wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 04:11 am BST

PDB ID	:	4V62
Title	:	Crystal Structure of cyanobacterial Photosystem II
Authors	:	Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on	:	2008-01-17
Resolution	:	2.90 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 following versions of software and data (see references (1)) were used in the production of this report:

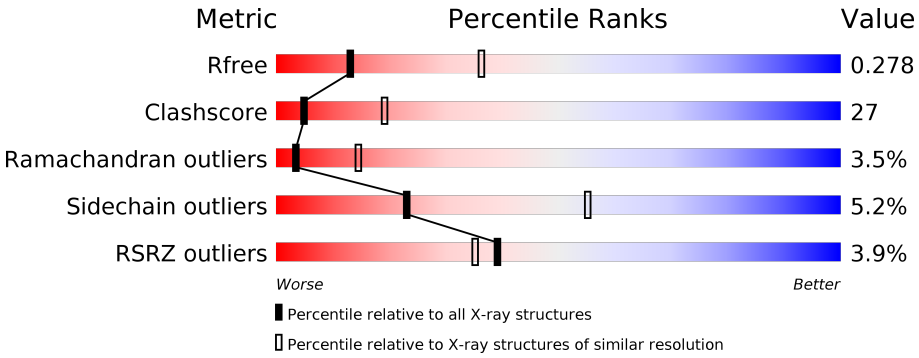
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	AA	344	2% 51% 42%
1	BA	344	2% 50% 43% 5%
2	AB	510	56% 35%
2	BB	510	2% 55% 36%
3	AC	473	2% 45% 43% 6% 5%
3	BC	473	4% 45% 44% 6% 5%

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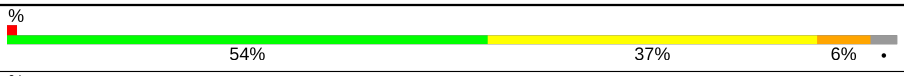
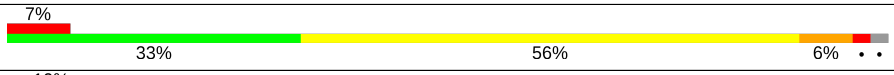
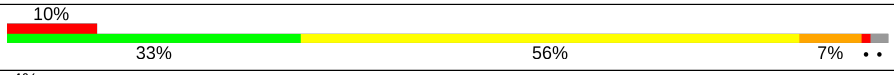
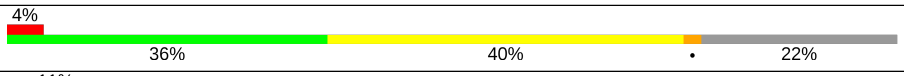
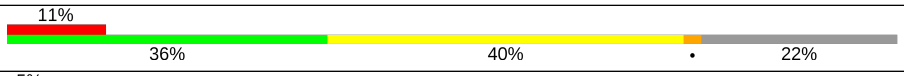
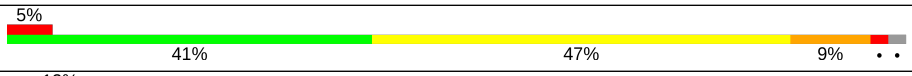
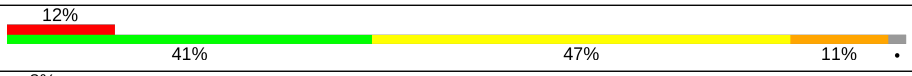
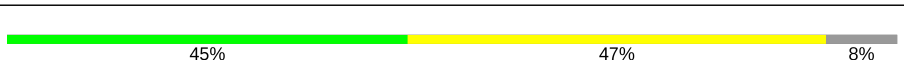
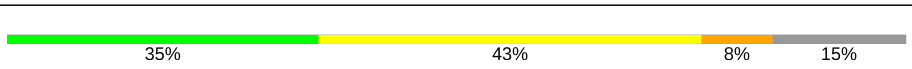
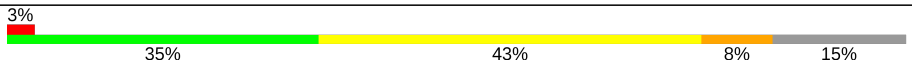
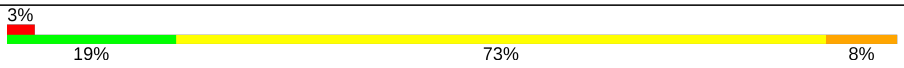
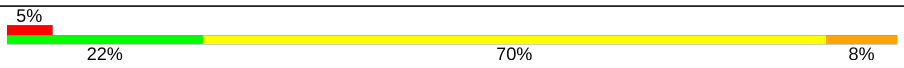
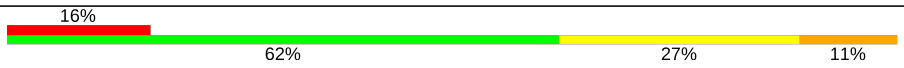
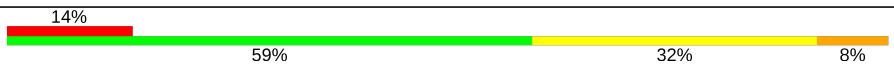
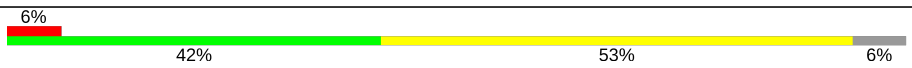
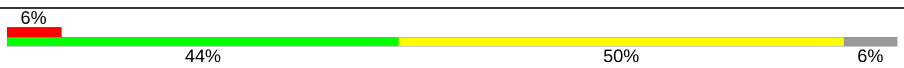
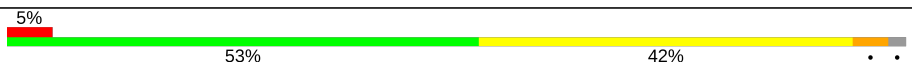
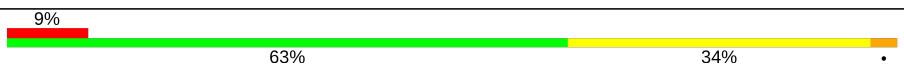
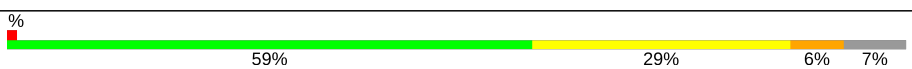
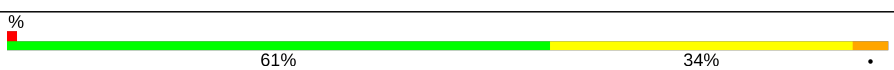
Mol	Chain	Length	Quality of chain
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	
16	AV	137	

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Mol	Chain	Length	Quality of chain
16	BV	137	6% 63% 33%
17	Ay	46	9% 48% 13% 39%
17	By	46	7% 48% 13% 39%
18	AX	50	4% 42% 20% 8% 26%
18	BX	50	12% 42% 20% 8% 26%
19	AY	28	75% 25%
19	BY	28	71% 29%
20	AZ	62	16% 37% 52% 11%
20	BZ	62	19% 35% 53% 11%

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
22	CLA	AA	402	X	-	-	-
22	CLA	AA	403	X	-	-	-
22	CLA	AA	404	X	-	-	-
22	CLA	AA	406	X	-	-	-
22	CLA	AB	601	X	-	-	-
22	CLA	AB	602	X	-	-	-
22	CLA	AB	603	X	-	-	-
22	CLA	AB	604	X	-	-	-
22	CLA	AB	605	X	-	-	-
22	CLA	AB	606	X	-	-	-
22	CLA	AB	607	X	-	-	-
22	CLA	AB	608	X	-	-	-
22	CLA	AB	609	X	-	-	-
22	CLA	AB	610	X	-	-	-
22	CLA	AB	611	X	-	-	-
22	CLA	AB	612	X	-	-	-
22	CLA	AB	613	X	-	-	-
22	CLA	AB	614	X	-	-	-
22	CLA	AB	615	X	-	-	-
22	CLA	AB	616	X	-	-	-
22	CLA	AC	501	X	-	-	-
22	CLA	AC	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	AC	503	X	-	-	-
22	CLA	AC	504	X	-	-	-
22	CLA	AC	505	X	-	-	-
22	CLA	AC	506	X	-	-	-
22	CLA	AC	507	X	-	-	-
22	CLA	AC	508	X	-	-	-
22	CLA	AC	509	X	-	-	-
22	CLA	AC	510	X	-	-	-
22	CLA	AC	511	X	-	-	-
22	CLA	AC	512	X	-	-	-
22	CLA	AC	513	X	-	-	-
22	CLA	AD	402	X	-	-	-
22	CLA	AD	404	X	-	-	-
22	CLA	BA	403	X	-	-	-
22	CLA	BA	404	X	-	-	-
22	CLA	BA	405	X	-	-	-
22	CLA	BA	407	X	-	-	-
22	CLA	BB	604	X	-	-	-
22	CLA	BB	605	X	-	-	-
22	CLA	BB	606	X	-	-	-
22	CLA	BB	607	X	-	-	-
22	CLA	BB	608	X	-	-	-
22	CLA	BB	609	X	-	-	-
22	CLA	BB	610	X	-	-	-
22	CLA	BB	611	X	-	-	-
22	CLA	BB	612	X	-	-	-
22	CLA	BB	613	X	-	-	-
22	CLA	BB	614	X	-	-	-
22	CLA	BB	615	X	-	-	-
22	CLA	BB	616	X	-	-	-
22	CLA	BB	617	X	-	-	-
22	CLA	BB	618	X	-	-	-
22	CLA	BB	619	X	-	-	-
22	CLA	BC	501	X	-	-	-
22	CLA	BC	502	X	-	-	-
22	CLA	BC	503	X	-	-	-
22	CLA	BC	504	X	-	-	-
22	CLA	BC	505	X	-	-	-
22	CLA	BC	506	X	-	-	-
22	CLA	BC	507	X	-	-	-
22	CLA	BC	508	X	-	-	-
22	CLA	BC	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	BC	510	X	-	-	-
22	CLA	BC	511	X	-	-	-
22	CLA	BC	512	X	-	-	-
22	CLA	BC	513	X	-	-	-
22	CLA	BD	402	X	-	-	-
22	CLA	BD	404	X	-	-	-
24	PL9	AJ	101	-	-	-	X
24	PL9	BJ	101	-	-	-	X
26	BCR	AJ	102	-	-	-	X
26	BCR	BJ	102	-	-	-	X
27	DGD	AA	410	X	-	-	-
27	DGD	AB	626	X	-	-	-
27	DGD	AC	516	X	-	-	-
27	DGD	AC	517	X	-	-	-
27	DGD	AC	518	X	-	-	-
27	DGD	AD	410	X	-	-	X
27	DGD	AH	102	X	-	-	-
27	DGD	BA	411	X	-	-	-
27	DGD	BB	602	X	-	-	-
27	DGD	BC	516	X	-	-	-
27	DGD	BC	517	X	-	-	-
27	DGD	BC	518	X	-	-	-
27	DGD	BD	410	X	-	-	X
27	DGD	BH	101	X	-	-	-
28	LHG	AC	521	-	-	-	X
28	LHG	BC	521	-	-	-	X
30	LMG	AA	413	X	-	-	-
30	LMG	AA	416	X	-	-	-
30	LMG	AB	621	X	-	-	-
30	LMG	AB	622	X	-	-	-
30	LMG	AB	623	X	-	-	-
30	LMG	AC	519	X	-	-	-
30	LMG	AC	520	X	-	-	X
30	LMG	AD	407	X	-	-	-
30	LMG	AD	408	X	-	-	-
30	LMG	AE	102	X	-	-	-
30	LMG	AI	101	X	-	-	X
30	LMG	AM	101	X	-	-	-
30	LMG	BA	414	X	-	-	-
30	LMG	BB	623	X	-	-	-
30	LMG	BB	624	X	-	-	-
30	LMG	BC	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMG	BC	520	X	-	-	X
30	LMG	BD	407	X	-	-	-
30	LMG	BD	408	X	-	-	-
30	LMG	BE	102	X	-	-	-
30	LMG	BI	101	X	-	-	-
30	LMG	BM	102	X	-	-	-
32	LMT	AB	624	-	-	-	X
32	LMT	AB	625	-	-	-	X
32	LMT	AB	627	-	-	-	X
32	LMT	AD	411	-	-	-	X
32	LMT	AI	102	-	-	-	X
32	LMT	BB	625	-	-	-	X
32	LMT	BD	411	-	-	-	X
32	LMT	BI	102	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50234 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	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	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
AC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
AC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
AC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
AC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
AC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8
BC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
BC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
BC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
BC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8
BC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
BC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
BC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	BD	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	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	BV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Ay	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	By	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

- Molecule 18 is a protein called Photosystem II PsbX protein.

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

- Molecule 19 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AY	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	BY	28	Total	C	N	O	0	0	0
			140	84	28	28			

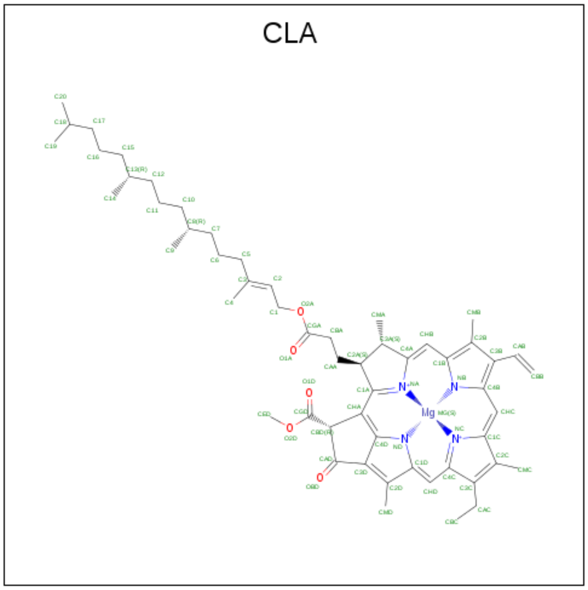
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	AA	1	Total	Fe	0	0
			1	1		
21	BA	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	AA	1	Total C Mg N O 65 55 1 4 5	0	0
22	AA	1	Total C Mg N O 65 55 1 4 5	0	0
22	AA	1	Total C Mg N O 65 55 1 4 5	0	0
22	AA	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AB	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AC	1	Total C Mg N O 65 55 1 4 5	0	0
22	AD	1	Total C Mg N O 65 55 1 4 5	0	0
22	AD	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	BA	1	Total C Mg N O 65 55 1 4 5	0	0
22	BA	1	Total C Mg N O 65 55 1 4 5	0	0
22	BA	1	Total C Mg N O 65 55 1 4 5	0	0
22	BA	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BB	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0

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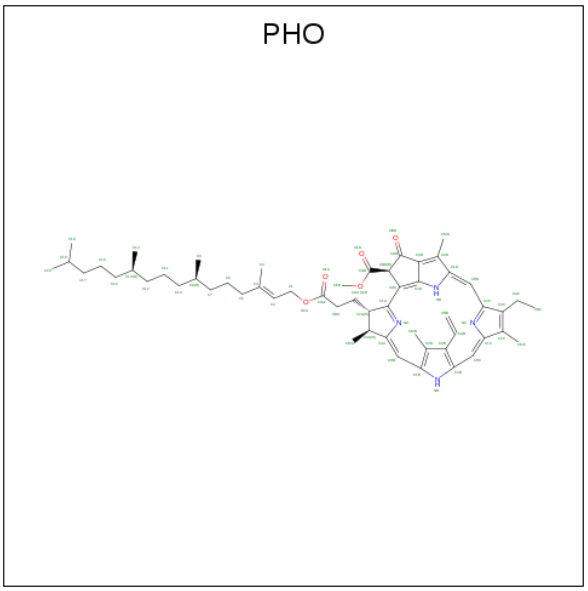
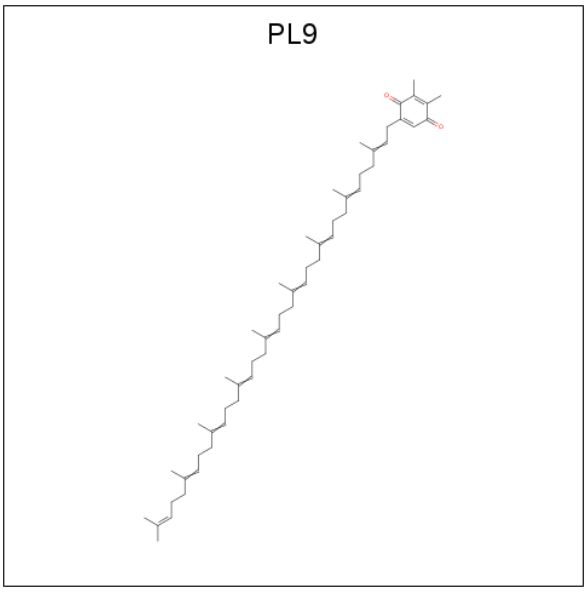
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BC	1	Total C Mg N O 65 55 1 4 5	0	0
22	BD	1	Total C Mg N O 65 55 1 4 5	0	0
22	BD	1	Total C Mg N O 65 55 1 4 5	0	0

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



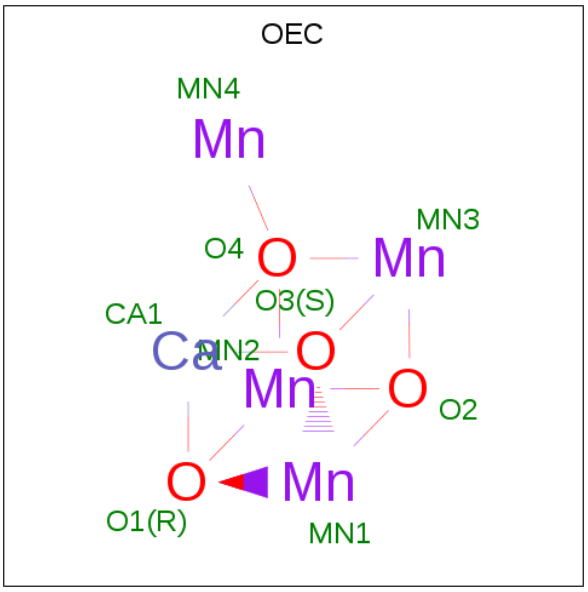
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	AA	1	Total	C	N	O	0	0
			64	55	4	5		
23	AD	1	Total	C	N	O	0	0
			64	55	4	5		
23	BA	1	Total	C	N	O	0	0
			64	55	4	5		
23	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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: $C_{53}H_{80}O_2$).



