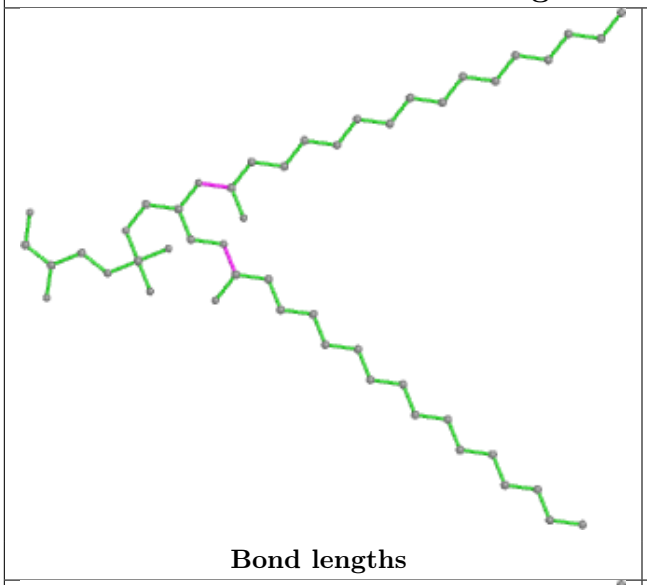


Torsions

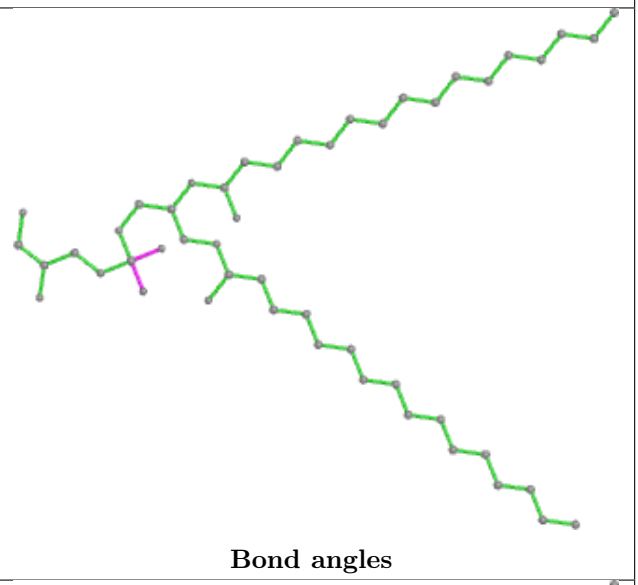


Rings

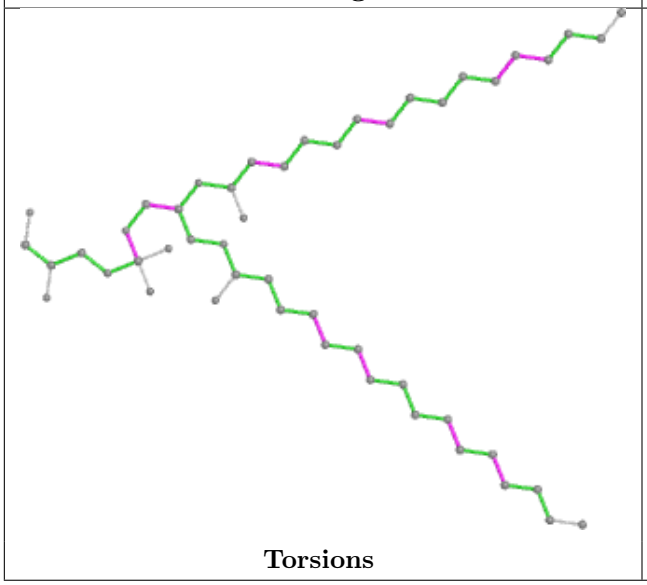
Ligand LHG l 302



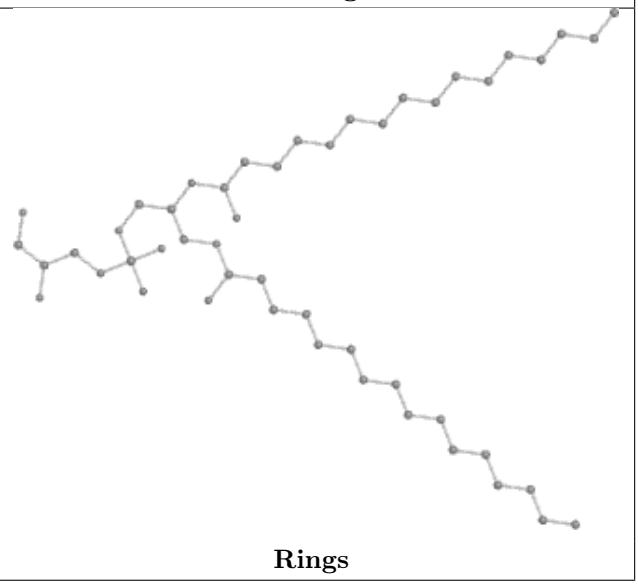
Bond lengths



Bond angles

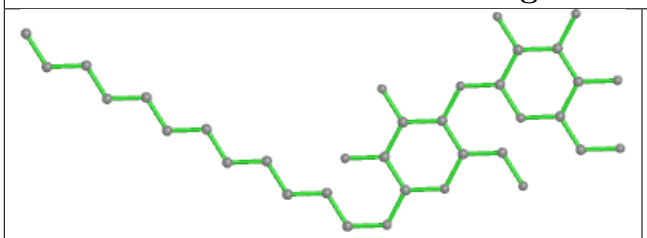


Torsions

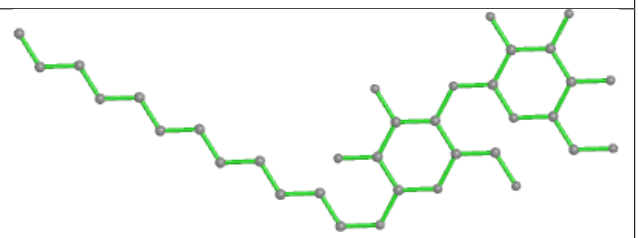


Rings

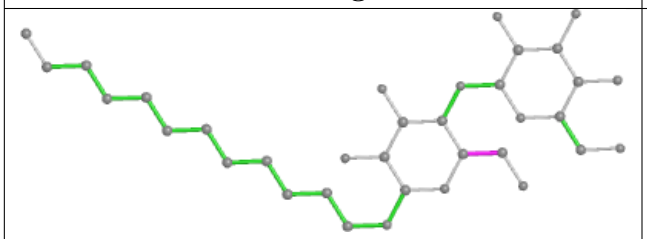
Ligand LMT m 103



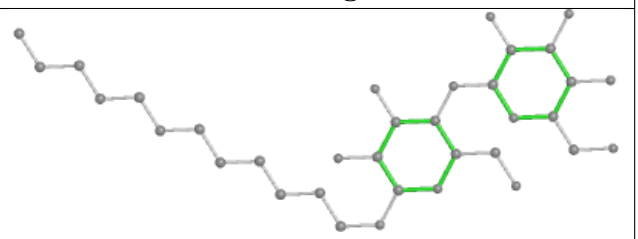
Bond lengths



Bond angles

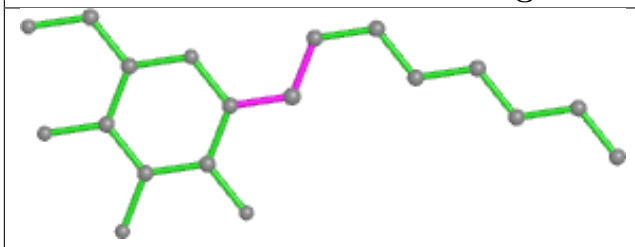


Torsions

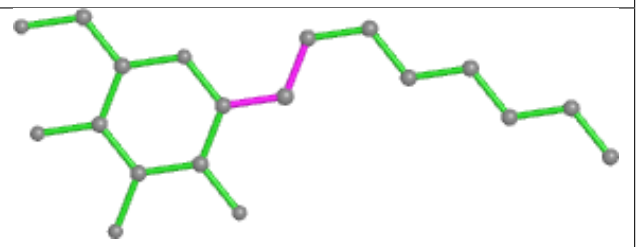


Rings

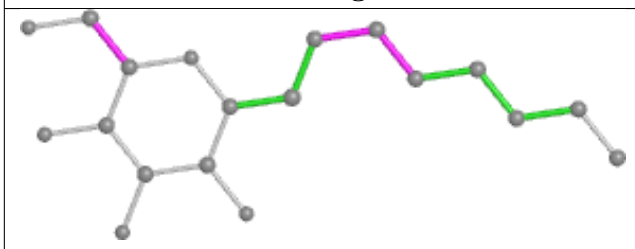
Ligand HTG h 1202



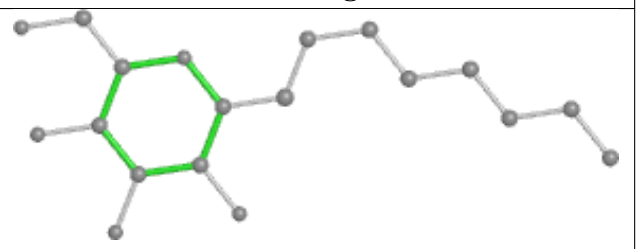
Bond lengths



Bond angles

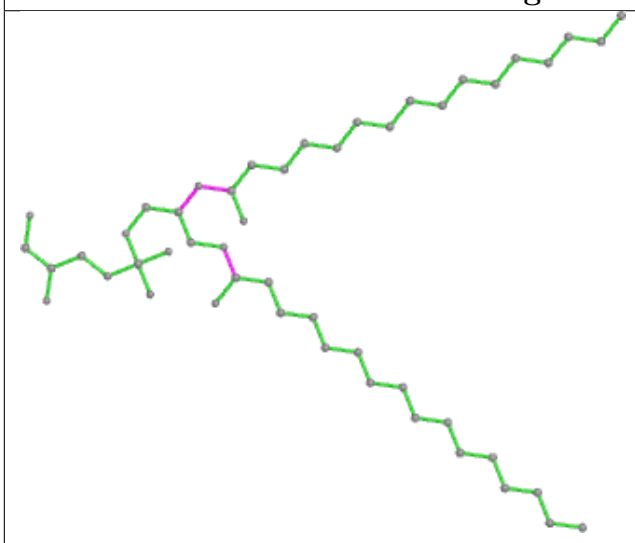


Torsions

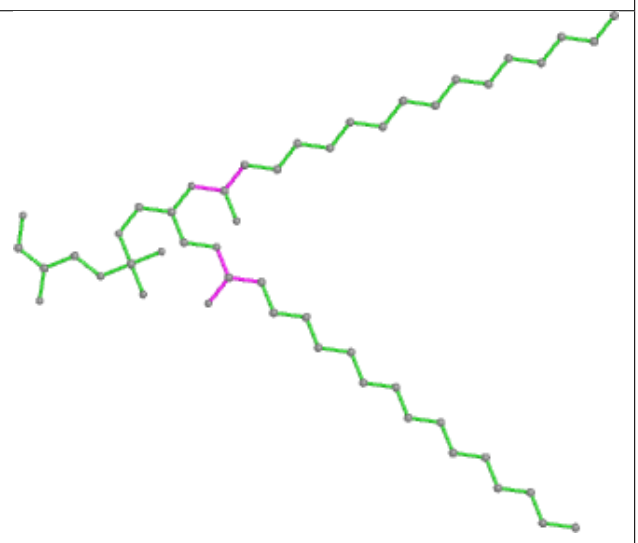


Rings

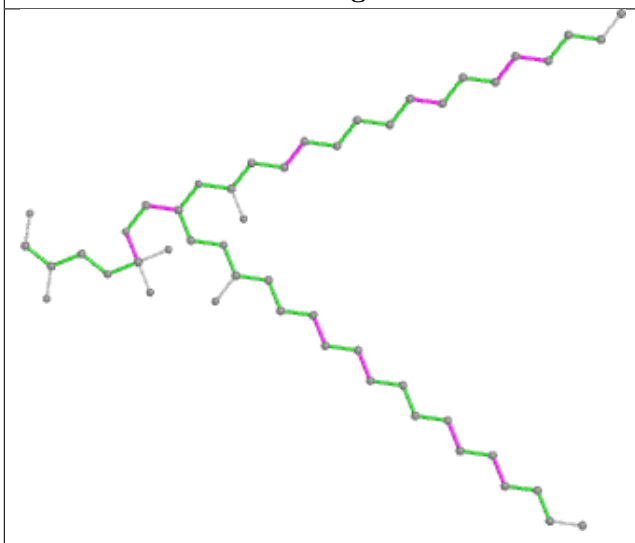
Ligand LHG B 640



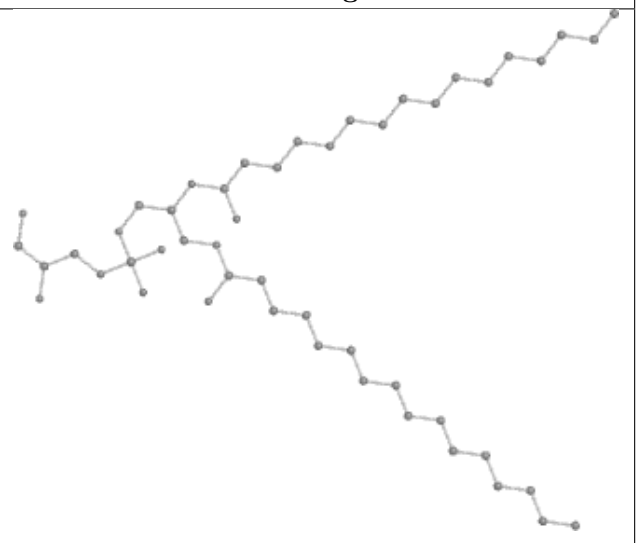
Bond lengths



Bond angles

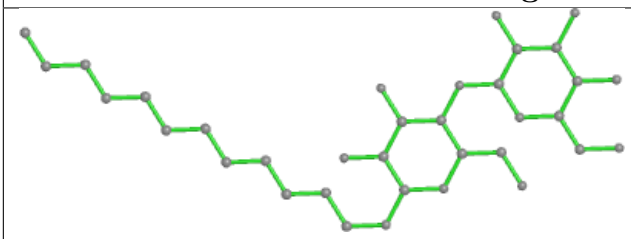


Torsions

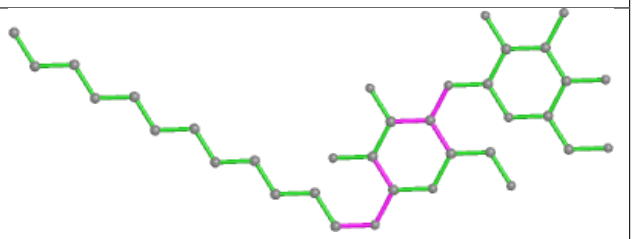


Rings

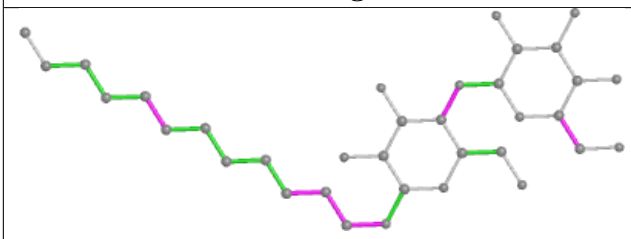
Ligand LMT B 622



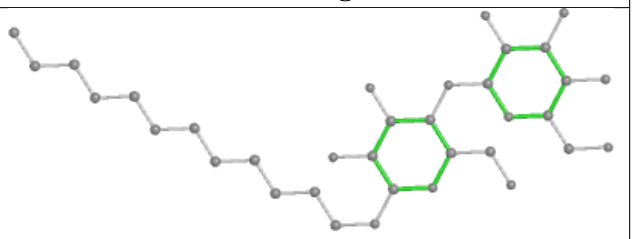
Bond lengths



Bond angles

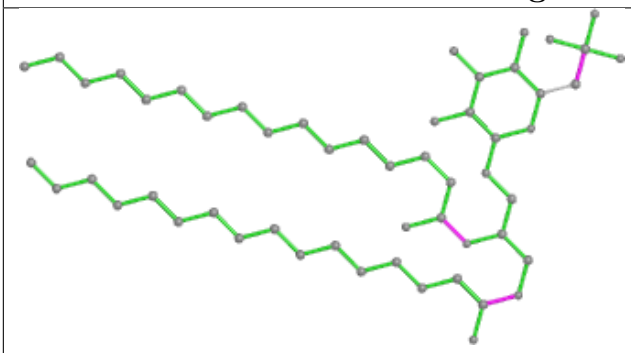


Torsions

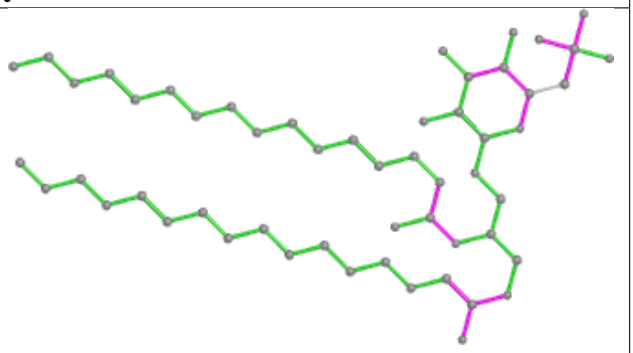


Rings

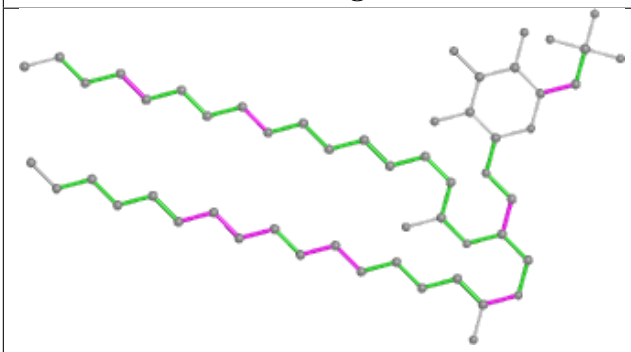
Ligand SQD a 401



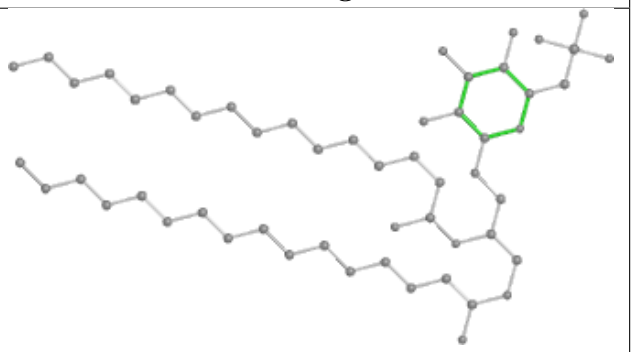
Bond lengths



Bond angles

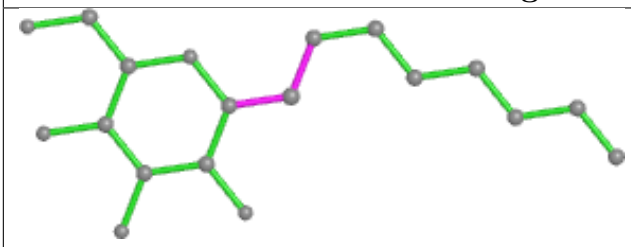


Torsions

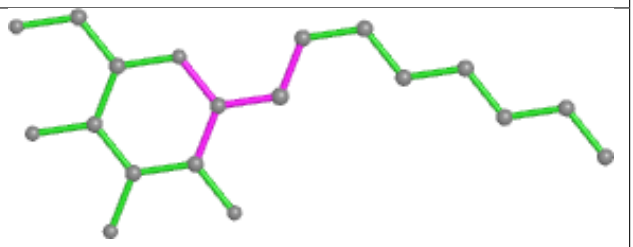


Rings

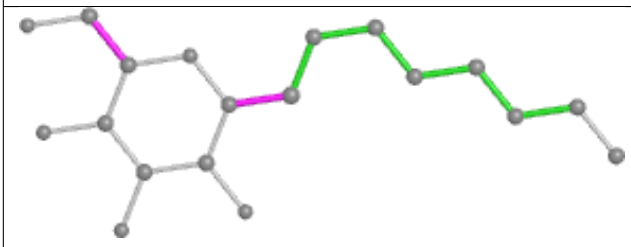
Ligand HTG B 624



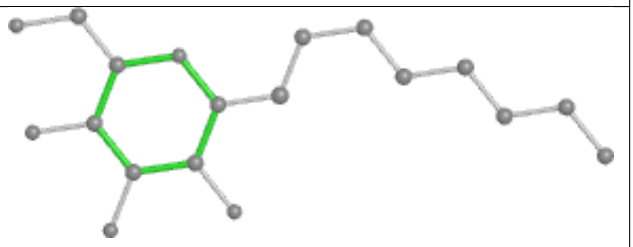
Bond lengths



Bond angles

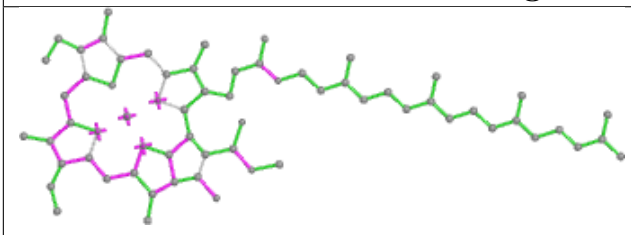


Torsions

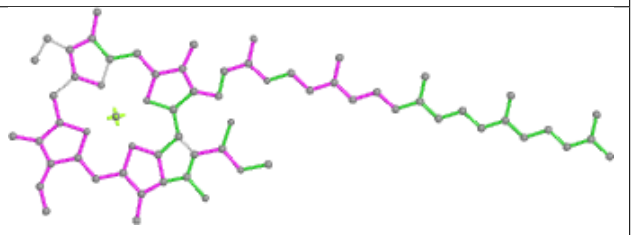


Rings

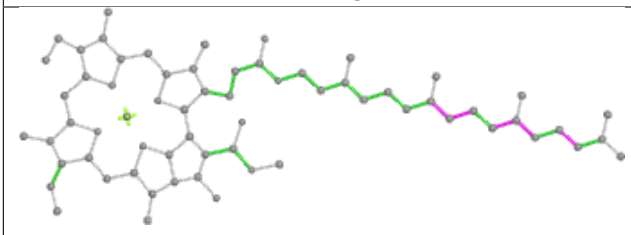
Ligand CLA A 409



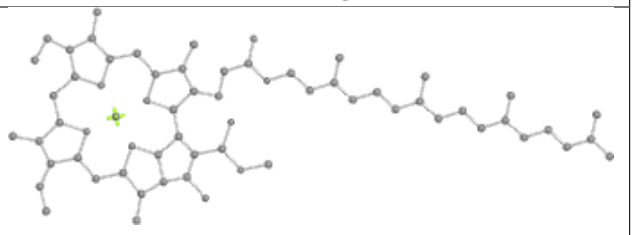
Bond lengths



Bond angles

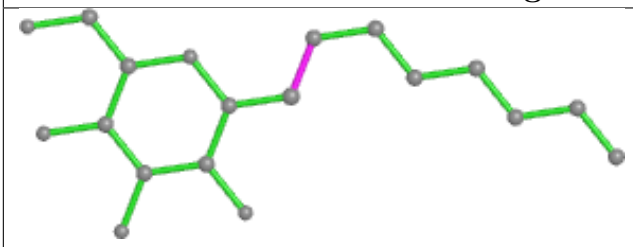


Torsions

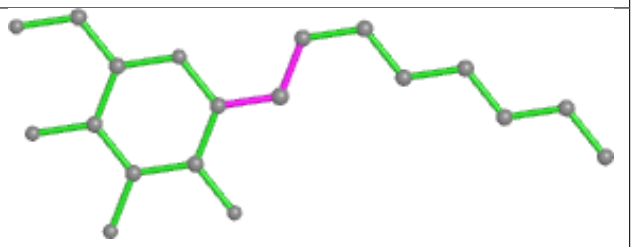


Rings

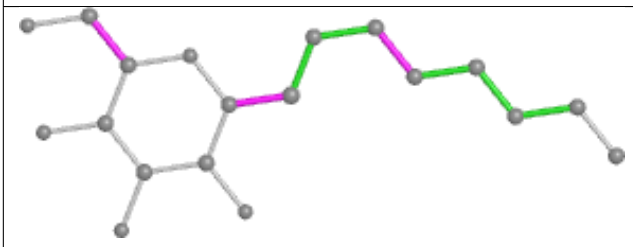
Ligand HTG b 626



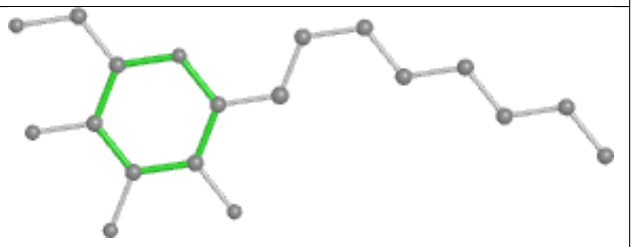
Bond lengths



Bond angles

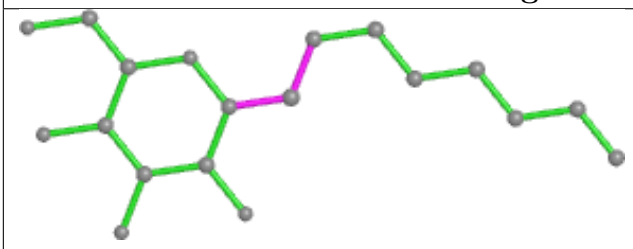


Torsions

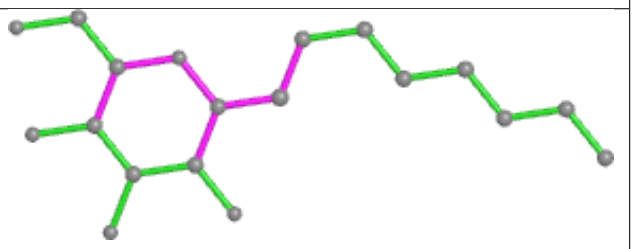


Rings

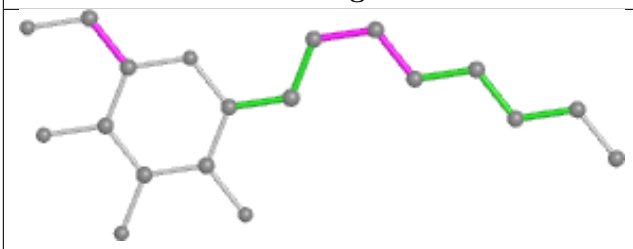
Ligand HTG C 523



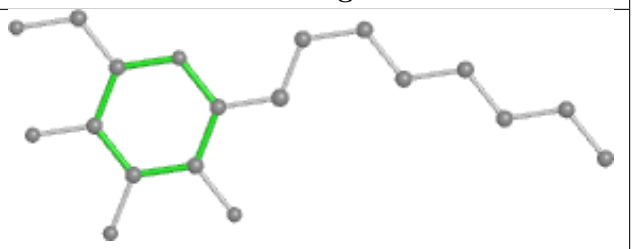
Bond lengths



Bond angles

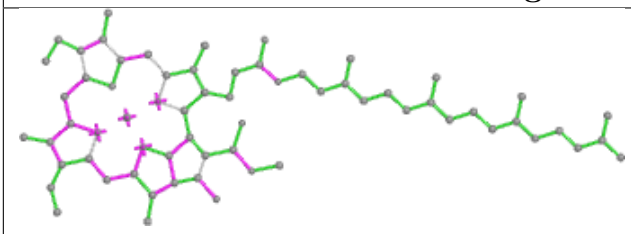


Torsions

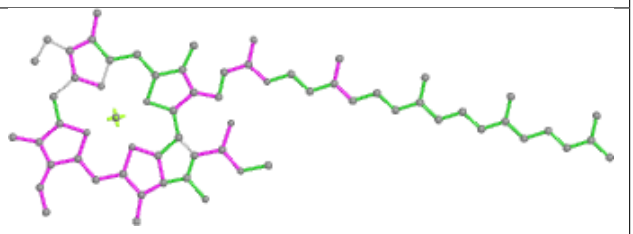


Rings

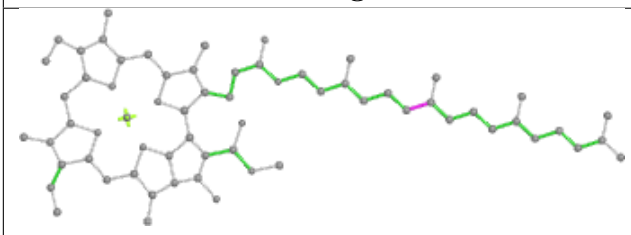
Ligand CLA B 604



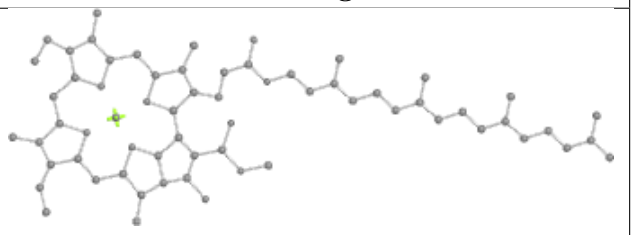
Bond lengths



Bond angles

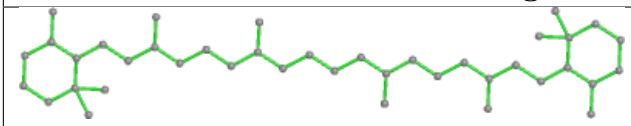


Torsions

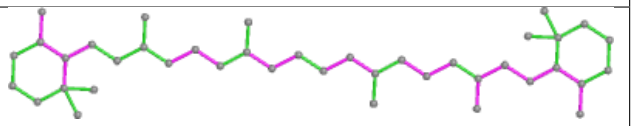


Rings

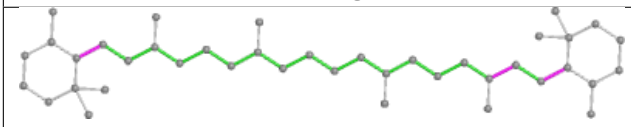
Ligand BCR Y 302



Bond lengths



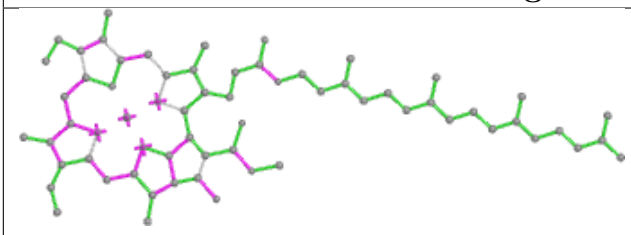
Bond angles



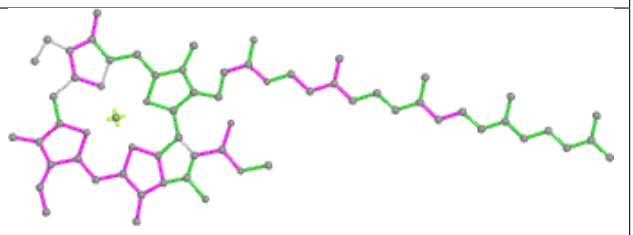
Torsions

Rings

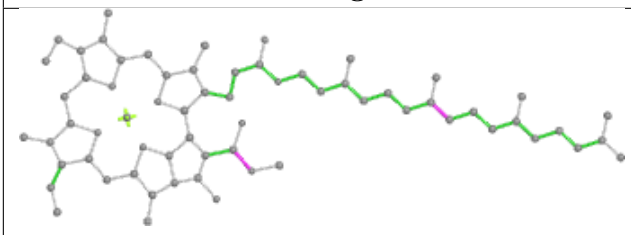
Ligand CLA C 514



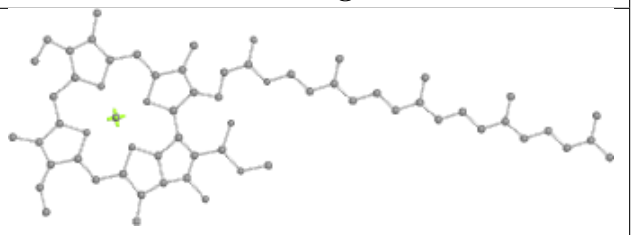
Bond lengths



Bond angles

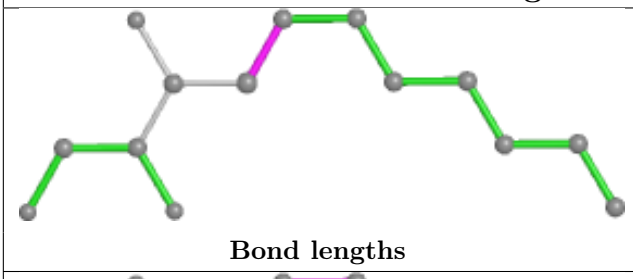


Torsions

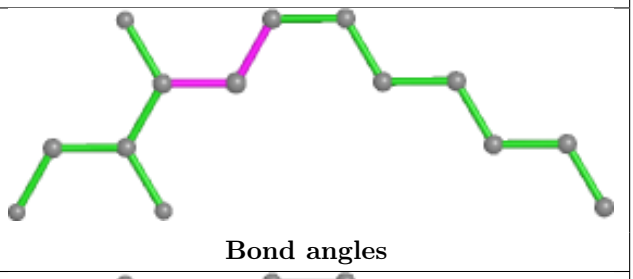


Rings

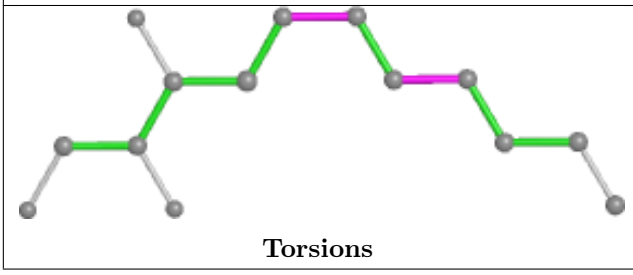
Ligand HTG u 201



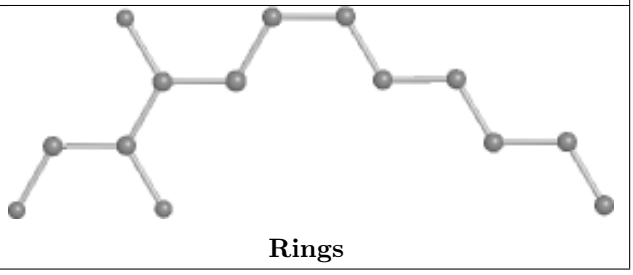
Bond lengths



Bond angles

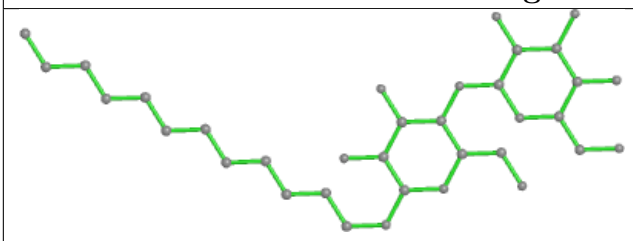


Torsions

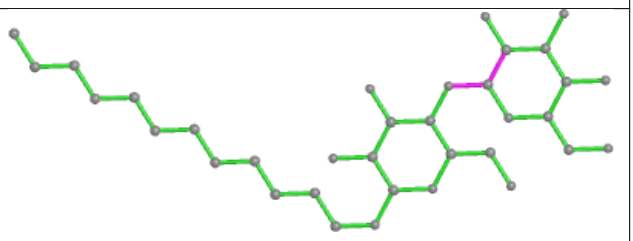


Rings

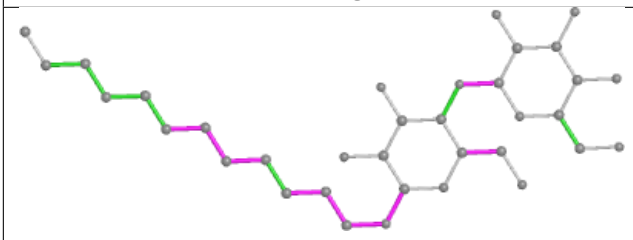
Ligand LMT Z 101



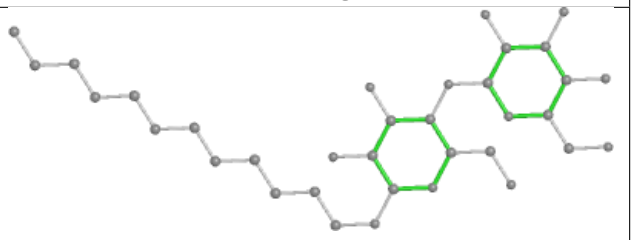
Bond lengths



Bond angles

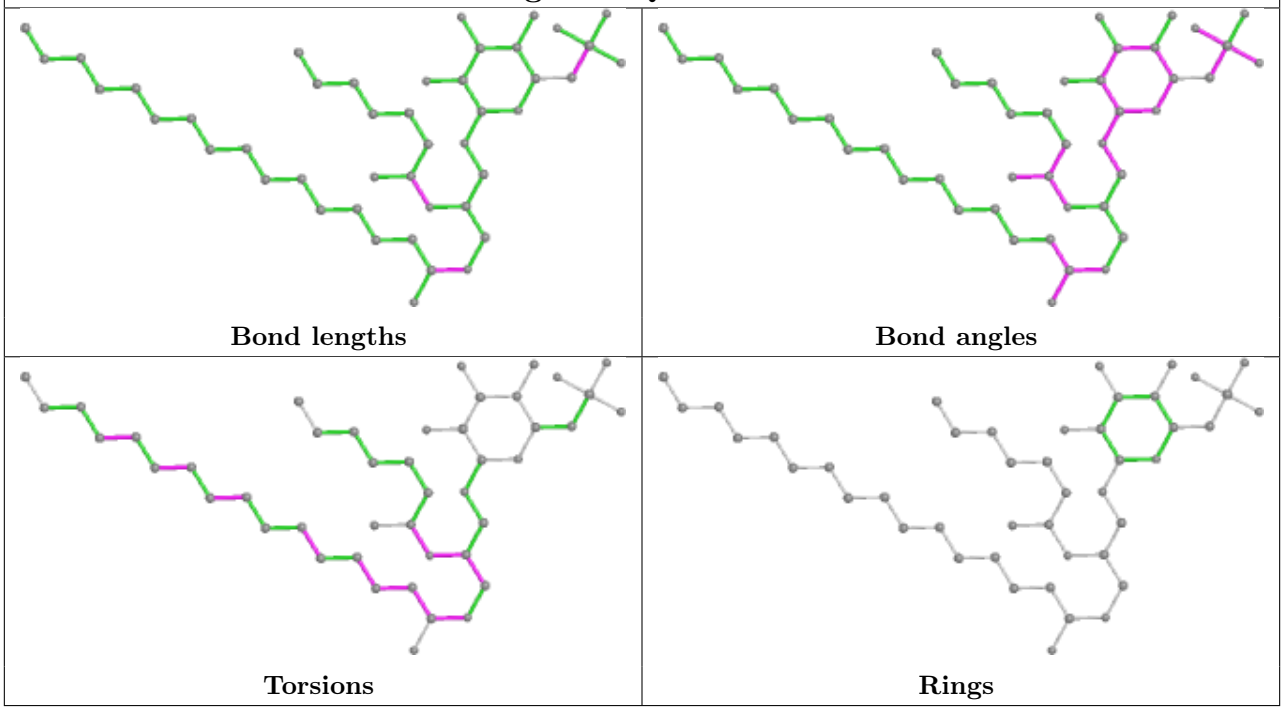


Torsions

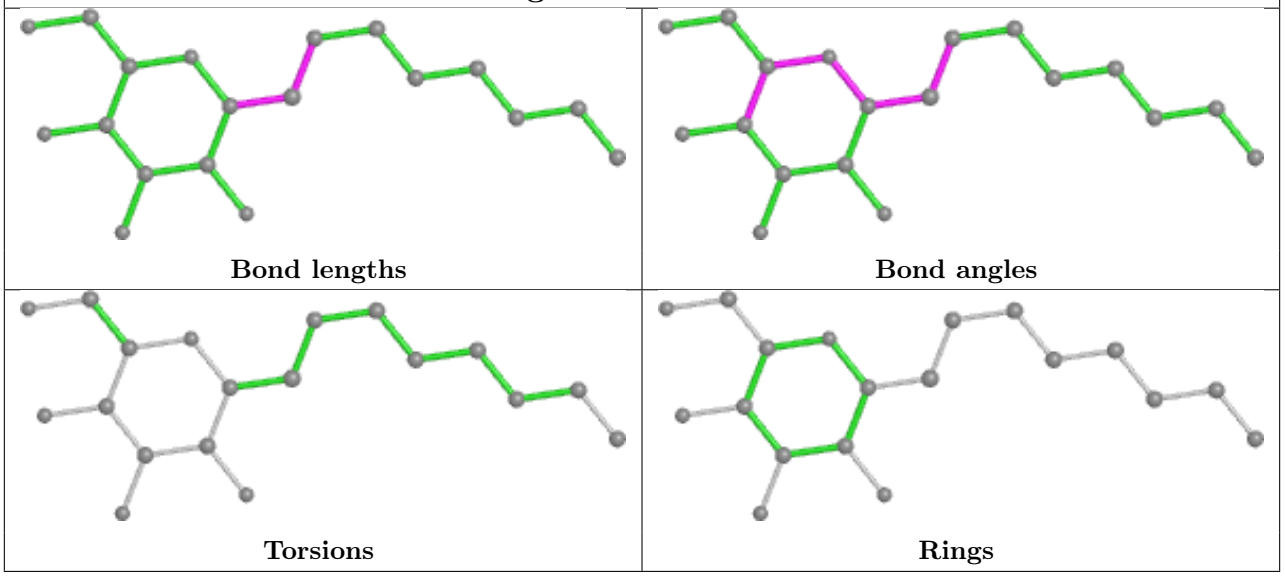


Rings

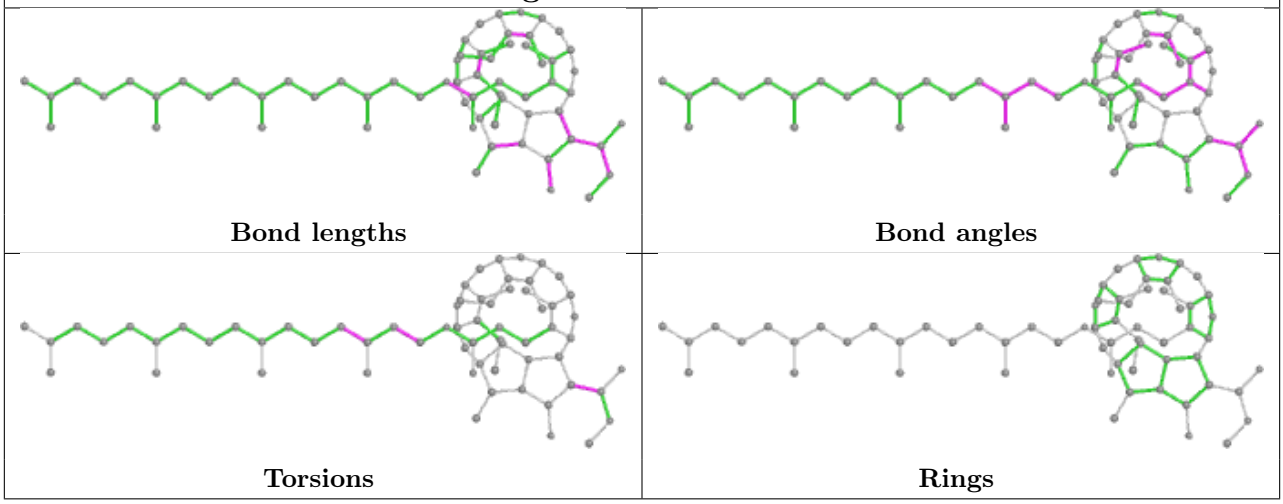
Ligand SQD D 408



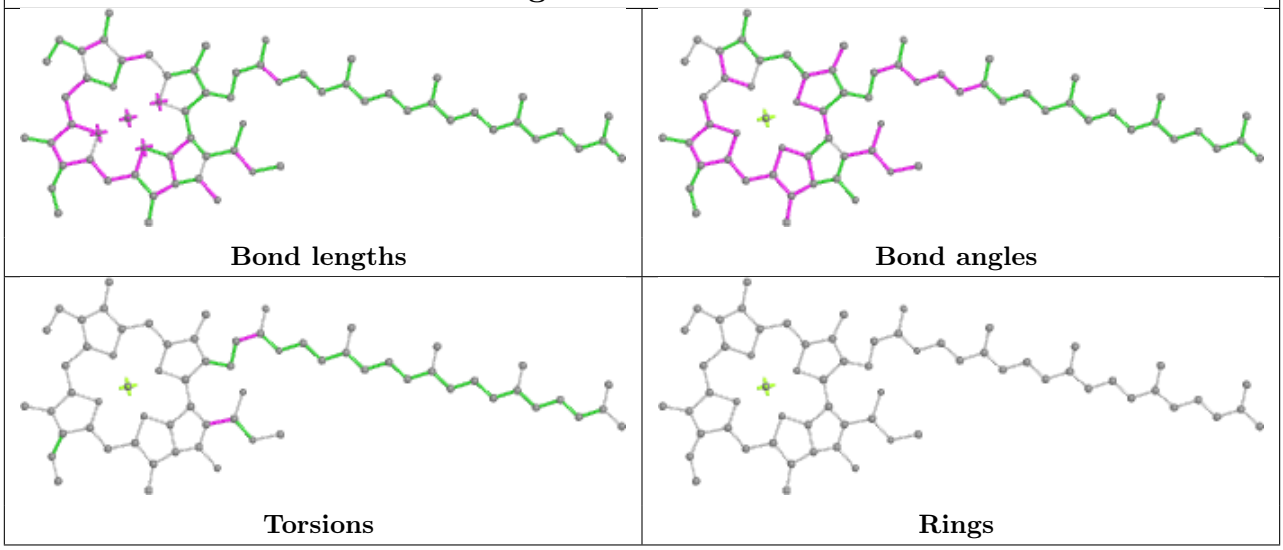
Ligand HTG c 525



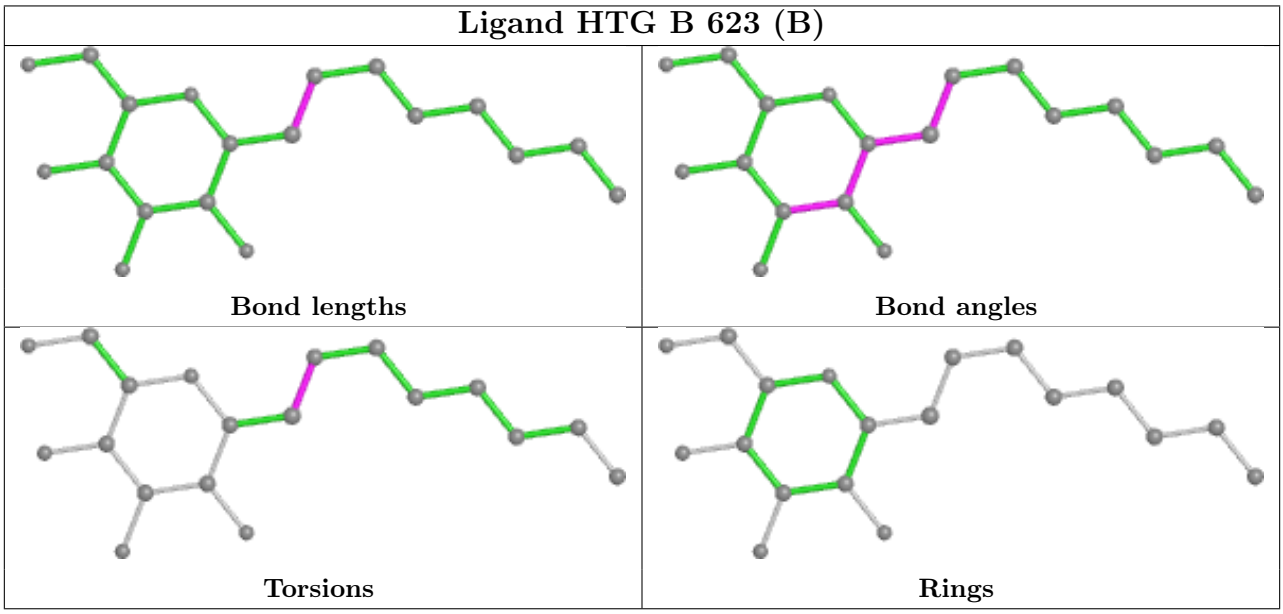
Ligand PHO A 408



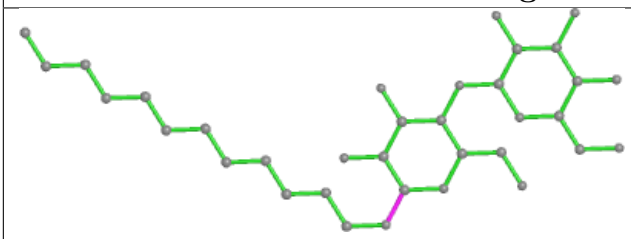
Ligand CLA b 616



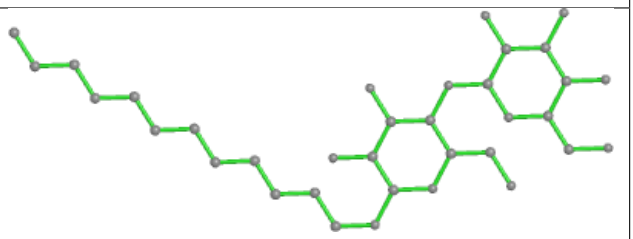
Ligand HTG B 623 (B)



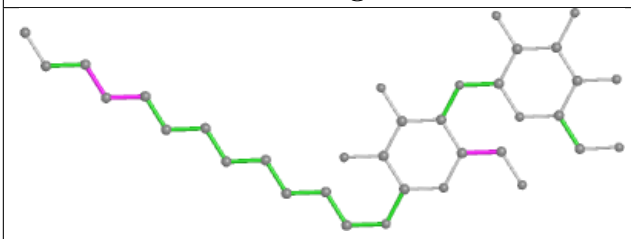
Ligand LMT m 101



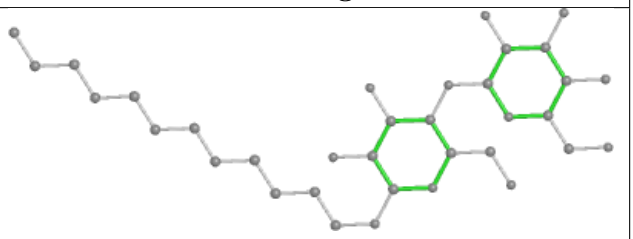
Bond lengths



Bond angles

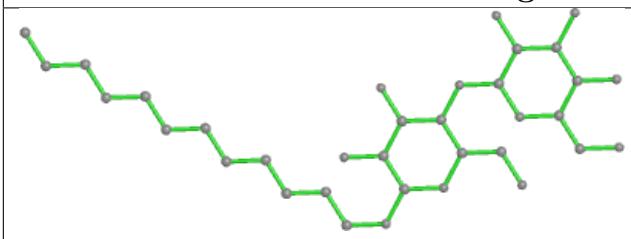


Torsions

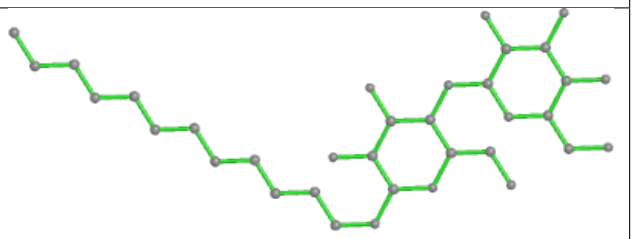


Rings

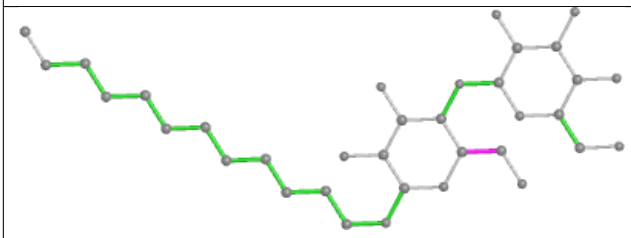
Ligand LMT M 101



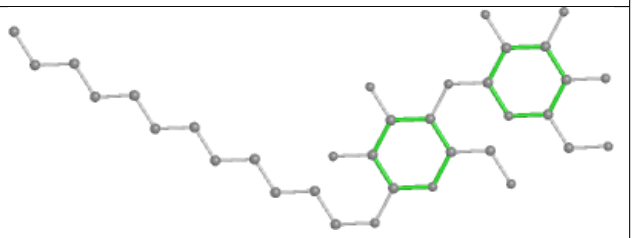
Bond lengths



Bond angles

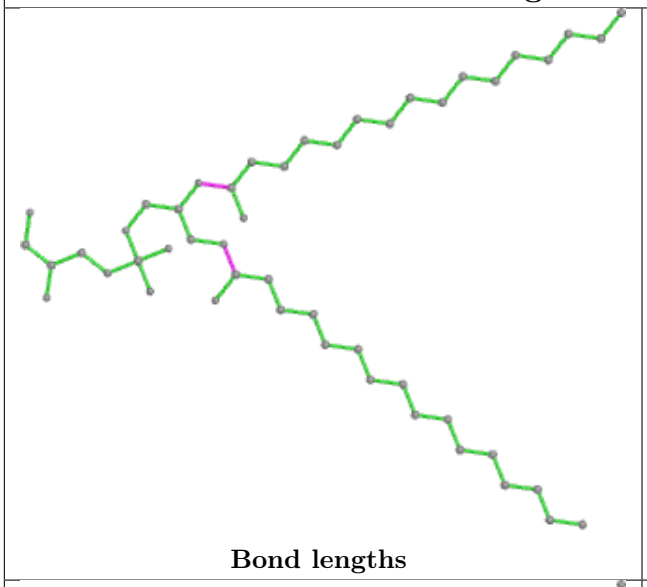


Torsions

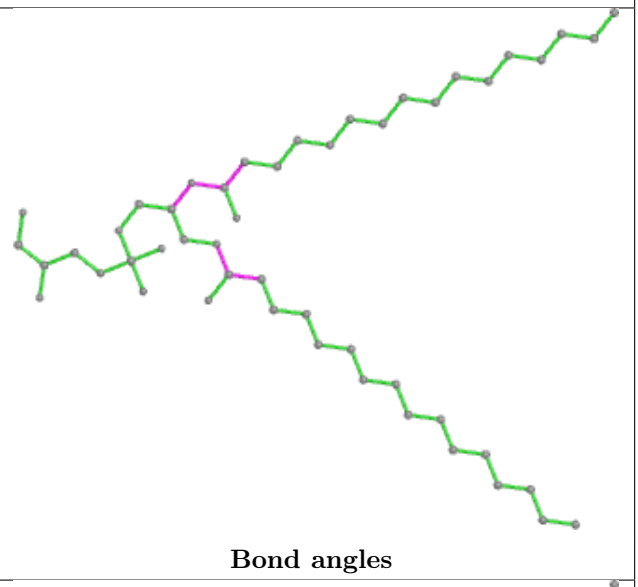


Rings

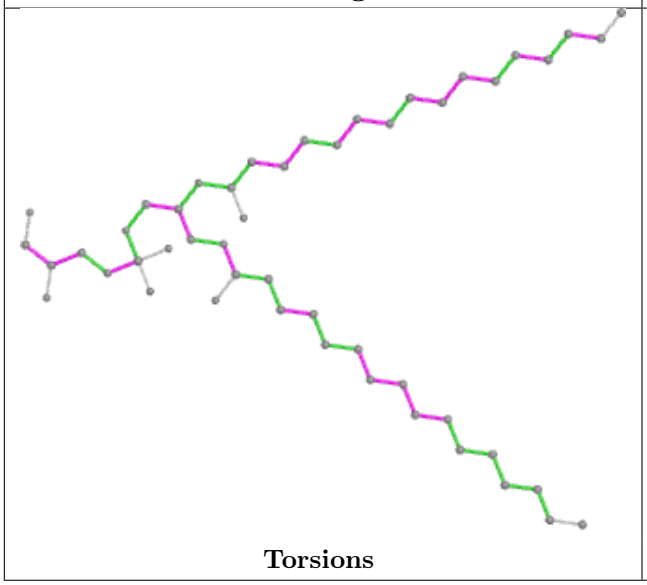
Ligand LHG E 101



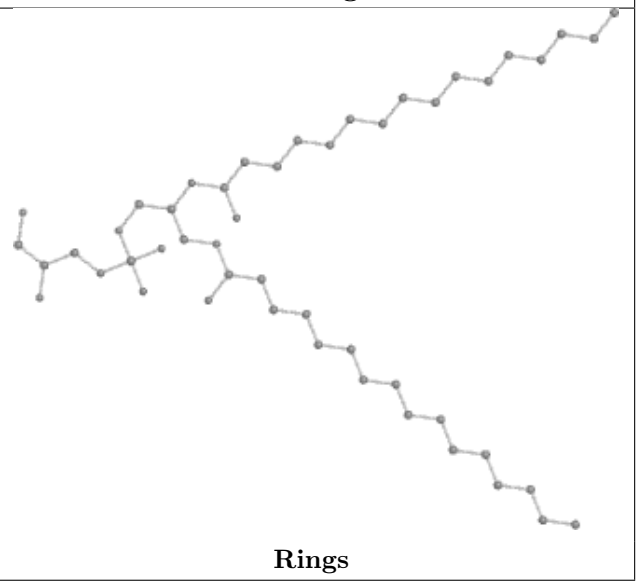
Bond lengths



Bond angles

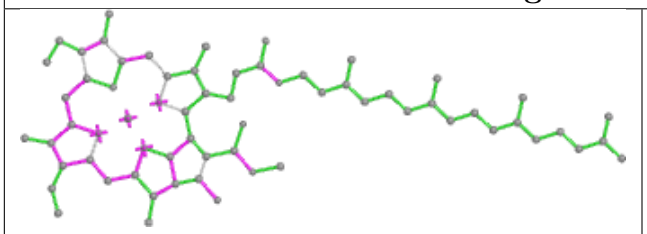


Torsions

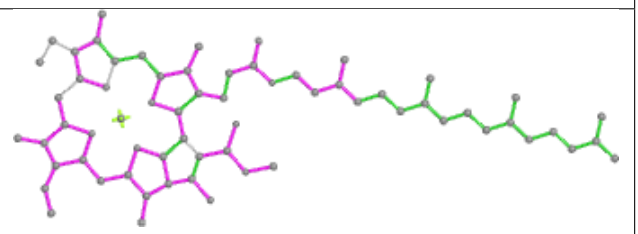


Rings

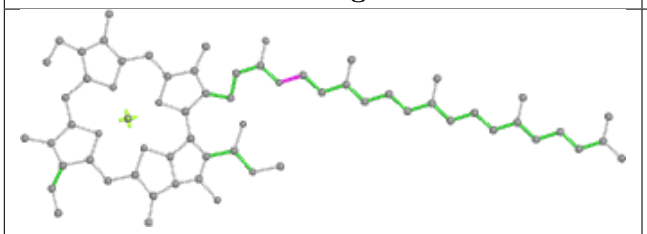
Ligand CLA D 403



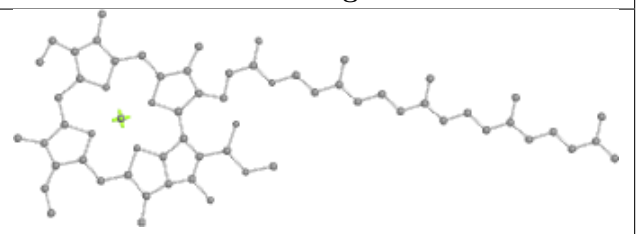
Bond lengths



Bond angles

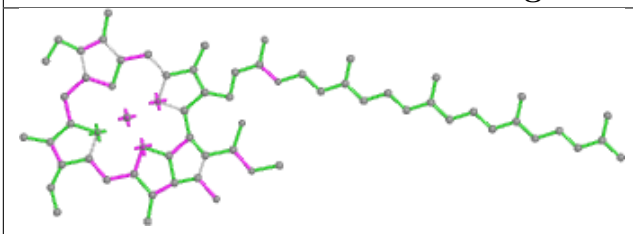


Torsions

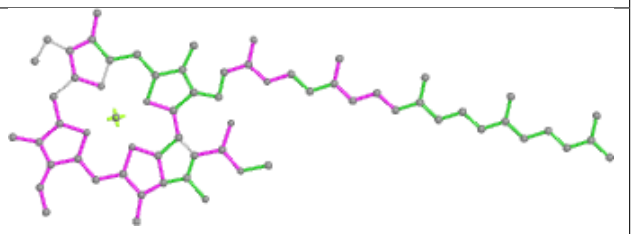


Rings

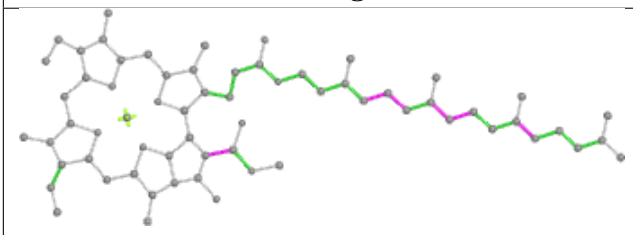
Ligand CLA B 615



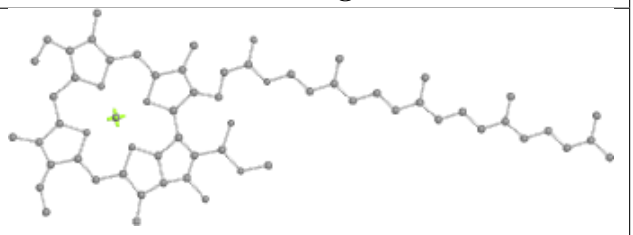
Bond lengths



Bond angles

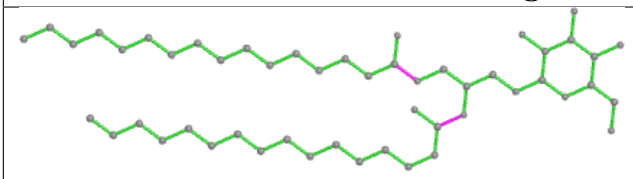


Torsions

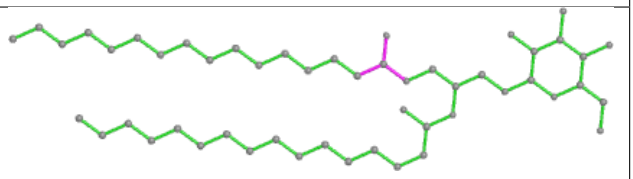


Rings

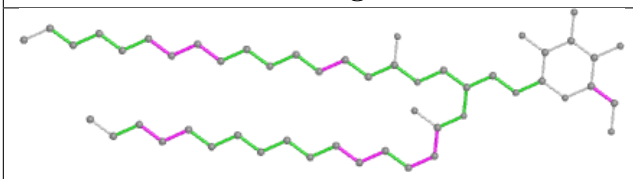
Ligand LMG d 411



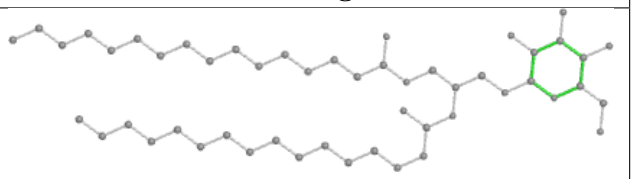
Bond lengths



Bond angles

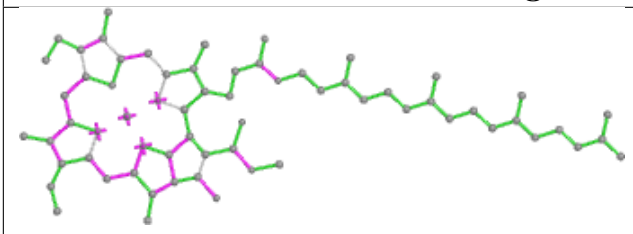


Torsions

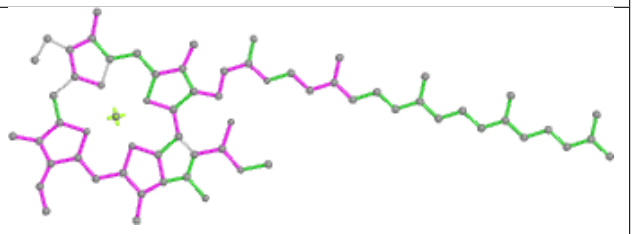


Rings

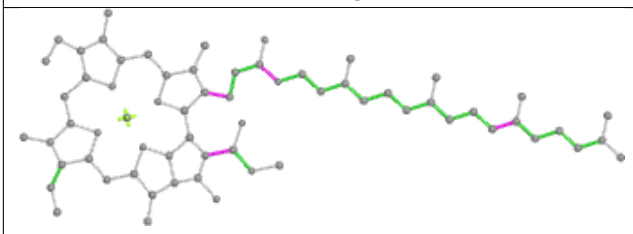
Ligand CLA C 513



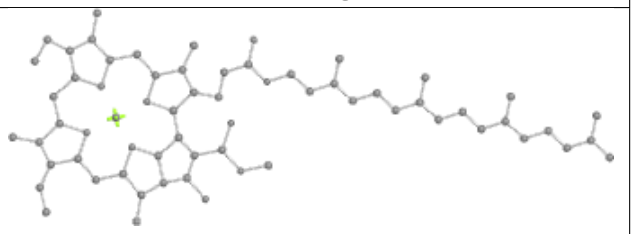
Bond lengths



Bond angles

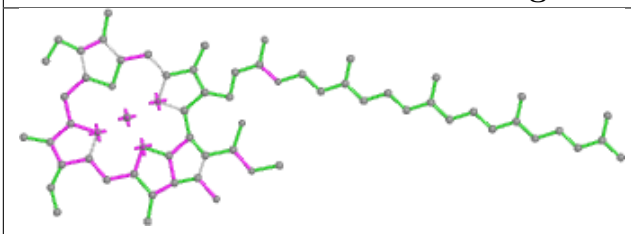


Torsions

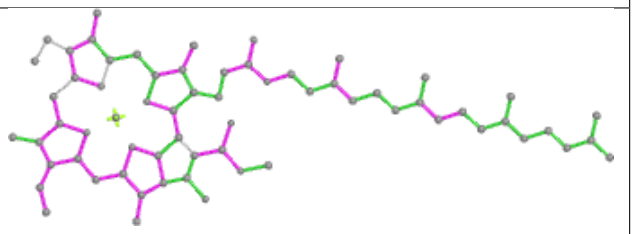


Rings

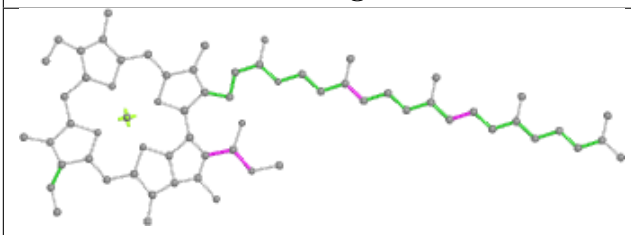
Ligand CLA c 512



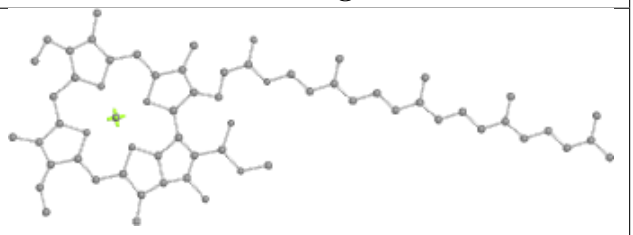
Bond lengths



Bond angles

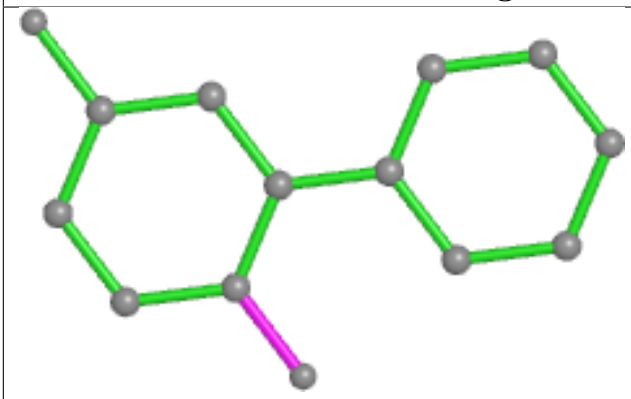


Torsions

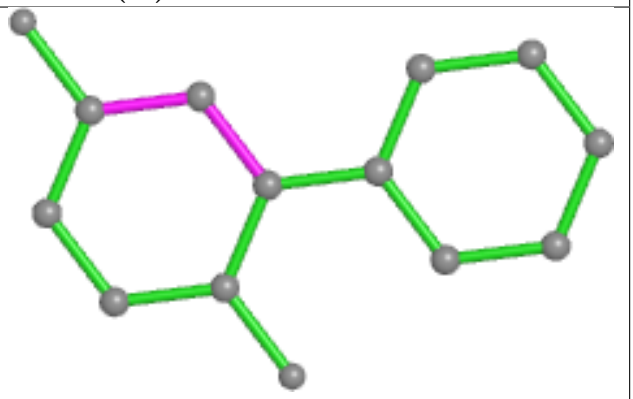


Rings

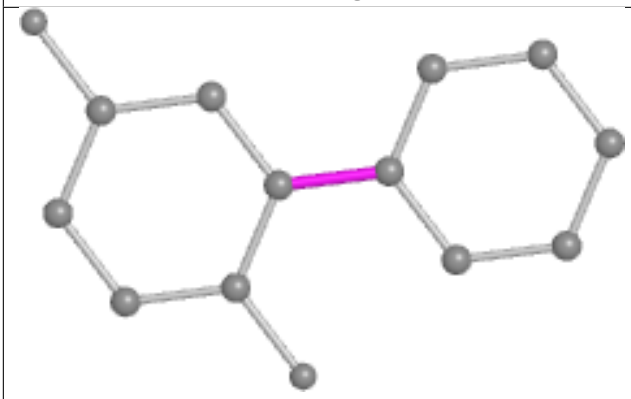
Ligand K3C a 424 (A)



