wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2023 – 08:52 PM EDT

PDB ID	:	4IXR
Title	:	RT fs X-ray diffraction of Photosystem II, first illuminated state
Authors	:	Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on	:	2013-01-27
Resolution	:	5.90 Å(reported)

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

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

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

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

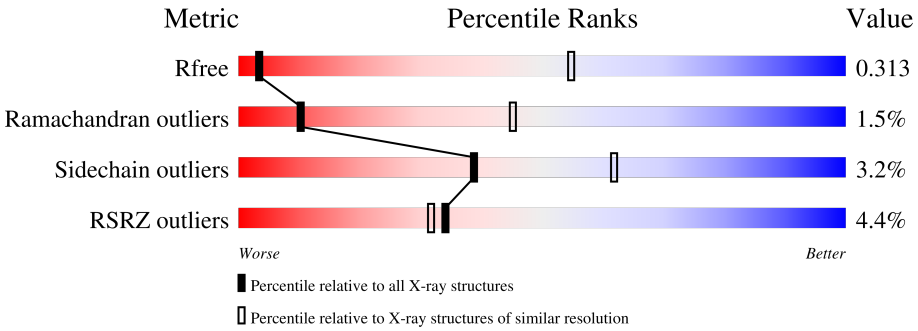
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 5.90 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	1016 (7.94-3.86)
Ramachandran outliers	138981	1011 (7.94-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)
RSRZ outliers	127900	1014 (8.00-3.78)

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	360	2% 90% · 7%
1	a	360	% 91% · 7%
2	B	510	5% 93% · ·

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Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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Mol	Chain	Length	Quality of chain
2	b	510	5% 93%
3	C	461	2% 93%
3	c	461	2% 92% 5%
4	D	352	% 92% 5%
4	d	352	% 92%
5	E	84	% 93%
5	e	84	4% 93%
6	F	45	4% 78% 22%
6	f	45	78% 22%
7	H	66	12% 88% 11%
7	h	66	5% 89% 9%
8	I	38	3% 84% 8% 8%
8	i	38	87% 5% 8%
9	J	40	2% 80% 5% 15%
9	j	40	2% 78% 8% 15%
10	K	46	76% 20%
10	k	46	7% 76% 20%
11	L	37	97%
11	l	37	97%
12	M	36	6% 94% 6%
12	m	36	8% 94% 6%
13	O	272	11% 87% 11%
13	o	272	7% 87% 11%
14	T	32	12% 94% 6%
14	t	32	94% 6%

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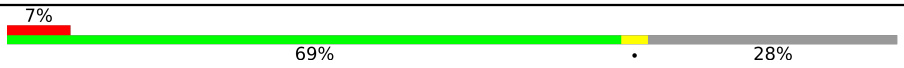
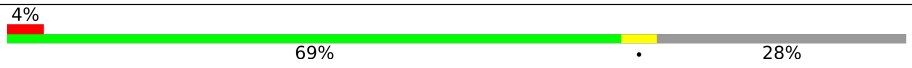
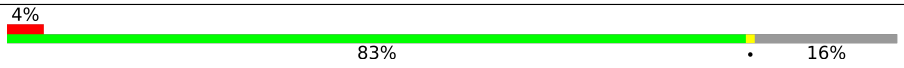
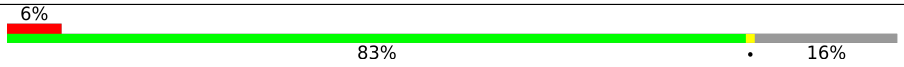
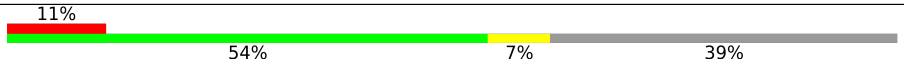
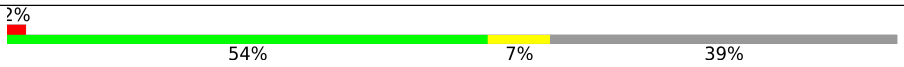
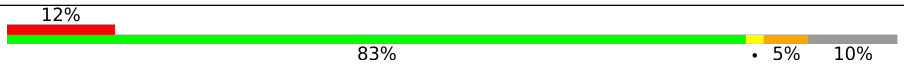
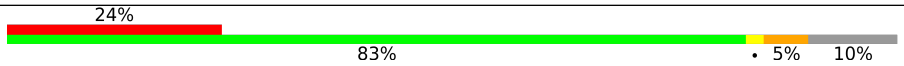
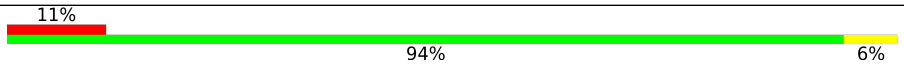
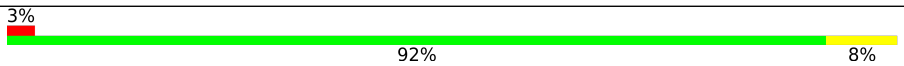
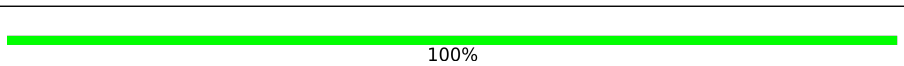
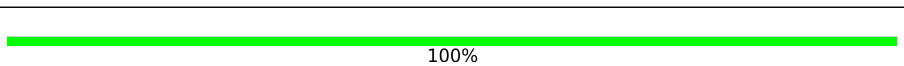
Mol	Chain	Length	Quality of chain
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	X
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	X
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	X
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	X
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	605	X	-	-	X
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	X
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	X
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	a	410	-	-	-	X
25	PL9	j	101	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	516	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	622	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	h	101	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	y	101	-	-	-	X
27	BCR	z	101	-	-	-	X
28	DGD	B	627	-	-	-	X
28	DGD	C	519	-	-	-	X
28	DGD	D	409	-	-	-	X
28	DGD	d	409	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	408	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	b	601	-	-	-	X
30	SQD	d	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	f	102	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	521	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	519	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
32	CL	A	416	-	-	-	X
32	CL	a	418	-	-	-	X
33	LMT	B	624	-	-	-	X
33	LMT	B	625	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	B	629	-	-	-	X
33	LMT	D	410	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	604	-	-	-	X
33	LMT	b	626	-	-	-	X
33	LMT	b	627	-	-	-	X
33	LMT	d	410	-	-	-	X
33	LMT	i	102	-	-	-	X
35	CA	K	101	-	-	-	X
35	CA	O	301	-	-	-	X
35	CA	k	101	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total 666	C 434	N 108	O 124	0	0	0
5	e	82	Total 666	C 434	N 108	O 124	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total 282	C 192	N 46	O 43	S 1	0	0	0
6	f	35	Total 282	C 192	N 46	O 43	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 507	C 338	N 81	O 86	S 2	0	0	0
7	h	65	Total 507	C 338	N 81	O 86	S 2	0	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 304	C 202	N 48	O 53	S 1	0	0	0
11	l	37	Total 304	C 202	N 48	O 53	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 267	C 178	N 40	O 48	S 1	0	0	0
12	m	34	Total 267	C 178	N 40	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0
13	o	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total 275	C 192	N 40	O 41	S 2	0	0	0
14	t	32	Total 275	C 192	N 40	O 41	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	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
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

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

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

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

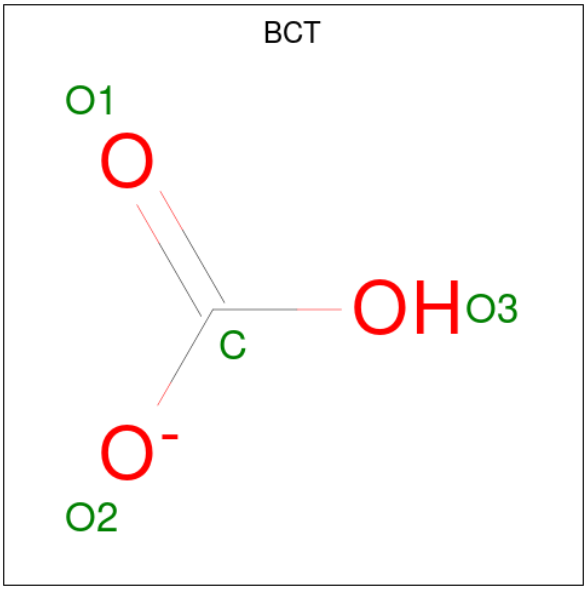
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	G	28	Total	C	N	O	0	0	0
			140	84	28	28			
20	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			

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

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

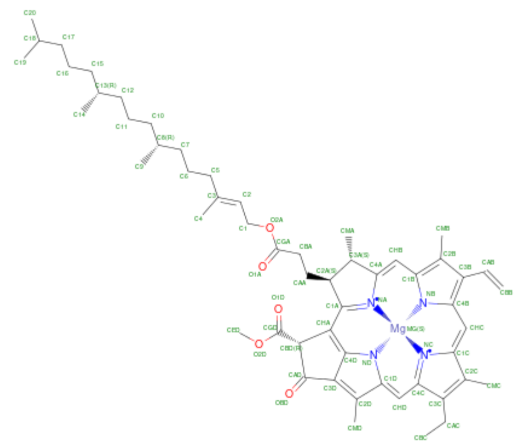
- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 4 1 3	0	0
22	d	1	Total C O 4 1 3	0	0

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

CLA



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

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

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

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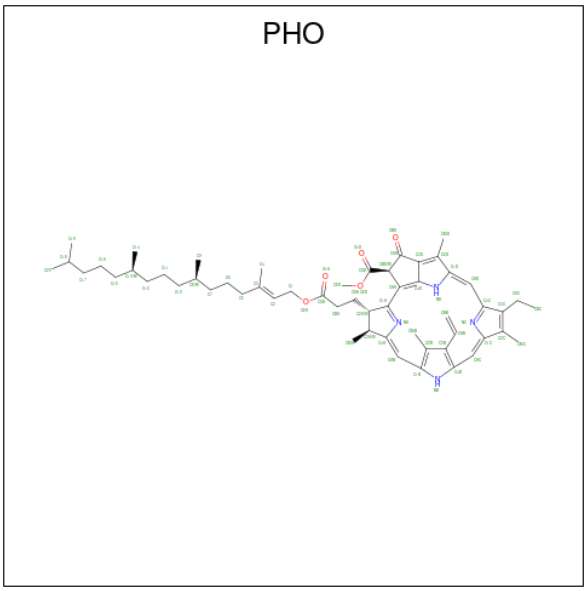
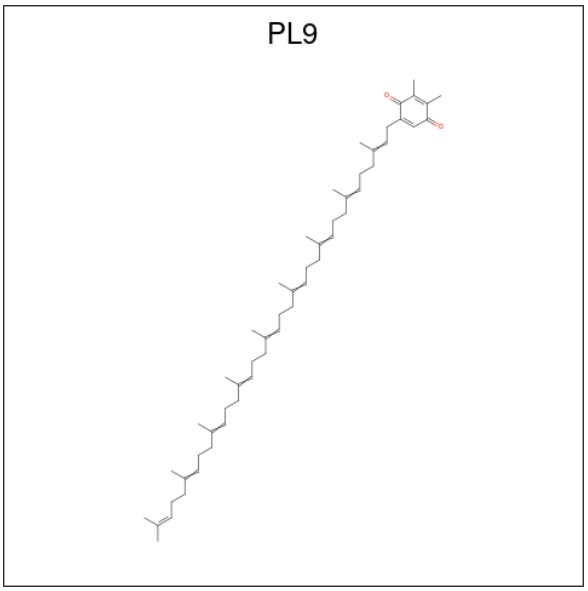
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4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

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



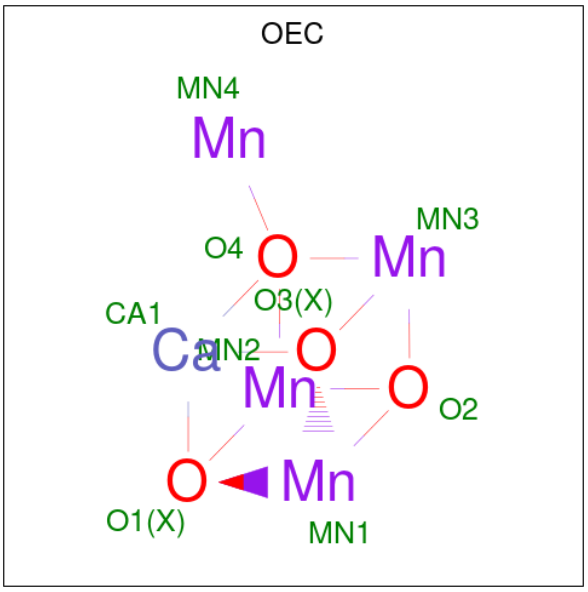
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C N O 64 55 4 5	0	0
24	D	1	Total C N O 64 55 4 5	0	0
24	a	1	Total C N O 64 55 4 5	0	0
24	a	1	Total C N O 64 55 4 5	0	0

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



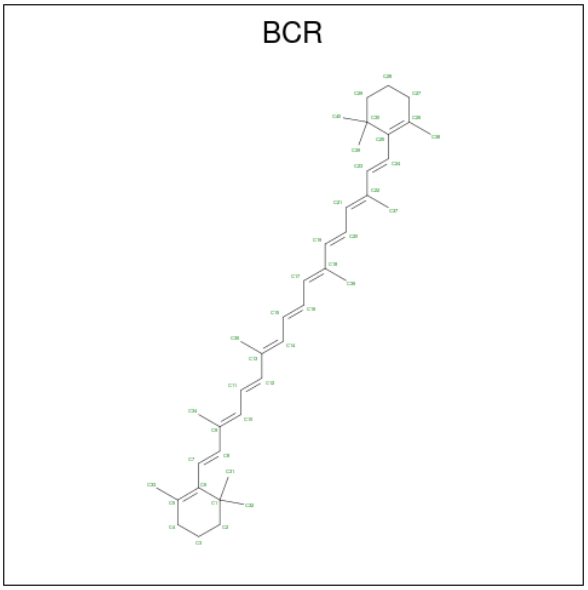
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 45 43 2	0	0
25	D	1	Total C O 55 53 2	0	0
25	J	1	Total C O 35 33 2	0	0
25	a	1	Total C O 45 43 2	0	0
25	d	1	Total C O 55 53 2	0	0
25	j	1	Total C O 35 33 2	0	0

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total Ca Mn 5 1 4	0	0
26	a	1	Total Ca Mn 5 1 4	0	0

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

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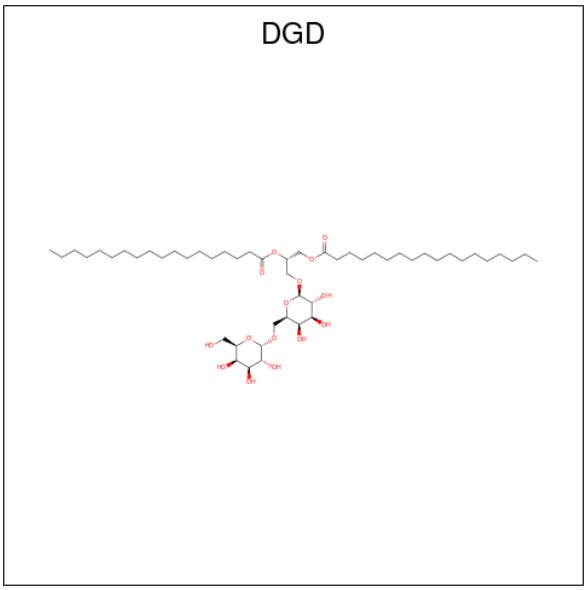
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	z	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52 37 15	0	0
28	b	1	Total C O 58 43 15	0	0

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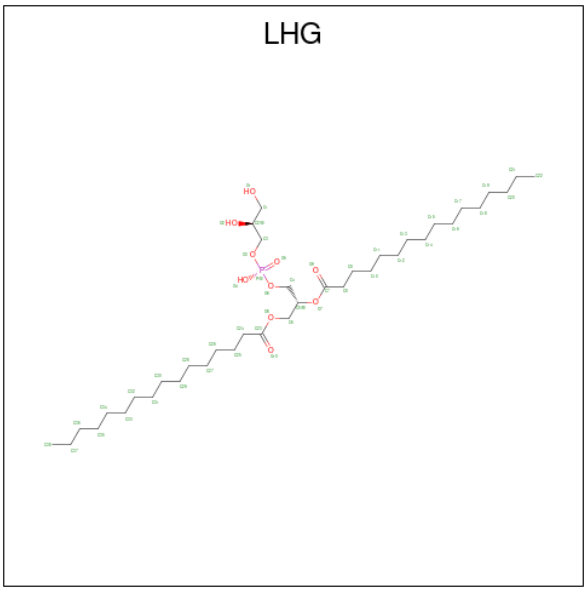
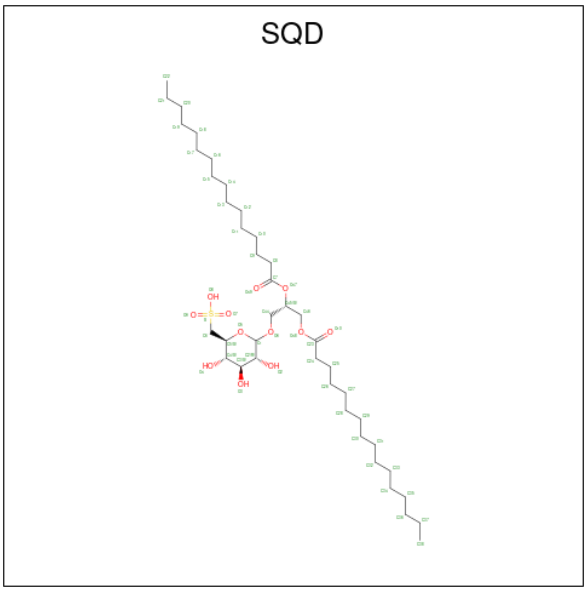
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O 53 38 15	0	0
28	c	1	Total C O 62 47 15	0	0
28	c	1	Total C O 66 51 15	0	0
28	d	1	Total C O 63 48 15	0	0

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



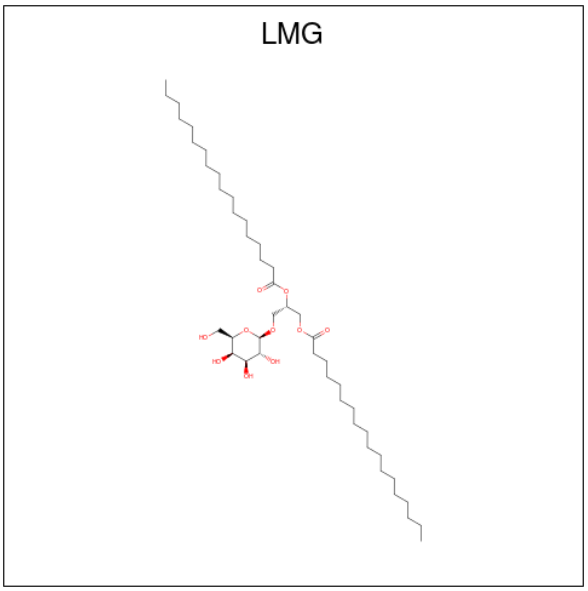
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O P 39 28 10 1	0	0
29	A	1	Total C O P 37 26 10 1	0	0
29	a	1	Total C O P 39 28 10 1	0	0
29	a	1	Total C O P 37 26 10 1	0	0

- Molecule 30 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
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 51 41 10	0	0
31	A	1	Total C O 42 32 10	0	0
31	B	1	Total C O 49 39 10	0	0
31	B	1	Total C O 49 39 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	C	1	Total C O 45 35 10	0	0
31	D	1	Total C O 46 36 10	0	0
31	D	1	Total C O 48 38 10	0	0
31	E	1	Total C O 44 34 10	0	0
31	I	1	Total C O 43 33 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	a	1	Total C O 42 32 10	0	0
31	a	1	Total C O 51 41 10	0	0
31	b	1	Total C O 49 39 10	0	0

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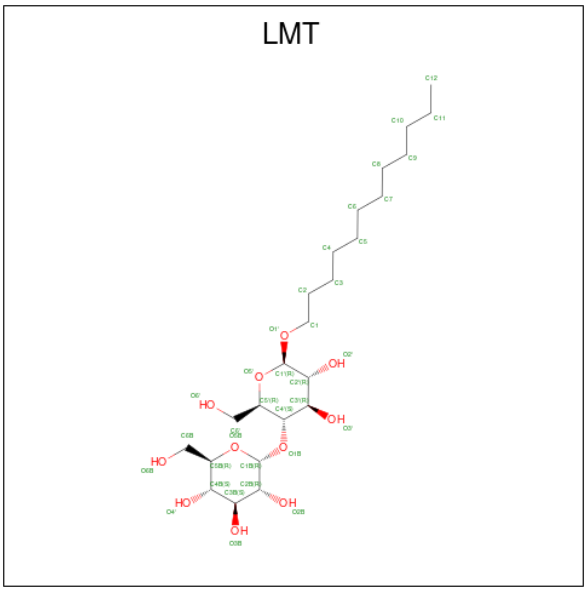
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C O 49 39 10	0	0
31	c	1	Total C O 45 35 10	0	0
31	d	1	Total C O 46 36 10	0	0
31	d	1	Total C O 48 38 10	0	0
31	e	1	Total C O 44 34 10	0	0
31	i	1	Total C O 43 33 10	0	0
31	k	1	Total C O 48 38 10	0	0
31	m	1	Total C O 42 32 10	0	0

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

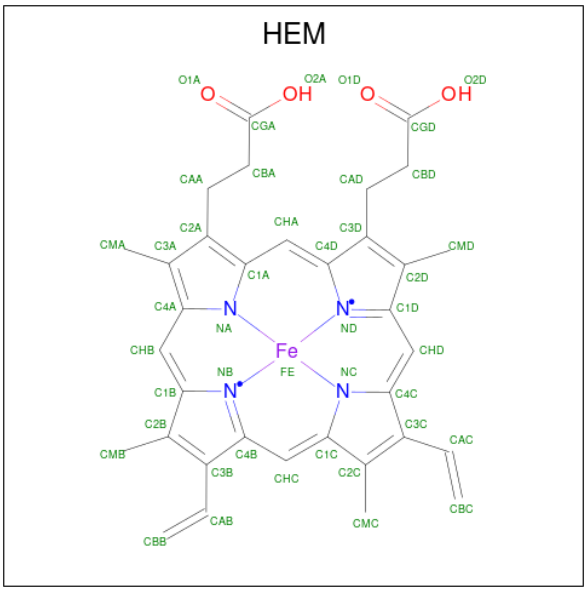
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Cl 1 1	0	0
32	a	1	Total Cl 1 1	0	0

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	D	1	Total C O 31 20 11	0	0
33	I	1	Total C O 35 24 11	0	0
33	M	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	d	1	Total C O 31 20 11	0	0
33	i	1	Total C O 35 24 11	0	0
33	m	1	Total C O 35 24 11	0	0

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



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

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

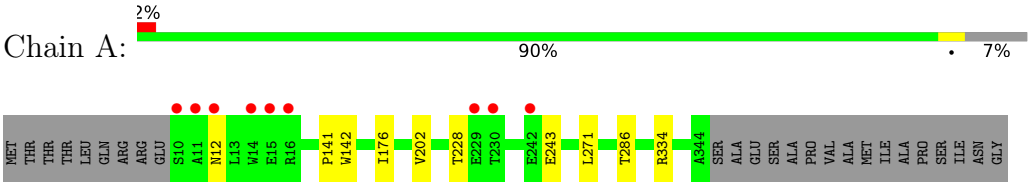
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

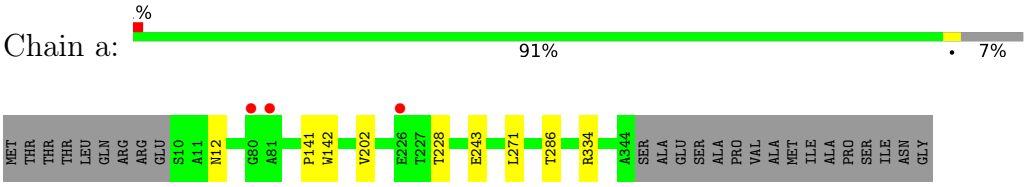
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



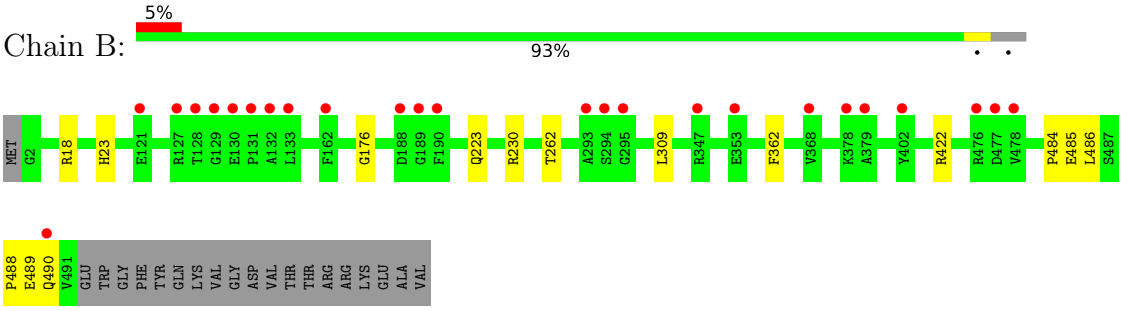
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



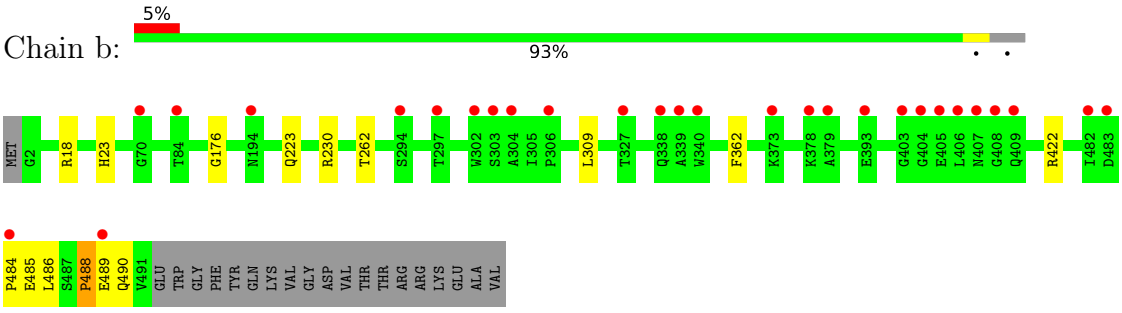
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



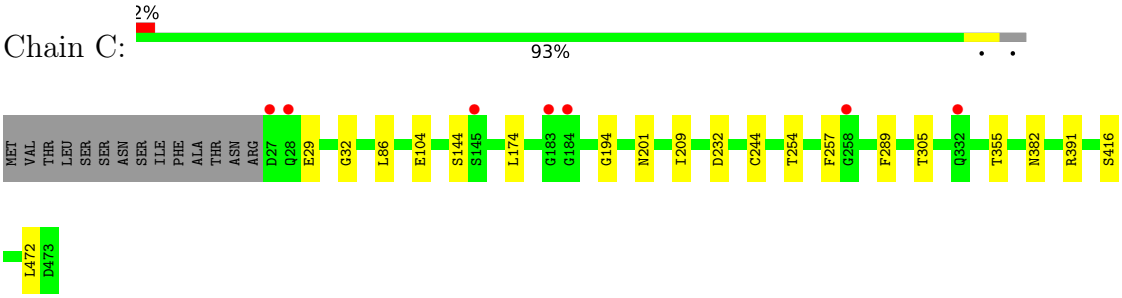
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



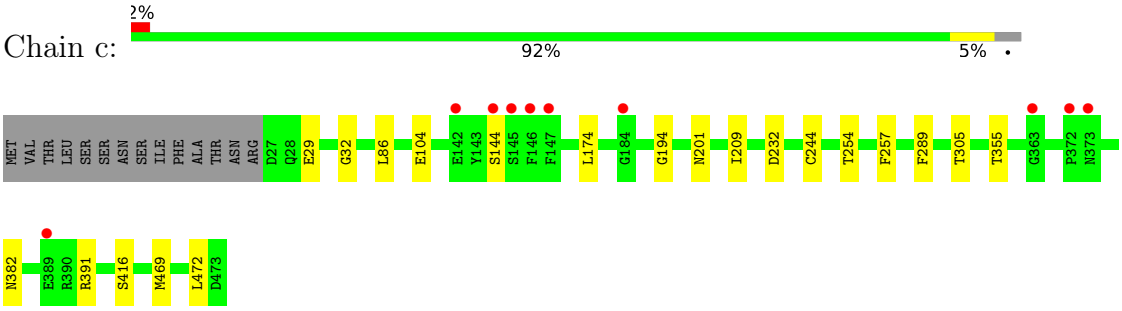
• Molecule 3: Photosystem II CP43 protein

Chain C:



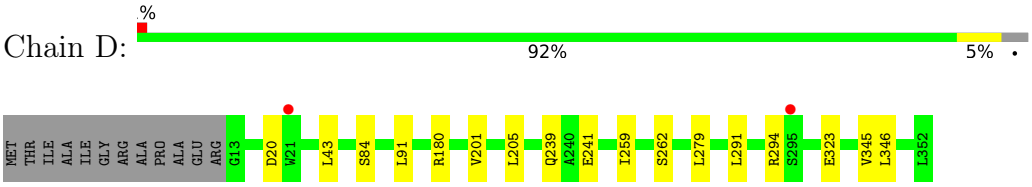
• Molecule 3: Photosystem II CP43 protein

Chain c:



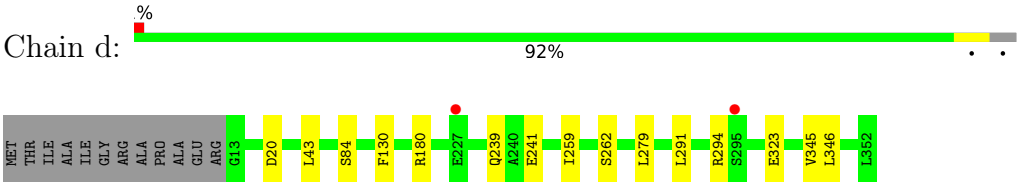
• Molecule 4: Photosystem II D2 protein

Chain D:



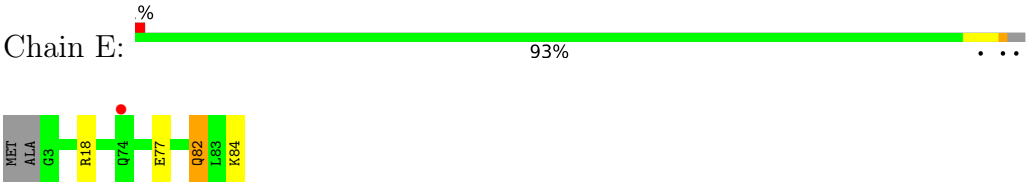
• Molecule 4: Photosystem II D2 protein

Chain d:



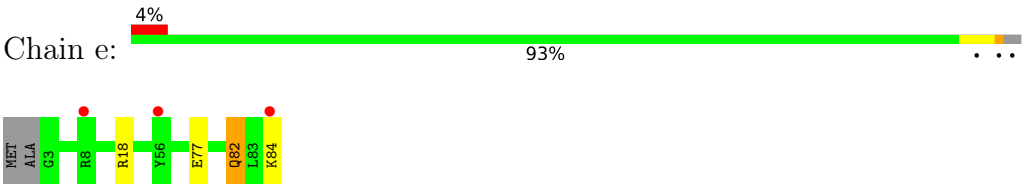
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



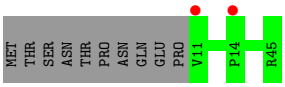
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



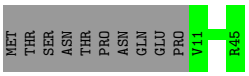
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



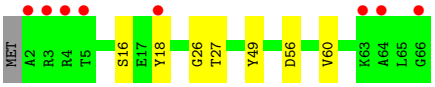
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



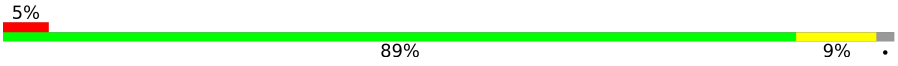
• Molecule 7: Photosystem II reaction center protein H

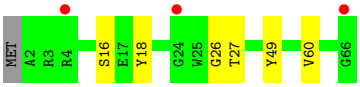
Chain H:



• Molecule 7: Photosystem II reaction center protein H

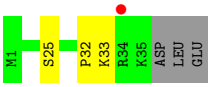
Chain h:





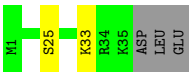
• Molecule 8: Photosystem II reaction center protein I

Chain I:



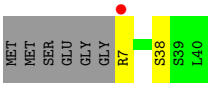
• Molecule 8: Photosystem II reaction center protein I

Chain i:



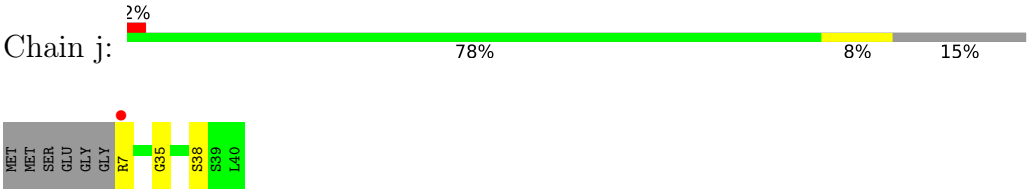
• Molecule 9: Photosystem II reaction center protein J

Chain J:



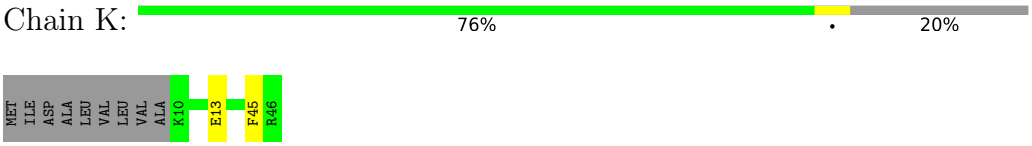
• Molecule 9: Photosystem II reaction center protein J

Chain j:



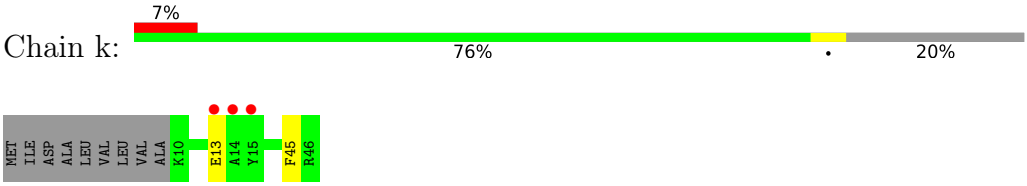
• Molecule 10: Photosystem II reaction center protein K

Chain K:



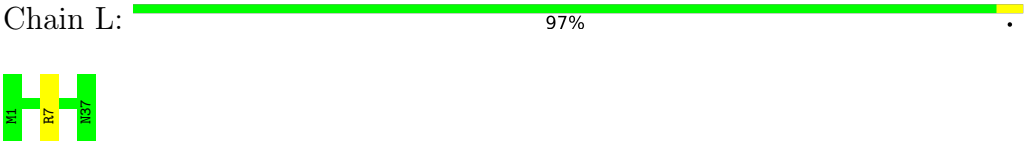
• Molecule 10: Photosystem II reaction center protein K

Chain k:



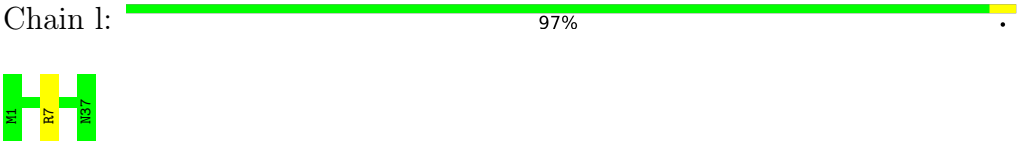
• Molecule 11: Photosystem II reaction center protein L

Chain L:



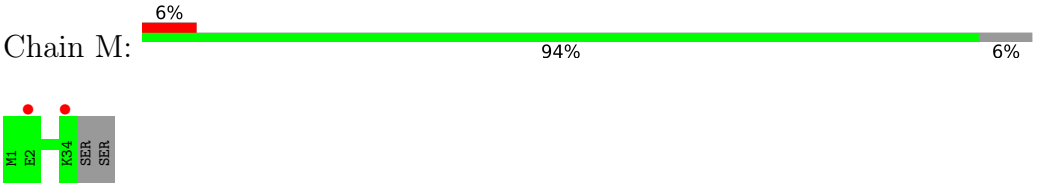
• Molecule 11: Photosystem II reaction center protein L

Chain l:



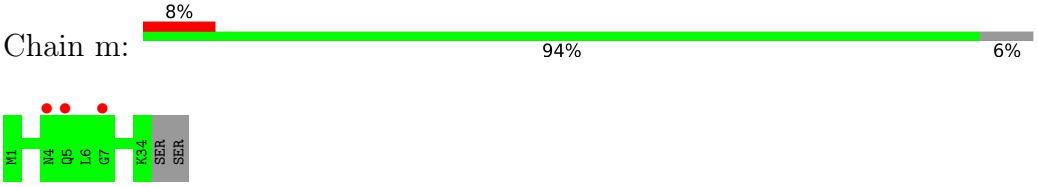
• Molecule 12: Photosystem II reaction center protein M

Chain M:



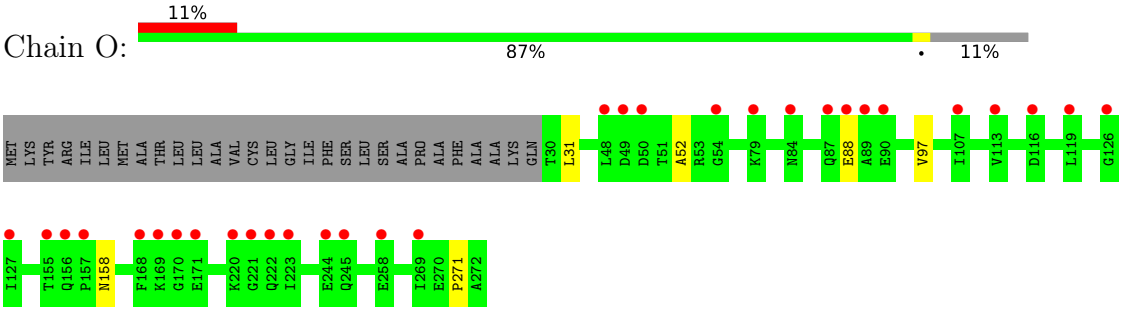
• Molecule 12: Photosystem II reaction center protein M

Chain m:



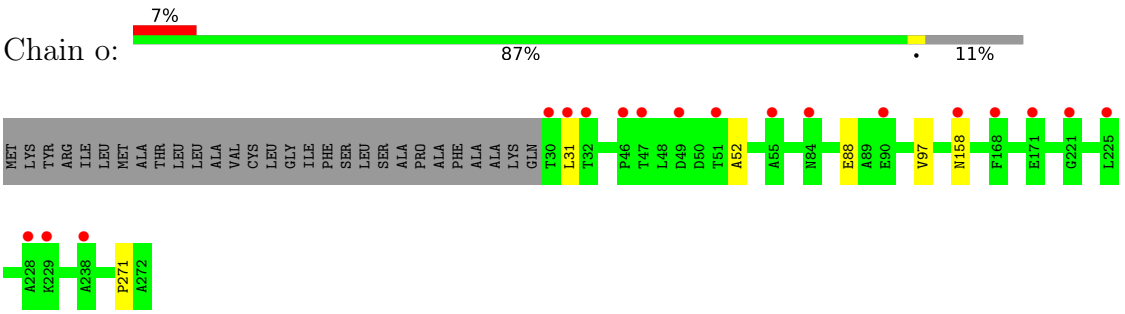
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



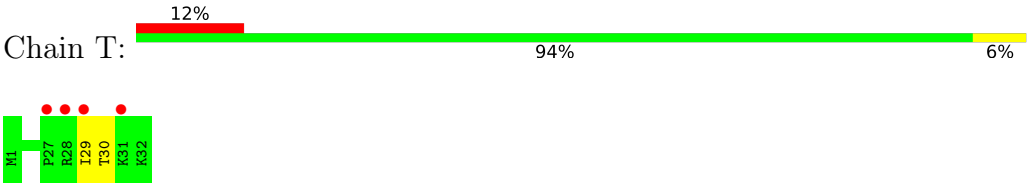
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



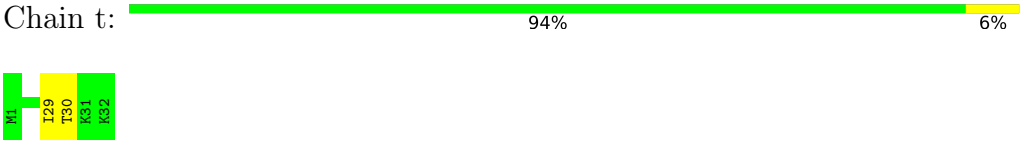
• Molecule 14: Photosystem II reaction center protein T

Chain T:



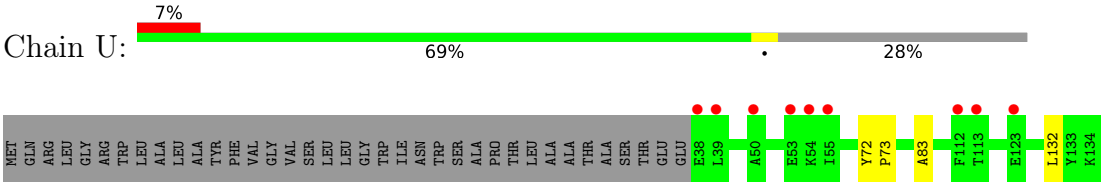
• Molecule 14: Photosystem II reaction center protein T

Chain t:



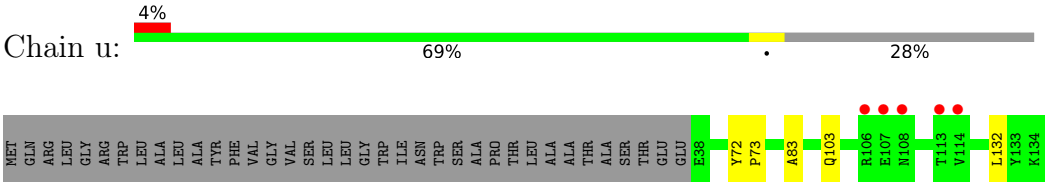
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



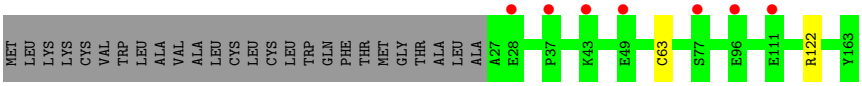
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



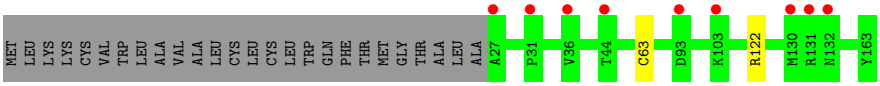
• Molecule 16: Cytochrome c-550

Chain V:



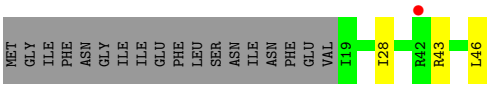
• Molecule 16: Cytochrome c-550

Chain v:



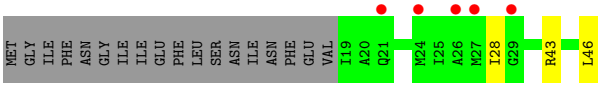
• Molecule 17: Photosystem II reaction center protein ycf12

Chain y:



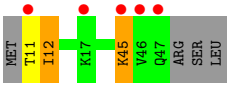
• Molecule 17: Photosystem II reaction center protein ycf12

Chain g:



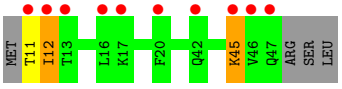
• Molecule 18: Photosystem II reaction center X protein

Chain X:



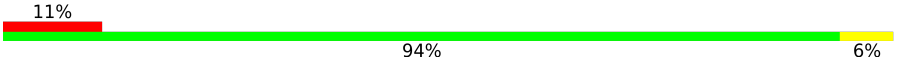
• Molecule 18: Photosystem II reaction center X protein

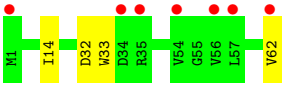
Chain x:



• Molecule 19: Photosystem II reaction center protein Z

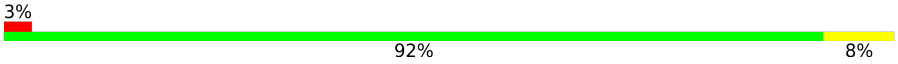
Chain Z:

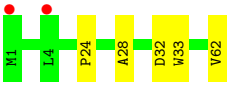




• Molecule 19: Photosystem II reaction center protein Z

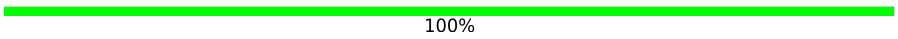
Chain z:





• Molecule 20: Photosystem II reaction center protein Y

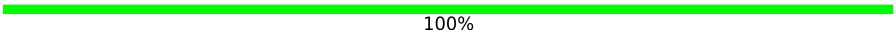
Chain G:



There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Y

Chain Y:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.5 (82.97-5.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.285 , 0.313 0.285 , 0.313	Depositor DCC
R_{free} test set	1200 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, BCT, DGD, FE2, CLA, PL9, OEC, CL, LMG, BCR, CA, LHG, HEM, PHO, SQD

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	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.28	0/3986	0.46	0/5433
3	C	0.28	0/3556	0.46	0/4842
3	c	0.27	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.29	0/685	0.48	0/933
5	e	0.28	0/685	0.48	0/933
6	F	0.28	0/291	0.45	0/397
6	f	0.26	0/291	0.45	0/397
7	H	0.26	0/520	0.49	0/709
7	h	0.27	0/520	0.50	0/709
8	I	0.28	0/293	0.48	0/395
8	i	0.32	0/293	0.49	0/395
9	J	0.29	0/255	0.46	0/346
9	j	0.28	0/255	0.44	0/346
10	K	0.29	0/303	0.52	0/416
10	k	0.28	0/303	0.53	0/416
11	L	0.25	0/311	0.43	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.65	0/367
12	m	0.41	0/270	0.65	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.36	0/284	0.49	0/381
14	t	0.35	0/284	0.47	0/381
15	U	0.27	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.30	0/1081	0.52	0/1468
16	v	0.26	0/1081	0.46	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	g	0.24	0/202	0.51	0/272
17	y	0.25	0/202	0.52	0/272
18	X	0.30	0/273	0.52	0/370
18	x	0.32	0/273	0.50	0/370
19	Z	0.30	0/490	0.50	0/669
19	z	0.28	0/490	0.48	0/669
All	All	0.29	0/41948	0.48	0/57100

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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	311 (93%)	17 (5%)	5 (2%)	10	45
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	13	50
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	15	54
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	15	54
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	12	48
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	12	48
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	25	65
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12 48
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12 48
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100 100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100 100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2 20
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2 20
8	I	33/38 (87%)	27 (82%)	4 (12%)	2 (6%)	1 16
8	i	33/38 (87%)	28 (85%)	4 (12%)	1 (3%)	4 28
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4 27
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	1 16
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1 18
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1 18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
13	O	241/272 (89%)	206 (86%)	31 (13%)	4 (2%)	9 42
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	9 42
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4 26
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4 26
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4 26
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4 26
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100 100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100 100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3 24
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3 24
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1 18
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1 18
19	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9 42
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	2 20
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	10 45

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA

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	271/291 (93%)	266 (98%)	5 (2%)	59 77
1	a	271/291 (93%)	266 (98%)	5 (2%)	59 77
2	B	390/407 (96%)	380 (97%)	10 (3%)	46 66
2	b	390/407 (96%)	379 (97%)	11 (3%)	43 65
3	C	347/362 (96%)	333 (96%)	14 (4%)	31 55
3	c	347/362 (96%)	332 (96%)	15 (4%)	29 54
4	D	275/283 (97%)	260 (94%)	15 (6%)	21 47
4	d	275/283 (97%)	262 (95%)	13 (5%)	26 51
5	E	72/73 (99%)	68 (94%)	4 (6%)	21 46
5	e	72/73 (99%)	68 (94%)	4 (6%)	21 46
6	F	29/39 (74%)	29 (100%)	0	100 100
6	f	29/39 (74%)	29 (100%)	0	100 100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13 38
7	h	53/55 (96%)	50 (94%)	3 (6%)	20 46
8	I	32/35 (91%)	31 (97%)	1 (3%)	40 62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40 62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30 54
9	j	24/28 (86%)	23 (96%)	1 (4%)	30 54
10	K	30/37 (81%)	30 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	k	30/37 (81%)	30 (100%)	0	100 100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42 64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42 64
12	M	31/33 (94%)	31 (100%)	0	100 100
12	m	31/33 (94%)	31 (100%)	0	100 100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76 86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76 86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37 60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37 60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71 84
15	u	84/112 (75%)	82 (98%)	2 (2%)	49 69
16	V	116/138 (84%)	114 (98%)	2 (2%)	60 78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60 78
17	g	20/37 (54%)	18 (90%)	2 (10%)	7 26
17	y	20/37 (54%)	18 (90%)	2 (10%)	7 26
18	X	30/34 (88%)	27 (90%)	3 (10%)	7 26
18	x	30/34 (88%)	27 (90%)	3 (10%)	7 26
19	Z	52/52 (100%)	49 (94%)	3 (6%)	20 45
19	z	52/52 (100%)	50 (96%)	2 (4%)	33 57
All	All	4244/4616 (92%)	4107 (97%)	137 (3%)	39 62

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	82	GLN
7	h	60	VAL
17	g	28	ILE
7	H	27	THR
5	E	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
17	y	45	ASN

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Mol	Chain	Res	Type
1	a	241	GLN
15	u	93	ASN
2	b	201	HIS
4	D	117	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	c	506	-	65,73,73	1.53	5 (7%)	76,113,113	1.45	8 (10%)
23	CLA	b	618	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	6 (7%)
33	LMT	B	628	-	36,36,36	0.45	0	47,47,47	0.77	1 (2%)
33	LMT	i	102	-	36,36,36	0.48	1 (2%)	47,47,47	0.67	0
28	DGD	b	623	-	59,59,67	1.20	7 (11%)	73,73,81	1.14	5 (6%)
29	LHG	A	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.08	2 (5%)
23	CLA	c	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	b	620	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	511	-	65,73,73	1.56	5 (7%)	76,113,113	1.37	8 (10%)
28	DGD	B	627	-	53,53,67	1.22	6 (11%)	67,67,81	1.43	9 (13%)
27	BCR	j	102	-	41,41,41	0.71	0	56,56,56	3.35	25 (44%)
28	DGD	c	516	-	54,54,67	1.24	6 (11%)	68,68,81	1.25	7 (10%)
33	LMT	d	410	-	32,32,36	0.49	1 (3%)	43,43,47	0.69	1 (2%)
23	CLA	b	617	-	65,73,73	1.48	6 (9%)	76,113,113	1.49	9 (11%)
24	PHO	D	402	-	51,69,69	1.04	5 (9%)	47,99,99	1.09	5 (10%)
31	LMG	A	414	-	51,51,55	1.15	6 (11%)	59,59,63	1.35	5 (8%)
34	HEM	f	101	6,5	41,50,50	1.97	6 (14%)	45,82,82	1.87	8 (17%)
23	CLA	c	510	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	6 (7%)
31	LMG	I	101	-	43,43,55	1.25	8 (18%)	51,51,63	1.31	7 (13%)
30	SQD	a	401	-	53,54,54	0.99	4 (7%)	62,65,65	1.66	10 (16%)
23	CLA	B	615	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
31	LMG	m	102	-	42,42,55	1.33	7 (16%)	50,50,63	1.57	7 (14%)
23	CLA	C	503	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	6 (7%)
27	BCR	T	102	-	41,41,41	0.70	0	56,56,56	2.24	16 (28%)
28	DGD	C	517	-	54,54,67	1.21	6 (11%)	68,68,81	1.25	6 (8%)
23	CLA	C	504	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	B	602	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	7 (9%)
28	DGD	c	517	-	63,63,67	1.21	10 (15%)	77,77,81	1.31	7 (9%)
28	DGD	A	411	-	57,57,67	1.23	7 (12%)	71,71,81	1.58	12 (16%)
31	LMG	a	416	-	51,51,55	1.11	6 (11%)	59,59,63	1.40	5 (8%)
29	LHG	a	417	-	36,36,48	1.09	2 (5%)	39,42,54	1.01	2 (5%)
23	CLA	C	511	3	65,73,73	1.50	6 (9%)	76,113,113	1.48	9 (11%)
25	PL9	a	410	-	45,45,55	1.25	7 (15%)	56,57,69	1.65	15 (26%)
27	BCR	C	515	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
23	CLA	B	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	7 (9%)
27	BCR	b	621	-	41,41,41	0.65	0	56,56,56	1.96	19 (33%)
23	CLA	C	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	9 (11%)
23	CLA	C	507	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.57	10 (16%)
28	DGD	C	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.28	7 (9%)
23	CLA	b	611	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	A	404	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	9 (11%)
23	CLA	C	513	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
27	BCR	y	101	-	41,41,41	0.73	0	56,56,56	1.94	14 (25%)
23	CLA	b	619	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)
34	HEM	F	101	6,5	41,50,50	1.94	5 (12%)	45,82,82	1.82	7 (15%)
33	LMT	B	624	-	36,36,36	0.42	0	47,47,47	0.69	0
23	CLA	b	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	a	406	-	65,73,73	1.52	6 (9%)	76,113,113	1.48	8 (10%)
23	CLA	c	512	-	65,73,73	1.51	6 (9%)	76,113,113	1.42	8 (10%)
31	LMG	E	101	-	44,44,55	1.19	7 (15%)	52,52,63	1.33	8 (15%)
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.67	0
23	CLA	B	616	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	6 (7%)
22	BCT	A	402	21	2,3,3	0.46	0	2,3,3	0.31	0
27	BCR	B	619	-	41,41,41	0.68	0	56,56,56	1.86	15 (26%)
33	LMT	M	102	-	36,36,36	0.44	0	47,47,47	0.67	0
31	LMG	c	519	-	45,45,55	1.21	7 (15%)	53,53,63	1.32	7 (13%)
23	CLA	c	507	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	9 (11%)
27	BCR	H	101	-	41,41,41	0.72	0	56,56,56	1.75	16 (28%)
25	PL9	j	101	-	35,35,55	1.19	5 (14%)	44,45,69	1.55	8 (18%)
33	LMT	b	627	-	36,36,36	0.43	0	47,47,47	0.65	0
31	LMG	a	402	-	42,42,55	1.23	6 (14%)	50,50,63	1.52	7 (14%)
23	CLA	b	609	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
23	CLA	B	601	-	65,73,73	1.54	5 (7%)	76,113,113	1.41	7 (9%)
28	DGD	b	602	-	53,53,67	1.23	6 (11%)	67,67,81	1.37	8 (11%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.30	7 (12%)
27	BCR	B	620	-	41,41,41	0.73	0	56,56,56	2.14	15 (26%)
23	CLA	c	502	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	8 (10%)
31	LMG	B	623	-	49,49,55	1.19	8 (16%)	57,57,63	1.38	9 (15%)
23	CLA	B	607	-	65,73,73	1.49	5 (7%)	76,113,113	1.51	10 (13%)
31	LMG	d	407	-	48,48,55	1.17	8 (16%)	56,56,63	1.47	7 (12%)
33	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
33	LMT	m	101	-	36,36,36	0.42	0	47,47,47	0.66	0
23	CLA	d	402	-	65,73,73	1.51	6 (9%)	76,113,113	1.48	8 (10%)
31	LMG	B	622	-	49,49,55	1.14	7 (14%)	57,57,63	1.30	6 (10%)
23	CLA	B	611	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	9 (11%)
34	HEM	V	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.61	4 (8%)
33	LMT	b	604	-	36,36,36	0.40	0	47,47,47	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMT	b	603	-	36,36,36	0.44	0	47,47,47	0.75	1 (2%)
23	CLA	D	403	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
31	LMG	D	406	-	46,46,55	1.17	6 (13%)	54,54,63	1.39	6 (11%)
24	PHO	a	407	-	51,69,69	1.03	5 (9%)	47,99,99	1.14	5 (10%)
27	BCR	a	412	-	41,41,41	0.74	0	56,56,56	1.90	12 (21%)
27	BCR	h	101	-	41,41,41	0.73	0	56,56,56	1.76	14 (25%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	53,56,65	1.67	10 (18%)
31	LMG	d	406	-	46,46,55	1.18	7 (15%)	54,54,63	1.33	6 (11%)
28	DGD	C	519	-	67,67,67	1.12	7 (10%)	81,81,81	1.43	10 (12%)
27	BCR	B	618	-	41,41,41	0.67	0	56,56,56	2.26	20 (35%)
31	LMG	C	520	-	48,48,55	1.13	6 (12%)	56,56,63	1.31	6 (10%)
23	CLA	B	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
27	BCR	C	514	-	41,41,41	0.73	0	56,56,56	2.34	21 (37%)
31	LMG	M	101	-	42,42,55	1.28	7 (16%)	50,50,63	1.51	6 (12%)
27	BCR	d	405	-	41,41,41	0.67	0	56,56,56	2.15	16 (28%)
31	LMG	A	418	-	42,42,55	1.22	6 (14%)	50,50,63	1.51	9 (18%)
27	BCR	b	622	-	41,41,41	0.72	0	56,56,56	2.20	17 (30%)
28	DGD	d	409	-	64,64,67	1.14	5 (7%)	78,78,81	1.42	12 (15%)
23	CLA	b	605	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	8 (10%)
28	DGD	a	413	-	57,57,67	1.19	7 (12%)	71,71,81	1.52	12 (16%)
23	CLA	B	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	7 (9%)
33	LMT	D	410	-	32,32,36	0.50	1 (3%)	43,43,47	0.69	1 (2%)
25	PL9	D	404	-	55,55,55	1.25	8 (14%)	68,69,69	1.63	18 (26%)
28	DGD	B	621	-	59,59,67	1.22	8 (13%)	73,73,81	1.10	5 (6%)
31	LMG	b	625	-	49,49,55	1.18	8 (16%)	57,57,63	1.42	10 (17%)
23	CLA	C	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
27	BCR	C	516	-	41,41,41	0.70	0	56,56,56	1.95	16 (28%)
23	CLA	b	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.31	8 (10%)
23	CLA	b	615	-	65,73,73	1.53	5 (7%)	76,113,113	1.39	7 (9%)
31	LMG	e	101	-	44,44,55	1.21	8 (18%)	52,52,63	1.35	9 (17%)
23	CLA	c	504	-	65,73,73	1.49	5 (7%)	76,113,113	1.44	7 (9%)
24	PHO	a	408	-	51,69,69	1.00	3 (5%)	47,99,99	1.13	3 (6%)
23	CLA	B	606	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	7 (9%)
23	CLA	B	612	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	6 (7%)
27	BCR	J	102	-	41,41,41	0.73	0	56,56,56	3.36	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	606	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	7 (9%)
23	CLA	b	612	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	C	502	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	6 (7%)
23	CLA	a	404	-	65,73,73	1.54	6 (9%)	76,113,113	1.45	9 (11%)
23	CLA	d	403	-	65,73,73	1.54	6 (9%)	76,113,113	1.36	8 (10%)
28	DGD	D	409	-	64,64,67	1.14	6 (9%)	78,78,81	1.41	9 (11%)
23	CLA	b	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
31	LMG	i	101	-	43,43,55	1.26	8 (18%)	51,51,63	1.31	6 (11%)
31	LMG	k	103	-	48,48,55	1.13	6 (12%)	56,56,63	1.27	7 (12%)
24	PHO	A	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.17	3 (6%)
25	PL9	A	408	-	45,45,55	1.28	7 (15%)	56,57,69	1.58	15 (26%)
23	CLA	C	509	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
23	CLA	D	401	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	A	403	-	65,73,73	1.53	6 (9%)	76,113,113	1.34	8 (10%)
30	SQD	f	102	-	44,45,54	1.02	4 (9%)	53,56,65	1.68	11 (20%)
23	CLA	a	405	-	65,73,73	1.52	5 (7%)	76,113,113	1.46	11 (14%)
23	CLA	B	605	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	C	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.40	8 (10%)
30	SQD	b	601	-	46,47,54	1.02	5 (10%)	55,58,65	1.62	9 (16%)
27	BCR	z	101	-	41,41,41	0.65	0	56,56,56	1.84	15 (26%)
27	BCR	k	102	-	41,41,41	0.74	0	56,56,56	1.96	16 (28%)
30	SQD	A	413	-	50,51,54	0.98	3 (6%)	59,62,65	1.54	10 (16%)
34	HEM	v	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.76	6 (13%)
23	CLA	c	513	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	B	608	-	65,73,73	1.52	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	c	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.46	9 (11%)
22	BCT	d	401	21	2,3,3	0.45	0	2,3,3	0.29	0
23	CLA	b	607	-	65,73,73	1.47	5 (7%)	76,113,113	1.38	9 (11%)
28	DGD	c	518	-	67,67,67	1.11	6 (8%)	81,81,81	1.47	13 (16%)
25	PL9	d	404	-	55,55,55	1.24	8 (14%)	68,69,69	1.72	19 (27%)
23	CLA	A	407	-	65,73,73	1.47	5 (7%)	76,113,113	1.36	6 (7%)
30	SQD	A	417	-	53,54,54	1.01	4 (7%)	62,65,65	1.63	12 (19%)
23	CLA	c	503	-	65,73,73	1.50	5 (7%)	76,113,113	1.31	7 (9%)
23	CLA	c	508	-	65,73,73	1.50	6 (9%)	76,113,113	1.43	9 (11%)
25	PL9	J	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.56	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SQD	D	408	-	42,43,54	1.11	5 (11%)	51,54,65	1.99	10 (19%)
27	BCR	T	101	-	41,41,41	0.70	0	56,56,56	1.78	13 (23%)
23	CLA	B	614	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	6 (7%)
23	CLA	C	506	-	65,73,73	1.52	5 (7%)	76,113,113	1.42	7 (9%)
27	BCR	B	617	-	41,41,41	0.71	0	56,56,56	1.85	13 (23%)
27	BCR	c	515	-	41,41,41	0.70	0	56,56,56	1.99	17 (30%)
23	CLA	b	616	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	6 (7%)
30	SQD	B	626	-	46,47,54	1.03	5 (10%)	55,58,65	1.57	10 (18%)
30	SQD	d	408	-	42,43,54	1.12	4 (9%)	51,54,65	1.98	10 (19%)
23	CLA	B	604	-	65,73,73	1.52	6 (9%)	76,113,113	1.36	8 (10%)
27	BCR	D	405	-	41,41,41	0.67	0	56,56,56	2.19	17 (30%)
33	LMT	B	629	-	36,36,36	0.46	0	47,47,47	0.65	0
23	CLA	C	510	-	65,73,73	1.52	6 (9%)	76,113,113	1.36	9 (11%)
23	CLA	C	512	-	65,73,73	1.50	5 (7%)	76,113,113	1.43	7 (9%)
23	CLA	A	405	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	9 (11%)
23	CLA	B	610	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	9 (11%)
27	BCR	c	514	-	41,41,41	0.71	0	56,56,56	2.37	20 (35%)
29	LHG	A	412	-	38,38,48	1.05	2 (5%)	41,44,54	0.98	2 (4%)
23	CLA	b	608	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	a	409	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	8 (10%)
23	CLA	c	509	-	65,73,73	1.55	5 (7%)	76,113,113	1.39	8 (10%)
31	LMG	D	407	-	48,48,55	1.18	8 (16%)	56,56,63	1.41	7 (12%)
27	BCR	A	410	-	41,41,41	0.74	0	56,56,56	1.89	11 (19%)
29	LHG	a	414	-	38,38,48	1.07	2 (5%)	41,44,54	1.00	2 (4%)
31	LMG	C	521	-	45,45,55	1.19	6 (13%)	53,53,63	1.36	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	-	1/1/15/20	17/37/115/115	-
23	CLA	b	618	-	1/1/15/20	16/37/115/115	-
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	b	623	-	-	19/47/87/95	0/2/2/2
29	LHG	A	415	-	-	13/41/41/53	-
23	CLA	c	501	-	1/1/15/20	13/37/115/115	-
23	CLA	b	620	-	1/1/15/20	18/37/115/115	-
23	CLA	c	511	-	1/1/15/20	16/37/115/115	-
28	DGD	B	627	-	-	16/41/81/95	0/2/2/2
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2
28	DGD	c	516	-	-	20/42/82/95	0/2/2/2
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
23	CLA	b	617	-	1/1/15/20	16/37/115/115	-
24	PHO	D	402	-	-	9/37/103/103	0/5/6/6
31	LMG	A	414	-	-	21/46/66/70	0/1/1/1
34	HEM	f	101	6,5	-	3/12/54/54	-
23	CLA	c	510	-	1/1/15/20	16/37/115/115	-
31	LMG	I	101	-	-	19/38/58/70	0/1/1/1
30	SQD	a	401	-	-	18/49/69/69	0/1/1/1
23	CLA	B	615	-	1/1/15/20	10/37/115/115	-
31	LMG	m	102	-	-	15/37/57/70	0/1/1/1
23	CLA	C	503	-	1/1/15/20	15/37/115/115	-
27	BCR	T	102	-	-	7/29/63/63	0/2/2/2
28	DGD	C	517	-	-	19/42/82/95	0/2/2/2
23	CLA	C	504	-	1/1/15/20	10/37/115/115	-
23	CLA	B	602	-	1/1/15/20	19/37/115/115	-
28	DGD	c	517	-	-	23/51/91/95	0/2/2/2
28	DGD	A	411	-	-	10/45/85/95	0/2/2/2
31	LMG	a	416	-	-	19/46/66/70	0/1/1/1
29	LHG	a	417	-	-	13/41/41/53	-
23	CLA	C	511	3	1/1/15/20	15/37/115/115	-
25	PL9	a	410	-	-	22/41/61/73	0/1/1/1
27	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	B	613	-	1/1/15/20	15/37/115/115	-
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/15/20	13/37/115/115	-
23	CLA	C	507	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	415	-	-	20/46/66/69	0/1/1/1
28	DGD	C	518	-	-	21/51/91/95	0/2/2/2
23	CLA	b	611	-	1/1/15/20	9/37/115/115	-
23	CLA	A	404	-	1/1/15/20	17/37/115/115	-
23	CLA	C	513	-	1/1/15/20	18/37/115/115	-
33	LMT	B	625	-	-	2/21/61/61	0/2/2/2
27	BCR	y	101	-	-	8/29/63/63	0/2/2/2
23	CLA	b	619	-	1/1/15/20	8/37/115/115	-
34	HEM	F	101	6,5	-	3/12/54/54	-
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
23	CLA	b	610	-	1/1/15/20	12/37/115/115	-
23	CLA	a	406	-	1/1/15/20	11/37/115/115	-
23	CLA	c	512	-	1/1/15/20	19/37/115/115	-
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
23	CLA	B	616	-	1/1/15/20	18/37/115/115	-
27	BCR	B	619	-	-	1/29/63/63	0/2/2/2
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMG	c	519	-	-	21/40/60/70	0/1/1/1
23	CLA	c	507	-	1/1/15/20	13/37/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
33	LMT	b	627	-	-	2/21/61/61	0/2/2/2
31	LMG	a	402	-	-	18/37/57/70	0/1/1/1
23	CLA	b	609	-	1/1/15/20	15/37/115/115	-
23	CLA	B	601	-	1/1/15/20	16/37/115/115	-
28	DGD	b	602	-	-	19/41/81/95	0/2/2/2
31	LMG	b	624	-	-	23/44/64/70	0/1/1/1
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
23	CLA	c	502	-	1/1/15/20	10/37/115/115	-
31	LMG	B	623	-	-	15/44/64/70	0/1/1/1
23	CLA	B	607	-	1/1/15/20	9/37/115/115	-
31	LMG	d	407	-	-	19/43/63/70	0/1/1/1
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	402	-	1/1/15/20	12/37/115/115	-
31	LMG	B	622	-	-	23/44/64/70	0/1/1/1
23	CLA	B	611	-	1/1/15/20	9/37/115/115	-
34	HEM	V	201	16	-	3/12/54/54	-
33	LMT	b	604	-	-	3/21/61/61	0/2/2/2
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
23	CLA	D	403	-	1/1/15/20	7/37/115/115	-
31	LMG	D	406	-	-	12/41/61/70	0/1/1/1
24	PHO	a	407	-	-	13/37/103/103	0/5/6/6
27	BCR	a	412	-	-	2/29/63/63	0/2/2/2
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
30	SQD	F	102	-	-	16/40/60/69	0/1/1/1
31	LMG	d	406	-	-	11/41/61/70	0/1/1/1
28	DGD	C	519	-	-	23/55/95/95	0/2/2/2
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
31	LMG	C	520	-	-	18/43/63/70	0/1/1/1
23	CLA	B	603	-	1/1/15/20	14/37/115/115	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2
31	LMG	A	418	-	-	16/37/57/70	0/1/1/1
27	BCR	b	622	-	-	3/29/63/63	0/2/2/2
28	DGD	d	409	-	-	31/52/92/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	14/37/115/115	-
28	DGD	a	413	-	-	12/45/85/95	0/2/2/2
23	CLA	B	609	-	1/1/15/20	11/37/115/115	-
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
25	PL9	D	404	-	-	13/53/73/73	0/1/1/1
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
31	LMG	b	625	-	-	16/44/64/70	0/1/1/1
23	CLA	C	505	-	1/1/15/20	18/37/115/115	-
27	BCR	C	516	-	-	8/29/63/63	0/2/2/2
23	CLA	b	613	-	1/1/15/20	11/37/115/115	-
23	CLA	b	615	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	c	504	-	1/1/15/20	10/37/115/115	-
24	PHO	a	408	-	-	14/37/103/103	0/5/6/6
23	CLA	B	606	-	1/1/15/20	10/37/115/115	-
23	CLA	B	612	-	1/1/15/20	10/37/115/115	-
27	BCR	J	102	-	-	6/29/63/63	0/2/2/2
23	CLA	b	606	-	1/1/15/20	19/37/115/115	-
23	CLA	b	612	-	1/1/15/20	15/37/115/115	-
23	CLA	C	502	-	1/1/15/20	11/37/115/115	-
23	CLA	a	404	-	1/1/15/20	8/37/115/115	-
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
28	DGD	D	409	-	-	30/52/92/95	0/2/2/2
23	CLA	b	614	-	1/1/15/20	18/37/115/115	-
31	LMG	i	101	-	-	19/38/58/70	0/1/1/1
31	LMG	k	103	-	-	18/43/63/70	0/1/1/1
24	PHO	A	406	-	-	13/37/103/103	0/5/6/6
25	PL9	A	408	-	-	23/41/61/73	0/1/1/1
23	CLA	C	509	-	1/1/15/20	16/37/115/115	-
23	CLA	D	401	-	1/1/15/20	12/37/115/115	-
23	CLA	A	403	-	1/1/15/20	8/37/115/115	-
30	SQD	f	102	-	-	15/40/60/69	0/1/1/1
23	CLA	a	405	-	1/1/15/20	17/37/115/115	-
23	CLA	B	605	-	1/1/15/20	15/37/115/115	-
23	CLA	C	508	-	1/1/15/20	15/37/115/115	-
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
27	BCR	z	101	-	-	4/29/63/63	0/2/2/2
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
34	HEM	v	201	16	-	3/12/54/54	-
23	CLA	c	513	-	1/1/15/20	18/37/115/115	-
23	CLA	B	608	-	1/1/15/20	15/37/115/115	-
23	CLA	c	505	-	1/1/15/20	18/37/115/115	-
23	CLA	b	607	-	1/1/15/20	15/37/115/115	-
28	DGD	c	518	-	-	21/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
23	CLA	A	407	-	1/1/15/20	7/37/115/115	-
30	SQD	A	417	-	-	16/49/69/69	0/1/1/1
23	CLA	c	503	-	1/1/15/20	15/37/115/115	-
23	CLA	c	508	-	1/1/15/20	14/37/115/115	-
25	PL9	J	101	-	-	11/29/49/73	0/1/1/1
30	SQD	D	408	-	-	12/38/58/69	0/1/1/1
27	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	614	-	1/1/15/20	16/37/115/115	-
23	CLA	C	506	-	1/1/15/20	17/37/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	BCR	c	515	-	-	8/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	14/37/115/115	-
30	SQD	B	626	-	-	14/42/62/69	0/1/1/1
30	SQD	d	408	-	-	12/38/58/69	0/1/1/1
23	CLA	B	604	-	1/1/15/20	9/37/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
33	LMT	B	629	-	-	3/21/61/61	0/2/2/2
23	CLA	C	510	-	1/1/15/20	16/37/115/115	-
23	CLA	C	512	-	1/1/15/20	19/37/115/115	-
23	CLA	A	405	-	1/1/15/20	12/37/115/115	-
23	CLA	B	610	-	1/1/15/20	17/37/115/115	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
29	LHG	A	412	-	-	17/43/43/53	-
23	CLA	b	608	-	1/1/15/20	7/37/115/115	-
23	CLA	a	409	-	1/1/15/20	7/37/115/115	-
23	CLA	c	509	-	1/1/15/20	16/37/115/115	-
31	LMG	D	407	-	-	20/43/63/70	0/1/1/1
27	BCR	A	410	-	-	2/29/63/63	0/2/2/2
29	LHG	a	414	-	-	18/43/43/53	-
31	LMG	C	521	-	-	20/40/60/70	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.38	1.54	1.36
34	V	201	HEM	C3D-C2D	8.16	1.54	1.36
34	f	101	HEM	C3D-C2D	8.10	1.54	1.36
23	A	403	CLA	C4B-NB	8.10	1.42	1.35
34	F	101	HEM	C3D-C2D	8.07	1.53	1.36

The worst 5 of 1459 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	j	102	BCR	C32-C1-C6	-13.66	88.14	110.30
27	J	102	BCR	C32-C1-C6	-13.37	88.62	110.30
27	T	102	BCR	C7-C8-C9	-8.78	112.96	126.23
27	B	618	BCR	C7-C8-C9	-8.64	113.18	126.23
27	J	102	BCR	C32-C1-C31	-8.46	82.55	108.53

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND

5 of 2130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C1A-C2A-CAA-CBA

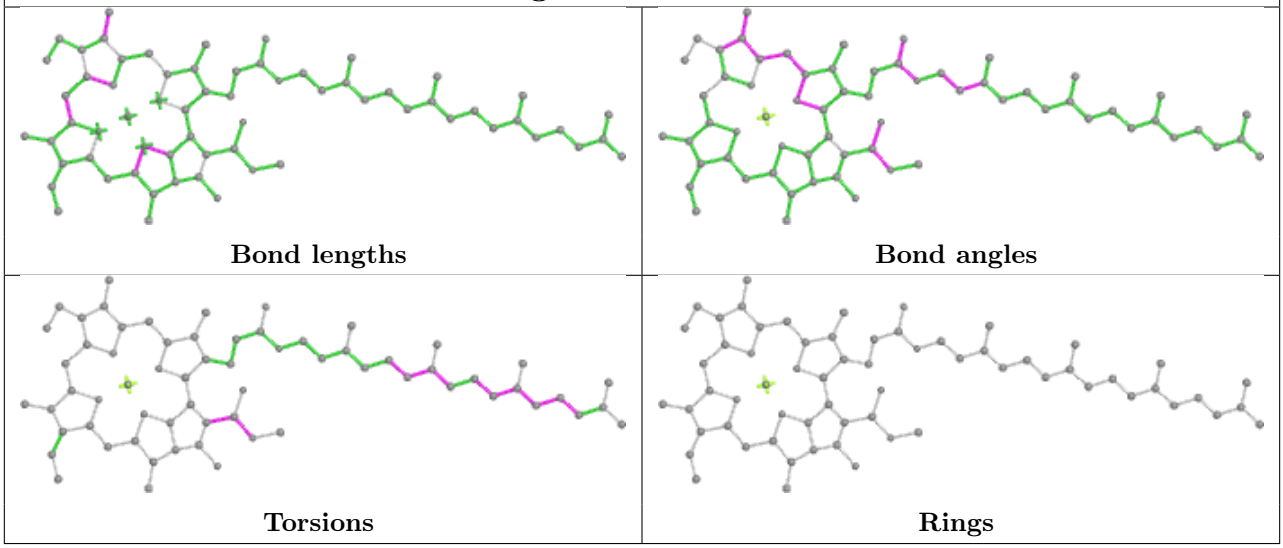
There are no ring outliers.

No monomer is involved in short contacts.

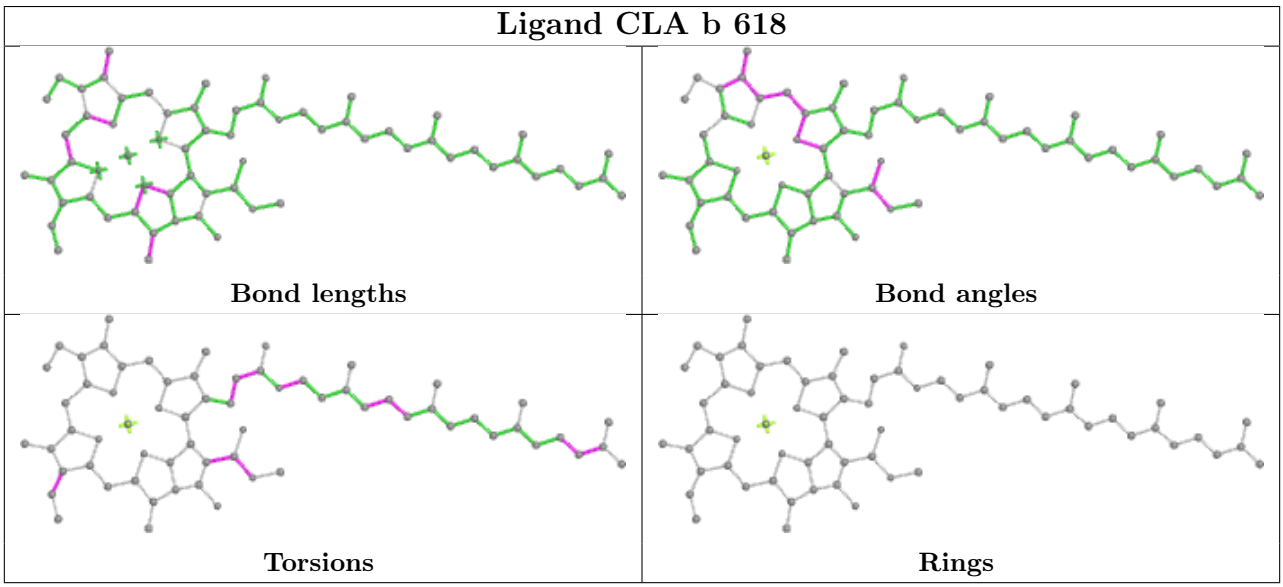
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

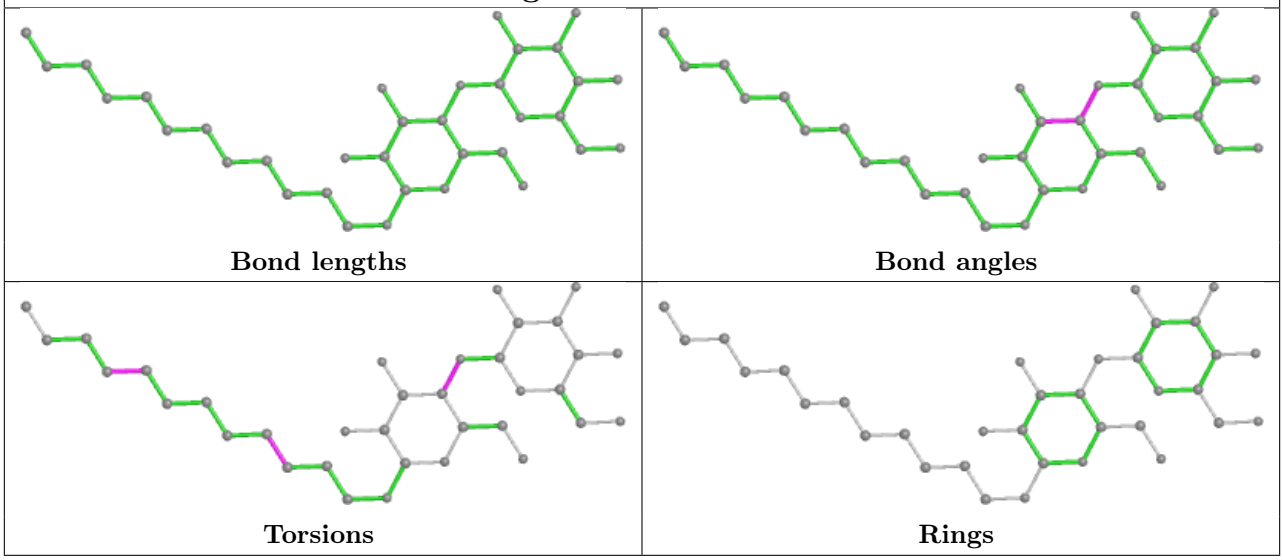
Ligand CLA c 506



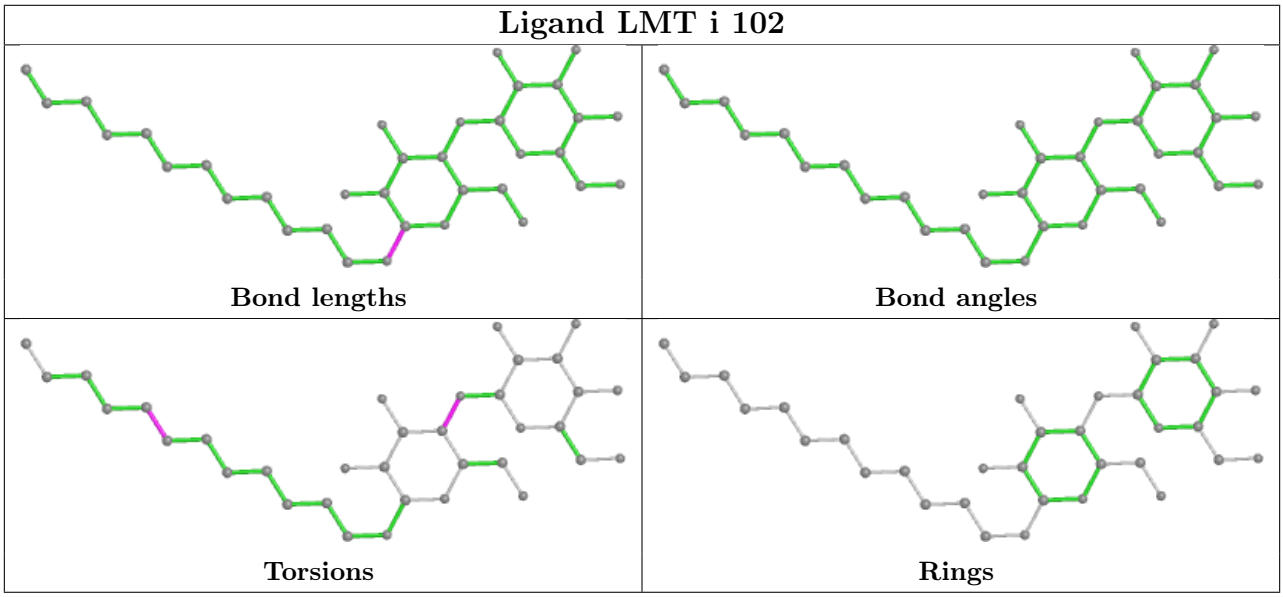
Ligand CLA b 618



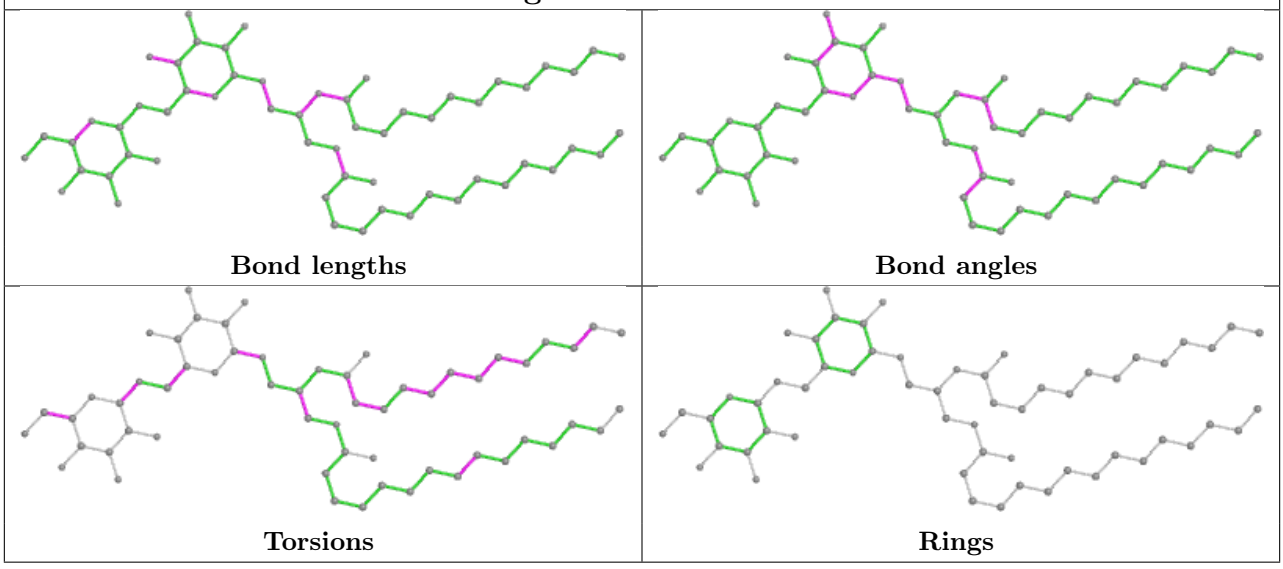
Ligand LMT B 628



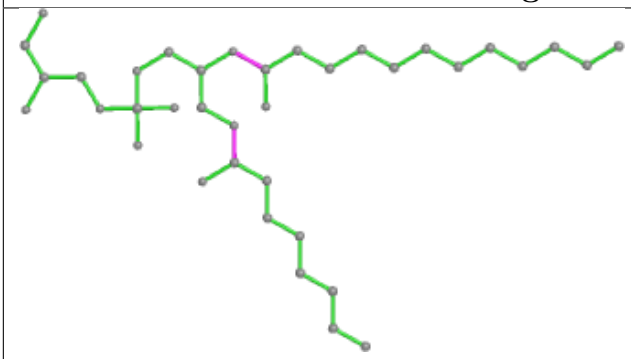
Ligand LMT i 102



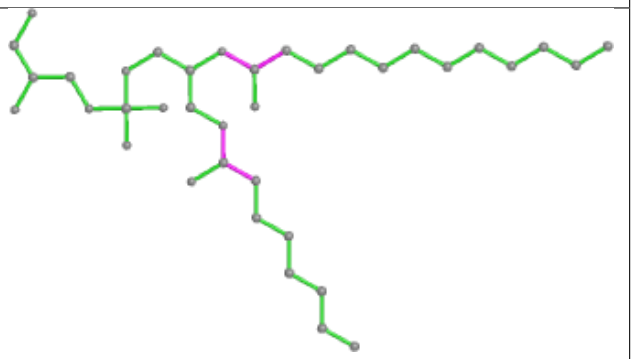
Ligand DGD b 623



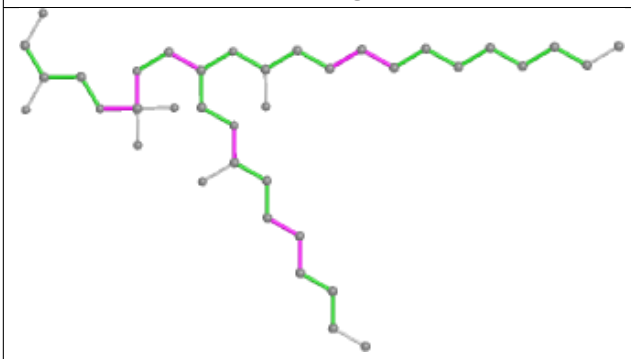
Ligand LHG A 415



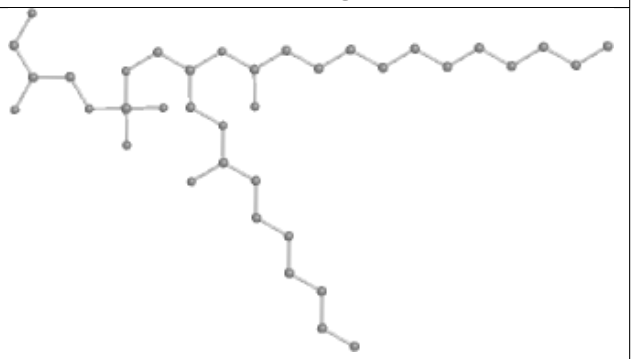
Bond lengths



Bond angles

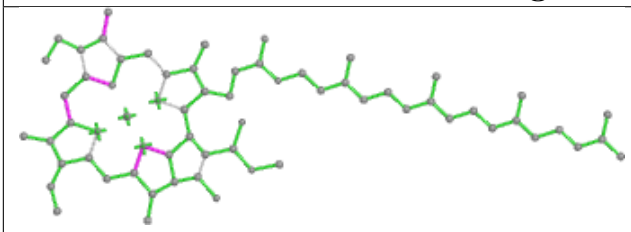


Torsions

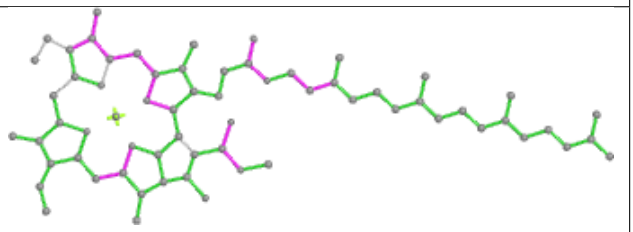


Rings

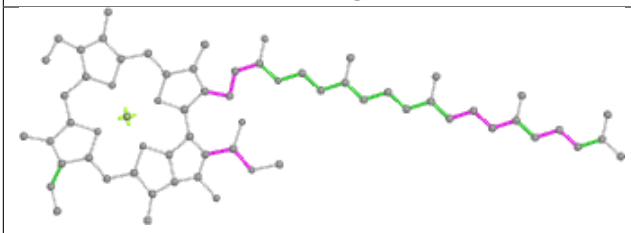
Ligand CLA c 501



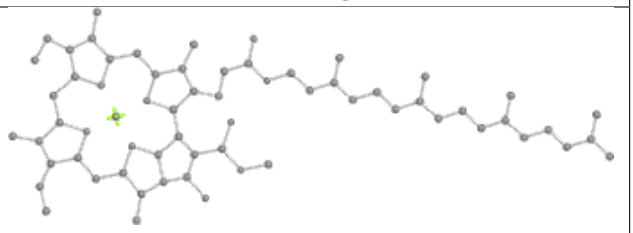
Bond lengths



Bond angles

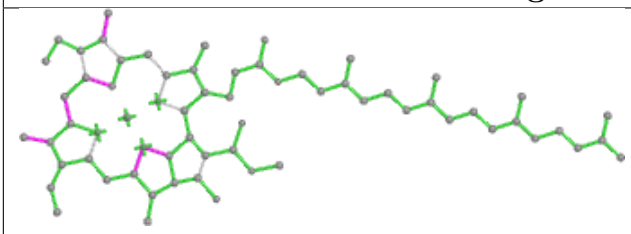


Torsions

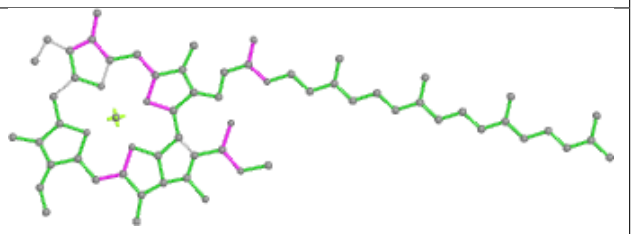


Rings

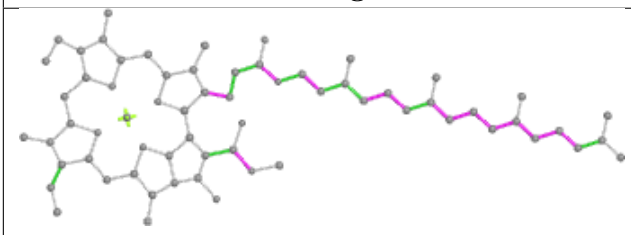
Ligand CLA b 620



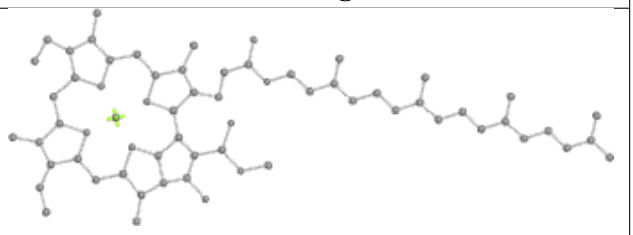
Bond lengths



Bond angles

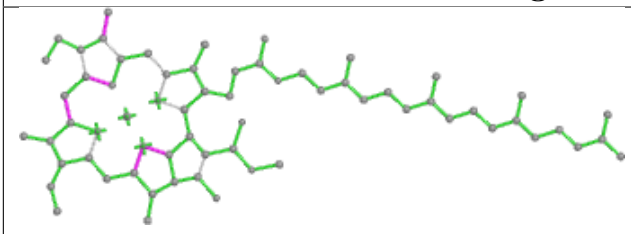


Torsions

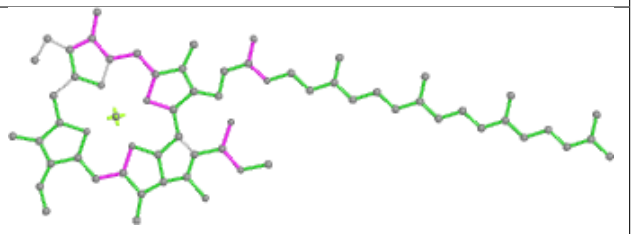


Rings

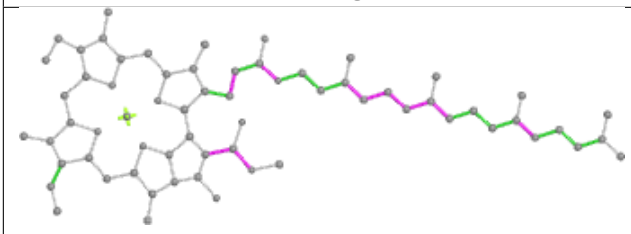
Ligand CLA c 511



Bond lengths



Bond angles



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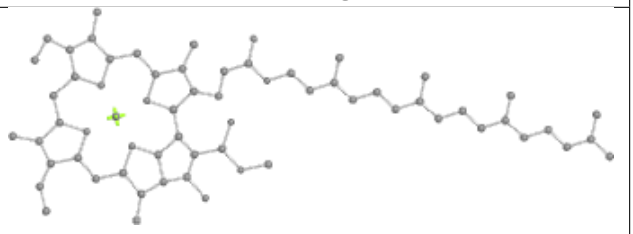
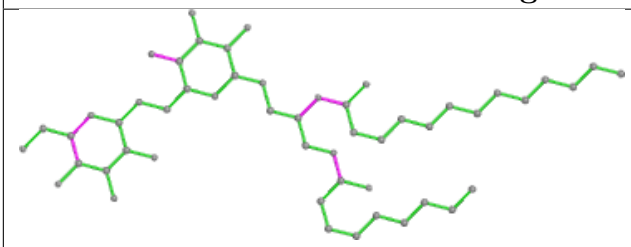


Rings

Ligand DGD B 627



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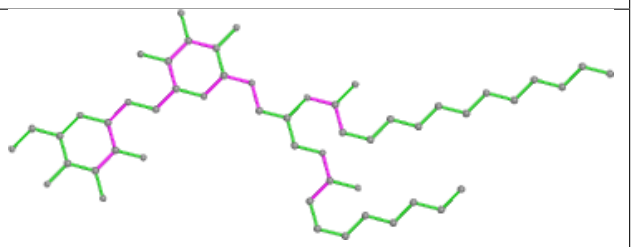
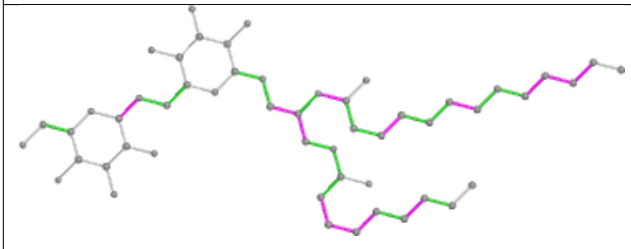


Bond angles



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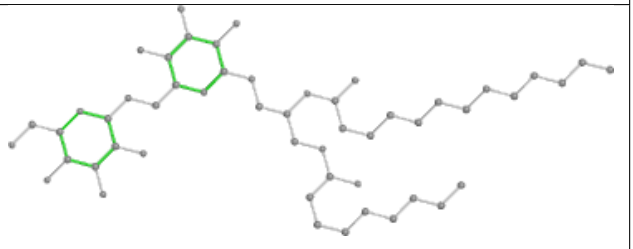
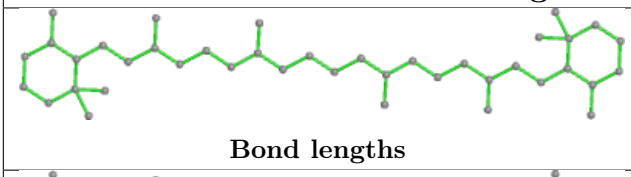


Rings

Ligand BCR j 102



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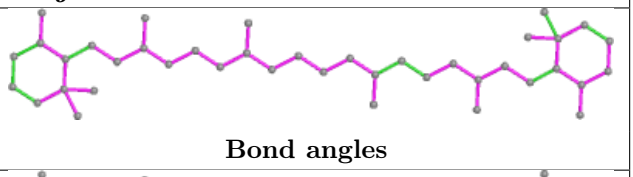
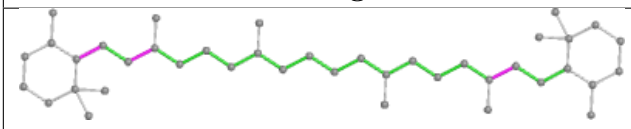
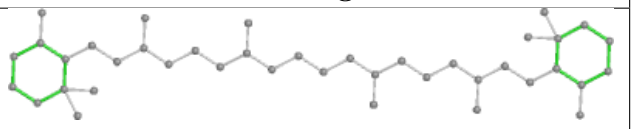


Bond angles

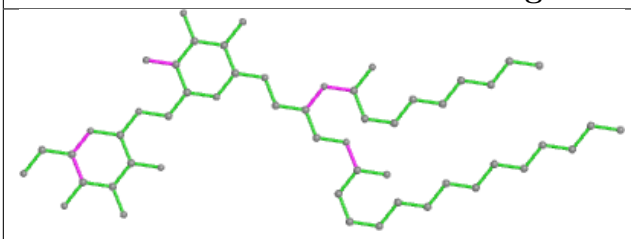


Torsions



Rings

Ligand DGD c 516



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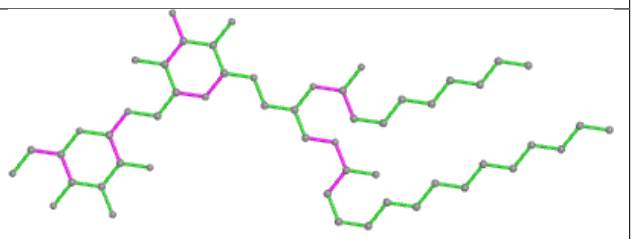
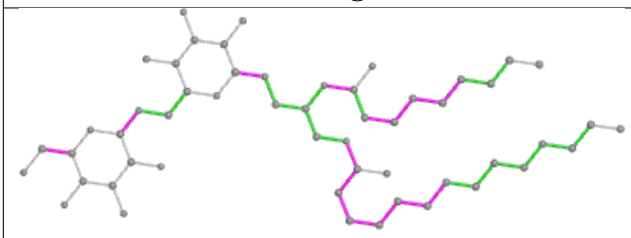


Bond angles



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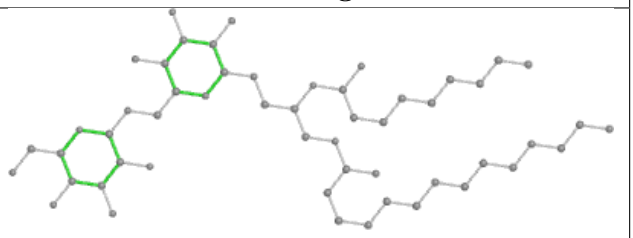
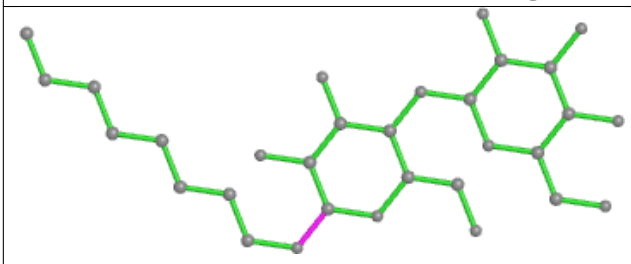
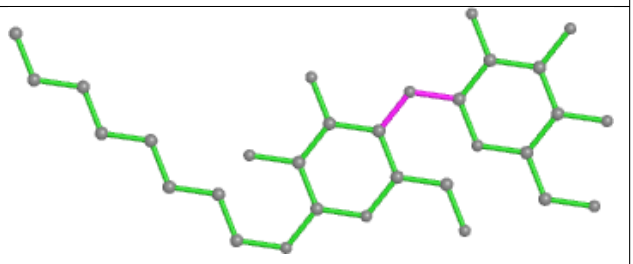


Rings

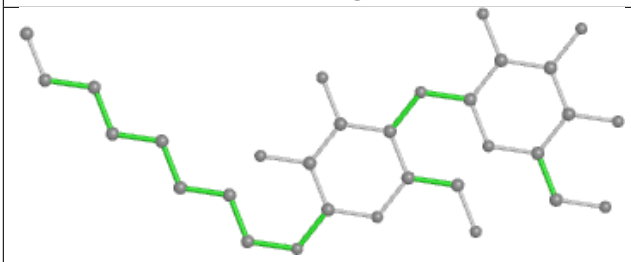
Ligand LMT d 410



Bond lengths



Bond angles



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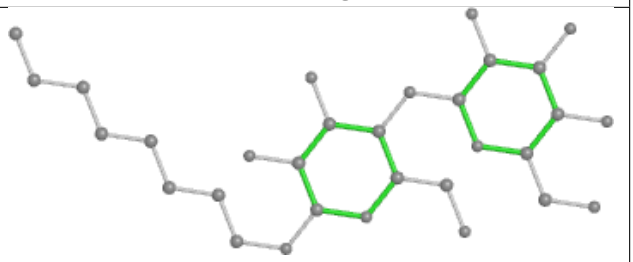
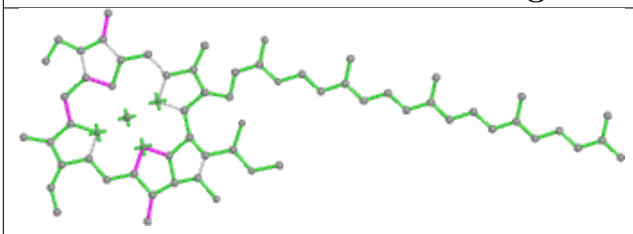


Rings

Ligand CLA b 617



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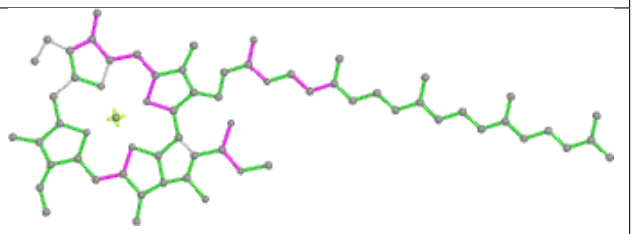
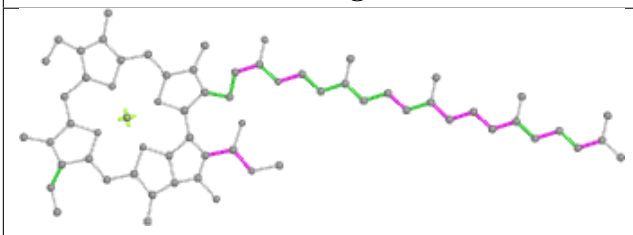


Bond angles



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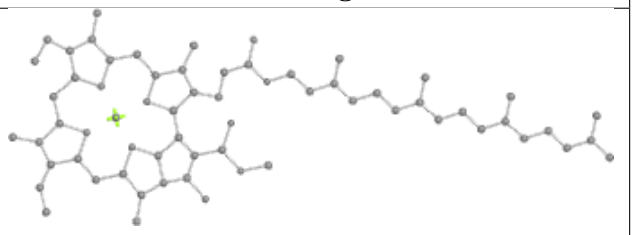
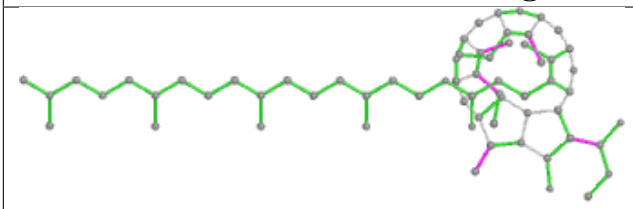


Rings

Ligand PHO D 402



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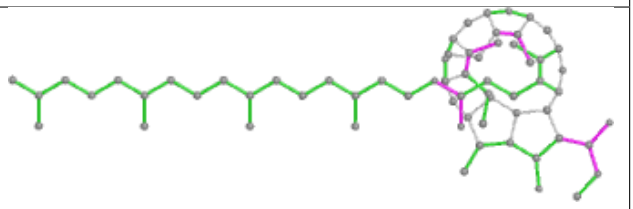
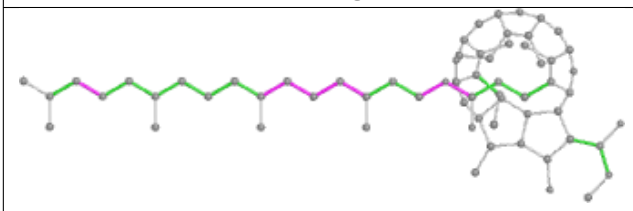
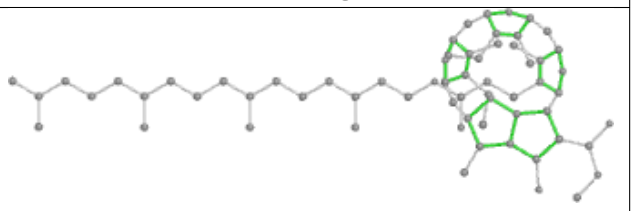


Bond angles

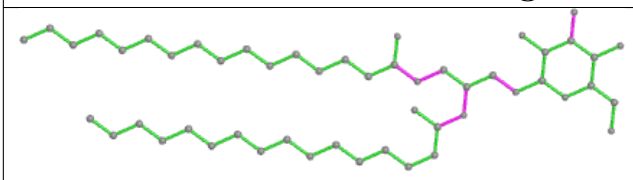


Torsions



Rings

Ligand LMG A 414



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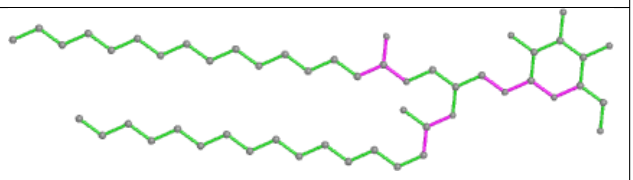
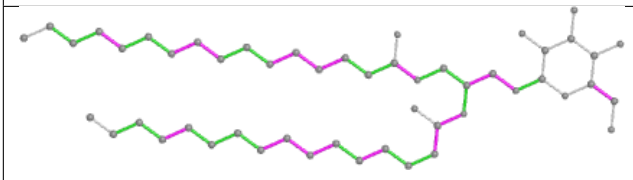
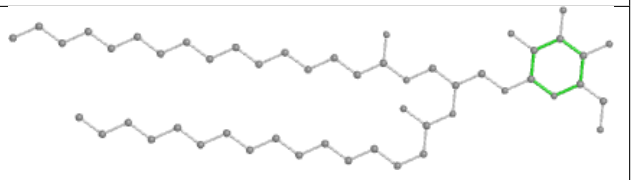