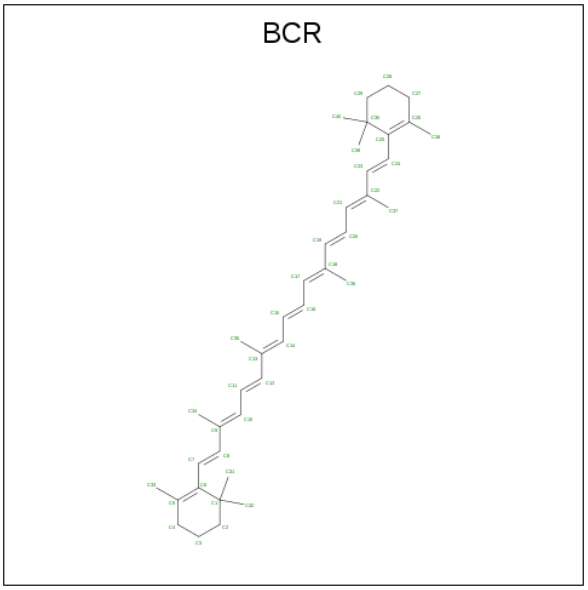
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	AA	1	Total C O 45 43 2	0	0
24	AD	1	Total C O 55 53 2	0	0
24	AJ	1	Total C O 35 33 2	0	0
24	BA	1	Total C O 45 43 2	0	0
24	BD	1	Total C O 55 53 2	0	0
24	BJ	1	Total C O 35 33 2	0	0

- Molecule 25 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	AA	1	Total Ca Mn 5 1 4	0	0
25	BA	1	Total Ca Mn 5 1 4	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AA	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AD	1	Total C 40 40	0	0
26	AH	1	Total C 40 40	0	0
26	AJ	1	Total C 40 40	0	0
26	AK	1	Total C 40 40	0	0
26	AT	1	Total C 40 40	0	0
26	AZ	1	Total C 40 40	0	0
26	BA	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BD	1	Total C 40 40	0	0
26	BJ	1	Total C 40 40	0	0
26	BK	1	Total C 40 40	0	0
26	BX	1	Total C 40 40	0	0

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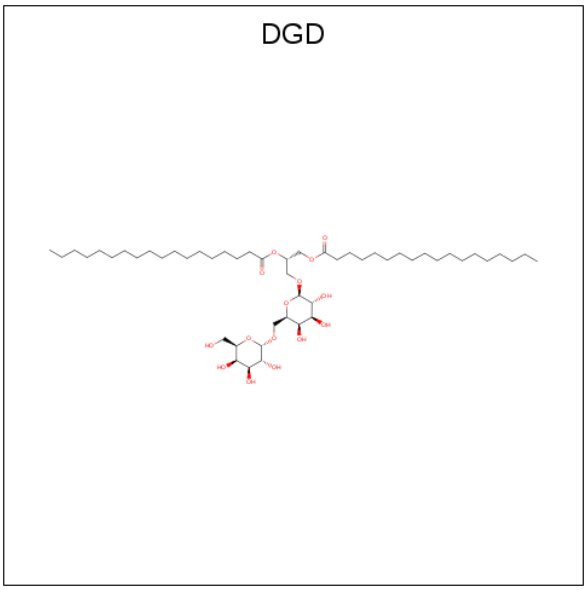
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	BZ	1	Total C 40 40	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C O 56 41 15	0	0
27	AB	1	Total C O 52 37 15	0	0
27	AC	1	Total C O 53 38 15	0	0
27	AC	1	Total C O 62 47 15	0	0
27	AC	1	Total C O 66 51 15	0	0
27	AD	1	Total C O 63 48 15	0	0
27	AH	1	Total C O 58 43 15	0	0
27	BA	1	Total C O 56 41 15	0	0
27	BB	1	Total C O 52 37 15	0	0
27	BC	1	Total C O 53 38 15	0	0

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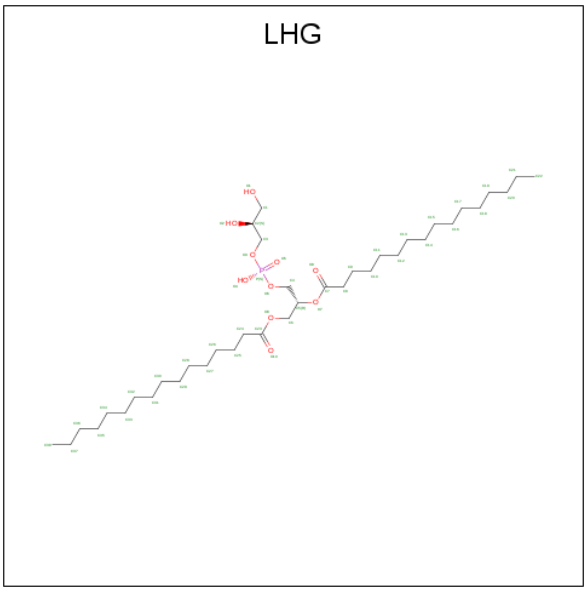
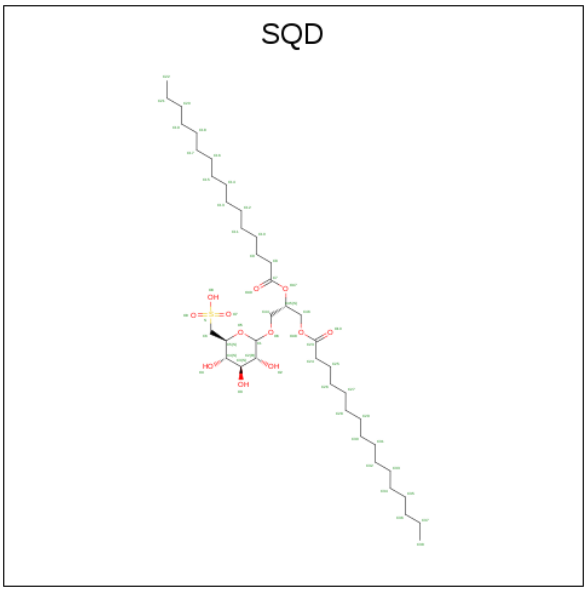
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BC	1	Total C O 62 47 15	0	0
27	BC	1	Total C O 66 51 15	0	0
27	BD	1	Total C O 63 48 15	0	0
27	BH	1	Total C O 58 43 15	0	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



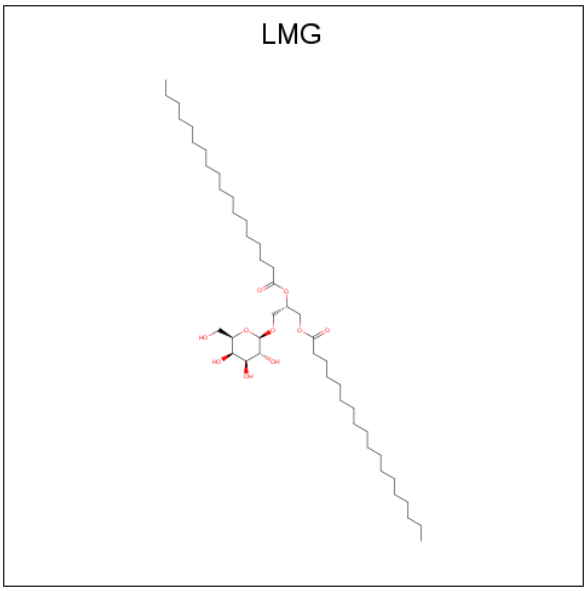
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	AA	1	Total C O P 39 28 10 1	0	0
28	AC	1	Total C O P 37 26 10 1	0	0
28	BA	1	Total C O P 39 28 10 1	0	0
28	BC	1	Total C O P 37 26 10 1	0	0

- Molecule 29 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
29	AA	1	Total	C	O	S	0	0
			51	38	12	1		
29	AA	1	Total	C	O	S	0	0
			54	41	12	1		
29	AD	1	Total	C	O	S	0	0
			43	30	12	1		
29	AF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BA	1	Total	C	O	S	0	0
			54	41	12	1		
29	BA	1	Total	C	O	S	0	0
			51	38	12	1		
29	BB	1	Total	C	O	S	0	0
			47	34	12	1		
29	BD	1	Total	C	O	S	0	0
			43	30	12	1		
29	BF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BL	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	AA	1	Total C O 51 41 10	0	0
30	AA	1	Total C O 42 32 10	0	0
30	AB	1	Total C O 49 39 10	0	0
30	AB	1	Total C O 49 39 10	0	0
30	AB	1	Total C O 42 32 10	0	0
30	AC	1	Total C O 48 38 10	0	0
30	AC	1	Total C O 45 35 10	0	0
30	AD	1	Total C O 46 36 10	0	0
30	AD	1	Total C O 48 38 10	0	0
30	AE	1	Total C O 44 34 10	0	0
30	AI	1	Total C O 43 33 10	0	0
30	AM	1	Total C O 42 32 10	0	0
30	BA	1	Total C O 51 41 10	0	0
30	BB	1	Total C O 49 39 10	0	0

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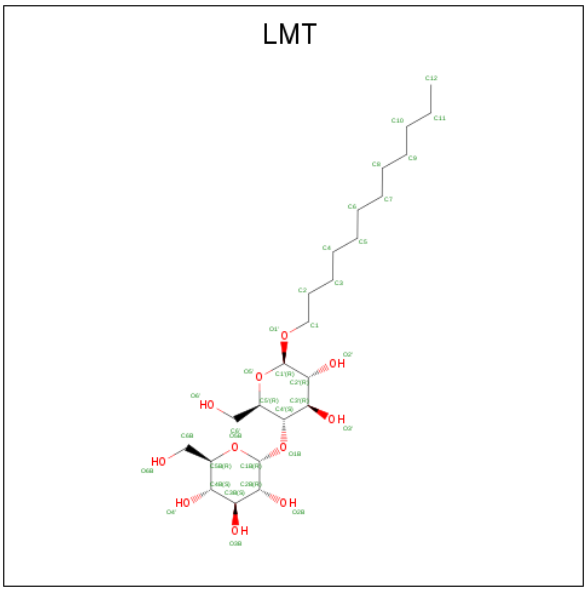
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	BB	1	Total C O 49 39 10	0	0
30	BC	1	Total C O 48 38 10	0	0
30	BC	1	Total C O 45 35 10	0	0
30	BD	1	Total C O 46 36 10	0	0
30	BD	1	Total C O 48 38 10	0	0
30	BE	1	Total C O 44 34 10	0	0
30	BI	1	Total C O 43 33 10	0	0
30	BM	1	Total C O 42 32 10	0	0

- Molecule 31 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

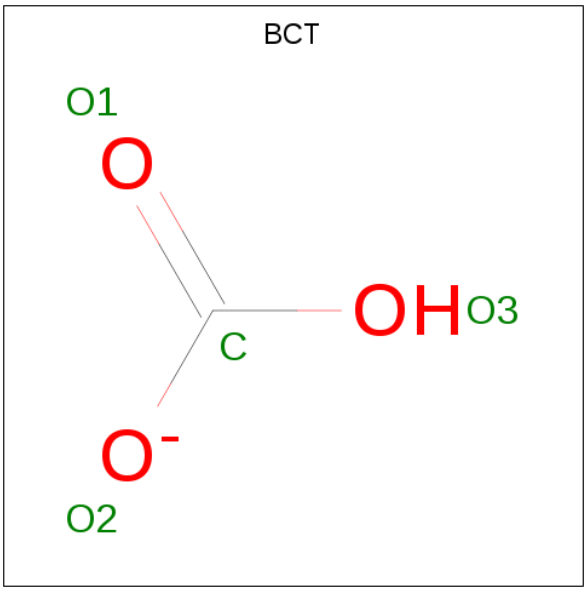
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	AA	1	Total Cl 1 1	0	0
31	BA	1	Total Cl 1 1	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



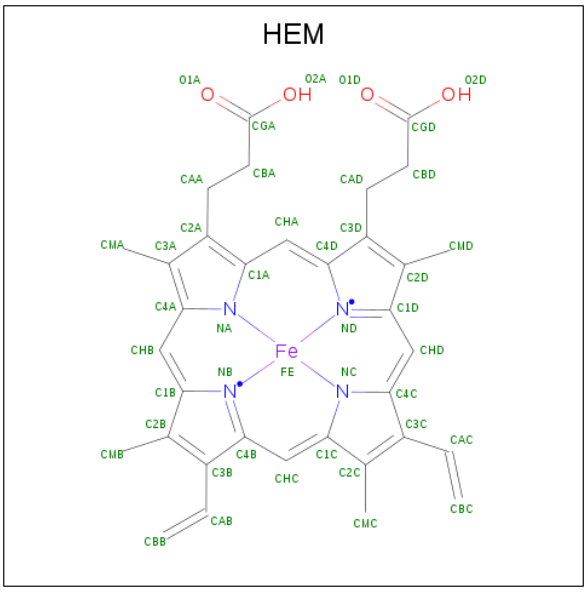
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AD	1	Total C O 31 20 11	0	0
32	AI	1	Total C O 35 24 11	0	0
32	AM	1	Total C O 35 24 11	0	0
32	AT	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BD	1	Total C O 31 20 11	0	0
32	BI	1	Total C O 35 24 11	0	0
32	BM	1	Total C O 35 24 11	0	0
32	BT	1	Total C O 35 24 11	0	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	AD	1	Total C O 4 1 3	0	0
33	BD	1	Total C O 4 1 3	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	AE	1	Total C Fe N O 43 34 1 4 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	AV	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	BE	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	BV	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

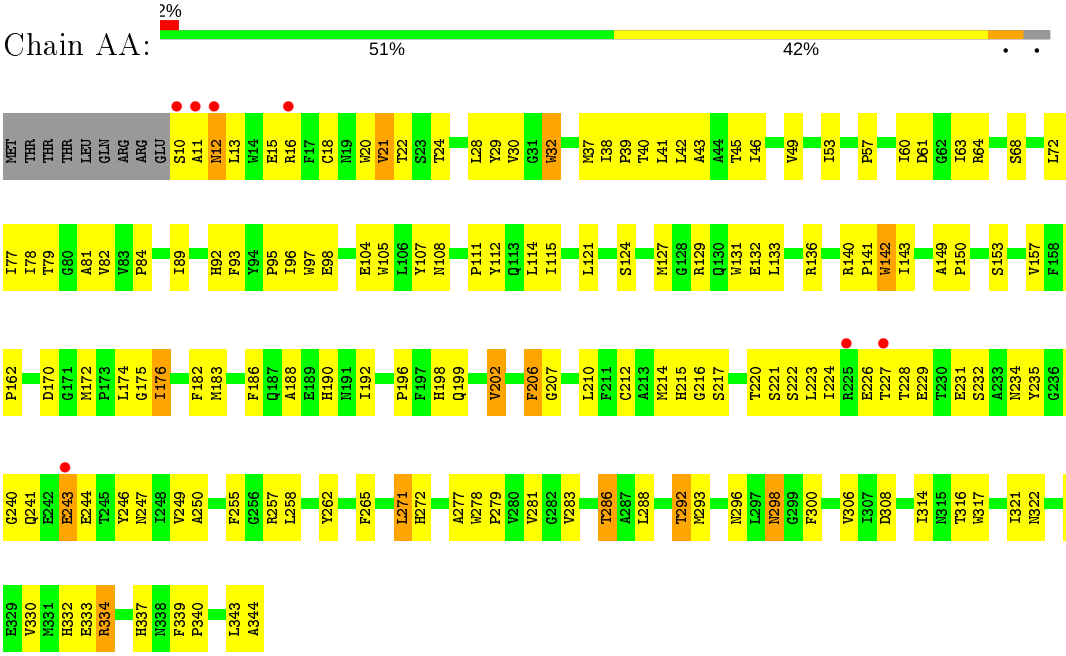
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	AO	1	Total	Ca	0	0
			1	1		
35	BO	1	Total	Ca	0	0
			1	1		
35	AK	1	Total	Ca	0	0
			1	1		
35	BK	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

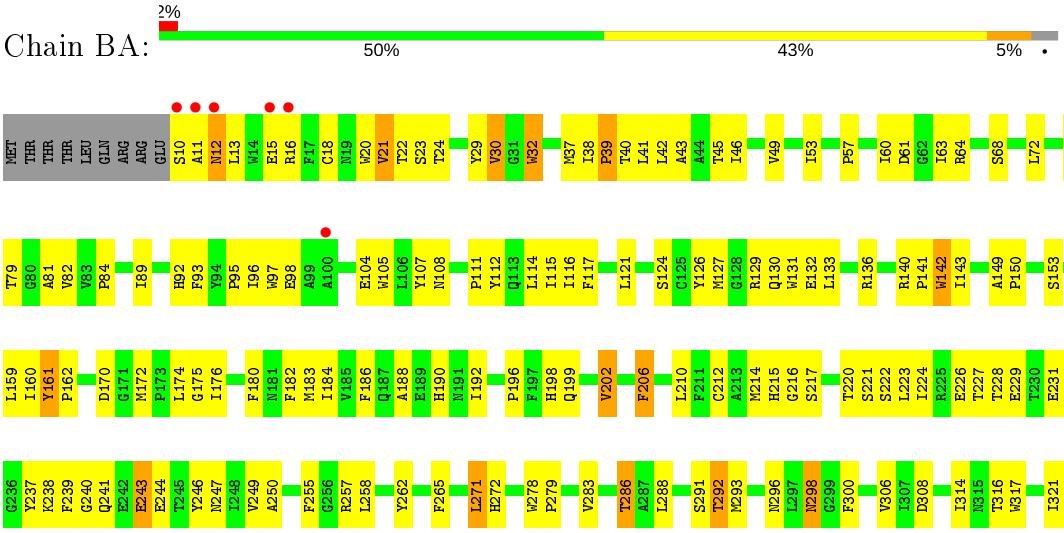
- Molecule 1: Photosystem Q(B) protein

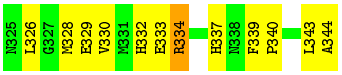
Chain AA:



- Molecule 1: Photosystem Q(B) protein

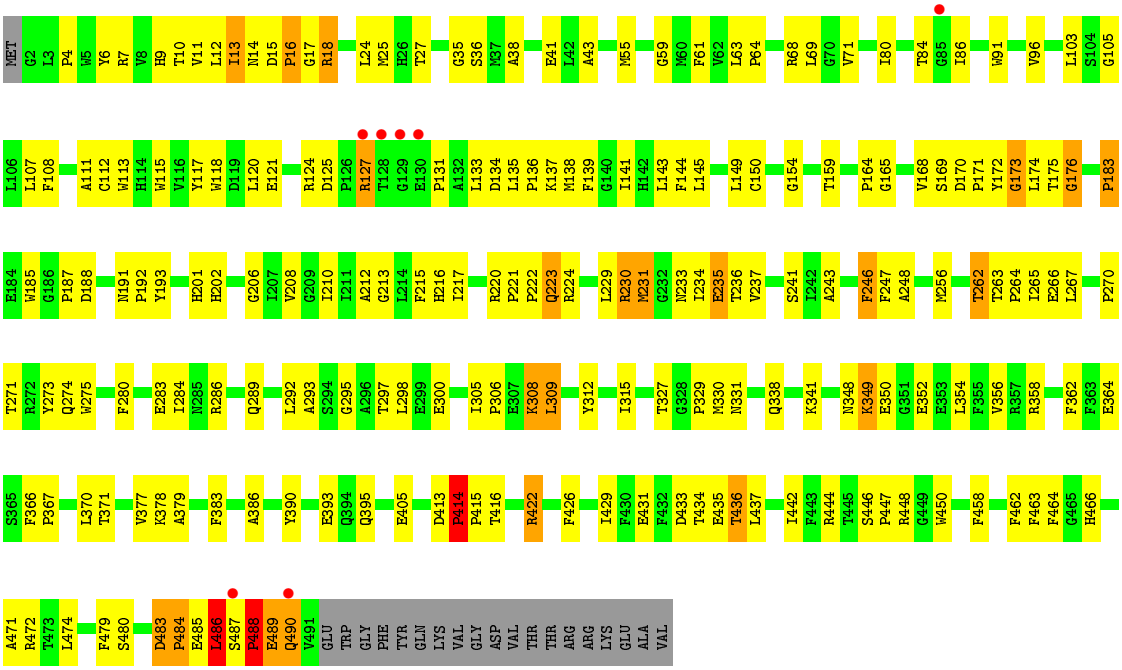
Chain BA:





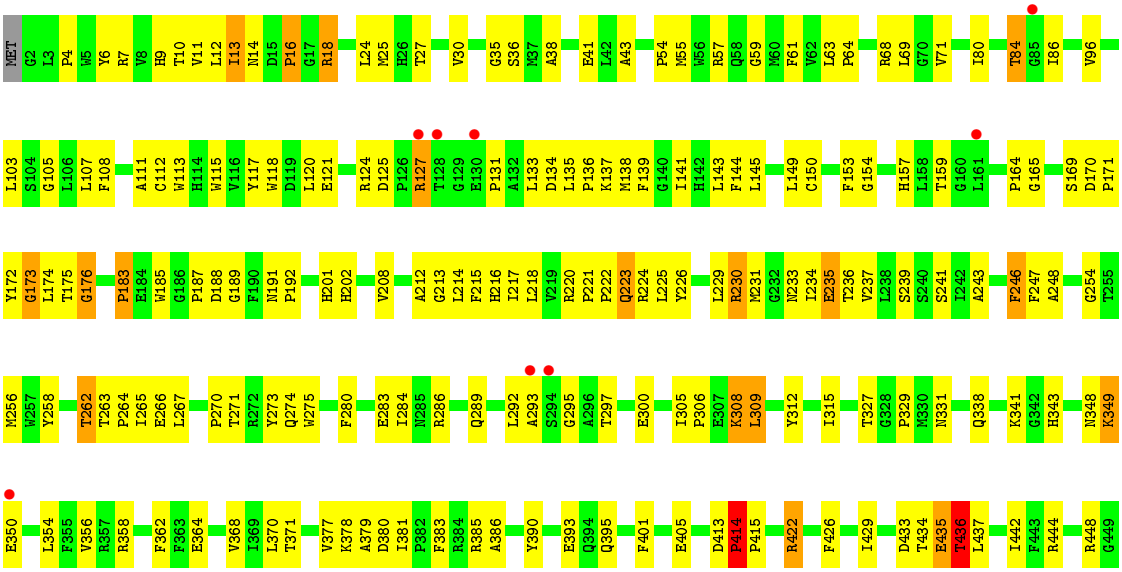
• Molecule 2: Photosystem II core light harvesting protein

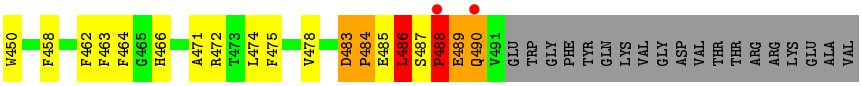
Chain AB:



• Molecule 2: Photosystem II core light harvesting protein

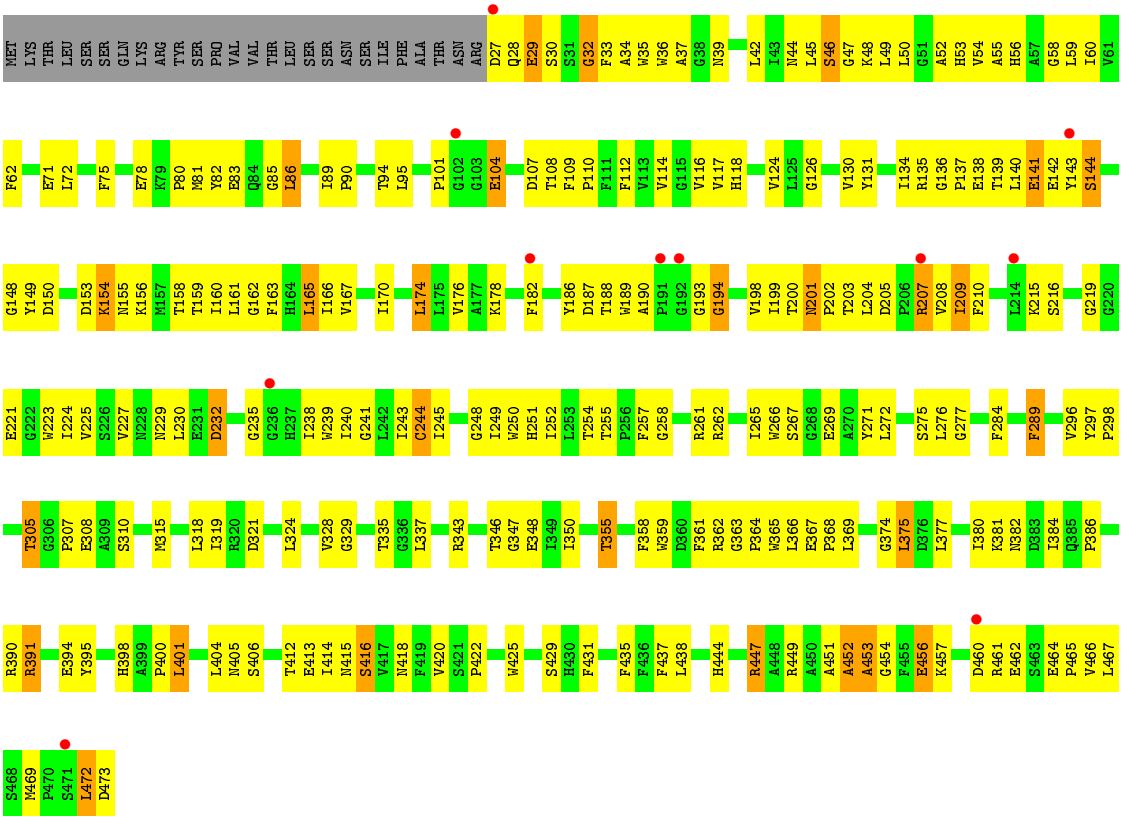
Chain BB:





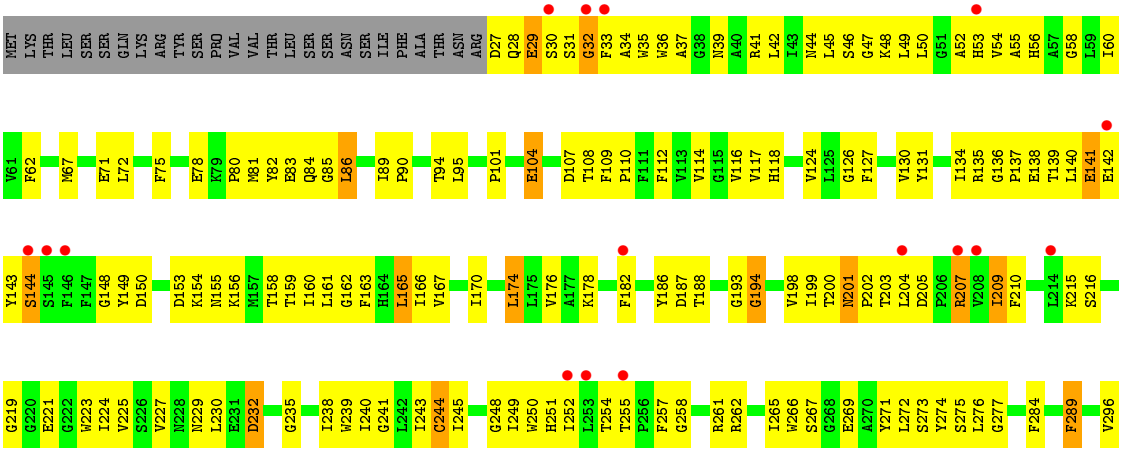
- Molecule 3: Photosystem II CP43 protein

Chain AC:



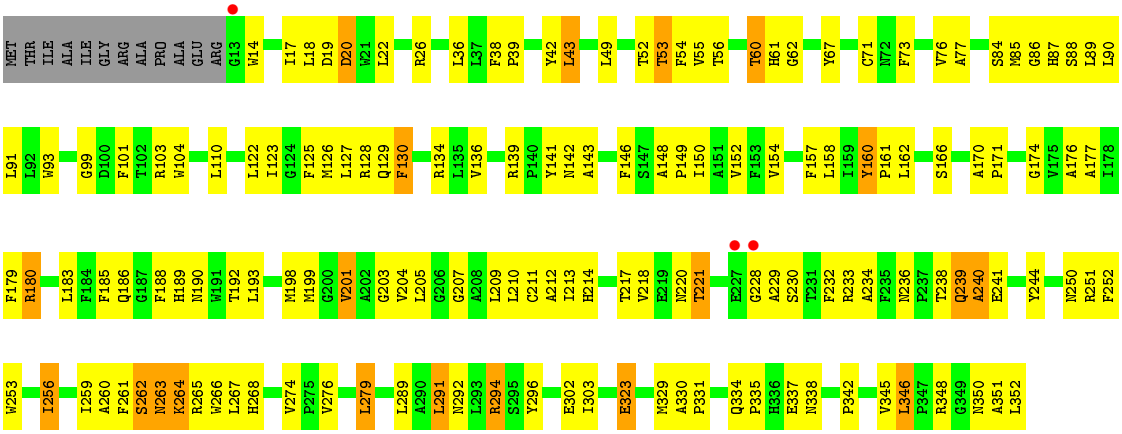
- Molecule 3: Photosystem II CP43 protein

Chain BC:



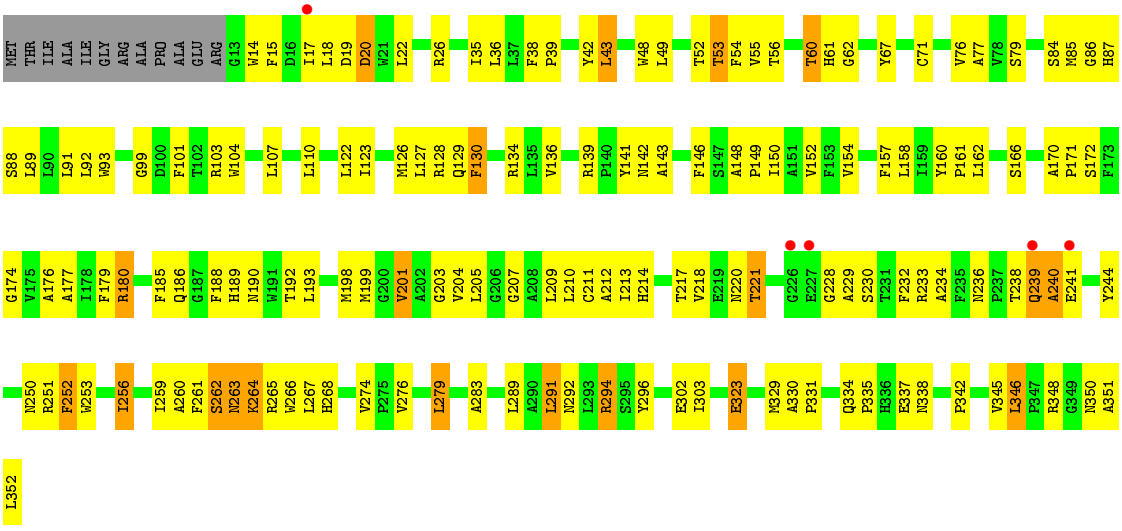
• Molecule 4: Photosystem II reaction center D2 protein

Chain AD:



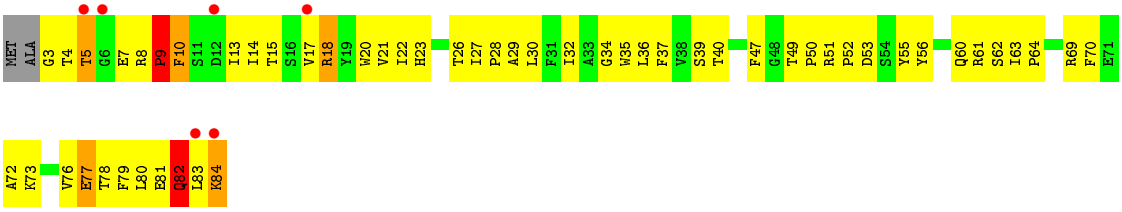
• Molecule 4: Photosystem II reaction center D2 protein

Chain BD:

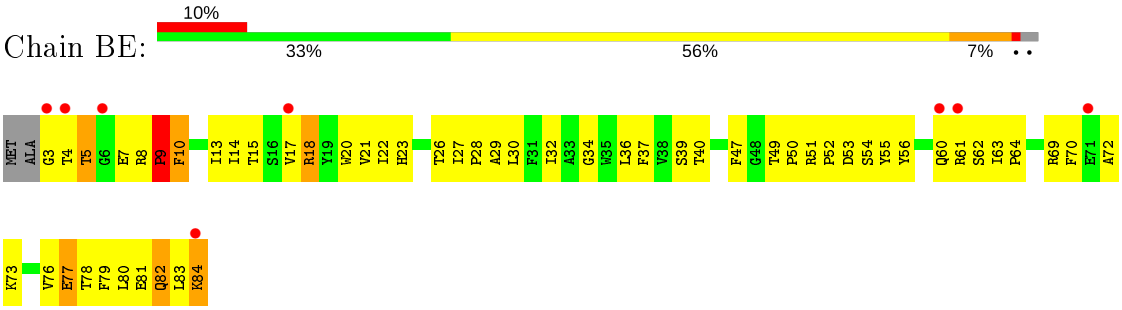


• Molecule 5: Cytochrome b559 subunit alpha

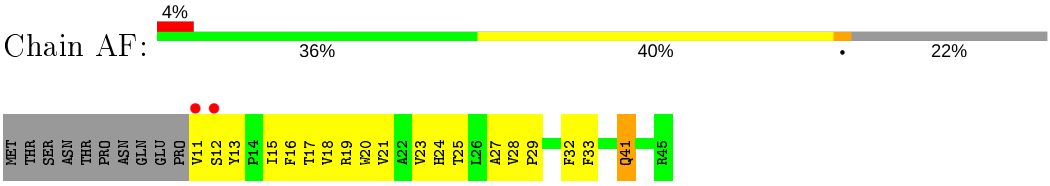
Chain AE:



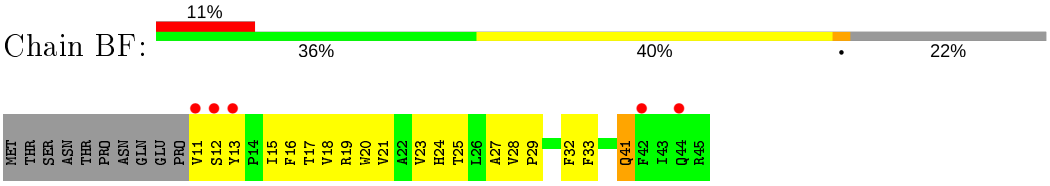
• Molecule 5: Cytochrome b559 subunit alpha