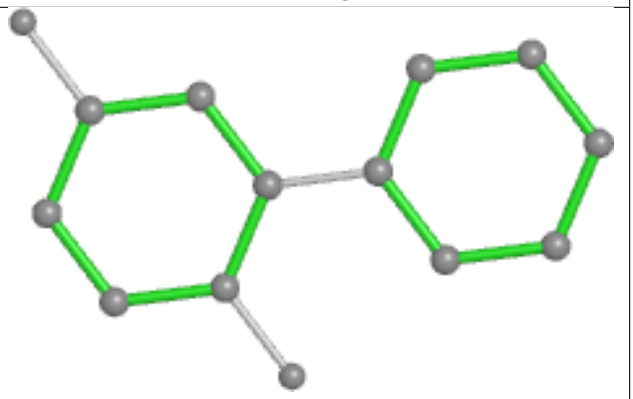
Bond lengths



Bond angles

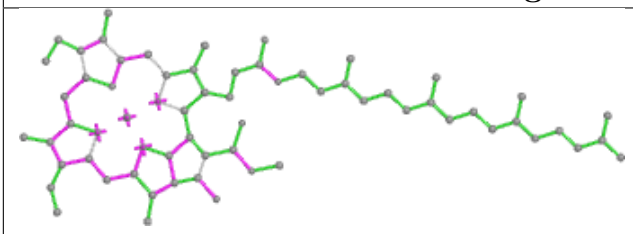


Torsions

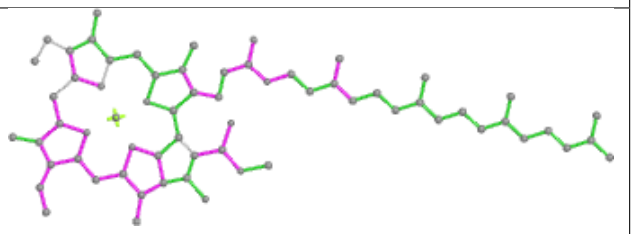


Rings

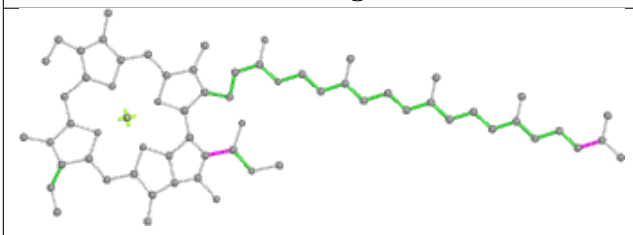
Ligand CLA B 608



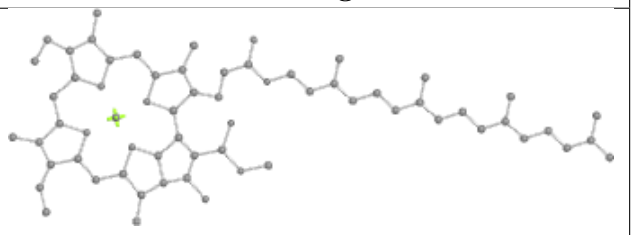
Bond lengths



Bond angles

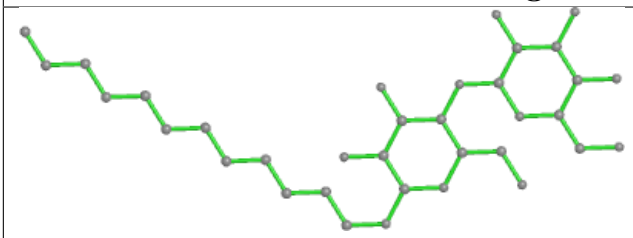


Torsions

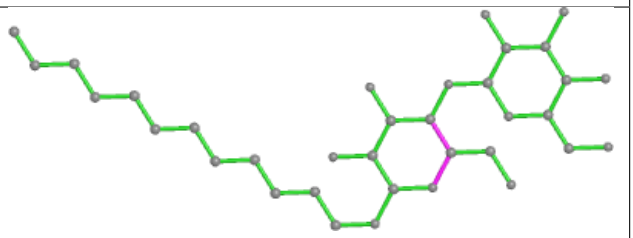


Rings

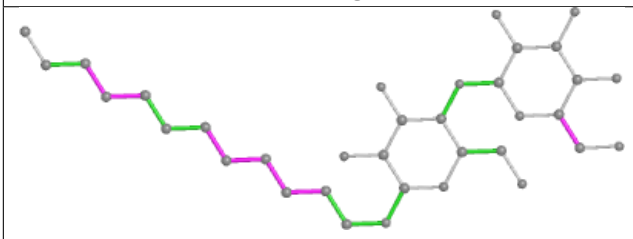
Ligand LMT a 402



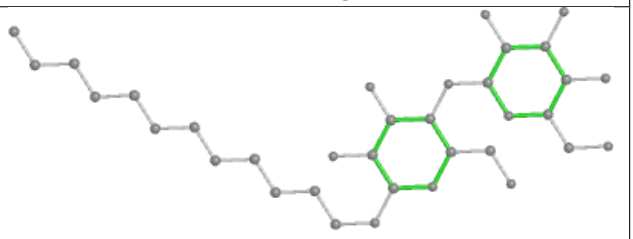
Bond lengths



Bond angles

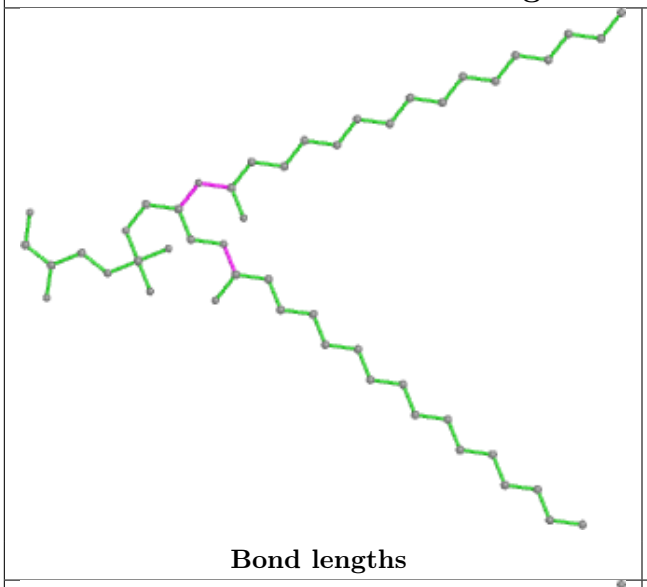


Torsions

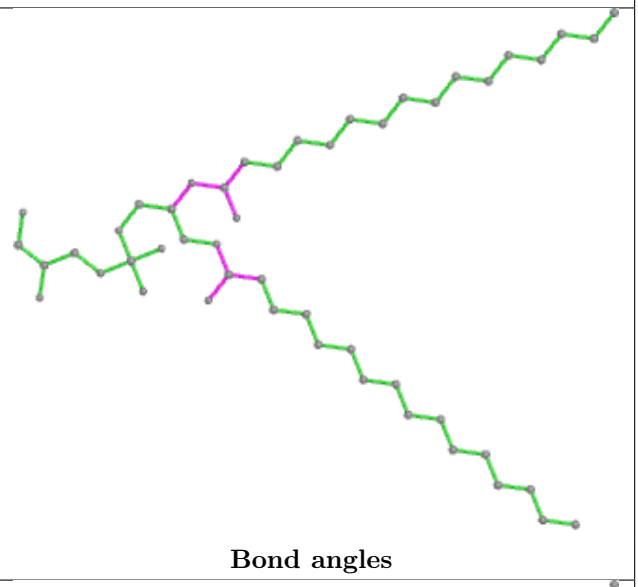


Rings

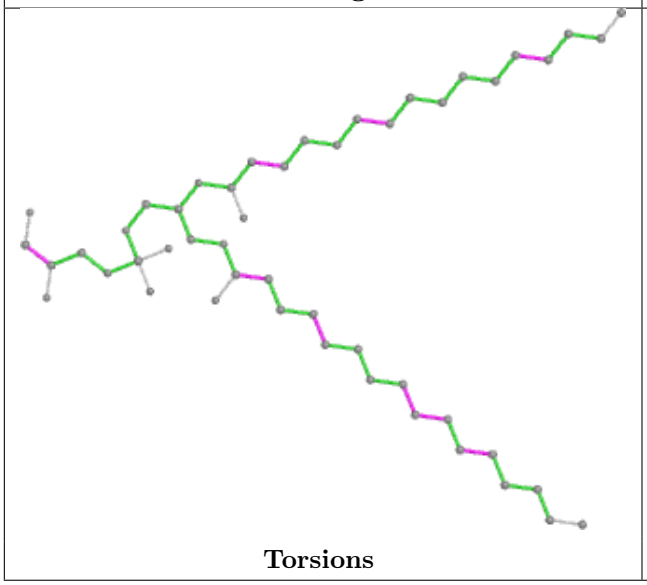
Ligand LHG D 409



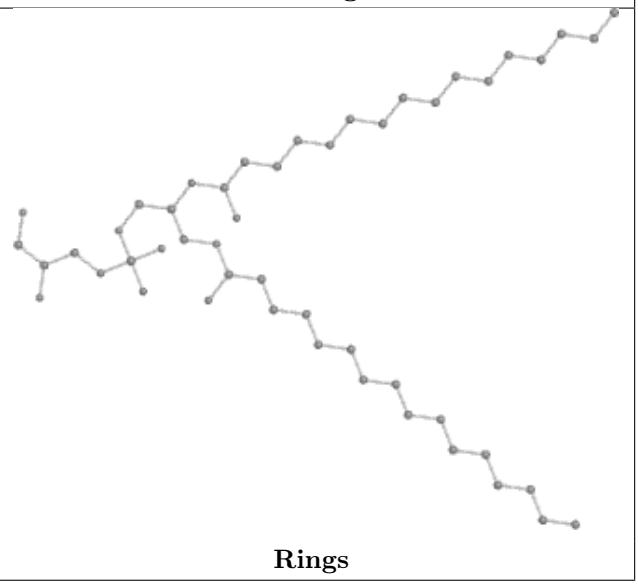
Bond lengths



Bond angles

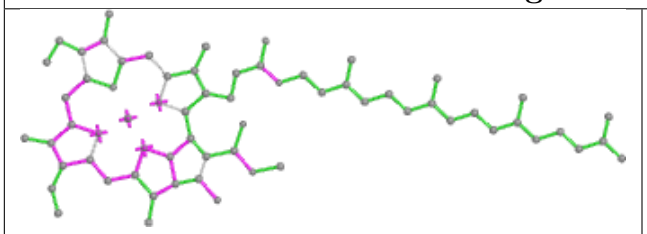


Torsions

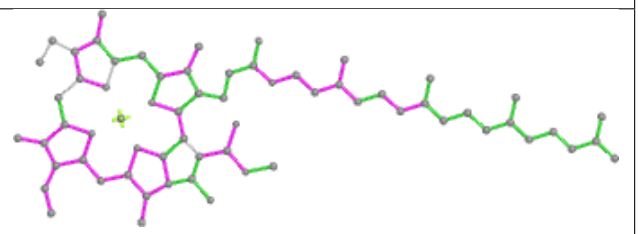


Rings

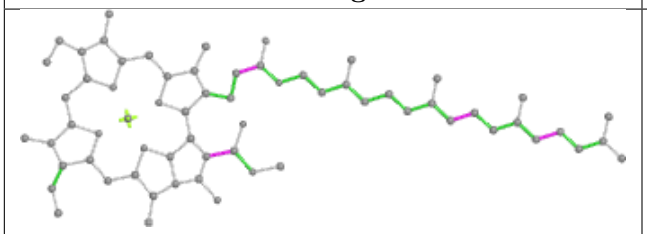
Ligand CLA C 511



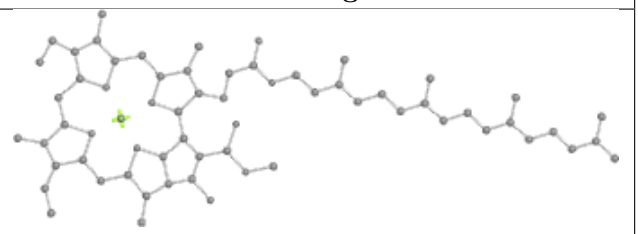
Bond lengths



Bond angles

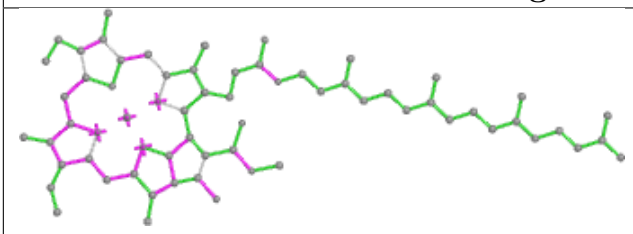


Torsions

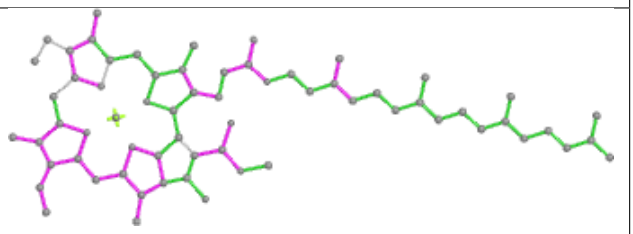


Rings

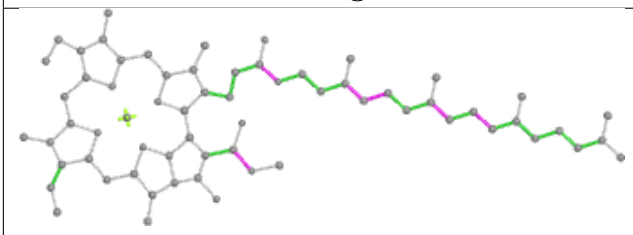
Ligand CLA c 515



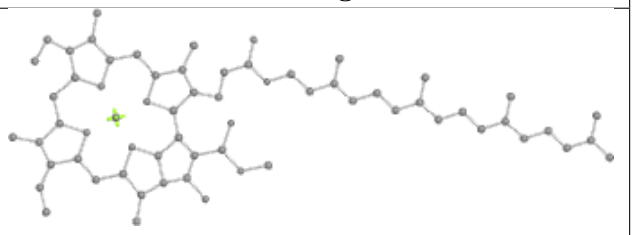
Bond lengths



Bond angles

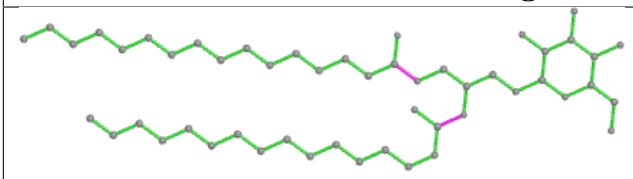


Torsions

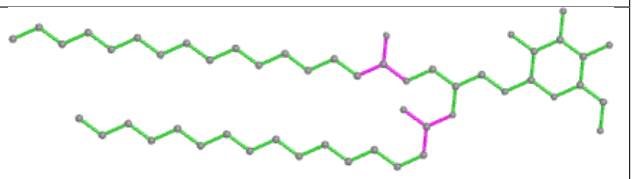


Rings

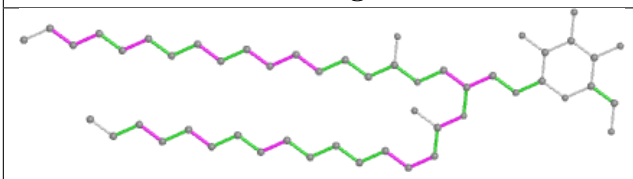
Ligand LMG C 520



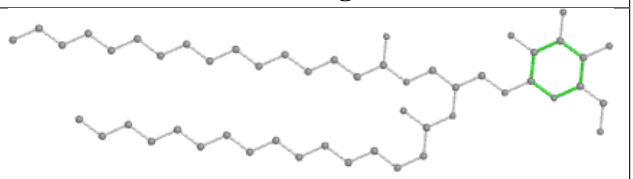
Bond lengths



Bond angles

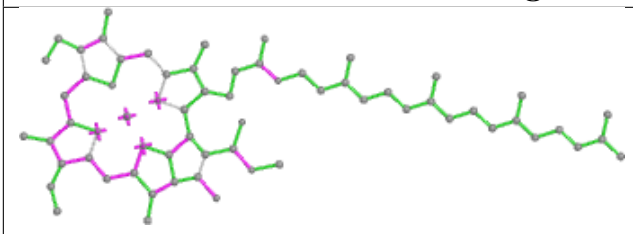


Torsions

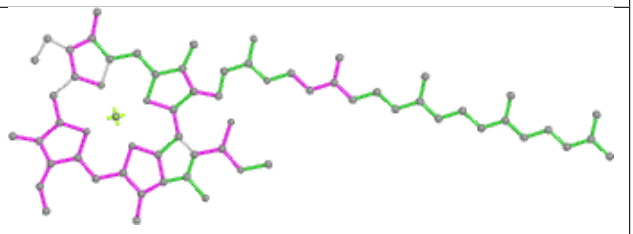


Rings

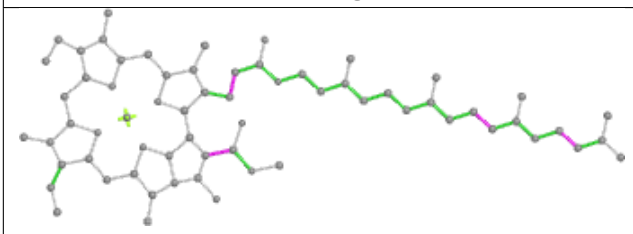
Ligand CLA B 607



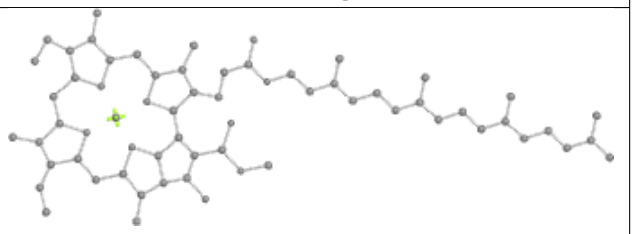
Bond lengths



Bond angles

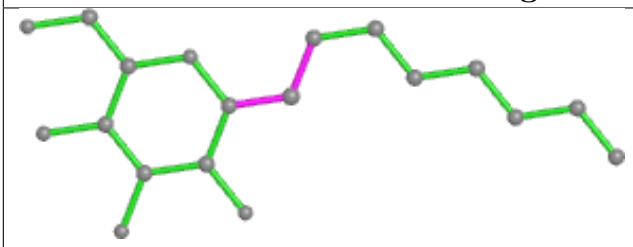


Torsions

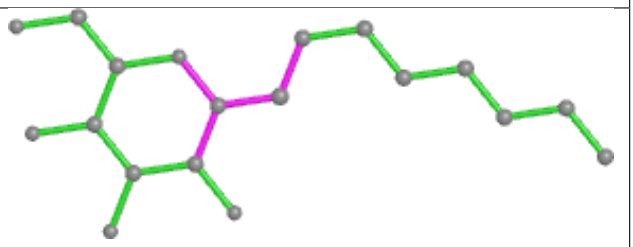


Rings

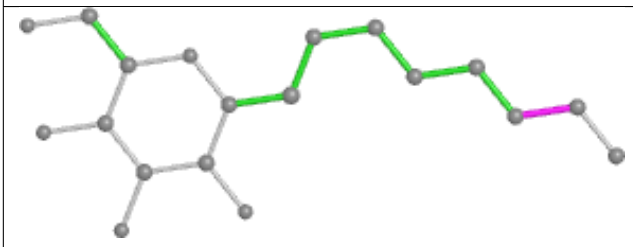
Ligand HTG D 413



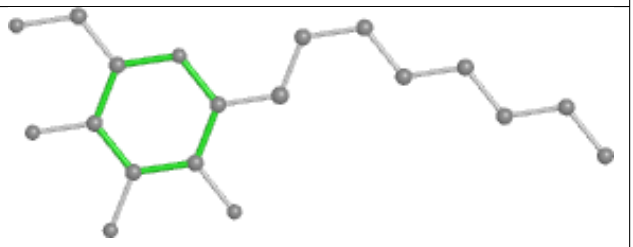
Bond lengths



Bond angles

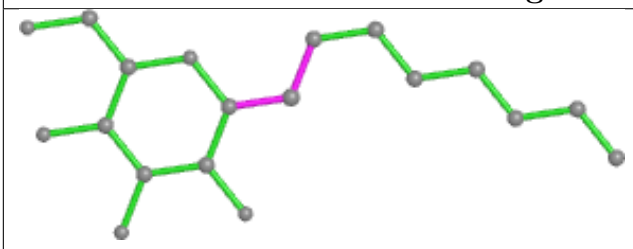


Torsions

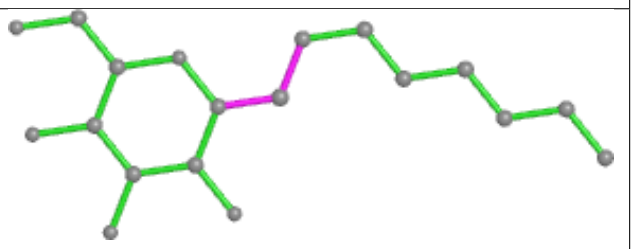


Rings

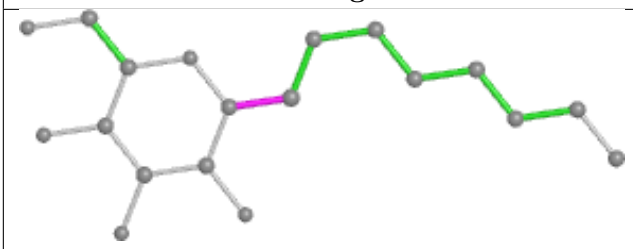
Ligand HTG c 524



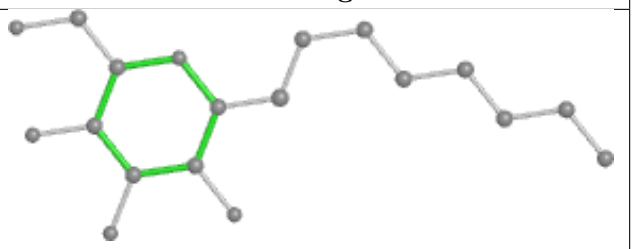
Bond lengths



Bond angles

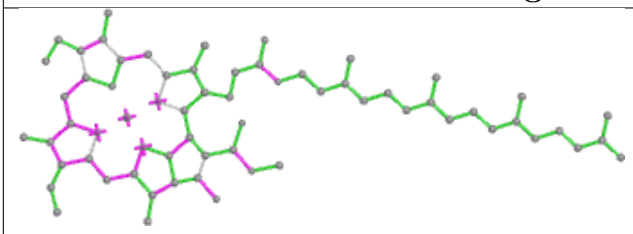


Torsions

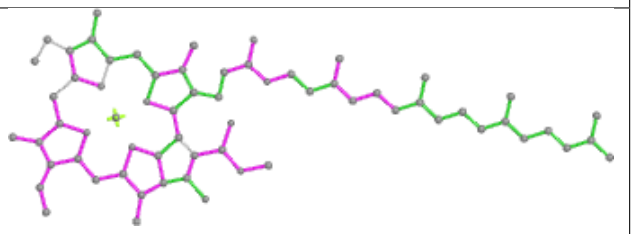


Rings

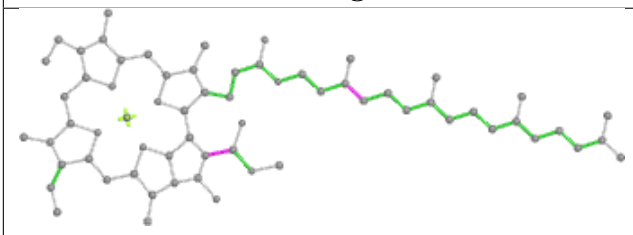
Ligand CLA B 610



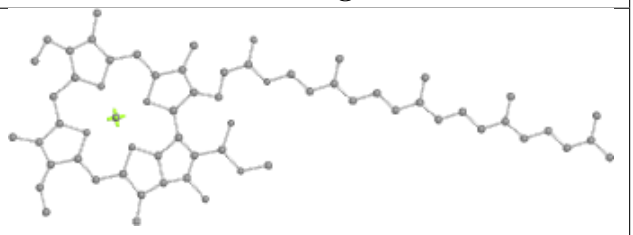
Bond lengths



Bond angles

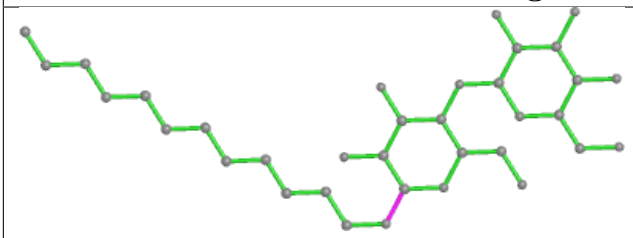


Torsions

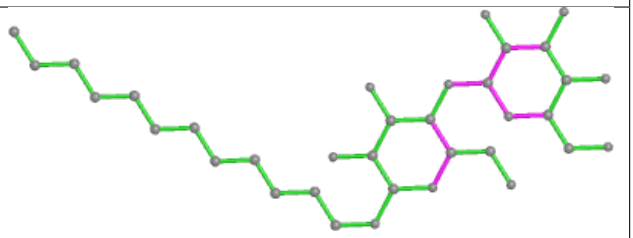


Rings

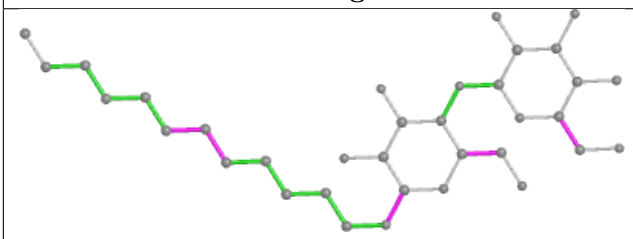
Ligand LMT c 523



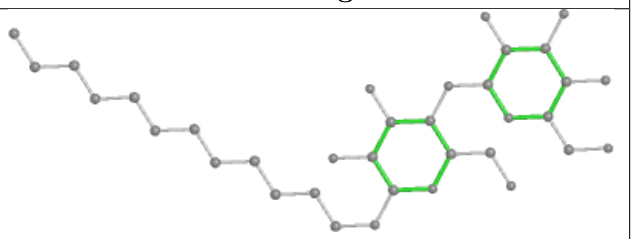
Bond lengths



Bond angles

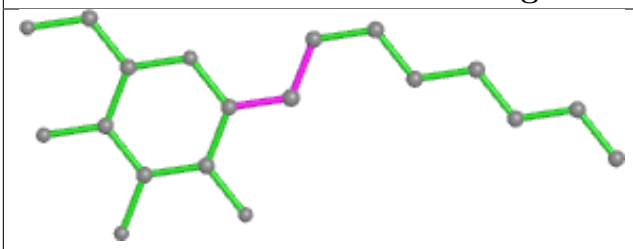


Torsions

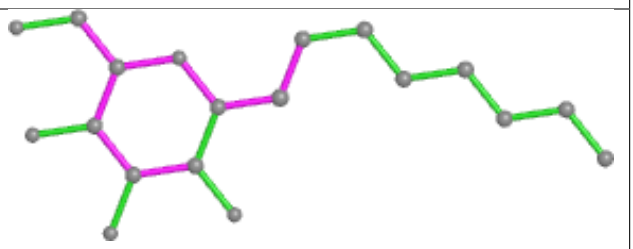


Rings

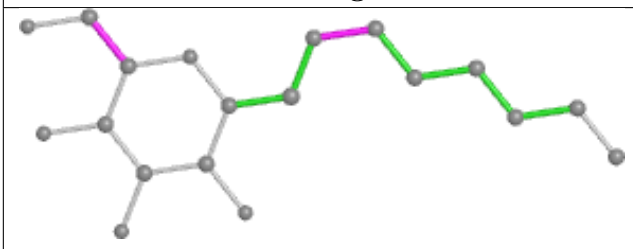
Ligand HTG B 626



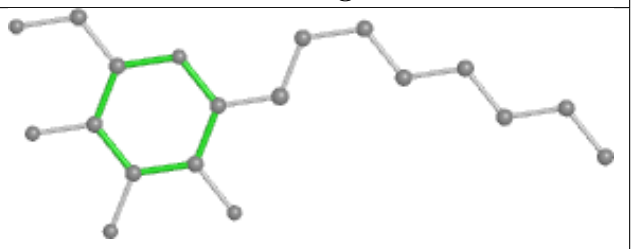
Bond lengths



Bond angles

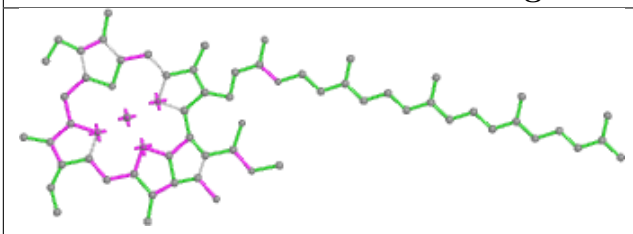


Torsions

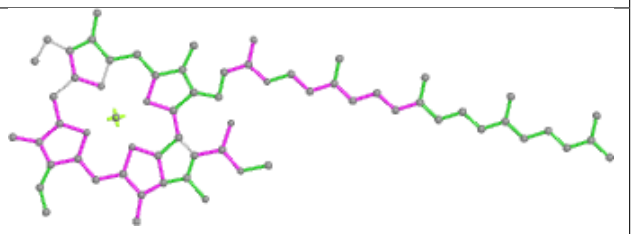


Rings

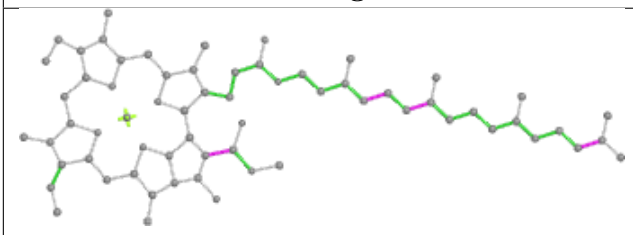
Ligand CLA B 605



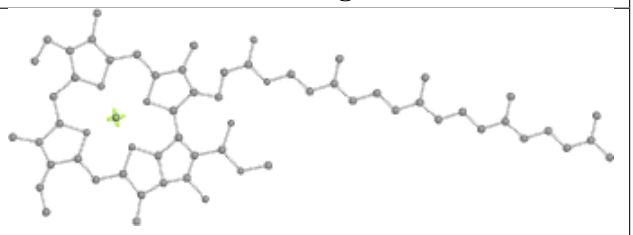
Bond lengths



Bond angles

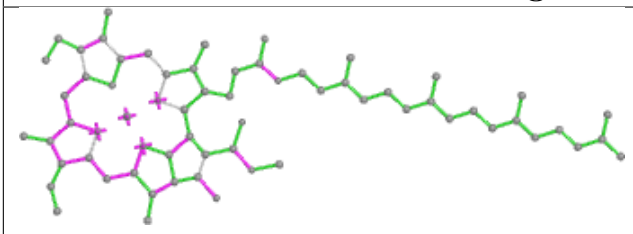


Torsions

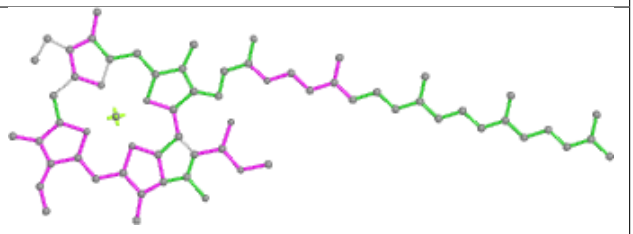


Rings

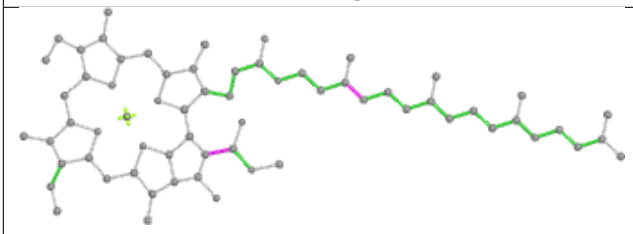
Ligand CLA b 612



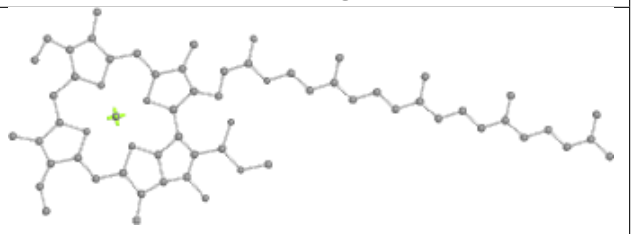
Bond lengths



Bond angles

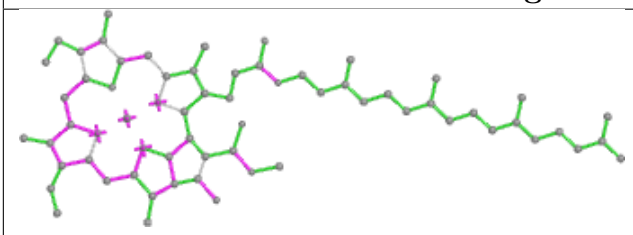


Torsions

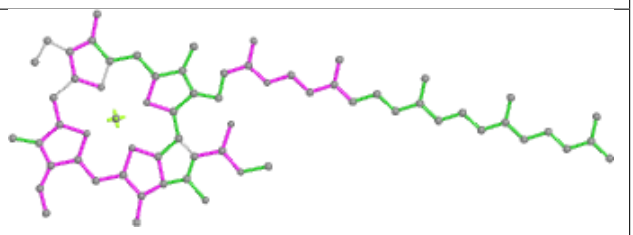


Rings

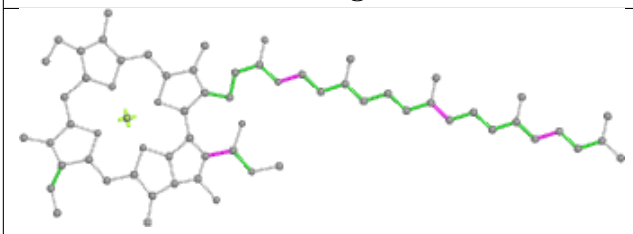
Ligand CLA C 510



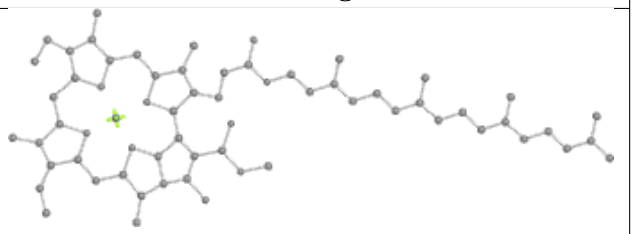
Bond lengths



Bond angles

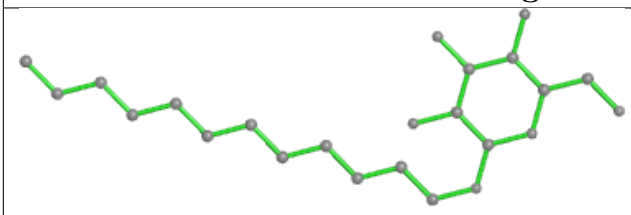


Torsions

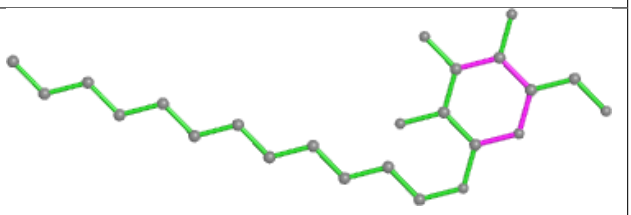


Rings

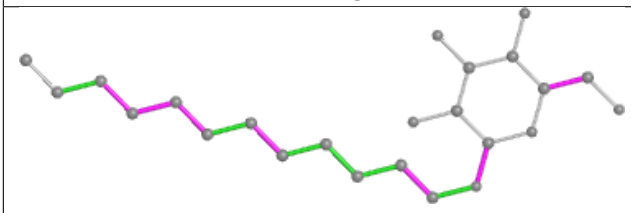
Ligand LMT T 104



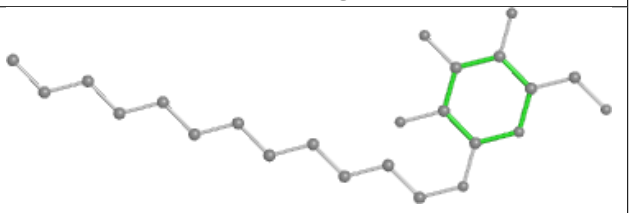
Bond lengths



Bond angles

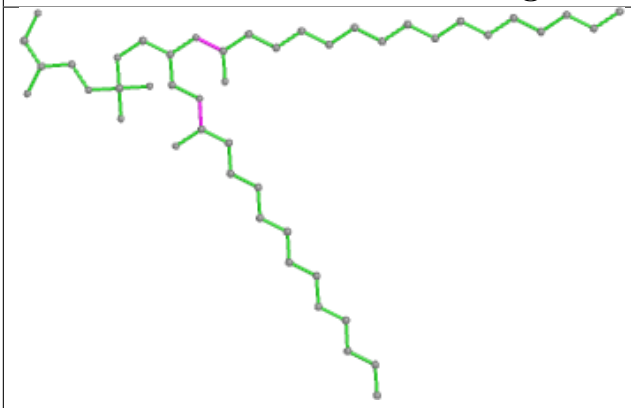


Torsions

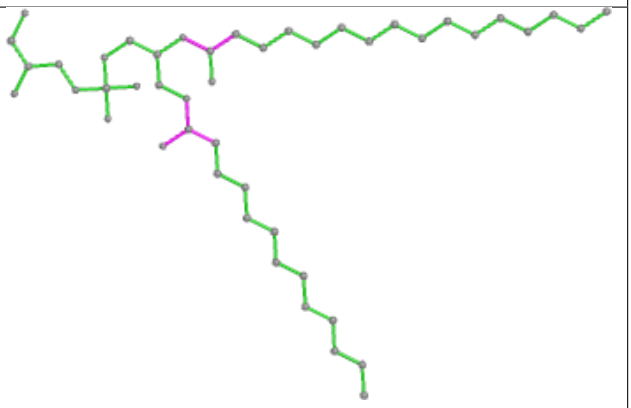


Rings

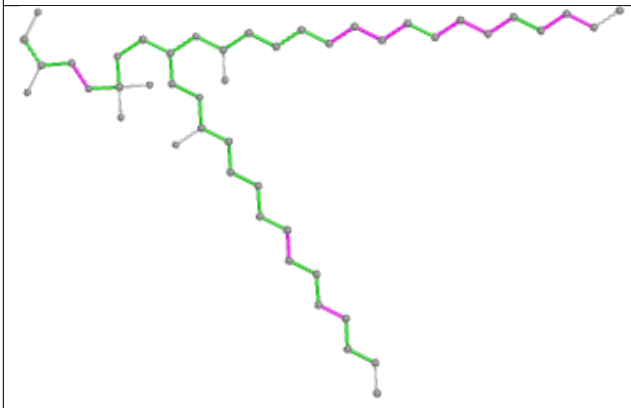
Ligand LHG D 411



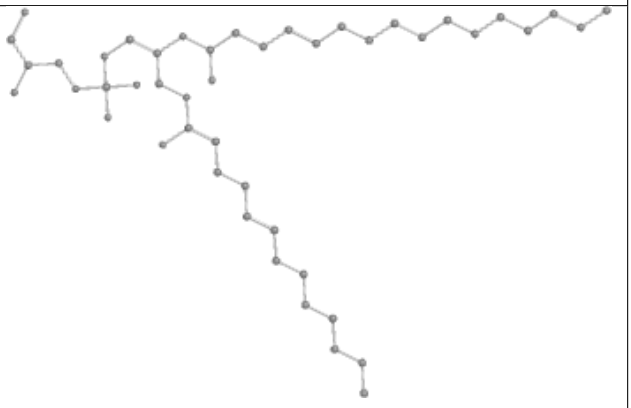
Bond lengths



Bond angles

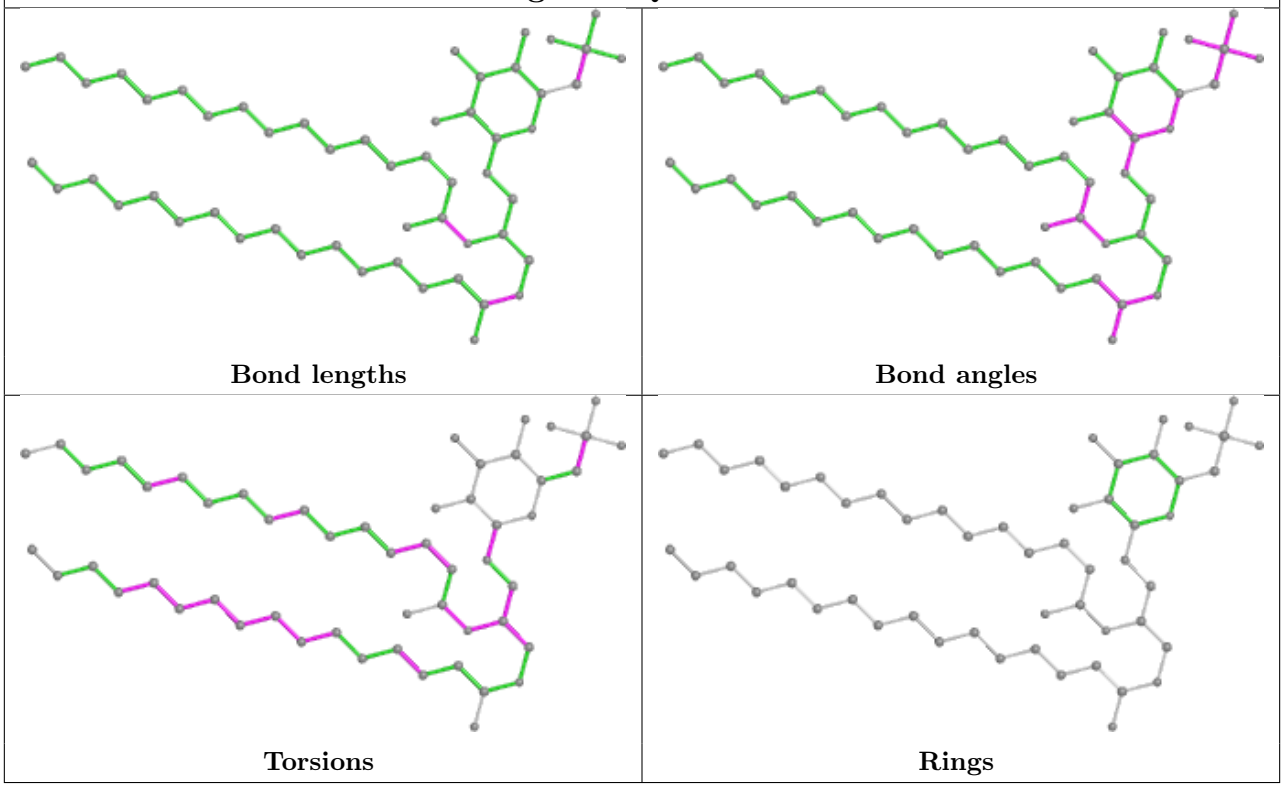


Torsions



Rings

Ligand SQD L 101



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%)	0.15	14 (4%) 36 45	31, 37, 60, 107	0
1	a	334/344 (97%)	0.44	36 (10%) 5 9	33, 39, 72, 113	0
2	B	505/505 (100%)	0.23	42 (8%) 11 17	32, 42, 68, 98	0
2	b	503/505 (99%)	0.34	56 (11%) 5 8	34, 45, 79, 146	0
3	C	451/455 (99%)	0.17	32 (7%) 16 24	35, 47, 64, 116	0
3	c	455/455 (100%)	0.35	38 (8%) 11 17	37, 51, 67, 121	0
4	D	341/342 (99%)	0.05	10 (2%) 51 60	30, 38, 53, 116	0
4	d	341/342 (99%)	0.04	12 (3%) 44 53	33, 42, 63, 115	0
5	E	81/83 (97%)	0.51	11 (13%) 3 4	41, 54, 77, 107	0
5	e	79/83 (95%)	1.12	19 (24%) 0 0	49, 63, 102, 131	0
6	F	34/44 (77%)	0.11	1 (2%) 51 60	41, 46, 66, 88	0
6	f	31/44 (70%)	0.06	2 (6%) 18 27	47, 54, 71, 107	0
7	H	63/63 (100%)	0.16	2 (3%) 47 57	39, 48, 62, 106	0
7	h	63/63 (100%)	0.50	8 (12%) 3 6	43, 54, 69, 103	0
8	I	35/38 (92%)	0.13	3 (8%) 10 16	44, 53, 98, 126	0
8	i	35/38 (92%)	0.42	1 (2%) 51 60	42, 51, 89, 144	0
9	J	36/40 (90%)	-0.17	2 (5%) 24 33	39, 51, 83, 101	0
9	j	39/40 (97%)	0.48	8 (20%) 1 1	46, 60, 129, 148	0
10	K	37/37 (100%)	-0.22	1 (2%) 54 63	44, 52, 68, 82	0
10	k	37/37 (100%)	0.22	3 (8%) 12 18	49, 59, 74, 90	0
11	L	37/37 (100%)	-0.12	1 (2%) 54 63	31, 36, 83, 113	0
11	l	37/37 (100%)	0.12	1 (2%) 54 63	33, 36, 85, 112	0
12	M	32/36 (88%)	-0.22	0 100 100	33, 37, 54, 85	0
12	m	33/36 (91%)	0.12	1 (3%) 50 59	33, 37, 59, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	0.67	51 (20%) 1 1	33, 50, 90, 139	0
13	o	243/244 (99%)	0.60	40 (16%) 1 2	36, 50, 96, 134	0
14	T	29/32 (90%)	-0.08	1 (3%) 45 55	32, 37, 71, 108	0
14	t	29/32 (90%)	0.45	3 (10%) 6 10	32, 37, 67, 88	0
15	U	97/104 (93%)	0.15	3 (3%) 49 58	39, 49, 73, 80	0
15	u	97/104 (93%)	-0.16	2 (2%) 63 72	41, 51, 71, 102	0
16	V	137/137 (100%)	-0.04	4 (2%) 51 60	37, 46, 62, 85	0
16	v	137/137 (100%)	0.54	20 (14%) 2 3	42, 56, 77, 107	0
17	Y	28/30 (93%)	1.63	10 (35%) 0 0	50, 62, 117, 138	0
17	y	28/30 (93%)	1.70	11 (39%) 0 0	59, 75, 110, 127	0
18	X	38/40 (95%)	0.50	6 (15%) 2 2	46, 56, 69, 91	0
18	x	37/40 (92%)	0.59	4 (10%) 5 9	52, 63, 101, 124	0
19	Z	61/62 (98%)	1.79	24 (39%) 0 0	52, 64, 100, 117	0
19	z	60/62 (96%)	2.66	36 (60%) 0 0	61, 74, 107, 118	0
20	R	34/41 (82%)	5.12	34 (100%) 0 0	68, 92, 107, 117	0
All	All	5272/5387 (97%)	0.36	553 (10%) 6 10	30, 46, 80, 148	0

The worst 5 of 553 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	34	LEU	11.4
20	R	18	TRP	10.8
17	Y	22	LEU	8.7
19	z	5	PHE	7.9
20	R	14	LEU	7.9

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
19	FME	Z	1	10/11	0.83	0.32	88,100,114,119	0
14	FME	t	1	10/11	0.93	0.11	34,38,57,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.95	0.15	43,48,54,55	0
14	FME	T	1	10/11	0.95	0.07	37,44,64,68	0
12	FME	m	1	10/11	0.96	0.13	42,50,78,87	0
12	FME	M	1	10/11	0.97	0.12	44,51,79,81	0
4	HSK	d	336[A]	10/12	0.97	0.10	46,49,54,56	7
4	HSK	d	336[B]	11/12	0.97	0.10	46,49,55,57	8
8	FME	I	1	10/11	0.98	0.08	44,49,54,54	0
4	HSK	D	336[A]	10/12	0.98	0.10	40,42,44,46	7
4	HSK	D	336[B]	11/12	0.98	0.10	40,41,43,45	8

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
31	UNL	B	639	15/-	0.42	0.45	88,95,108,108	0
31	UNL	A	419	10/-	0.45	0.34	79,90,94,95	0
30	GOL	h	1206	6/6	0.49	0.31	95,104,105,109	0
31	UNL	b	633	15/-	0.49	0.26	80,90,106,106	0
31	UNL	E	103	15/-	0.52	0.41	76,79,90,95	0
36	HTG	b	626	19/19	0.52	0.34	74,133,142,142	0
39	DGD	D	407	53/66	0.53	0.31	76,89,137,139	0
31	UNL	B	635	13/-	0.54	0.23	78,94,106,107	0
31	UNL	b	635	15/-	0.54	0.45	89,106,109,110	0
31	UNL	I	104	15/-	0.56	0.35	87,94,102,103	0
31	UNL	a	423	10/-	0.56	0.38	94,98,104,104	0
31	UNL	k	301	16/-	0.57	0.20	82,118,131,131	0
31	UNL	A	417	40/-	0.58	0.34	74,94,119,122	0
36	HTG	D	413	19/19	0.58	0.41	71,120,132,134	0
31	UNL	a	419	40/-	0.59	0.43	78,107,124,132	0
38	DMS	b	636	4/4	0.61	0.34	134,135,138,139	0
38	DMS	o	309	4/4	0.61	0.21	140,142,142,143	0
29	LMT	C	521	35/35	0.61	0.44	76,138,158,160	0
38	DMS	a	426	4/4	0.63	0.32	144,146,147,147	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	UNL	D	415	12/-	0.63	0.35	79,86,92,94	0
31	UNL	B	638	9/-	0.64	0.39	67,73,84,86	0
31	UNL	h	1201	15/-	0.65	0.53	87,104,123,123	0
31	UNL	e	102	15/-	0.65	0.34	76,82,97,98	0
29	LMT	f	104	35/35	0.66	0.40	90,115,143,147	0
33	PL9	A	422[B]	55/55	0.66	0.44	54,80,96,98	55
35	CA	B	601	1/1	0.66	0.10	110,110,110,110	0
38	DMS	o	307	4/4	0.67	0.32	121,123,123,124	0
36	HTG	d	414	19/19	0.68	0.23	71,103,114,118	19
30	GOL	b	630	6/6	0.68	0.18	57,75,76,76	0
31	UNL	A	418	15/-	0.68	0.60	85,88,97,98	0
31	UNL	b	632	15/-	0.69	0.29	71,86,107,108	0
27	SQD	L	101	54/54	0.69	0.27	55,83,128,132	0
36	HTG	h	1202	19/19	0.69	0.37	89,109,120,121	0
31	UNL	x	802	18/-	0.69	0.21	60,74,107,110	0
36	HTG	I	102	19/19	0.70	0.24	73,112,128,132	0
31	UNL	J	104	16/-	0.70	0.29	76,87,94,96	0
31	UNL	x	801	12/-	0.70	0.26	77,89,94,95	0
31	UNL	j	1302	16/-	0.70	0.33	69,82,99,100	0
38	DMS	B	644	4/4	0.70	0.18	136,138,138,138	0
38	DMS	o	304	4/4	0.71	0.24	101,113,115,116	0
31	UNL	E	102	15/-	0.71	0.33	77,85,99,99	0
30	GOL	a	418	6/6	0.71	0.24	69,82,85,86	0
31	UNL	Y	301	12/-	0.71	0.23	82,91,97,98	0
31	UNL	c	531	11/-	0.72	0.20	84,96,105,106	0
29	LMT	m	101	35/35	0.72	0.23	49,71,97,101	0
29	LMT	b	624	25/35	0.72	0.22	69,95,125,130	0
31	UNL	B	637	10/-	0.72	0.19	89,96,99,100	0
28	LMG	C	532	51/55	0.72	0.28	64,117,127,130	0
38	DMS	B	645	4/4	0.72	0.29	129,130,130,130	0
29	LMT	M	101	35/35	0.73	0.22	47,71,83,85	0
31	UNL	J	103	15/-	0.73	0.25	76,86,98,99	0
33	PL9	a	425[B]	55/55	0.73	0.53	41,71,125,126	55
38	DMS	C	533	4/4	0.73	0.25	99,102,107,111	0
31	UNL	i	103	40/-	0.73	0.42	73,93,120,123	0
31	UNL	c	529	12/-	0.74	0.18	93,97,103,105	0
30	GOL	C	527	6/6	0.74	0.18	80,86,90,90	0
38	DMS	B	643	4/4	0.74	0.16	87,99,102,103	0
31	UNL	d	403	40/-	0.74	0.28	57,83,114,117	0
36	HTG	b	602	19/19	0.74	0.17	70,114,131,134	0
30	GOL	T	103	6/6	0.74	0.27	116,117,119,120	0
31	UNL	C	526	15/-	0.75	0.22	80,91,111,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	E	104	24/35	0.75	0.30	84,98,107,112	0
31	UNL	h	1207	12/-	0.75	0.46	67,87,101,103	0
38	DMS	E	106	4/4	0.75	0.30	109,113,116,119	0
29	LMT	J	102	24/35	0.75	0.22	65,86,117,122	0
29	LMT	m	103	35/35	0.75	0.21	57,74,104,105	0
30	GOL	c	532	6/6	0.75	0.24	59,87,90,93	0
29	LMT	c	523	35/35	0.75	0.45	103,134,152,153	0
30	GOL	k	304	6/6	0.75	0.22	101,105,108,118	0
30	GOL	v	1601	6/6	0.75	0.25	70,85,94,98	0
31	UNL	h	1203	12/-	0.76	0.28	80,88,90,93	0
31	UNL	a	422	11/-	0.76	0.38	87,91,95,96	0
29	LMT	T	104	24/35	0.76	0.31	44,71,113,118	0
36	HTG	u	201	14/19	0.77	0.28	73,89,104,111	0
31	UNL	C	501	40/-	0.77	0.30	68,92,106,108	0
29	LMT	Z	101	35/35	0.77	0.24	54,108,130,136	0
38	DMS	z	102	4/4	0.77	0.18	141,143,143,144	0
31	UNL	A	420	9/-	0.77	0.31	98,100,108,110	0
36	HTG	C	523	19/19	0.78	0.34	72,102,110,111	0
29	LMT	m	102	35/35	0.78	0.24	39,58,71,73	0
32	K3C	a	424[A]	14/14	0.78	0.27	116,122,125,126	14
30	GOL	v	1607	6/6	0.78	0.25	56,68,79,84	0
30	GOL	E	105	6/6	0.78	0.38	100,107,109,110	0
36	HTG	c	525	19/19	0.78	0.42	69,92,102,104	19
31	UNL	C	531	18/-	0.78	0.28	69,93,106,107	0
29	LMT	B	642	24/35	0.79	0.33	51,69,117,121	0
31	UNL	c	501	40/-	0.79	0.26	76,101,136,137	0
36	HTG	b	625	19/19	0.79	0.32	47,59,82,86	0
28	LMG	c	522	51/55	0.79	0.25	58,121,129,132	0
31	UNL	b	634	9/-	0.79	0.29	67,85,95,96	0
31	UNL	X	101	16/-	0.80	0.21	55,63,78,84	0
38	DMS	o	308	4/4	0.80	0.26	77,78,84,97	0
36	HTG	B	626	19/19	0.80	0.19	55,122,127,128	0
31	UNL	B	634	18/-	0.80	0.21	73,82,96,99	0
31	UNL	I	103	16/-	0.80	0.31	66,83,91,91	0
37	LHG	e	101	40/49	0.81	0.29	90,135,148,150	0
30	GOL	A	416	6/6	0.81	0.21	55,78,82,86	0
38	DMS	b	637	4/4	0.81	0.28	89,93,97,99	0
38	DMS	d	415	4/4	0.81	0.34	114,118,118,119	0
31	UNL	a	420	12/-	0.81	0.50	75,89,106,107	0
35	CA	b	603	1/1	0.82	0.13	142,142,142,142	0
38	DMS	B	646	4/4	0.82	0.42	108,110,113,115	0
27	SQD	a	401	54/54	0.82	0.20	54,73,95,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
38	DMS	D	416	4/4	0.82	0.38	91,98,102,102	0
31	UNL	B	636	18/-	0.82	0.16	56,74,98,108	0
28	LMG	a	415	51/55	0.83	0.21	58,75,87,90	0
31	UNL	j	1301	18/-	0.83	0.16	66,81,110,112	0
32	K3C	A	421[A]	14/14	0.83	0.20	84,85,87,88	14
29	LMT	B	622	35/35	0.83	0.16	59,89,115,120	0
38	DMS	B	647	4/4	0.83	0.20	122,122,122,123	0
30	GOL	d	402	6/6	0.83	0.10	83,103,103,106	0
41	RRX	h	1204	41/41	0.83	0.17	41,53,65,73	0
38	DMS	Y	303	4/4	0.84	0.15	141,143,145,146	0
31	UNL	t	101	8/-	0.84	0.61	70,80,85,86	0
38	DMS	C	525	4/4	0.84	0.17	111,114,116,117	0
30	GOL	O	303	6/6	0.84	0.25	73,77,82,88	0
37	LHG	E	101	49/49	0.84	0.23	53,87,108,115	0
30	GOL	a	416	6/6	0.84	0.15	43,53,57,59	0
30	GOL	v	1605	6/6	0.85	0.21	46,56,63,65	0
38	DMS	i	104	4/4	0.85	0.21	107,108,109,109	0
30	GOL	d	413	6/6	0.85	0.11	74,93,98,99	0
27	SQD	L	102	54/54	0.85	0.19	52,76,113,120	0
30	GOL	L	103	6/6	0.85	0.22	58,69,79,82	0
31	UNL	c	530	11/-	0.85	0.15	85,92,105,108	0
36	HTG	B	624	19/19	0.85	0.40	62,98,106,108	19
31	UNL	i	102	15/-	0.85	0.14	70,79,106,106	0
29	LMT	a	402	35/35	0.85	0.20	49,68,83,93	0
30	GOL	T	101	6/6	0.86	0.22	37,55,59,63	0
31	UNL	B	632	16/-	0.86	0.23	59,74,97,97	0
38	DMS	c	535	4/4	0.86	0.37	112,112,112,113	0
30	GOL	B	631	6/6	0.86	0.15	49,60,67,73	0
30	GOL	o	305	6/6	0.86	0.21	60,85,88,89	0
41	RRX	H	101	41/41	0.86	0.15	40,50,61,71	0
36	HTG	U	201	9/19	0.86	0.27	71,84,122,126	0
28	LMG	b	623	51/55	0.87	0.19	45,56,76,79	0
38	DMS	c	536	4/4	0.87	0.23	105,108,109,111	0
28	LMG	A	412	51/55	0.87	0.20	51,73,97,101	0
36	HTG	B	623[A]	19/19	0.87	0.20	39,52,67,67	19
36	HTG	B	623[B]	19/19	0.87	0.20	31,50,67,70	19
30	GOL	C	528	6/6	0.87	0.19	66,81,86,93	0
30	GOL	C	529	6/6	0.87	0.20	93,95,101,107	0
29	LMT	z	101	32/35	0.87	0.15	63,112,129,131	0
38	DMS	v	1608	4/4	0.87	0.22	118,122,124,126	0
28	LMG	C	520	51/55	0.87	0.19	43,80,103,106	0
31	UNL	b	631	16/-	0.87	0.14	58,63,74,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	GOL	B	629	6/6	0.87	0.17	50,65,76,78	0
36	HTG	b	601	19/19	0.87	0.15	57,68,82,86	0
30	GOL	A	415	6/6	0.88	0.17	44,54,55,58	0
38	DMS	o	306	4/4	0.88	0.27	113,116,117,117	0
26	BCR	k	303	40/40	0.88	0.17	49,56,65,67	0
30	GOL	v	1602	6/6	0.88	0.48	64,75,79,86	0
30	GOL	a	421	6/6	0.88	0.19	90,97,107,111	0
31	UNL	D	402	40/-	0.88	0.15	55,72,101,107	0
30	GOL	v	1606	6/6	0.88	0.27	74,86,91,98	0
30	GOL	b	629	6/6	0.88	0.16	58,68,71,77	0
24	CLA	B	610	65/65	0.88	0.13	37,42,47,54	0
30	GOL	o	302	6/6	0.88	0.18	61,71,78,85	0
36	HTG	c	524	19/19	0.89	0.26	87,102,108,110	0
30	GOL	B	627	6/6	0.89	0.19	53,58,67,78	0
28	LMG	c	521	51/55	0.89	0.18	48,80,115,117	0
38	DMS	d	416	4/4	0.89	0.22	88,90,90,93	0
28	LMG	B	621	51/55	0.89	0.18	45,52,69,84	0
30	GOL	c	526	6/6	0.90	0.15	58,80,93,98	0
38	DMS	b	638	4/4	0.90	0.22	79,91,95,98	0
38	DMS	c	533	4/4	0.90	0.30	100,104,104,105	0
27	SQD	A	413	54/54	0.90	0.17	54,72,100,102	0
31	UNL	I	101	16/-	0.90	0.15	50,63,75,76	0
38	DMS	V	207	4/4	0.90	0.12	97,105,106,109	0
30	GOL	u	202	6/6	0.90	0.34	76,100,104,106	0
39	DGD	H	102	62/66	0.90	0.21	36,46,58,64	0
39	DGD	h	1205	62/66	0.90	0.18	41,49,62,76	0
27	SQD	f	102	33/54	0.90	0.14	74,97,122,123	0
37	LHG	l	302	49/49	0.90	0.20	38,47,66,78	0
29	LMT	A	414	35/35	0.91	0.15	52,73,95,108	0
26	BCR	c	516	40/40	0.91	0.16	58,70,74,76	0
36	HTG	B	625	19/19	0.91	0.13	52,73,95,96	0
31	UNL	i	101	16/-	0.91	0.15	59,67,82,84	0
30	GOL	V	205	6/6	0.91	0.34	72,87,90,100	0
24	CLA	c	514	65/65	0.91	0.16	49,60,88,94	0
30	GOL	c	527	6/6	0.91	0.34	65,68,78,86	0
37	LHG	D	409	49/49	0.91	0.19	40,49,57,62	0
31	UNL	T	105	9/-	0.91	0.49	72,78,85,88	0
26	BCR	K	101	40/40	0.91	0.12	39,49,56,59	0
31	UNL	H	103	8/-	0.91	0.17	71,78,81,83	0
31	UNL	d	412	16/-	0.92	0.31	54,71,95,97	0
30	GOL	V	204	6/6	0.92	0.17	42,53,56,57	0
36	HTG	V	203	13/19	0.92	0.21	65,71,107,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CA	f	103	1/1	0.92	0.24	86,86,86,86	0
26	BCR	b	622	40/40	0.92	0.13	41,49,61,68	0
30	GOL	B	633	6/6	0.92	0.15	41,52,57,58	6
30	GOL	a	417	6/6	0.92	0.17	54,63,66,70	0
24	CLA	b	605	65/65	0.92	0.14	39,46,56,58	0
39	DGD	C	518	62/66	0.92	0.16	36,47,91,102	0
27	SQD	D	408	45/54	0.92	0.24	50,85,118,127	0
36	HTG	C	522	19/19	0.92	0.22	82,86,95,97	0
38	DMS	c	537	4/4	0.92	0.14	93,100,100,103	0
30	GOL	B	630	6/6	0.92	0.14	51,60,67,75	0
30	GOL	V	201	6/6	0.92	0.25	56,73,76,84	0
30	GOL	b	627	6/6	0.93	0.18	64,66,69,84	0
37	LHG	d	408	49/49	0.93	0.26	38,52,66,74	0
24	CLA	C	507	65/65	0.93	0.12	43,58,101,104	0
27	SQD	a	414	54/54	0.93	0.17	54,73,92,96	0
26	BCR	a	413	40/40	0.93	0.11	29,39,45,46	0
31	UNL	l	301	16/-	0.93	0.21	58,76,110,111	0
24	CLA	C	514	65/65	0.93	0.16	46,59,99,100	0
24	CLA	B	603	65/65	0.93	0.15	34,41,47,53	0
24	CLA	b	612	65/65	0.93	0.11	41,48,55,60	0
24	CLA	c	505	65/65	0.93	0.19	41,51,59,71	0
24	CLA	B	612	65/65	0.93	0.19	28,35,51,61	0
24	CLA	c	515	65/65	0.93	0.18	50,64,103,106	0
25	PHO	D	401	64/64	0.93	0.18	28,36,44,47	0
24	CLA	b	604	65/65	0.94	0.20	48,66,112,120	0
28	LMG	D	412	51/55	0.94	0.18	37,51,102,112	0
26	BCR	T	102	40/40	0.94	0.15	35,47,58,59	0
38	DMS	O	304	4/4	0.94	0.14	83,99,100,102	0
36	HTG	O	302	19/19	0.94	0.11	42,46,68,71	0
24	CLA	B	615	65/65	0.94	0.14	28,38,94,99	0
24	CLA	b	609	65/65	0.94	0.10	36,46,76,79	0
24	CLA	C	504	65/65	0.94	0.13	40,47,56,67	0
28	LMG	d	411	51/55	0.94	0.13	45,53,108,114	0
26	BCR	c	517	40/40	0.94	0.11	45,52,66,72	0
26	BCR	d	406	40/40	0.94	0.11	42,51,76,82	0
30	GOL	c	528	6/6	0.94	0.15	38,45,47,47	0
26	BCR	k	302	40/40	0.94	0.10	48,56,67,70	0
24	CLA	b	617	65/65	0.94	0.19	32,41,97,106	0
24	CLA	b	618	65/65	0.94	0.11	34,47,69,75	0
36	HTG	o	301	19/19	0.94	0.11	40,48,64,67	0
24	CLA	b	619	65/65	0.94	0.13	40,47,113,115	0
37	LHG	B	640	49/49	0.94	0.16	37,46,65,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	PL9	d	407	55/55	0.94	0.17	30,39,49,52	0
30	GOL	C	530	6/6	0.94	0.31	44,50,54,61	6
35	CA	F	102	1/1	0.94	0.19	77,77,77,77	0
37	LHG	d	409	49/49	0.94	0.15	34,41,59,70	0
24	CLA	c	503	65/65	0.94	0.13	41,50,64,71	0
24	CLA	c	504	65/65	0.94	0.22	38,47,62,70	0
24	CLA	B	602	65/65	0.94	0.19	38,58,106,113	0
24	CLA	c	508	65/65	0.94	0.12	47,57,86,89	0
24	CLA	C	513	65/65	0.94	0.11	45,57,86,95	0
39	DGD	c	518	62/66	0.94	0.15	38,49,91,96	0
39	DGD	c	519	62/66	0.94	0.20	43,53,110,123	0
24	CLA	B	607	65/65	0.94	0.12	33,41,67,79	0
24	CLA	D	404	65/65	0.94	0.12	36,42,98,100	0
26	BCR	C	515	40/40	0.94	0.12	47,62,66,73	0
24	CLA	C	512	65/65	0.95	0.10	39,50,56,58	0
24	CLA	d	405	65/65	0.95	0.11	43,49,94,101	0
24	CLA	b	615	65/65	0.95	0.18	34,40,51,58	0
26	BCR	B	619	40/40	0.95	0.19	34,41,56,63	0
26	BCR	B	620	40/40	0.95	0.10	38,44,58,60	0
30	GOL	V	206	6/6	0.95	0.35	55,56,63,63	0
26	BCR	B	641	40/40	0.95	0.13	35,47,61,62	0
24	CLA	C	503	65/65	0.95	0.15	36,42,59,65	0
26	BCR	C	516	40/40	0.95	0.12	42,52,57,59	0
26	BCR	D	405	40/40	0.95	0.20	36,45,76,77	0
24	CLA	B	611	65/65	0.95	0.18	35,41,52,64	0
30	GOL	b	628	6/6	0.95	0.16	47,58,62,64	0
24	CLA	D	403	65/65	0.95	0.15	25,32,50,54	0
26	BCR	Y	302	40/40	0.95	0.10	44,50,58,64	0
30	GOL	B	628	6/6	0.95	0.11	44,49,50,52	0
35	CA	c	502	1/1	0.95	0.05	61,61,61,61	0
24	CLA	C	505	65/65	0.95	0.14	36,43,80,86	0
26	BCR	b	621	40/40	0.95	0.21	34,46,59,63	0
24	CLA	a	412	65/65	0.95	0.13	33,41,113,114	0
24	CLA	B	617	65/65	0.95	0.14	35,45,111,116	0
31	UNL	D	414	16/-	0.95	0.24	46,62,78,84	0
24	CLA	c	506	65/65	0.95	0.19	40,48,77,80	0
24	CLA	C	508	65/65	0.95	0.12	41,49,68,71	0
24	CLA	c	509	65/65	0.95	0.12	41,49,68,77	0
24	CLA	c	510	65/65	0.95	0.20	38,47,105,126	0
27	SQD	A	411	54/54	0.95	0.15	40,69,91,94	0
24	CLA	c	513	65/65	0.95	0.12	42,53,62,67	0
24	CLA	C	511	65/65	0.95	0.15	38,44,61,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	605	65/65	0.96	0.23	27,35,72,80	0
24	CLA	A	409	65/65	0.96	0.12	33,39,118,122	0
24	CLA	b	607	65/65	0.96	0.19	29,39,83,87	0
24	CLA	b	608	65/65	0.96	0.15	33,39,56,62	0
38	DMS	c	534	4/4	0.96	0.19	62,74,78,78	0
24	CLA	c	507	65/65	0.96	0.11	35,45,62,67	0
37	LHG	D	411	46/49	0.96	0.14	36,44,100,104	0
24	CLA	B	608	65/65	0.96	0.14	28,34,48,53	0
24	CLA	b	610	65/65	0.96	0.13	30,38,49,52	0
24	CLA	B	604	65/65	0.96	0.17	32,40,49,53	0
37	LHG	d	410	39/49	0.96	0.17	40,46,97,100	0
30	GOL	M	102	6/6	0.96	0.11	36,38,61,71	0
26	BCR	b	620	40/40	0.96	0.18	37,43,49,51	0
24	CLA	c	512	65/65	0.96	0.26	39,48,60,71	0
24	CLA	b	613	65/65	0.96	0.12	35,46,54,70	0
24	CLA	b	614	65/65	0.96	0.22	32,38,57,65	0
24	CLA	C	502	65/65	0.96	0.14	38,47,64,75	0
24	CLA	b	616	65/65	0.96	0.23	32,38,68,71	0
25	PHO	A	408	64/64	0.96	0.12	28,34,38,40	0
39	DGD	C	519	62/66	0.96	0.13	34,43,85,94	0
24	CLA	C	509	65/65	0.96	0.14	35,43,95,116	0
30	GOL	v	1604	6/6	0.96	0.10	49,57,59,60	0
33	PL9	D	406	55/55	0.96	0.11	31,37,47,49	0
26	BCR	B	618	40/40	0.96	0.17	34,40,47,48	0
39	DGD	c	520	62/66	0.96	0.15	39,50,80,95	0
24	CLA	a	410	65/65	0.96	0.17	34,40,104,109	0
34	BCT	A	423	4/4	0.96	0.07	38,39,48,52	0
24	CLA	C	510	65/65	0.96	0.14	39,46,70,77	0
24	CLA	B	614	65/65	0.97	0.24	30,36,67,81	0
24	CLA	a	408	65/65	0.97	0.16	31,35,43,64	0
35	CA	O	301	1/1	0.97	0.20	70,70,70,70	0
24	CLA	a	409	65/65	0.97	0.13	29,34,43,53	0
24	CLA	c	511	65/65	0.97	0.26	42,50,66,70	0
24	CLA	A	405	65/65	0.97	0.12	27,32,41,63	0
24	CLA	B	616	65/65	0.97	0.12	36,42,65,71	0
24	CLA	B	609	65/65	0.97	0.15	31,39,47,50	0
24	CLA	A	406	65/65	0.97	0.10	26,32,38,53	0
24	CLA	d	404	65/65	0.97	0.17	28,36,58,65	0
39	DGD	C	517	62/66	0.97	0.19	36,47,90,91	0
24	CLA	b	606	65/65	0.97	0.13	37,44,54,57	0
37	LHG	D	410	49/49	0.97	0.12	32,42,65,78	0
24	CLA	B	606	65/65	0.97	0.18	30,37,51,54	0

Continued on next page...

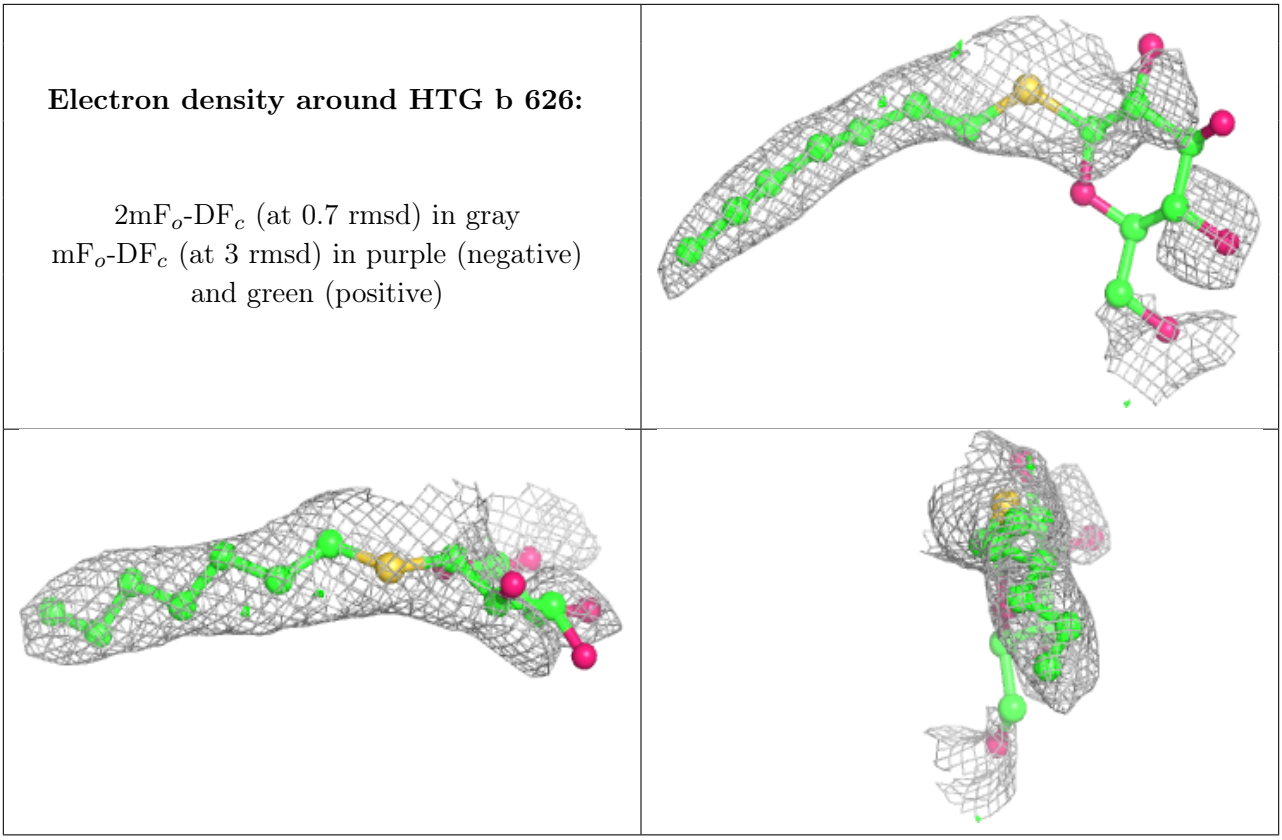
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	A	407	65/65	0.97	0.15	29,35,98,100	0
25	PHO	a	411	64/64	0.97	0.16	31,37,41,47	0
25	PHO	d	401	64/64	0.97	0.15	33,41,50,54	0
26	BCR	A	410	40/40	0.97	0.15	32,40,45,47	0
24	CLA	B	613	65/65	0.97	0.18	28,37,46,53	0
40	HEM	F	101	43/43	0.97	0.08	42,52,61,65	0
40	HEM	f	101	43/43	0.97	0.16	55,66,96,113	0
24	CLA	C	506	65/65	0.97	0.14	36,46,65,70	0
24	CLA	b	611	65/65	0.97	0.15	37,44,52,58	0
34	BCT	a	407	4/4	0.98	0.07	45,48,53,58	0
23	CL	a	405	1/1	0.98	0.04	44,44,44,44	0
30	GOL	C	524	6/6	0.98	0.15	36,41,43,44	0
35	CA	o	303	1/1	0.98	0.05	67,67,67,67	0
23	CL	a	406	1/1	0.98	0.13	41,41,41,41	0
42	MG	j	1303	1/1	0.98	0.23	52,52,52,52	0
43	HEC	v	1603	43/43	0.98	0.13	40,49,54,55	0
23	CL	A	404	1/1	0.99	0.15	38,38,38,38	0
21	OEX	A	401	10/10	0.99	0.10	35,37,41,42	0
21	OEX	a	403	10/10	0.99	0.09	38,40,42,42	0
42	MG	J	101	1/1	0.99	0.09	43,43,43,43	0
22	FE2	A	402	1/1	0.99	0.06	39,39,39,39	0
43	HEC	V	202	43/43	0.99	0.07	36,42,45,49	0
23	CL	A	403	1/1	0.99	0.04	38,38,38,38	0
22	FE2	a	404	1/1	1.00	0.06	42,42,42,42	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.

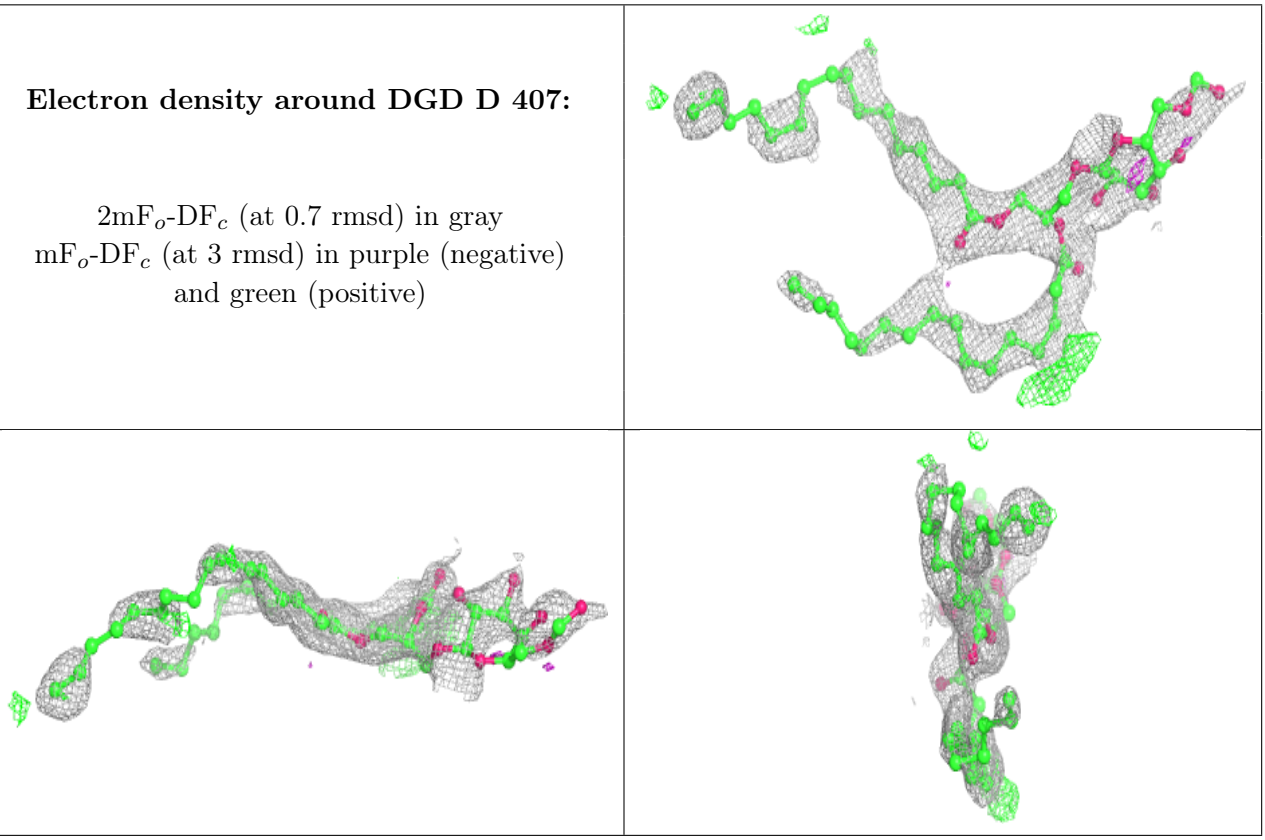
Electron density around HTG b 626:

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



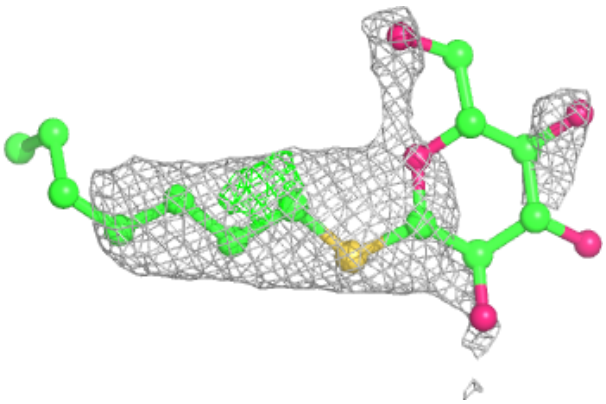
Electron density around DGD D 407:

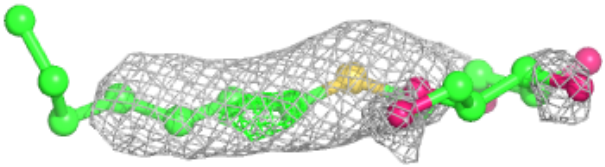
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

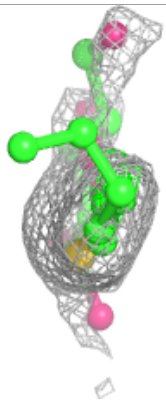


Electron density around HTG D 413:

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

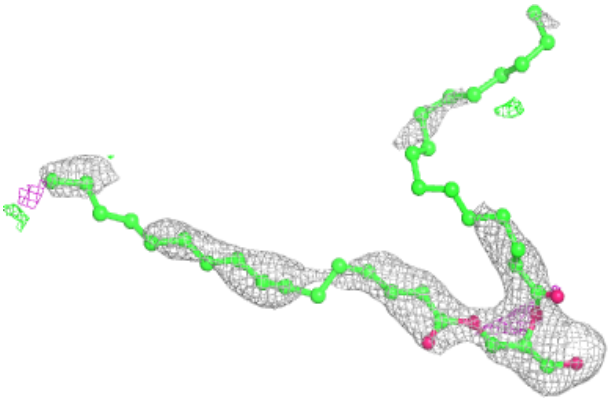


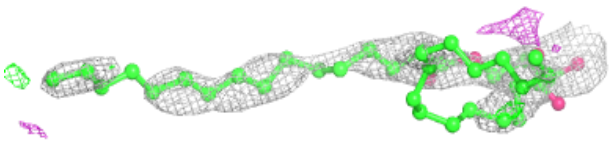


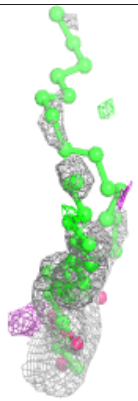


Electron density around UNL a 419:

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

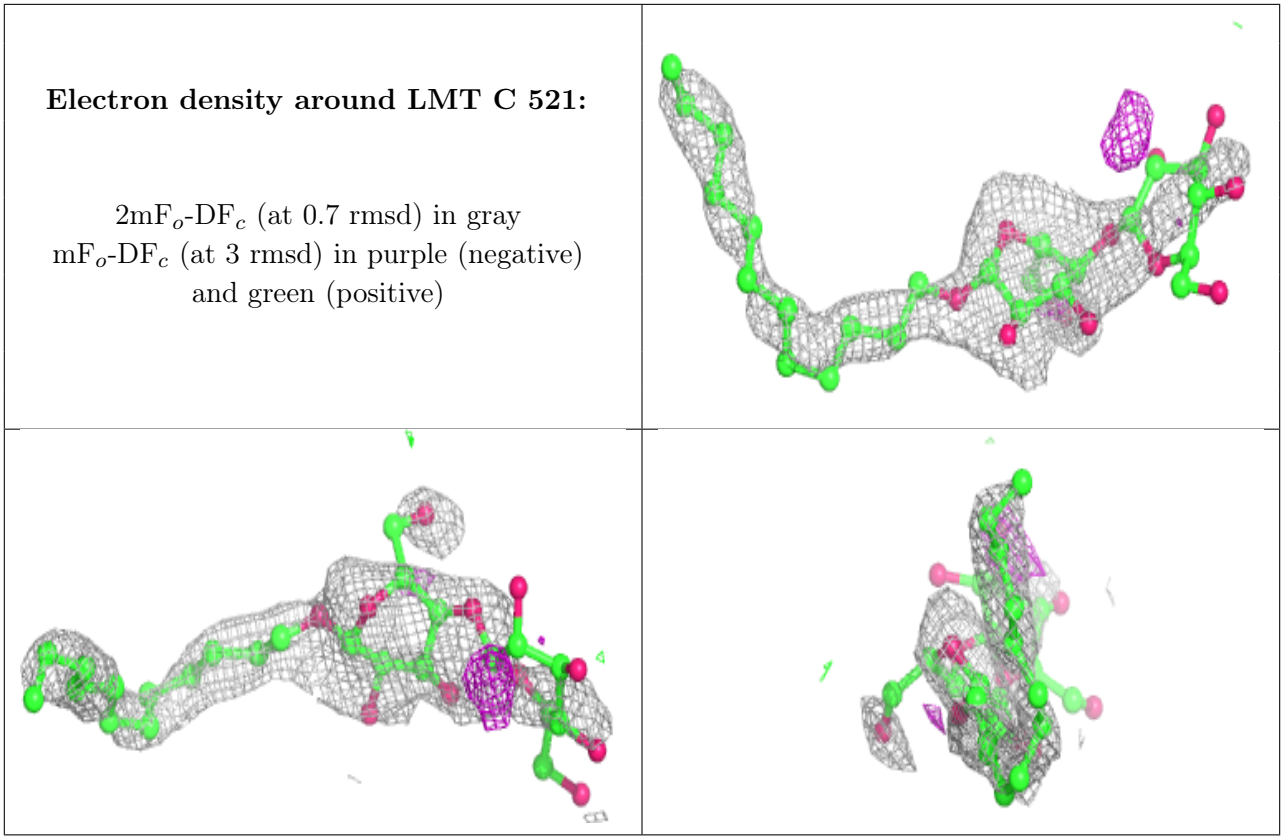






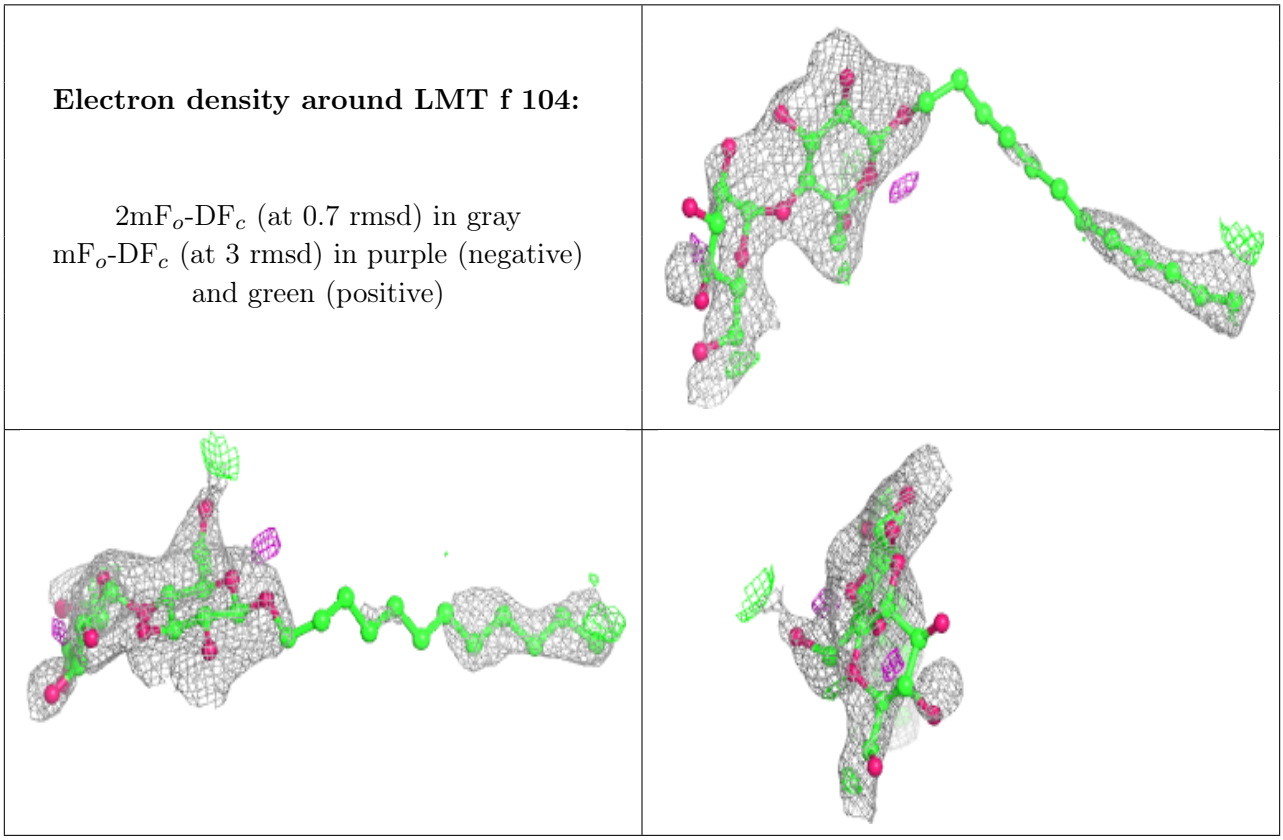
Electron density around LMT C 521:

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



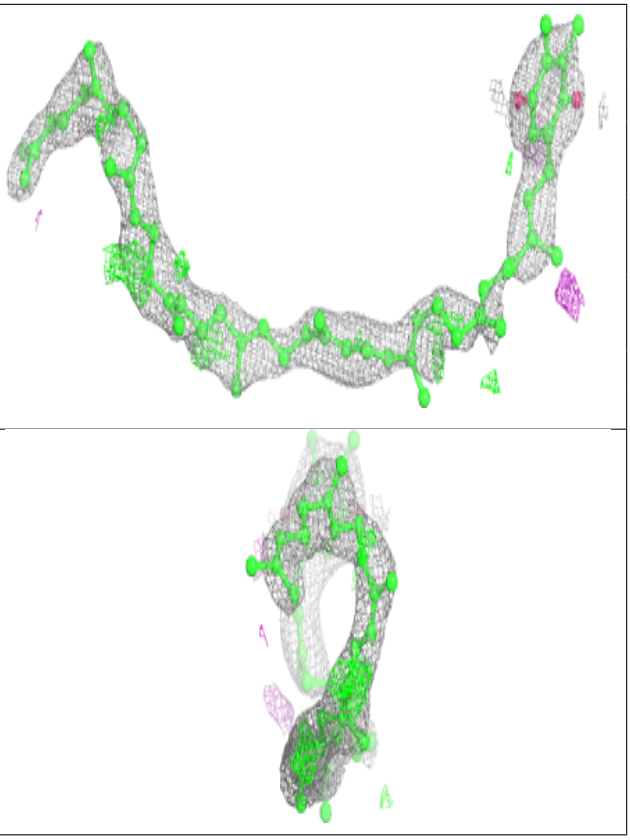
Electron density around LMT f 104:

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



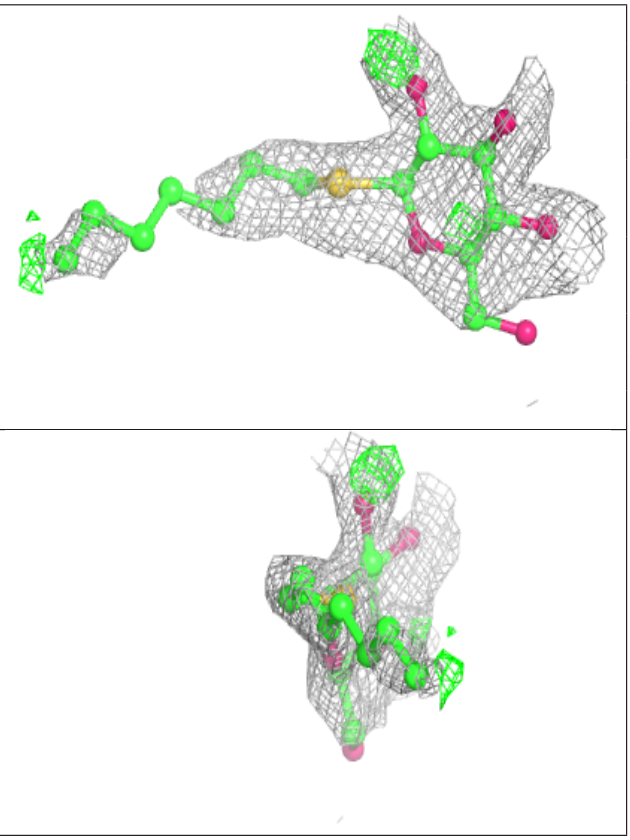
Electron density around PL9 A 422 (B):

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



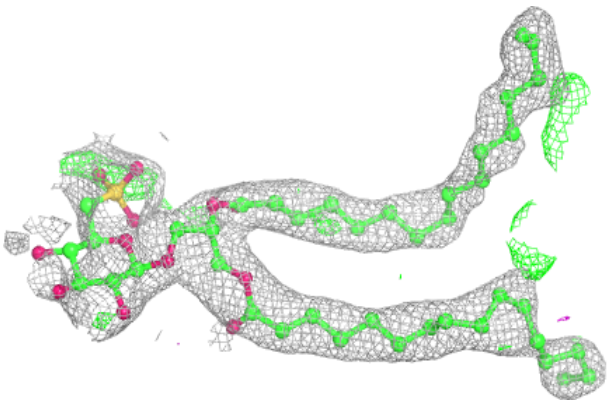
Electron density around HTG d 414:

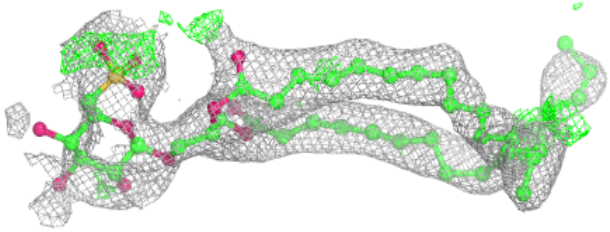
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

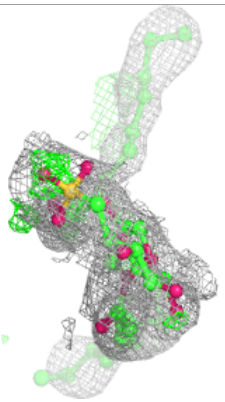


Electron density around SQD L 101:

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

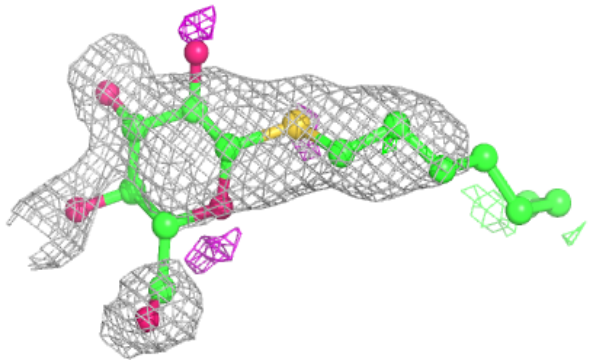


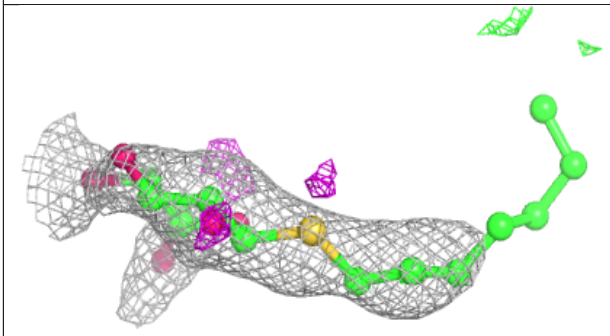


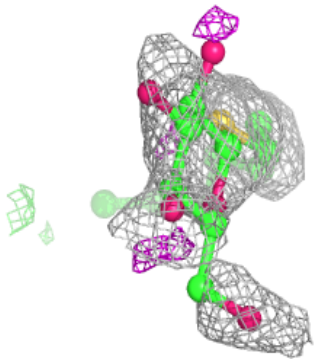


Electron density around HTG h 1202:

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

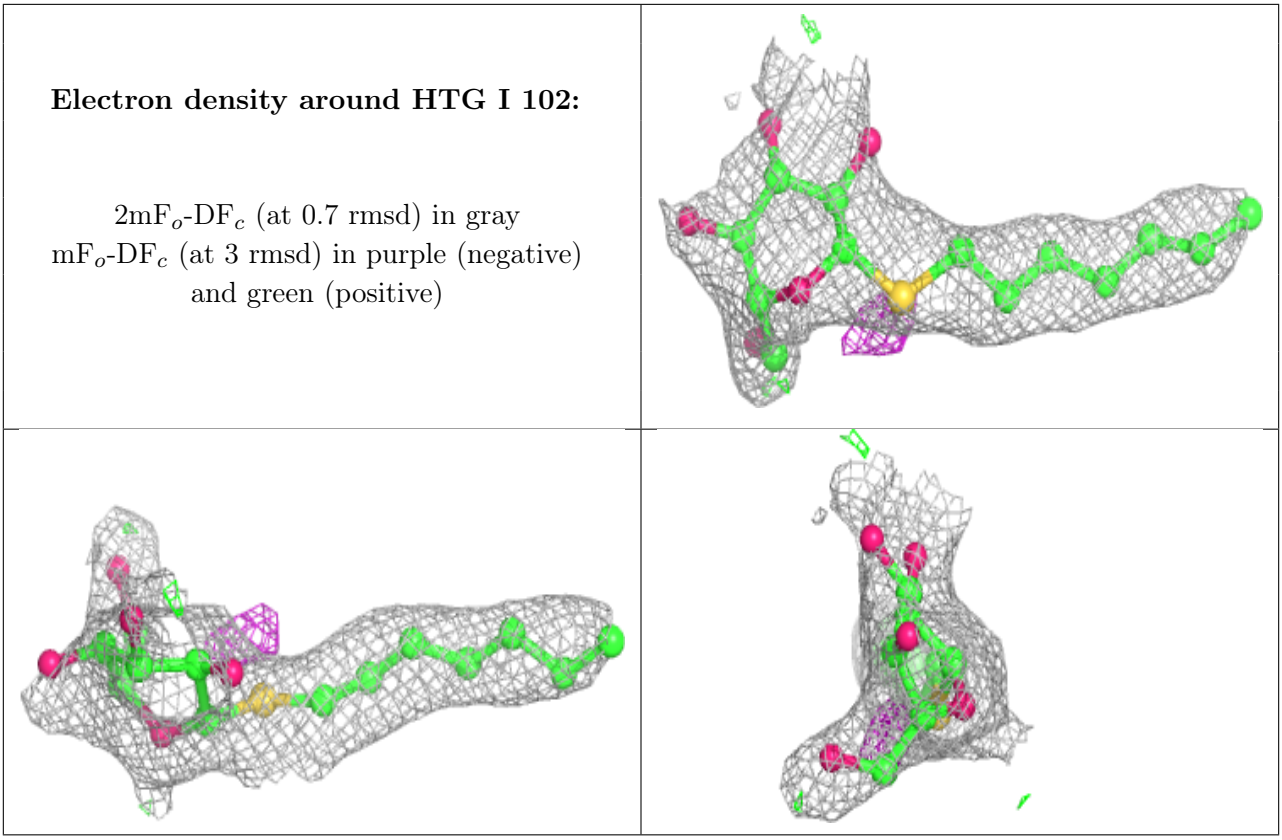






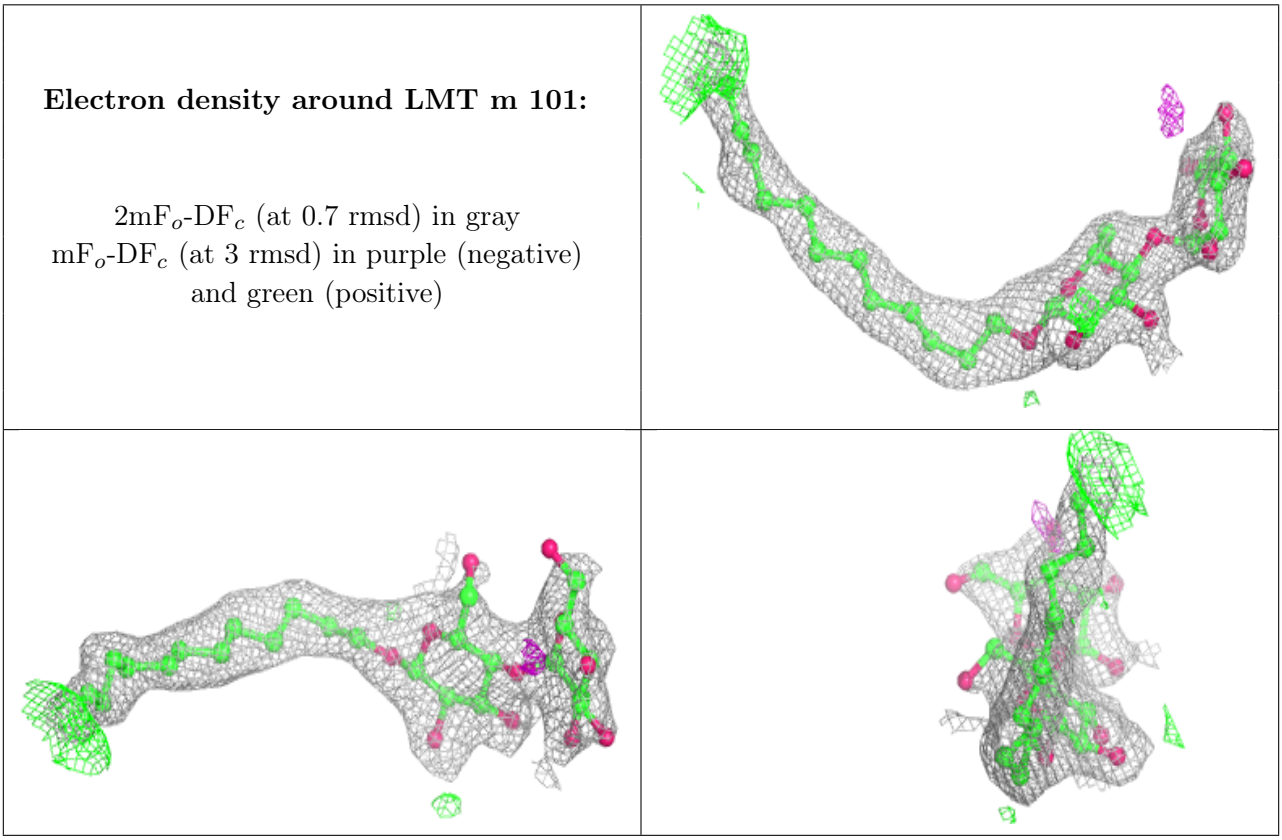
Electron density around HTG I 102:

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



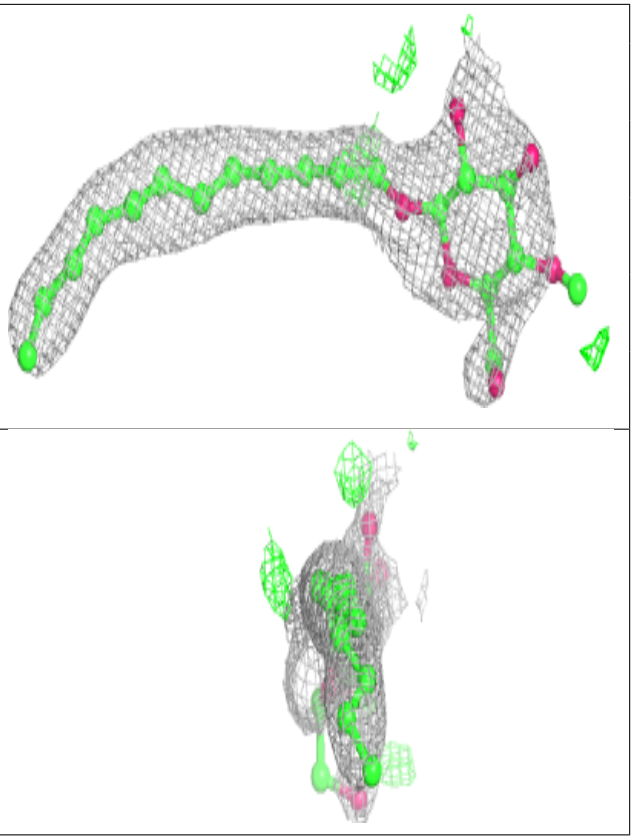
Electron density around LMT m 101:

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



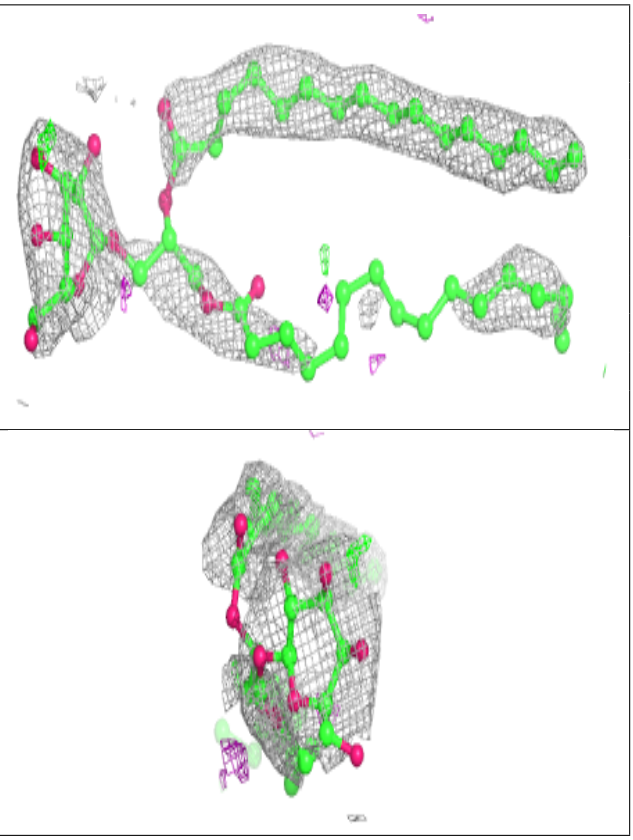
Electron density around LMT b 624:

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



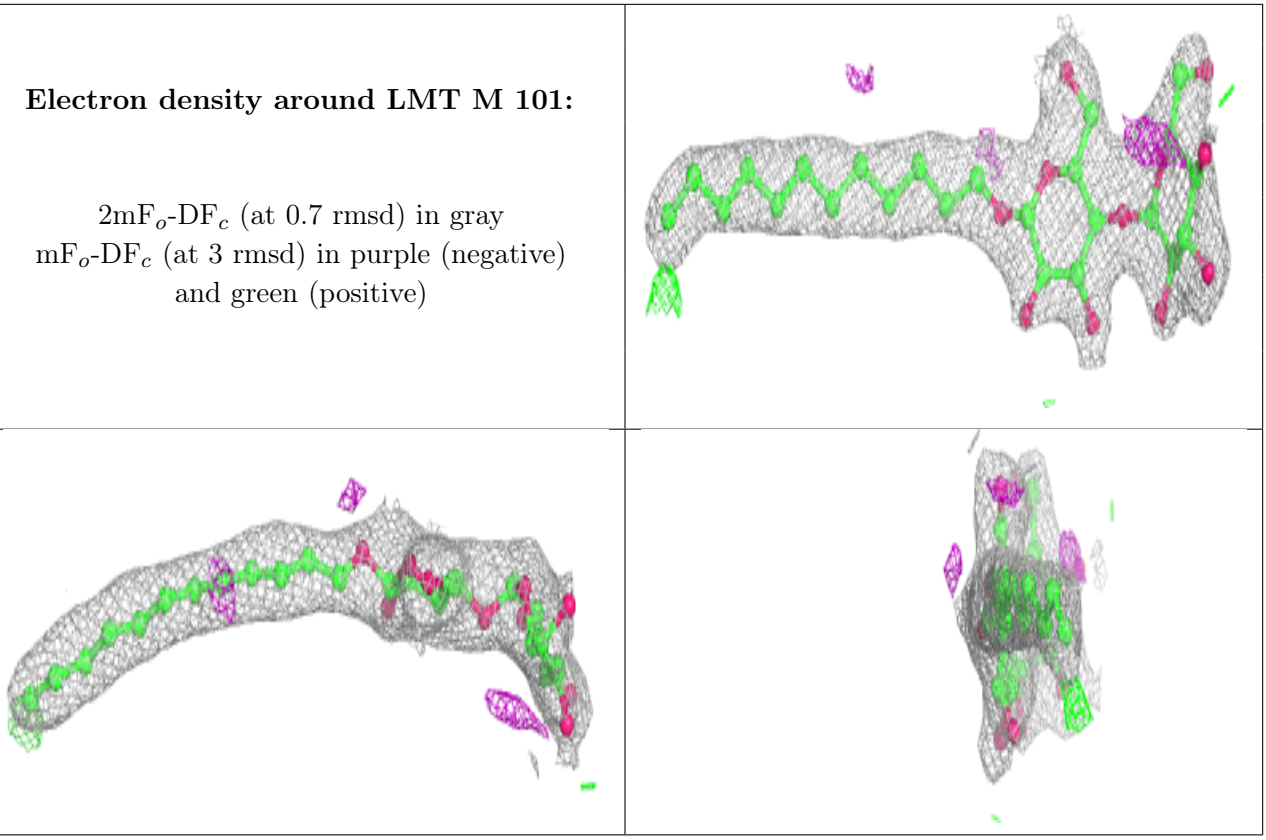
Electron density around LMG C 532:

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



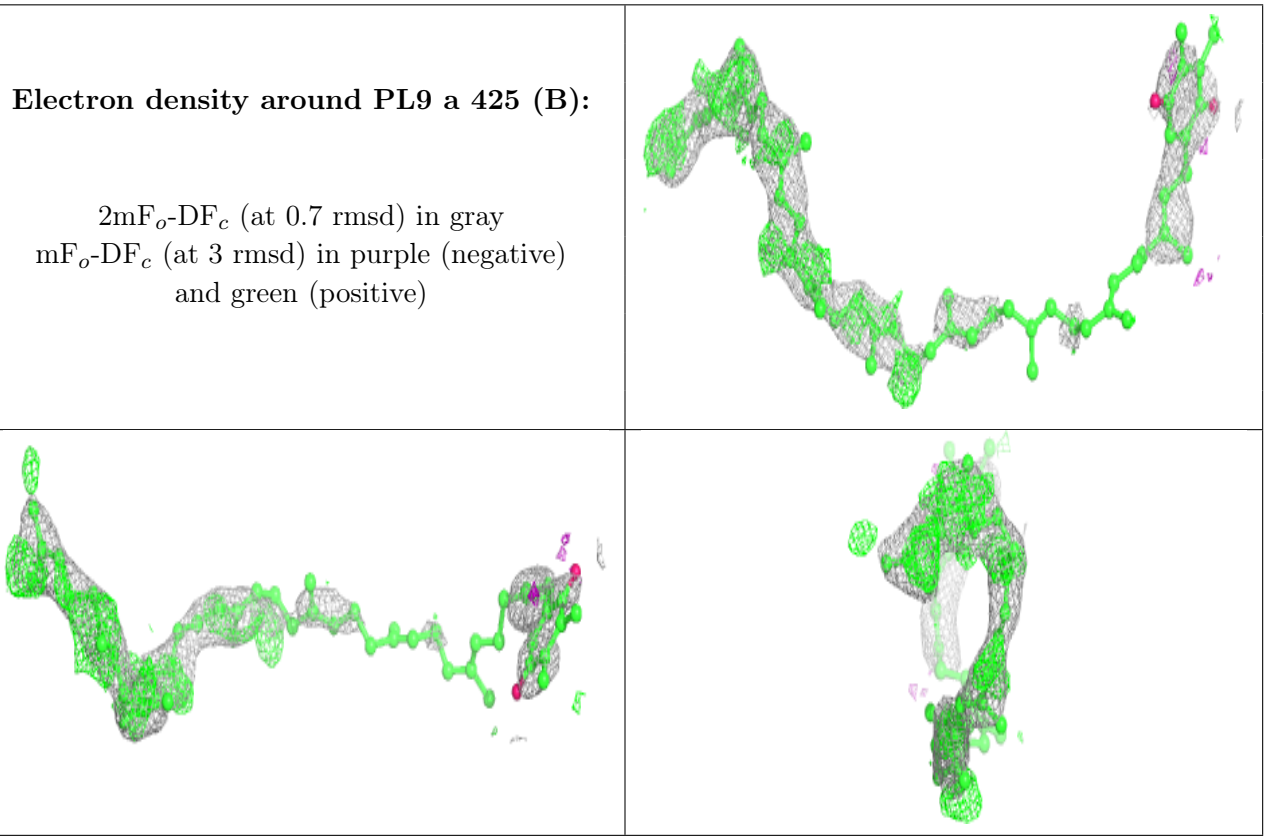
Electron density around LMT M 101:

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



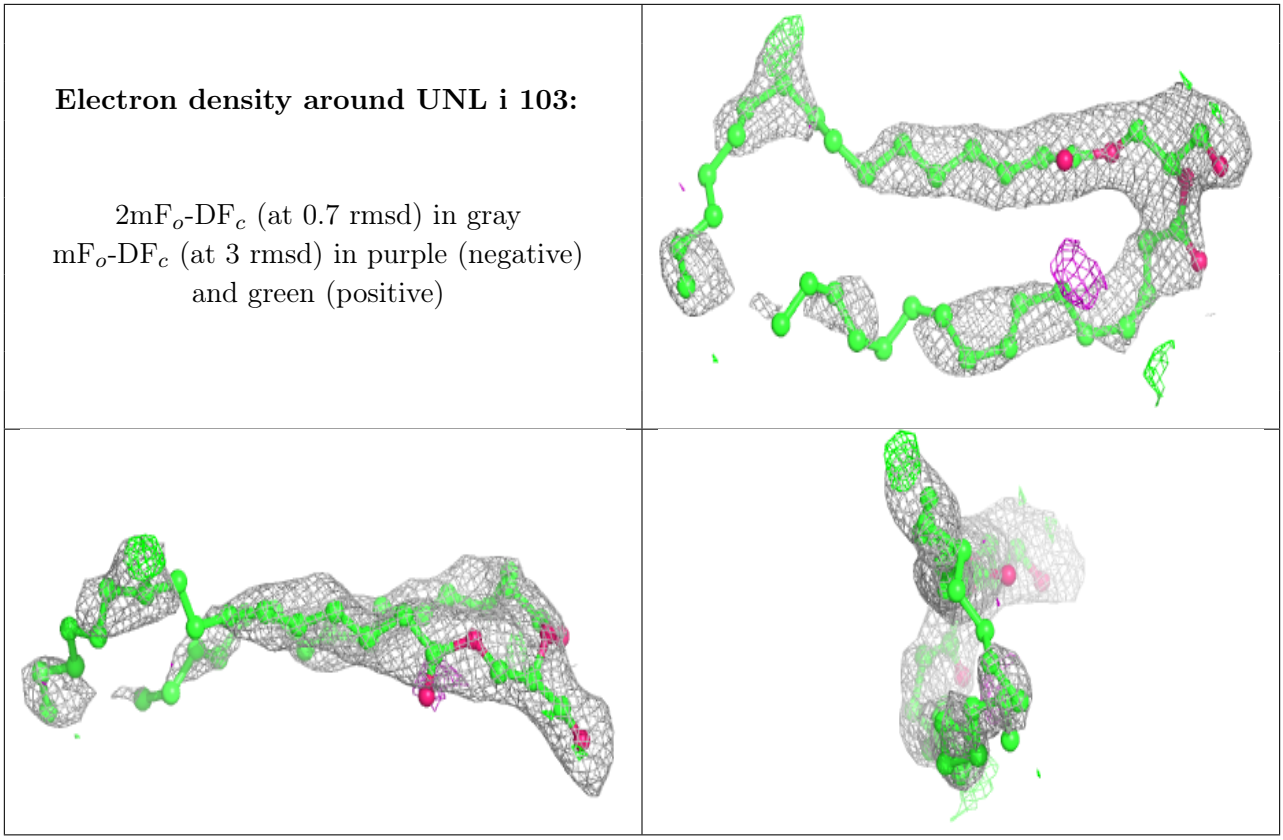
Electron density around PL9 a 425 (B):

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



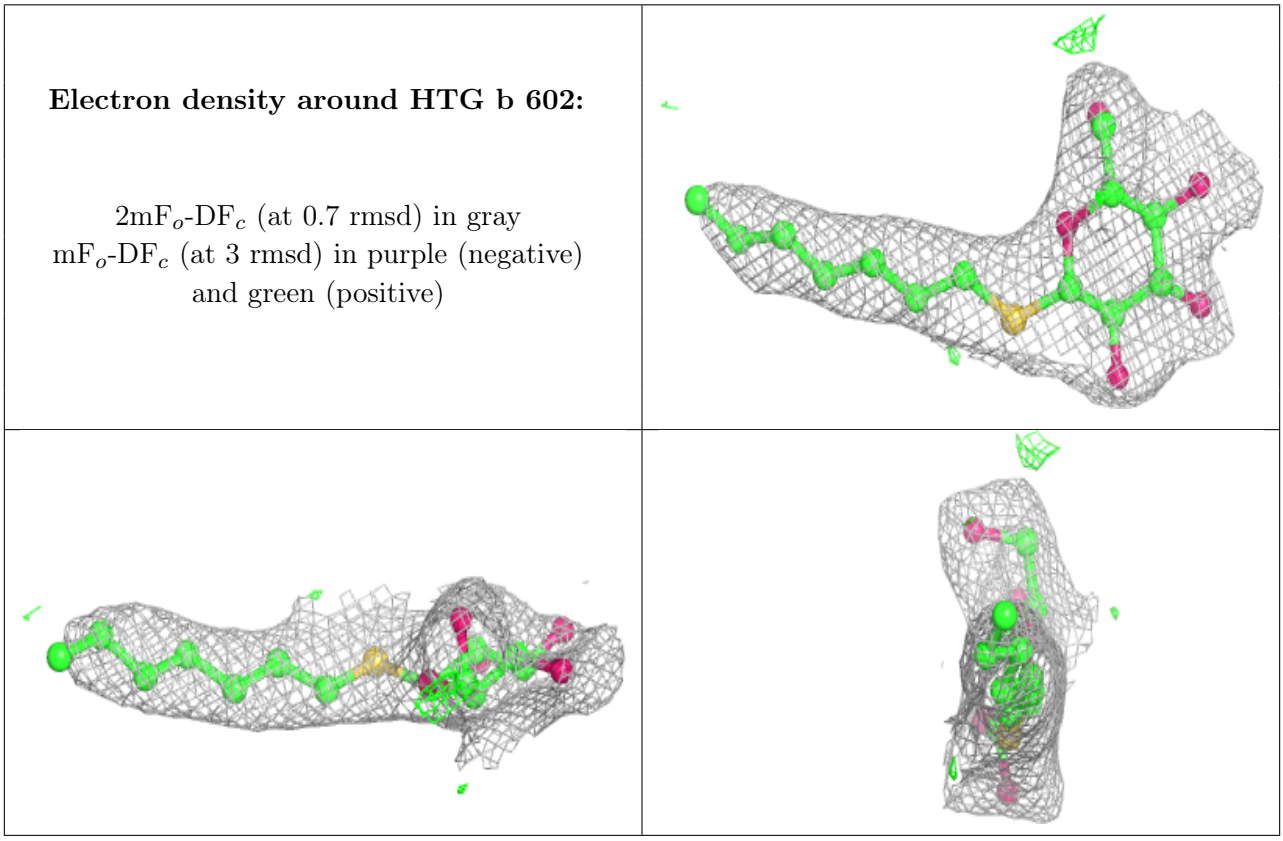
Electron density around UNL i 103:

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



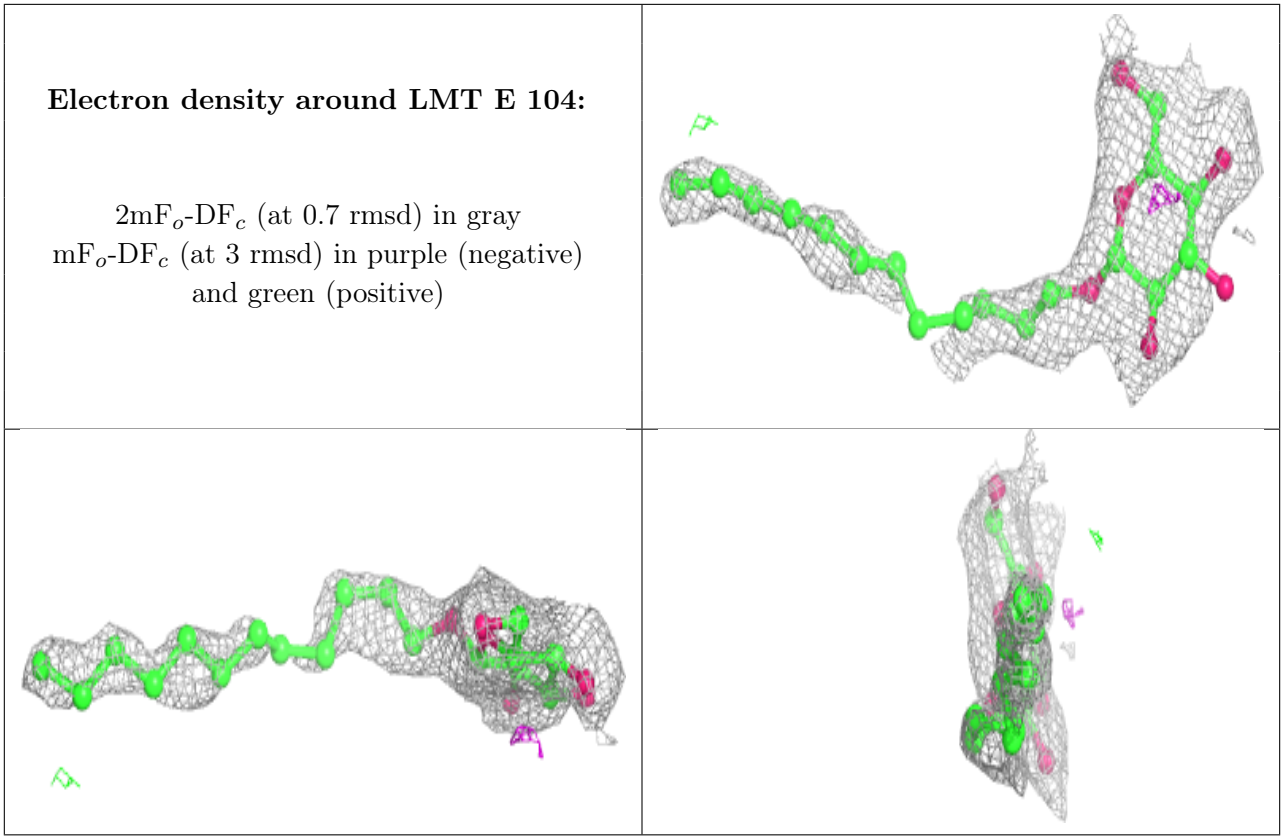
Electron density around HTG b 602:

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



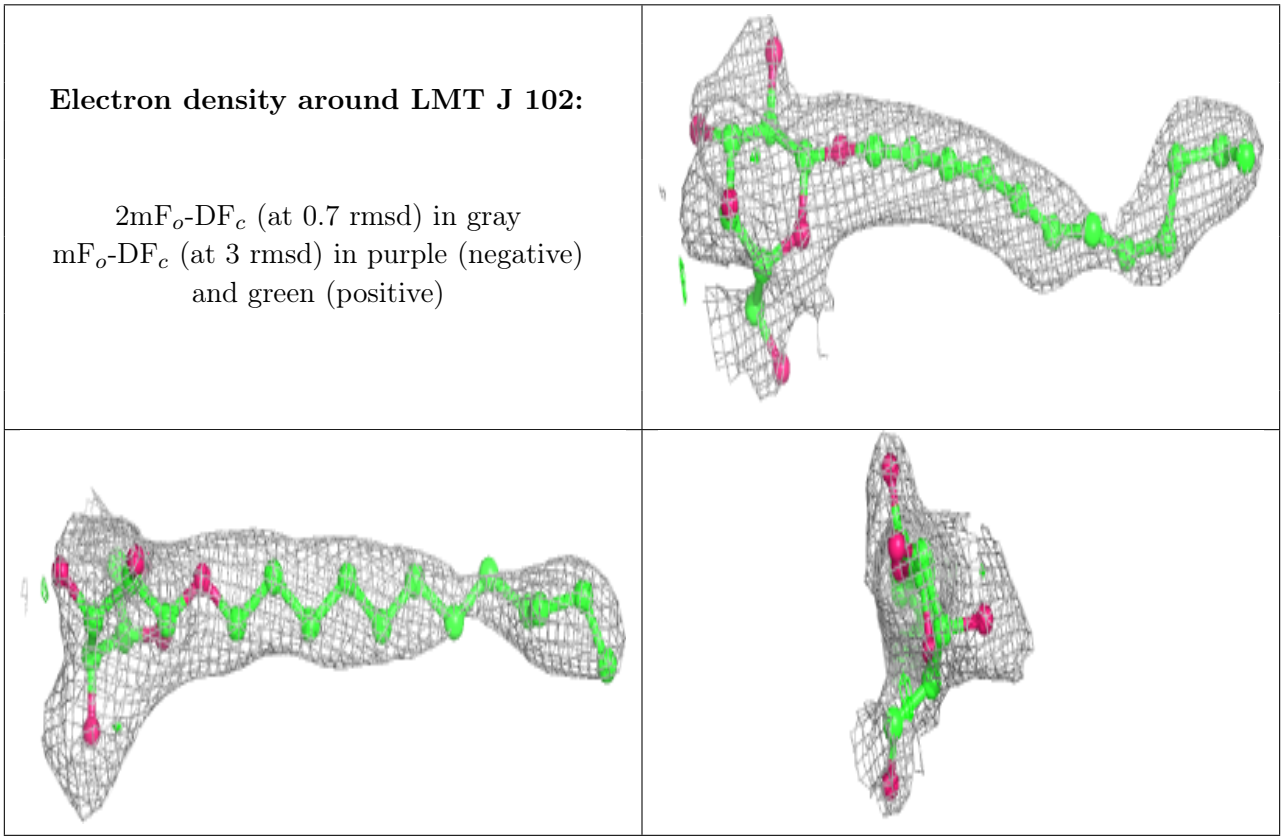
Electron density around LMT E 104:

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



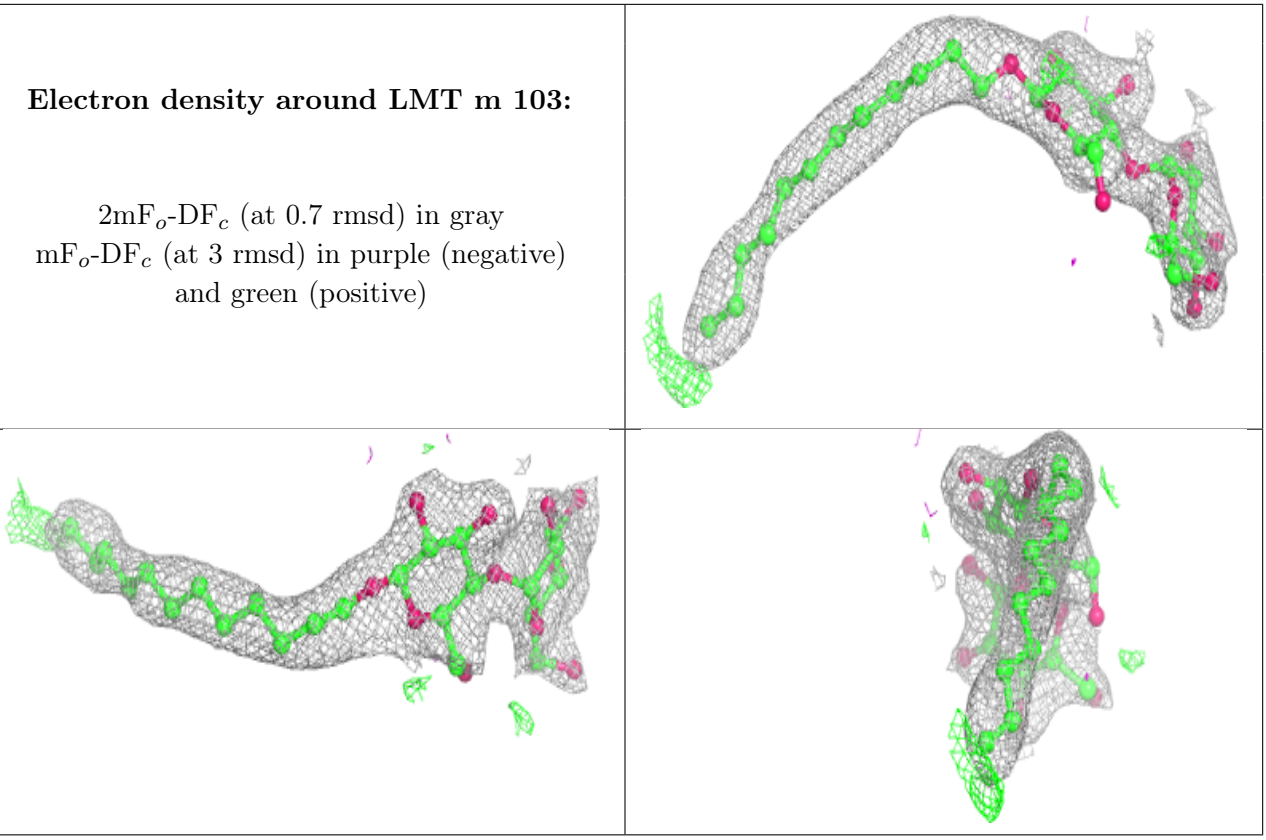
Electron density around LMT J 102:

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



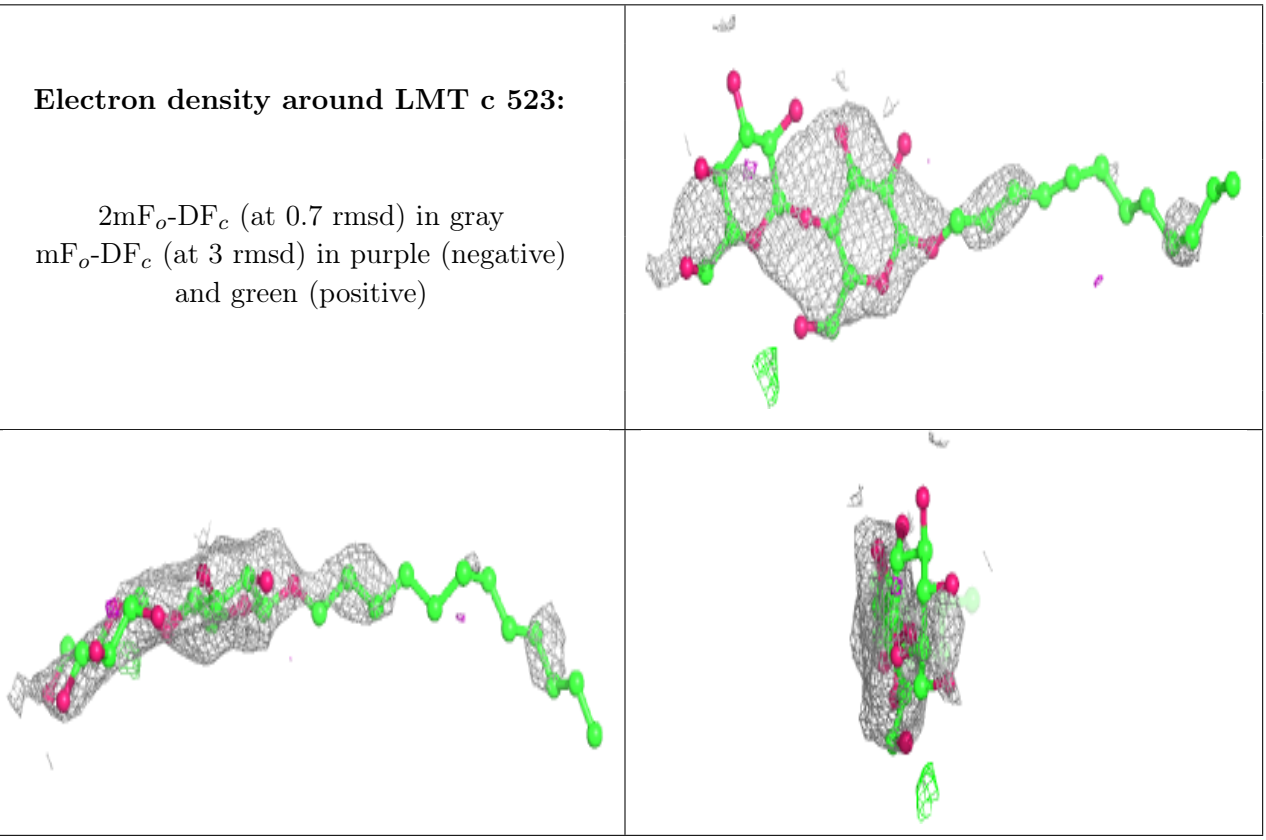
Electron density around LMT m 103:

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



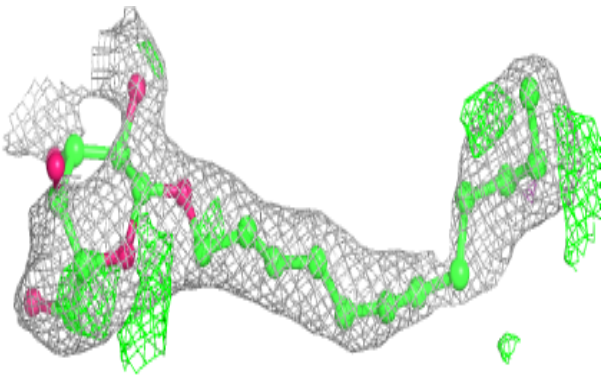
Electron density around LMT c 523:

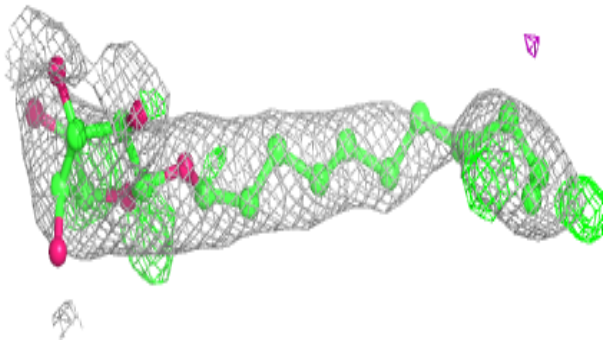
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

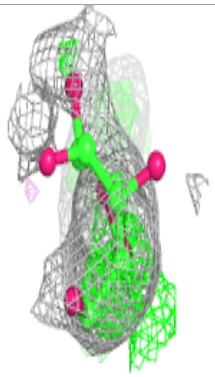


Electron density around LMT T 104:

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

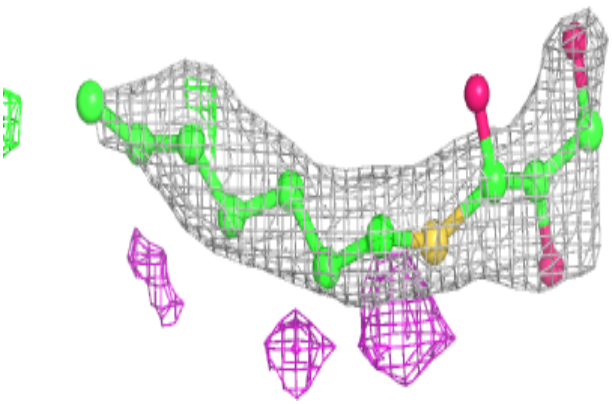


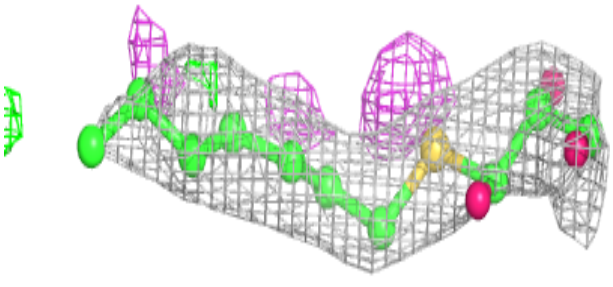


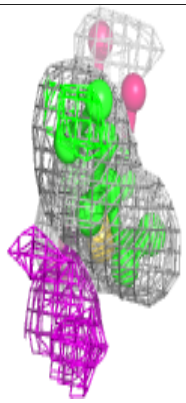


Electron density around HTG u 201:

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

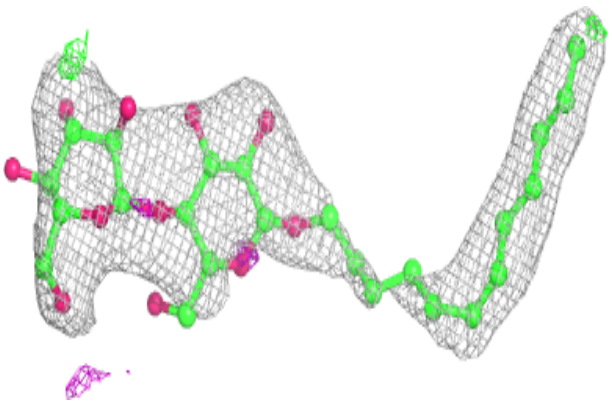


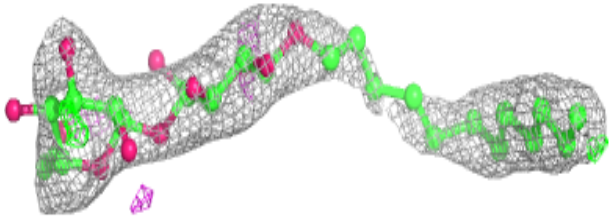


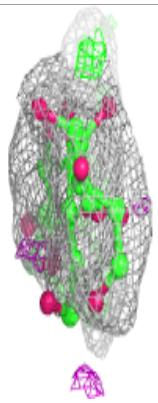


Electron density around LMT Z 101:

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

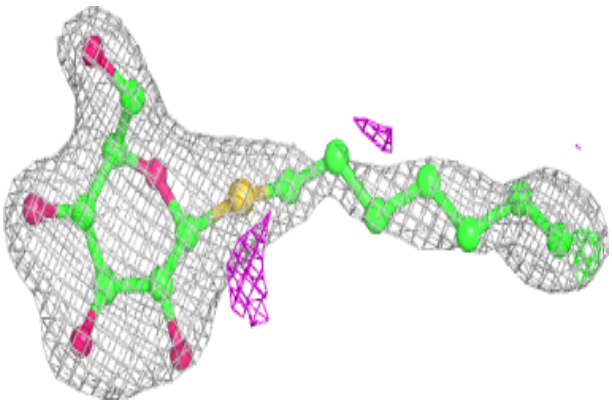


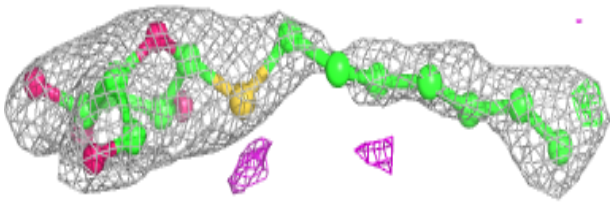


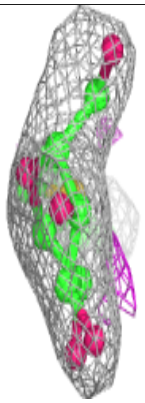


Electron density around HTG C 523:

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

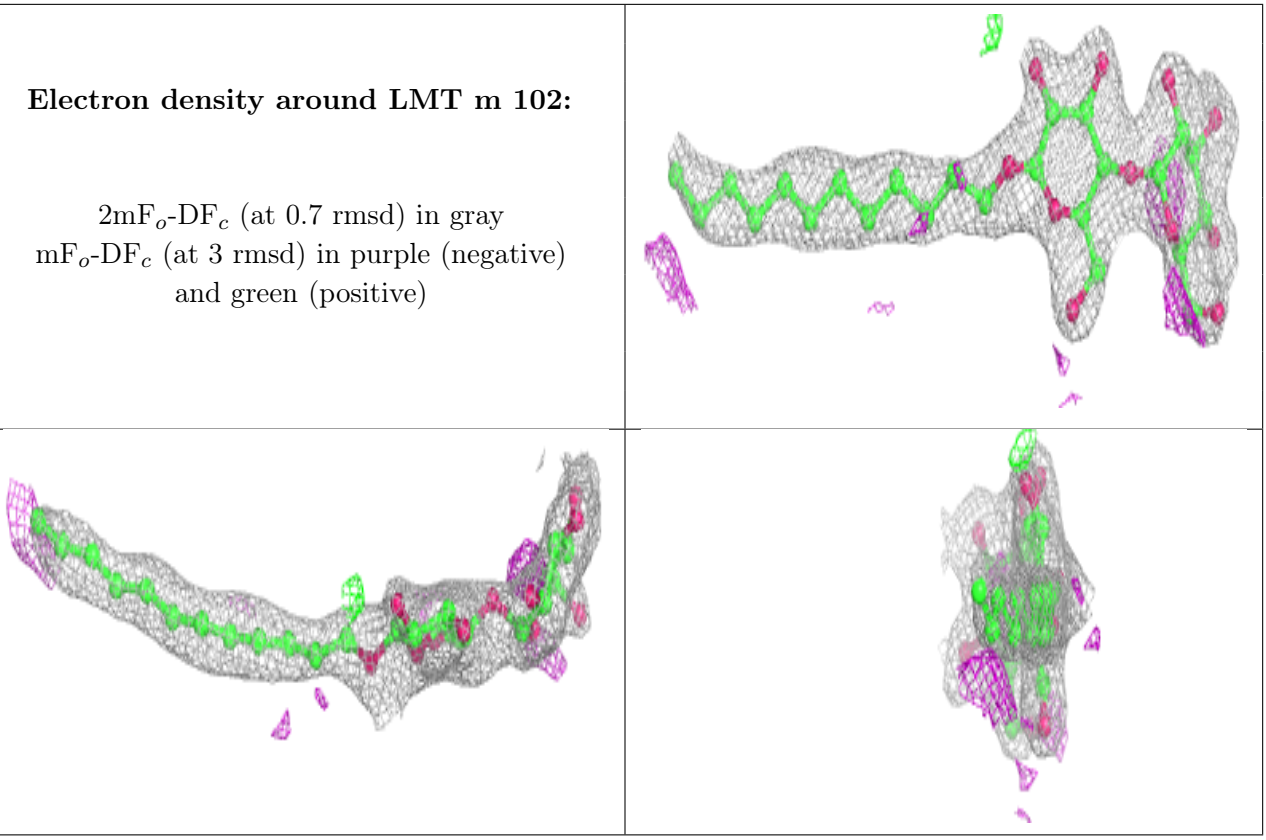






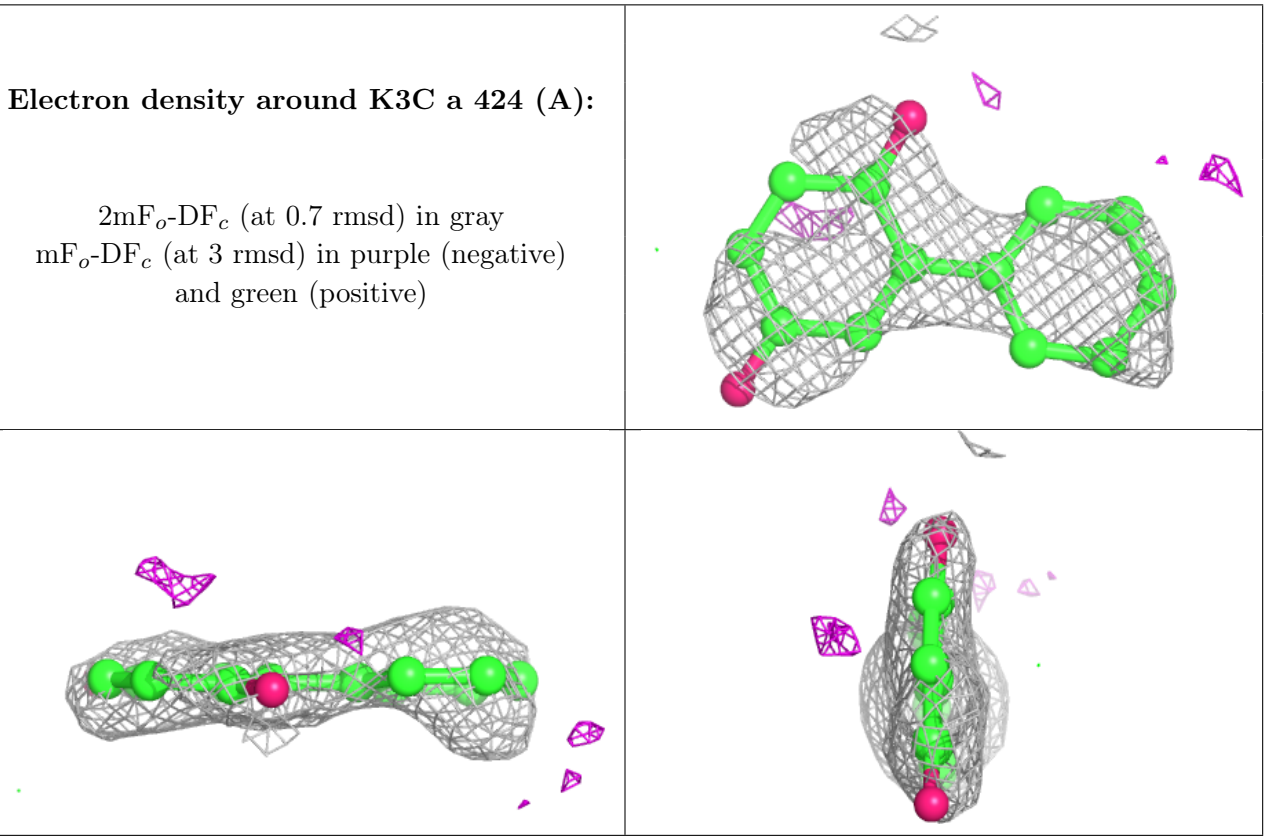
Electron density around LMT m 102:

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



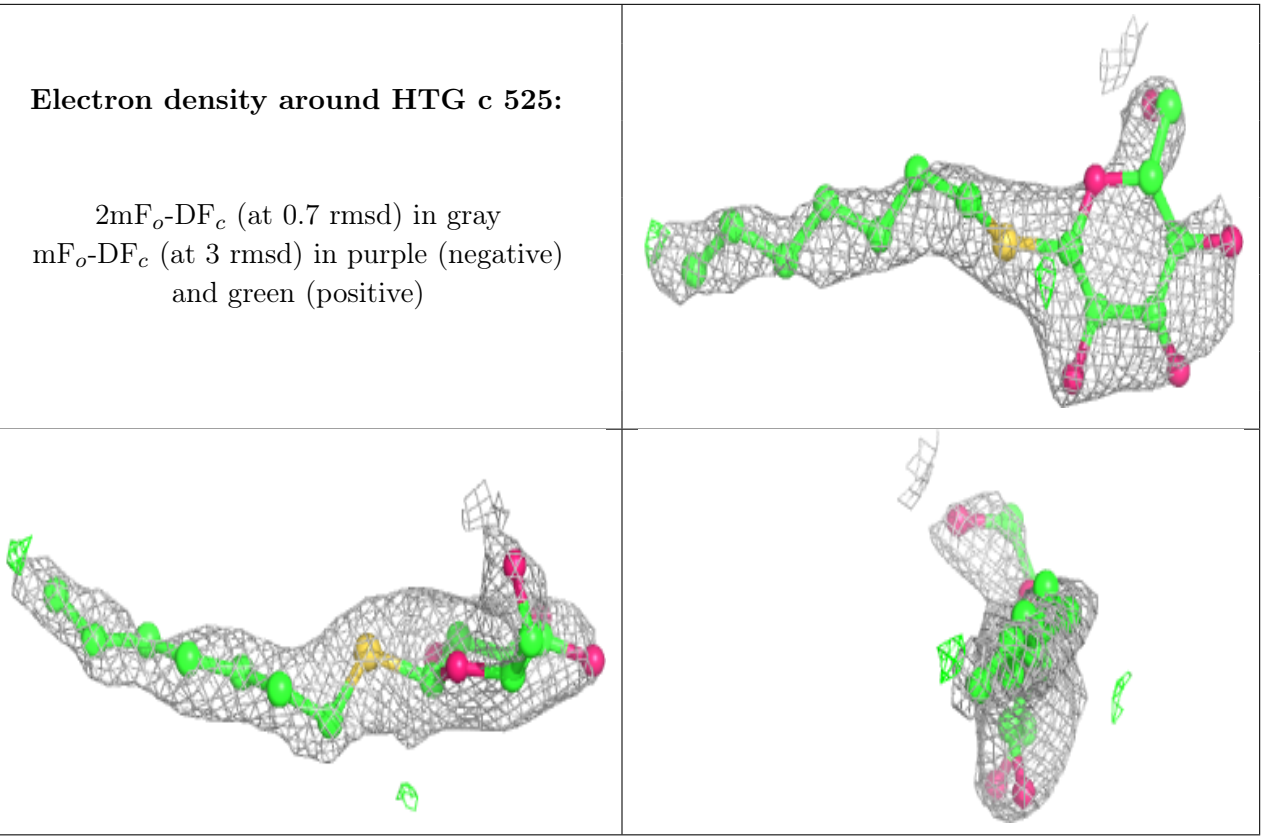
Electron density around K3C a 424 (A):

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



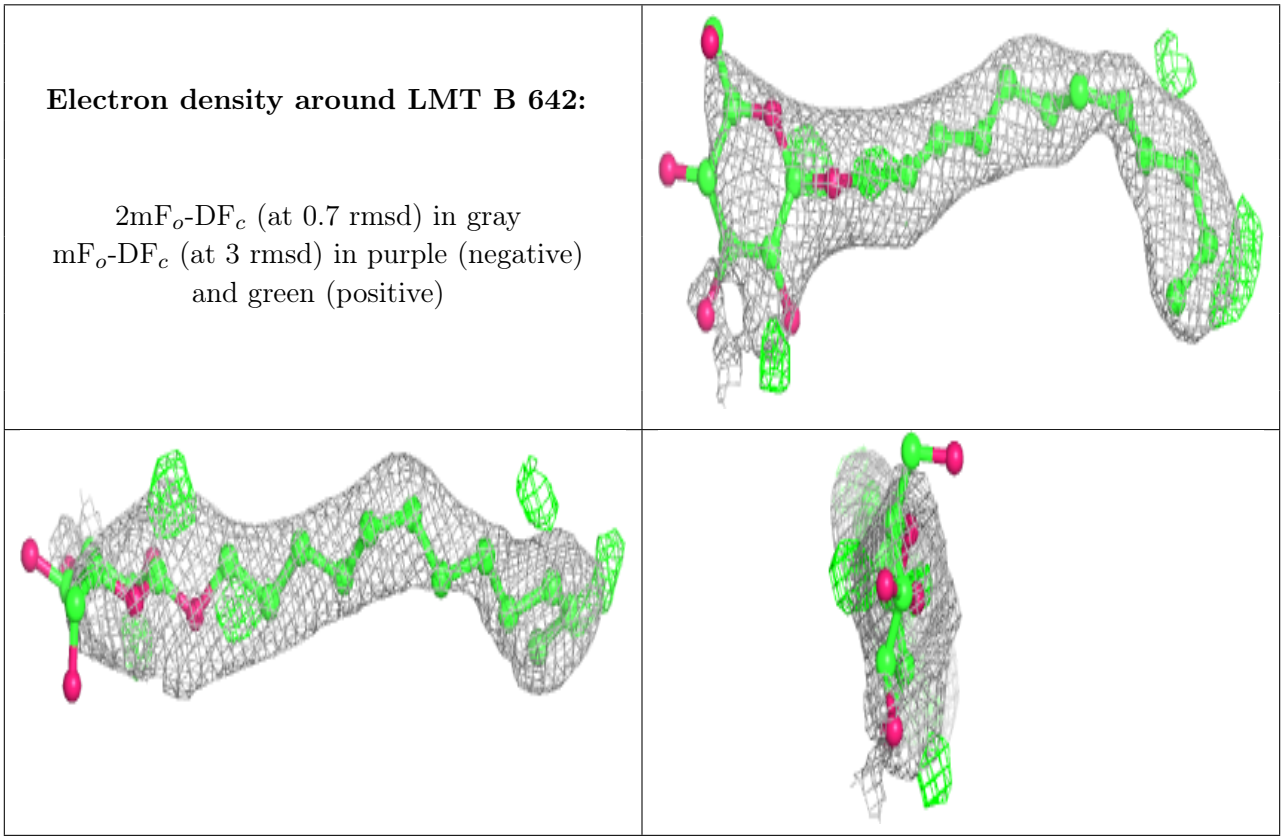
Electron density around HTG c 525:

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



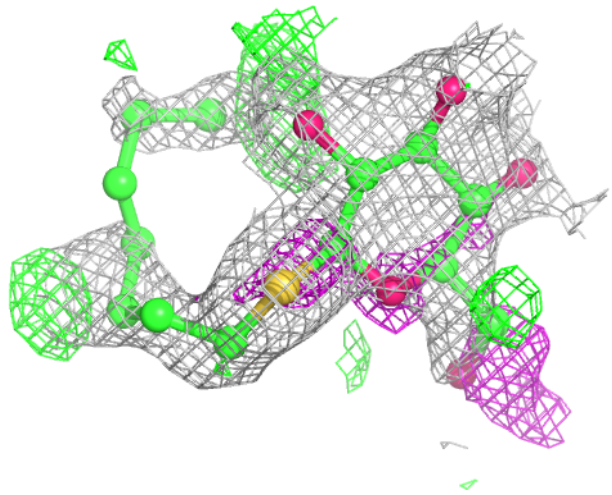
Electron density around LMT B 642:

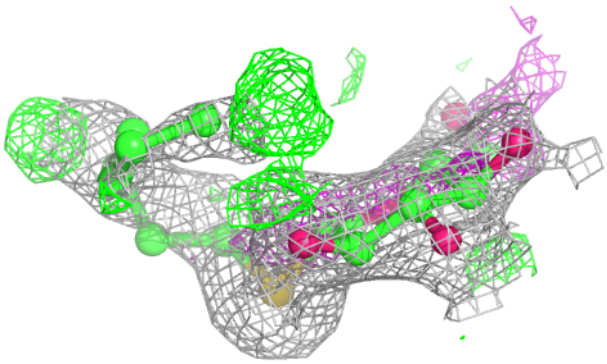
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

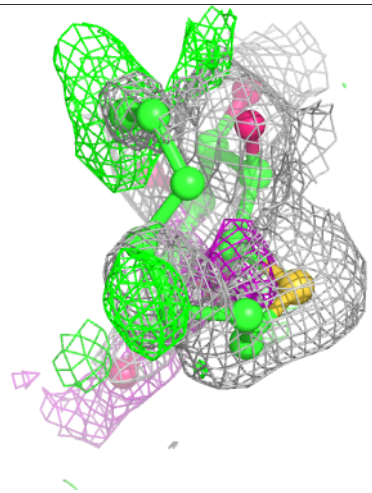


Electron density around HTG b 625:

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

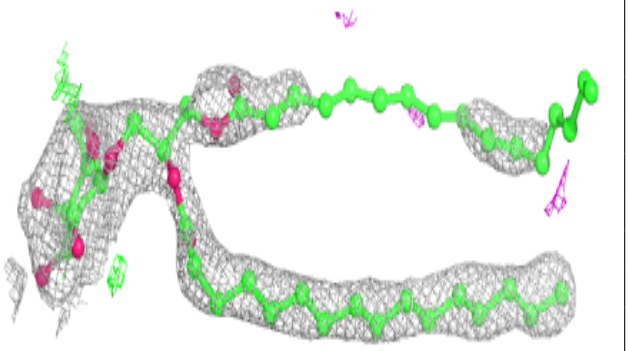


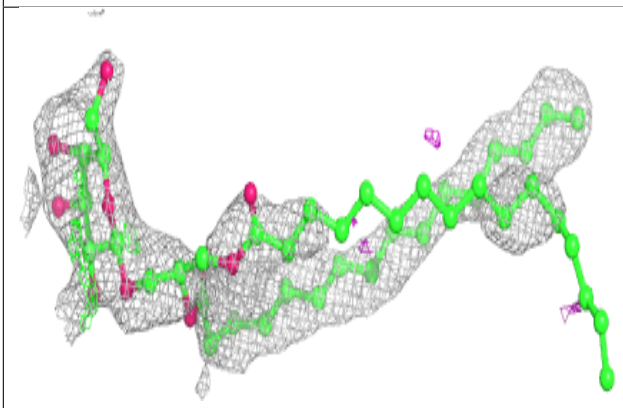


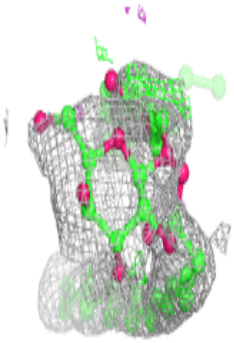


Electron density around LMG c 522:

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

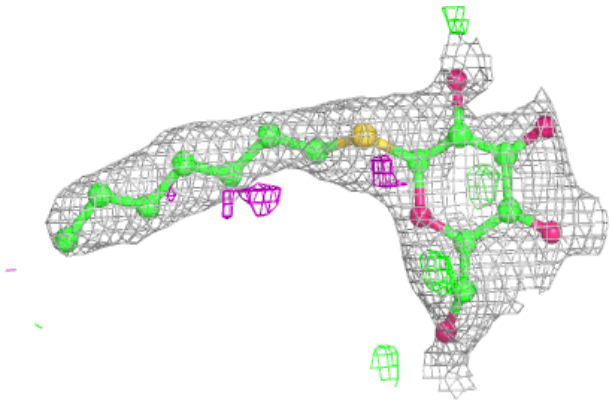


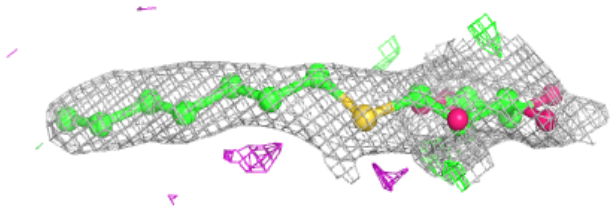


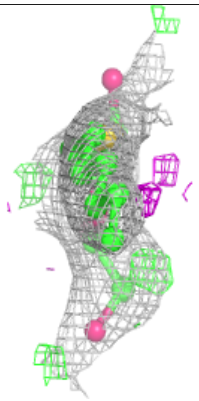


Electron density around HTG B 626:

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

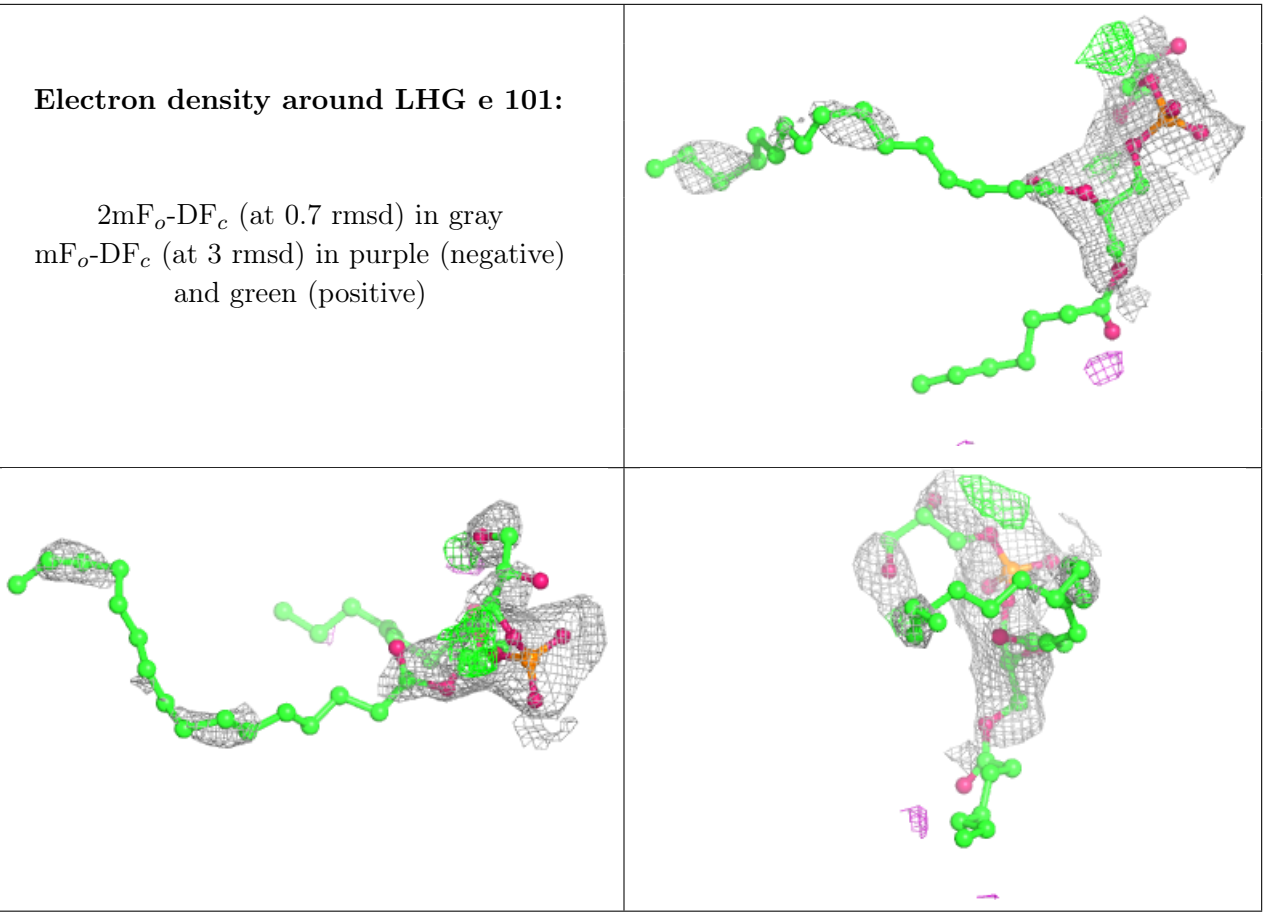






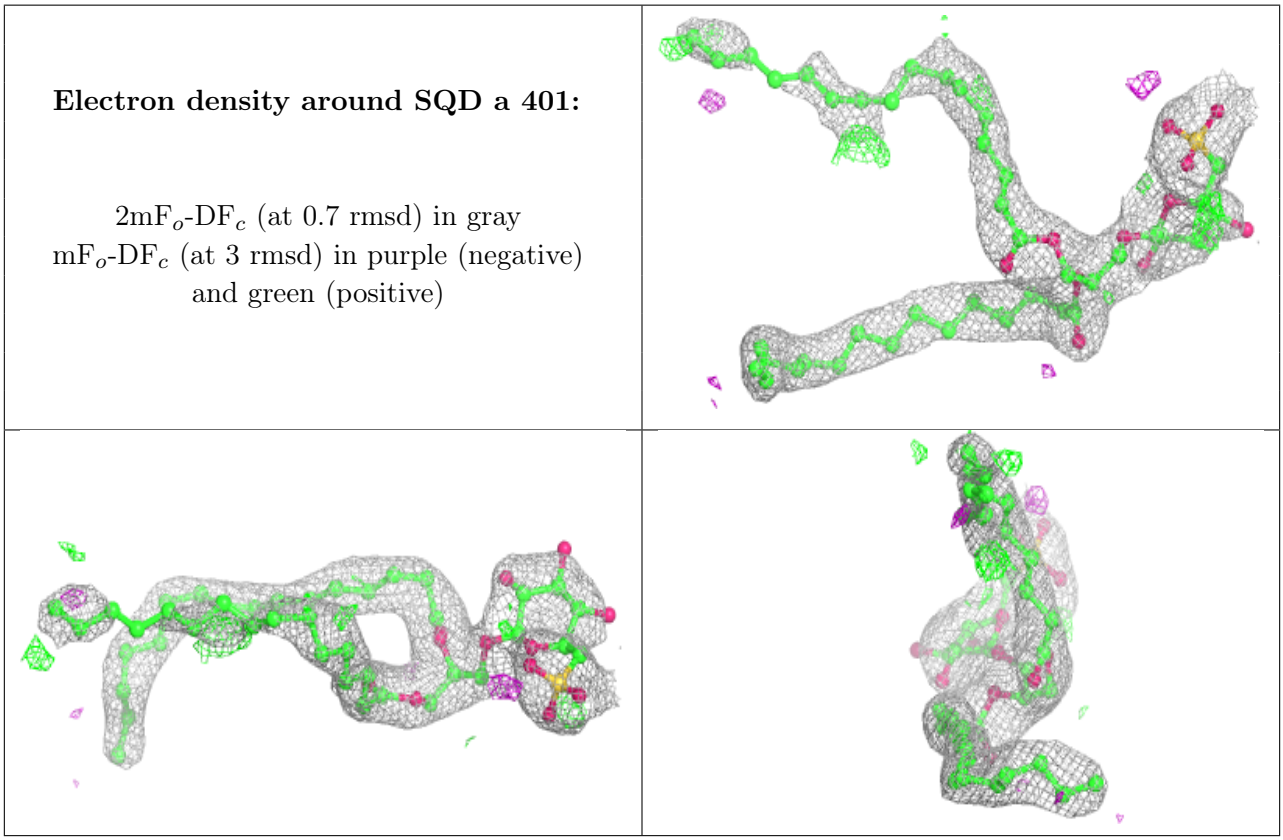
Electron density around LHG e 101:

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



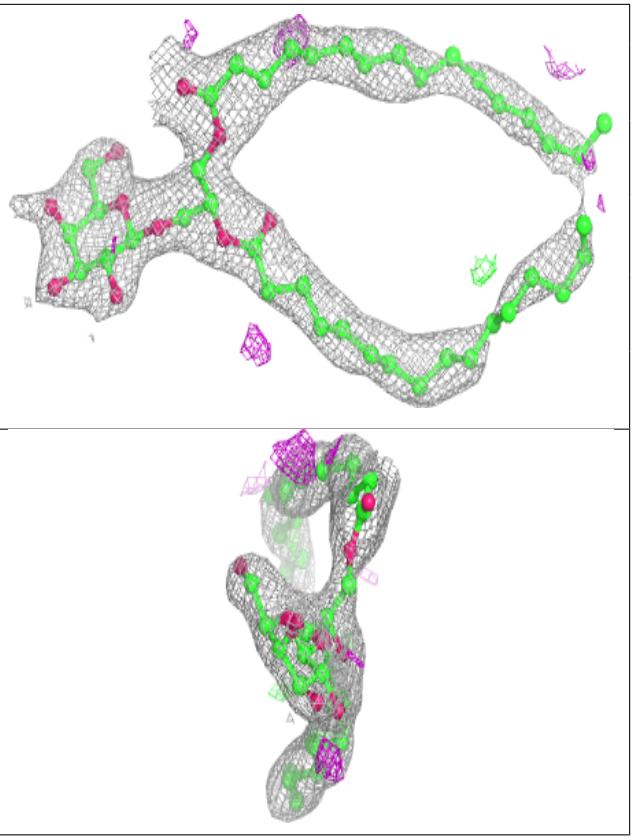
Electron density around SQD a 401:

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



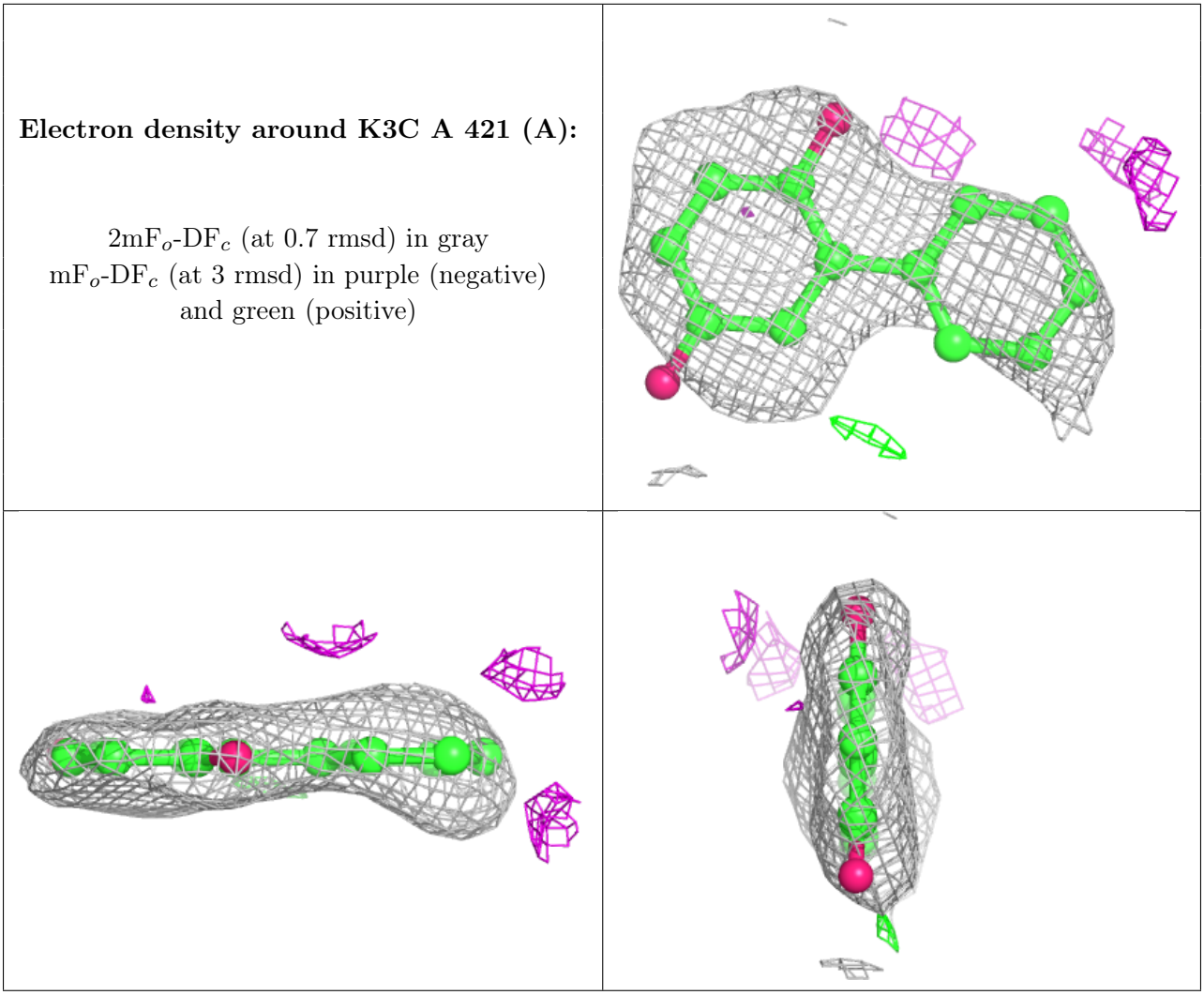
Electron density around LMG a 415:

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



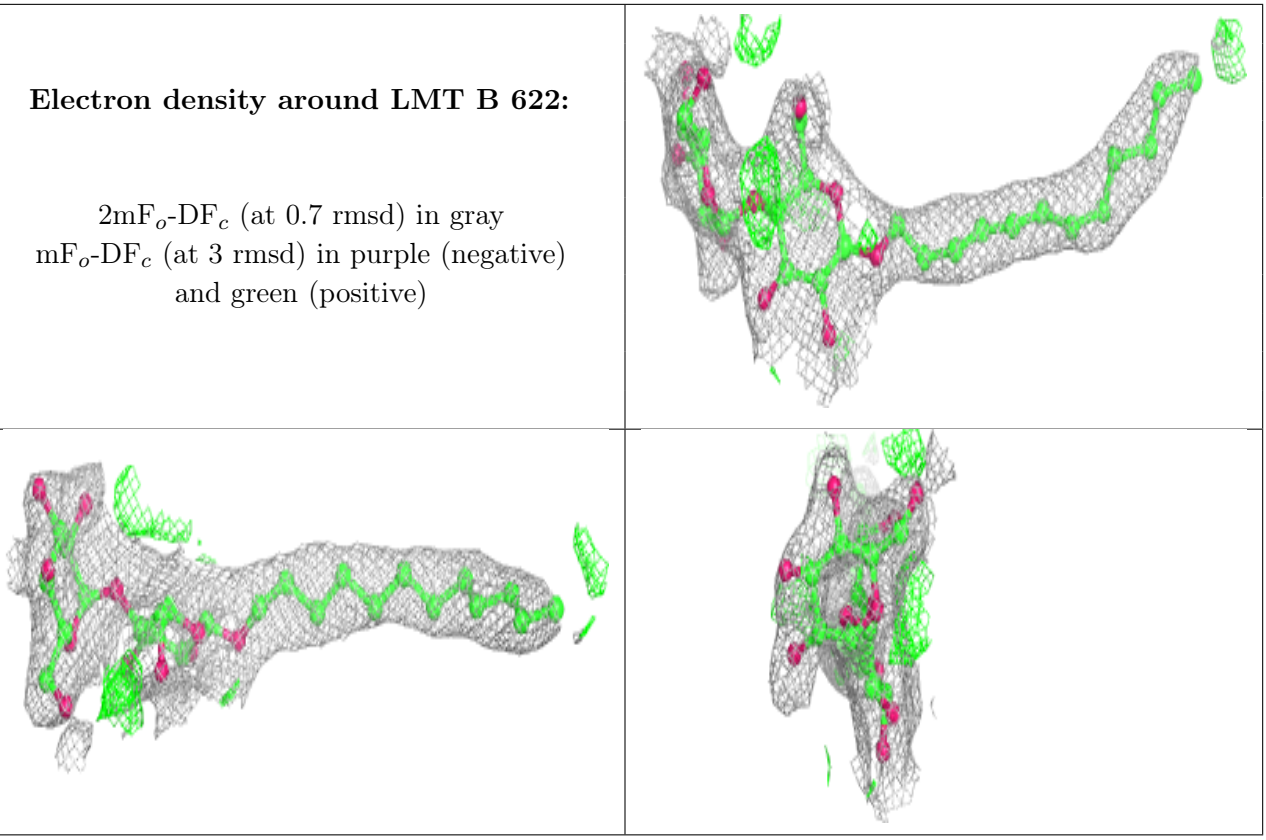
Electron density around K3C A 421 (A):

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



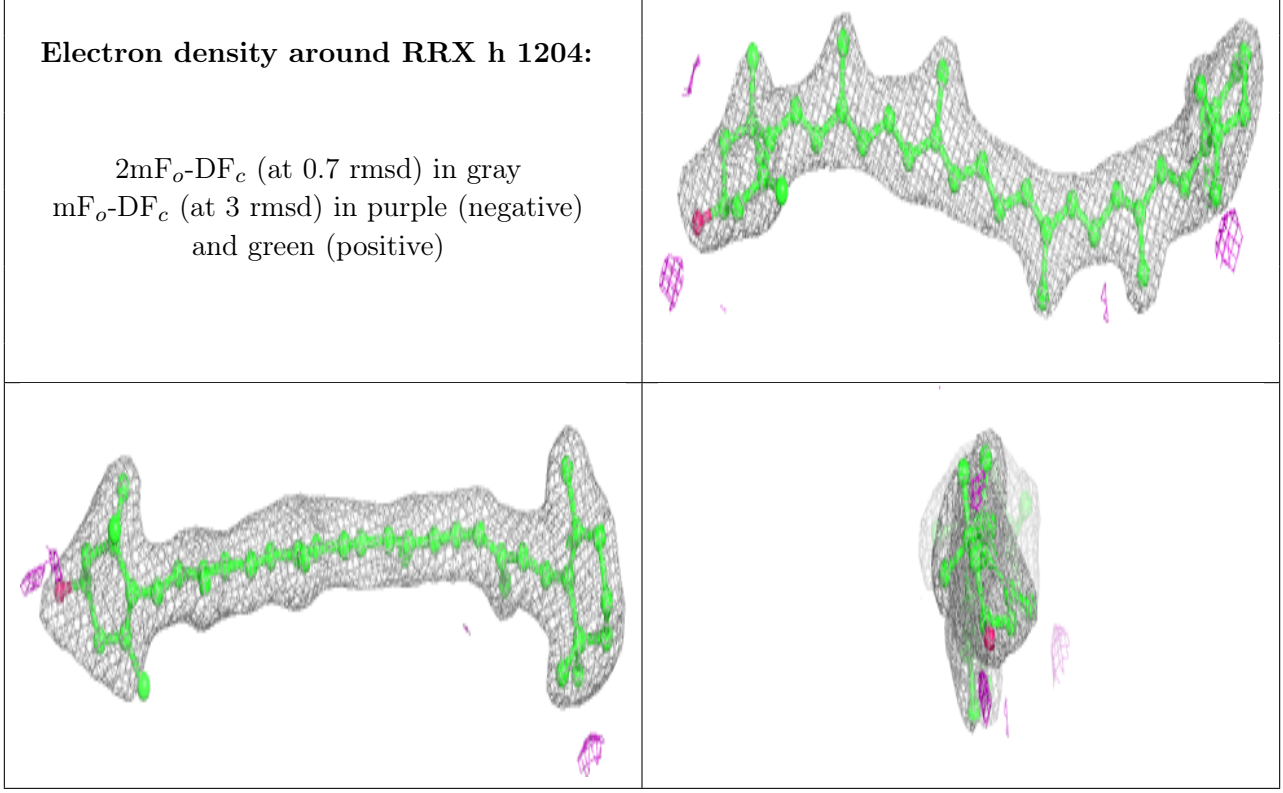
Electron density around LMT B 622:

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



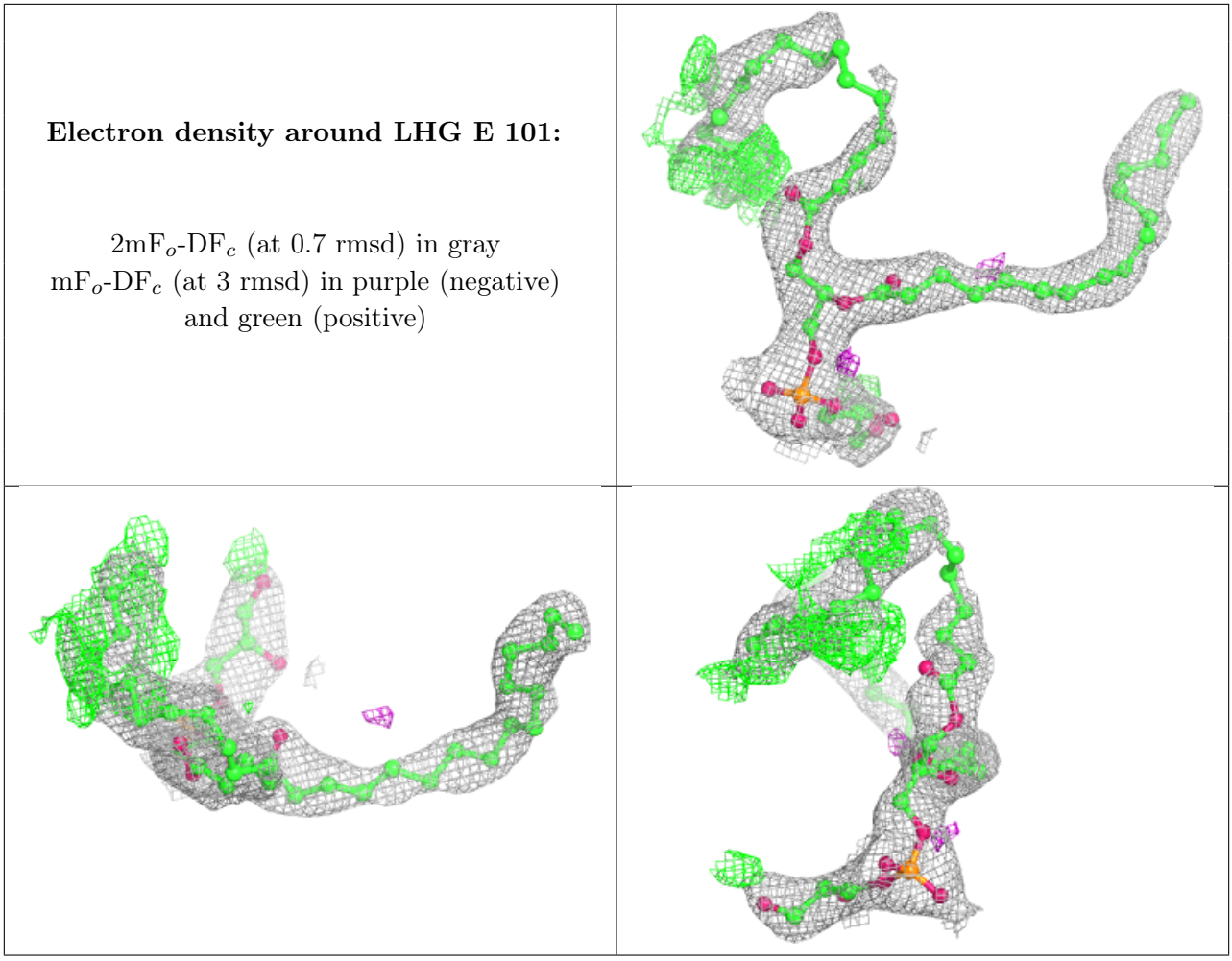
Electron density around RRX h 1204:

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



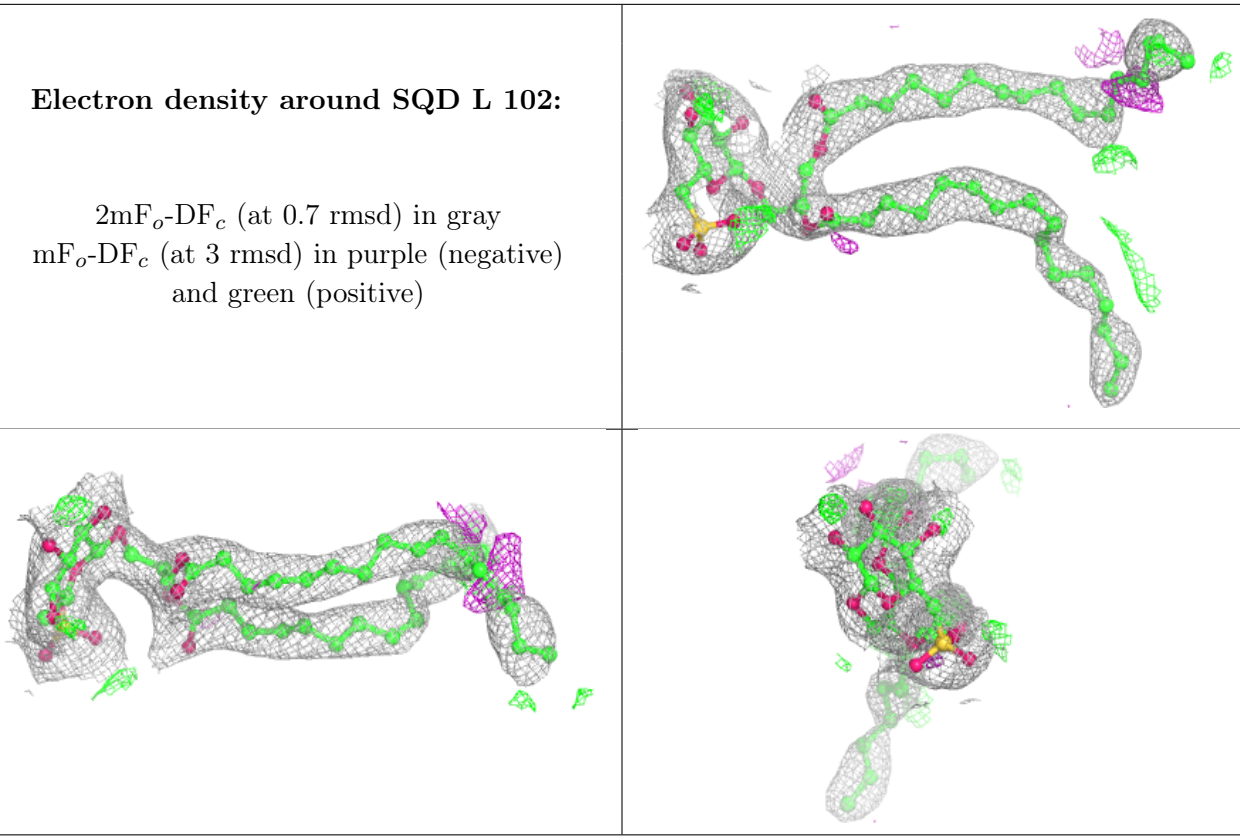
Electron density around LHG E 101:

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



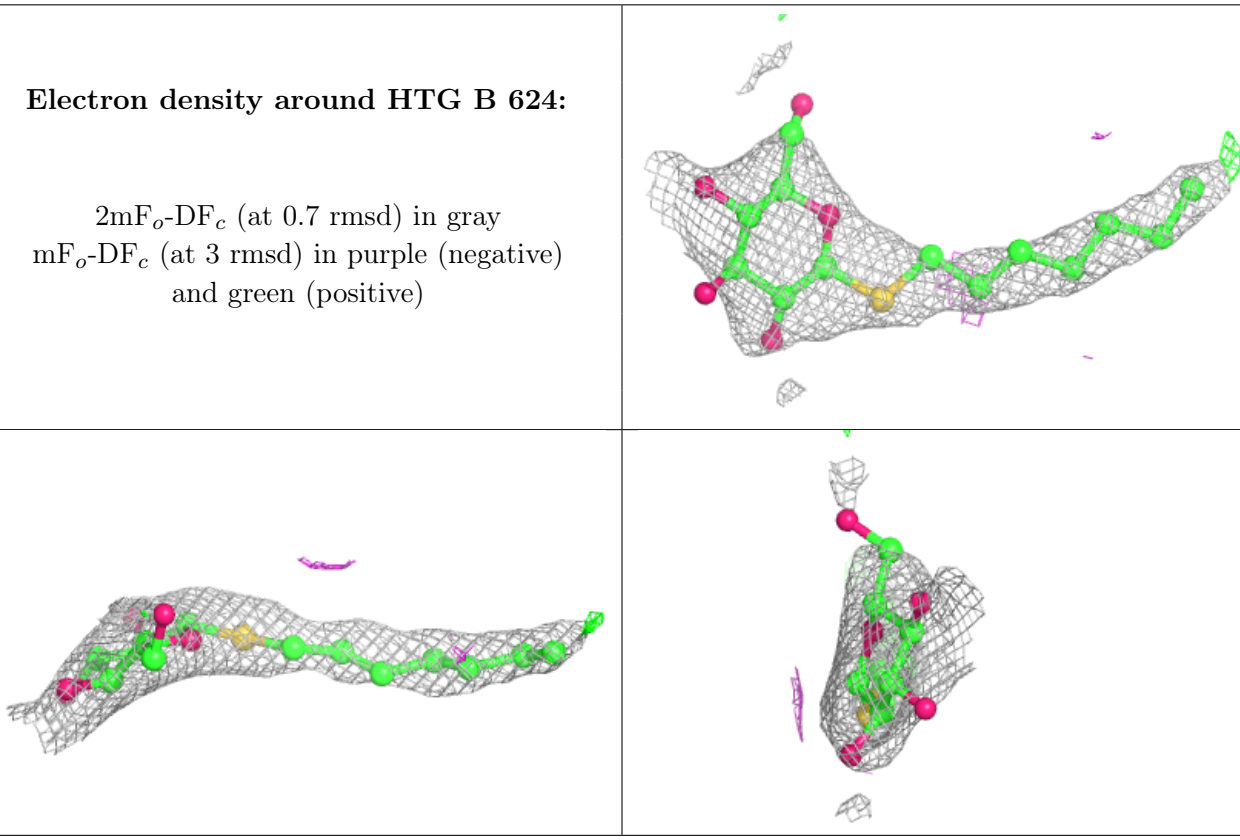
Electron density around SQD L 102:

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



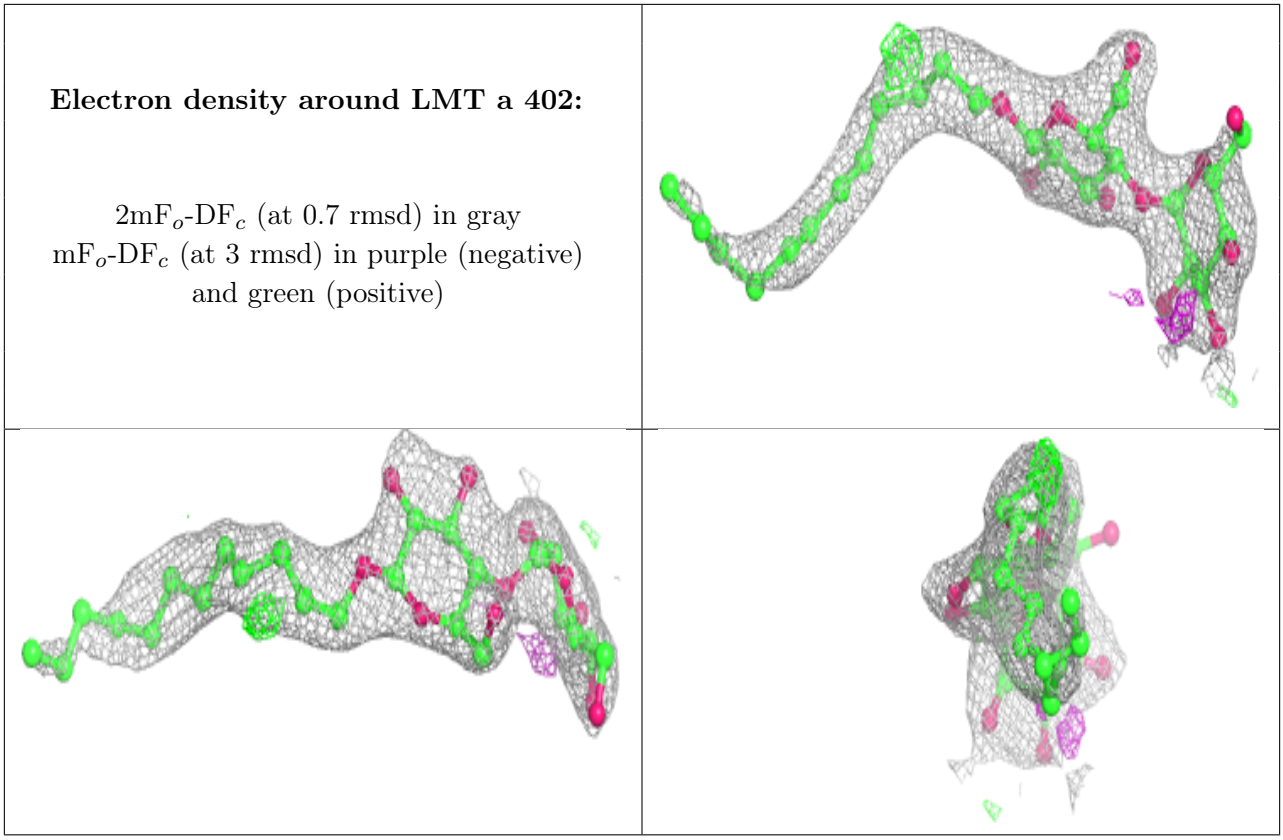
Electron density around HTG B 624:

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



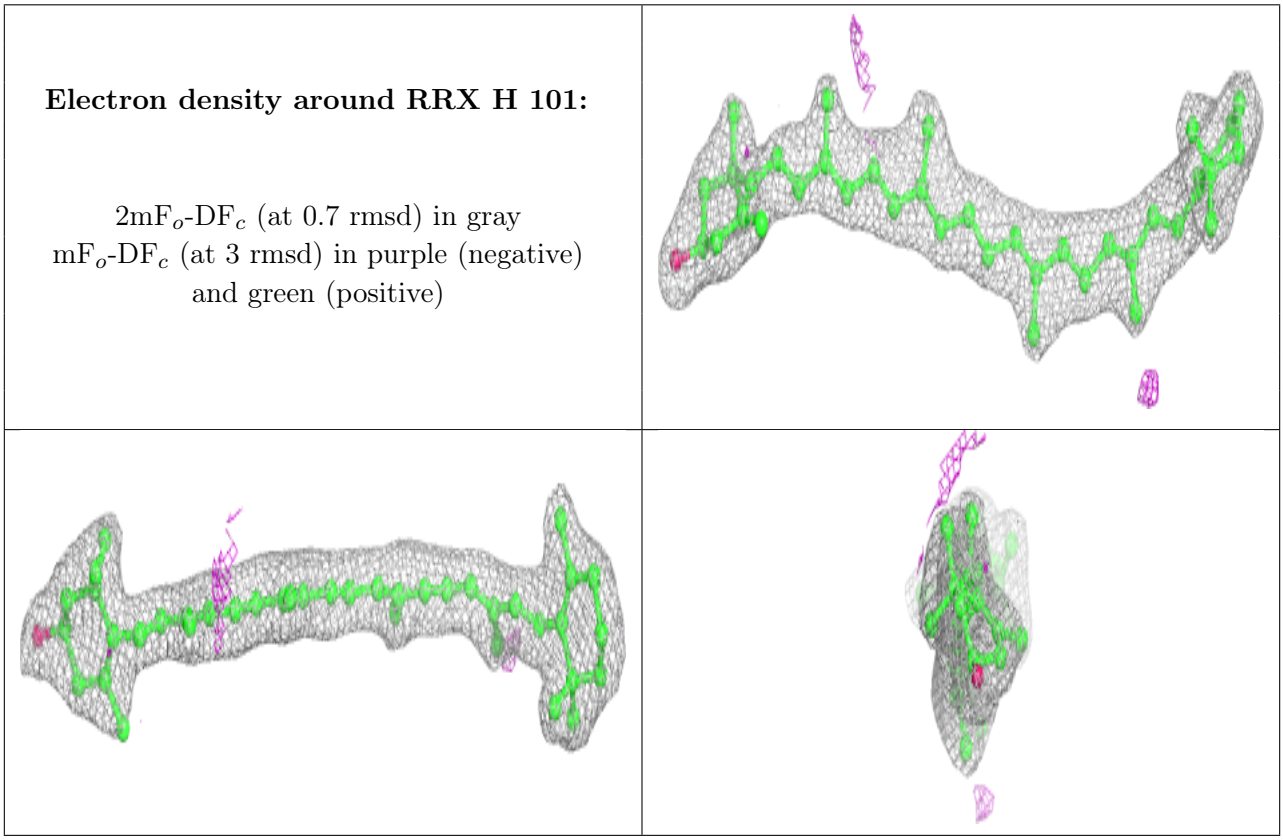
Electron density around LMT a 402:

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



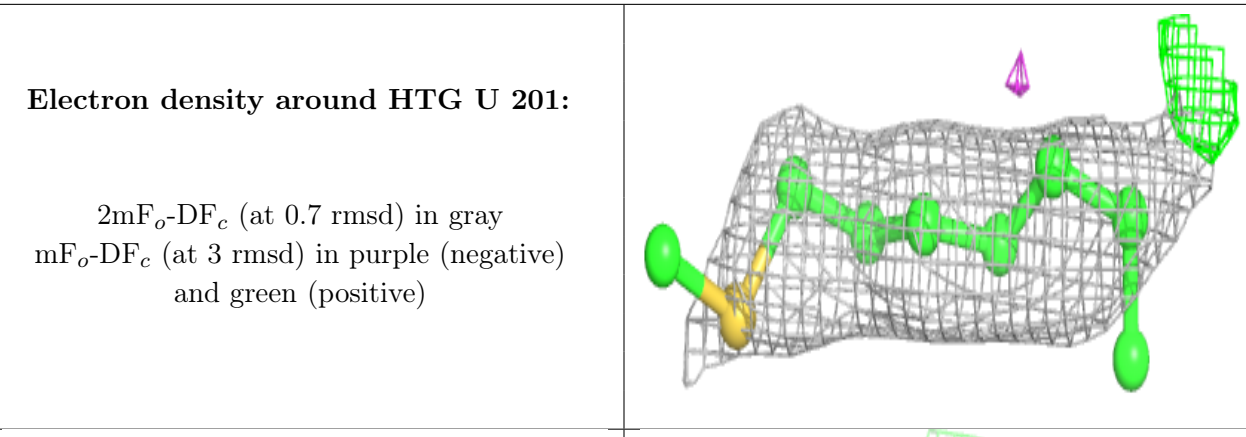
Electron density around RRX H 101:

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



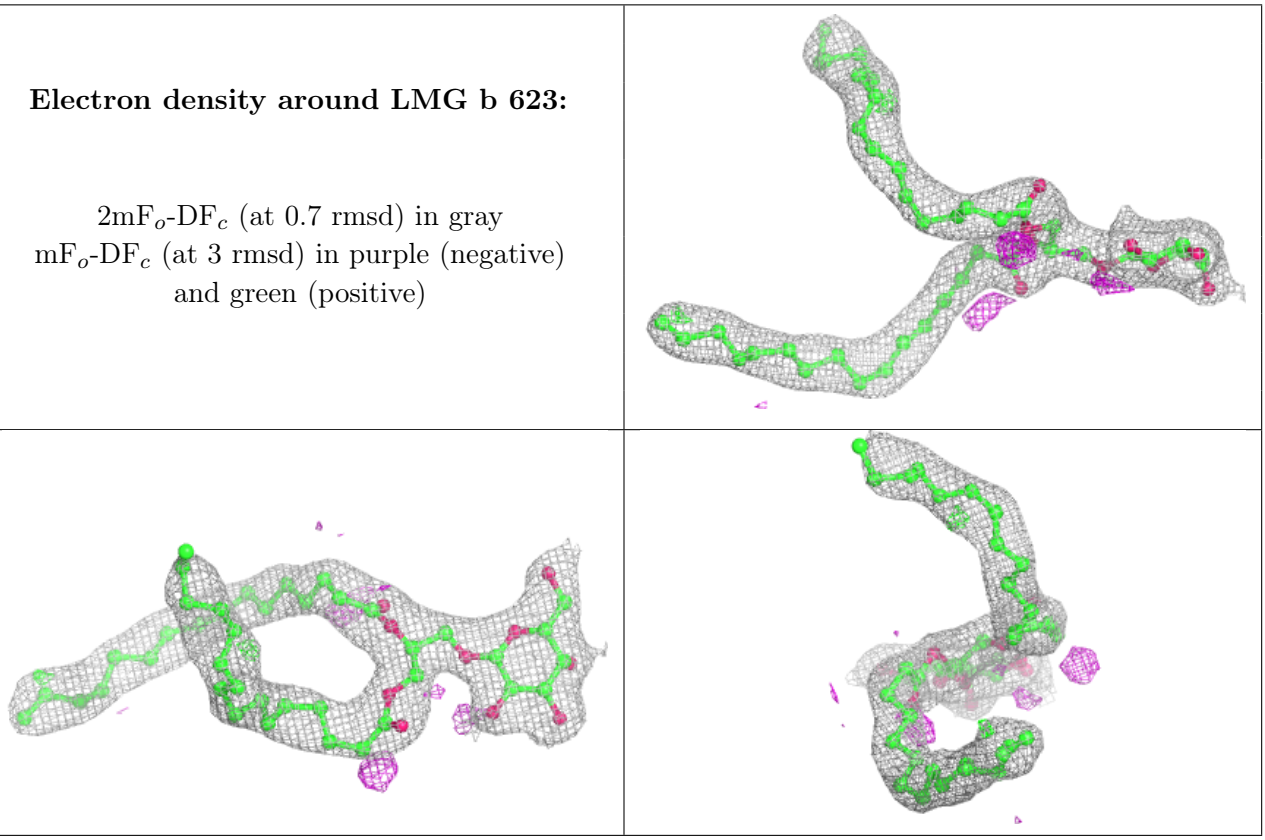
Electron density around HTG U 201:

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



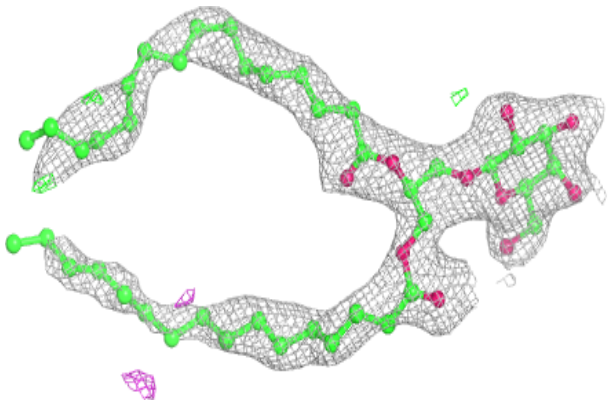
Electron density around LMG b 623:

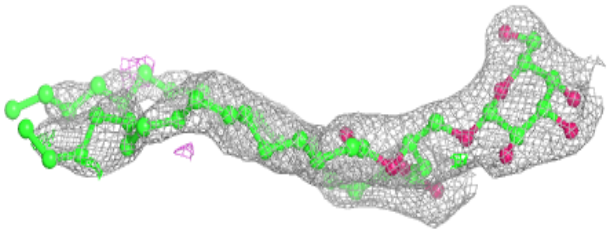
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

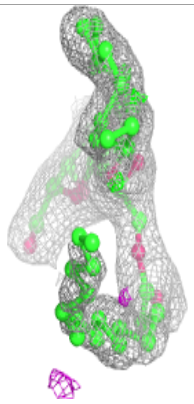


Electron density around LMG A 412:

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

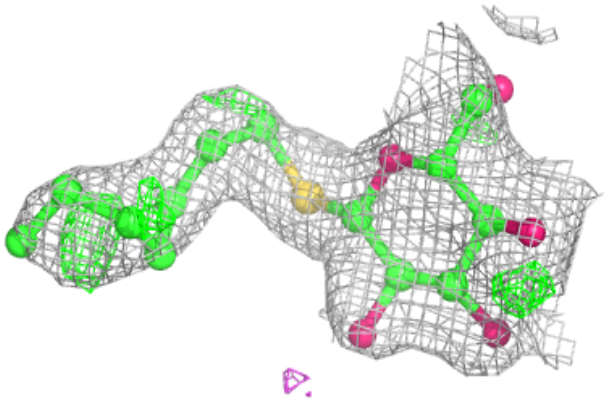


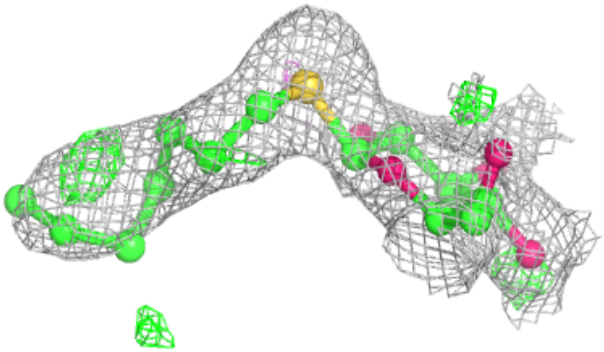


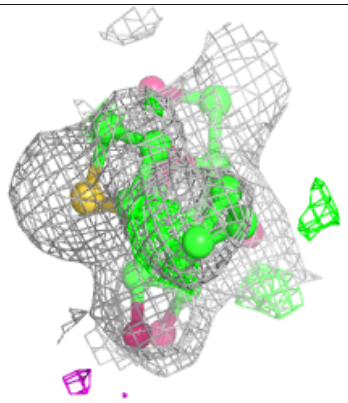


Electron density around HTG B 623 (A):

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

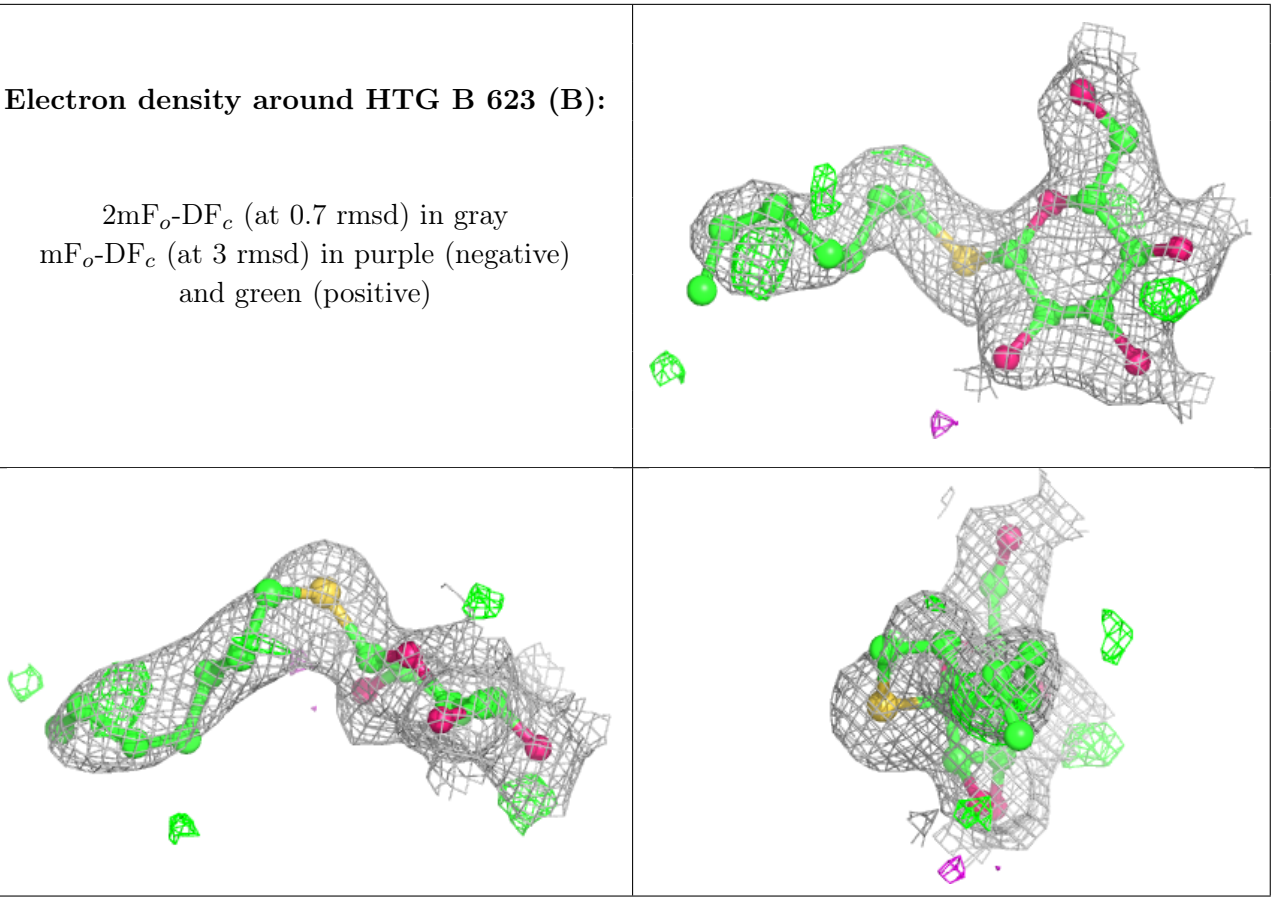






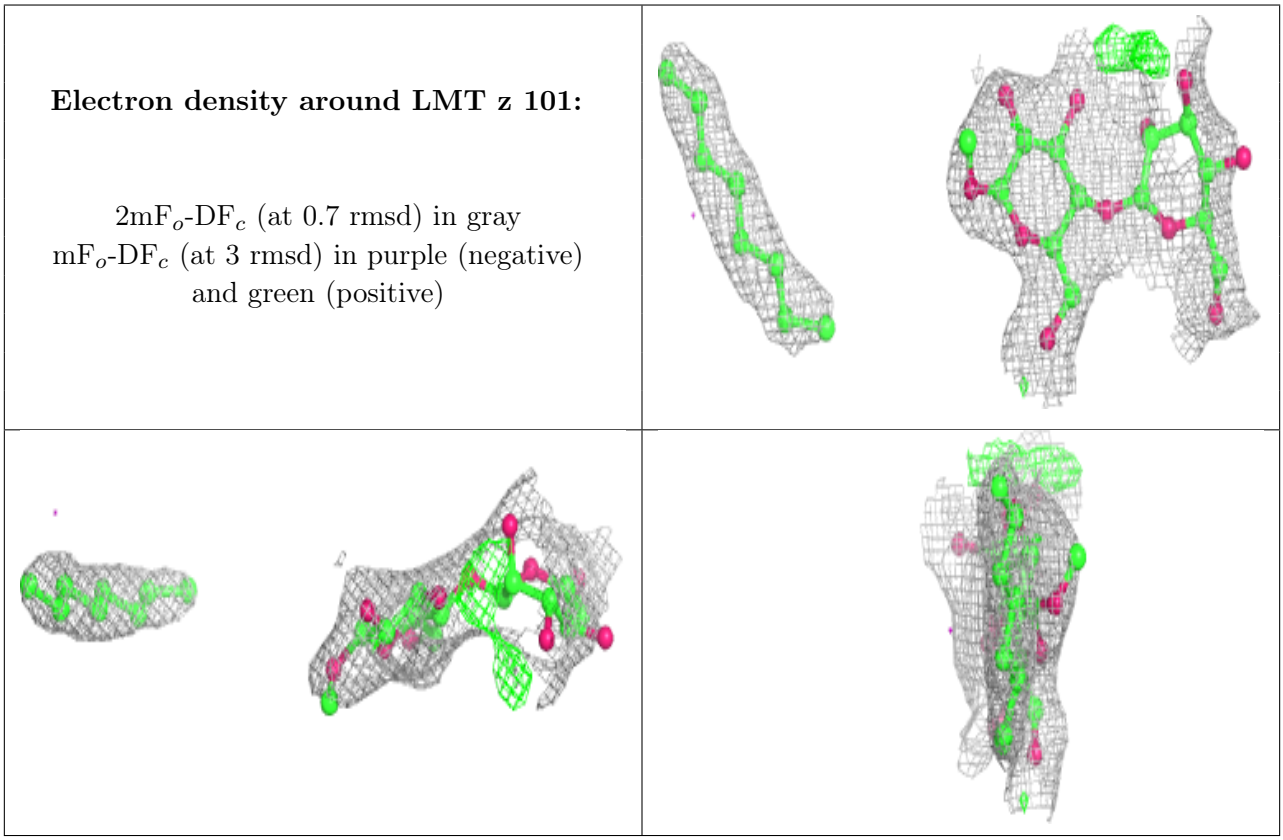
Electron density around HTG B 623 (B):

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



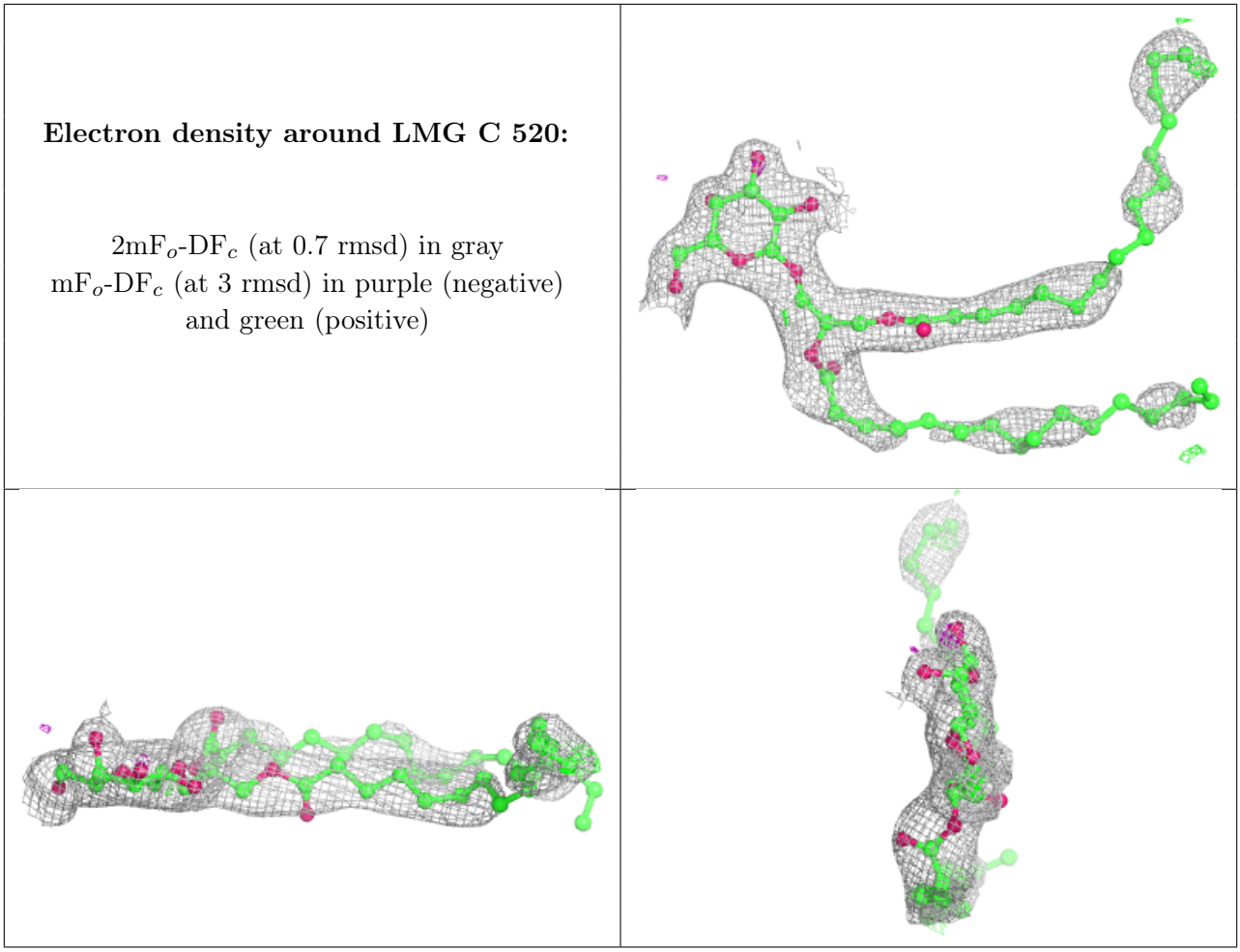
Electron density around LMT z 101:

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



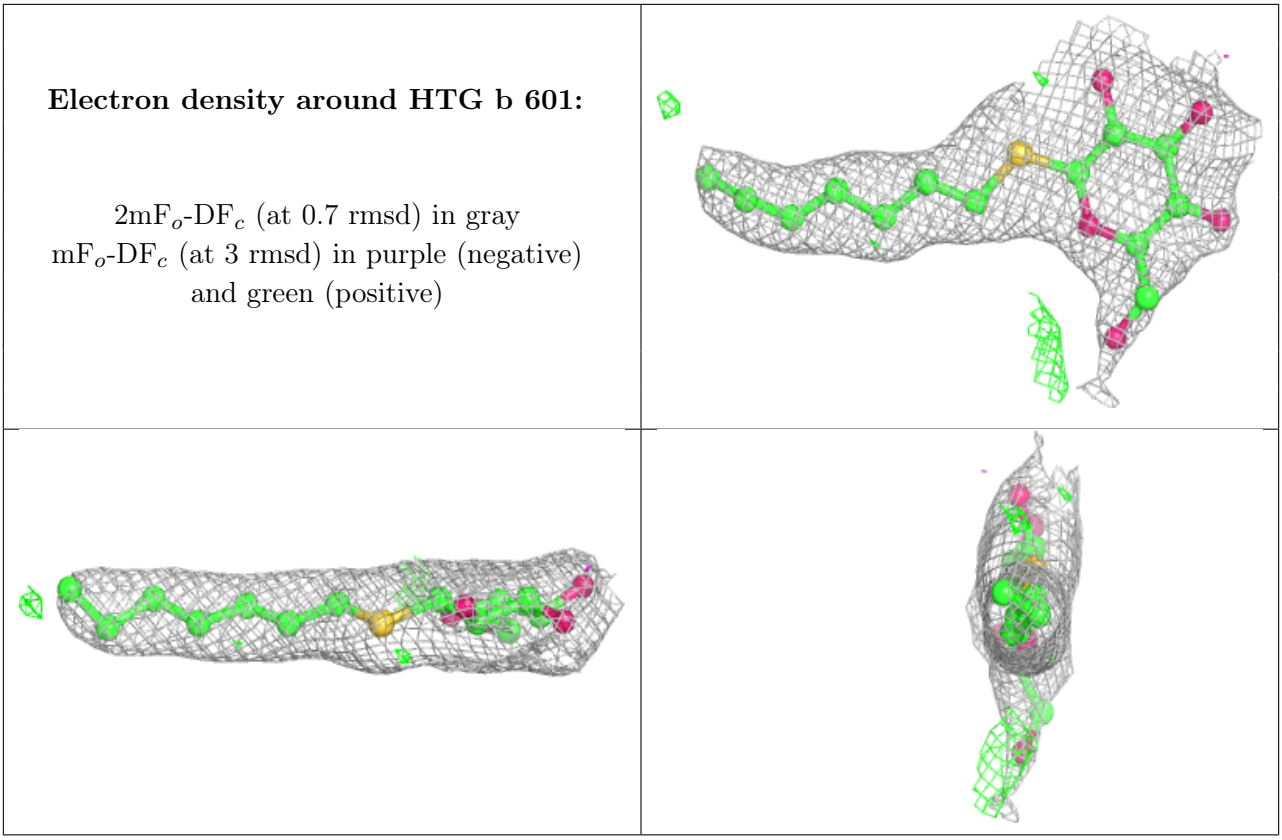
Electron density around LMG C 520:

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



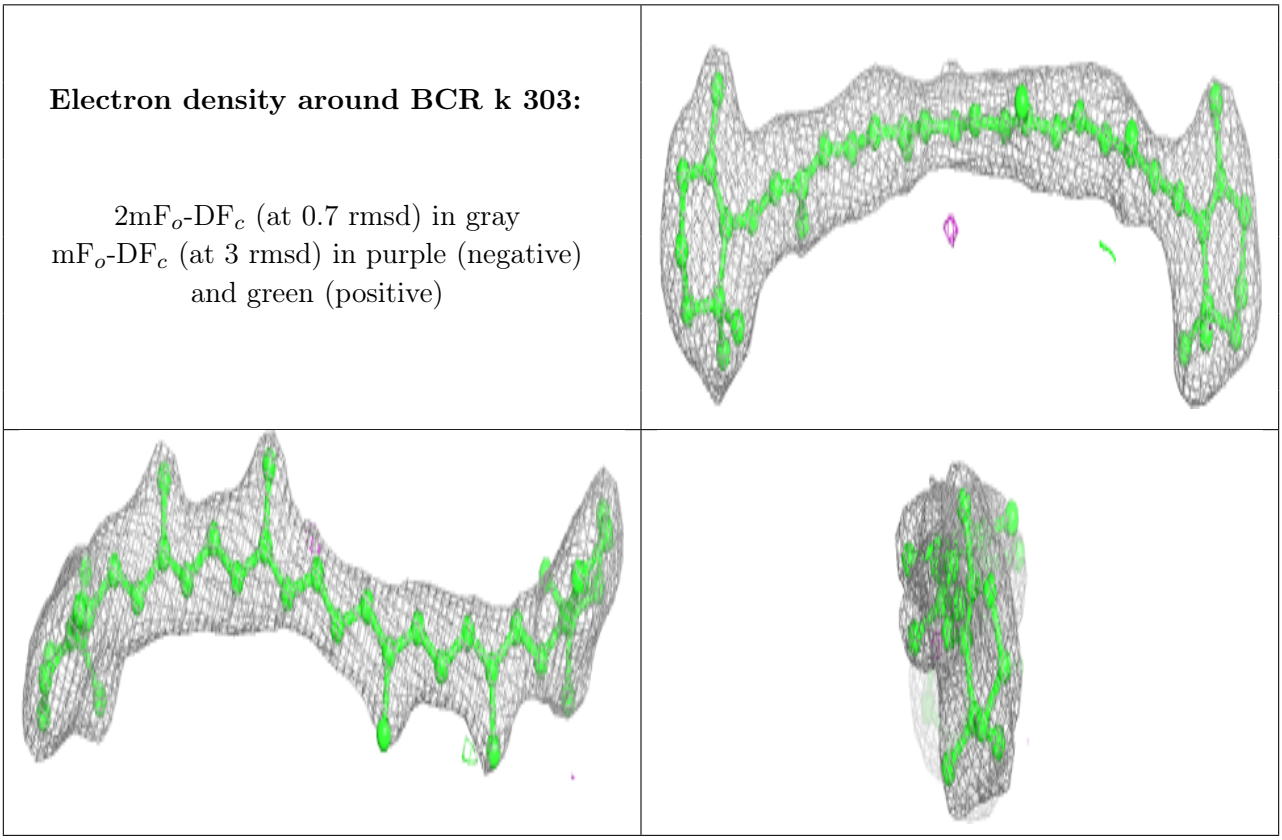
Electron density around HTG b 601:

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



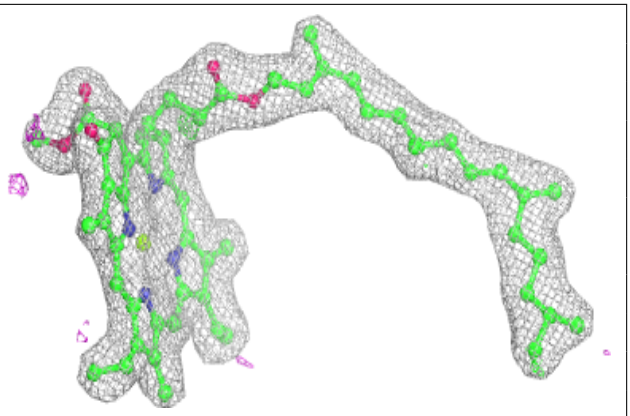
Electron density around BCR k 303:

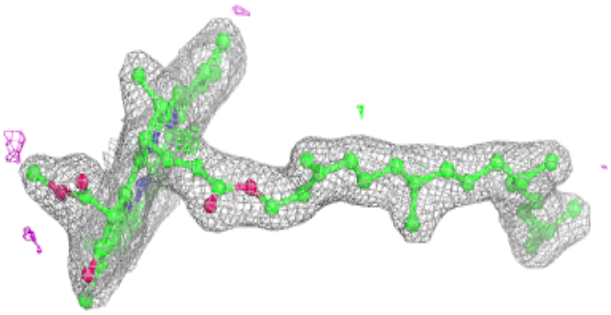
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

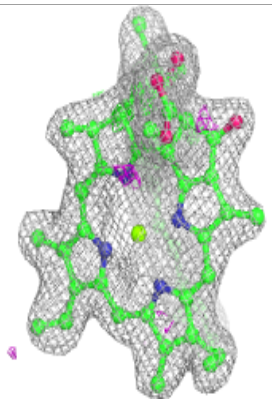


Electron density around CLA B 610:

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

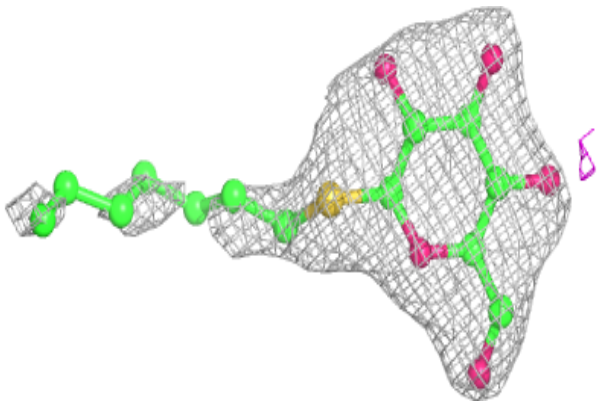


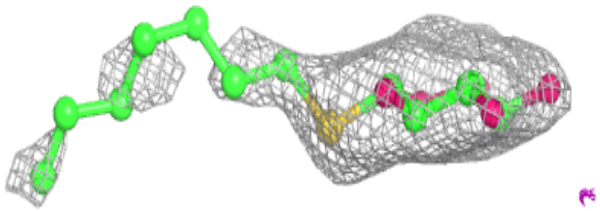


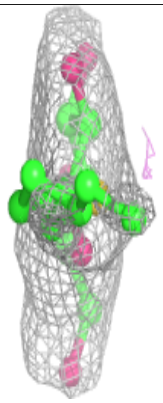


Electron density around HTG c 524:

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

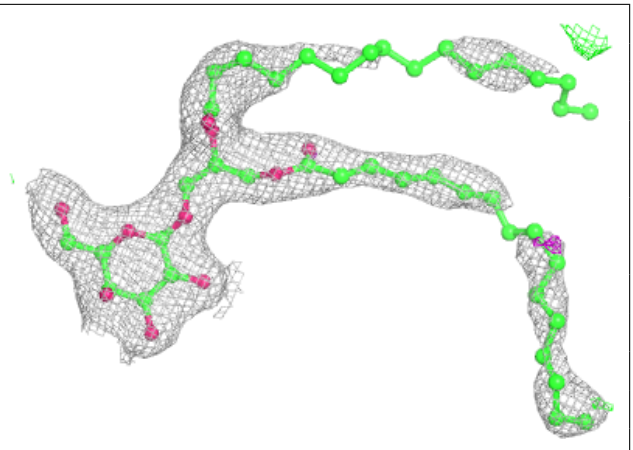


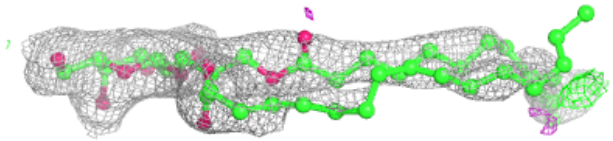


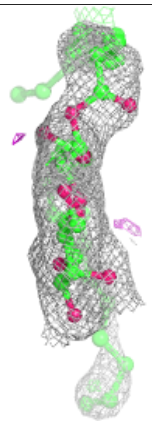


Electron density around LMG c 521:

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

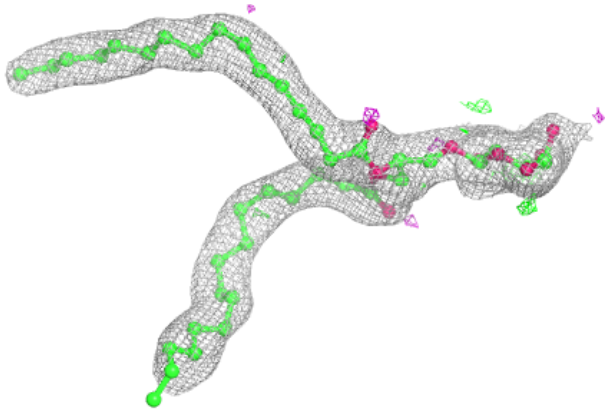


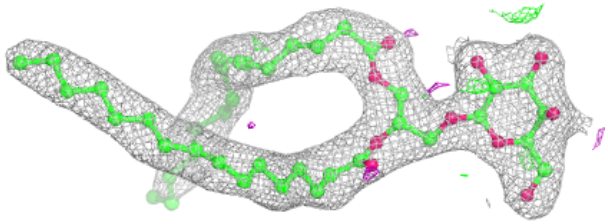


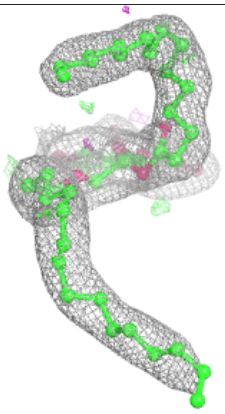


Electron density around LMG B 621:

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

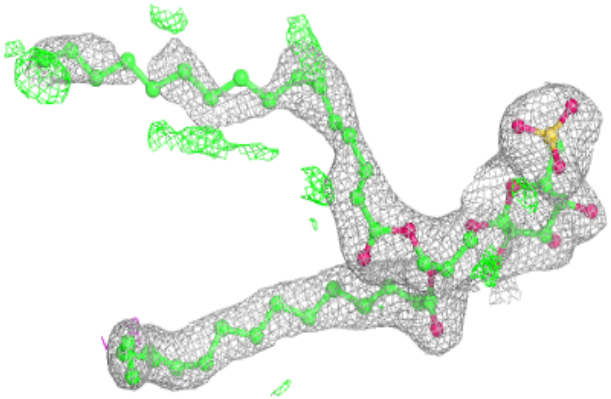


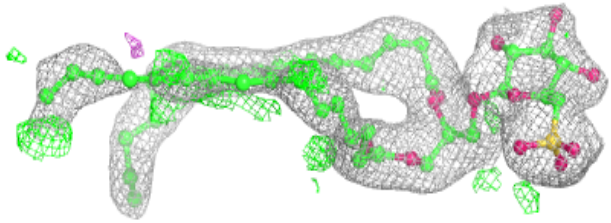


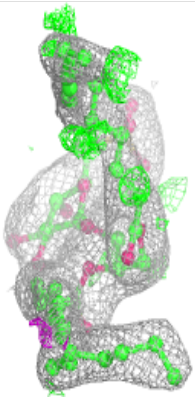


Electron density around SQD A 413:

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

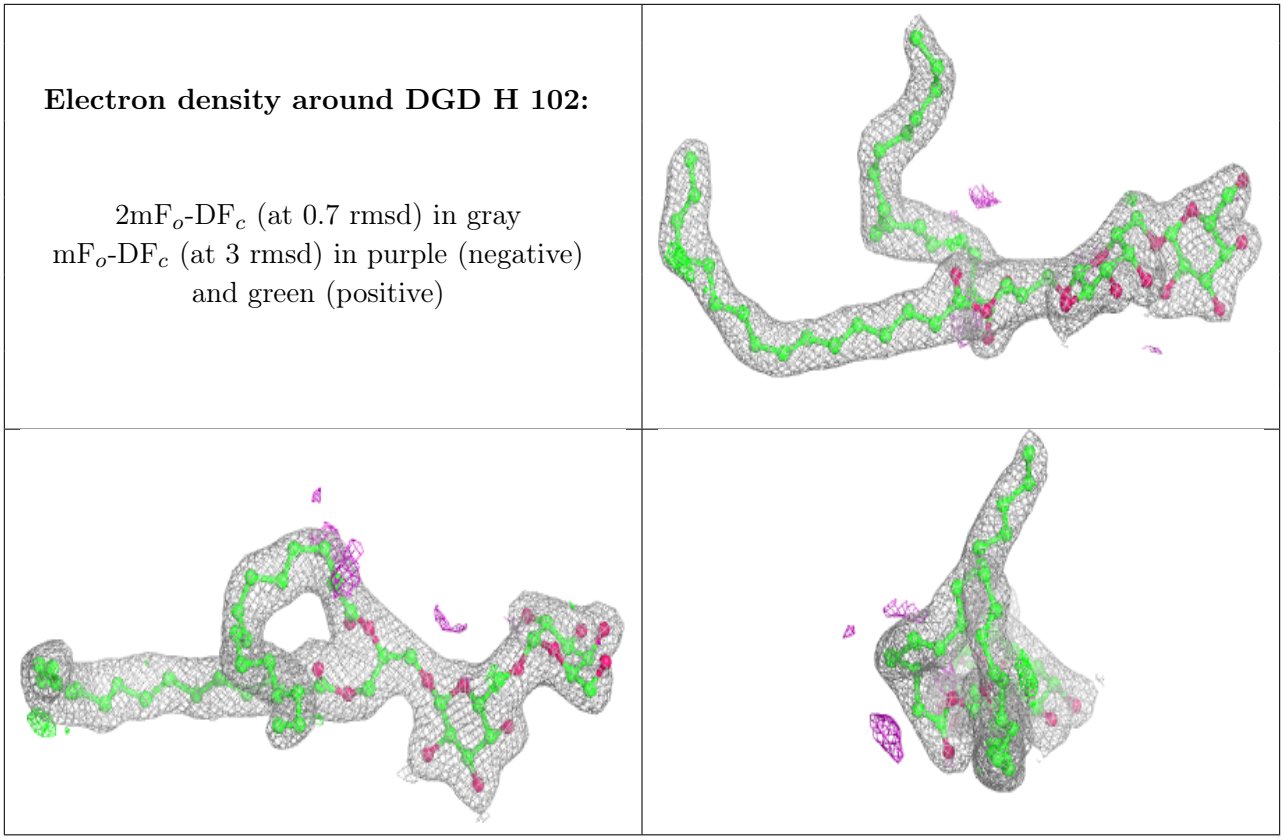






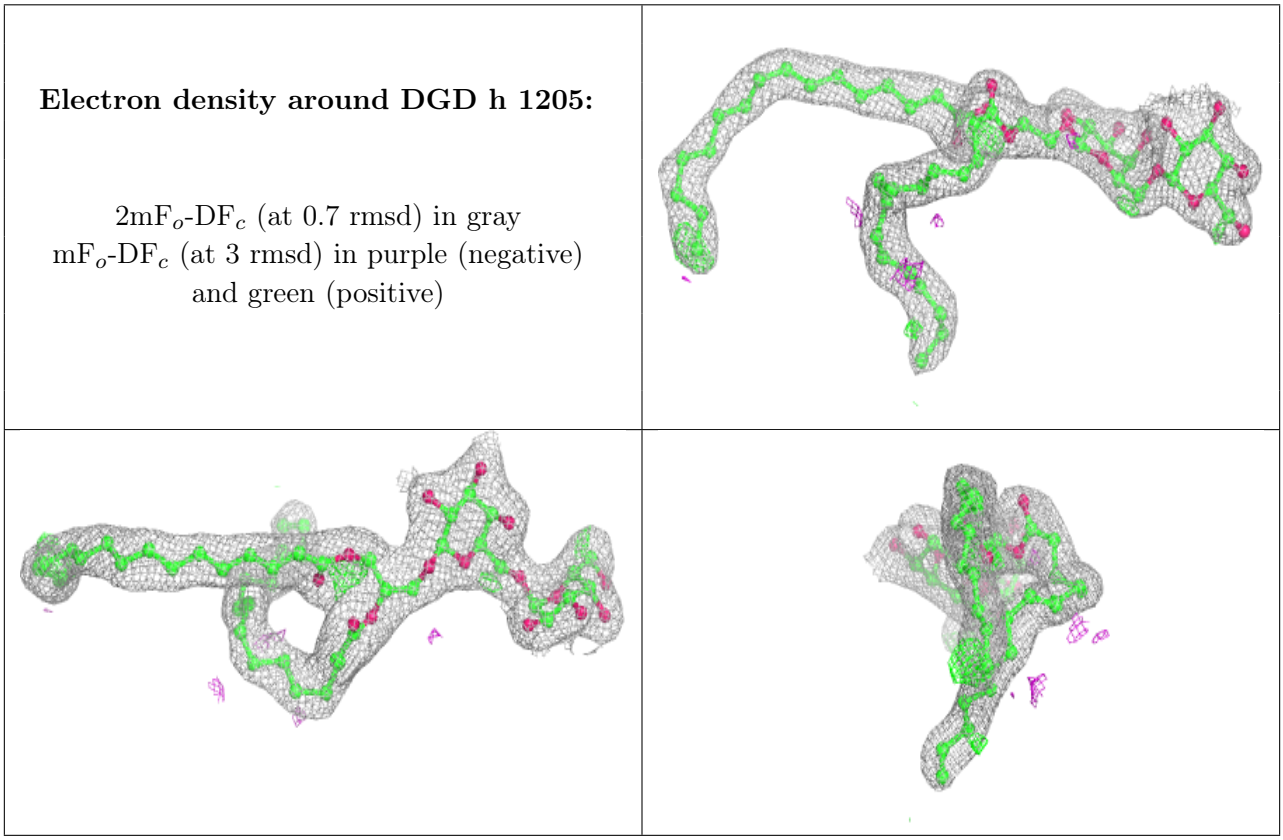
Electron density around DGD H 102:

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



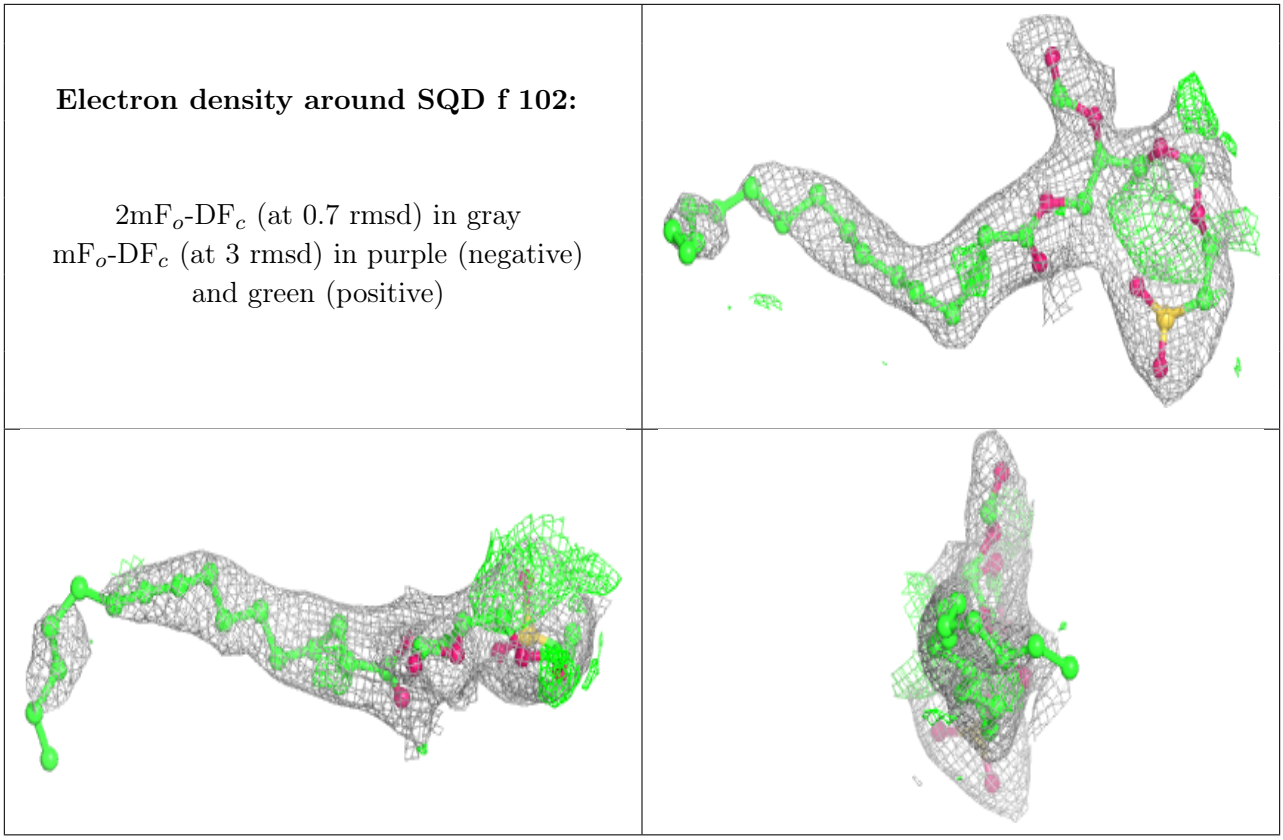
Electron density around DGD h 1205:

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



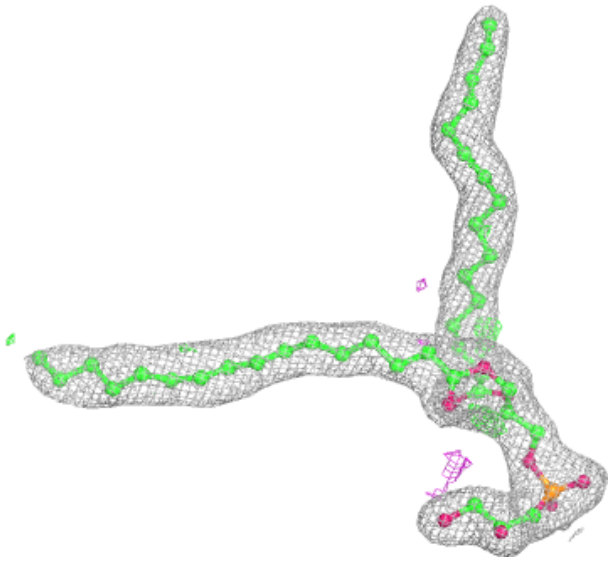
Electron density around SQD f 102:

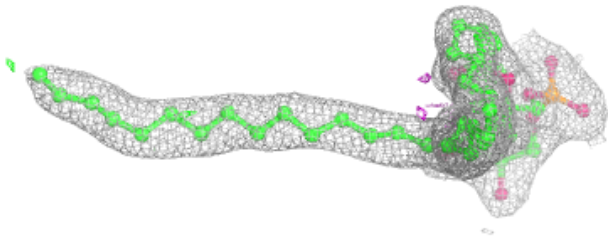
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

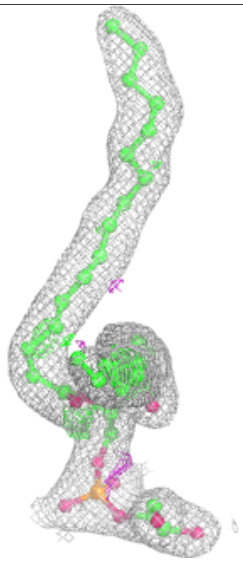


Electron density around LHG l 302:

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

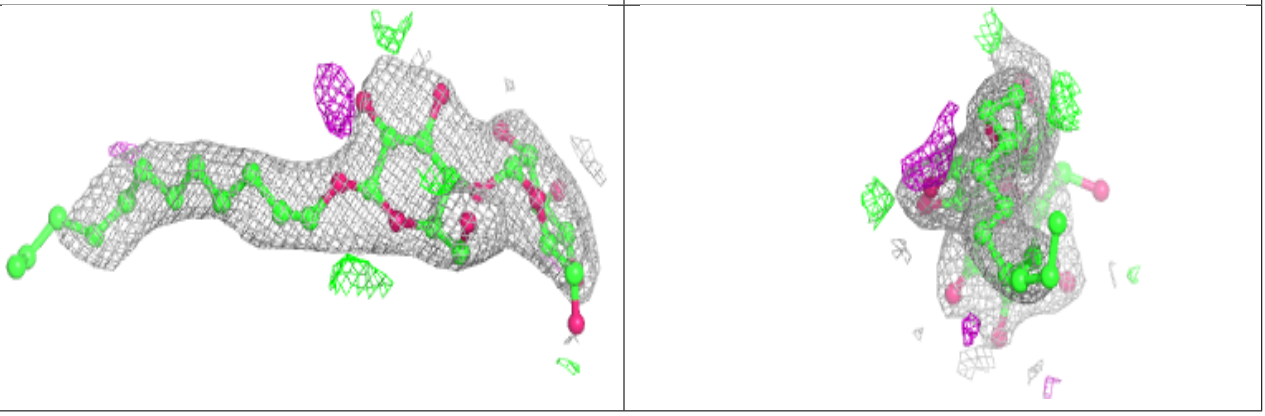






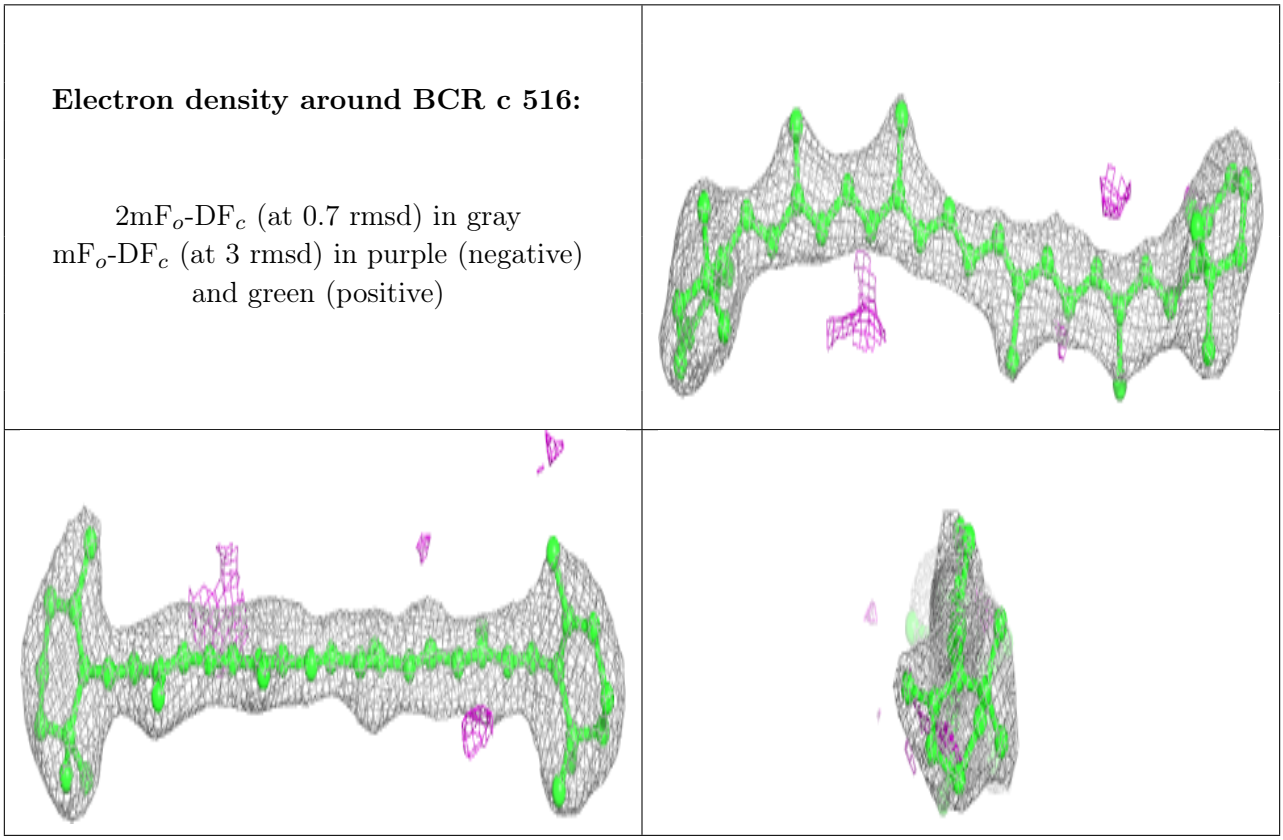
Electron density around LMT A 414:

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



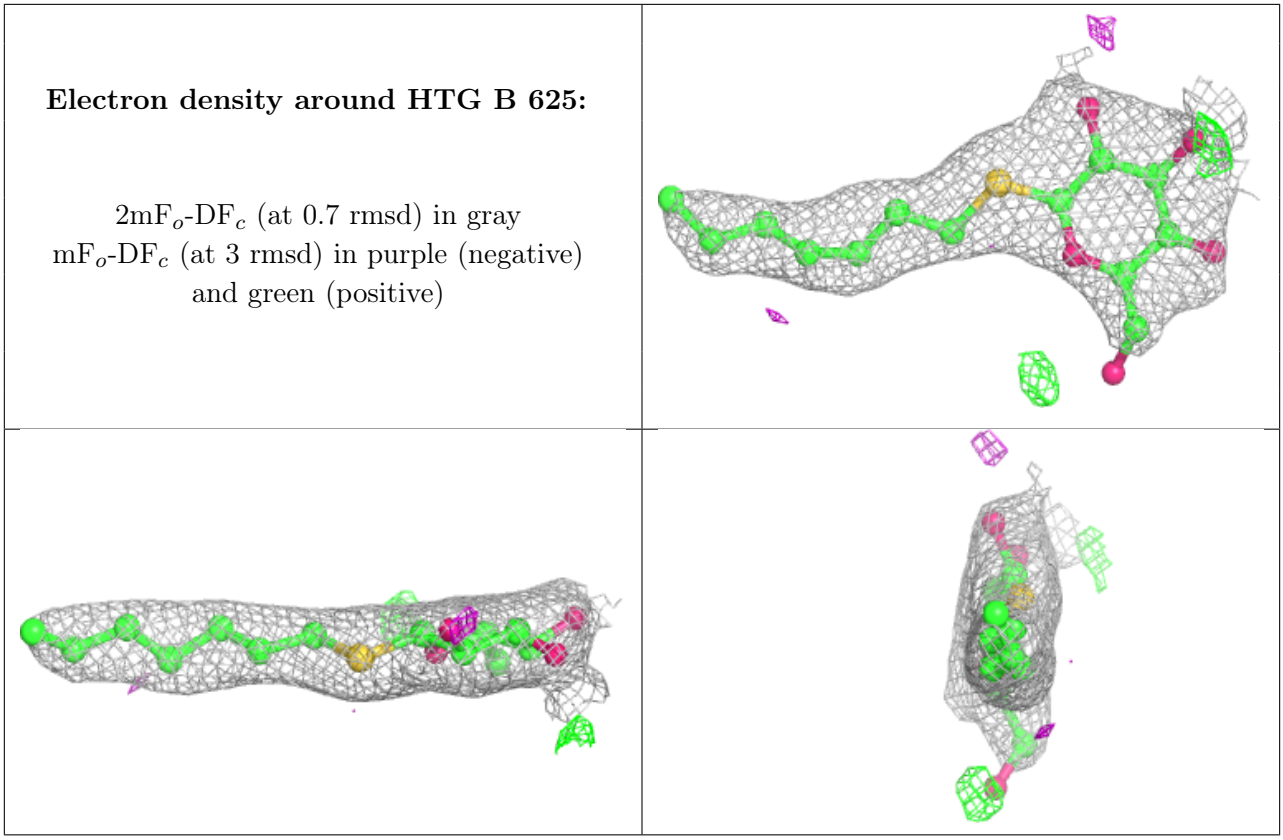
Electron density around BCR c 516:

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



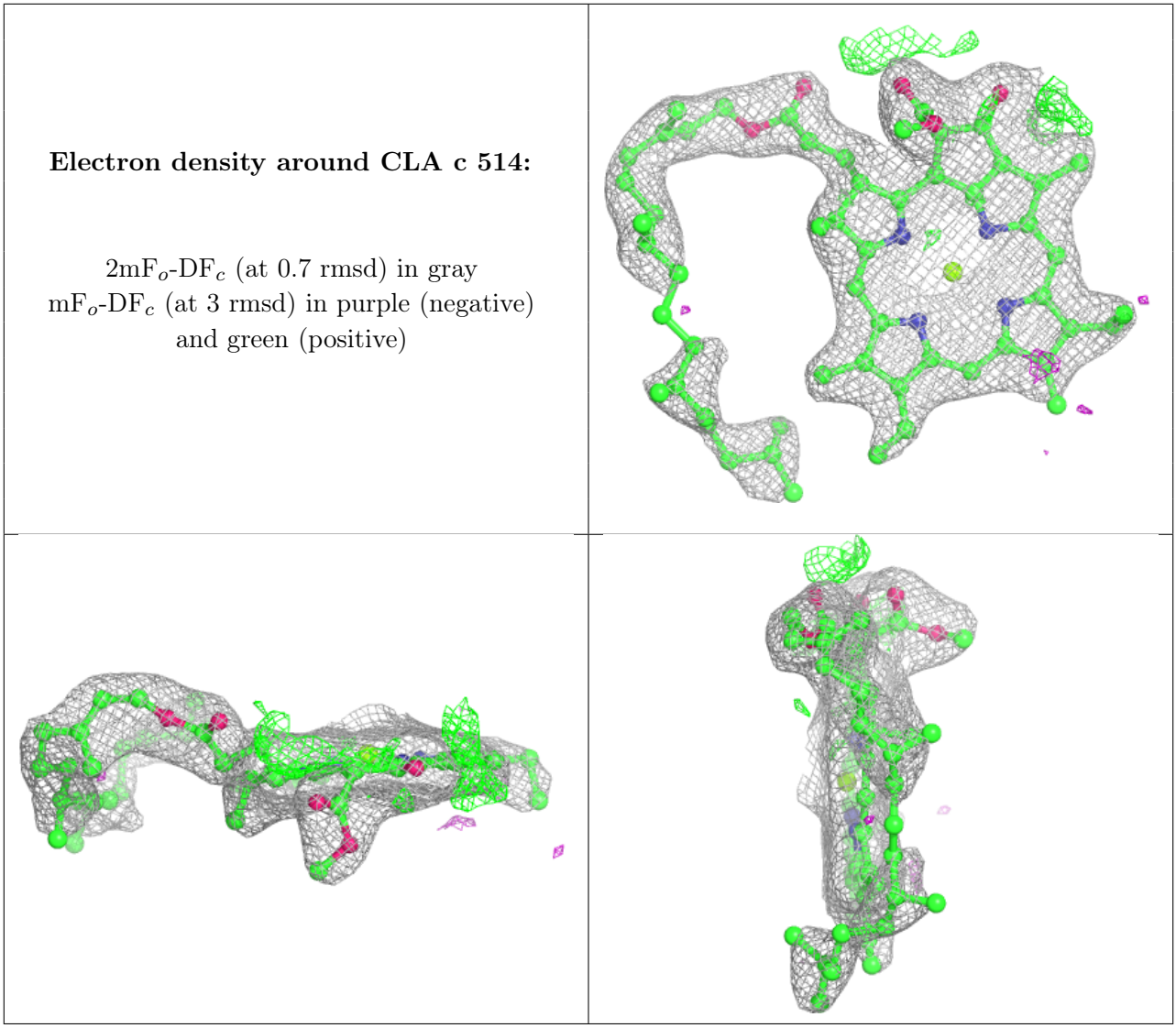
Electron density around HTG B 625:

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



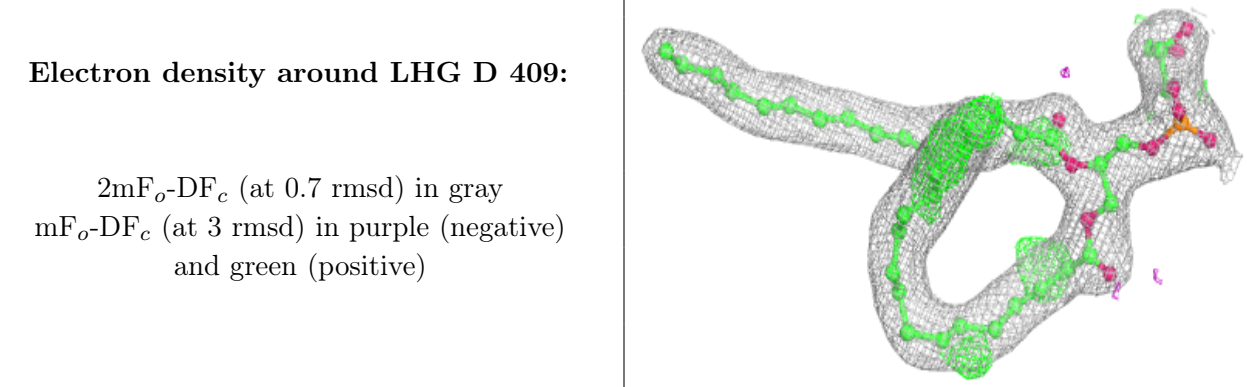
Electron density around CLA c 514:

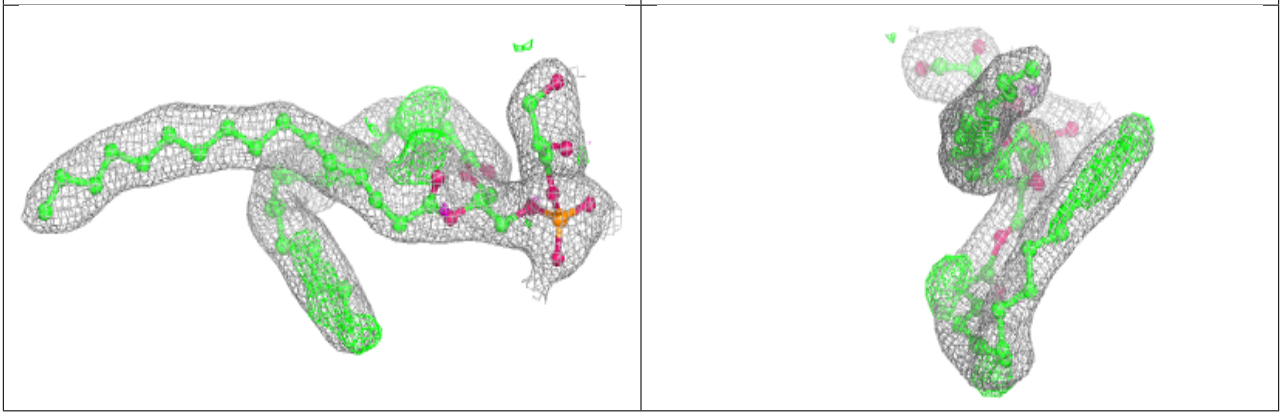
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG D 409:

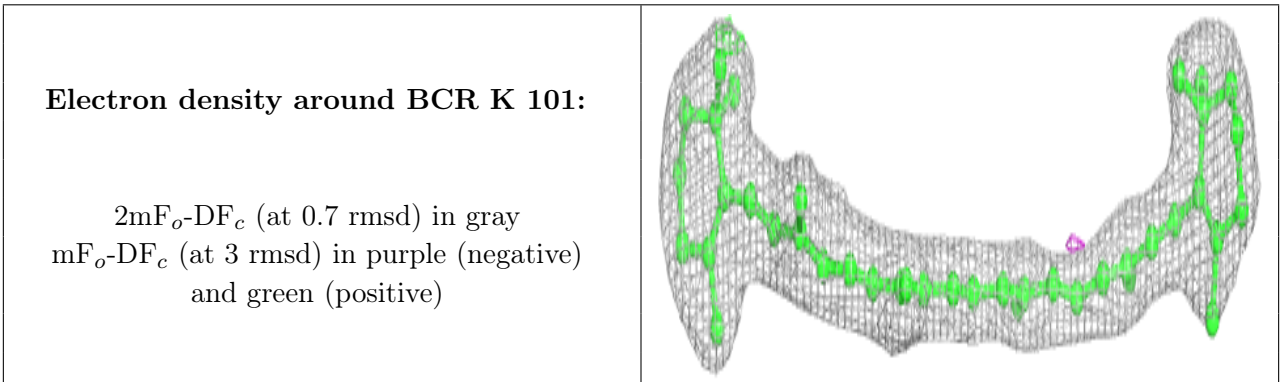
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

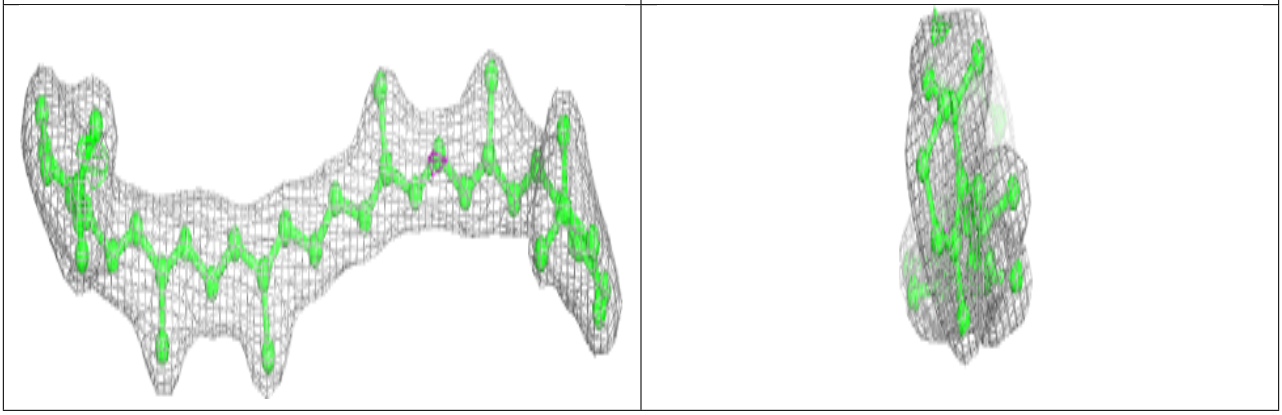




Electron density around BCR K 101:

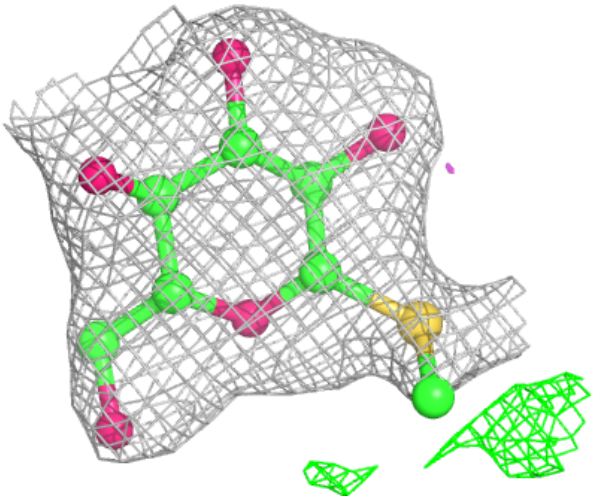
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

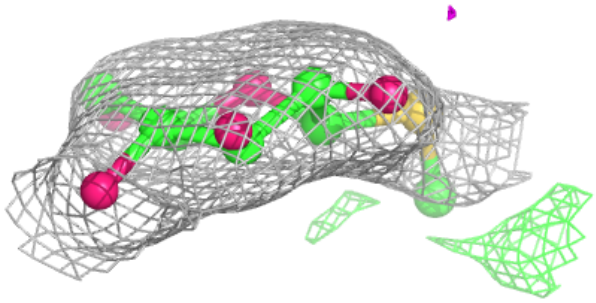


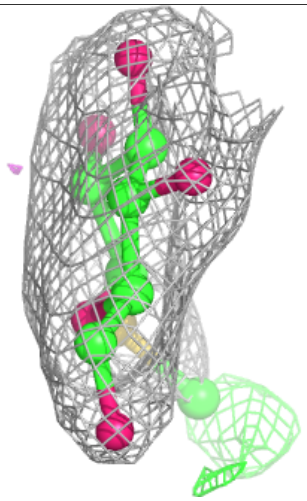


Electron density around HTG V 203:

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

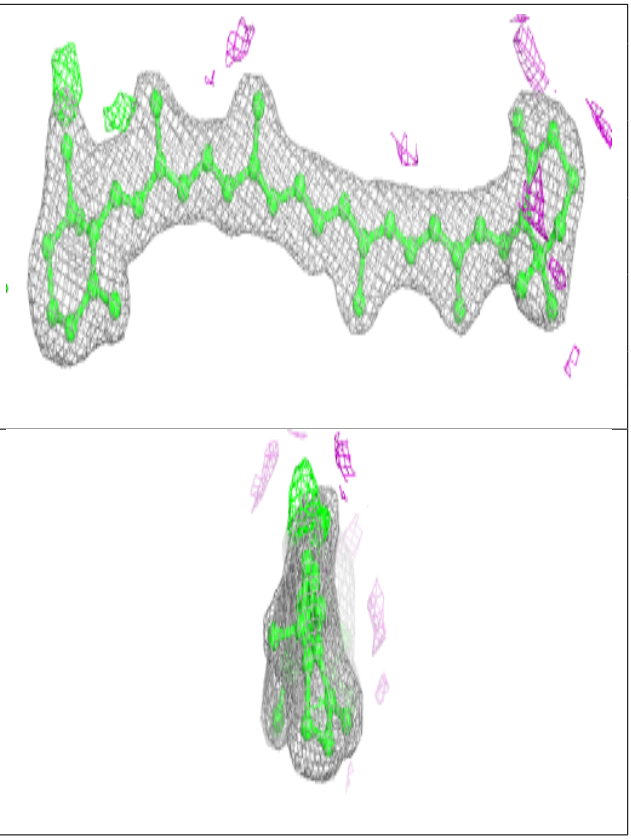






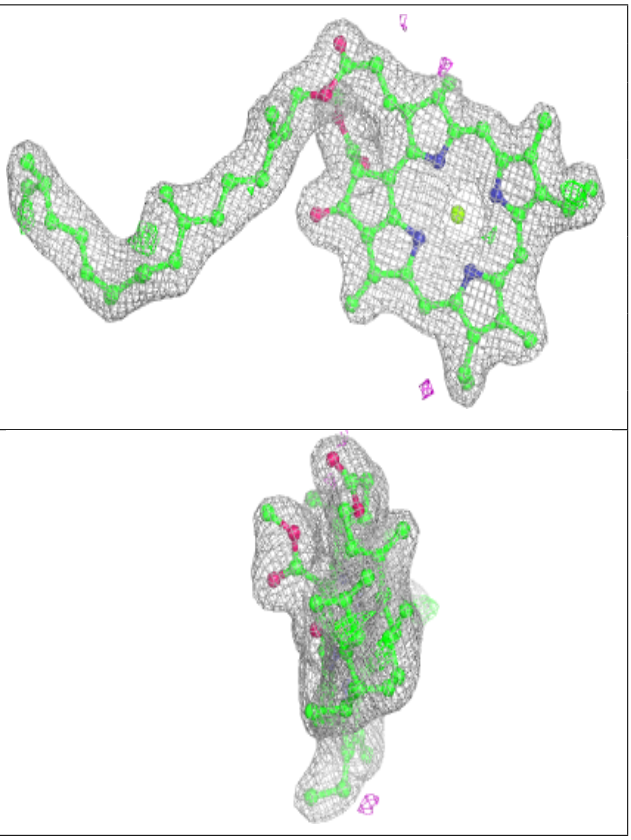
Electron density around BCR b 622:

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



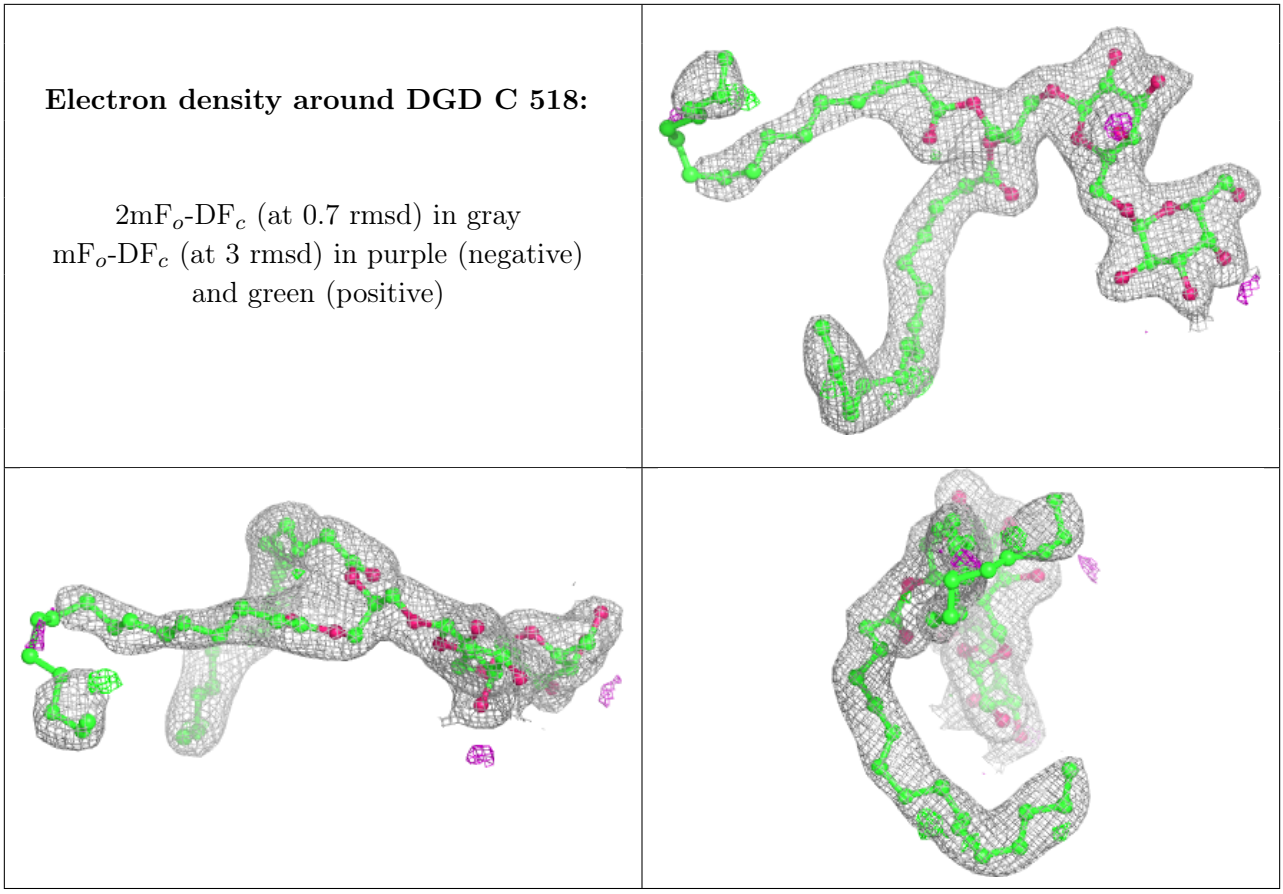
Electron density around CLA b 605:

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



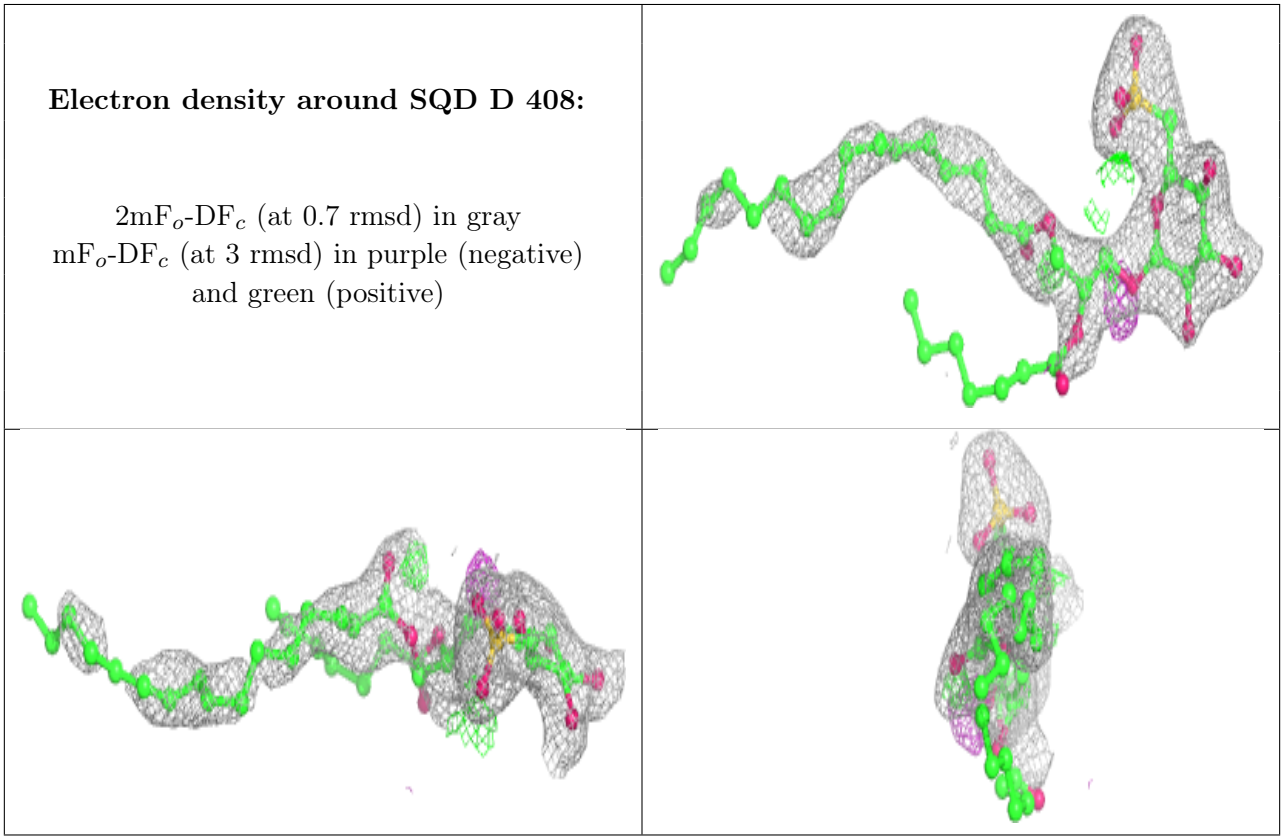
Electron density around DGD C 518:

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



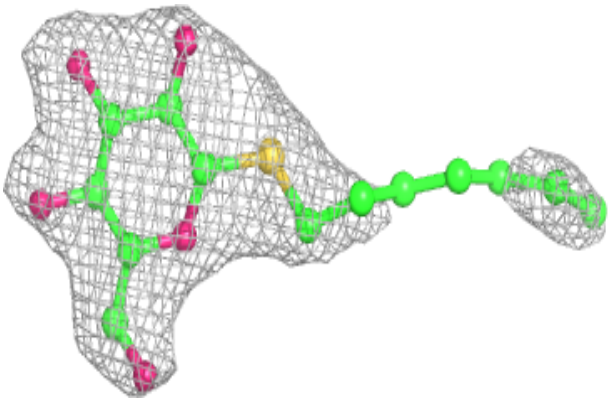
Electron density around SQD D 408:

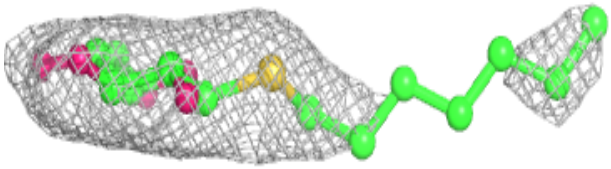
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

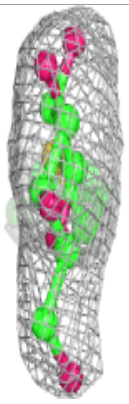


Electron density around HTG C 522:

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

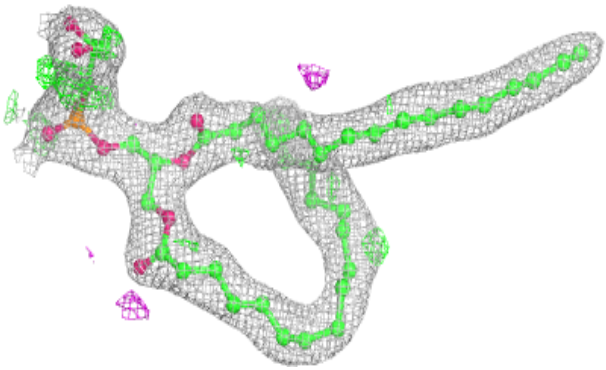


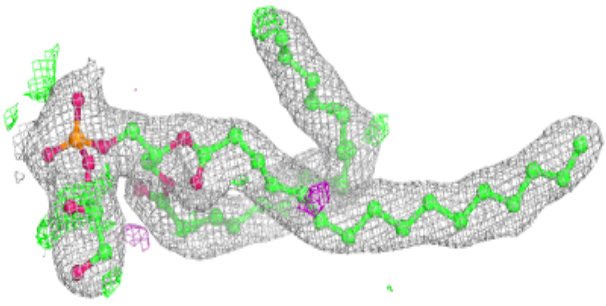


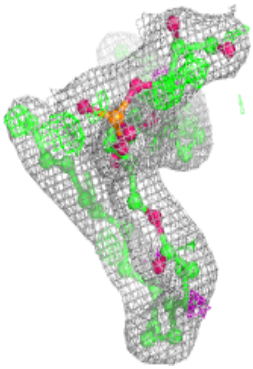


Electron density around LHG d 408:

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

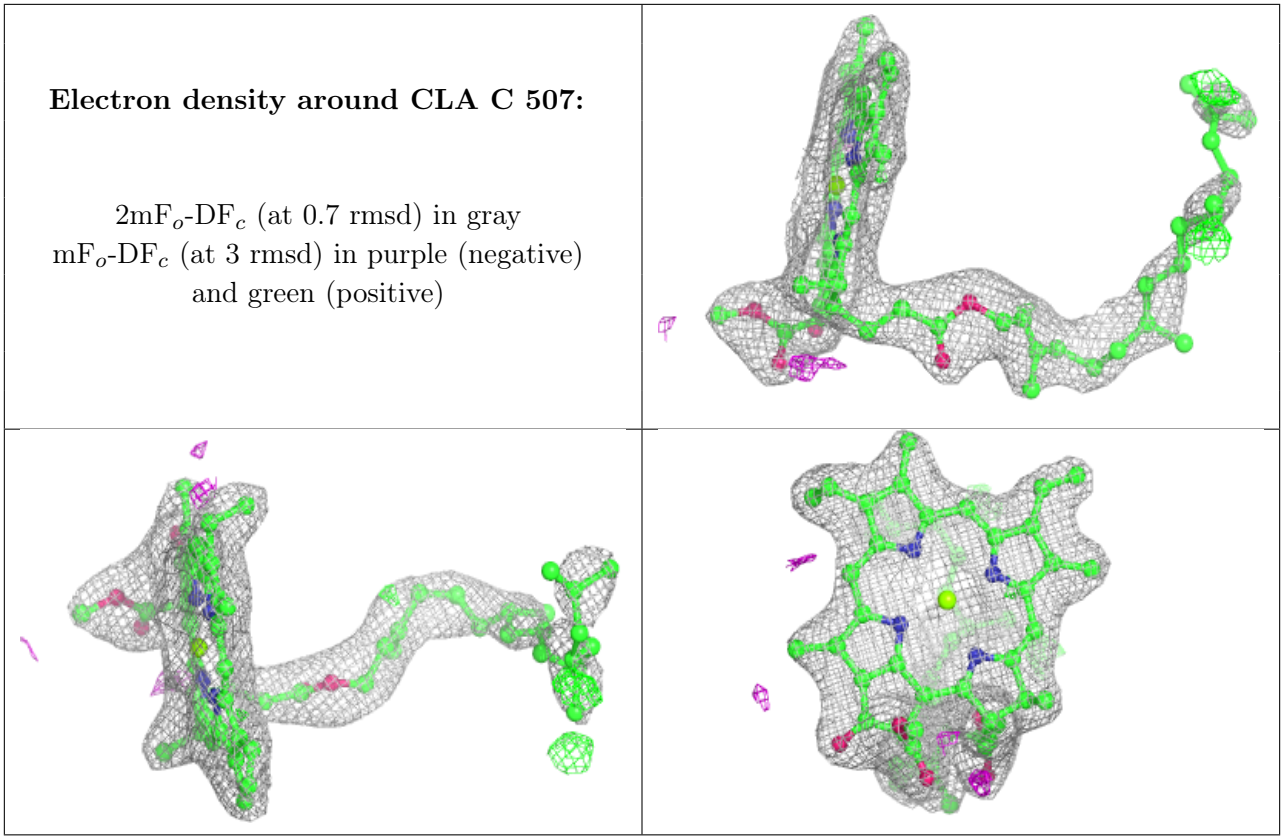






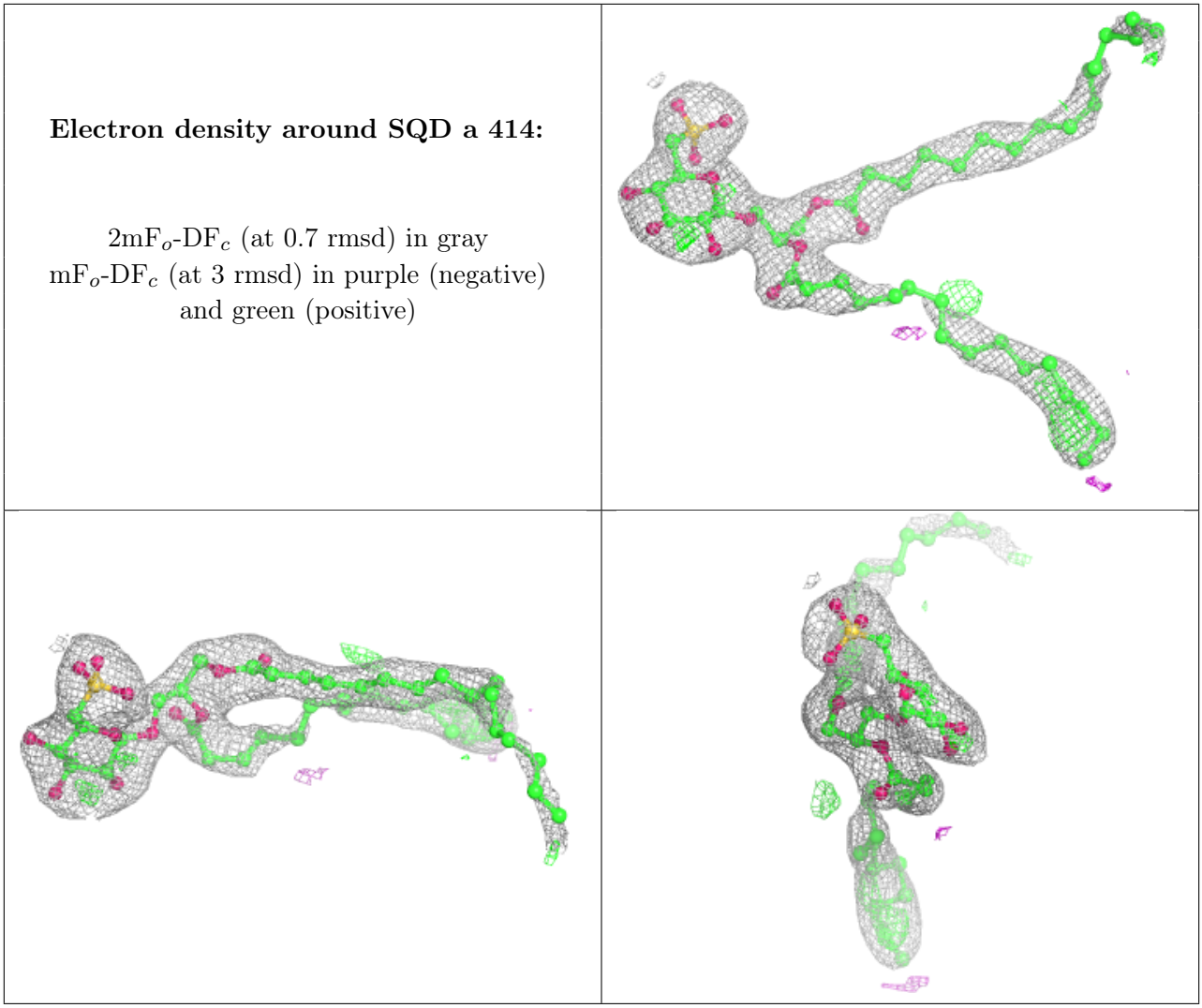
Electron density around CLA C 507:

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



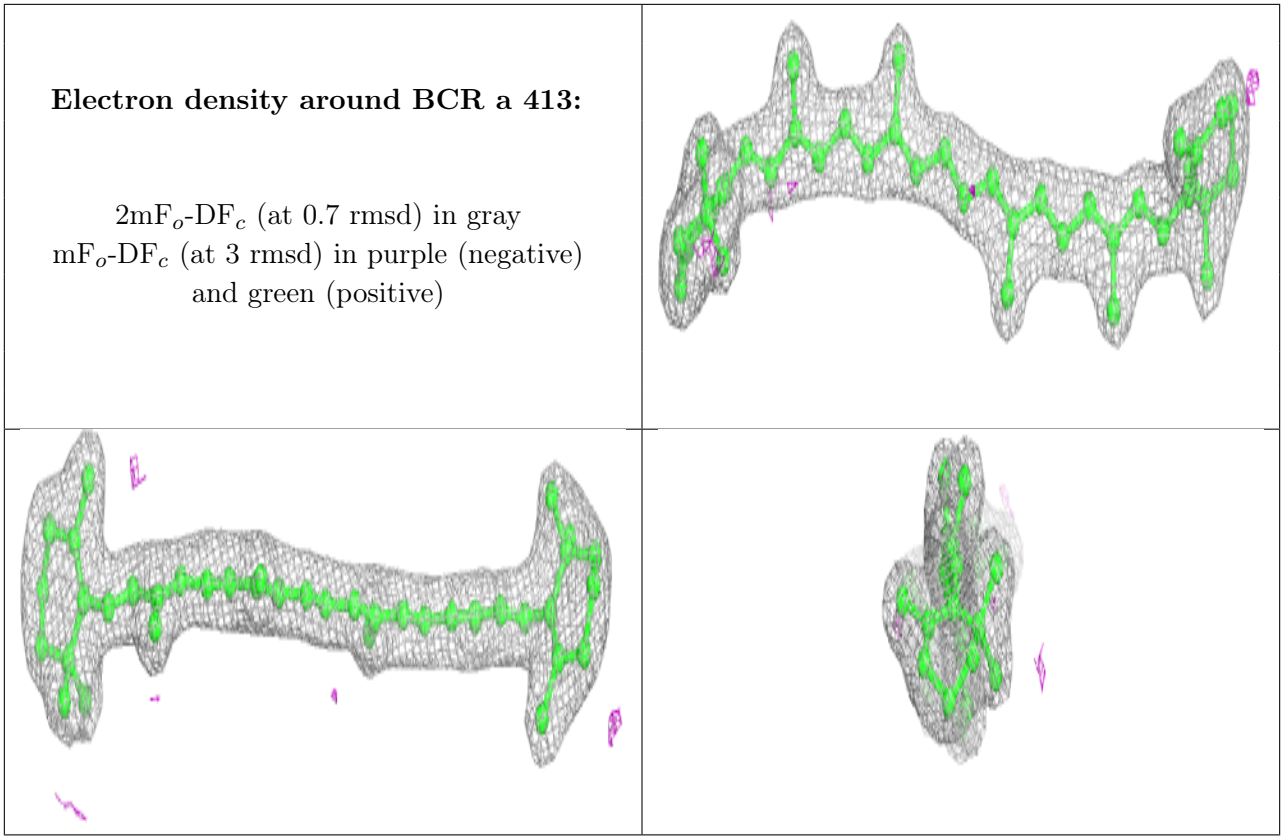
Electron density around SQD a 414:

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



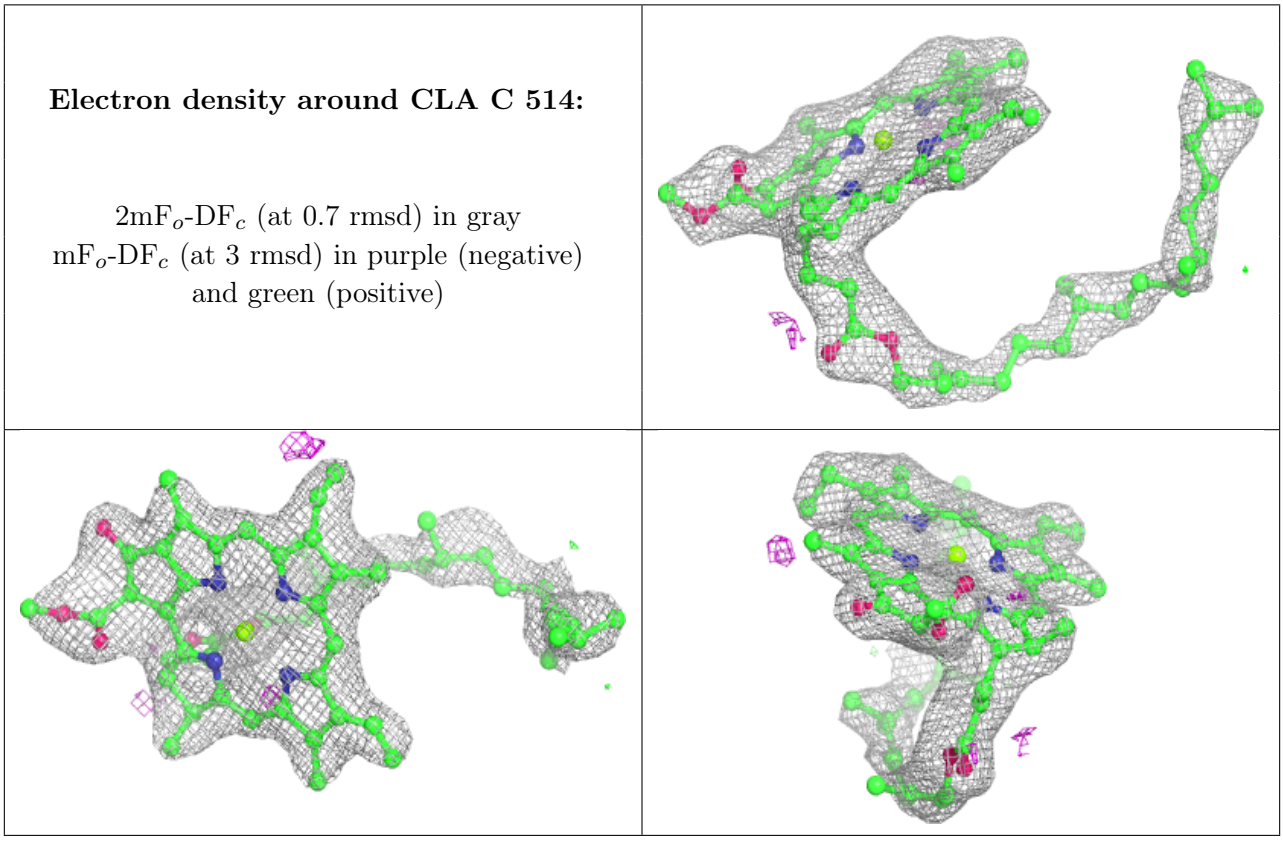
Electron density around BCR a 413:

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



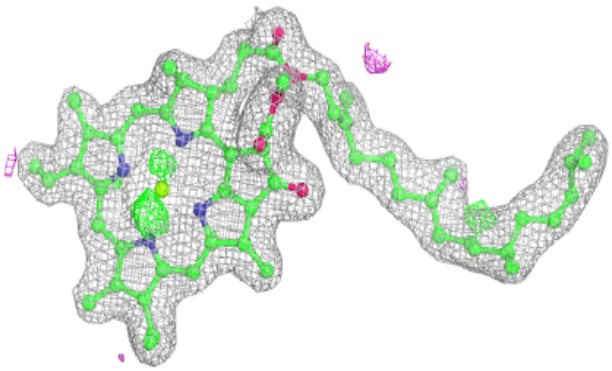
Electron density around CLA C 514:

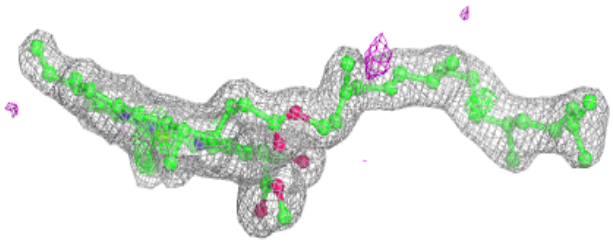
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

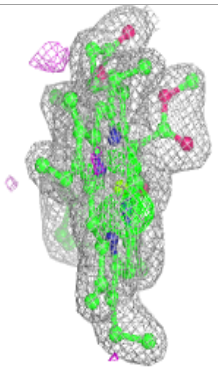


Electron density around CLA B 603:

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

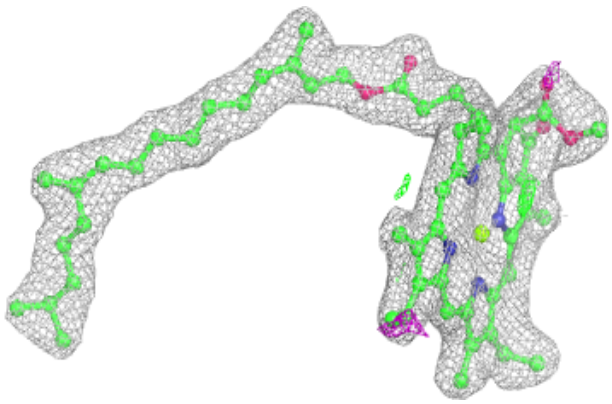


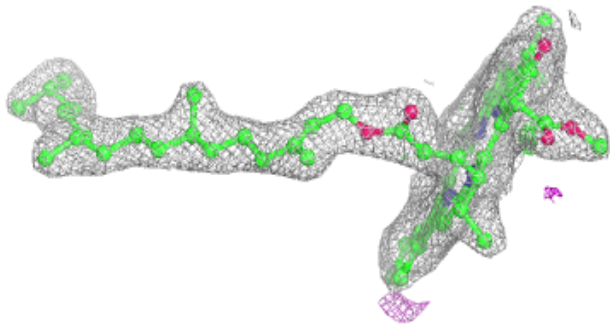


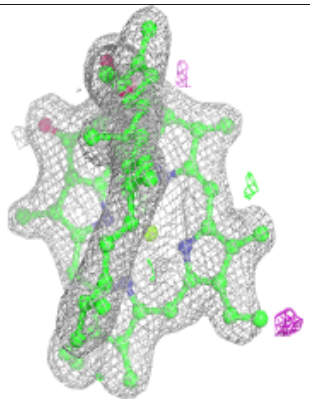


Electron density around CLA b 612:

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

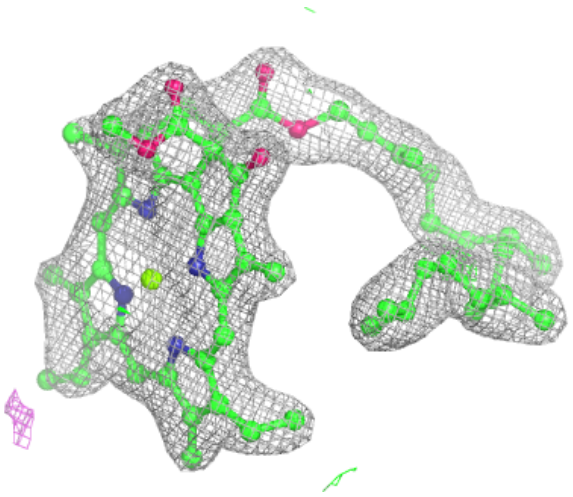


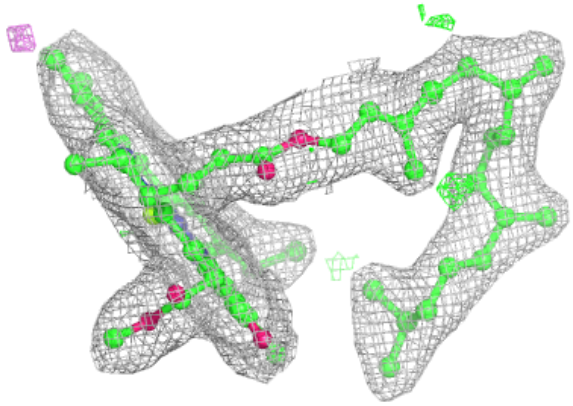


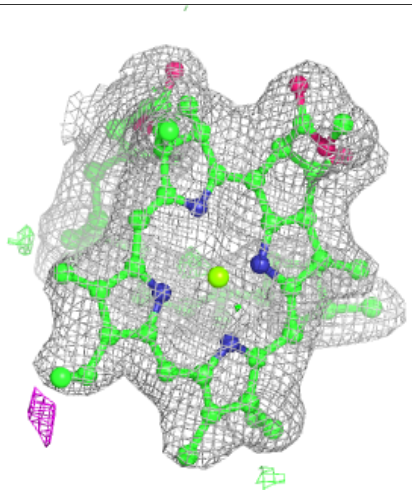


Electron density around CLA c 505:

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

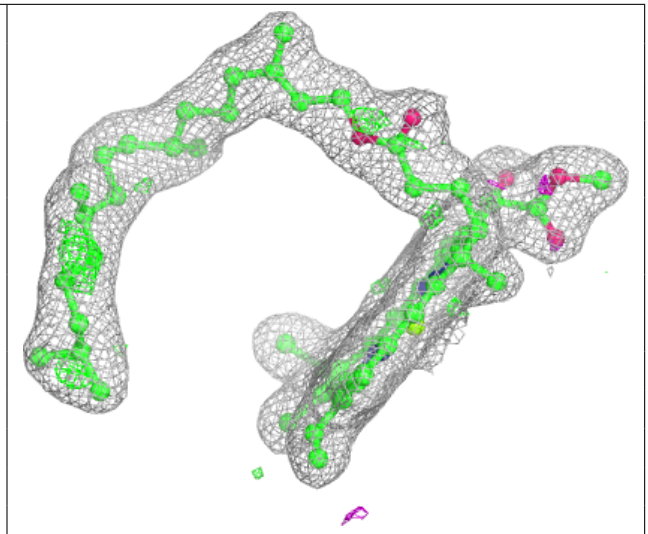


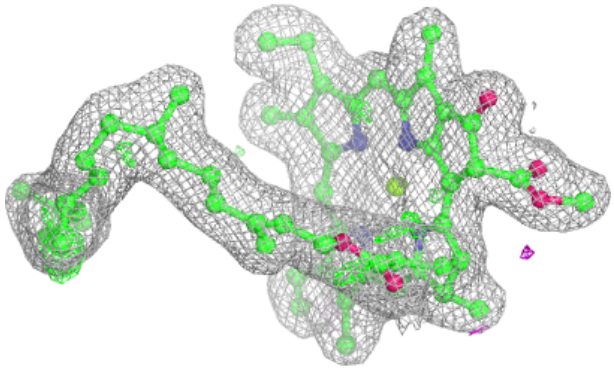


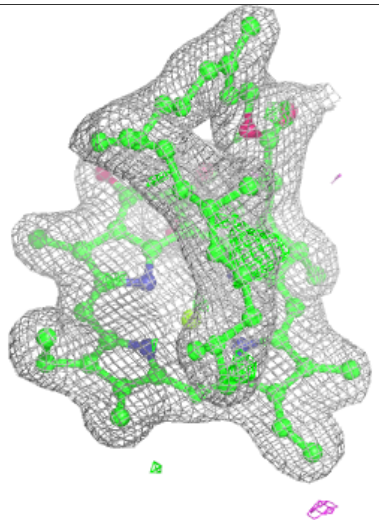


Electron density around CLA B 612:

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

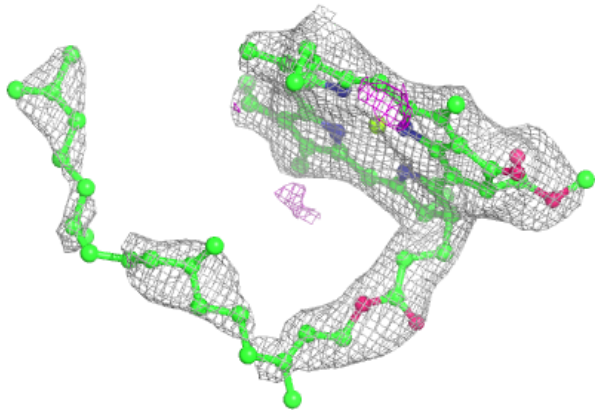


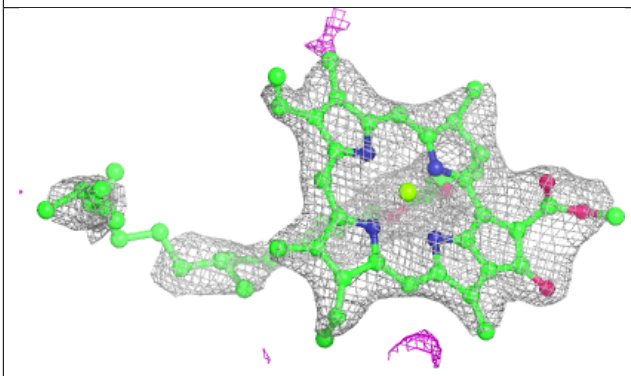


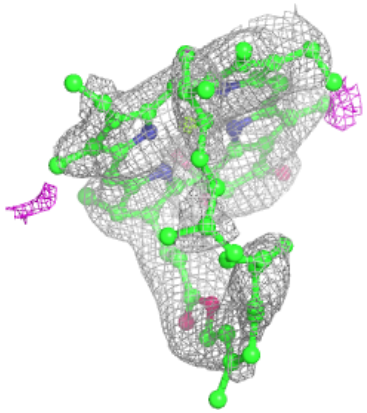


Electron density around CLA c 515:

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

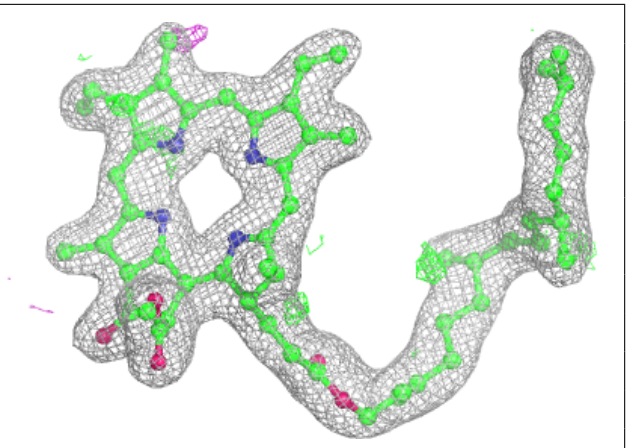


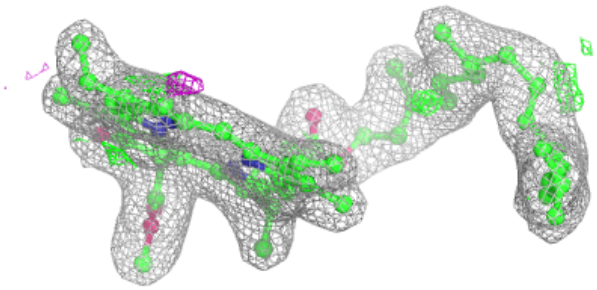


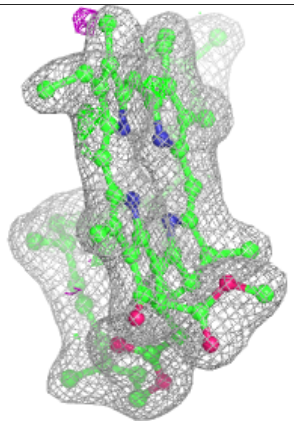


Electron density around PHO D 401:

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

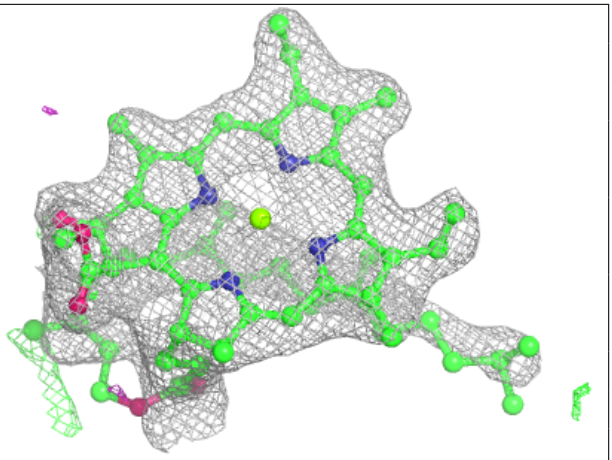


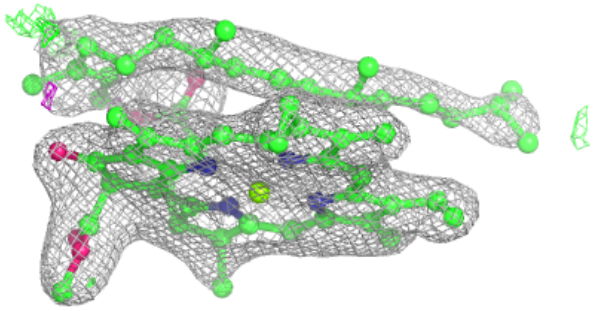


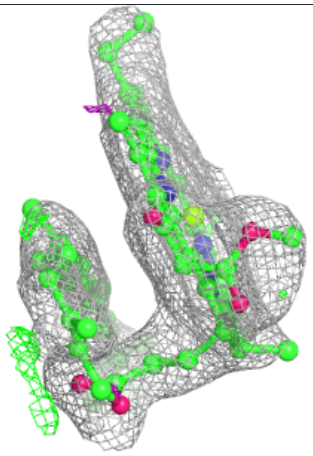


Electron density around CLA b 604:

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

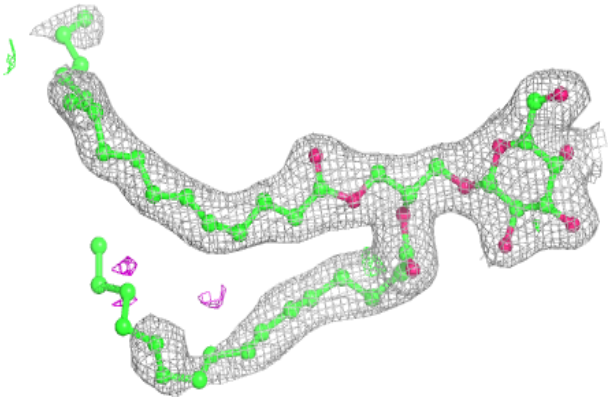


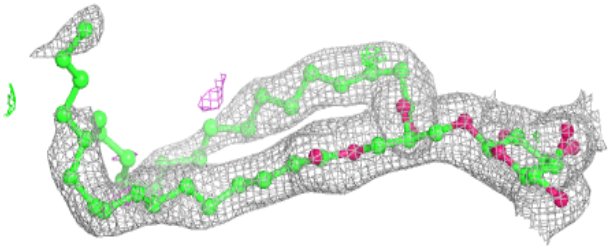


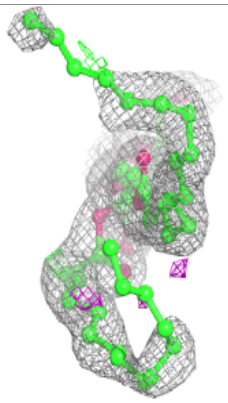


Electron density around LMG D 412:

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

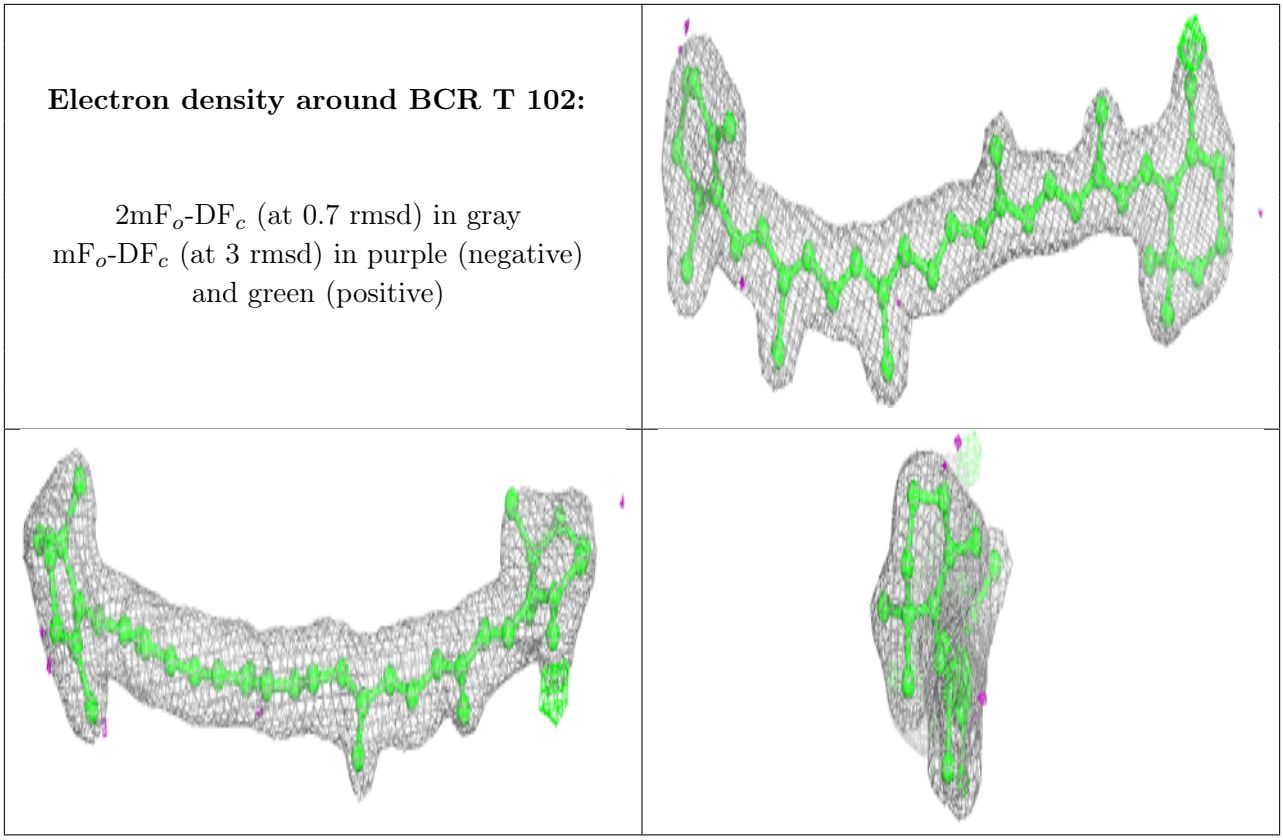






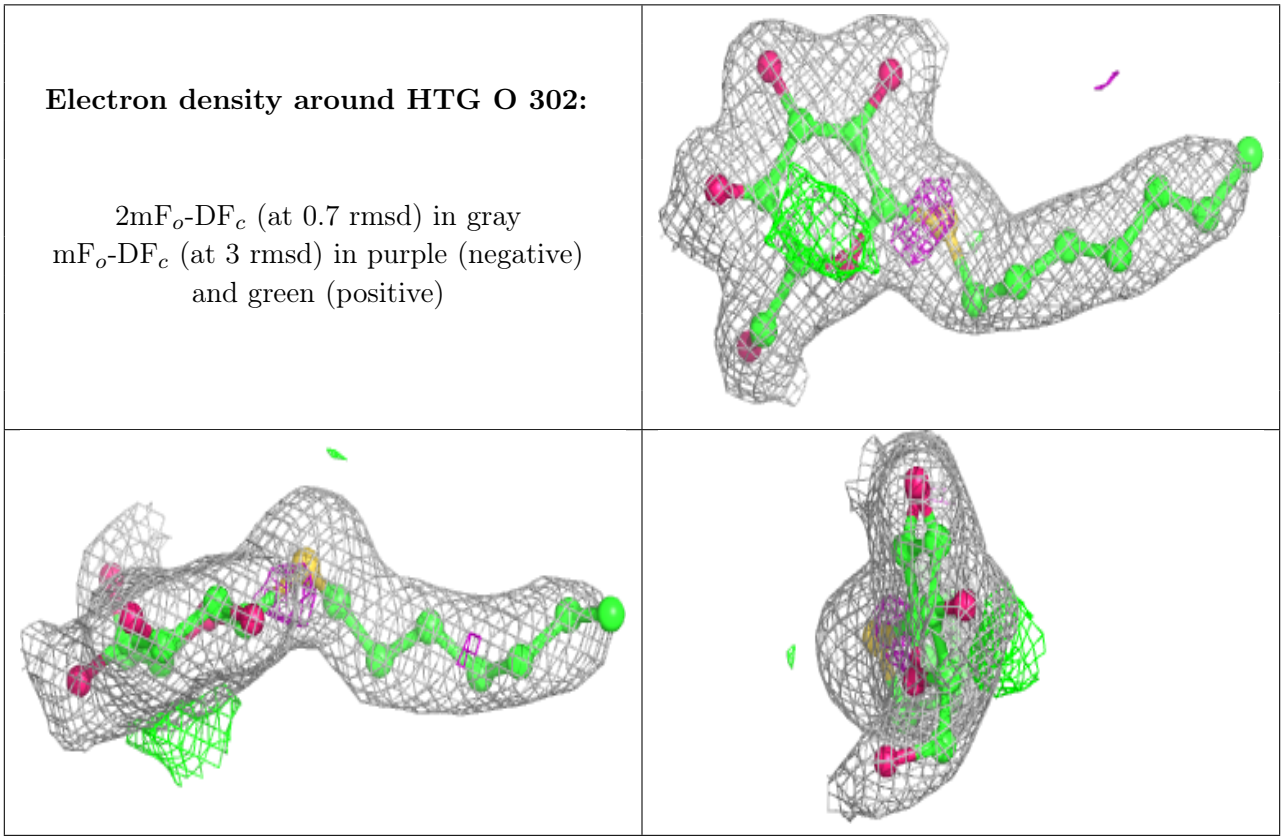
Electron density around BCR T 102:

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



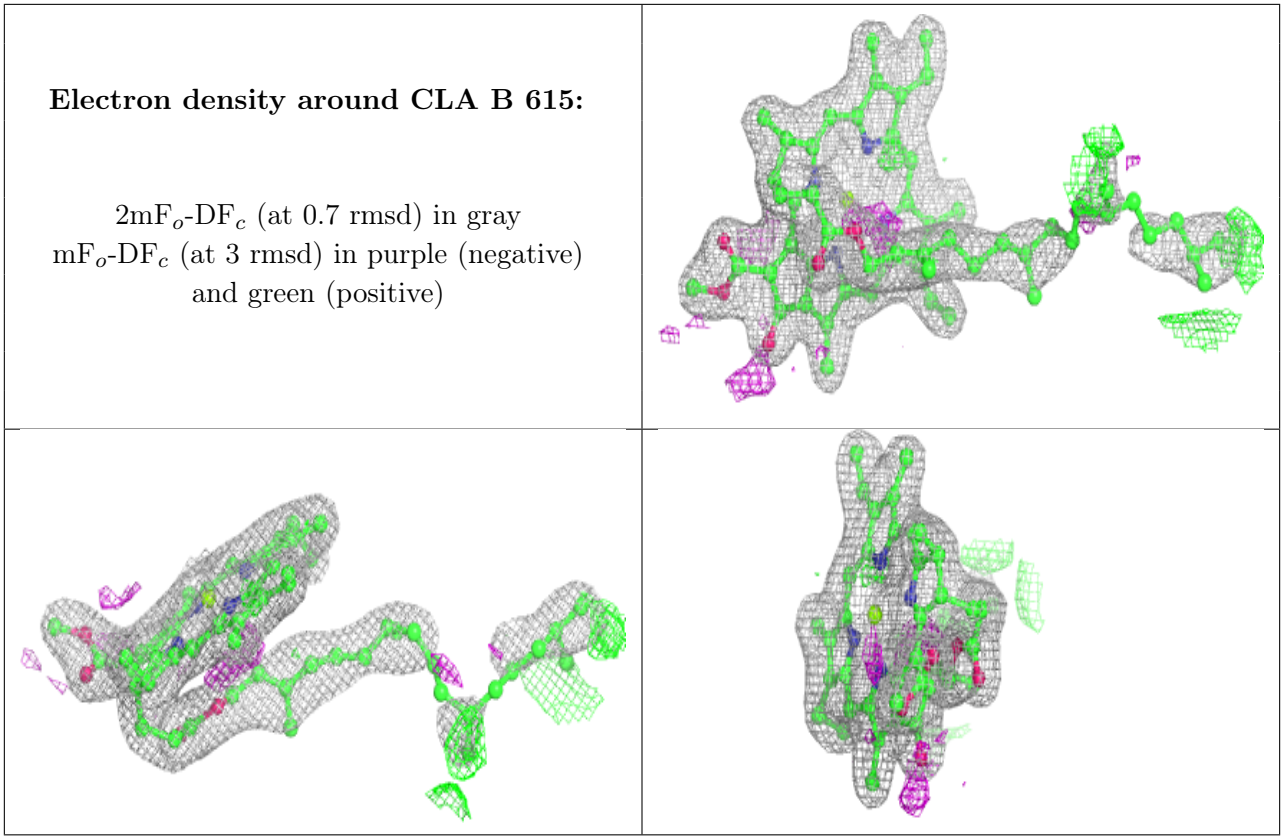
Electron density around HTG O 302:

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



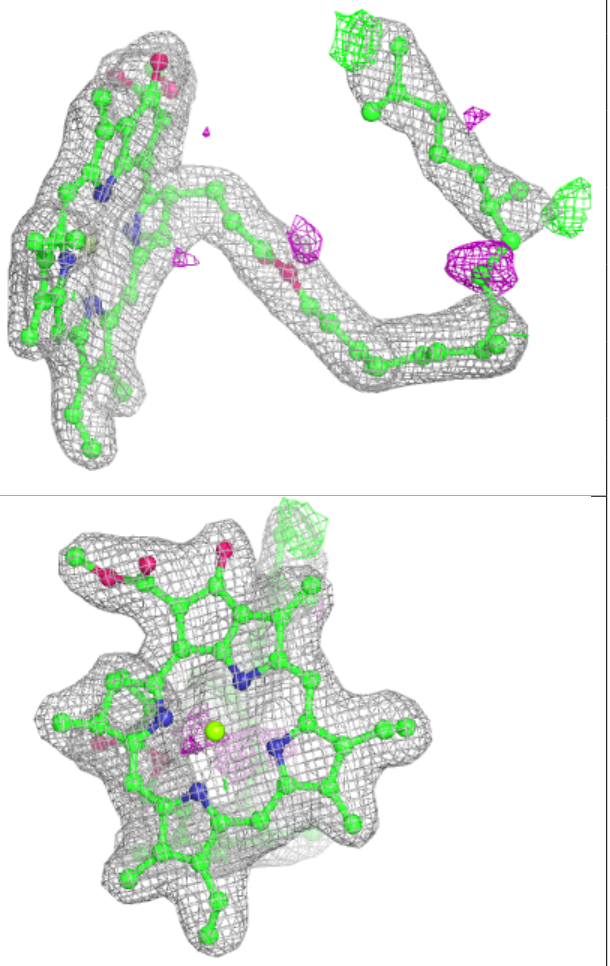
Electron density around CLA B 615:

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



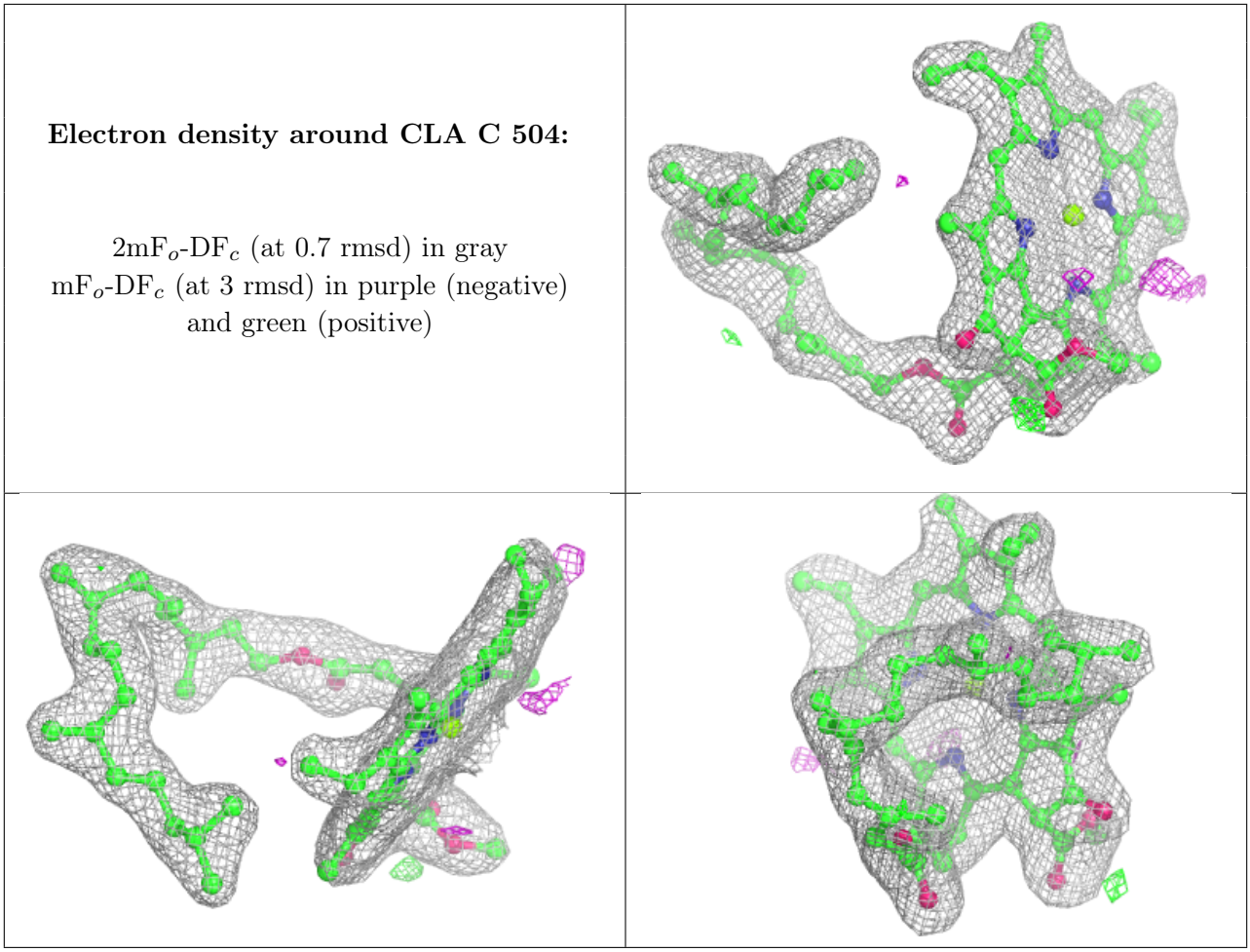
Electron density around CLA b 609:

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



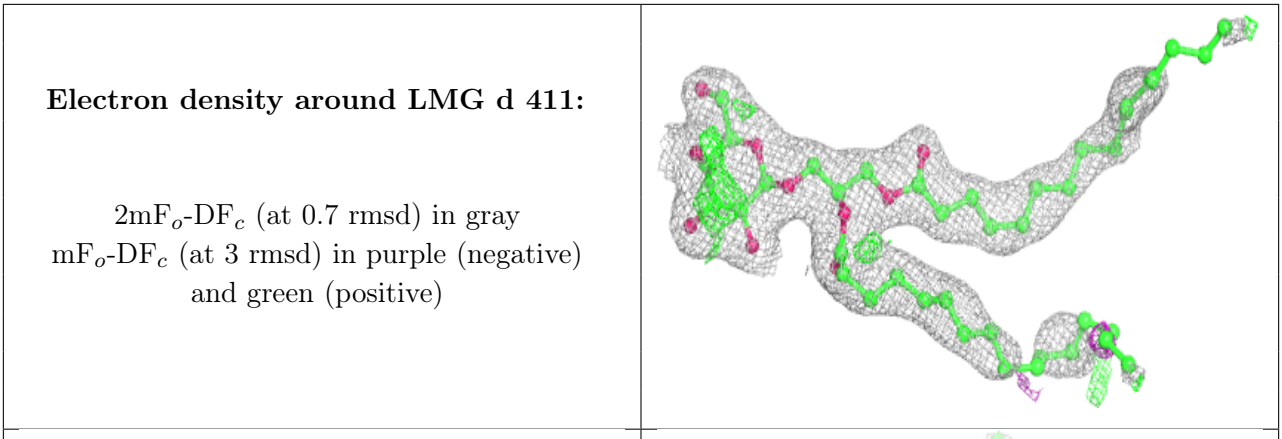
Electron density around CLA C 504:

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



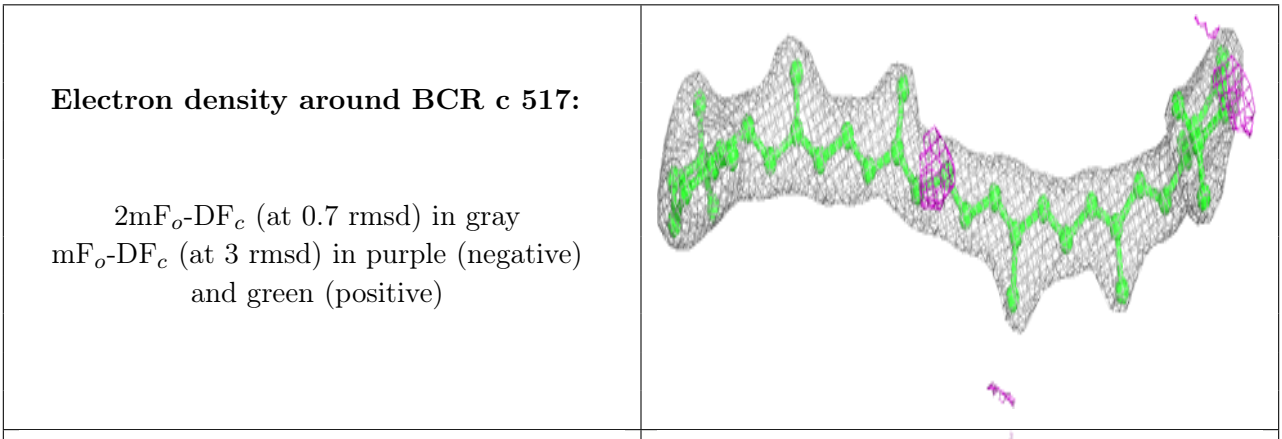
Electron density around LMG d 411:

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



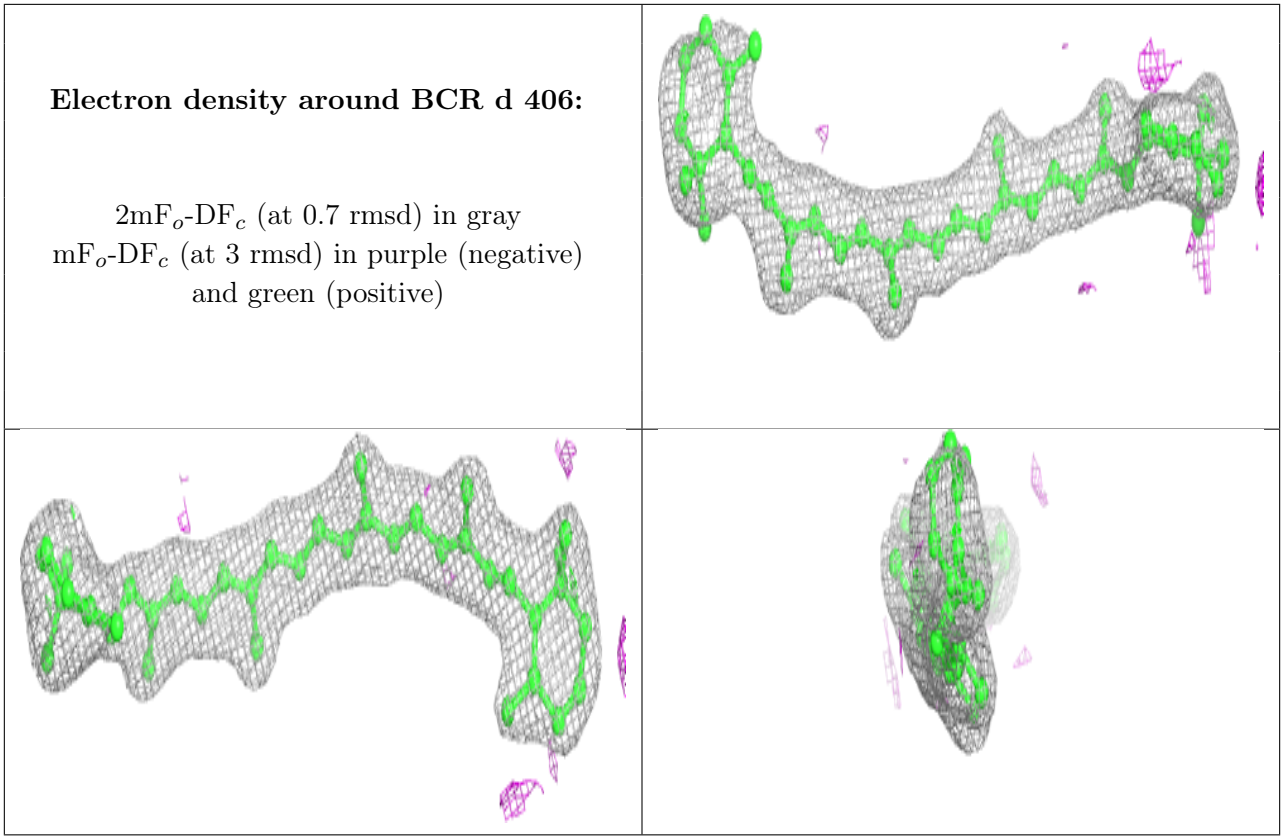
Electron density around BCR c 517:

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



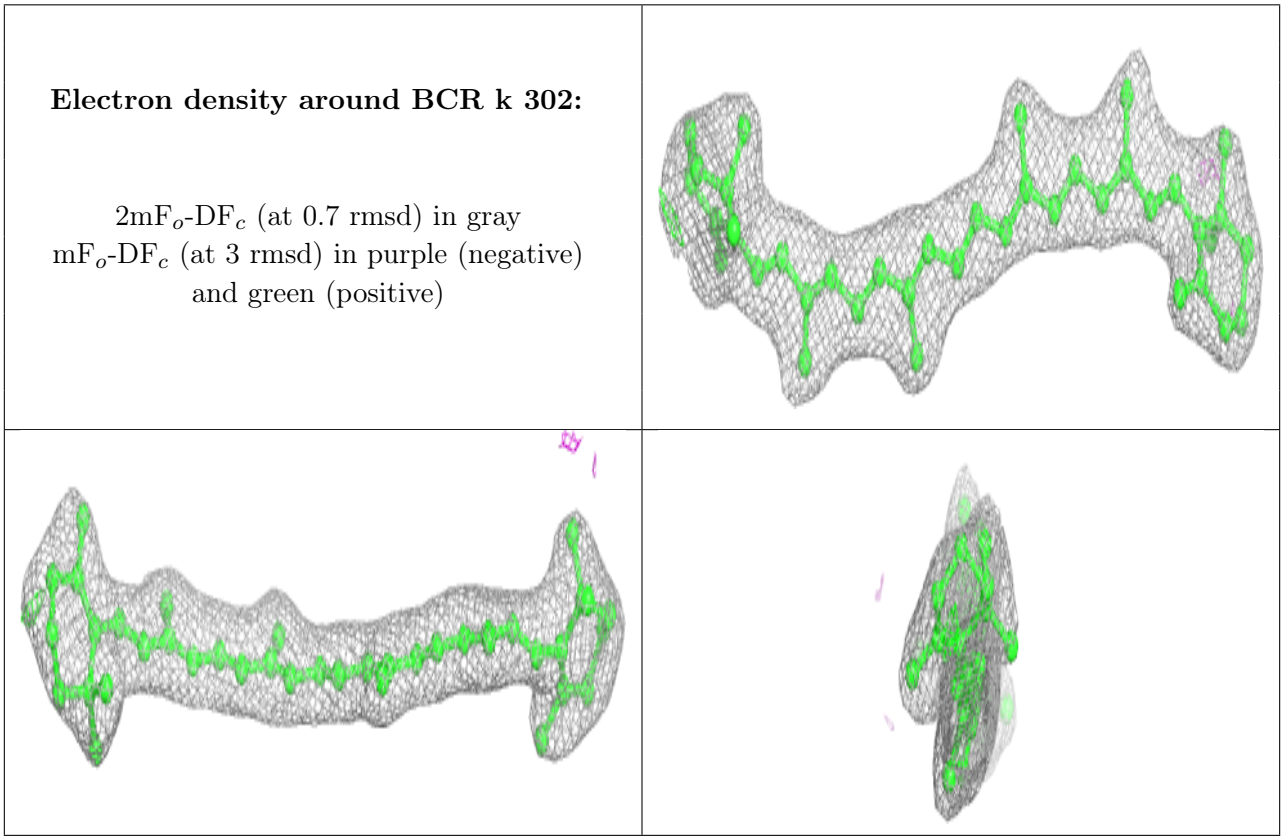
Electron density around BCR d 406:

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



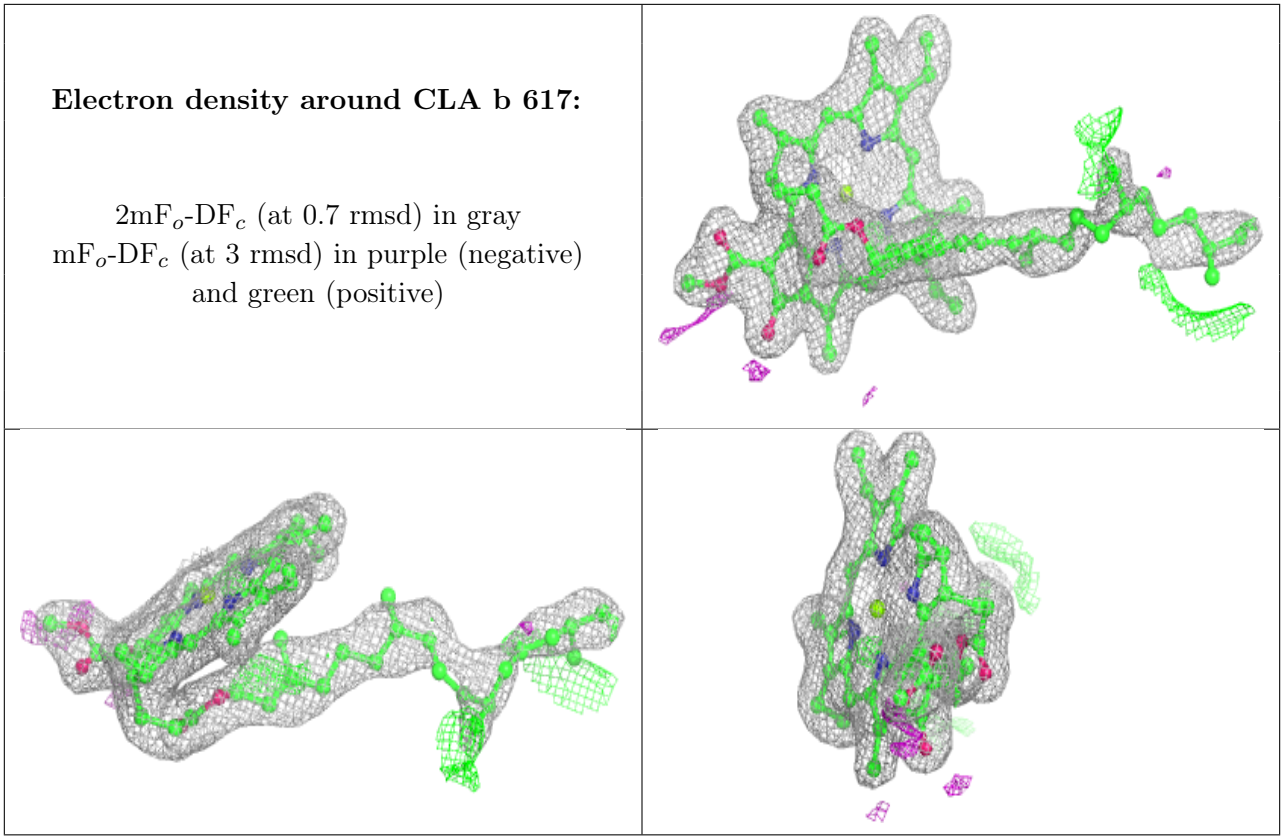
Electron density around BCR k 302:

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



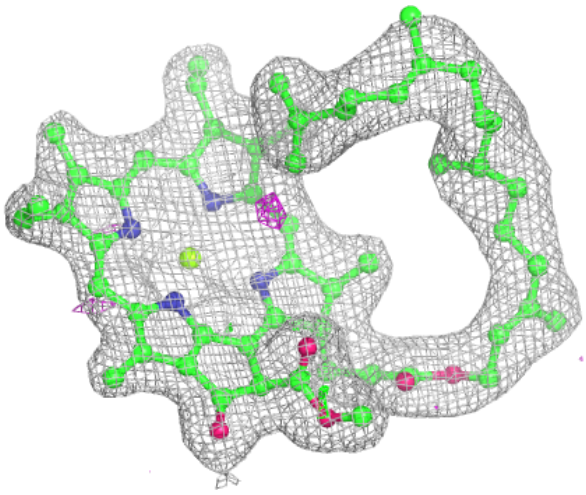
Electron density around CLA b 617:

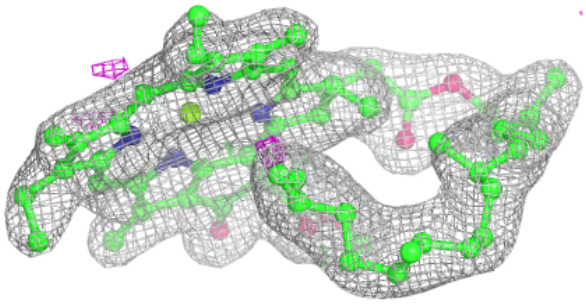
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

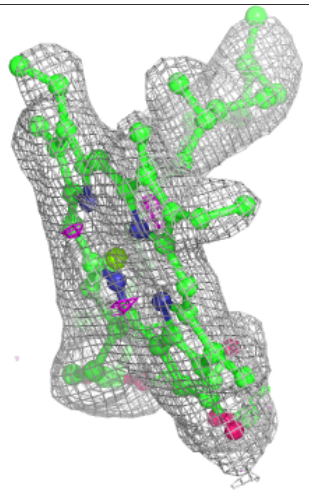


Electron density around CLA b 618:

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

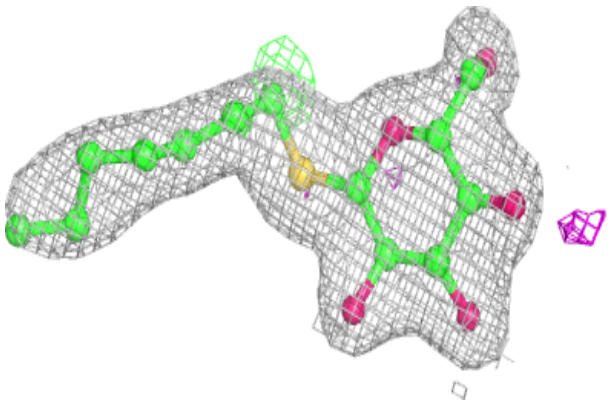


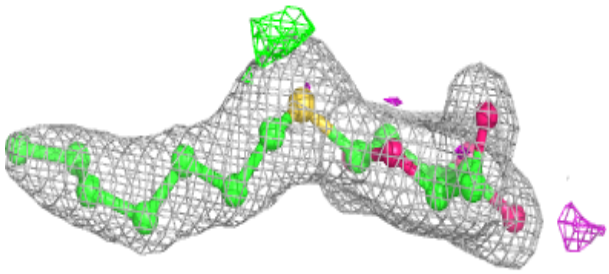


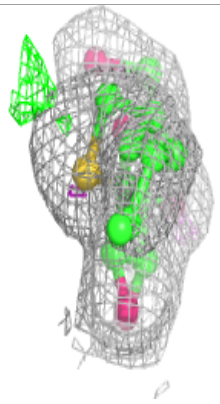


Electron density around HTG o 301:

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

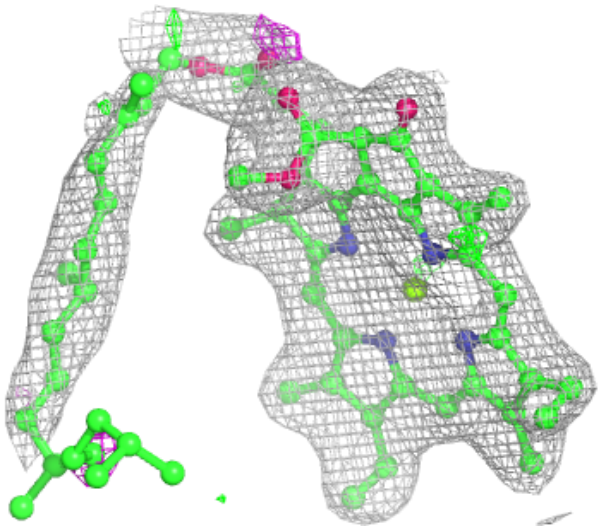


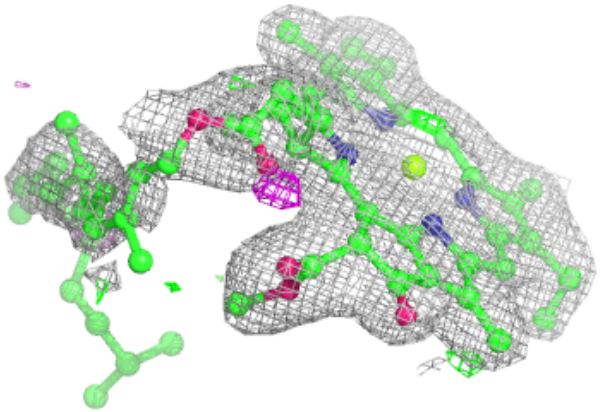


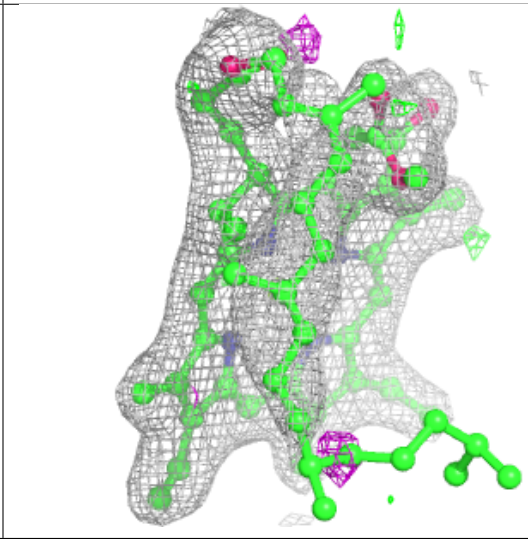


Electron density around CLA b 619:

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

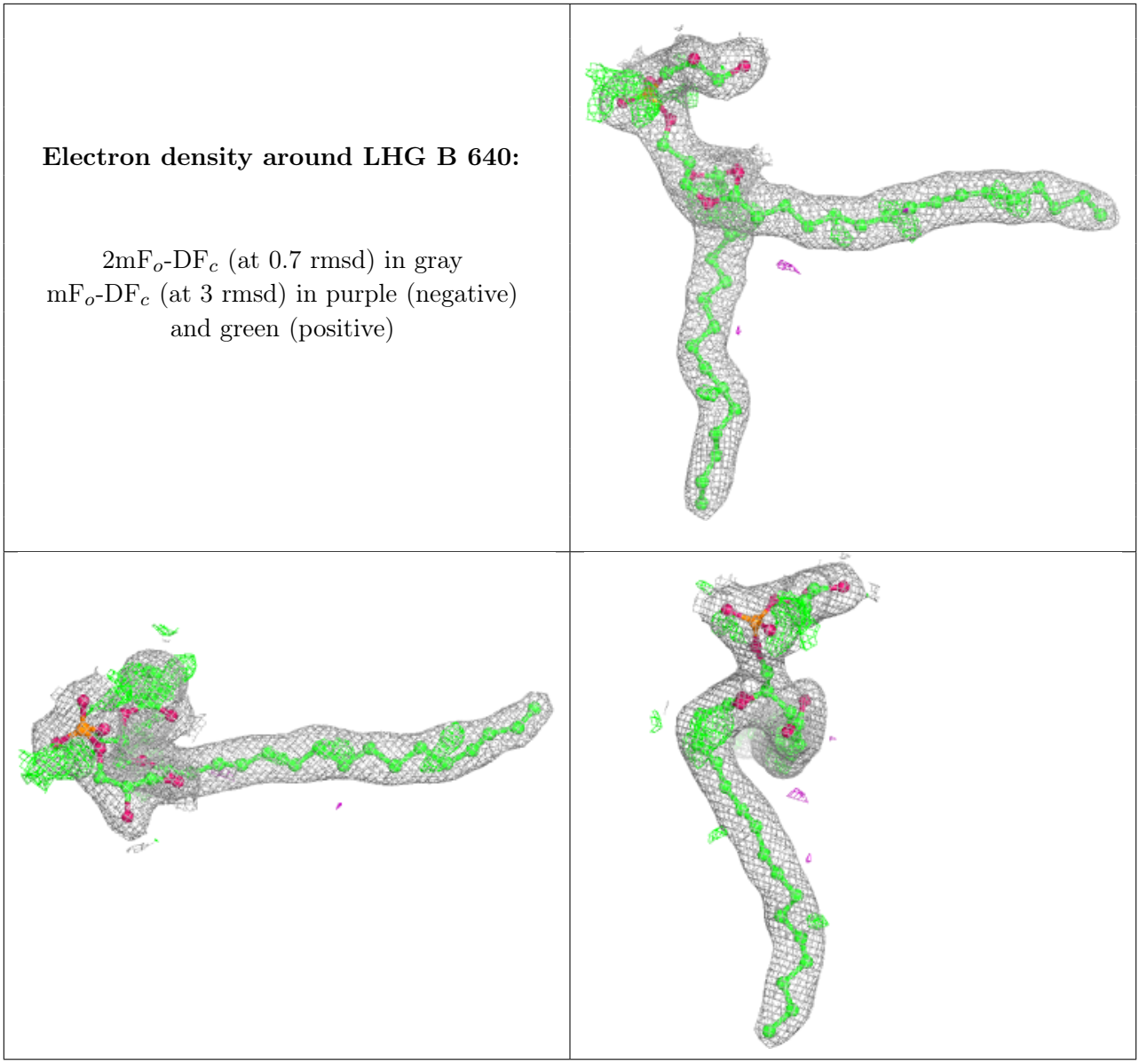






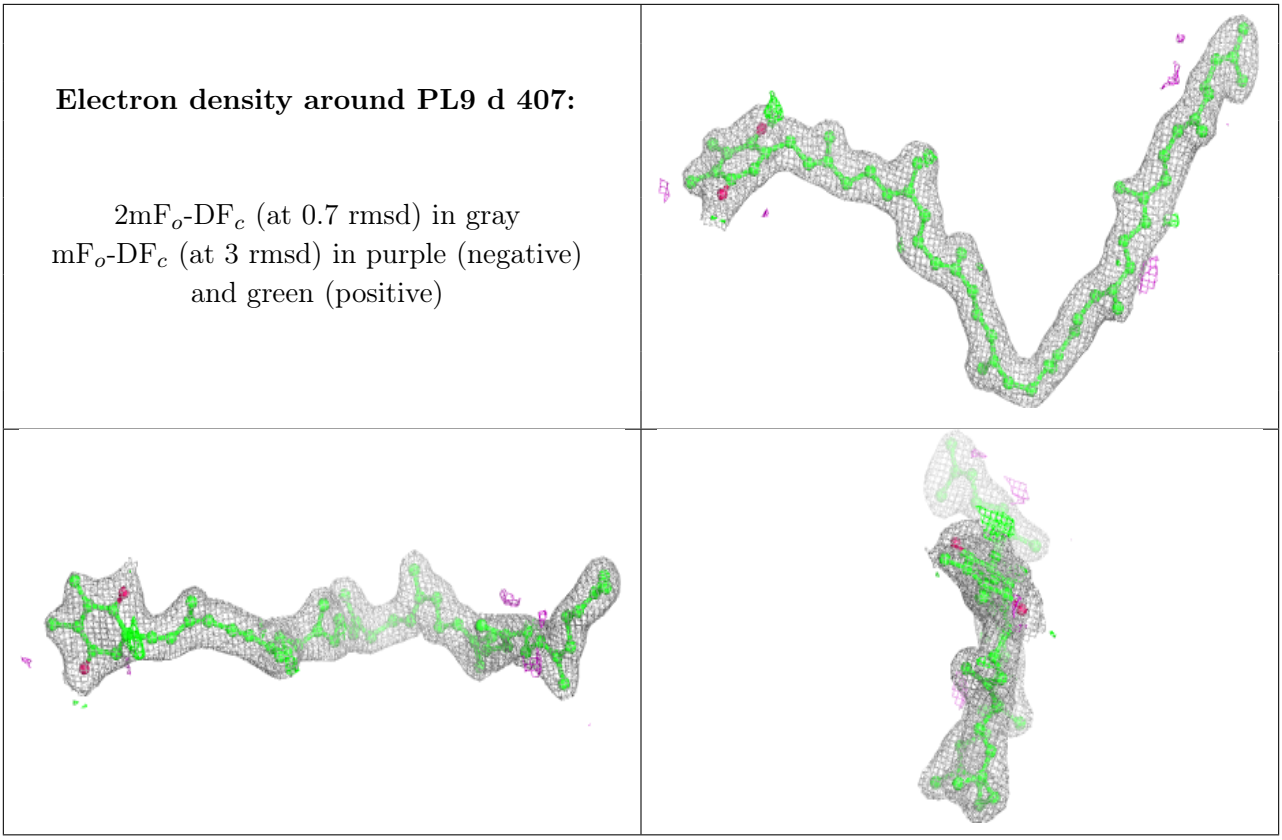
Electron density around LHG B 640:

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



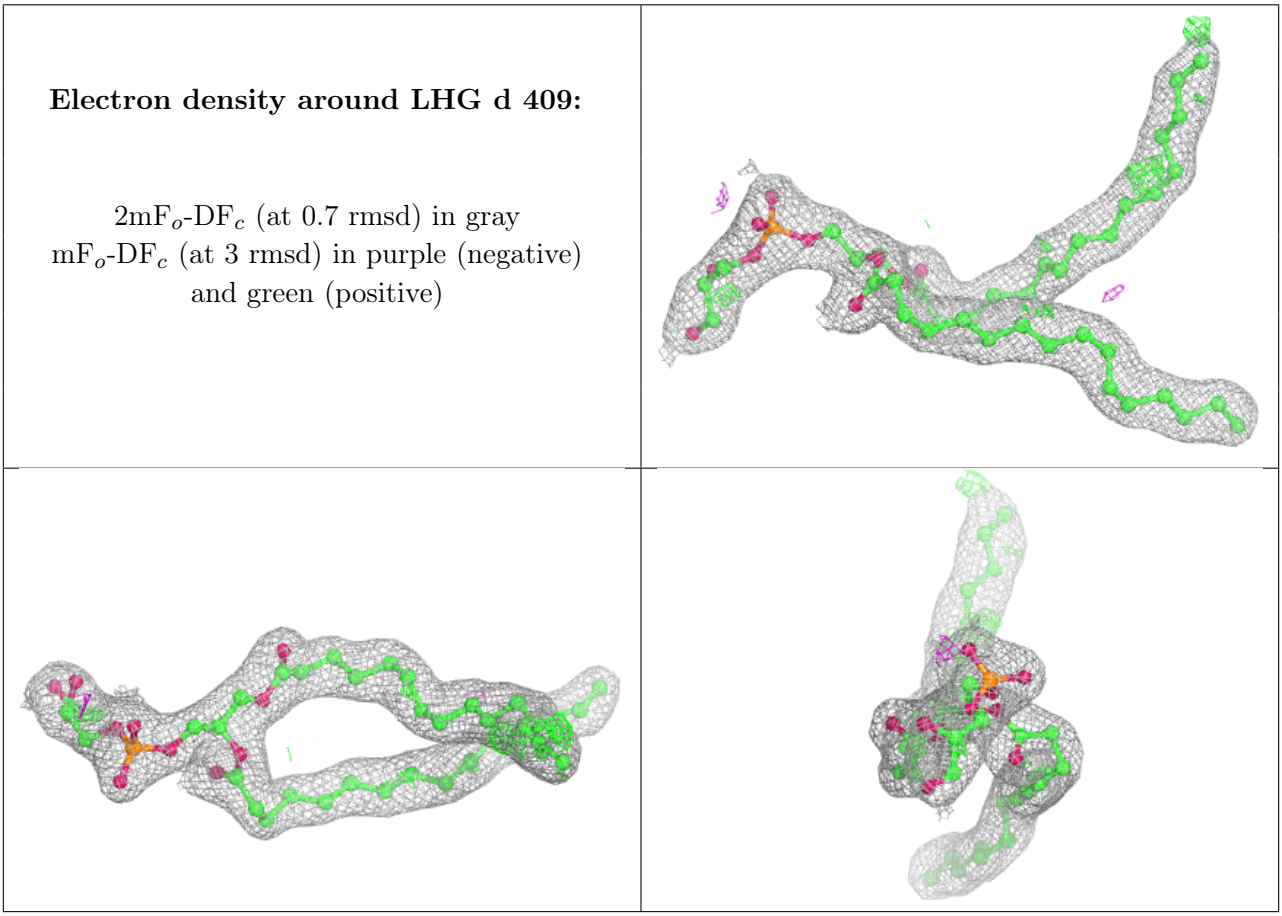
Electron density around PL9 d 407:

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



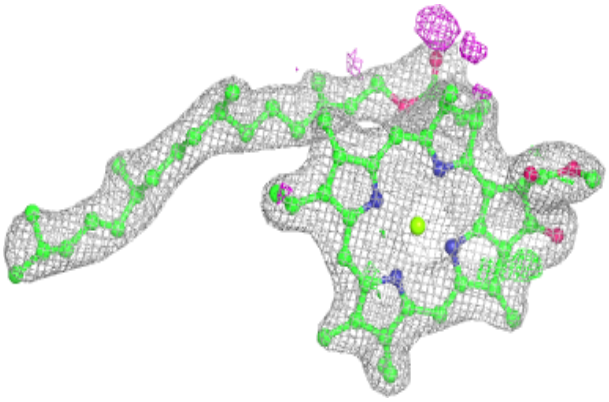
Electron density around LHG d 409:

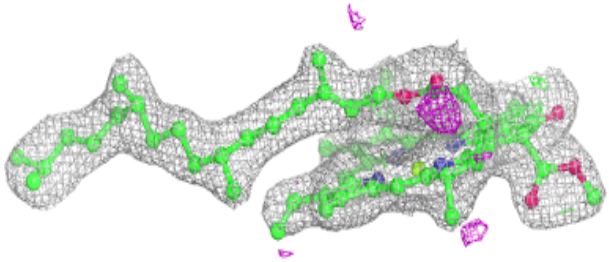
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

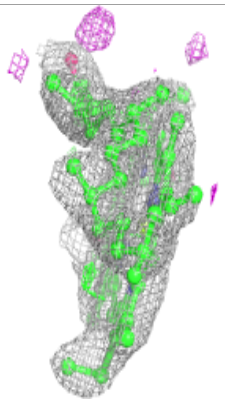


Electron density around CLA c 503:

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

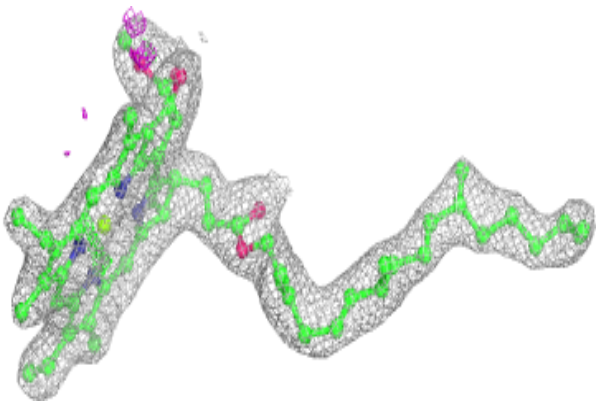


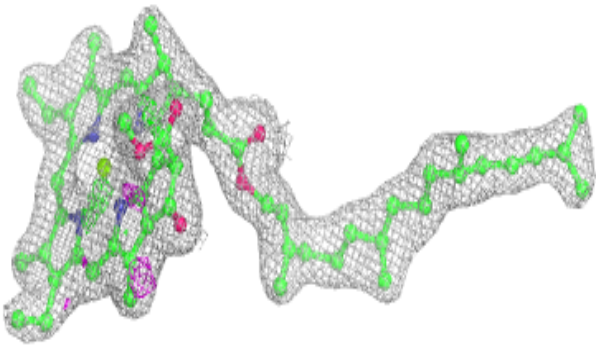


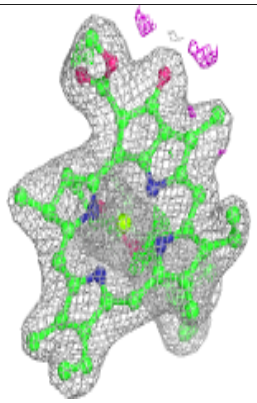


Electron density around CLA c 504:

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

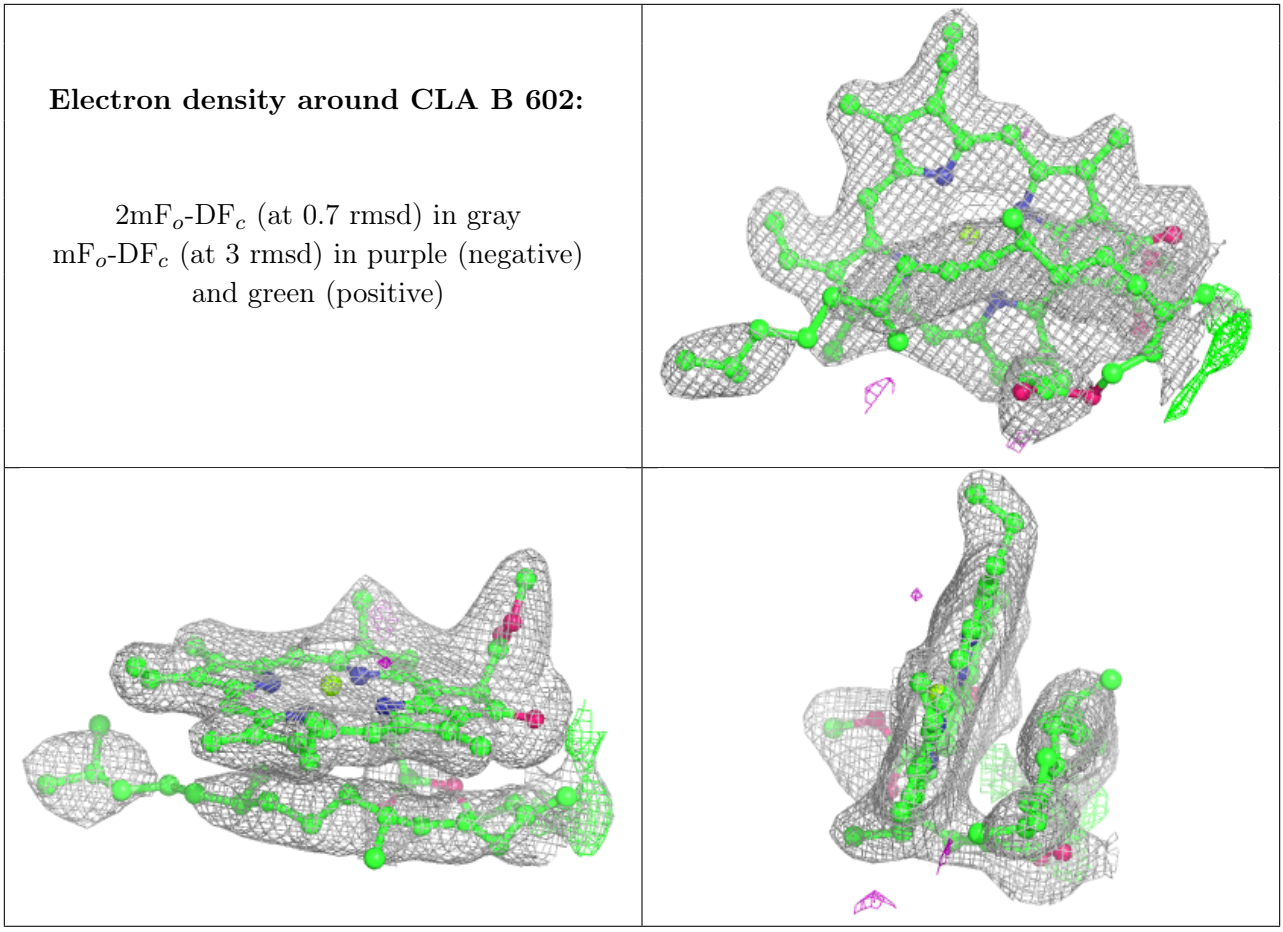






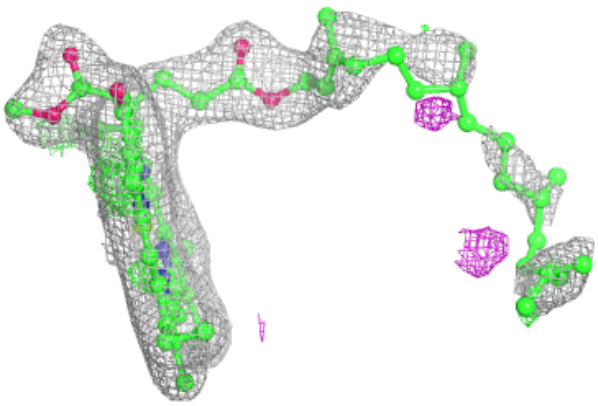
Electron density around CLA B 602:

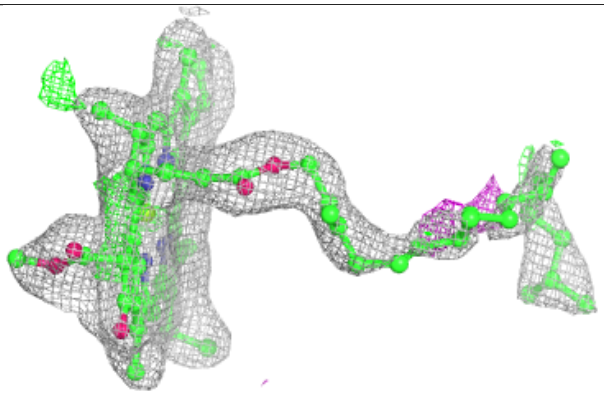
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

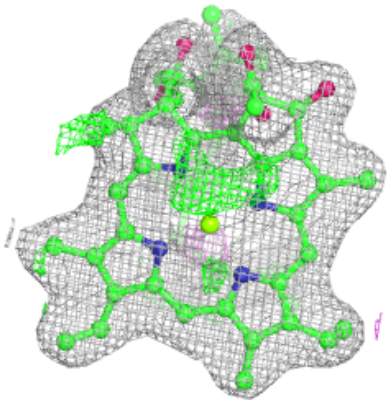


Electron density around CLA c 508:

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

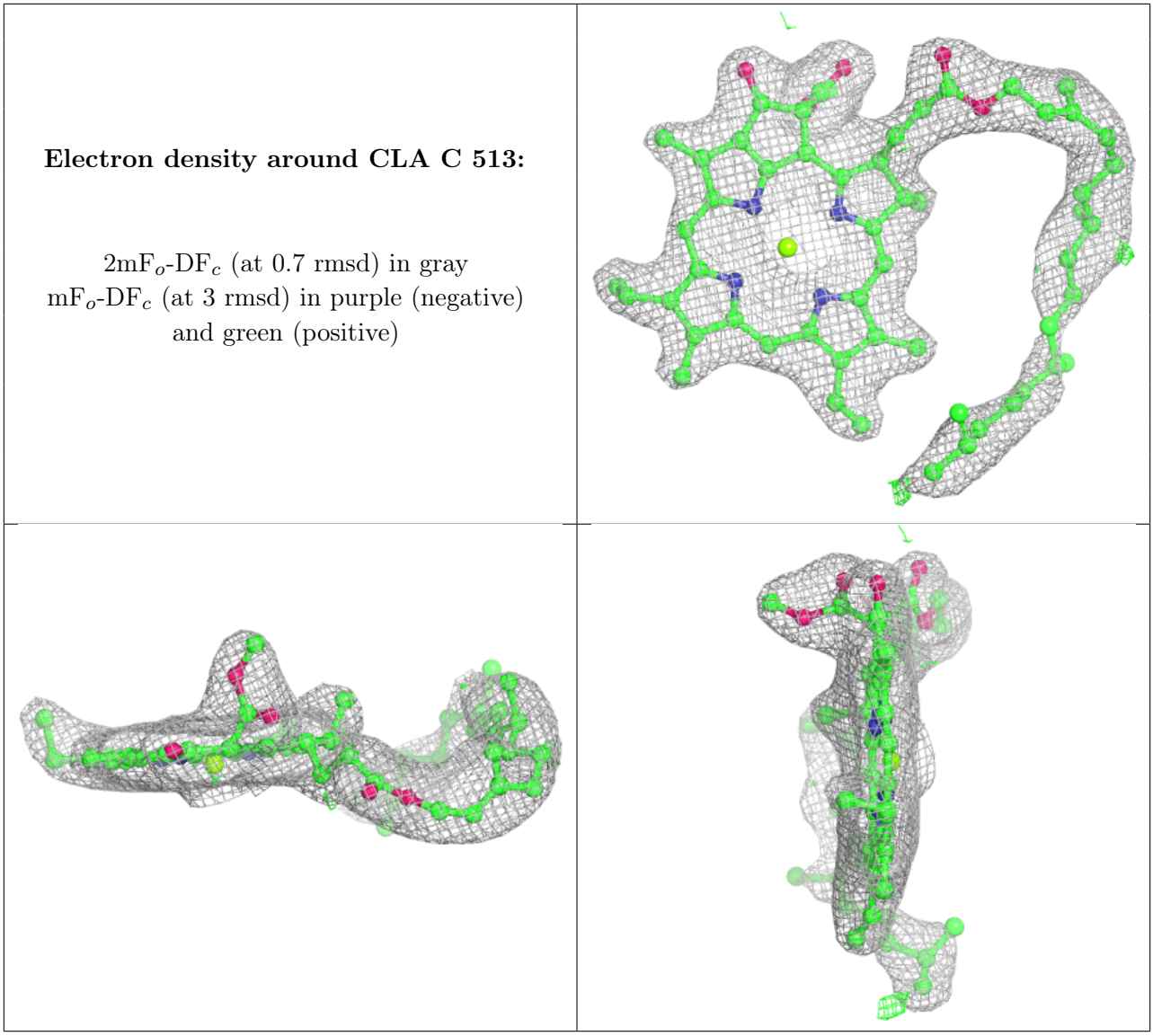






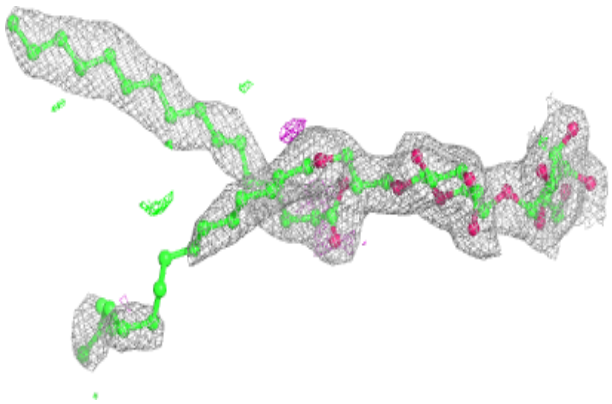
Electron density around CLA C 513:

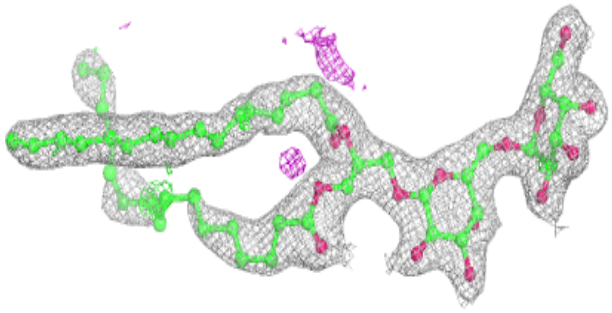
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

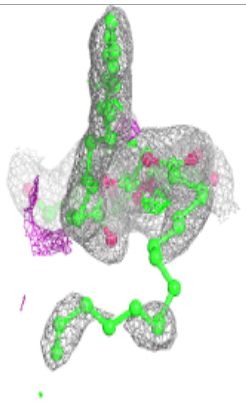


Electron density around DGD c 518:

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

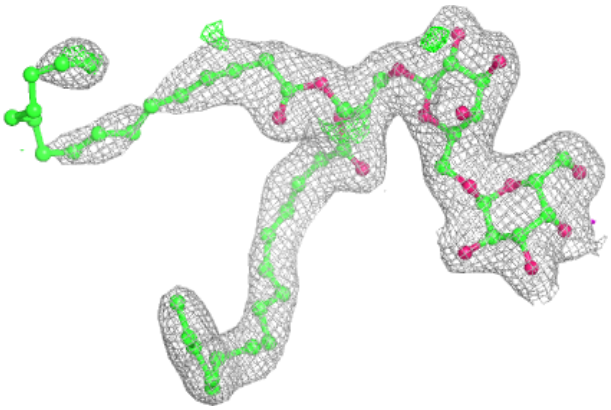


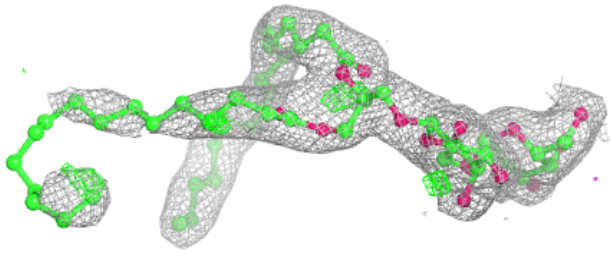


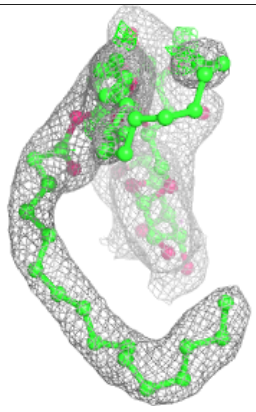


Electron density around DGD c 519:

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

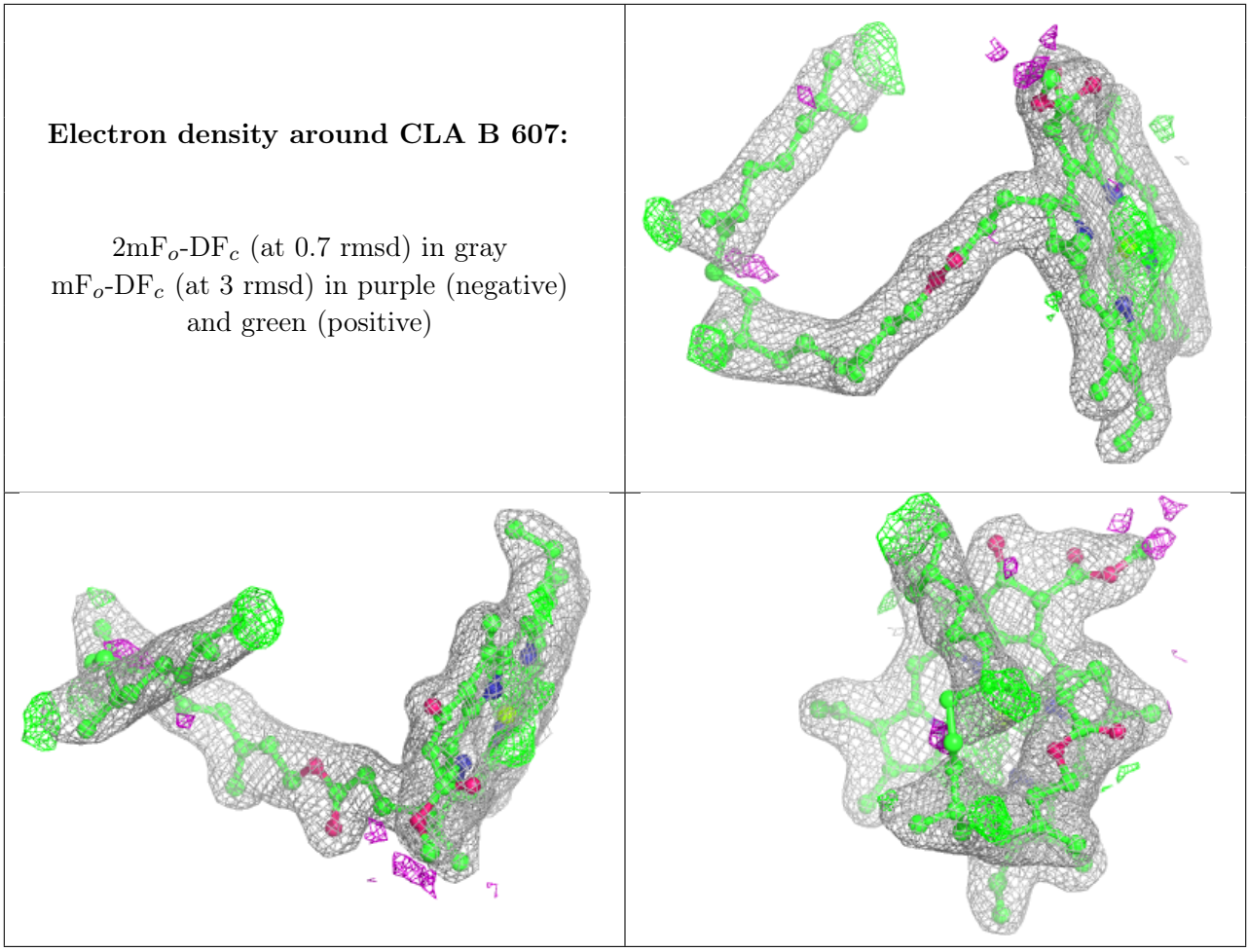






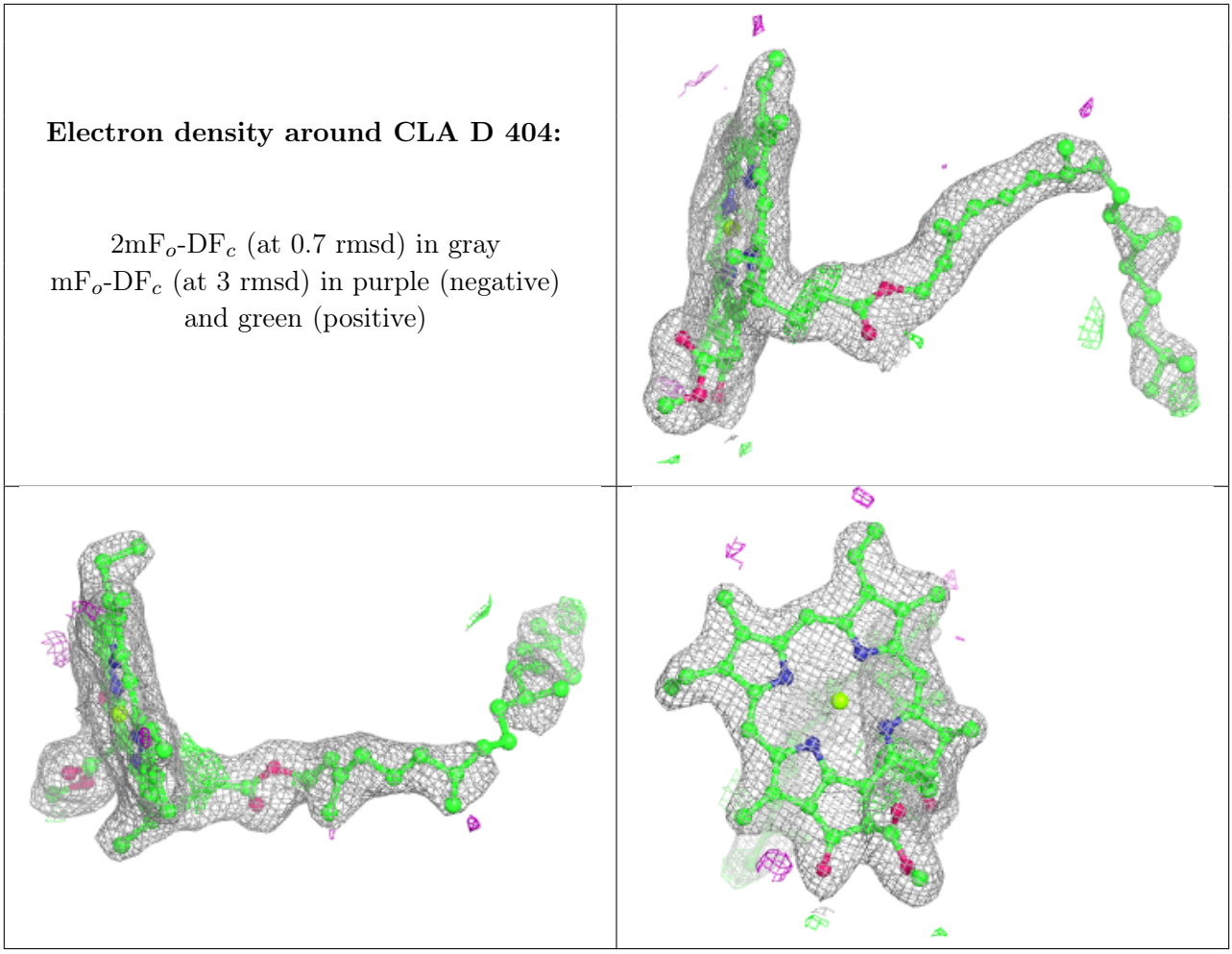
Electron density around CLA B 607:

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



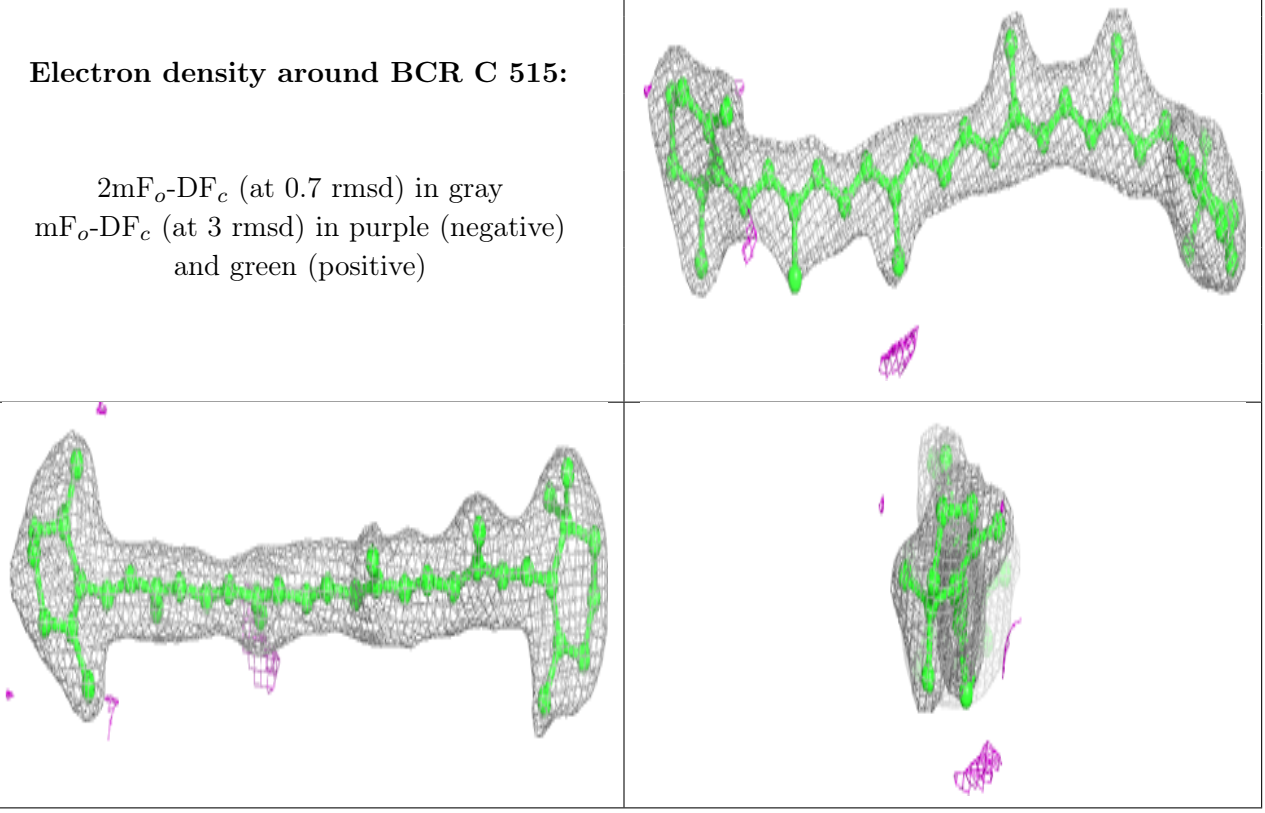
Electron density around CLA D 404:

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



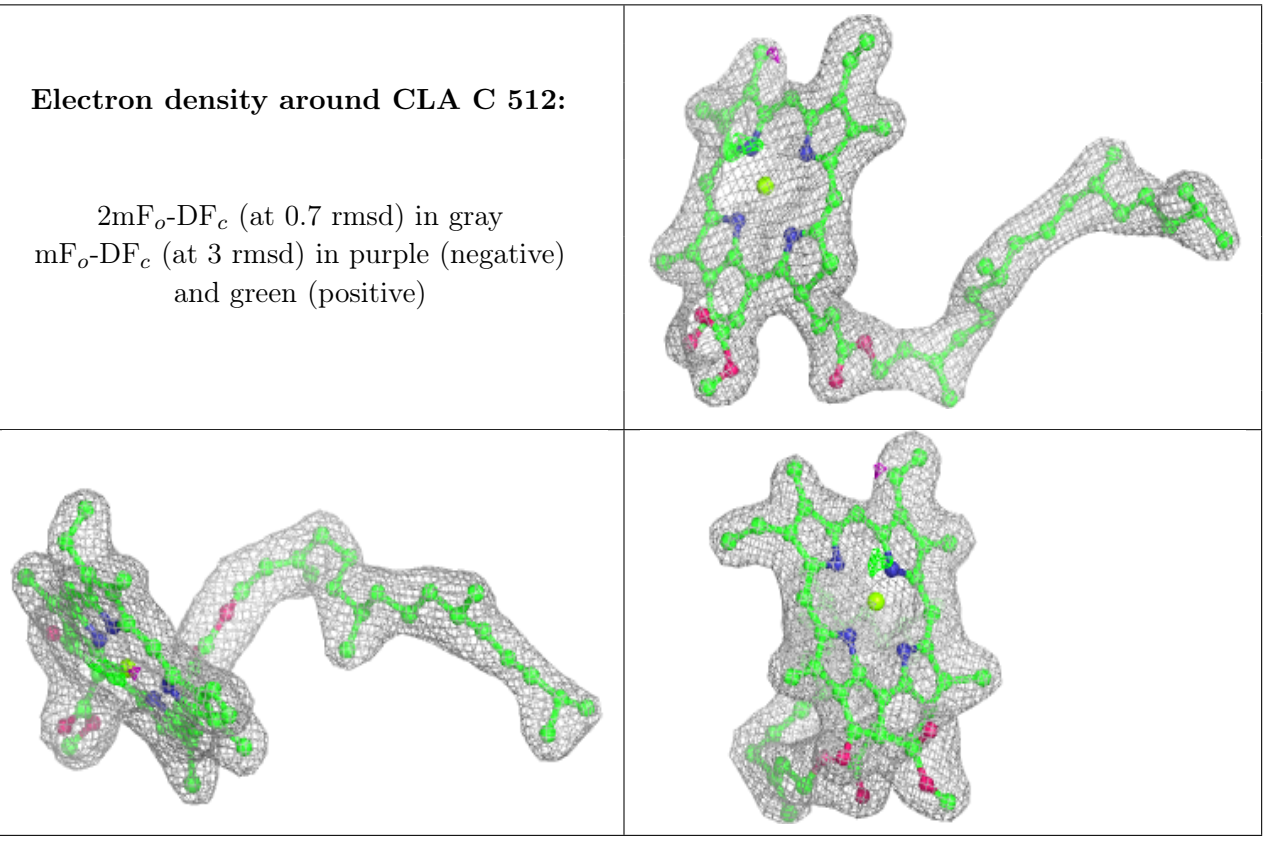
Electron density around BCR C 515:

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



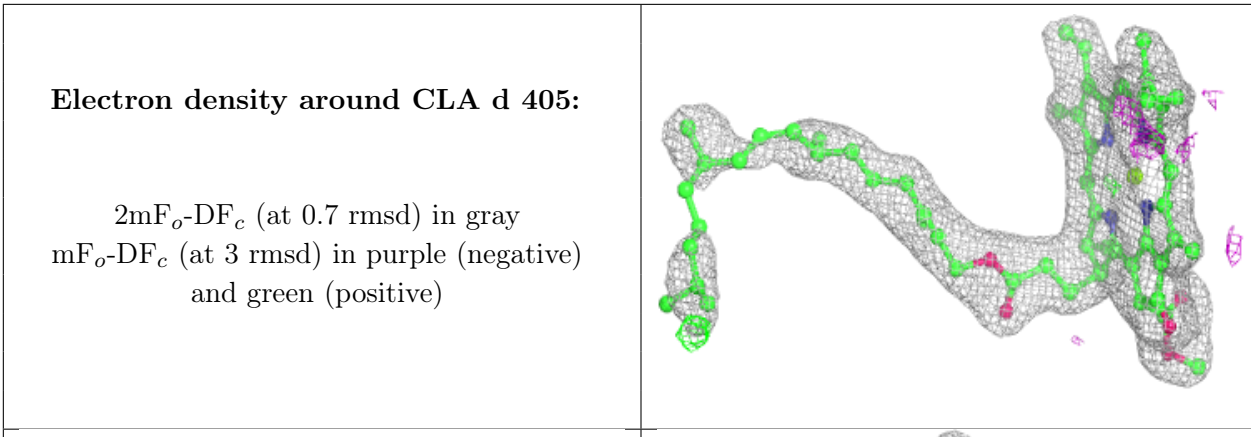
Electron density around CLA C 512:

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



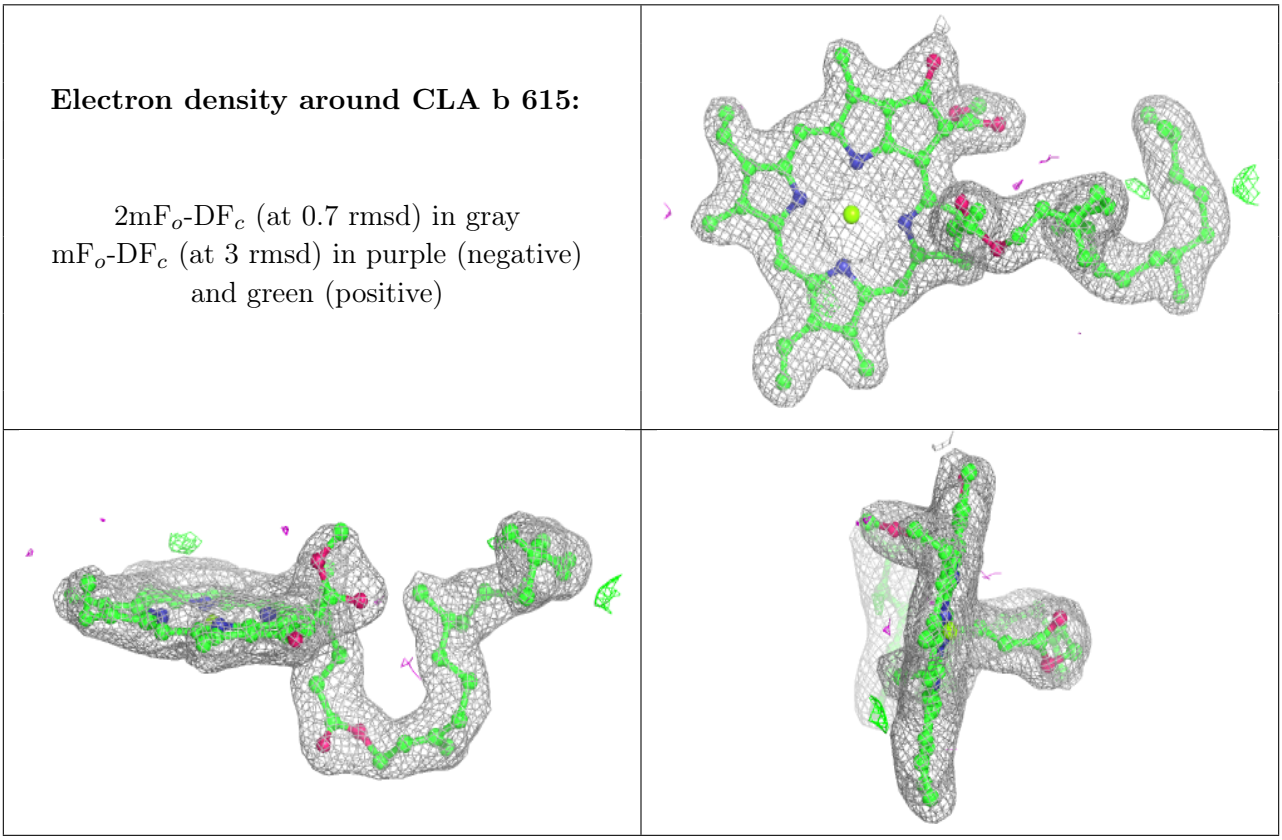
Electron density around CLA d 405:

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



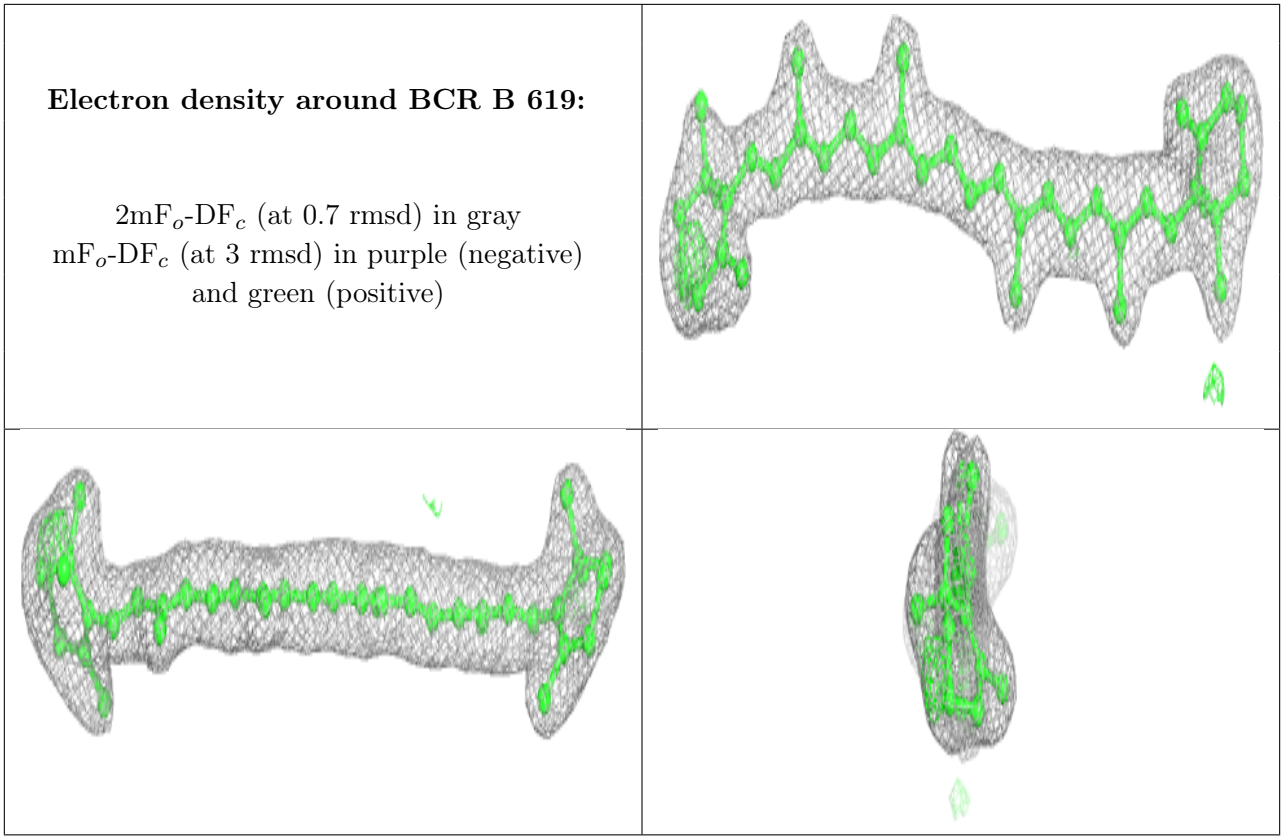
Electron density around CLA b 615:

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



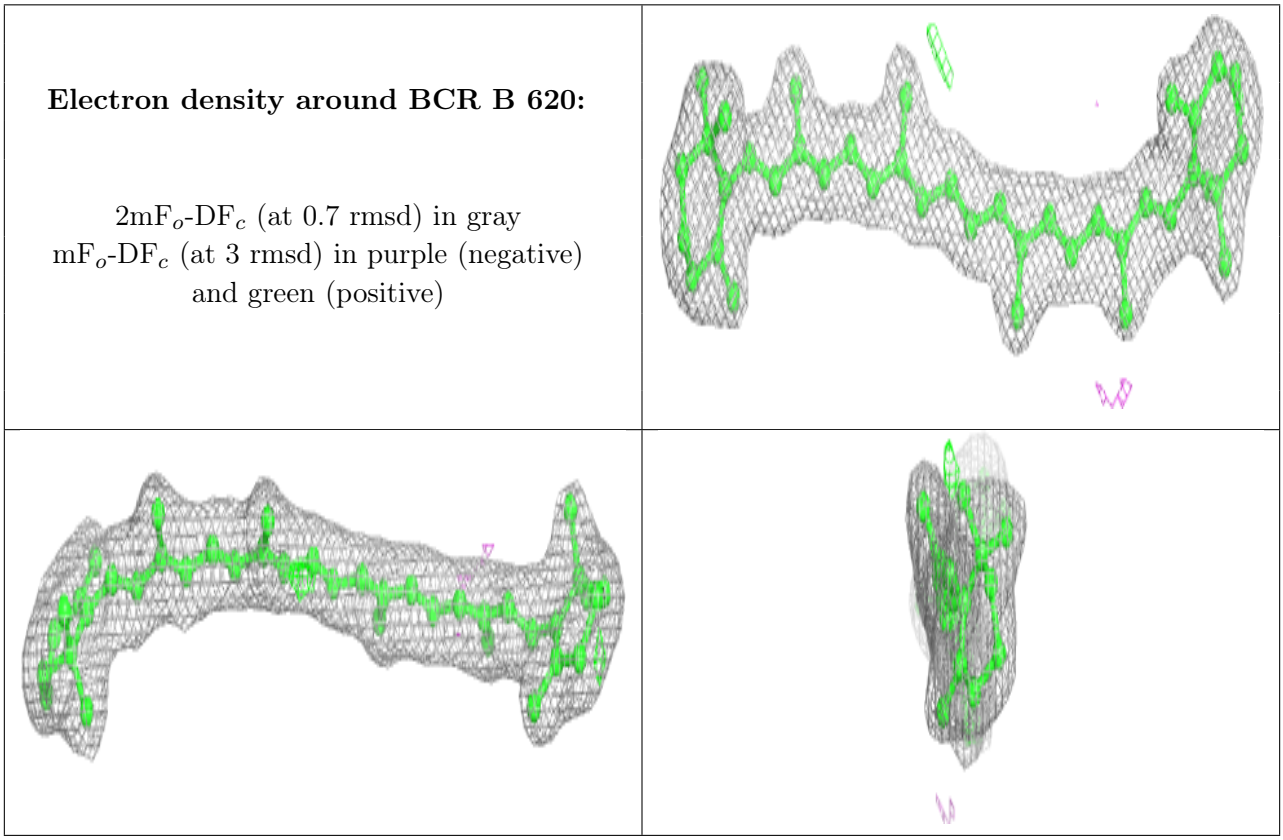
Electron density around BCR B 619:

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



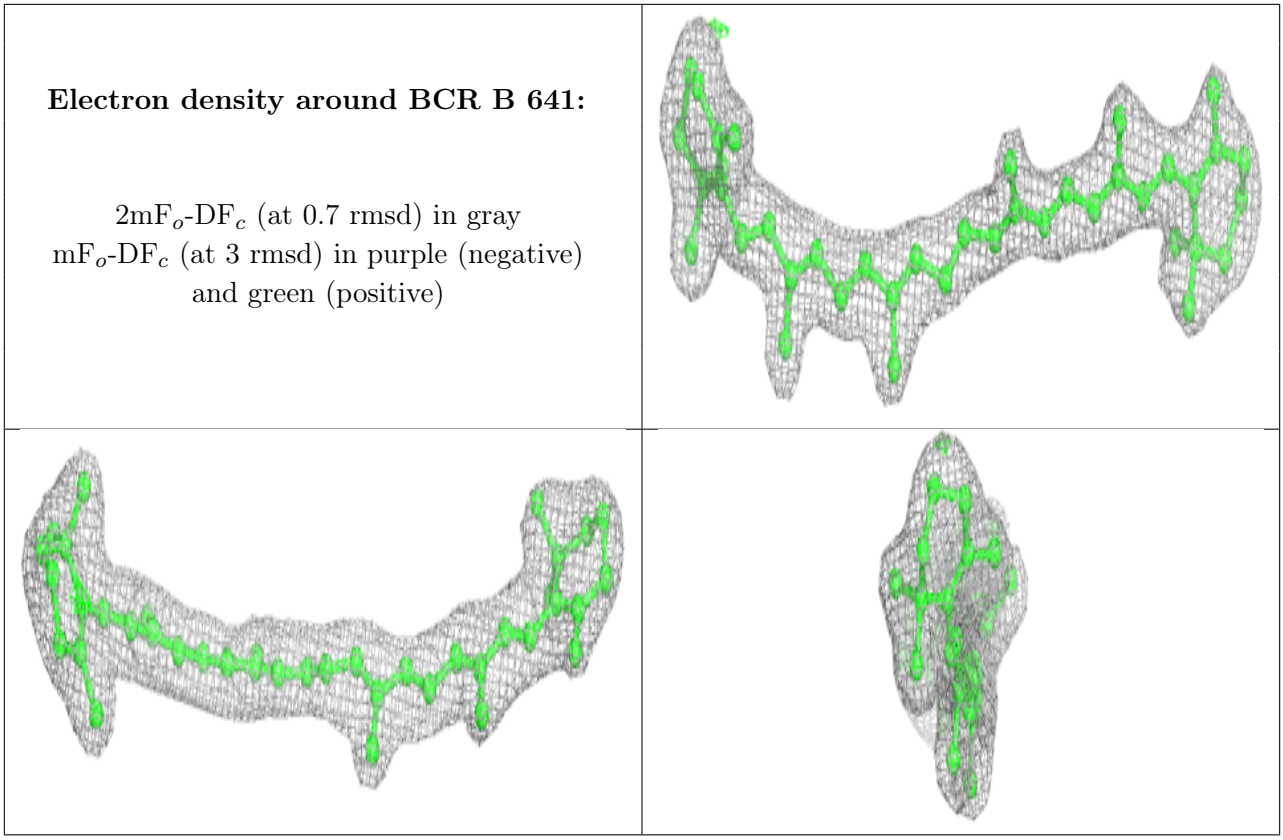
Electron density around BCR B 620:

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



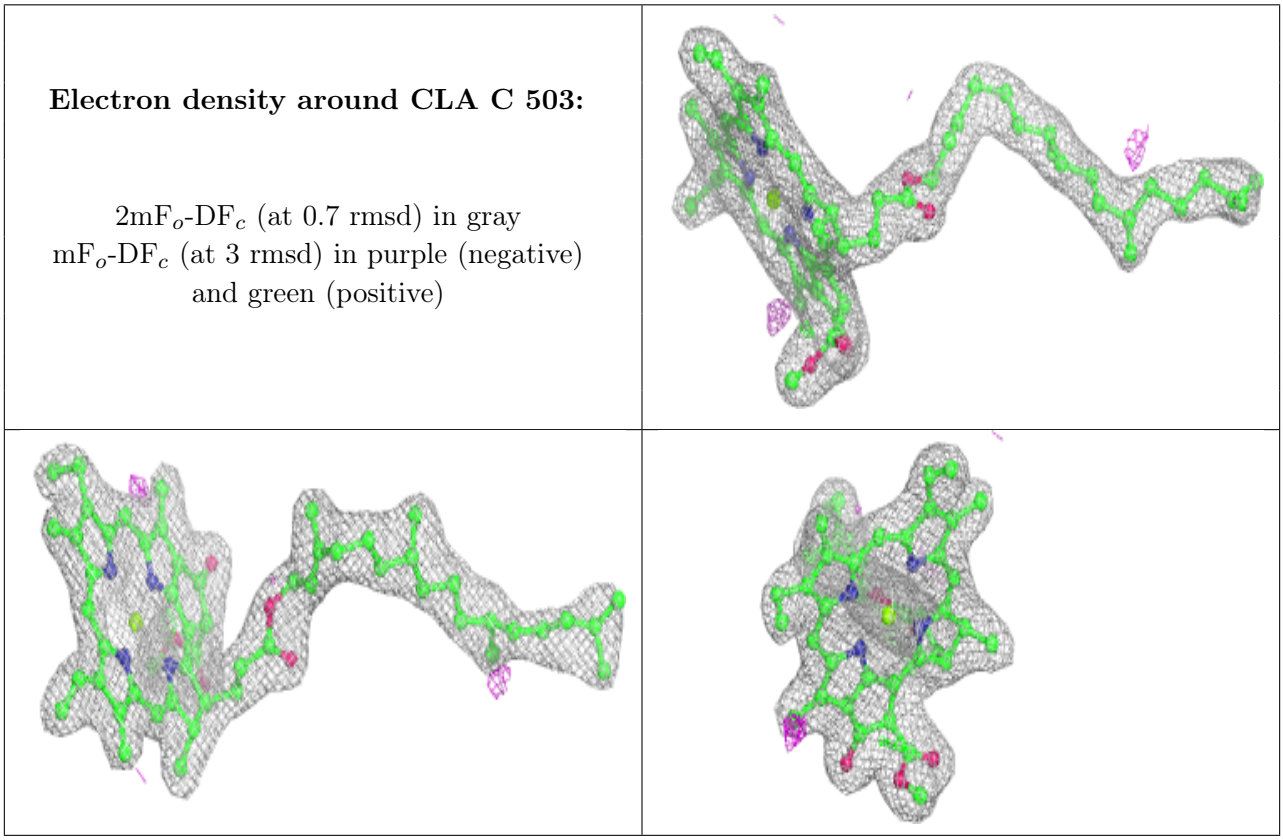
Electron density around BCR B 641:

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



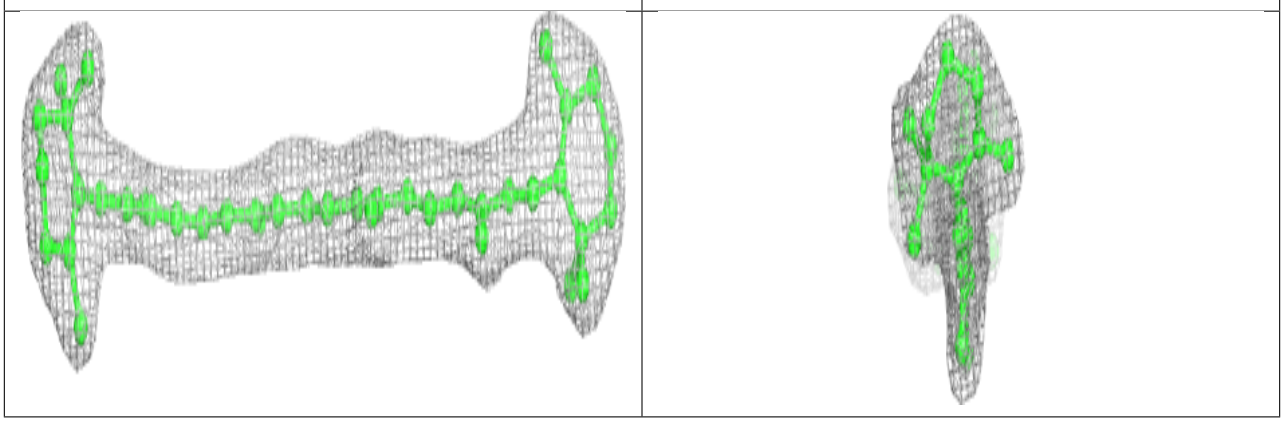
Electron density around CLA C 503:

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



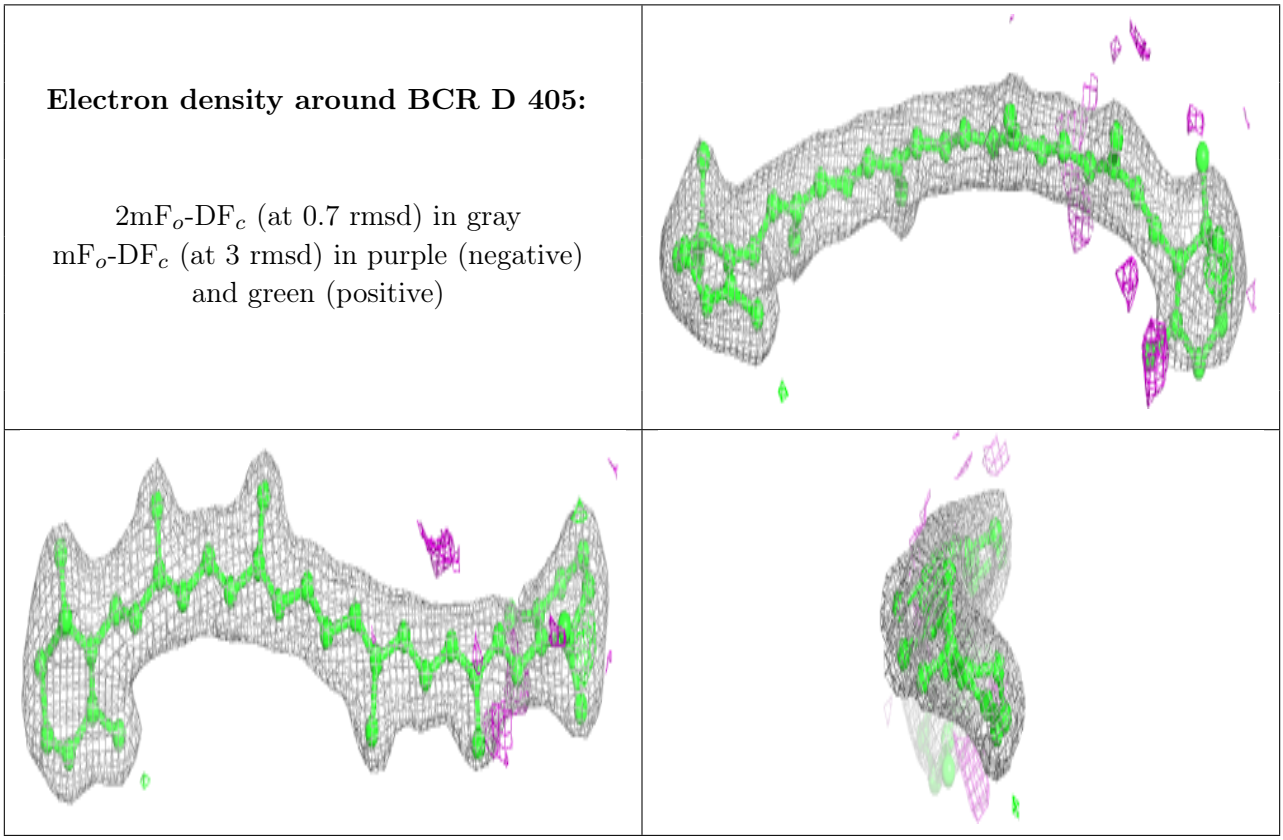
Electron density around BCR C 516:

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



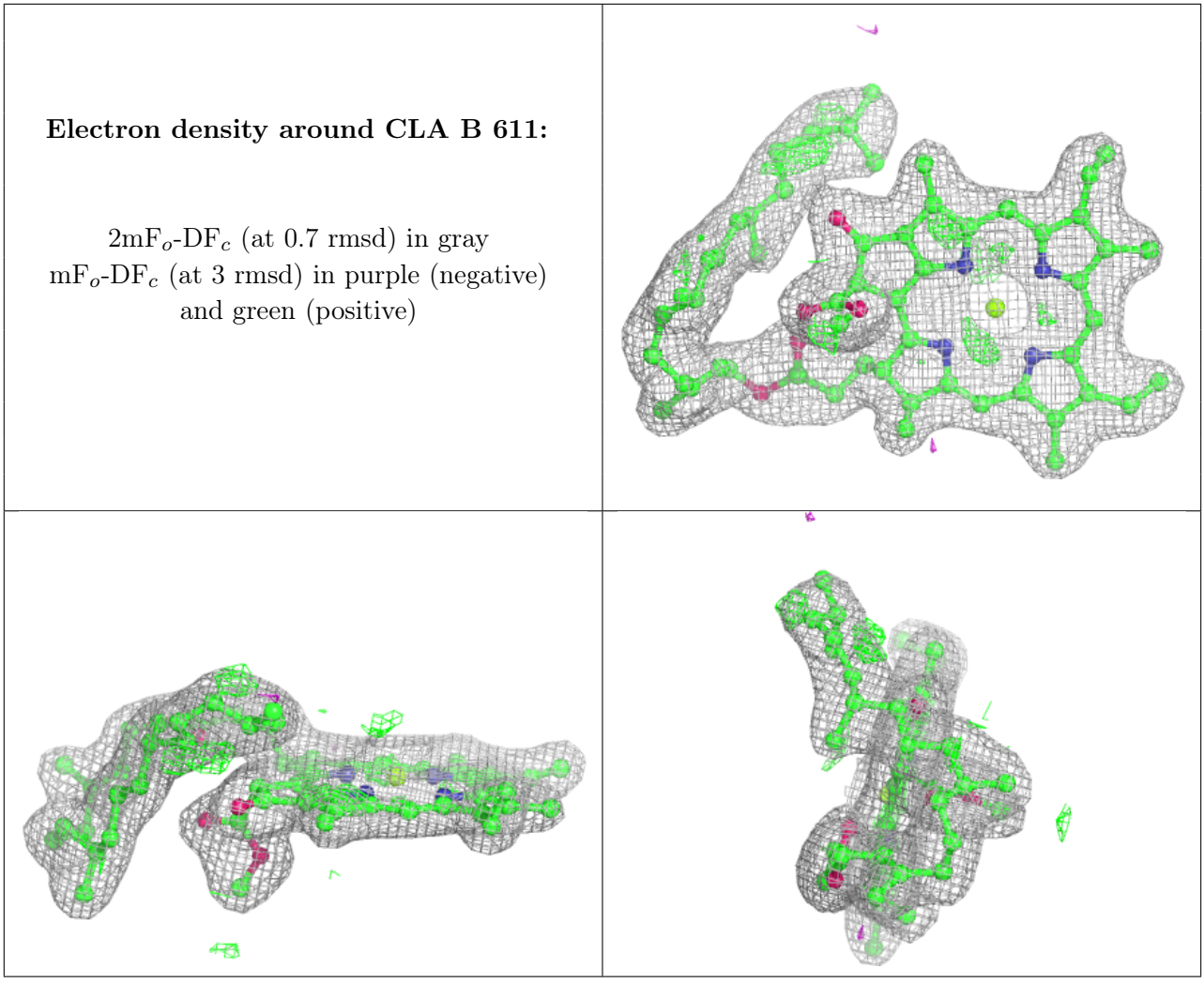
Electron density around BCR D 405:

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



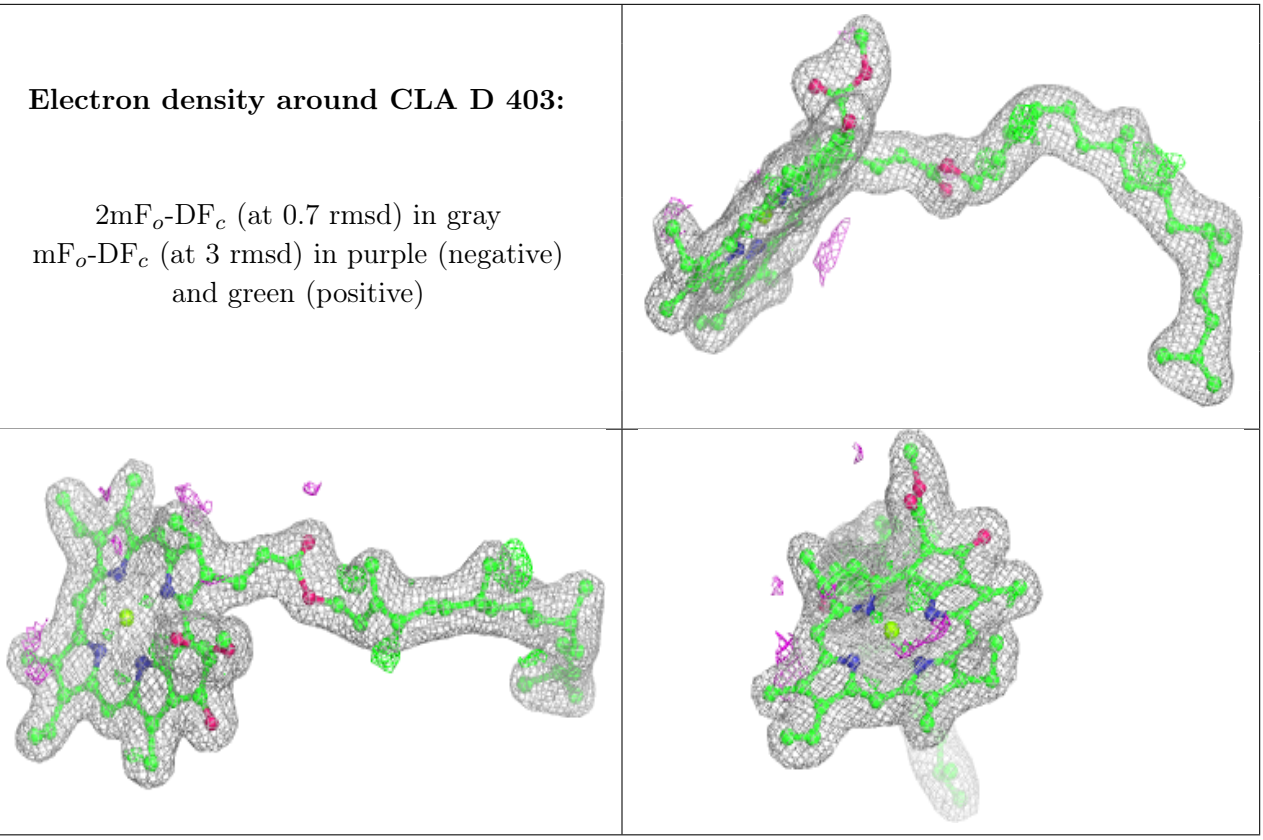
Electron density around CLA B 611:

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



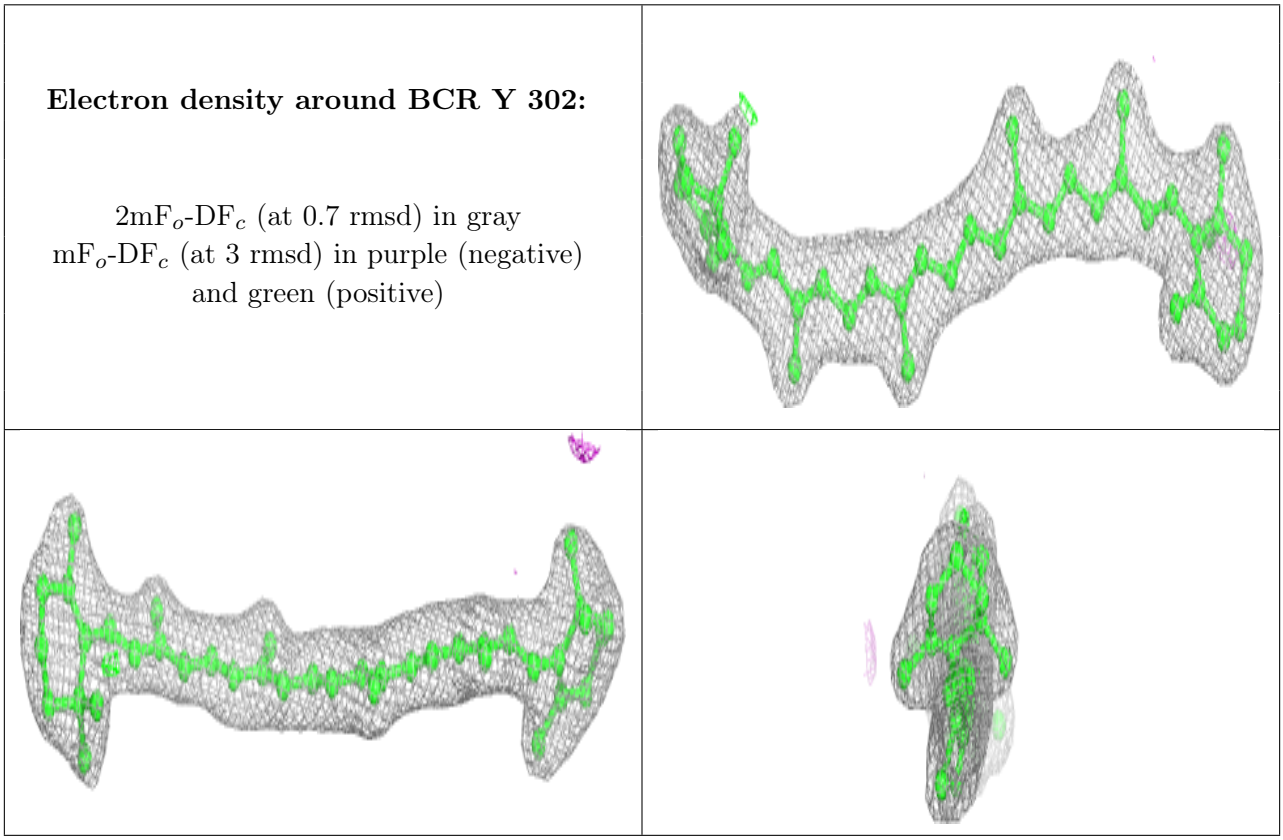
Electron density around CLA D 403:

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



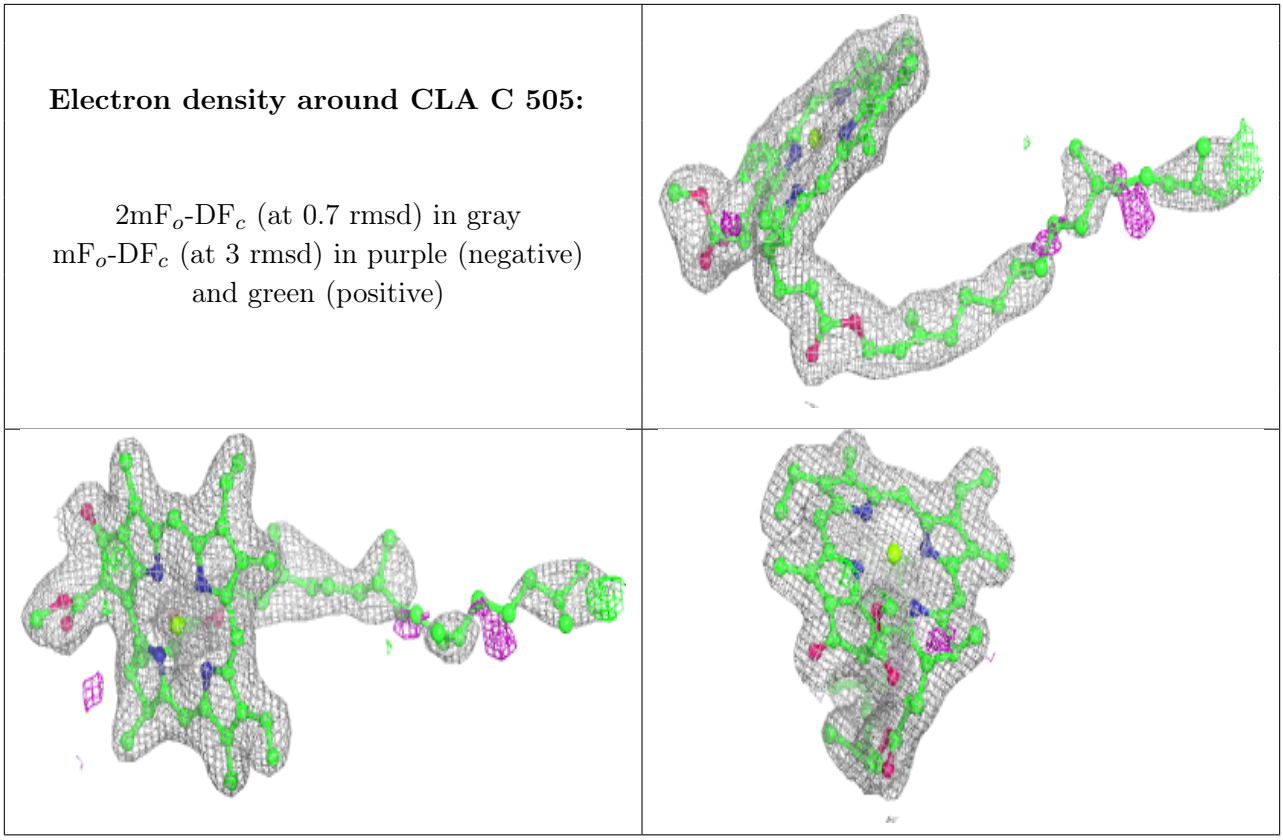
Electron density around BCR Y 302:

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



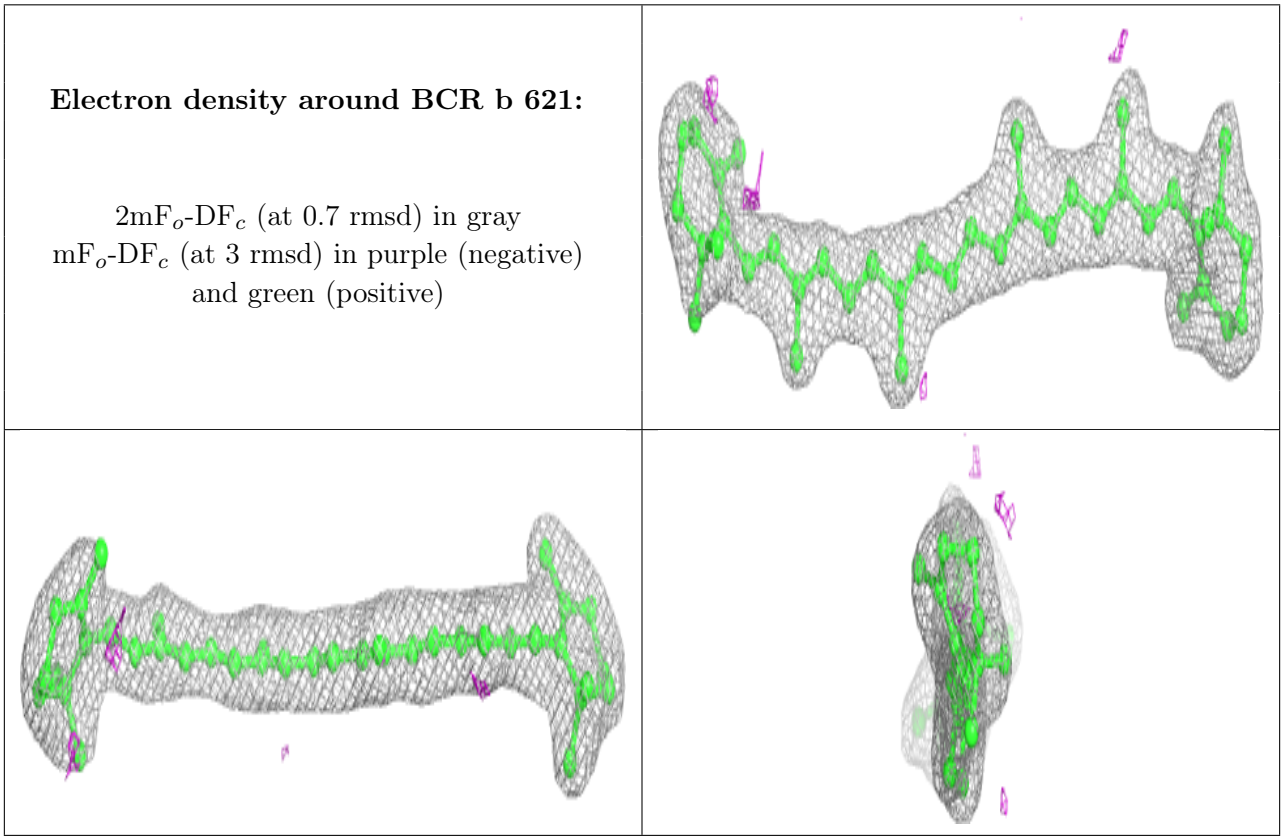
Electron density around CLA C 505:

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



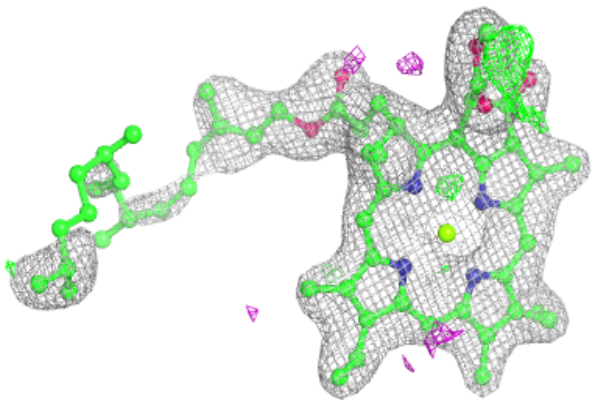
Electron density around BCR b 621:

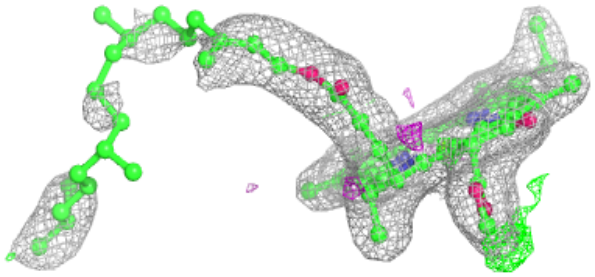
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

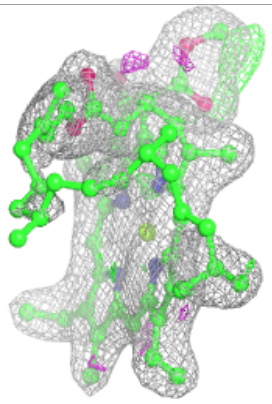


Electron density around CLA a 412:

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

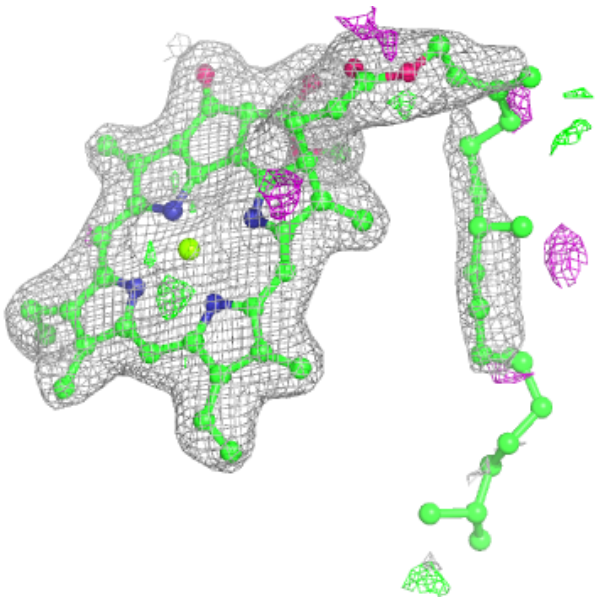


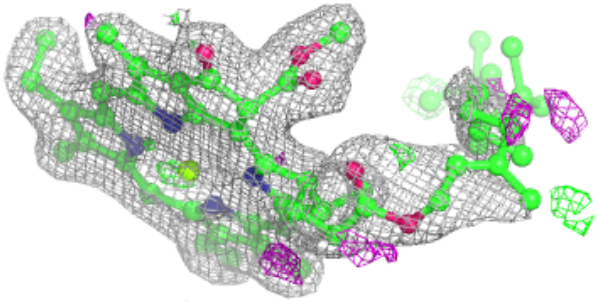


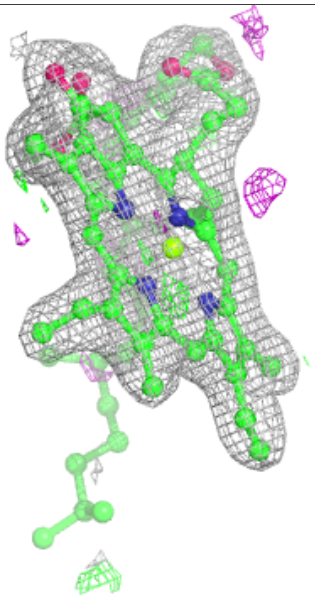


Electron density around CLA B 617:

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

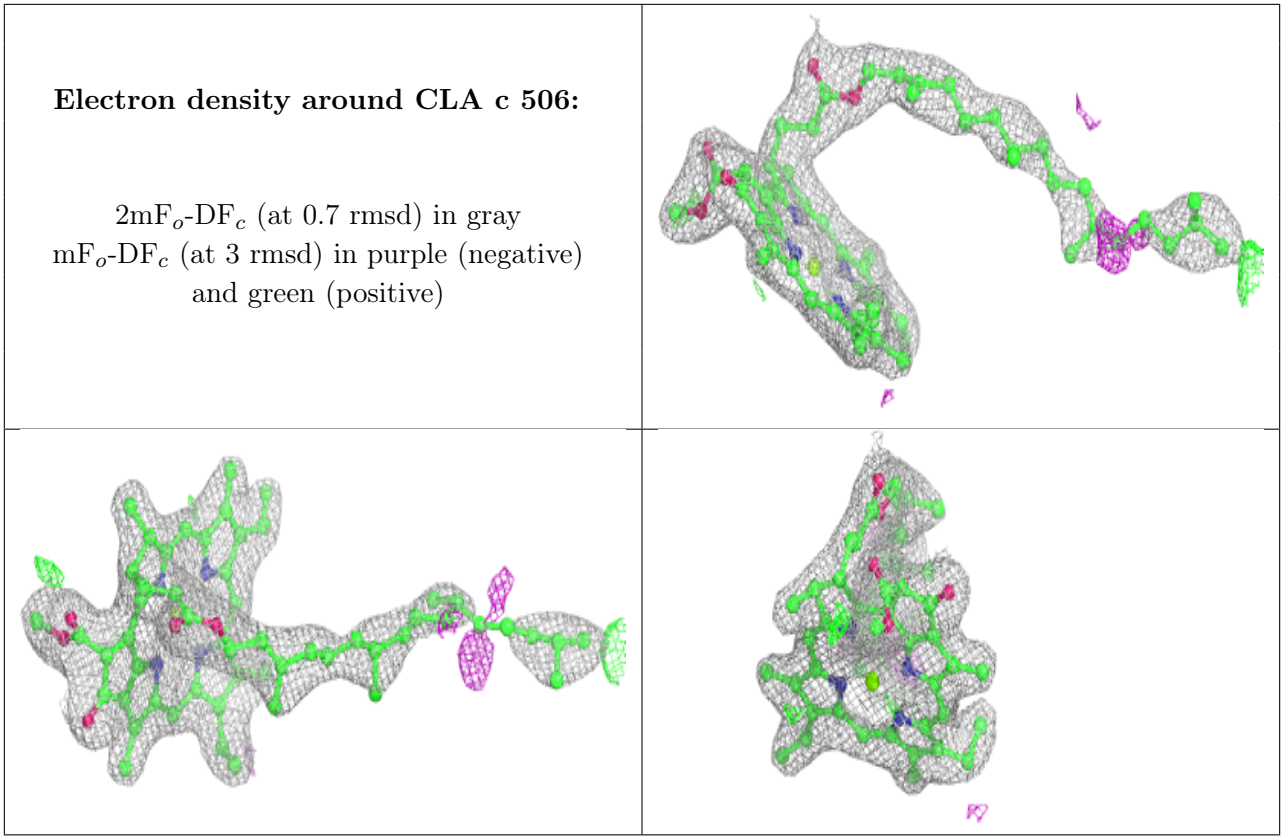






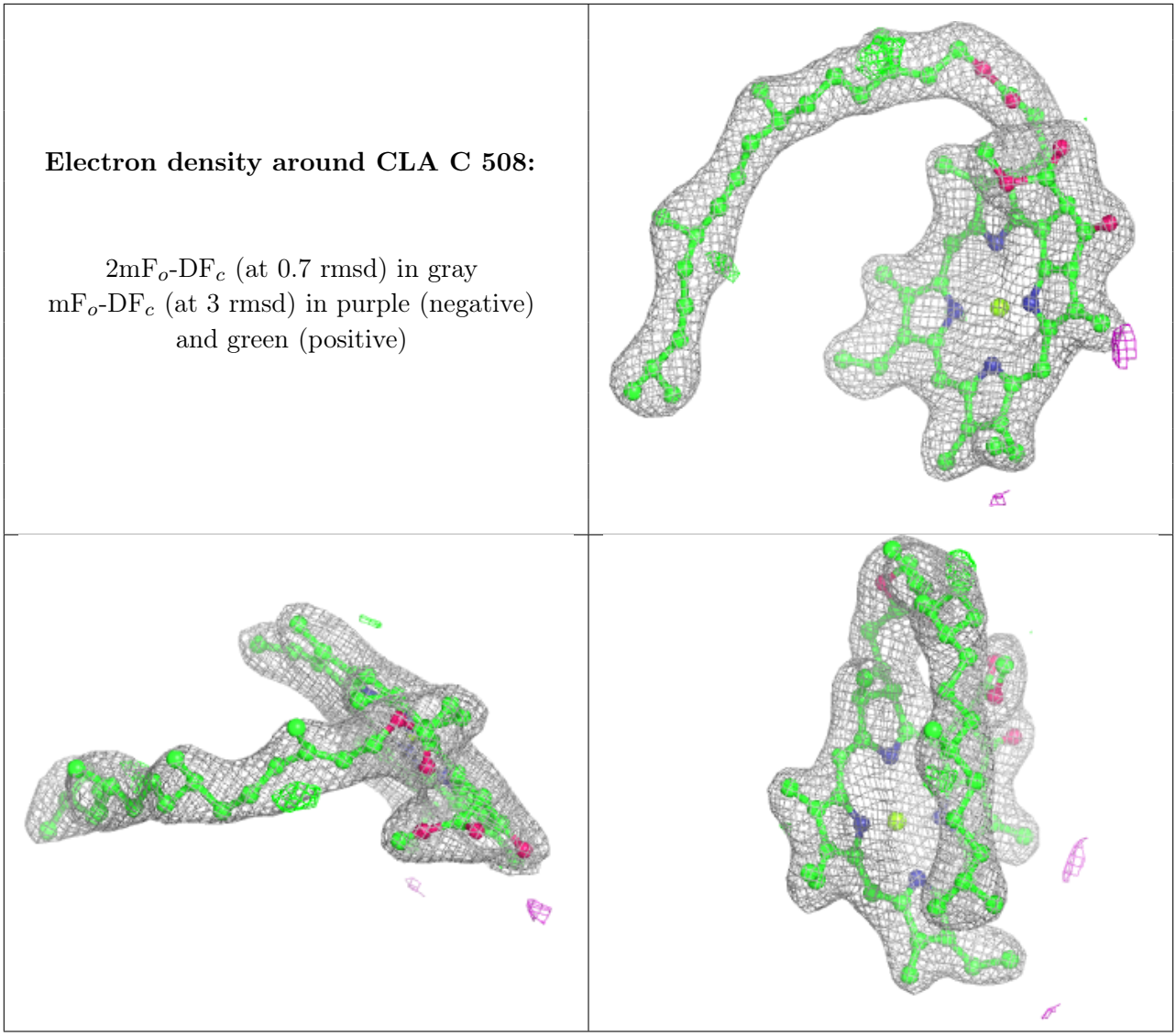
Electron density around CLA c 506:

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



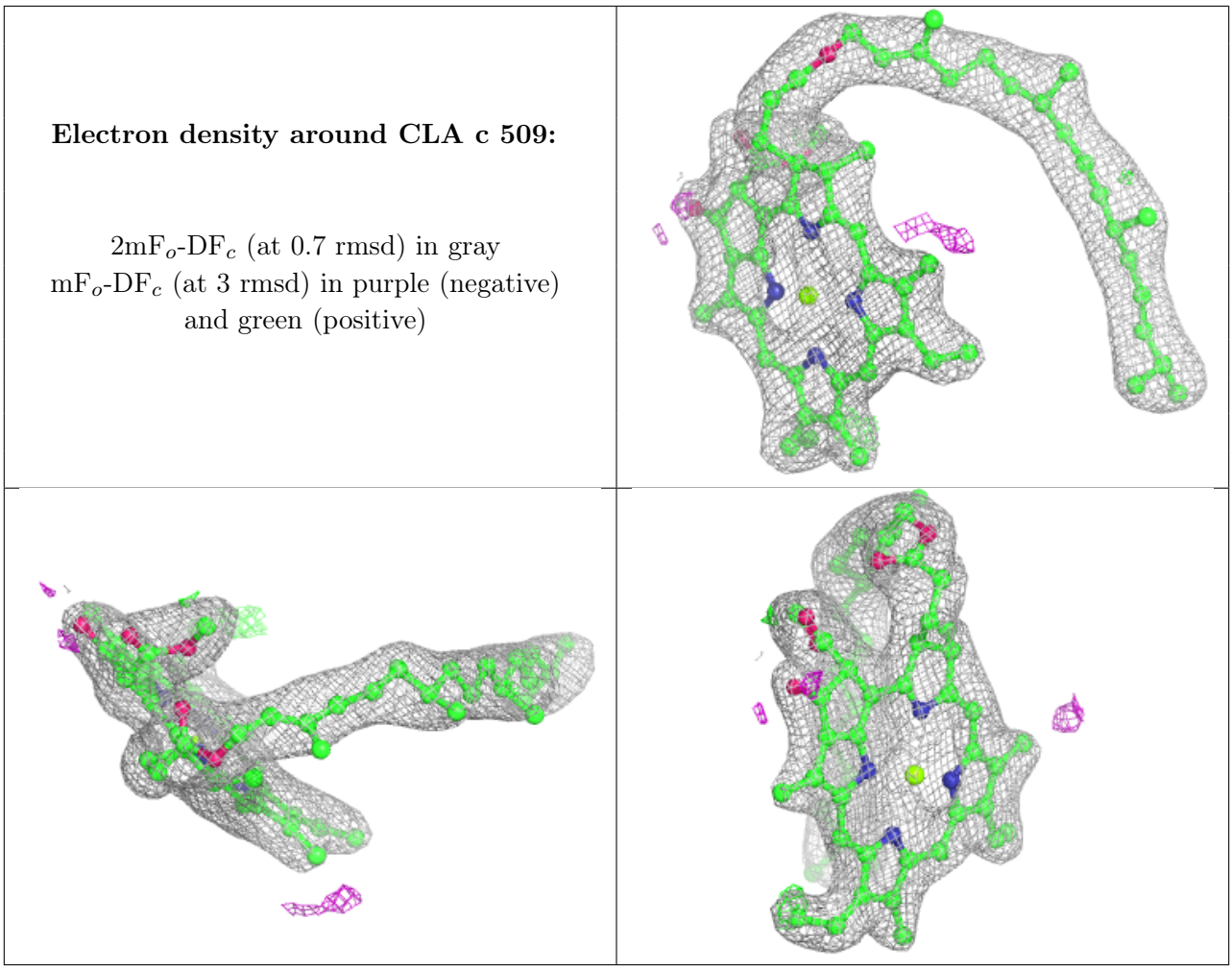
Electron density around CLA C 508:

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



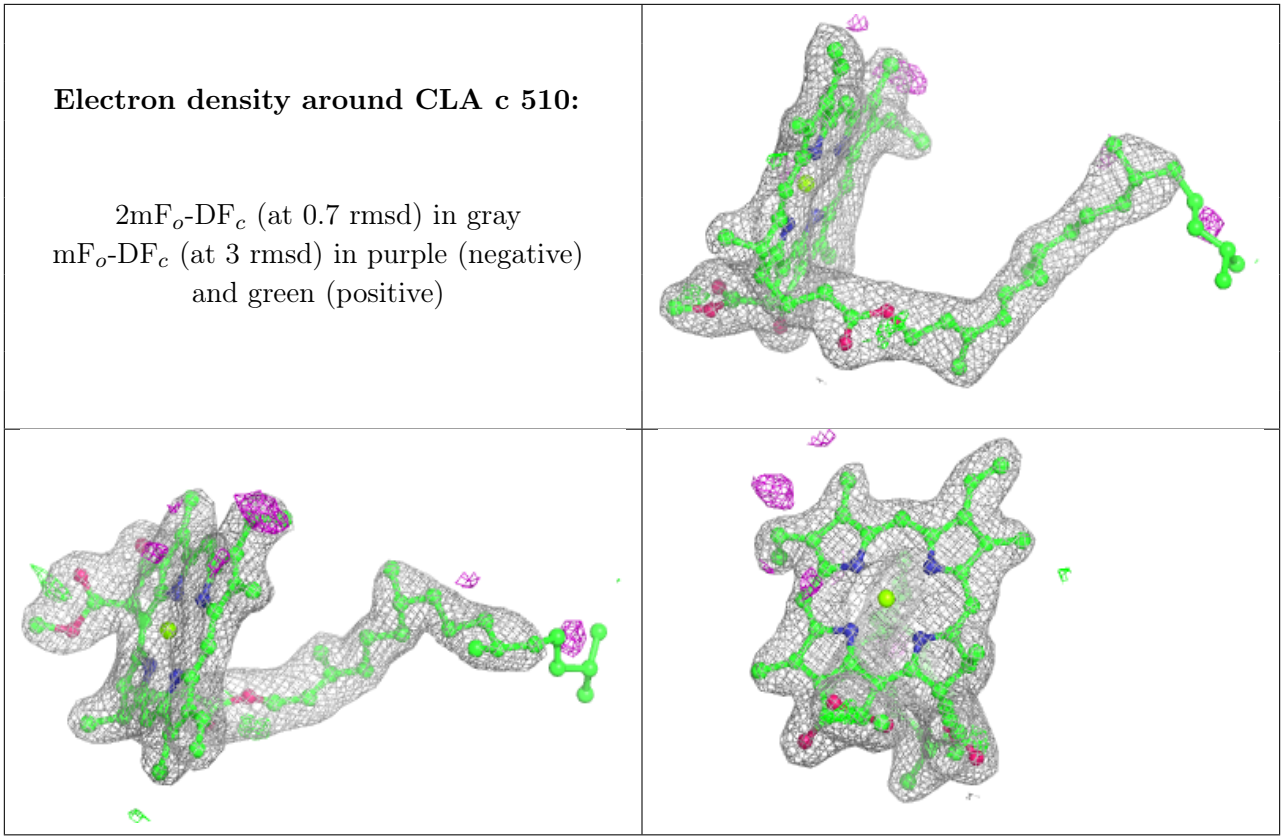
Electron density around CLA c 509:

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



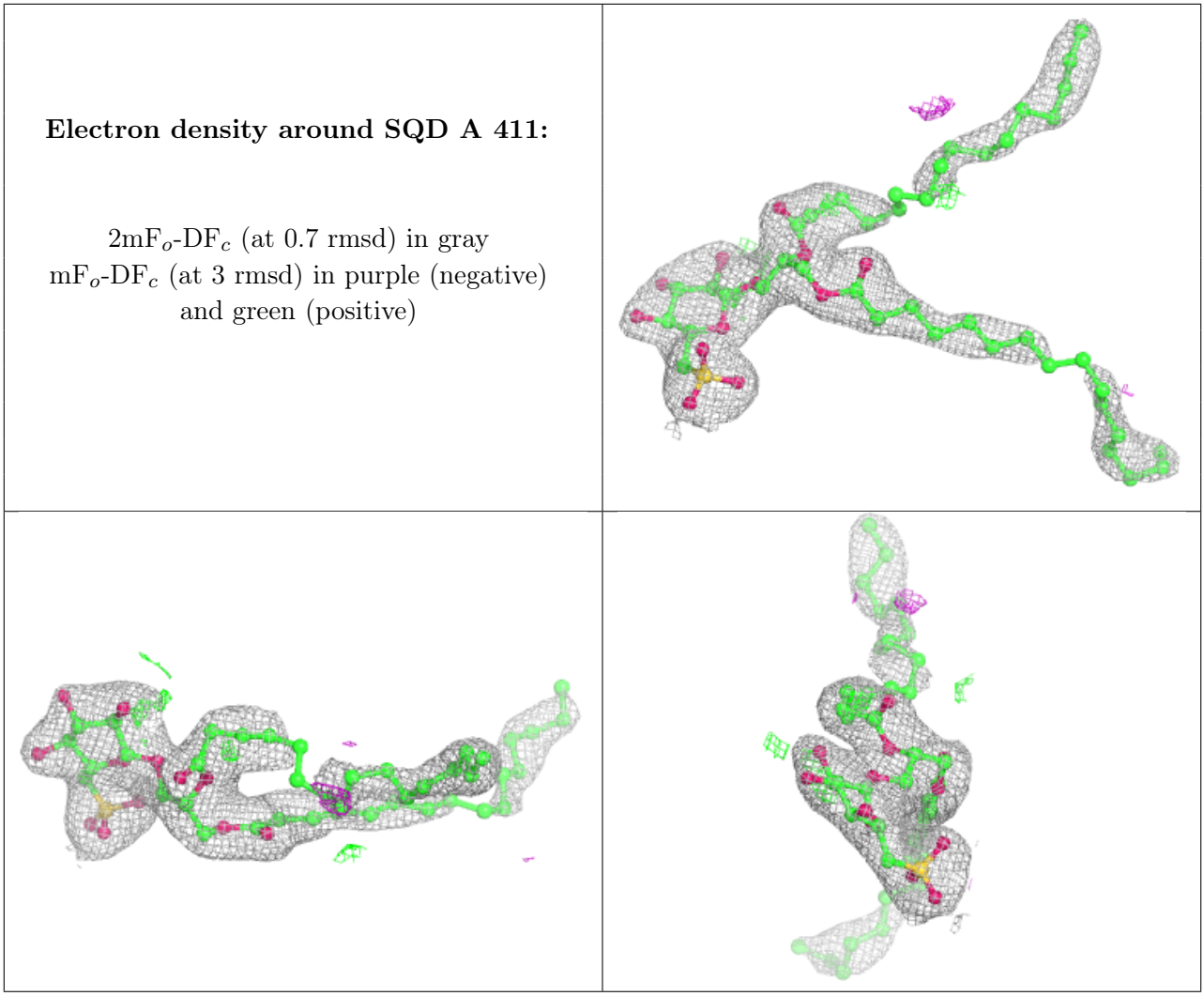
Electron density around CLA c 510:

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



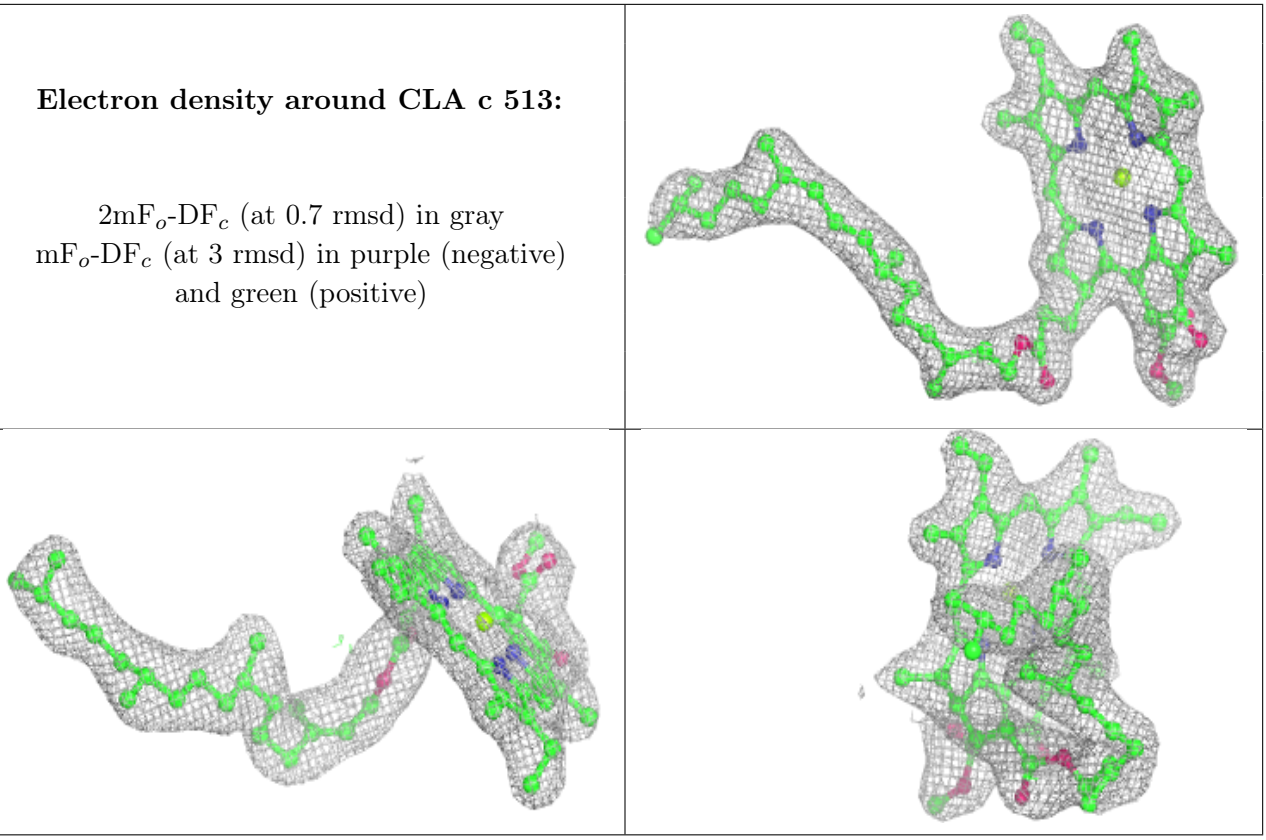
Electron density around SQD A 411:

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



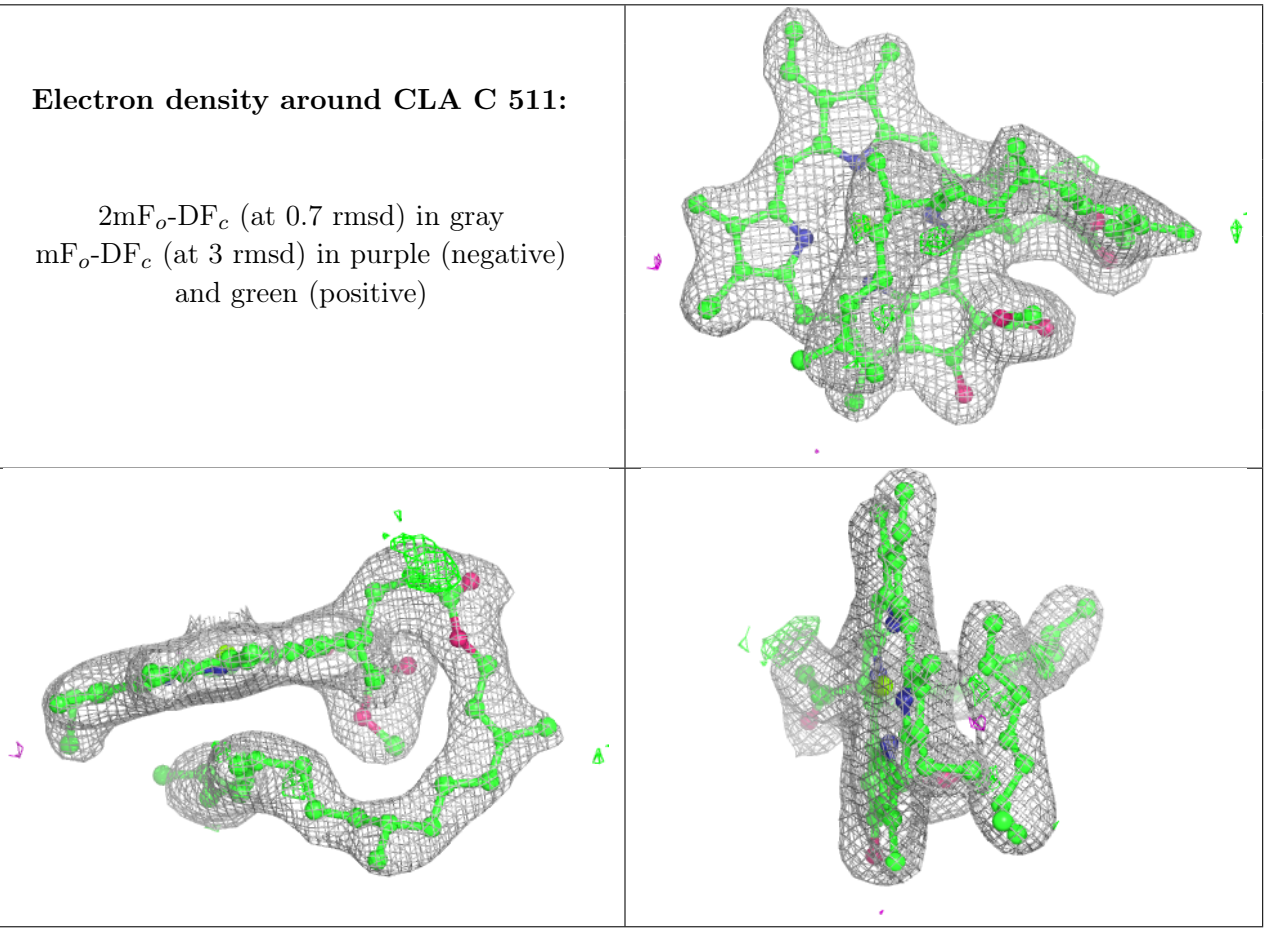
Electron density around CLA c 513:

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



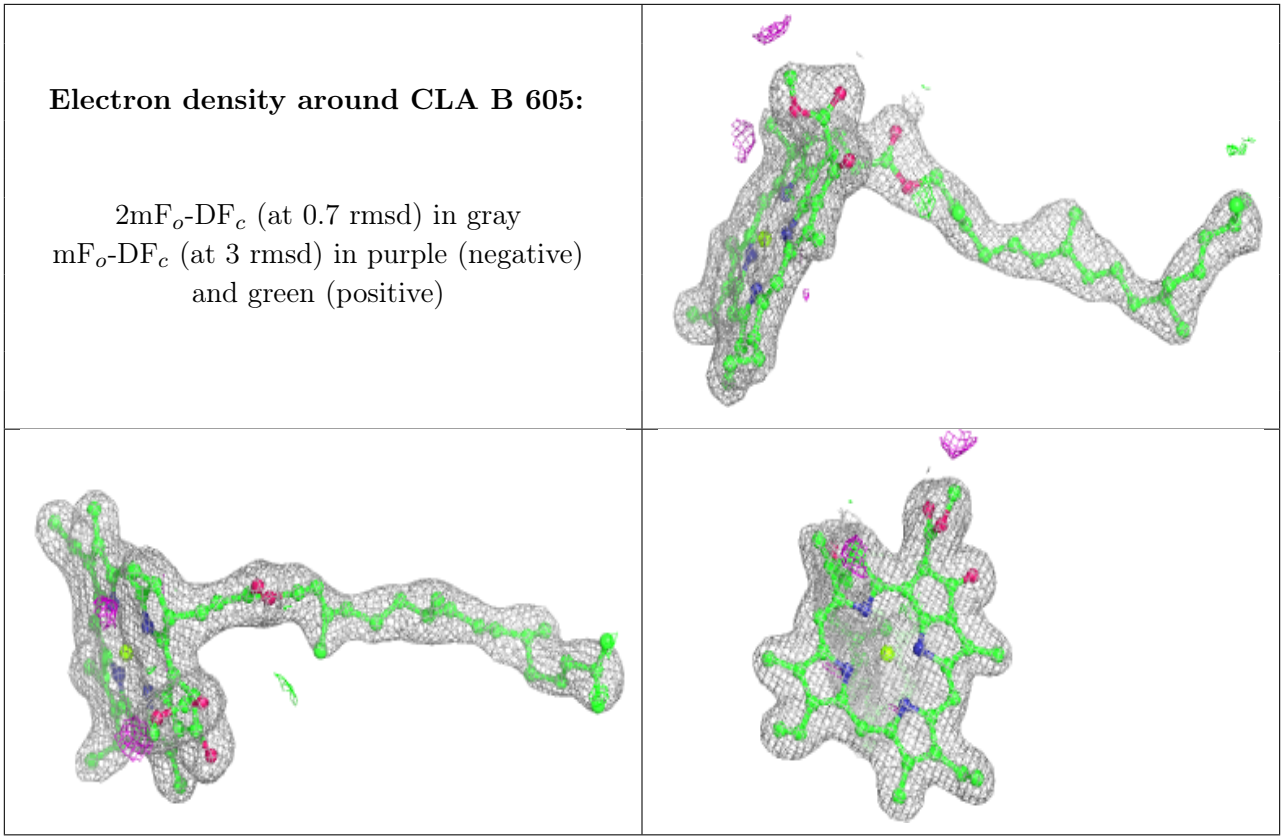
Electron density around CLA C 511:

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



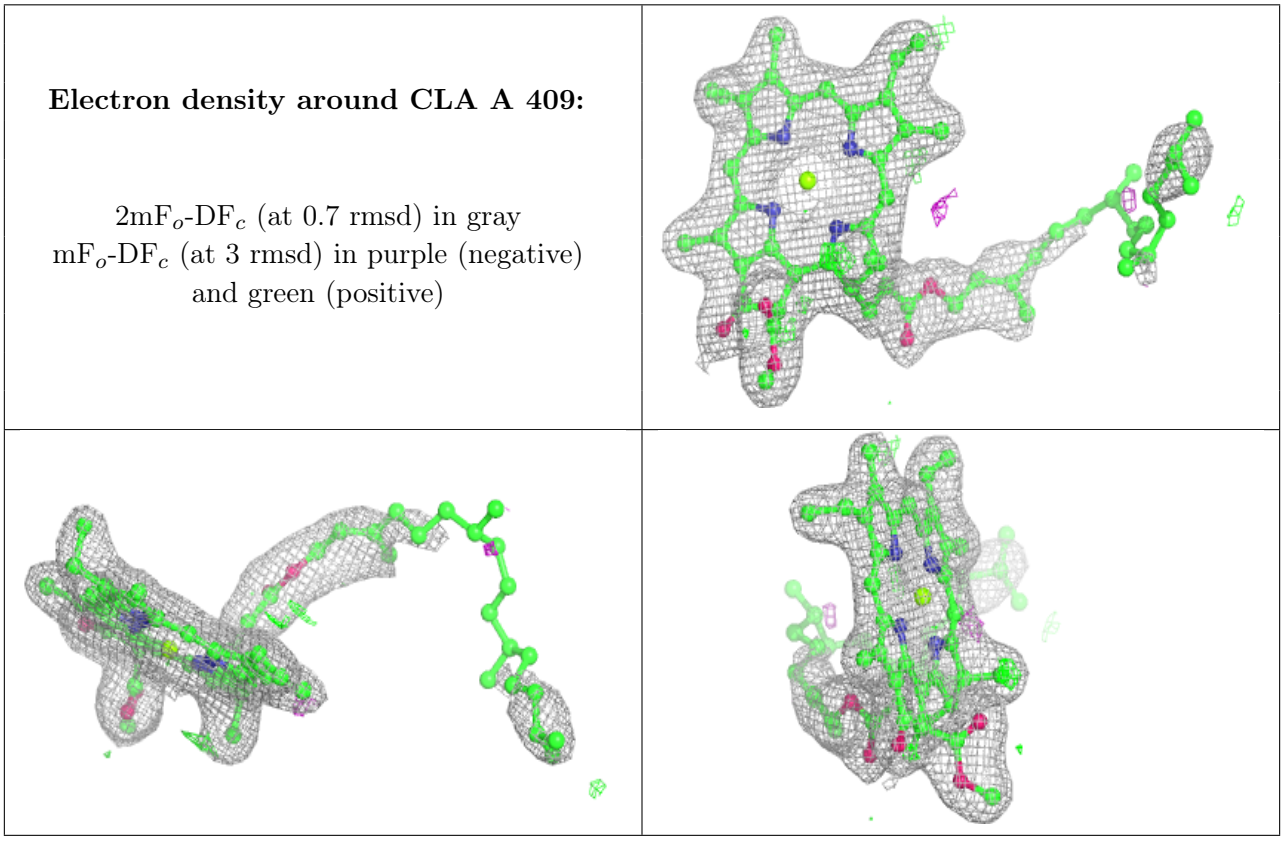
Electron density around CLA B 605:

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



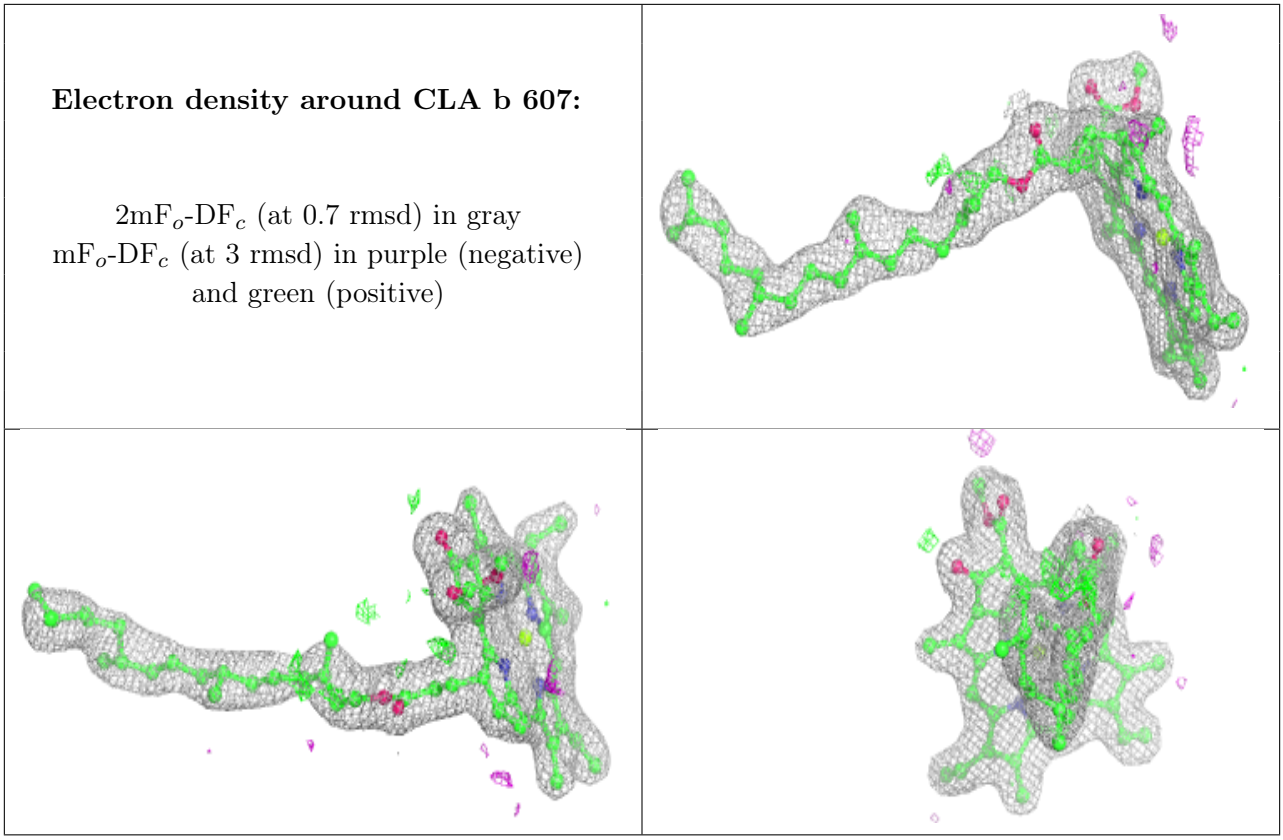
Electron density around CLA A 409:

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



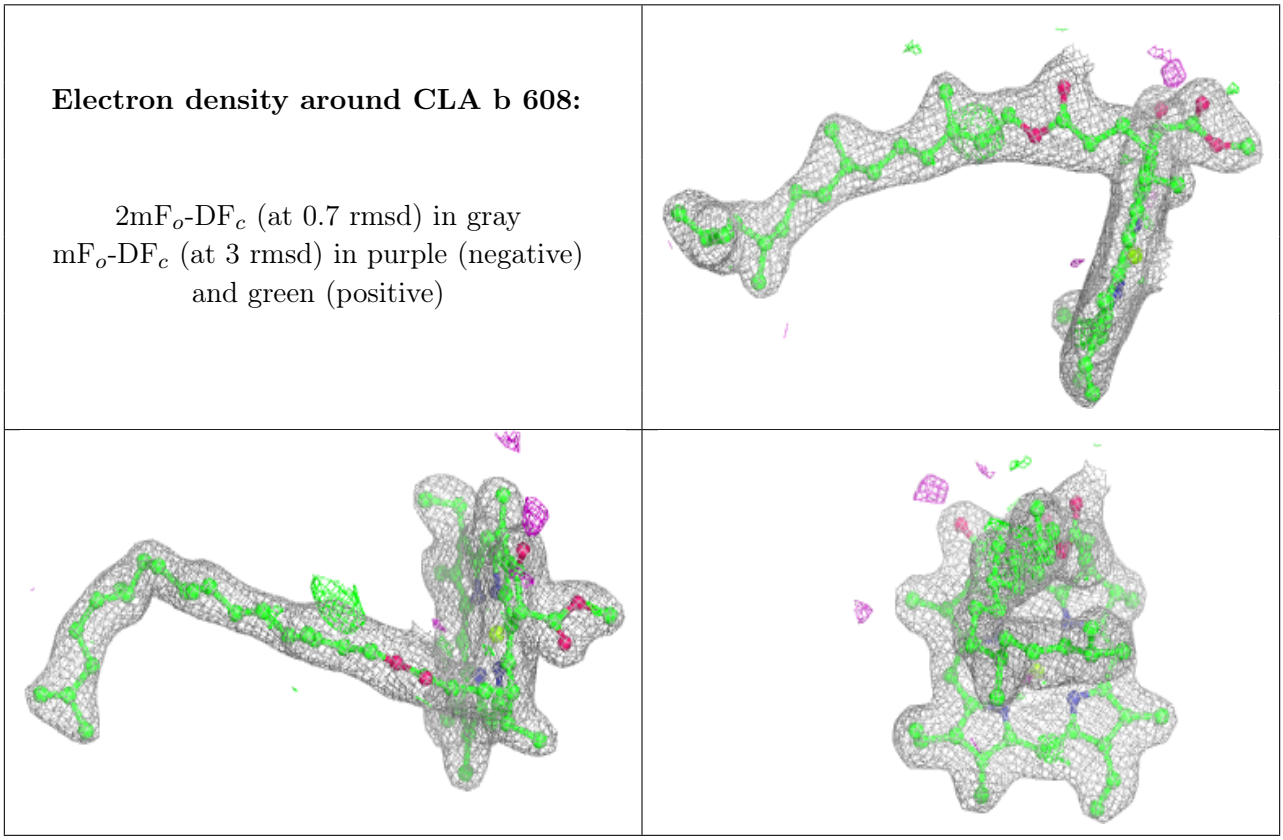
Electron density around CLA b 607:

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



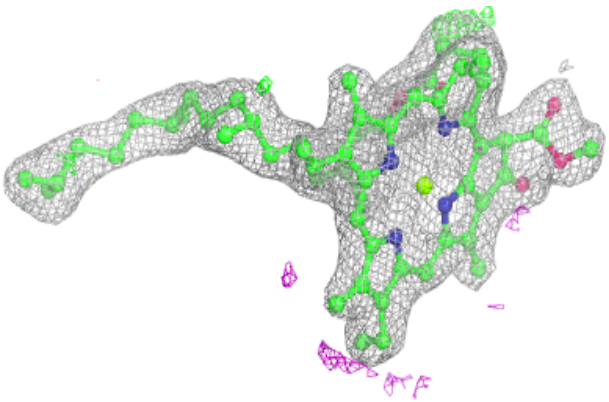
Electron density around CLA b 608:

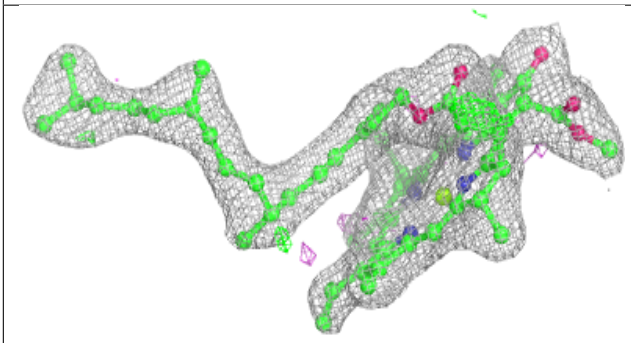
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

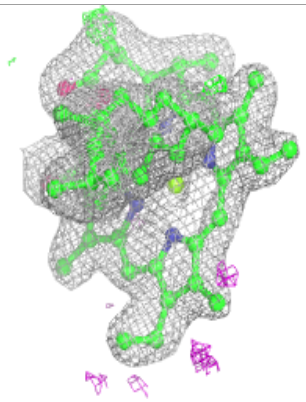


Electron density around CLA c 507:

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

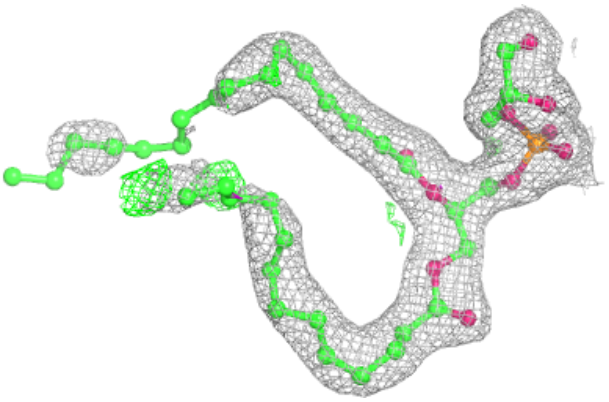


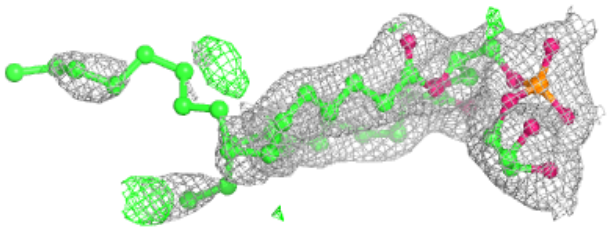


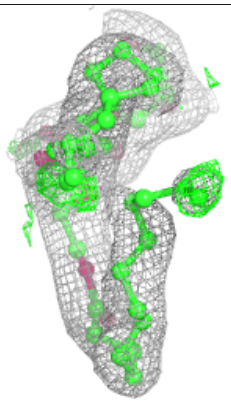


Electron density around LHG D 411:

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

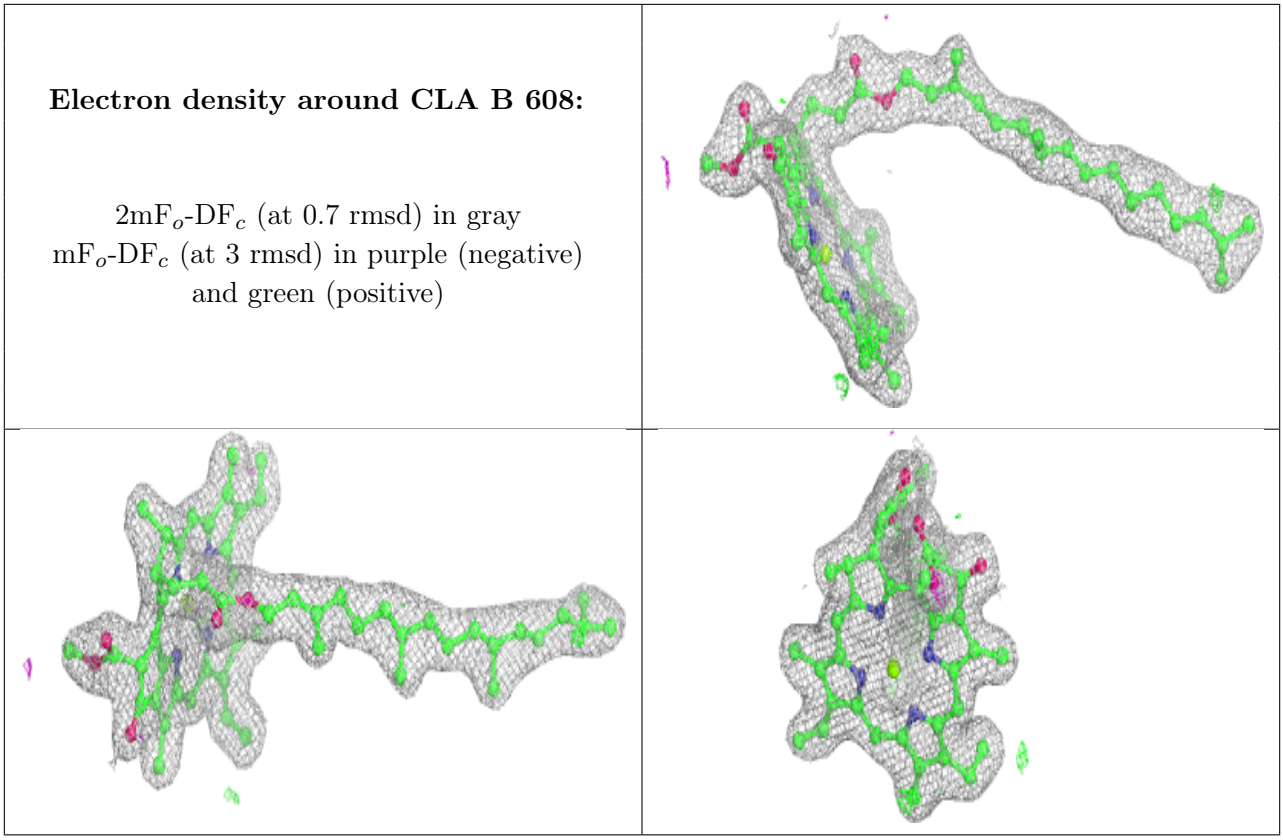






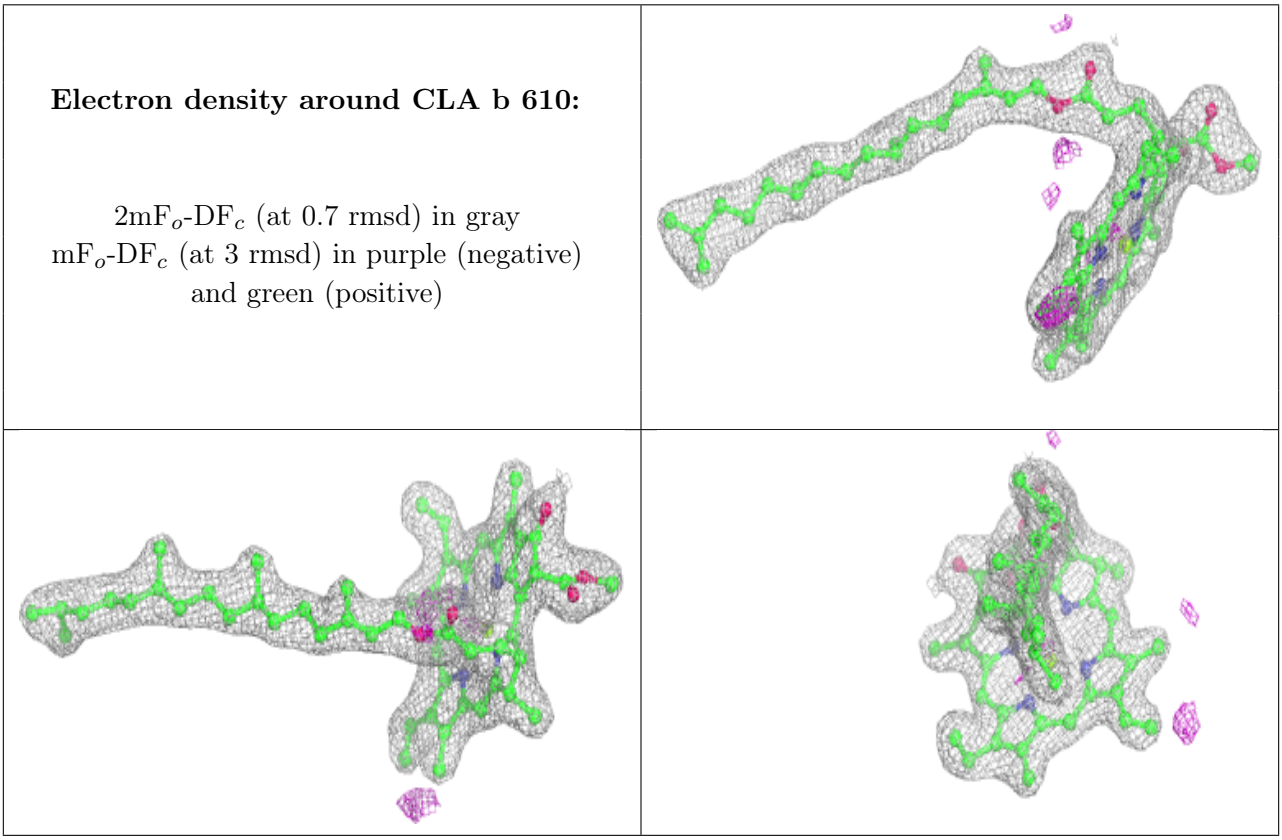
Electron density around CLA B 608:

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



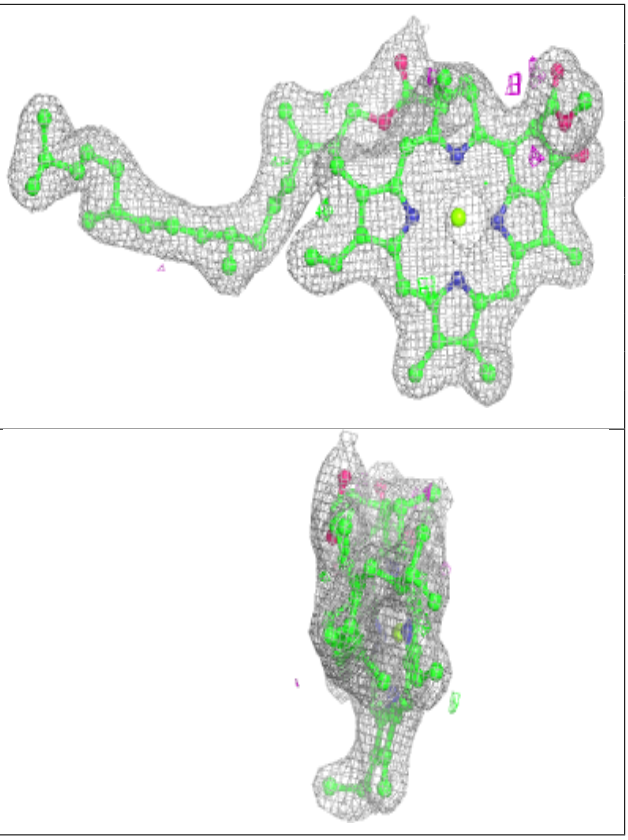
Electron density around CLA b 610:

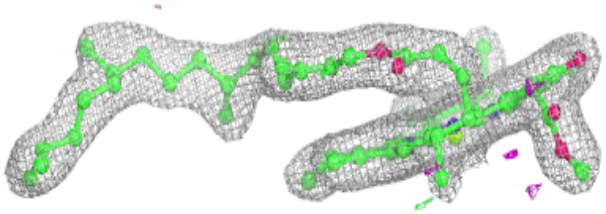
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 604:

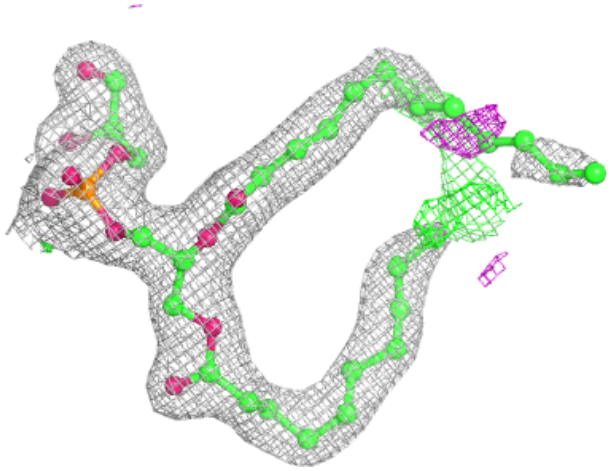
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

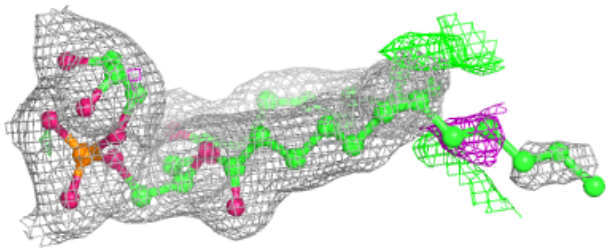


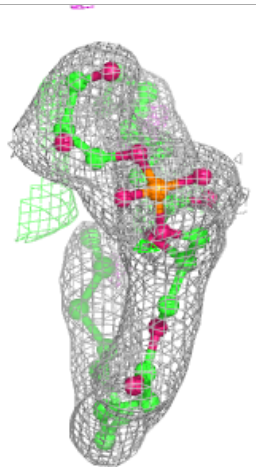


Electron density around LHG d 410:

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

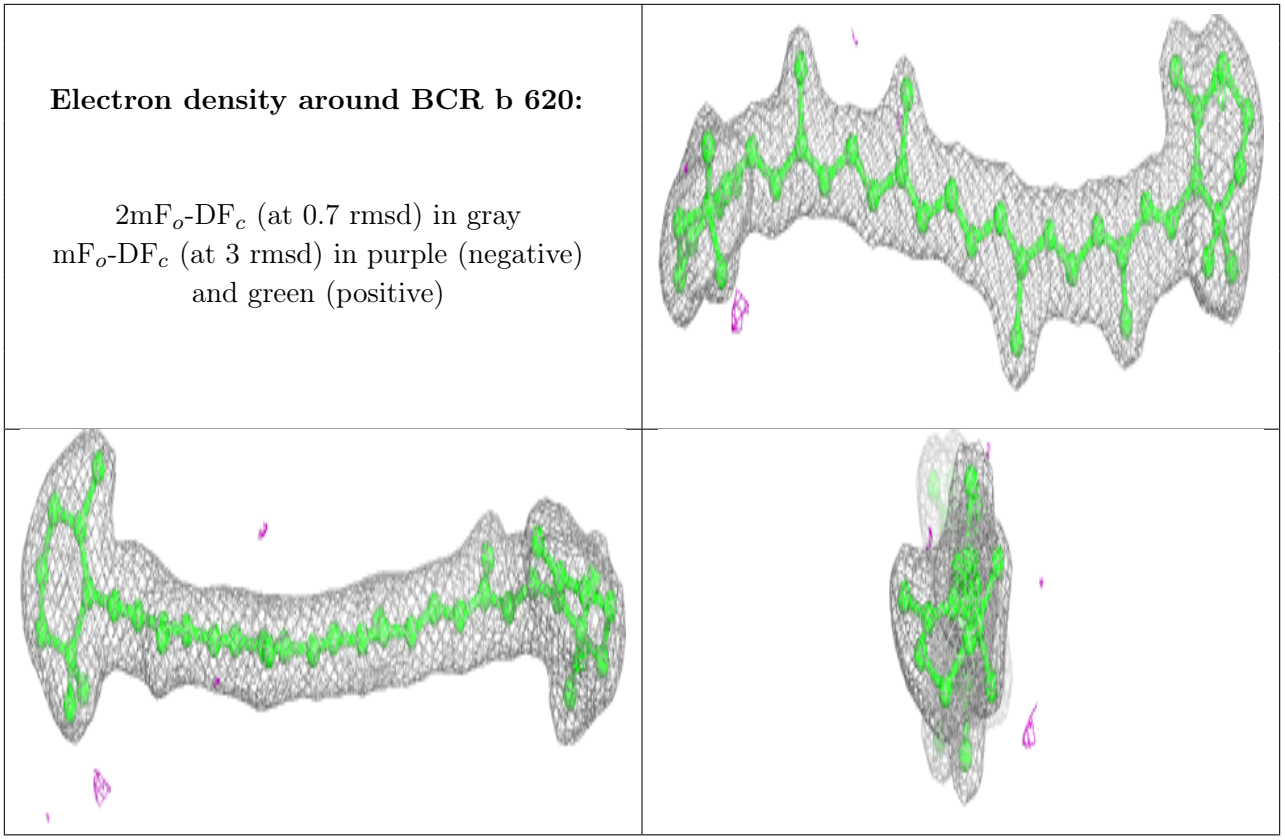






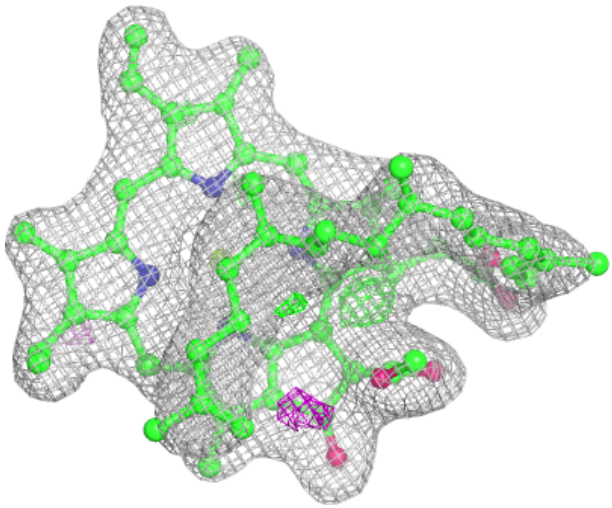
Electron density around BCR b 620:

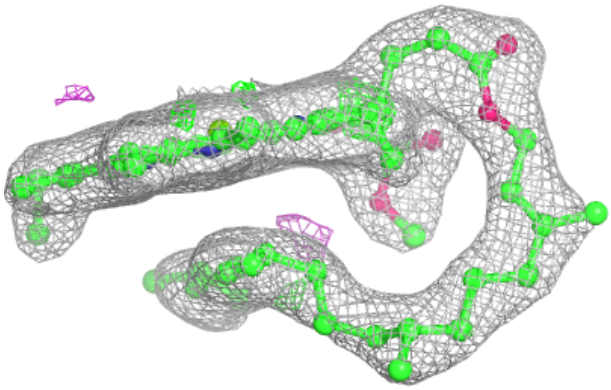
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA c 512:

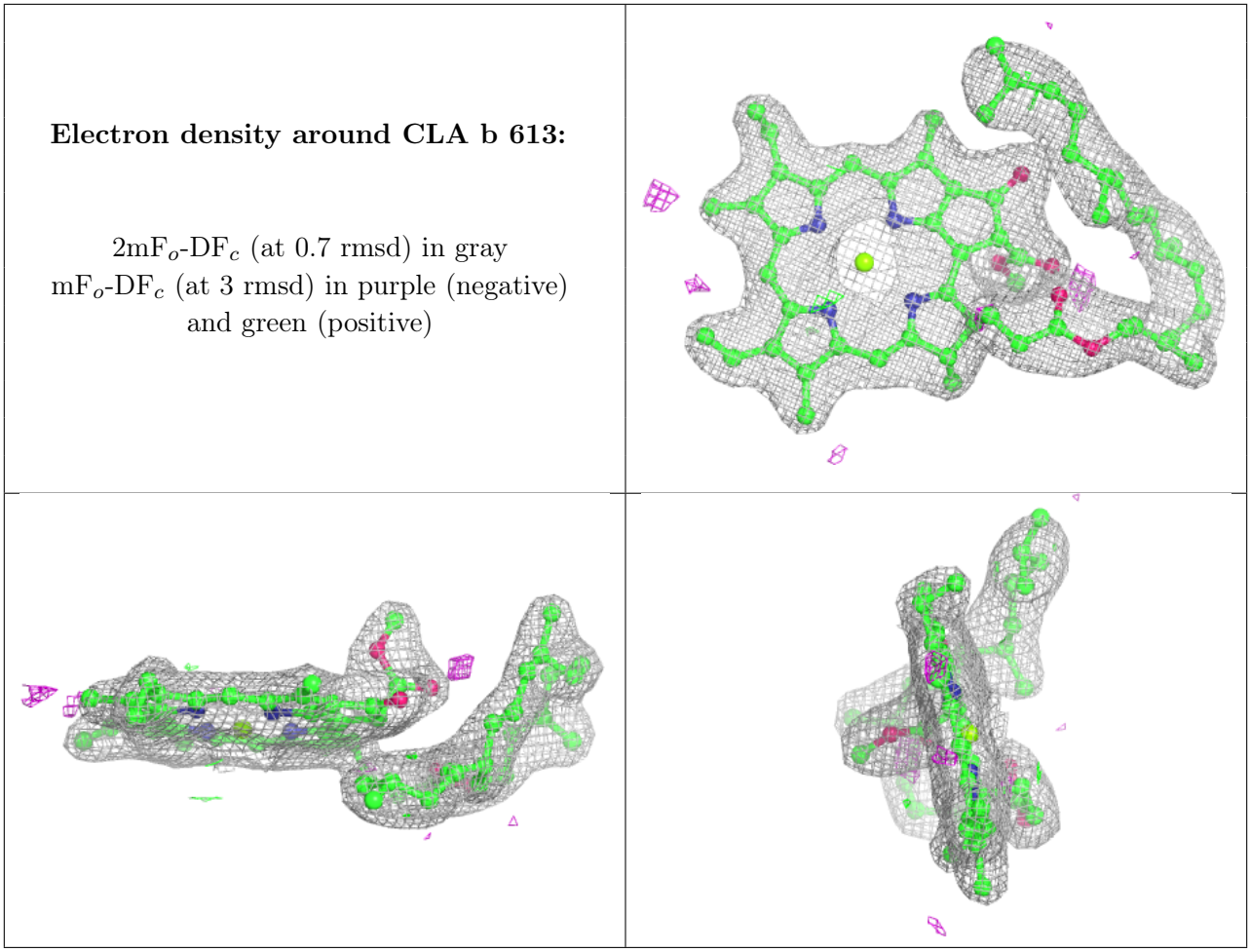
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





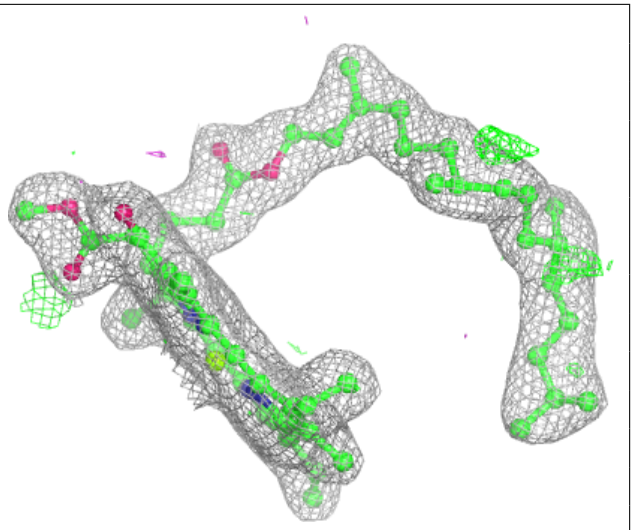
Electron density around CLA b 613:

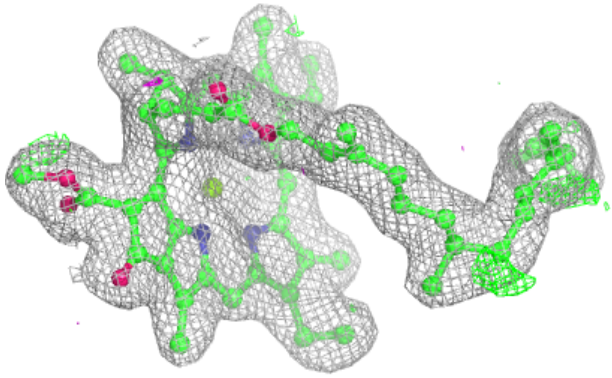
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

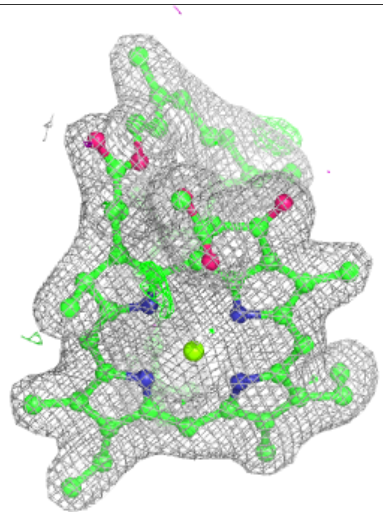


Electron density around CLA b 614:

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

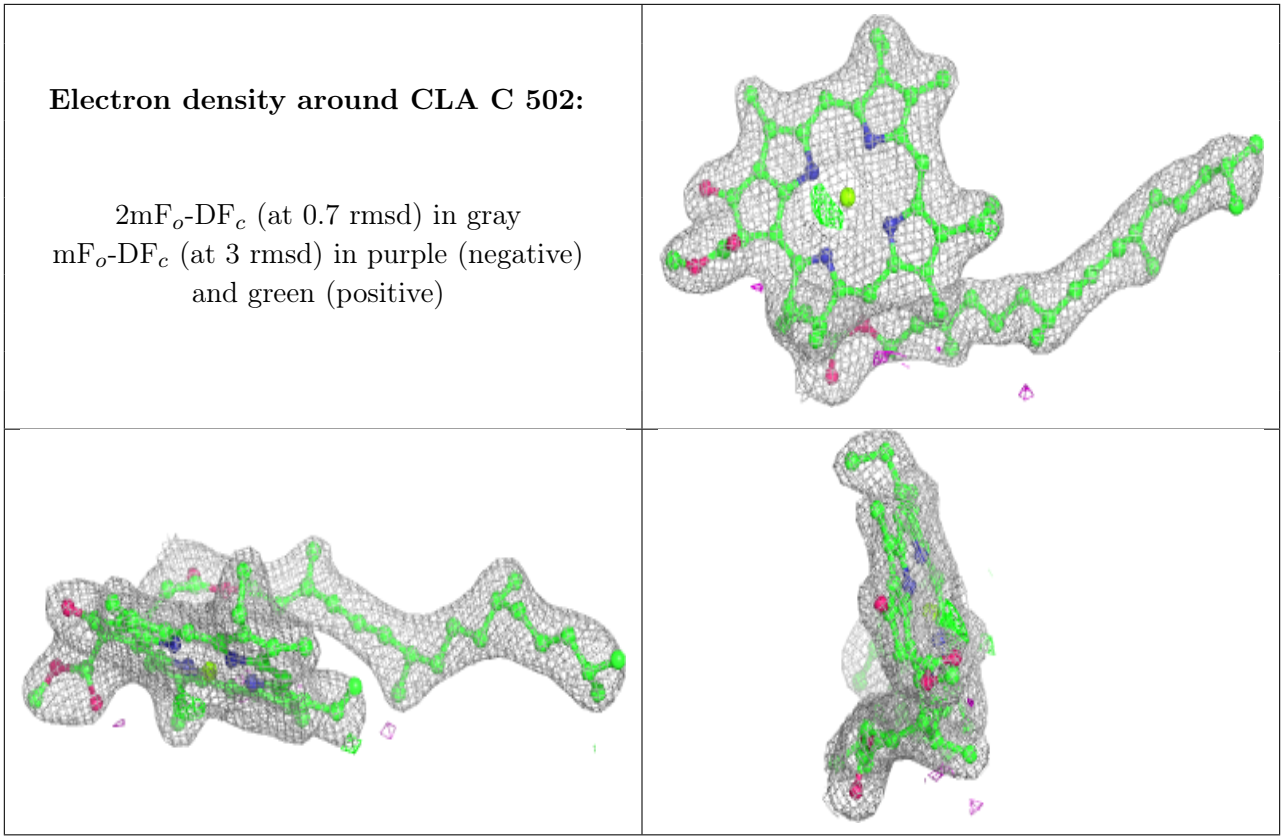






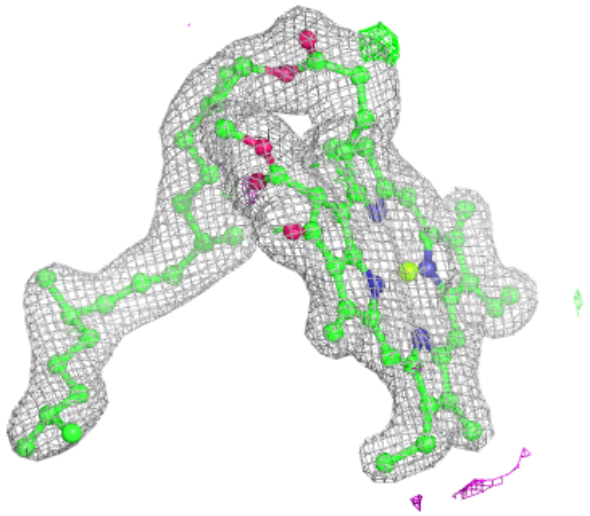
Electron density around CLA C 502:

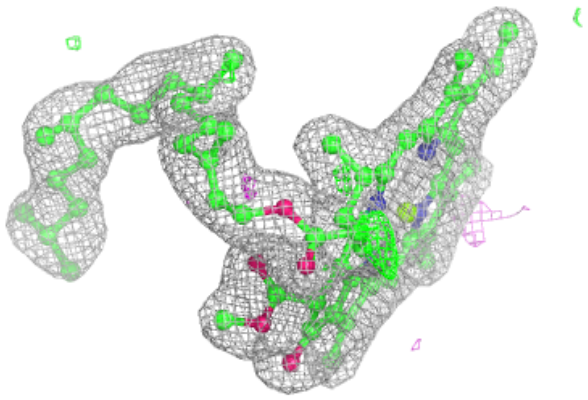
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

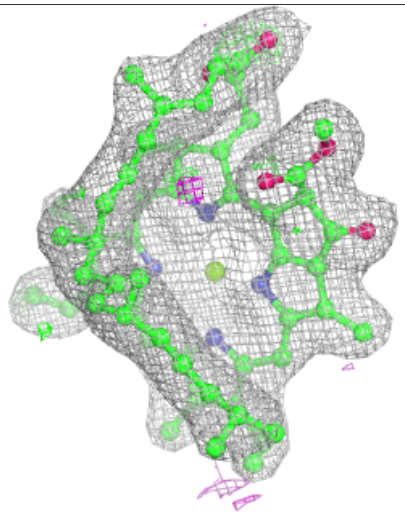


Electron density around CLA b 616:

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

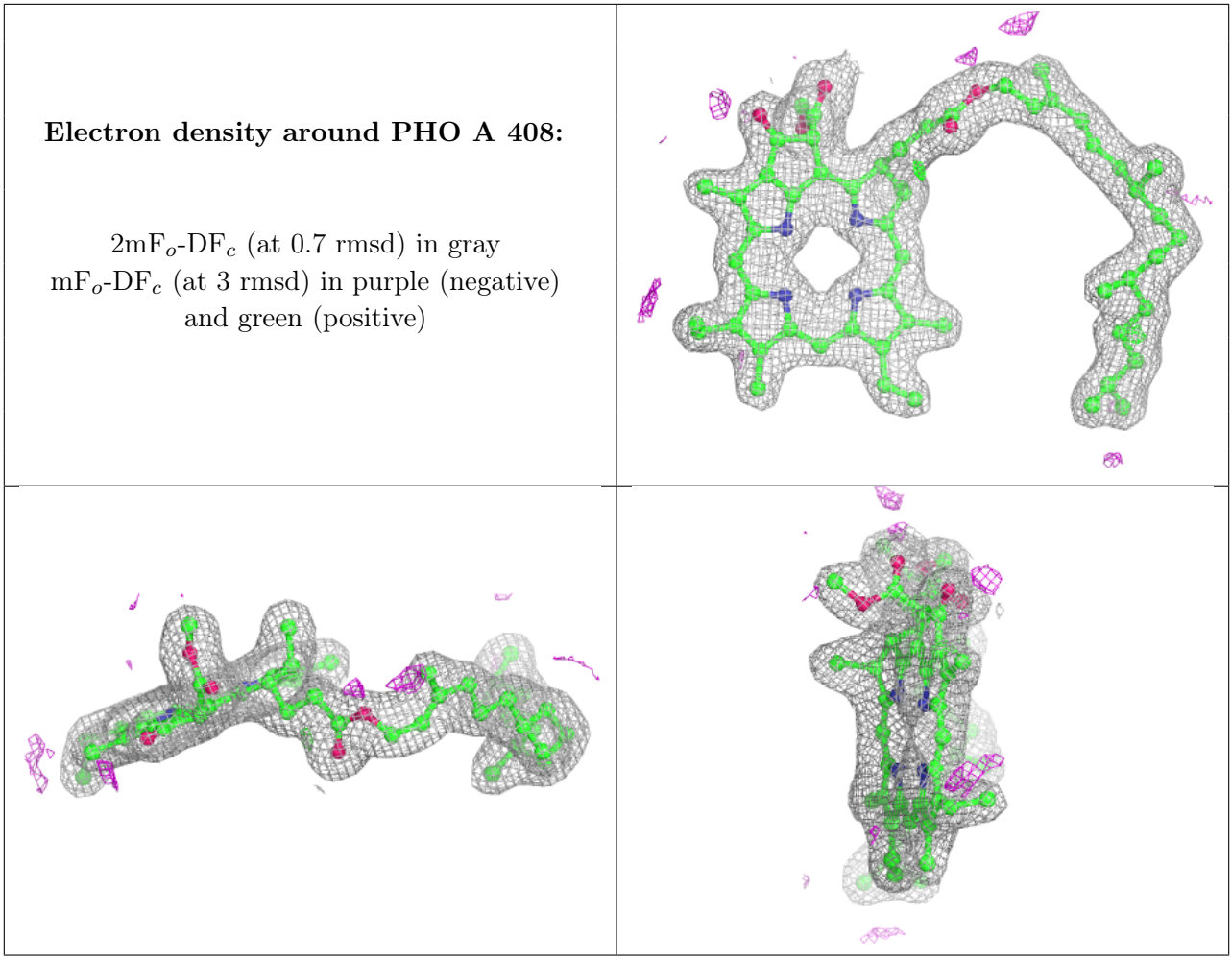






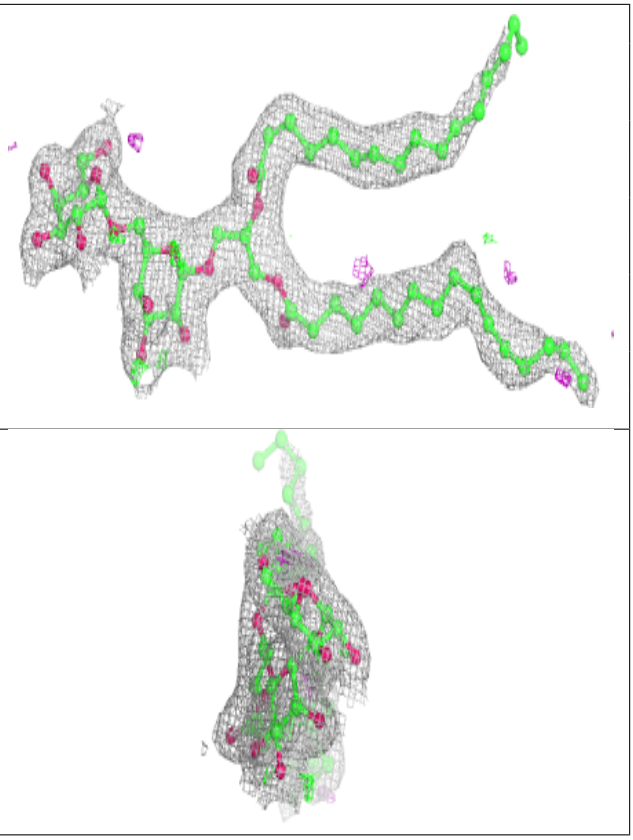
Electron density around PHO A 408:

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



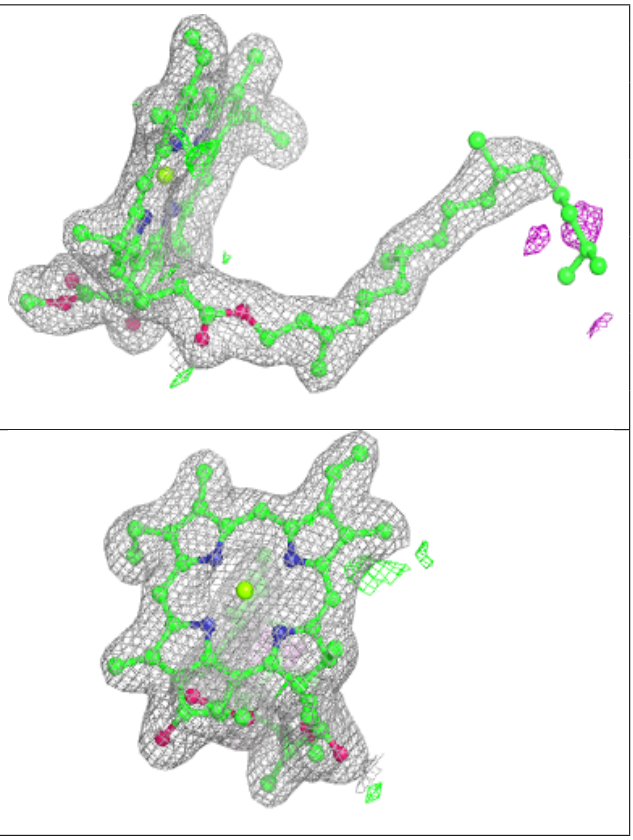
Electron density around DGD C 519:

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



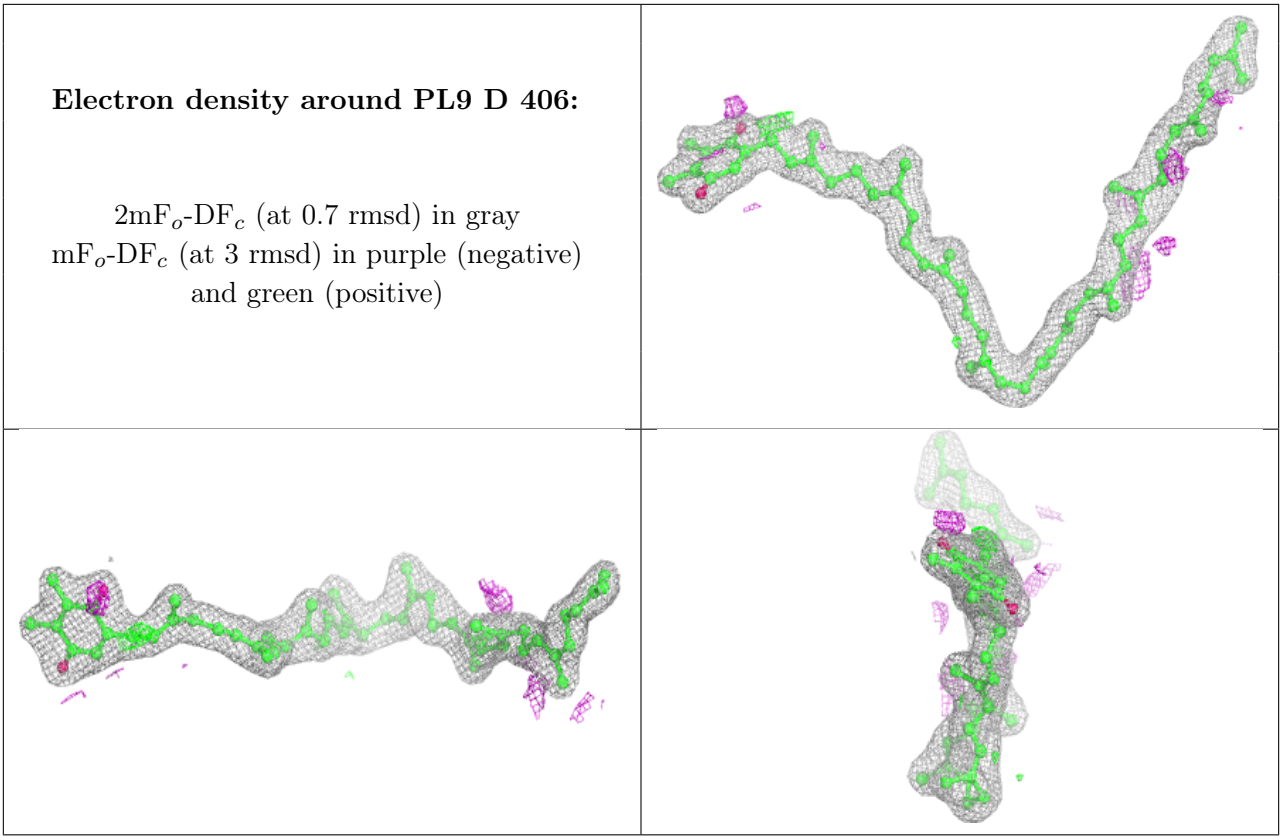
Electron density around CLA C 509:

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



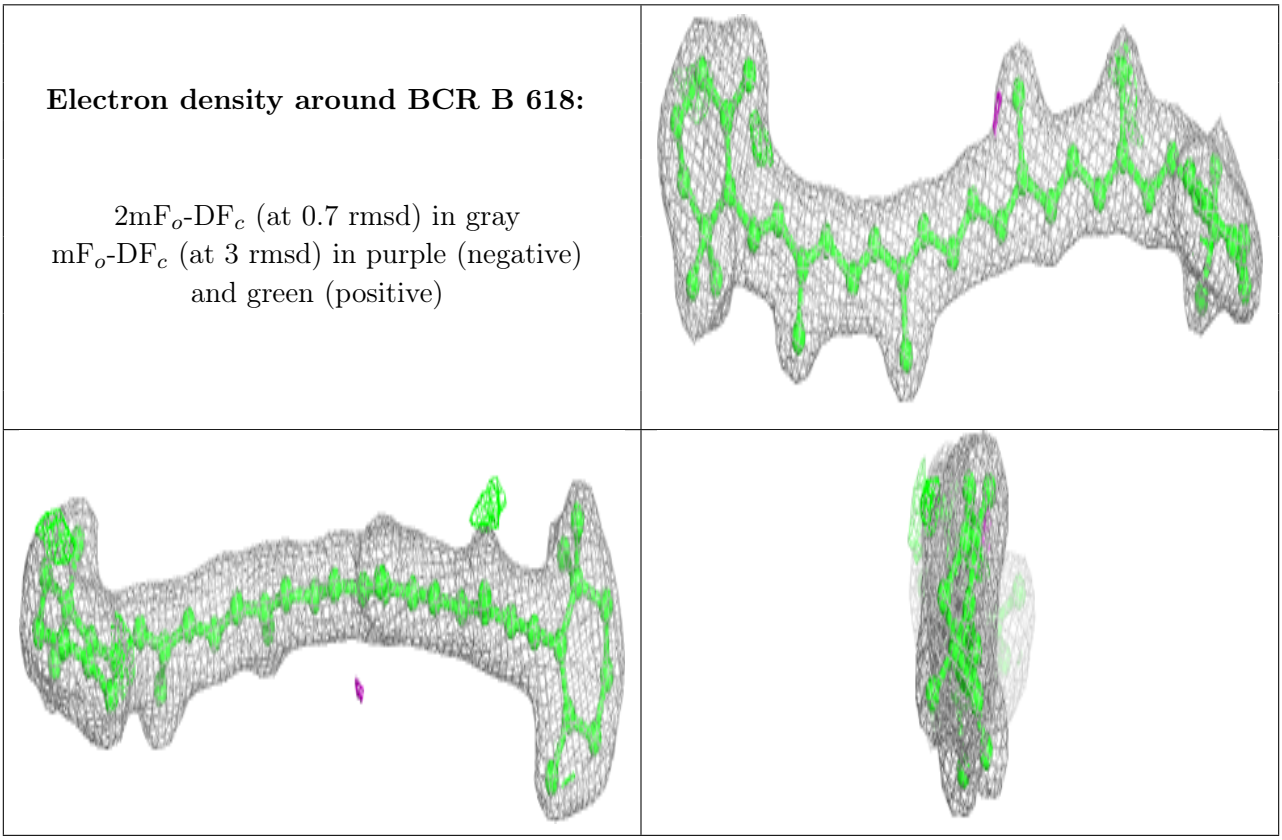
Electron density around PL9 D 406:

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



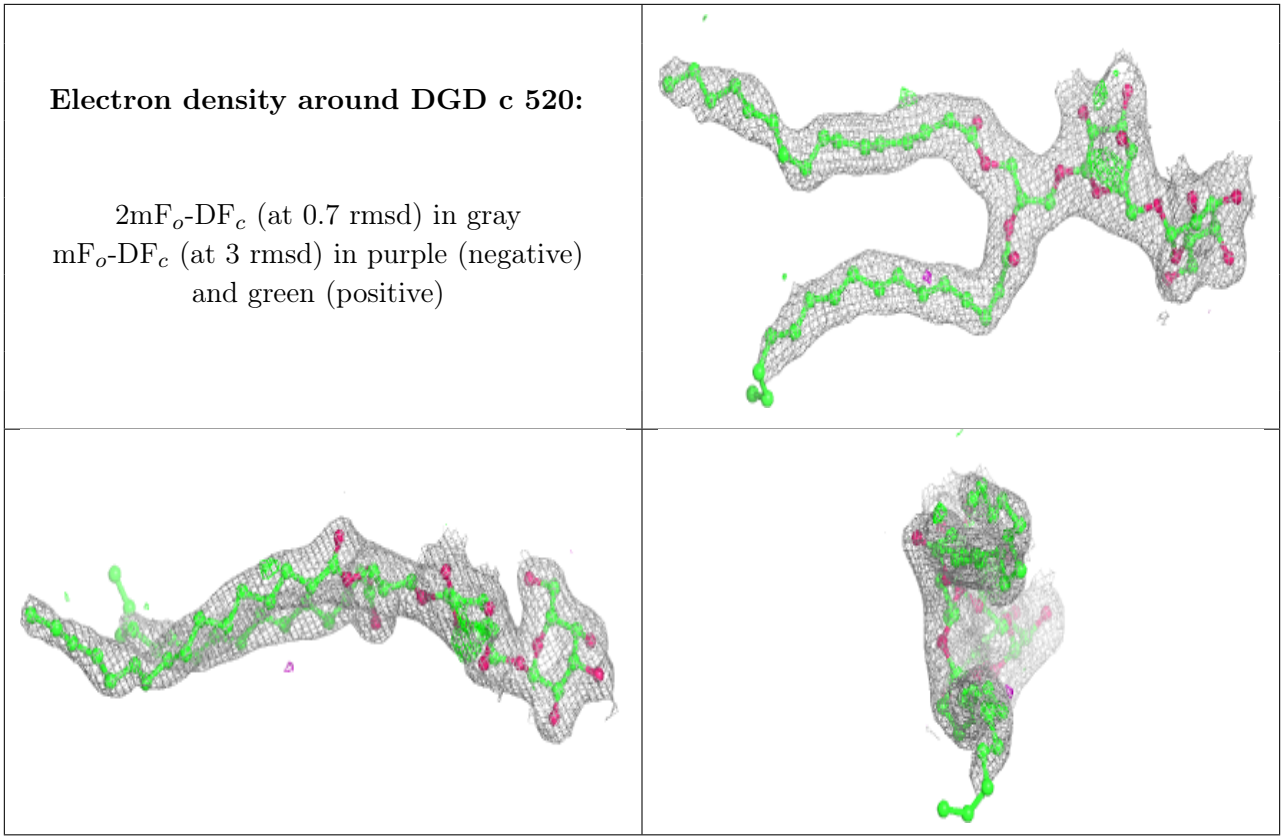
Electron density around BCR B 618:

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



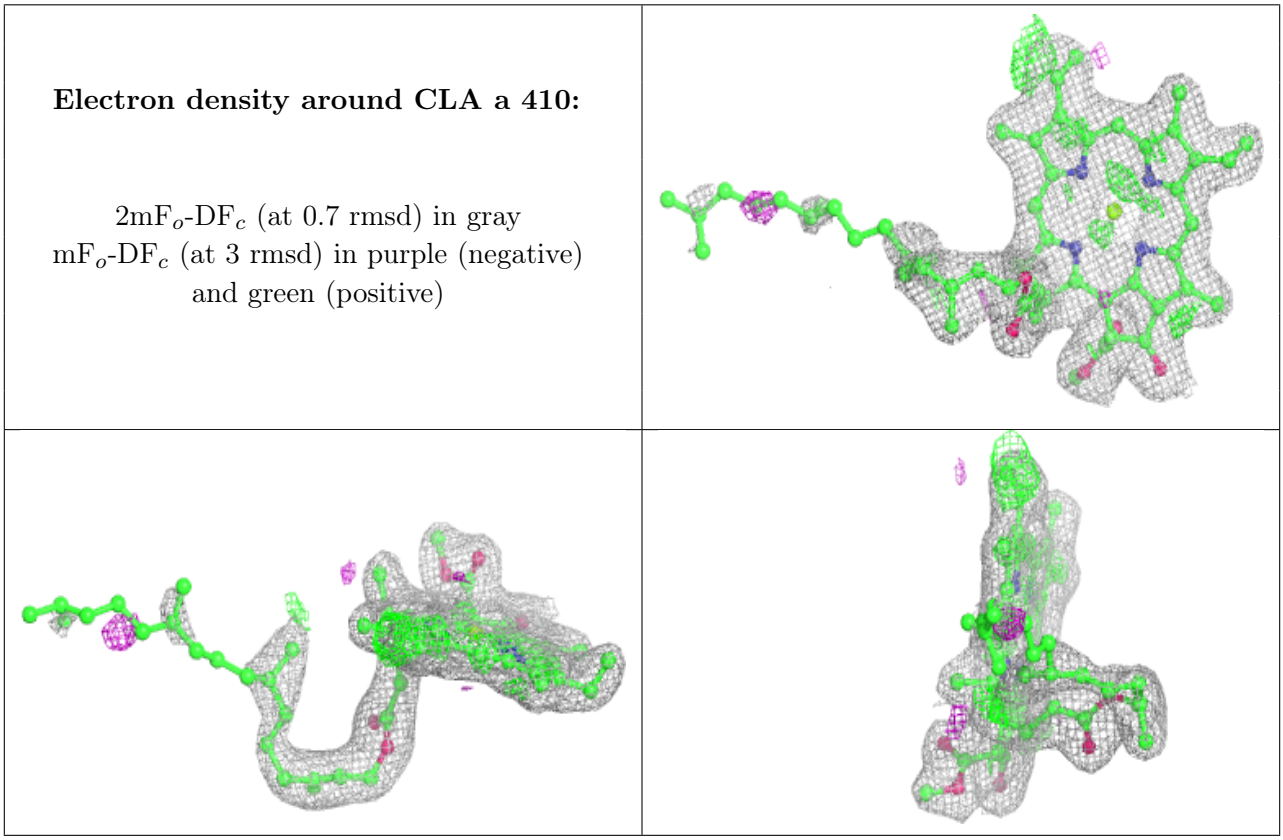
Electron density around DGD c 520:

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



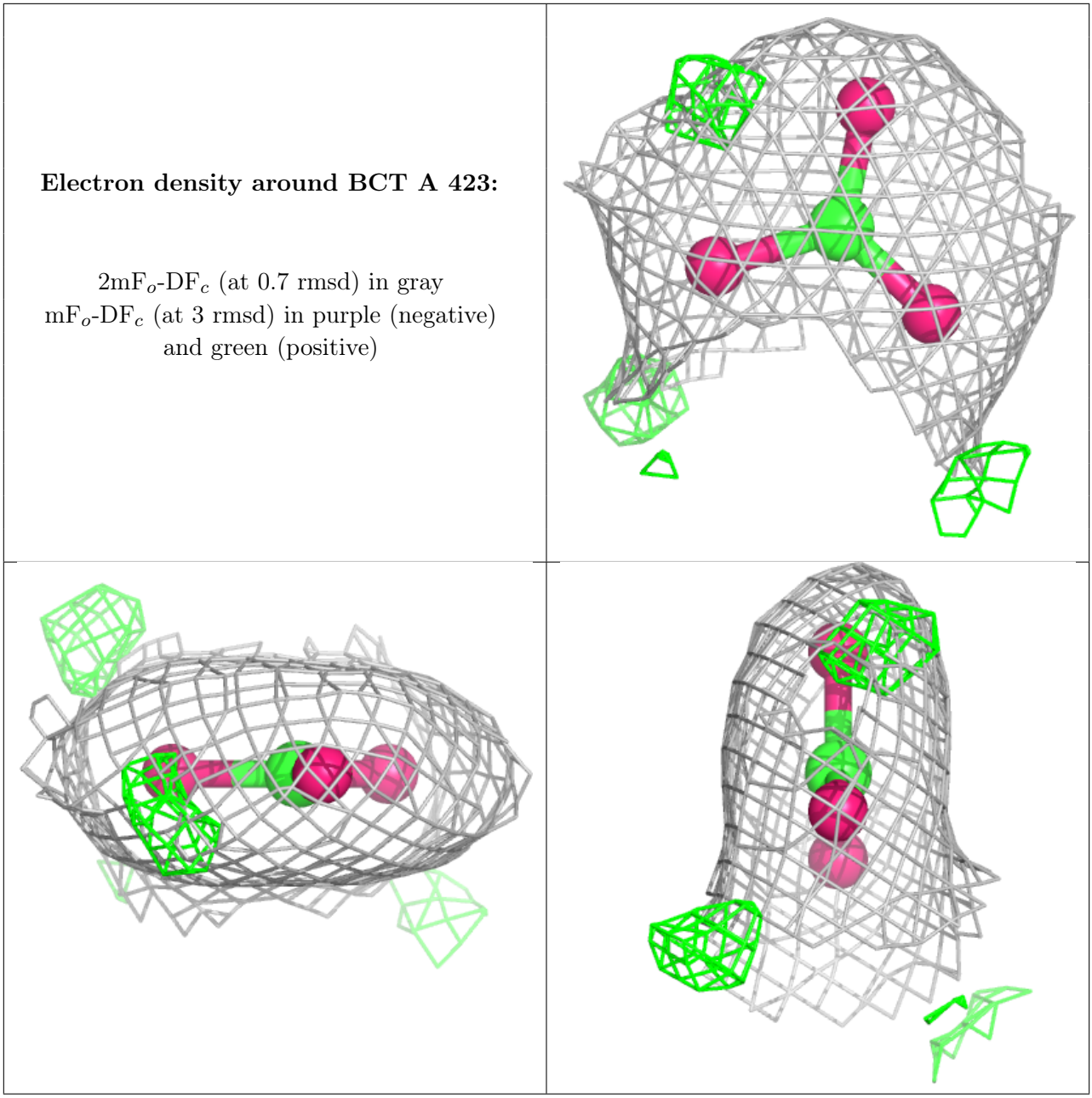
Electron density around CLA a 410:

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



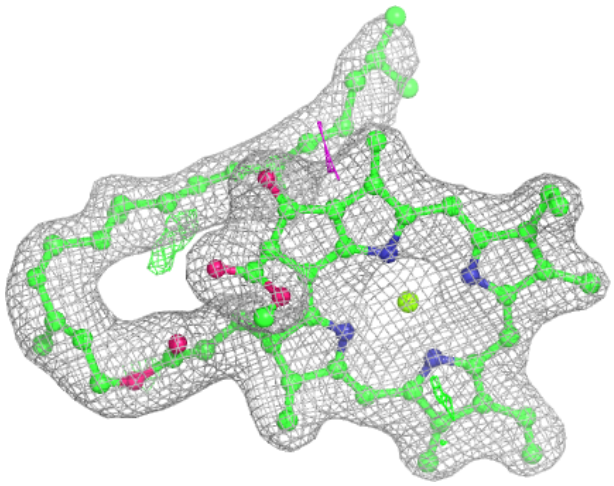
Electron density around BCT A 423:

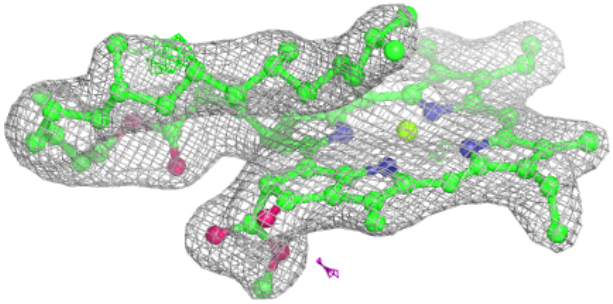
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

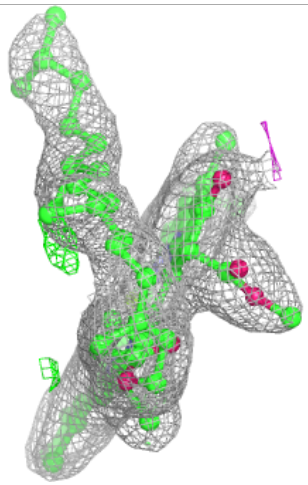


Electron density around CLA C 510:

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

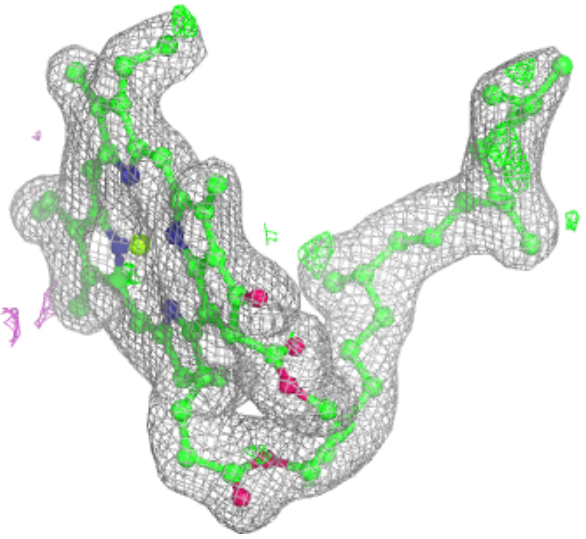


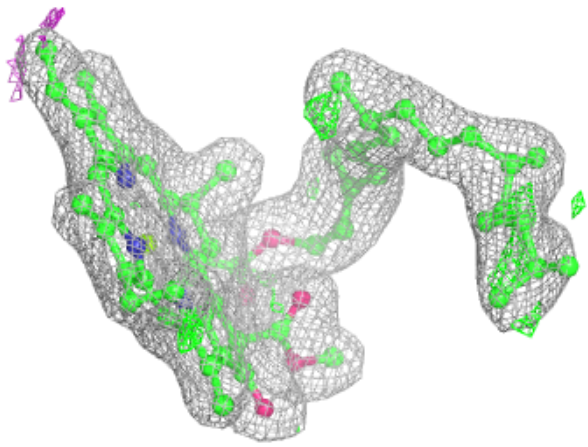


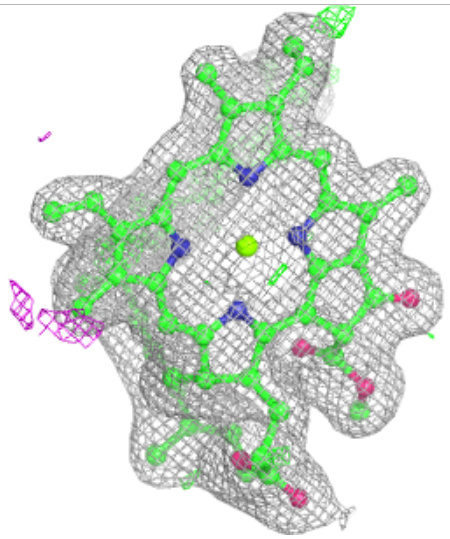


Electron density around CLA B 614:

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

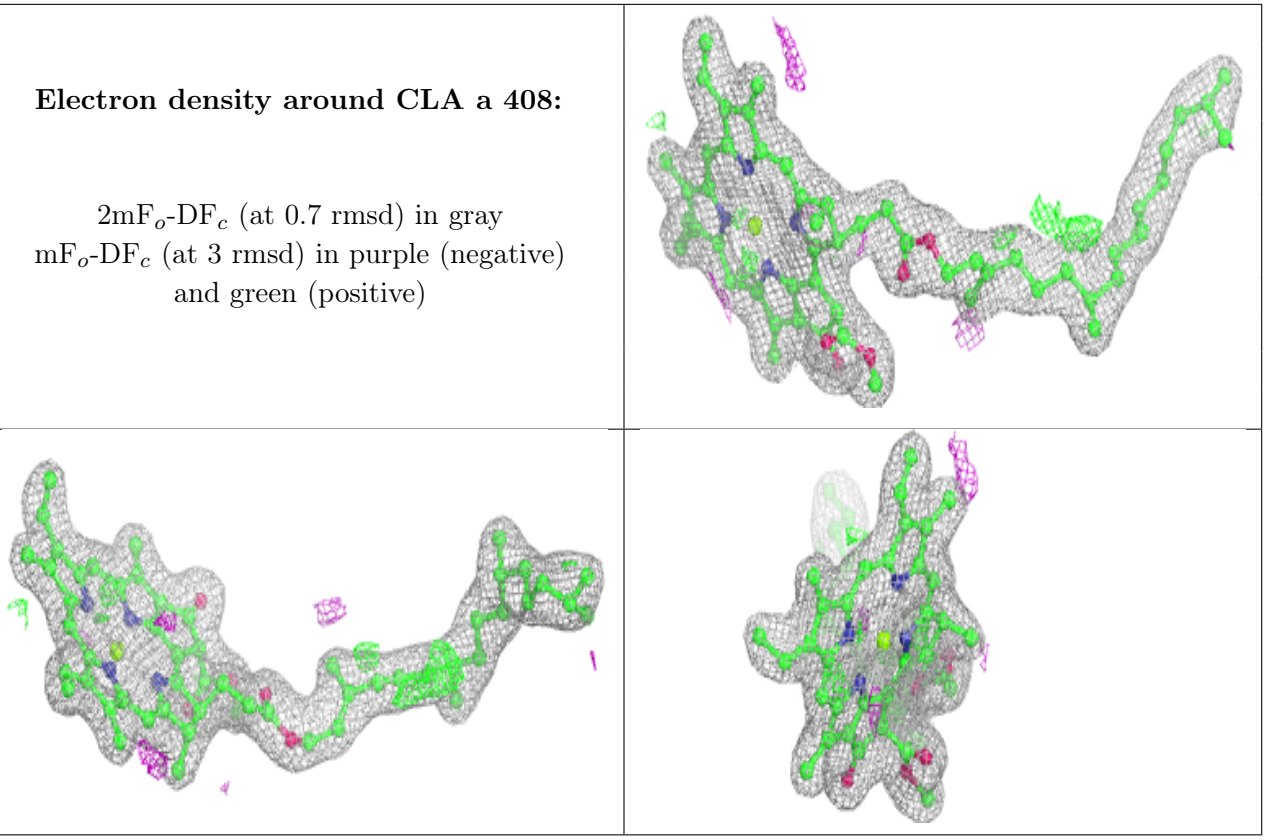






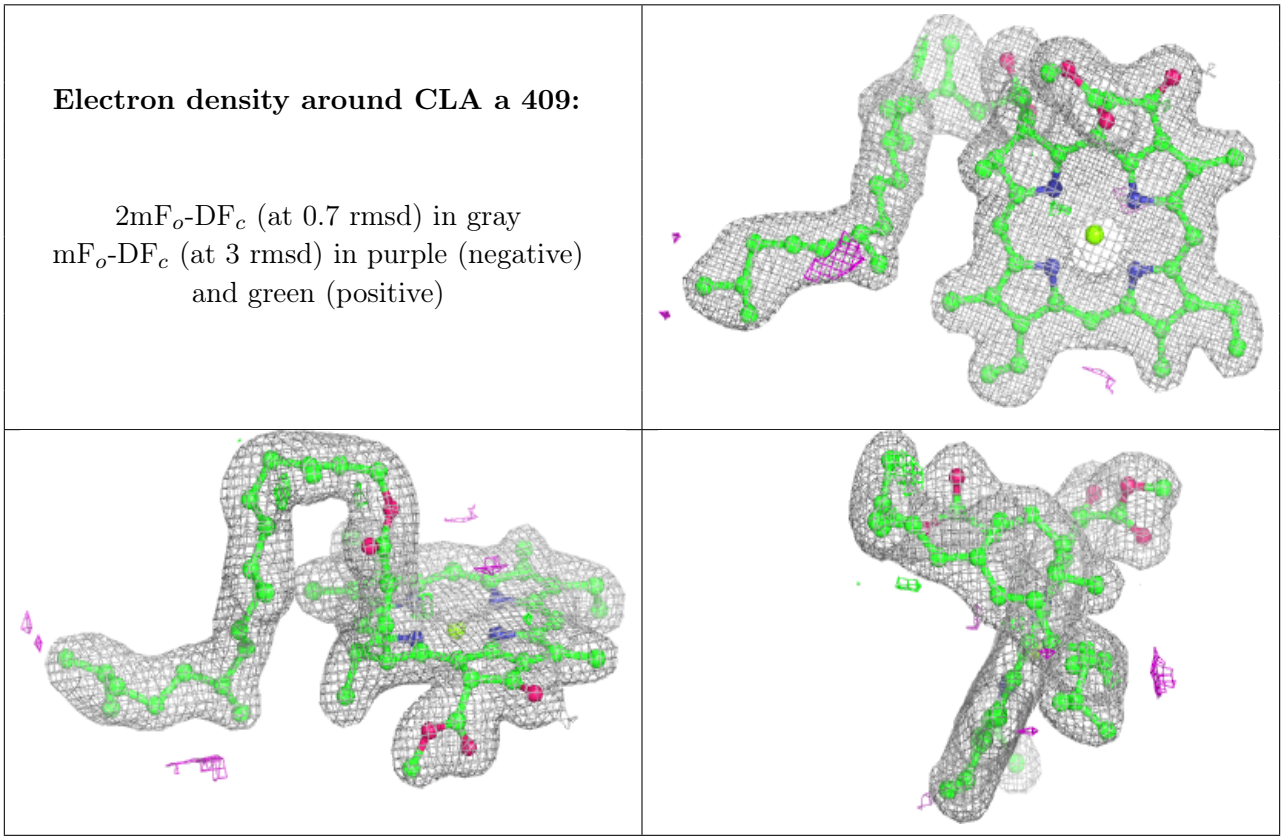
Electron density around CLA a 408:

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



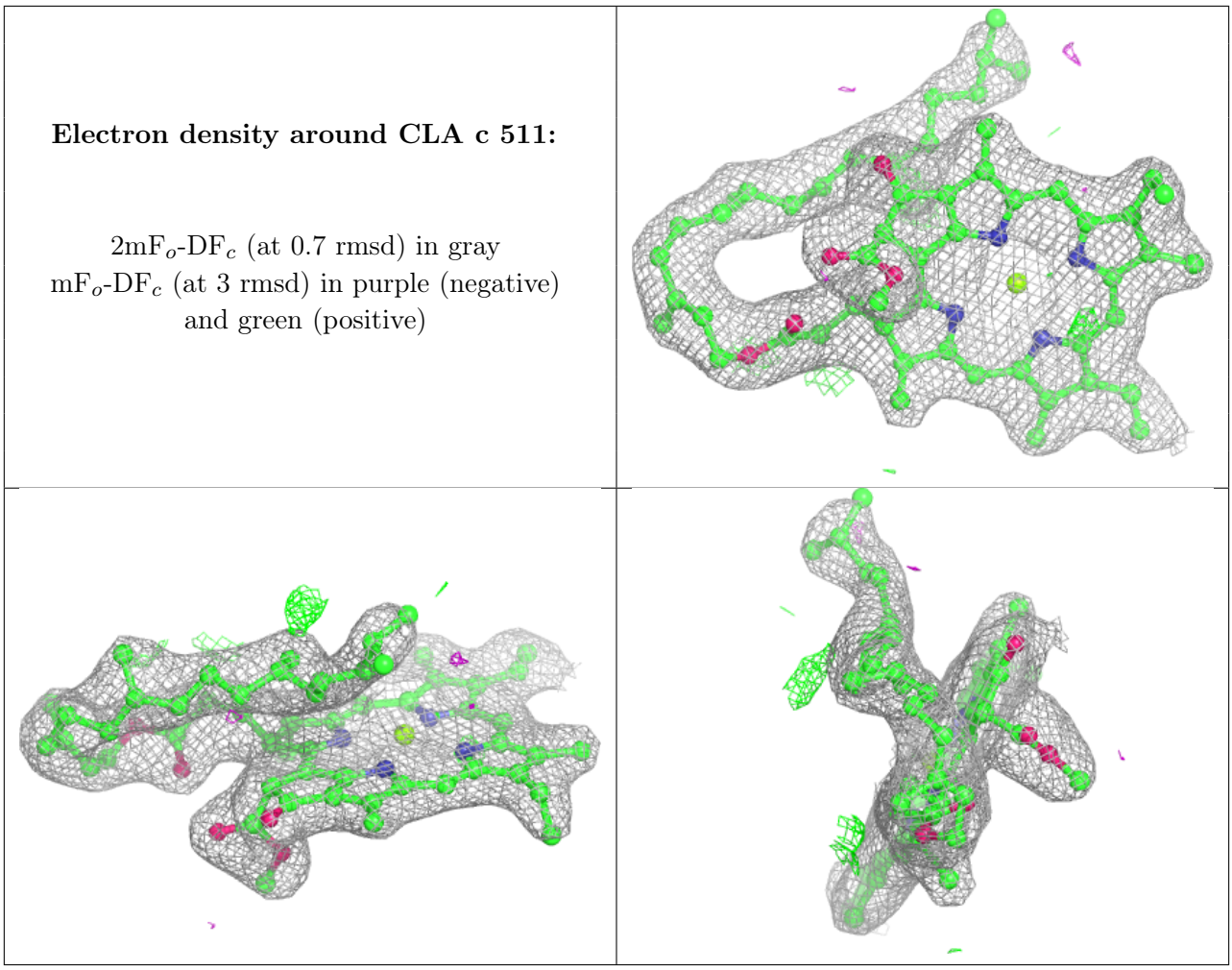
Electron density around CLA a 409:

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



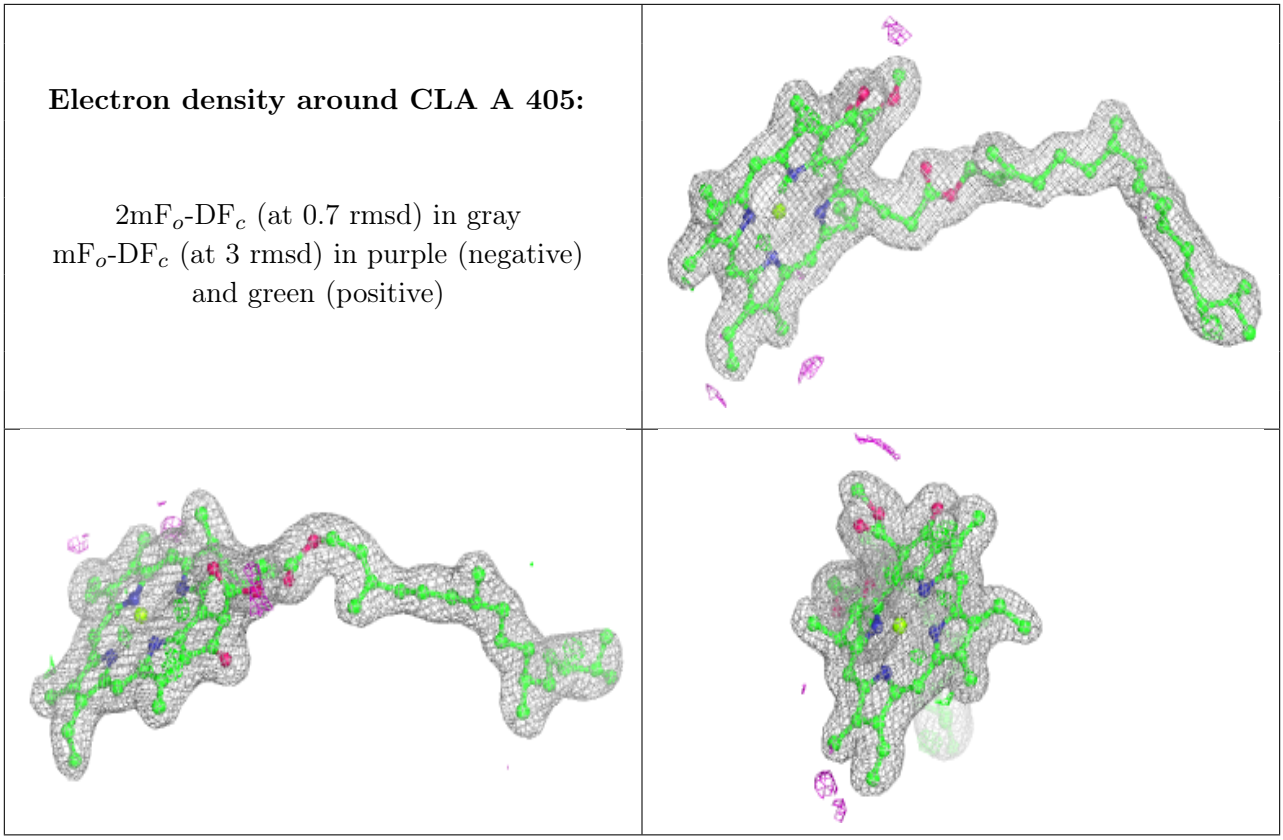
Electron density around CLA c 511:

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



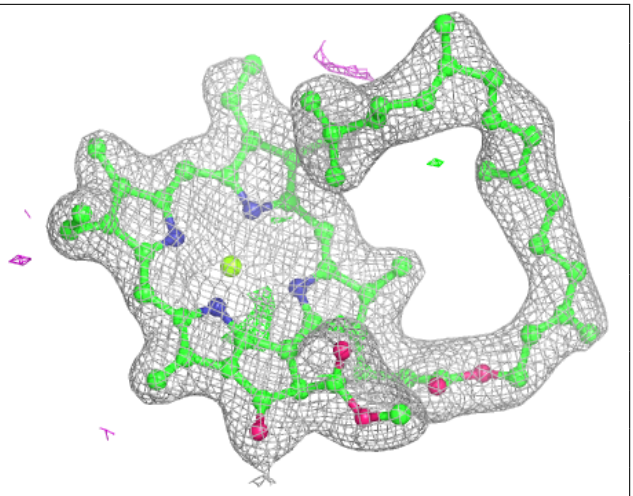
Electron density around CLA A 405:

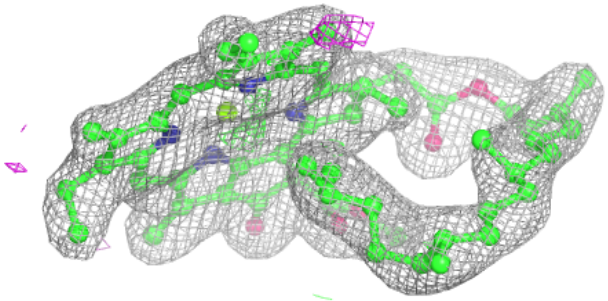
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

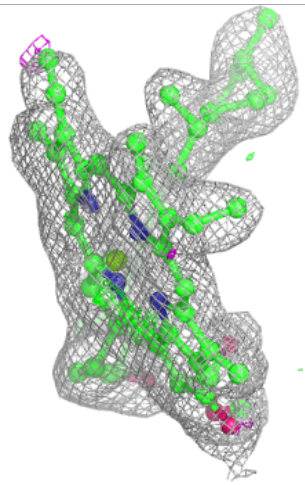


Electron density around CLA B 616:

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

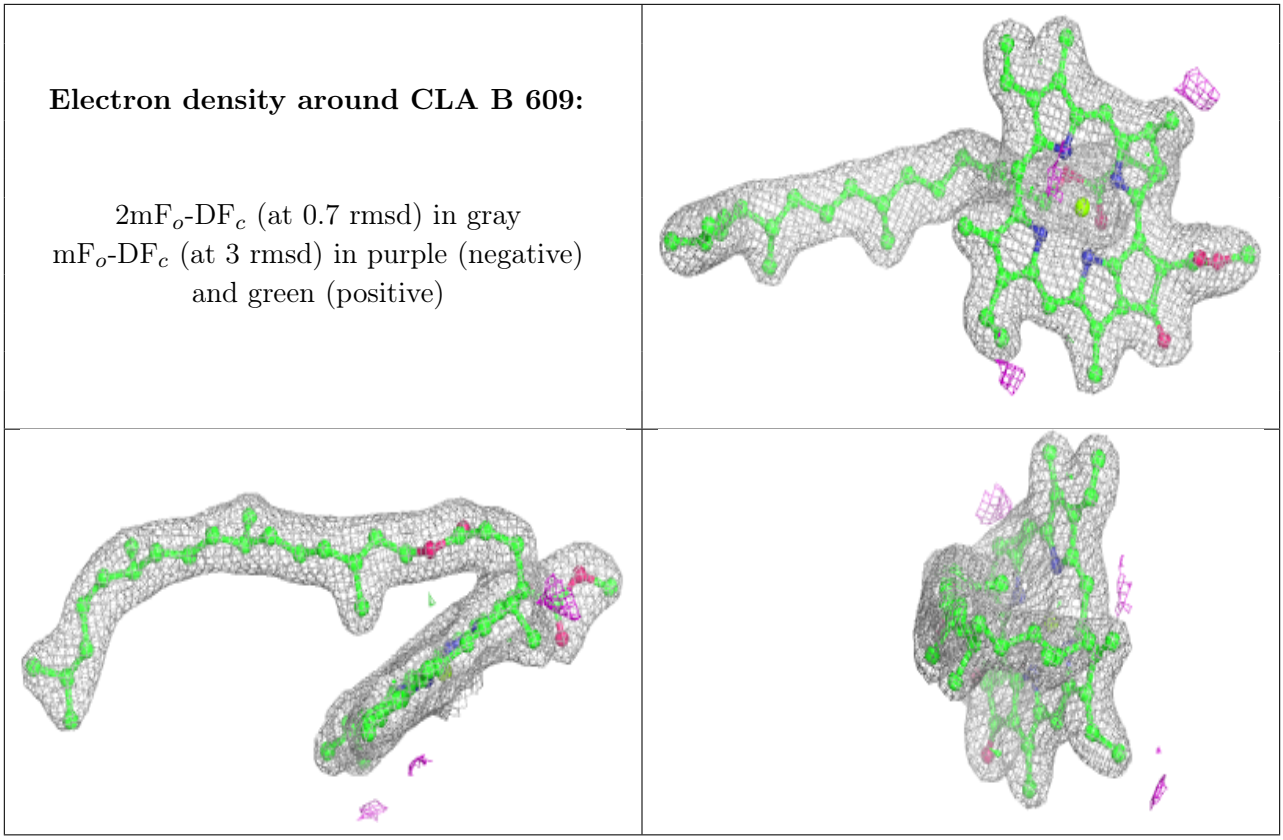






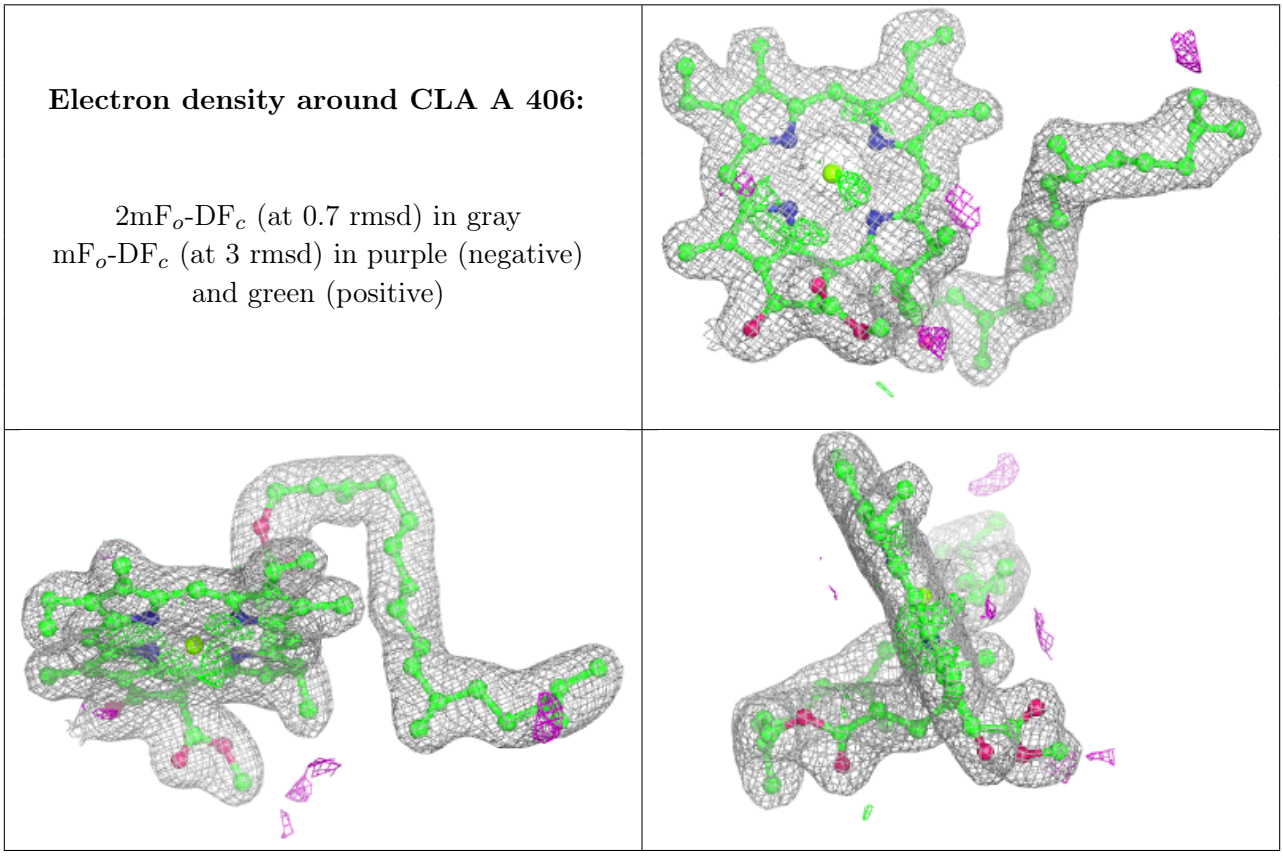
Electron density around CLA B 609:

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



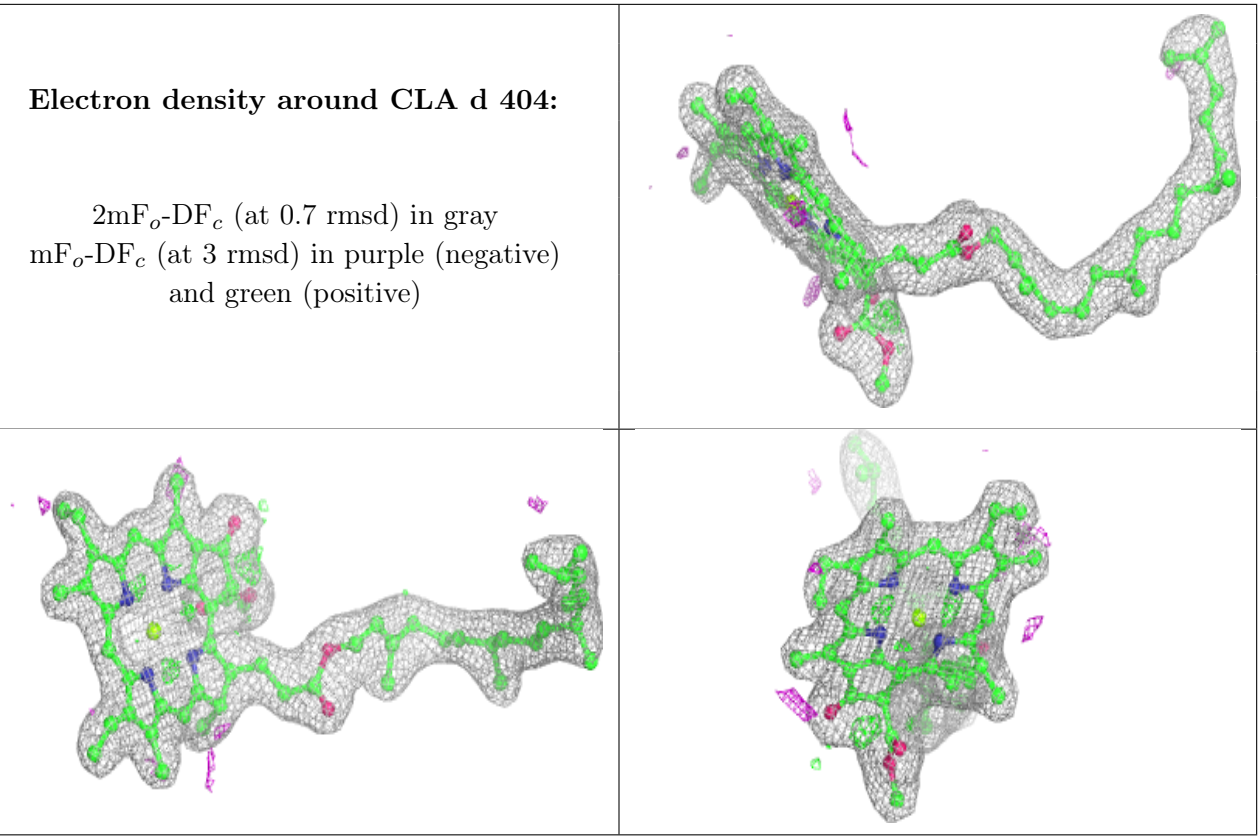
Electron density around CLA A 406:

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



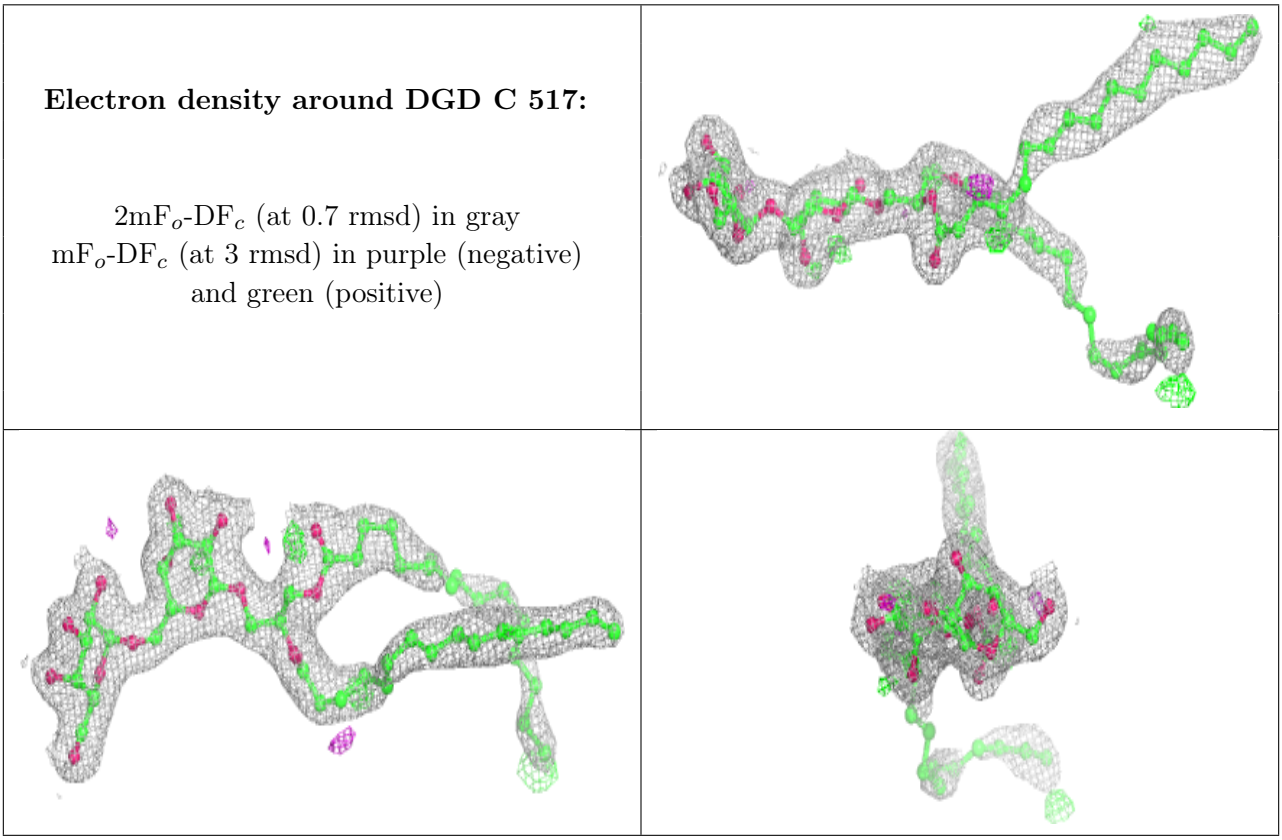
Electron density around CLA d 404:

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



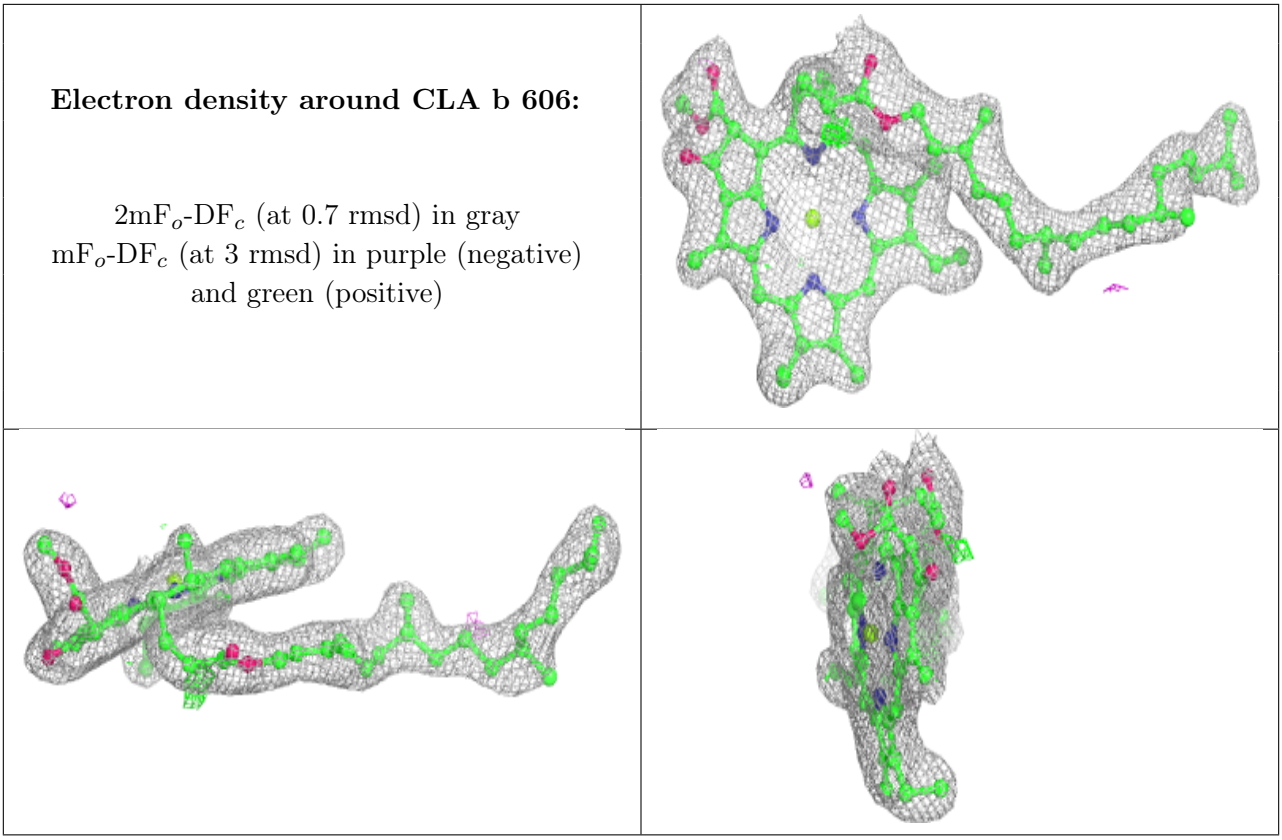
Electron density around DGD C 517:

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



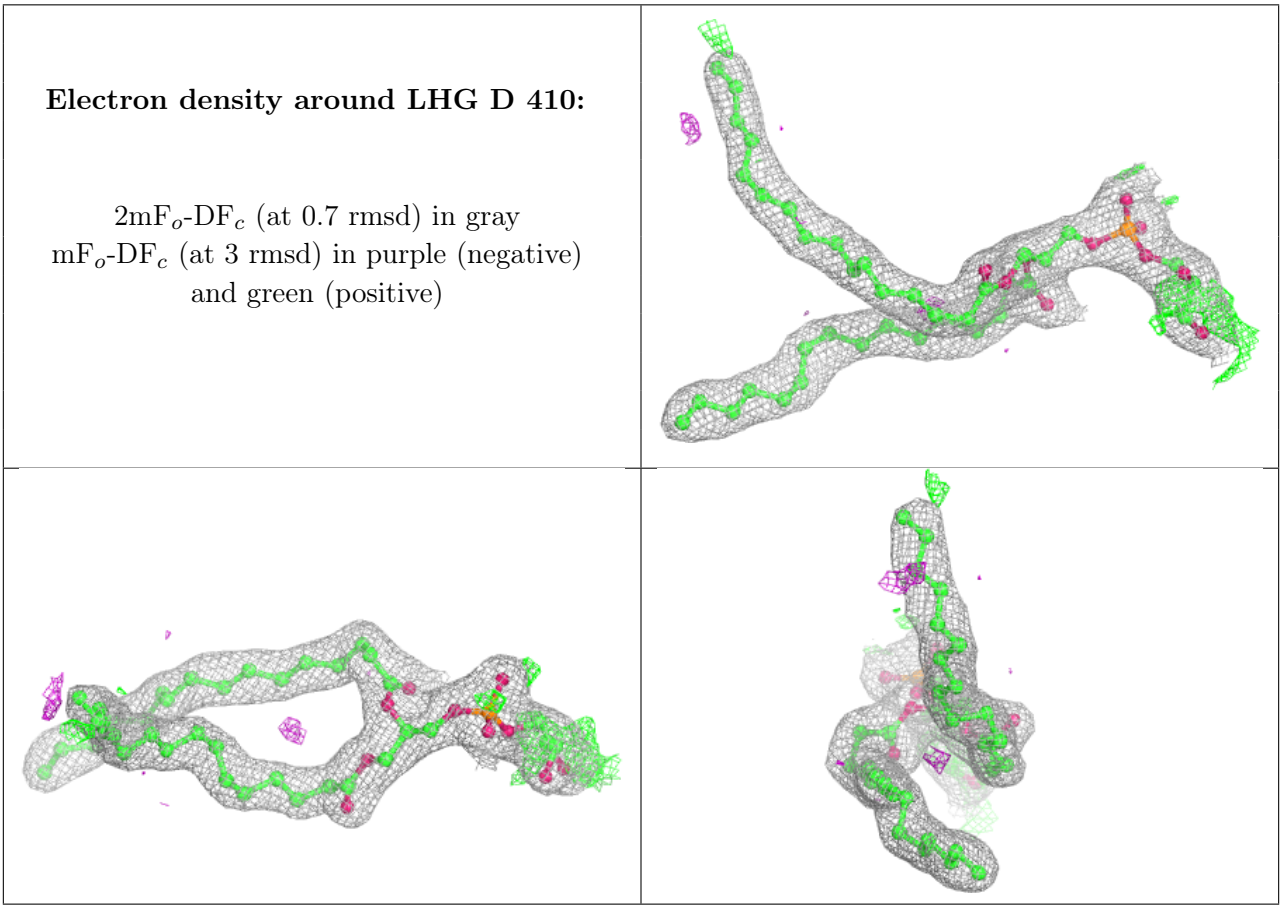
Electron density around CLA b 606:

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



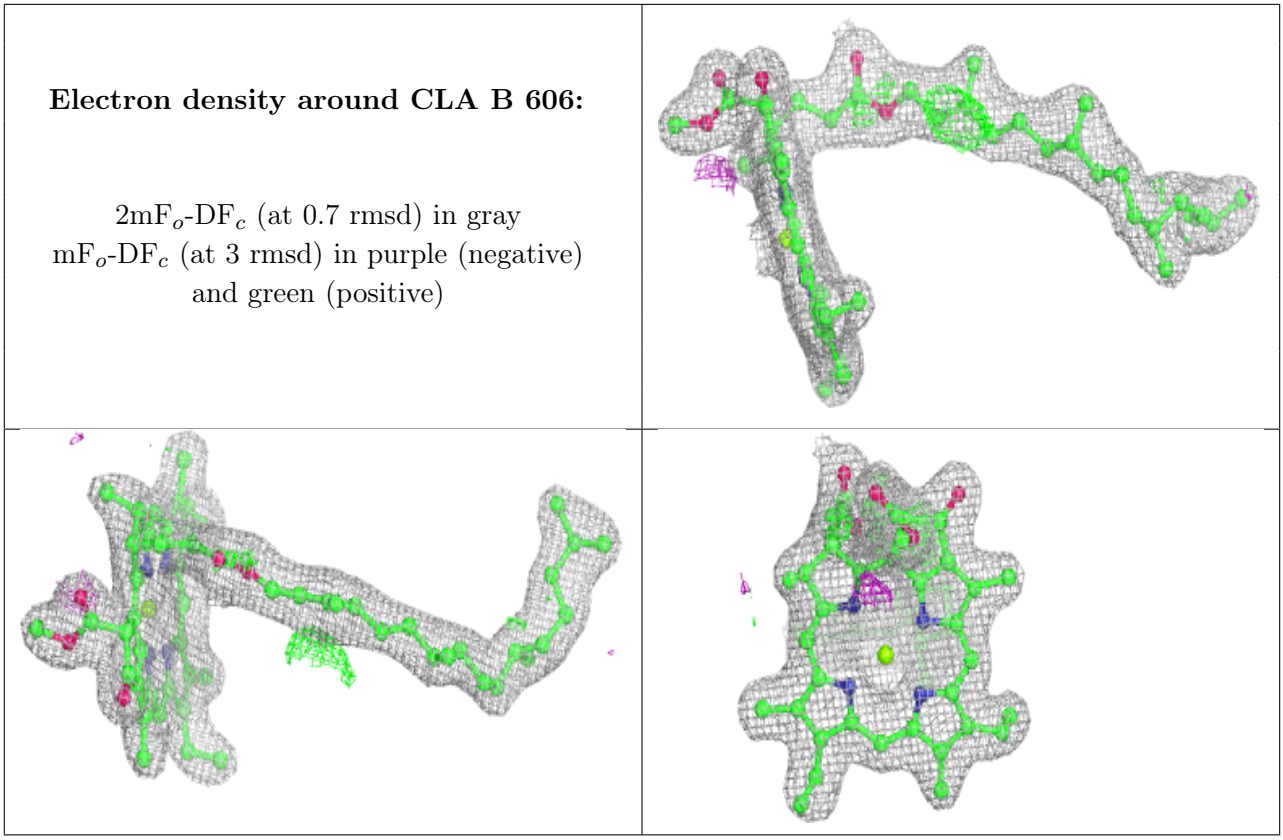
Electron density around LHG D 410:

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



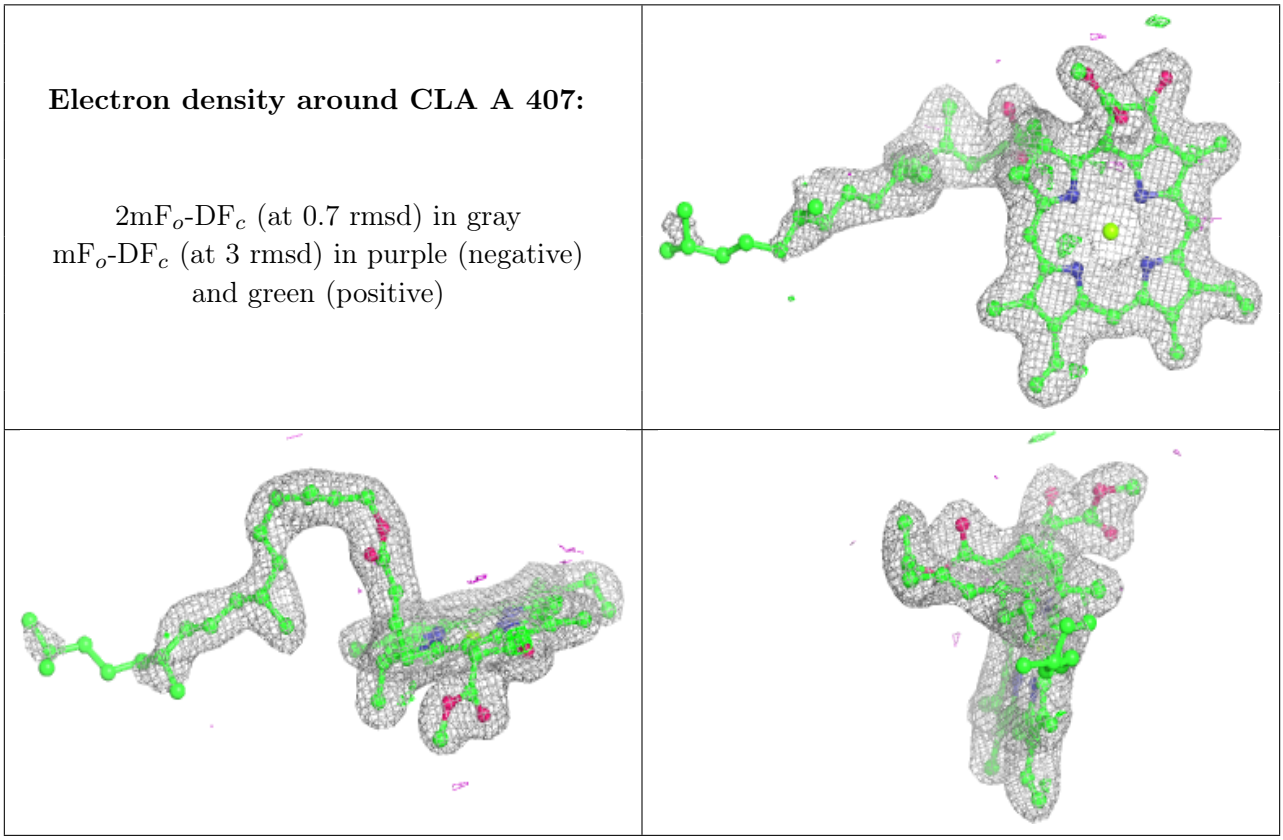
Electron density around CLA B 606:

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



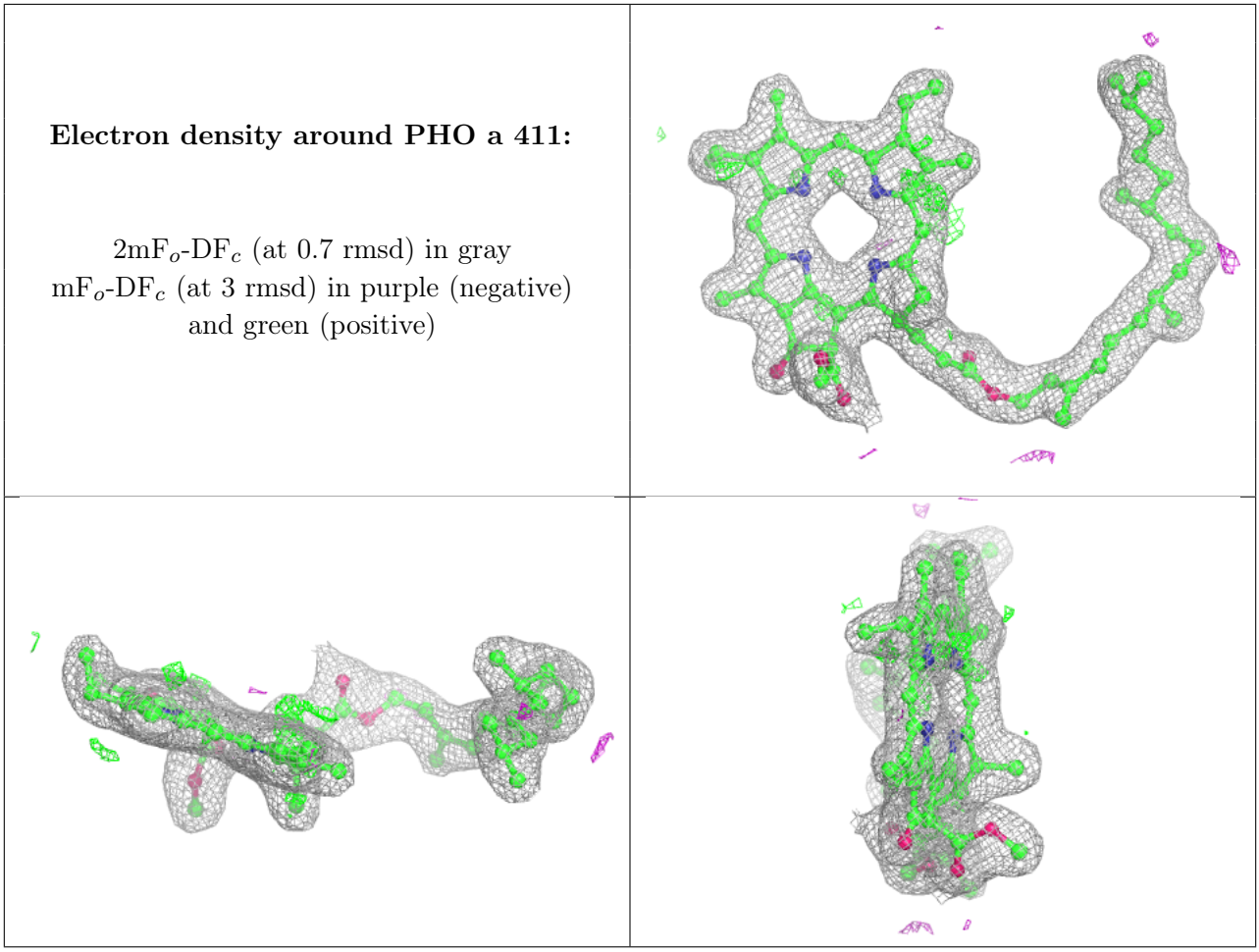
Electron density around CLA A 407:

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



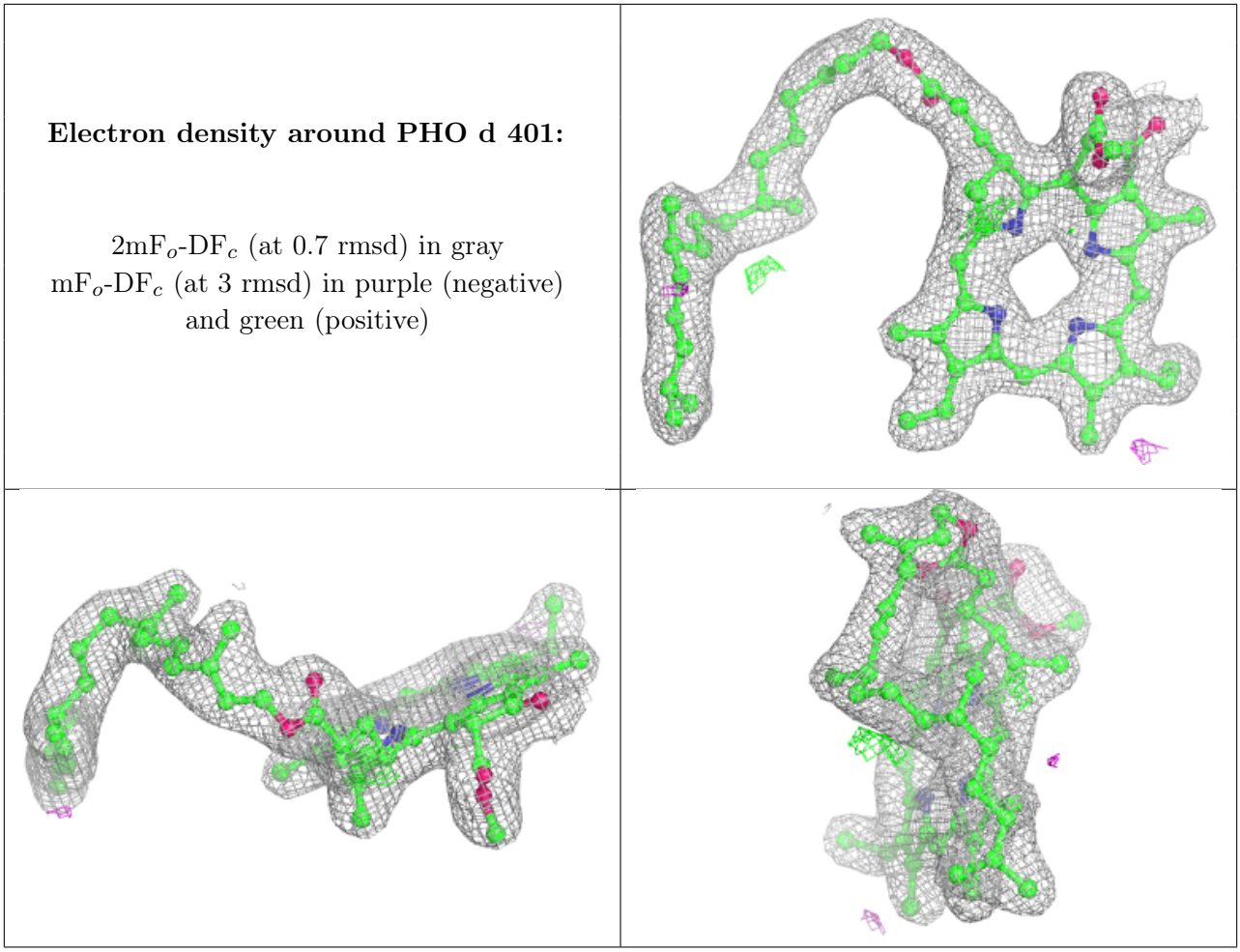
Electron density around PHO a 411:

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



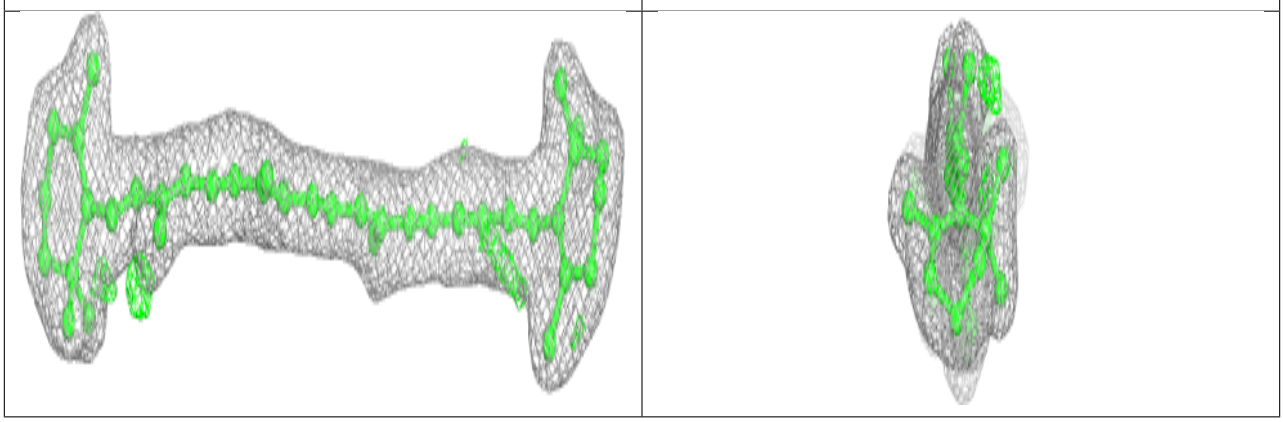
Electron density around PHO d 401:

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



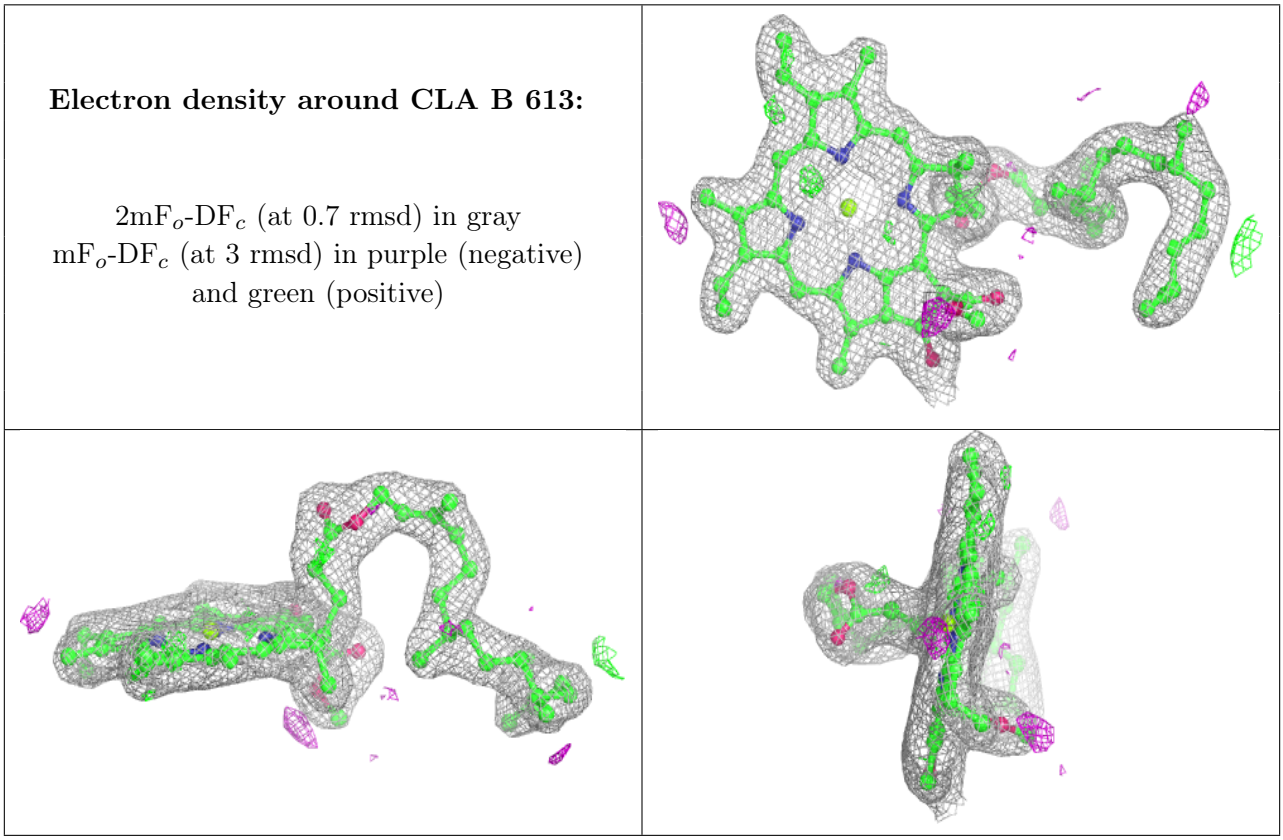
Electron density around BCR A 410:

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



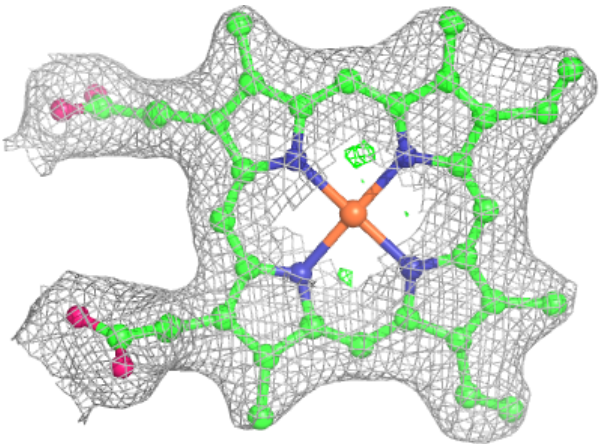
Electron density around CLA B 613:

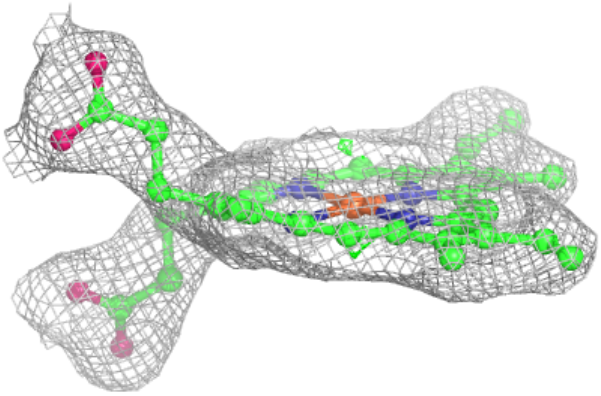
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

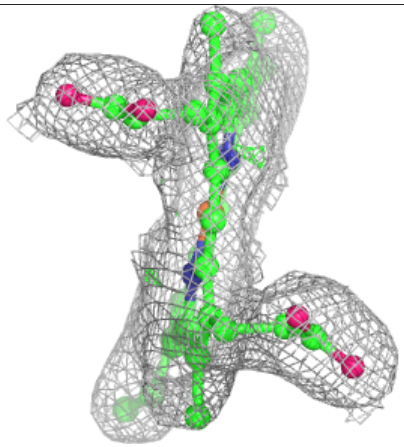


Electron density around HEM F 101:

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

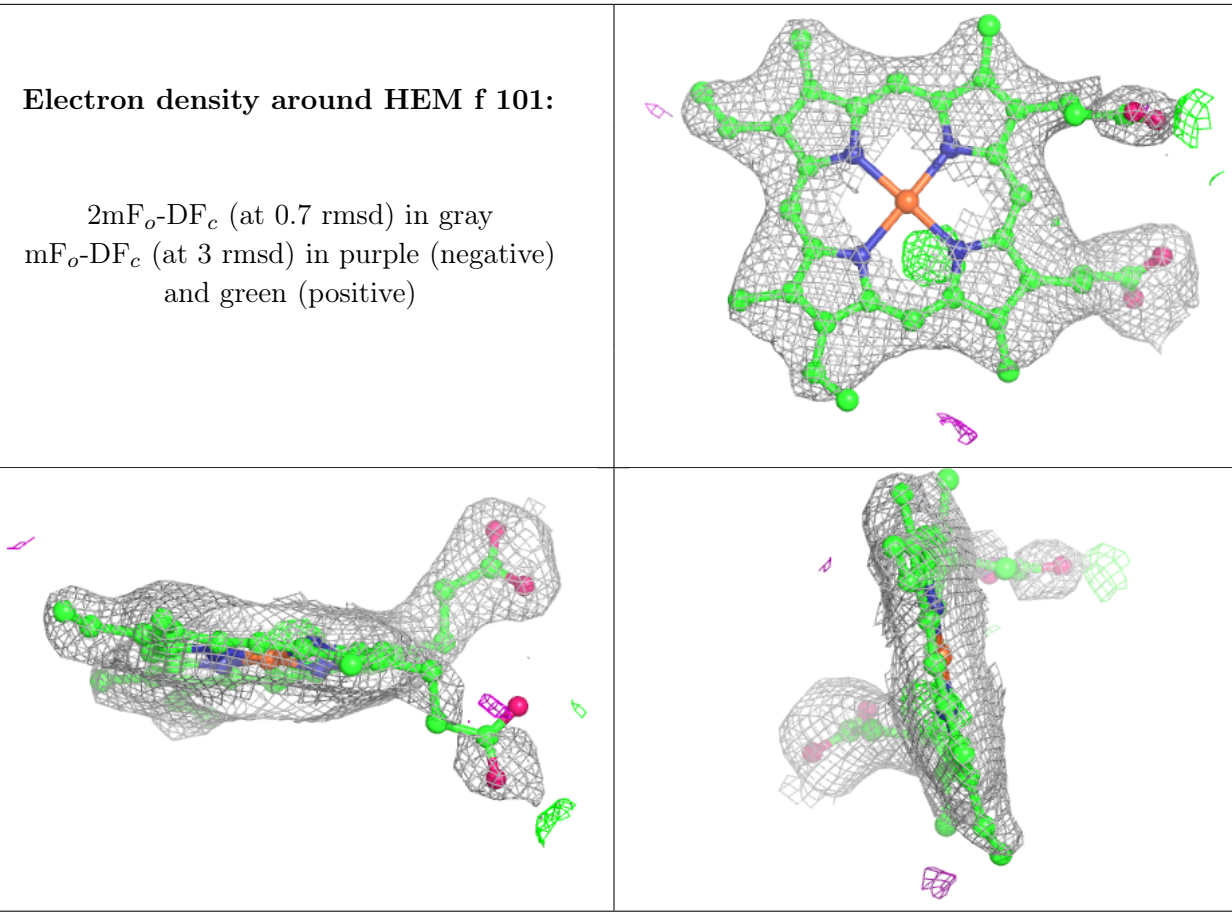






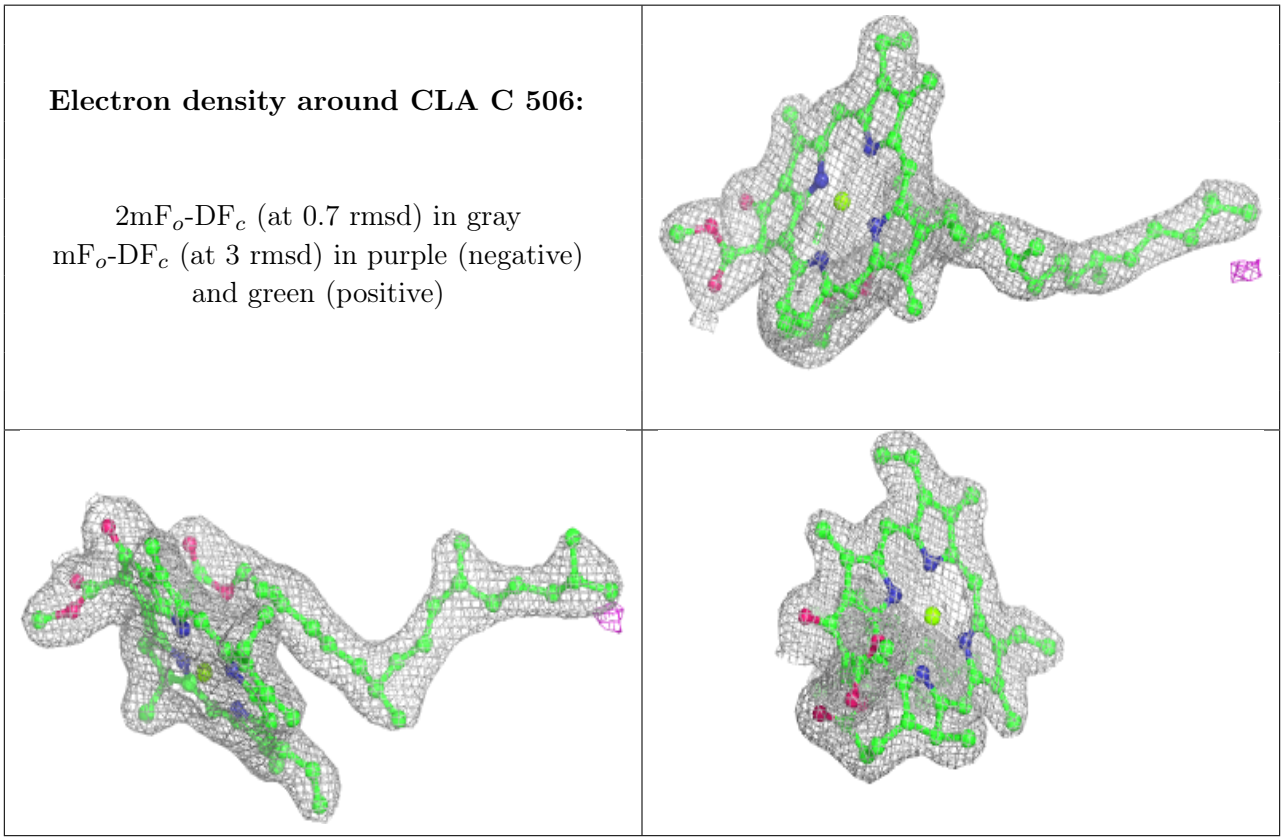
Electron density around HEM f 101:

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



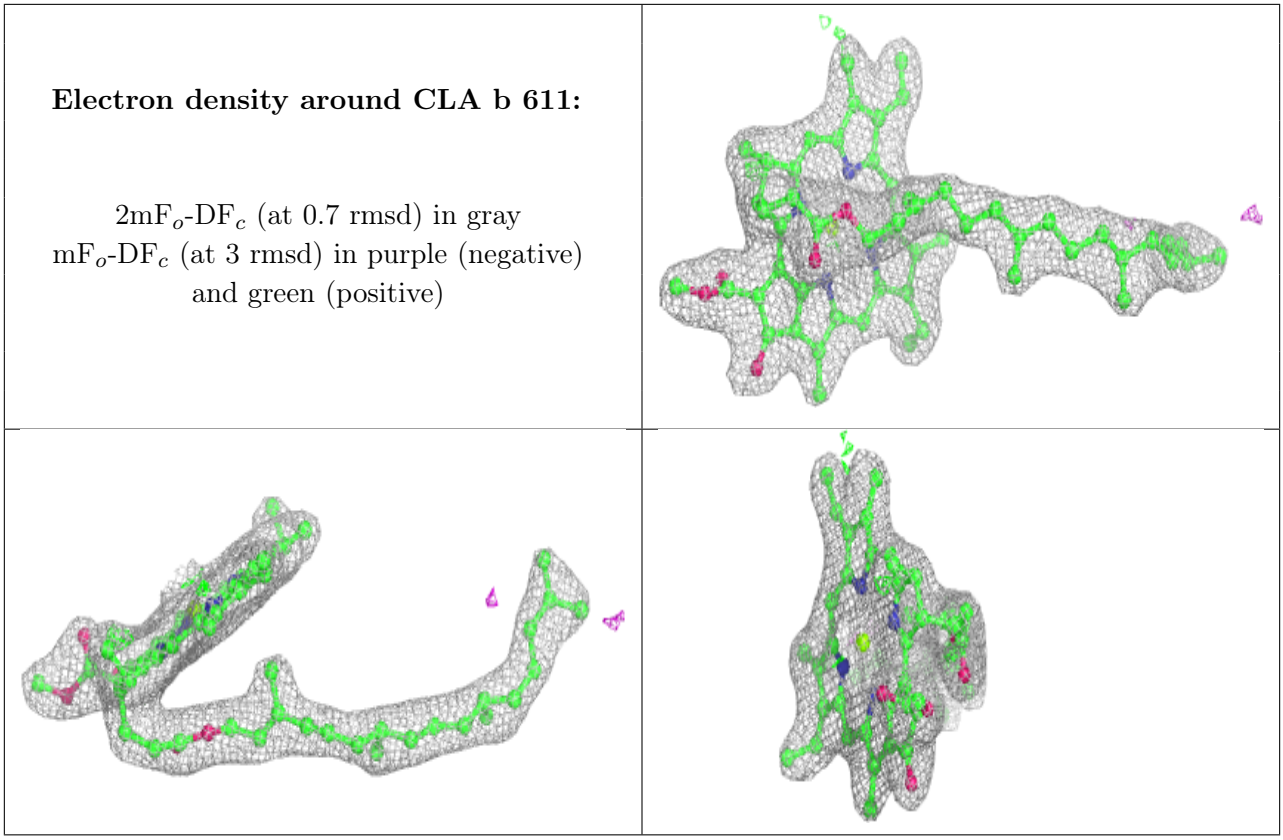
Electron density around CLA C 506:

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



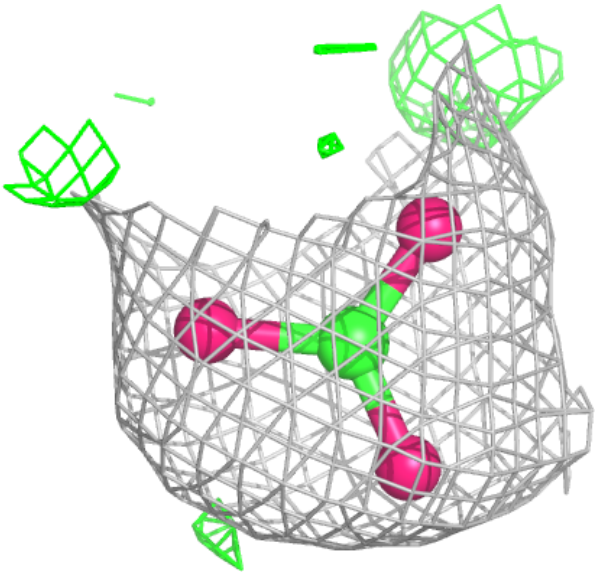
Electron density around CLA b 611:

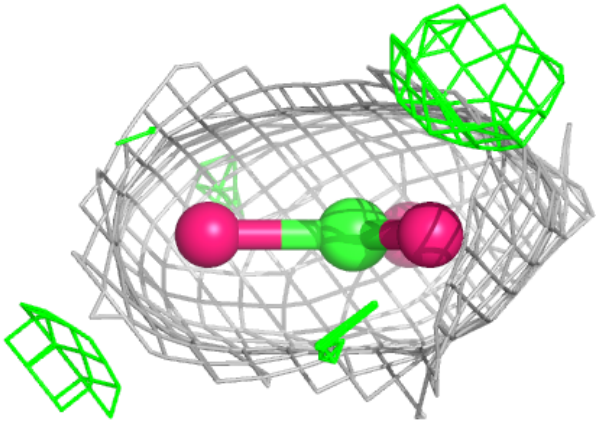
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

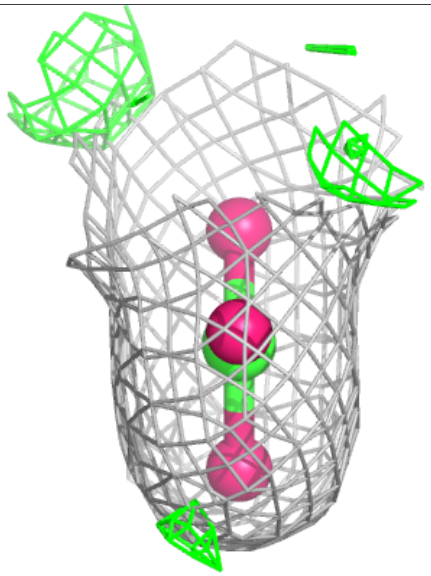


Electron density around BCT a 407:

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

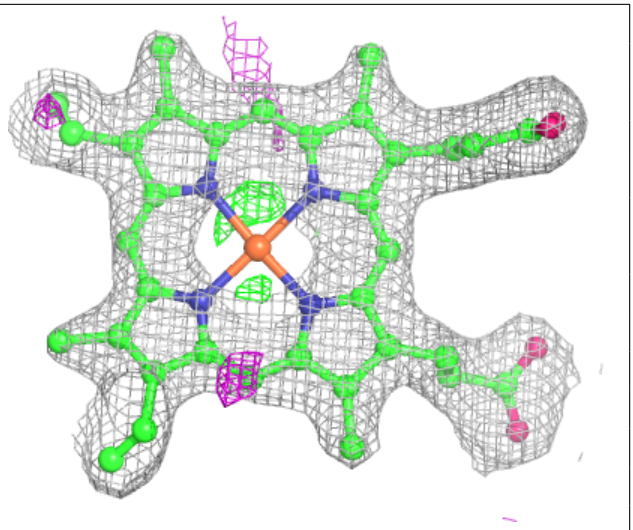


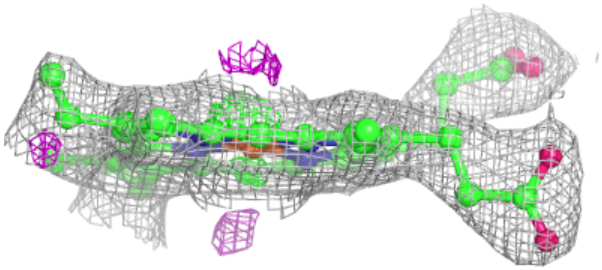


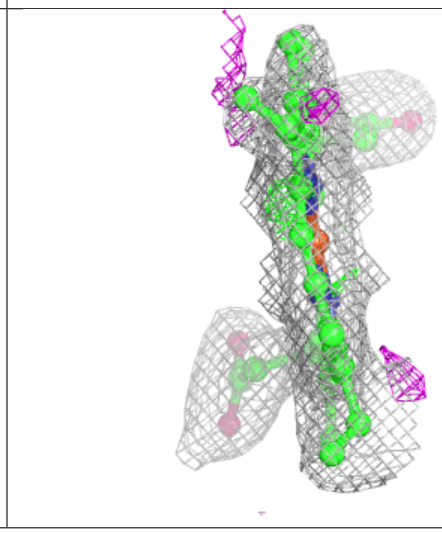


Electron density around HEC v 1603:

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

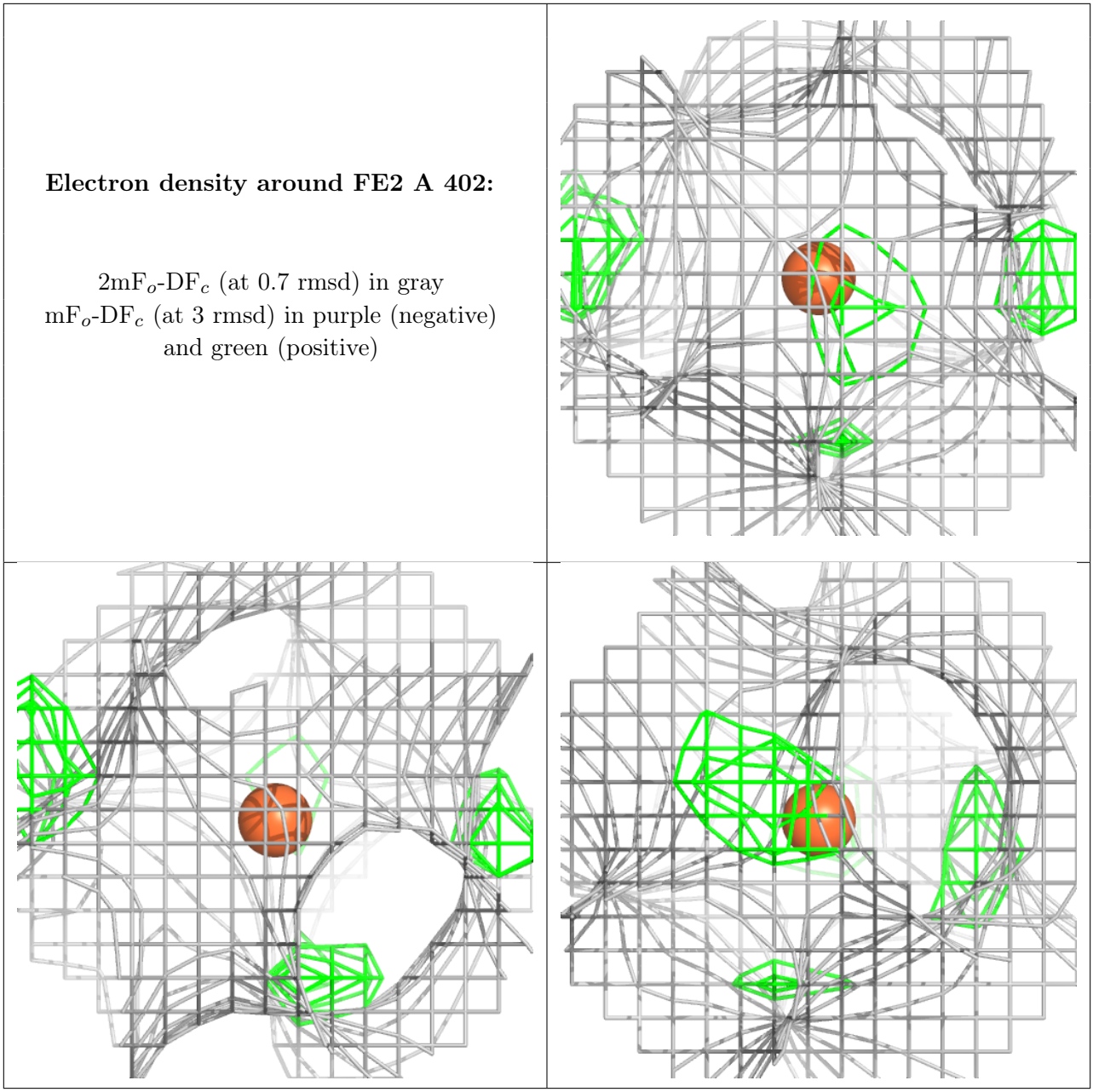






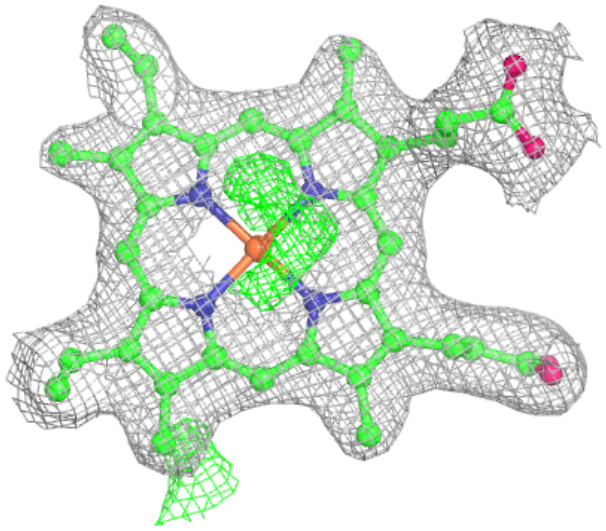
Electron density around FE2 A 402:

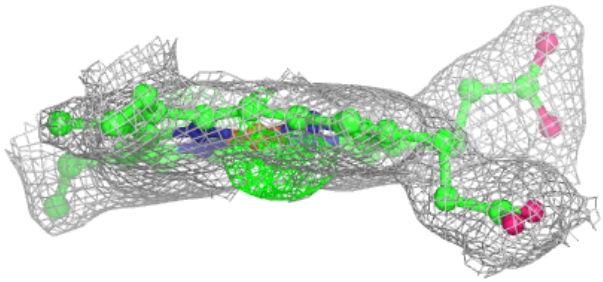
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

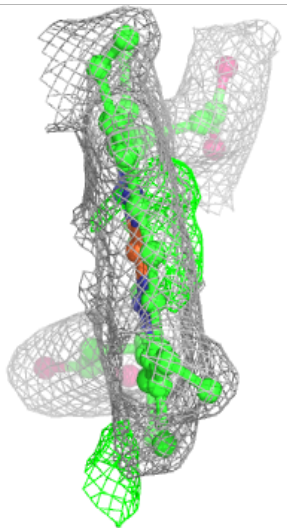


Electron density around HEC V 202:

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

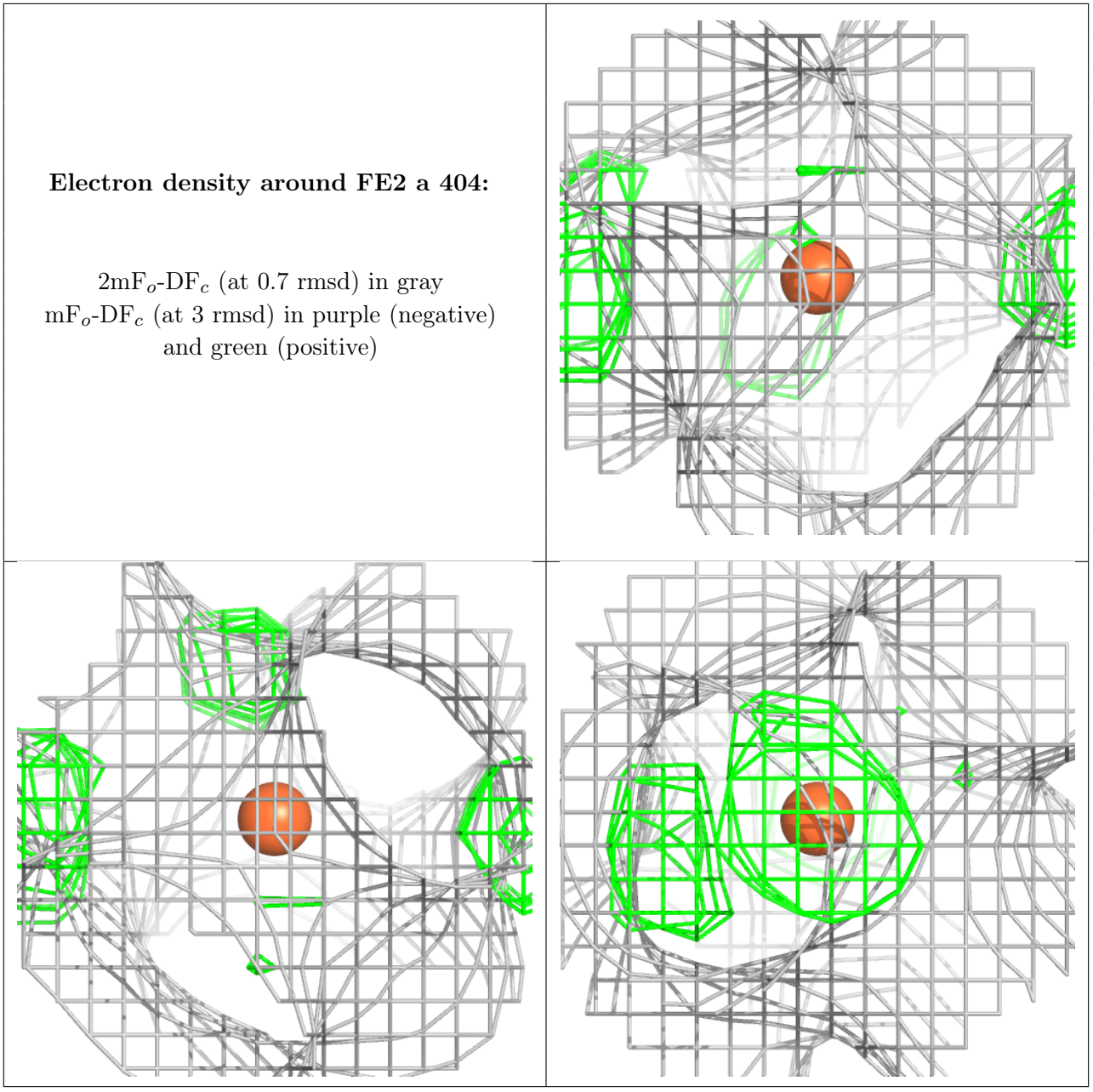






Electron density around FE2 a 404:

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



6.5 Other polymers

There are no such residues in this entry.