Bond angles

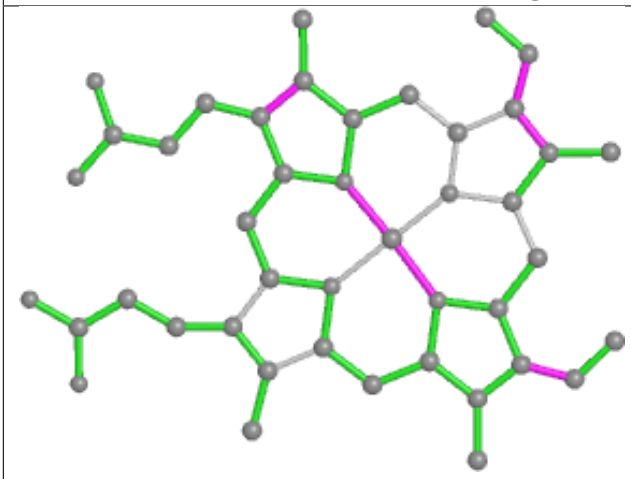


Torsions

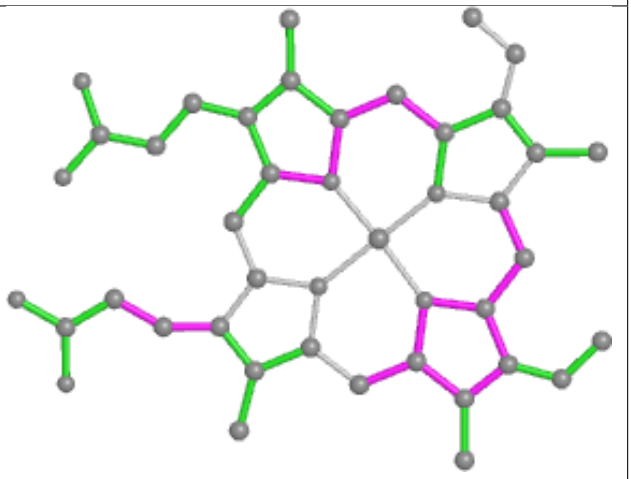


Rings

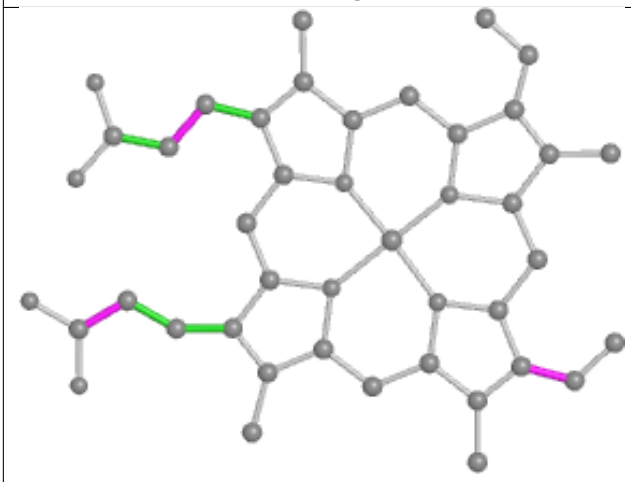
Ligand HEM f 101



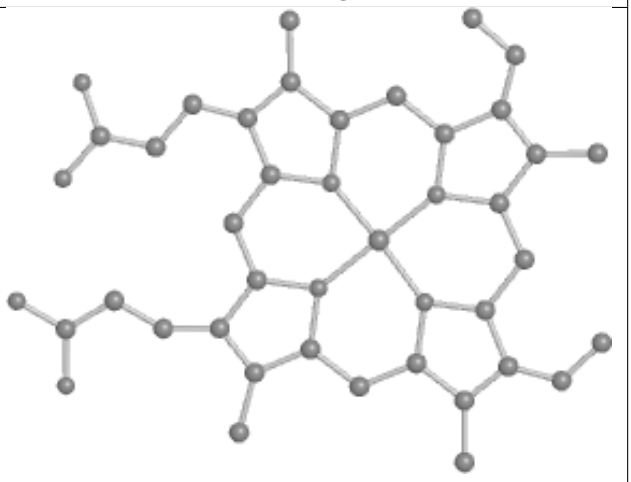
Bond lengths



Bond angles

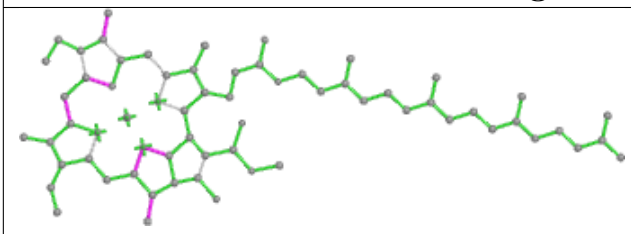


Torsions

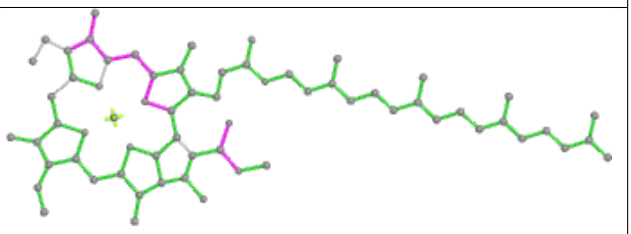


Rings

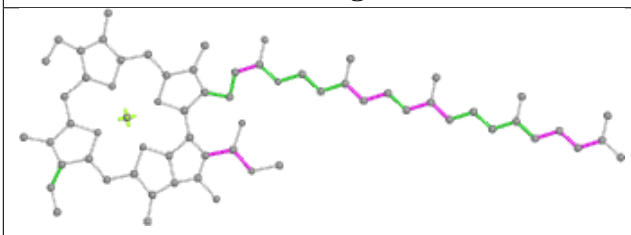
Ligand CLA c 510



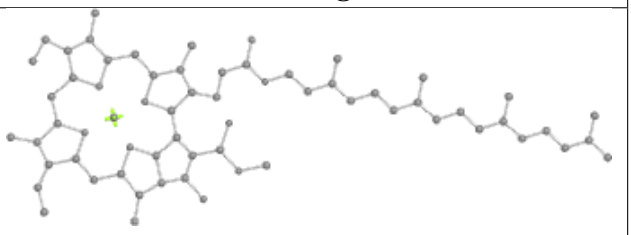
Bond lengths



Bond angles

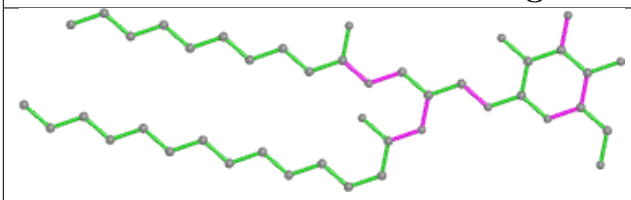


Torsions

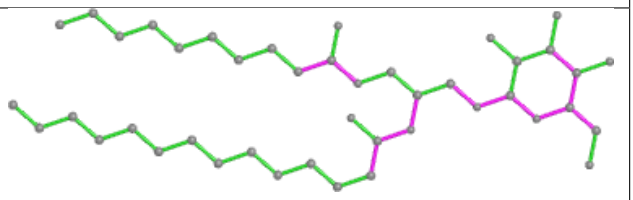


Rings

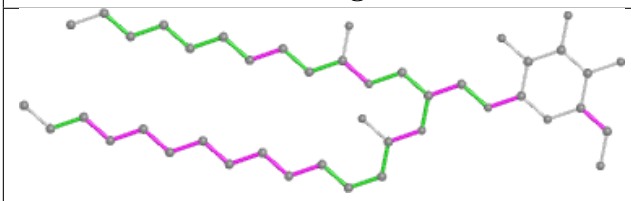
Ligand LMG I 101



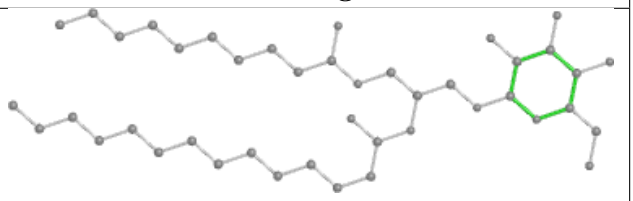
Bond lengths



Bond angles

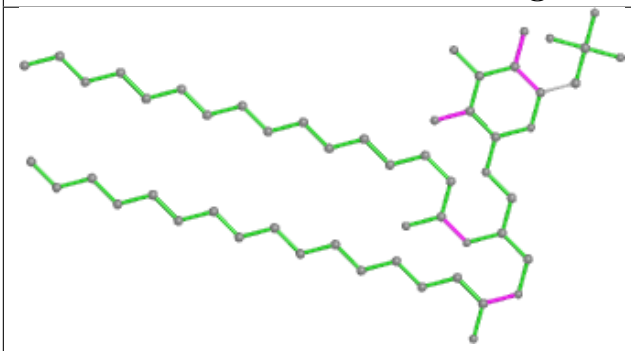


Torsions

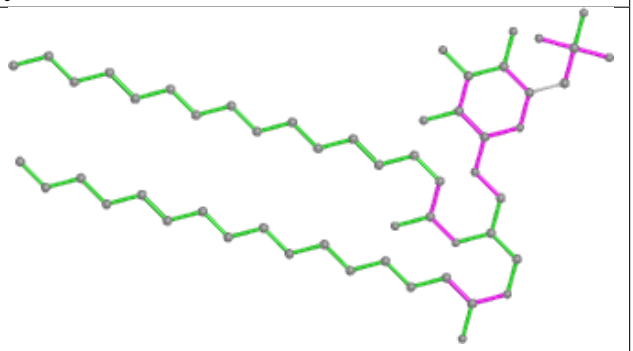


Rings

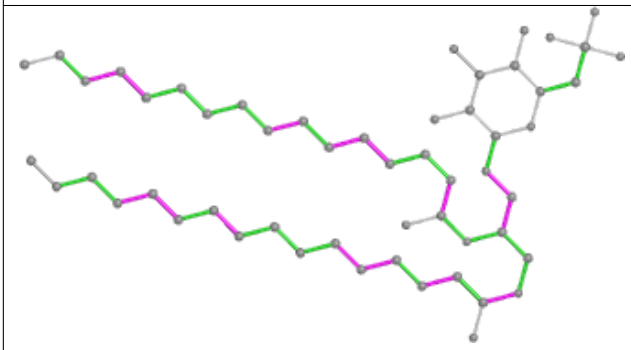
Ligand SQD a 401



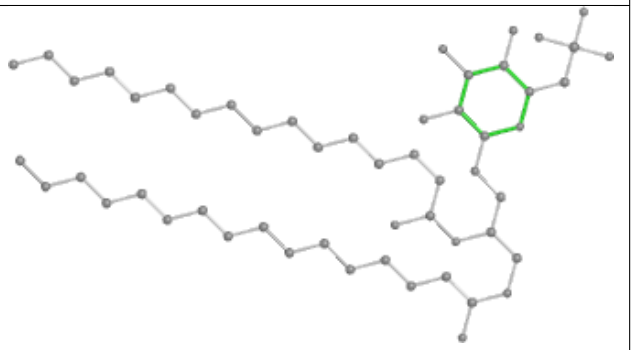
Bond lengths



Bond angles

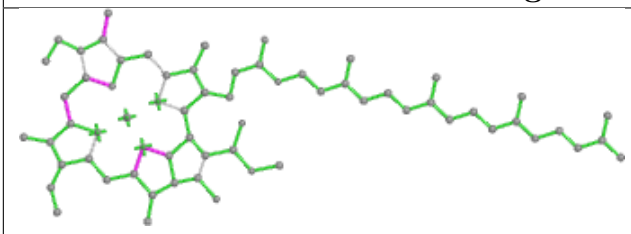


Torsions

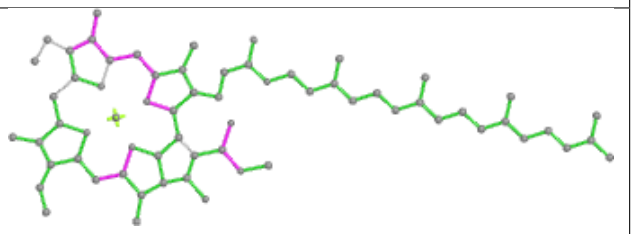


Rings

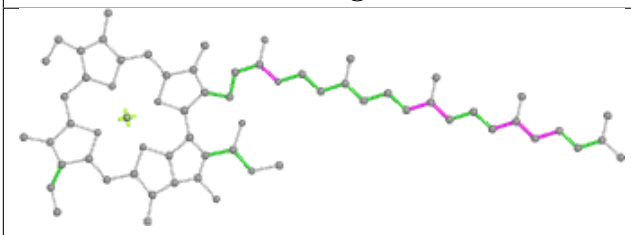
Ligand CLA B 615



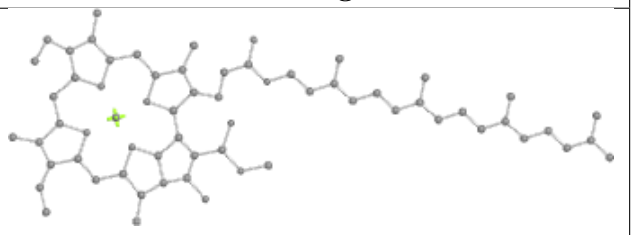
Bond lengths



Bond angles

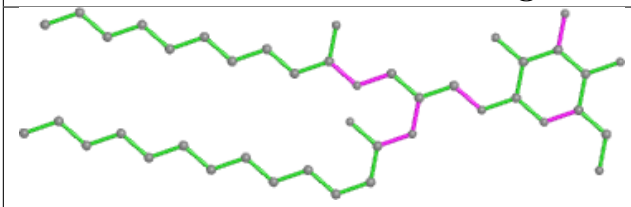


Torsions

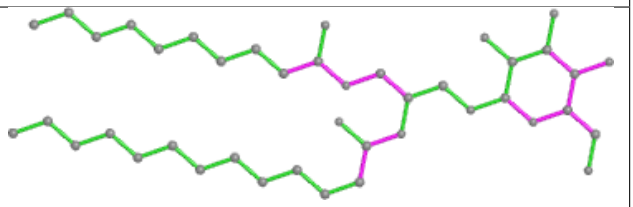


Rings

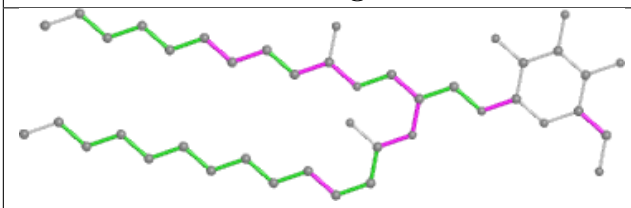
Ligand LMG m 102



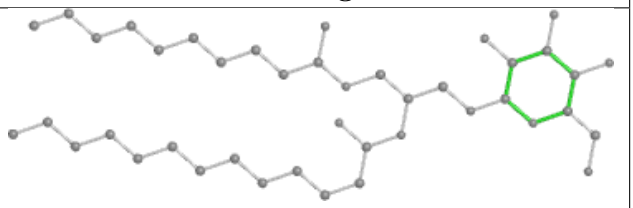
Bond lengths



Bond angles

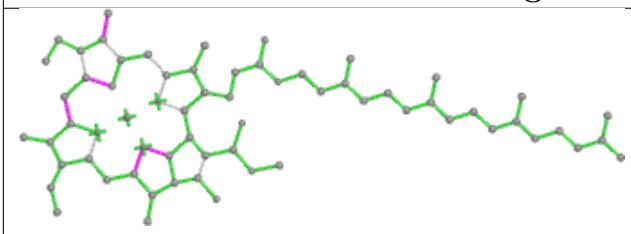


Torsions

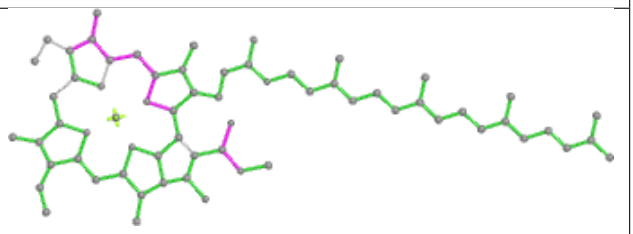


Rings

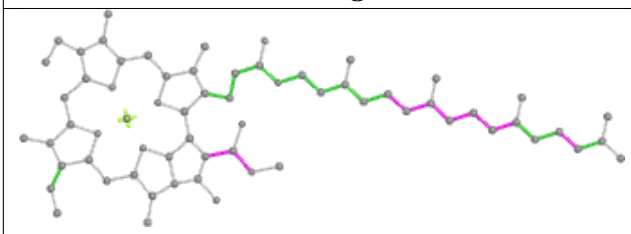
Ligand CLA C 503



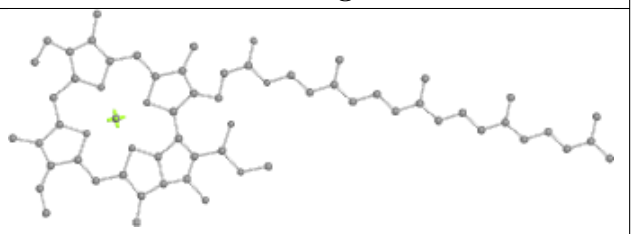
Bond lengths



Bond angles

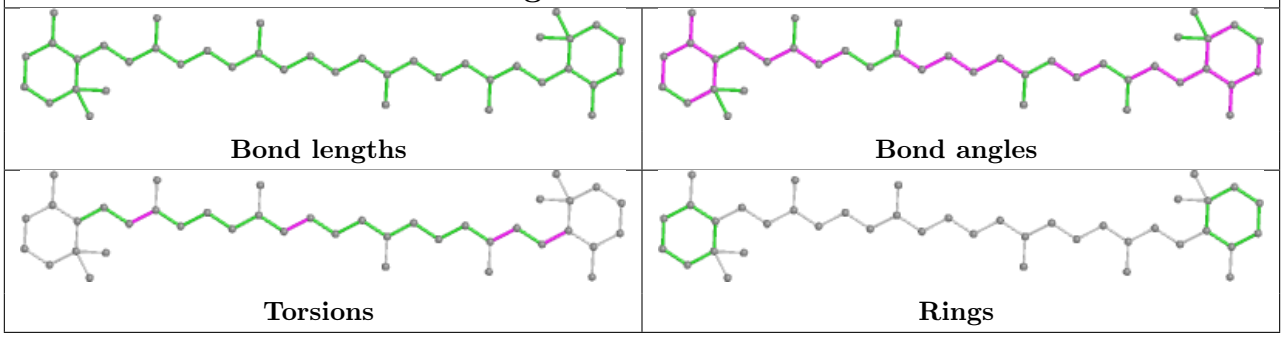


Torsions

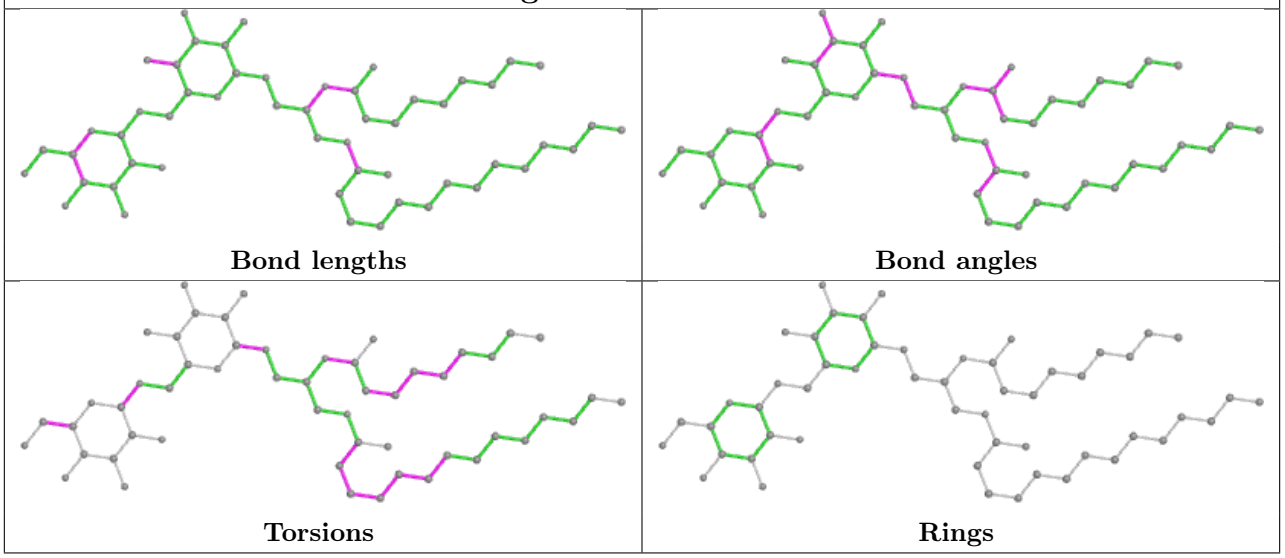


Rings

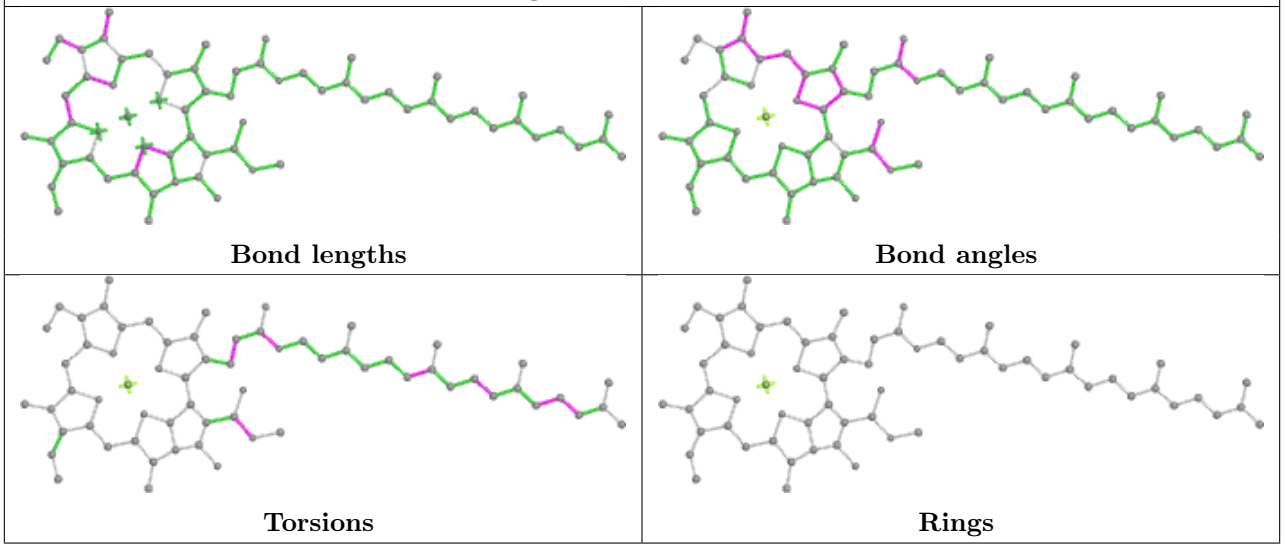
Ligand BCR T 102



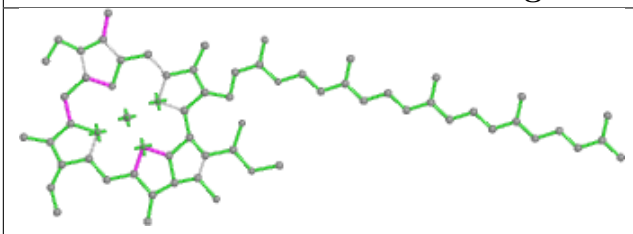
Ligand DGD C 517



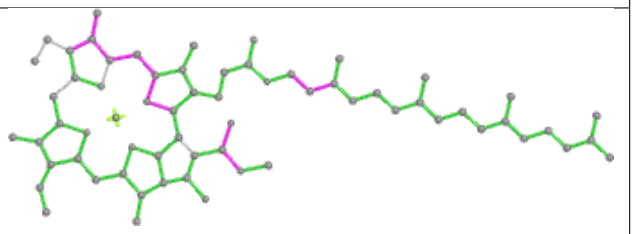
Ligand CLA C 504



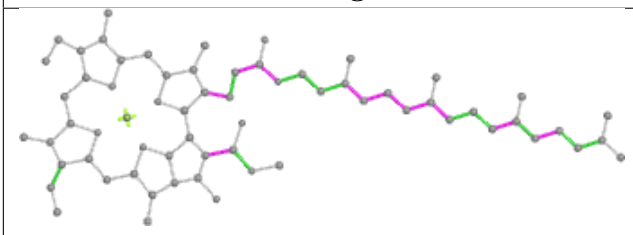
Ligand CLA B 602



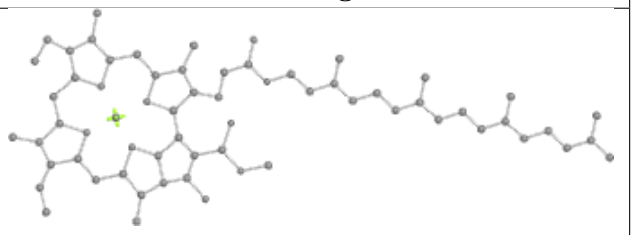
Bond lengths



Bond angles

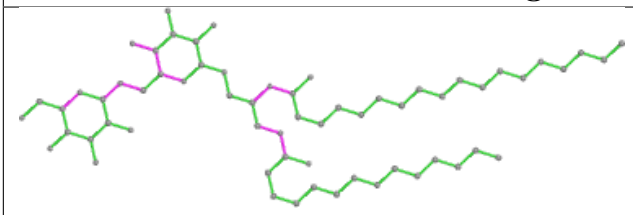


Torsions

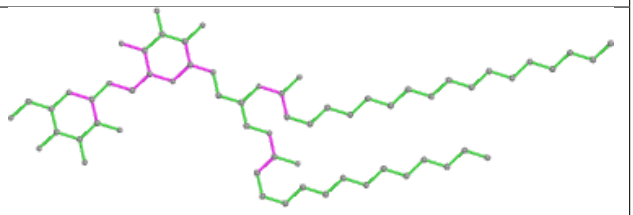


Rings

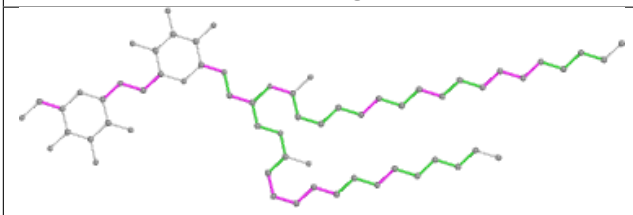
Ligand DGD c 517



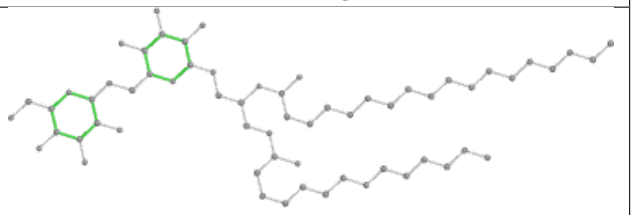
Bond lengths



Bond angles

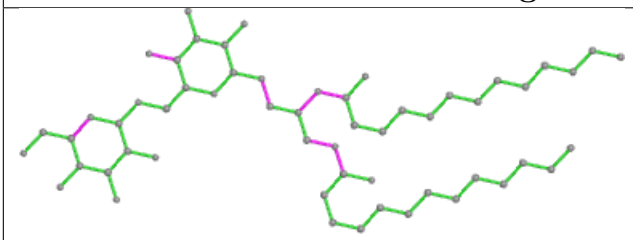


Torsions

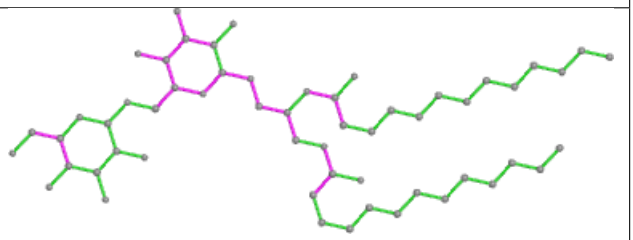


Rings

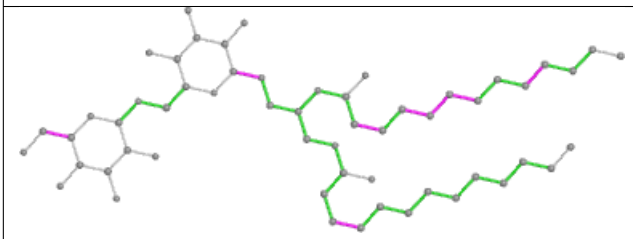
Ligand DGD A 411



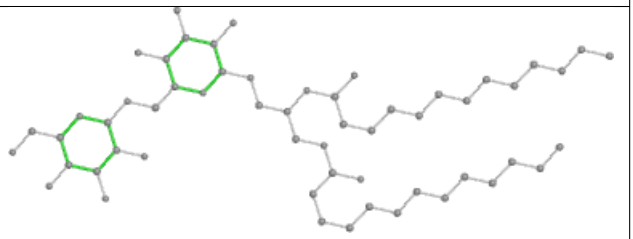
Bond lengths



Bond angles

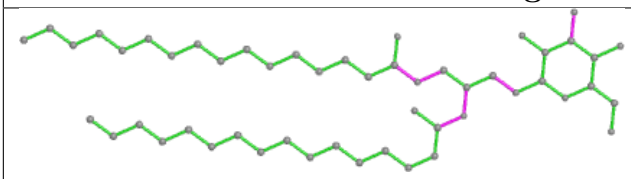


Torsions

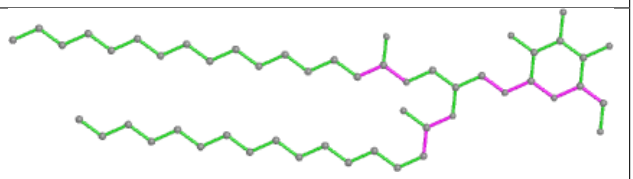


Rings

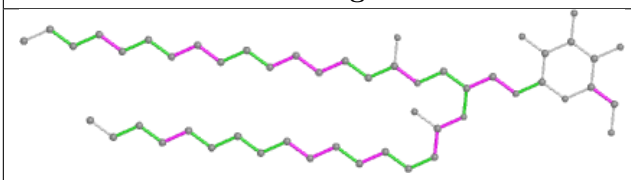
Ligand LMG a 416



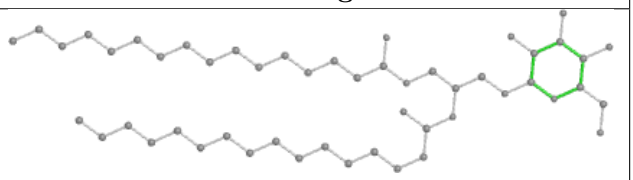
Bond lengths



Bond angles

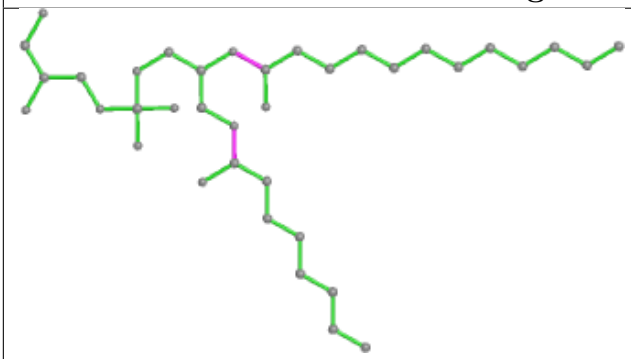


Torsions

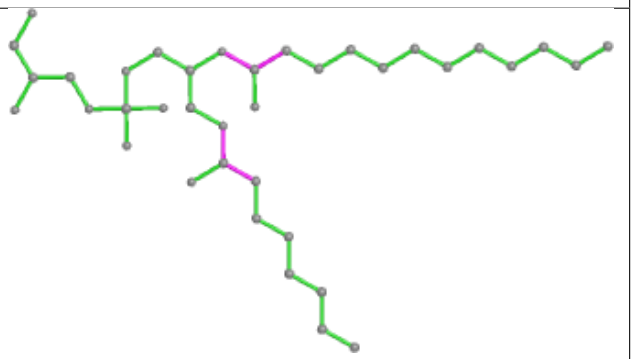


Rings

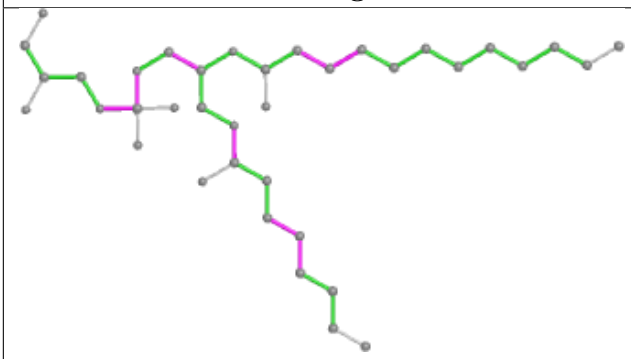
Ligand LHG a 417



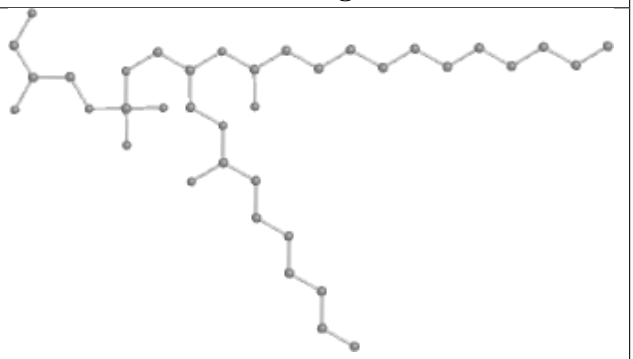
Bond lengths



Bond angles

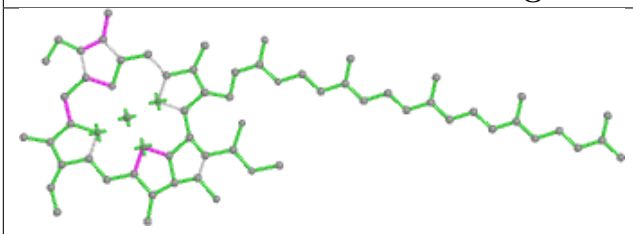


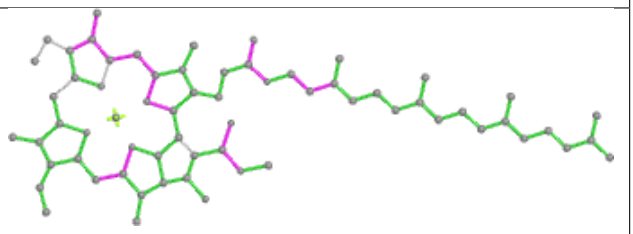
Torsions

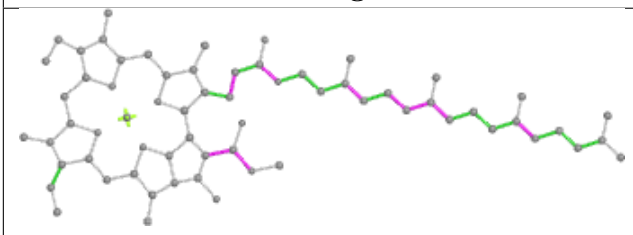


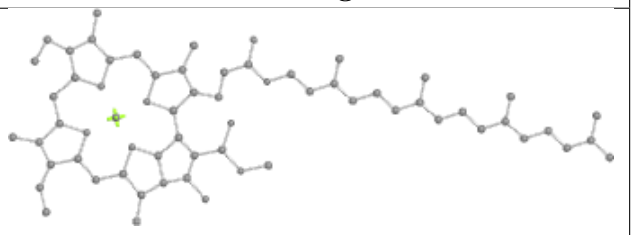
Rings

Ligand CLA C 511

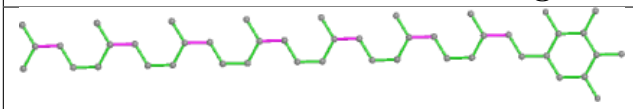

Bond lengths

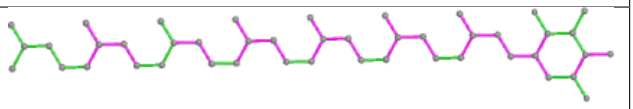

Bond angles

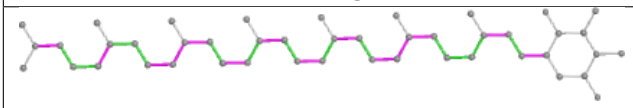

Torsions

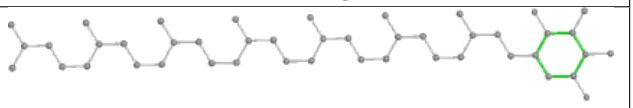

Rings

Ligand PL9 a 410

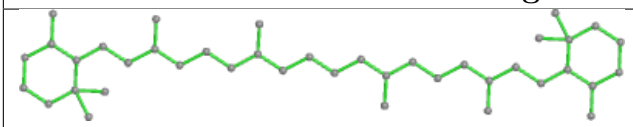

Bond lengths

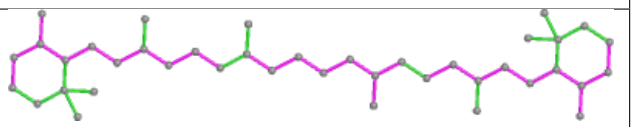

Bond angles

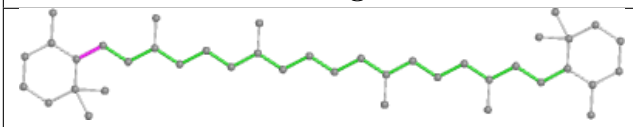

Torsions


Rings

Ligand BCR C 515

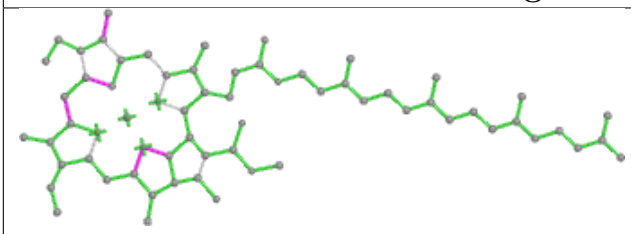

Bond lengths


Bond angles

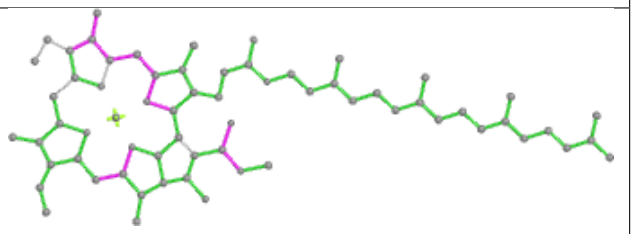

Torsions


Rings

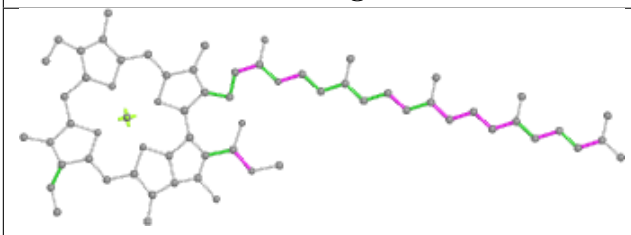
Ligand CLA B 613



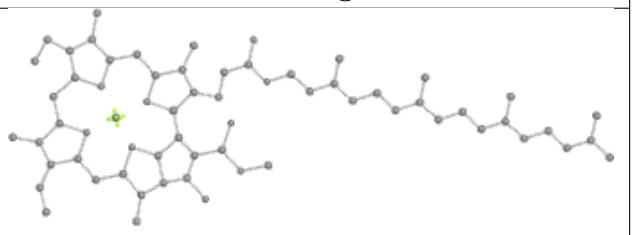
Bond lengths



Bond angles

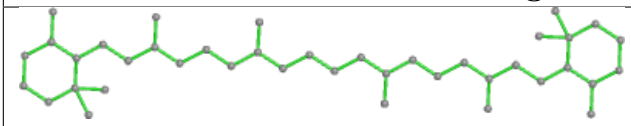


Torsions

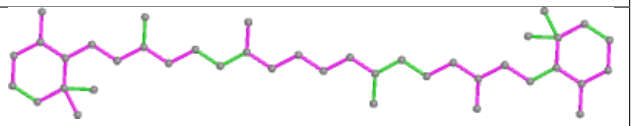


Rings

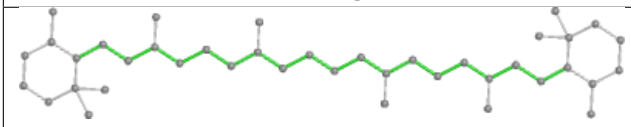
Ligand BCR b 621



Bond lengths



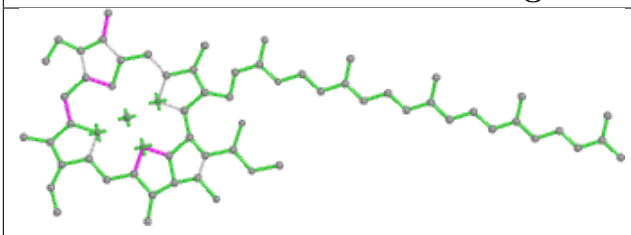
Bond angles



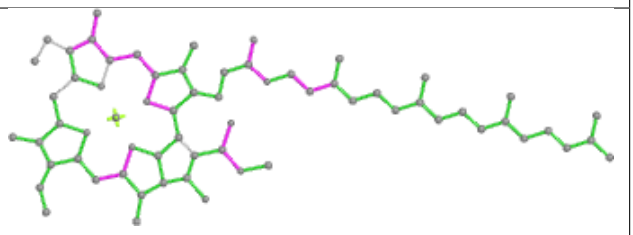
Torsions

Rings

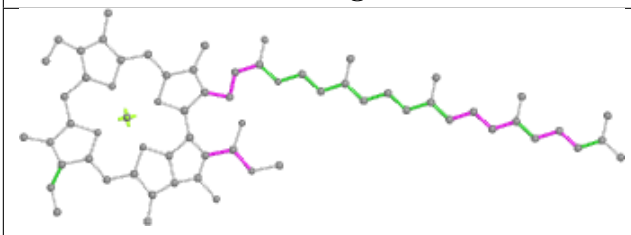
Ligand CLA C 501



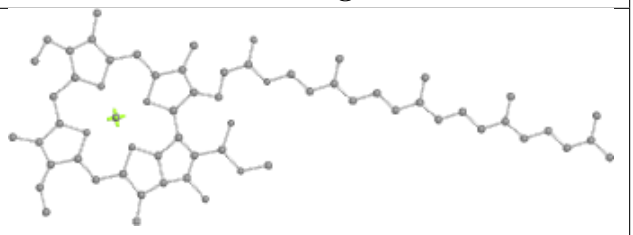
Bond lengths



Bond angles

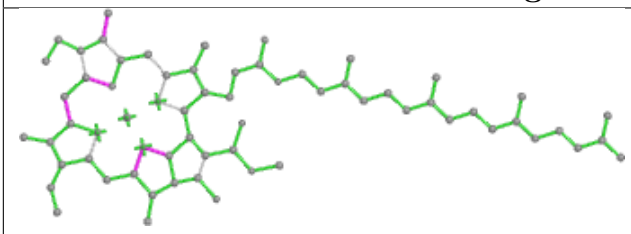


Torsions

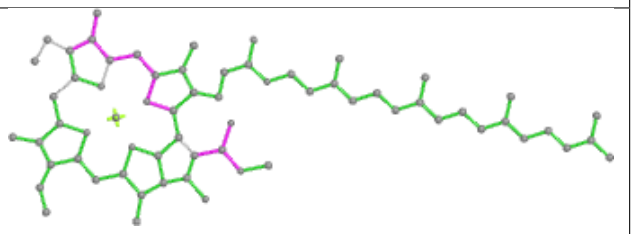


Rings

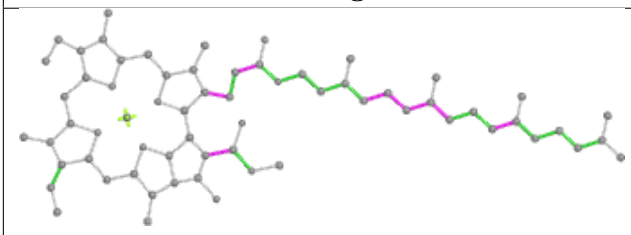
Ligand CLA C 507



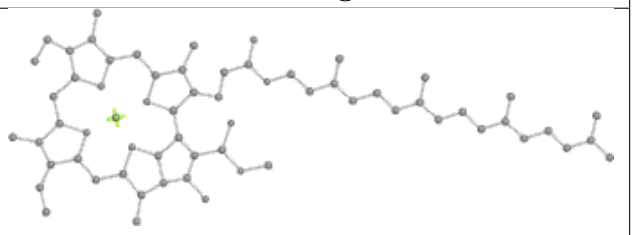
Bond lengths



Bond angles

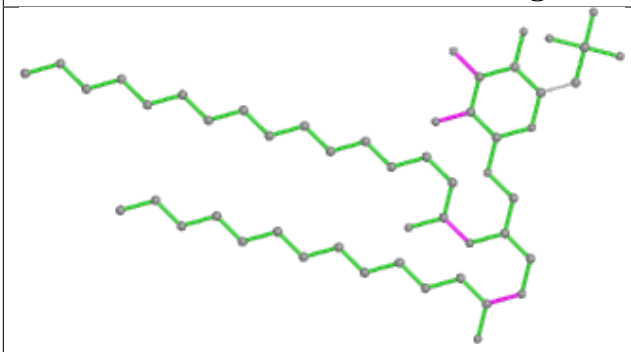


Torsions

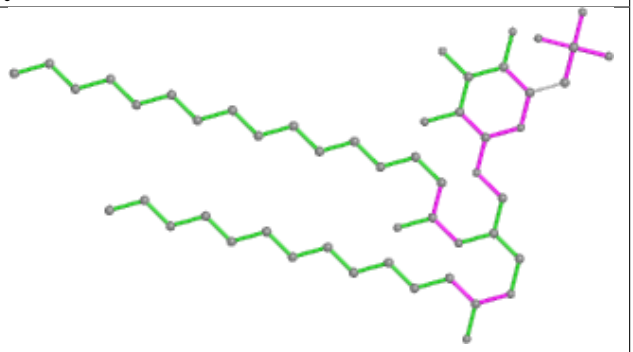


Rings

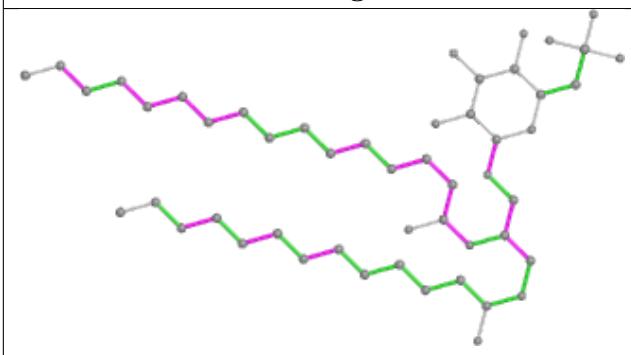
Ligand SQD a 415



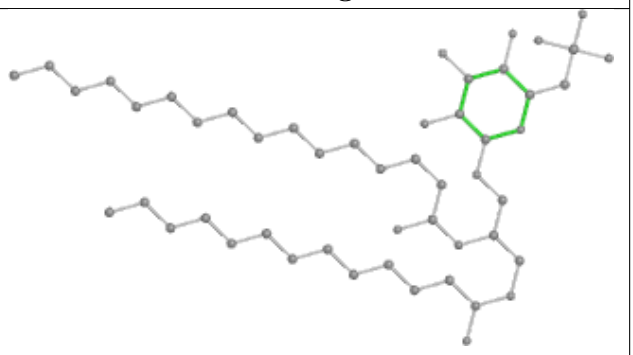
Bond lengths



Bond angles

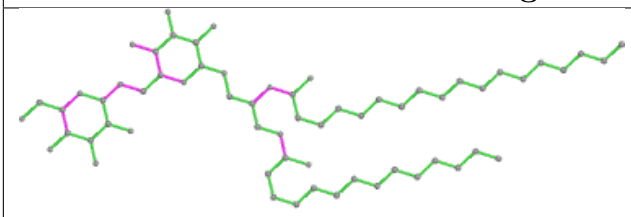


Torsions

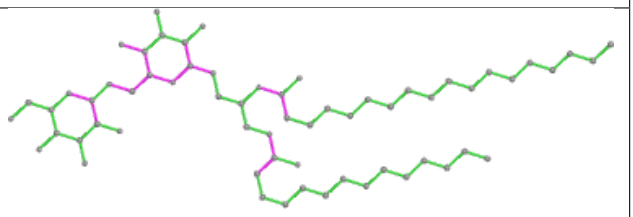


Rings

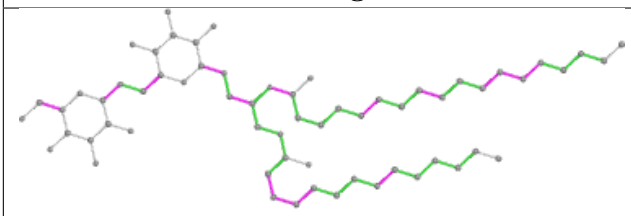
Ligand DGD C 518



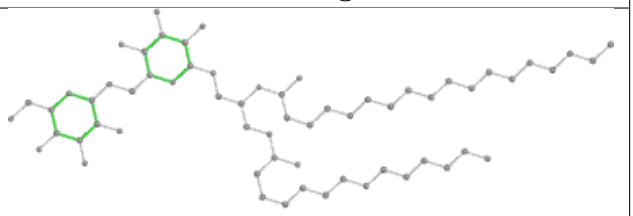
Bond lengths



Bond angles

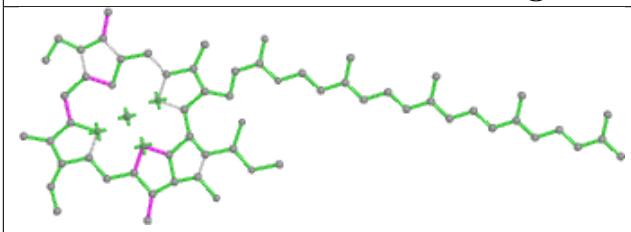


Torsions



Rings

Ligand CLA b 611



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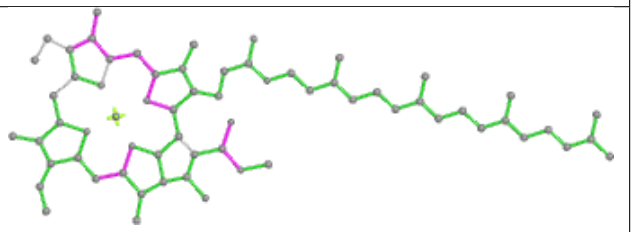
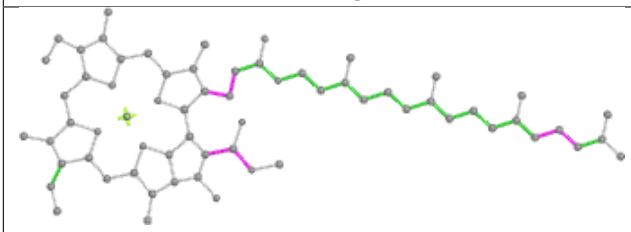
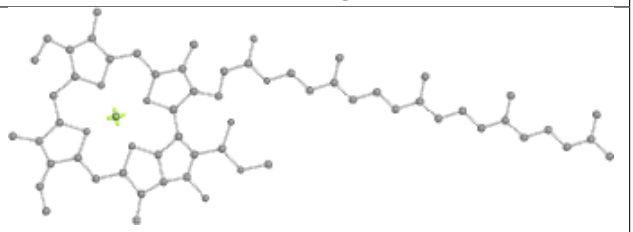


Bond angles

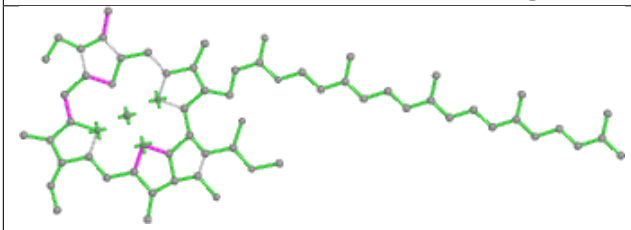


Torsions



Rings

Ligand CLA A 404



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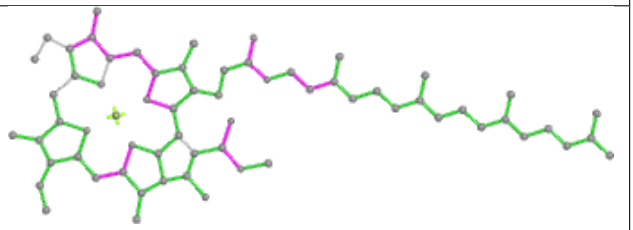
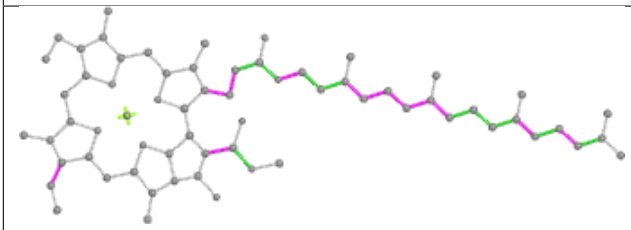


Bond angles



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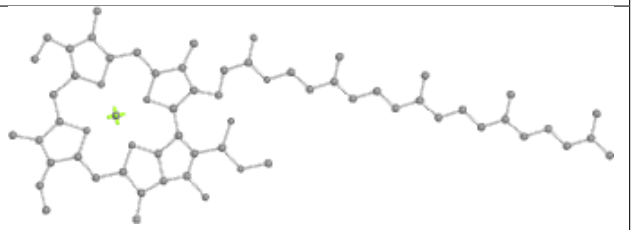
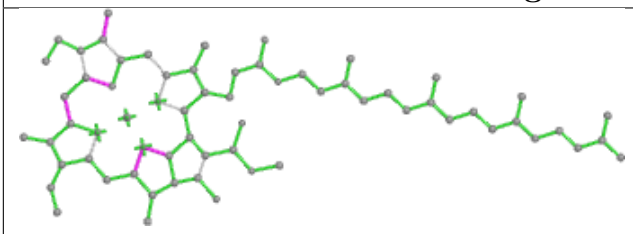


Rings

Ligand CLA C 513



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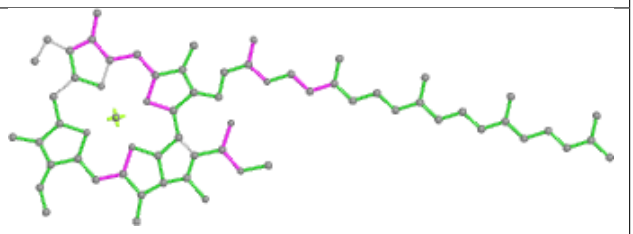
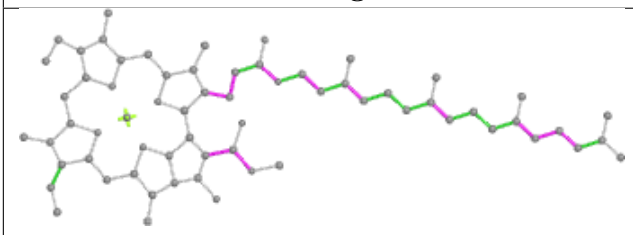


Bond angles



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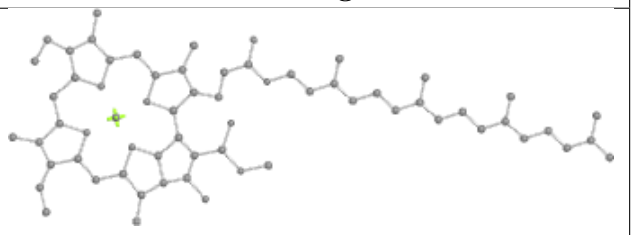
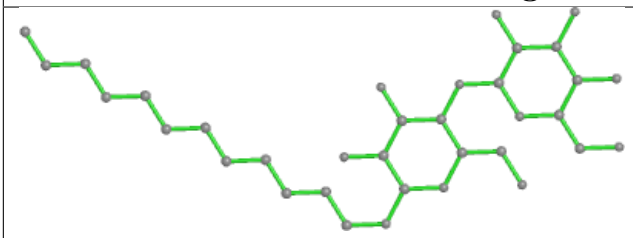


Rings

Ligand LMT B 625



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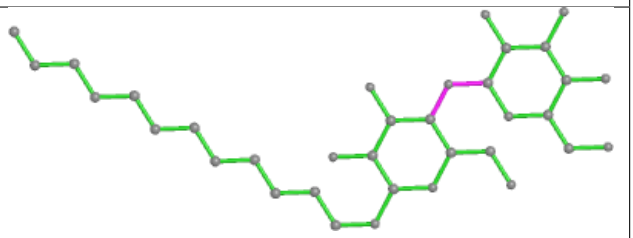
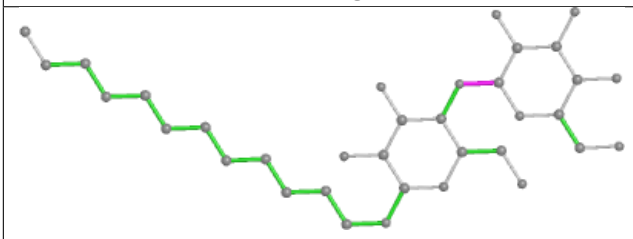
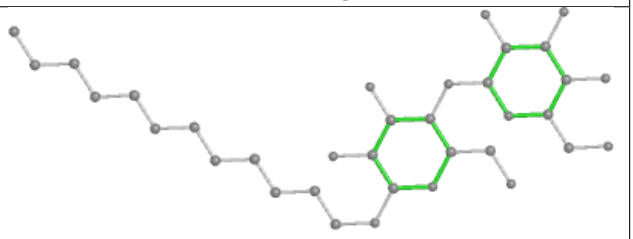


Bond angles

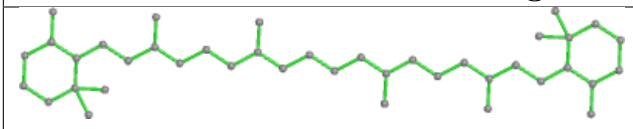


Torsions

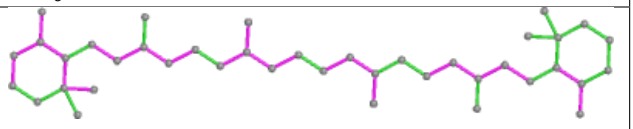


Rings

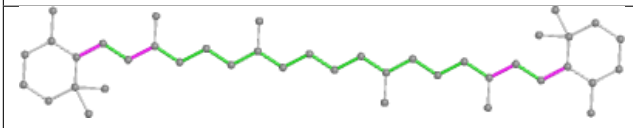
Ligand BCR y 101



Bond lengths



Bond angles



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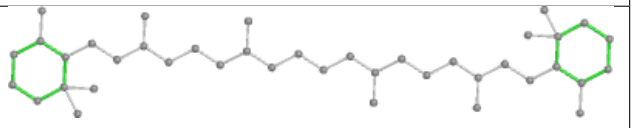
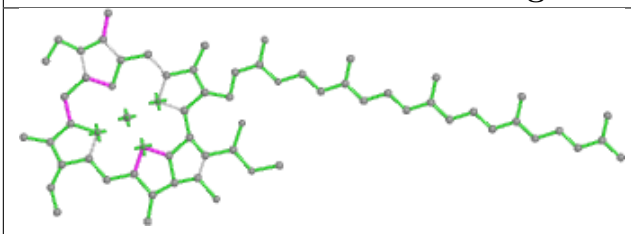


Rings

Ligand CLA b 619



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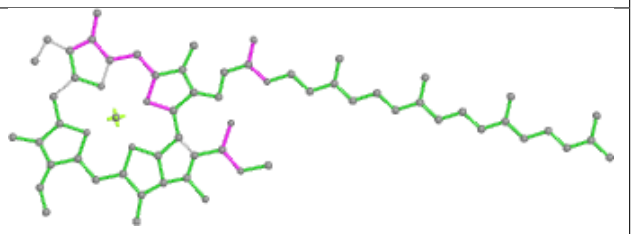
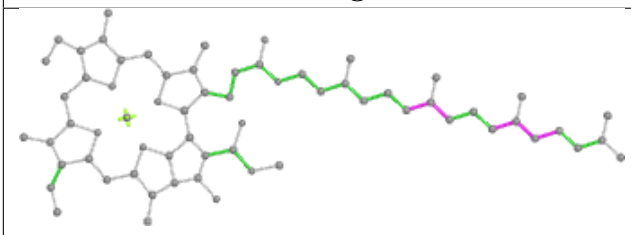
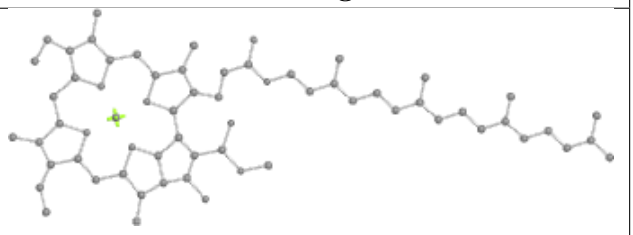


Bond angles

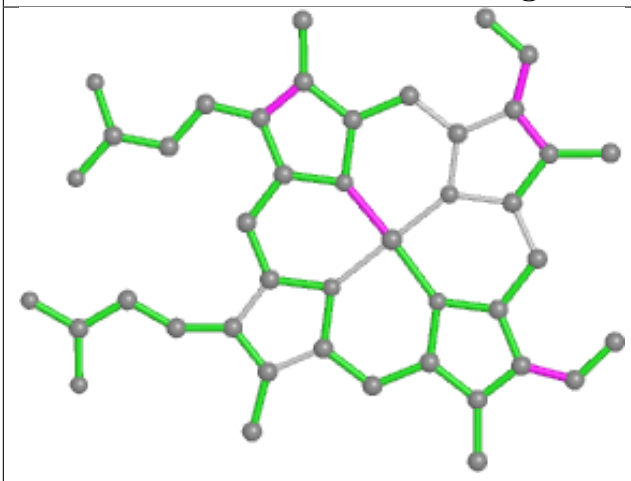


Torsions



Rings

Ligand HEM F 101



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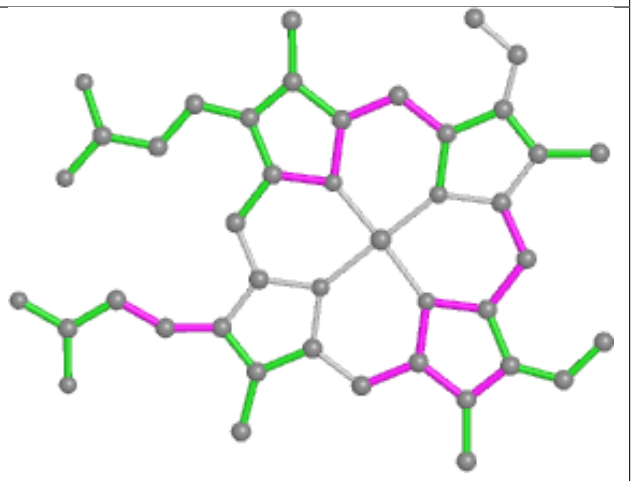
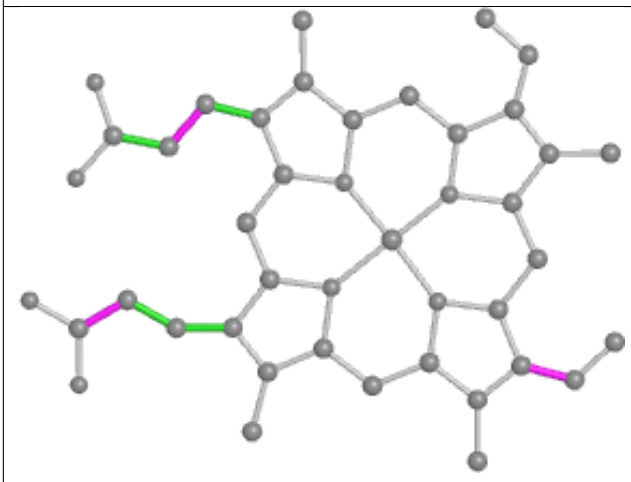
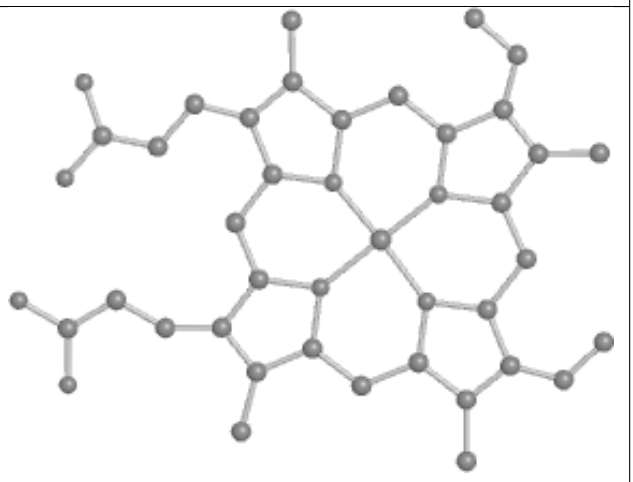


Bond angles

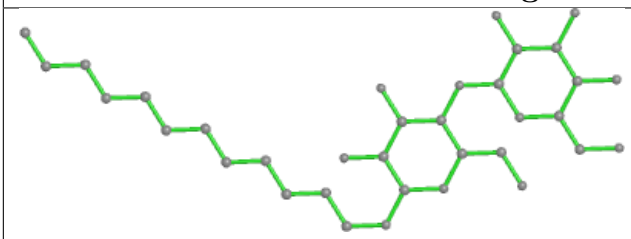


Torsions



Rings

Ligand LMT B 624



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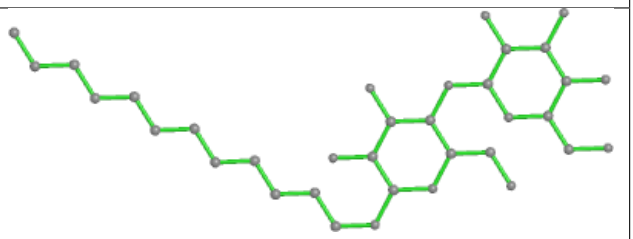
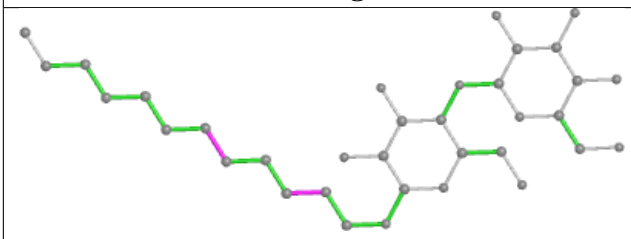


Bond angles



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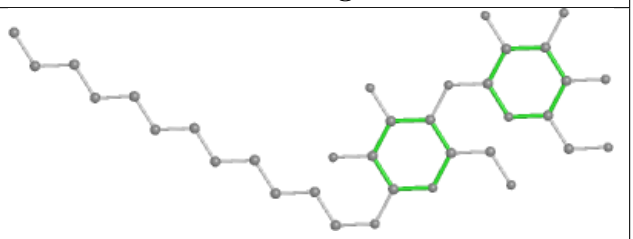
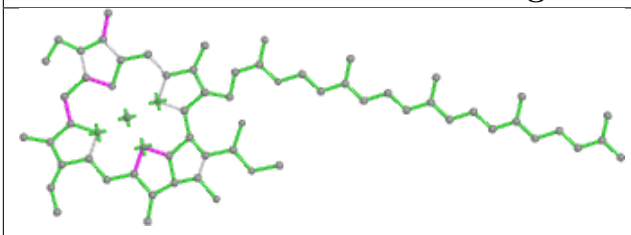


Rings

Ligand CLA b 610



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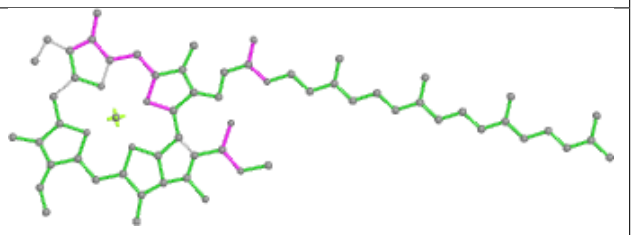
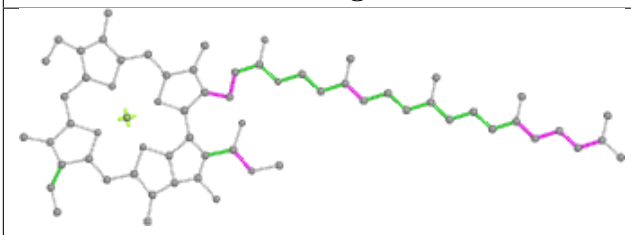
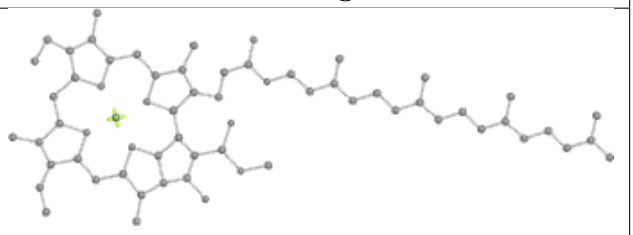


Bond angles

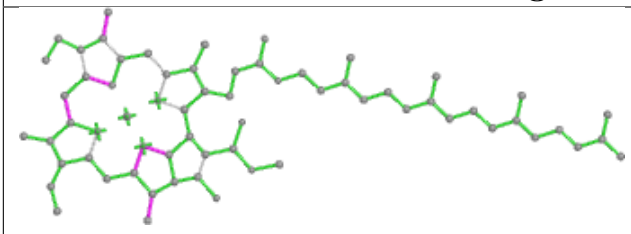


Torsions



Rings

Ligand CLA a 406



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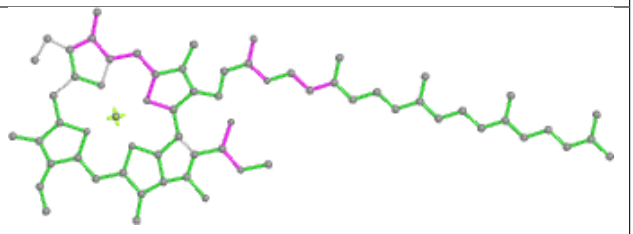
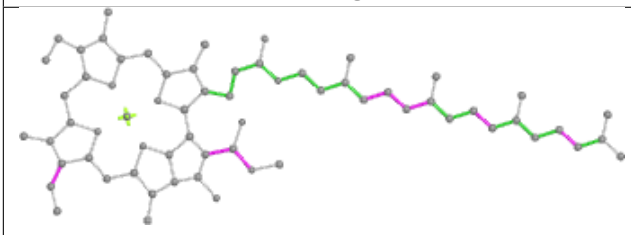
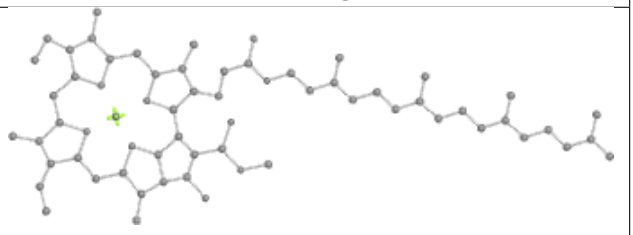


Bond angles

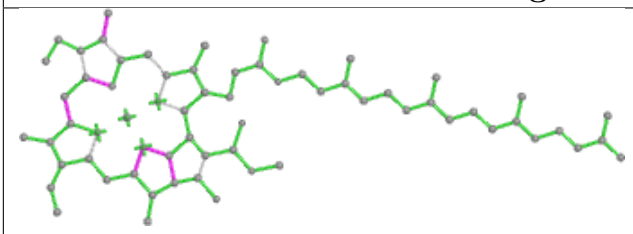


Torsions

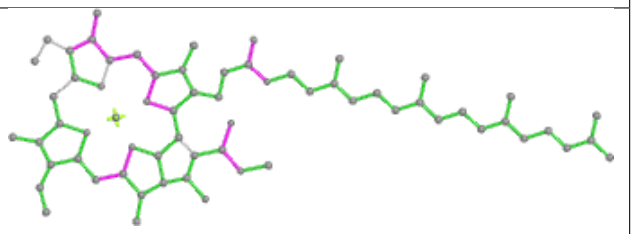


Rings

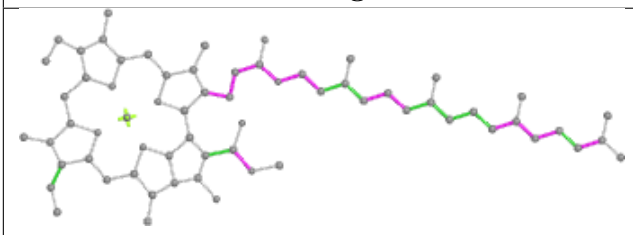
Ligand CLA c 512



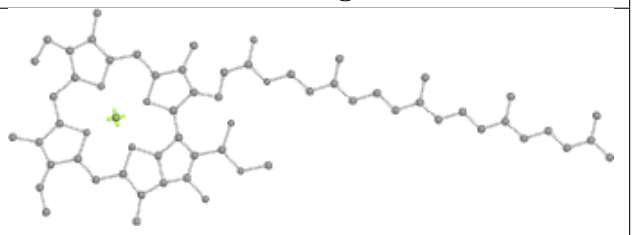
Bond lengths



Bond angles

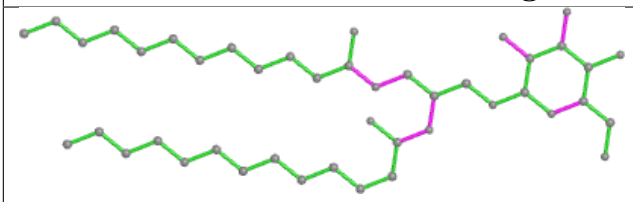


Torsions

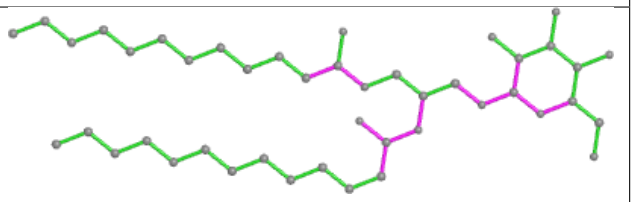


Rings

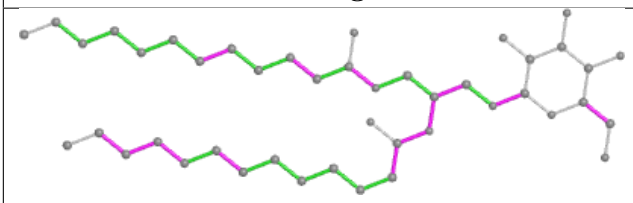
Ligand LMG E 101



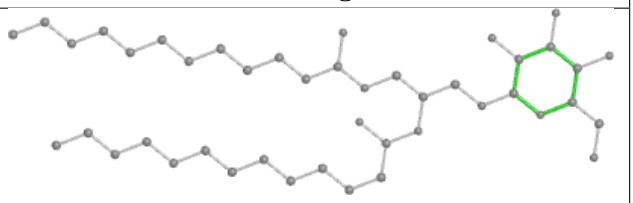
Bond lengths



Bond angles

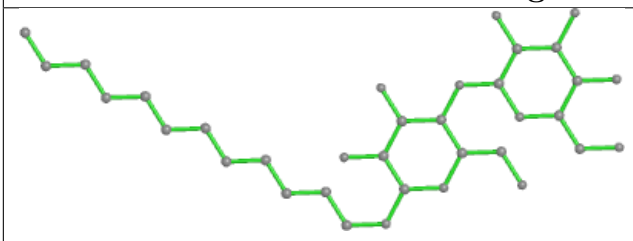


Torsions

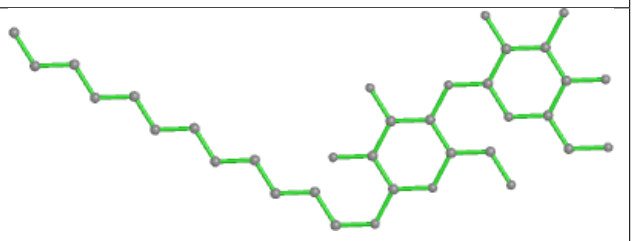


Rings

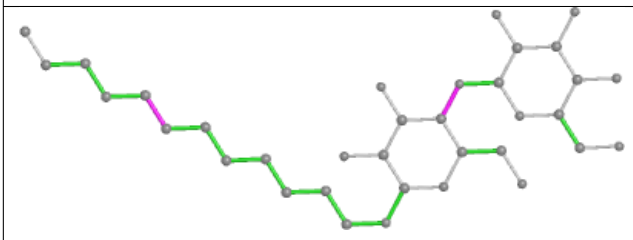
Ligand LMT I 102



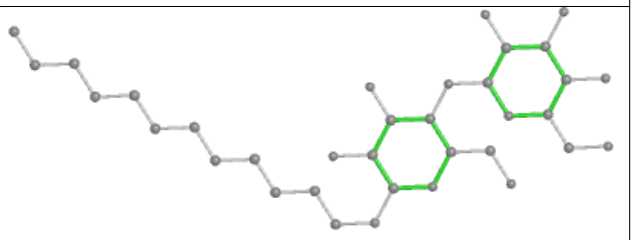
Bond lengths



Bond angles

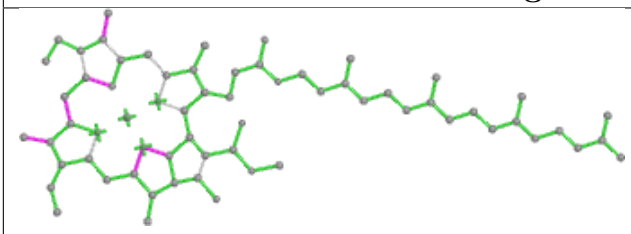


Torsions

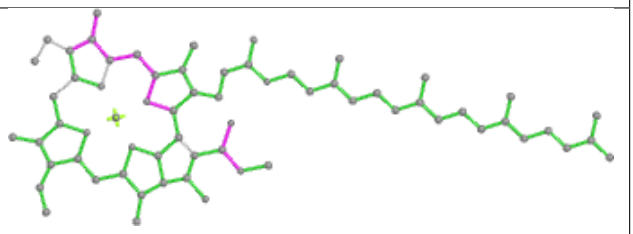


Rings

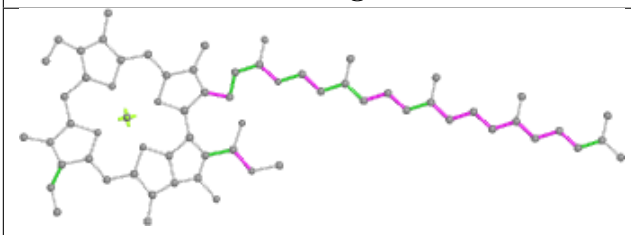
Ligand CLA B 616



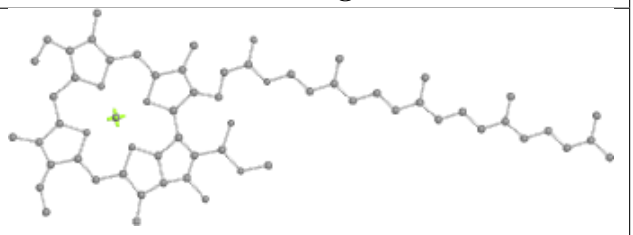
Bond lengths



Bond angles

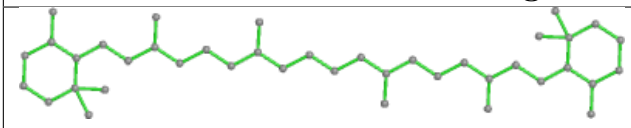


Torsions

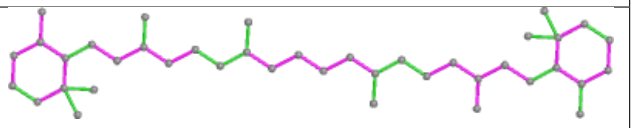


Rings

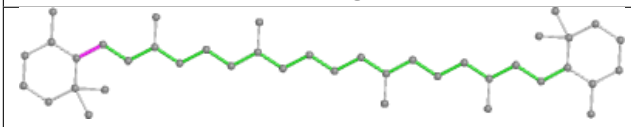
Ligand BCR B 619



Bond lengths



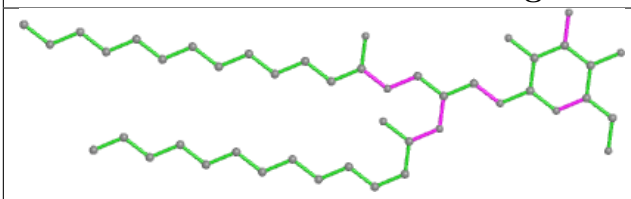
Bond angles



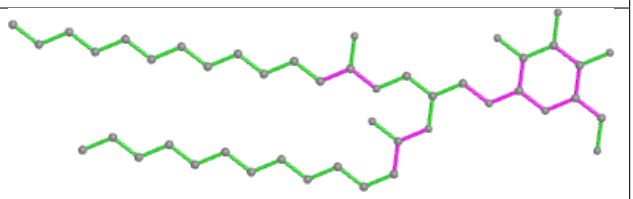
Torsions

Rings

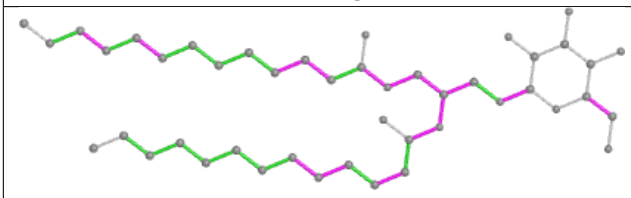
Ligand LMG c 519



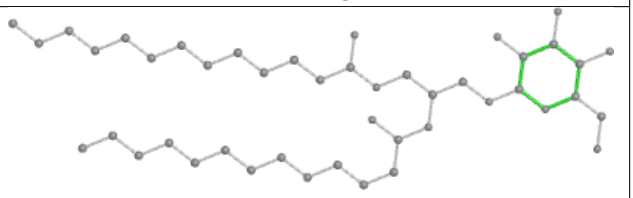
Bond lengths



Bond angles

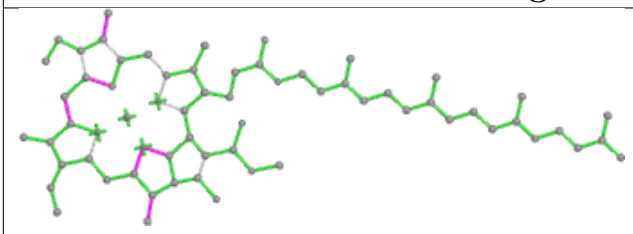


Torsions

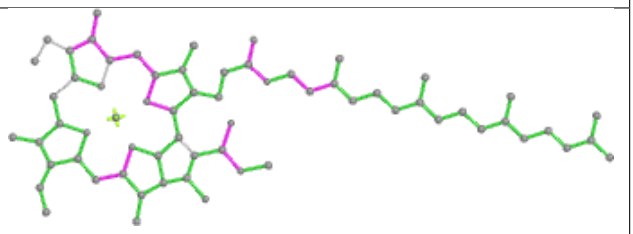


Rings

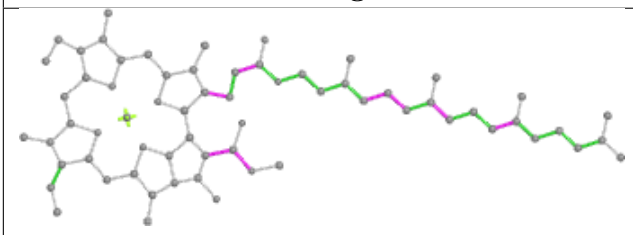
Ligand CLA c 507



Bond lengths



Bond angles



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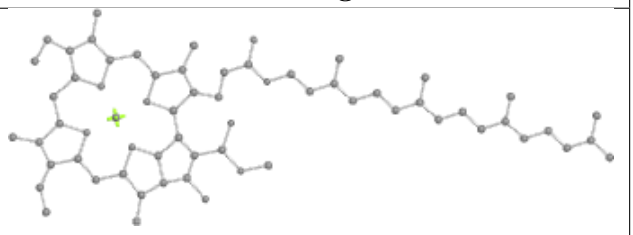
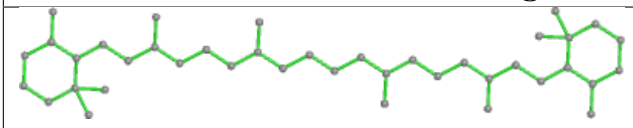
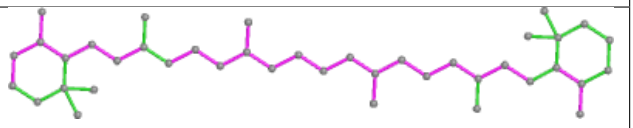


Rings

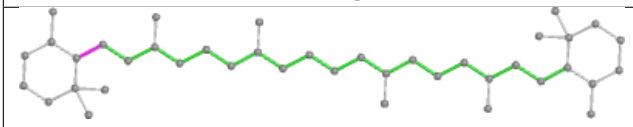
Ligand BCR H 101



Bond lengths



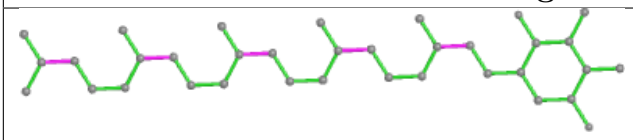
Bond angles



Torsions

Rings

Ligand PL9 j 101



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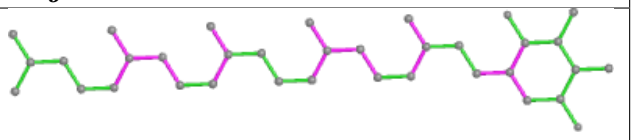
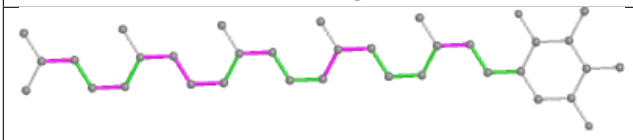
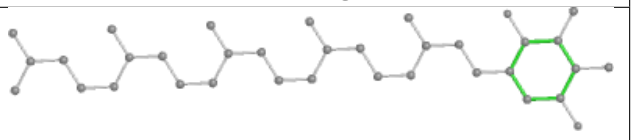


Bond angles

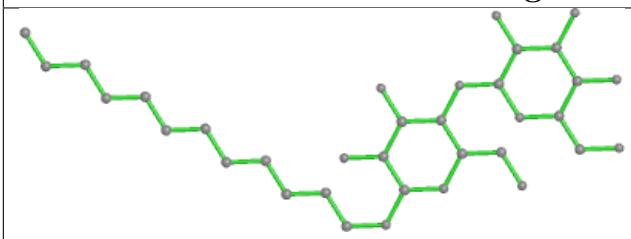


Torsions



Rings

Ligand LMT b 627



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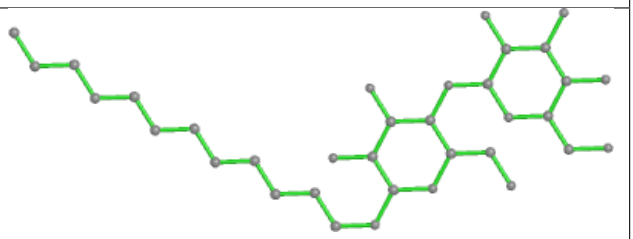
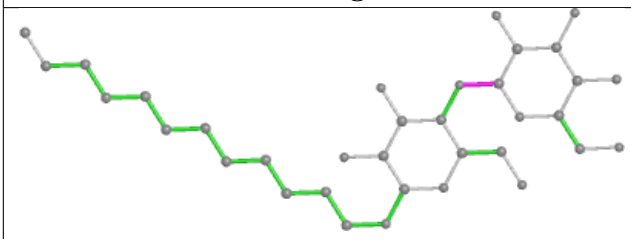
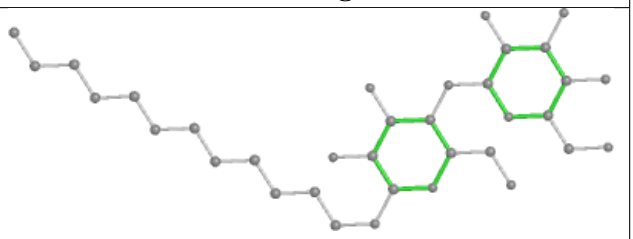


Bond angles

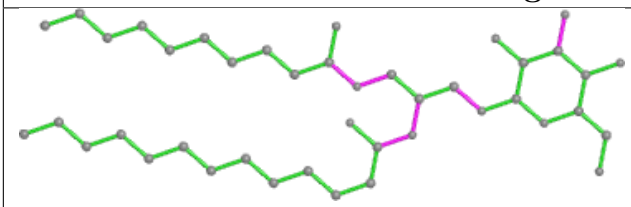


Torsions

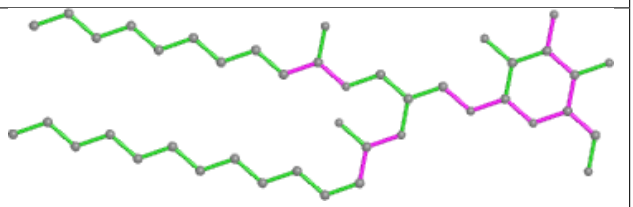


Rings

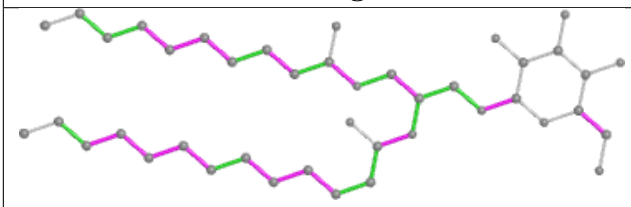
Ligand LMG a 402



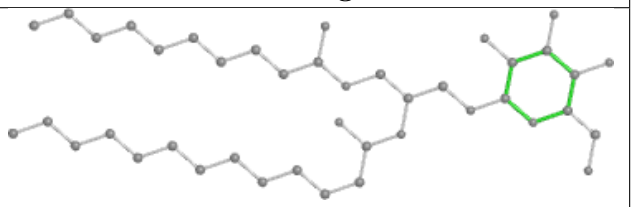
Bond lengths



Bond angles

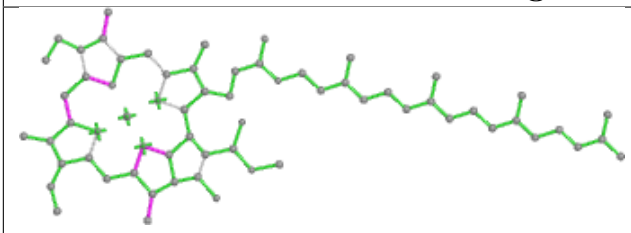


Torsions



Rings

Ligand CLA b 609



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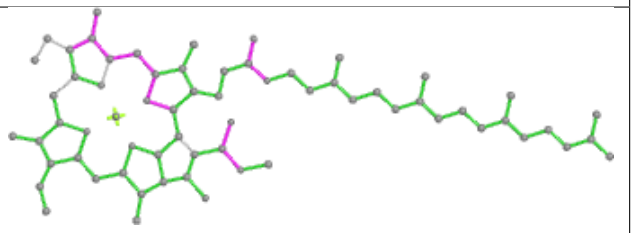
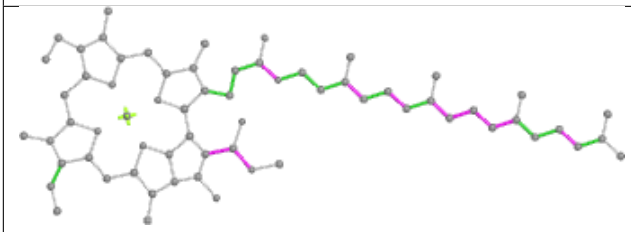
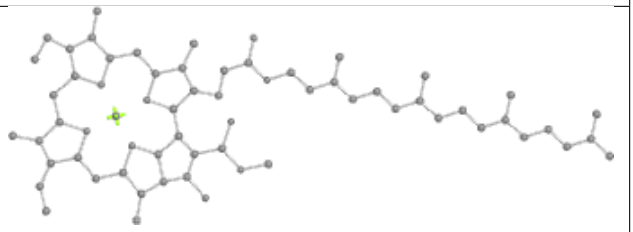


Bond angles

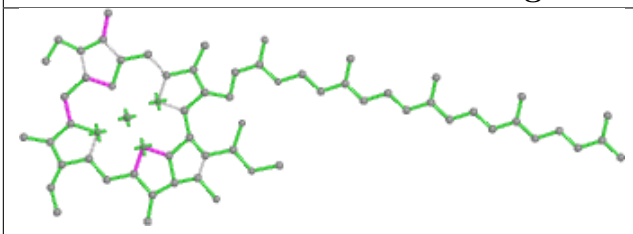


Torsions

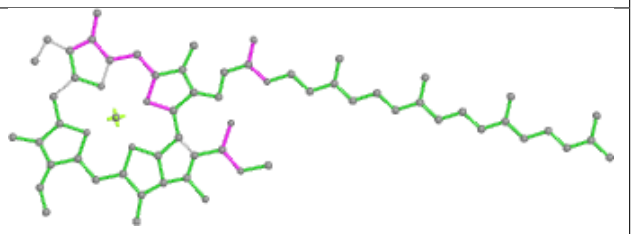


Rings

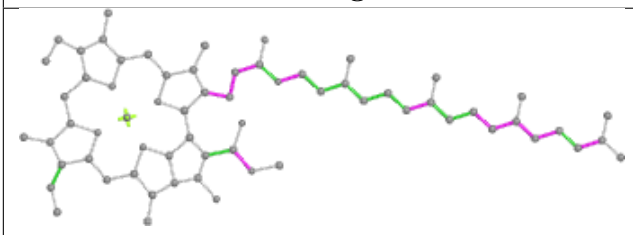
Ligand CLA B 601



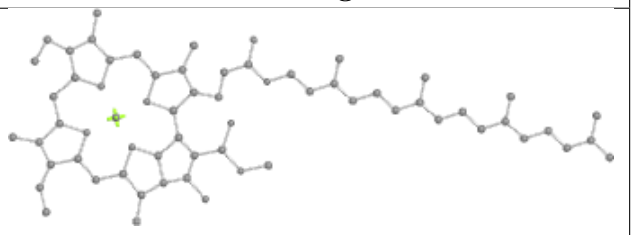
Bond lengths



Bond angles

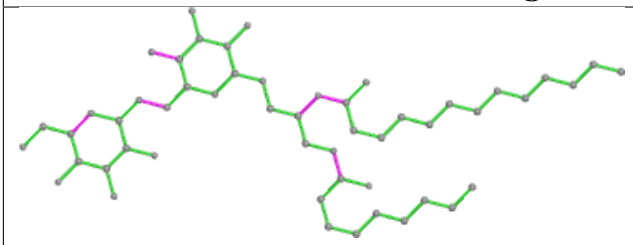


Torsions



Rings

Ligand DGD b 602



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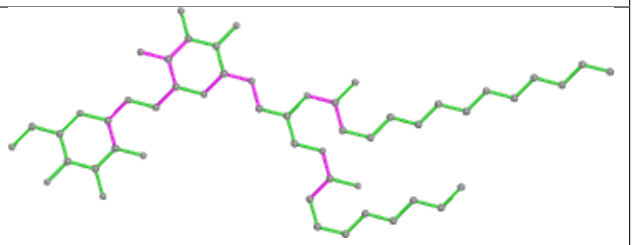
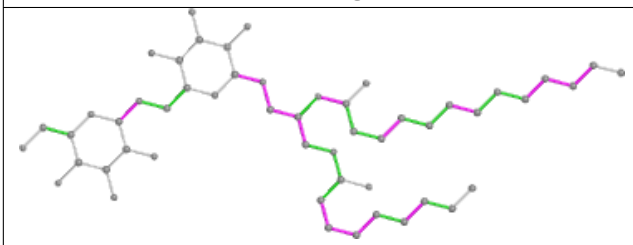
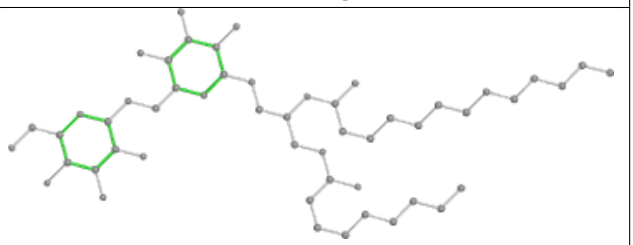


Bond angles

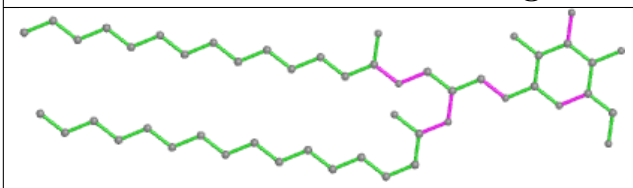


Torsions

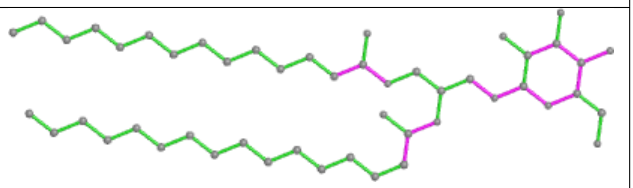


Rings

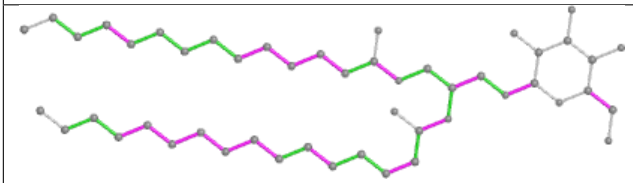
Ligand LMG b 624



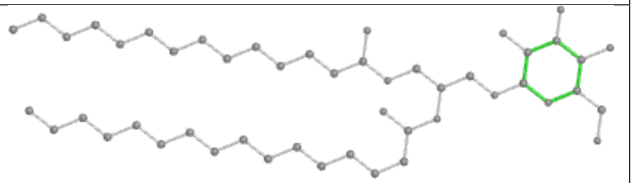
Bond lengths



Bond angles

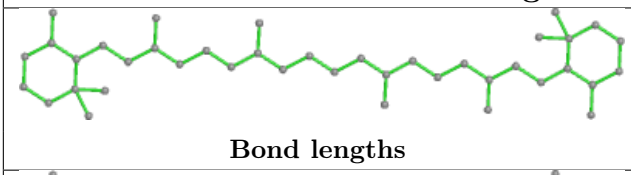


Torsions

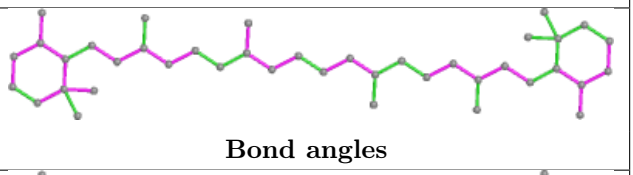


Rings

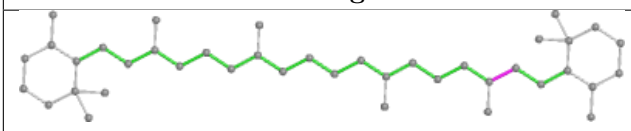
Ligand BCR B 620



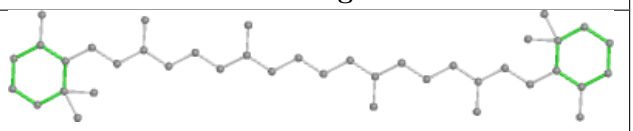
Bond lengths



Bond angles

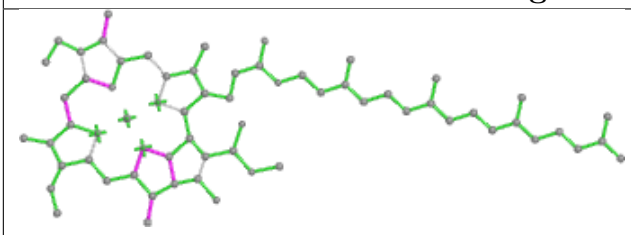


Torsions

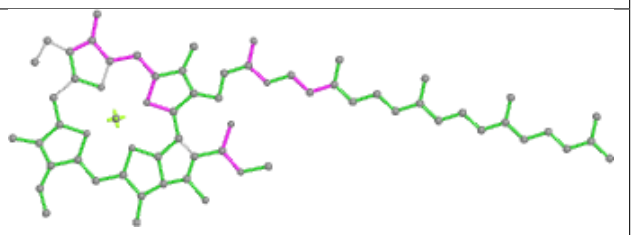


Rings

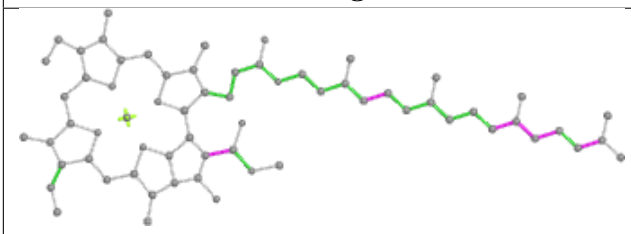
Ligand CLA c 502



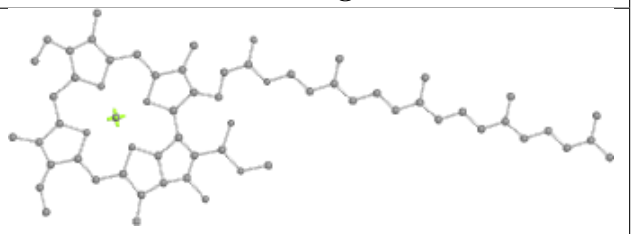
Bond lengths



Bond angles

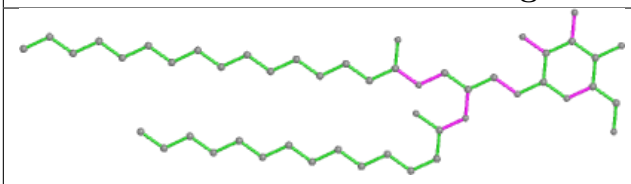


Torsions

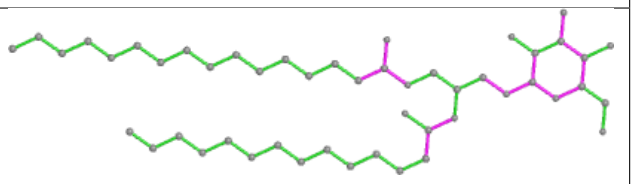


Rings

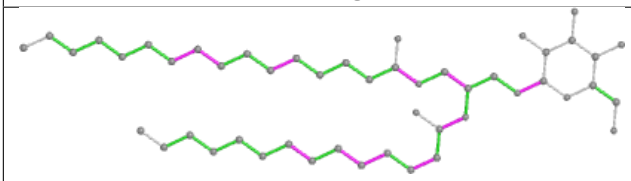
Ligand LMG B 623



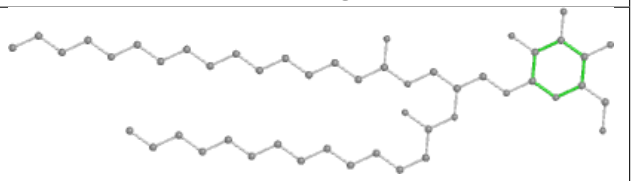
Bond lengths



Bond angles

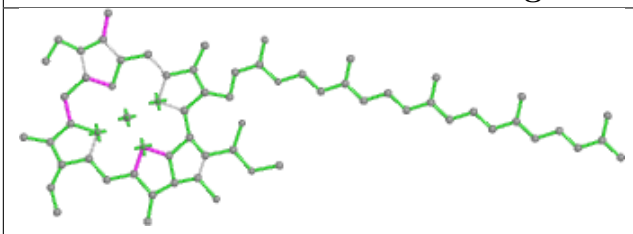


Torsions

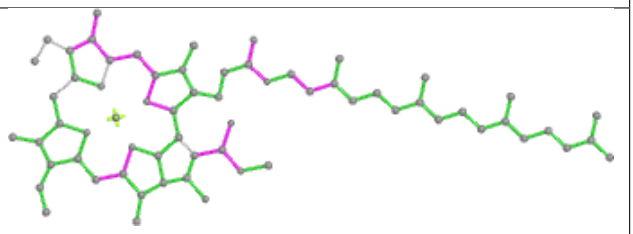


Rings

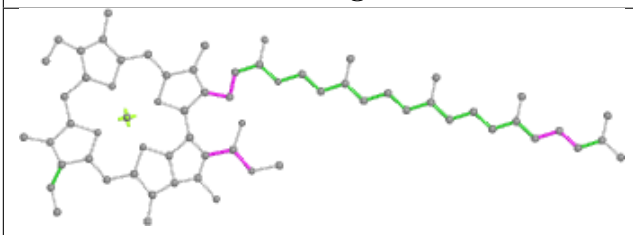
Ligand CLA B 607



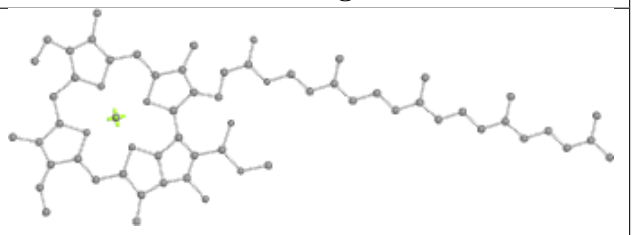
Bond lengths



Bond angles

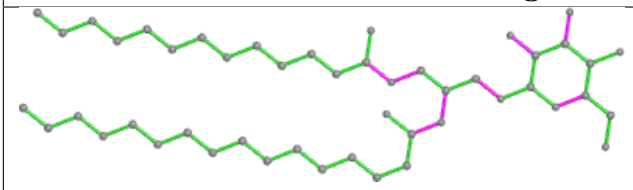


Torsions



Rings

Ligand LMG d 407



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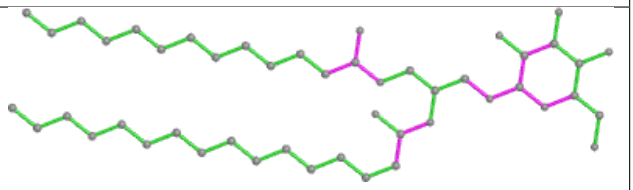
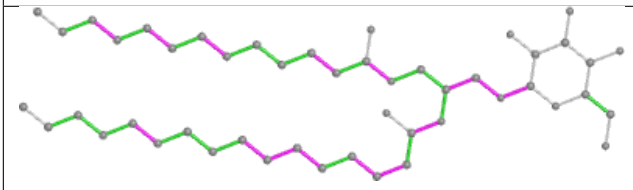
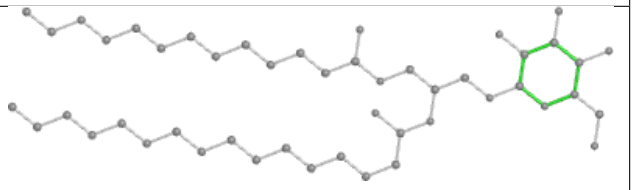


Bond angles

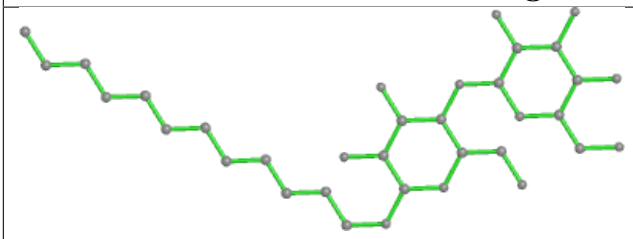


Torsions



Rings

Ligand LMT b 626



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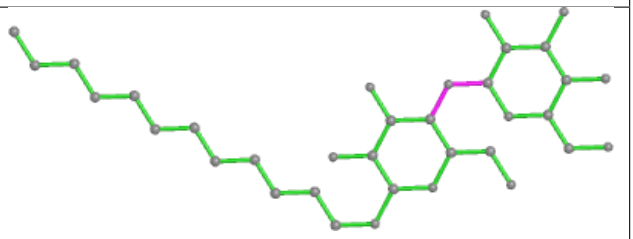
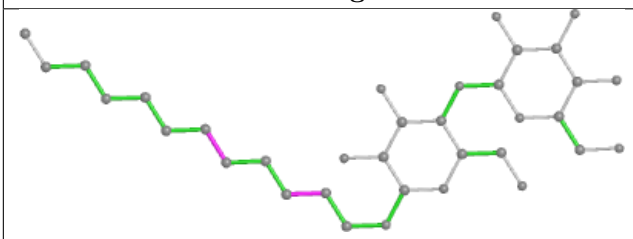
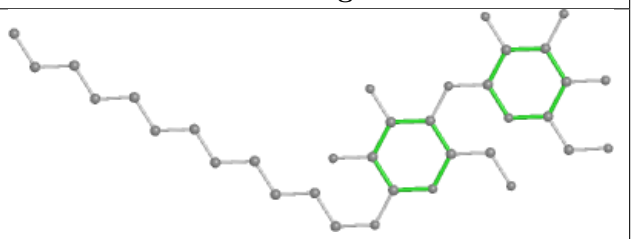


Bond angles

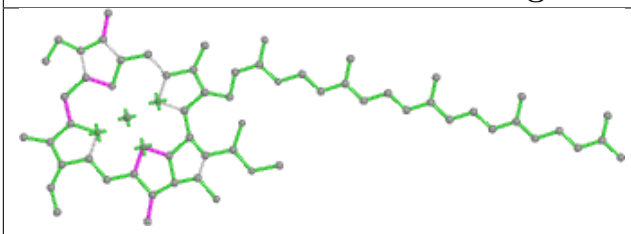


Torsions



Rings

Ligand CLA d 402



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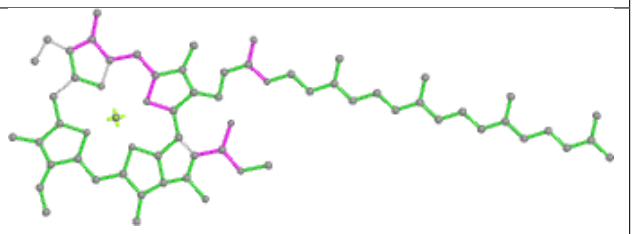
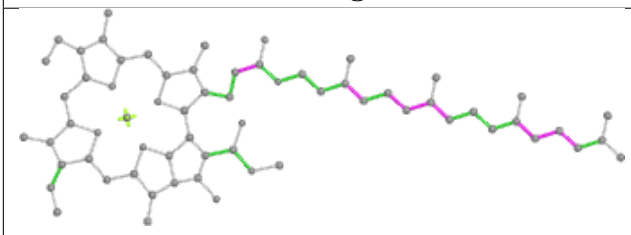
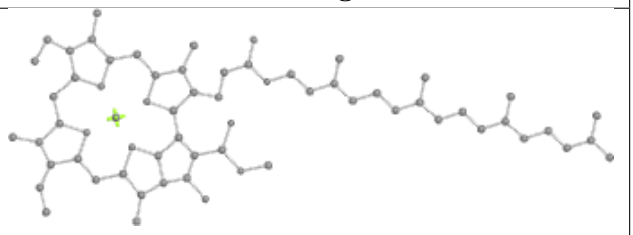


Bond angles

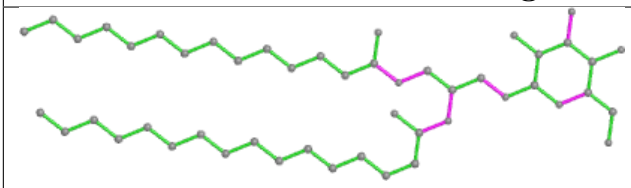


Torsions

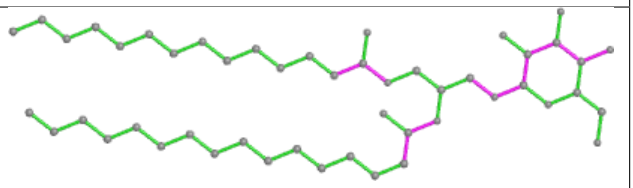


Rings

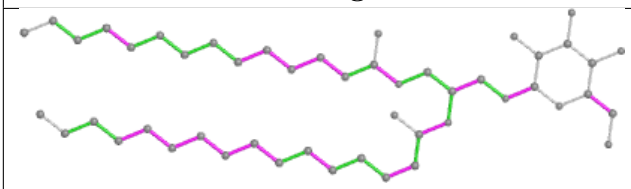
Ligand LMG B 622



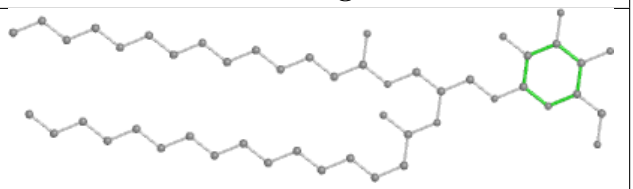
Bond lengths



Bond angles

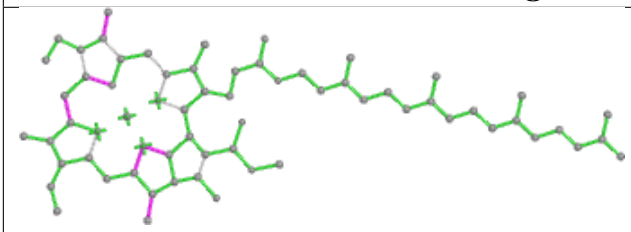


Torsions



Rings

Ligand CLA B 611



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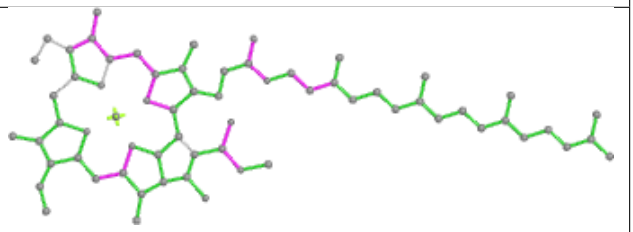
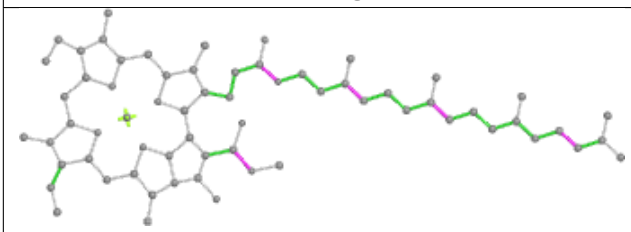
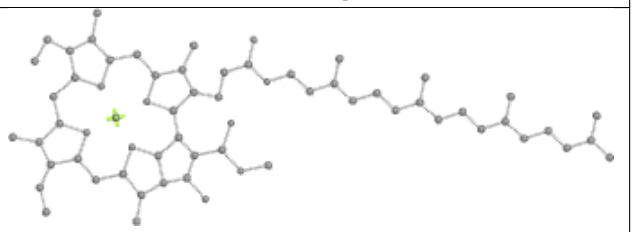


Bond angles

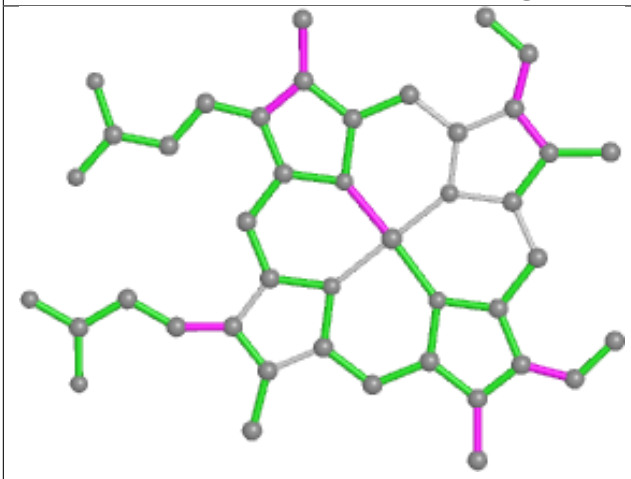


Torsions

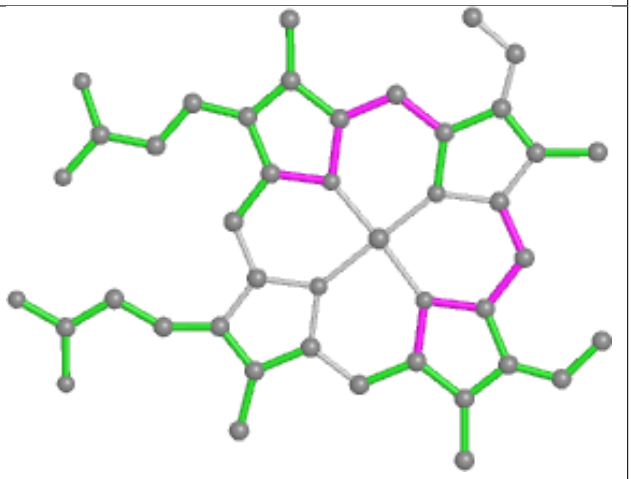


Rings

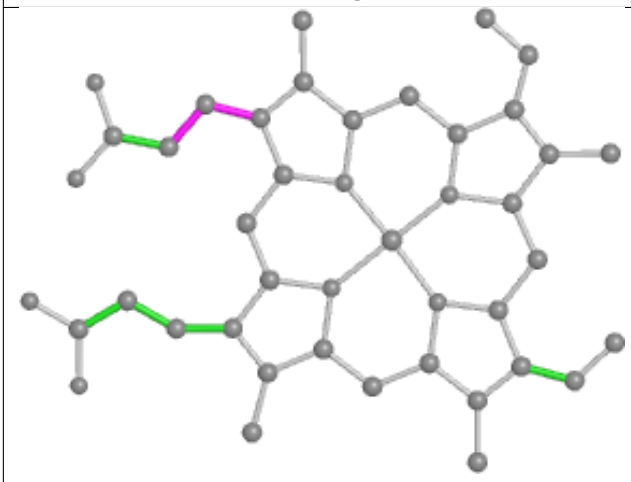
Ligand HEM V 201



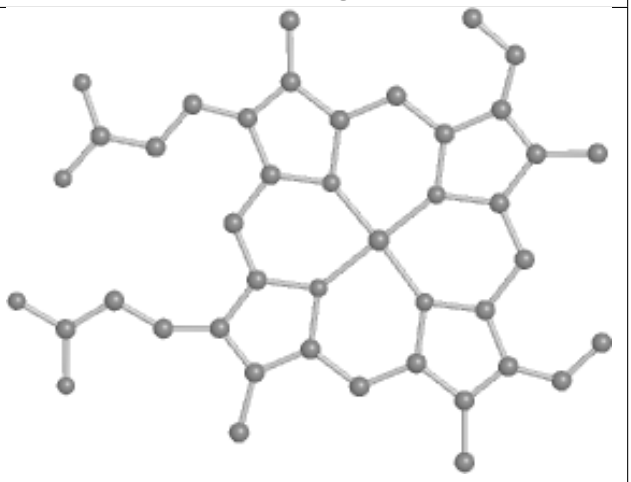
Bond lengths



Bond angles

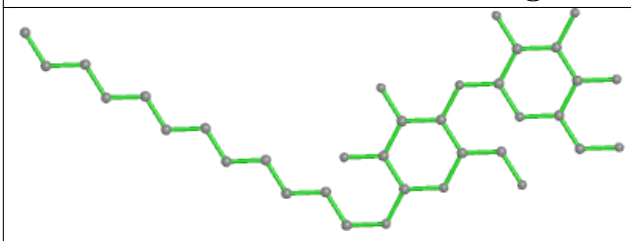


Torsions

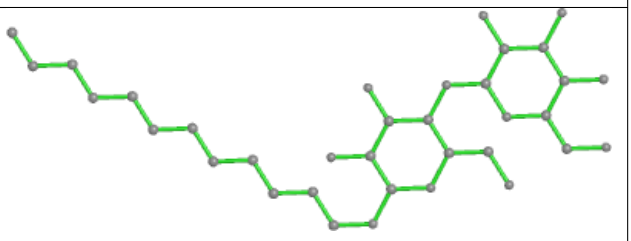


Rings

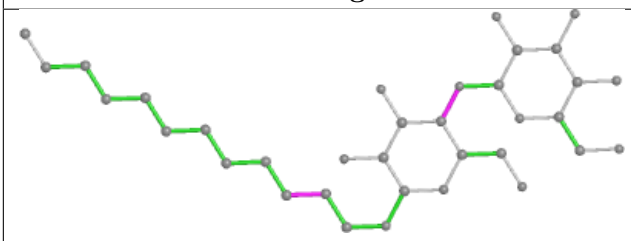
Ligand LMT b 604



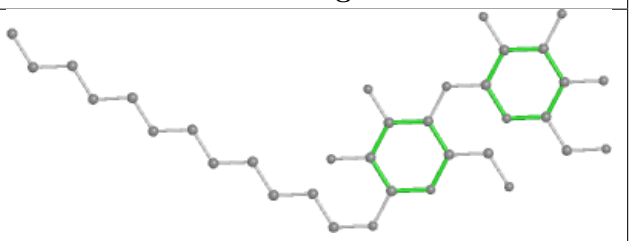
Bond lengths



Bond angles

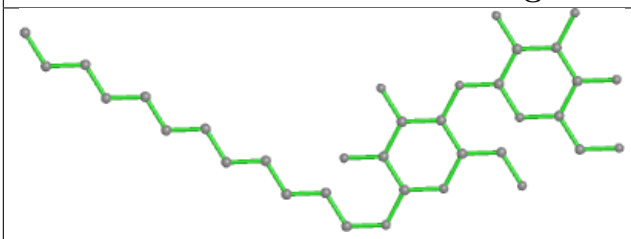


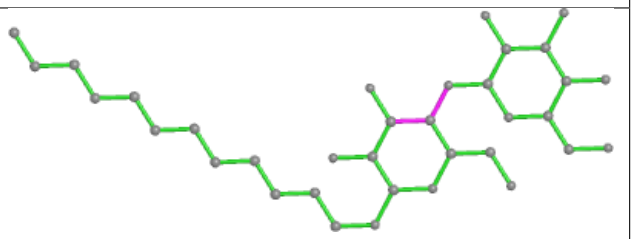
Torsions

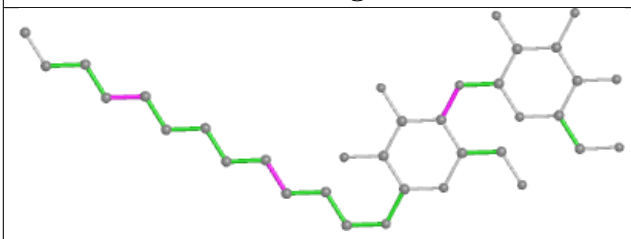


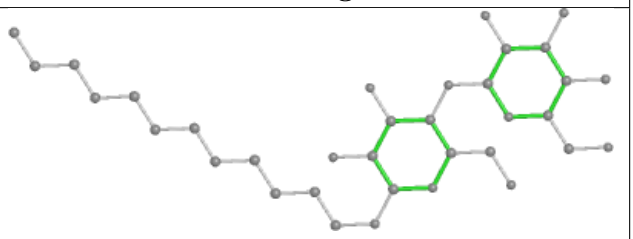
Rings

Ligand LMT b 603

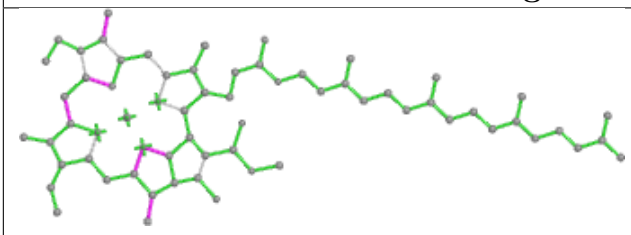

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA D 403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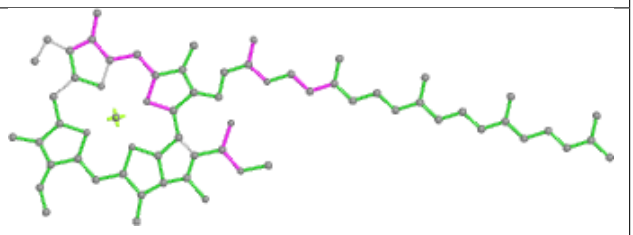
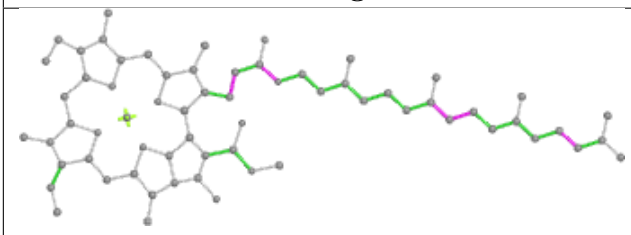
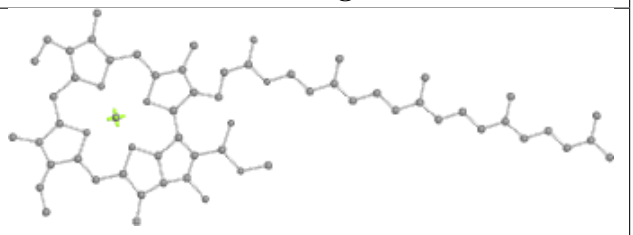
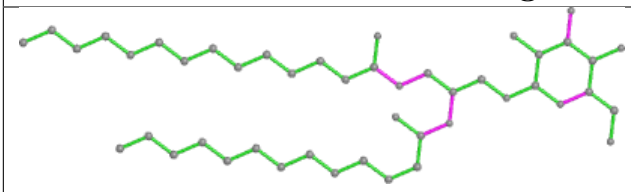
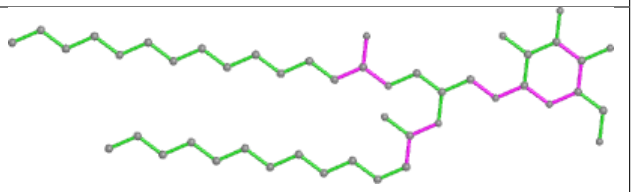