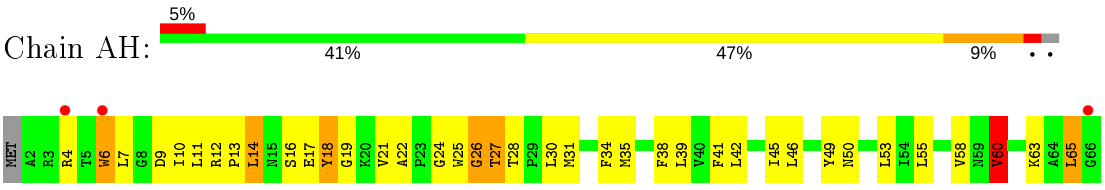
• Molecule 6: Cytochrome b559 subunit beta



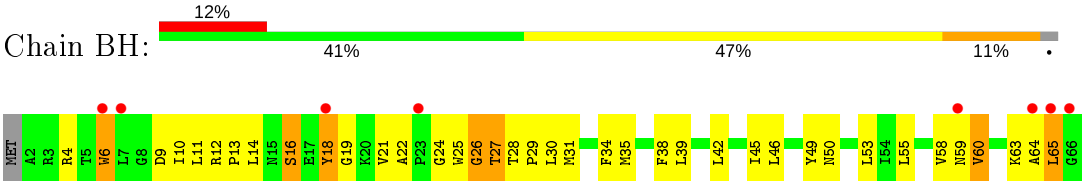
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H

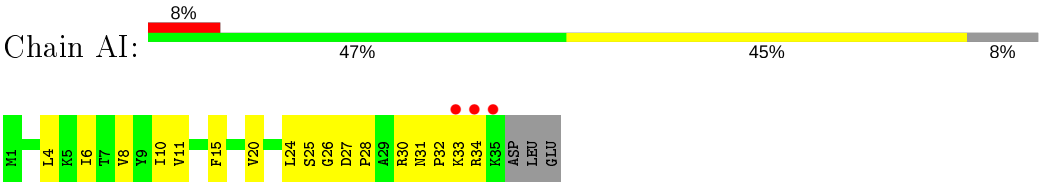


• Molecule 7: Photosystem II reaction center protein H



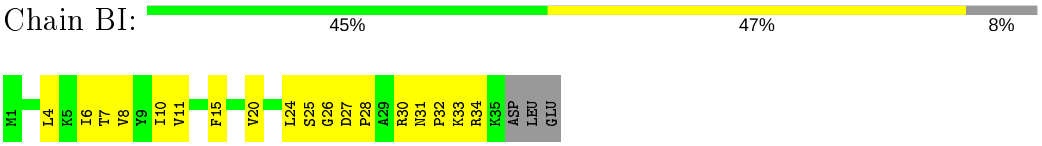
• Molecule 8: Photosystem II reaction center protein I

Chain AI:



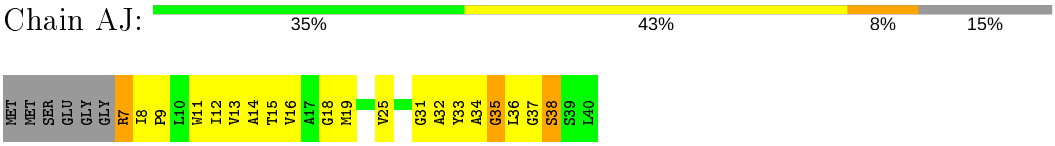
• Molecule 8: Photosystem II reaction center protein I

Chain BI:



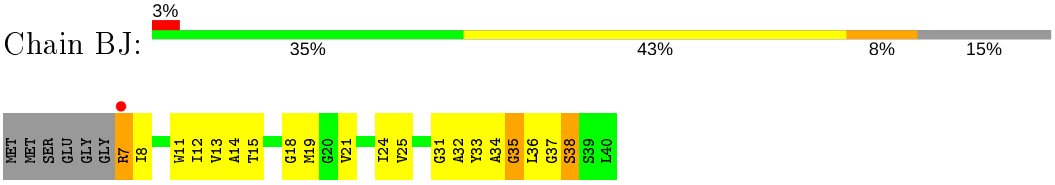
• Molecule 9: Photosystem II reaction center protein J

Chain AJ:



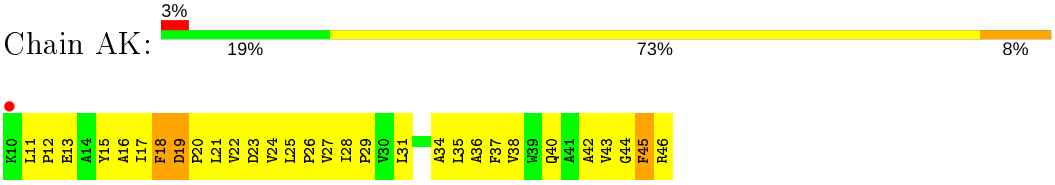
• Molecule 9: Photosystem II reaction center protein J

Chain BJ:



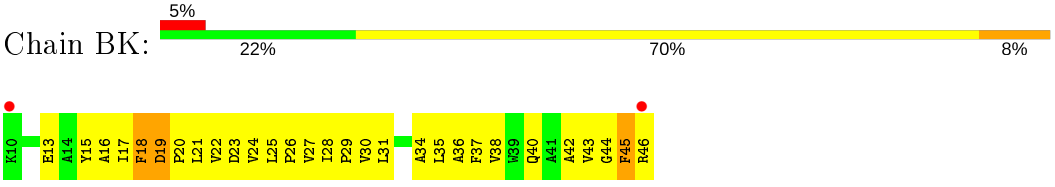
• Molecule 10: Photosystem II reaction center protein K

Chain AK:



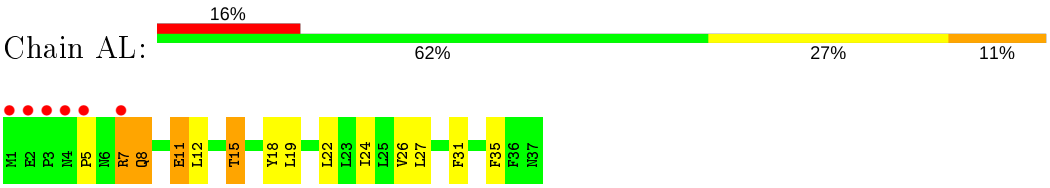
• Molecule 10: Photosystem II reaction center protein K

Chain BK:



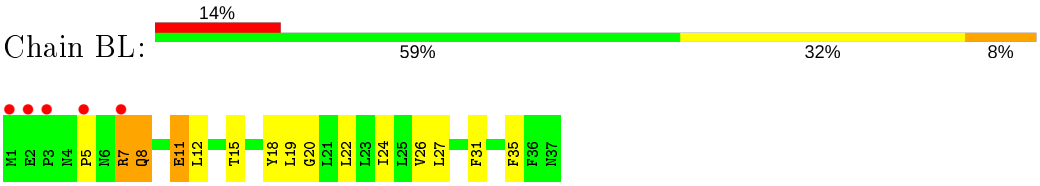
• Molecule 11: Photosystem II reaction center protein L

Chain AL:



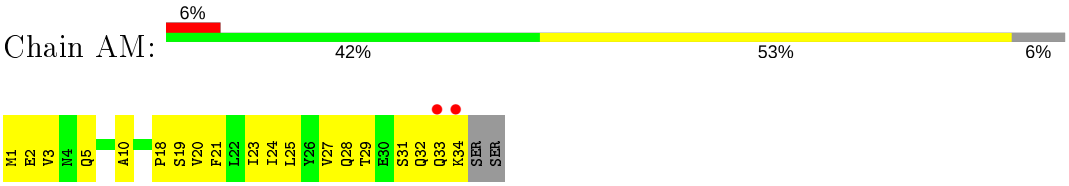
• Molecule 11: Photosystem II reaction center protein L

Chain BL:



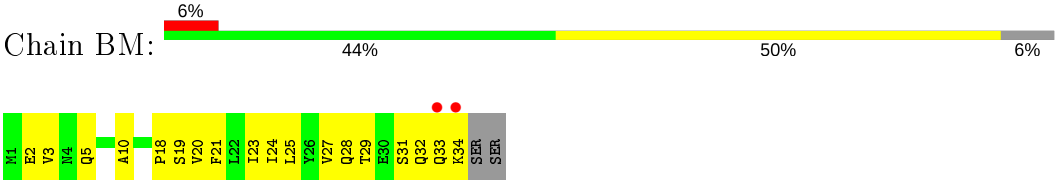
• Molecule 12: Photosystem II reaction center protein M

Chain AM:



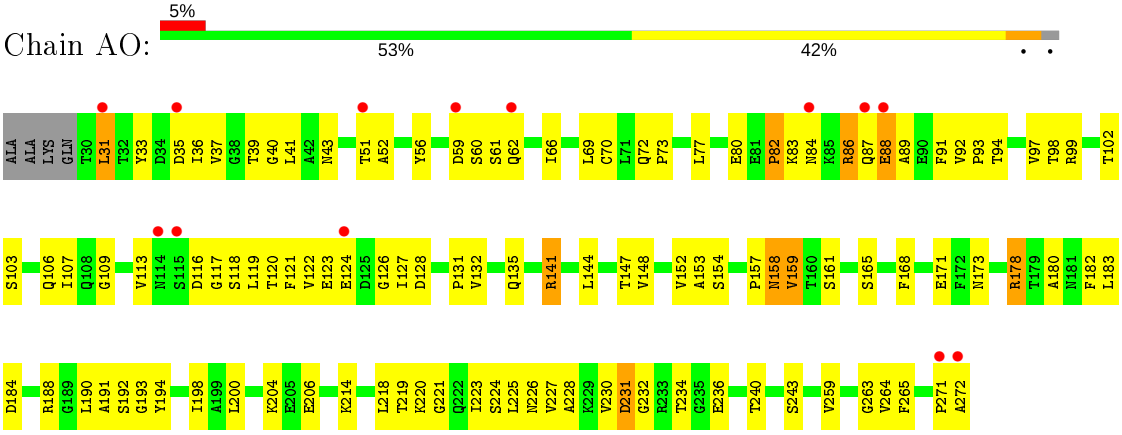
• Molecule 12: Photosystem II reaction center protein M

Chain BM:



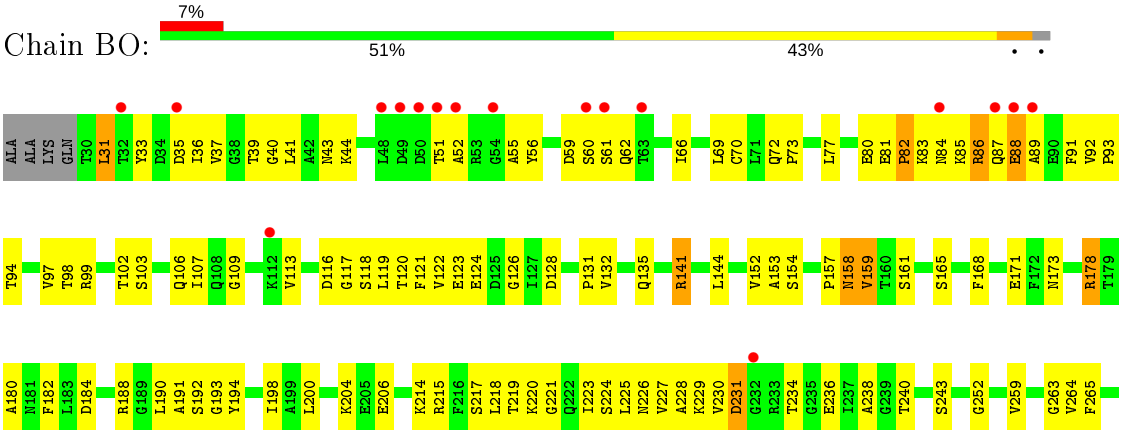
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO:



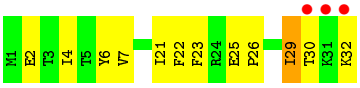
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain BO:



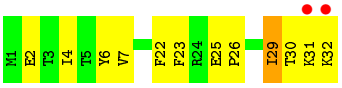
• Molecule 14: Photosystem II reaction center protein T

Chain AT:



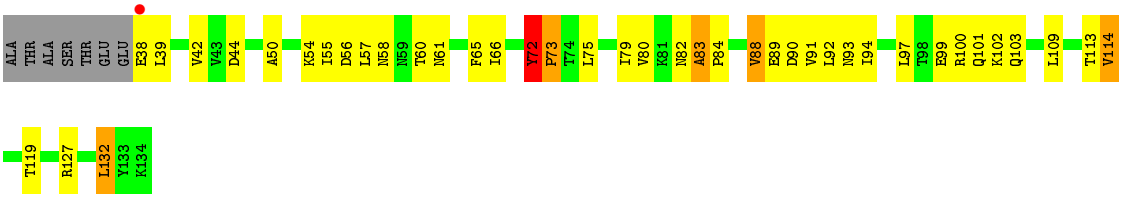
• Molecule 14: Photosystem II reaction center protein T

Chain BT:



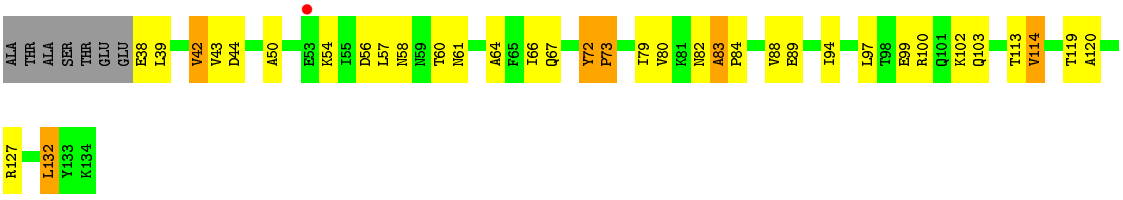
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain AU:



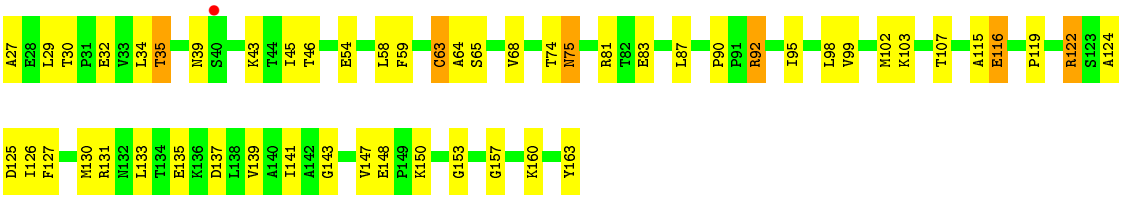
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain BU:



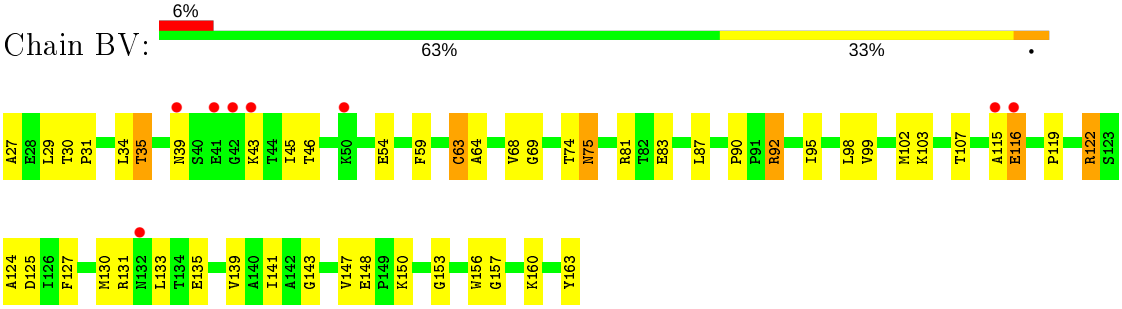
• Molecule 16: Cytochrome c-550

Chain AV:



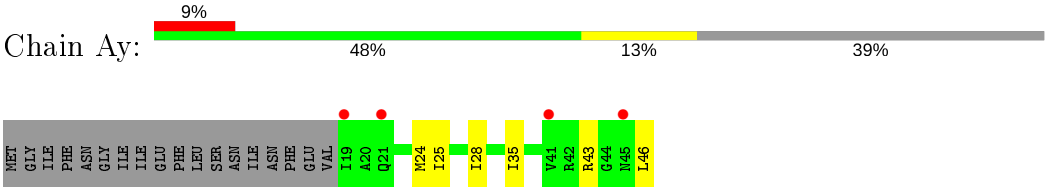
• Molecule 16: Cytochrome c-550

Chain BV:



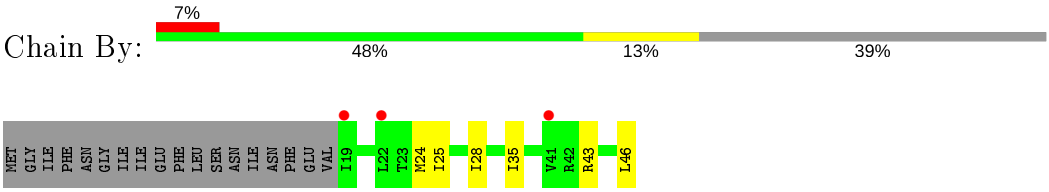
• Molecule 17: Protein ycf12

Chain Ay:



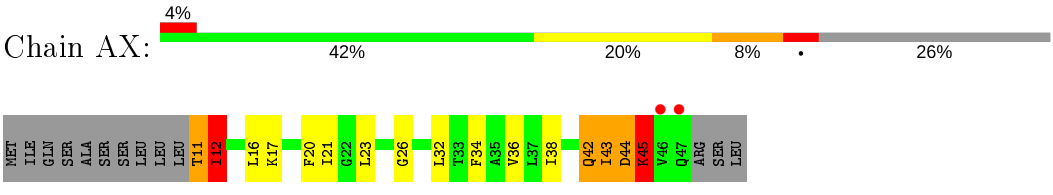
• Molecule 17: Protein ycf12

Chain By:



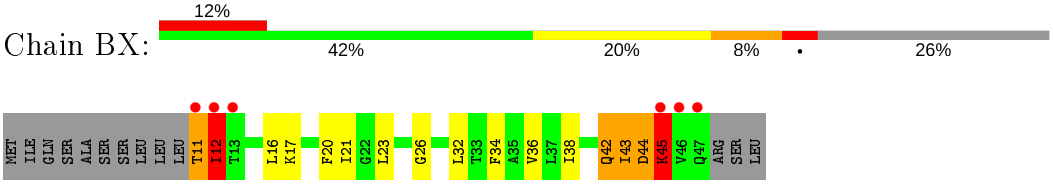
• Molecule 18: Photosystem II PsbX protein

Chain AX:



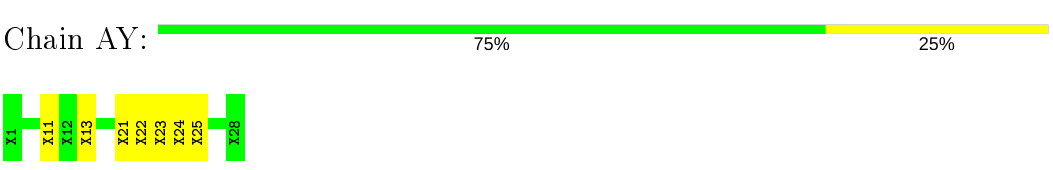
• Molecule 18: Photosystem II PsbX protein

Chain BX:



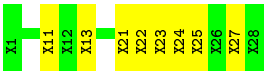
• Molecule 19: Photosystem II protein Y

Chain AY:



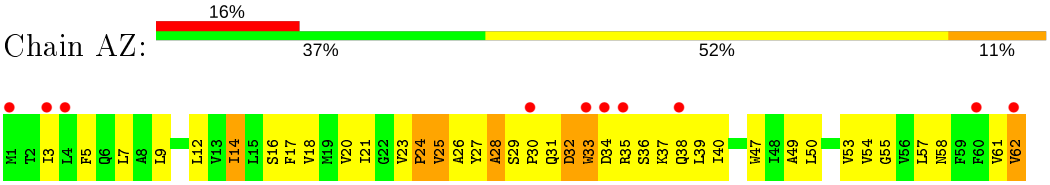
• Molecule 19: Photosystem II protein Y

Chain BY:



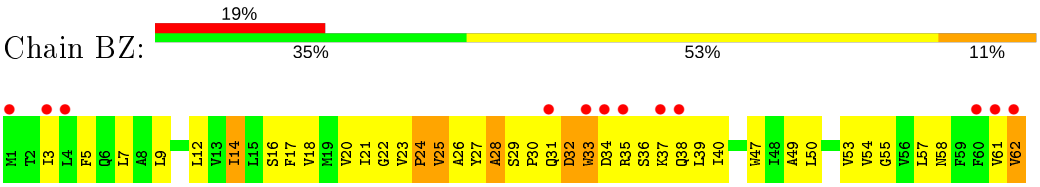
• Molecule 20: Photosystem II reaction center protein Z

Chain AZ:



• Molecule 20: Photosystem II reaction center protein Z

Chain BZ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.90) 99.3 (20.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292 0.242 , 0.278	Depositor DCC
R_{free} test set	3869 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 71.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: LHG, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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	AA	0.44	0/2713	0.66	0/3700
1	BA	0.43	0/2713	0.65	0/3700
2	AB	0.44	0/3986	0.67	3/5433 (0.1%)
2	BB	0.43	0/3986	0.66	3/5433 (0.1%)
3	AC	0.41	0/3556	0.64	1/4842 (0.0%)
3	BC	0.39	0/3556	0.63	1/4842 (0.0%)
4	AD	0.47	0/2801	0.65	0/3818
4	BD	0.45	0/2801	0.65	0/3818
5	AE	0.45	0/685	0.71	0/933
5	BE	0.45	0/685	0.70	0/933
6	AF	0.45	0/291	0.59	0/397
6	BF	0.47	0/291	0.57	0/397
7	AH	0.42	0/520	0.73	1/709 (0.1%)
7	BH	0.40	0/520	0.72	1/709 (0.1%)
8	AI	0.51	0/293	0.68	0/395
8	BI	0.50	0/293	0.67	0/395
9	AJ	0.43	0/255	0.69	0/346
9	BJ	0.45	0/255	0.66	0/346
10	AK	0.43	0/303	0.63	0/416
10	BK	0.44	0/303	0.61	0/416
11	AL	0.39	0/311	0.65	0/422
11	BL	0.41	0/311	0.65	0/422
12	AM	0.44	0/270	0.70	0/367
12	BM	0.45	0/270	0.67	0/367
13	AO	0.44	0/1876	0.70	0/2548
13	BO	0.43	0/1876	0.70	0/2548
14	AT	0.50	0/284	0.62	0/381
14	BT	0.48	0/284	0.62	0/381
15	AU	0.42	0/785	0.73	1/1064 (0.1%)
15	BU	0.40	0/785	0.73	0/1064
16	AV	0.38	0/1081	0.65	0/1468
16	BV	0.37	0/1081	0.64	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Ay	0.46	0/202	0.73	0/272
17	By	0.41	0/202	0.74	0/272
18	AX	0.43	0/273	0.63	0/370
18	BX	0.41	0/273	0.63	0/370
20	AZ	0.45	0/490	0.69	0/669
20	BZ	0.47	0/490	0.70	0/669
All	All	0.43	0/41950	0.66	11/57100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
1	BA	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BB	486	LEU	CA-CB-CG	7.12	131.67	115.30
2	AB	486	LEU	CA-CB-CG	6.99	131.39	115.30
2	AB	488	PRO	N-CA-C	5.86	127.33	112.10
2	AB	489	GLU	N-CA-C	5.76	126.56	111.00
7	AH	65	LEU	CA-CB-CG	5.72	128.45	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	161	TYR	Sidechain
1	BA	161	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2628	0	2524	179	0
1	BA	2628	0	2524	179	0
2	AB	3850	0	3718	224	0
2	BB	3850	0	3718	227	0
3	AC	3444	0	3365	258	0
3	BC	3444	0	3365	263	0
4	AD	2706	0	2608	177	0
4	BD	2706	0	2608	184	0
5	AE	666	0	651	71	0
5	BE	666	0	651	74	0
6	AF	282	0	291	28	0
6	BF	282	0	291	29	0
7	AH	507	0	521	52	0
7	BH	507	0	521	50	0
8	AI	286	0	308	15	0
8	BI	286	0	308	18	0
9	AJ	249	0	262	28	0
9	BJ	249	0	262	26	0
10	AK	293	0	305	42	0
10	BK	293	0	305	44	0
11	AL	304	0	316	15	0
11	BL	304	0	316	17	0
12	AM	267	0	289	27	0
12	BM	267	0	289	26	0
13	AO	1845	0	1801	115	0
13	BO	1845	0	1801	118	0
14	AT	275	0	288	21	0
14	BT	275	0	288	20	0
15	AU	774	0	773	46	0
15	BU	774	0	773	42	0
16	AV	1060	0	1068	42	0
16	BV	1060	0	1068	39	0
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	27	0
18	BX	270	0	299	25	0
19	AY	140	0	32	4	0
19	BY	140	0	32	6	0
20	AZ	479	0	516	54	0
20	BZ	479	0	516	55	0
21	AA	1	0	0	0	0
21	BA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AA	260	0	288	18	0
22	AB	1040	0	1152	77	0
22	AC	845	0	936	61	0
22	AD	130	0	144	11	0
22	BA	260	0	288	18	0
22	BB	1040	0	1152	83	0
22	BC	845	0	936	62	0
22	BD	130	0	144	12	0
23	AA	64	0	74	5	0
23	AD	64	0	74	2	0
23	BA	64	0	74	5	0
23	BD	64	0	74	5	0
24	AA	45	0	61	5	0
24	AD	55	0	80	9	0
24	AJ	35	0	45	0	0
24	BA	45	0	61	6	0
24	BD	55	0	80	8	0
24	BJ	35	0	45	0	0
25	AA	5	0	0	0	0
25	BA	5	0	0	0	0
26	AA	40	0	56	6	0
26	AB	160	0	224	10	0
26	AC	80	0	112	15	0
26	AD	40	0	56	3	0
26	AH	40	0	56	5	0
26	AJ	40	0	56	5	0
26	AK	40	0	56	13	0
26	AT	40	0	56	8	0
26	AZ	40	0	56	5	0
26	BA	40	0	56	3	0
26	BB	120	0	168	5	0
26	BC	80	0	112	17	0
26	BD	40	0	56	3	0
26	BJ	40	0	56	5	0
26	BK	40	0	56	13	0
26	BX	40	0	56	6	0
26	BZ	40	0	56	5	0
27	AA	56	0	70	0	0
27	AB	52	0	62	3	0
27	AC	181	0	245	19	0
27	AD	63	0	87	0	0
27	AH	58	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BA	56	0	70	0	0
27	BB	52	0	62	3	0
27	BC	181	0	245	21	0
27	BD	63	0	87	0	0
27	BH	58	0	74	1	0
28	AA	39	0	51	3	0
28	AC	37	0	44	5	0
28	BA	39	0	51	4	0
28	BC	37	0	44	4	0
29	AA	105	0	145	10	0
29	AD	43	0	49	2	0
29	AF	45	0	53	2	0
29	BA	105	0	145	6	0
29	BB	47	0	60	2	0
29	BD	43	0	49	2	0
29	BF	45	0	53	1	0
29	BL	47	0	60	2	0
30	AA	93	0	126	5	0
30	AB	140	0	190	4	0
30	AC	93	0	126	6	0
30	AD	94	0	128	9	0
30	AE	44	0	58	4	0
30	AI	43	0	56	3	0
30	AM	42	0	54	4	0
30	BA	51	0	72	2	0
30	BB	98	0	136	2	0
30	BC	93	0	126	8	0
30	BD	94	0	128	10	0
30	BE	44	0	58	4	0
30	BI	43	0	56	3	0
30	BM	42	0	54	4	0
31	AA	1	0	0	0	0
31	BA	1	0	0	0	0
32	AB	105	0	138	6	0
32	AD	31	0	35	2	0
32	AI	35	0	46	4	0
32	AM	35	0	46	1	0
32	AT	35	0	46	3	0
32	BB	105	0	138	5	0
32	BD	31	0	35	1	0
32	BI	35	0	46	3	0
32	BM	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BT	35	0	46	3	0
33	AD	4	0	0	1	0
33	BD	4	0	0	1	0
34	AE	43	0	30	5	0
34	AV	43	0	30	3	0
34	BE	43	0	30	6	0
34	BV	43	0	30	3	0
35	AK	1	0	0	0	0
35	AO	1	0	0	0	0
35	BK	1	0	0	0	0
35	BO	1	0	0	0	0
All	All	50234	0	51364	2715	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 2715 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:63:CYS:SG	34:AV:201:HEM:HAB	1.85	1.16
15:BU:83:ALA:HB1	15:BU:84:PRO:HD2	1.23	1.16
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.23	1.16
16:BV:63:CYS:SG	34:BV:201:HEM:HAB	1.85	1.15
9:BJ:15:THR:HG21	10:BK:38:VAL:HG13	1.24	1.13

There are no symmetry-related clashes.

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	AA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	7 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	7 26
2	AB	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	4 18
2	BB	488/510 (96%)	422 (86%)	52 (11%)	14 (3%)	4 18
3	AC	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	3 14
3	BC	445/473 (94%)	372 (84%)	56 (13%)	17 (4%)	3 13
4	AD	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	5 19
4	BD	338/352 (96%)	288 (85%)	42 (12%)	8 (2%)	6 22
5	AE	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	2 7
5	BE	80/84 (95%)	70 (88%)	6 (8%)	4 (5%)	2 7
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	4 17
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	4 17
7	AH	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	0 1
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	1 4
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1 4
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	1 4
9	AJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1 4
9	BJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1 4
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 5
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 5
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	AM	32/36 (89%)	23 (72%)	9 (28%)	0	100 100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100 100
13	AO	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	2 7
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	2 9
14	AT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4 15
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4 15
15	AU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3 10
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3 10
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	22 54
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	22 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Ay	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
17	By	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
18	AX	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	0	1
18	BX	35/50 (70%)	27 (77%)	4 (11%)	4 (11%)	0	1
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	7
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	7
All	All	5138/5480 (94%)	4278 (83%)	679 (13%)	181 (4%)	3	14

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG

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	AA	271/280 (97%)	258 (95%)	13 (5%)	25	58
1	BA	271/280 (97%)	259 (96%)	12 (4%)	28	61
2	AB	390/407 (96%)	374 (96%)	16 (4%)	30	64
2	BB	390/407 (96%)	373 (96%)	17 (4%)	28	61
3	AC	347/374 (93%)	329 (95%)	18 (5%)	23	55
3	BC	347/374 (93%)	329 (95%)	18 (5%)	23	55
4	AD	275/283 (97%)	256 (93%)	19 (7%)	15	41
4	BD	275/283 (97%)	256 (93%)	19 (7%)	15	41
5	AE	72/73 (99%)	66 (92%)	6 (8%)	11	32
5	BE	72/73 (99%)	66 (92%)	6 (8%)	11	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	29/39 (74%)	29 (100%)	0	100	100
6	BF	29/39 (74%)	29 (100%)	0	100	100
7	AH	53/55 (96%)	50 (94%)	3 (6%)	20	51
7	BH	53/55 (96%)	50 (94%)	3 (6%)	20	51
8	AI	32/35 (91%)	31 (97%)	1 (3%)	40	74
8	BI	32/35 (91%)	31 (97%)	1 (3%)	40	74
9	AJ	24/28 (86%)	23 (96%)	1 (4%)	30	63
9	BJ	24/28 (86%)	23 (96%)	1 (4%)	30	63
10	AK	30/30 (100%)	28 (93%)	2 (7%)	16	43
10	BK	30/30 (100%)	28 (93%)	2 (7%)	16	43
11	AL	35/35 (100%)	31 (89%)	4 (11%)	5	17
11	BL	35/35 (100%)	32 (91%)	3 (9%)	10	30
12	AM	31/33 (94%)	31 (100%)	0	100	100
12	BM	31/33 (94%)	31 (100%)	0	100	100
13	AO	202/208 (97%)	195 (96%)	7 (4%)	36	70
13	BO	202/208 (97%)	194 (96%)	8 (4%)	31	65
14	AT	29/29 (100%)	28 (97%)	1 (3%)	37	71
14	BT	29/29 (100%)	28 (97%)	1 (3%)	37	71
15	AU	84/89 (94%)	80 (95%)	4 (5%)	25	58
15	BU	84/89 (94%)	80 (95%)	4 (5%)	25	58
16	AV	116/117 (99%)	111 (96%)	5 (4%)	29	62
16	BV	116/117 (99%)	111 (96%)	5 (4%)	29	62
17	Ay	20/37 (54%)	18 (90%)	2 (10%)	7	23
17	By	20/37 (54%)	18 (90%)	2 (10%)	7	23
18	AX	30/42 (71%)	26 (87%)	4 (13%)	4	11
18	BX	30/42 (71%)	26 (87%)	4 (13%)	4	11
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	8	25
20	BZ	52/52 (100%)	47 (90%)	5 (10%)	8	25
All	All	4244/4492 (94%)	4022 (95%)	222 (5%)	23	55

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Ay	28	ILE
2	BB	18	ARG
15	BU	132	LEU
18	AX	12	ILE
1	BA	32	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
15	AU	93	ASN
1	BA	241	GLN
13	BO	222	GLN
17	Ay	21	GLN
1	BA	12	ASN

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 carbohydrates 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	$\#\|Z\|>2$
32	LMT	AI	102	-	36,36,36	1.44	4 (11%)	47,47,47	0.96	1 (2%)
28	LHG	AA	411	-	38,38,48	1.99	5 (13%)	41,44,54	1.40	4 (9%)
22	CLA	AB	614	2	59,73,73	1.49	9 (15%)	67,113,113	2.09	16 (23%)
32	LMT	BI	102	-	36,36,36	1.54	4 (11%)	47,47,47	0.97	2 (4%)
22	CLA	BB	617	2	59,73,73	1.44	7 (11%)	67,113,113	2.04	15 (22%)
26	BCR	AK	102	-	41,41,41	1.85	7 (17%)	56,56,56	2.52	24 (42%)
26	BCR	BB	621	-	41,41,41	1.86	6 (14%)	56,56,56	2.12	16 (28%)
26	BCR	AB	617	-	41,41,41	1.69	8 (19%)	56,56,56	1.98	14 (25%)
22	CLA	BC	501	3	59,73,73	1.44	7 (11%)	67,113,113	2.01	13 (19%)
22	CLA	AC	510	-	59,73,73	1.29	8 (13%)	67,113,113	1.90	11 (16%)
22	CLA	AA	403	-	59,73,73	1.34	7 (11%)	67,113,113	1.98	15 (22%)
22	CLA	BB	615	-	59,73,73	1.36	7 (11%)	67,113,113	1.98	13 (19%)
22	CLA	AB	613	-	59,73,73	1.22	6 (10%)	67,113,113	1.96	11 (16%)
30	LMG	AC	520	-	45,45,55	1.54	9 (20%)	53,53,63	1.01	4 (7%)
27	DGD	AB	626	-	53,53,67	1.88	17 (32%)	67,67,81	1.58	8 (11%)
26	BCR	AH	101	-	41,41,41	1.86	8 (19%)	56,56,56	2.25	22 (39%)
27	DGD	AH	102	-	59,59,67	1.28	9 (15%)	73,73,81	1.43	7 (9%)
22	CLA	BB	611	2	59,73,73	1.42	9 (15%)	67,113,113	1.96	16 (23%)
22	CLA	BA	407	1	59,73,73	1.29	7 (11%)	67,113,113	1.89	11 (16%)
26	BCR	BA	410	-	41,41,41	1.71	7 (17%)	56,56,56	2.07	23 (41%)
33	BCT	AD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
30	LMG	AB	623	-	42,42,55	1.50	8 (19%)	50,50,63	1.00	3 (6%)
22	CLA	BC	504	-	59,73,73	1.33	8 (13%)	67,113,113	1.93	12 (17%)
30	LMG	AM	101	-	42,42,55	1.63	7 (16%)	50,50,63	1.16	5 (10%)
22	CLA	AD	404	-	59,73,73	1.46	7 (11%)	67,113,113	1.99	12 (17%)
22	CLA	BB	608	2	59,73,73	1.35	7 (11%)	67,113,113	1.92	11 (16%)
32	LMT	BB	625	-	36,36,36	1.57	9 (25%)	47,47,47	1.25	3 (6%)
22	CLA	BC	512	-	59,73,73	1.59	7 (11%)	67,113,113	2.07	13 (19%)
34	HEM	BV	201	16	27,50,50	1.99	8 (29%)	17,82,82	2.25	5 (29%)
27	DGD	AC	517	-	63,63,67	1.07	5 (7%)	77,77,81	1.62	10 (12%)
29	SQD	BD	409	-	42,43,54	2.66	19 (45%)	51,54,65	2.96	15 (29%)
22	CLA	AB	605	-	59,73,73	1.43	7 (11%)	67,113,113	1.93	12 (17%)
22	CLA	AC	503	3	59,73,73	1.58	9 (15%)	67,113,113	2.07	9 (13%)
30	LMG	AB	622	-	49,49,55	1.08	6 (12%)	57,57,63	1.03	3 (5%)
29	SQD	AD	409	-	42,43,54	2.69	19 (45%)	51,54,65	2.97	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	AB	611	2	59,73,73	1.25	6 (10%)	67,113,113	1.94	12 (17%)
28	LHG	BC	521	-	36,36,48	1.08	2 (5%)	39,42,54	1.13	3 (7%)
32	LMT	BM	101	-	36,36,36	1.21	3 (8%)	47,47,47	0.96	2 (4%)
30	LMG	BA	414	-	51,51,55	0.93	4 (7%)	59,59,63	1.01	4 (6%)
22	CLA	AB	606	2	59,73,73	1.43	6 (10%)	67,113,113	1.93	11 (16%)
22	CLA	AB	603	2	59,73,73	1.37	8 (13%)	67,113,113	1.96	14 (20%)
34	HEM	BE	101	5,6	27,50,50	2.07	7 (25%)	17,82,82	2.51	5 (29%)
26	BCR	AZ	101	-	41,41,41	1.85	7 (17%)	56,56,56	2.09	18 (32%)
22	CLA	BB	612	2	59,73,73	1.52	7 (11%)	67,113,113	1.95	14 (20%)
22	CLA	BB	618	-	59,73,73	1.28	7 (11%)	67,113,113	2.05	12 (17%)
29	SQD	BA	401	-	53,54,54	2.55	28 (52%)	62,65,65	2.71	22 (35%)
26	BCR	BB	620	-	41,41,41	1.57	8 (19%)	56,56,56	1.99	15 (26%)
30	LMG	BE	102	-	44,44,55	1.36	6 (13%)	52,52,63	1.07	5 (9%)
22	CLA	BA	404	-	59,73,73	1.34	7 (11%)	67,113,113	2.06	14 (20%)
27	DGD	AA	410	-	57,57,67	1.51	12 (21%)	71,71,81	1.46	9 (12%)
23	PHO	AD	403	-	67,69,69	1.08	5 (7%)	85,99,99	1.41	13 (15%)
29	SQD	AA	412	-	50,51,54	2.39	24 (48%)	59,62,65	2.78	19 (32%)
22	CLA	BB	605	2	59,73,73	1.31	7 (11%)	67,113,113	1.84	13 (19%)
27	DGD	AC	518	-	67,67,67	1.05	6 (8%)	81,81,81	1.27	4 (4%)
22	CLA	BC	508	3	59,73,73	1.51	8 (13%)	67,113,113	2.03	12 (17%)
22	CLA	BA	405	-	59,73,73	1.28	6 (10%)	67,113,113	1.96	12 (17%)
26	BCR	AB	618	-	41,41,41	1.71	6 (14%)	56,56,56	2.20	26 (46%)
24	PL9	BA	408	-	45,45,55	1.00	2 (4%)	56,57,69	1.64	16 (28%)
29	SQD	BL	101	-	46,47,54	2.63	22 (47%)	55,58,65	2.69	15 (27%)
22	CLA	AC	506	3	59,73,73	1.41	7 (11%)	67,113,113	2.02	12 (17%)
32	LMT	AB	624	-	36,36,36	1.46	8 (22%)	47,47,47	1.23	3 (6%)
30	LMG	BB	623	-	49,49,55	1.09	5 (10%)	57,57,63	1.05	4 (7%)
22	CLA	BB	604	-	59,73,73	1.71	10 (16%)	67,113,113	2.06	13 (19%)
22	CLA	BB	607	2	59,73,73	1.57	8 (13%)	67,113,113	2.05	11 (16%)
27	DGD	BC	516	-	54,54,67	1.36	9 (16%)	68,68,81	1.50	6 (8%)
26	BCR	AA	409	-	41,41,41	1.64	7 (17%)	56,56,56	2.08	20 (35%)
22	CLA	AC	509	-	59,73,73	1.38	7 (11%)	67,113,113	1.99	14 (20%)
26	BCR	AC	514	-	41,41,41	1.77	8 (19%)	56,56,56	2.12	22 (39%)
27	DGD	BD	410	-	64,64,67	1.78	16 (25%)	78,78,81	1.36	7 (8%)
32	LMT	BB	603	-	36,36,36	1.45	7 (19%)	47,47,47	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LMG	BI	101	-	43,43,55	1.57	8 (18%)	51,51,63	1.08	4 (7%)
34	HEM	AV	201	16	27,50,50	2.02	9 (33%)	17,82,82	2.20	6 (35%)
22	CLA	AB	601	-	59,73,73	1.62	8 (13%)	67,113,113	2.05	13 (19%)
27	DGD	BC	517	-	63,63,67	1.11	6 (9%)	77,77,81	1.62	8 (10%)
22	CLA	BB	610	-	59,73,73	1.48	8 (13%)	67,113,113	2.02	11 (16%)
22	CLA	AB	616	-	59,73,73	1.39	10 (16%)	67,113,113	2.02	13 (19%)
24	PL9	BD	405	-	55,55,55	0.54	0	68,69,69	1.72	19 (27%)
33	BCT	BD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
26	BCR	AJ	102	-	41,41,41	2.04	9 (21%)	56,56,56	3.34	22 (39%)
22	CLA	BC	505	3	59,73,73	1.67	9 (15%)	67,113,113	2.10	14 (20%)
29	SQD	AF	101	-	44,45,54	2.46	20 (45%)	53,56,65	2.85	19 (35%)
26	BCR	BZ	101	-	41,41,41	1.96	9 (21%)	56,56,56	2.07	19 (33%)
27	DGD	BA	411	-	57,57,67	1.64	13 (22%)	71,71,81	1.45	8 (11%)
26	BCR	BC	514	-	41,41,41	1.91	8 (19%)	56,56,56	2.11	20 (35%)
22	CLA	BC	506	3	59,73,73	1.37	8 (13%)	67,113,113	1.97	10 (14%)
30	LMG	AA	413	-	51,51,55	0.91	3 (5%)	59,59,63	1.00	4 (6%)
27	DGD	BH	101	-	59,59,67	1.23	9 (15%)	73,73,81	1.43	6 (8%)
22	CLA	AB	615	-	59,73,73	1.35	7 (11%)	67,113,113	2.09	12 (17%)
30	LMG	BD	408	-	48,48,55	1.15	4 (8%)	56,56,63	0.99	2 (3%)
22	CLA	AA	406	1	59,73,73	1.29	6 (10%)	67,113,113	1.92	10 (14%)
22	CLA	BB	609	2	59,73,73	1.48	7 (11%)	67,113,113	1.98	12 (17%)
22	CLA	AB	609	2	59,73,73	1.51	8 (13%)	67,113,113	1.92	14 (20%)
32	LMT	AB	627	-	36,36,36	1.47	6 (16%)	47,47,47	1.03	3 (6%)
22	CLA	BB	614	2	59,73,73	1.20	6 (10%)	67,113,113	1.87	11 (16%)
26	BCR	AC	515	-	41,41,41	1.69	6 (14%)	56,56,56	2.16	19 (33%)
26	BCR	BK	102	-	41,41,41	1.86	7 (17%)	56,56,56	2.52	25 (44%)
22	CLA	AB	604	2	59,73,73	1.54	8 (13%)	67,113,113	2.07	11 (16%)
30	LMG	AB	621	-	49,49,55	1.04	5 (10%)	57,57,63	1.02	4 (7%)
26	BCR	AD	406	-	41,41,41	1.83	7 (17%)	56,56,56	2.30	20 (35%)
22	CLA	AC	513	3	59,73,73	1.65	9 (15%)	67,113,113	2.01	13 (19%)
29	SQD	AA	415	-	53,54,54	2.50	26 (49%)	62,65,65	2.68	20 (32%)
30	LMG	BC	520	-	45,45,55	1.57	10 (22%)	53,53,63	1.03	4 (7%)
22	CLA	BB	606	2	59,73,73	1.33	8 (13%)	67,113,113	1.95	12 (17%)
22	CLA	BC	503	3	59,73,73	1.60	7 (11%)	67,113,113	2.03	11 (16%)
22	CLA	BC	513	3	59,73,73	1.60	9 (15%)	67,113,113	2.00	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	SQD	BA	413	-	50,51,54	2.42	22 (44%)	59,62,65	2.73	19 (32%)
23	PHO	BA	406	-	67,69,69	1.03	4 (5%)	85,99,99	1.40	15 (17%)
28	LHG	AC	521	-	36,36,48	1.08	2 (5%)	39,42,54	1.12	3 (7%)
30	LMG	AE	102	-	44,44,55	1.35	6 (13%)	52,52,63	1.07	5 (9%)
26	BCR	AB	619	-	41,41,41	1.93	8 (19%)	56,56,56	2.08	14 (25%)
23	PHO	AA	405	-	67,69,69	1.02	2 (2%)	85,99,99	1.41	15 (17%)
30	LMG	AC	519	-	48,48,55	1.26	5 (10%)	56,56,63	0.83	2 (3%)
30	LMG	BB	624	-	49,49,55	1.06	5 (10%)	57,57,63	1.02	3 (5%)
22	CLA	BC	510	-	59,73,73	1.23	7 (11%)	67,113,113	1.94	11 (16%)
26	BCR	BJ	102	-	41,41,41	2.15	9 (21%)	56,56,56	3.35	23 (41%)
24	PL9	AJ	101	-	35,35,55	1.39	4 (11%)	44,45,69	1.74	12 (27%)
27	DGD	AC	516	-	54,54,67	1.24	8 (14%)	68,68,81	1.52	7 (10%)
24	PL9	AA	407	-	45,45,55	0.96	1 (2%)	56,57,69	1.70	15 (26%)
32	LMT	BD	411	-	32,32,36	1.43	4 (12%)	43,43,47	0.96	2 (4%)
22	CLA	BC	502	3	59,73,73	1.42	7 (11%)	67,113,113	2.01	12 (17%)
32	LMT	AD	411	-	32,32,36	1.53	5 (15%)	43,43,47	1.00	2 (4%)
30	LMG	AA	416	-	42,42,55	1.52	7 (16%)	50,50,63	0.98	3 (6%)
22	CLA	AC	505	3	59,73,73	1.58	9 (15%)	67,113,113	2.05	12 (17%)
22	CLA	AB	602	2	59,73,73	1.31	6 (10%)	67,113,113	1.84	13 (19%)
34	HEM	AE	101	5,6	27,50,50	2.05	7 (25%)	17,82,82	2.48	5 (29%)
24	PL9	BJ	101	-	35,35,55	1.44	5 (14%)	44,45,69	1.69	13 (29%)
22	CLA	AA	404	-	59,73,73	1.25	7 (11%)	67,113,113	1.94	14 (20%)
25	OEC	AA	408	1,3	0,0,13	0.00	-	-		
22	CLA	AD	402	4	59,73,73	1.59	9 (15%)	67,113,113	2.10	14 (20%)
26	BCR	AB	620	-	41,41,41	1.85	8 (19%)	56,56,56	2.05	18 (32%)
29	SQD	BB	601	-	46,47,54	2.57	22 (47%)	55,58,65	2.68	16 (29%)
25	OEC	BA	409	1,3	0,0,13	0.00	-	-		
27	DGD	AD	410	-	64,64,67	1.84	16 (25%)	78,78,81	1.37	7 (8%)
22	CLA	AA	402	1	59,73,73	1.38	8 (13%)	67,113,113	1.94	11 (16%)
22	CLA	AB	608	2	59,73,73	1.36	7 (11%)	67,113,113	1.97	14 (20%)
22	CLA	BC	509	-	59,73,73	1.47	10 (16%)	67,113,113	2.03	13 (19%)
26	BCR	BX	101	-	41,41,41	1.84	8 (19%)	56,56,56	2.26	22 (39%)
22	CLA	AC	502	3	59,73,73	1.43	8 (13%)	67,113,113	1.97	12 (17%)
26	BCR	AT	102	-	41,41,41	1.63	6 (14%)	56,56,56	2.20	25 (44%)
29	SQD	BF	101	-	44,45,54	2.54	19 (43%)	53,56,65	2.82	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMT	BB	626	-	36,36,36	1.38	5 (13%)	47,47,47	0.94	1 (2%)
22	CLA	AC	512	-	59,73,73	1.60	9 (15%)	67,113,113	2.06	13 (19%)
26	BCR	BB	622	-	41,41,41	1.83	8 (19%)	56,56,56	2.04	17 (30%)
22	CLA	AB	612	-	59,73,73	1.35	7 (11%)	67,113,113	1.96	12 (17%)
30	LMG	BD	407	-	46,46,55	1.04	4 (8%)	54,54,63	0.91	2 (3%)
22	CLA	BD	404	-	59,73,73	1.47	8 (13%)	67,113,113	1.95	12 (17%)
22	CLA	AB	610	-	59,73,73	1.33	9 (15%)	67,113,113	2.03	15 (22%)
22	CLA	BC	511	3	59,73,73	1.60	8 (13%)	67,113,113	2.08	12 (17%)
30	LMG	BM	102	-	42,42,55	1.66	8 (19%)	50,50,63	1.11	5 (10%)
22	CLA	AC	508	3	59,73,73	1.48	8 (13%)	67,113,113	2.10	12 (17%)
22	CLA	BB	613	-	59,73,73	1.39	11 (18%)	67,113,113	2.02	15 (22%)
30	LMG	AD	408	-	48,48,55	1.07	3 (6%)	56,56,63	0.99	2 (3%)
30	LMG	BC	519	-	48,48,55	1.28	6 (12%)	56,56,63	0.83	2 (3%)
22	CLA	BC	507	-	59,73,73	1.33	7 (11%)	67,113,113	2.03	13 (19%)
32	LMT	AM	102	-	36,36,36	1.21	2 (5%)	47,47,47	0.95	2 (4%)
27	DGD	BB	602	-	53,53,67	1.88	17 (32%)	67,67,81	1.57	8 (11%)
22	CLA	BB	616	-	59,73,73	1.17	7 (11%)	67,113,113	1.96	11 (16%)
27	DGD	BC	518	-	67,67,67	1.18	6 (8%)	81,81,81	1.27	4 (4%)
22	CLA	BD	402	4	59,73,73	1.59	10 (16%)	67,113,113	2.07	13 (19%)
24	PL9	AD	405	-	55,55,55	0.56	0	68,69,69	1.71	18 (26%)
22	CLA	AC	507	-	59,73,73	1.29	6 (10%)	67,113,113	2.02	14 (20%)
30	LMG	AI	101	-	43,43,55	1.51	8 (18%)	51,51,63	1.06	3 (5%)
22	CLA	AC	511	3	59,73,73	1.62	7 (11%)	67,113,113	2.07	13 (19%)
32	LMT	AT	101	-	36,36,36	1.37	5 (13%)	47,47,47	1.08	4 (8%)
22	CLA	AB	607	-	59,73,73	1.44	9 (15%)	67,113,113	1.99	11 (16%)
26	BCR	BC	515	-	41,41,41	1.82	7 (17%)	56,56,56	2.14	19 (33%)
30	LMG	AD	407	-	46,46,55	0.97	4 (8%)	54,54,63	0.90	2 (3%)
22	CLA	AC	504	-	59,73,73	1.34	7 (11%)	67,113,113	1.90	12 (17%)
22	CLA	AC	501	3	59,73,73	1.38	7 (11%)	67,113,113	1.99	13 (19%)
22	CLA	BA	403	1	59,73,73	1.44	8 (13%)	67,113,113	1.91	10 (14%)
22	CLA	BB	619	-	59,73,73	1.40	9 (15%)	67,113,113	2.08	12 (17%)
32	LMT	AB	625	-	36,36,36	1.40	7 (19%)	47,47,47	0.96	2 (4%)
23	PHO	BD	403	-	67,69,69	1.06	5 (7%)	85,99,99	1.45	14 (16%)
26	BCR	BD	406	-	41,41,41	1.92	8 (19%)	56,56,56	2.28	21 (37%)
28	LHG	BA	412	-	38,38,48	1.95	6 (15%)	41,44,54	1.39	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMT	BT	101	-	36,36,36	1.32	5 (13%)	47,47,47	1.05	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	AI	102	-	-	4/21/61/61	0/2/2/2
28	LHG	AA	411	-	-	15/43/43/53	-
22	CLA	AB	614	2	3/3/20/25	19/37/135/135	-
32	LMT	BI	102	-	-	4/21/61/61	0/2/2/2
22	CLA	BB	617	2	3/3/20/25	18/37/135/135	-
26	BCR	AK	102	-	-	4/29/63/63	0/2/2/2
26	BCR	BB	621	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	617	-	-	1/29/63/63	0/2/2/2
22	CLA	BC	501	3	3/3/20/25	12/37/135/135	-
22	CLA	AC	510	-	3/3/20/25	12/37/135/135	-
22	CLA	AA	403	-	3/3/20/25	17/37/135/135	-
22	CLA	BB	615	-	3/3/20/25	12/37/135/135	-
22	CLA	AB	613	-	3/3/20/25	15/37/135/135	-
30	LMG	AC	520	-	2/2/8/8	19/40/60/70	0/1/1/1
27	DGD	AB	626	-	3/3/13/13	24/41/81/95	0/2/2/2
26	BCR	AH	101	-	-	2/29/63/63	0/2/2/2
27	DGD	AH	102	-	3/3/13/13	18/47/87/95	0/2/2/2
24	PL9	AA	407	-	-	16/41/61/73	0/1/1/1
30	LMG	BD	408	-	2/2/8/8	25/43/63/70	0/1/1/1
26	BCR	BA	410	-	-	4/29/63/63	0/2/2/2
30	LMG	AB	623	-	2/2/8/8	17/37/57/70	0/1/1/1
30	LMG	AM	101	-	2/2/8/8	16/37/57/70	0/1/1/1
22	CLA	AC	502	3	3/3/20/25	11/37/135/135	-
22	CLA	BB	608	2	3/3/20/25	17/37/135/135	-
32	LMT	BB	625	-	-	4/21/61/61	0/2/2/2
22	CLA	BC	512	-	3/3/20/25	21/37/135/135	-
34	HEM	BV	201	16	-	0/6/54/54	-
27	DGD	AC	517	-	3/3/13/13	29/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	BD	409	-	-	12/38/58/69	0/1/1/1
22	CLA	AB	605	-	3/3/20/25	15/37/135/135	-
22	CLA	AC	503	3	3/3/20/25	15/37/135/135	-
30	LMG	AB	622	-	2/2/8/8	19/44/64/70	0/1/1/1
29	SQD	AD	409	-	-	12/38/58/69	0/1/1/1
22	CLA	AB	611	2	3/3/20/25	14/37/135/135	-
28	LHG	BC	521	-	-	16/41/41/53	-
32	LMT	BM	101	-	-	1/21/61/61	0/2/2/2
30	LMG	BA	414	-	2/2/8/8	28/46/66/70	0/1/1/1
22	CLA	AB	606	2	3/3/20/25	14/37/135/135	-
22	CLA	AB	603	2	3/3/20/25	11/37/135/135	-
34	HEM	BE	101	5,6	-	0/6/54/54	-
22	CLA	BC	504	-	3/3/20/25	10/37/135/135	-
22	CLA	BB	612	2	3/3/20/25	10/37/135/135	-
32	LMT	BD	411	-	-	0/17/57/61	0/2/2/2
22	CLA	BB	618	-	3/3/20/25	9/37/135/135	-
29	SQD	BA	401	-	-	20/49/69/69	0/1/1/1
26	BCR	BB	620	-	-	1/29/63/63	0/2/2/2
30	LMG	BE	102	-	2/2/8/8	19/39/59/70	0/1/1/1
22	CLA	BA	404	-	3/3/20/25	17/37/135/135	-
27	DGD	AA	410	-	3/3/13/13	18/45/85/95	0/2/2/2
22	CLA	BC	503	3	3/3/20/25	16/37/135/135	-
29	SQD	AA	412	-	-	17/46/66/69	0/1/1/1
22	CLA	BB	605	2	3/3/20/25	21/37/135/135	-
27	DGD	AC	518	-	3/3/13/13	21/55/95/95	0/2/2/2
22	CLA	BC	508	3	3/3/20/25	12/37/135/135	-
22	CLA	BA	405	-	3/3/20/25	14/37/135/135	-
26	BCR	AB	618	-	-	3/29/63/63	0/2/2/2
24	PL9	BA	408	-	-	16/41/61/73	0/1/1/1
29	SQD	BL	101	-	-	17/42/62/69	0/1/1/1
22	CLA	AC	506	3	3/3/20/25	16/37/135/135	-
32	LMT	AB	624	-	-	4/21/61/61	0/2/2/2
30	LMG	BB	623	-	2/2/8/8	22/44/64/70	0/1/1/1
22	CLA	BB	604	-	3/3/20/25	20/37/135/135	-
22	CLA	BB	607	2	3/3/20/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	BC	516	-	3/3/13/13	18/42/82/95	0/2/2/2
26	BCR	AA	409	-	-	4/29/63/63	0/2/2/2
26	BCR	AZ	101	-	-	3/29/63/63	0/2/2/2
22	CLA	AC	509	-	3/3/20/25	11/37/135/135	-
26	BCR	AC	514	-	-	5/29/63/63	0/2/2/2
27	DGD	BD	410	-	3/3/13/13	33/52/92/95	0/2/2/2
32	LMT	BB	603	-	-	4/21/61/61	0/2/2/2
30	LMG	BI	101	-	2/2/8/8	20/38/58/70	0/1/1/1
34	HEM	AV	201	16	-	0/6/54/54	-
22	CLA	AB	601	-	3/3/20/25	20/37/135/135	-
27	DGD	BC	517	-	3/3/13/13	29/51/91/95	0/2/2/2
22	CLA	BB	610	-	3/3/20/25	15/37/135/135	-
27	DGD	BC	518	-	3/3/13/13	21/55/95/95	0/2/2/2
24	PL9	BD	405	-	-	17/53/73/73	0/1/1/1
23	PHO	AD	403	-	-	15/53/103/103	0/5/6/6
26	BCR	AJ	102	-	-	5/29/63/63	0/2/2/2
22	CLA	BC	505	3	3/3/20/25	18/37/135/135	-
29	SQD	AF	101	-	-	14/40/60/69	0/1/1/1
26	BCR	BZ	101	-	-	3/29/63/63	0/2/2/2
27	DGD	BA	411	-	3/3/13/13	18/45/85/95	0/2/2/2
26	BCR	BC	514	-	-	5/29/63/63	0/2/2/2
22	CLA	BC	506	3	3/3/20/25	17/37/135/135	-
30	LMG	AA	413	-	2/2/8/8	29/46/66/70	0/1/1/1
27	DGD	BH	101	-	3/3/13/13	18/47/87/95	0/2/2/2
22	CLA	AB	615	-	3/3/20/25	9/37/135/135	-
22	CLA	BA	407	1	3/3/20/25	10/37/135/135	-
22	CLA	AA	406	1	3/3/20/25	11/37/135/135	-
22	CLA	BB	609	2	3/3/20/25	14/37/135/135	-
22	CLA	AB	609	2	3/3/20/25	10/37/135/135	-
32	LMT	AB	627	-	-	4/21/61/61	0/2/2/2
22	CLA	BB	614	2	3/3/20/25	14/37/135/135	-
26	BCR	AC	515	-	-	4/29/63/63	0/2/2/2
26	BCR	BK	102	-	-	4/29/63/63	0/2/2/2
22	CLA	AB	604	2	3/3/20/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	AB	621	-	2/2/8/8	22/44/64/70	0/1/1/1
26	BCR	AD	406	-	-	3/29/63/63	0/2/2/2
22	CLA	AC	513	3	3/3/20/25	20/37/135/135	-
29	SQD	AA	415	-	-	21/49/69/69	0/1/1/1
30	LMG	BC	520	-	2/2/8/8	18/40/60/70	0/1/1/1
22	CLA	BB	606	2	3/3/20/25	11/37/135/135	-
30	LMG	AC	519	-	2/2/8/8	24/43/63/70	0/1/1/1
22	CLA	BC	513	3	3/3/20/25	20/37/135/135	-
29	SQD	BA	413	-	-	18/46/66/69	0/1/1/1
23	PHO	BA	406	-	-	15/53/103/103	0/5/6/6
28	LHG	AC	521	-	-	16/41/41/53	-
30	LMG	AE	102	-	2/2/8/8	19/39/59/70	0/1/1/1
26	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
23	PHO	AA	405	-	-	15/53/103/103	0/5/6/6
30	LMG	BB	624	-	2/2/8/8	17/44/64/70	0/1/1/1
22	CLA	BC	510	-	3/3/20/25	12/37/135/135	-
26	BCR	BJ	102	-	-	5/29/63/63	0/2/2/2
24	PL9	AJ	101	-	-	10/29/49/73	0/1/1/1
27	DGD	AC	516	-	3/3/13/13	17/42/82/95	0/2/2/2
22	CLA	BB	611	2	3/3/20/25	18/37/135/135	-
22	CLA	AB	608	2	3/3/20/25	18/37/135/135	-
22	CLA	BC	502	3	3/3/20/25	12/37/135/135	-
32	LMT	AD	411	-	-	0/17/57/61	0/2/2/2
30	LMG	AA	416	-	2/2/8/8	17/37/57/70	0/1/1/1
22	CLA	AC	505	3	3/3/20/25	18/37/135/135	-
22	CLA	AB	602	2	3/3/20/25	21/37/135/135	-
34	HEM	AE	101	5,6	-	0/6/54/54	-
24	PL9	BJ	101	-	-	10/29/49/73	0/1/1/1
22	CLA	AA	404	-	3/3/20/25	14/37/135/135	-
22	CLA	AD	402	4	2/2/20/25	12/37/135/135	-
26	BCR	AB	620	-	-	2/29/63/63	0/2/2/2
29	SQD	BB	601	-	-	17/42/62/69	0/1/1/1
25	OEC	BA	409	1,3	-	-	0/1/0/5
27	DGD	AD	410	-	3/3/13/13	34/52/92/95	0/2/2/2
22	CLA	AA	402	1	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BC	509	-	3/3/20/25	11/37/135/135	-
26	BCR	BX	101	-	-	2/29/63/63	0/2/2/2
22	CLA	AD	404	-	3/3/20/25	10/37/135/135	-
26	BCR	AT	102	-	-	3/29/63/63	0/2/2/2
29	SQD	BF	101	-	-	14/40/60/69	0/1/1/1
32	LMT	BB	626	-	-	2/21/61/61	0/2/2/2
22	CLA	AC	512	-	3/3/20/25	21/37/135/135	-
26	BCR	BB	622	-	-	2/29/63/63	0/2/2/2
22	CLA	AB	612	-	3/3/20/25	11/37/135/135	-
30	LMG	BD	407	-	2/2/8/8	17/41/61/70	0/1/1/1
22	CLA	BD	404	-	3/3/20/25	9/37/135/135	-
22	CLA	AB	610	-	3/3/20/25	16/37/135/135	-
22	CLA	BC	511	3	3/3/20/25	14/37/135/135	-
23	PHO	BD	403	-	-	16/53/103/103	0/5/6/6
22	CLA	AC	508	3	3/3/20/25	12/37/135/135	-
22	CLA	BB	613	-	3/3/20/25	16/37/135/135	-
30	LMG	AD	408	-	2/2/8/8	25/43/63/70	0/1/1/1
30	LMG	BC	519	-	2/2/8/8	24/43/63/70	0/1/1/1
22	CLA	BC	507	-	3/3/20/25	12/37/135/135	-
32	LMT	AM	102	-	-	1/21/61/61	0/2/2/2
27	DGD	BB	602	-	3/3/13/13	24/41/81/95	0/2/2/2
22	CLA	BB	616	-	3/3/20/25	15/37/135/135	-
22	CLA	AB	616	-	3/3/20/25	16/37/135/135	-
22	CLA	BD	402	4	2/2/20/25	11/37/135/135	-
24	PL9	AD	405	-	-	15/53/73/73	0/1/1/1
22	CLA	AC	507	-	3/3/20/25	12/37/135/135	-
30	LMG	AI	101	-	2/2/8/8	19/38/58/70	0/1/1/1
22	CLA	AC	511	3	3/3/20/25	14/37/135/135	-
32	LMT	AT	101	-	-	4/21/61/61	0/2/2/2
22	CLA	AB	607	-	3/3/20/25	13/37/135/135	-
26	BCR	BC	515	-	-	4/29/63/63	0/2/2/2
30	LMG	AD	407	-	2/2/8/8	17/41/61/70	0/1/1/1
22	CLA	AC	504	-	3/3/20/25	10/37/135/135	-
22	CLA	AC	501	3	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BA	403	1	3/3/20/25	5/37/135/135	-
22	CLA	BB	619	-	3/3/20/25	15/37/135/135	-
32	LMT	AB	625	-	-	2/21/61/61	0/2/2/2
30	LMG	BM	102	-	2/2/8/8	16/37/57/70	0/1/1/1
26	BCR	BD	406	-	-	3/29/63/63	0/2/2/2
28	LHG	BA	412	-	-	15/43/43/53	-
32	LMT	BT	101	-	-	4/21/61/61	0/2/2/2