Bond angles

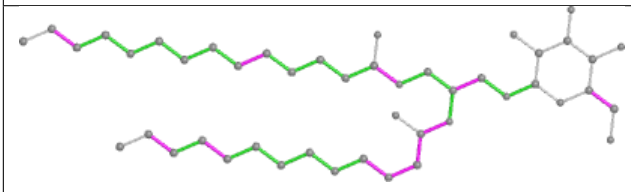

Torsions

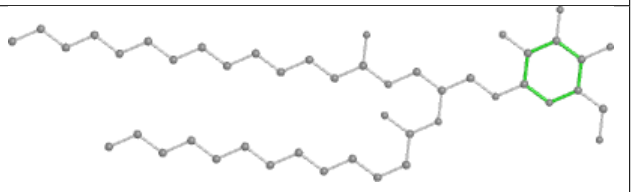

Rings

Ligand LMG D 406

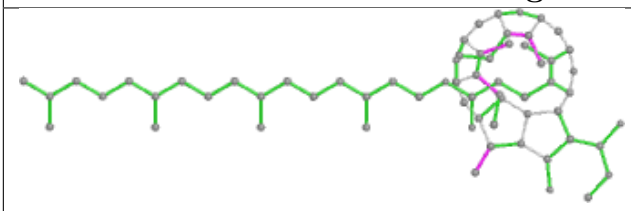

Bond lengths


Bond angles

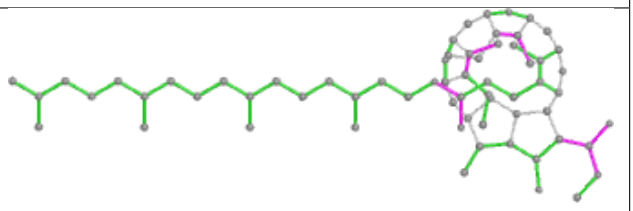

Torsions


Rings

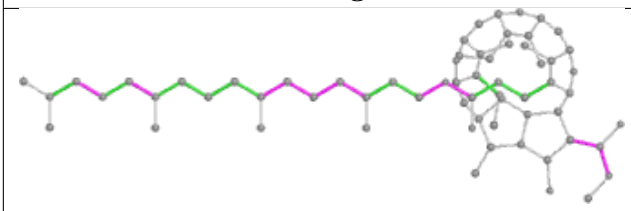
Ligand PHO a 407



Bond lengths



Bond angles



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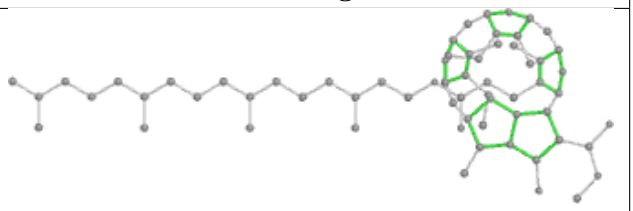
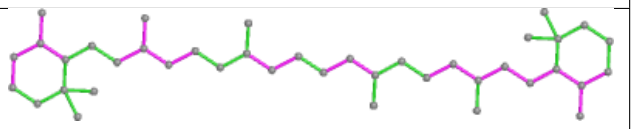


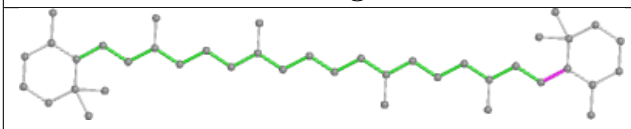
Rings

Ligand BCR a 412

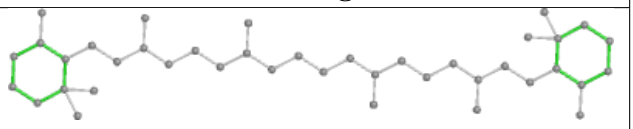
Bond lengths



Bond angles



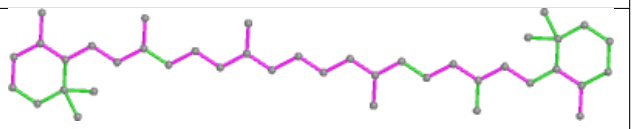
Torsions



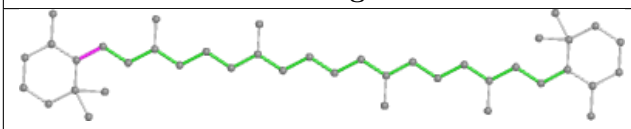
Rings

Ligand BCR h 101

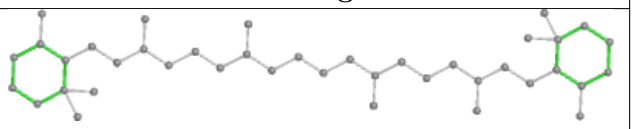
Bond lengths



Bond angles

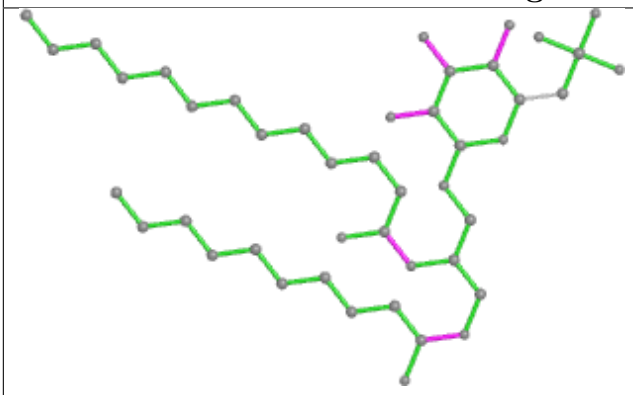


Torsions

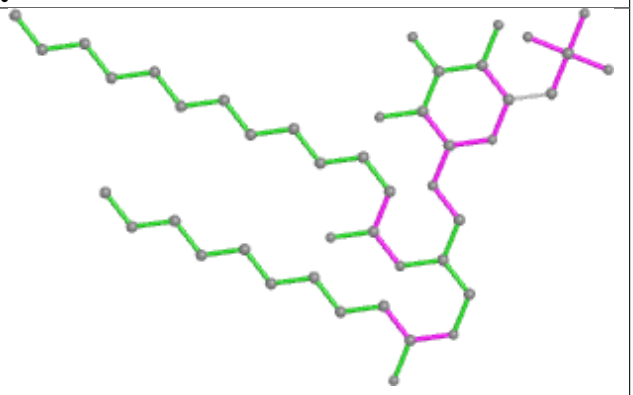


Rings

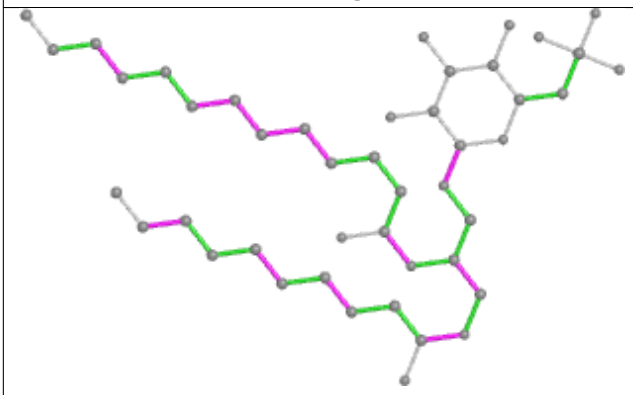
Ligand SQD F 102



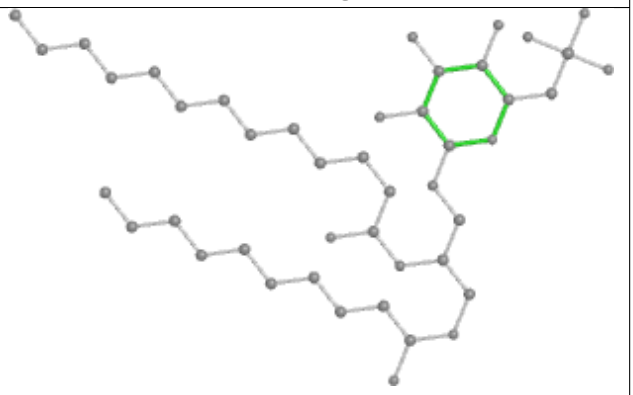
Bond lengths



Bond angles

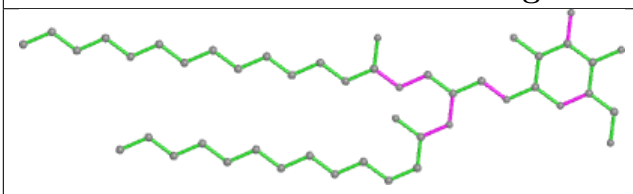


Torsions

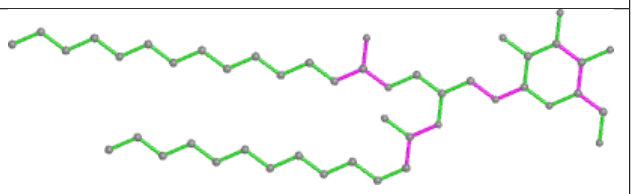


Rings

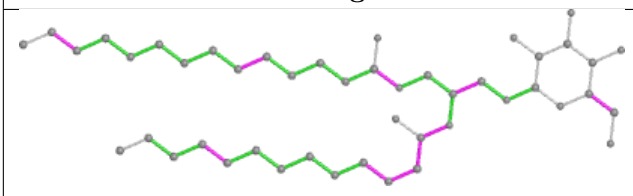
Ligand LMG d 406



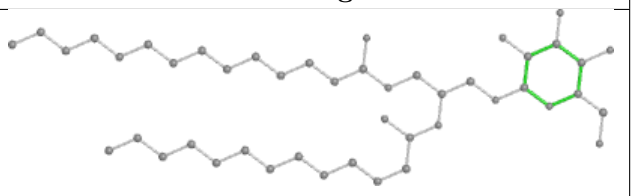
Bond lengths



Bond angles

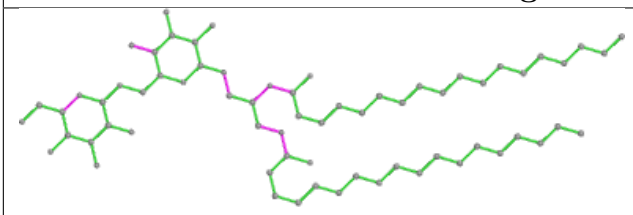


Torsions



Rings

Ligand DGD C 519



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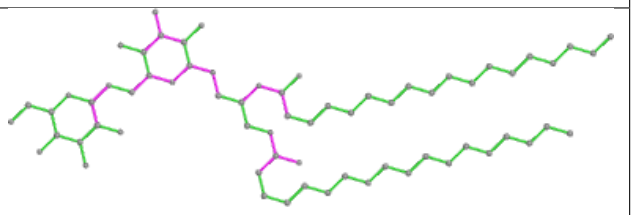
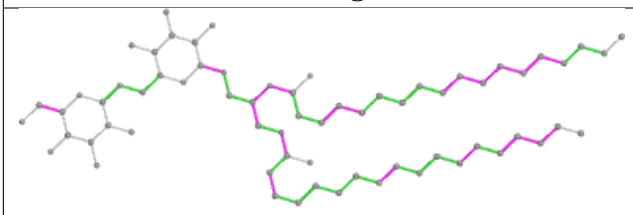
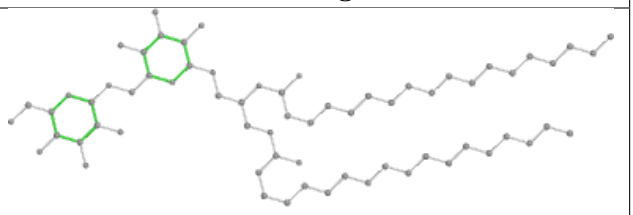


Bond angles

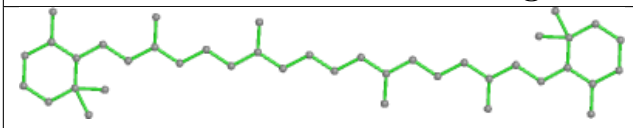


Torsions

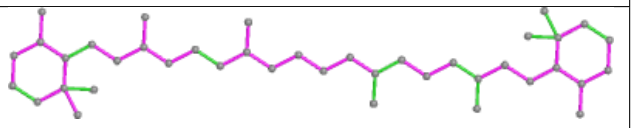


Rings

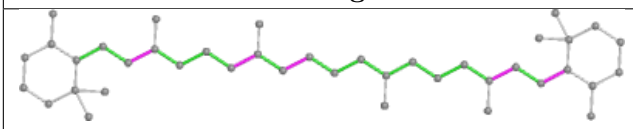
Ligand BCR B 618



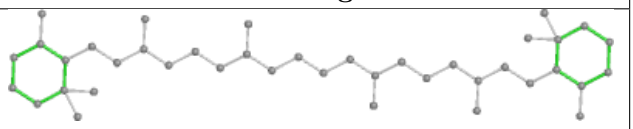
Bond lengths



Bond angles

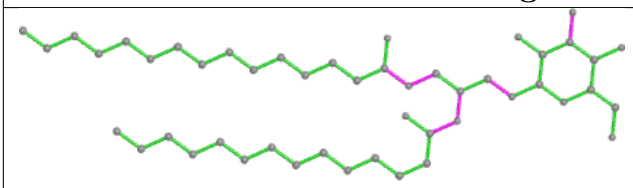


Torsions

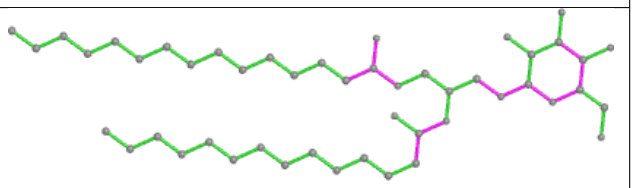


Rings

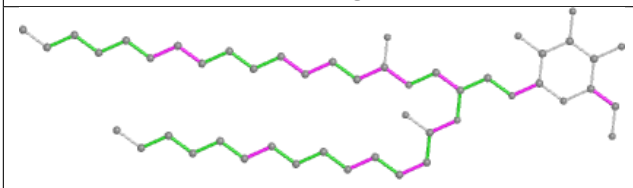
Ligand LMG C 520



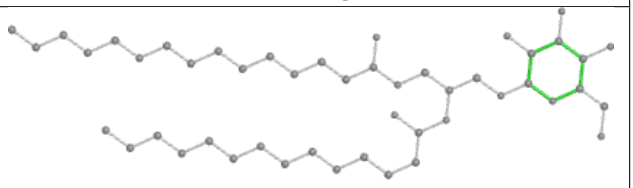
Bond lengths



Bond angles

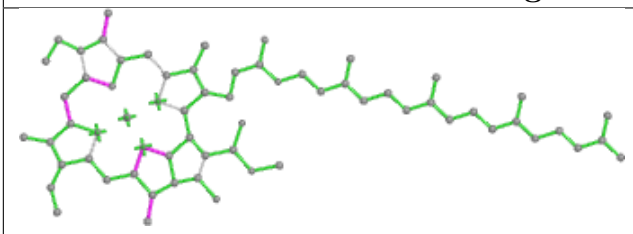


Torsions

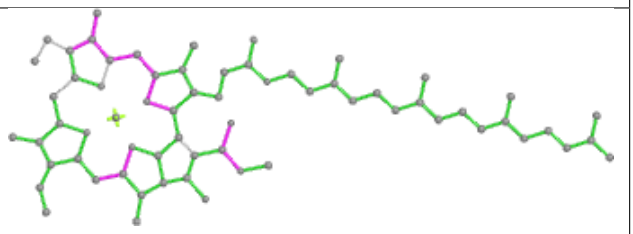


Rings

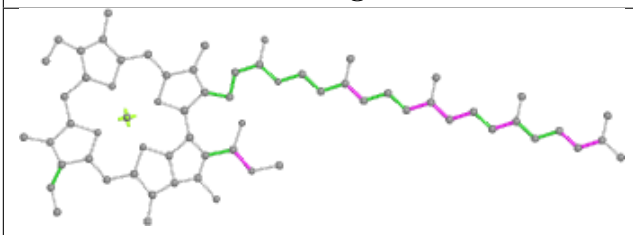
Ligand CLA B 603



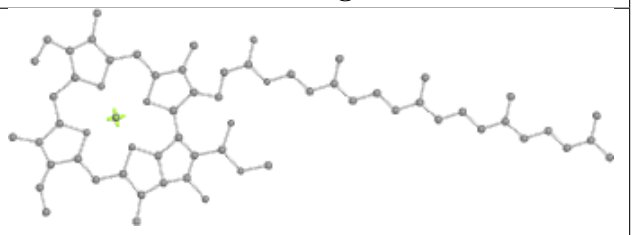
Bond lengths



Bond angles

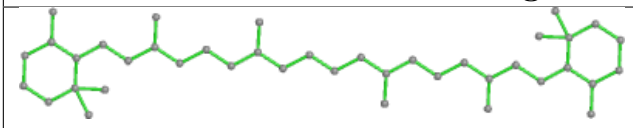


Torsions

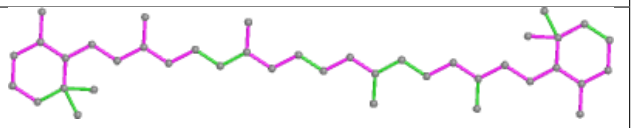


Rings

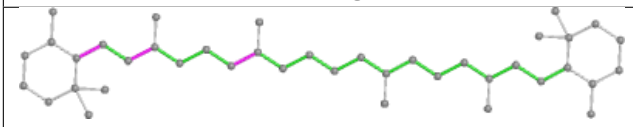
Ligand BCR C 514



Bond lengths



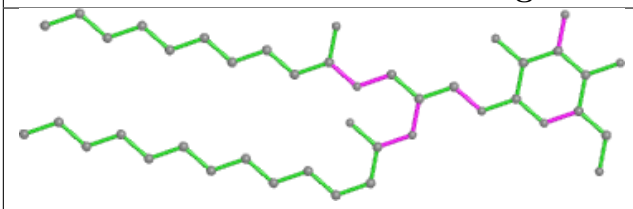
Bond angles



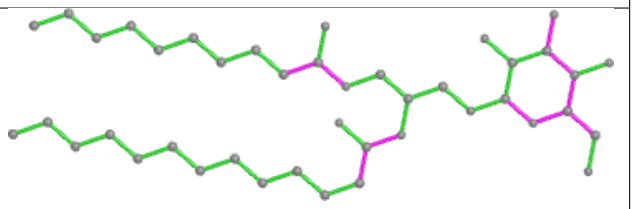
Torsions

Rings

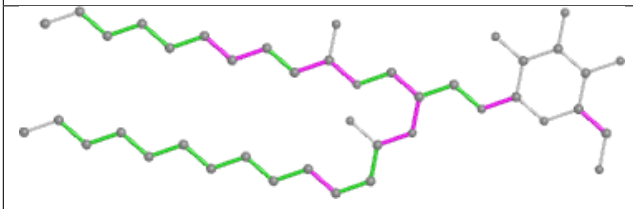
Ligand LMG M 101



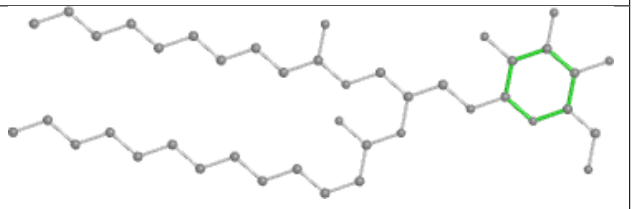
Bond lengths



Bond angles

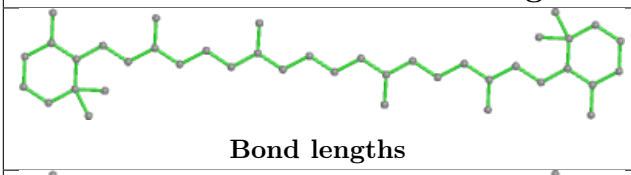


Torsions

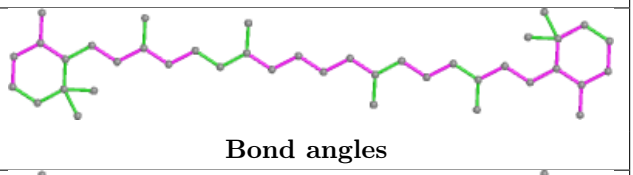


Rings

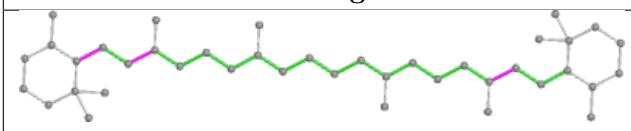
Ligand BCR d 405



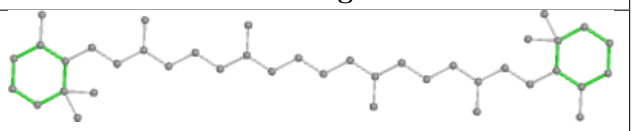
Bond lengths



Bond angles

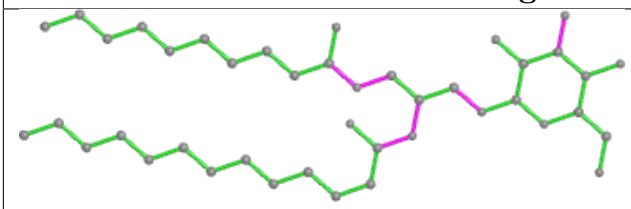


Torsions

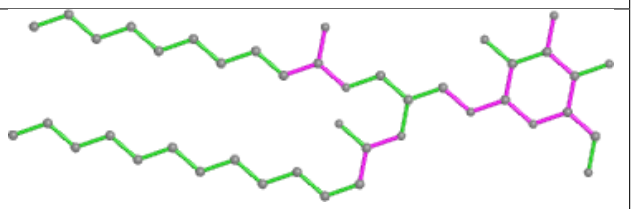


Rings

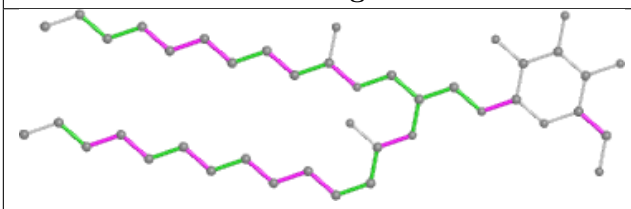
Ligand LMG A 418



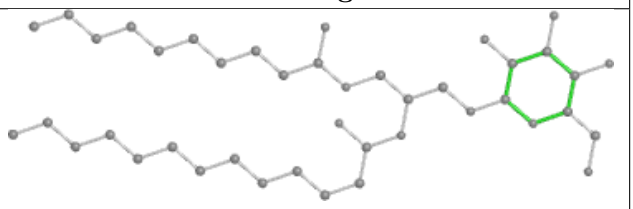
Bond lengths



Bond angles

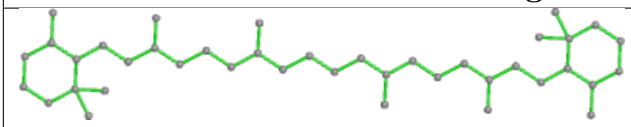


Torsions

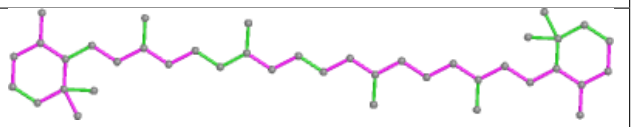


Rings

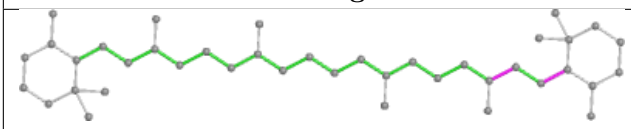
Ligand BCR b 622



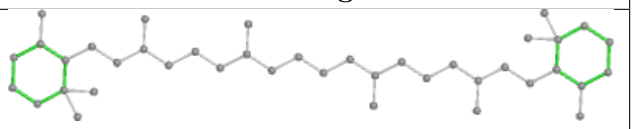
Bond lengths



Bond angles

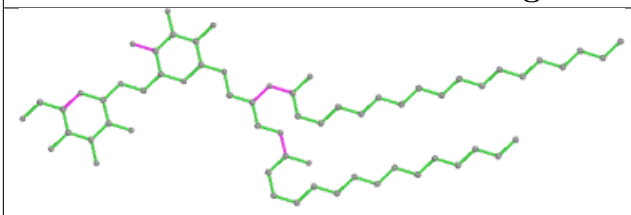


Torsions

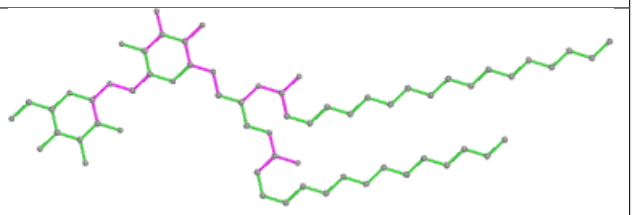


Rings

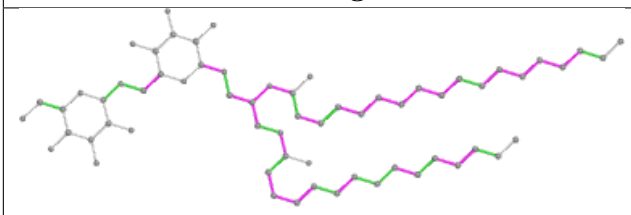
Ligand DGD d 409



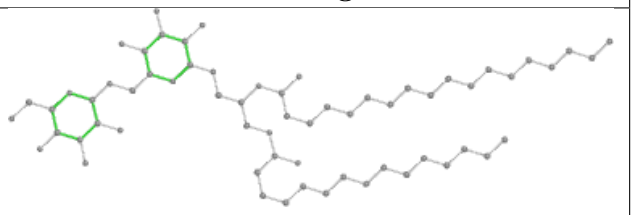
Bond lengths



Bond angles

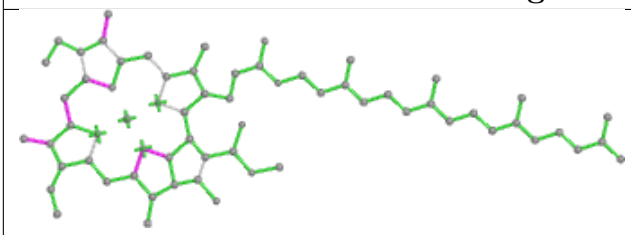


Torsions

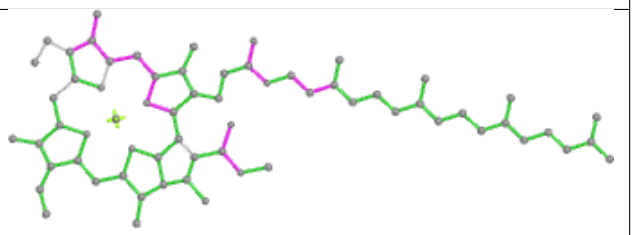


Rings

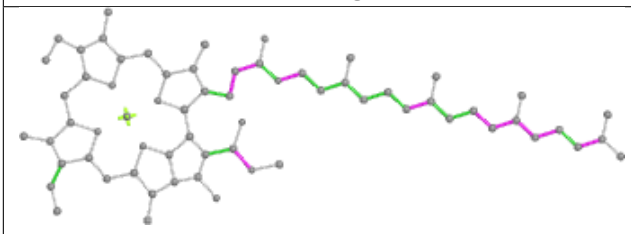
Ligand CLA b 605



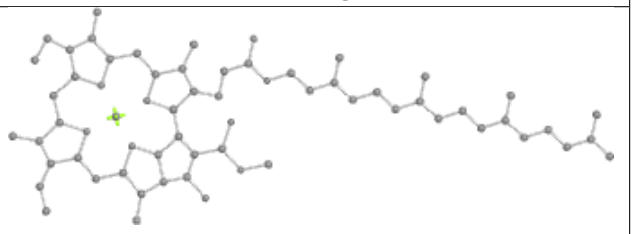
Bond lengths



Bond angles

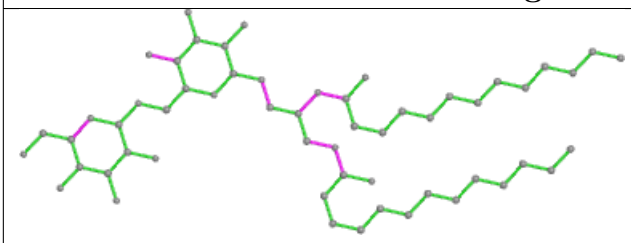


Torsions

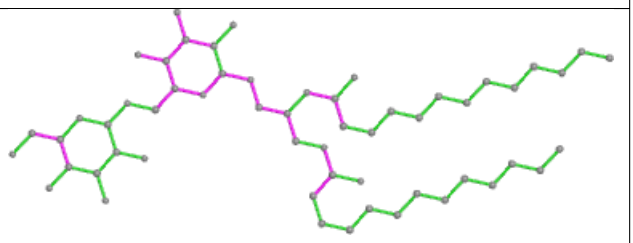


Rings

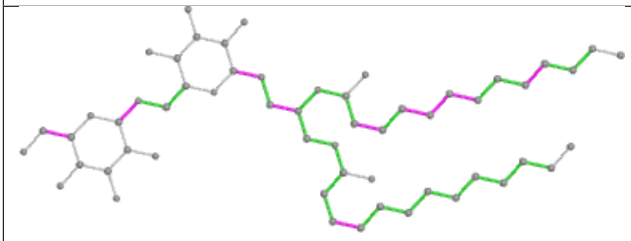
Ligand DGD a 413



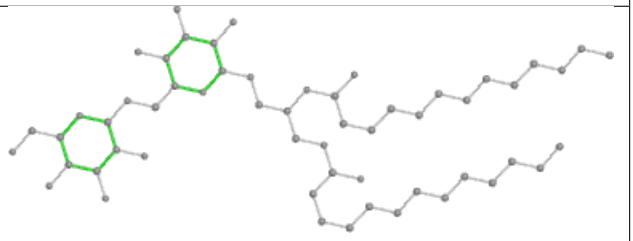
Bond lengths



Bond angles

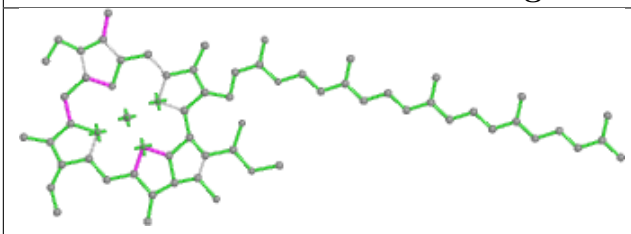


Torsions

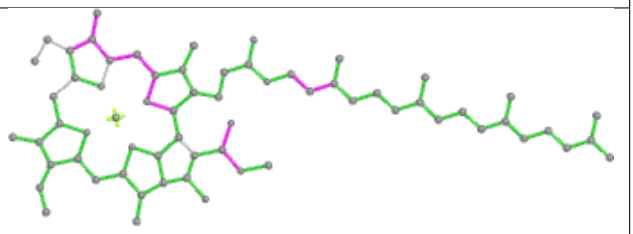


Rings

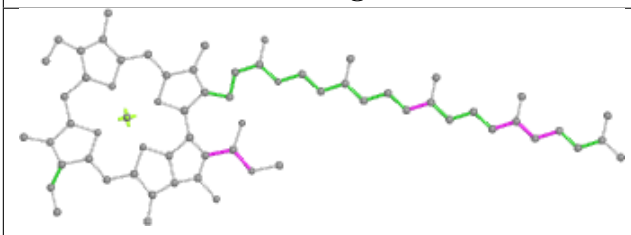
Ligand CLA B 609



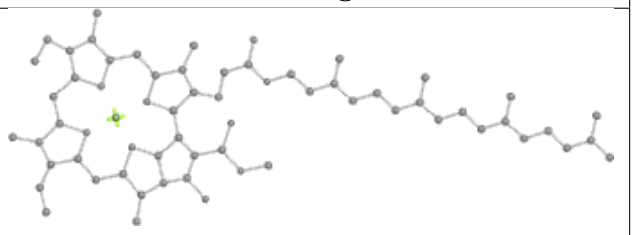
Bond lengths



Bond angles

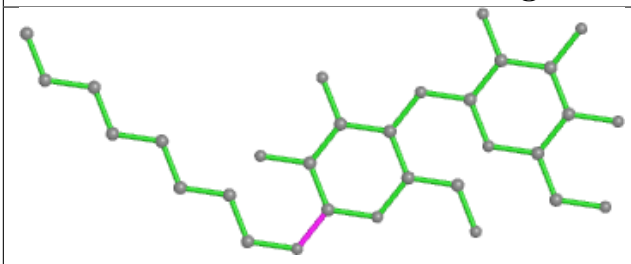


Torsions



Rings

Ligand LMT D 410



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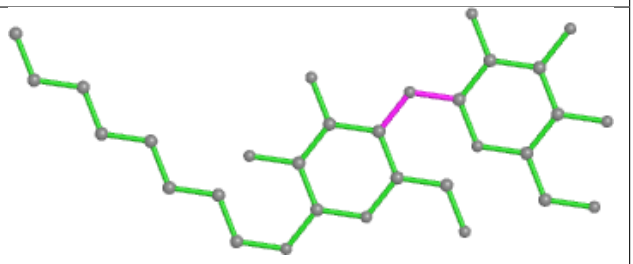
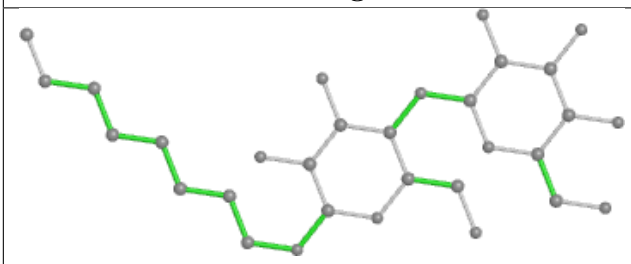


Bond angles



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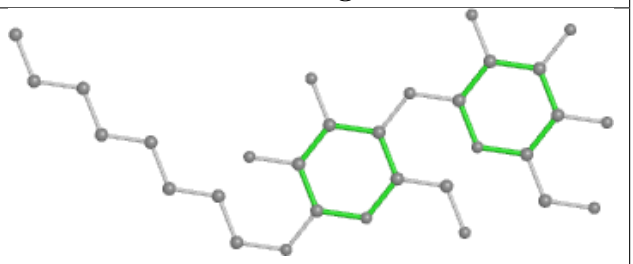
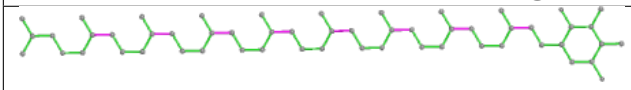


Rings

Ligand PL9 D 404



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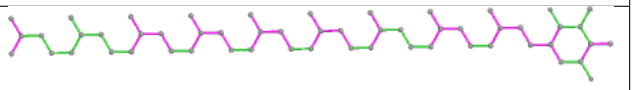
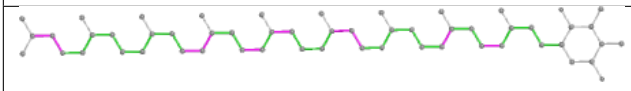


Bond angles



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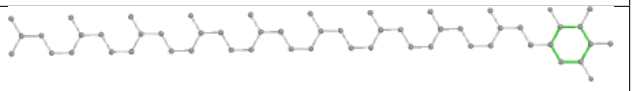
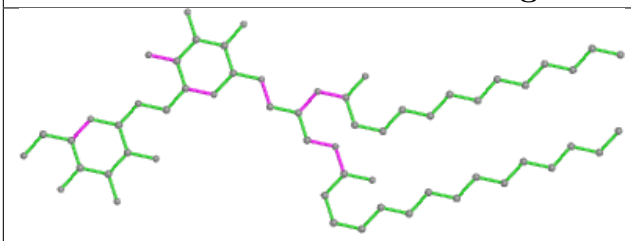
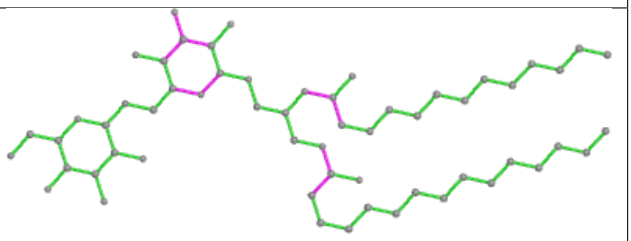


Rings

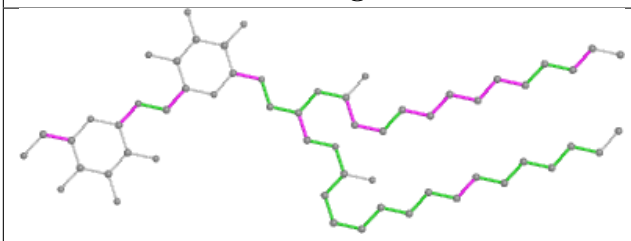
Ligand DGD B 621



Bond lengths



Bond angles



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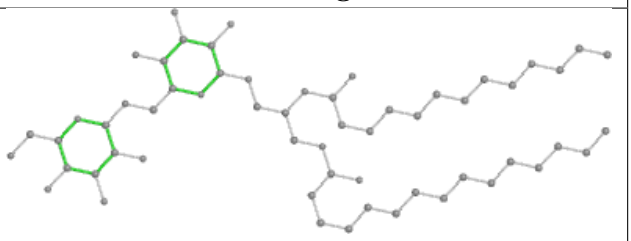
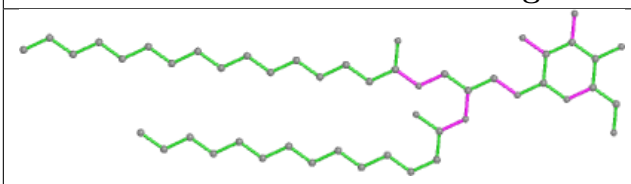
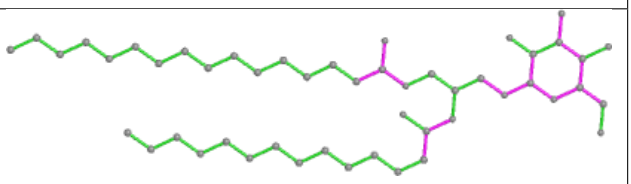


Rings

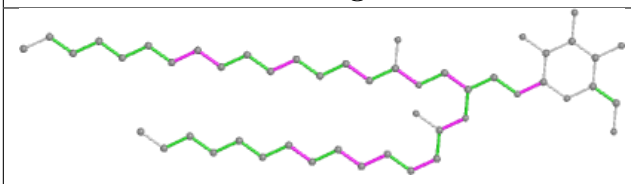
Ligand LMG b 625



Bond lengths



Bond angles



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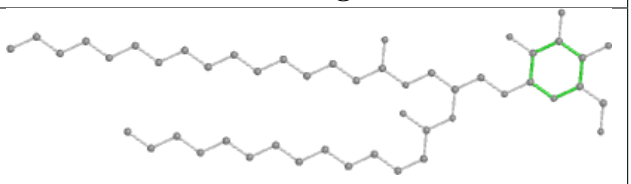
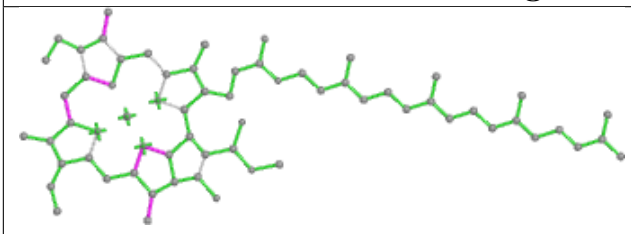


Rings

Ligand CLA C 505



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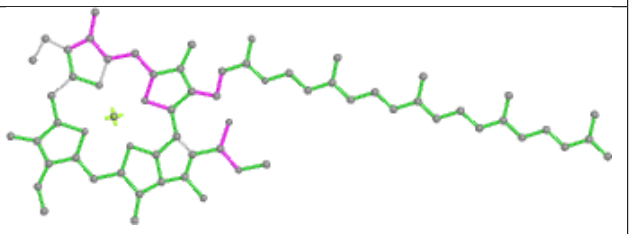
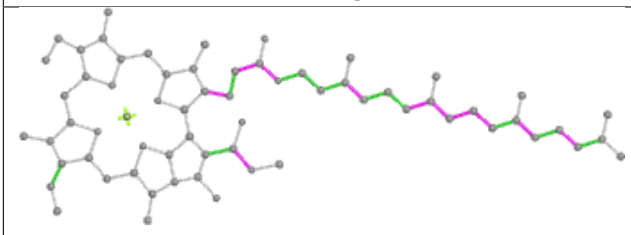


Bond angles



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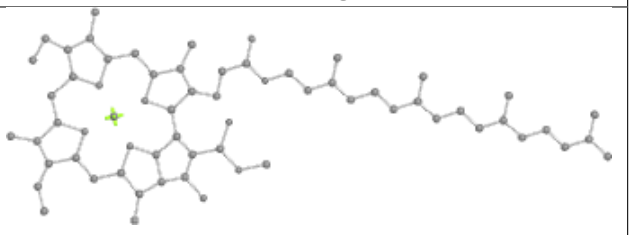
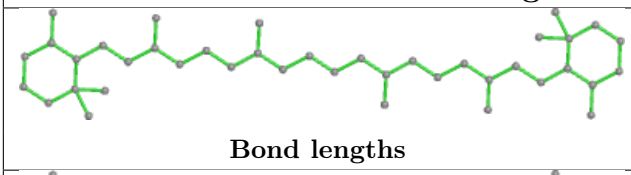


Rings

Ligand BCR C 516



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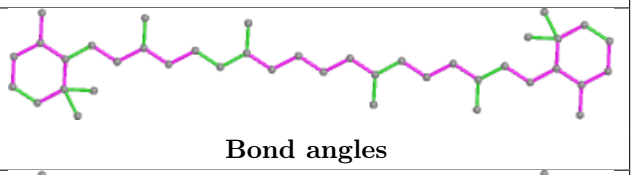
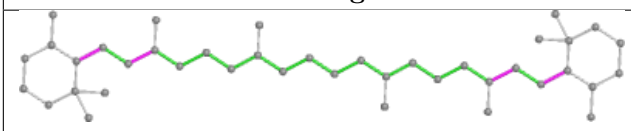


Bond angles



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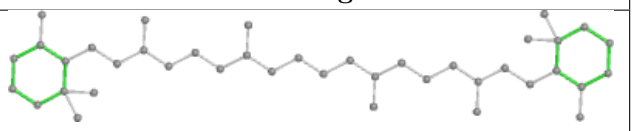
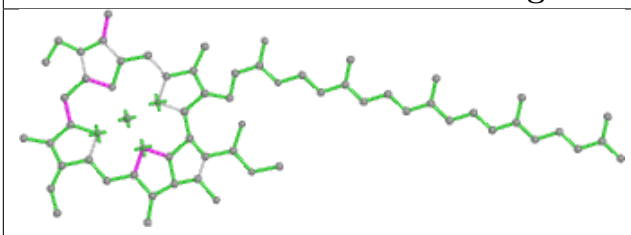


Rings

Ligand CLA b 613



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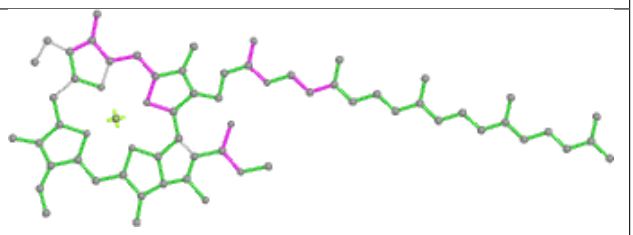
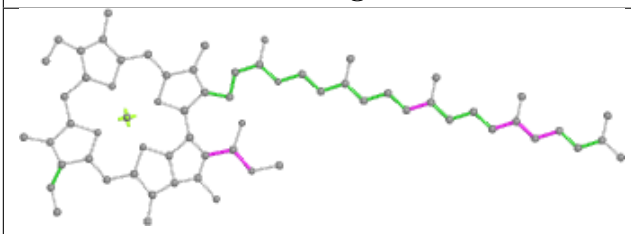


Bond angles



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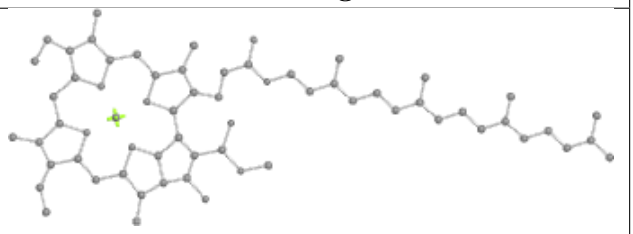
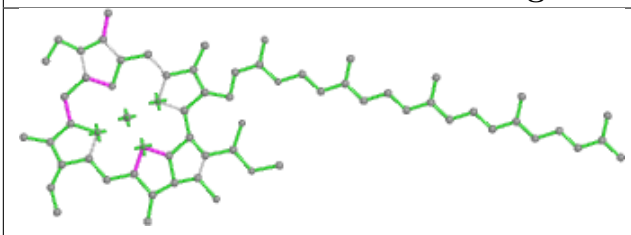


Rings

Ligand CLA b 615



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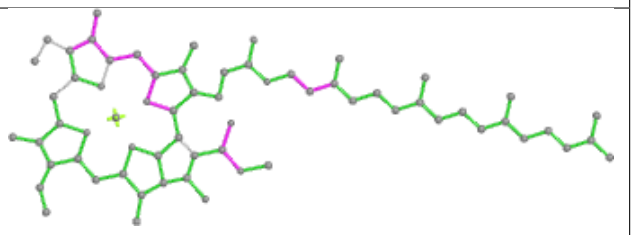
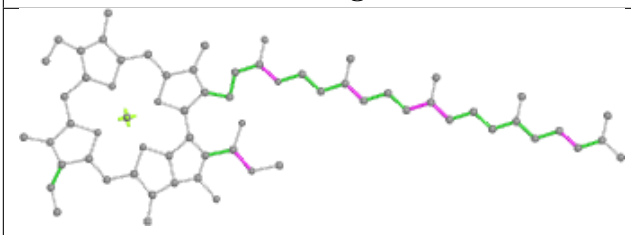
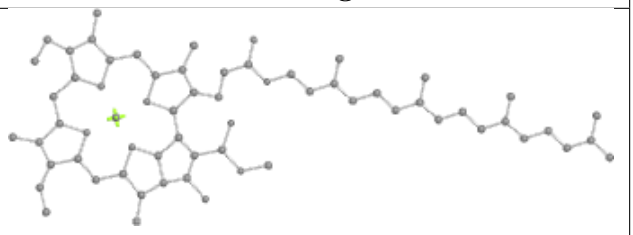


Bond angles

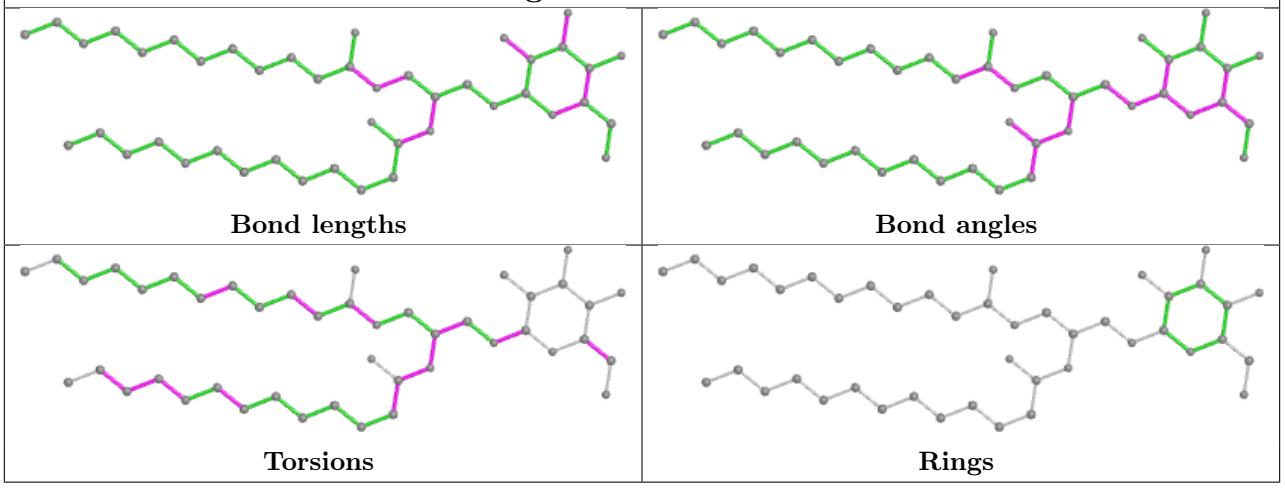


Torsions

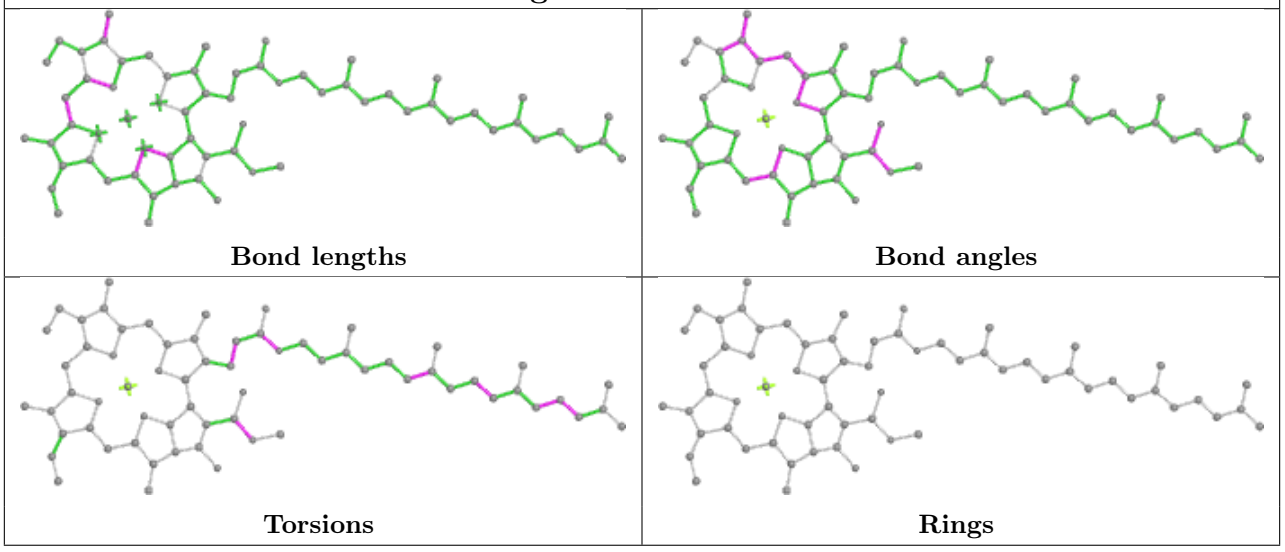


Rings

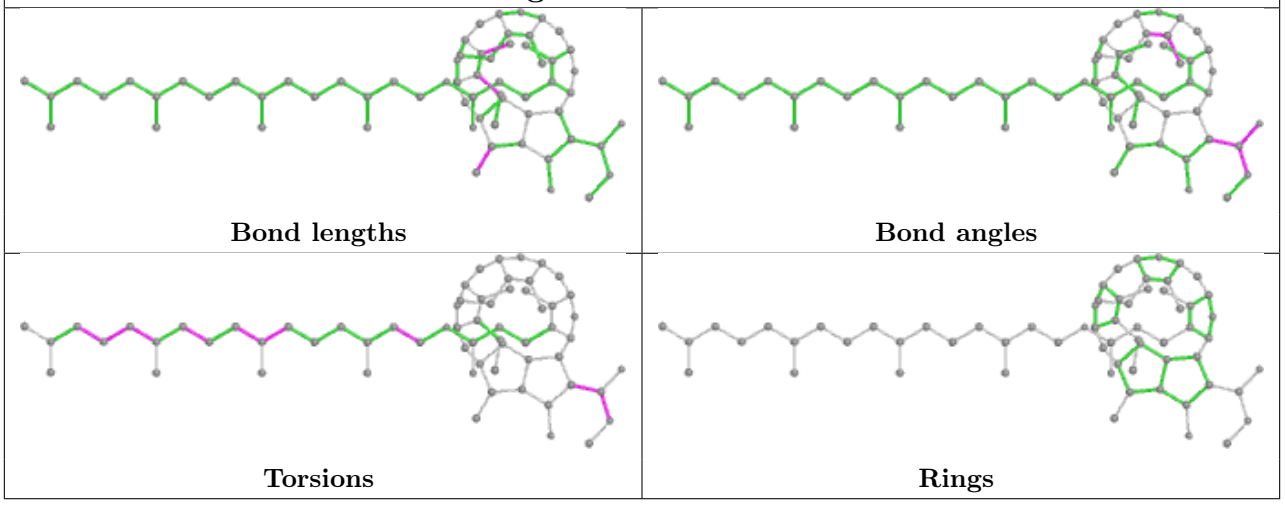
Ligand LMG e 101



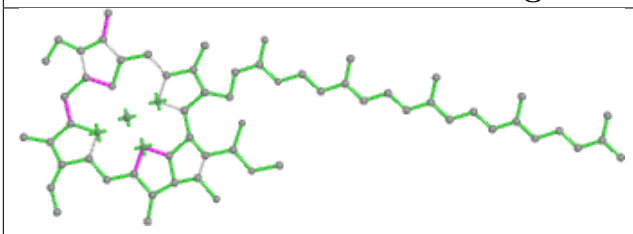
Ligand CLA c 504



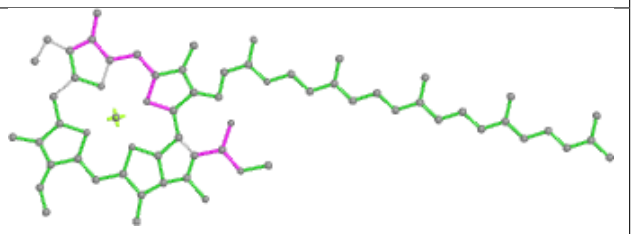
Ligand PHO a 408



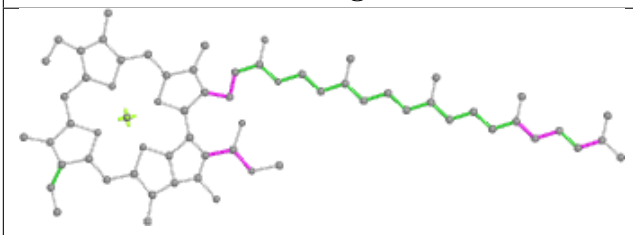
Ligand CLA B 606



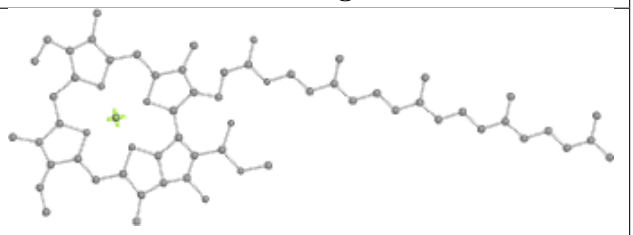
Bond lengths



Bond angles

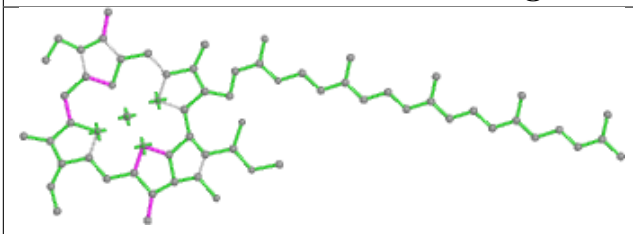


Torsions



Rings

Ligand CLA B 612



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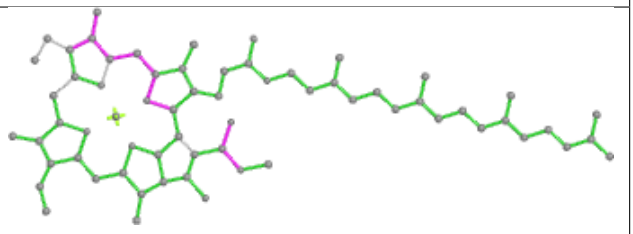
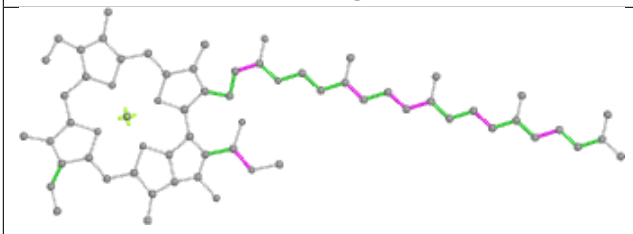


Bond angles



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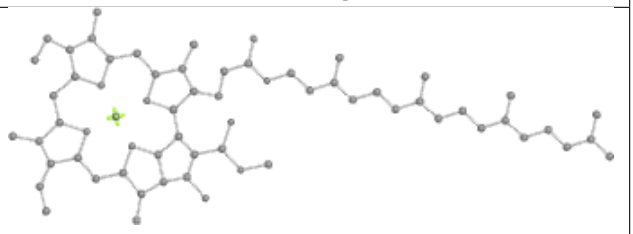
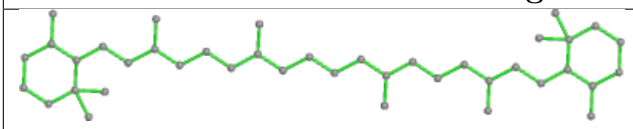
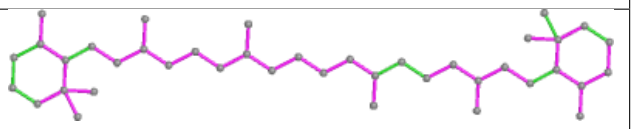


Rings

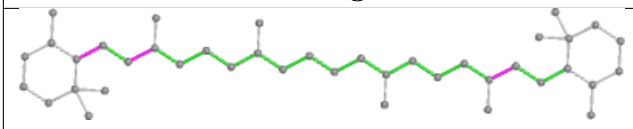
Ligand BCR J 102



Bond lengths



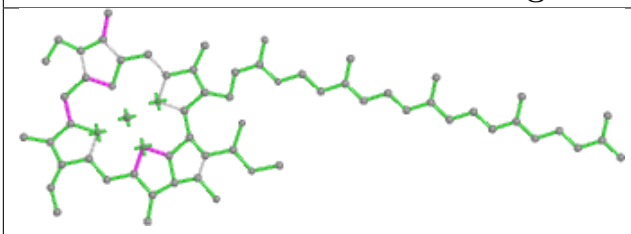
Bond angles



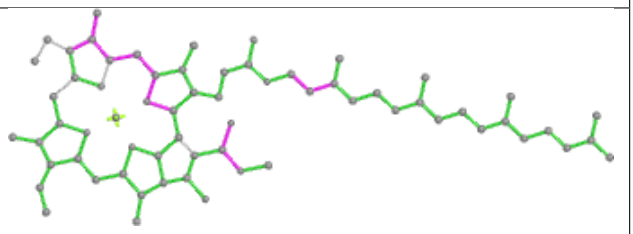
Torsions

Rings

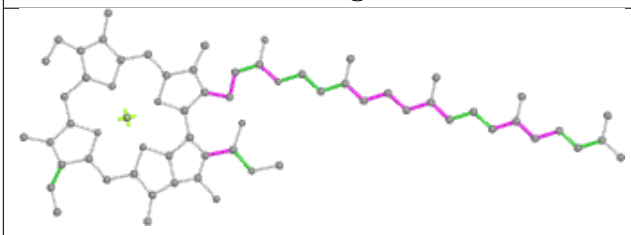
Ligand CLA b 606



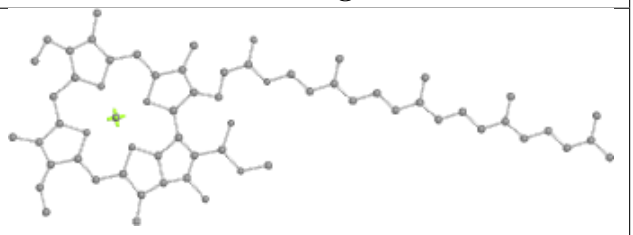
Bond lengths



Bond angles

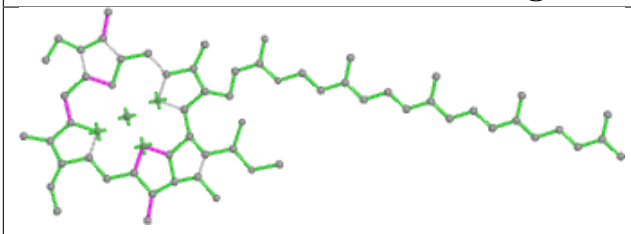


Torsions

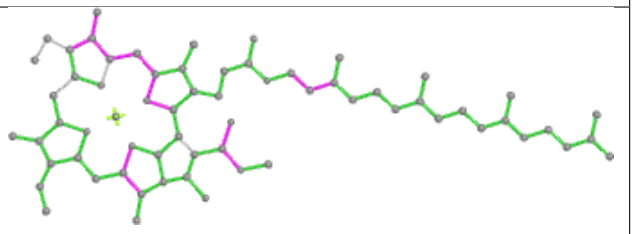


Rings

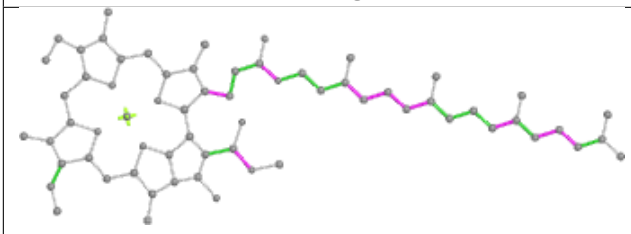
Ligand CLA b 612



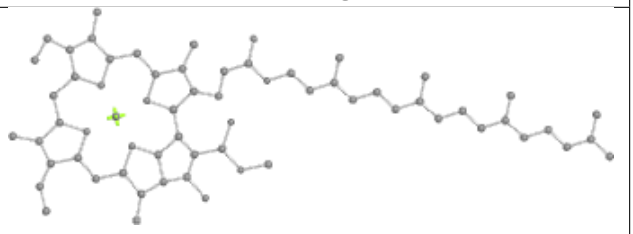
Bond lengths



Bond angles

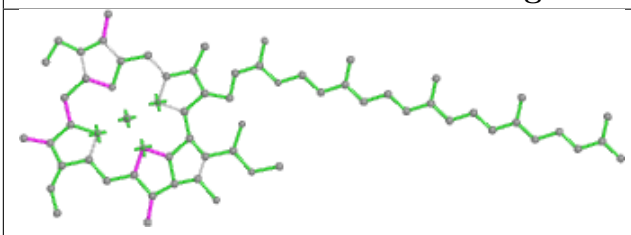


Torsions

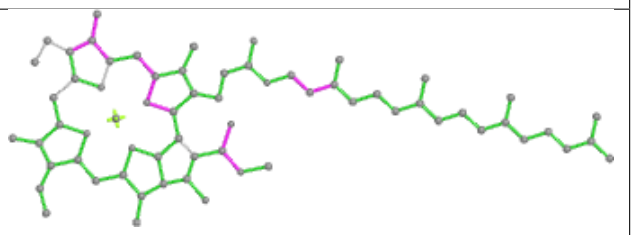


Rings

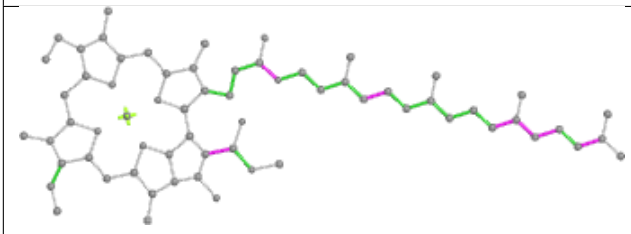
Ligand CLA C 502



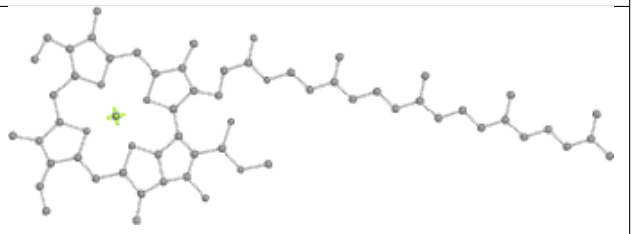
Bond lengths



Bond angles

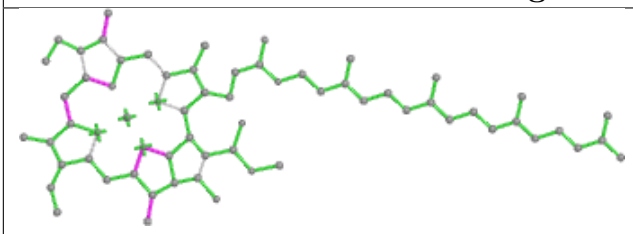


Torsions



Rings

Ligand CLA a 404



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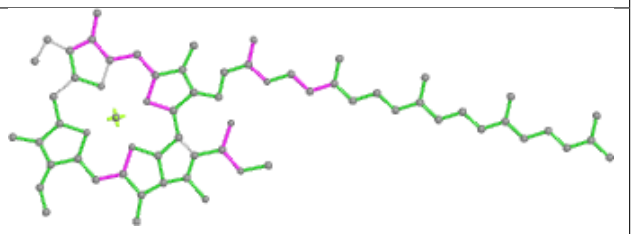

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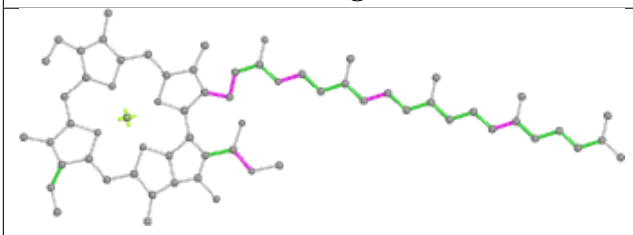

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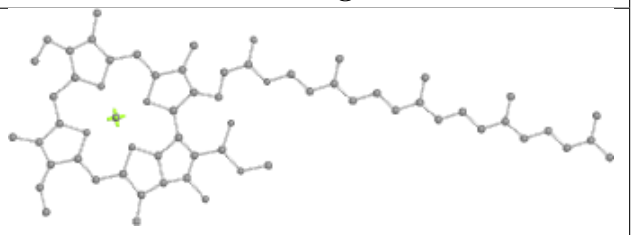
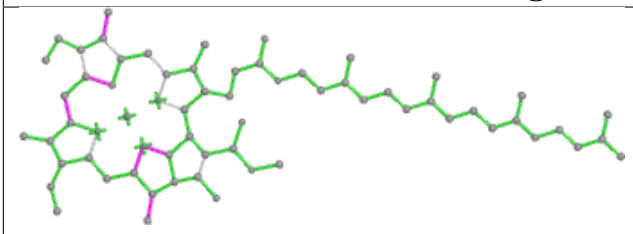


Rings

Ligand CLA d 403



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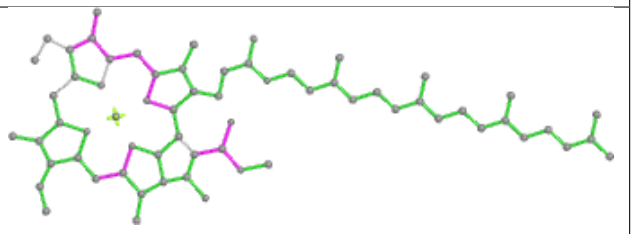
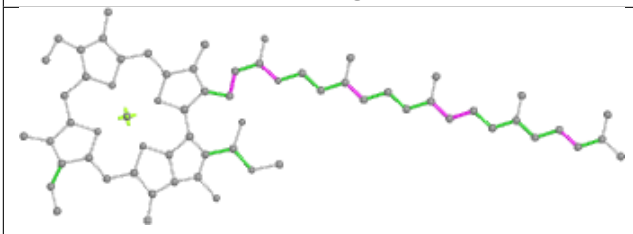


Bond angles



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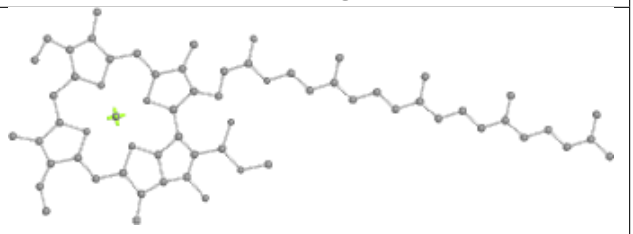
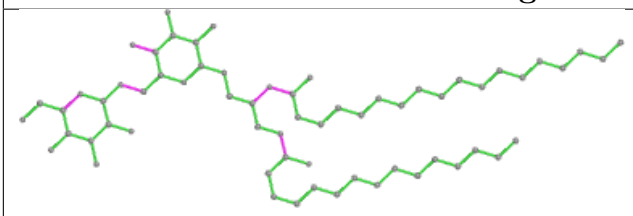


Rings

Ligand DGD D 409



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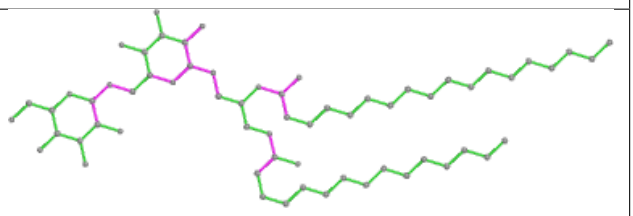

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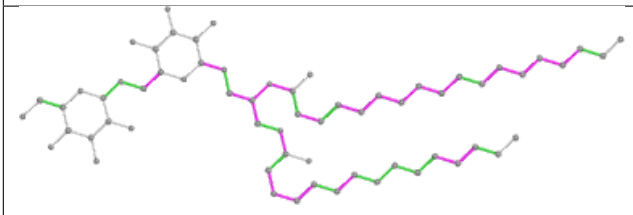

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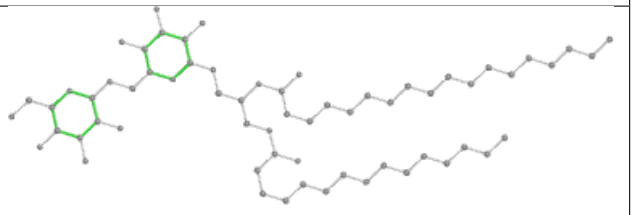
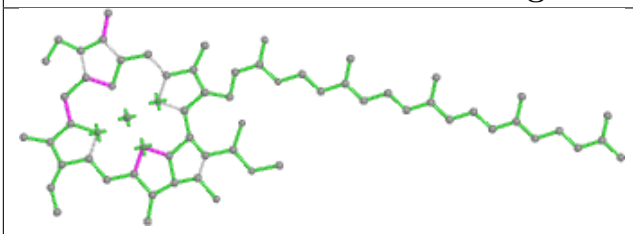


Rings

Ligand CLA b 614



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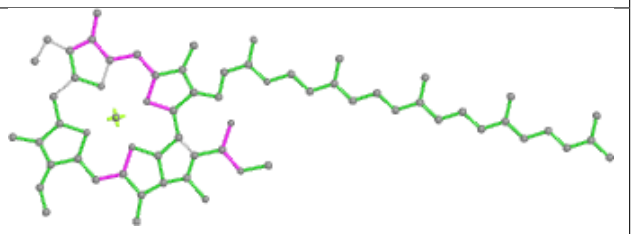
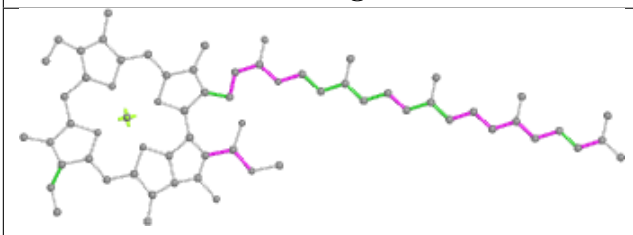


Bond angles



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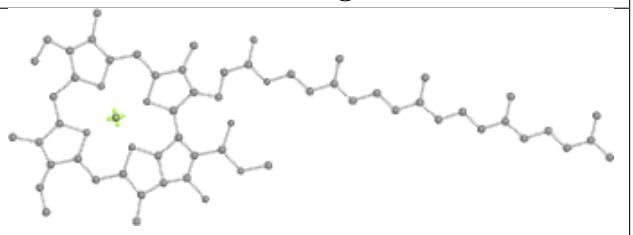
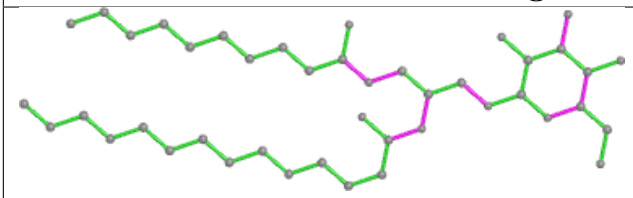


Rings

Ligand LMG i 101



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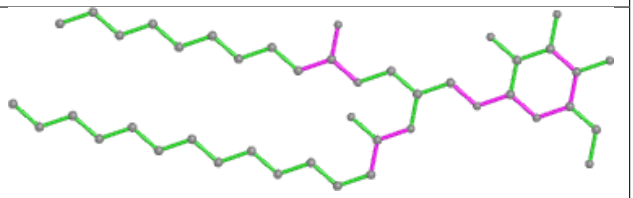
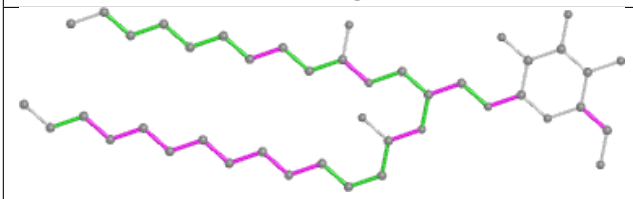


Bond angles



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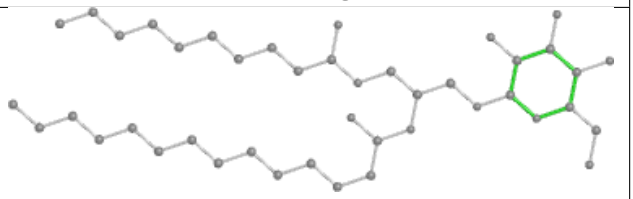
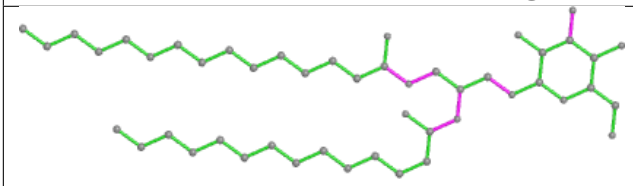


Rings

Ligand LMG k 103



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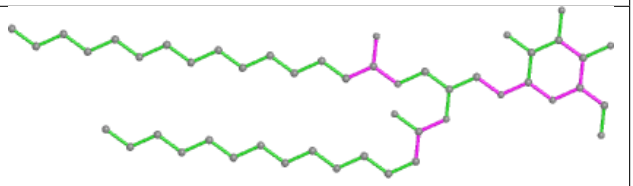
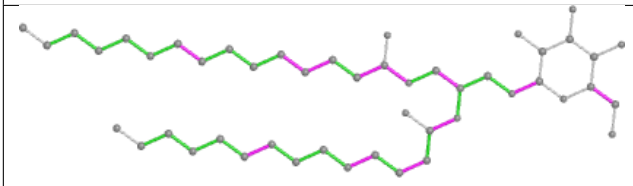


Bond angles



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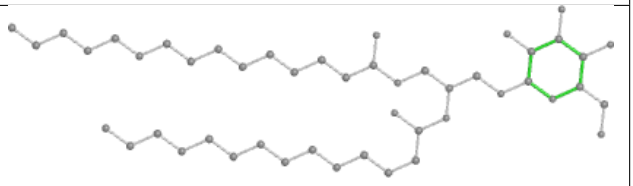
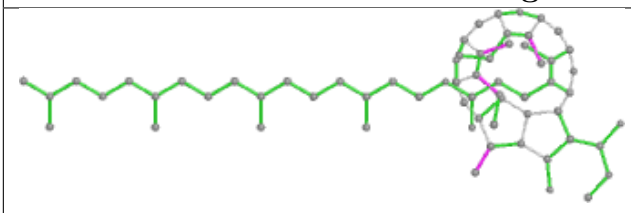


Rings

Ligand PHO A 406



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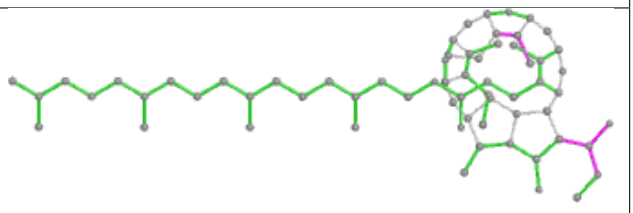
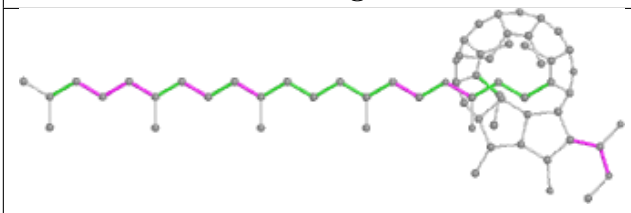


Bond angles



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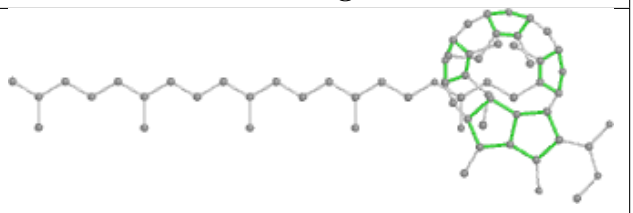
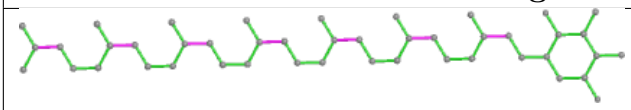


Rings

Ligand PL9 A 408



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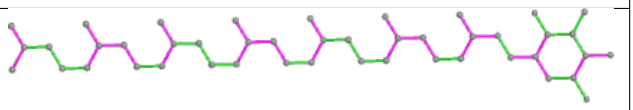
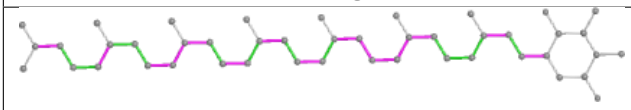
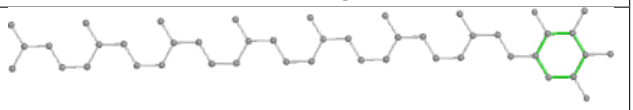


Bond angles

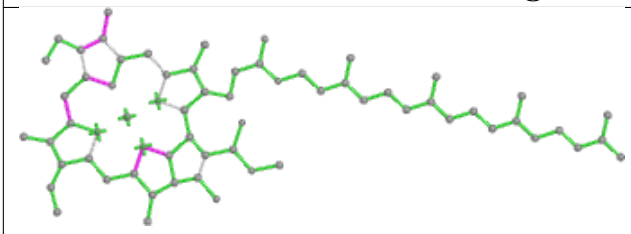


Torsions



Rings

Ligand CLA C 509



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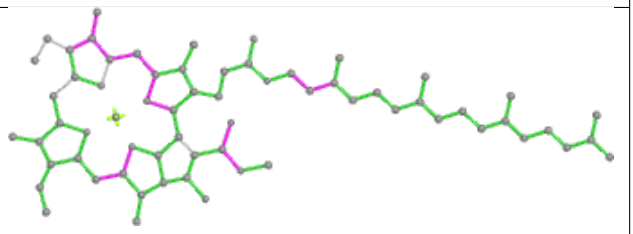
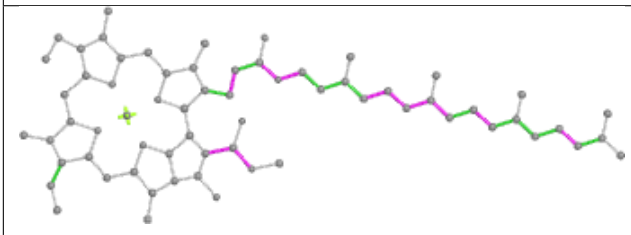


Bond angles



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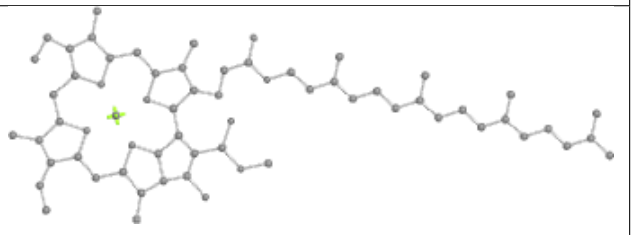
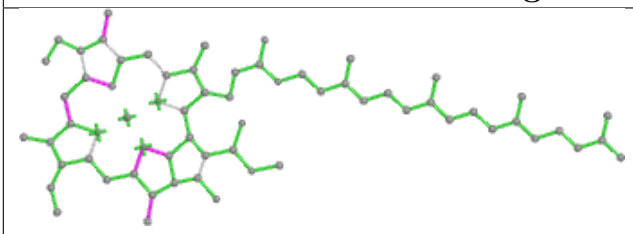


Rings

Ligand CLA D 401



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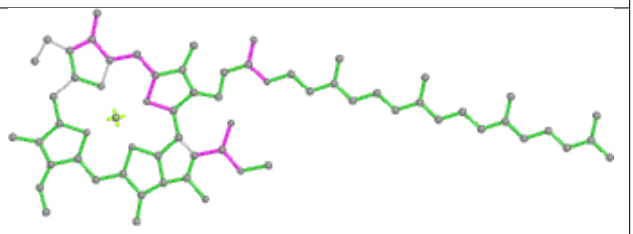
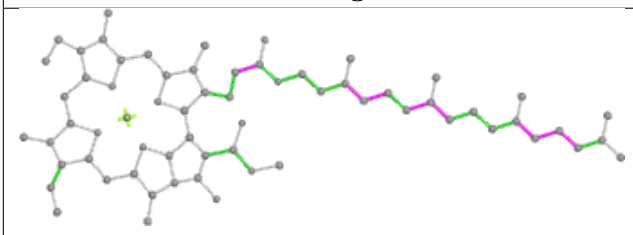


Bond angles



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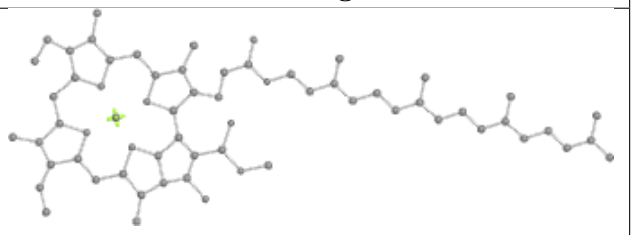
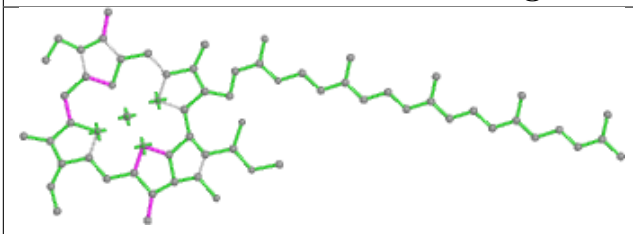


Rings

Ligand CLA A 403



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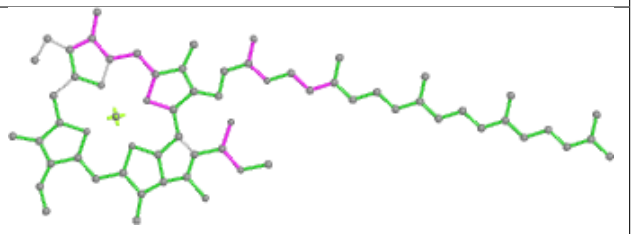
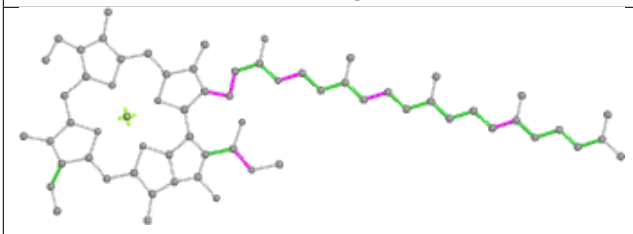


Bond angles



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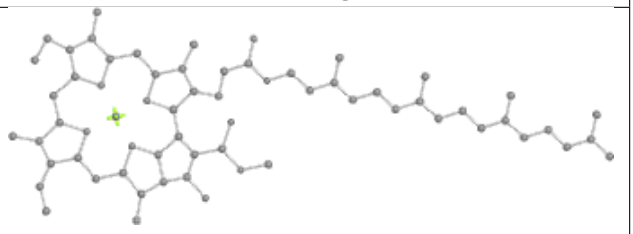
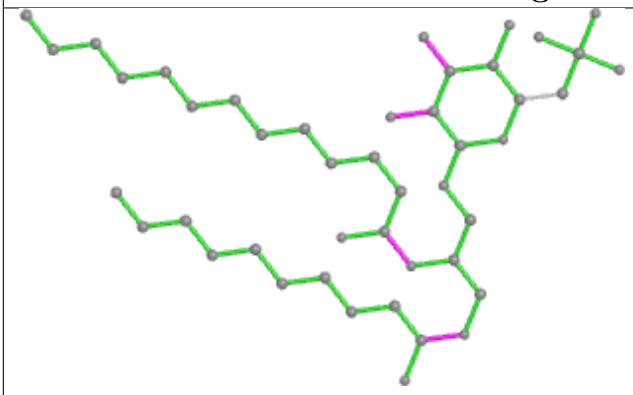
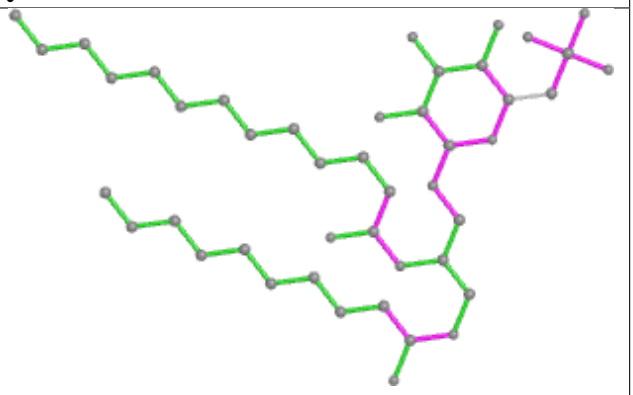


Rings

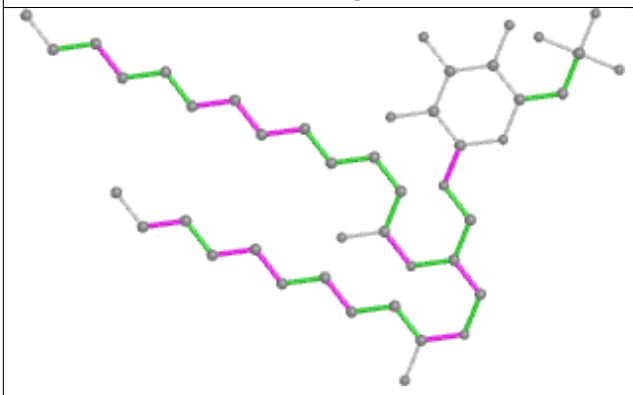
Ligand SQD f 102



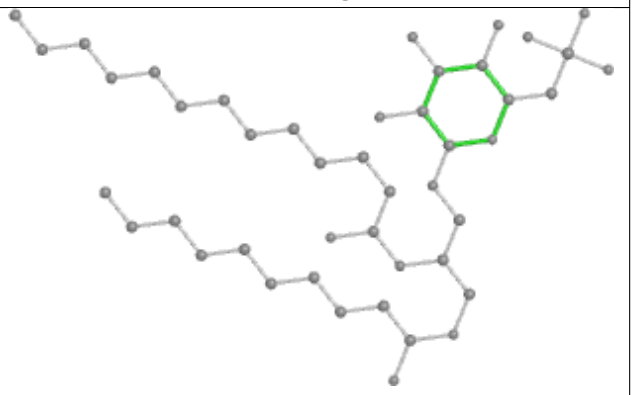
Bond lengths



Bond angles

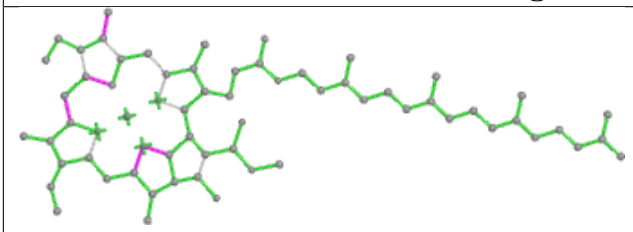


Torsions

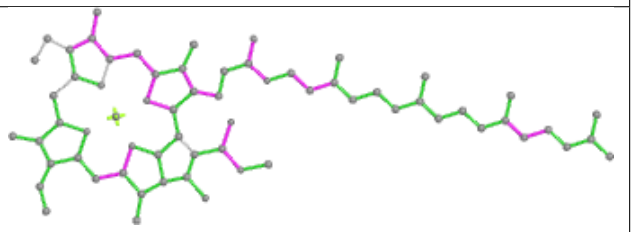


Rings

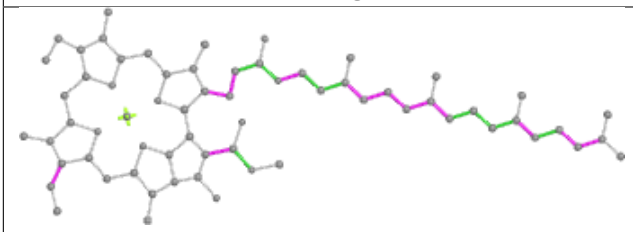
Ligand CLA a 405



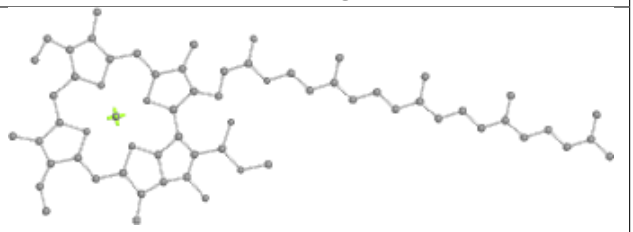
Bond lengths



Bond angles

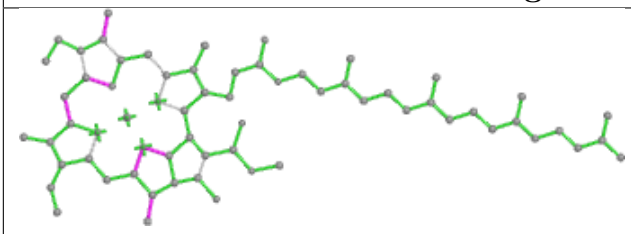


Torsions

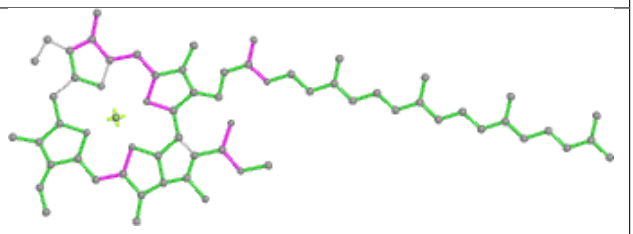


Rings

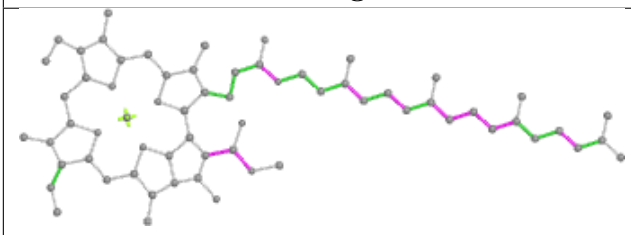
Ligand CLA B 605



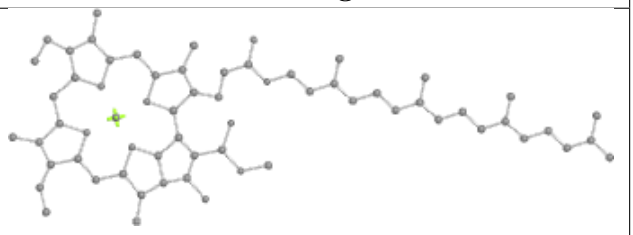
Bond lengths



Bond angles

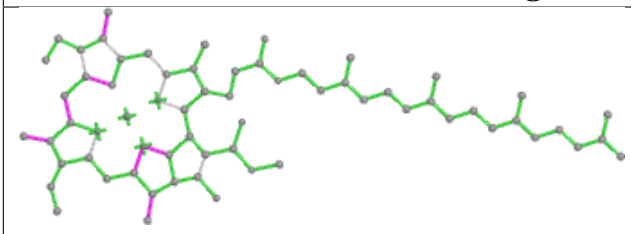


Torsions

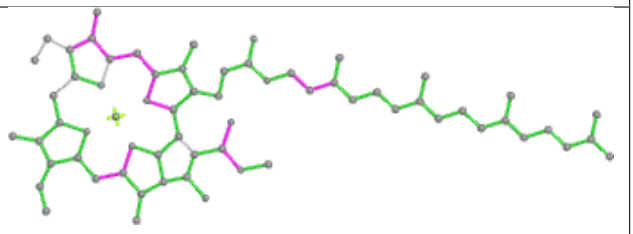


Rings

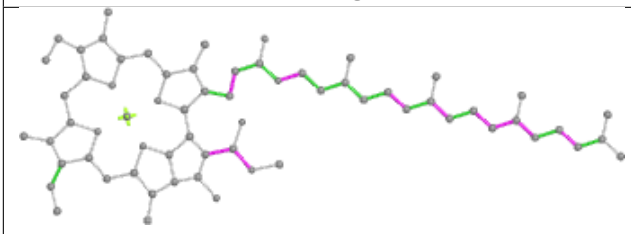
Ligand CLA C 508



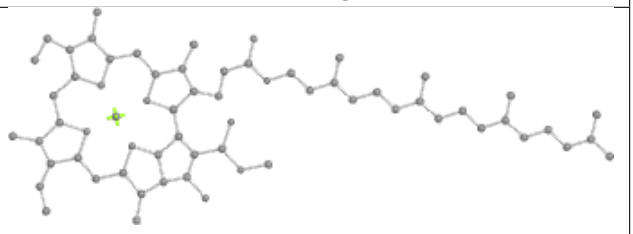
Bond lengths



Bond angles

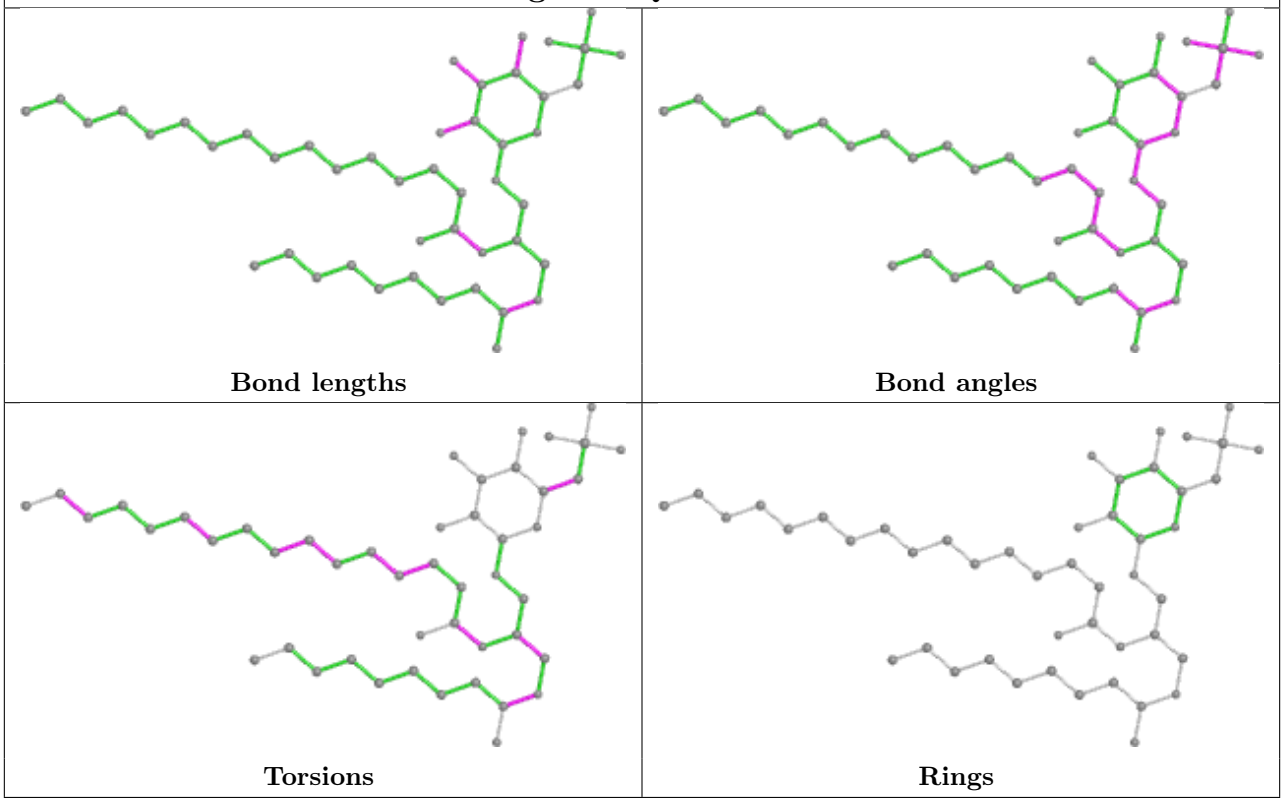


Torsions

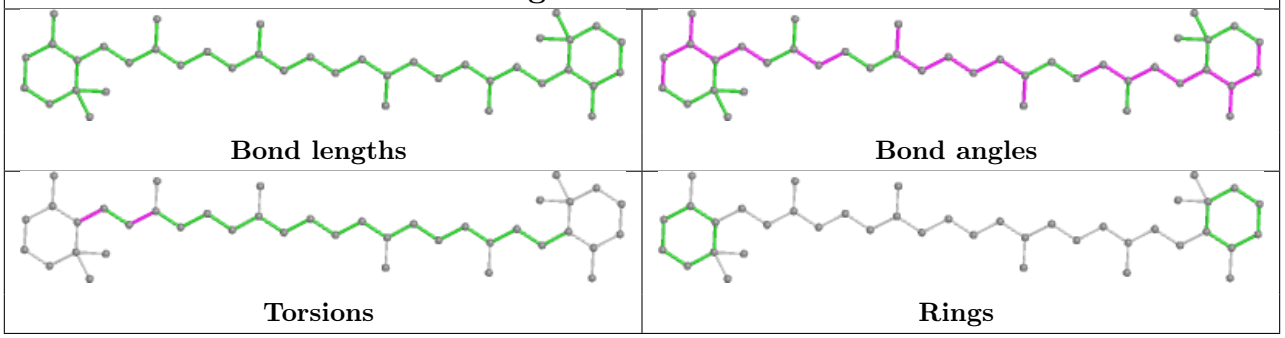


Rings

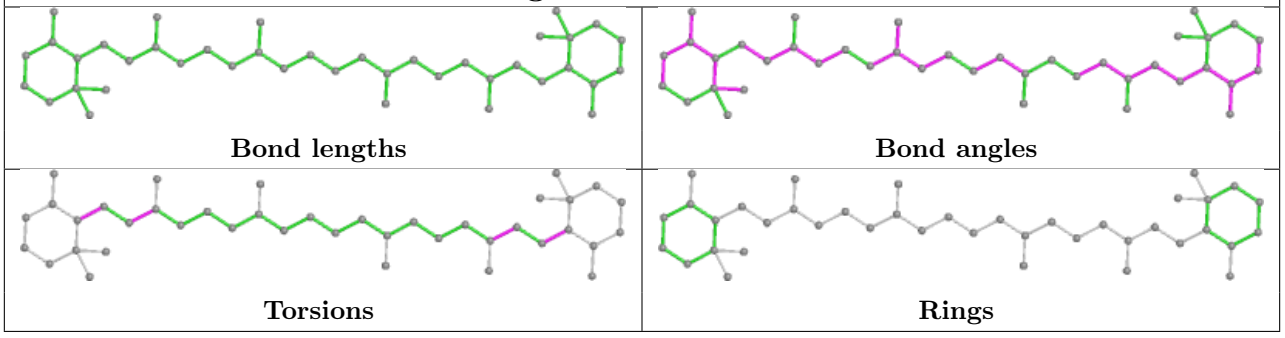
Ligand SQD b 601



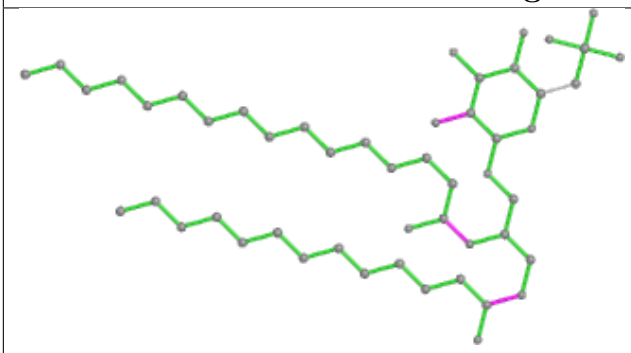
Ligand BCR z 101



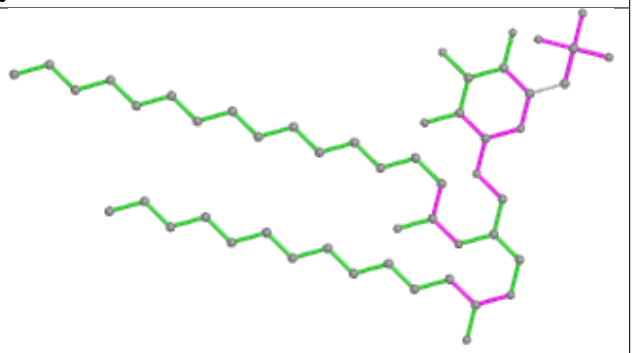
Ligand BCR k 102



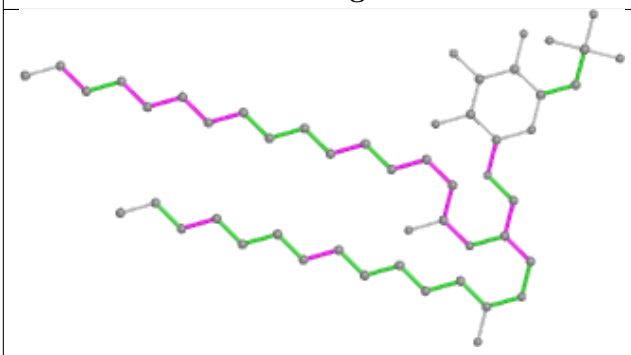
Ligand SQD A 413



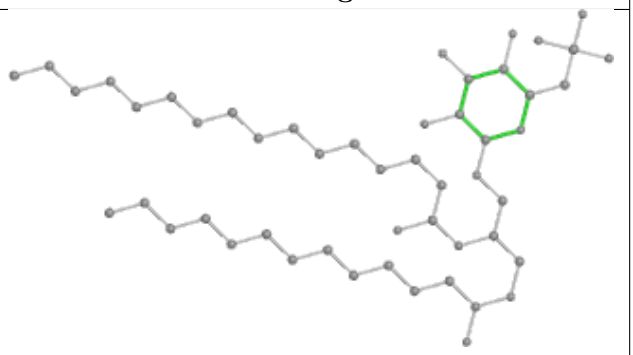
Bond lengths



Bond angles

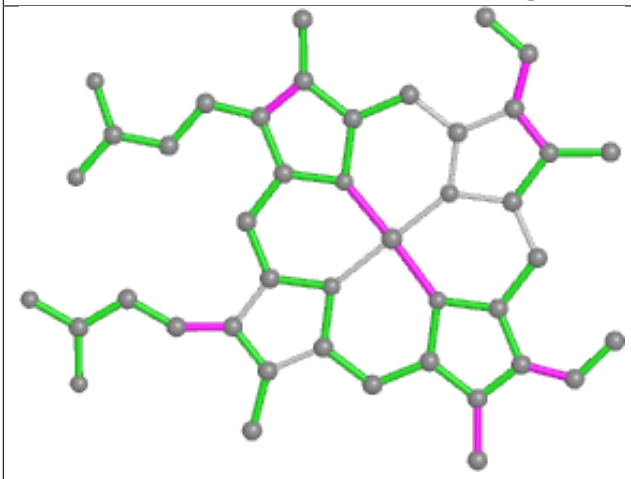


Torsions

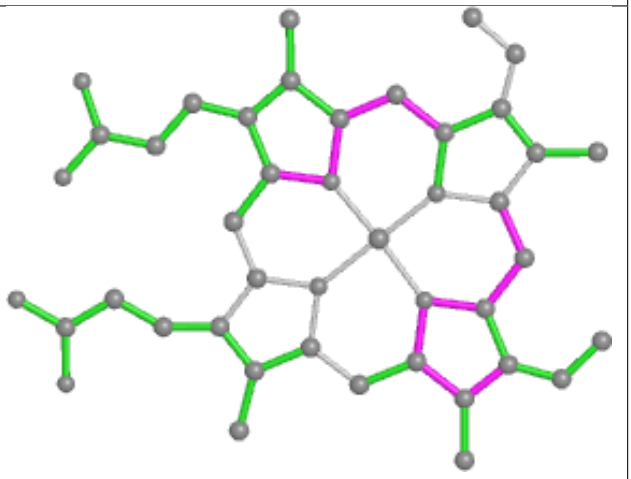


Rings

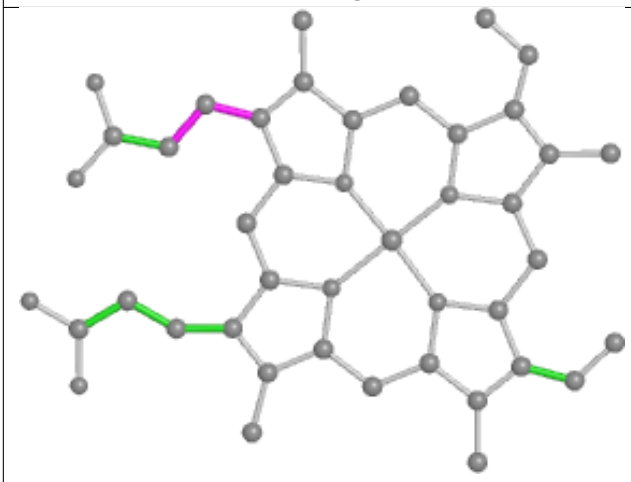
Ligand HEM v 201



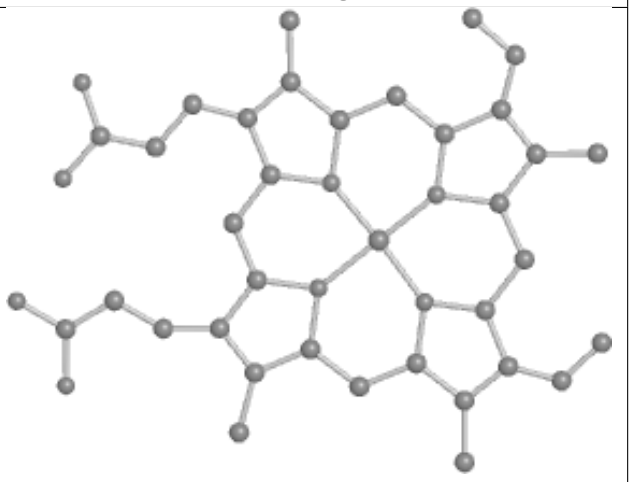
Bond lengths



Bond angles

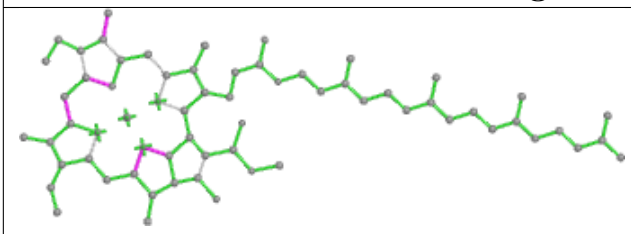


Torsions

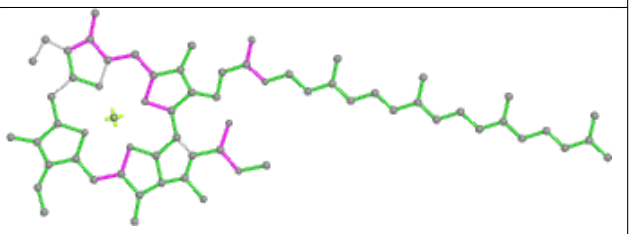


Rings

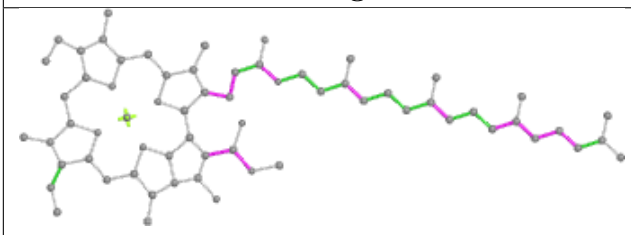
Ligand CLA c 513



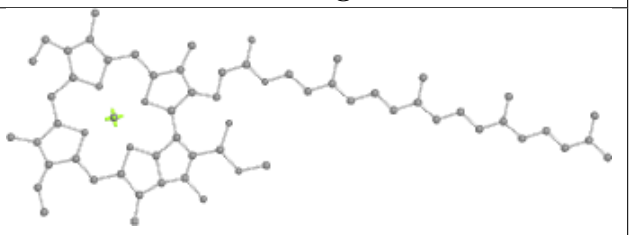
Bond lengths



Bond angles

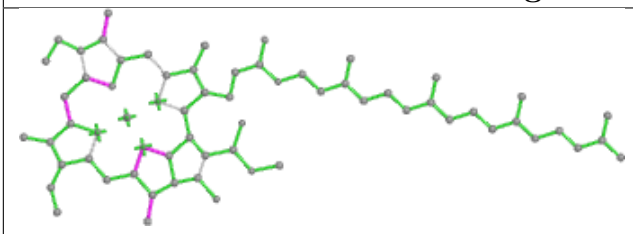


Torsions

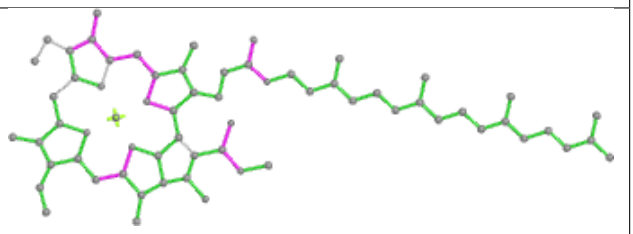


Rings

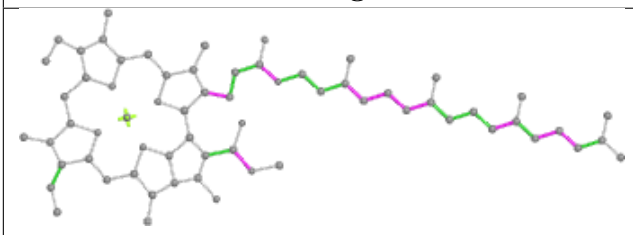
Ligand CLA B 608



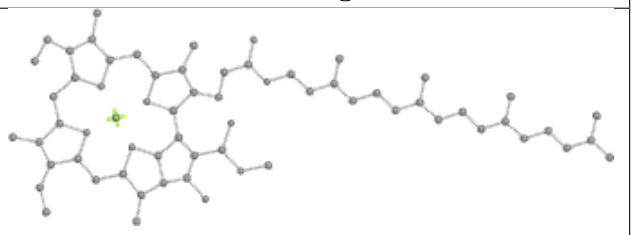
Bond lengths



Bond angles

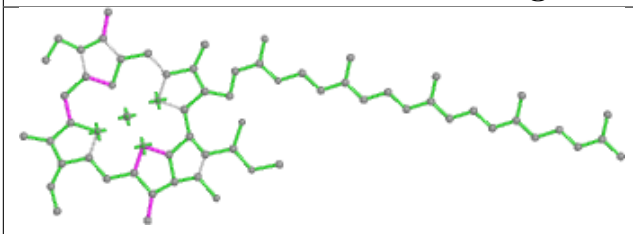


Torsions

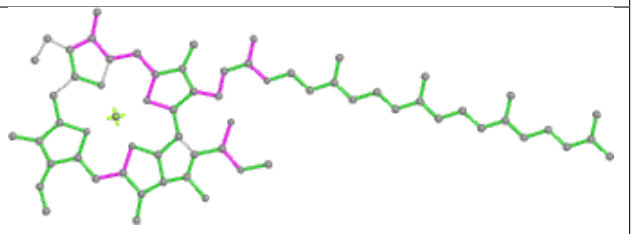


Rings

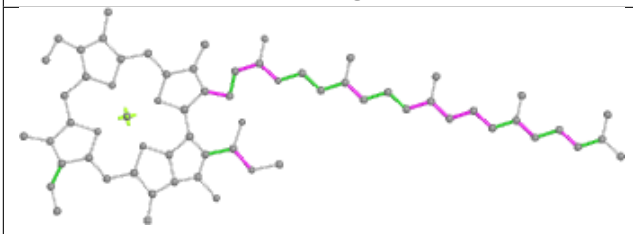
Ligand CLA c 505



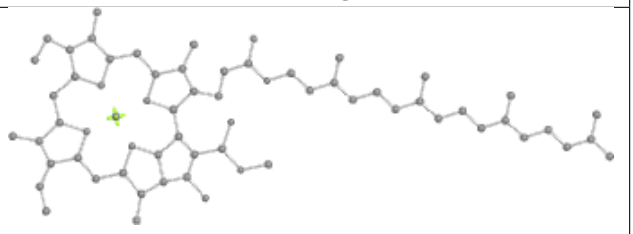
Bond lengths



Bond angles

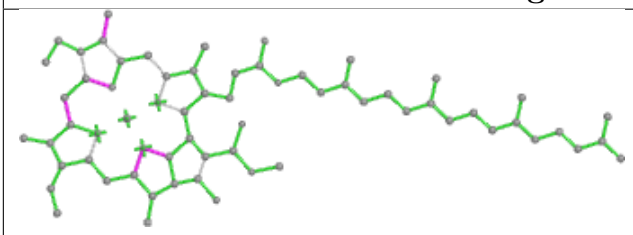


Torsions

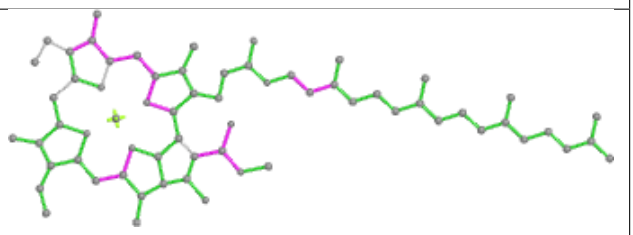


Rings

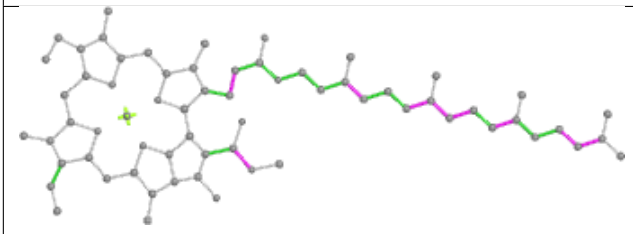
Ligand CLA b 607



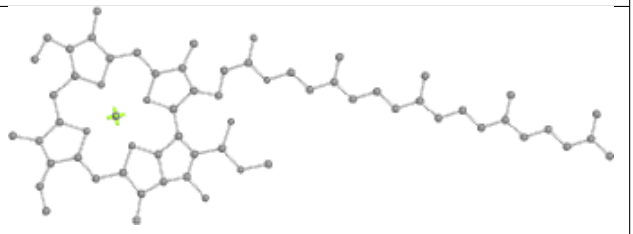
Bond lengths



Bond angles

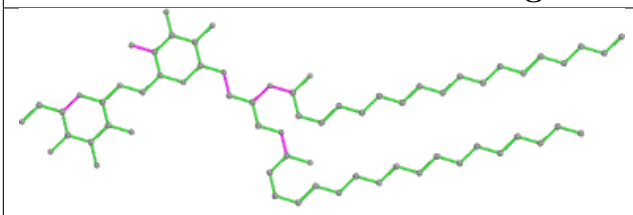


Torsions

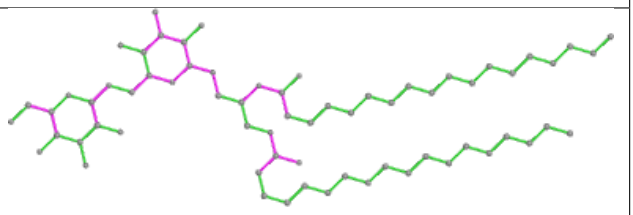


Rings

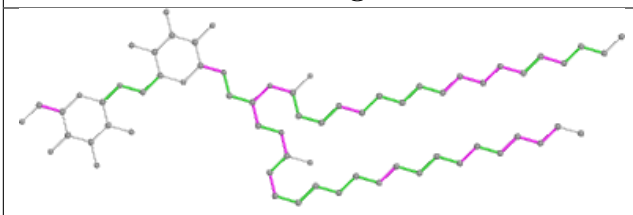
Ligand DGD c 518



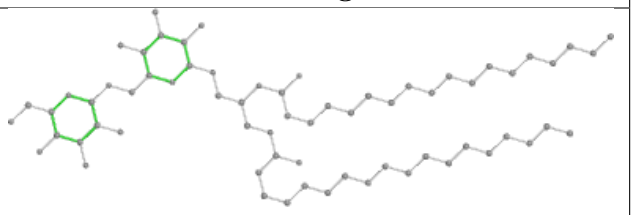
Bond lengths



Bond angles

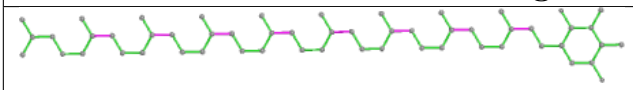


Torsions

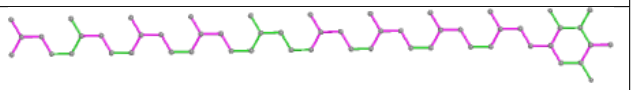


Rings

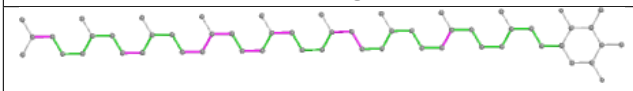
Ligand PL9 d 404



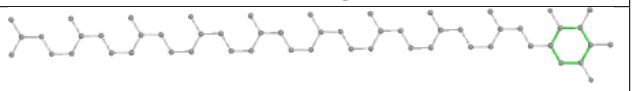
Bond lengths



Bond angles

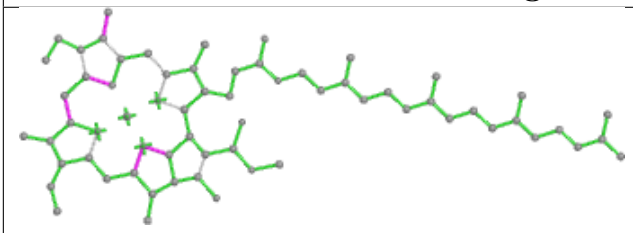


Torsions

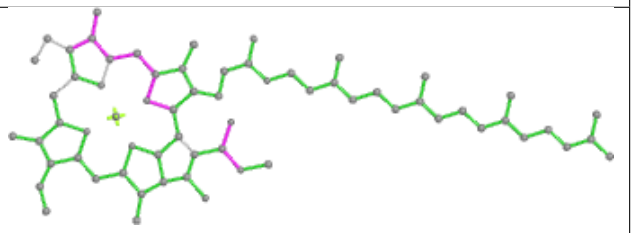


Rings

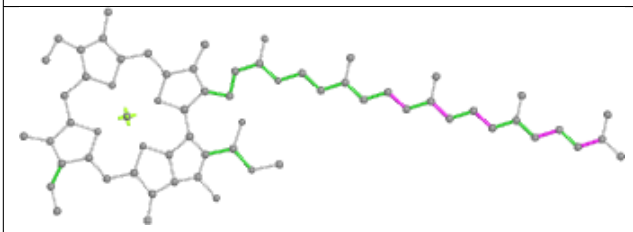
Ligand CLA A 407



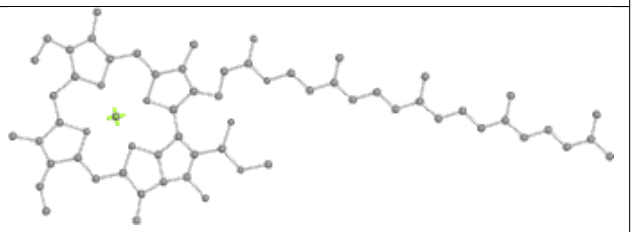
Bond lengths



Bond angles

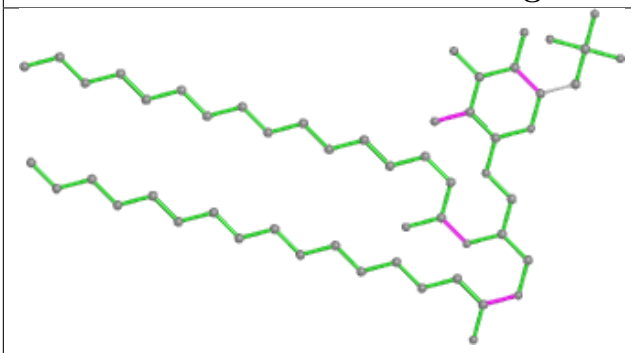


Torsions

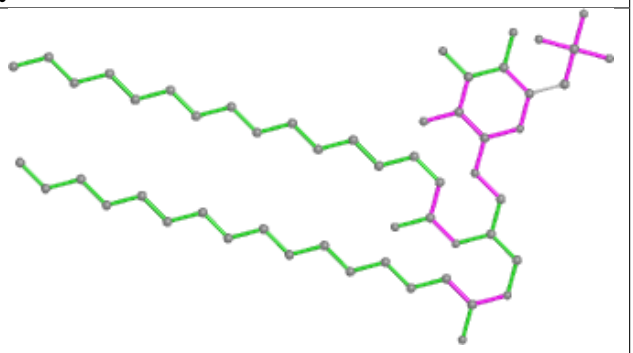


Rings

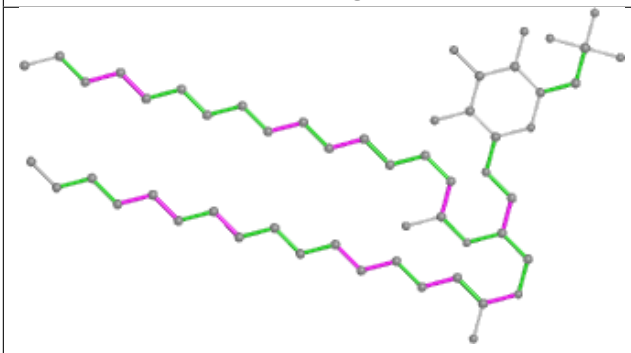
Ligand SQD A 417



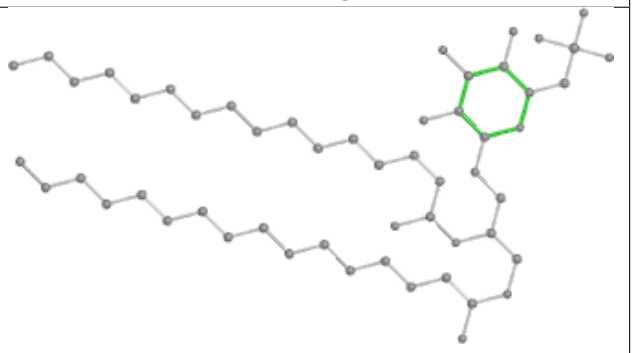
Bond lengths



Bond angles

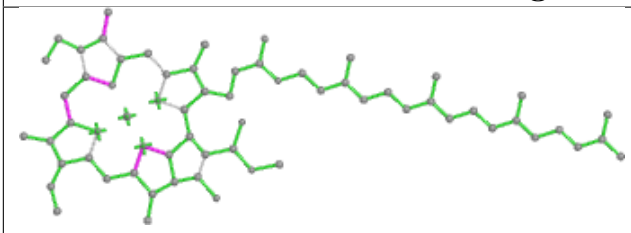


Torsions

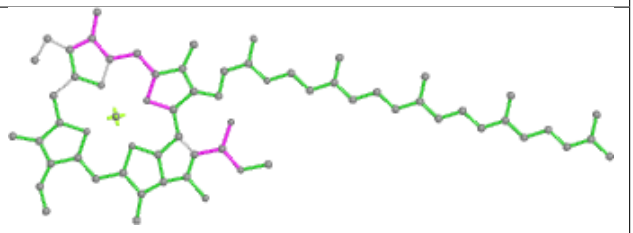


Rings

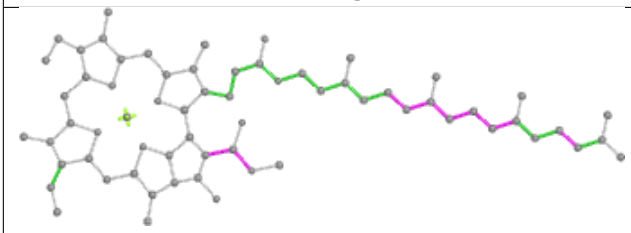
Ligand CLA c 503



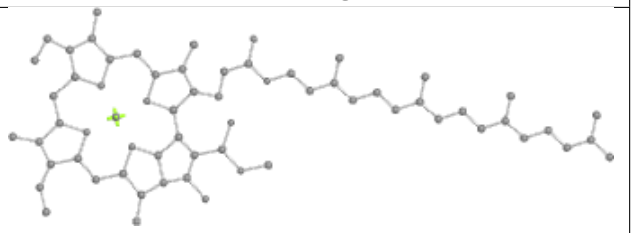
Bond lengths



Bond angles

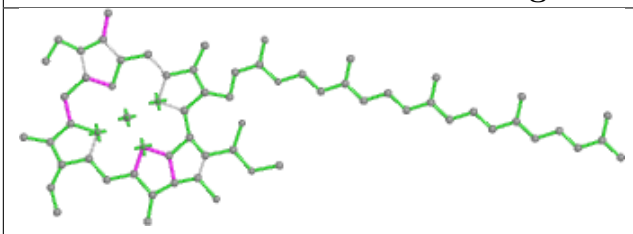


Torsions

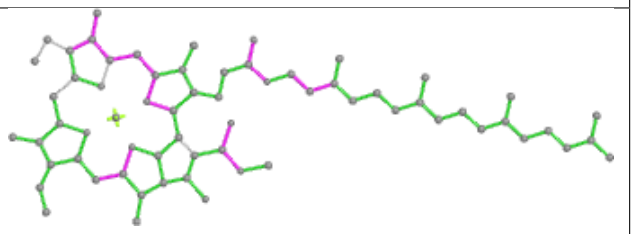


Rings

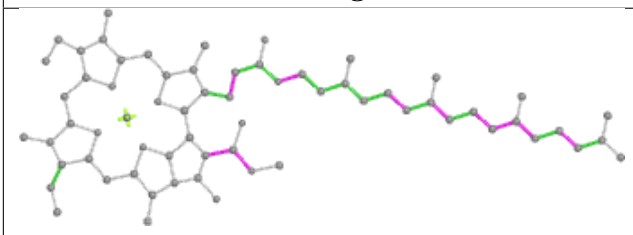
Ligand CLA c 508



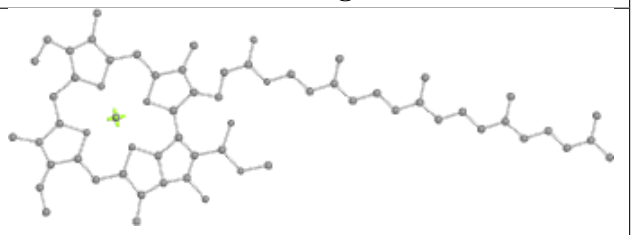
Bond lengths



Bond angles

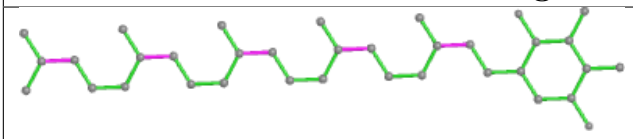


Torsions

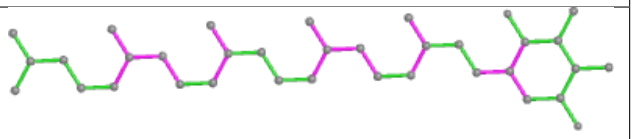


Rings

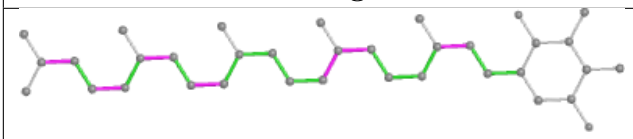
Ligand PL9 J 101



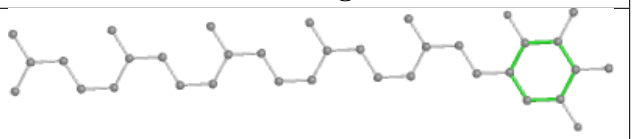
Bond lengths



Bond angles

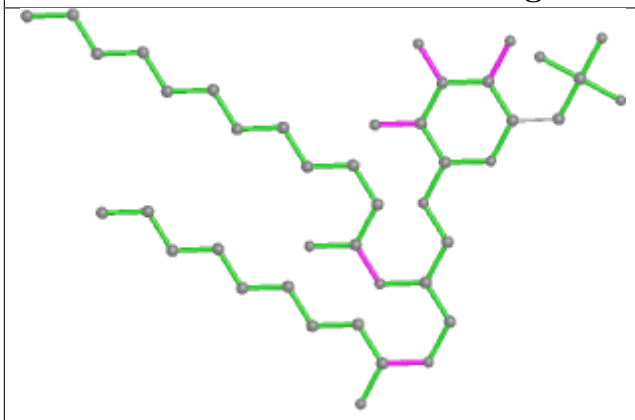


Torsions



Rings

Ligand SQD D 408



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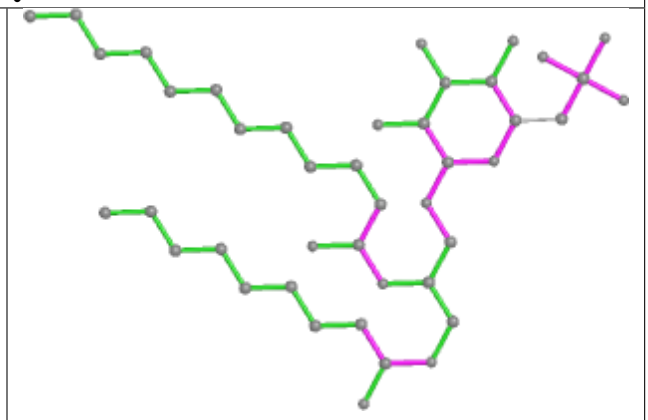
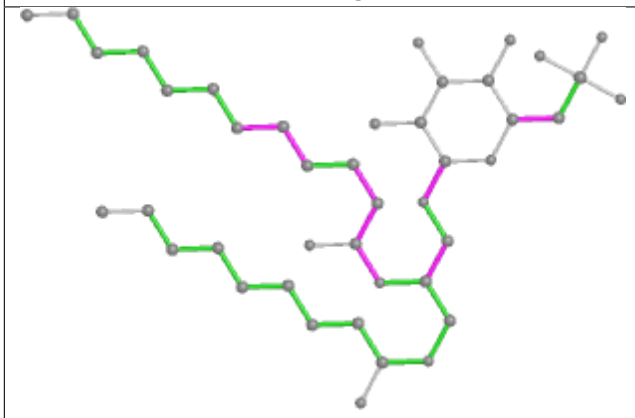
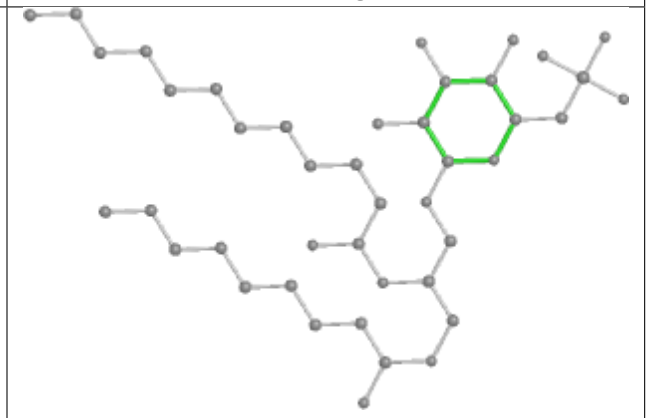


Bond angles

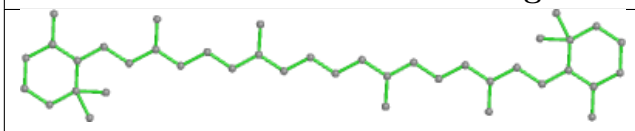


Torsions

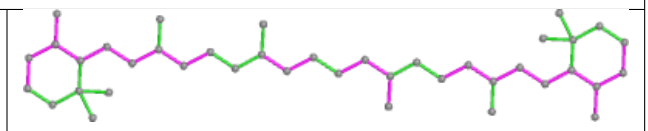


Rings

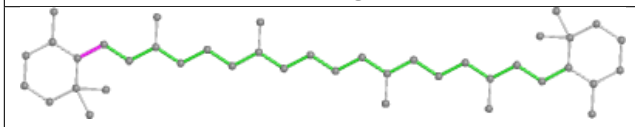
Ligand BCR T 101



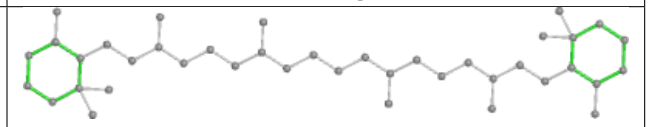
Bond lengths



Bond angles

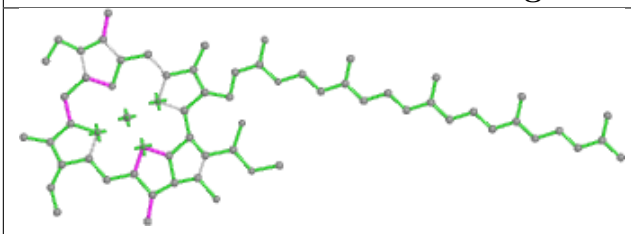


Torsions

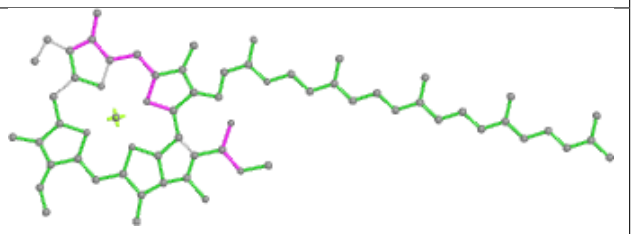


Rings

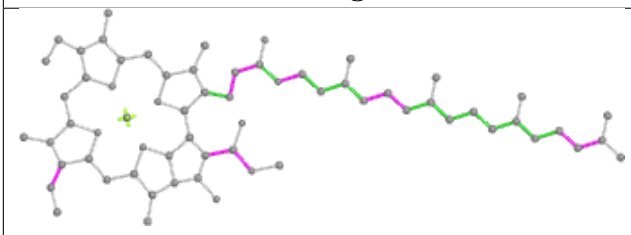
Ligand CLA B 614



Bond lengths



Bond angles



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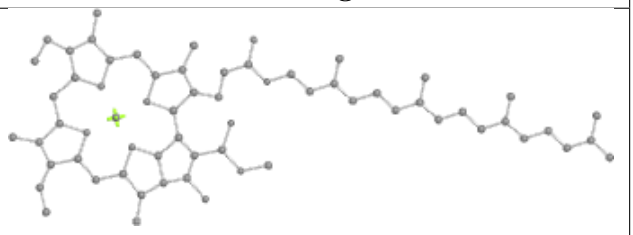
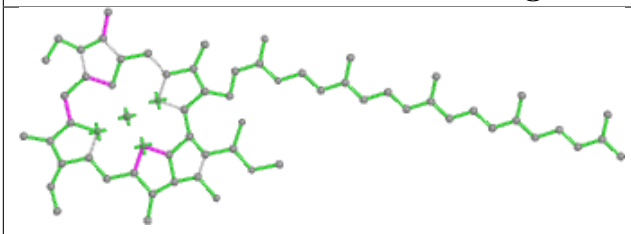
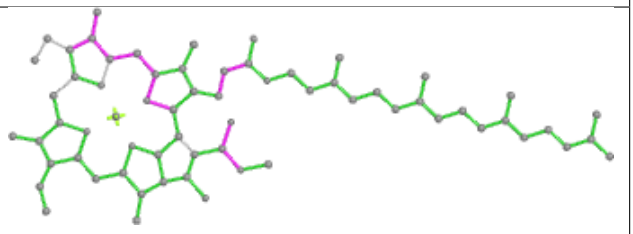


Rings

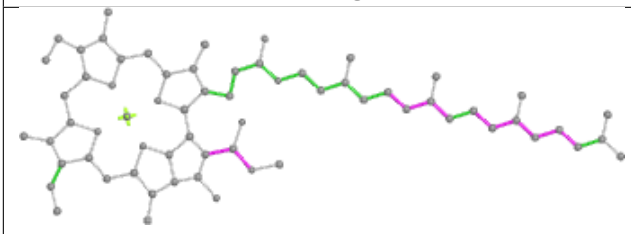
Ligand CLA C 506



Bond lengths



Bond angles



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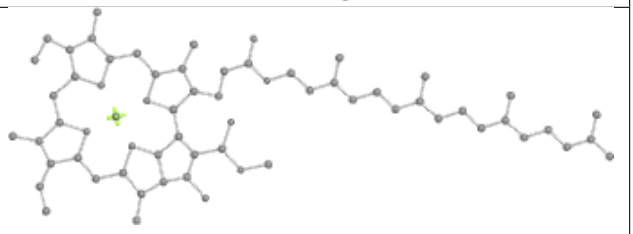
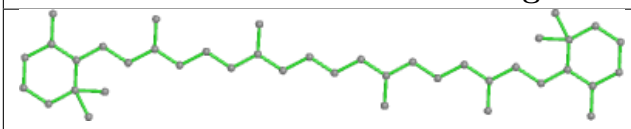
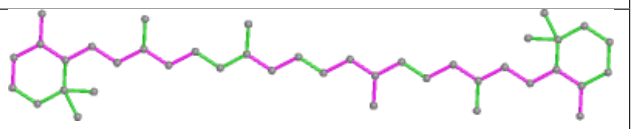


Rings

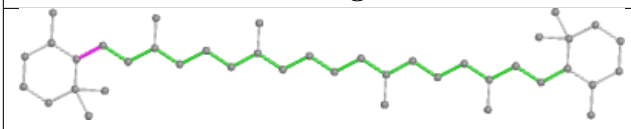
Ligand BCR B 617



Bond lengths



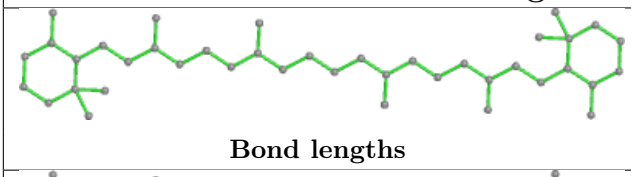
Bond angles



Torsions

Rings

Ligand BCR c 515



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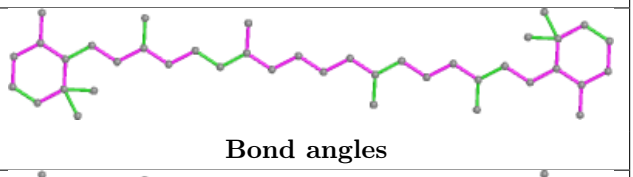
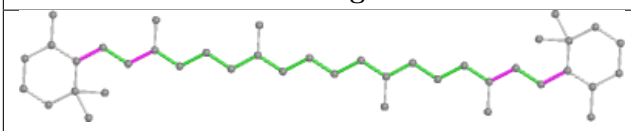
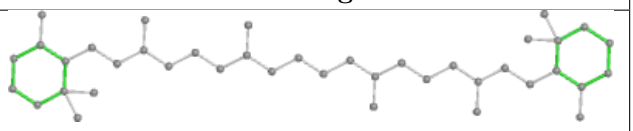


Bond angles

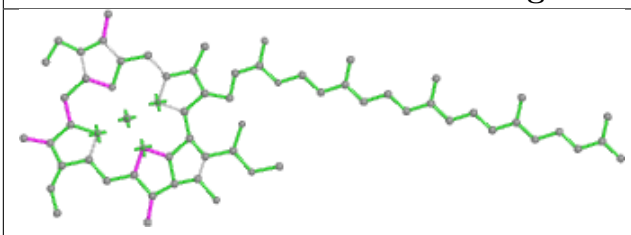


Torsions

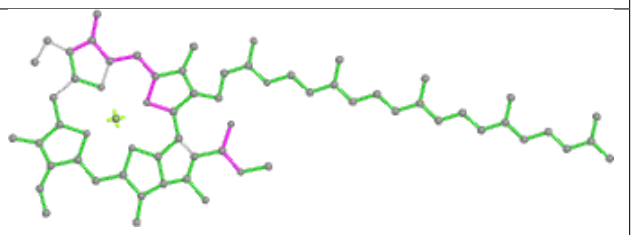


Rings

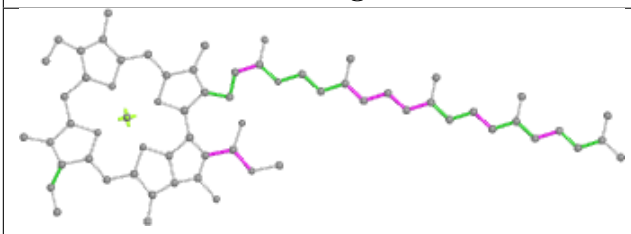
Ligand CLA b 616



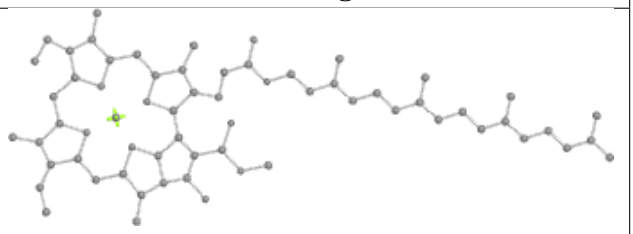
Bond lengths



Bond angles

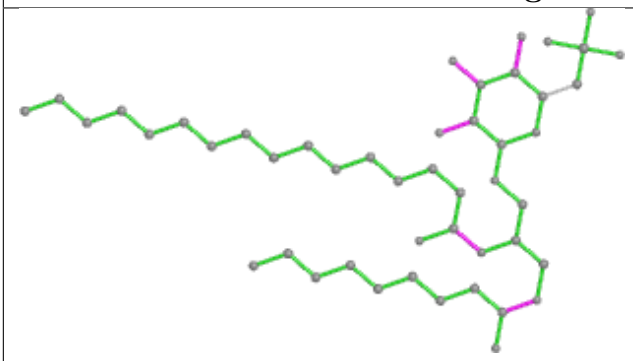


Torsions

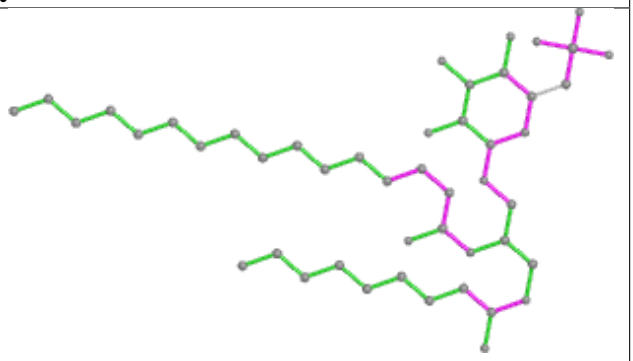


Rings

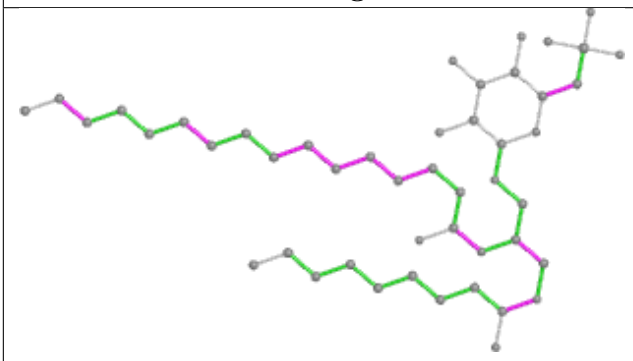
Ligand SQD B 626



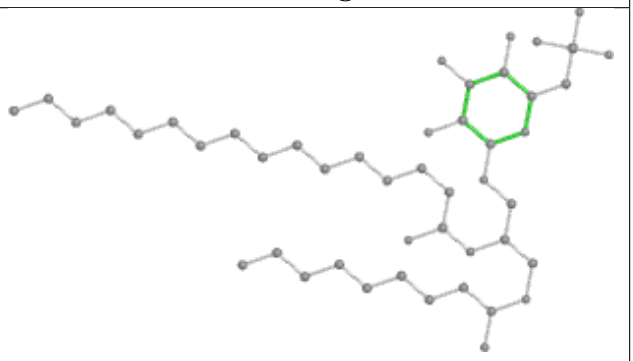
Bond lengths



Bond angles

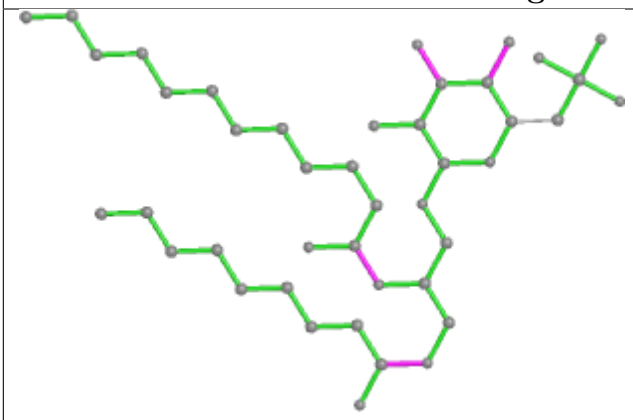


Torsions

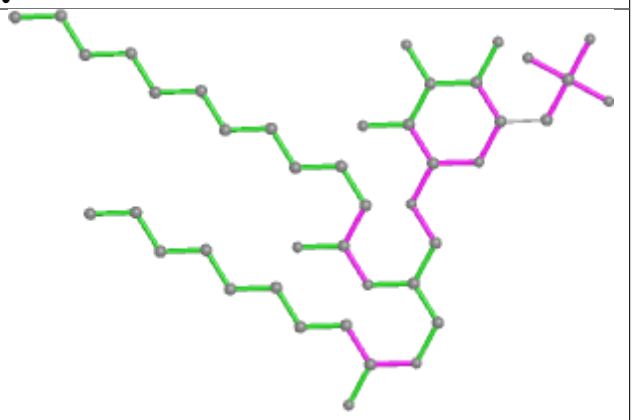


Rings

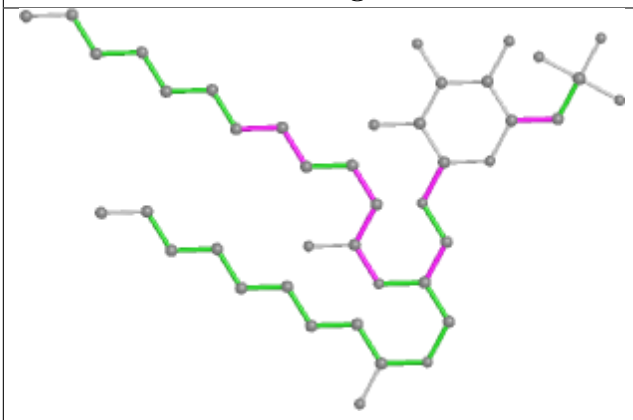
Ligand SQD d 408



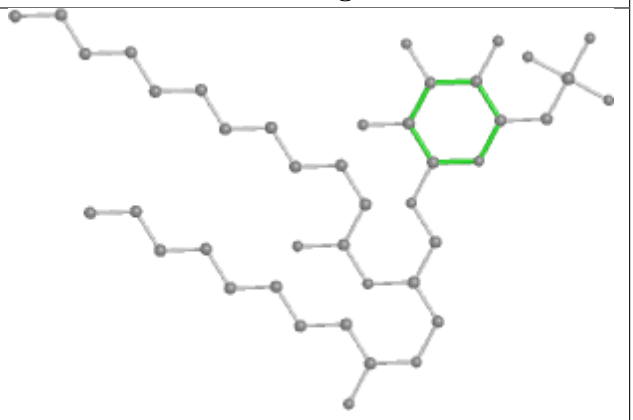
Bond lengths



Bond angles

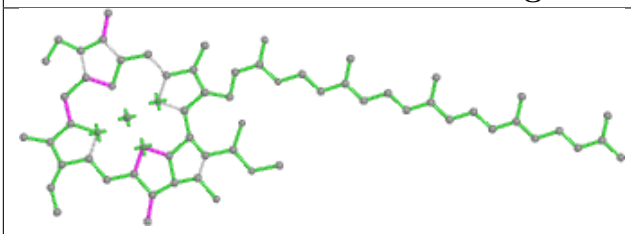


Torsions

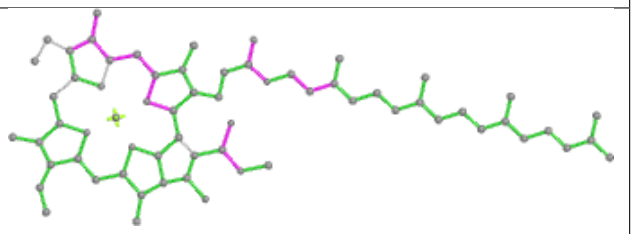


Rings

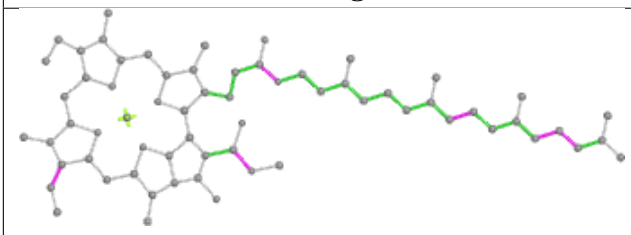
Ligand CLA B 604



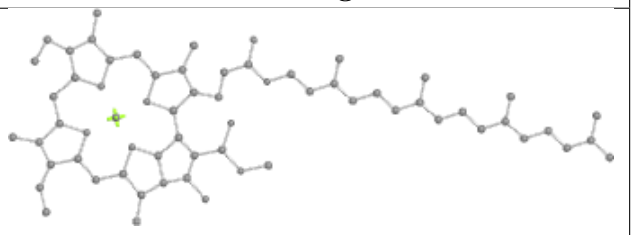
Bond lengths



Bond angles

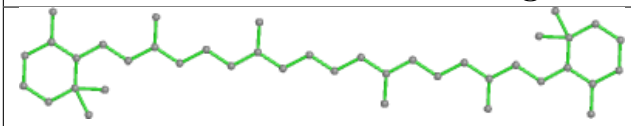


Torsions

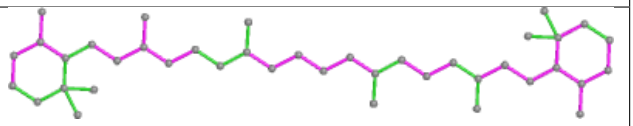


Rings

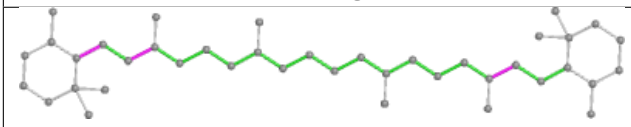
Ligand BCR D 405



Bond lengths



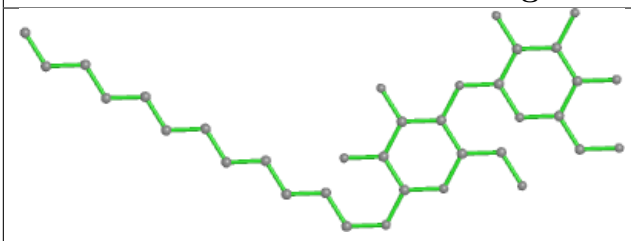
Bond angles



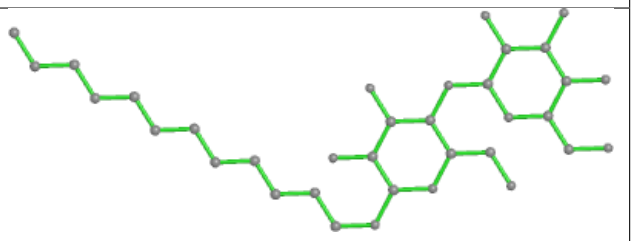
Torsions

Rings

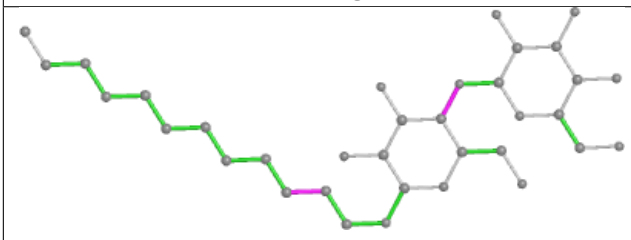
Ligand LMT B 629



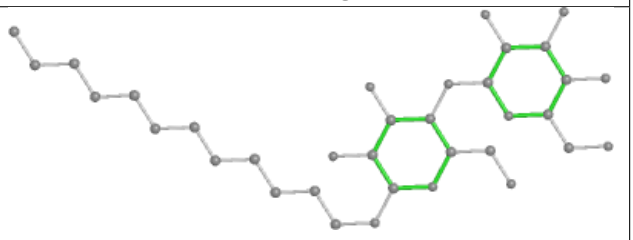
Bond lengths



Bond angles

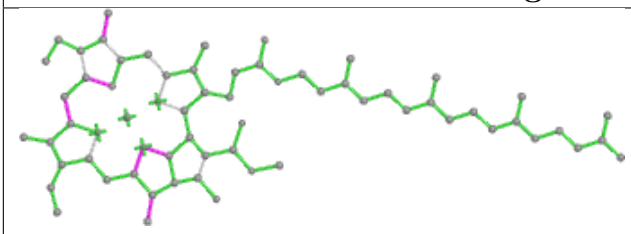


Torsions

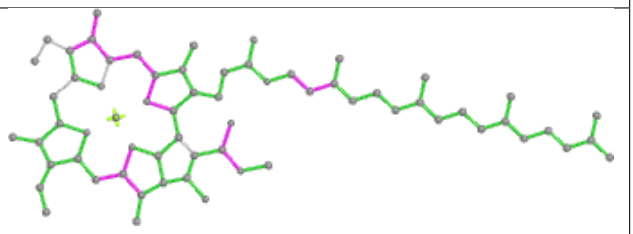


Rings

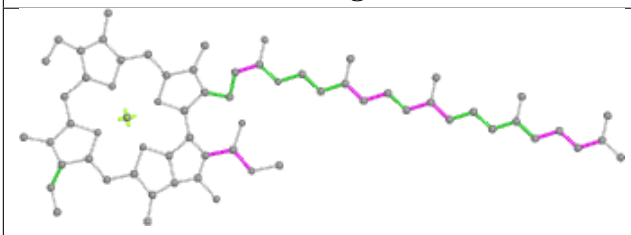
Ligand CLA C 510



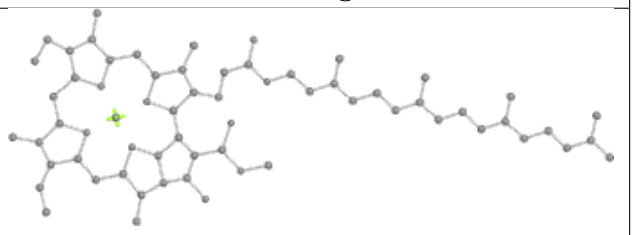
Bond lengths



Bond angles

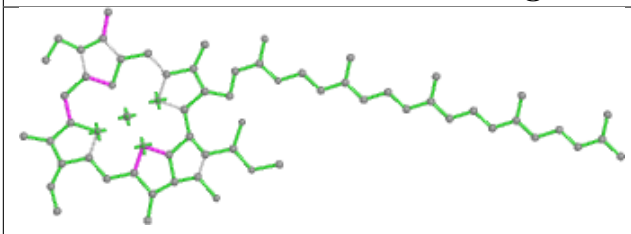


Torsions

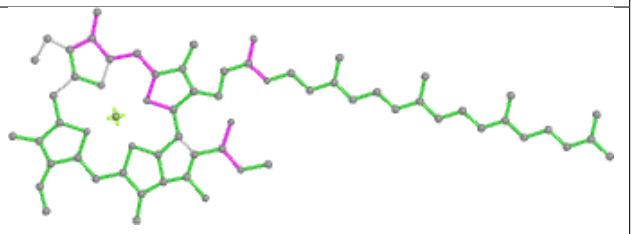


Rings

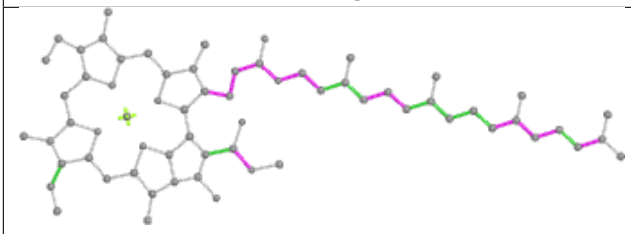
Ligand CLA C 512



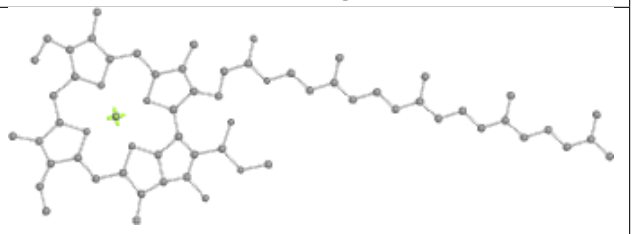
Bond lengths



Bond angles

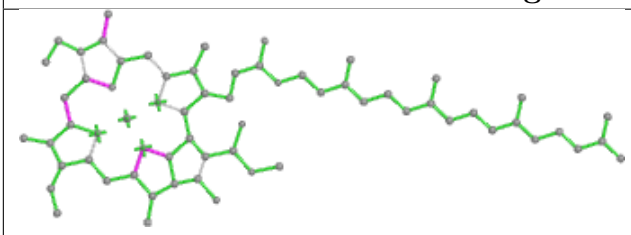


Torsions

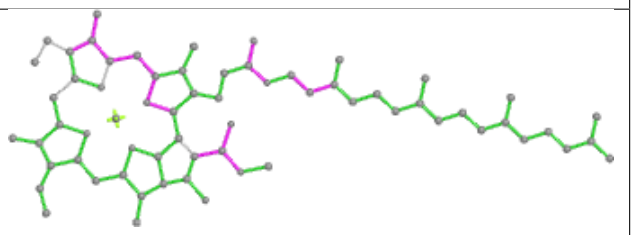


Rings

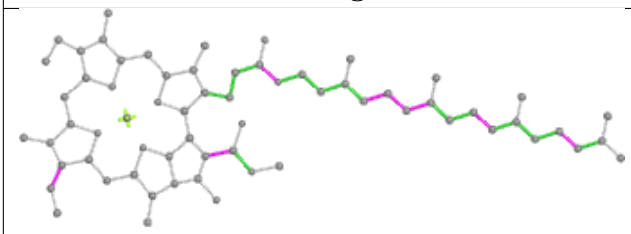
Ligand CLA A 405



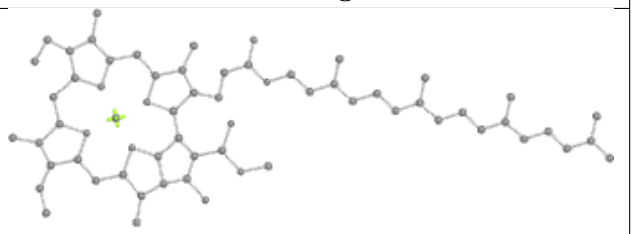
Bond lengths



Bond angles

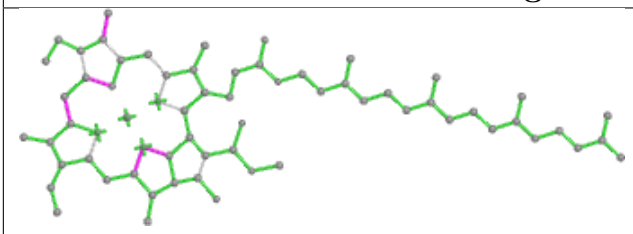


Torsions

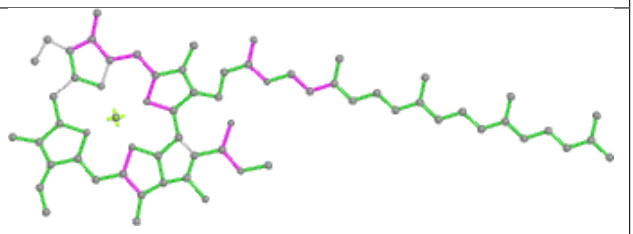


Rings

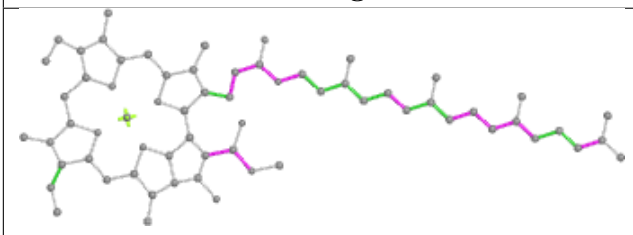
Ligand CLA B 610



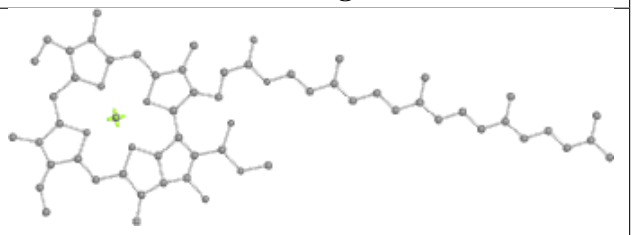
Bond lengths



Bond angles

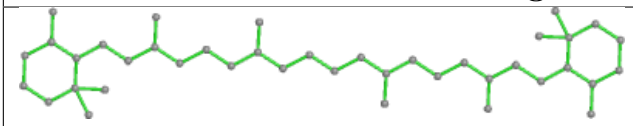


Torsions

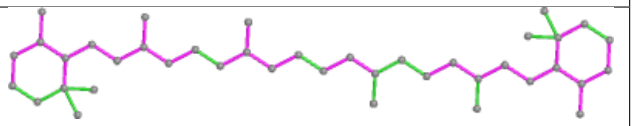


Rings

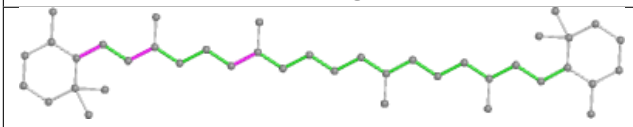
Ligand BCR c 514



Bond lengths



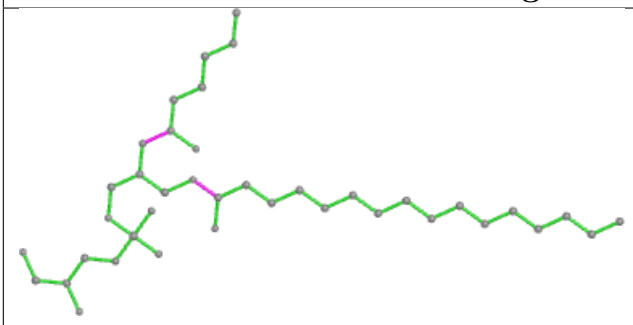
Bond angles



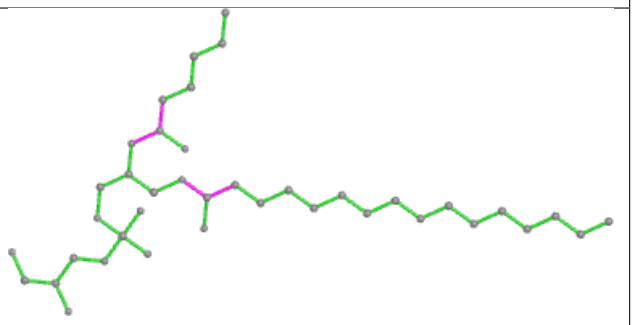
Torsions

Rings

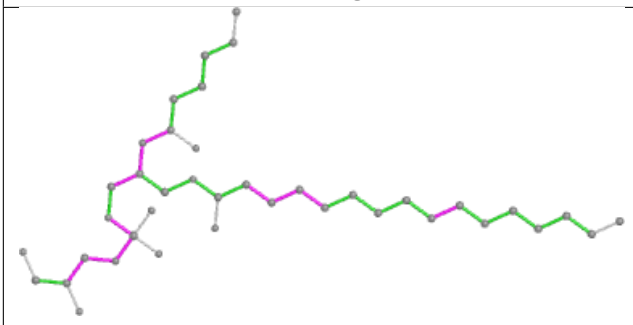
Ligand LHG A 412



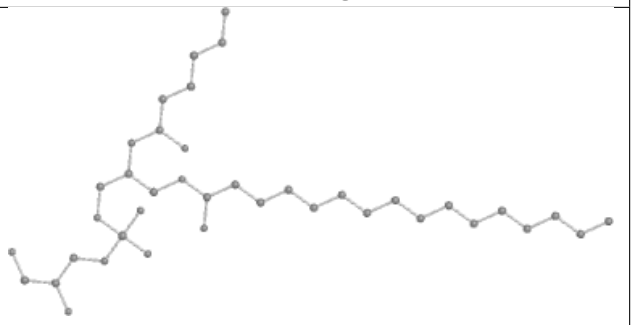
Bond lengths



Bond angles

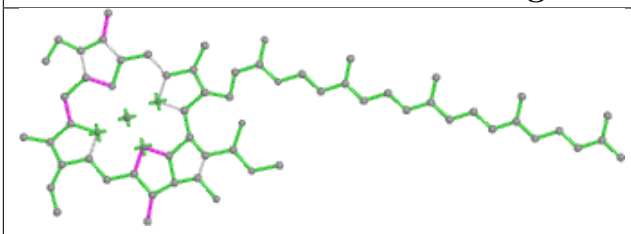


Torsions

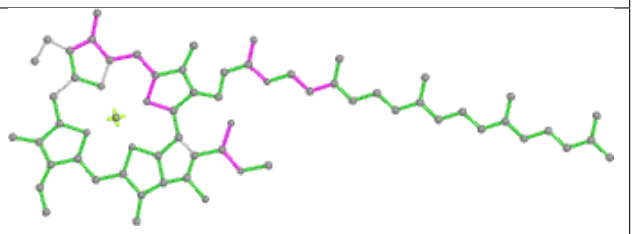


Rings

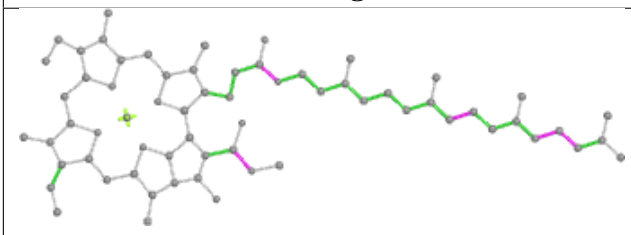
Ligand CLA b 608



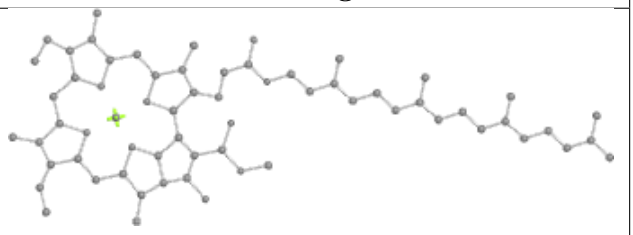
Bond lengths



Bond angles

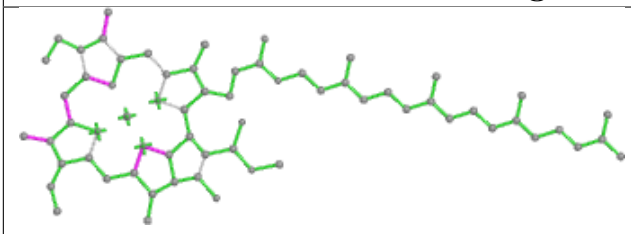


Torsions

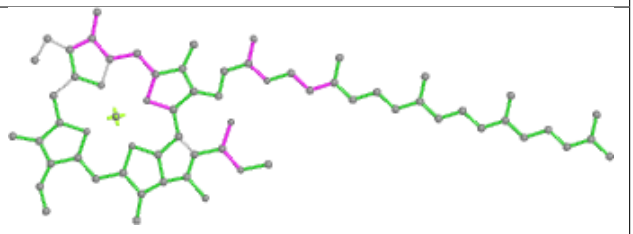


Rings

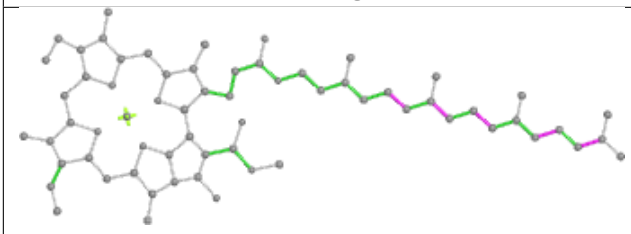
Ligand CLA a 409



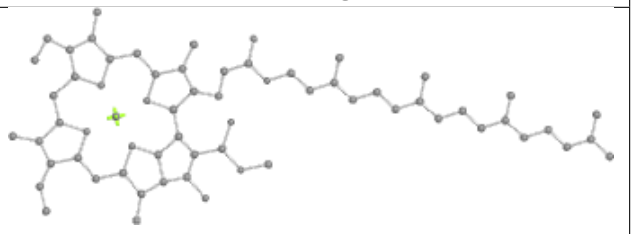
Bond lengths



Bond angles

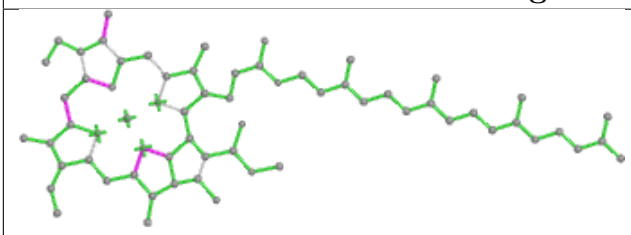


Torsions

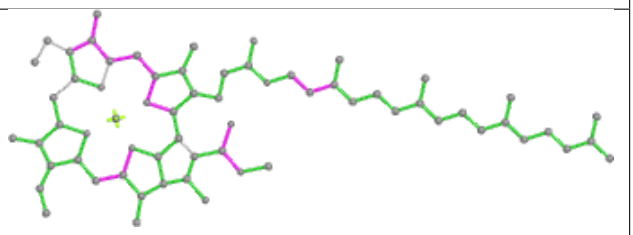


Rings

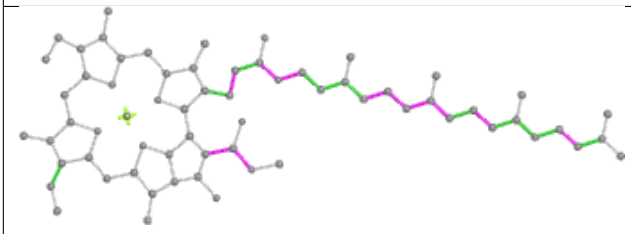
Ligand CLA c 509



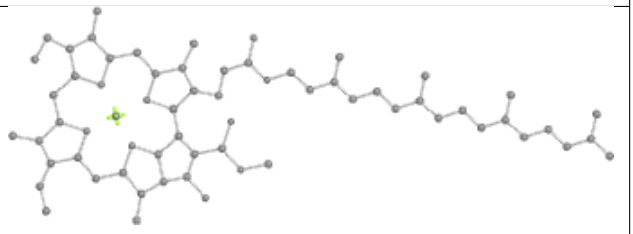
Bond lengths



Bond angles

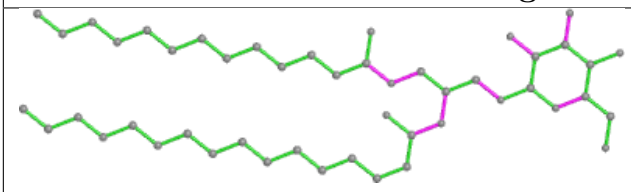


Torsions

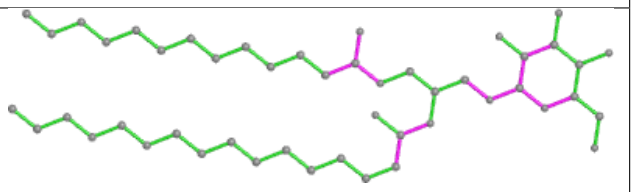


Rings

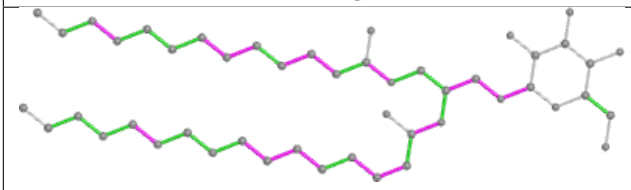
Ligand LMG D 407



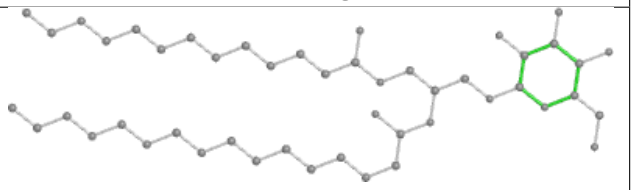
Bond lengths



Bond angles

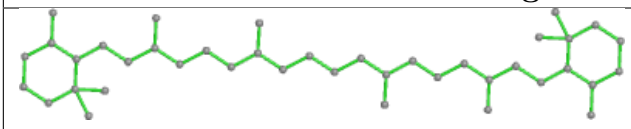


Torsions

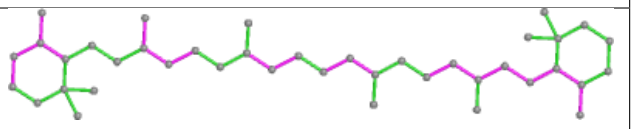


Rings

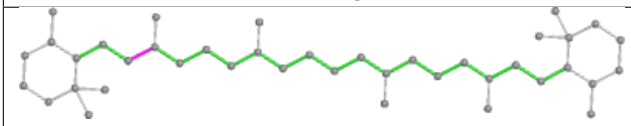
Ligand BCR A 410



Bond lengths



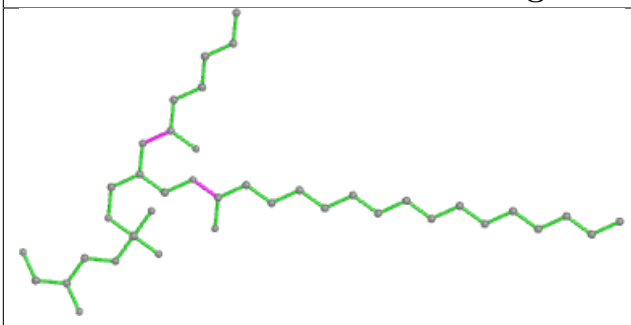
Bond angles



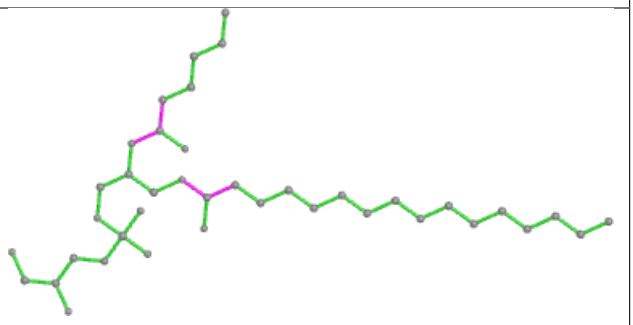
Torsions

Rings

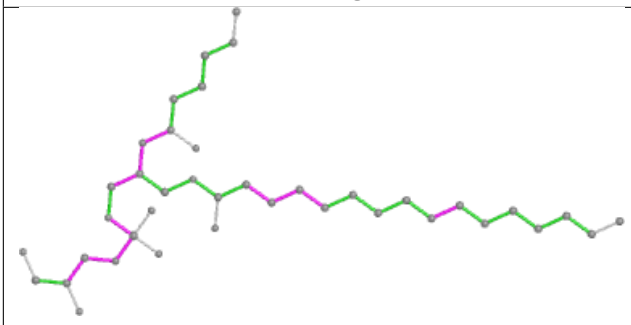
Ligand LHG a 414



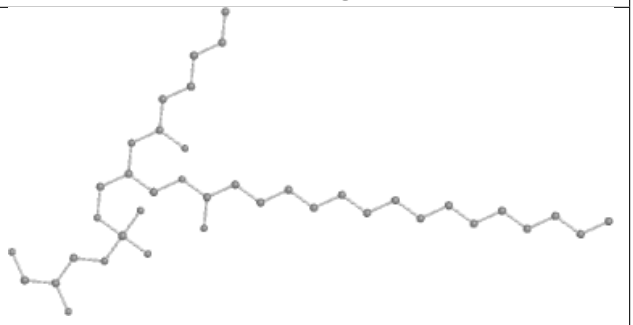
Bond lengths



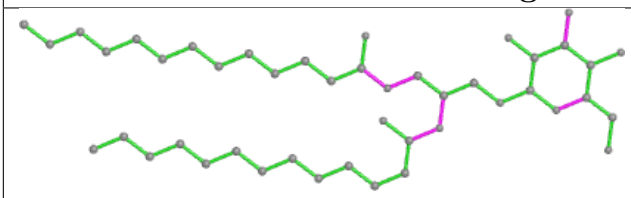
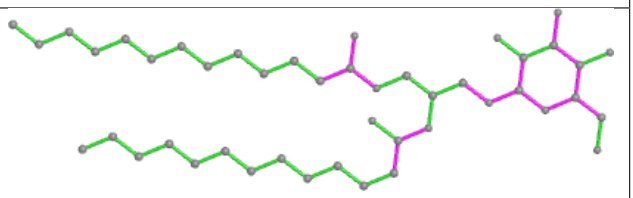
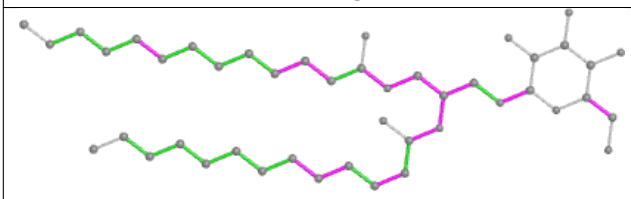
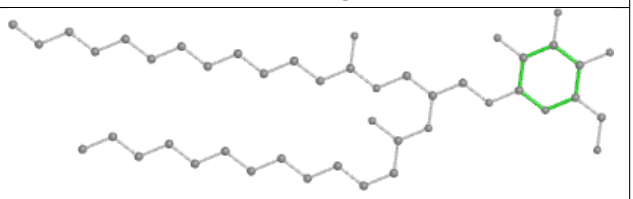
Bond angles



Torsions



Rings

Ligand LMG C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/360 (93%)	0.09	9 (2%) 54 47	43, 64, 104, 149	0
1	a	335/360 (93%)	-0.12	3 (0%) 84 77	44, 65, 106, 149	0
2	B	490/510 (96%)	0.32	25 (5%) 28 27	46, 69, 103, 159	0
2	b	490/510 (96%)	0.30	28 (5%) 23 23	47, 71, 104, 159	0
3	C	447/461 (96%)	0.05	7 (1%) 72 64	54, 79, 106, 132	0
3	c	447/461 (96%)	0.19	10 (2%) 62 54	56, 81, 105, 135	0
4	D	340/352 (96%)	-0.04	2 (0%) 89 84	44, 66, 103, 137	0
4	d	340/352 (96%)	-0.08	2 (0%) 89 84	45, 66, 102, 134	0
5	E	82/84 (97%)	0.06	1 (1%) 79 71	68, 92, 125, 130	0
5	e	82/84 (97%)	0.36	3 (3%) 41 37	70, 92, 125, 129	0
6	F	35/45 (77%)	0.03	2 (5%) 23 23	68, 84, 119, 139	0
6	f	35/45 (77%)	0.31	0 100 100	73, 85, 120, 141	0
7	H	65/66 (98%)	0.76	8 (12%) 4 8	77, 94, 122, 138	0
7	h	65/66 (98%)	0.58	3 (4%) 32 30	73, 93, 120, 144	0
8	I	35/38 (92%)	0.16	1 (2%) 51 44	65, 79, 107, 118	0
8	i	35/38 (92%)	0.01	0 100 100	66, 81, 106, 120	0
9	J	34/40 (85%)	0.01	1 (2%) 51 44	69, 85, 95, 112	0
9	j	34/40 (85%)	-0.25	1 (2%) 51 44	74, 88, 95, 116	0
10	K	37/46 (80%)	0.10	0 100 100	77, 87, 101, 122	0
10	k	37/46 (80%)	0.25	3 (8%) 12 13	73, 88, 108, 123	0
11	L	37/37 (100%)	-0.02	0 100 100	48, 62, 128, 156	0
11	l	37/37 (100%)	-0.13	0 100 100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.08	2 (5%) 22 22	56, 71, 110, 164	0
12	m	34/36 (94%)	0.24	3 (8%) 10 12	55, 69, 108, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.82	31 (12%) 3 7	50, 78, 122, 169	0
13	o	243/272 (89%)	0.59	18 (7%) 14 15	52, 78, 121, 167	0
14	T	32/32 (100%)	0.27	4 (12%) 3 7	55, 67, 158, 174	0
14	t	32/32 (100%)	-0.09	0 100 100	54, 69, 159, 168	0
15	U	97/134 (72%)	0.90	9 (9%) 8 11	56, 71, 92, 108	0
15	u	97/134 (72%)	0.74	5 (5%) 27 27	55, 71, 90, 111	0
16	V	137/163 (84%)	0.31	7 (5%) 28 27	53, 71, 86, 101	0
16	v	137/163 (84%)	0.72	9 (6%) 18 17	59, 72, 88, 95	0
17	g	28/46 (60%)	0.78	5 (17%) 1 4	95, 108, 126, 132	0
17	y	28/46 (60%)	0.29	1 (3%) 42 38	89, 107, 126, 131	0
18	X	37/41 (90%)	0.93	5 (13%) 3 6	76, 93, 124, 140	0
18	x	37/41 (90%)	0.90	10 (27%) 0 2	75, 90, 126, 141	0
19	Z	62/62 (100%)	1.06	7 (11%) 5 8	86, 104, 168, 185	0
19	z	62/62 (100%)	0.68	2 (3%) 47 41	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.26	227 (4%) 34 32	43, 75, 115, 187	0

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	170	GLY	5.8
2	B	129	GLY	5.3
13	o	84	ASN	4.2
2	b	483	ASP	4.1
15	U	54	LYS	4.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	PL9	J	101	35/55	0.30	0.53	119,157,178,182	0
31	LMG	C	521	45/55	0.32	1.13	84,119,143,175	0
25	PL9	j	101	35/55	0.33	0.42	120,160,178,182	0
35	CA	k	101	1/1	0.33	0.52	103,103,103,103	0
35	CA	O	301	1/1	0.35	0.47	112,112,112,112	0
33	LMT	d	410	31/35	0.38	0.88	83,134,157,157	0
33	LMT	B	628	35/35	0.39	0.61	72,126,141,144	0
33	LMT	i	102	35/35	0.39	1.06	99,137,146,152	0
32	CL	A	416	1/1	0.45	1.00	49,49,49,49	0
31	LMG	E	101	44/55	0.47	0.64	87,123,132,139	0
33	LMT	B	629	35/35	0.49	0.67	70,137,165,168	0
27	BCR	j	102	40/40	0.50	0.50	110,128,180,184	0
23	CLA	b	605	65/65	0.50	0.91	88,108,124,137	0
33	LMT	B	624	35/35	0.50	0.82	80,142,170,171	0
23	CLA	B	601	65/65	0.53	0.99	92,108,131,137	0
31	LMG	c	519	45/55	0.55	0.97	86,119,142,171	0
28	DGD	D	409	63/66	0.56	0.74	104,127,181,188	0
27	BCR	B	620	40/40	0.57	0.94	75,86,98,103	0
33	LMT	b	627	35/35	0.57	0.88	100,140,152,154	0
27	BCR	J	102	40/40	0.58	0.45	108,125,177,180	0
33	LMT	b	603	35/35	0.60	0.48	73,119,136,138	0
28	DGD	d	409	63/66	0.60	0.61	106,128,181,190	0
33	LMT	D	410	31/35	0.60	0.94	83,133,154,159	0
33	LMT	b	626	35/35	0.62	0.66	76,139,174,176	0
29	LHG	A	415	37/49	0.62	0.57	104,133,190,202	0
27	BCR	B	618	40/40	0.62	0.36	75,82,94,95	0
31	LMG	A	418	42/55	0.63	0.44	81,105,123,147	0
35	CA	K	101	1/1	0.63	0.53	86,86,86,86	0
30	SQD	d	408	43/54	0.64	0.74	67,109,152,157	0
27	BCR	k	102	40/40	0.64	0.77	72,80,109,111	0
25	PL9	a	410	45/55	0.64	0.46	82,103,121,125	0
27	BCR	D	405	40/40	0.65	0.52	68,81,105,110	0
33	LMT	I	102	35/35	0.65	0.69	99,135,144,145	0
35	CA	o	301	1/1	0.65	0.47	98,98,98,98	0
27	BCR	b	622	40/40	0.66	0.64	72,83,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DGD	C	519	66/66	0.66	0.43	55,72,100,114	0
23	CLA	c	513	65/65	0.66	1.07	93,109,142,148	0
31	LMG	a	402	42/55	0.66	0.52	72,100,119,143	0
27	BCR	z	101	40/40	0.67	1.32	86,96,112,115	0
23	CLA	C	506	65/65	0.67	0.60	79,91,125,133	0
30	SQD	B	626	47/54	0.68	0.42	75,100,144,148	0
30	SQD	b	601	47/54	0.68	0.41	81,103,147,151	0
27	BCR	y	101	40/40	0.68	0.79	79,86,106,109	0
31	LMG	e	101	44/55	0.68	0.43	91,122,132,136	0
25	PL9	A	408	45/55	0.68	0.48	89,101,119,127	0
33	LMT	b	604	35/35	0.68	0.49	69,133,158,160	0
23	CLA	c	502	65/65	0.68	0.61	63,75,100,106	0
30	SQD	F	102	45/54	0.69	0.76	87,127,149,152	0
29	LHG	a	417	37/49	0.70	0.37	110,135,197,206	0
27	BCR	A	410	40/40	0.70	0.47	52,68,85,90	0
23	CLA	B	616	65/65	0.70	0.71	79,93,147,152	0
27	BCR	T	102	40/40	0.71	0.33	71,79,86,86	0
27	BCR	B	619	40/40	0.71	0.34	62,75,83,86	0
28	DGD	B	627	52/66	0.71	0.50	75,105,178,180	0
27	BCR	H	101	40/40	0.71	1.03	83,96,130,131	0
23	CLA	b	620	65/65	0.71	0.58	75,98,145,147	0
30	SQD	a	415	51/54	0.71	0.39	88,101,128,129	0
30	SQD	D	408	43/54	0.72	0.66	71,103,148,152	0
33	LMT	B	625	35/35	0.72	0.74	95,139,149,152	0
28	DGD	A	411	56/66	0.72	0.38	77,102,146,153	0
27	BCR	b	621	40/40	0.72	0.28	63,73,84,87	0
27	BCR	a	412	40/40	0.73	0.42	54,71,84,87	0
30	SQD	A	413	51/54	0.73	0.39	81,99,128,131	0
31	LMG	i	101	43/55	0.73	0.66	84,120,162,177	0
23	CLA	B	614	65/65	0.73	0.41	63,83,125,129	0
27	BCR	h	101	40/40	0.74	0.94	85,94,124,127	0
31	LMG	I	101	43/55	0.74	0.56	73,118,166,178	0
31	LMG	M	101	42/55	0.74	0.35	83,111,135,144	0
23	CLA	C	507	65/65	0.74	0.67	79,93,100,104	0
31	LMG	B	622	49/55	0.75	0.33	61,79,105,117	0
28	DGD	a	413	56/66	0.75	0.38	76,100,145,148	0
23	CLA	C	513	65/65	0.75	0.94	95,109,142,149	0
31	LMG	k	103	48/55	0.75	0.43	79,100,112,115	0
27	BCR	C	516	40/40	0.75	0.57	74,86,95,100	0
30	SQD	f	102	45/54	0.75	0.60	88,133,148,152	0
25	PL9	d	404	55/55	0.75	0.32	45,65,78,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	SQD	a	401	54/54	0.76	0.43	76,114,149,152	0
23	CLA	c	512	65/65	0.77	1.06	83,104,146,152	0
25	PL9	D	404	55/55	0.77	0.32	42,61,71,77	0
31	LMG	m	102	42/55	0.77	0.38	73,111,128,138	0
28	DGD	c	518	66/66	0.77	0.33	54,73,105,118	0
30	SQD	A	417	54/54	0.78	0.37	77,113,147,154	0
27	BCR	c	515	40/40	0.78	0.80	75,86,95,101	0
23	CLA	C	504	65/65	0.78	0.36	62,83,138,145	0
21	FE2	A	401	1/1	0.78	0.17	64,64,64,64	0
32	CL	a	418	1/1	0.78	0.49	49,49,49,49	0
23	CLA	a	406	65/65	0.78	0.36	55,71,140,147	0
27	BCR	B	617	40/40	0.78	0.33	67,74,81,84	0
23	CLA	B	602	65/65	0.79	0.63	68,87,95,96	0
23	CLA	B	606	65/65	0.79	0.72	67,81,110,121	0
27	BCR	d	405	40/40	0.79	0.37	69,82,102,106	0
27	BCR	T	101	40/40	0.79	0.31	68,75,82,83	0
23	CLA	c	506	65/65	0.79	0.49	78,92,122,128	0
23	CLA	C	502	65/65	0.79	0.50	59,75,108,111	0
23	CLA	B	608	65/65	0.79	0.64	64,75,93,97	0
23	CLA	C	505	65/65	0.79	0.41	69,77,86,91	0
23	CLA	C	510	65/65	0.80	0.38	67,74,83,93	0
31	LMG	D	406	46/55	0.80	0.33	58,73,116,129	0
23	CLA	b	612	65/65	0.80	0.51	63,75,95,98	0
29	LHG	a	414	39/49	0.80	0.41	60,78,94,102	0
27	BCR	c	514	40/40	0.80	1.10	76,82,88,89	0
23	CLA	C	511	65/65	0.80	0.55	74,88,102,109	0
31	LMG	a	416	51/55	0.80	0.33	62,80,93,100	0
28	DGD	b	602	52/66	0.80	0.41	79,107,180,186	0
28	DGD	b	623	58/66	0.80	0.36	57,74,99,107	0
27	BCR	C	515	40/40	0.80	1.05	85,92,115,116	0
23	CLA	a	409	65/65	0.81	0.46	55,67,129,133	0
33	LMT	m	101	35/35	0.81	0.41	68,93,112,114	0
31	LMG	b	625	49/55	0.81	0.31	51,75,86,89	0
31	LMG	C	520	48/55	0.81	0.29	89,100,109,112	0
23	CLA	b	613	65/65	0.81	0.73	65,93,104,114	0
23	CLA	b	619	65/65	0.81	0.59	85,97,108,116	0
23	CLA	b	618	65/65	0.82	0.32	60,82,123,130	0
31	LMG	d	407	48/55	0.82	0.36	58,70,85,120	0
28	DGD	c	516	53/66	0.82	0.31	63,77,96,103	0
28	DGD	C	518	62/66	0.82	0.34	58,81,134,144	0
23	CLA	c	507	65/65	0.82	0.67	83,93,105,111	0
23	CLA	c	511	65/65	0.82	0.68	75,91,102,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMT	M	102	35/35	0.82	0.52	69,96,112,115	0
23	CLA	B	615	65/65	0.82	0.83	83,96,106,116	0
23	CLA	c	505	65/65	0.82	0.35	70,77,83,85	0
23	CLA	B	604	65/65	0.83	0.58	59,67,104,124	0
23	CLA	C	512	65/65	0.83	0.84	89,101,144,149	0
29	LHG	A	412	39/49	0.83	0.29	59,79,89,93	0
23	CLA	d	402	65/65	0.83	0.37	49,57,81,95	0
31	LMG	B	623	49/55	0.83	0.31	58,76,84,87	0
23	CLA	d	403	65/65	0.83	0.67	72,88,121,128	0
23	CLA	c	503	65/65	0.83	0.81	77,89,97,103	0
23	CLA	c	504	65/65	0.83	0.34	75,83,133,138	0
23	CLA	A	407	65/65	0.84	0.49	56,66,127,129	0
27	BCR	C	514	40/40	0.84	1.00	73,80,87,94	0
23	CLA	b	614	65/65	0.84	0.60	66,82,88,91	0
34	HEM	v	201	43/43	0.84	0.51	57,68,75,76	0
31	LMG	A	414	51/55	0.84	0.26	63,77,92,95	0
23	CLA	b	607	65/65	0.84	0.77	68,82,92,103	0
23	CLA	B	610	65/65	0.84	0.67	69,81,88,92	0
24	PHO	A	406	64/64	0.84	0.36	50,69,77,81	0
23	CLA	C	501	65/65	0.85	0.48	69,82,90,95	0
23	CLA	c	501	65/65	0.85	0.82	67,82,92,94	0
23	CLA	A	405	65/65	0.85	0.30	44,69,140,145	0
34	HEM	V	201	43/43	0.85	0.47	58,69,74,76	0
23	CLA	c	509	65/65	0.85	0.51	67,85,91,97	0
23	CLA	b	608	65/65	0.85	0.40	61,68,107,117	0
28	DGD	B	621	58/66	0.85	0.38	46,71,101,105	0
23	CLA	C	509	65/65	0.85	0.62	62,81,95,98	0
28	DGD	c	517	62/66	0.85	0.30	64,84,132,141	0
24	PHO	a	408	64/64	0.86	0.33	58,68,79,86	0
23	CLA	D	403	65/65	0.86	0.88	74,87,123,124	0
23	CLA	b	606	65/65	0.86	0.47	70,87,96,97	0
22	BCT	d	401	4/4	0.86	0.49	87,91,92,94	0
23	CLA	B	607	65/65	0.86	0.28	52,66,82,85	0
31	LMG	b	624	49/55	0.86	0.27	59,82,102,113	0
31	LMG	D	407	48/55	0.86	0.26	54,72,81,120	0
23	CLA	B	605	65/65	0.87	0.66	58,78,86,92	0
21	FE2	a	403	1/1	0.87	0.16	72,72,72,72	0
23	CLA	b	609	65/65	0.87	0.51	61,76,84,88	0
23	CLA	b	610	65/65	0.87	0.52	70,83,112,126	0
28	DGD	C	517	53/66	0.87	0.29	61,79,96,101	0
23	CLA	b	611	65/65	0.87	0.32	54,64,89,92	0
23	CLA	B	611	65/65	0.87	0.31	63,72,80,87	0

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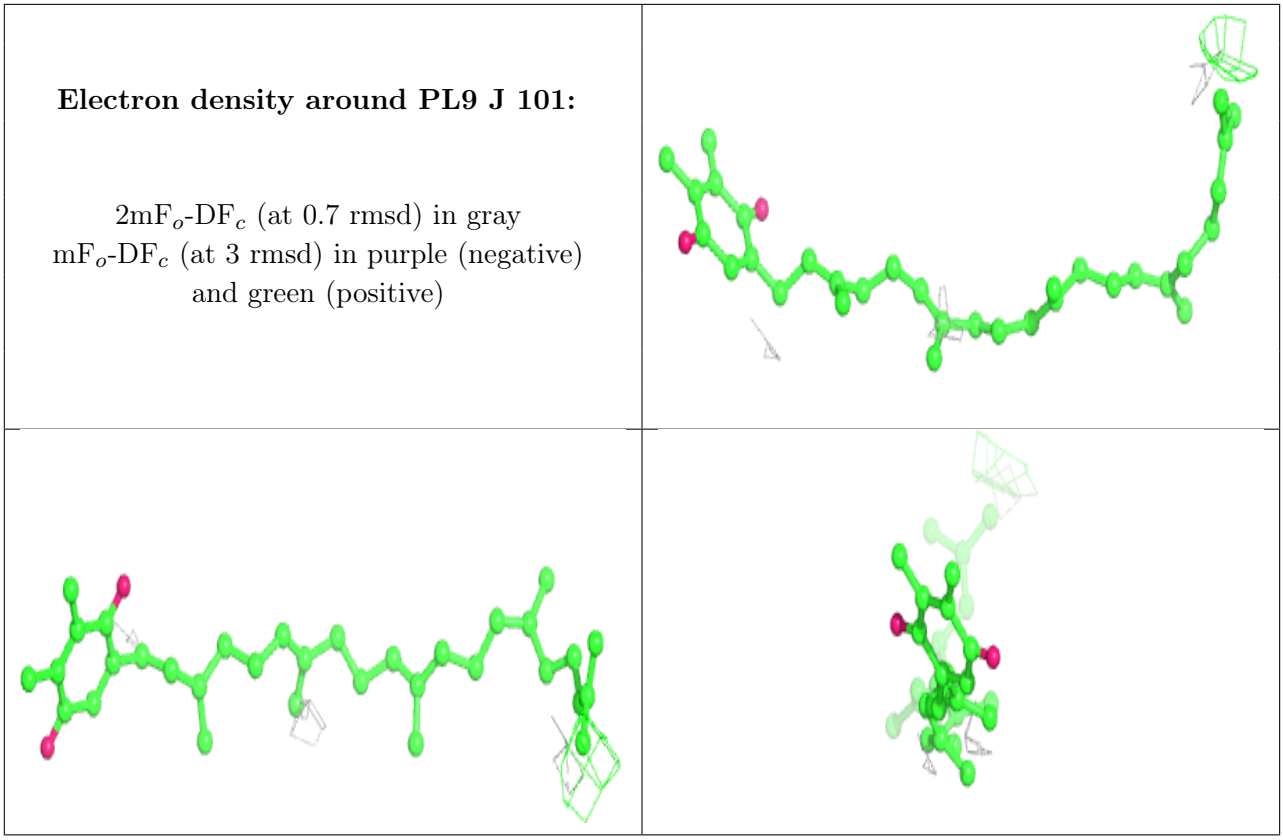
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	a	405	65/65	0.87	0.31	44,53,69,73	0
23	CLA	C	508	65/65	0.87	0.32	71,86,117,132	0
23	CLA	B	613	65/65	0.87	0.30	46,64,88,93	0
23	CLA	C	503	65/65	0.87	0.49	71,88,99,105	0
22	BCT	A	402	4/4	0.87	0.32	85,90,90,94	0
24	PHO	a	407	64/64	0.88	0.28	53,63,70,73	0
34	HEM	F	101	43/43	0.88	0.45	89,105,127,130	0
23	CLA	D	401	65/65	0.88	0.28	49,59,87,97	0
24	PHO	D	402	64/64	0.88	0.29	51,62,72,74	0
23	CLA	B	603	65/65	0.89	0.66	65,81,94,109	0
23	CLA	B	612	65/65	0.89	0.50	61,72,82,86	0
34	HEM	f	101	43/43	0.89	0.50	89,105,124,126	0
31	LMG	d	406	46/55	0.89	0.24	63,73,116,130	0
23	CLA	a	404	65/65	0.90	0.33	53,60,67,74	0
23	CLA	c	510	65/65	0.90	0.42	67,75,84,89	0
23	CLA	A	404	65/65	0.90	0.29	44,54,67,74	0
23	CLA	B	609	65/65	0.90	0.74	74,89,104,106	0
23	CLA	c	508	65/65	0.90	0.36	70,85,118,134	0
23	CLA	A	403	65/65	0.91	0.29	52,58,66,70	0
23	CLA	b	615	65/65	0.91	0.28	54,72,80,87	0
23	CLA	b	616	65/65	0.91	0.34	61,73,83,86	0
23	CLA	b	617	65/65	0.92	0.27	57,67,91,93	0
26	OEC	a	411	5/9	0.92	0.35	35,44,62,68	0
26	OEC	A	409	5/9	0.94	0.43	35,44,57,62	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.

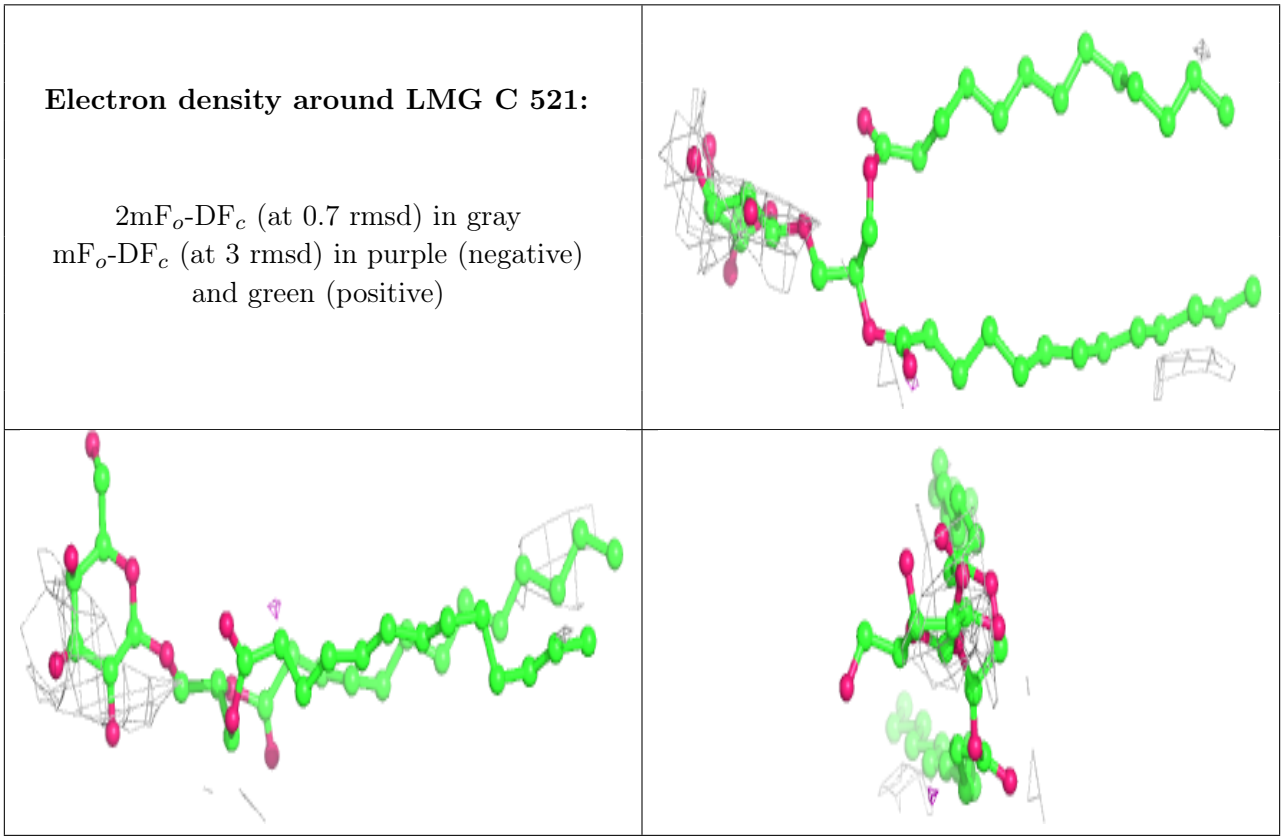
Electron density around PL9 J 101:

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



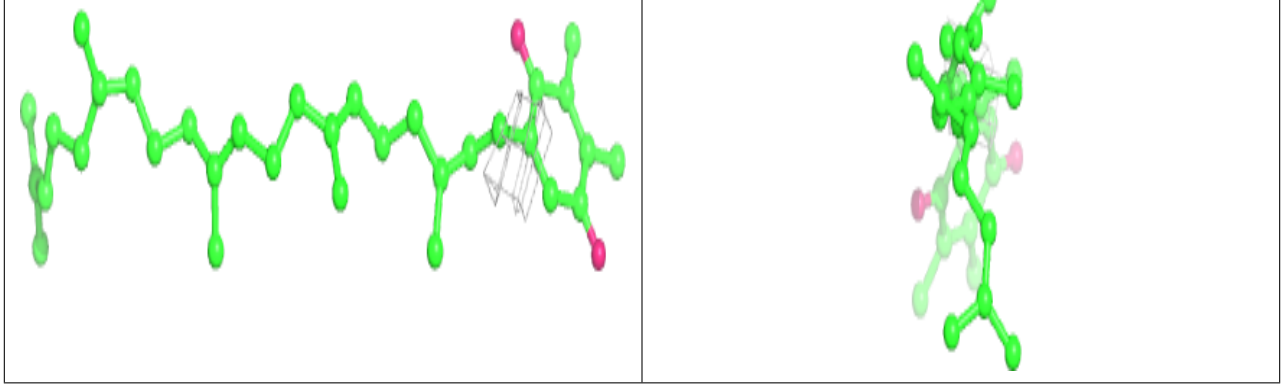
Electron density around LMG C 521:

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



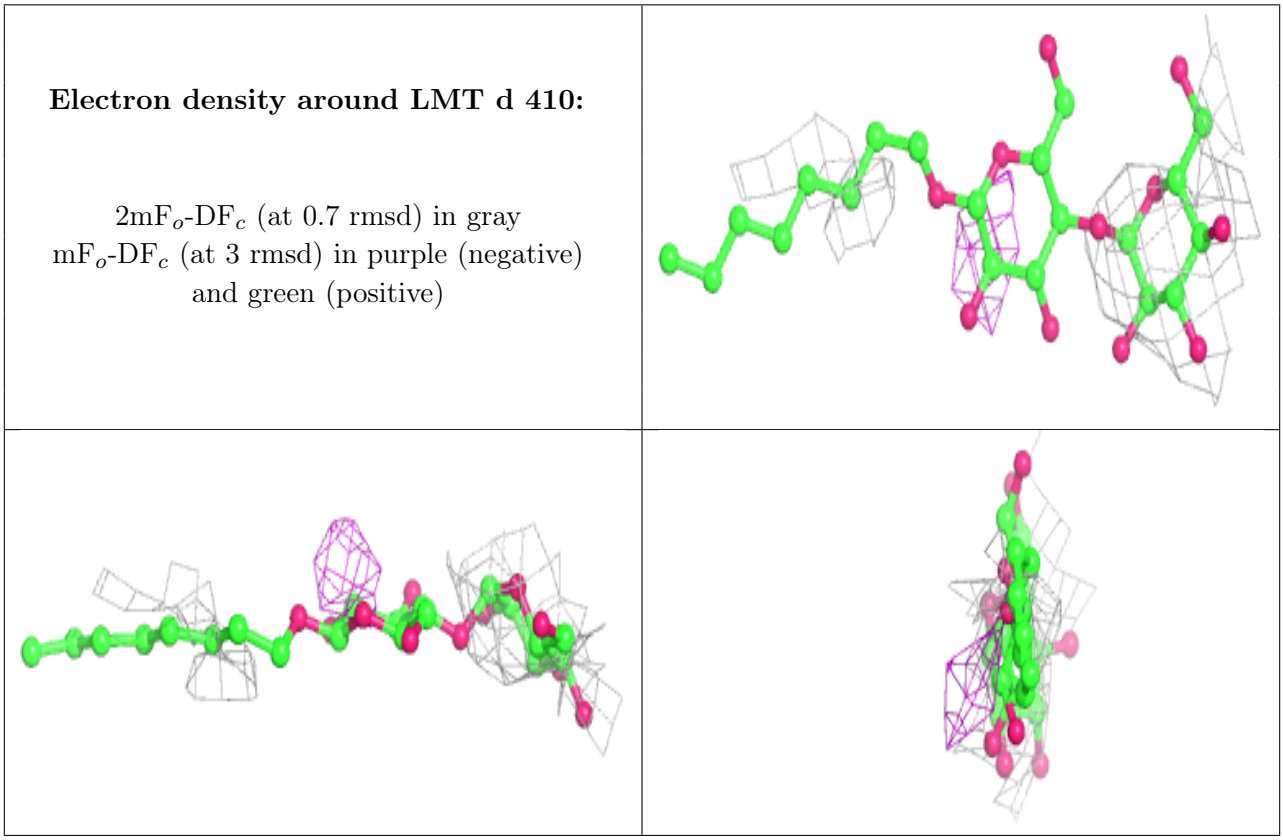
Electron density around PL9 j 101:

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



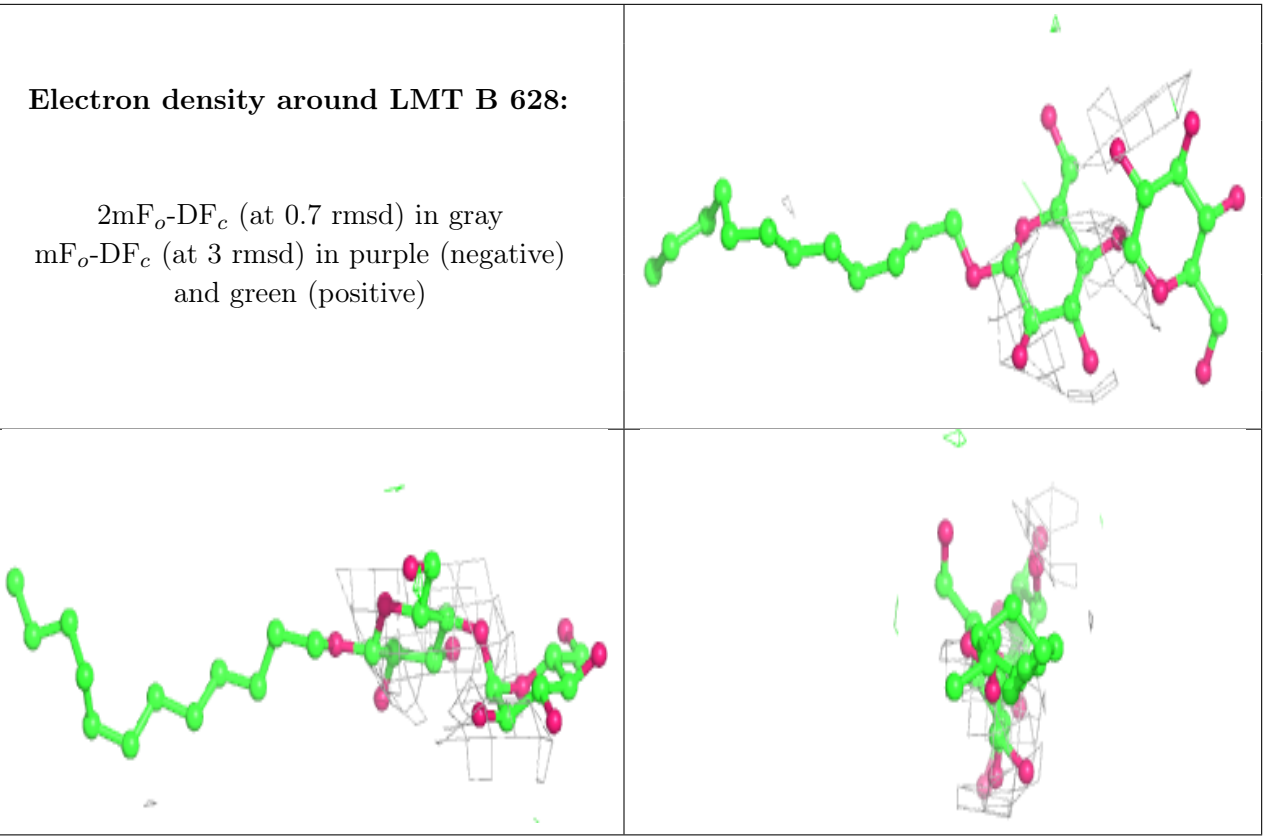
Electron density around LMT d 410:

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



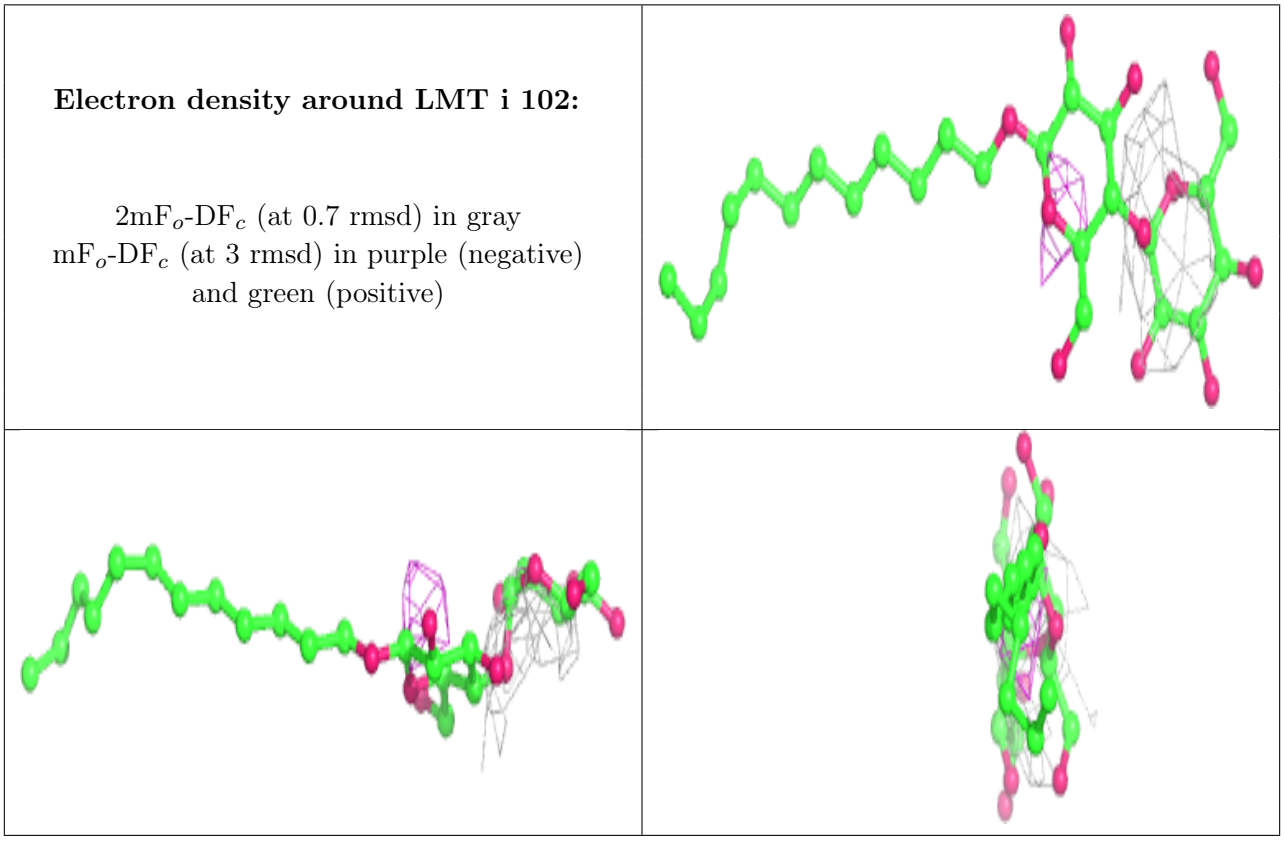
Electron density around LMT B 628:

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



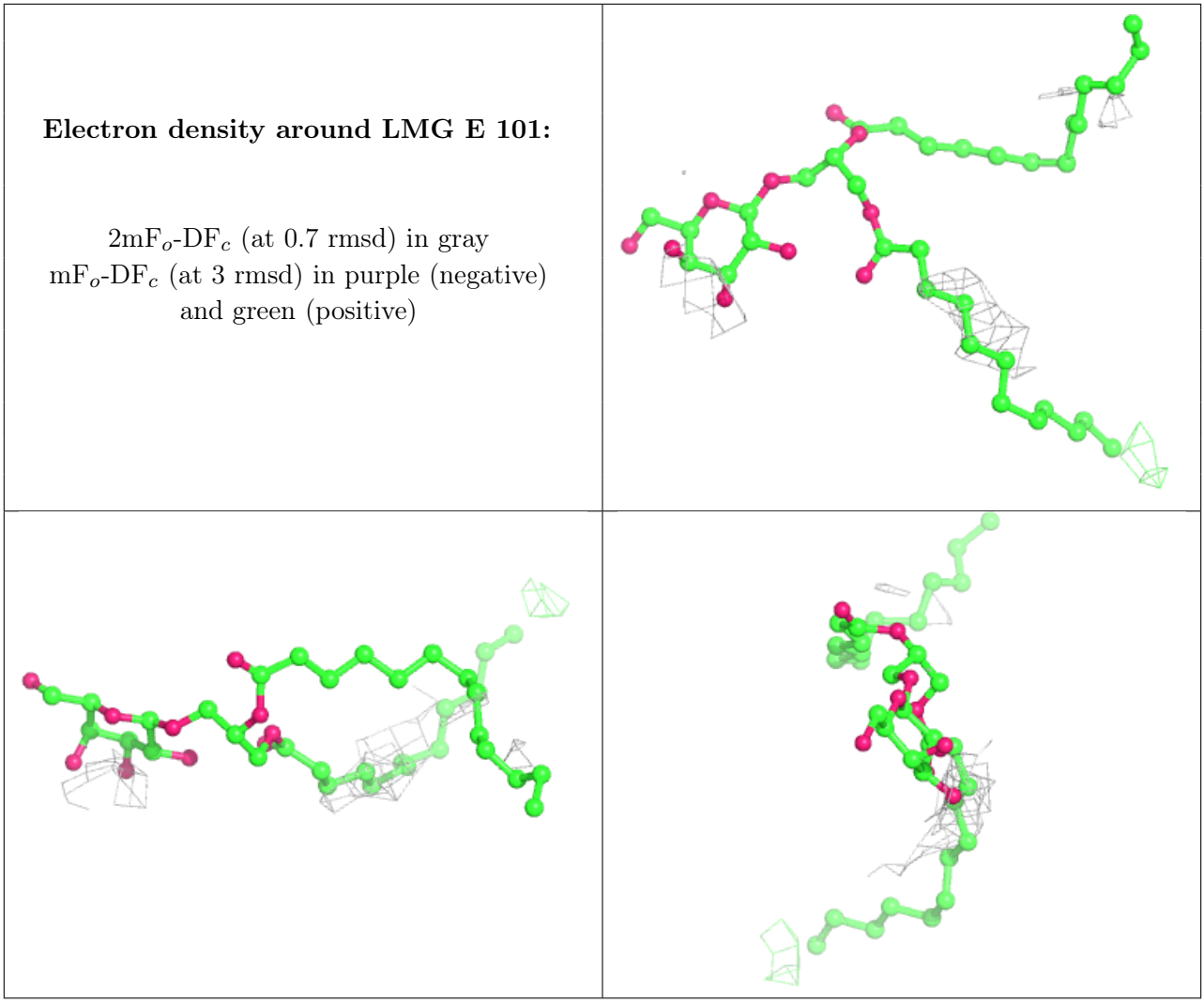
Electron density around LMT i 102:

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



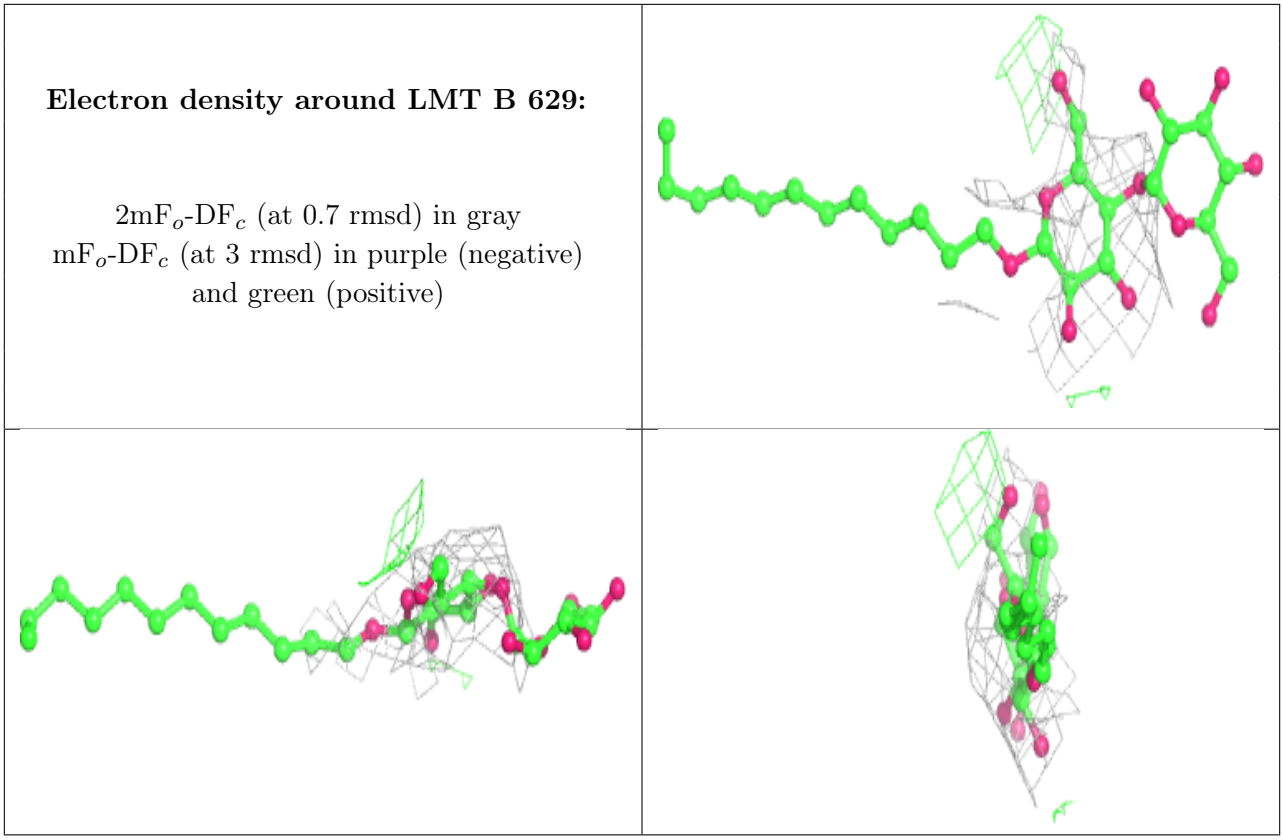
Electron density around LMG E 101:

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



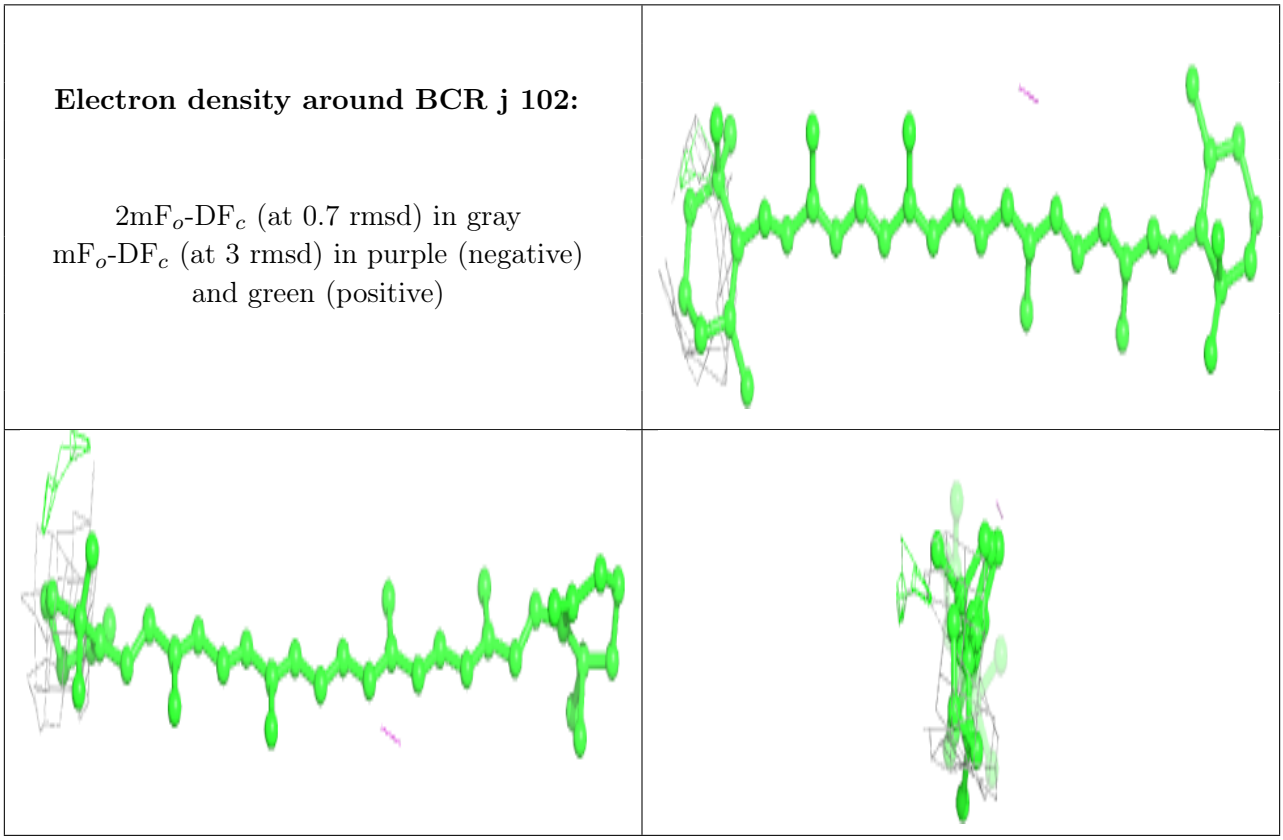
Electron density around LMT B 629:

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



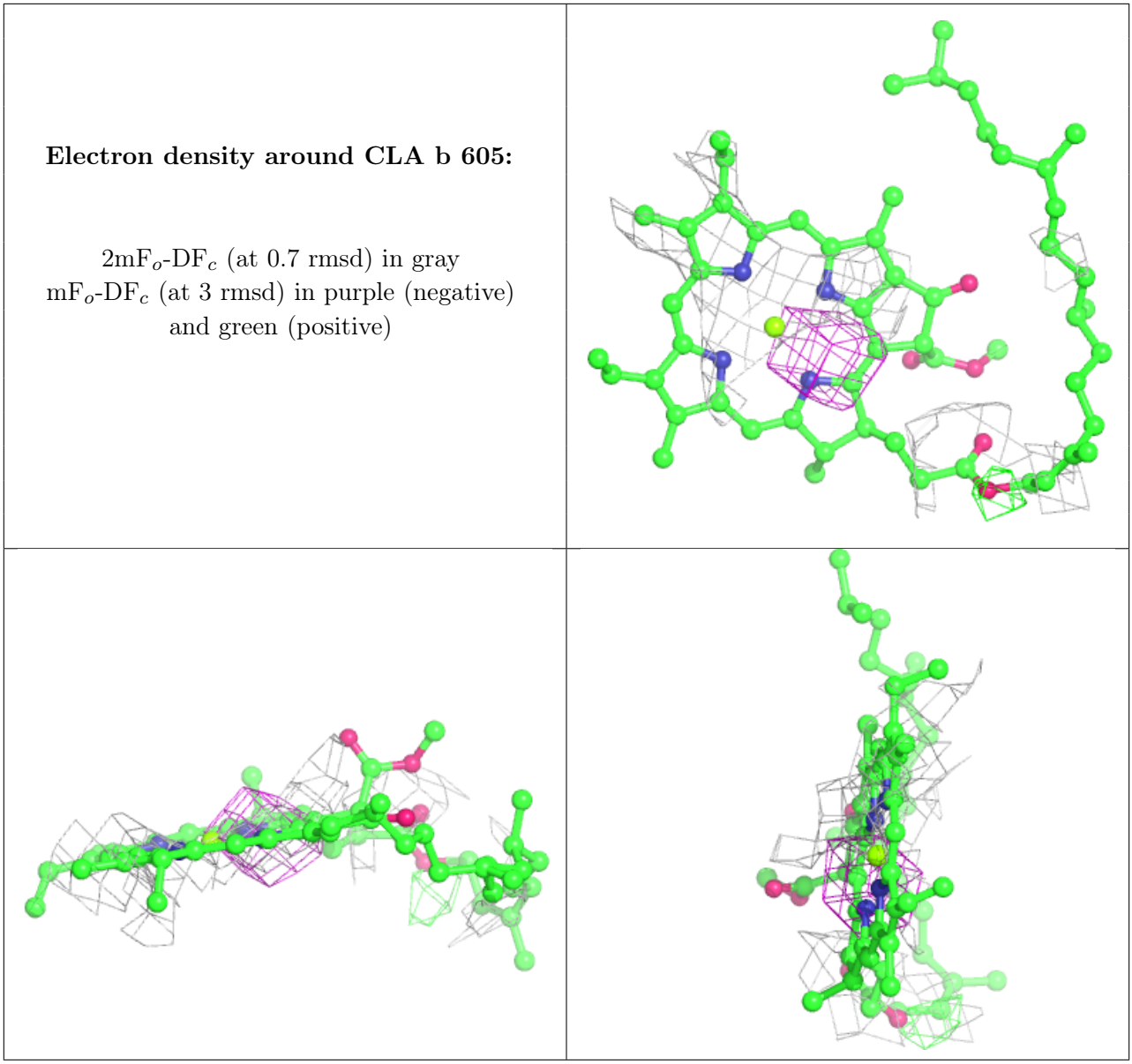
Electron density around BCR j 102:

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



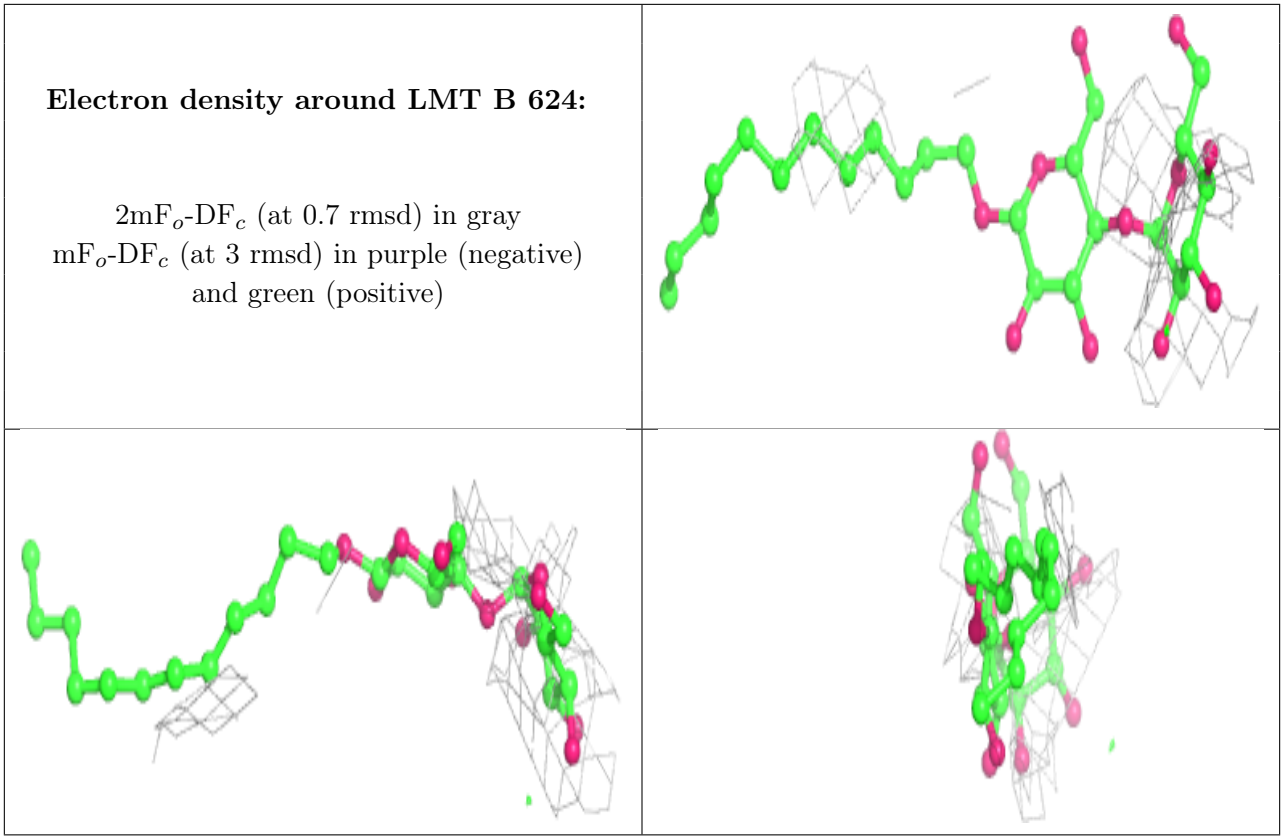
Electron density around CLA b 605:

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



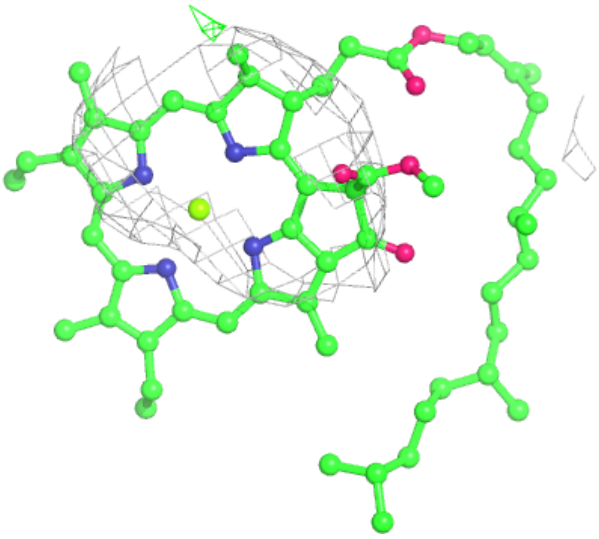
Electron density around LMT B 624:

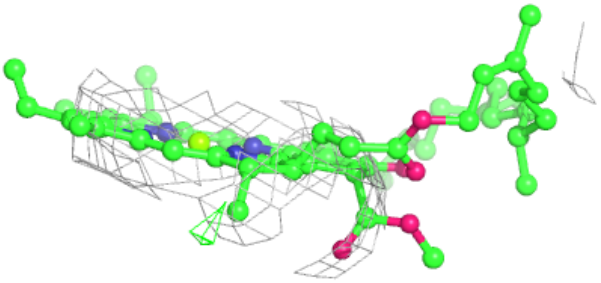
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

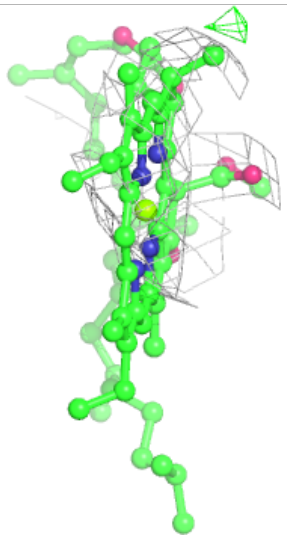


Electron density around CLA B 601:

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

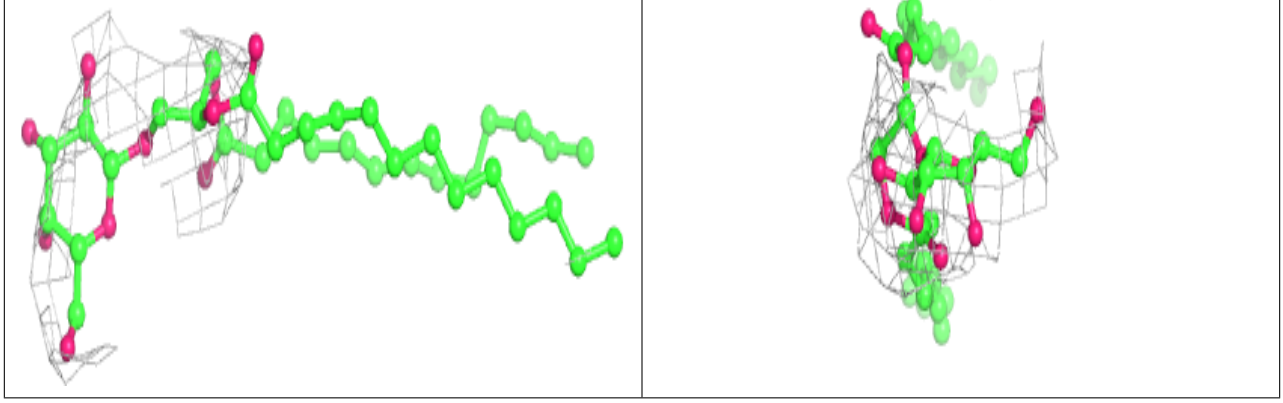






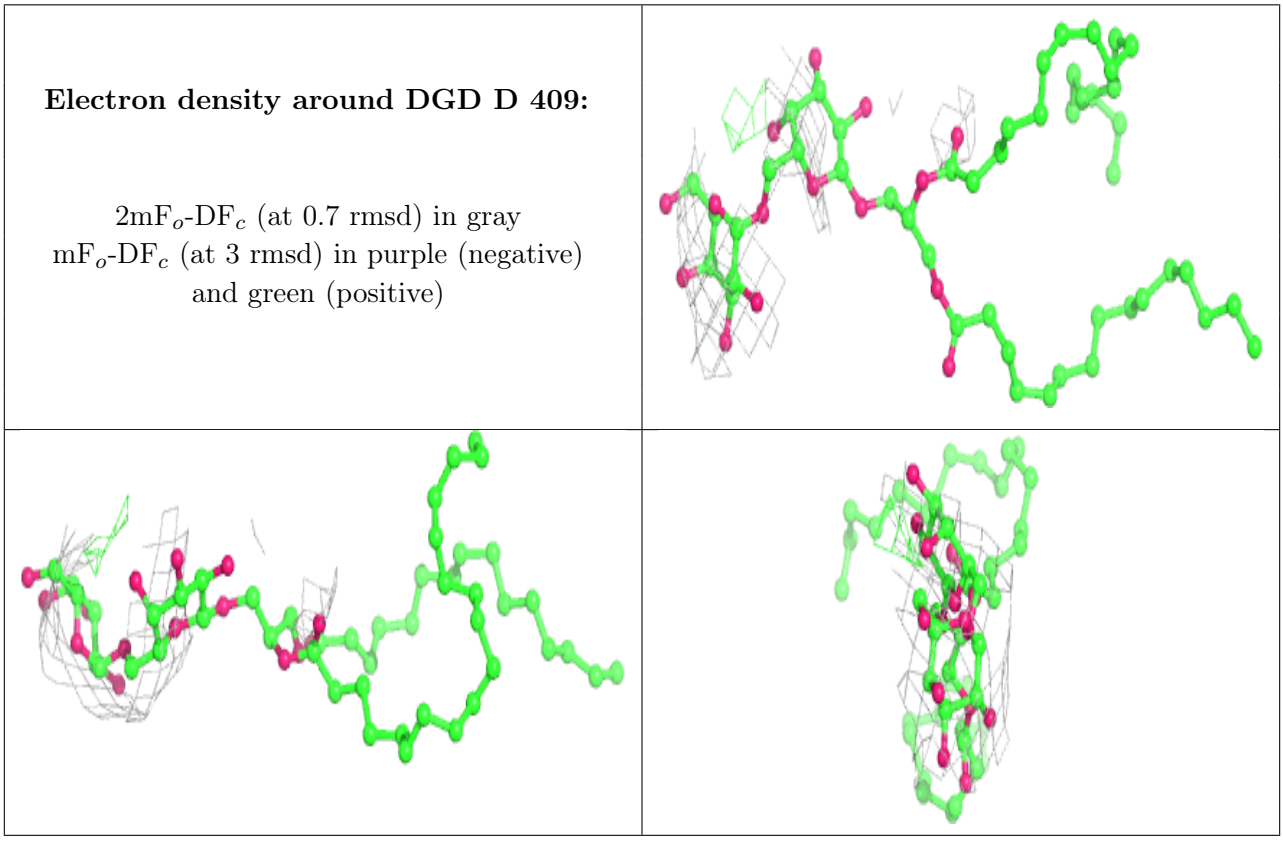
Electron density around LMG c 519:

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



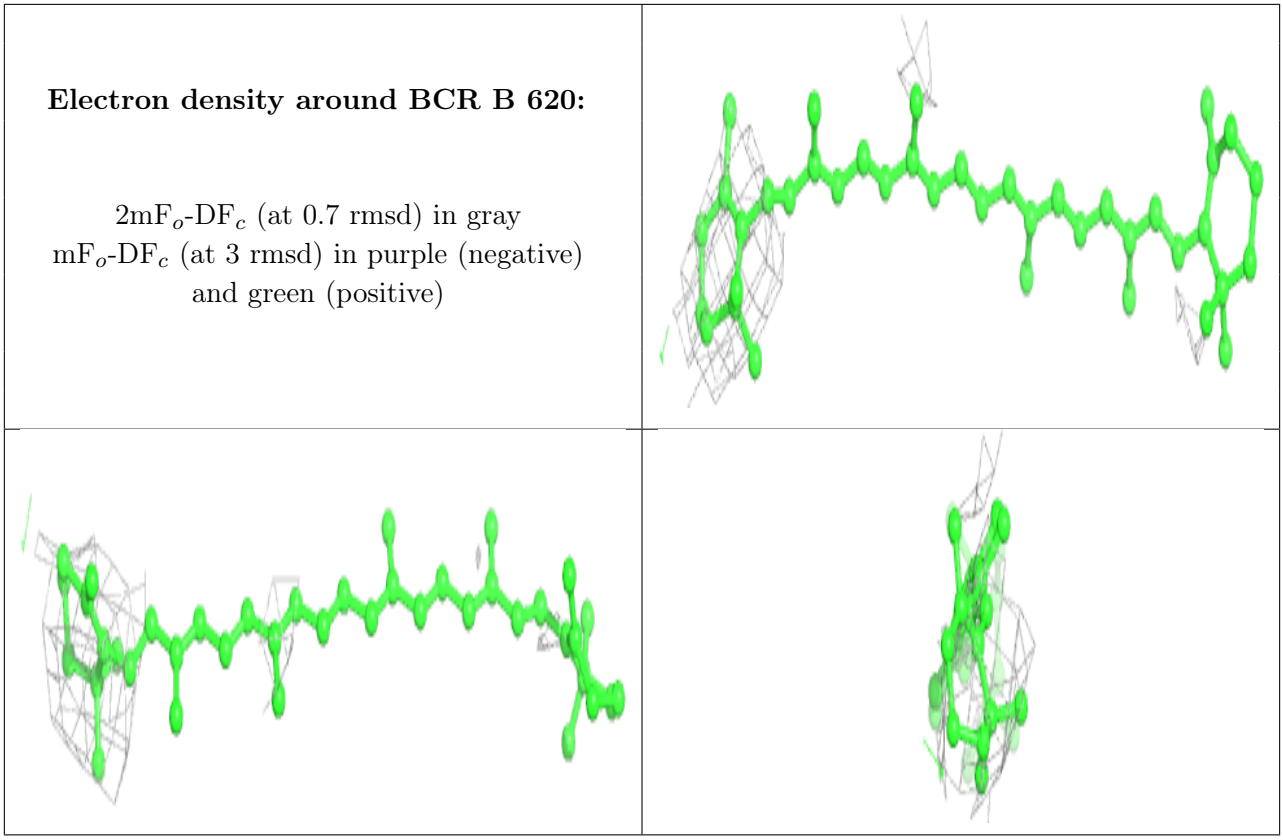
Electron density around DGD D 409:

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



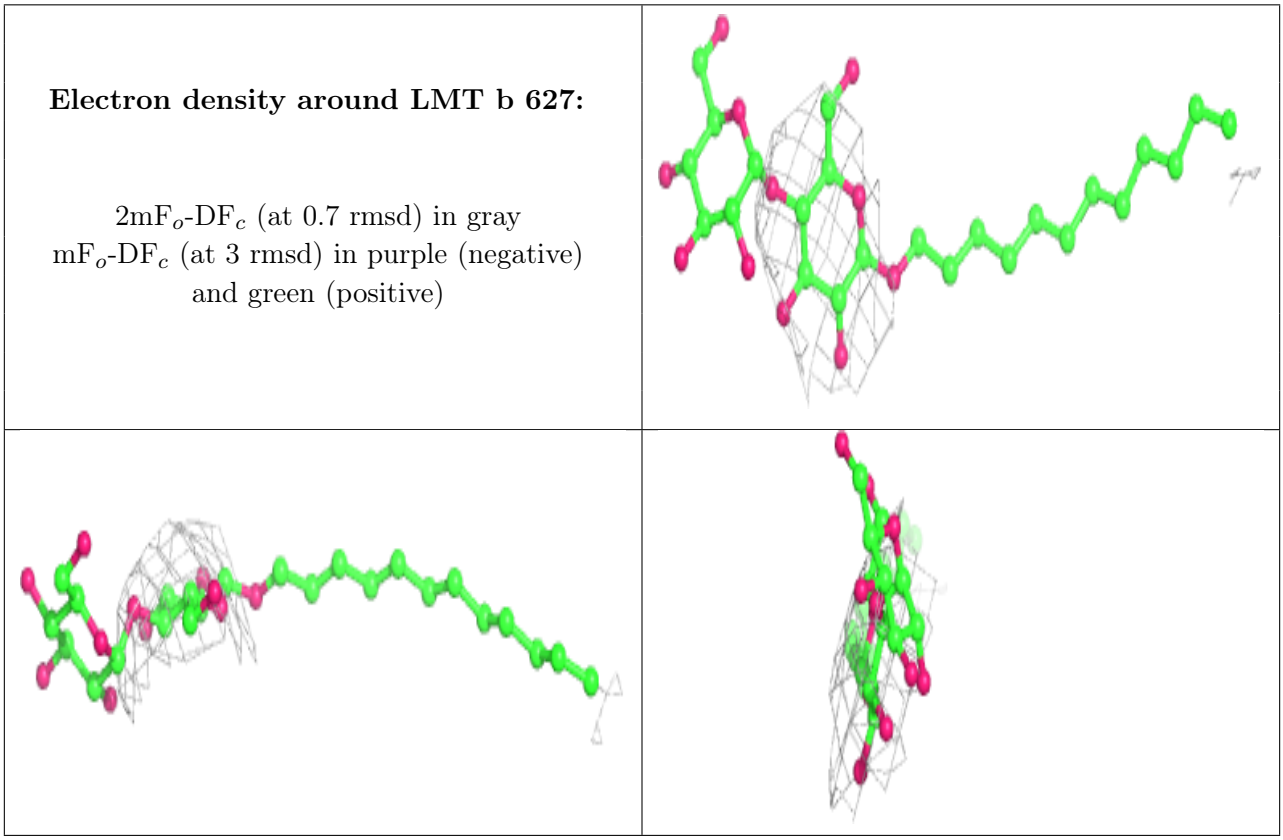
Electron density around BCR B 620:

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



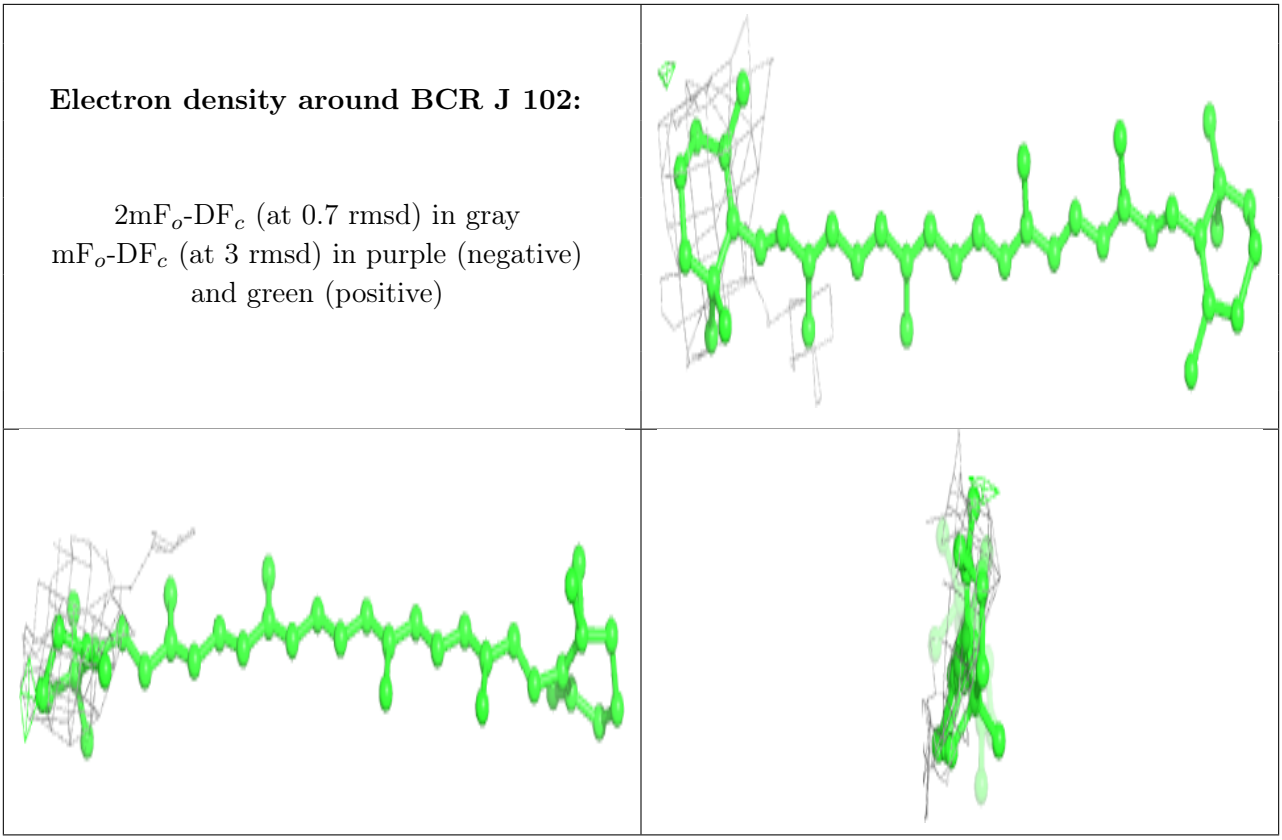
Electron density around LMT b 627:

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



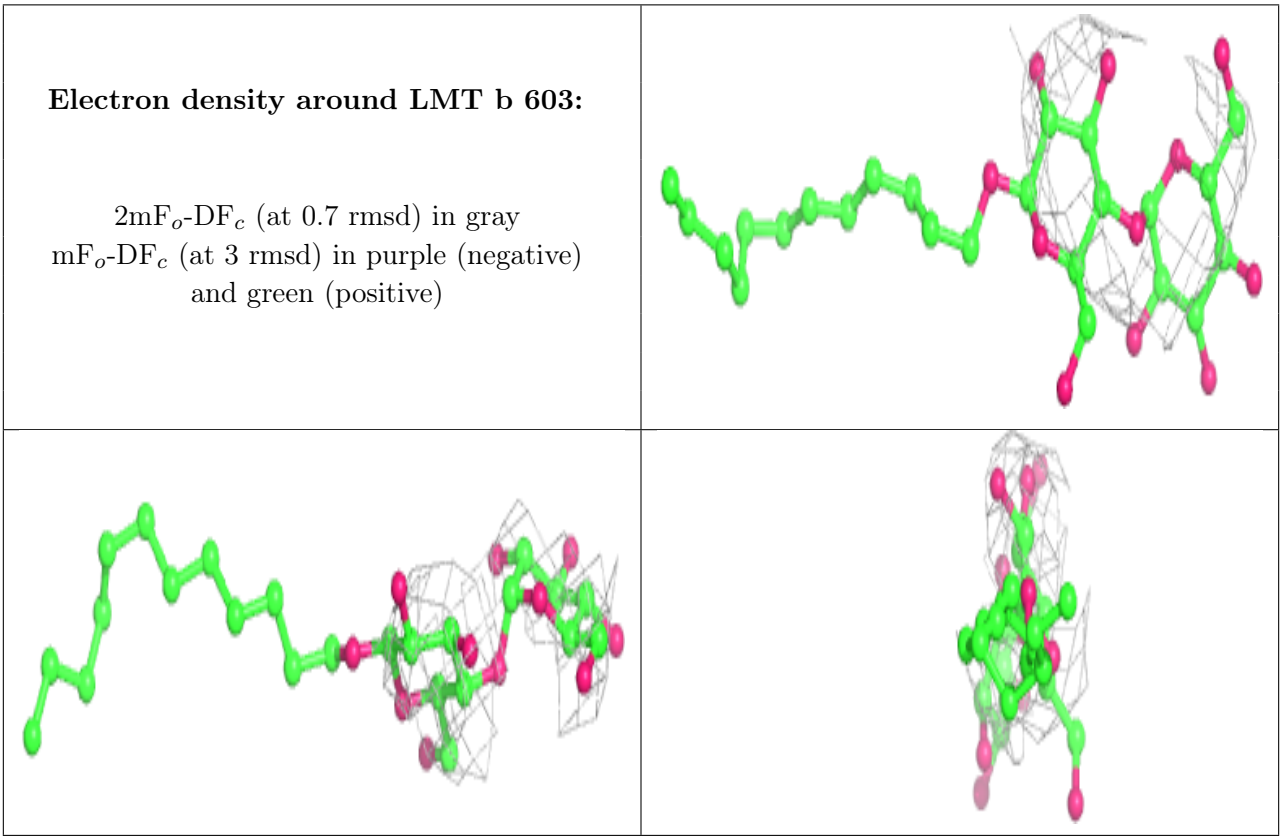
Electron density around BCR J 102:

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



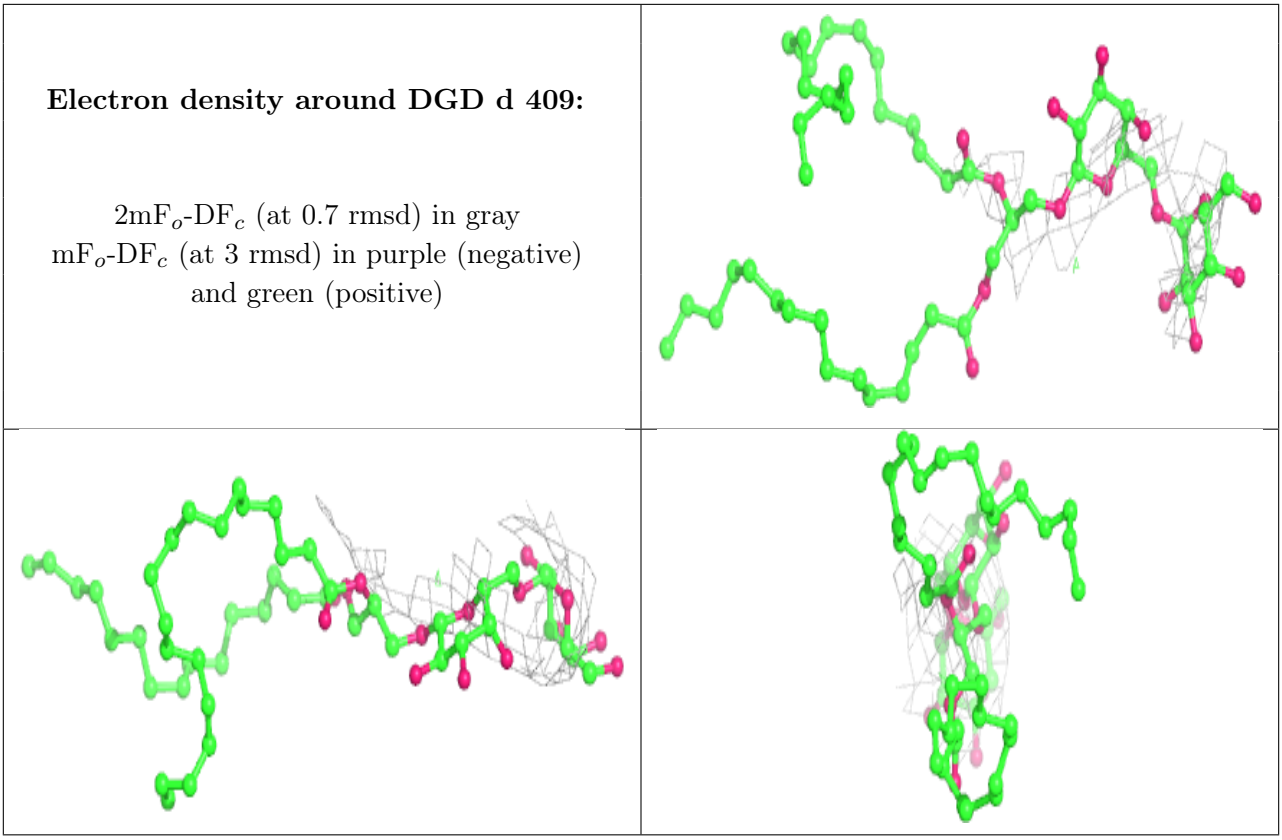
Electron density around LMT b 603:

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



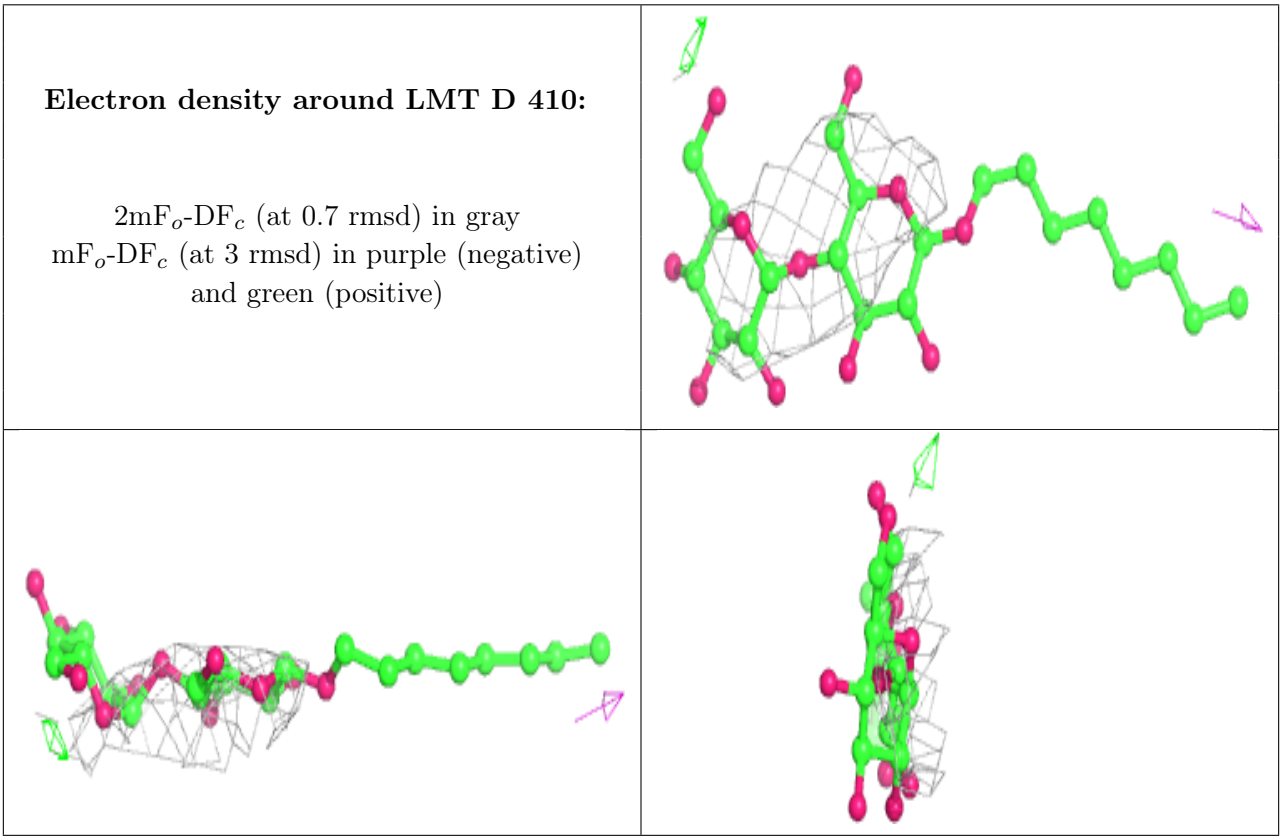
Electron density around DGD d 409:

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



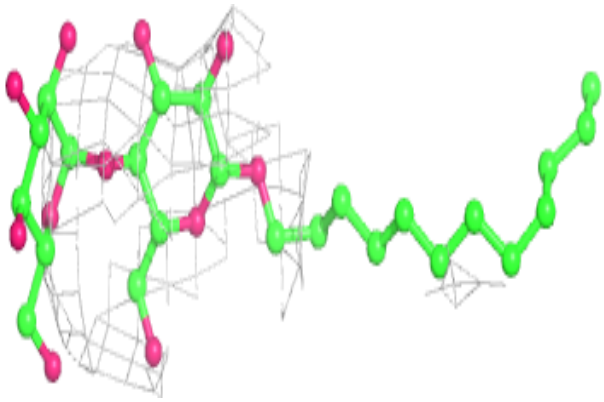
Electron density around LMT D 410:

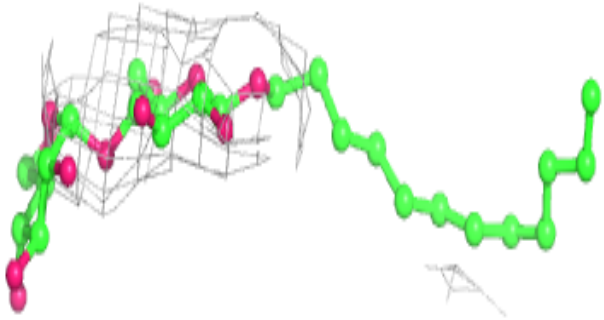
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT b 626:

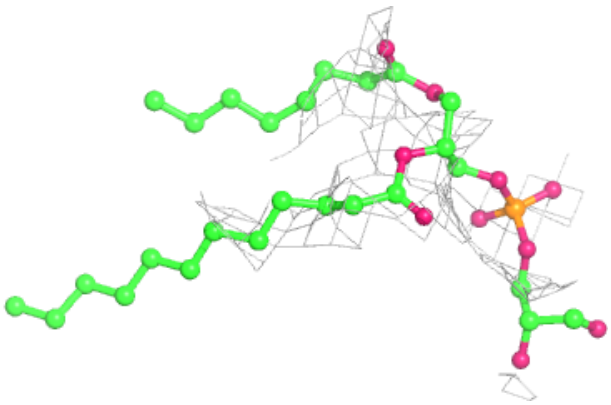
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

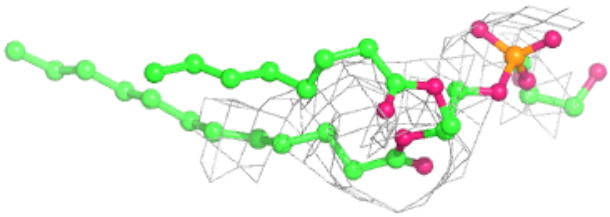


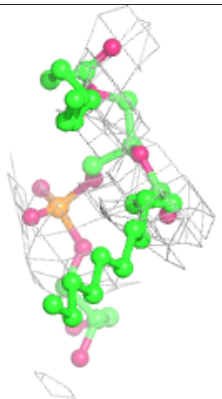


Electron density around LHG A 415:

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

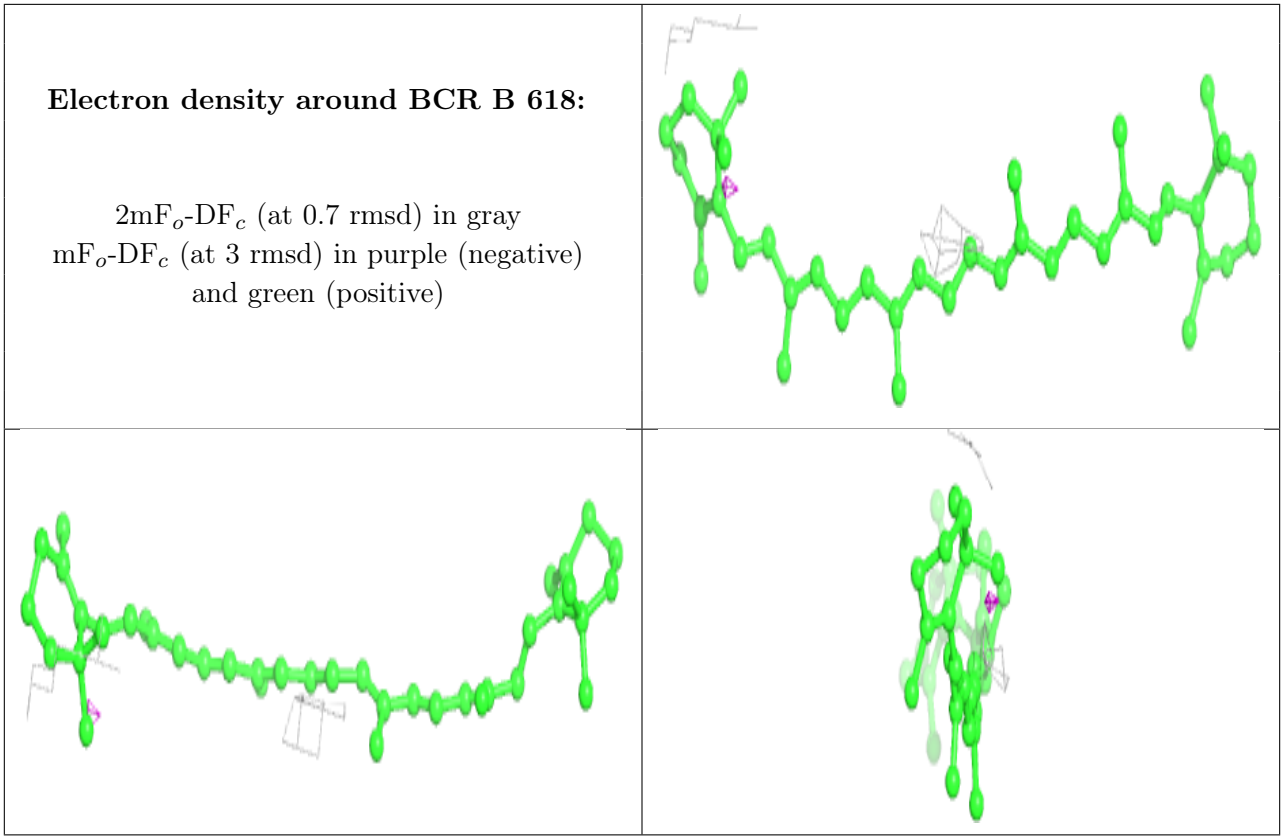






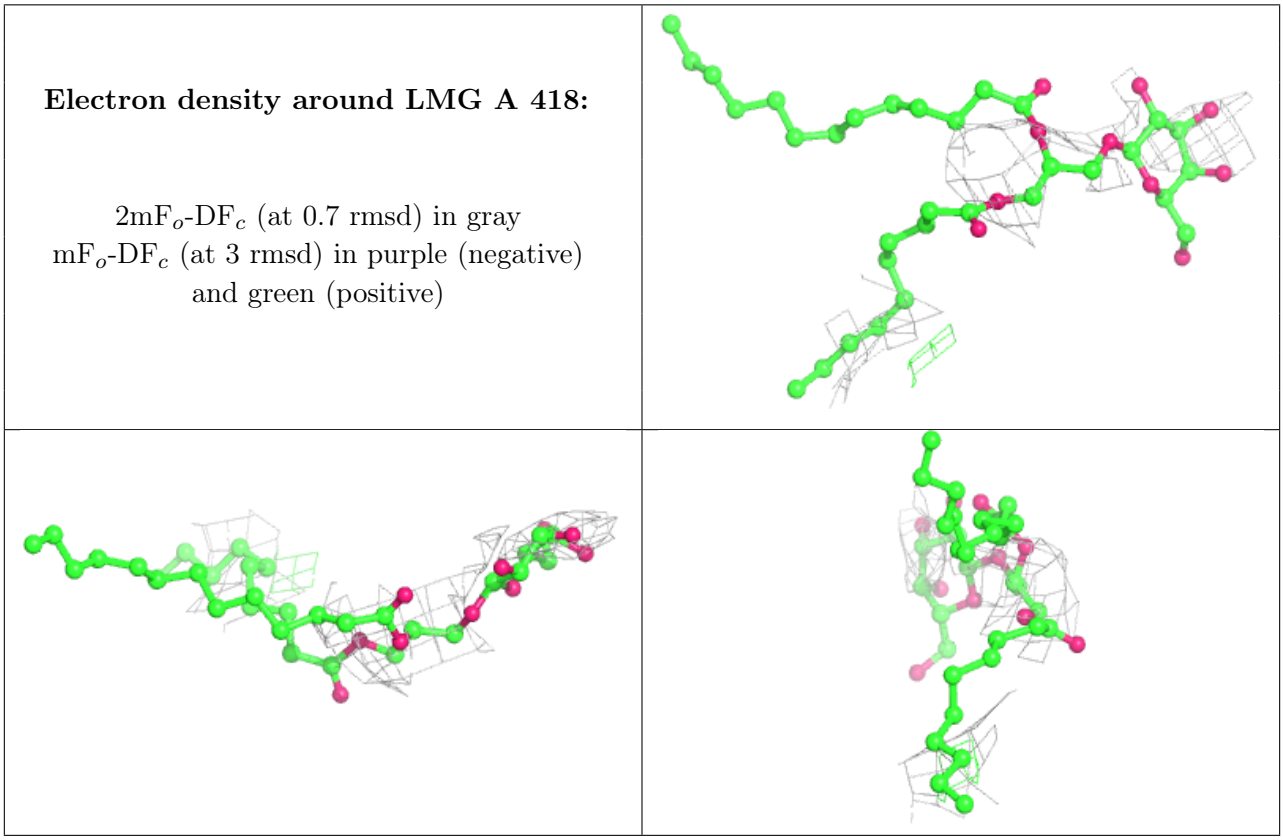
Electron density around BCR B 618:

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



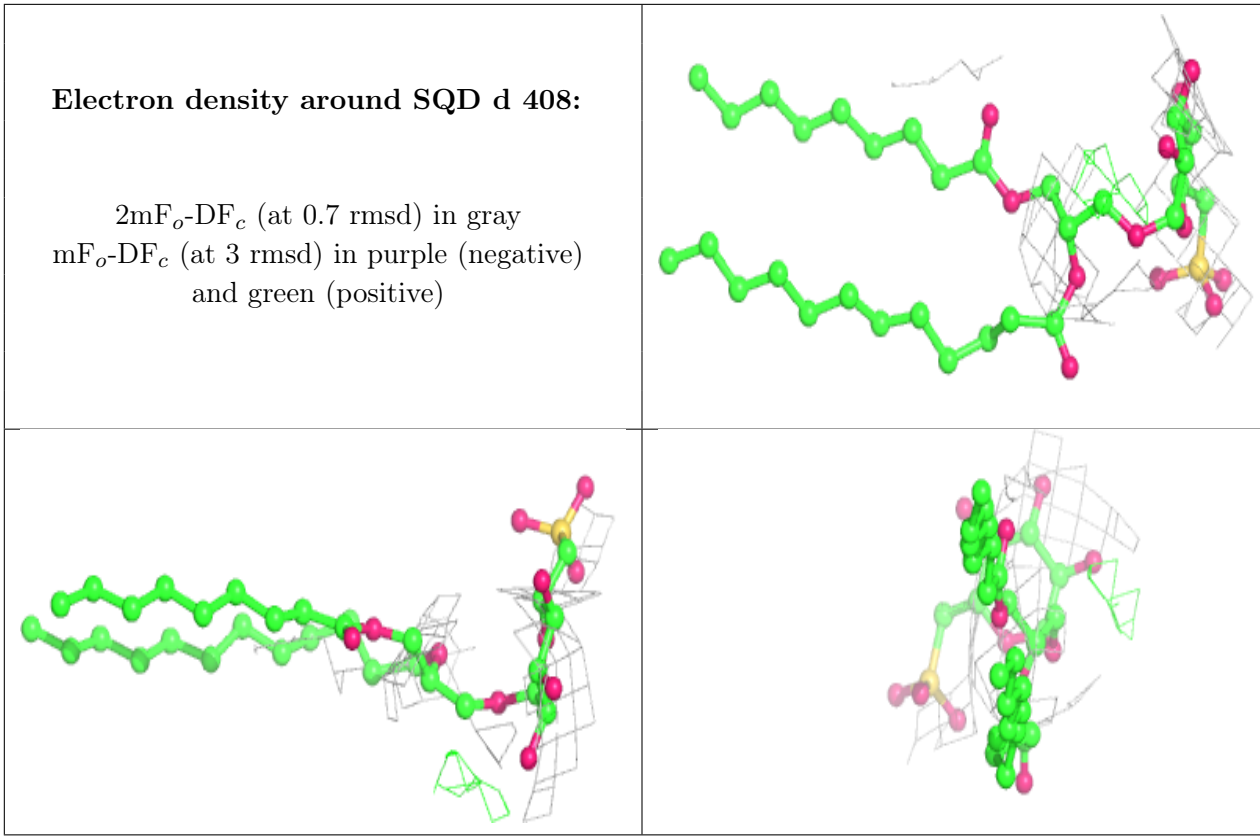
Electron density around LMG A 418:

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



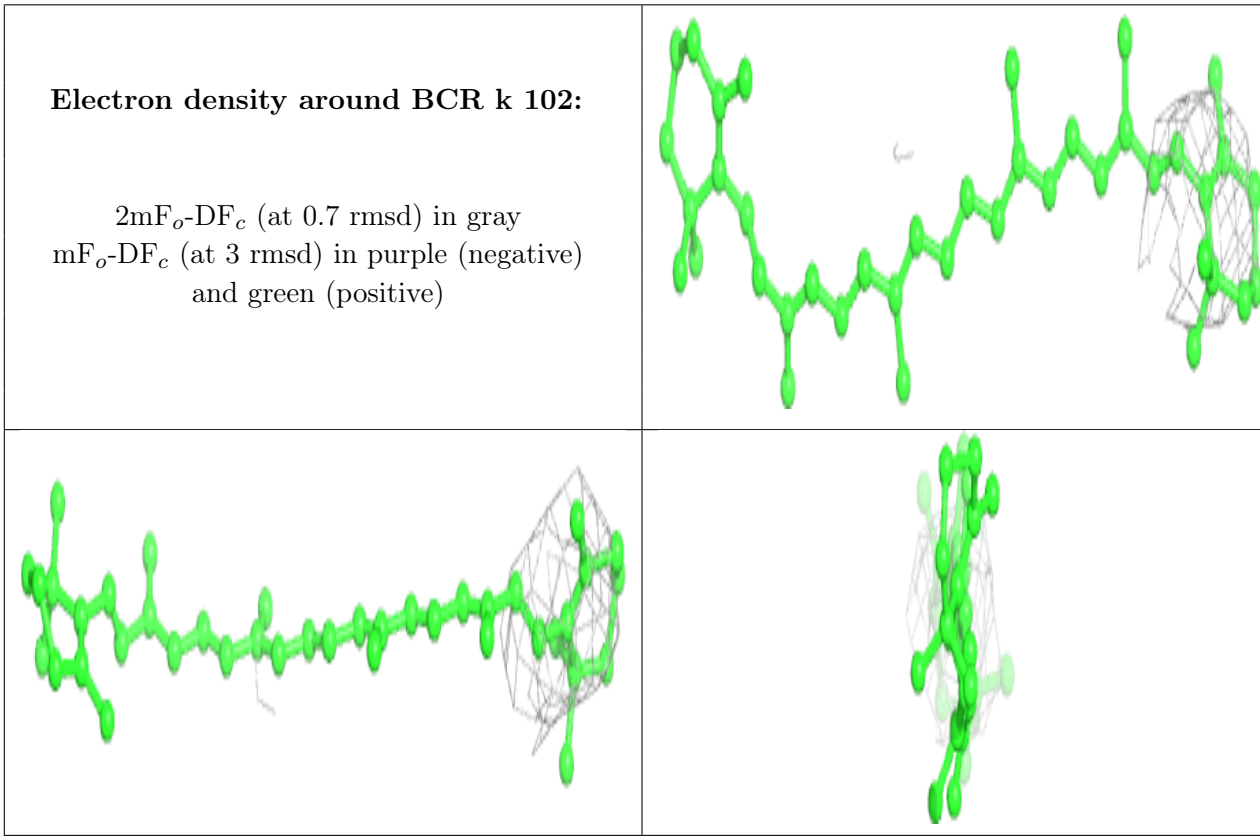
Electron density around SQD d 408:

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



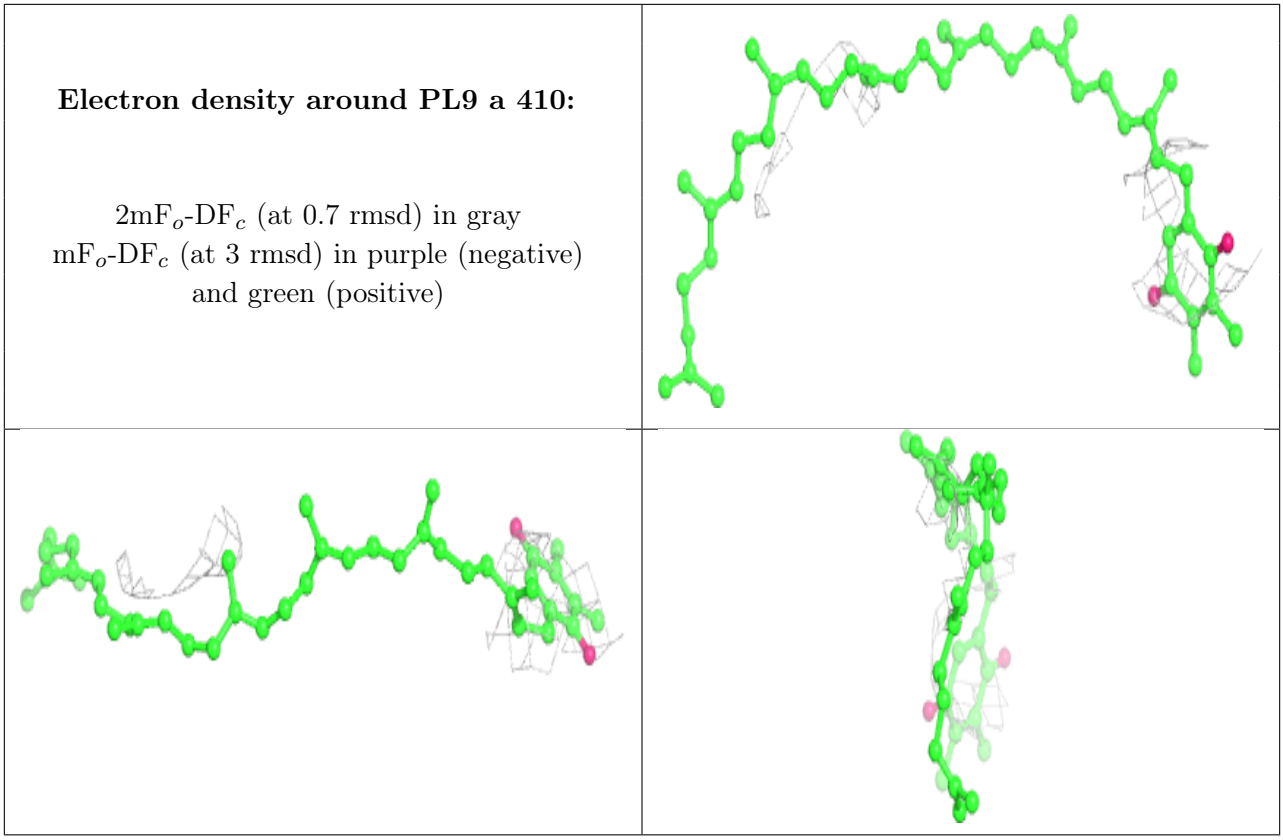
Electron density around BCR k 102:

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



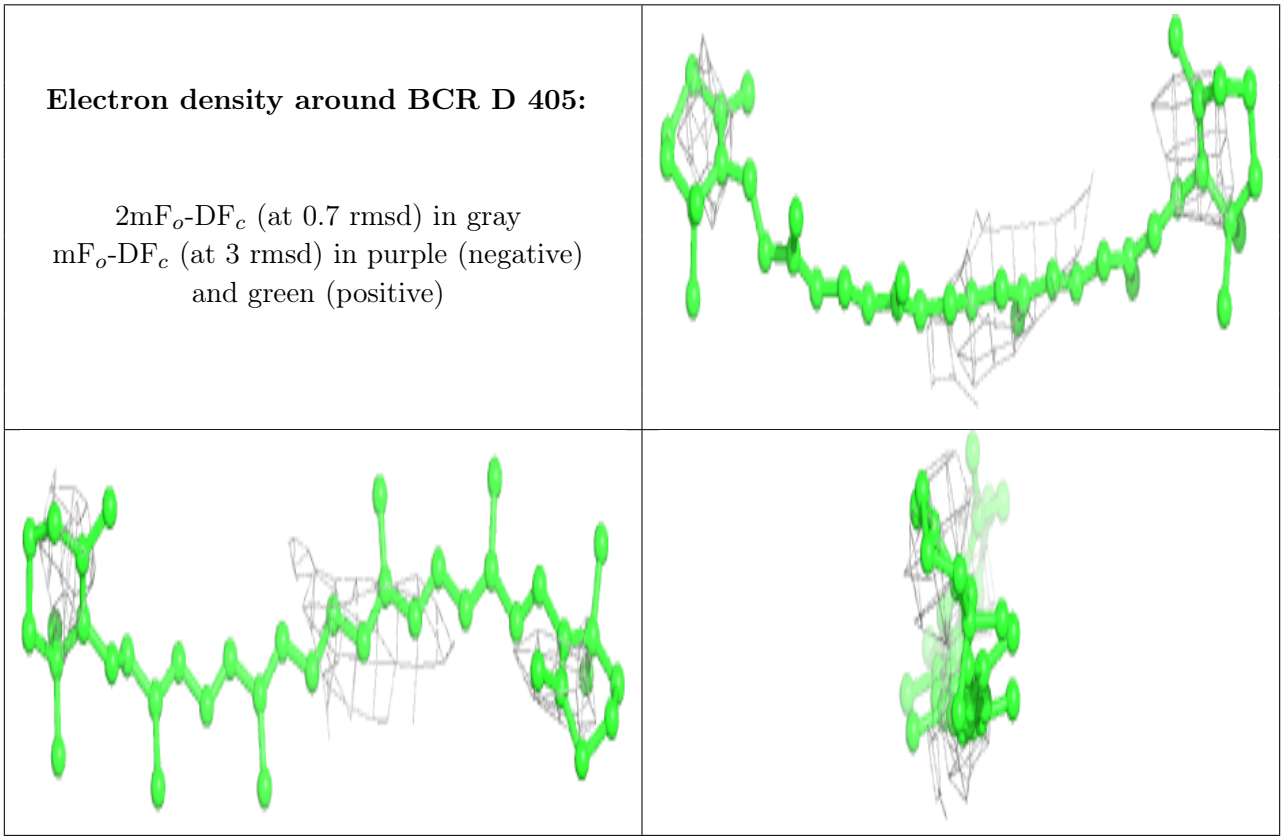
Electron density around PL9 a 410:

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



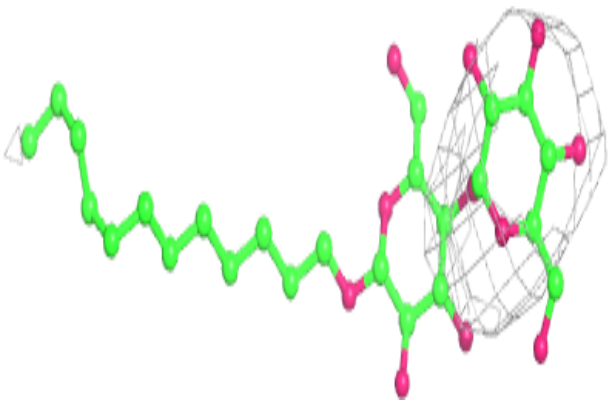
Electron density around BCR D 405:

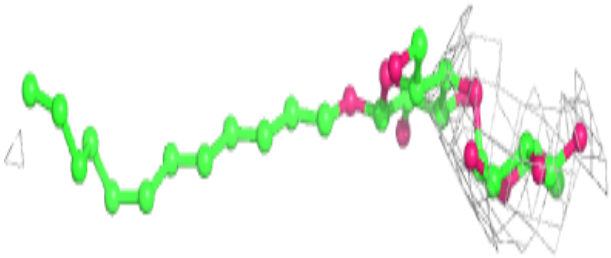
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

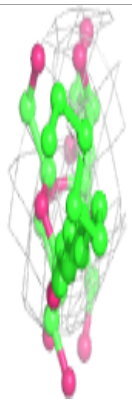


Electron density around LMT I 102:

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

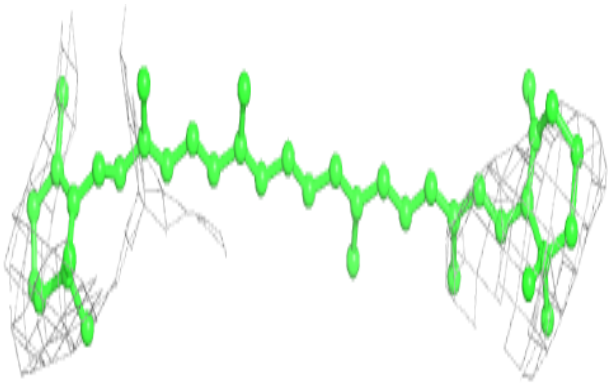


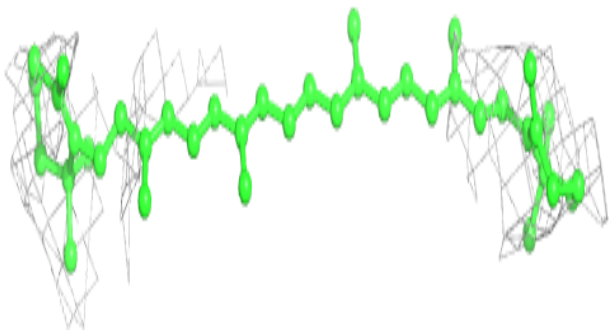


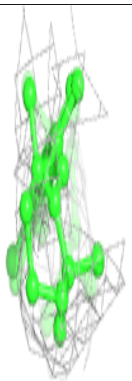


Electron density around BCR b 622:

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

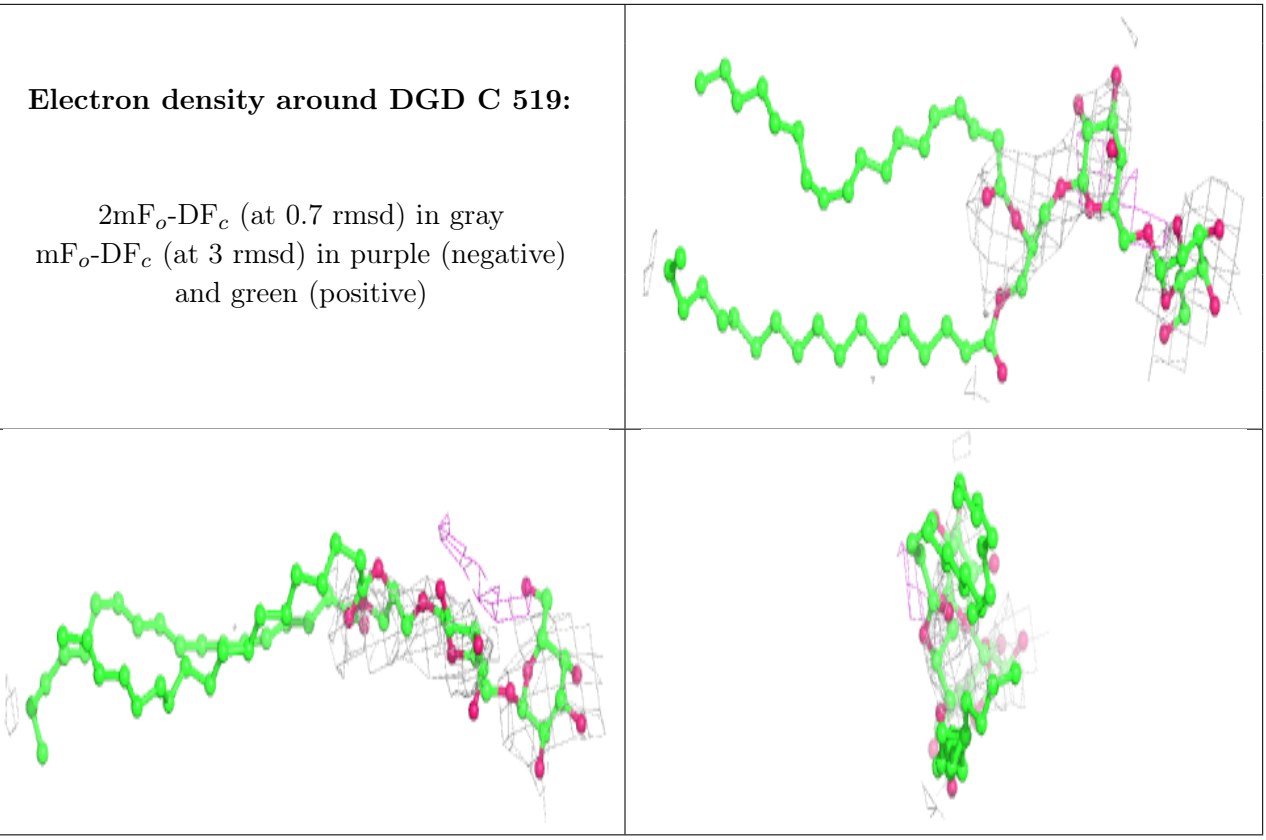






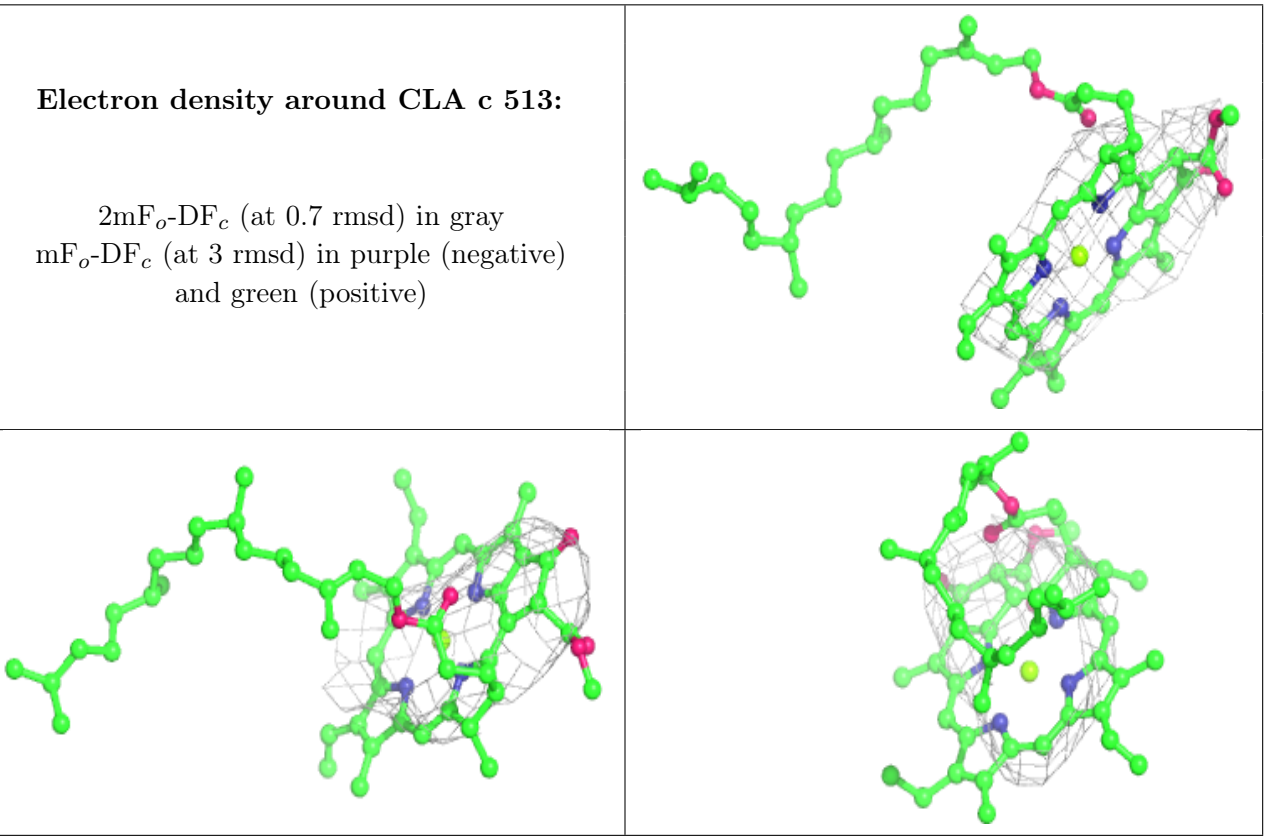
Electron density around DGD C 519:

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



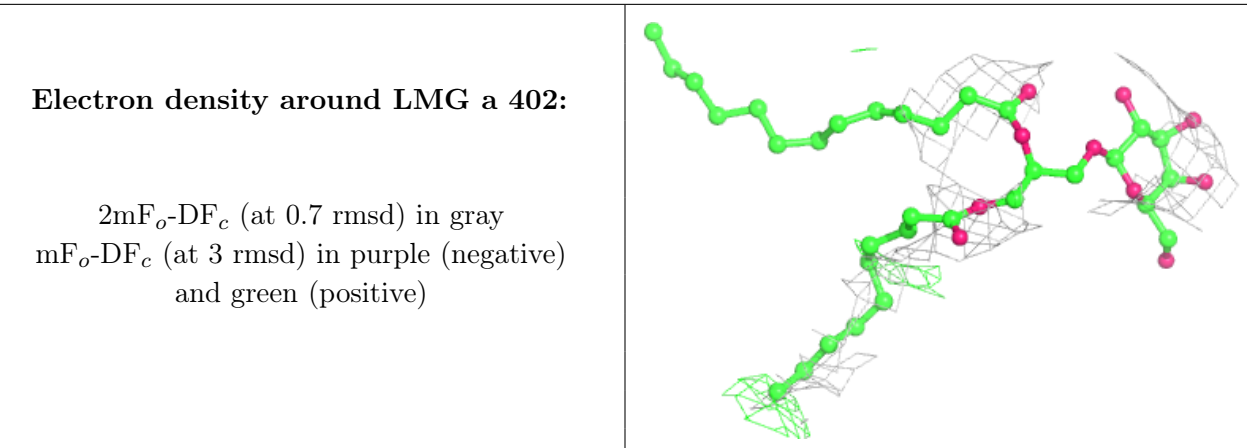
Electron density around CLA c 513:

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



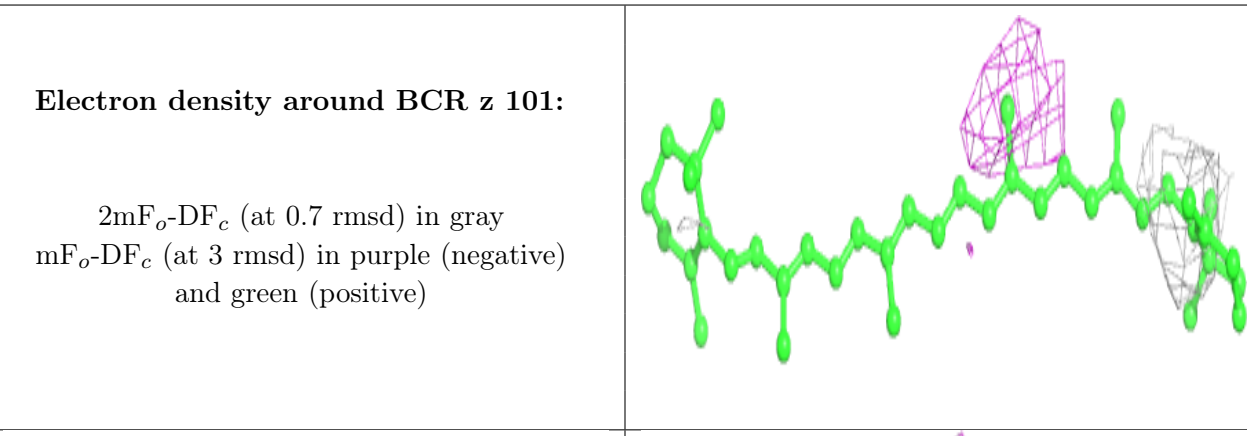
Electron density around LMG a 402:

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



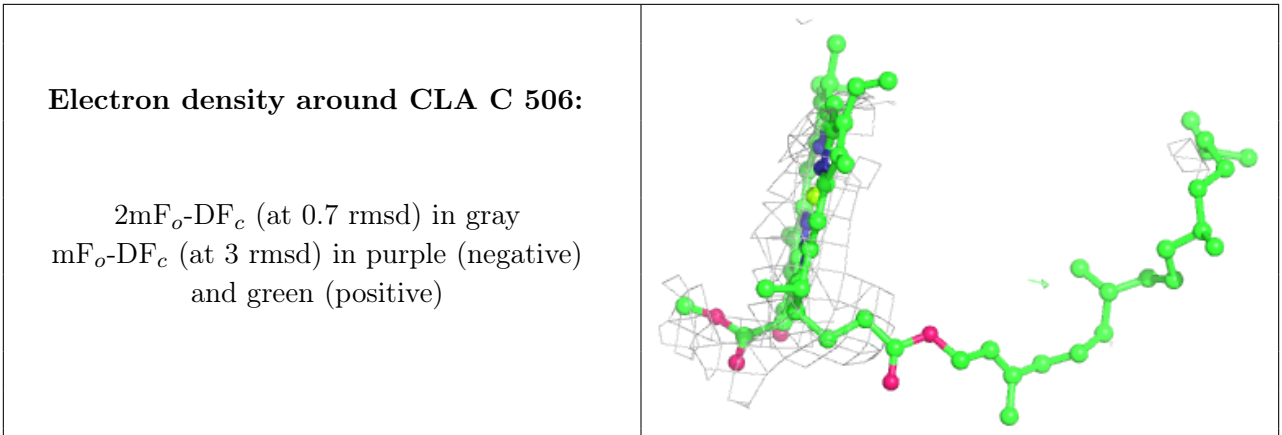
Electron density around BCR z 101:

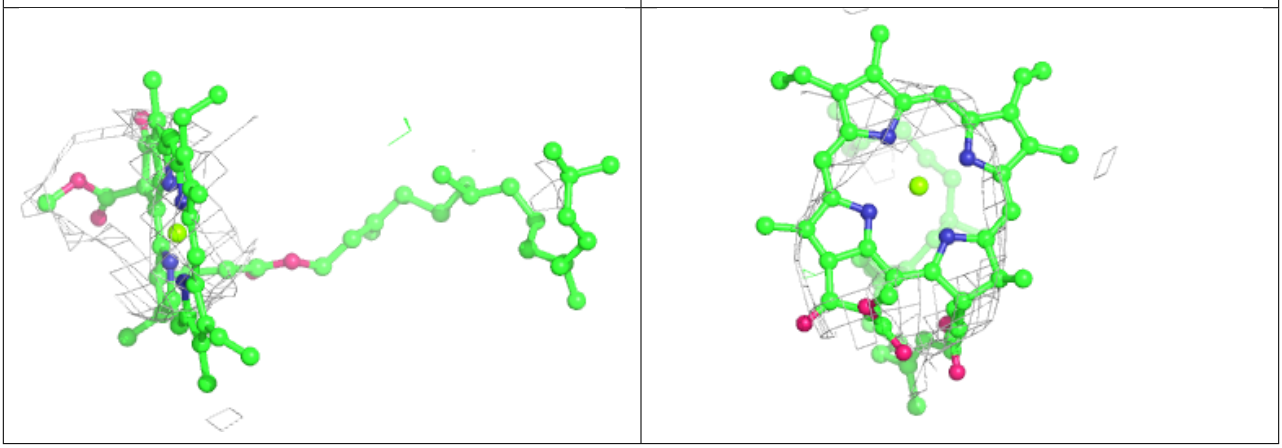
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 506:

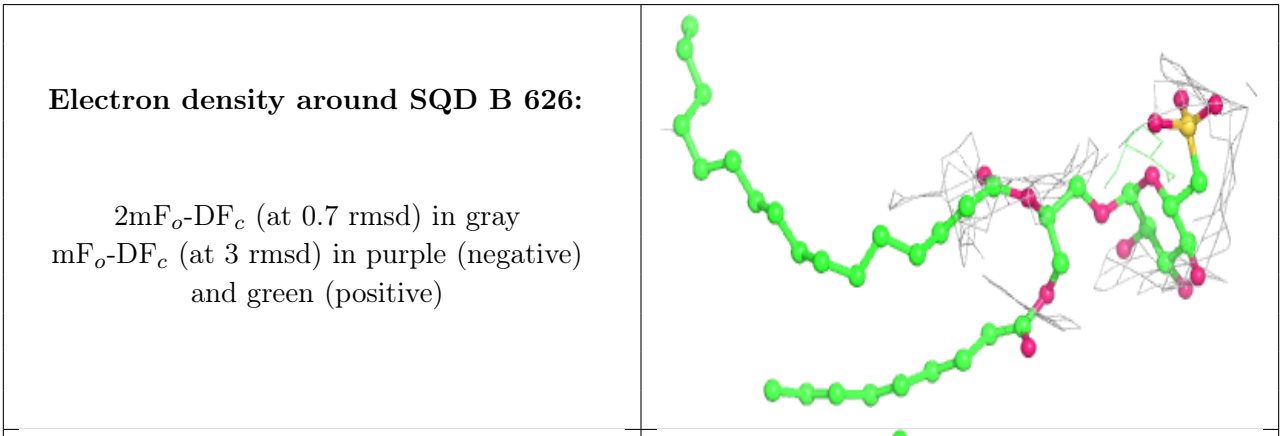
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

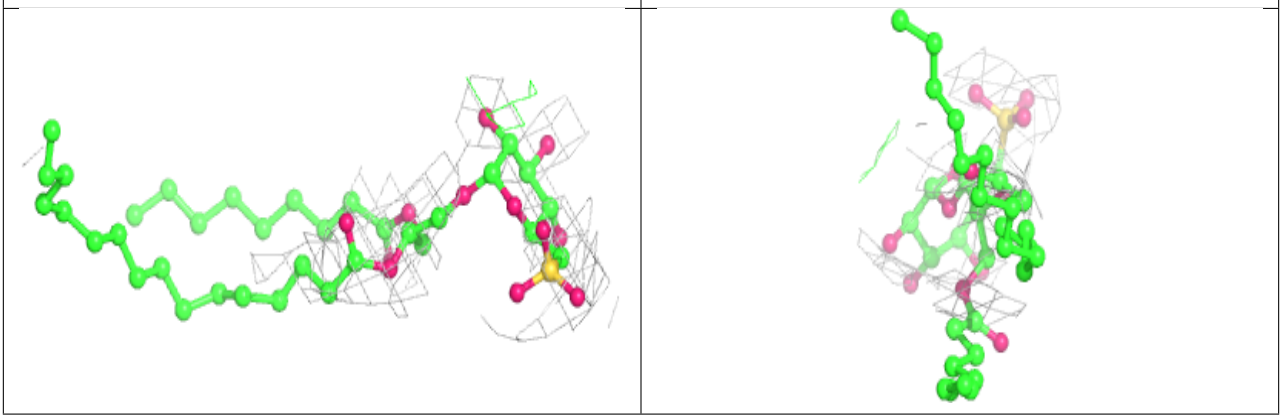




Electron density around SQD B 626:

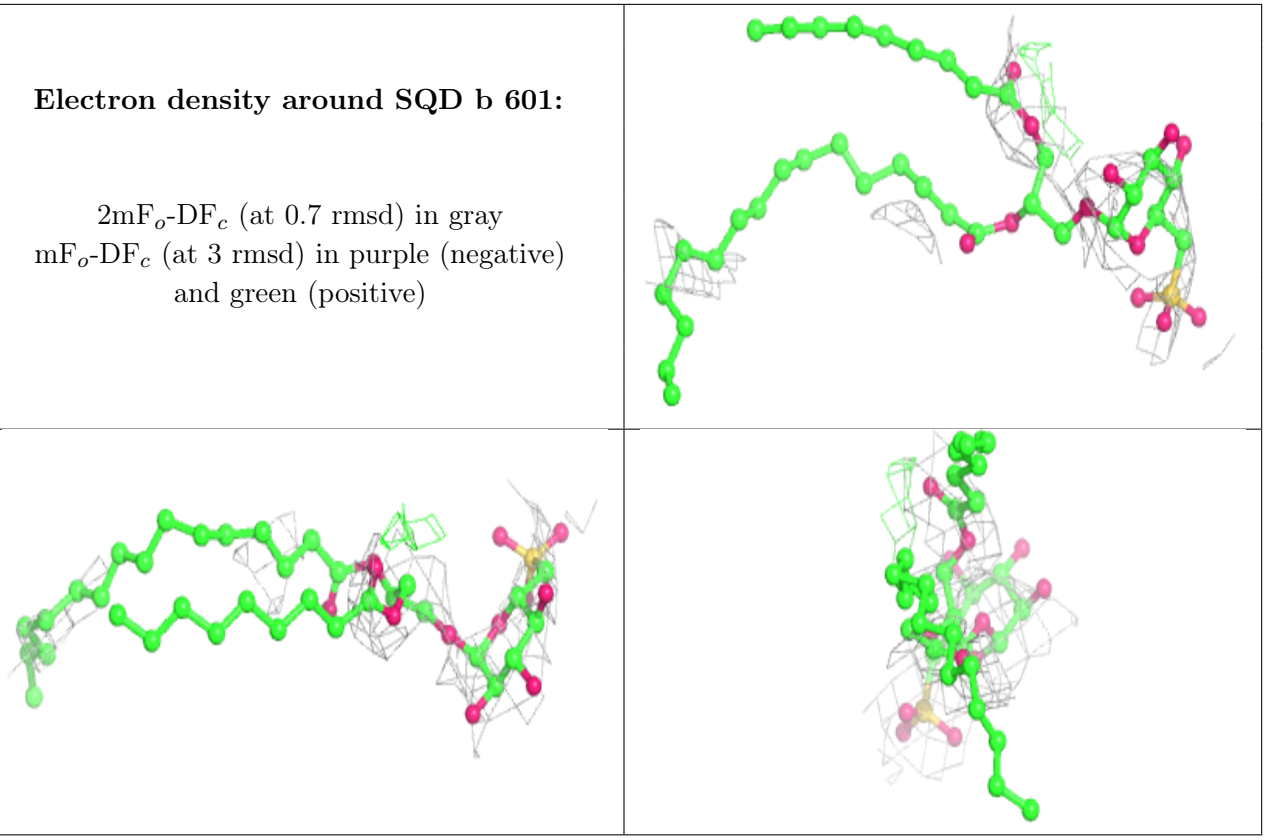
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





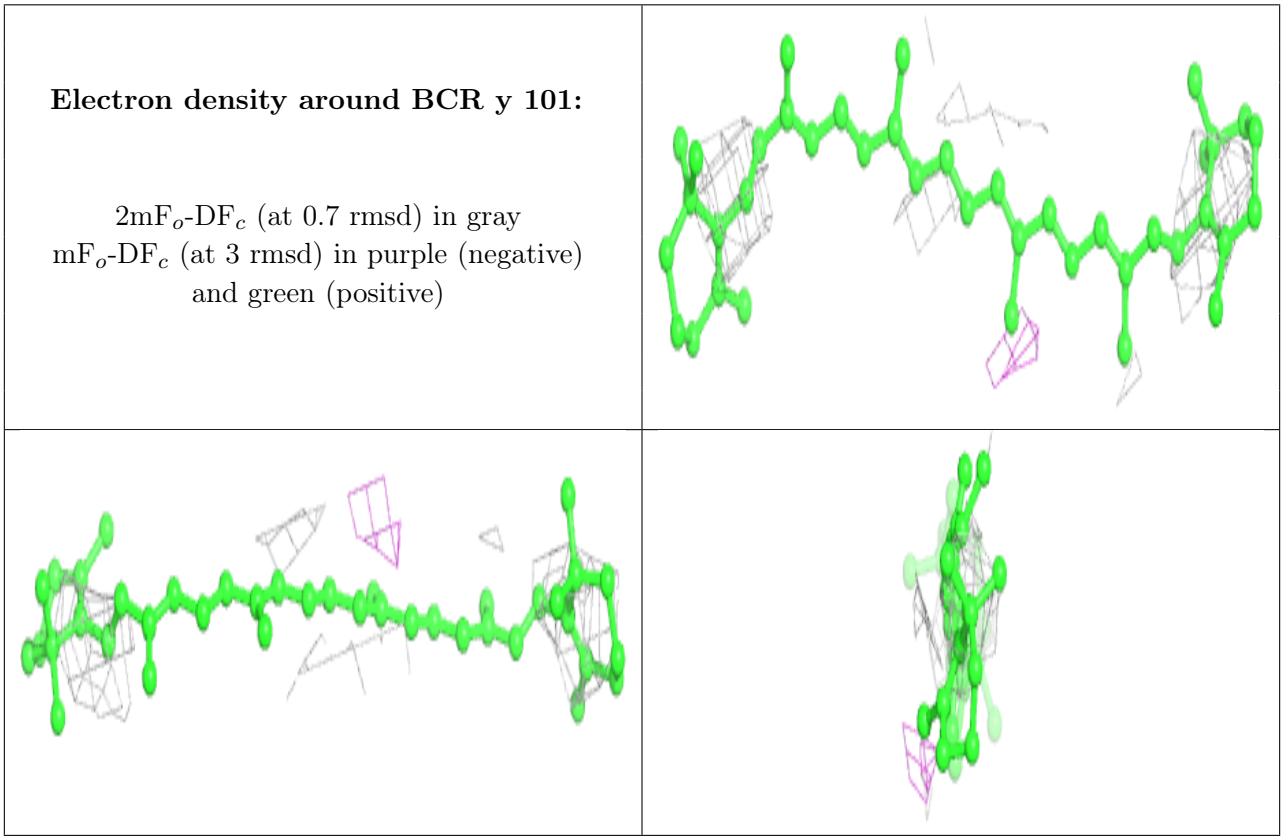
Electron density around SQD b 601:

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



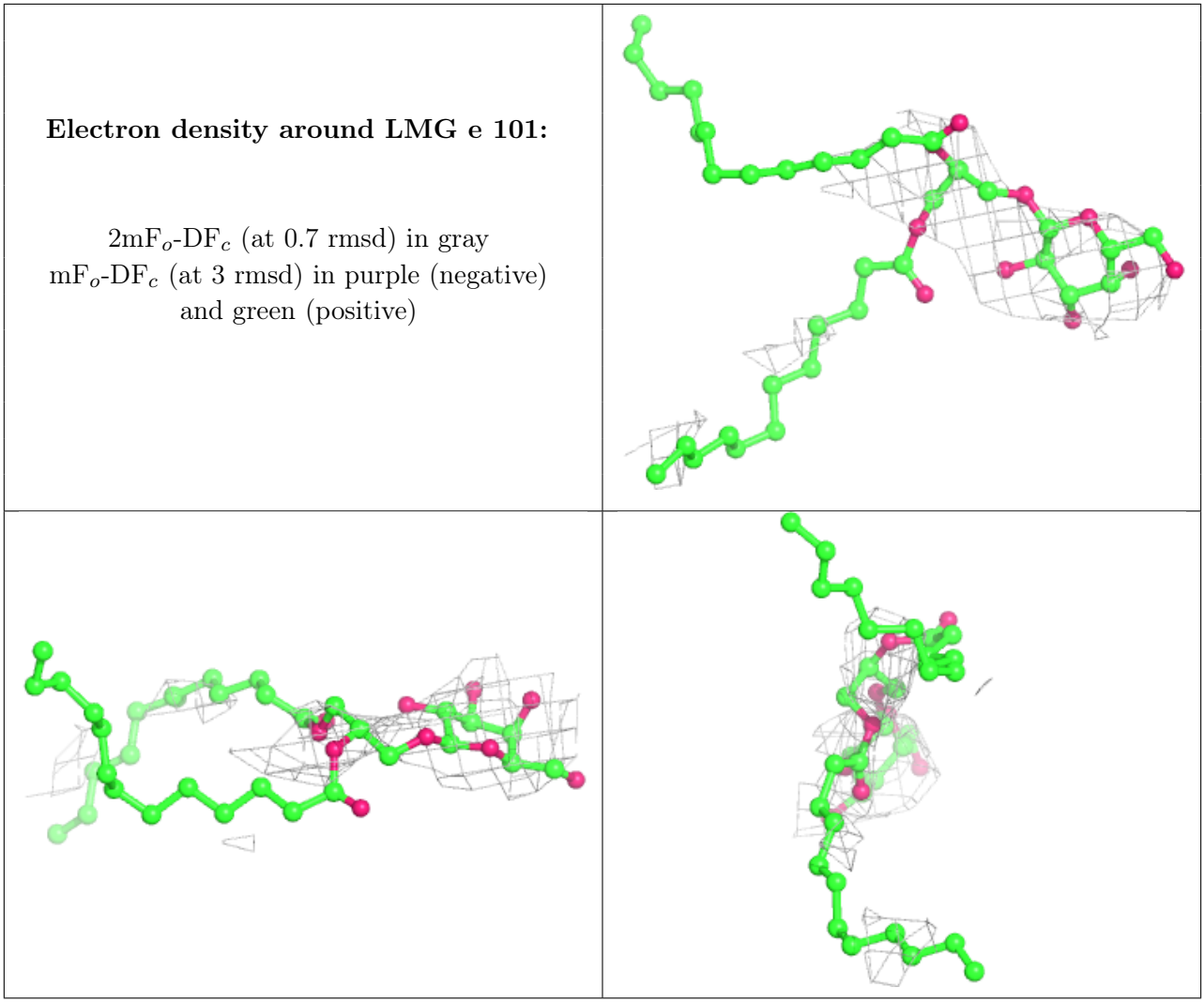
Electron density around BCR y 101:

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



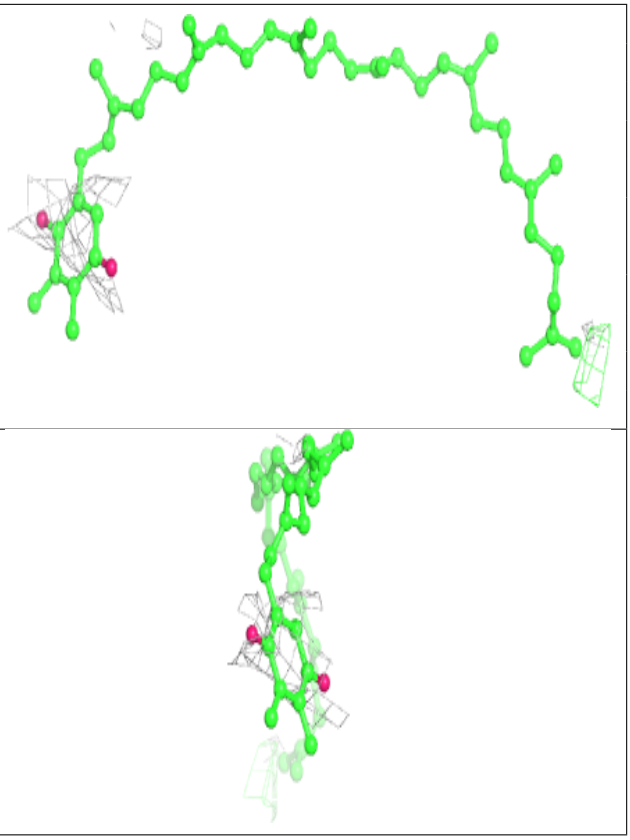
Electron density around LMG e 101:

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



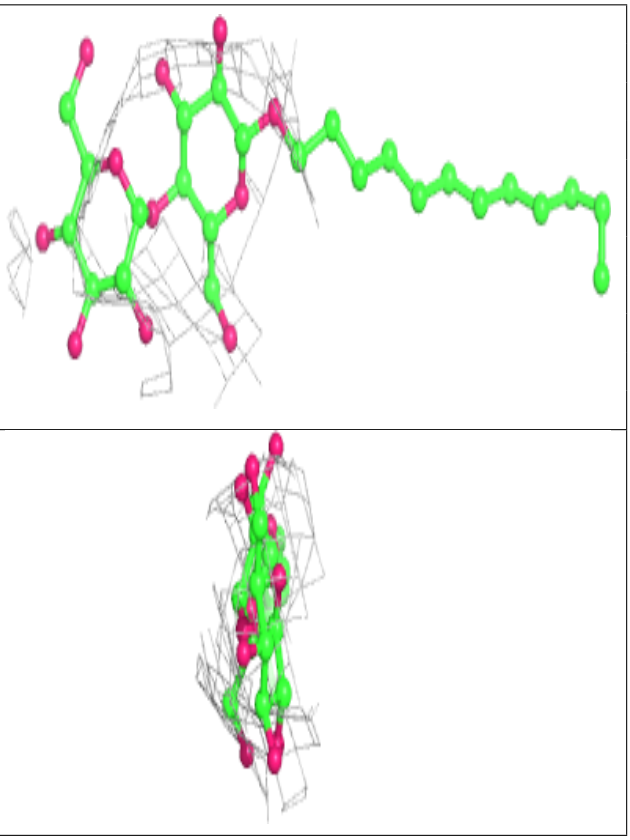
Electron density around PL9 A 408:

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



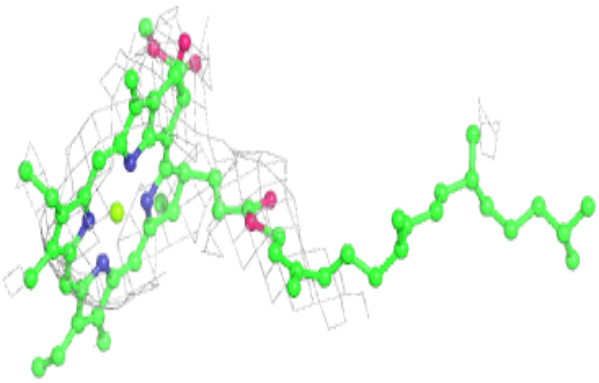
Electron density around LMT b 604:

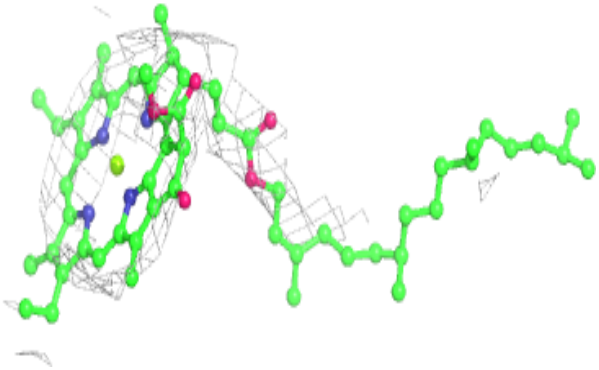
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

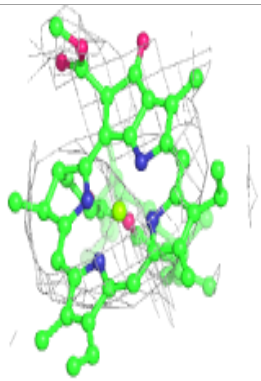


Electron density around CLA c 502:

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

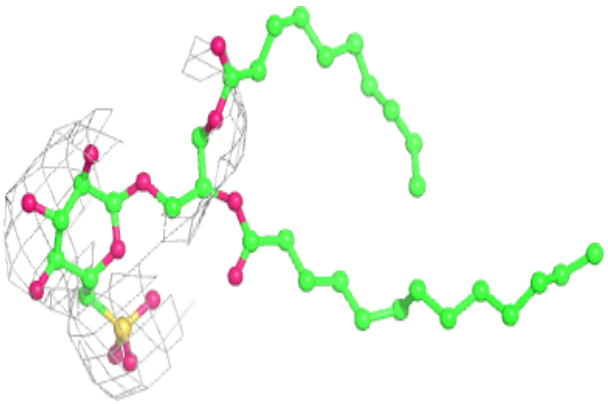


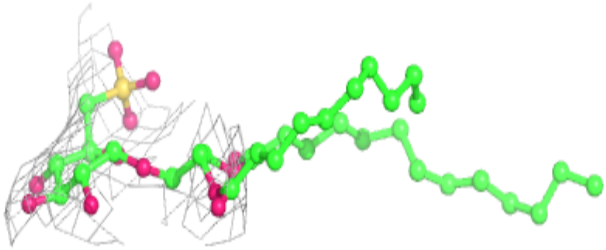


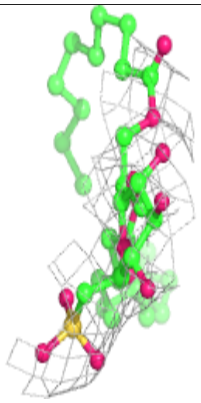


Electron density around SQD F 102:

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

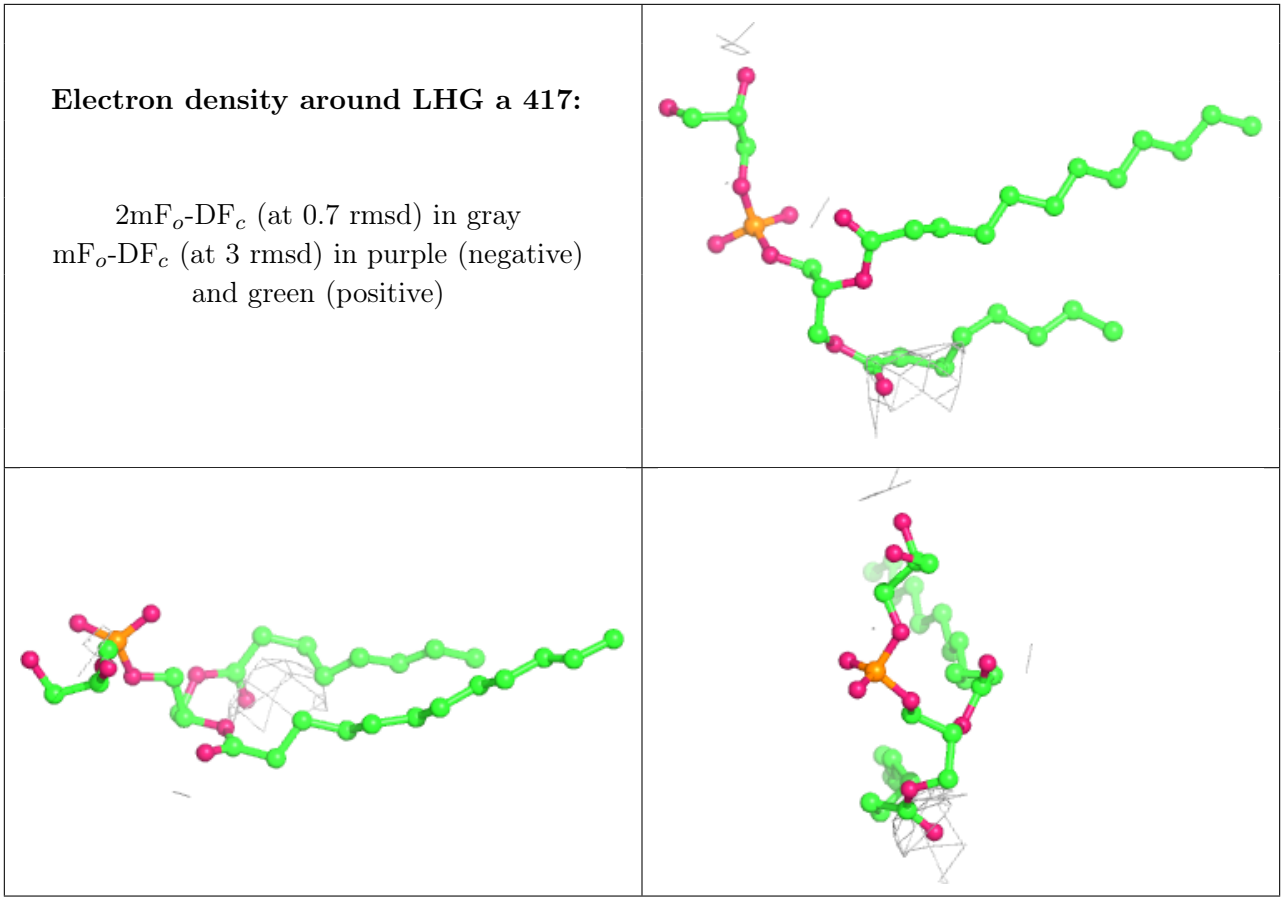






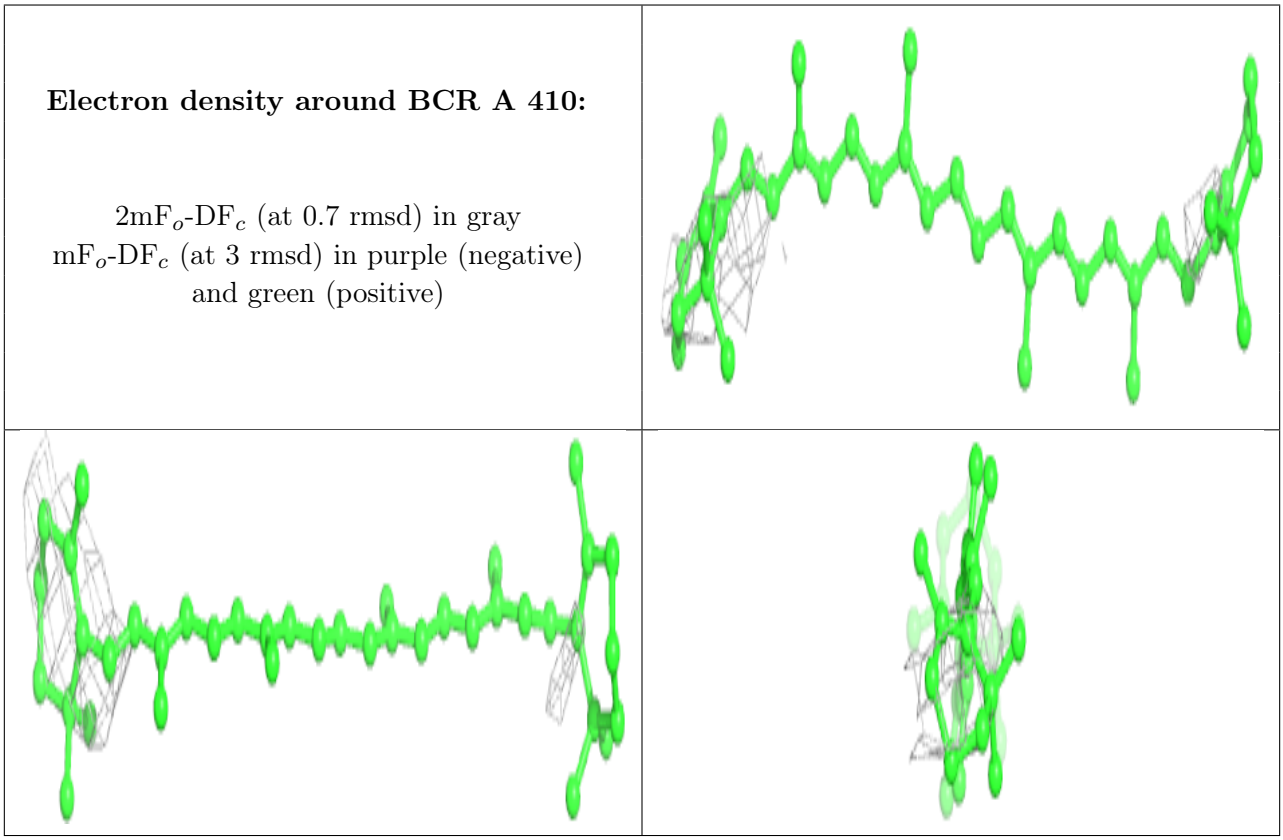
Electron density around LHG a 417:

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



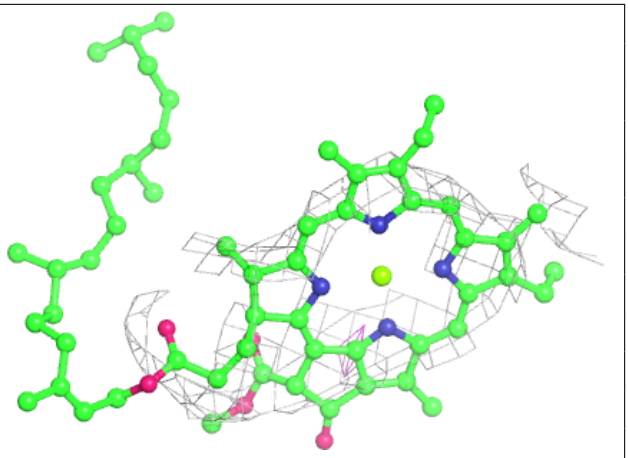
Electron density around BCR A 410:

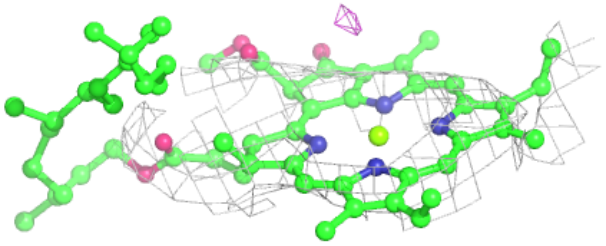
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

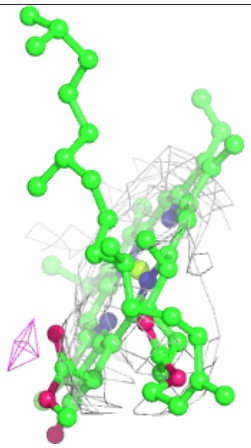


Electron density around CLA B 616:

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

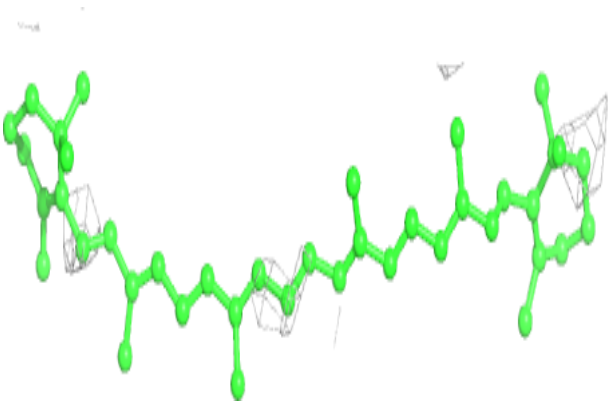


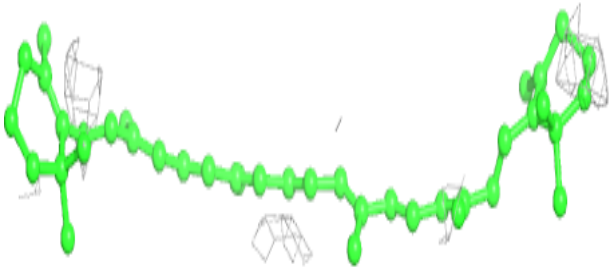


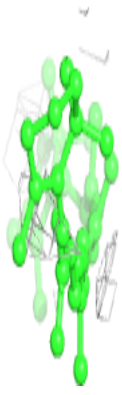


Electron density around BCR T 102:

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

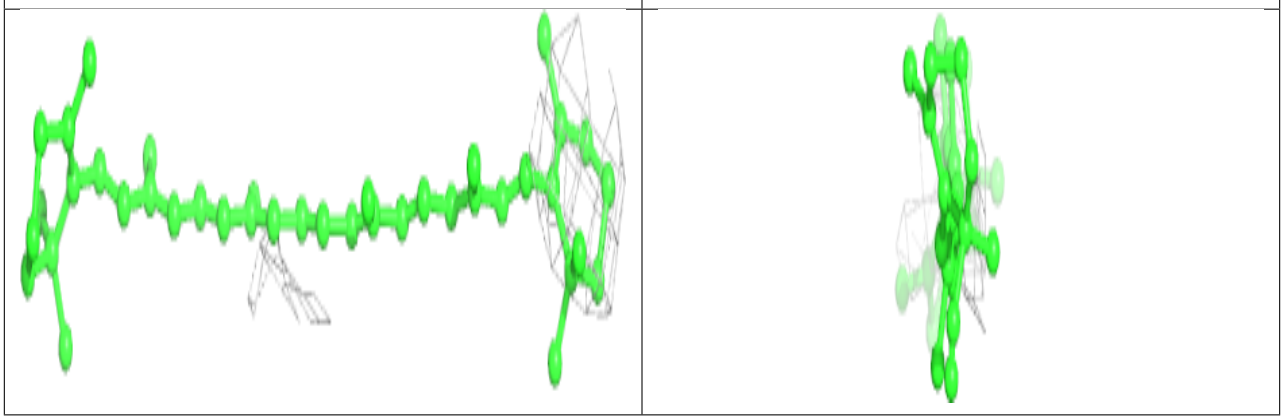






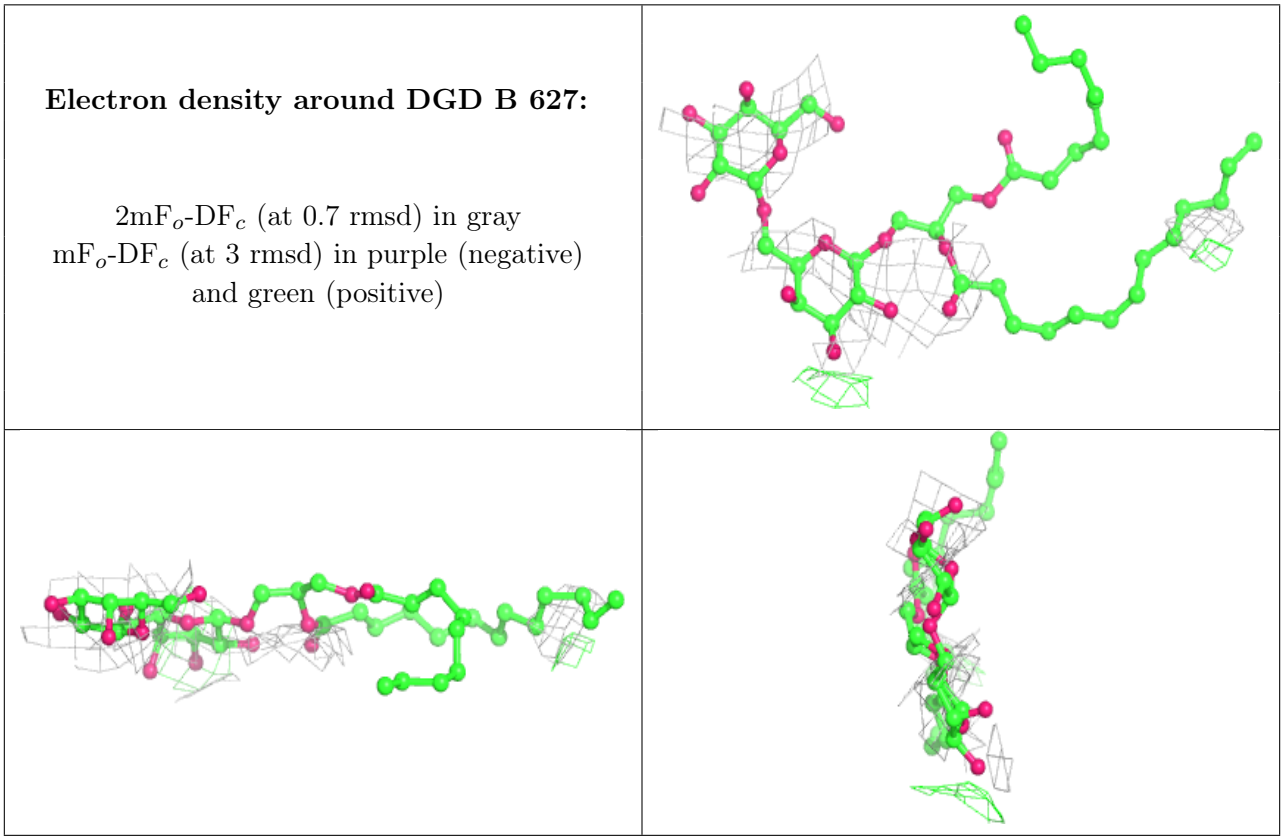
Electron density around BCR B 619:

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



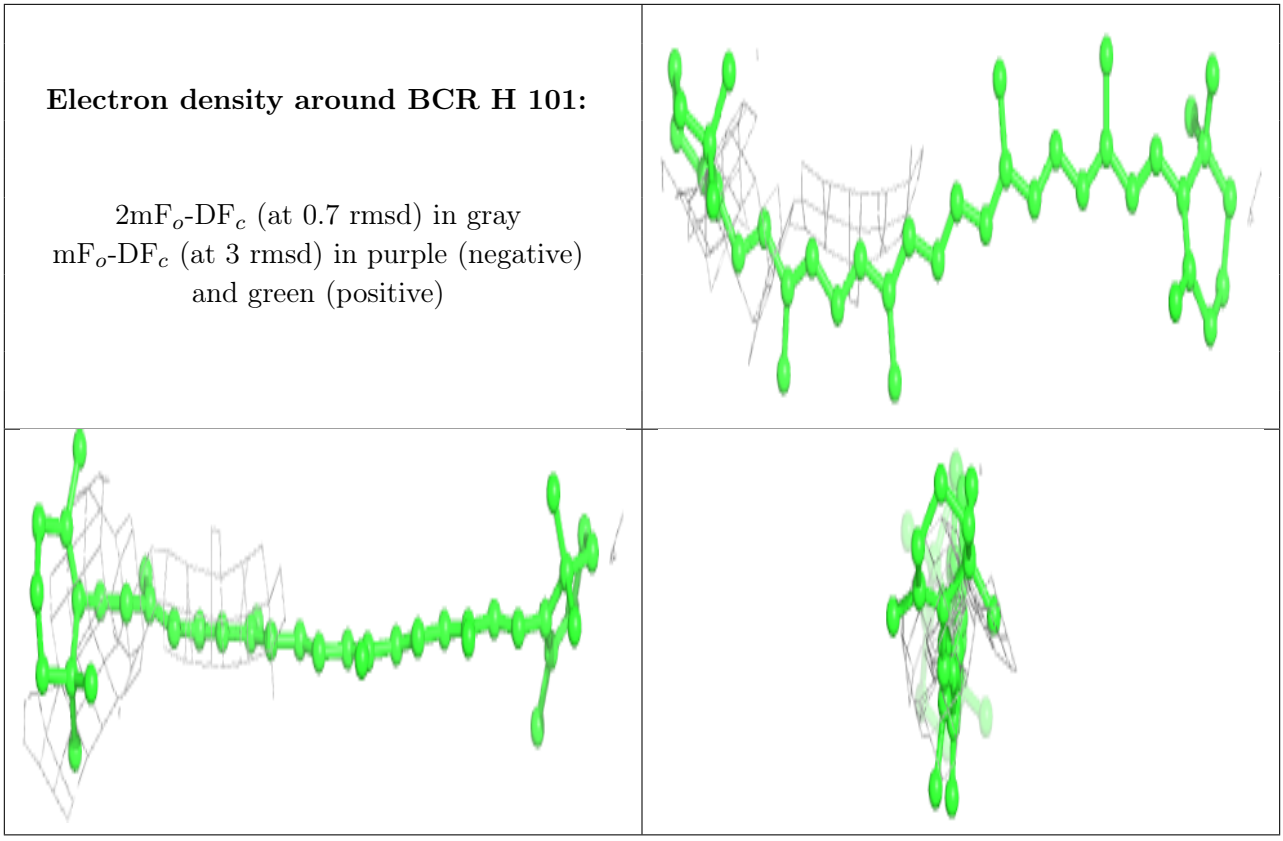
Electron density around DGD B 627:

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



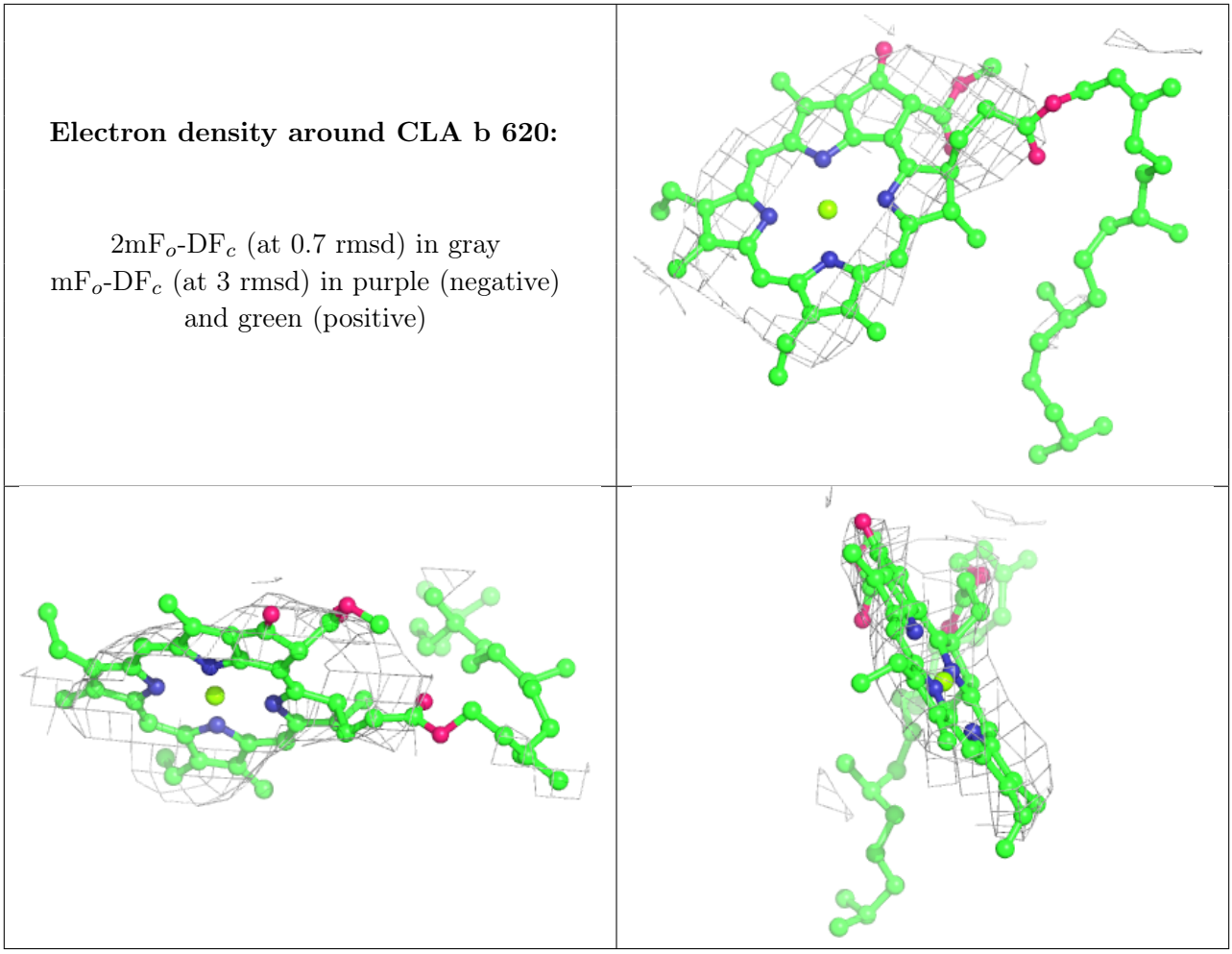
Electron density around BCR H 101:

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



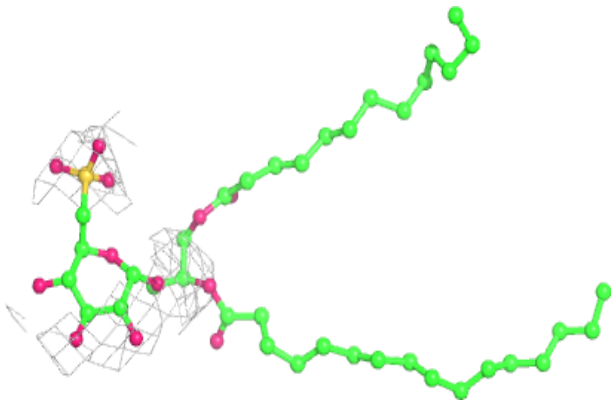
Electron density around CLA b 620:

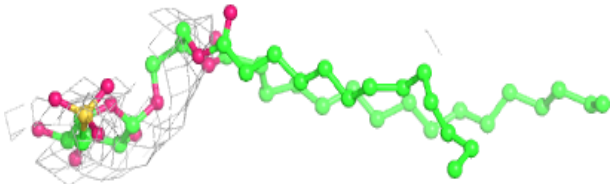
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

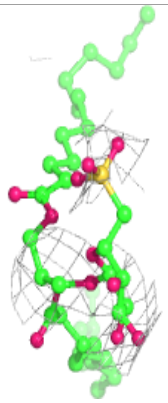


Electron density around SQD a 415:

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

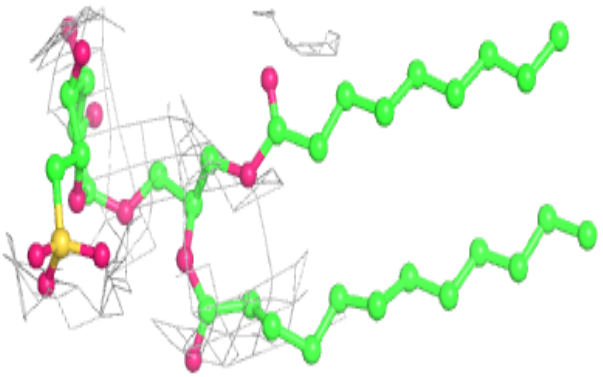


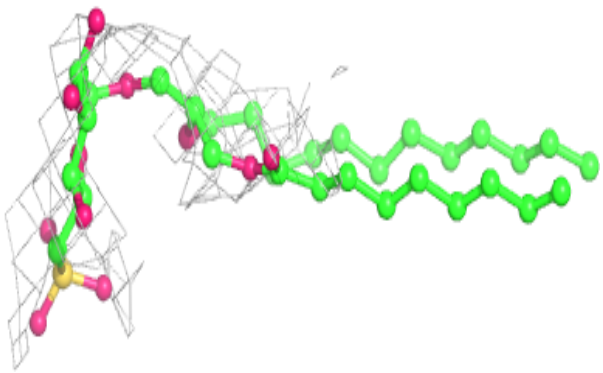


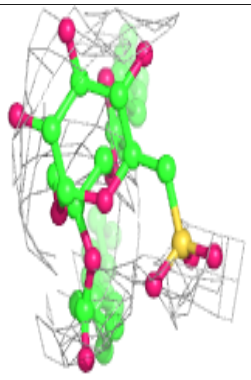


Electron density around SQD D 408:

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

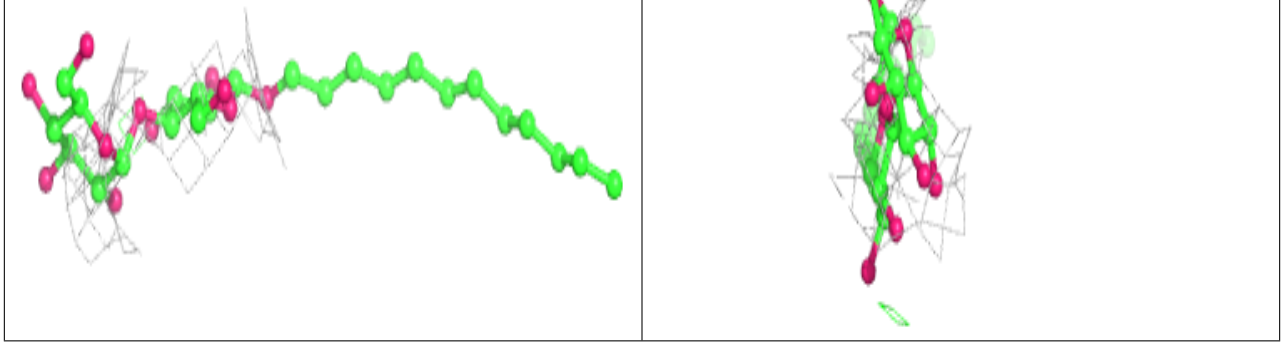






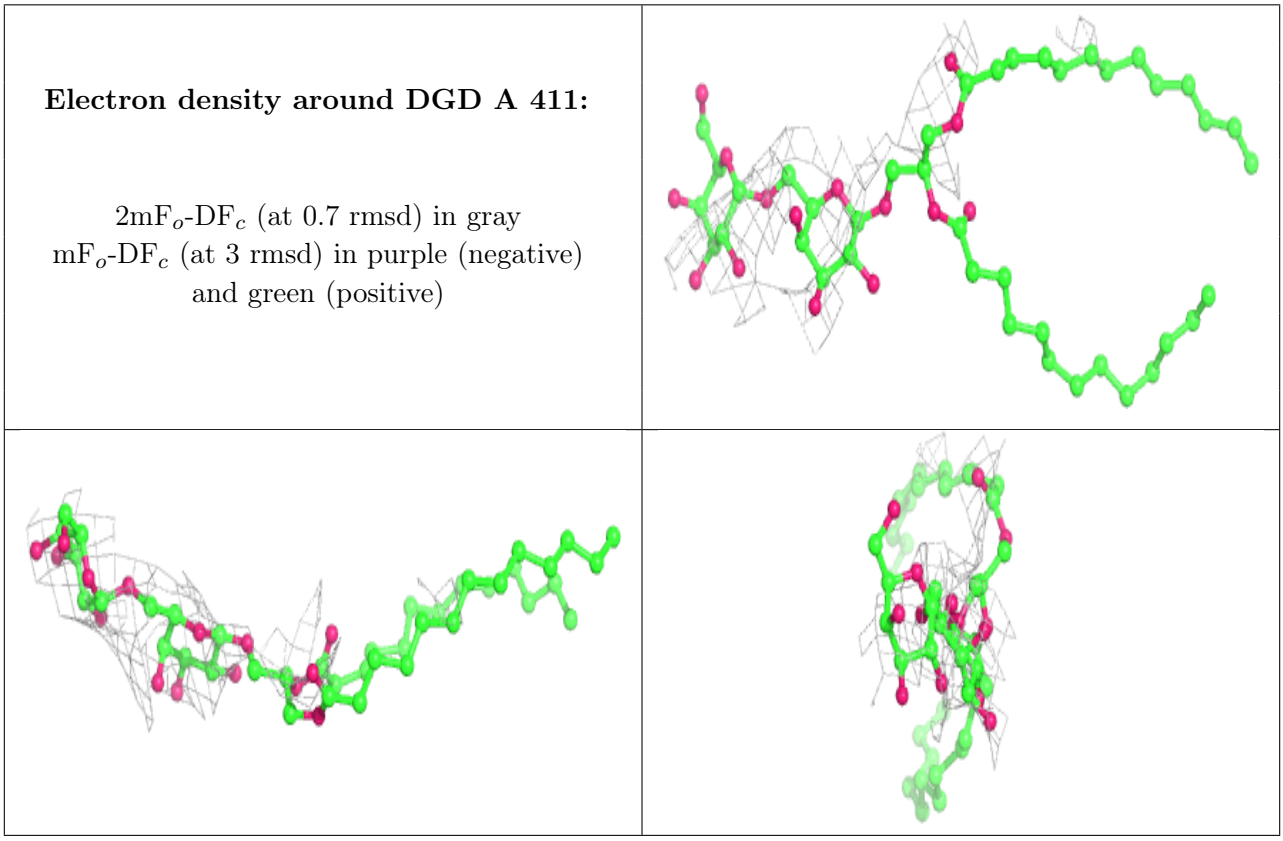
Electron density around LMT B 625:

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



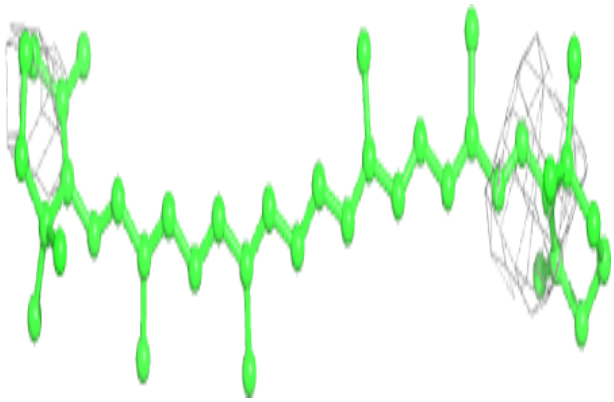
Electron density around DGD A 411:

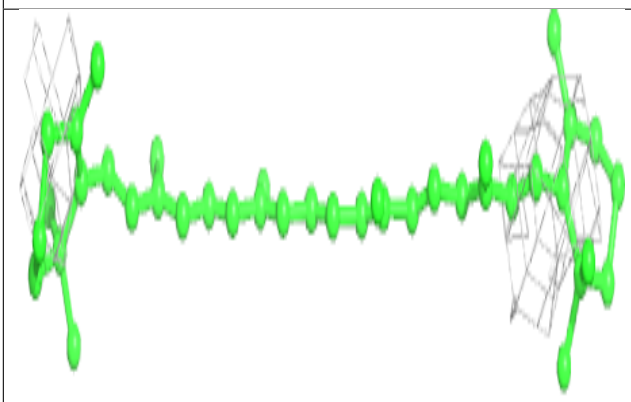
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

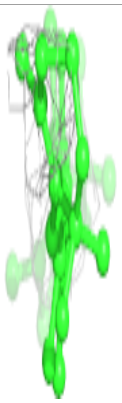


Electron density around BCR b 621:

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

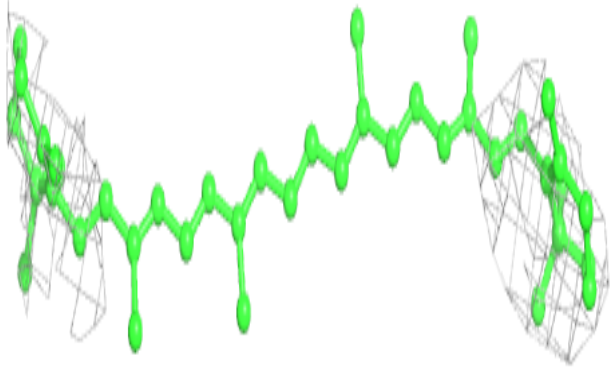


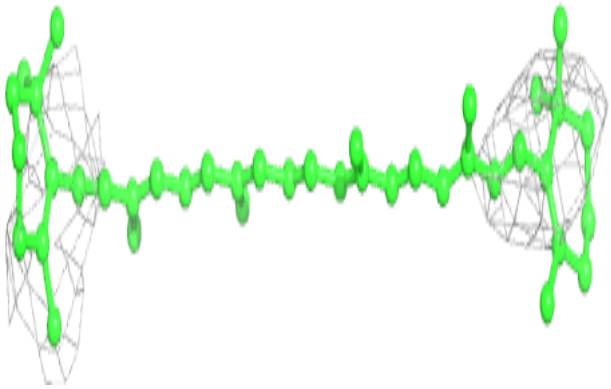


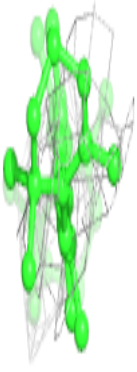


Electron density around BCR a 412:

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

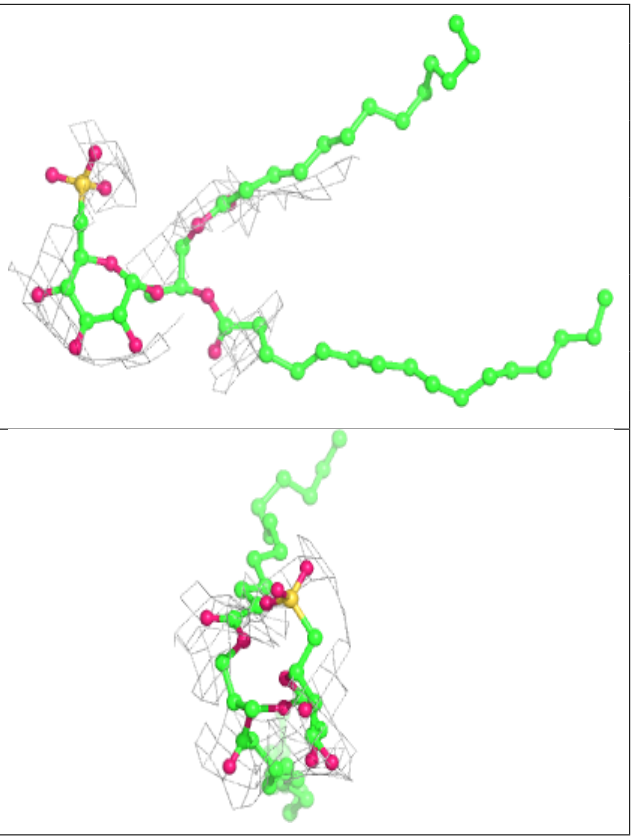






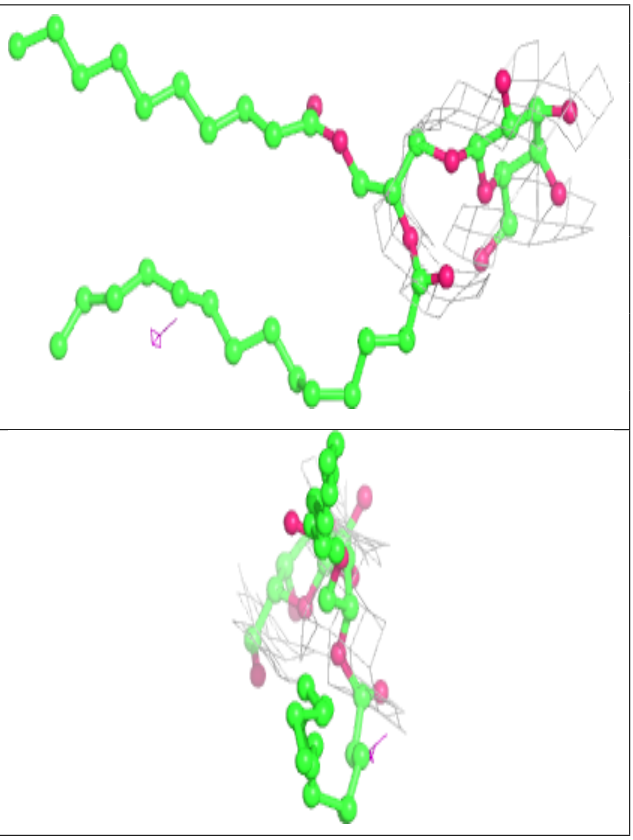
Electron density around SQD A 413:

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



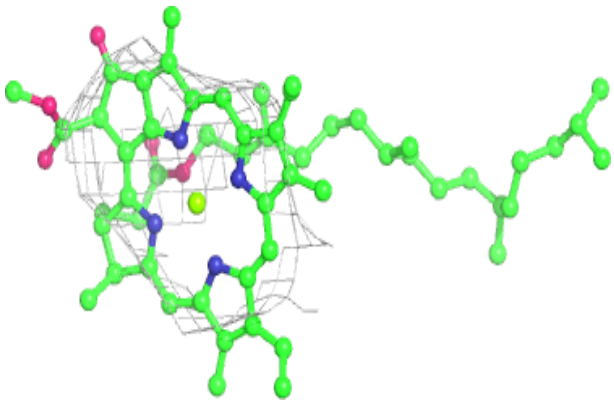
Electron density around LMG i 101:

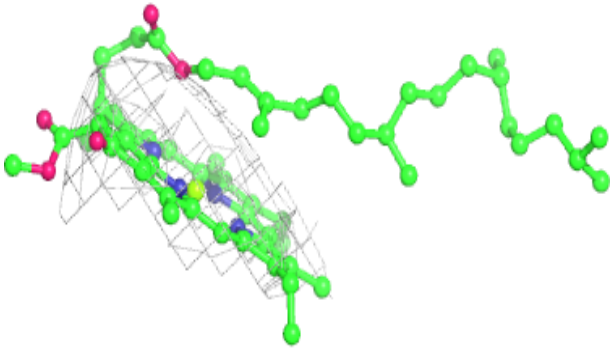
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

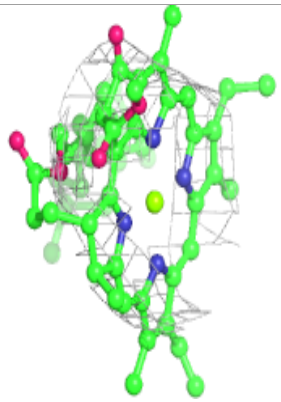


Electron density around CLA B 614:

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

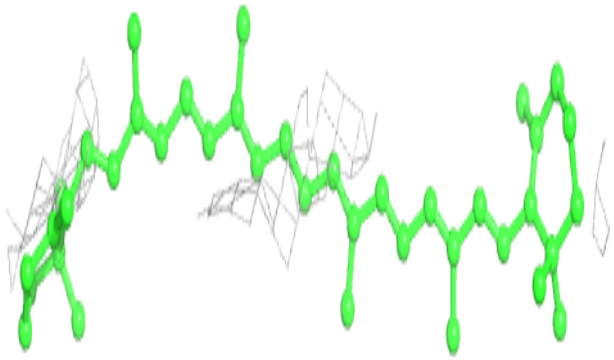


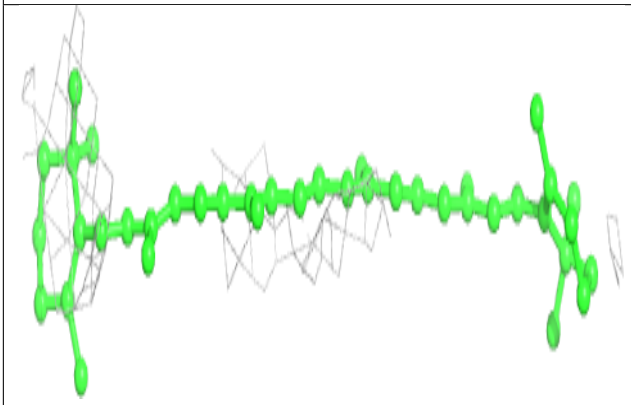


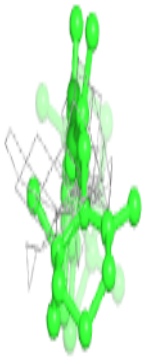


Electron density around BCR h 101:

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

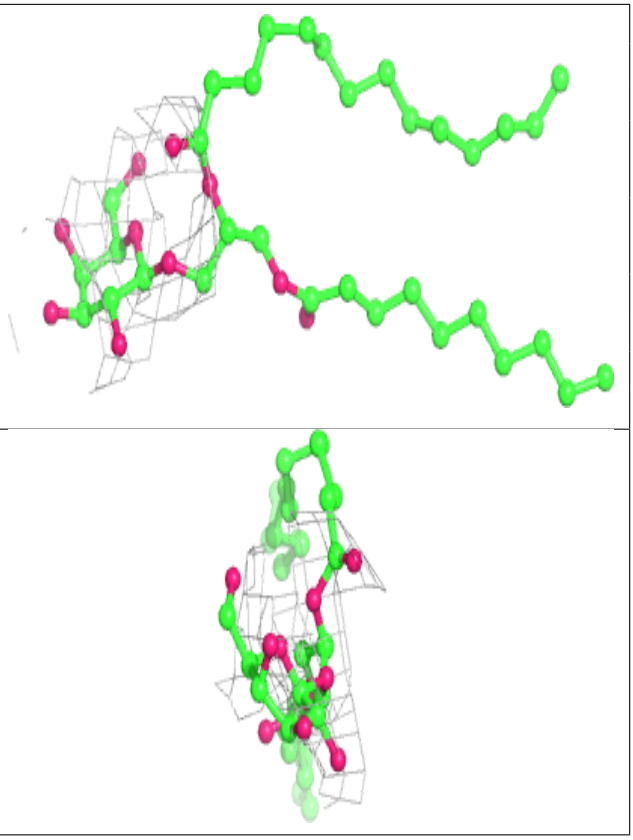






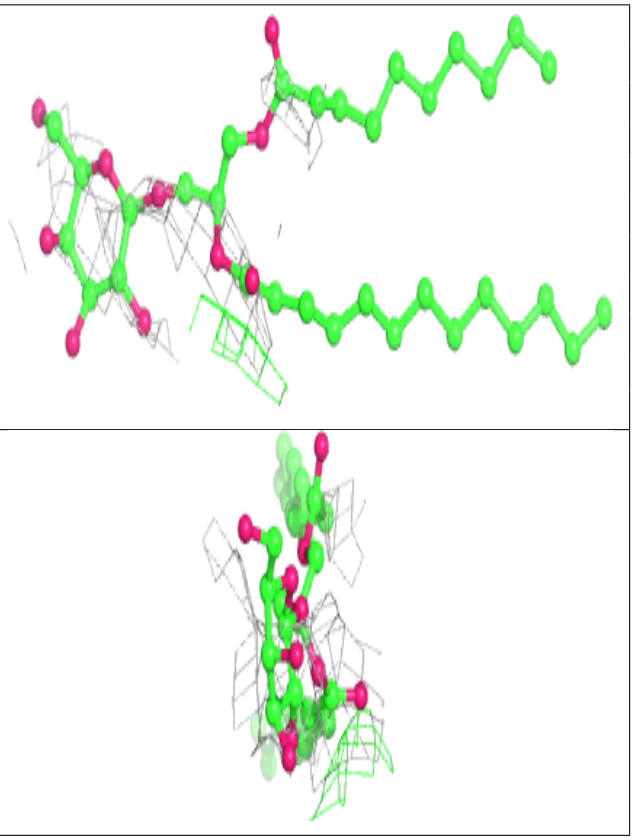
Electron density around LMG I 101:

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



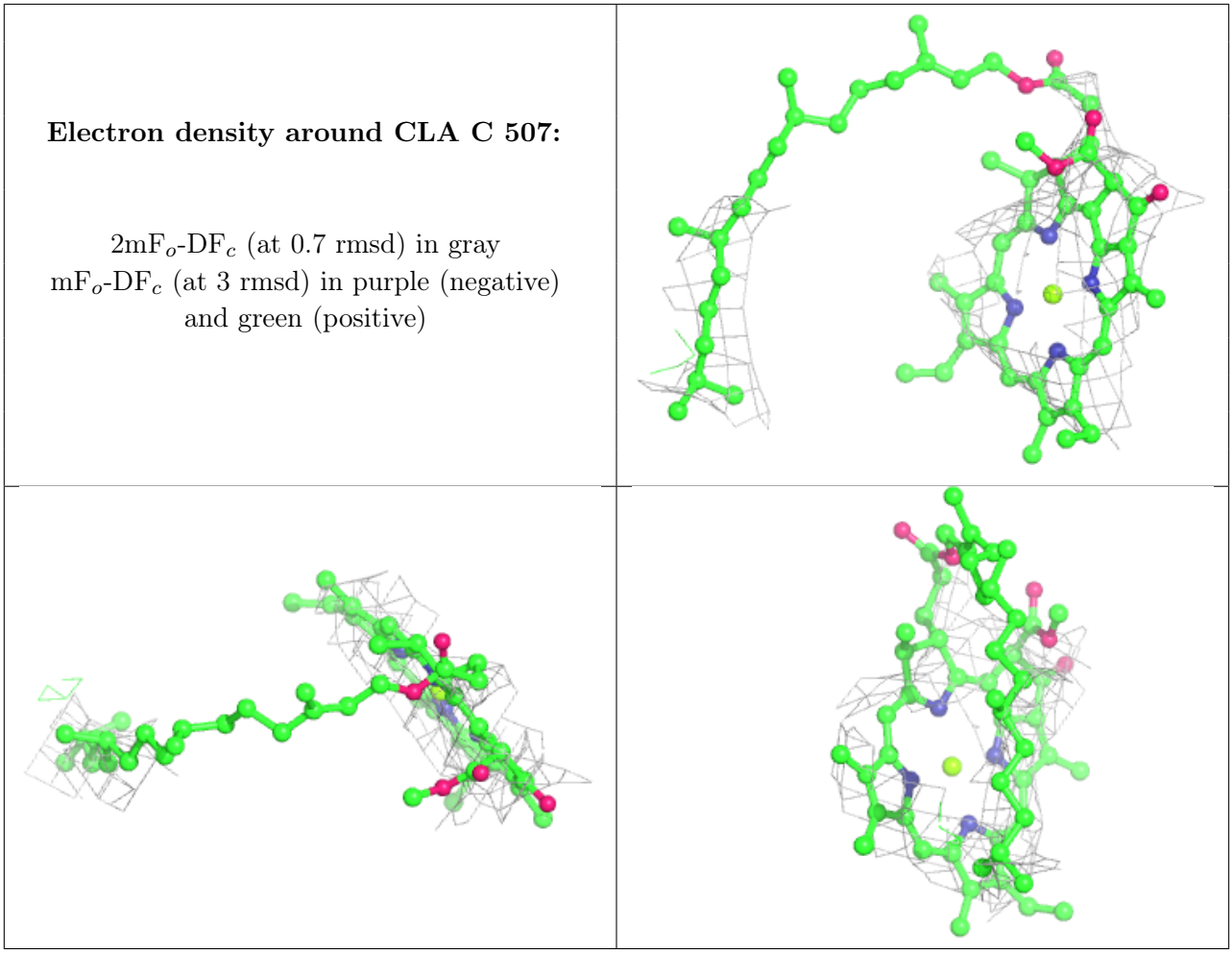
Electron density around LMG M 101:

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



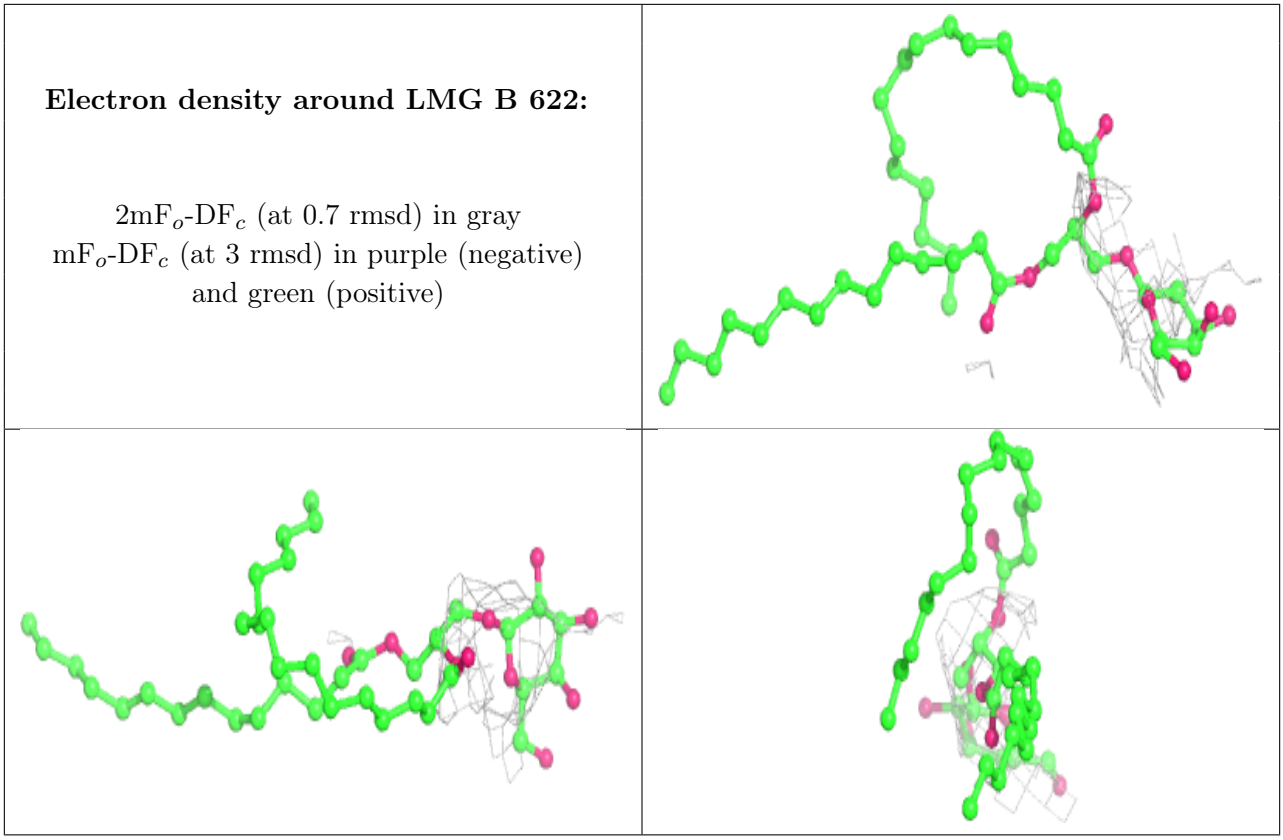
Electron density around CLA C 507:

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



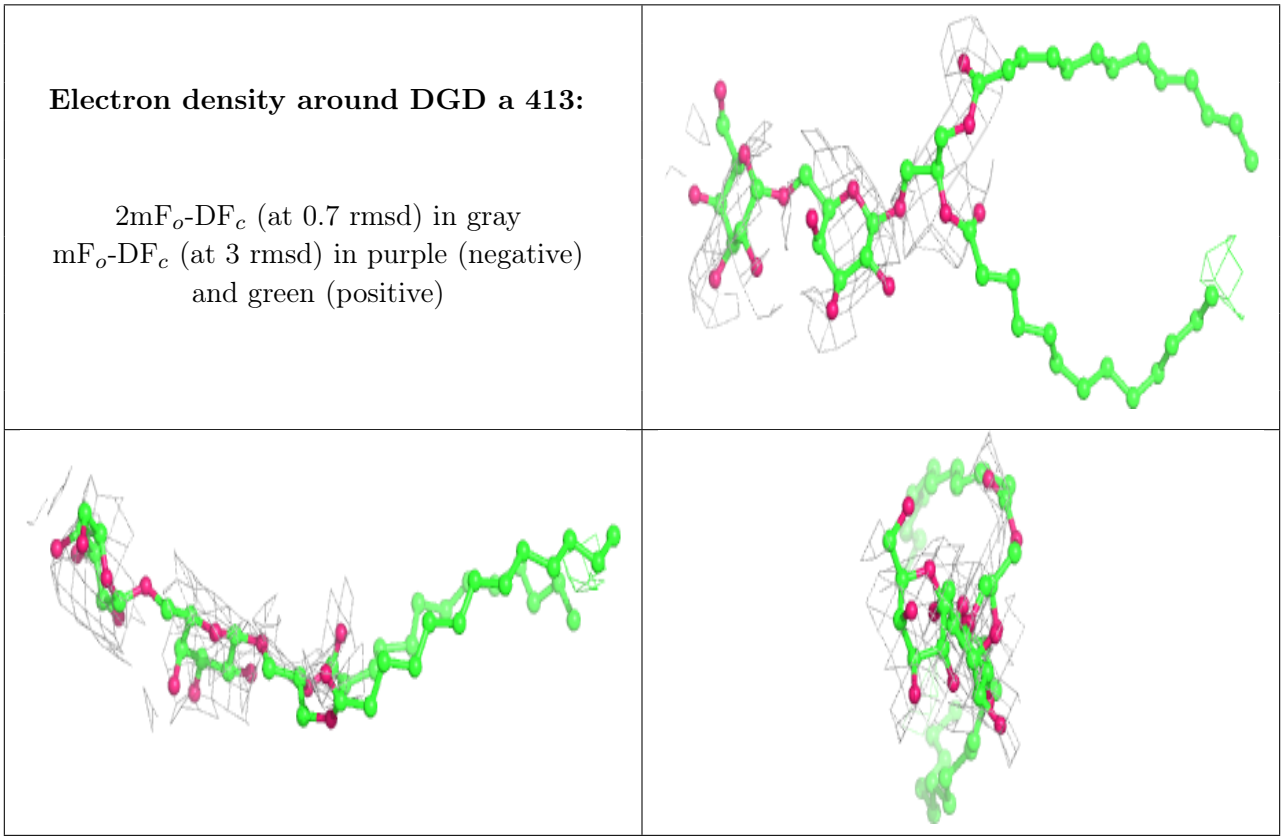
Electron density around LMG B 622:

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



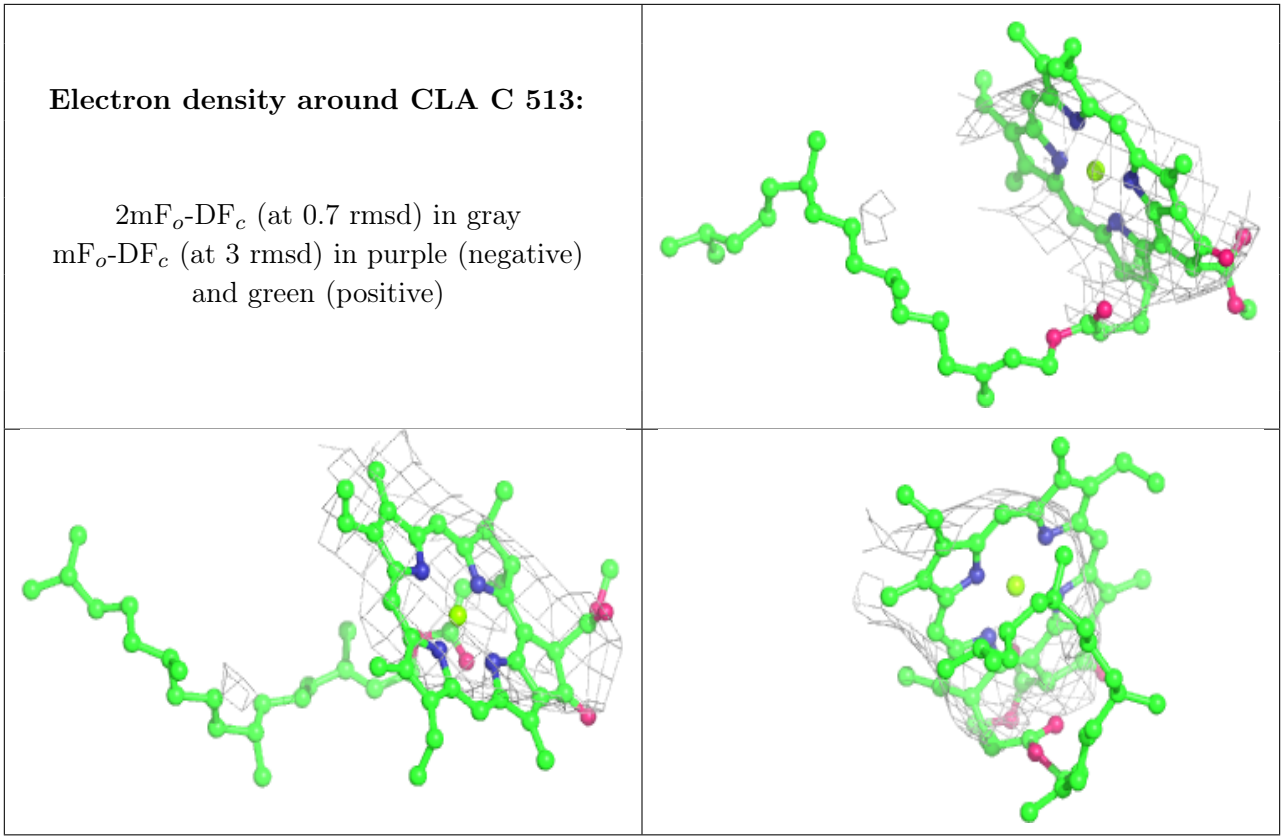
Electron density around DGD a 413:

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



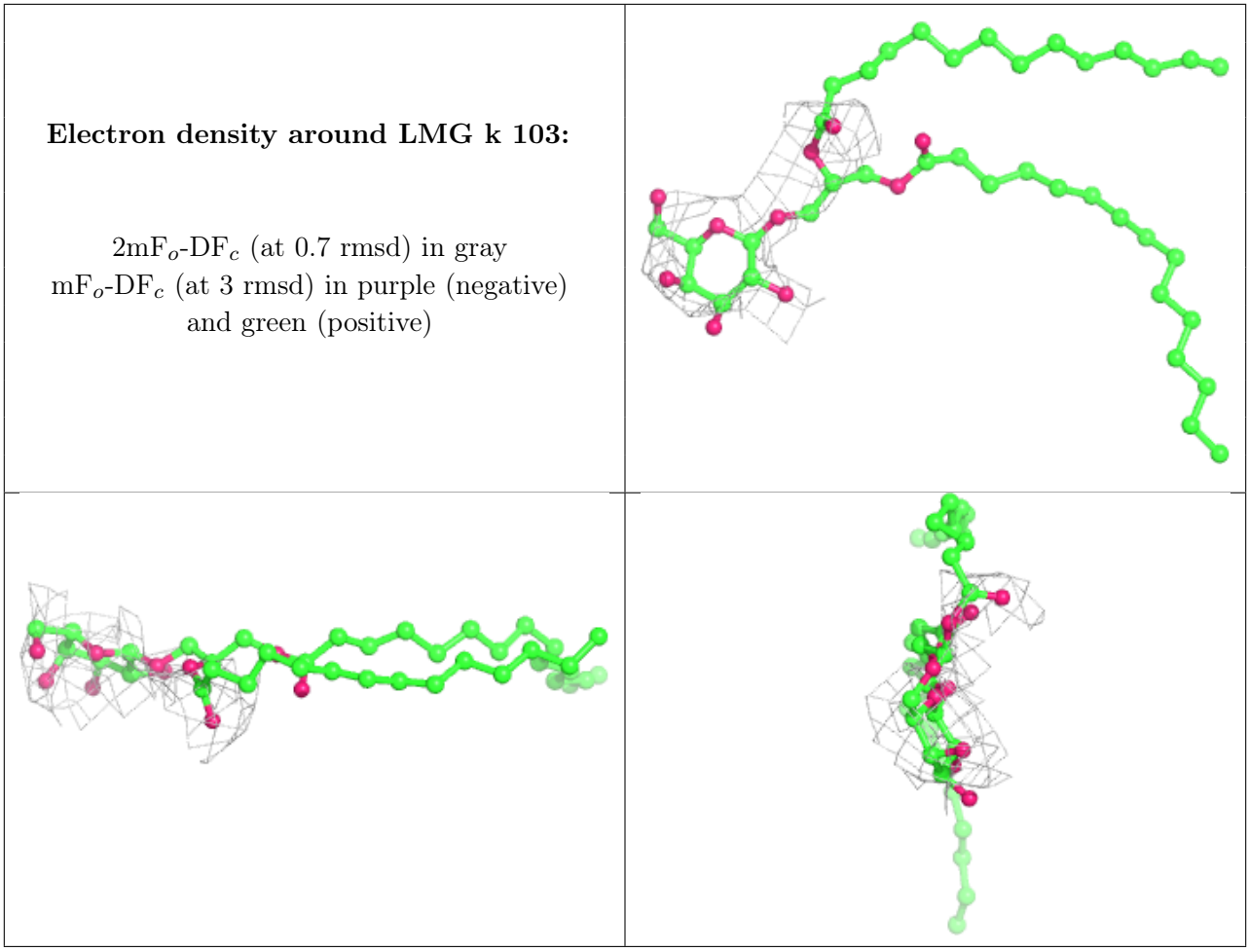
Electron density around CLA C 513:

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



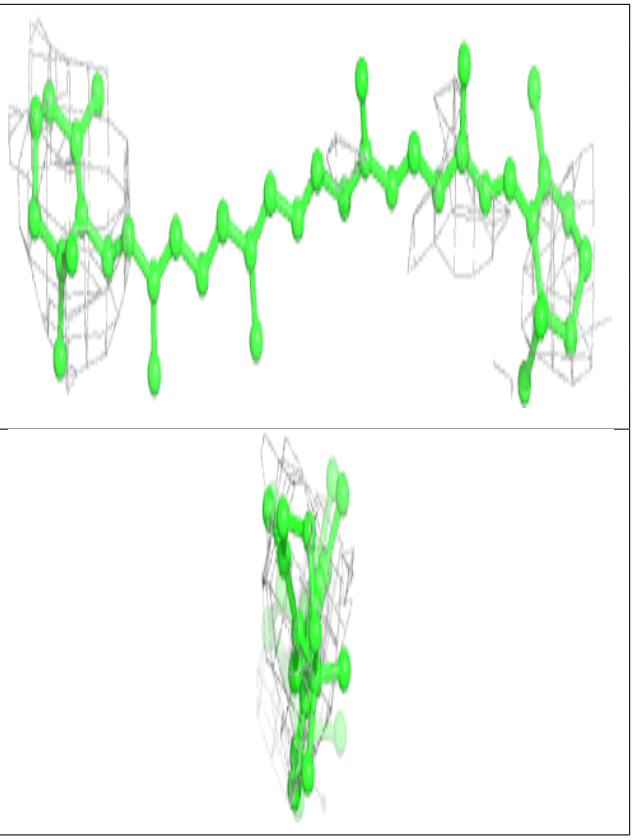
Electron density around LMG k 103:

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



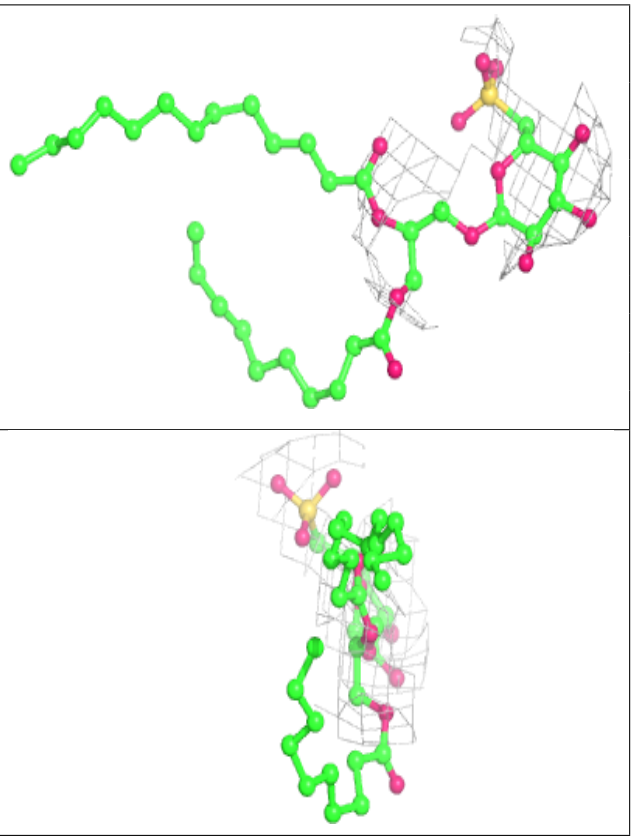
Electron density around BCR C 516:

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



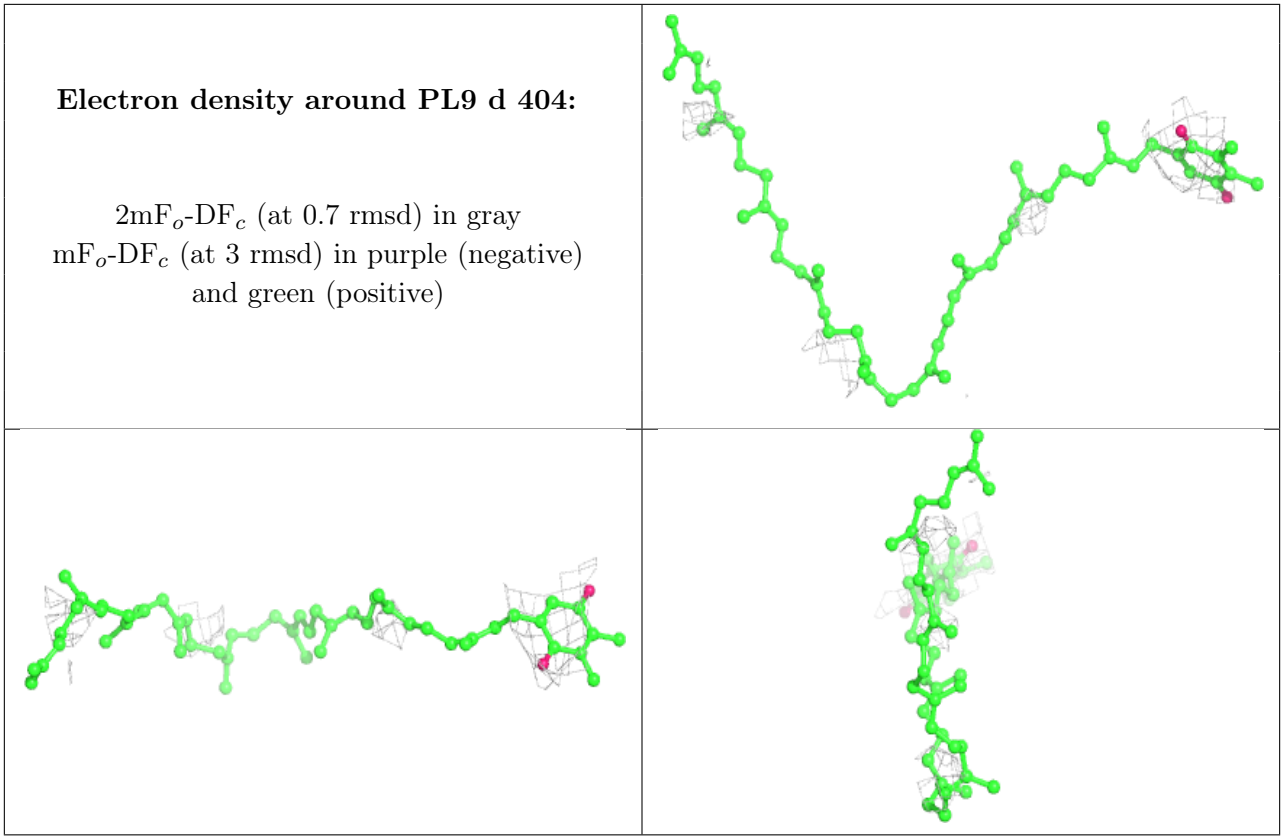
Electron density around SQD f 102:

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



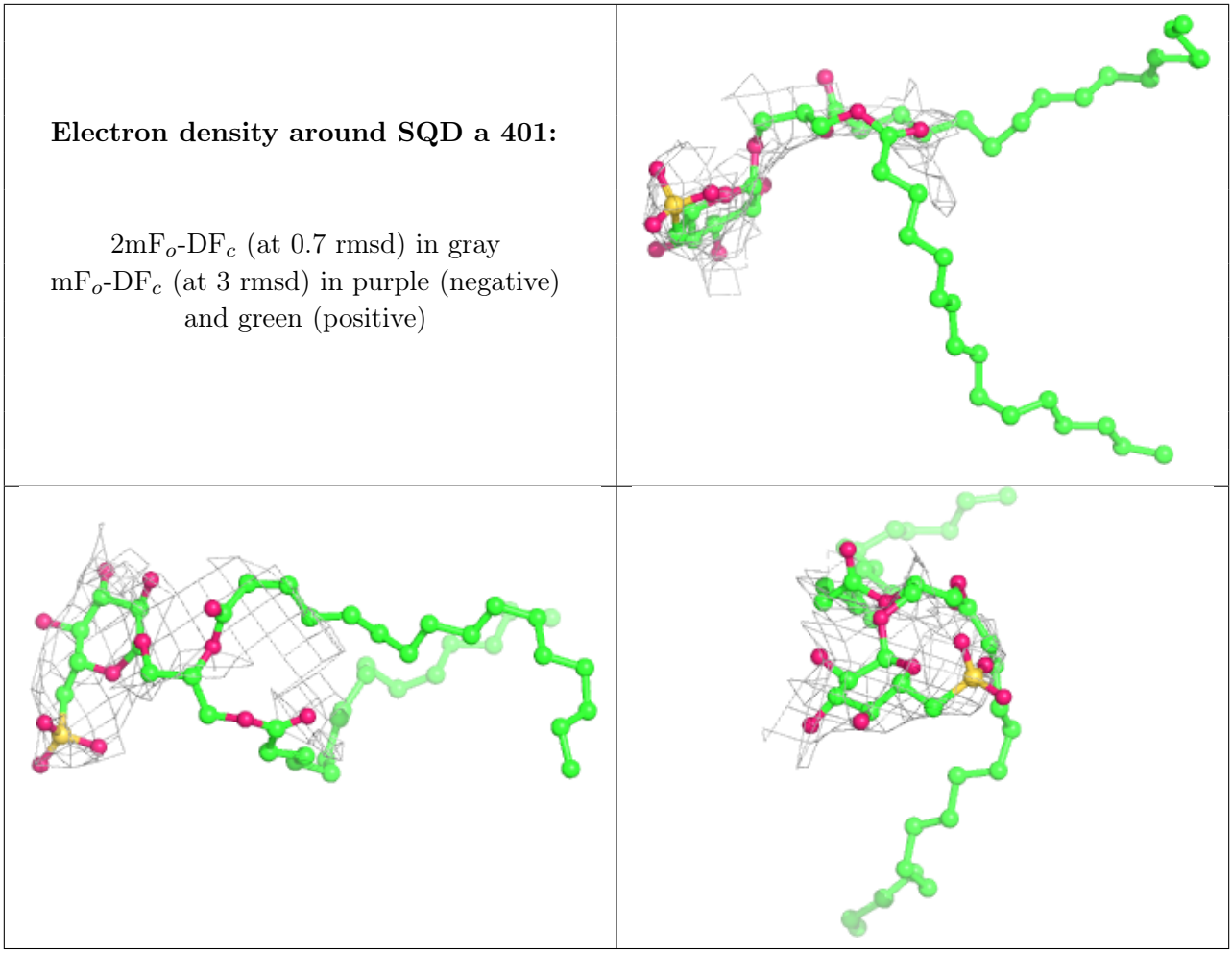
Electron density around PL9 d 404:

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



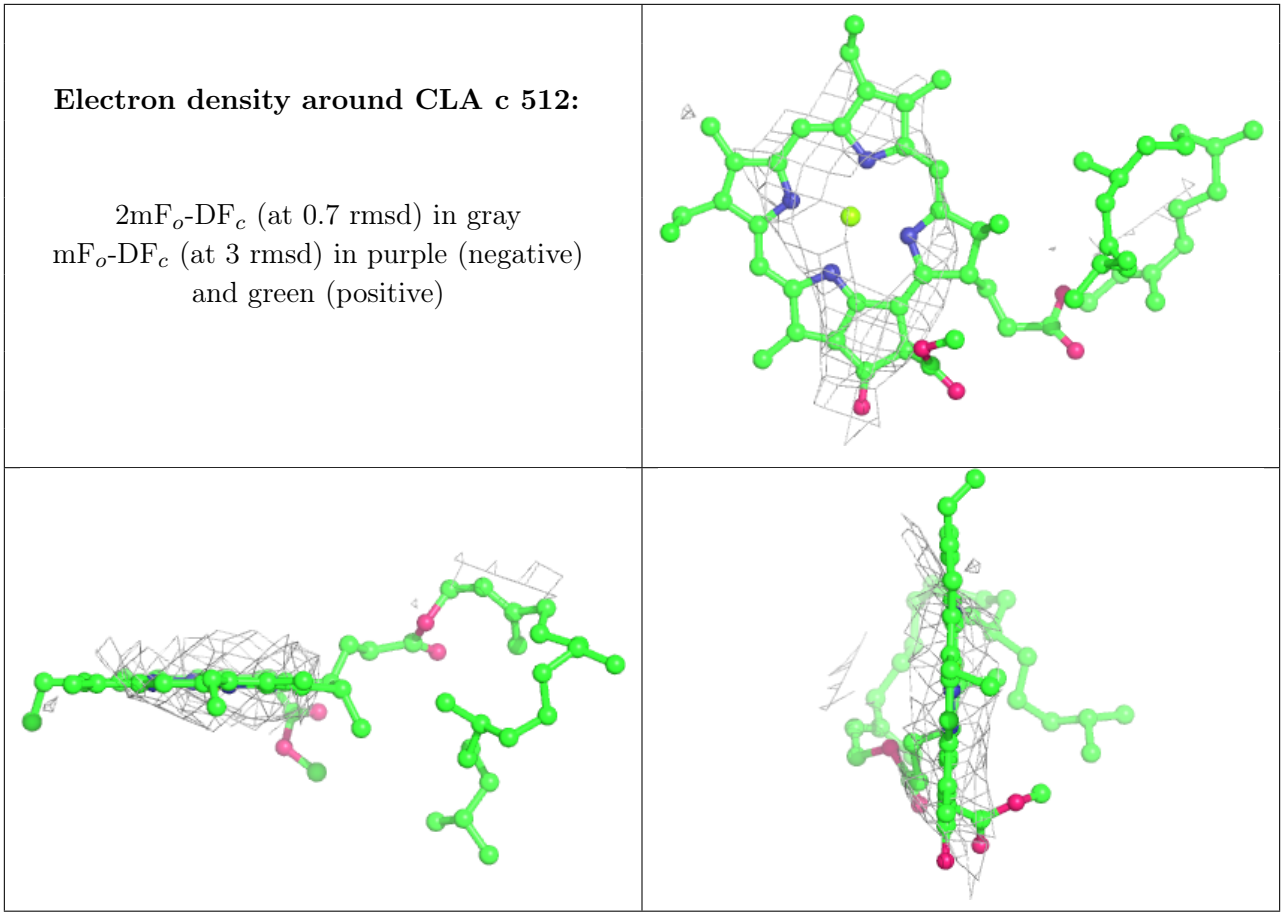
Electron density around SQD a 401:

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



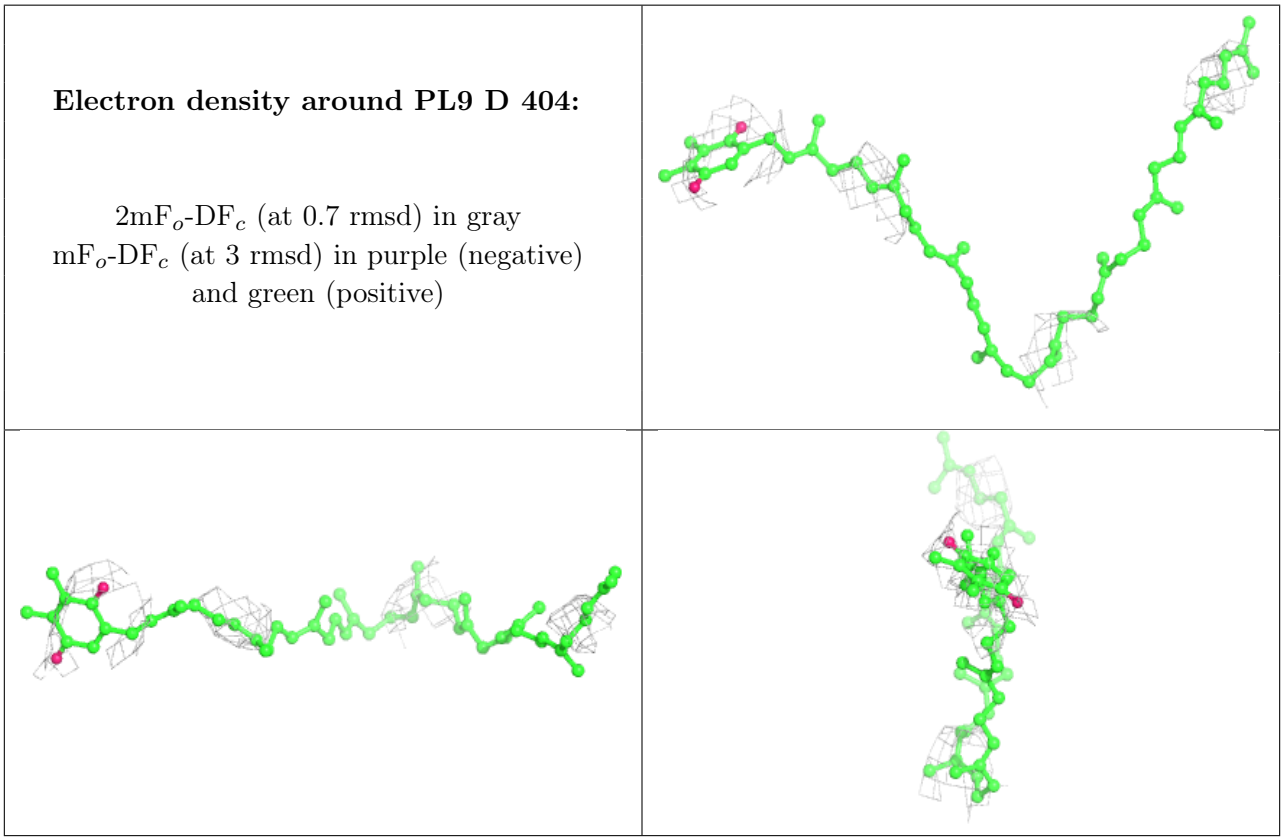
Electron density around CLA c 512:

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



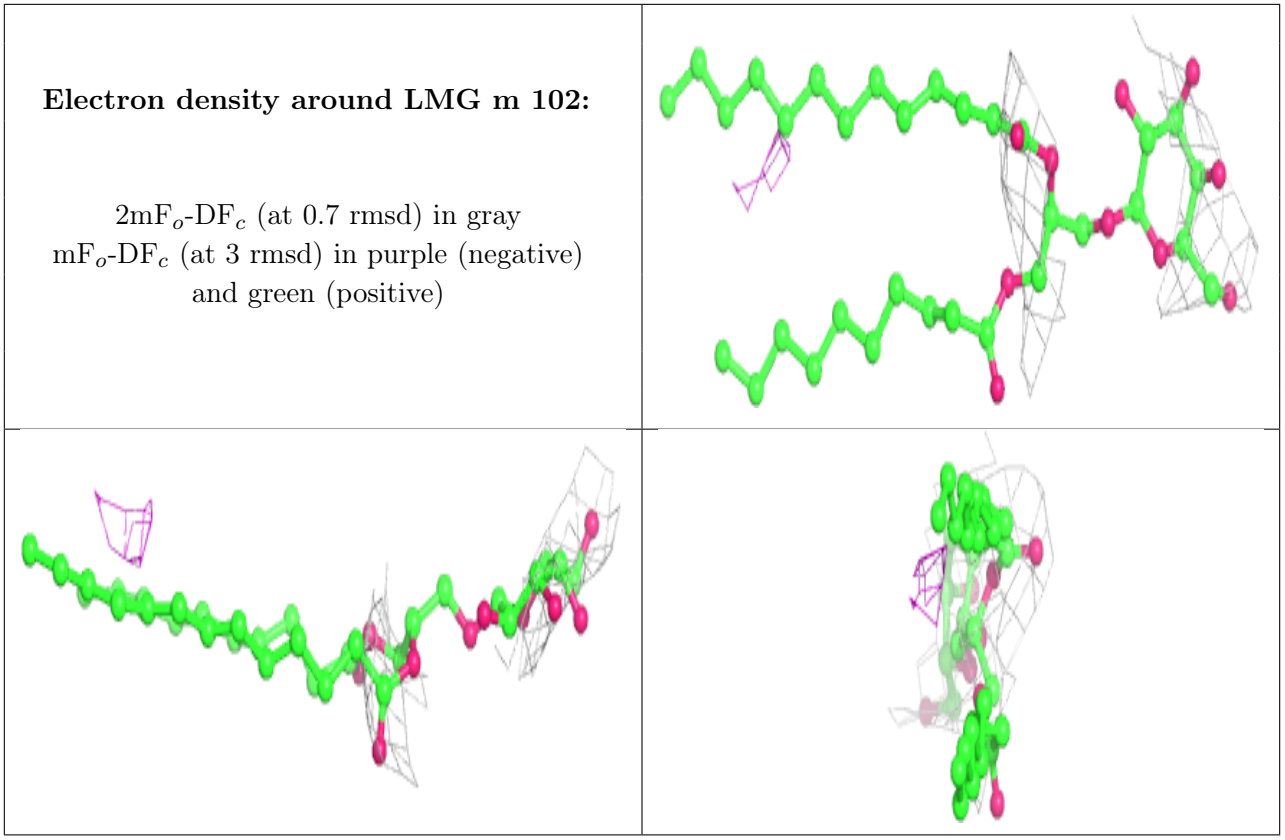
Electron density around PL9 D 404:

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



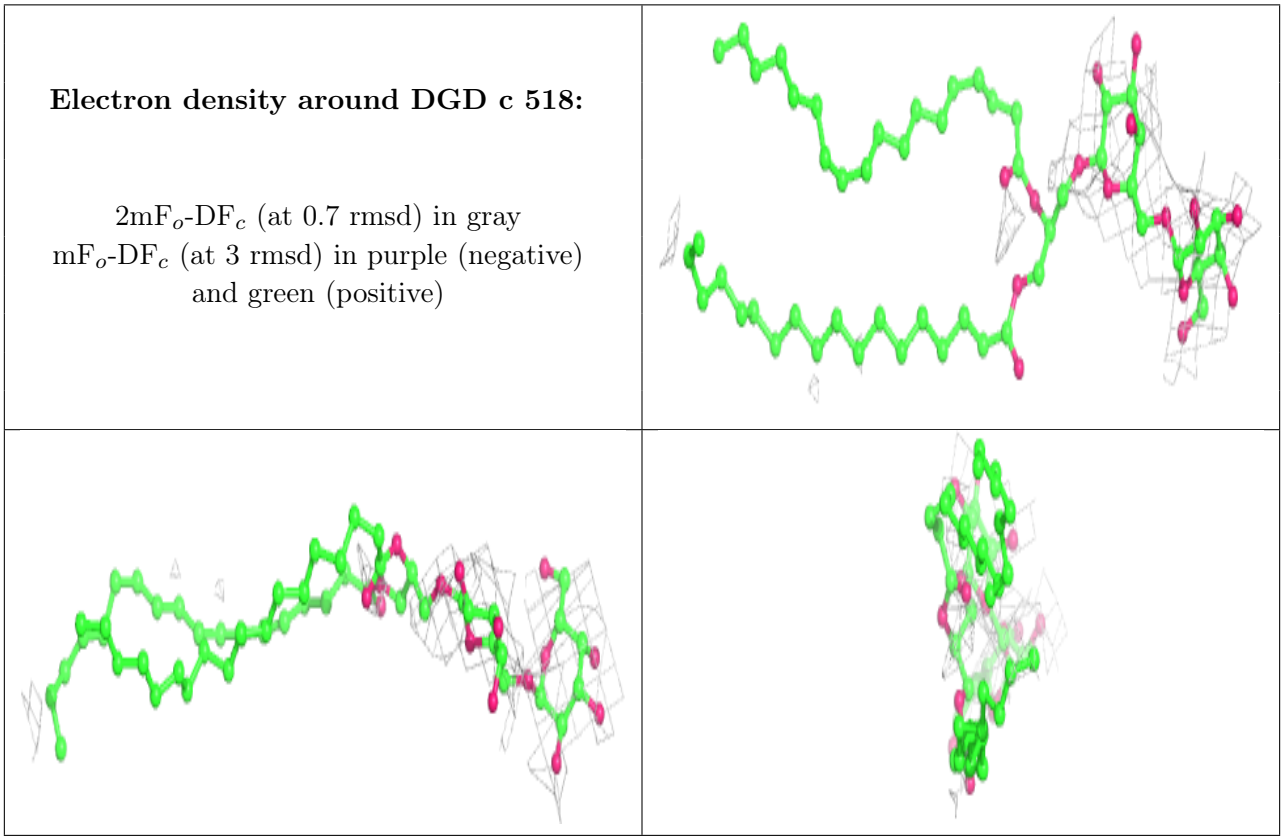
Electron density around LMG m 102:

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



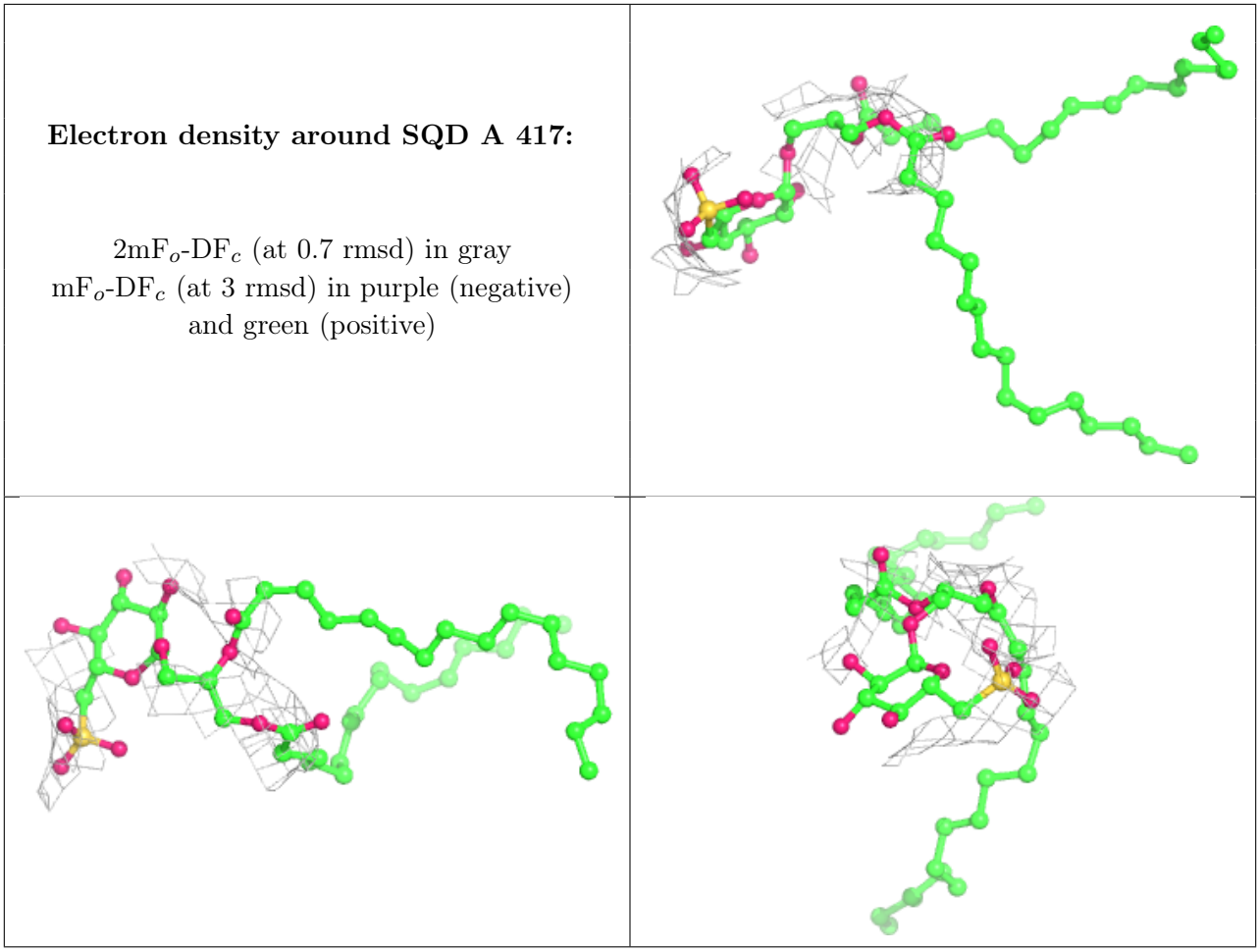
Electron density around DGD c 518:

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



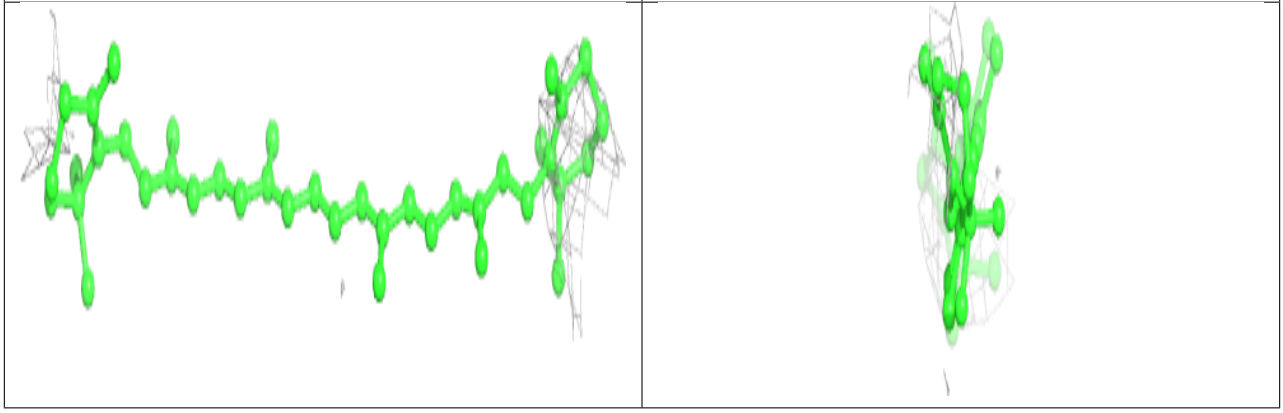
Electron density around SQD A 417:

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



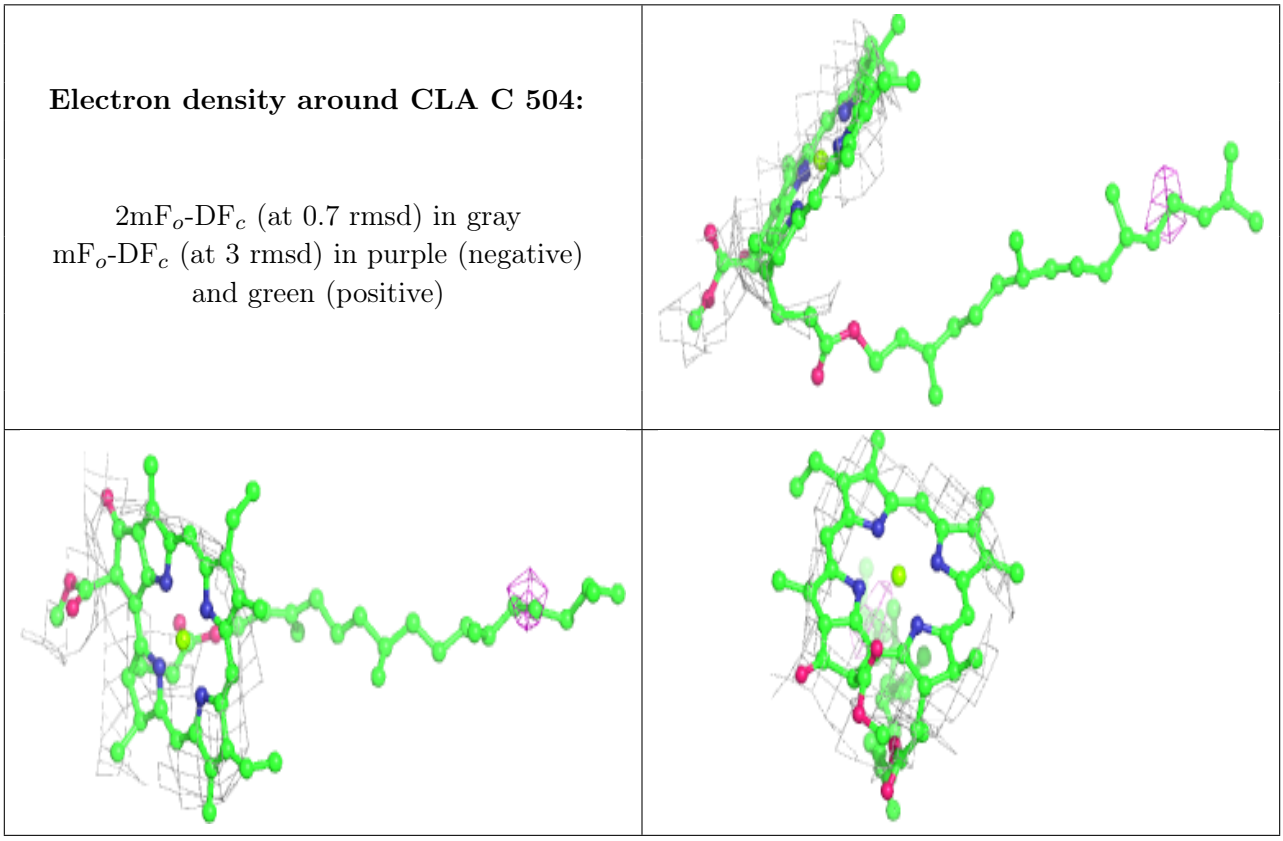
Electron density around BCR c 515:

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



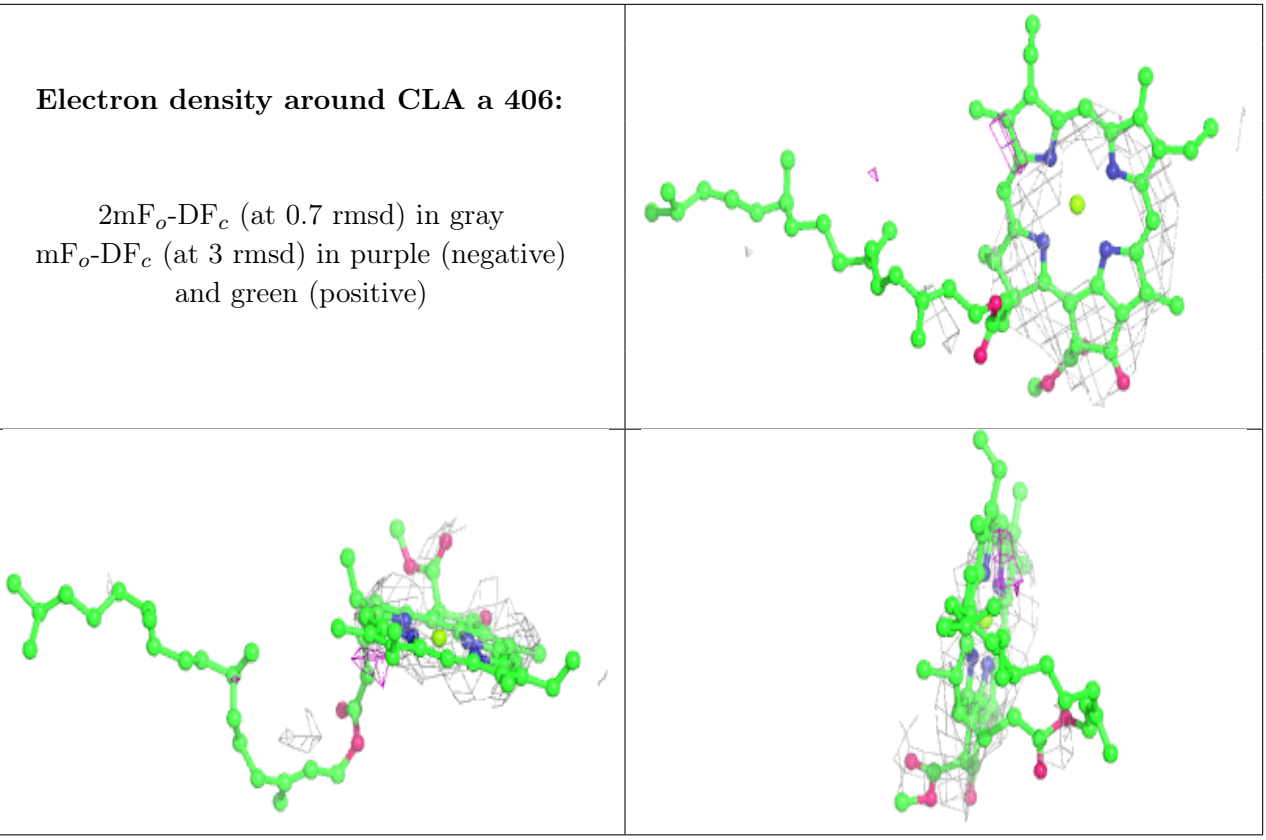
Electron density around CLA C 504:

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



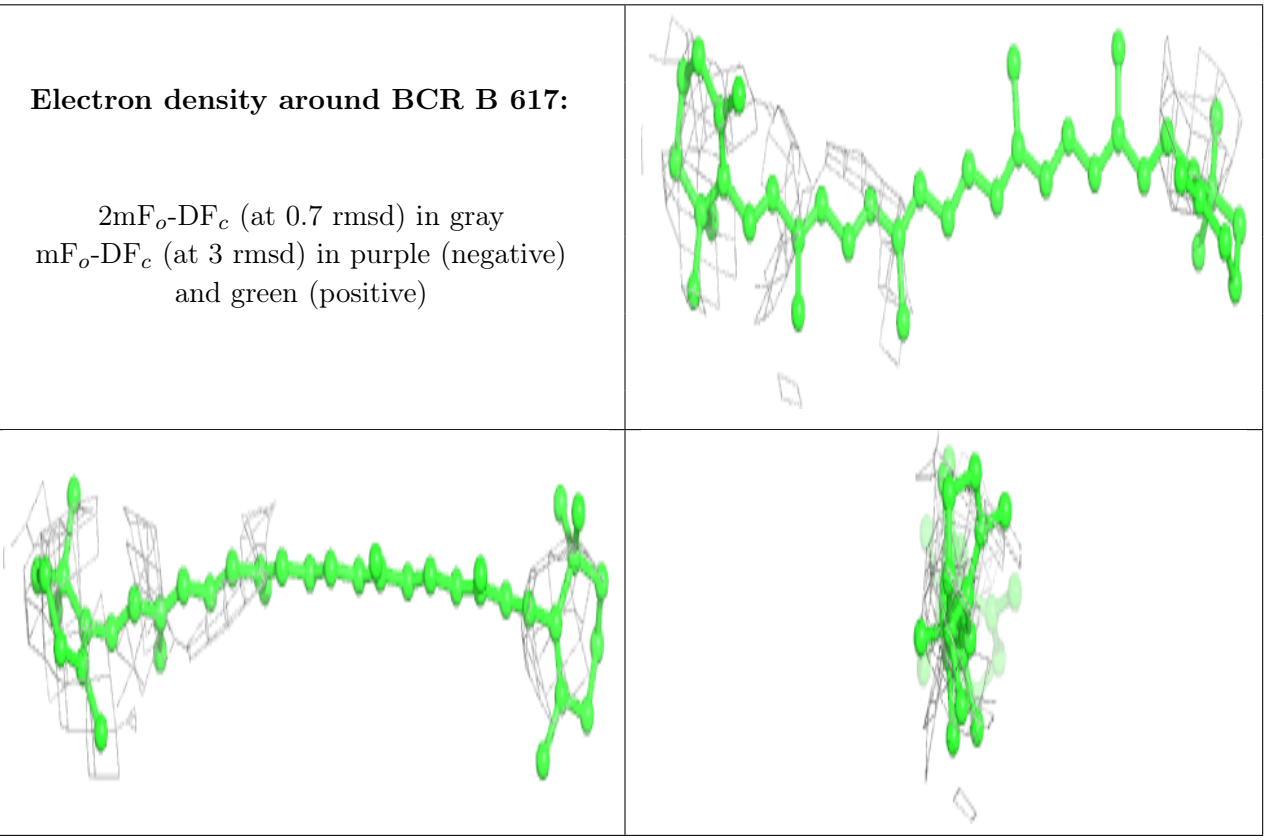
Electron density around CLA a 406:

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



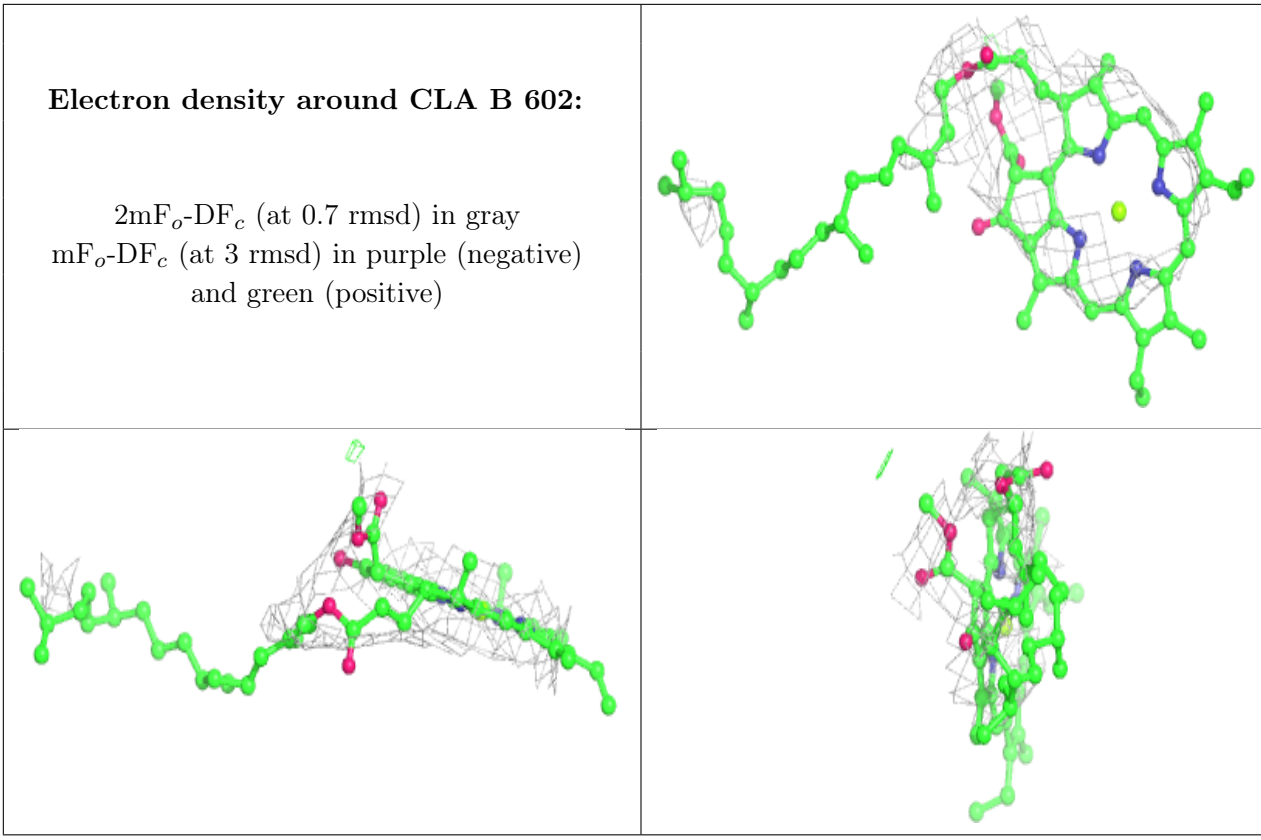
Electron density around BCR B 617:

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



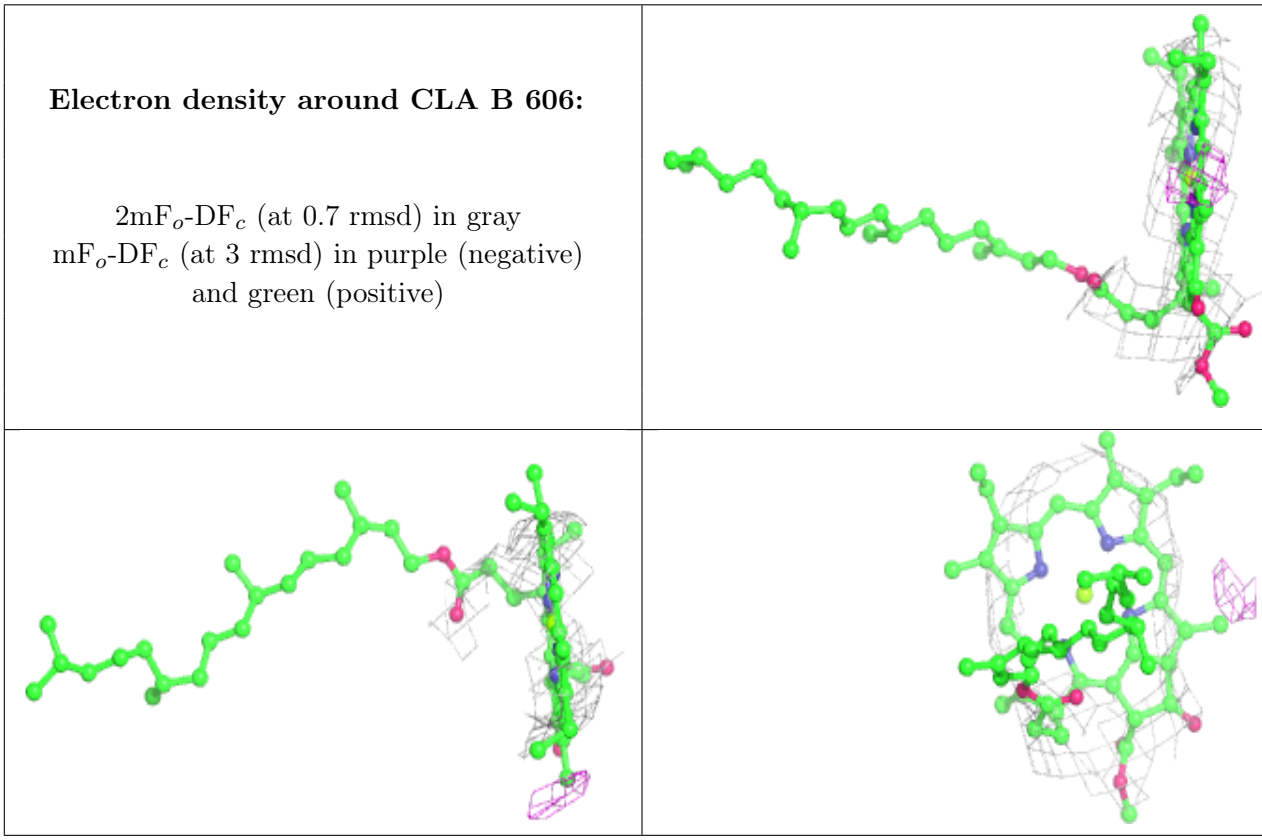
Electron density around CLA B 602:

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



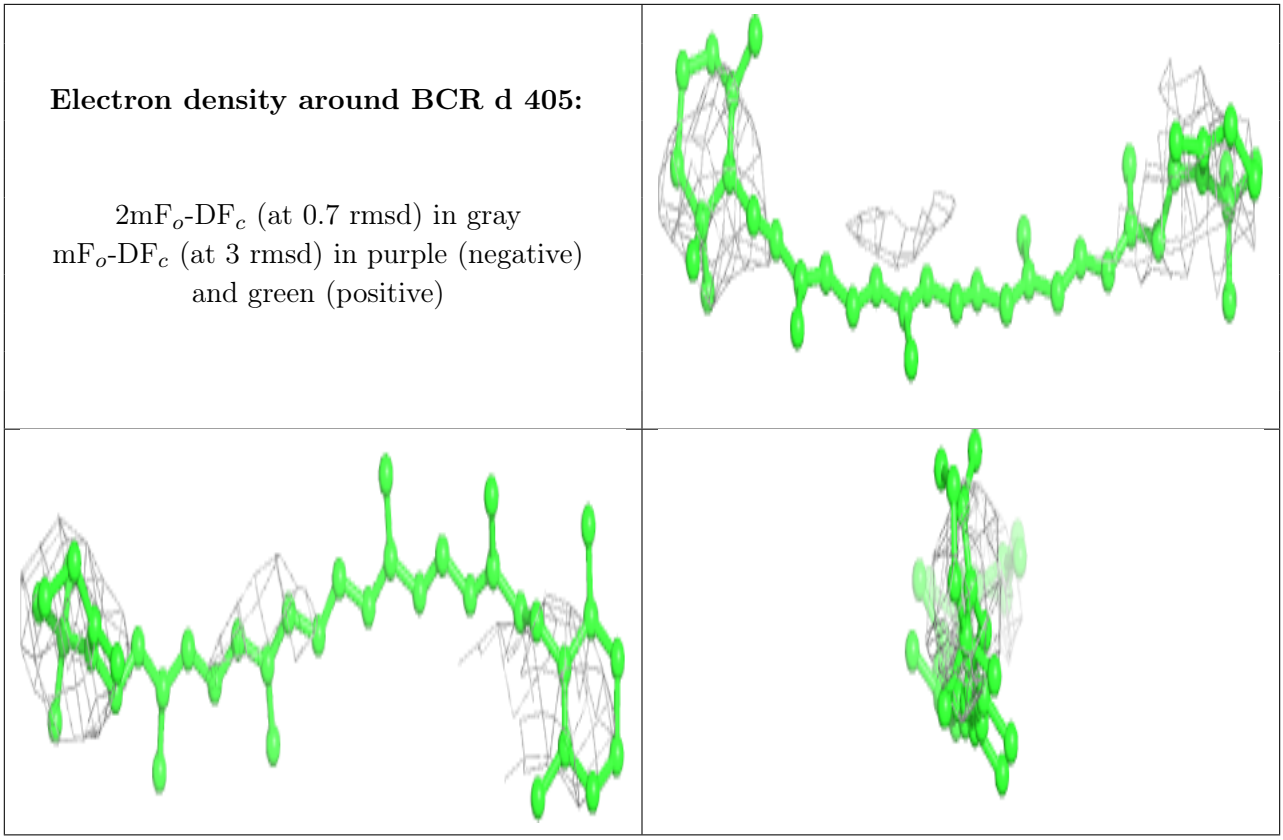
Electron density around CLA B 606:

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



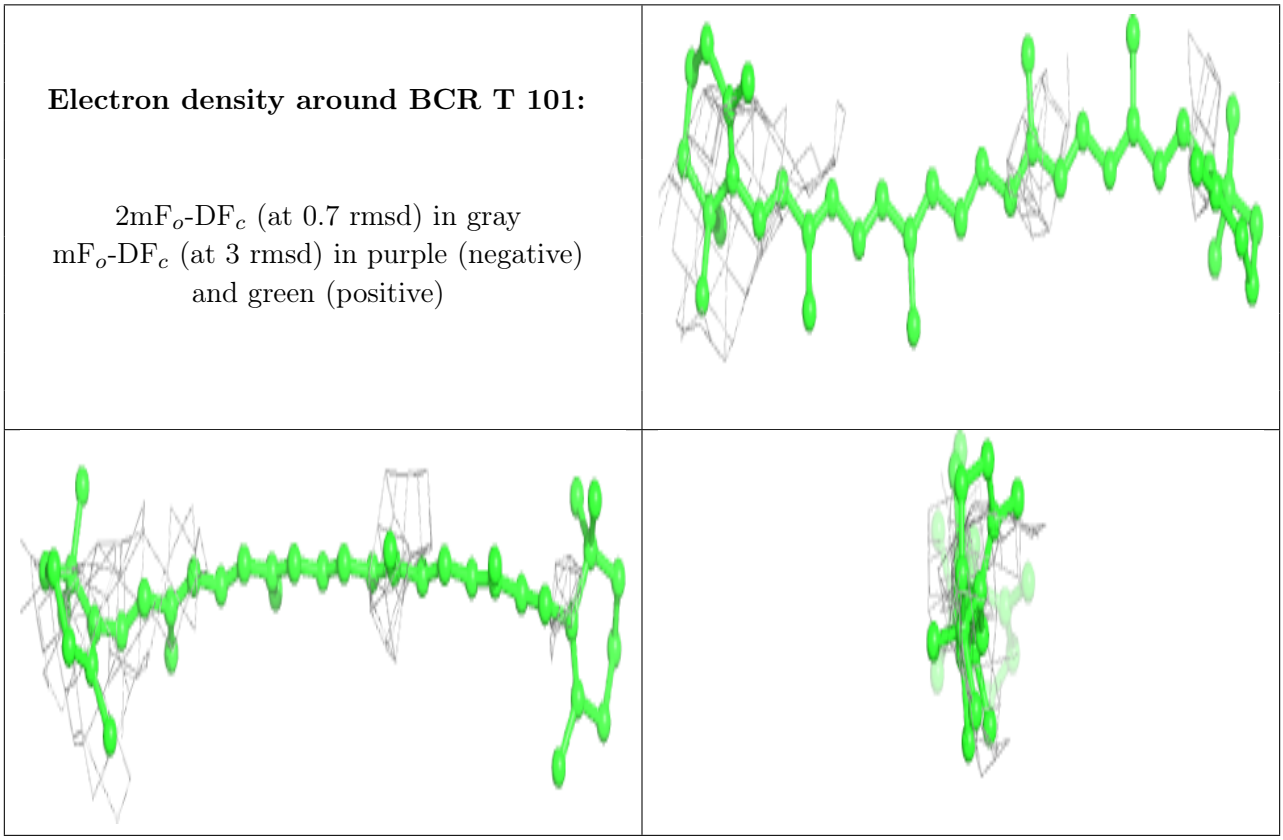
Electron density around BCR d 405:

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



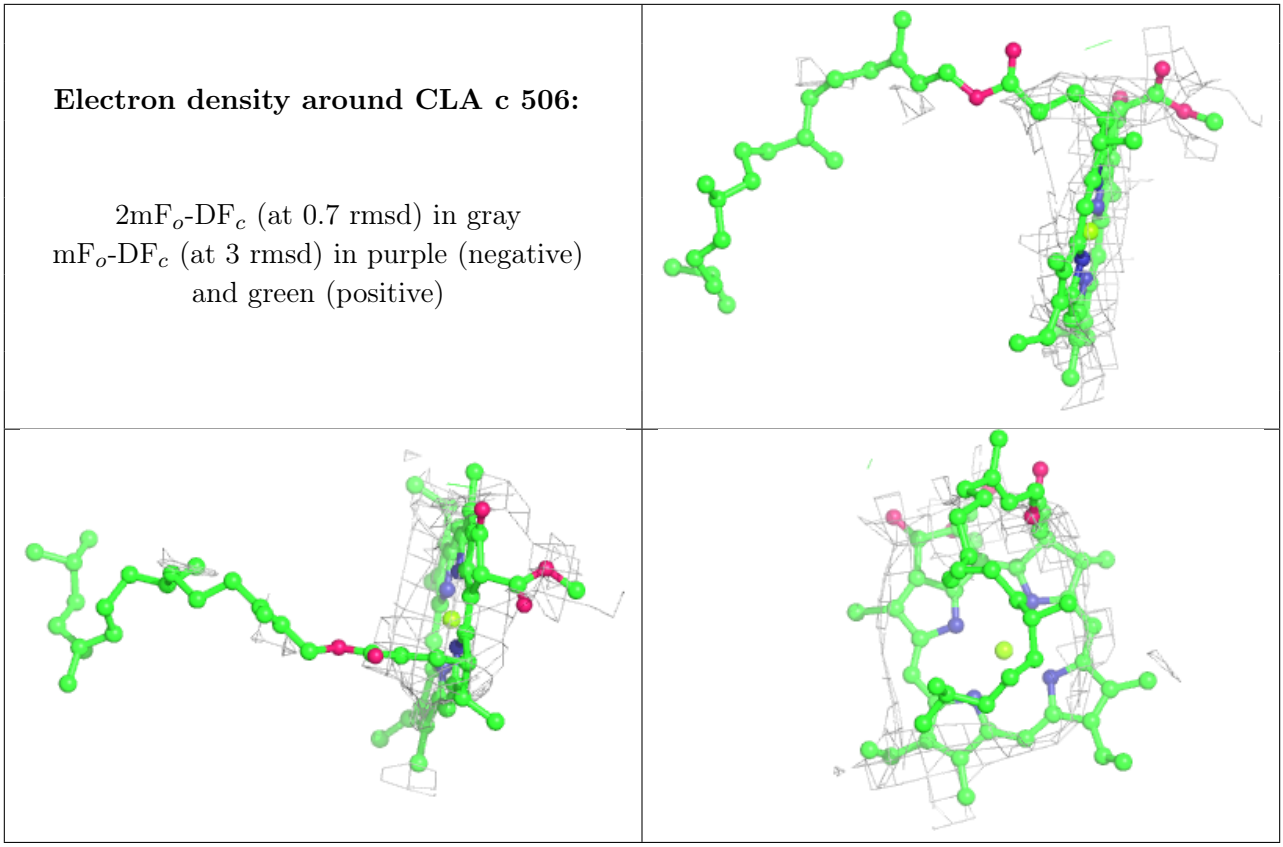
Electron density around BCR T 101:

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



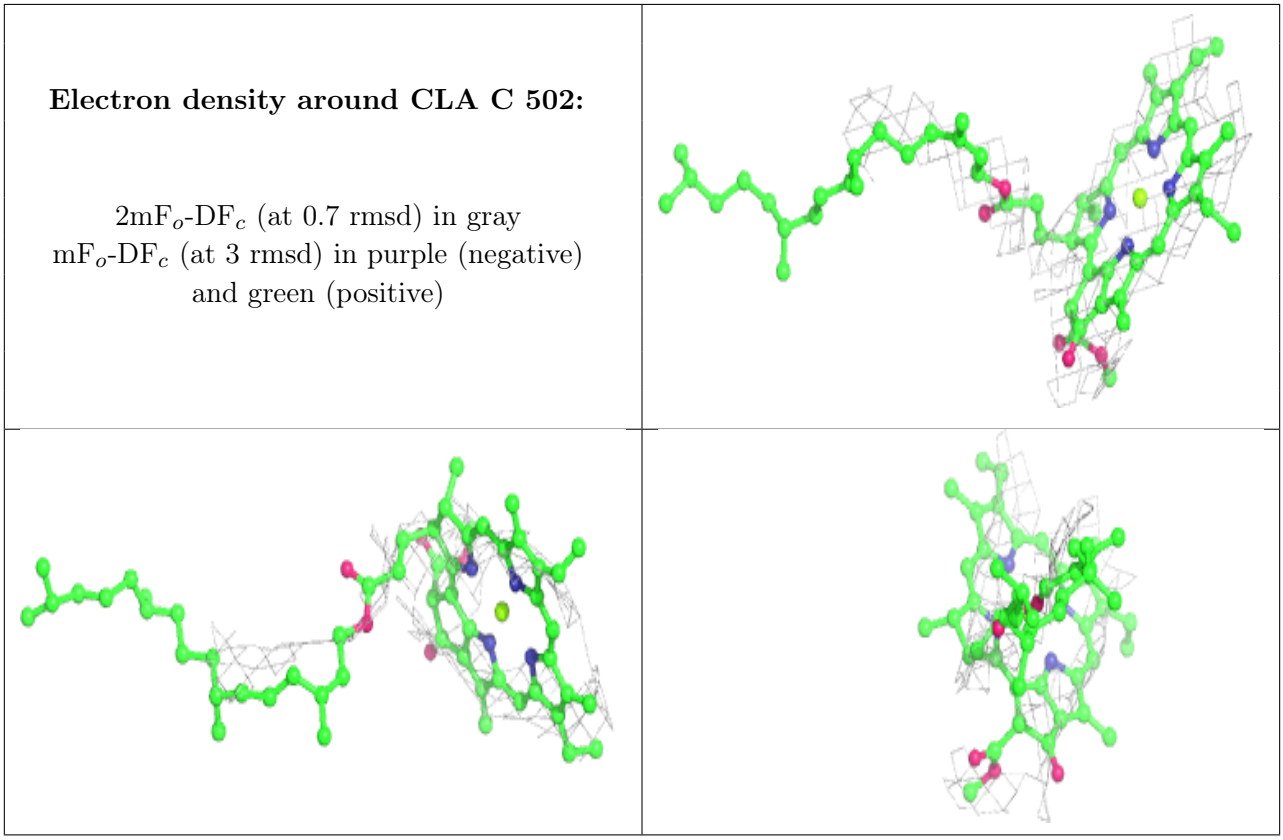
Electron density around CLA c 506:

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



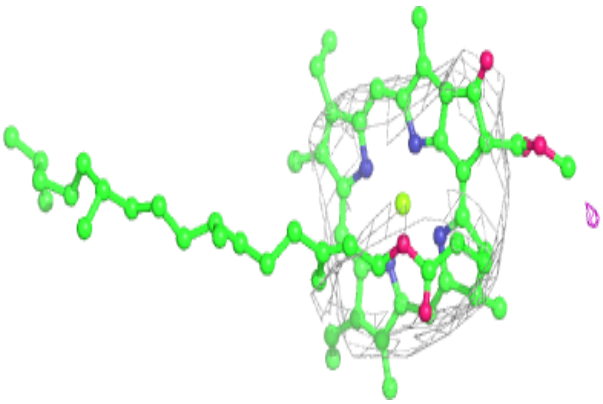
Electron density around CLA C 502:

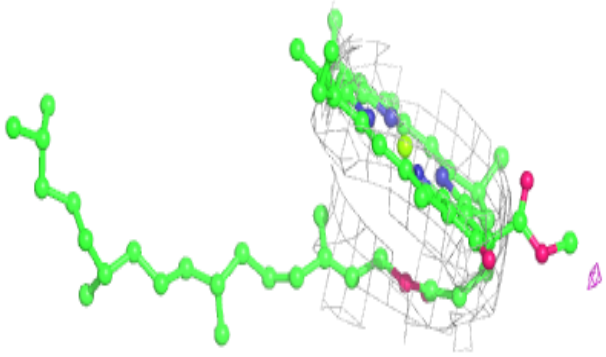
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

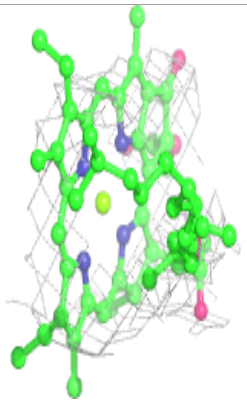


Electron density around CLA B 608:

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

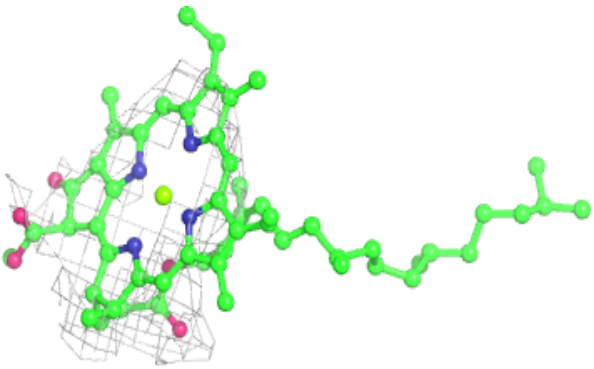


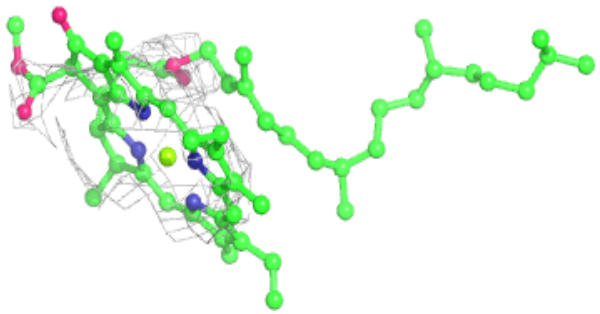


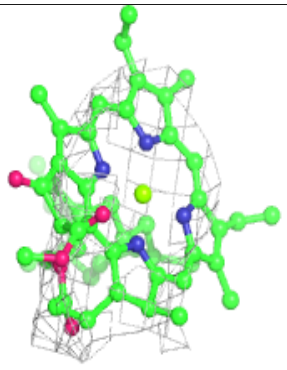


Electron density around CLA C 505:

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

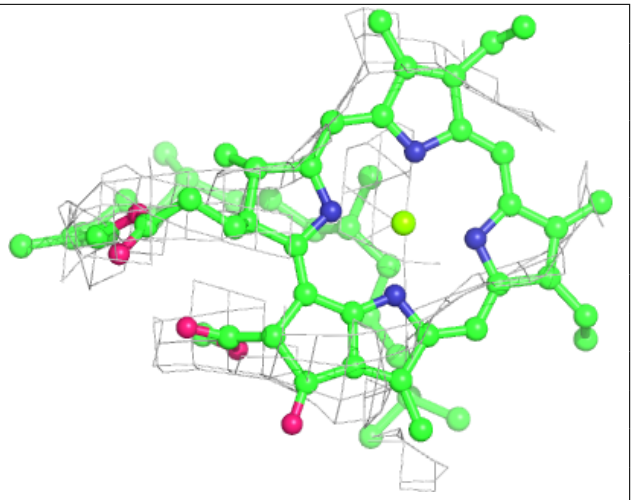


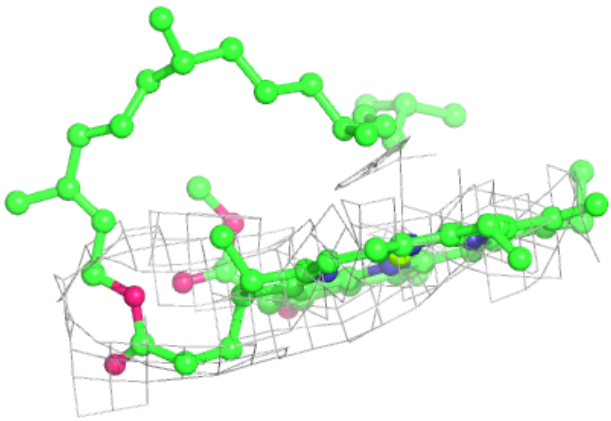


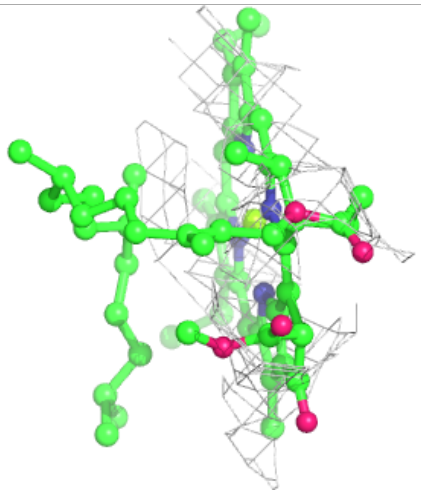


Electron density around CLA C 510:

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

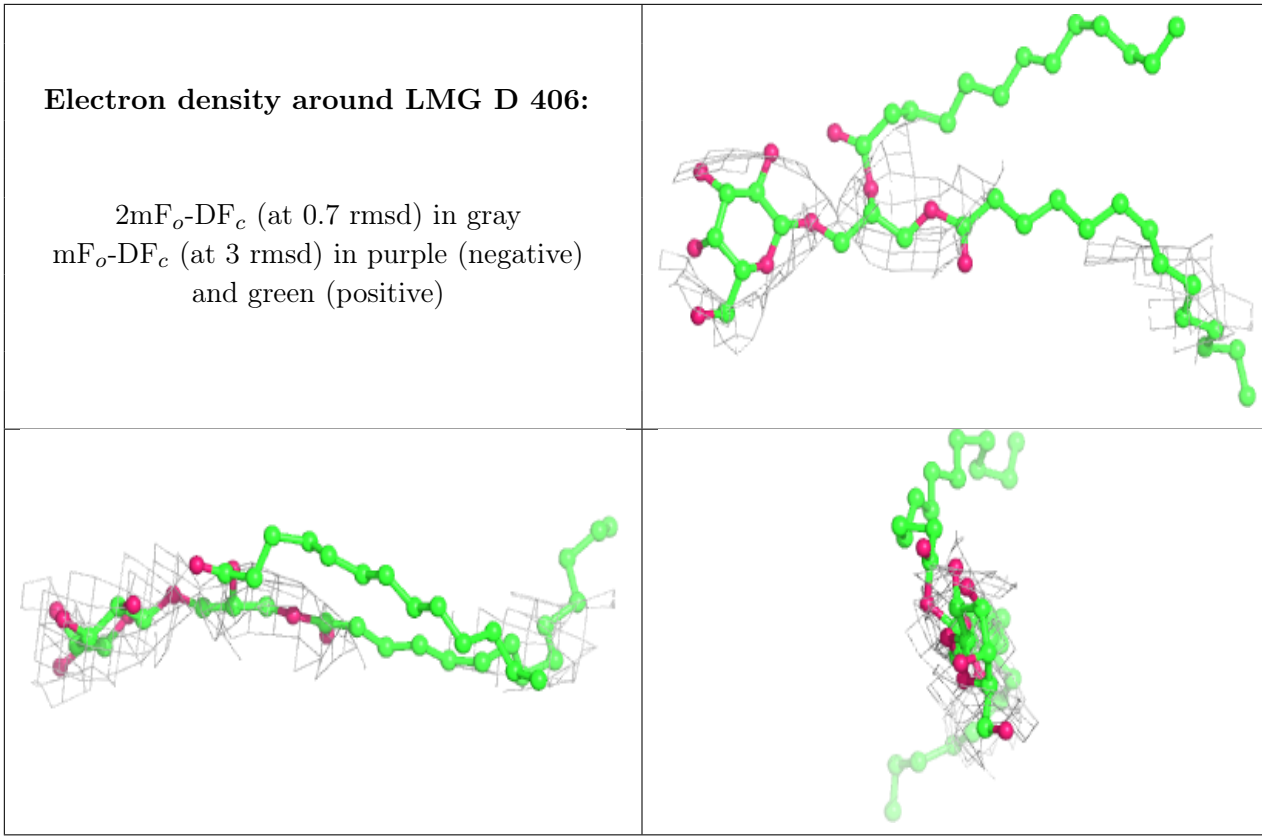






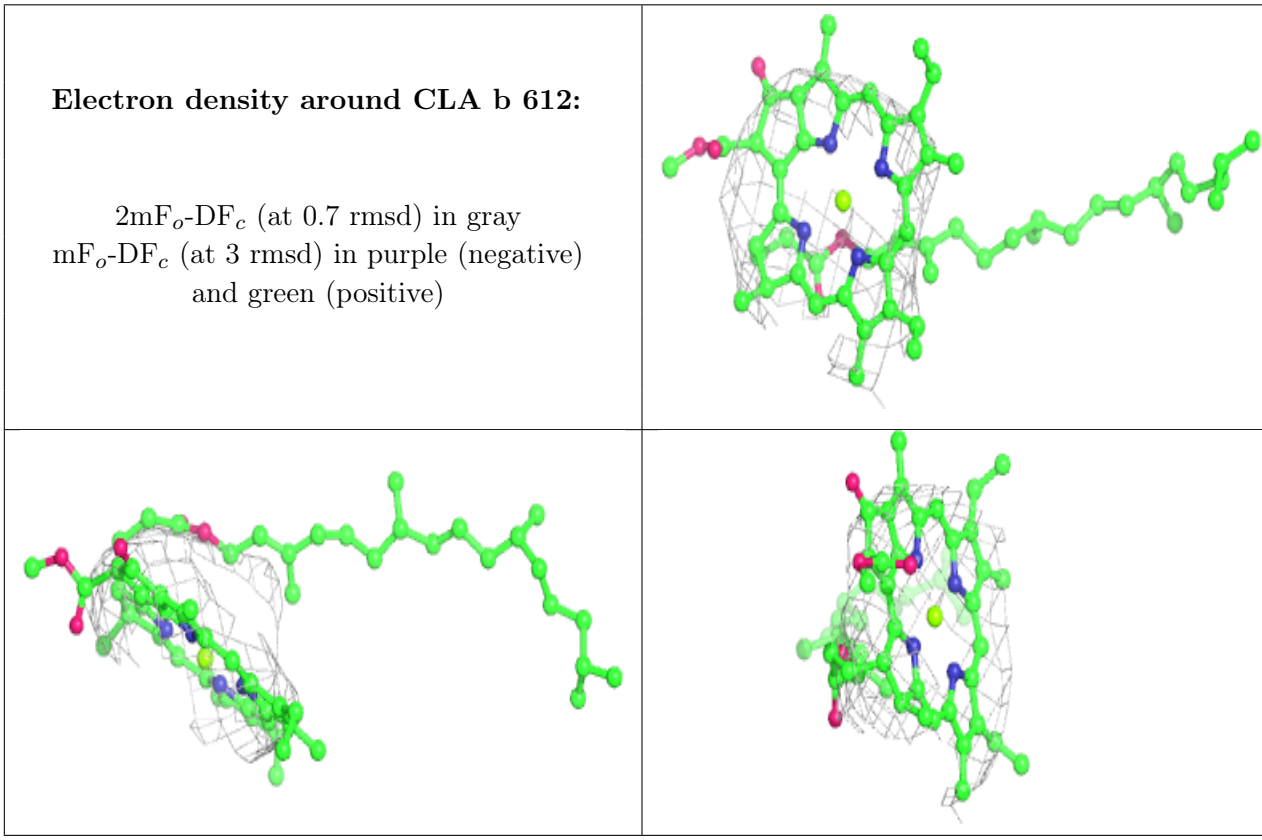
Electron density around LMG D 406:

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



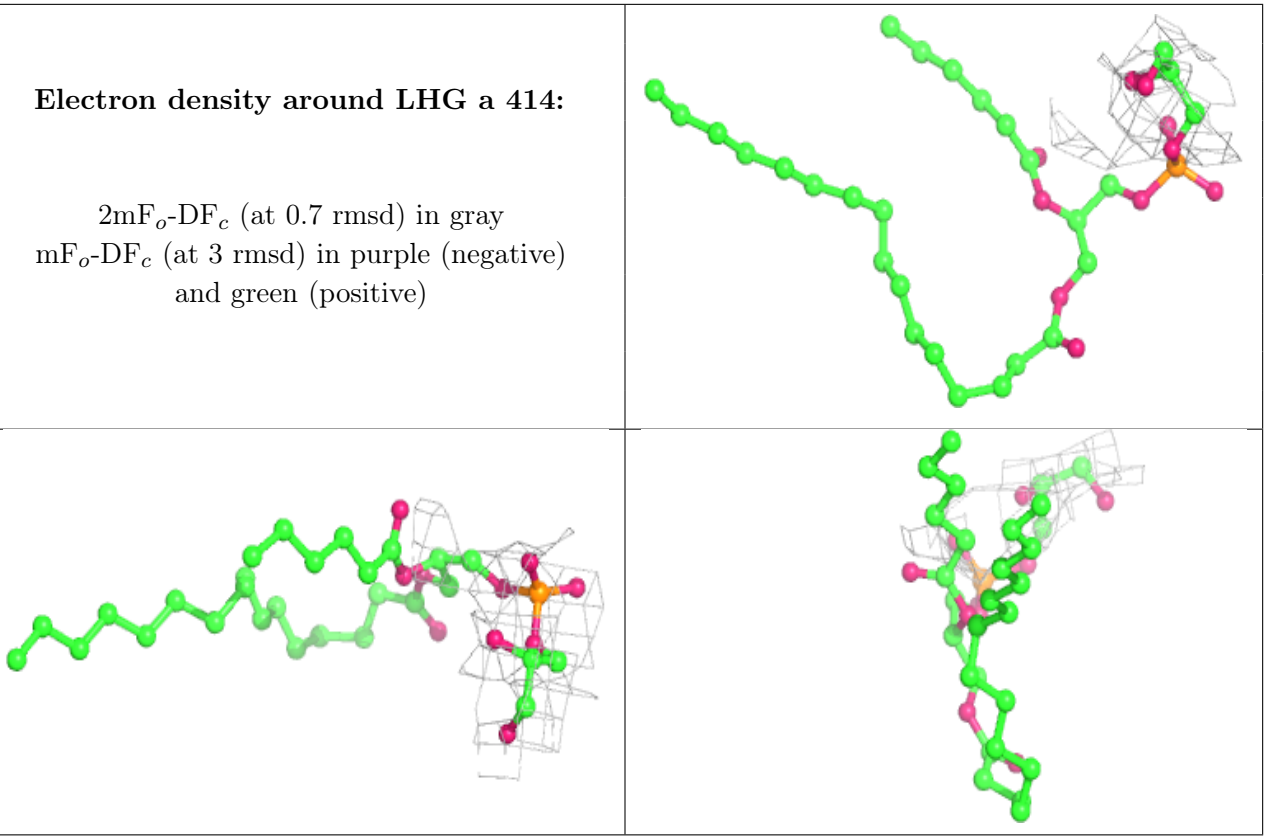
Electron density around CLA b 612:

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



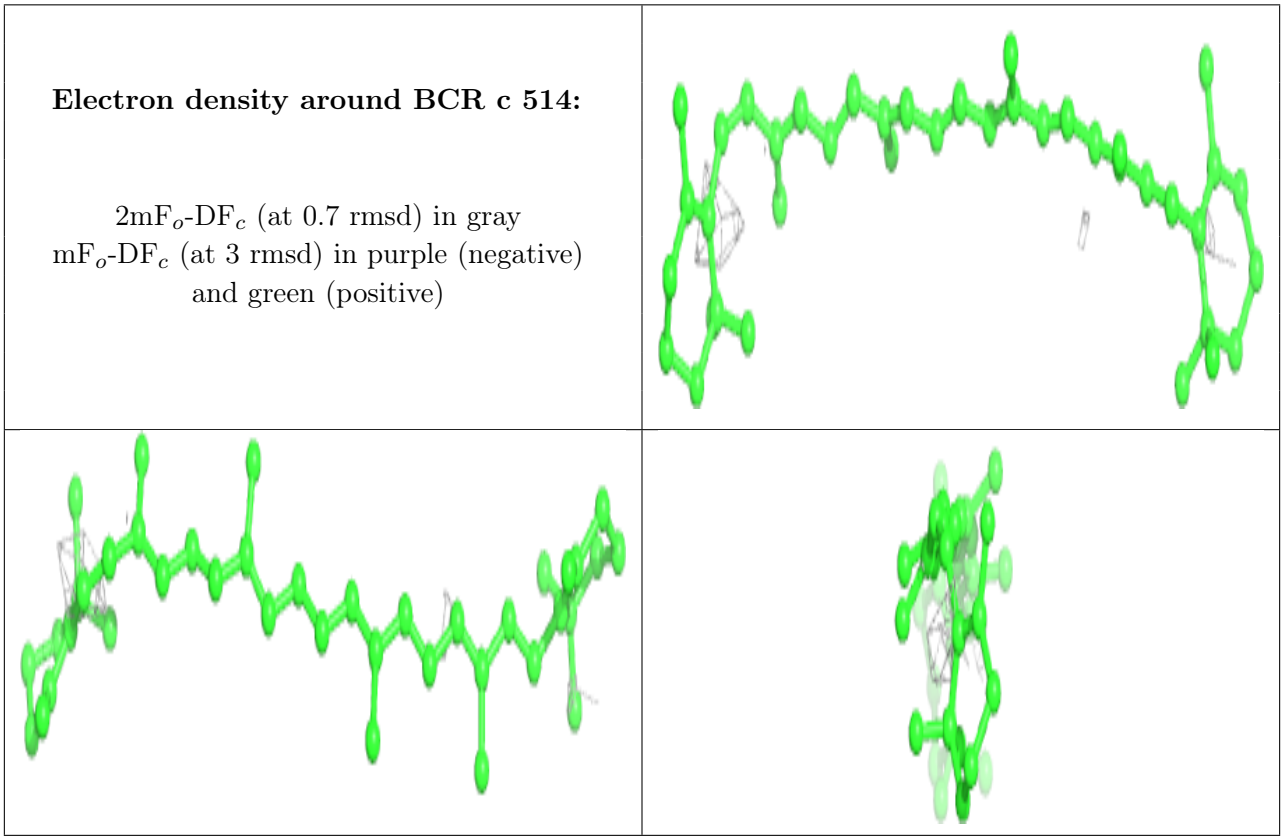
Electron density around LHG a 414:

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



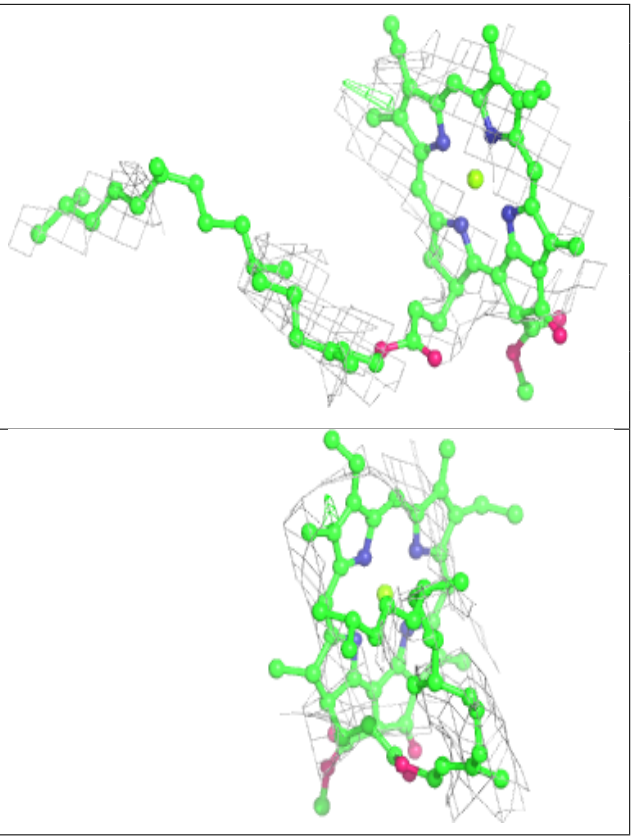
Electron density around BCR c 514:

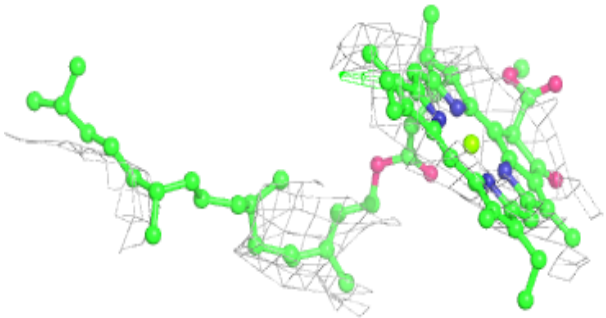
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 511:

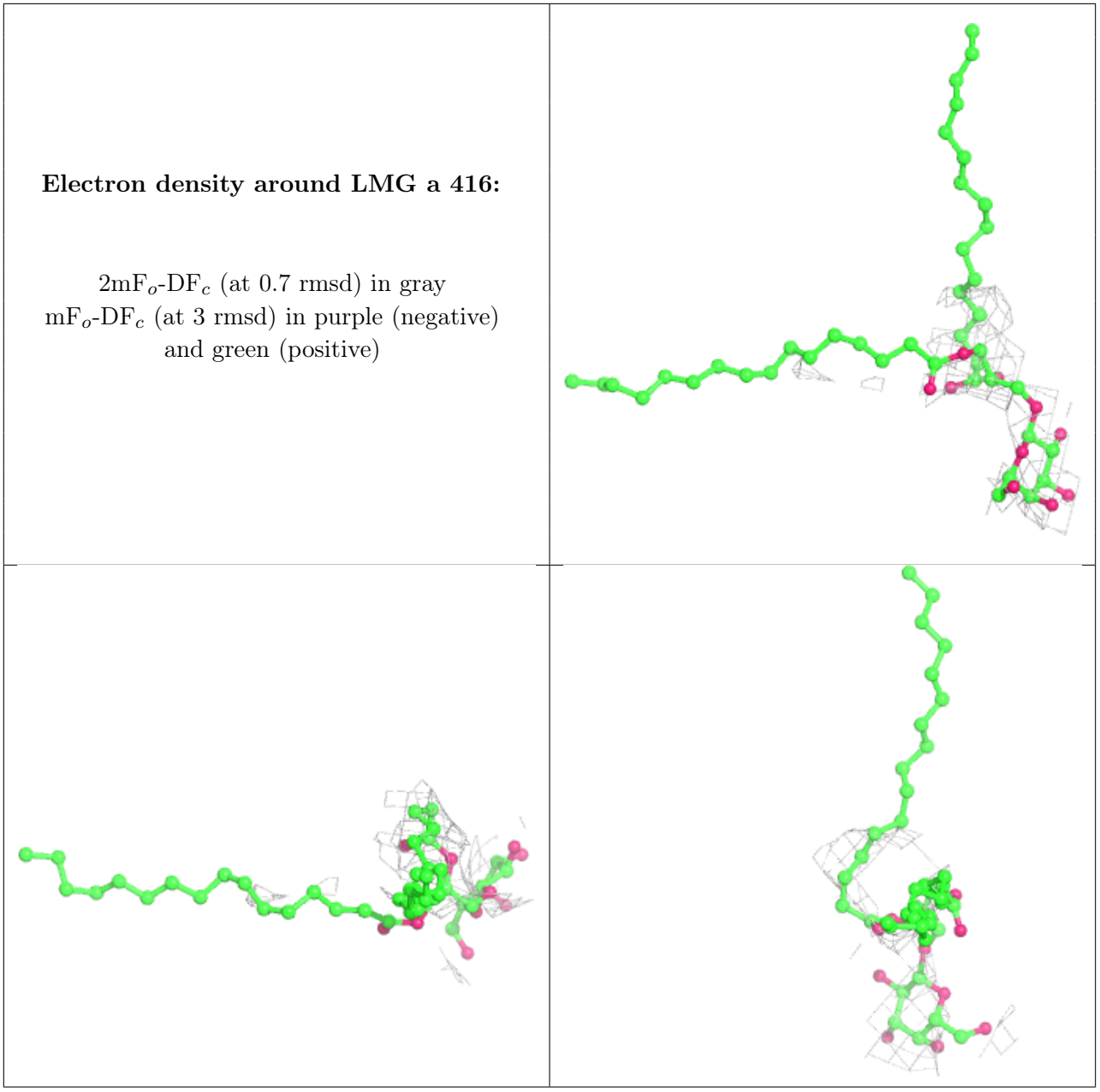
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





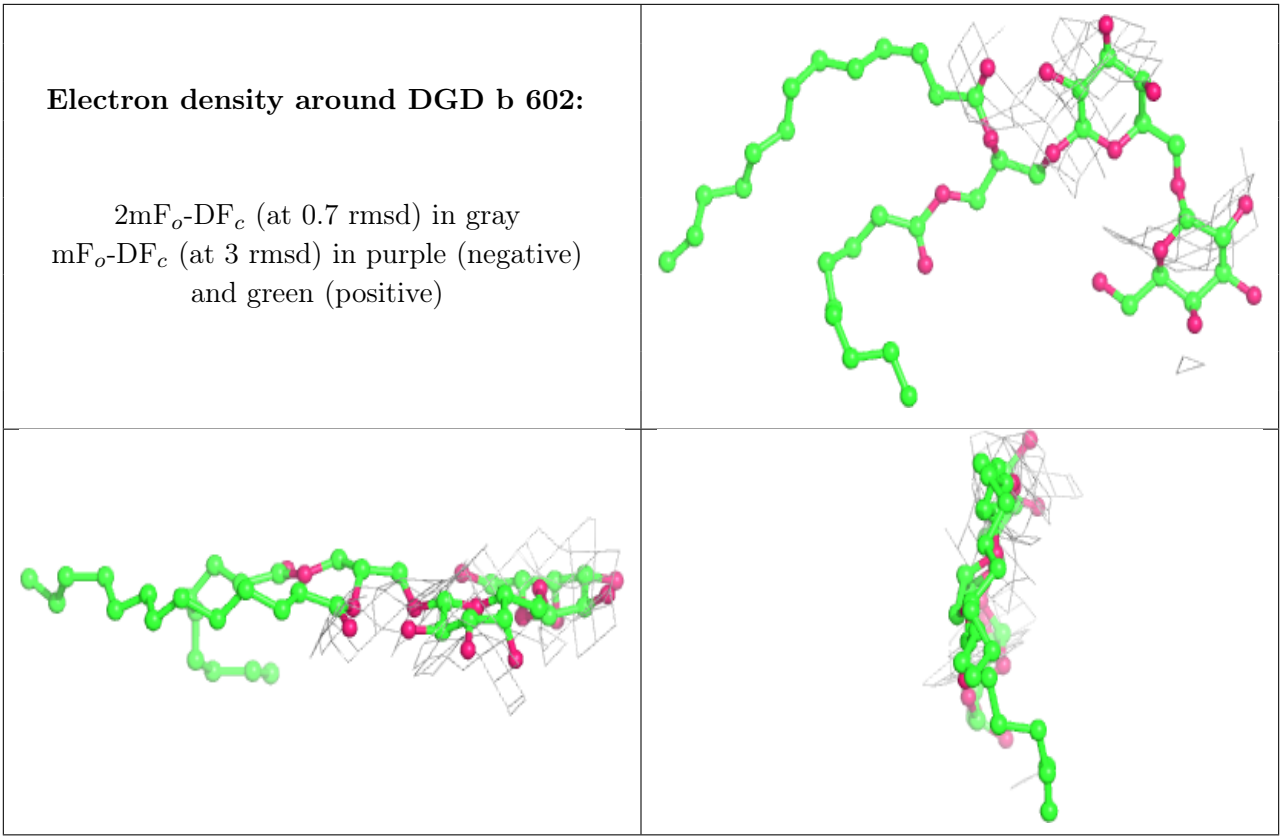
Electron density around LMG a 416:

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



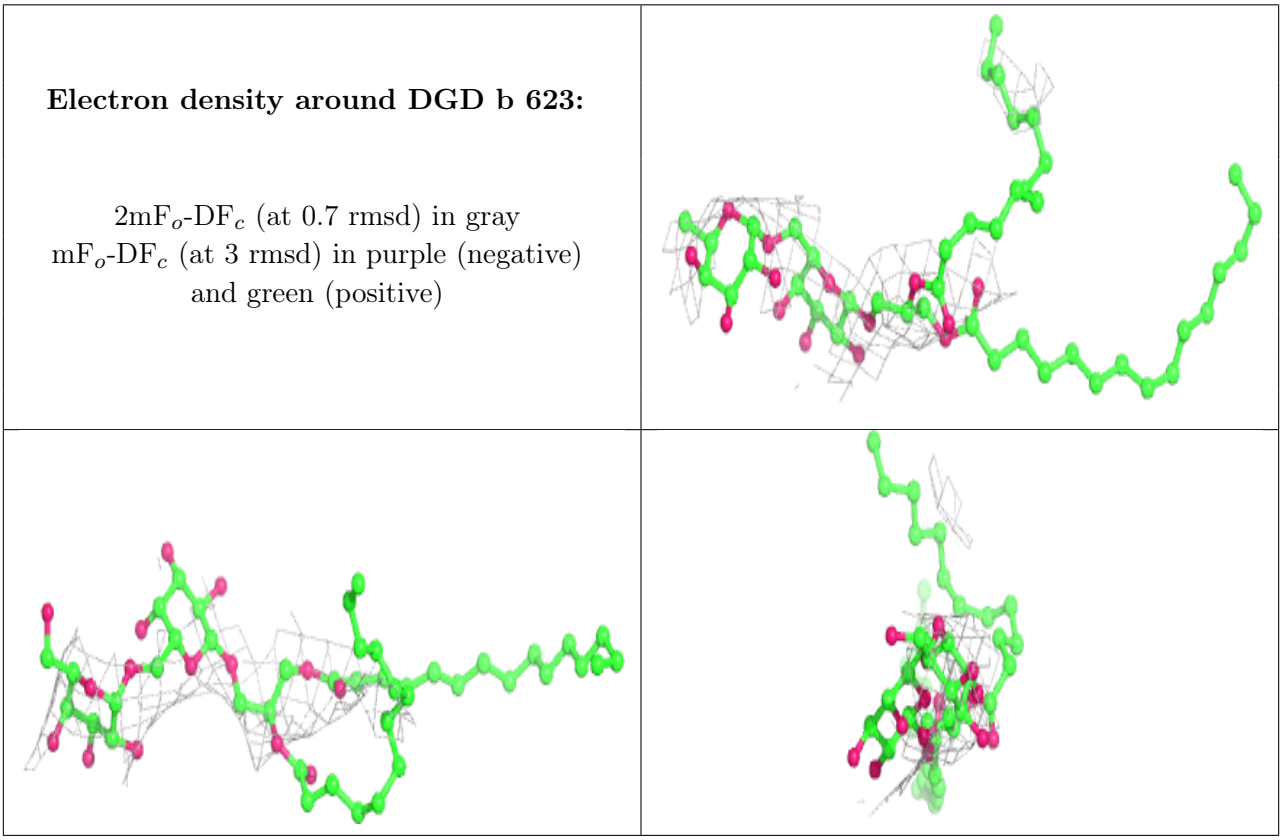
Electron density around DGD b 602:

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



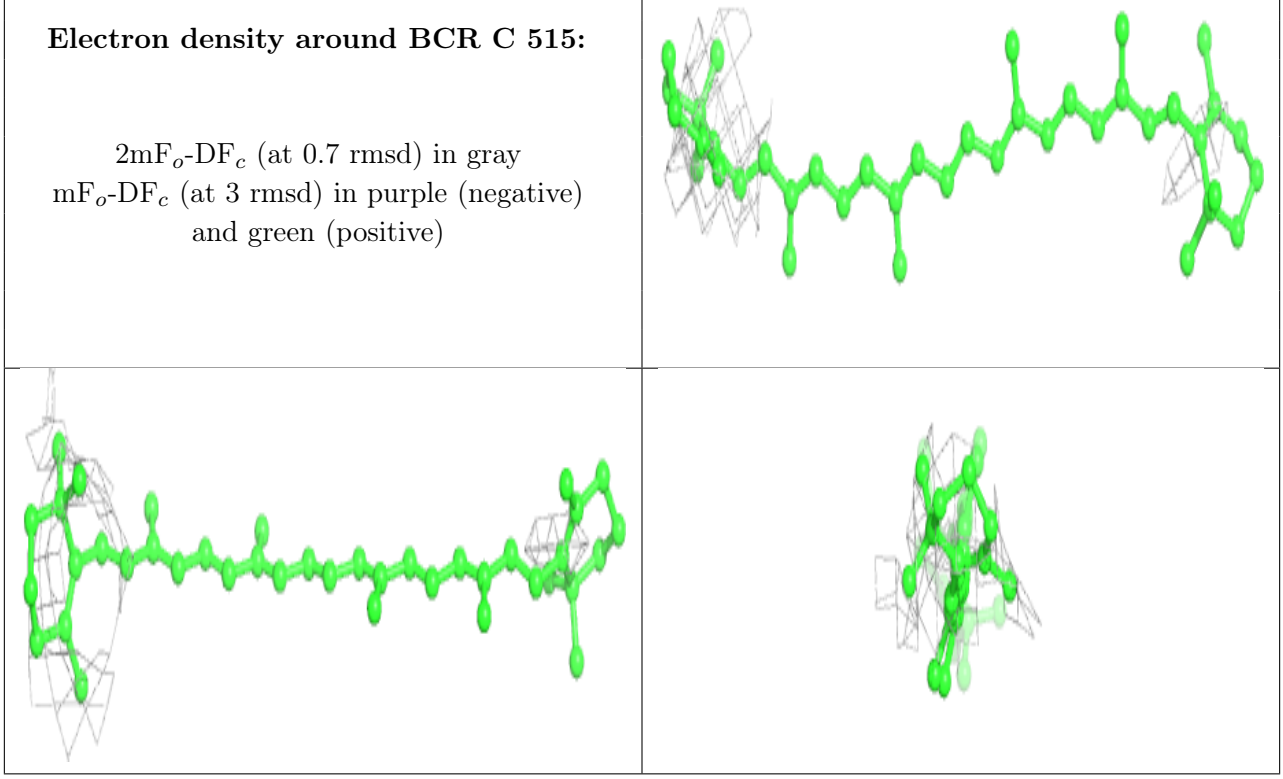
Electron density around DGD b 623:

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



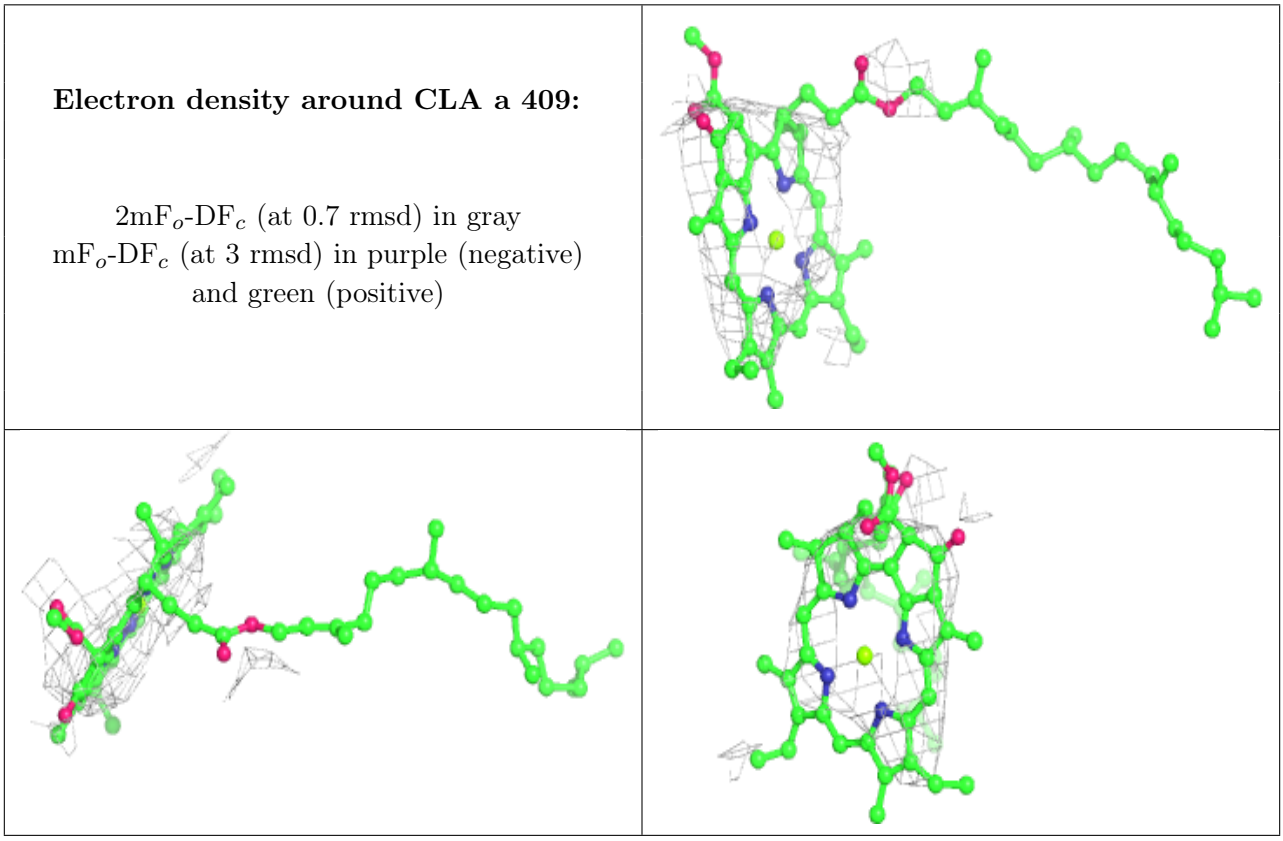
Electron density around BCR C 515:

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



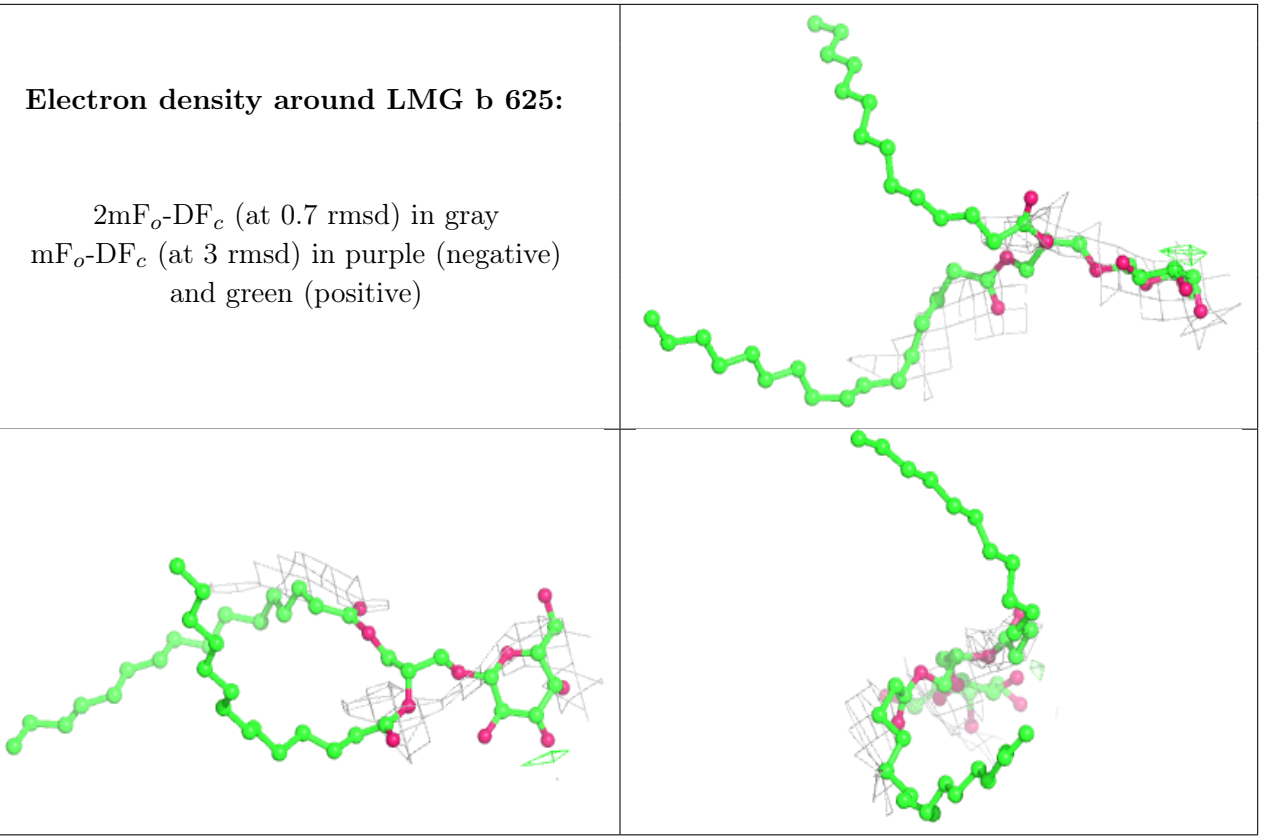
Electron density around CLA a 409:

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



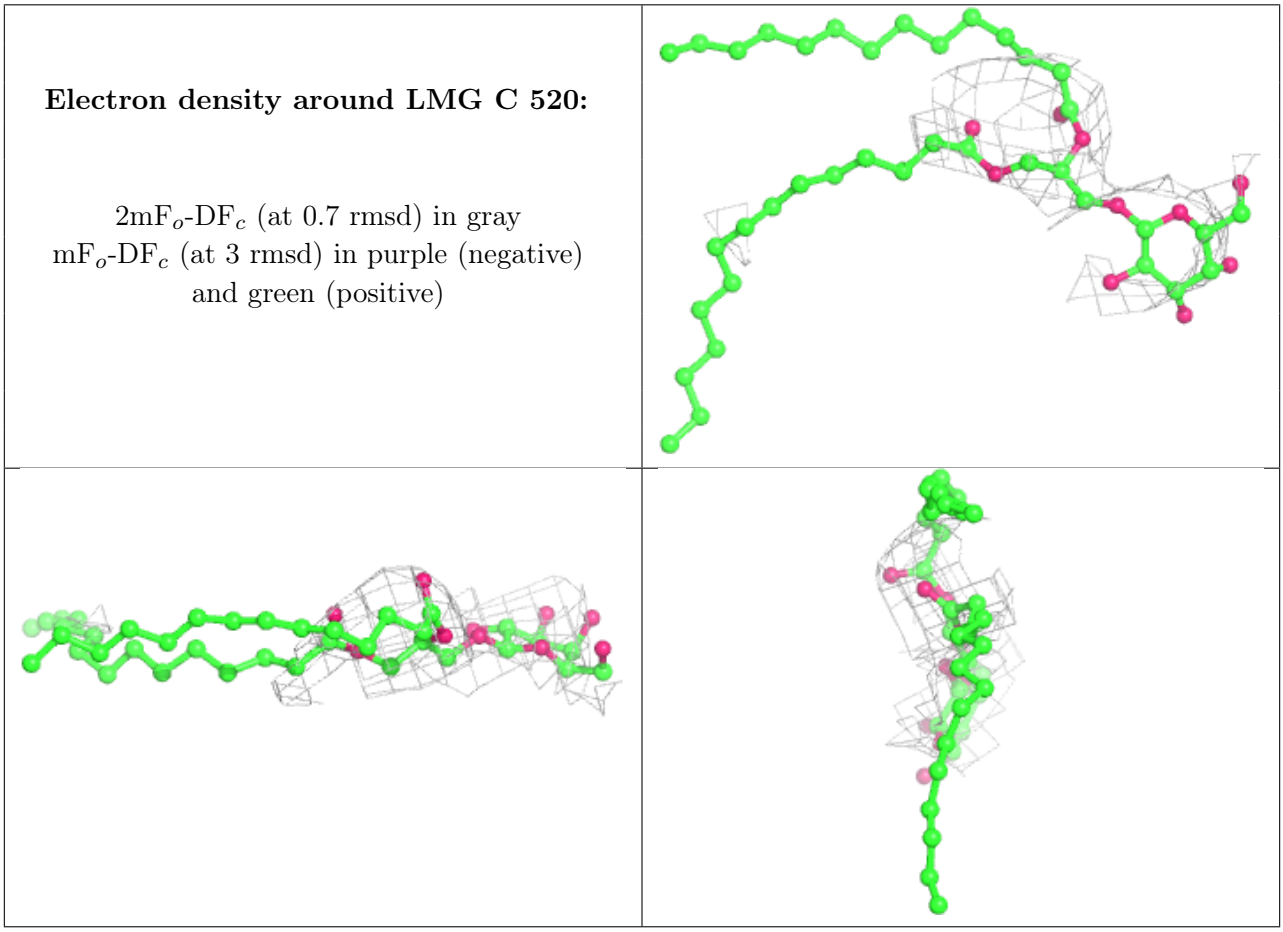
Electron density around LMG b 625:

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



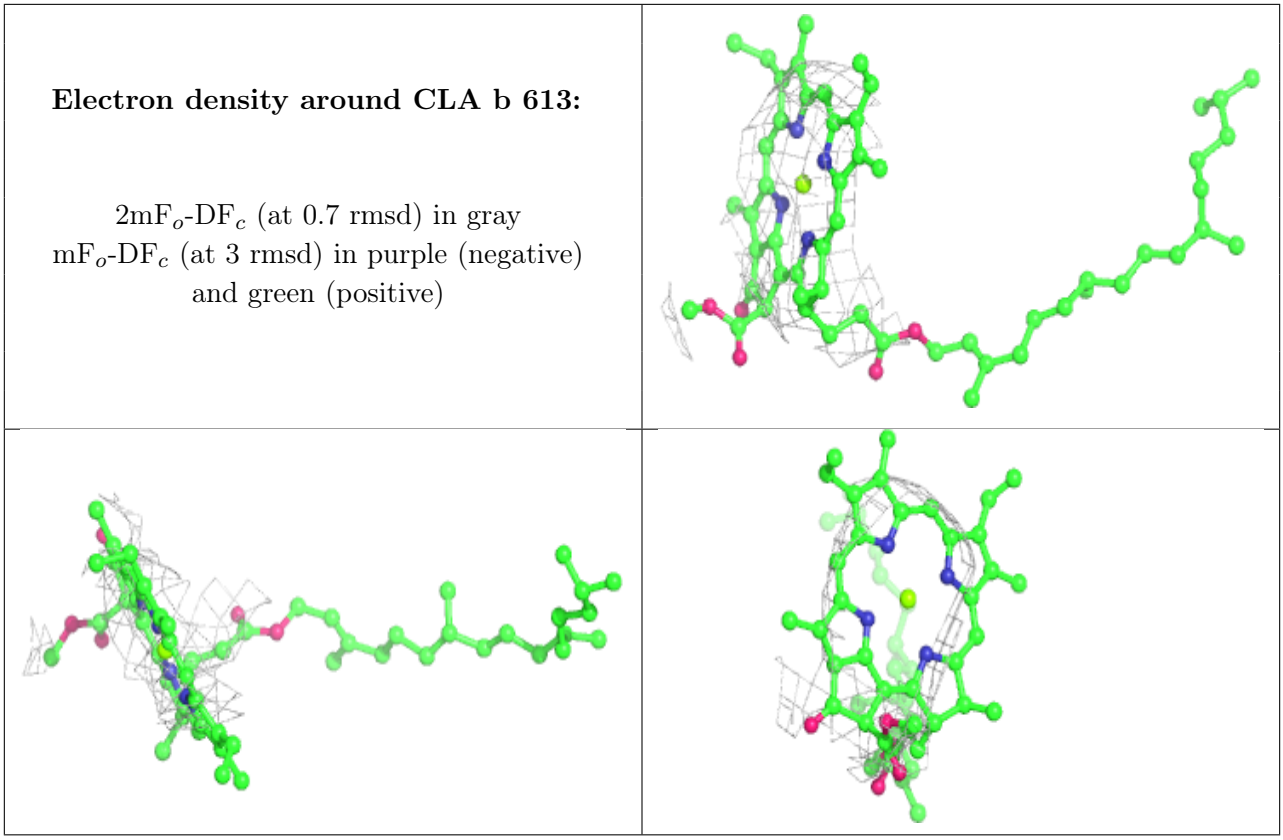
Electron density around LMG C 520:

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



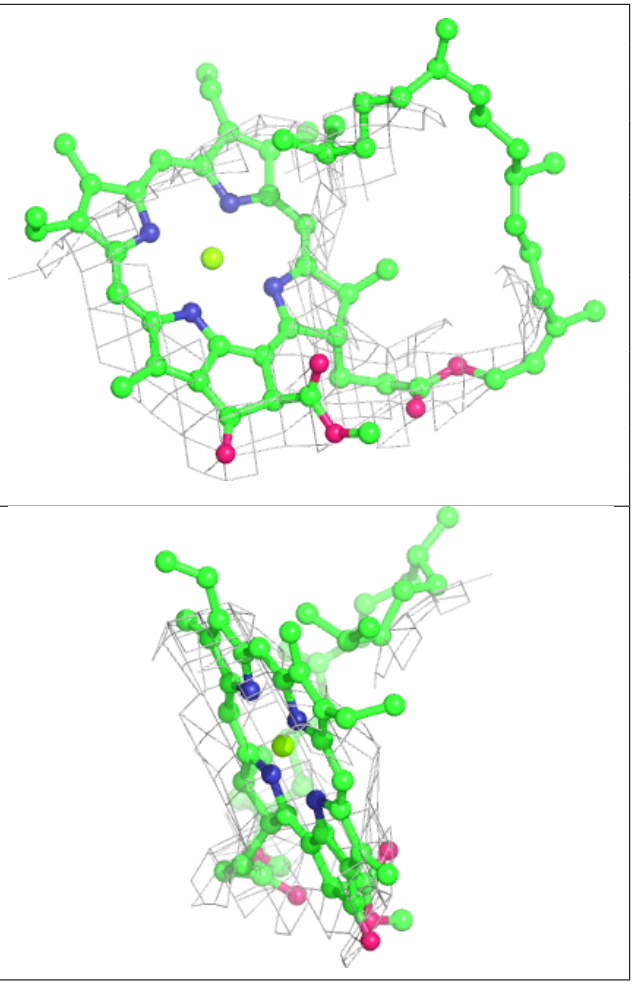
Electron density around CLA b 613:

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



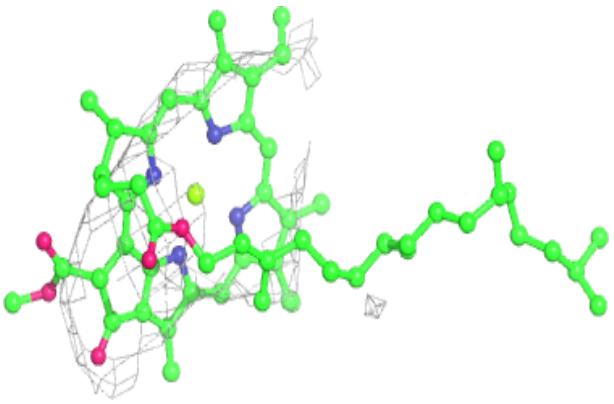
Electron density around CLA b 619:

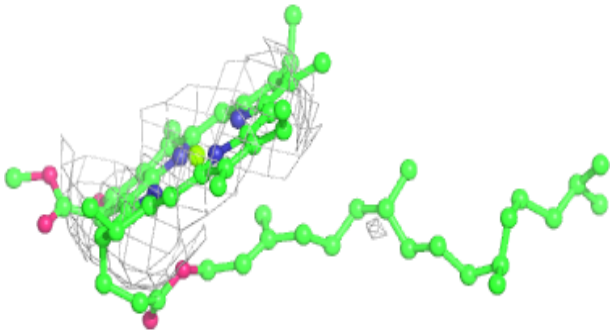
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

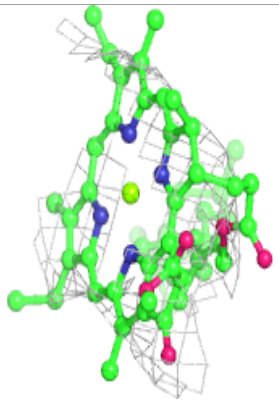


Electron density around CLA b 618:

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

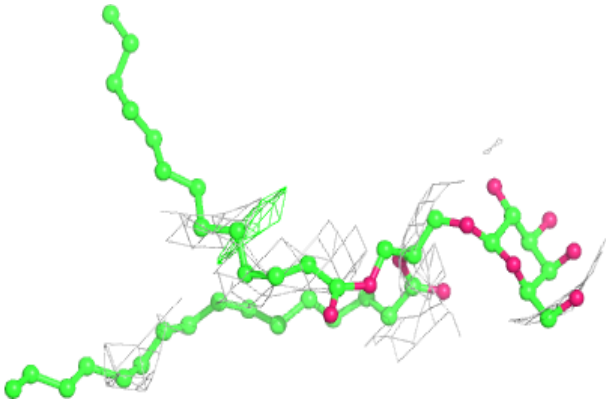


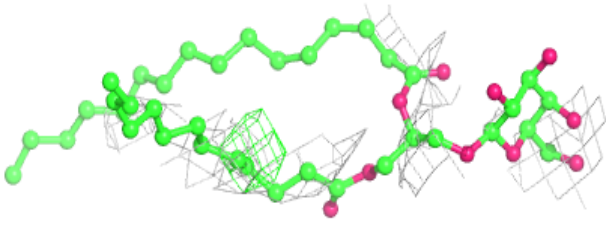


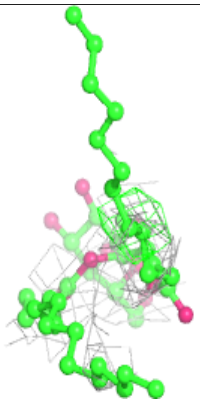


Electron density around LMG d 407:

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

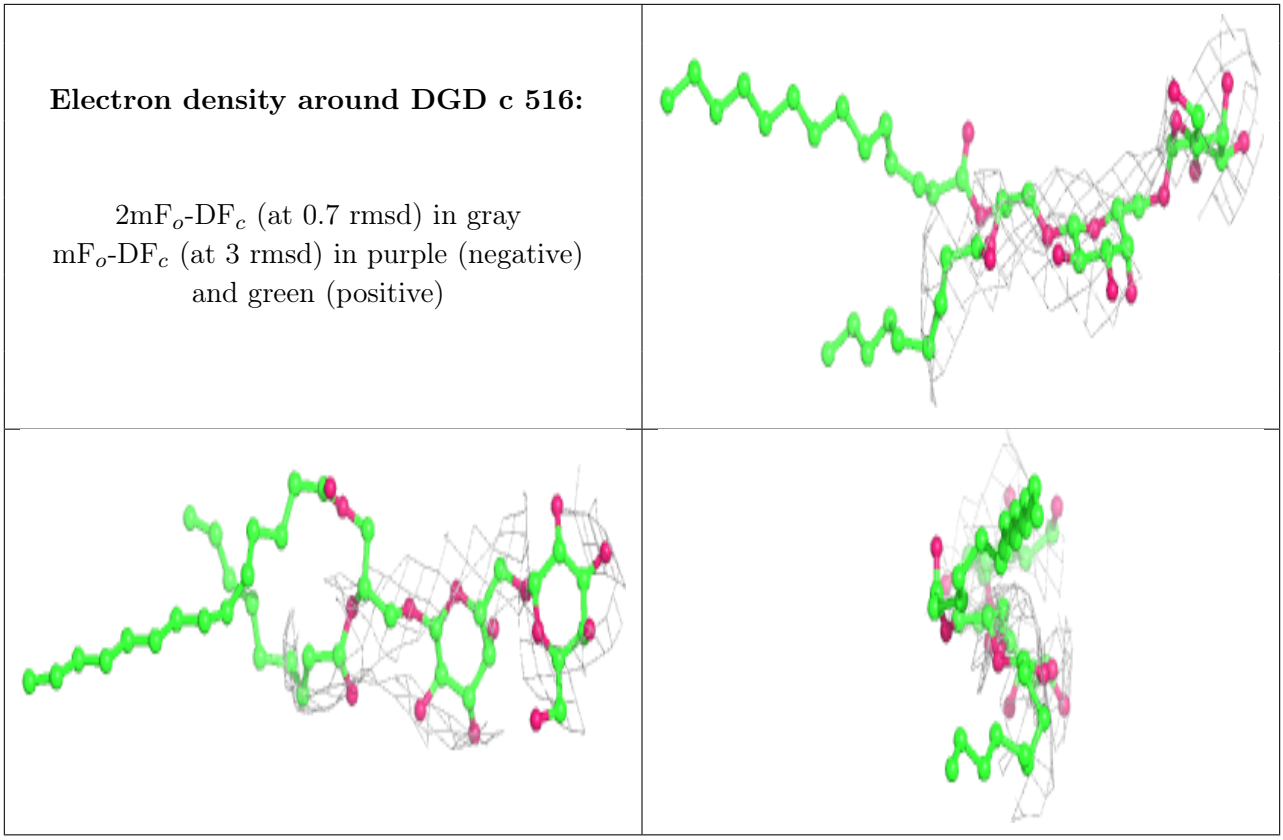






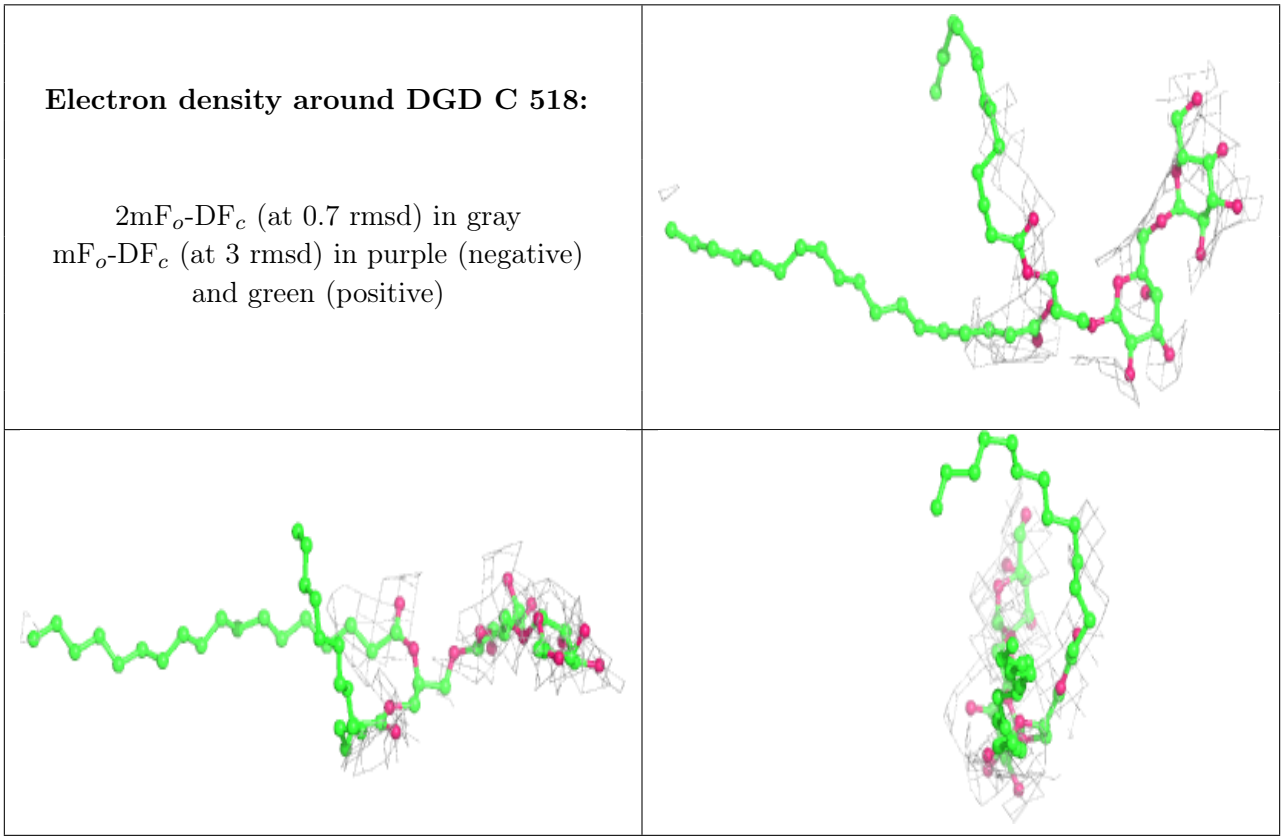
Electron density around DGD c 516:

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



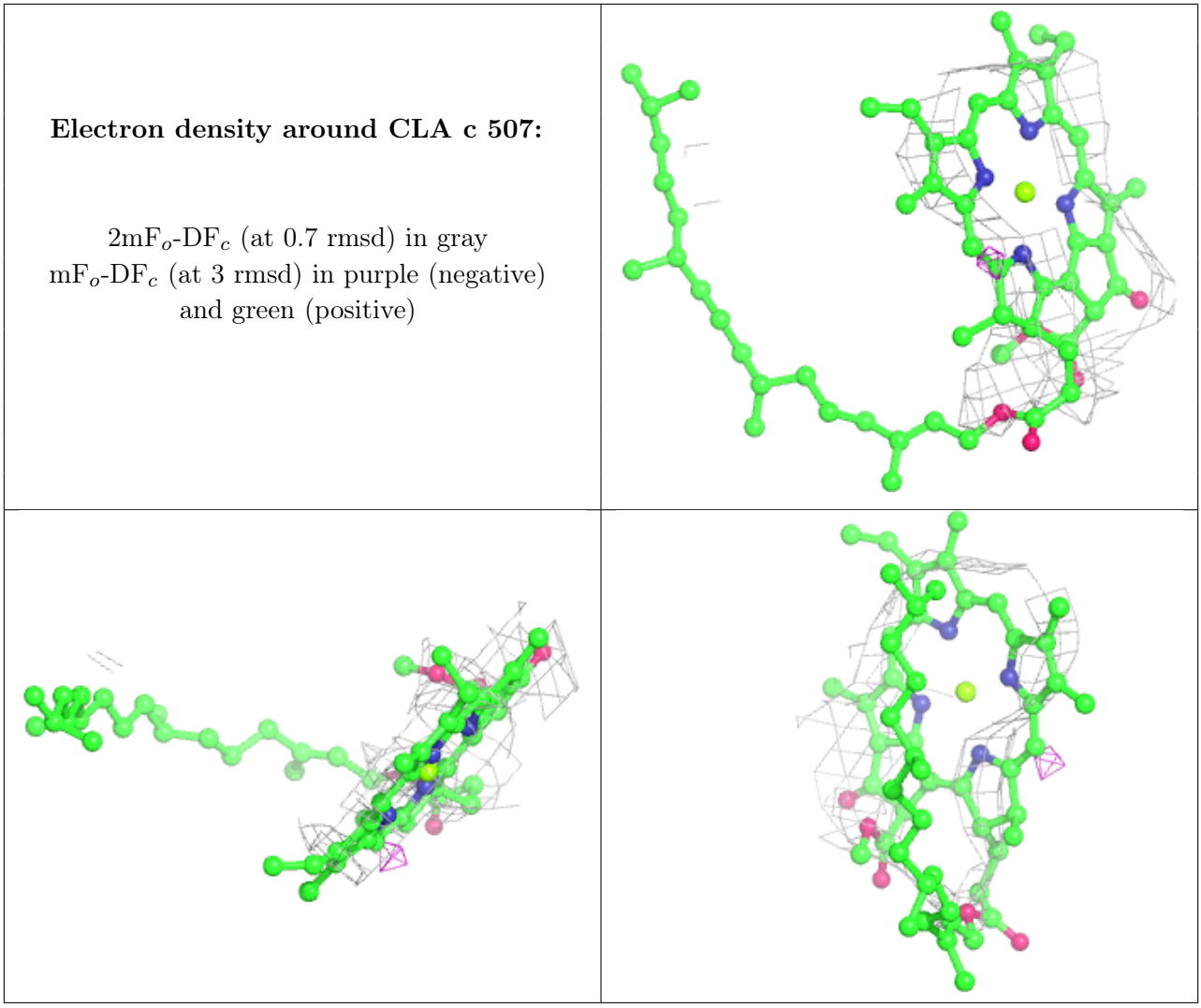
Electron density around DGD C 518:

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



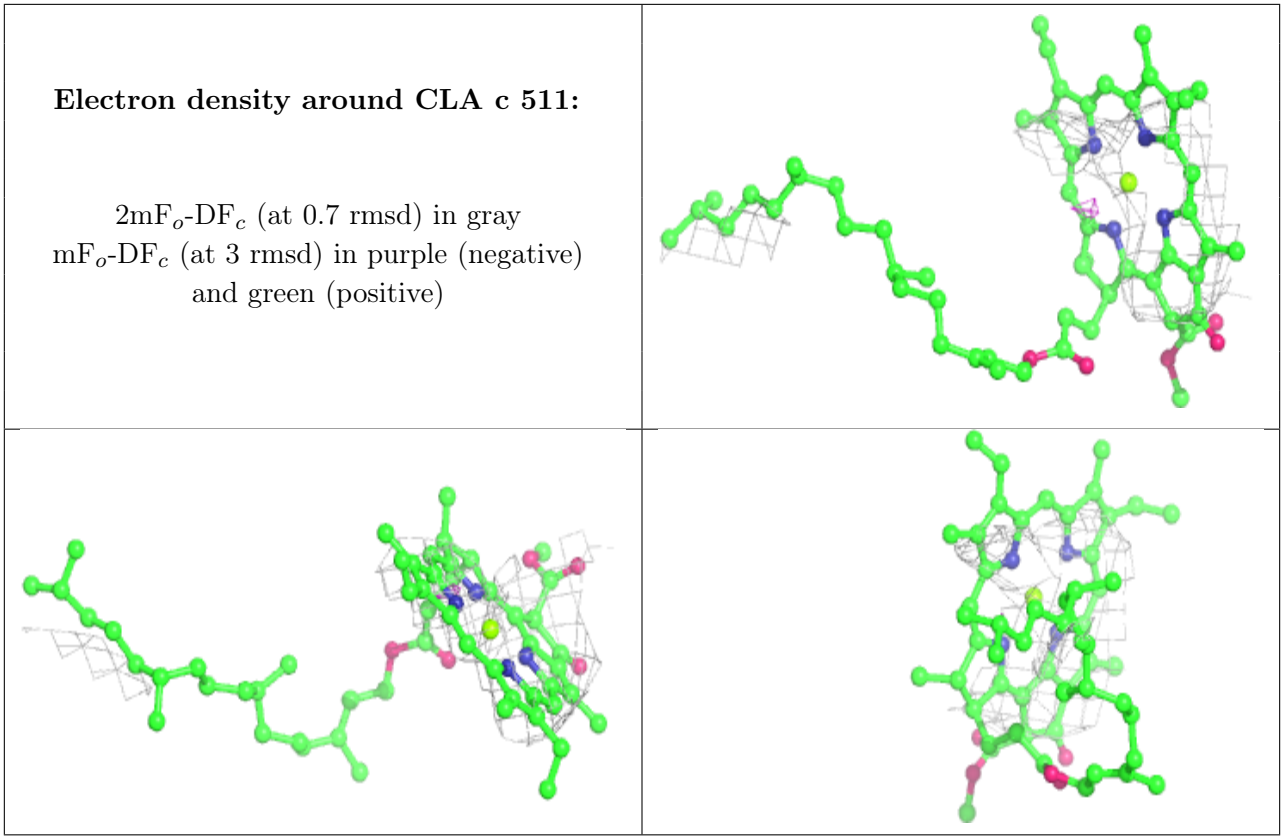
Electron density around CLA c 507:

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



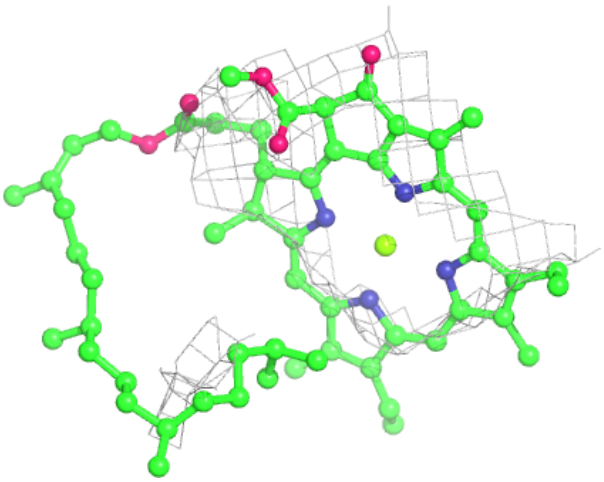
Electron density around CLA c 511:

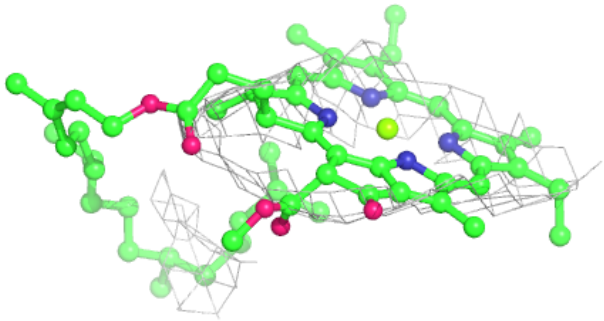
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

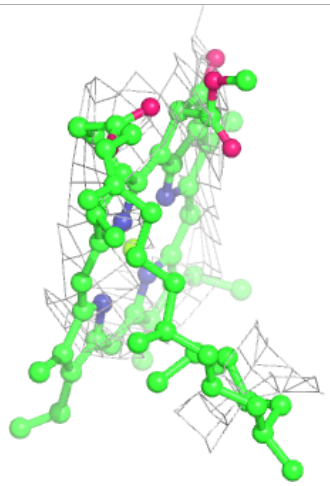


Electron density around CLA B 615:

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

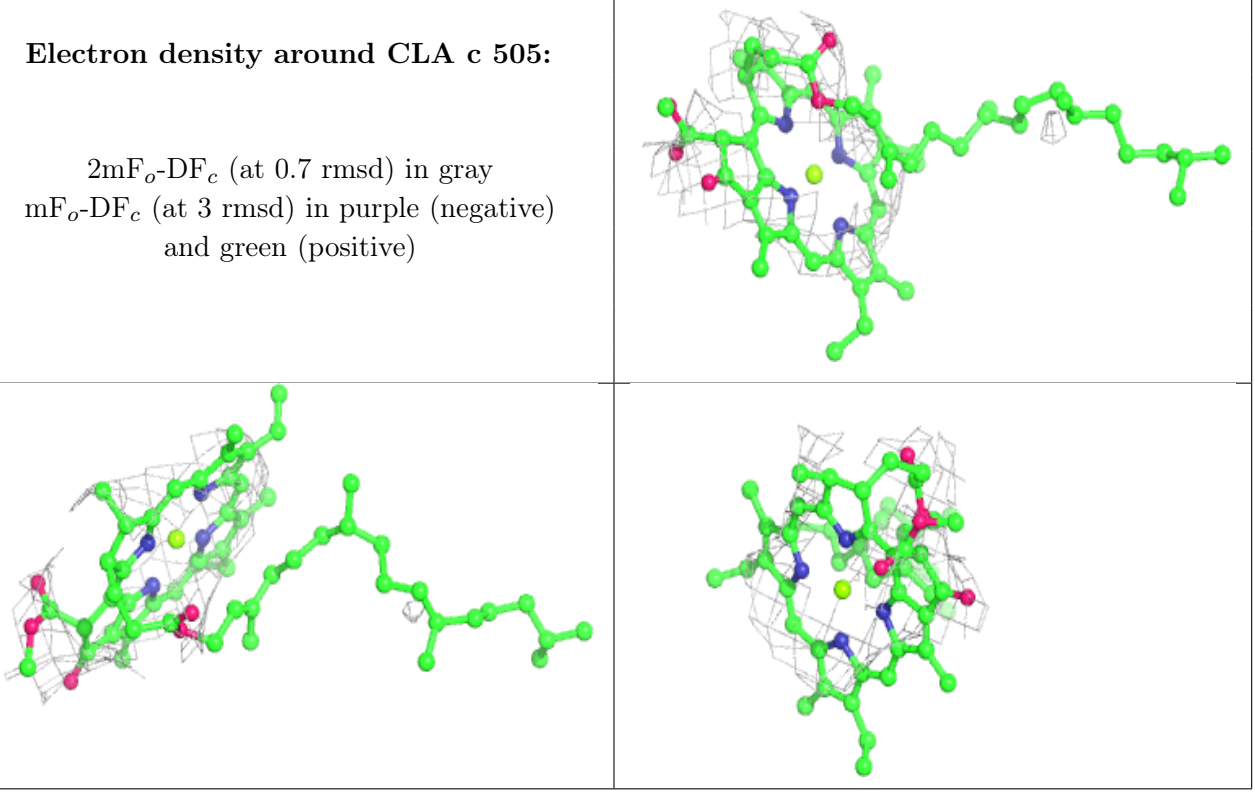






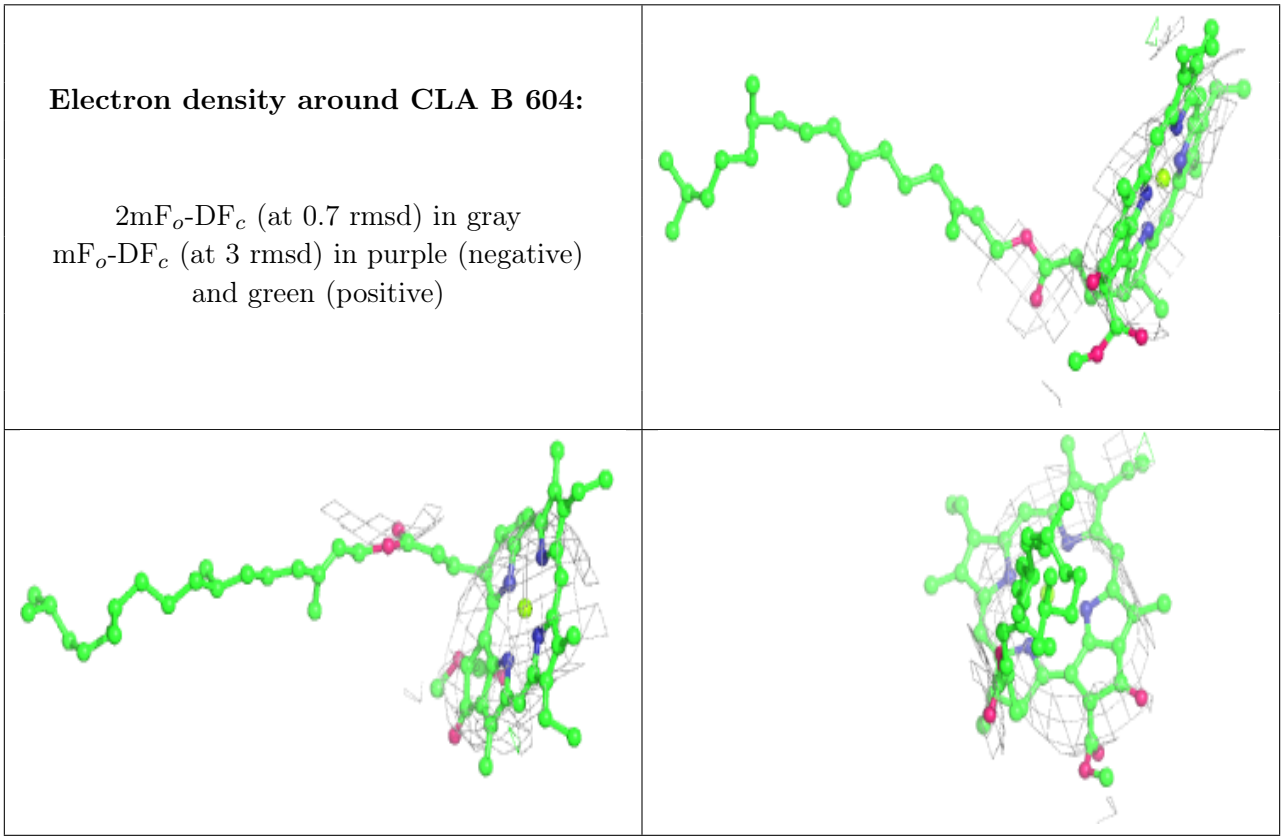
Electron density around CLA c 505:

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



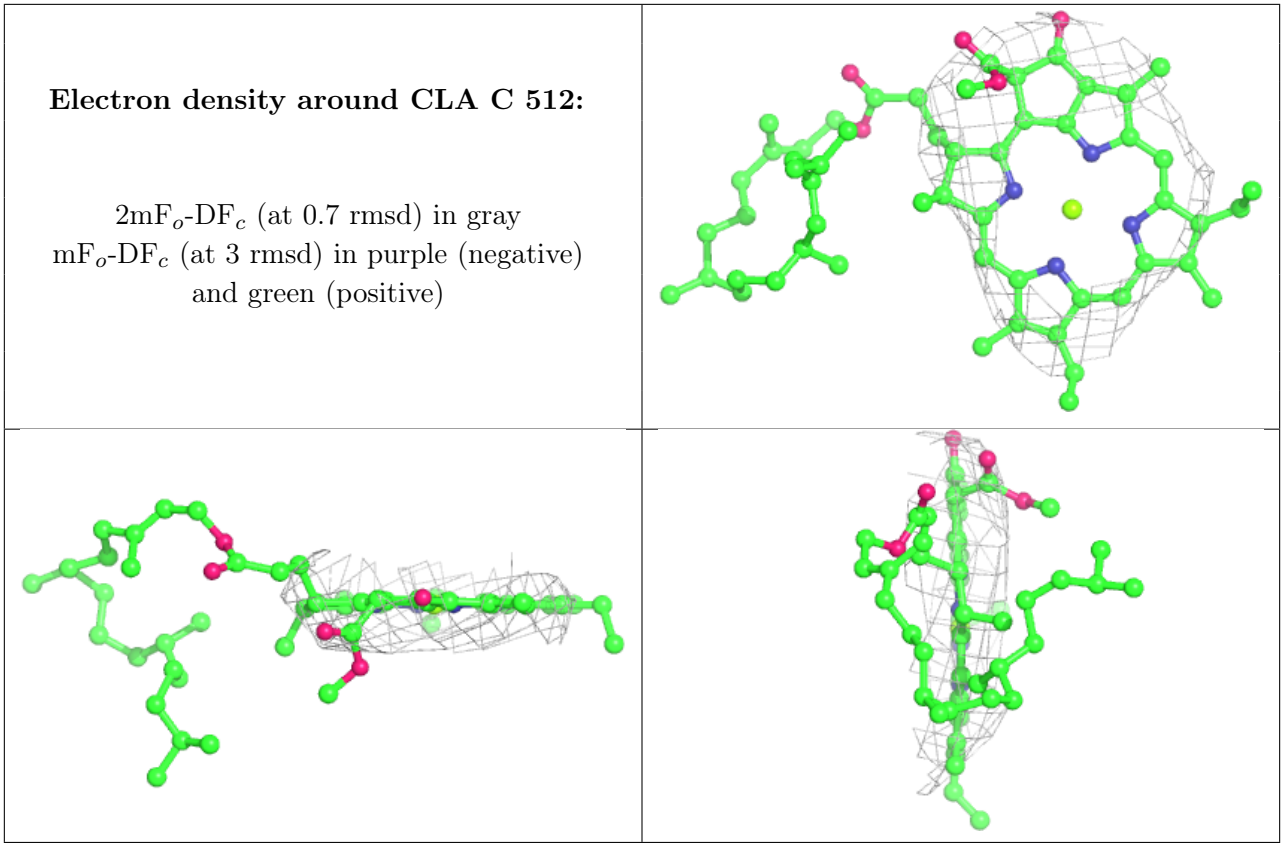
Electron density around CLA B 604:

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



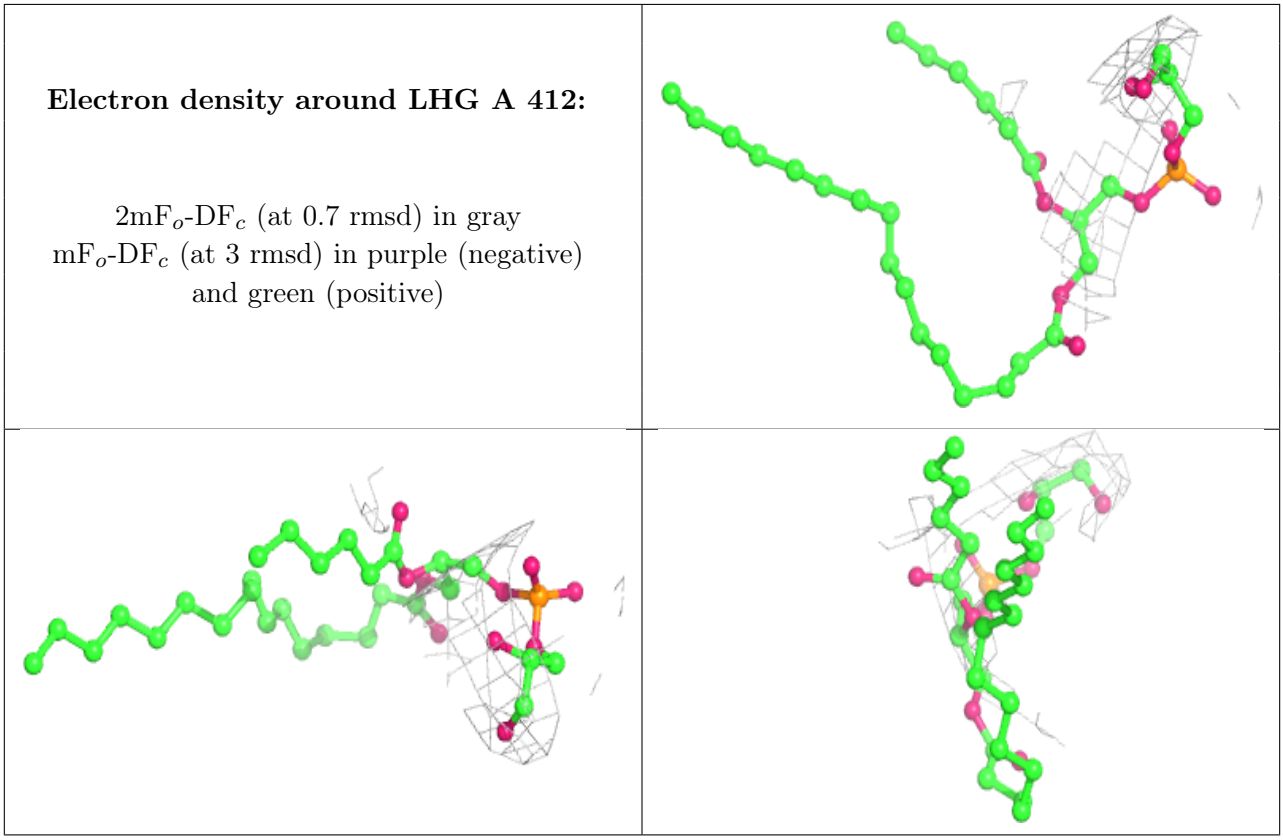
Electron density around CLA C 512:

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



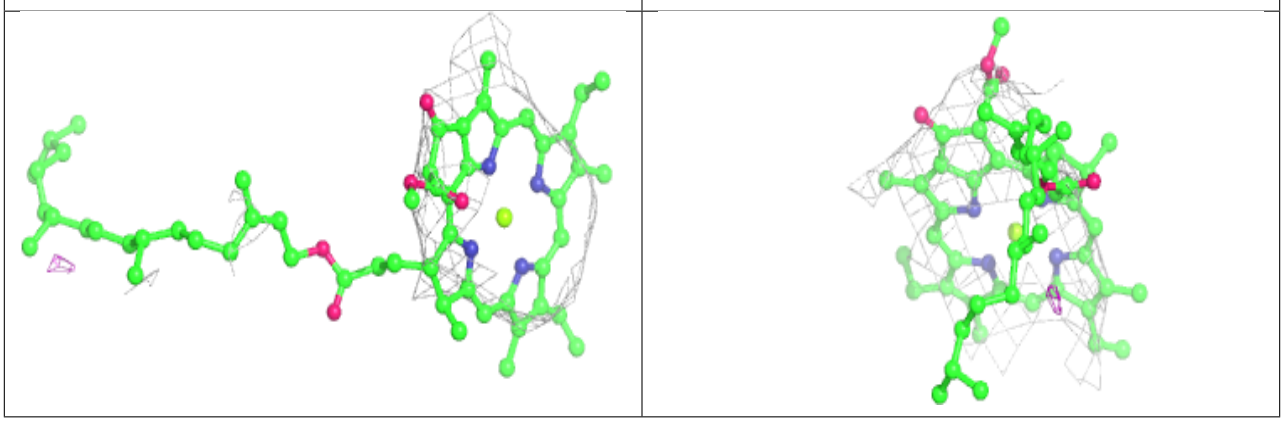
Electron density around LHG A 412:

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



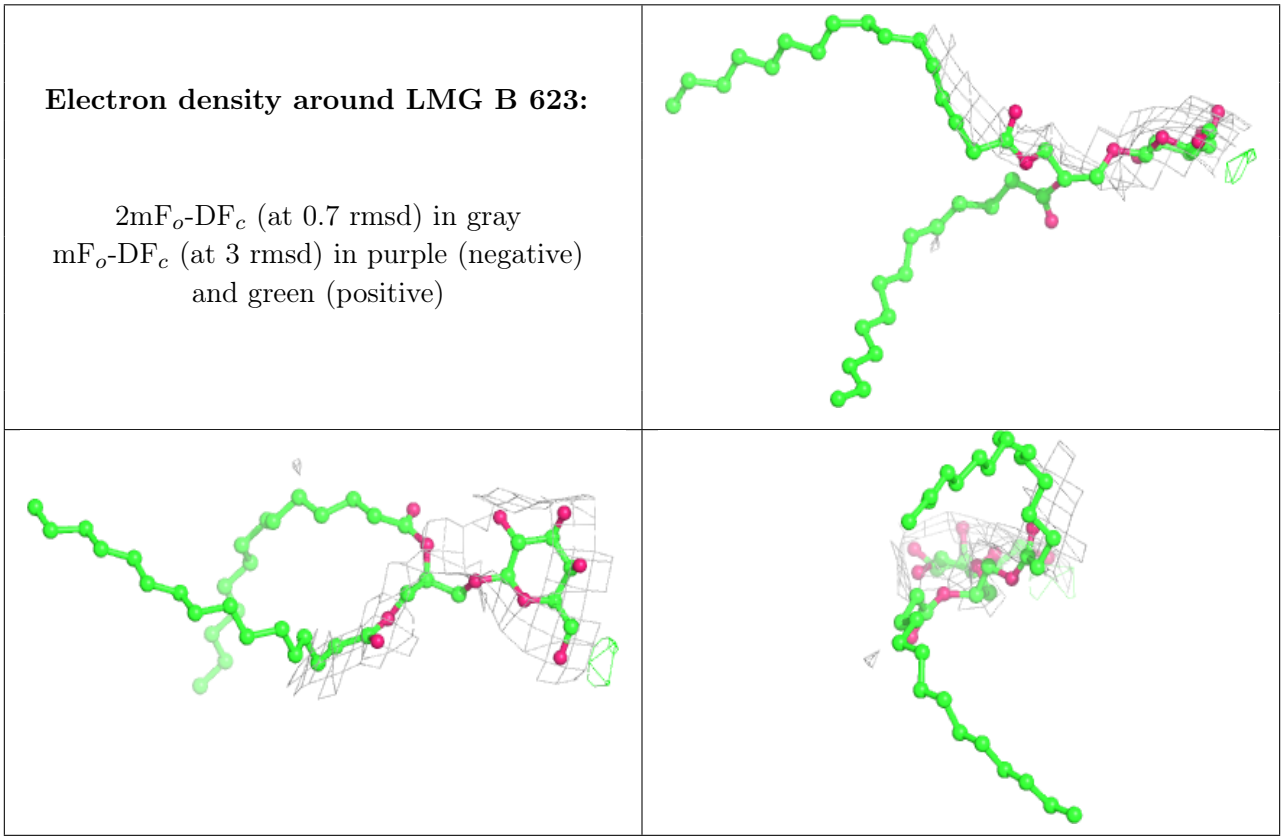
Electron density around CLA d 402:

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



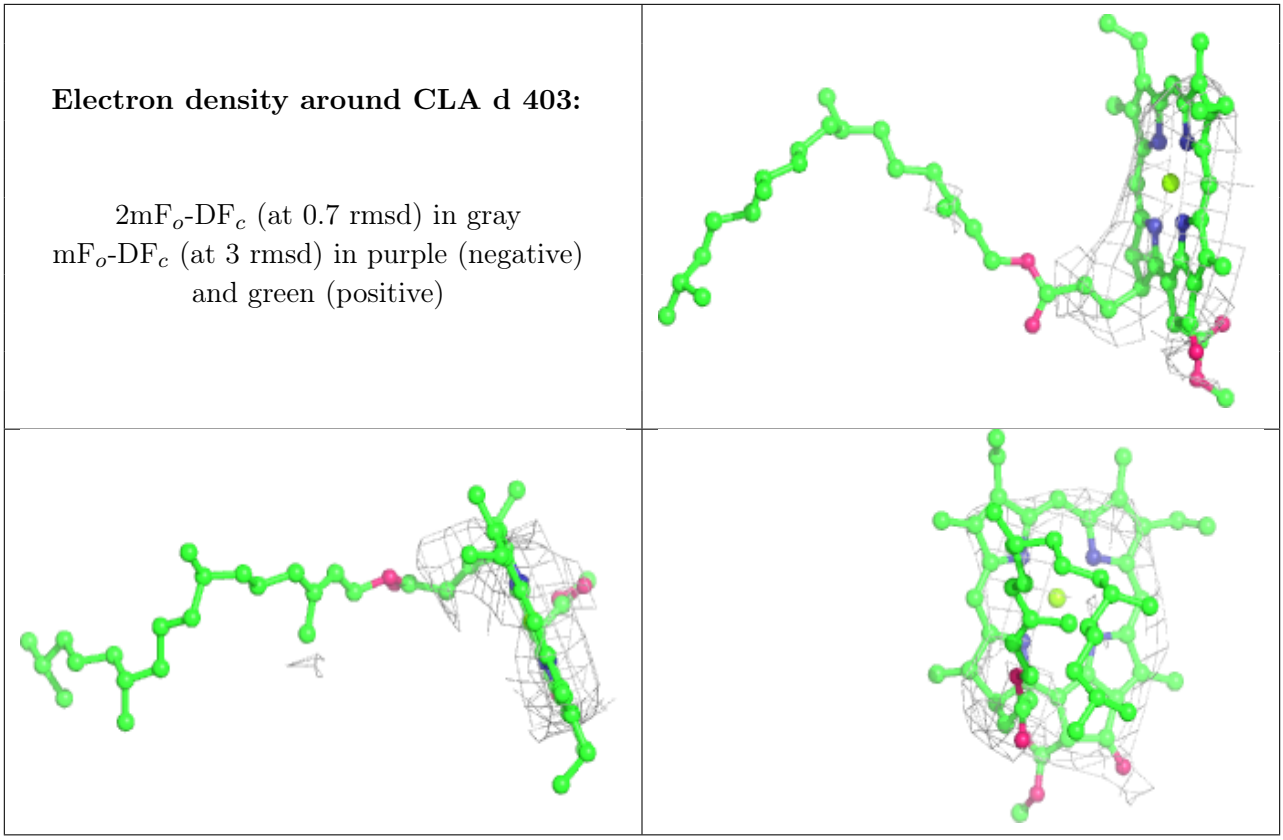
Electron density around LMG B 623:

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



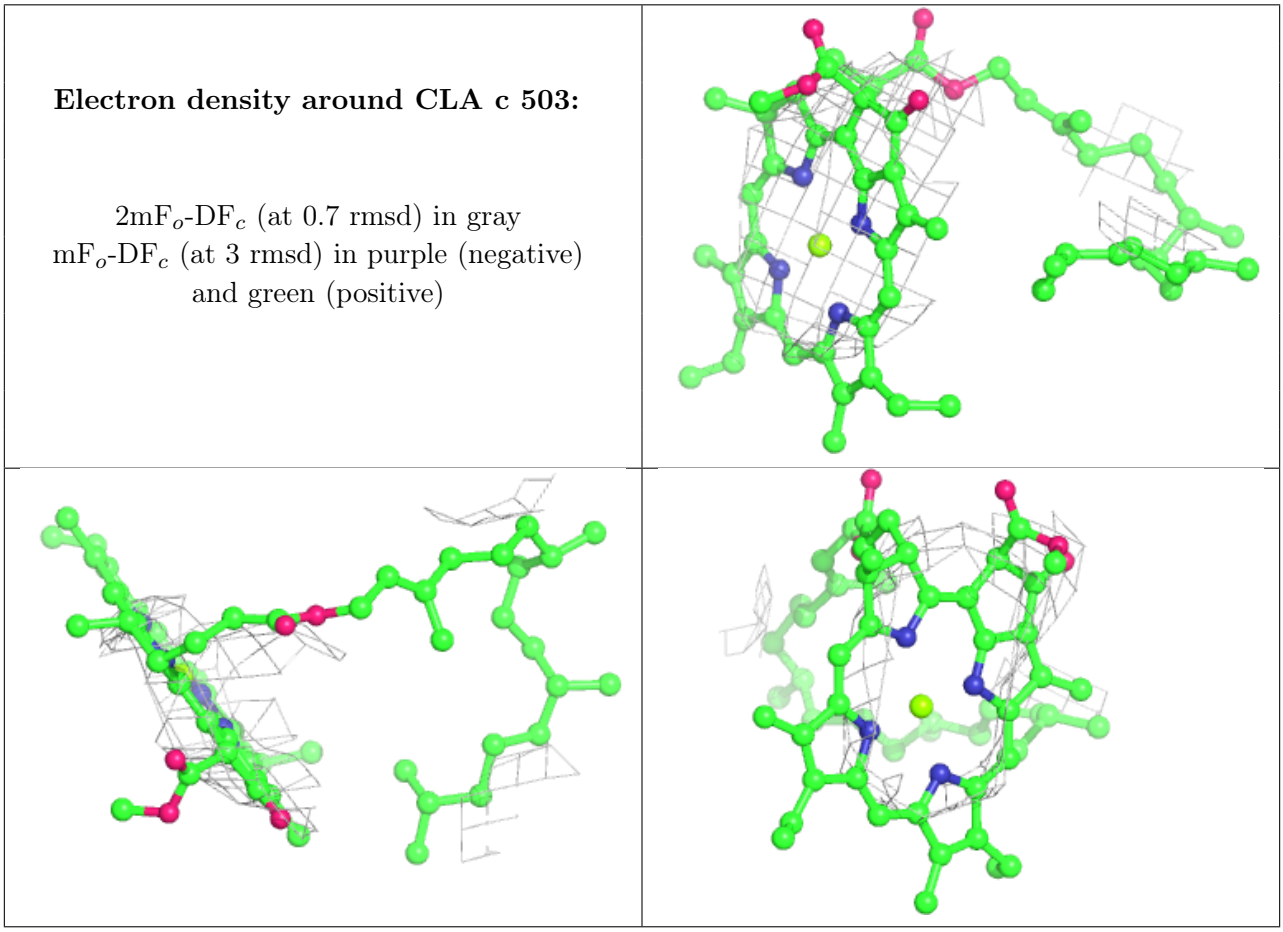
Electron density around CLA d 403:

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



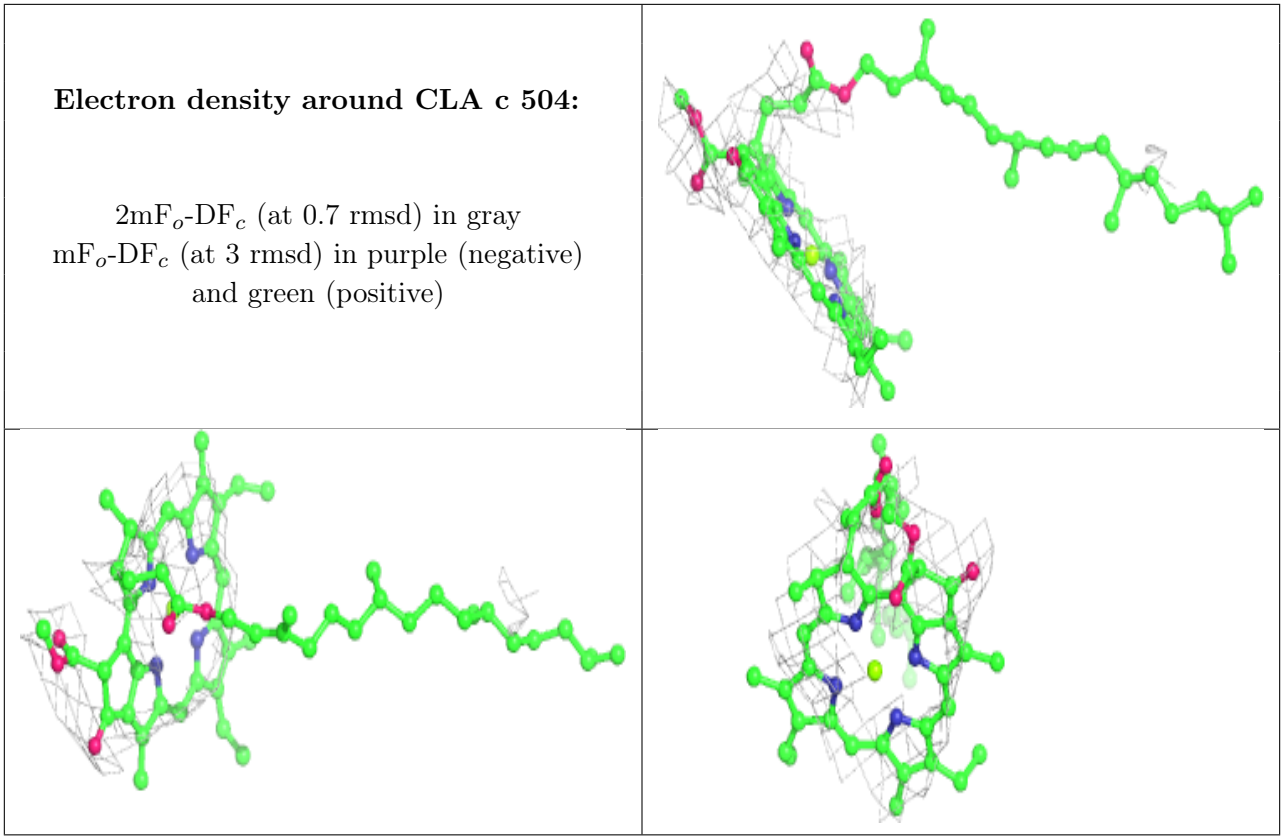
Electron density around CLA c 503:

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



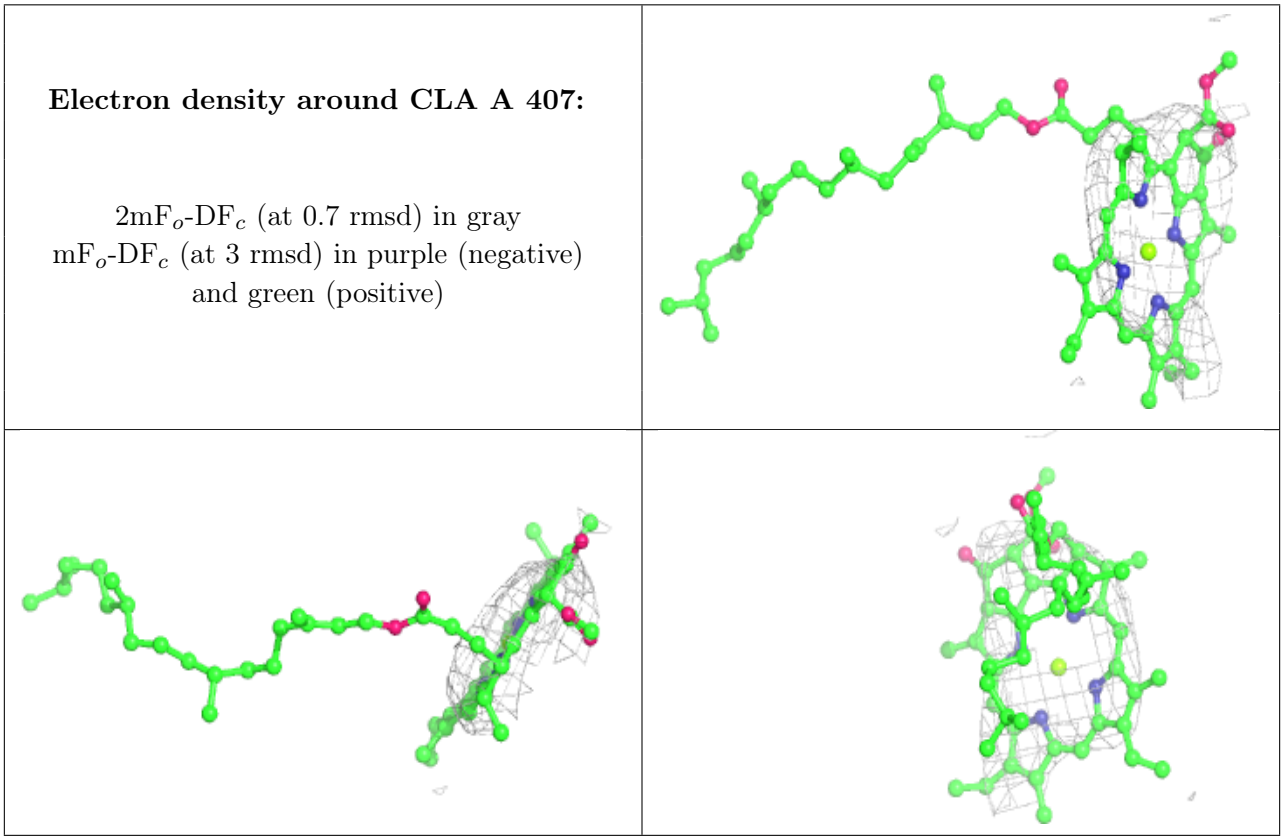
Electron density around CLA c 504:

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



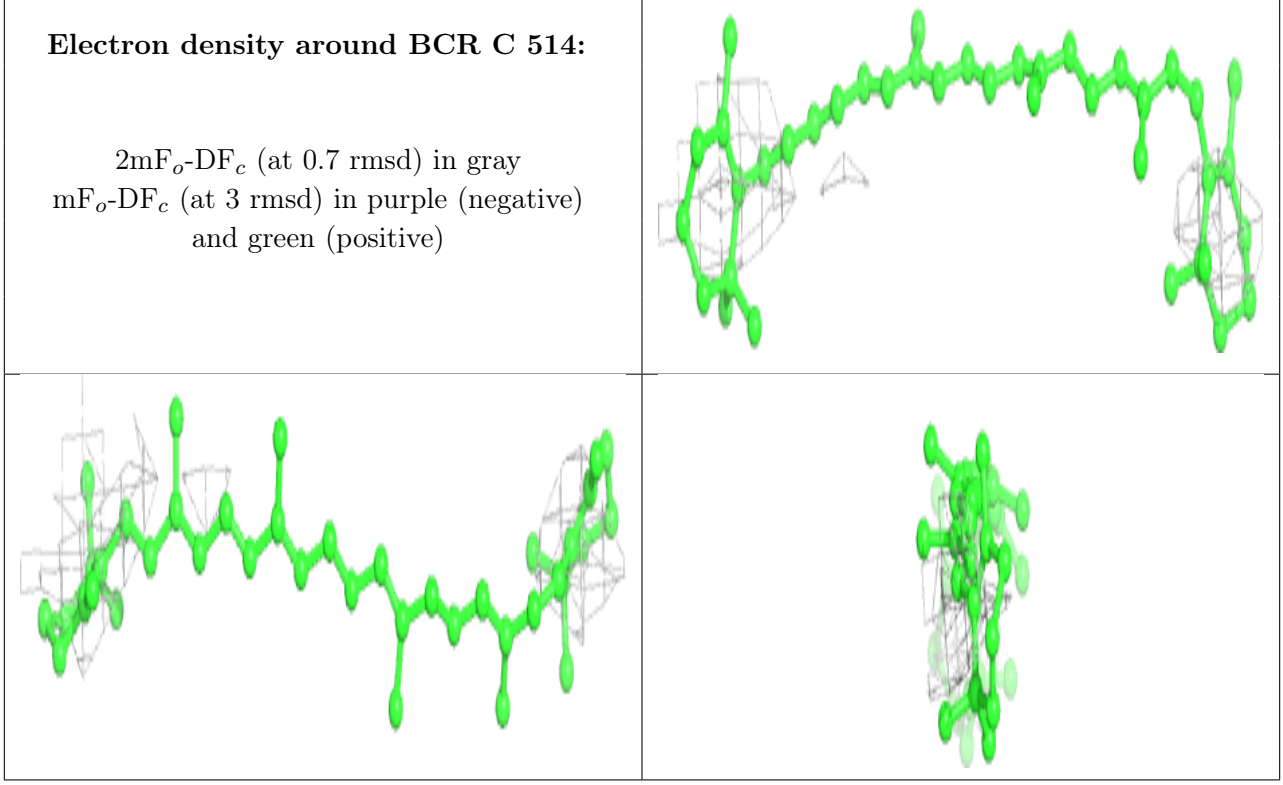
Electron density around CLA A 407:

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



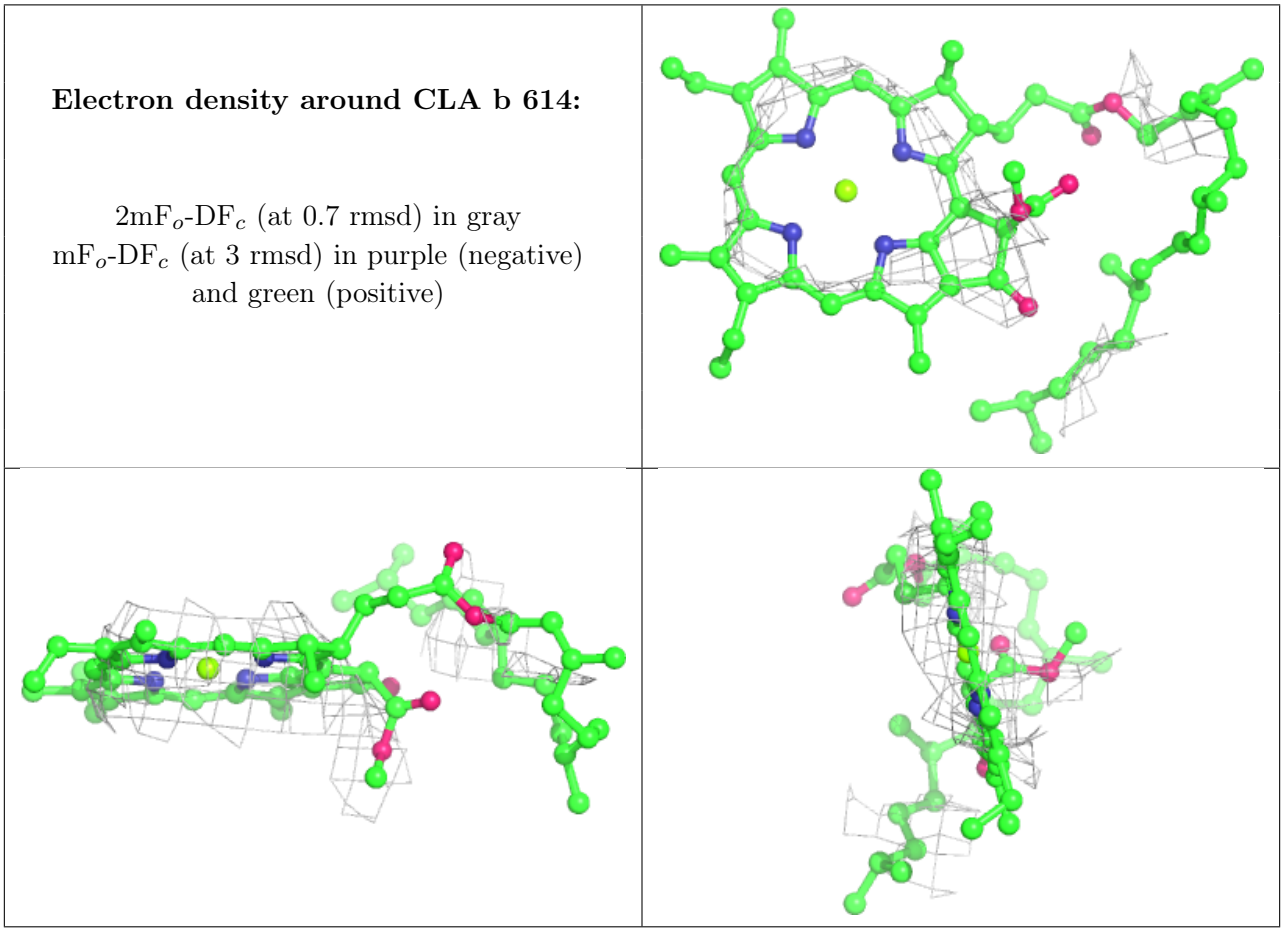
Electron density around BCR C 514:

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



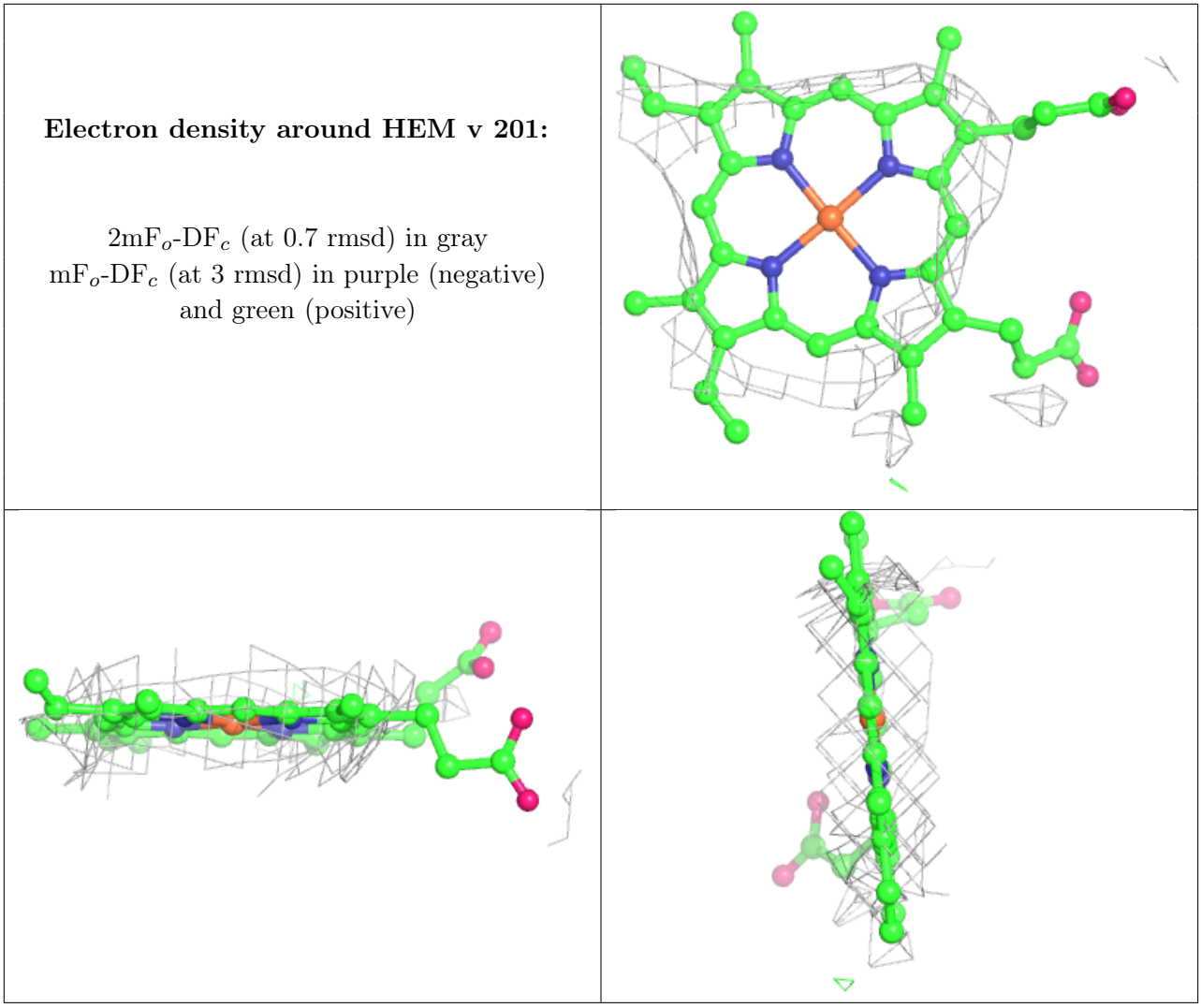
Electron density around CLA b 614:

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



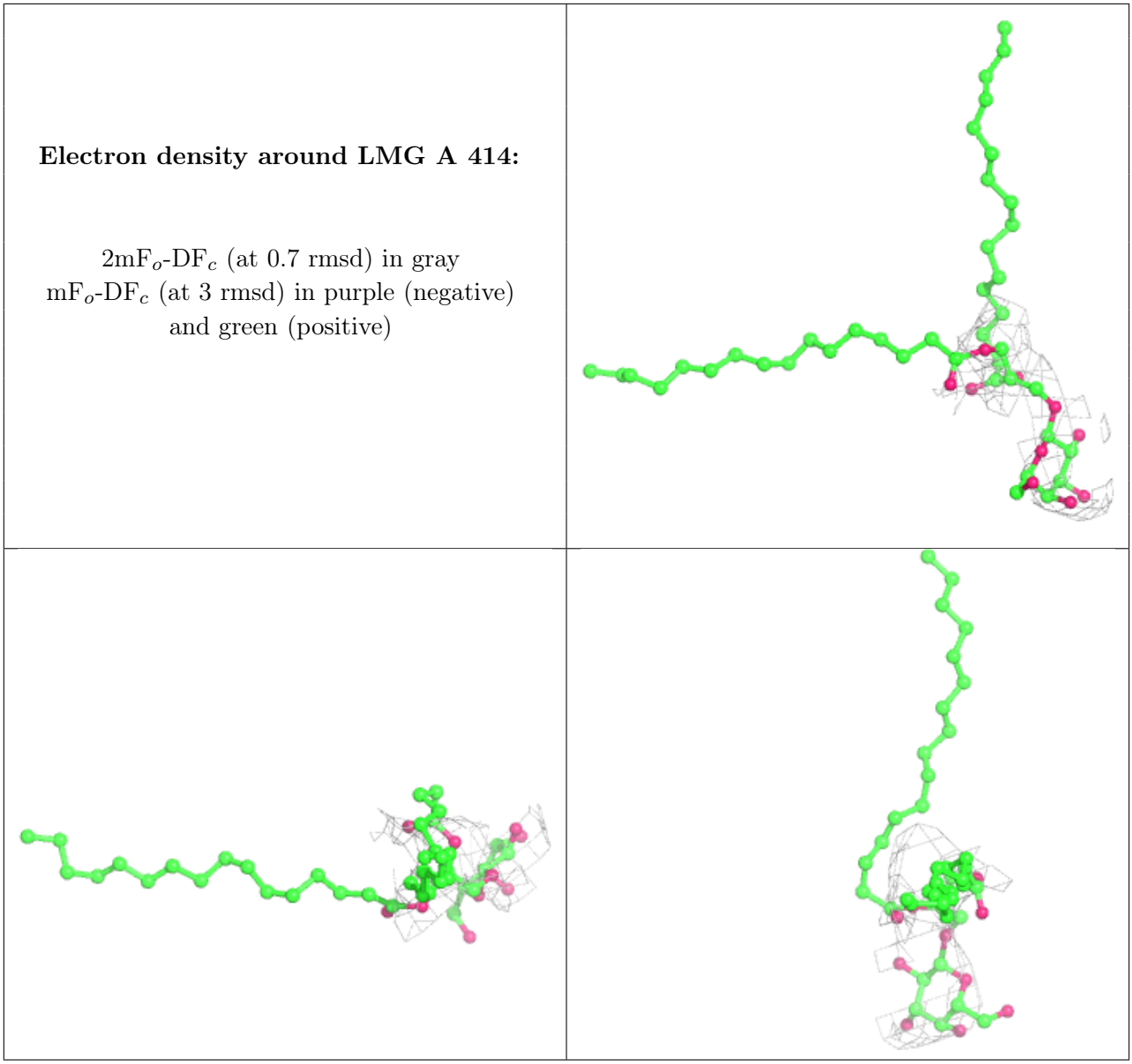
Electron density around HEM v 201:

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



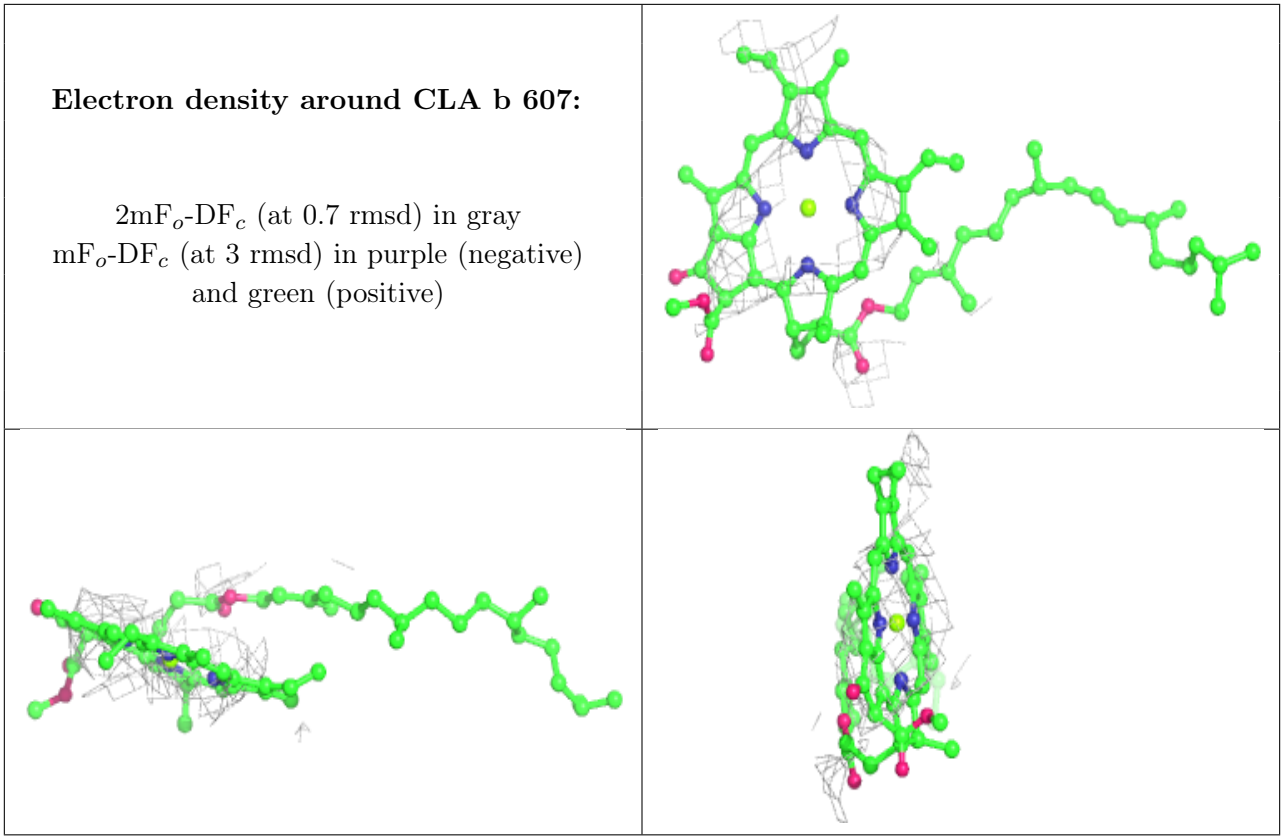
Electron density around LMG A 414:

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



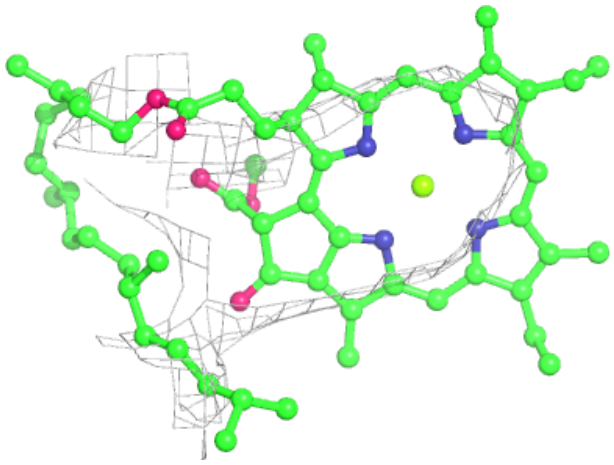
Electron density around CLA b 607:

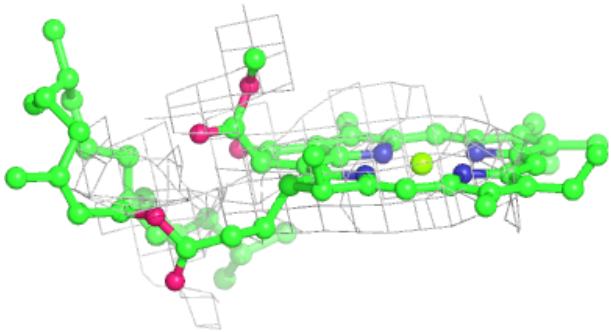
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

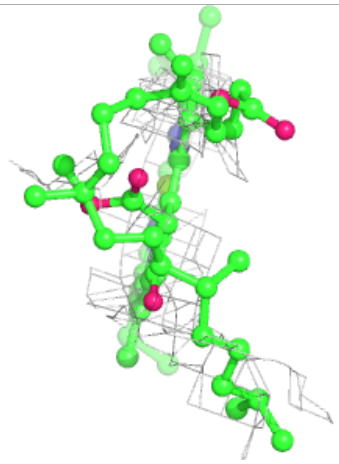


Electron density around CLA B 610:

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

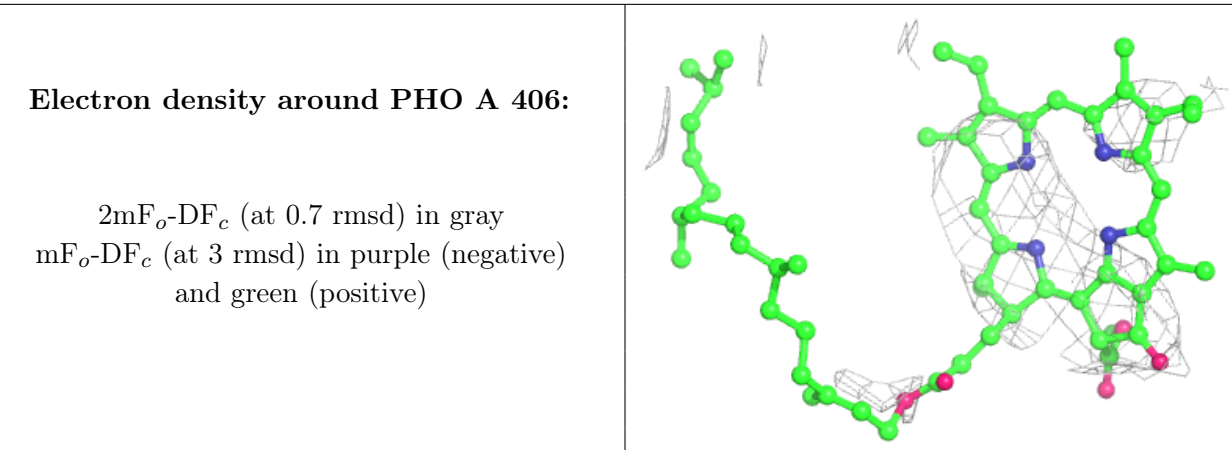






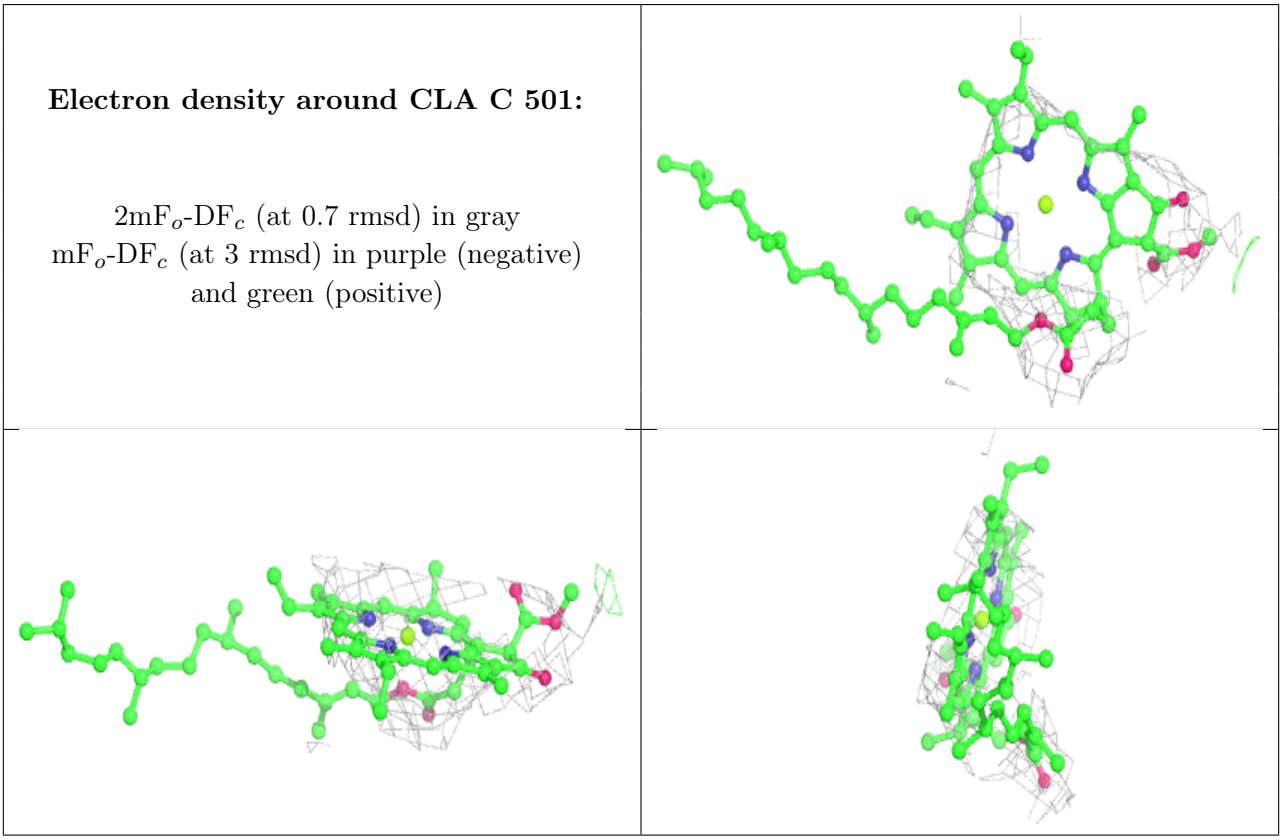
Electron density around PHO A 406:

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



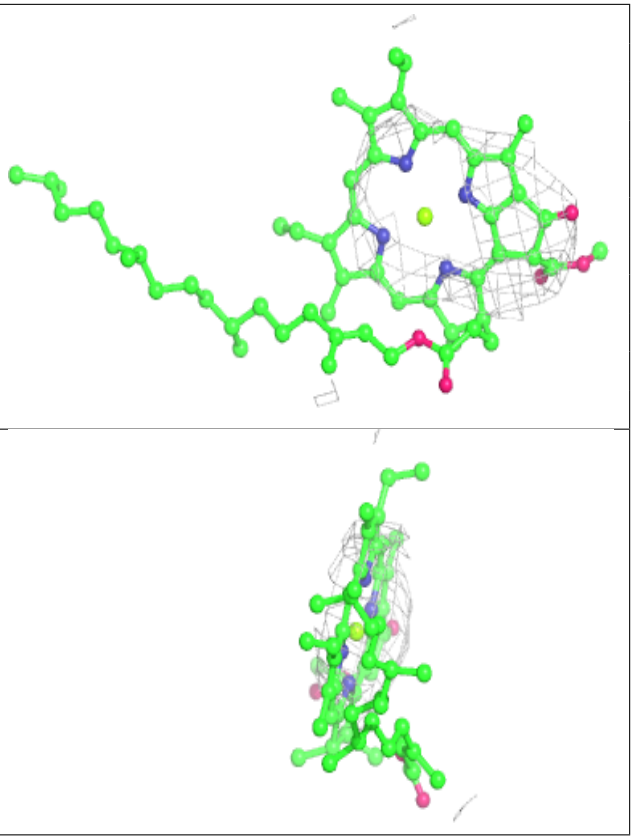
Electron density around CLA C 501:

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



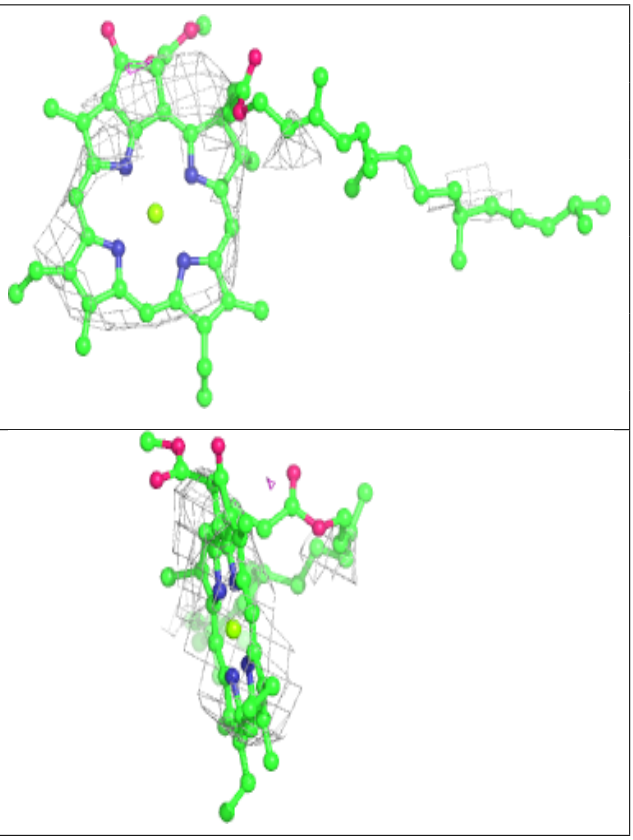
Electron density around CLA c 501:

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



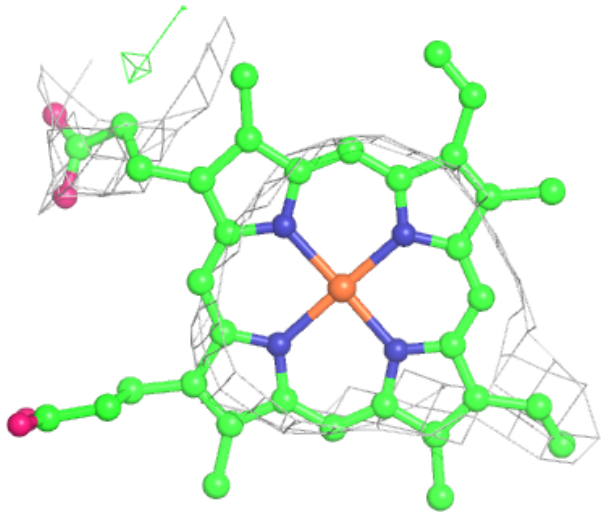
Electron density around CLA A 405:

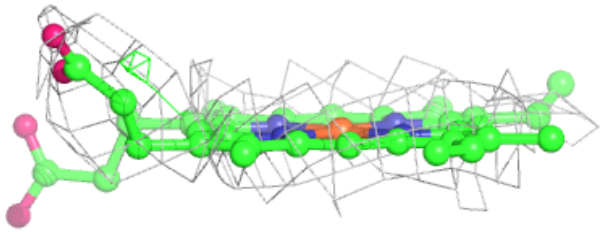
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

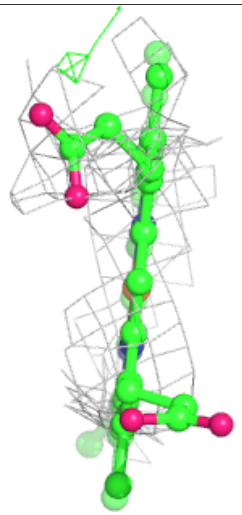


Electron density around HEM V 201:

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

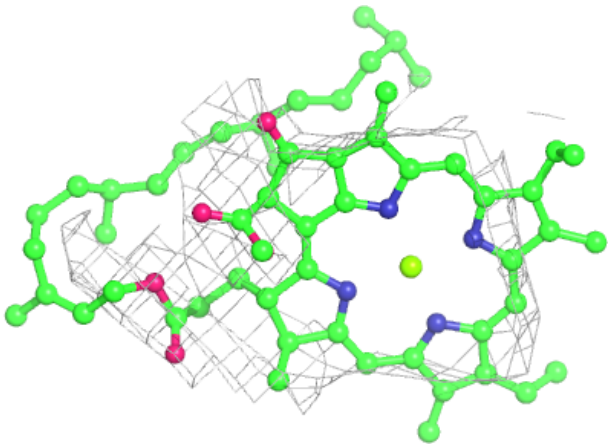


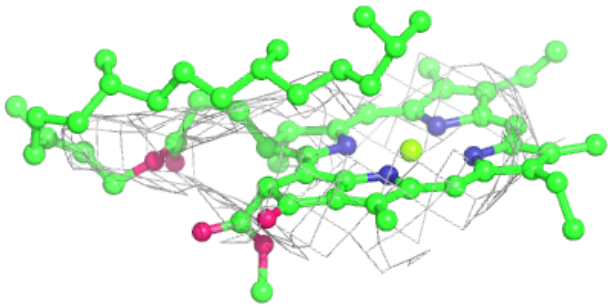


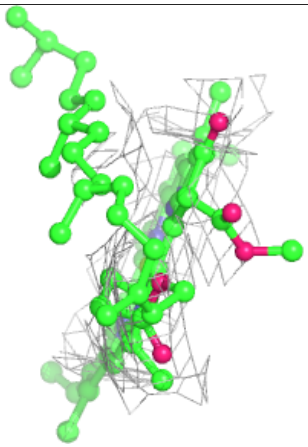


Electron density around CLA c 509:

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

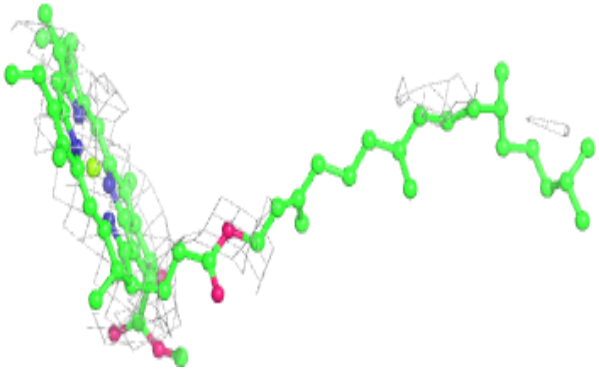


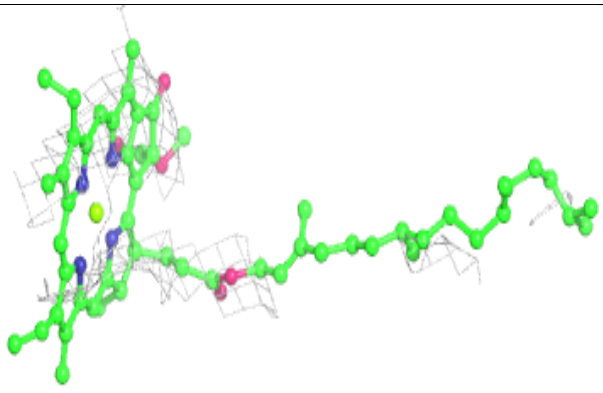


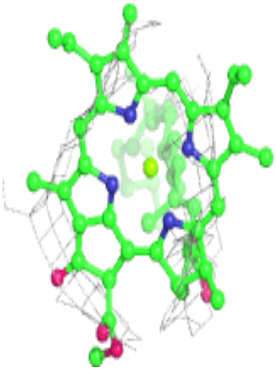


Electron density around CLA b 608:

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

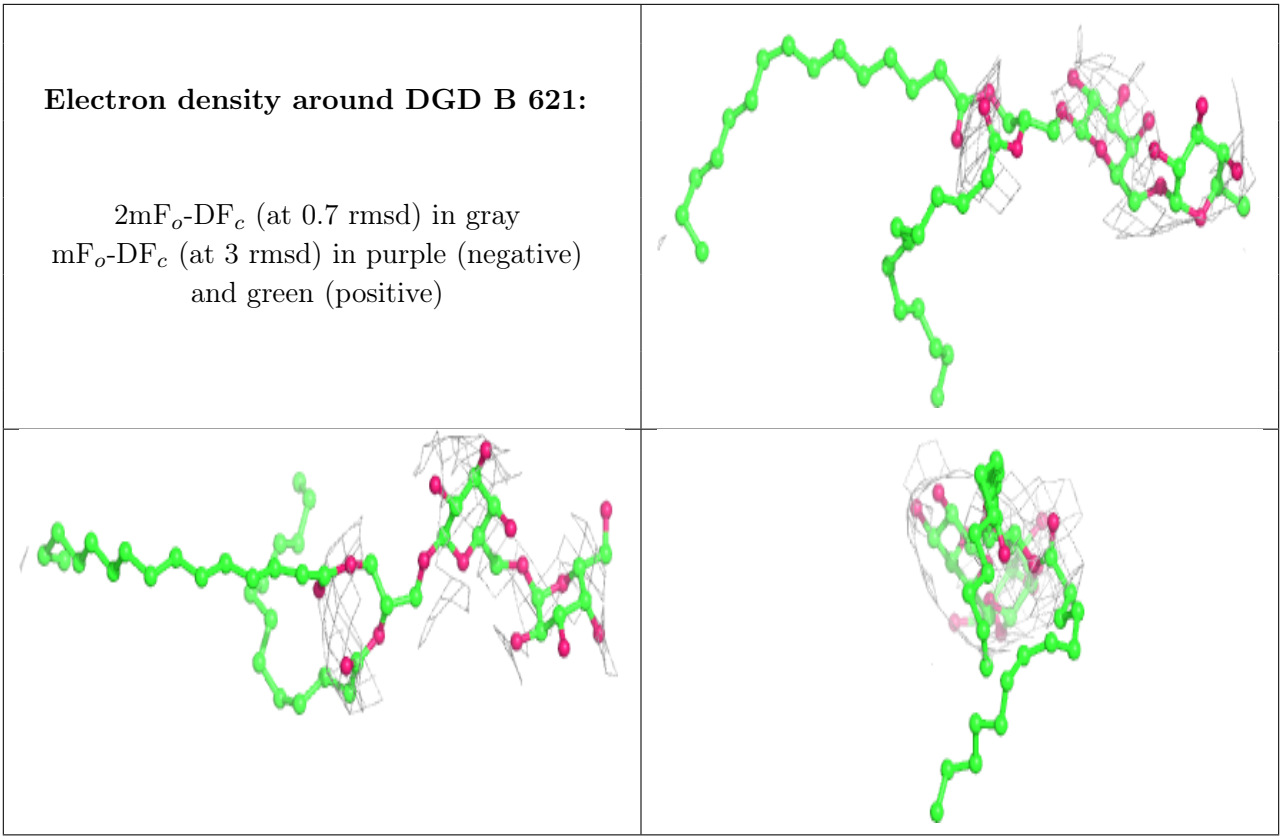






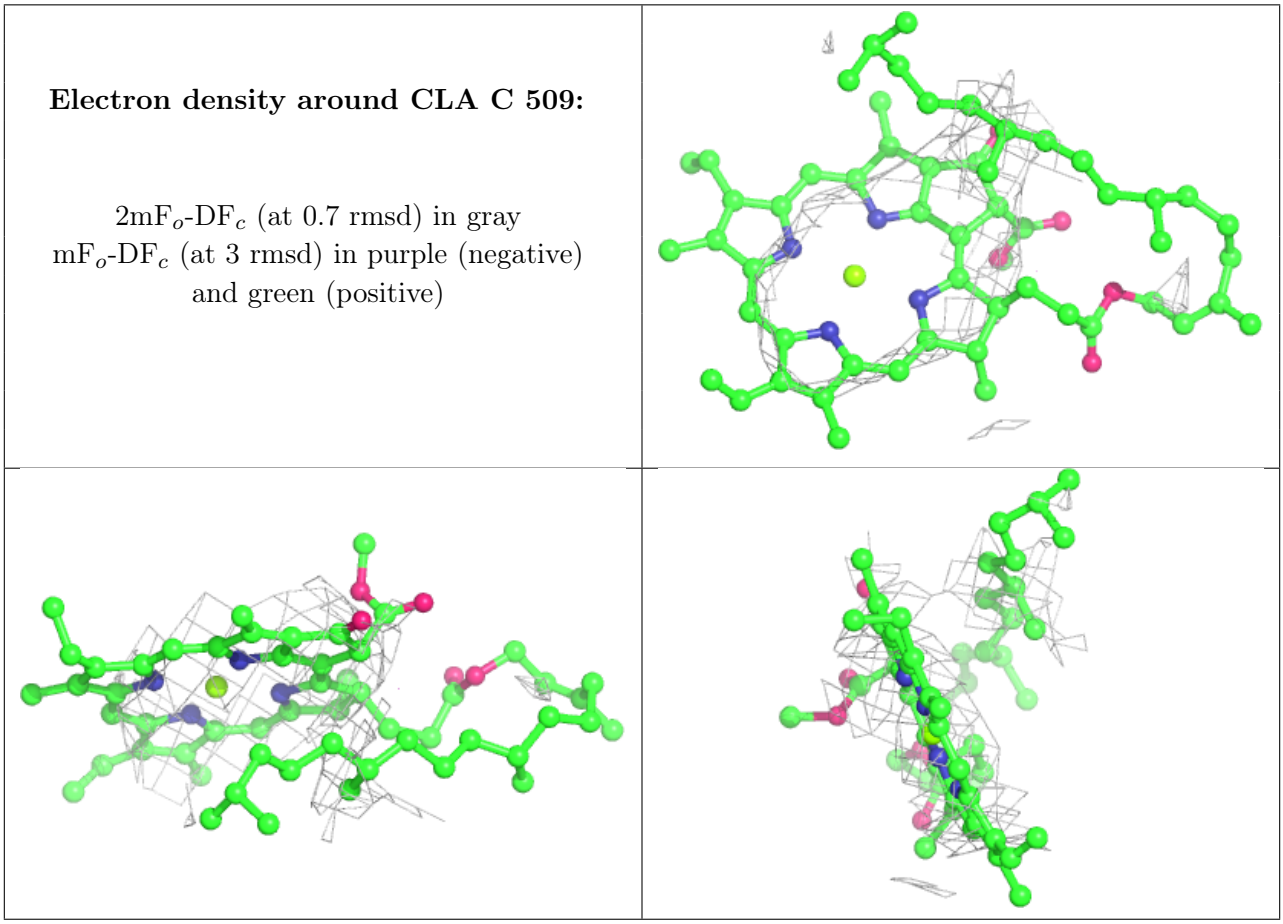
Electron density around DGD B 621:

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



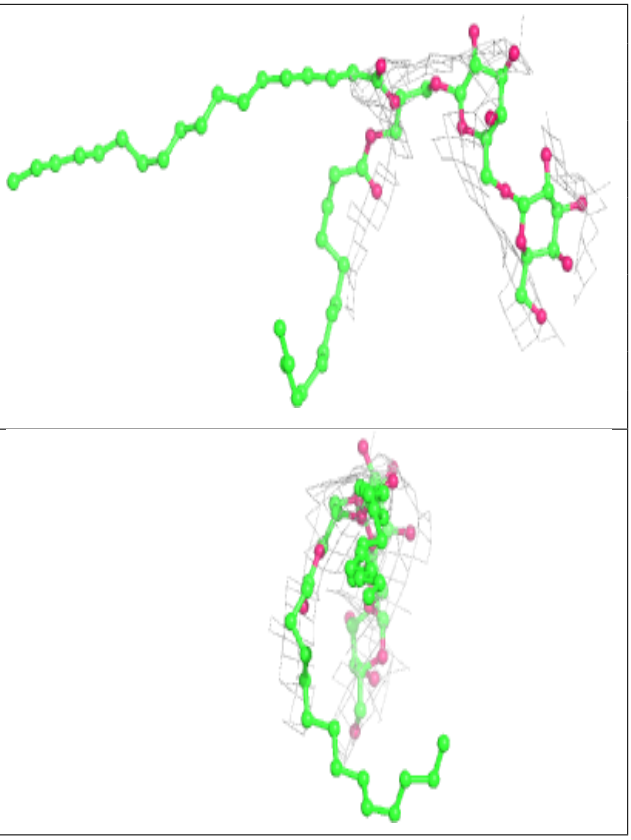
Electron density around CLA C 509:

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



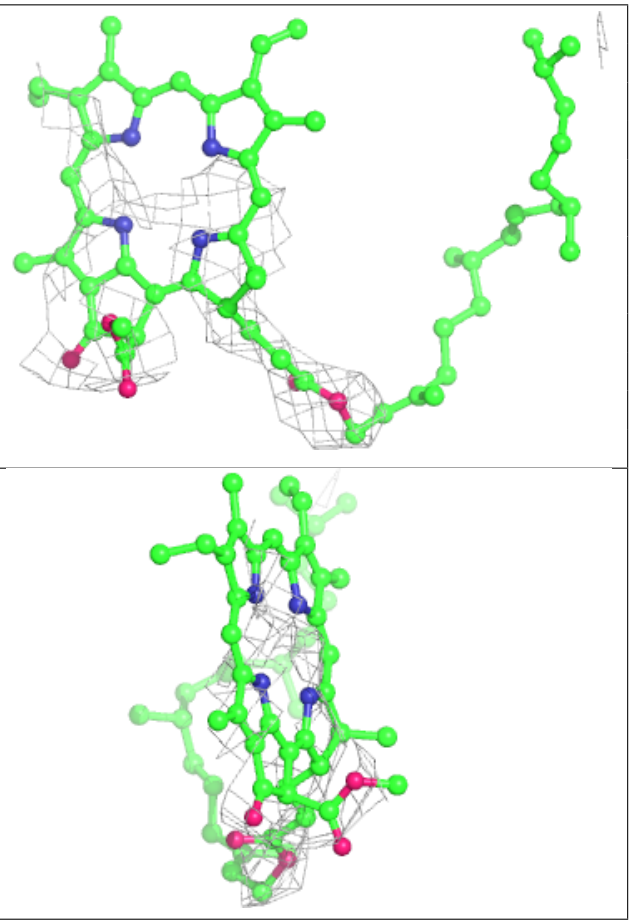
Electron density around DGD c 517:

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



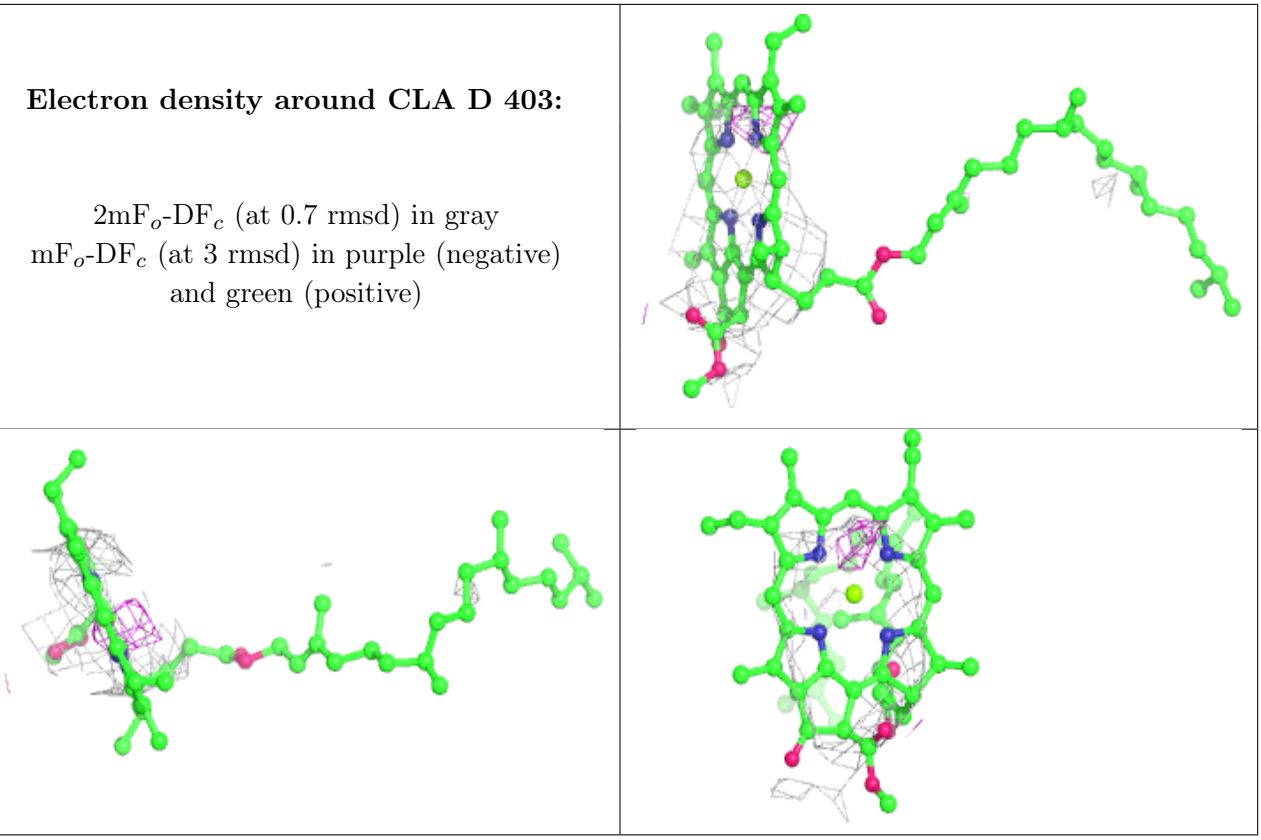
Electron density around PHO a 408:

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



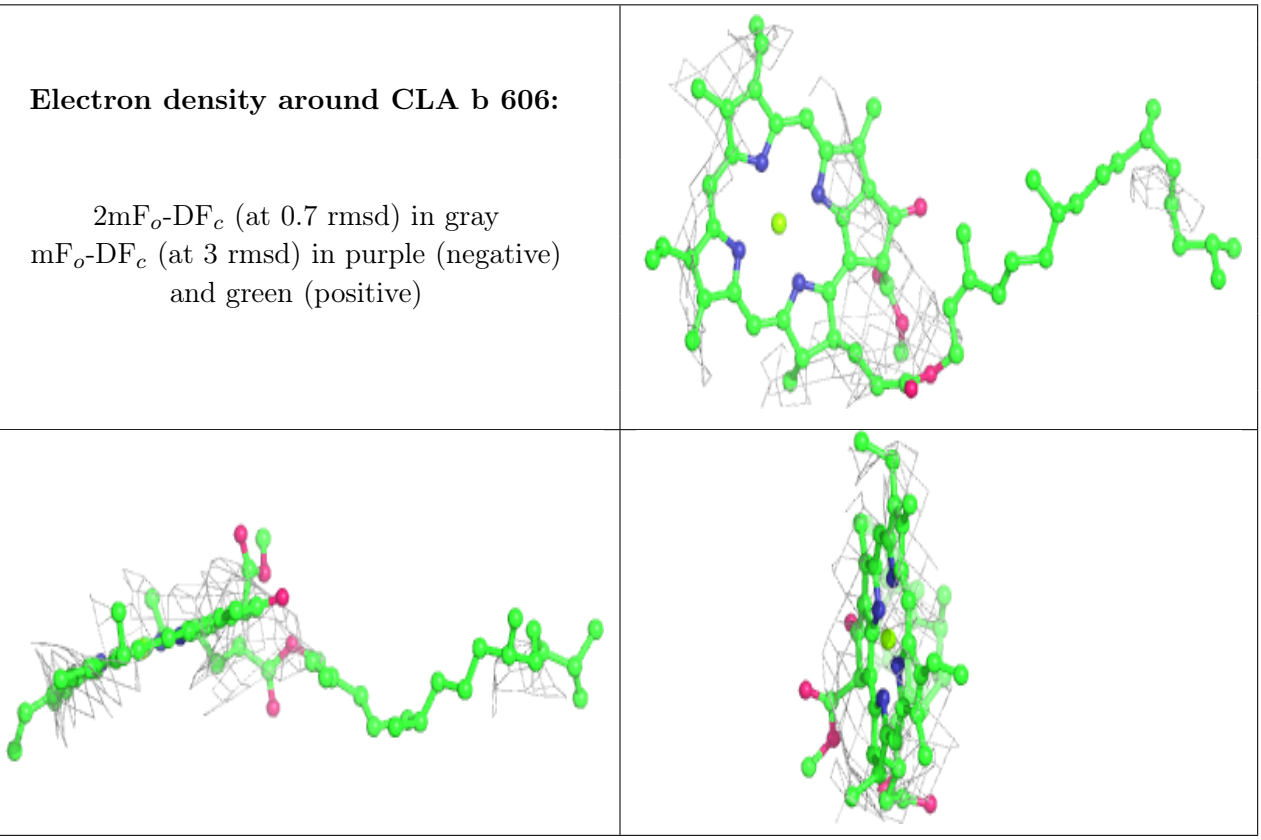
Electron density around CLA D 403:

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



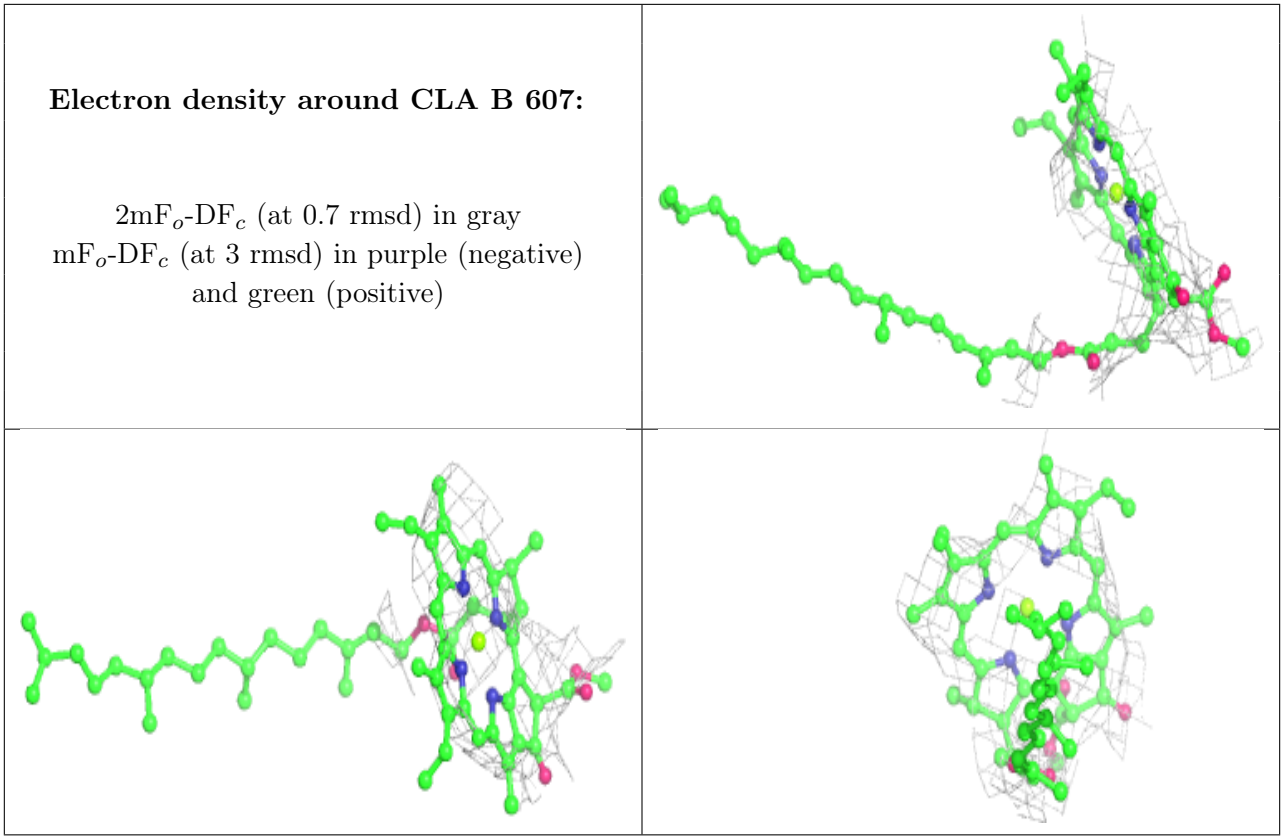
Electron density around CLA b 606:

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



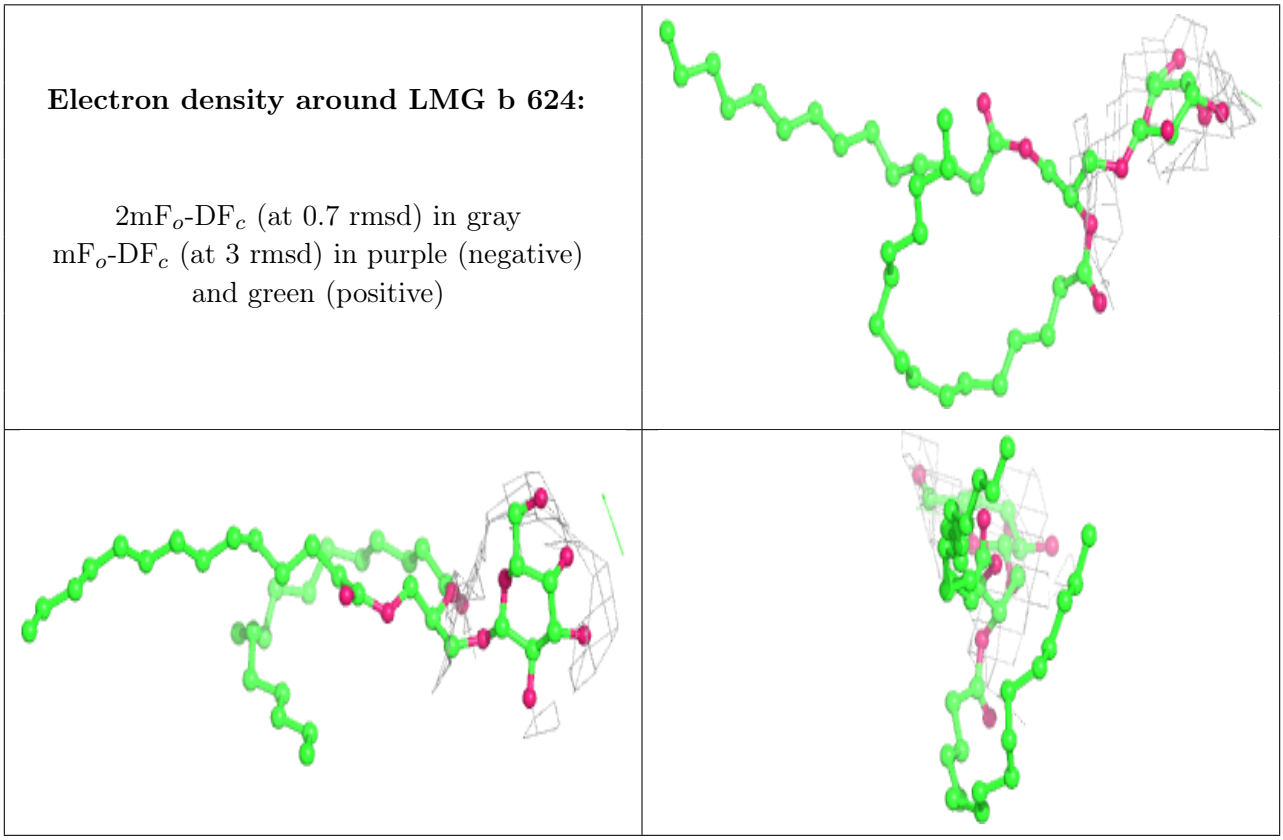
Electron density around CLA B 607:

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



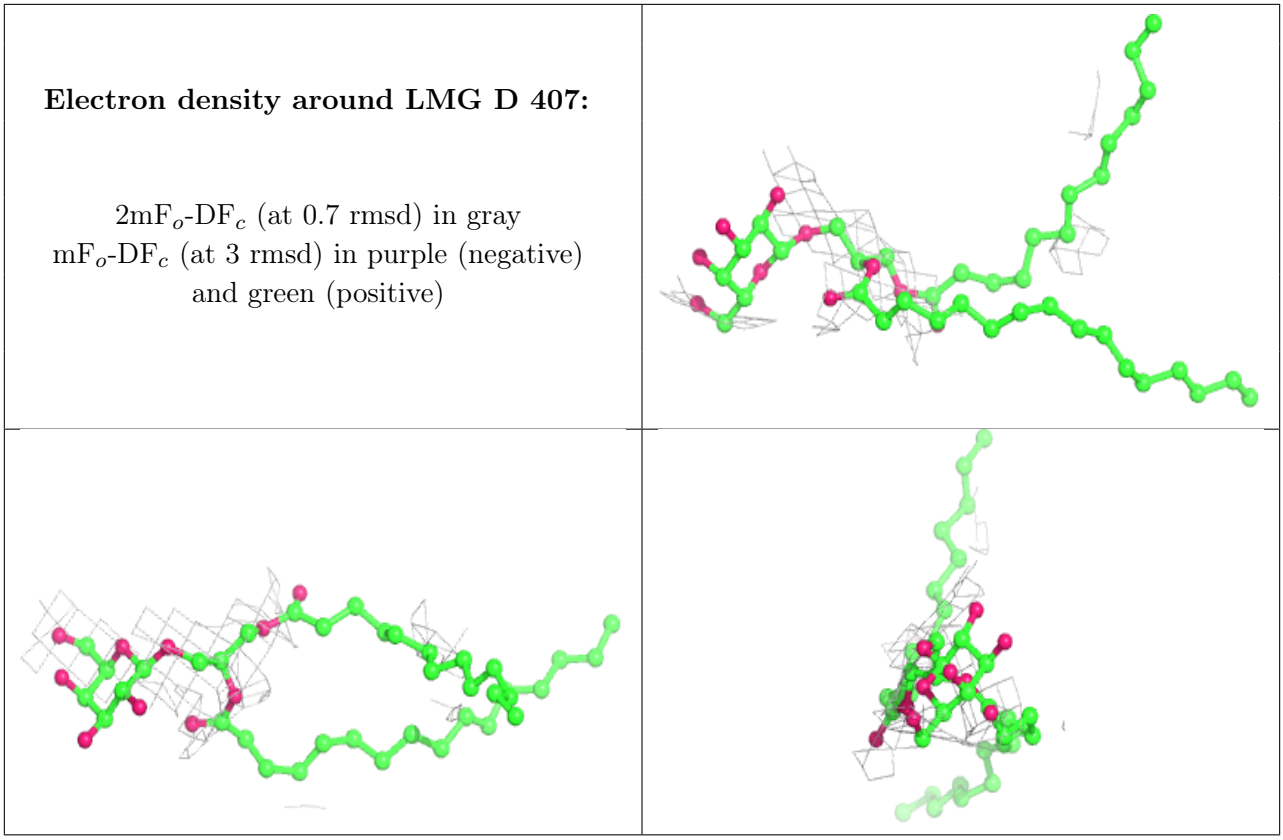
Electron density around LMG b 624:

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



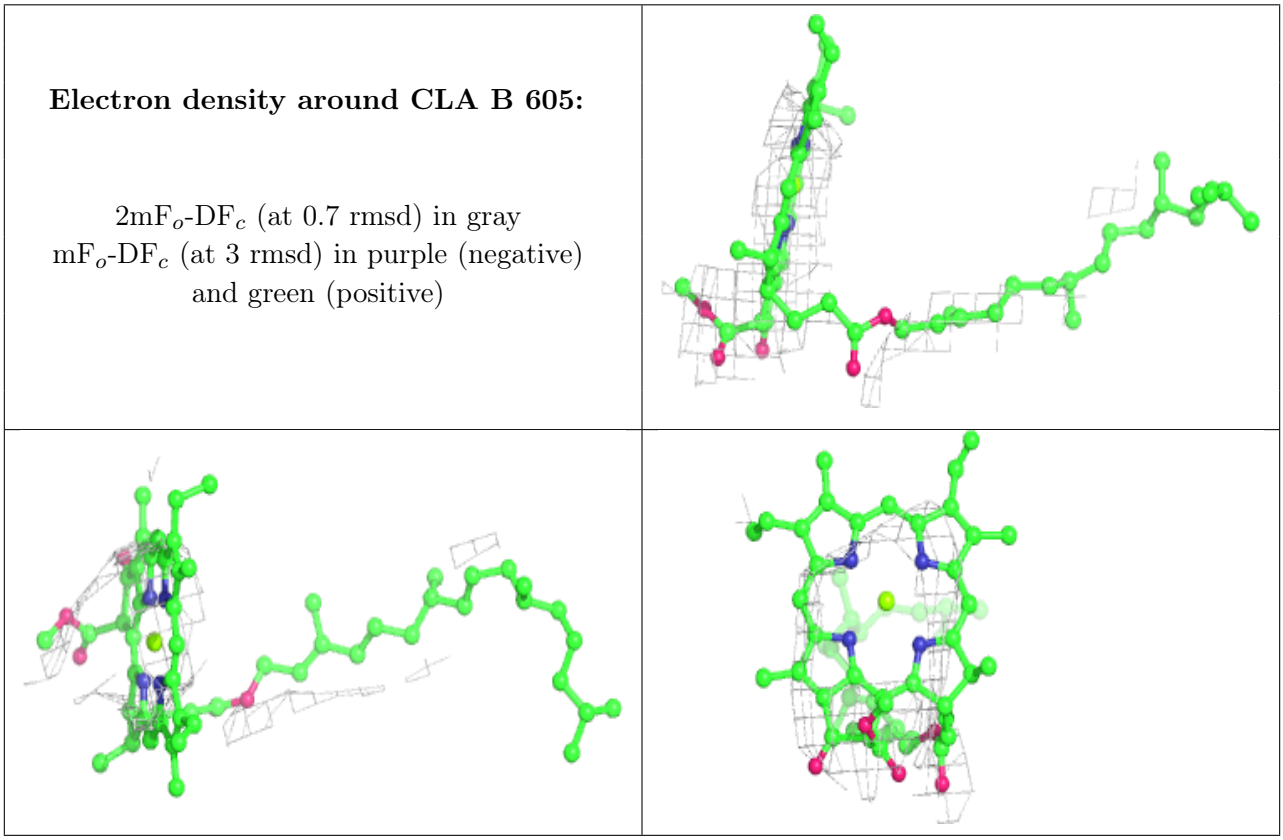
Electron density around LMG D 407:

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



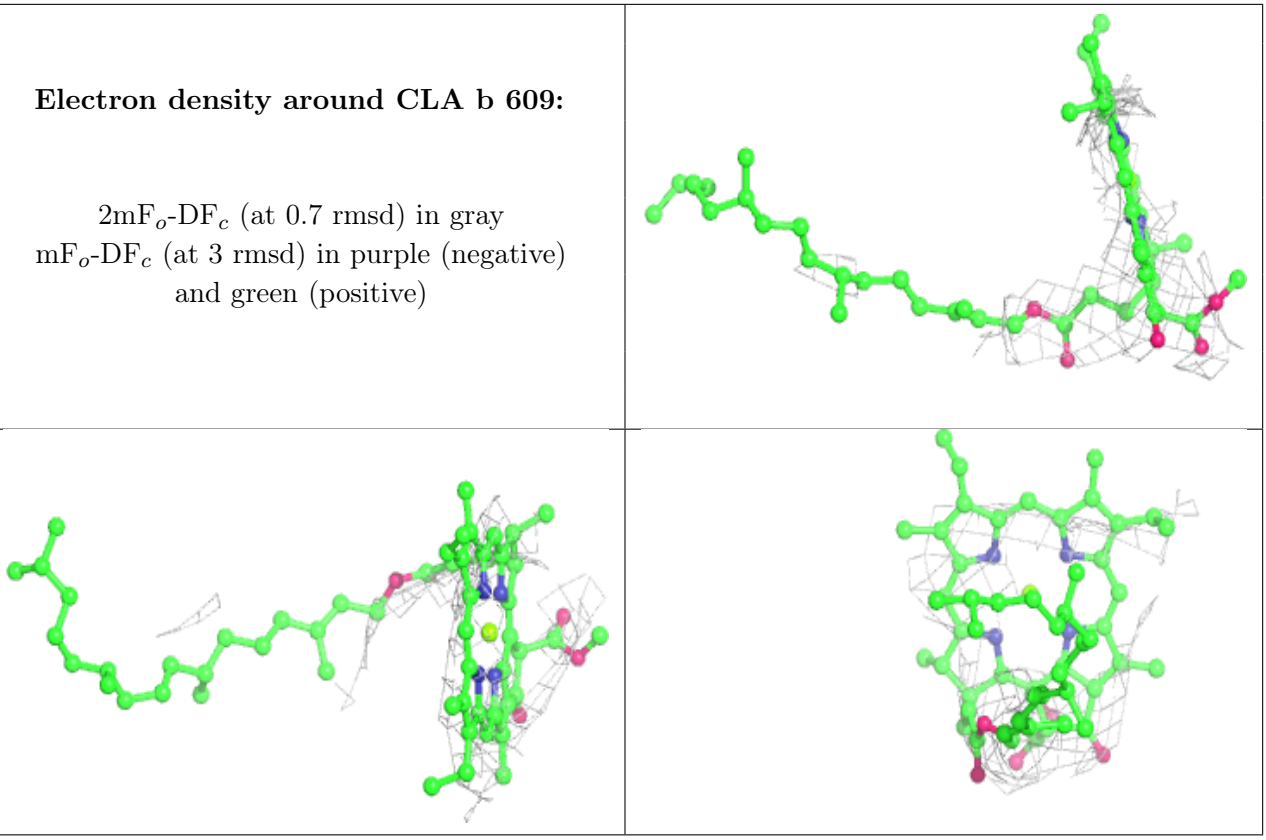
Electron density around CLA B 605:

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



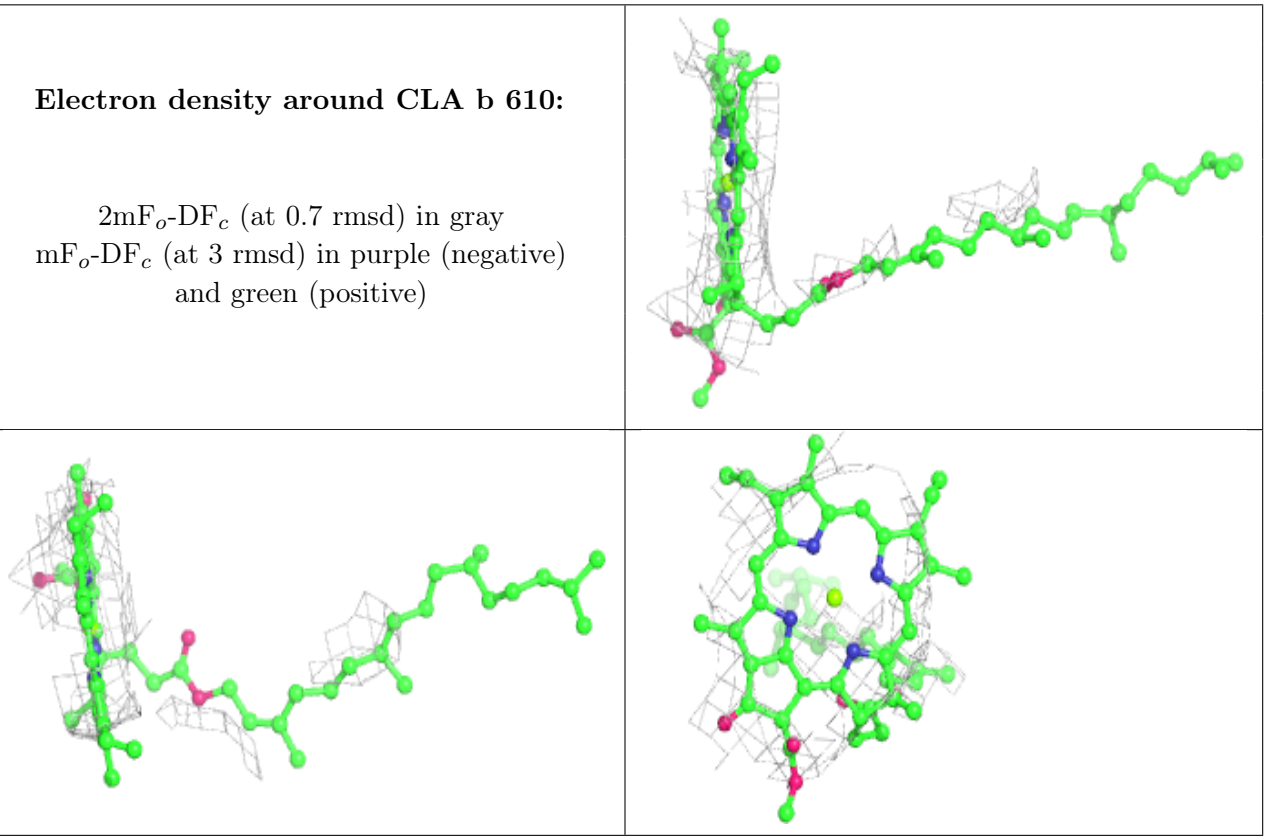
Electron density around CLA b 609:

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



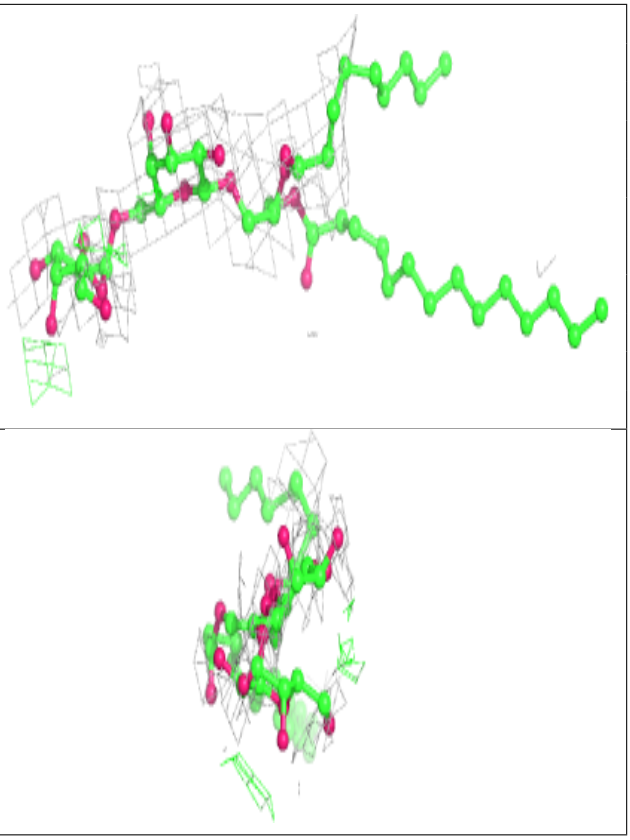
Electron density around CLA b 610:

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



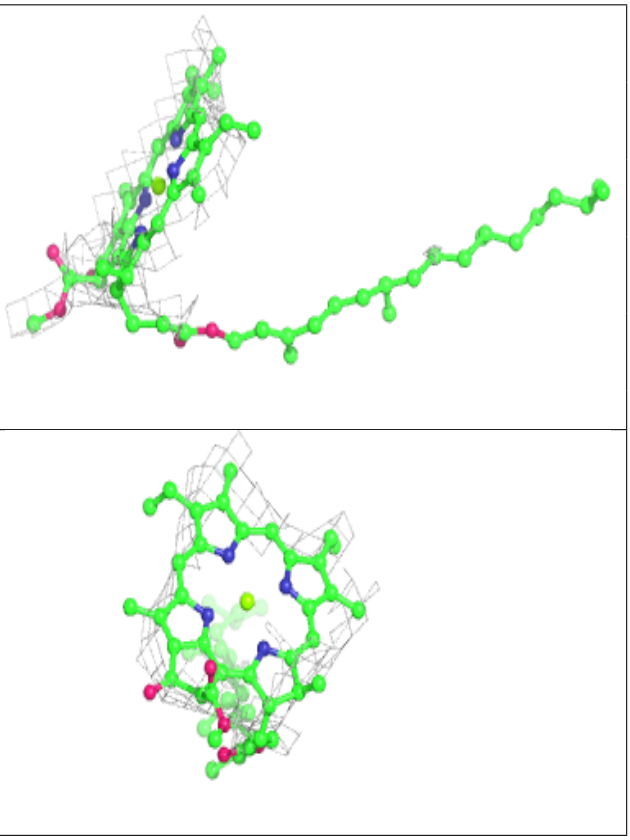
Electron density around DGD C 517:

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



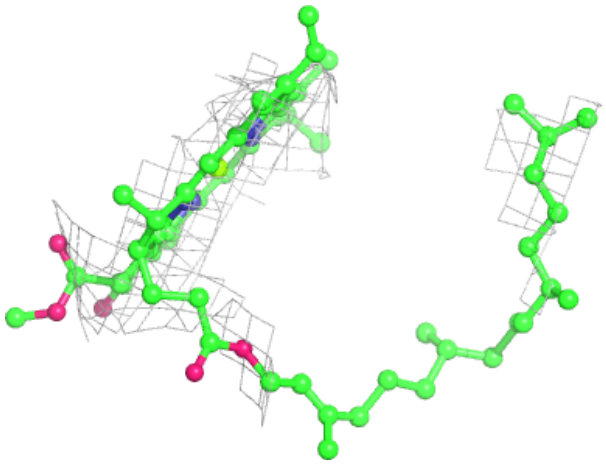
Electron density around CLA b 611:

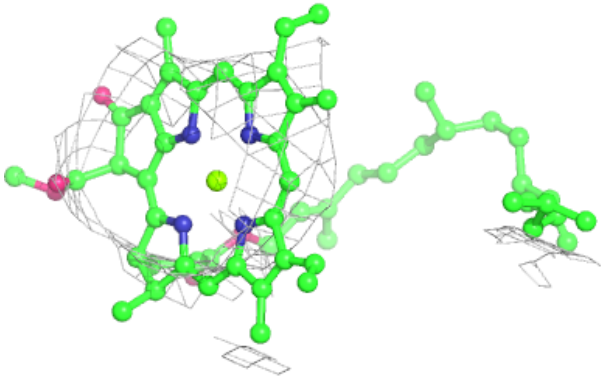
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

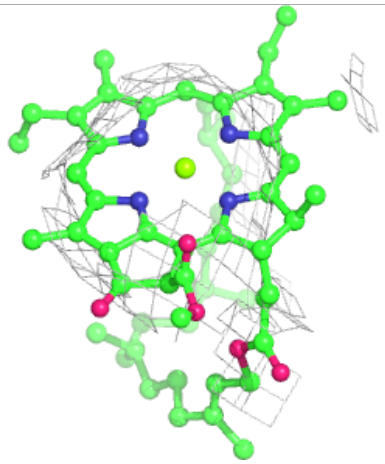


Electron density around CLA B 611:

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

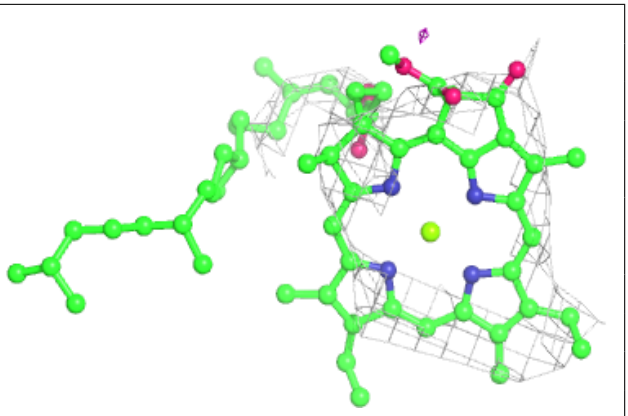


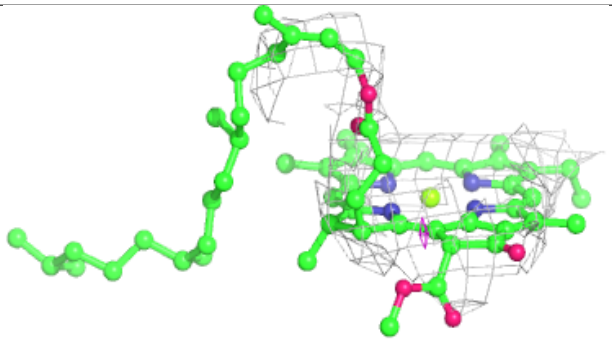


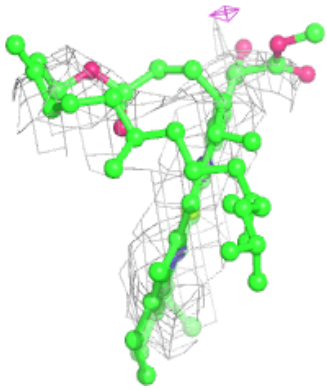


Electron density around CLA a 405:

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

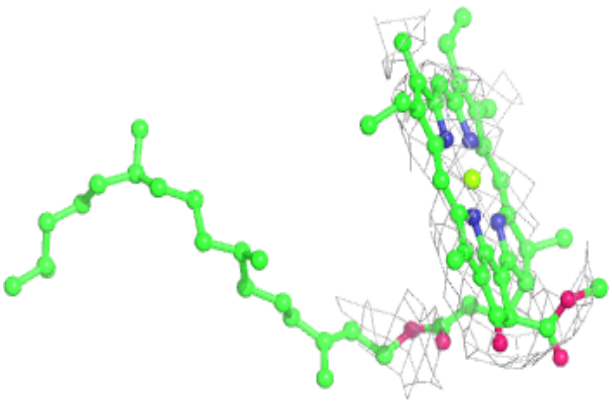


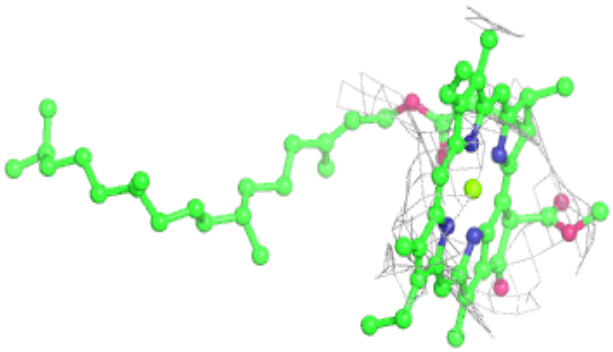


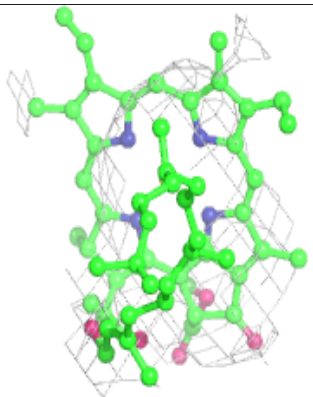


Electron density around CLA C 508:

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

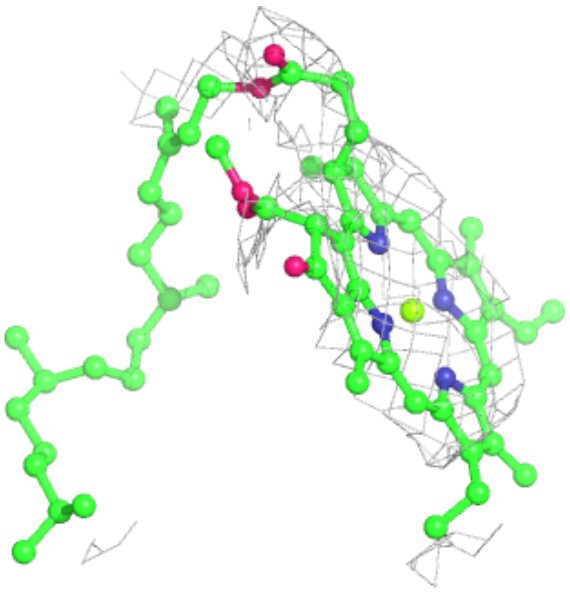


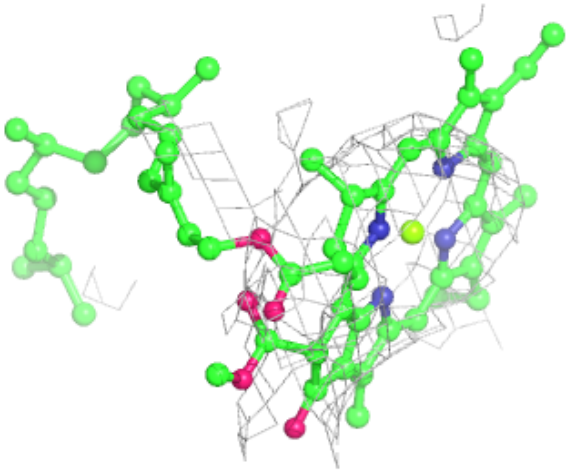


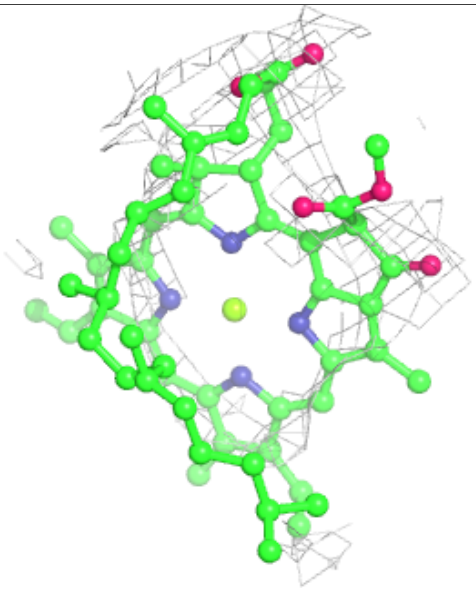


Electron density around CLA B 613:

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

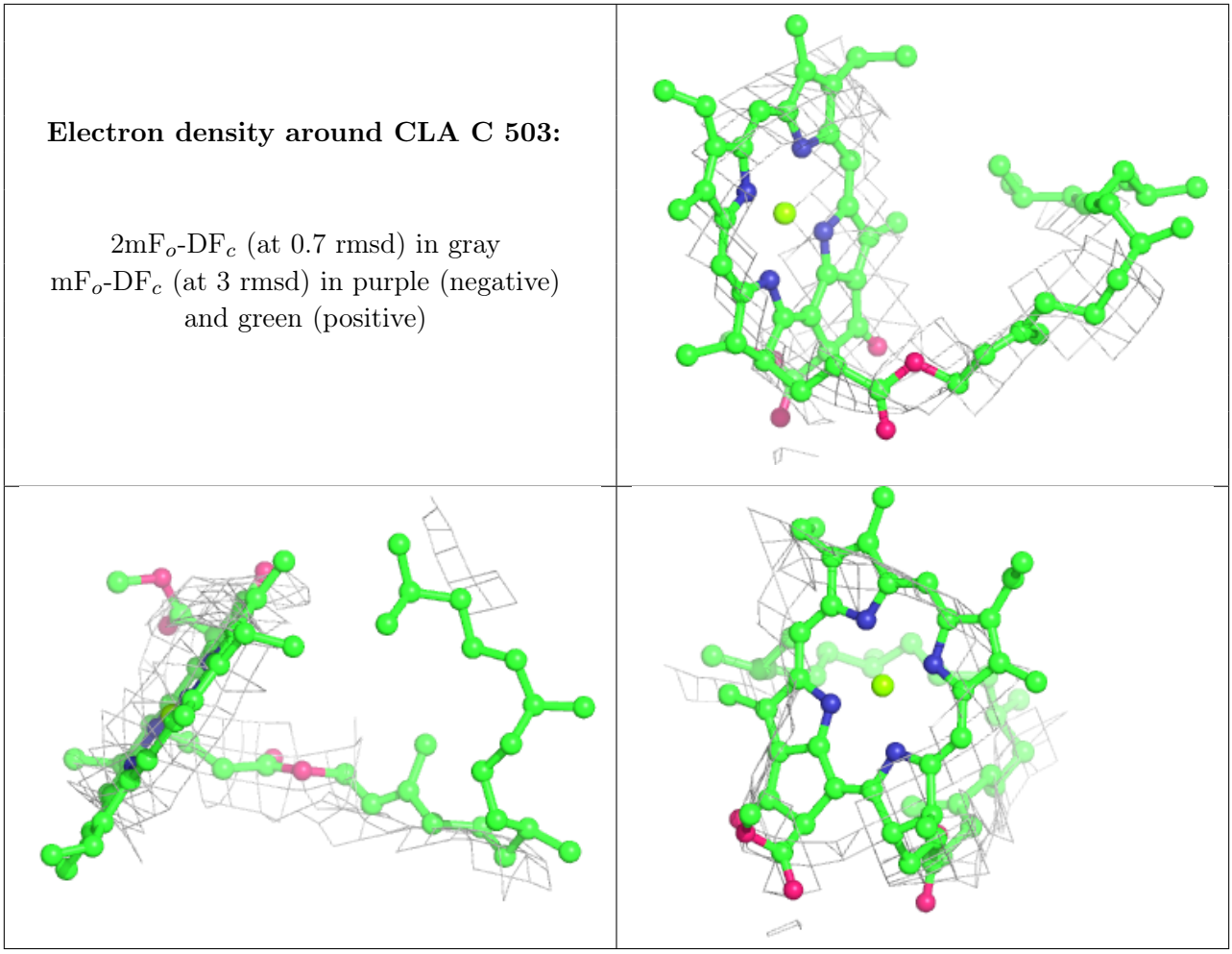






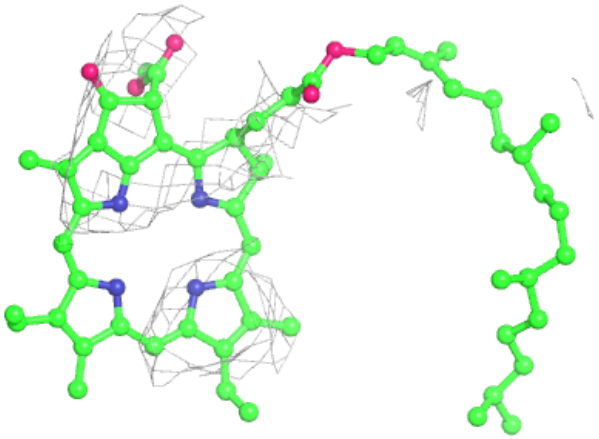
Electron density around CLA C 503:

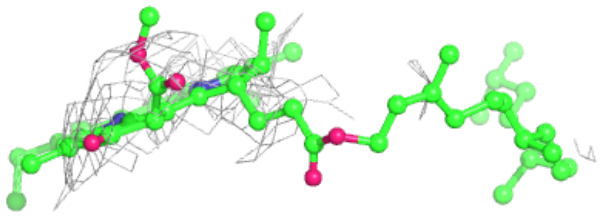
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

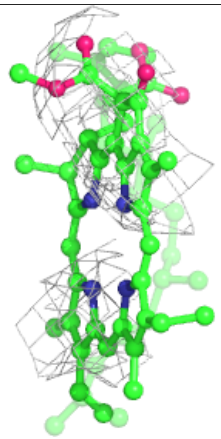


Electron density around PHO a 407:

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

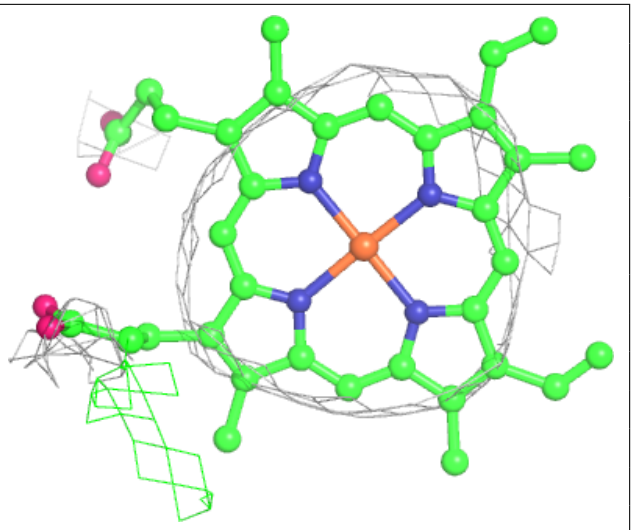


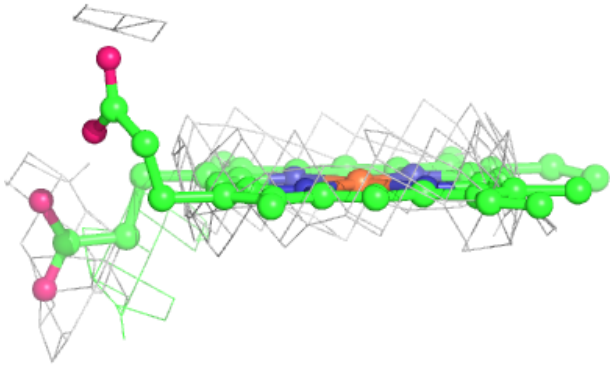


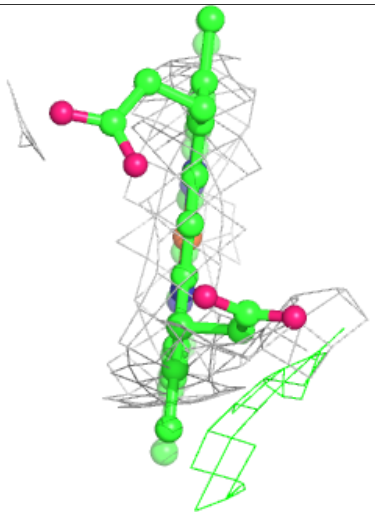


Electron density around HEM F 101:

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

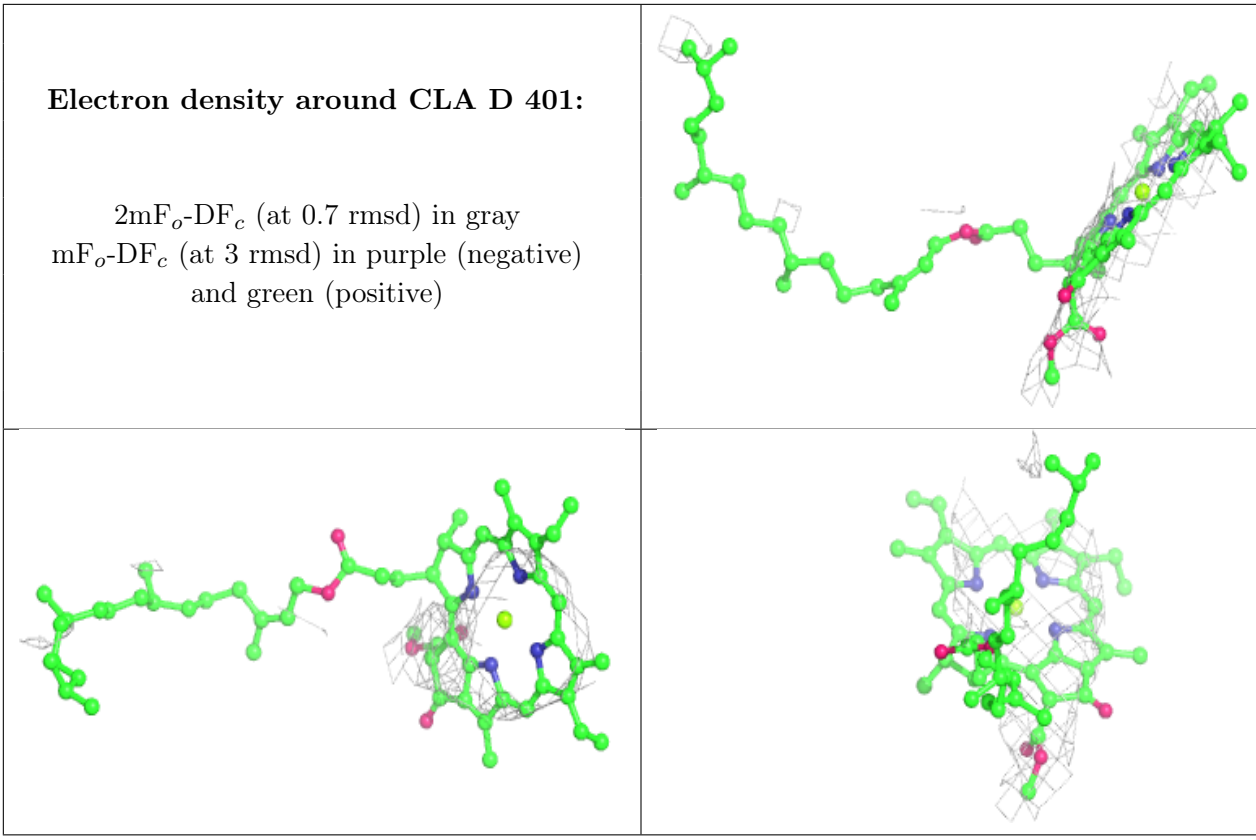






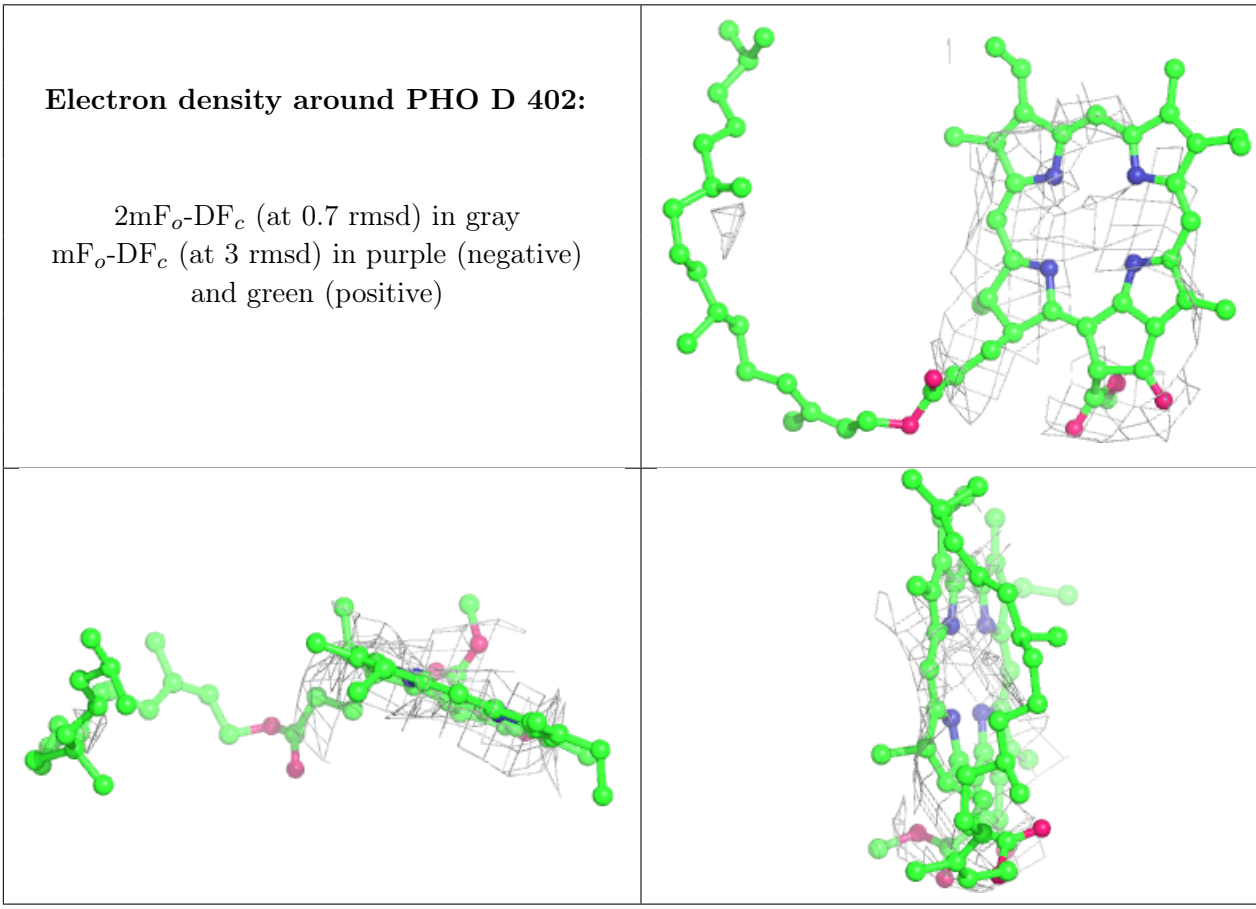
Electron density around CLA D 401:

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



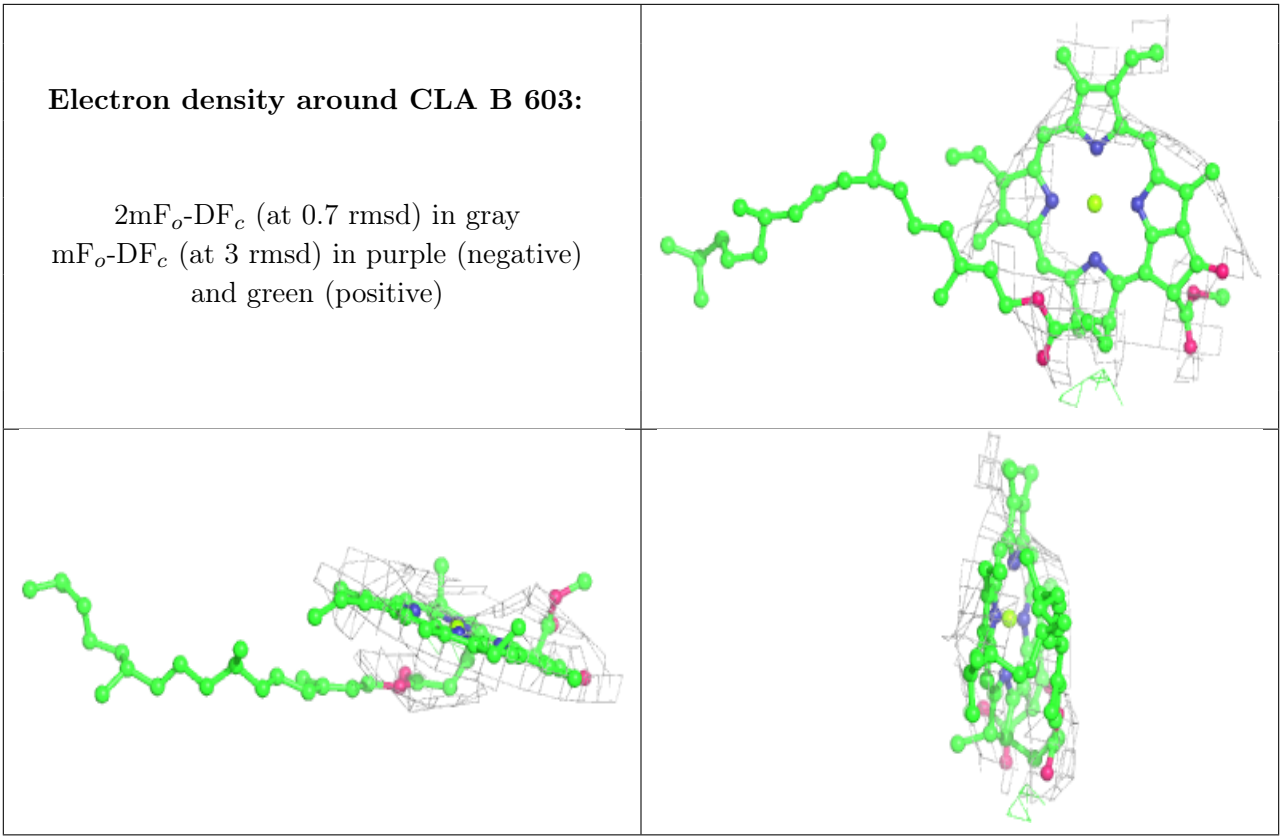
Electron density around PHO D 402:

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



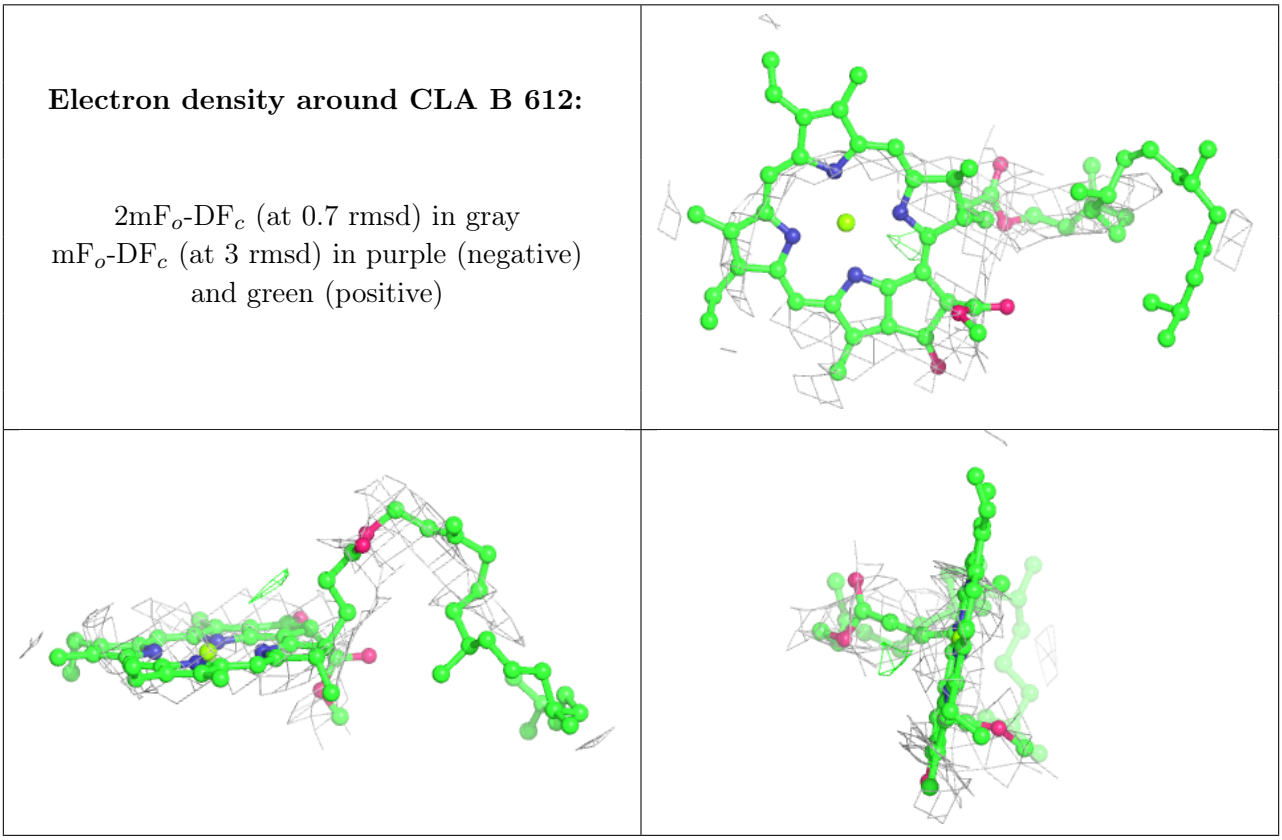
Electron density around CLA B 603:

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



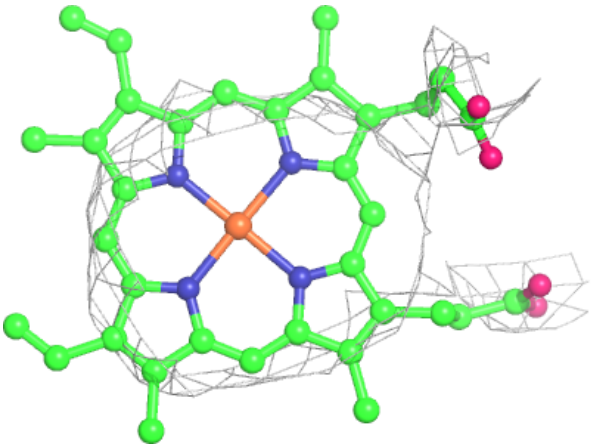
Electron density around CLA B 612:

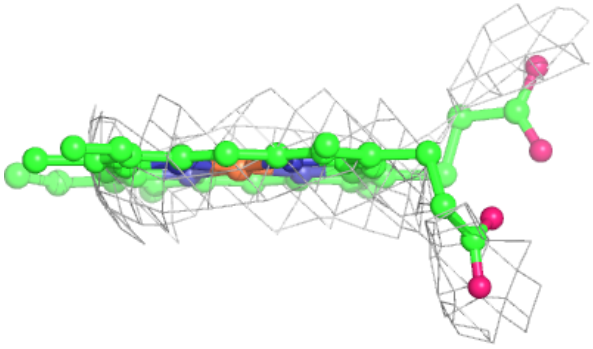
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

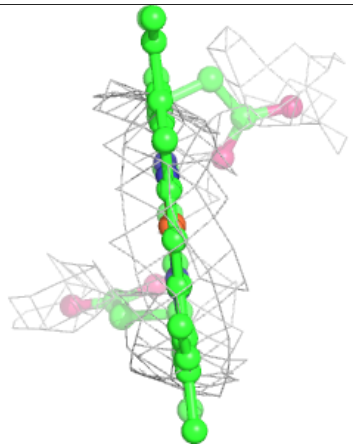


Electron density around HEM f 101:

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

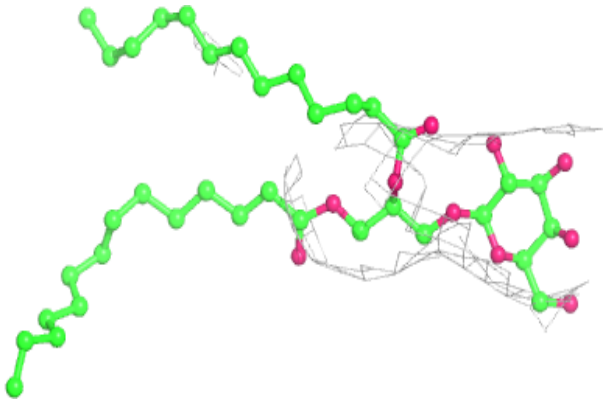


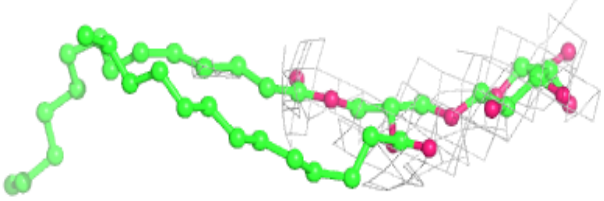


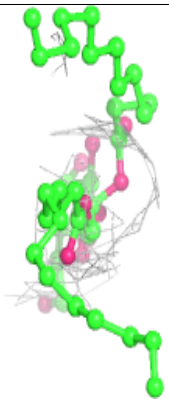


Electron density around LMG d 406:

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

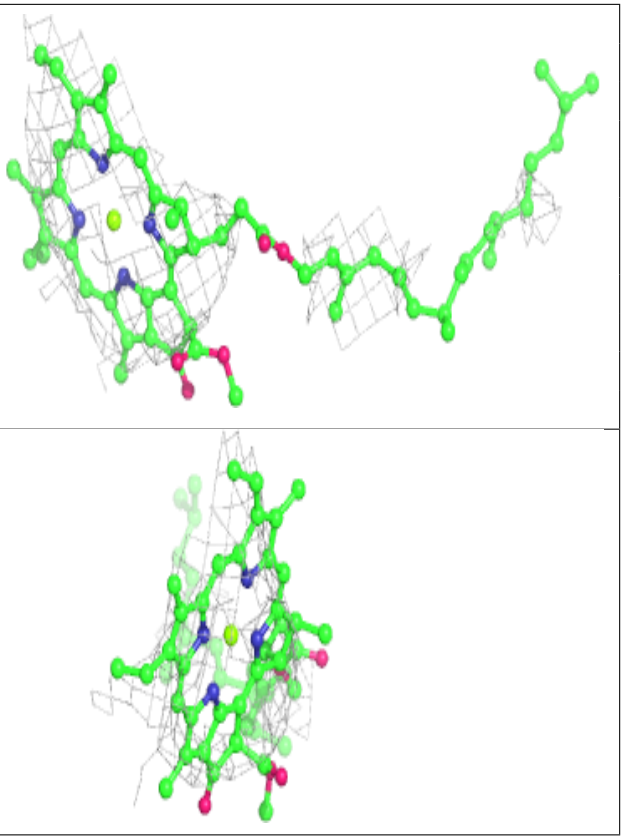


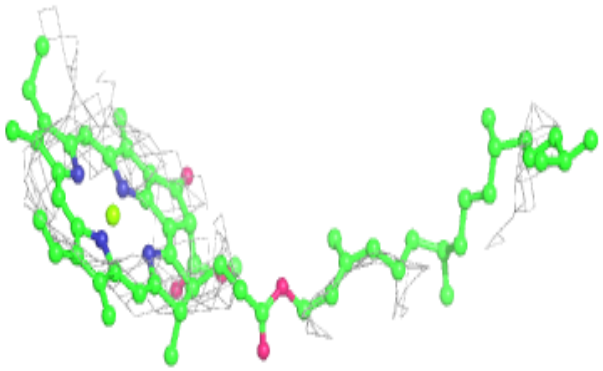




Electron density around CLA a 404:

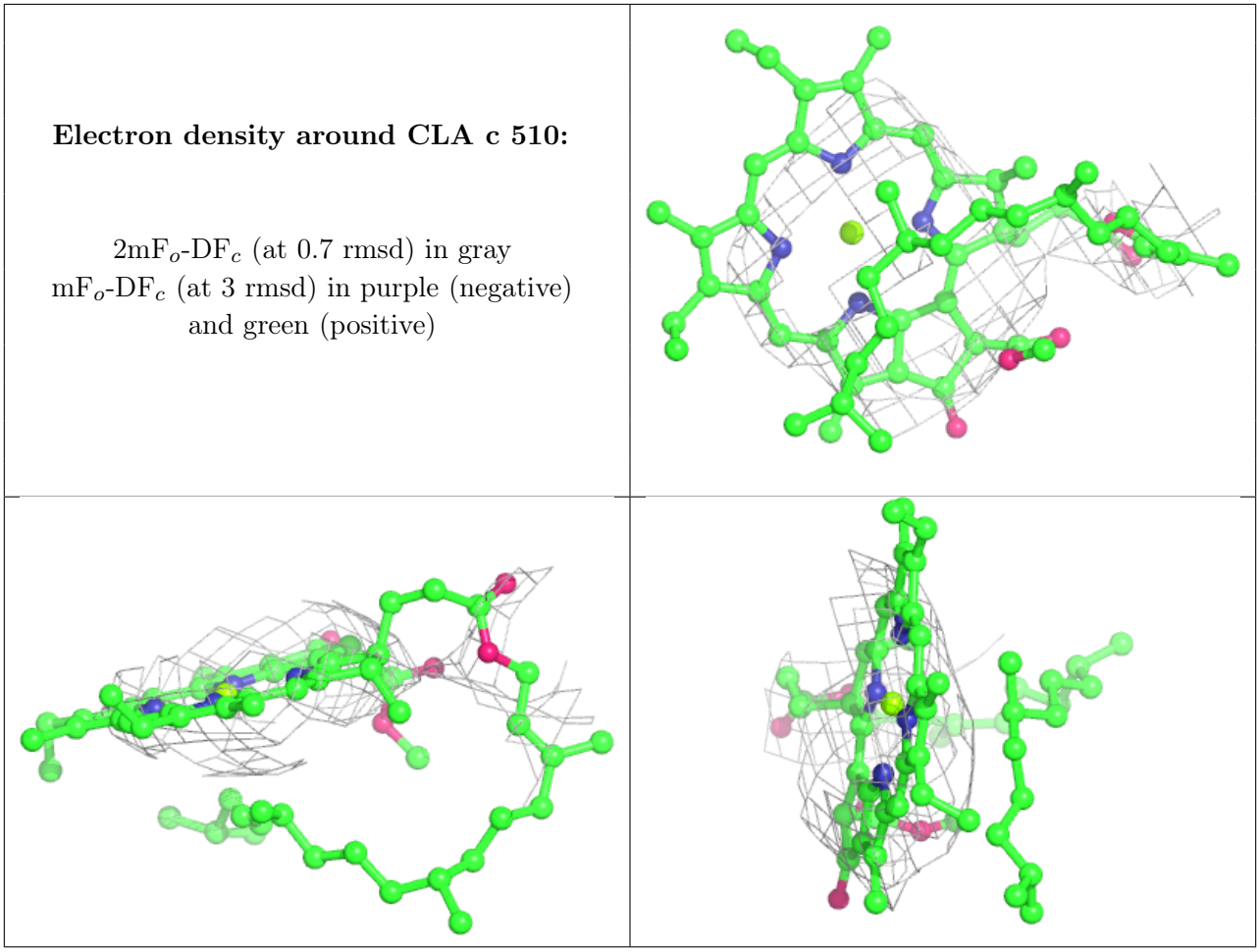
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





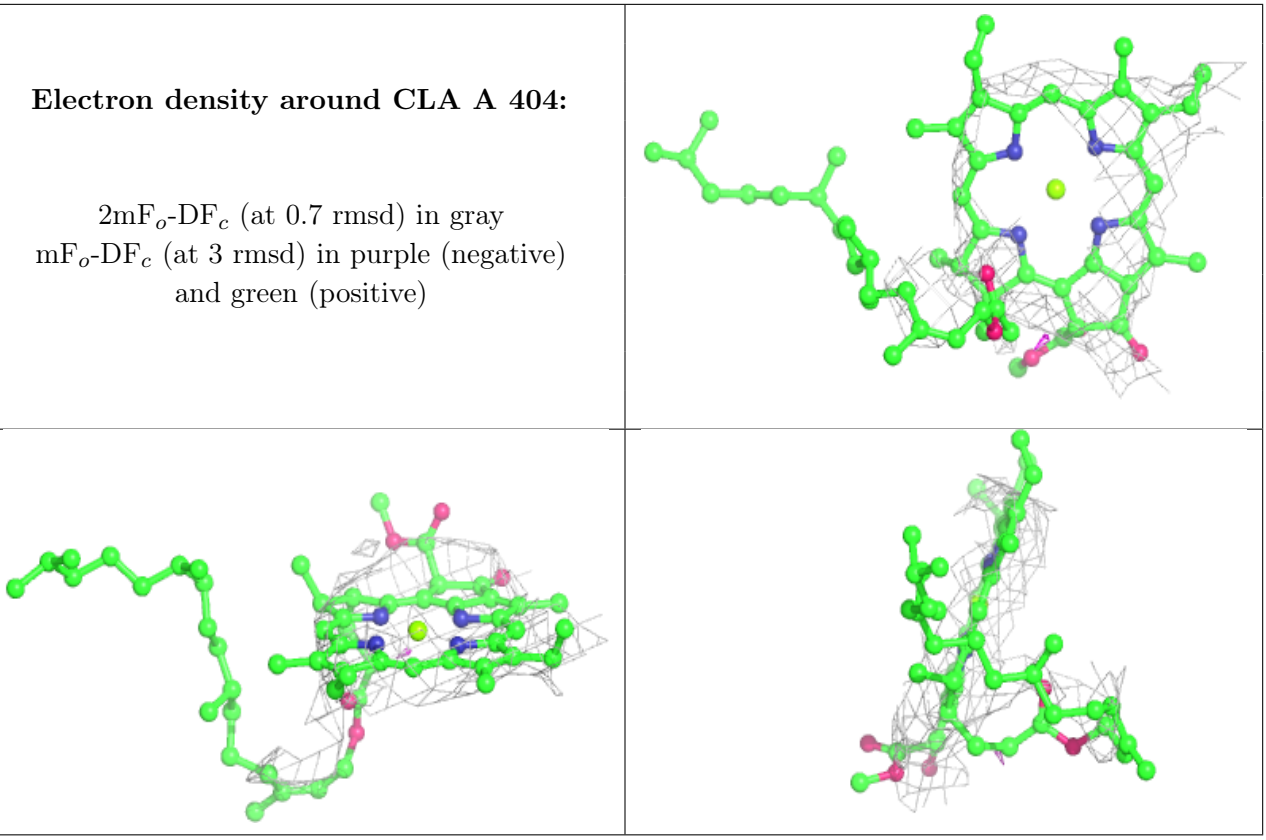
Electron density around CLA c 510:

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



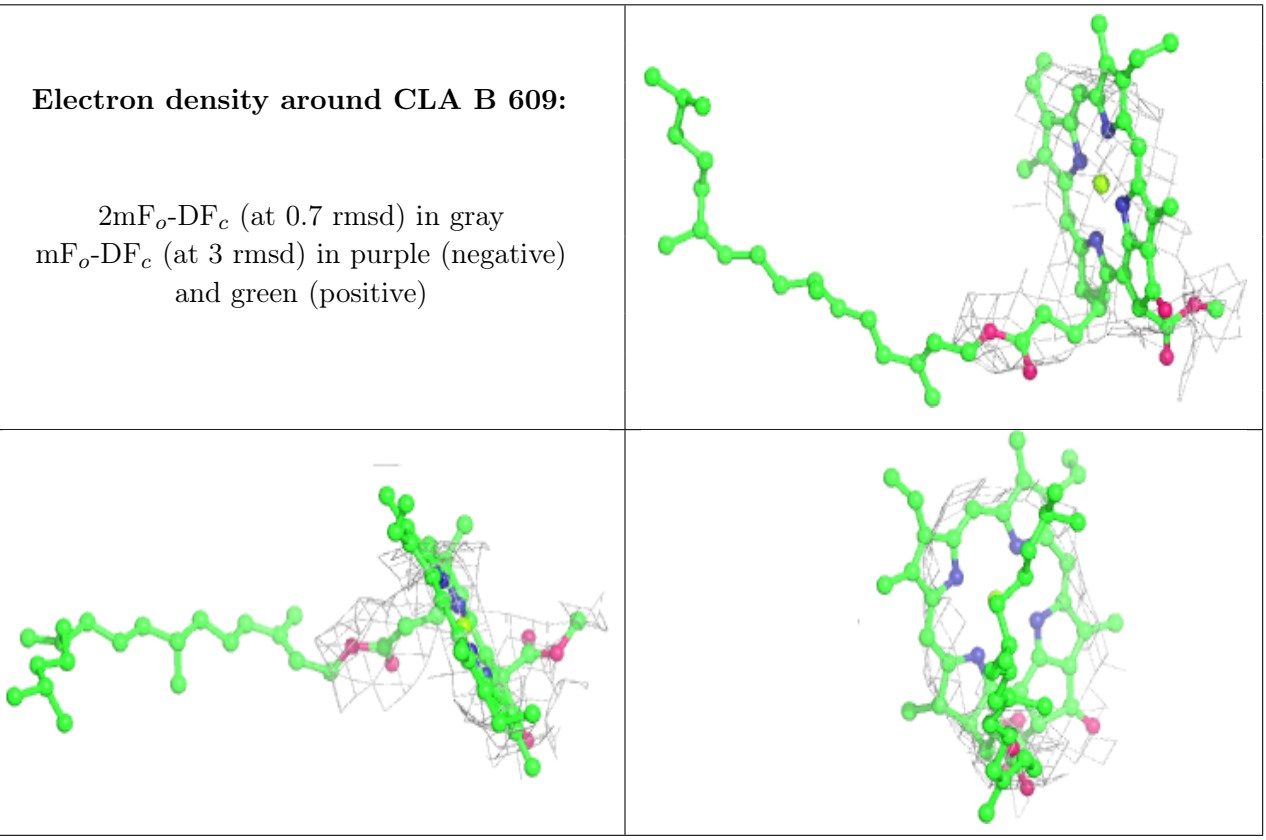
Electron density around CLA A 404:

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



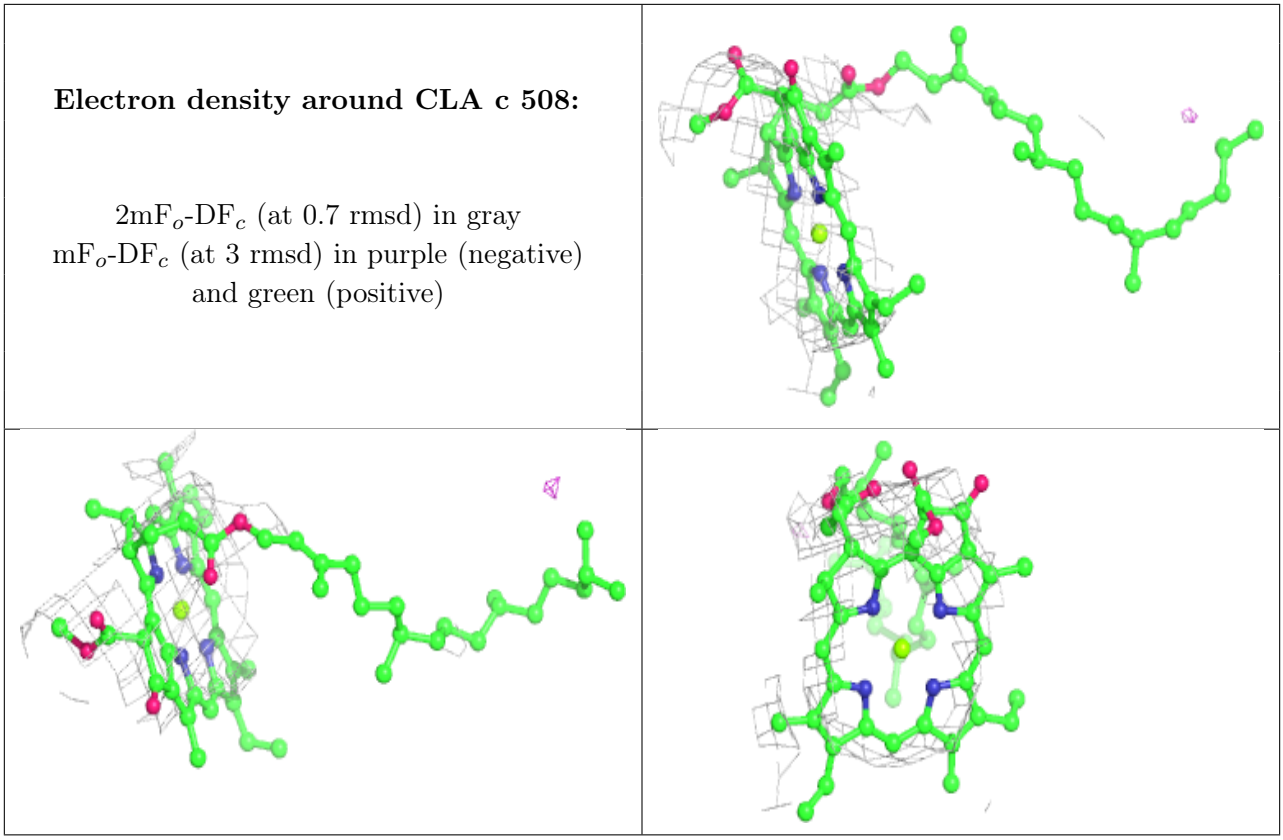
Electron density around CLA B 609:

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



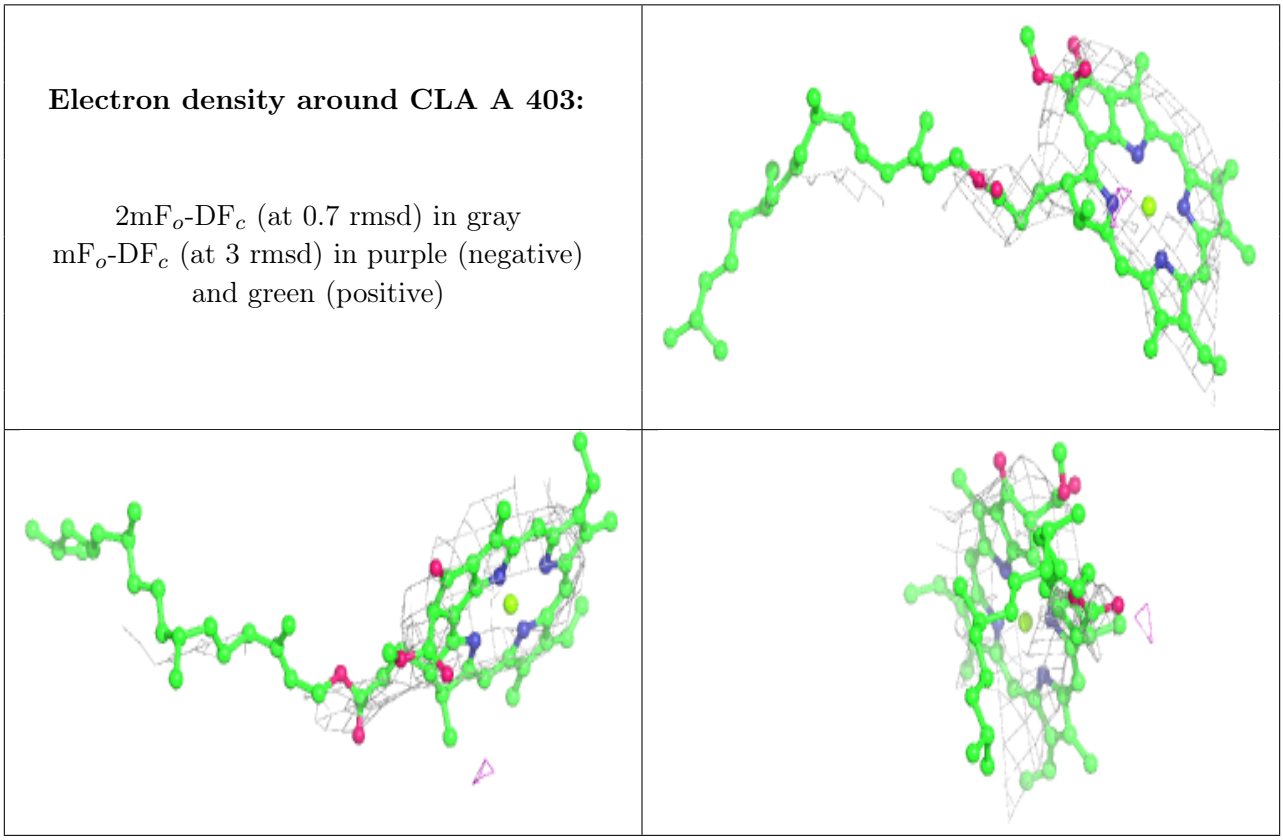
Electron density around CLA c 508:

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



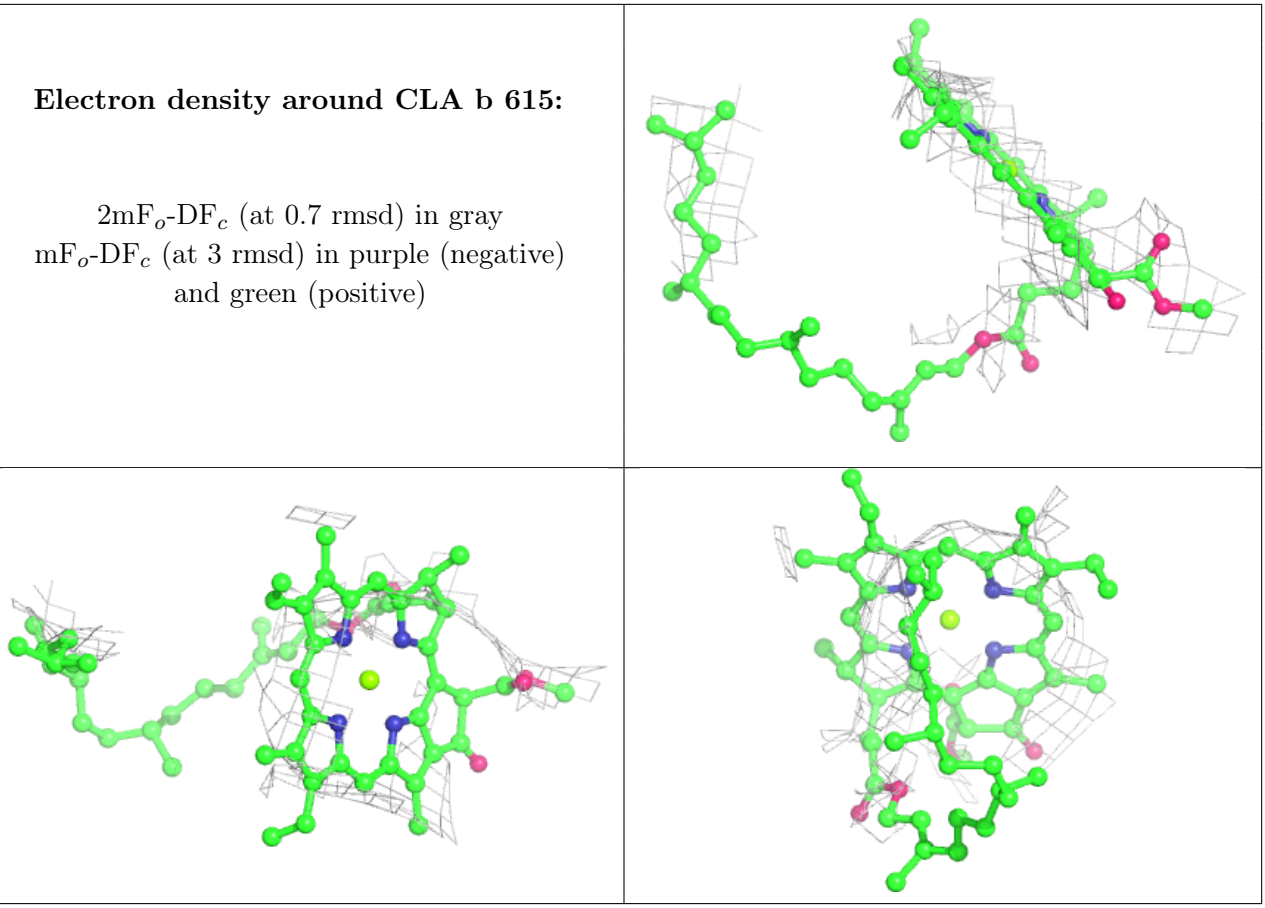
Electron density around CLA A 403:

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



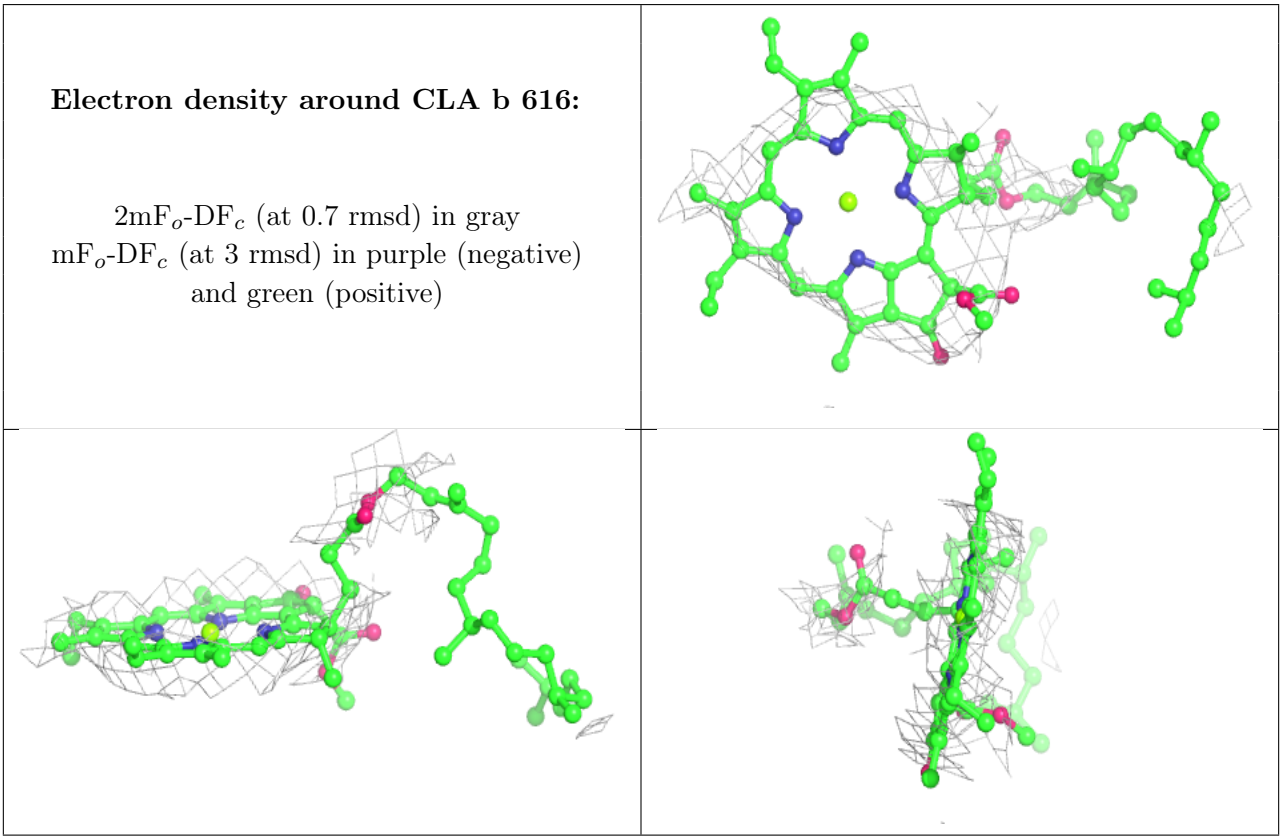
Electron density around CLA b 615:

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



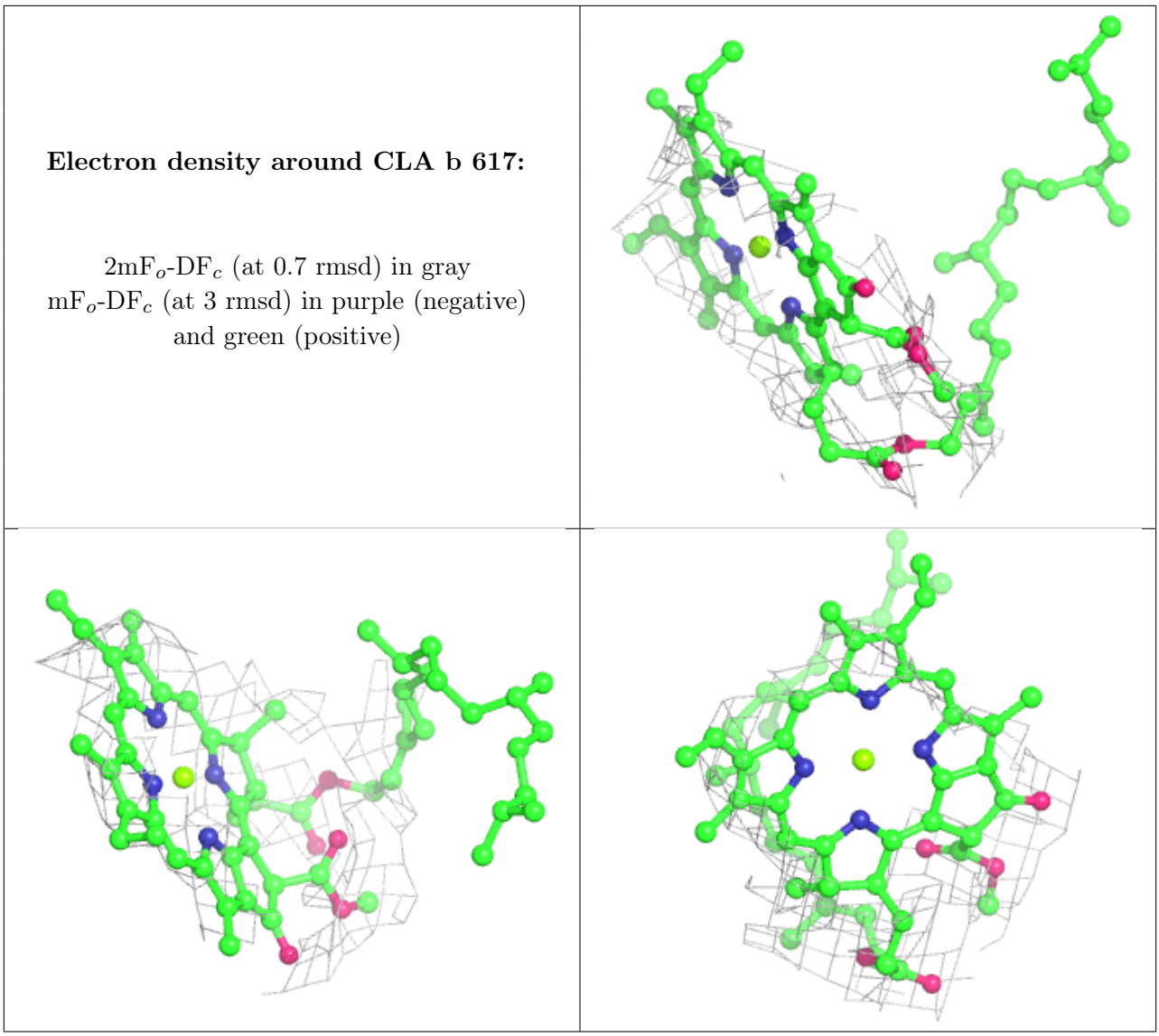
Electron density around CLA b 616:

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



Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.