The worst 5 of 1368 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BL	101	SQD	C4-C3	8.57	1.74	1.52
22	BC	505	CLA	MG-NA	8.49	2.26	2.06
28	AA	411	LHG	P-O5	8.17	1.79	1.50
29	BB	601	SQD	C4-C3	8.03	1.72	1.52
29	AA	412	SQD	C4-C3	7.97	1.72	1.52

The worst 5 of 1924 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AB	604	CLA	C4A-NA-C1A	13.27	112.67	106.71
22	BB	607	CLA	C4A-NA-C1A	13.12	112.61	106.71
22	AC	508	CLA	C4A-NA-C1A	13.02	112.56	106.71
22	BC	511	CLA	C4A-NA-C1A	12.89	112.50	106.71
22	AC	503	CLA	C4A-NA-C1A	12.83	112.47	106.71

5 of 294 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AB	614	CLA	NC
22	AB	614	CLA	ND
22	AB	614	CLA	NA
22	BB	617	CLA	NC
22	BB	617	CLA	ND

5 of 2221 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	AA	411	LHG	C1-C2-C3-O3
22	AB	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	AB	614	CLA	CHA-CBD-CGD-O2D
22	BB	617	CLA	CHA-CBD-CGD-O1D
22	BB	617	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

165 monomers are involved in 627 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	AI	102	LMT	4	0
28	AA	411	LHG	3	0
22	AB	614	CLA	1	0
32	BI	102	LMT	3	0
22	BB	617	CLA	2	0
26	AK	102	BCR	13	0
26	AB	617	BCR	3	0
22	BC	501	CLA	3	0
22	AC	510	CLA	4	0
22	AA	403	CLA	7	0
22	BB	615	CLA	5	0
22	AB	613	CLA	3	0
30	AC	520	LMG	4	0
27	AB	626	DGD	3	0
26	AH	101	BCR	5	0
27	AH	102	DGD	1	0
22	BB	611	CLA	9	0
22	BA	407	CLA	3	0
26	BA	410	BCR	3	0
33	AD	401	BCT	1	0
30	AB	623	LMG	2	0
22	BC	504	CLA	6	0
30	AM	101	LMG	4	0
22	AD	404	CLA	4	0
22	BB	608	CLA	5	0
22	BC	512	CLA	7	0
34	BV	201	HEM	3	0
27	AC	517	DGD	8	0
29	BD	409	SQD	2	0
22	AB	605	CLA	5	0
22	AC	503	CLA	4	0
30	AB	622	LMG	1	0
29	AD	409	SQD	2	0
22	AB	611	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	BC	521	LHG	4	0
32	BM	101	LMT	1	0
30	BA	414	LMG	2	0
22	AB	606	CLA	5	0
22	AB	603	CLA	7	0
34	BE	101	HEM	6	0
26	AZ	101	BCR	5	0
22	BB	612	CLA	7	0
22	BB	618	CLA	6	0
29	BA	401	SQD	2	0
26	BB	620	BCR	3	0
30	BE	102	LMG	4	0
22	BA	404	CLA	6	0
23	AD	403	PHO	2	0
29	AA	412	SQD	5	0
22	BB	605	CLA	6	0
27	AC	518	DGD	8	0
22	BC	508	CLA	7	0
22	BA	405	CLA	3	0
26	AB	618	BCR	5	0
24	BA	408	PL9	6	0
29	BL	101	SQD	2	0
22	AC	506	CLA	3	0
32	AB	624	LMT	1	0
30	BB	623	LMG	1	0
22	BB	604	CLA	1	0
22	BB	607	CLA	5	0
27	BC	516	DGD	3	0
26	AA	409	BCR	6	0
22	AC	509	CLA	2	0
26	AC	514	BCR	9	0
32	BB	603	LMT	3	0
30	BI	101	LMG	3	0
34	AV	201	HEM	3	0
22	AB	601	CLA	2	0
27	BC	517	DGD	10	0
22	BB	610	CLA	14	0
22	AB	616	CLA	4	0
24	BD	405	PL9	8	0
33	BD	401	BCT	1	0
26	AJ	102	BCR	5	0
22	BC	505	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	AF	101	SQD	2	0
26	BZ	101	BCR	5	0
26	BC	514	BCR	10	0
22	BC	506	CLA	3	0
30	AA	413	LMG	1	0
27	BH	101	DGD	1	0
22	AB	615	CLA	7	0
30	BD	408	LMG	8	0
22	AA	406	CLA	3	0
22	BB	609	CLA	6	0
22	AB	609	CLA	6	0
32	AB	627	LMT	3	0
22	BB	614	CLA	7	0
26	AC	515	BCR	6	0
26	BK	102	BCR	13	0
22	AB	604	CLA	5	0
30	AB	621	LMG	1	0
26	AD	406	BCR	3	0
22	AC	513	CLA	3	0
29	AA	415	SQD	5	0
30	BC	520	LMG	5	0
22	BB	606	CLA	7	0
22	BC	503	CLA	5	0
22	BC	513	CLA	4	0
29	BA	413	SQD	4	0
23	BA	406	PHO	5	0
28	AC	521	LHG	5	0
30	AE	102	LMG	4	0
23	AA	405	PHO	5	0
30	AC	519	LMG	2	0
30	BB	624	LMG	1	0
22	BC	510	CLA	3	0
26	BJ	102	BCR	5	0
27	AC	516	DGD	3	0
24	AA	407	PL9	5	0
32	BD	411	LMT	1	0
22	BC	502	CLA	4	0
32	AD	411	LMT	2	0
30	AA	416	LMG	4	0
22	AC	505	CLA	10	0
22	AB	602	CLA	5	0
34	AE	101	HEM	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AA	404	CLA	2	0
22	AD	402	CLA	7	0
26	AB	620	BCR	2	0
29	BB	601	SQD	2	0
22	AA	402	CLA	7	0
22	AB	608	CLA	9	0
22	BC	509	CLA	2	0
26	BX	101	BCR	6	0
22	AC	502	CLA	4	0
26	AT	102	BCR	8	0
29	BF	101	SQD	1	0
32	BB	626	LMT	2	0
22	AC	512	CLA	9	0
26	BB	622	BCR	2	0
22	AB	612	CLA	5	0
30	BD	407	LMG	2	0
22	BD	404	CLA	4	0
22	AB	610	CLA	3	0
22	BC	511	CLA	11	0
30	BM	102	LMG	4	0
22	AC	508	CLA	8	0
22	BB	613	CLA	3	0
30	AD	408	LMG	7	0
30	BC	519	LMG	3	0
22	BC	507	CLA	4	0
32	AM	102	LMT	1	0
27	BB	602	DGD	3	0
22	BB	616	CLA	3	0
27	BC	518	DGD	8	0
22	BD	402	CLA	8	0
24	AD	405	PL9	9	0
22	AC	507	CLA	4	0
30	AI	101	LMG	3	0
22	AC	511	CLA	9	0
32	AT	101	LMT	3	0
22	AB	607	CLA	15	0
26	BC	515	BCR	7	0
30	AD	407	LMG	2	0
22	AC	504	CLA	5	0
22	AC	501	CLA	3	0
22	BA	403	CLA	7	0
22	BB	619	CLA	6	0

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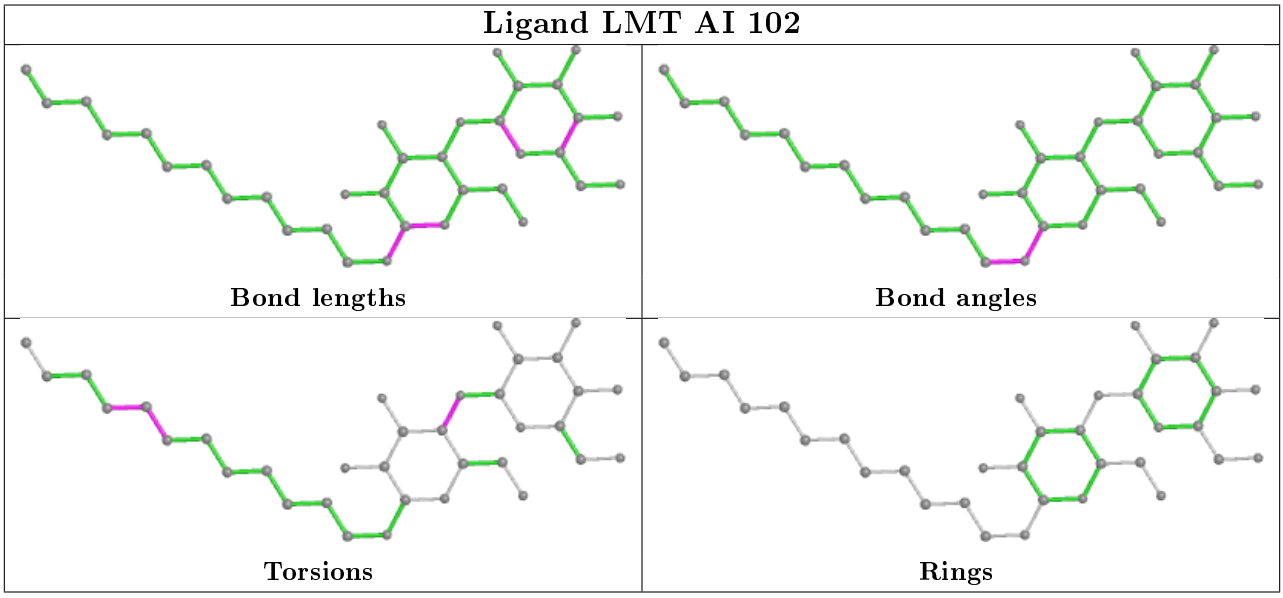
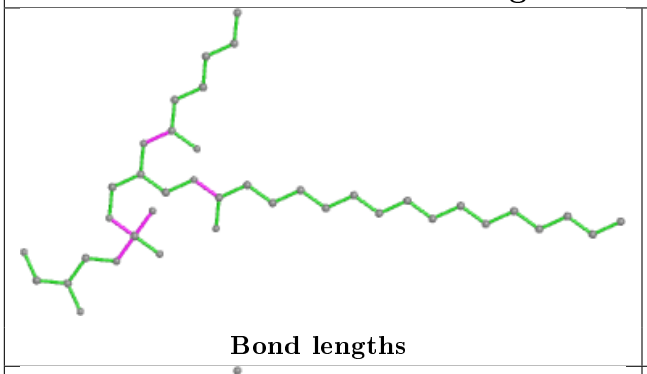
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	AB	625	LMT	2	0
23	BD	403	PHO	5	0
26	BD	406	BCR	3	0
28	BA	412	LHG	4	0
32	BT	101	LMT	3	0

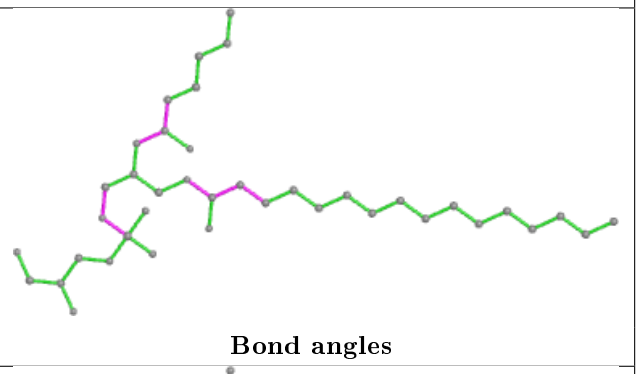
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



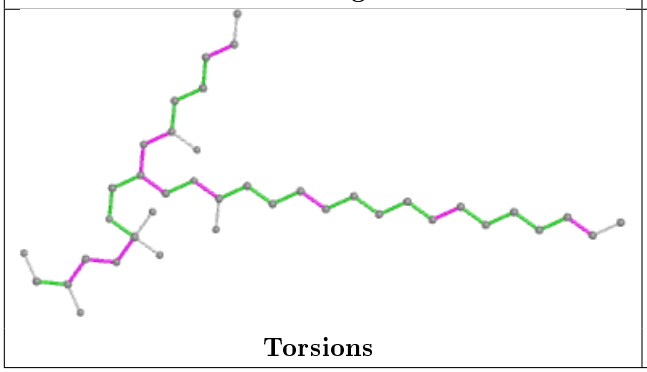
Ligand LHG AA 411



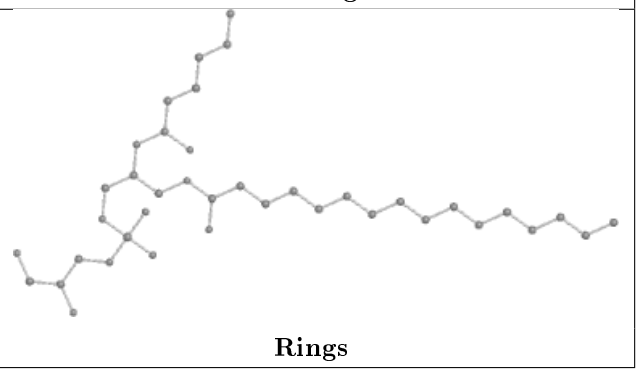
Bond lengths



Bond angles

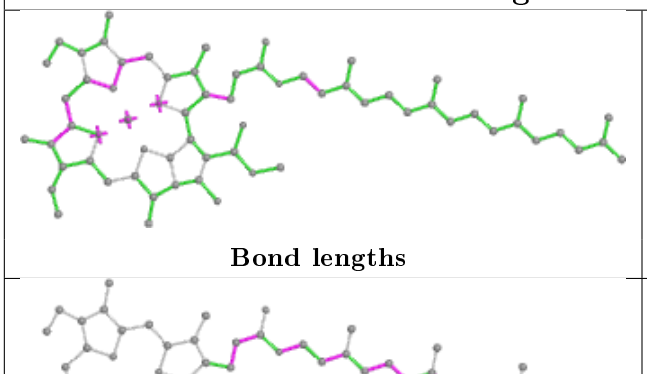


Torsions

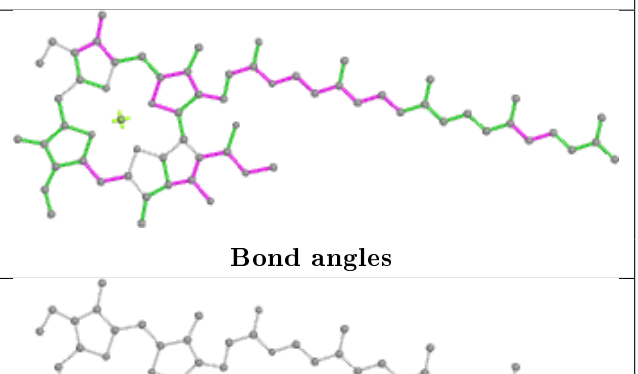


Rings

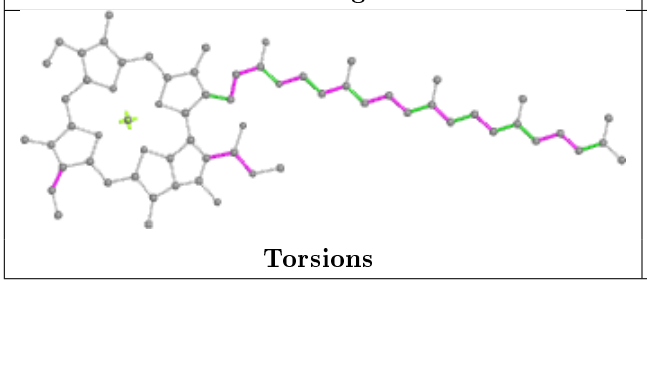
Ligand CLA AB 614



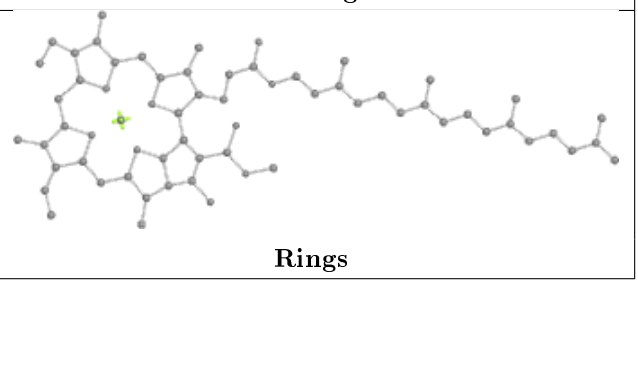
Bond lengths



Bond angles

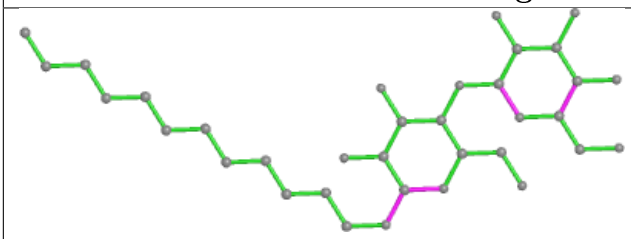


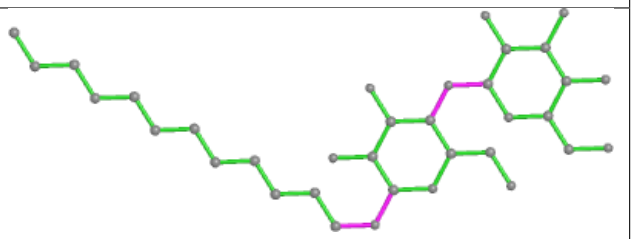
Torsions

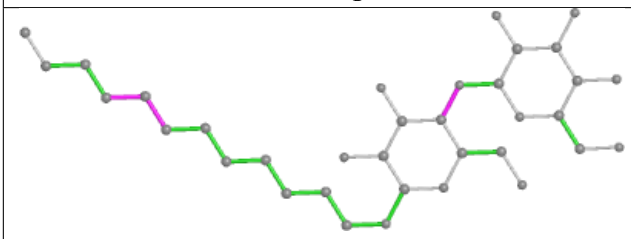


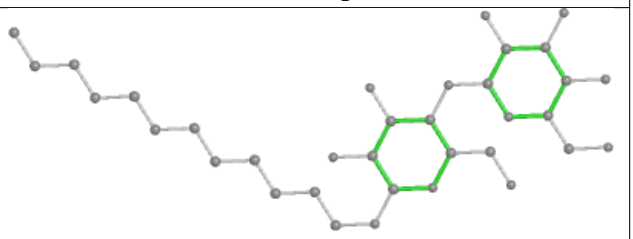
Rings

Ligand LMT BI 102

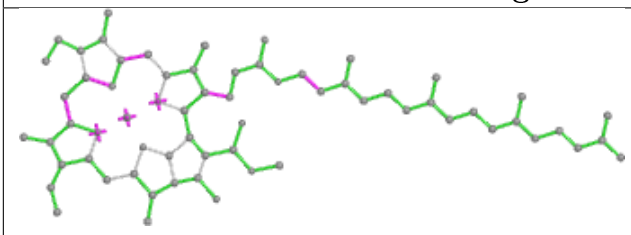

Bond lengths

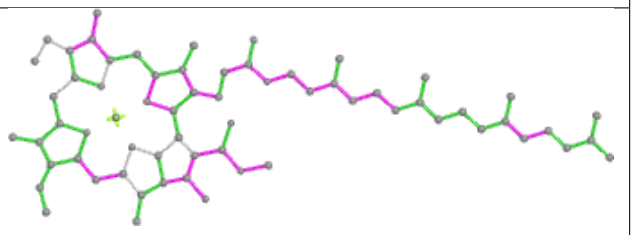

Bond angles

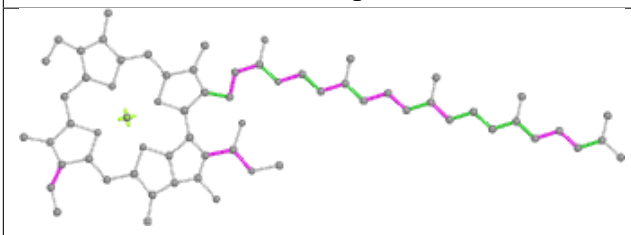

Torsions

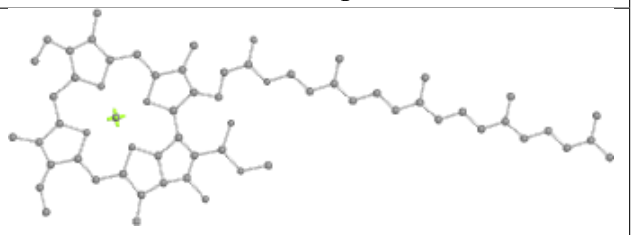

Rings

Ligand CLA BB 617

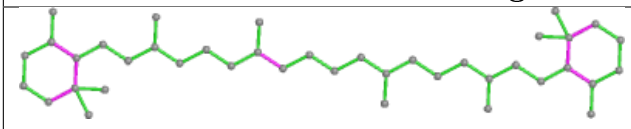

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR AK 102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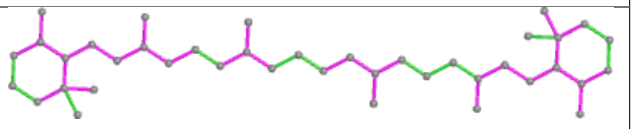
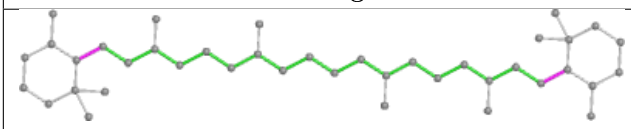
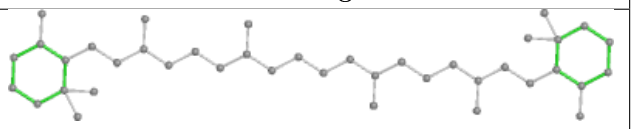
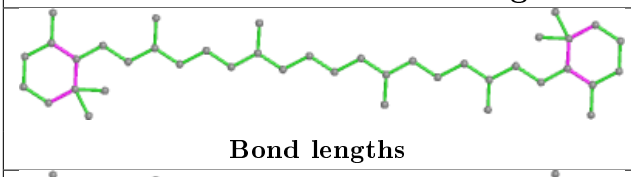

Bond angles


Torsions


Rings

Ligand BCR BB 621



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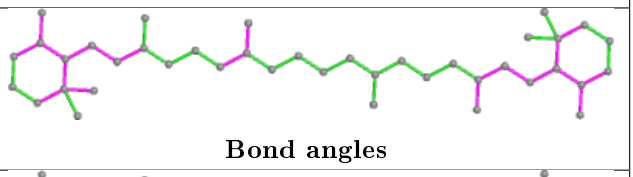
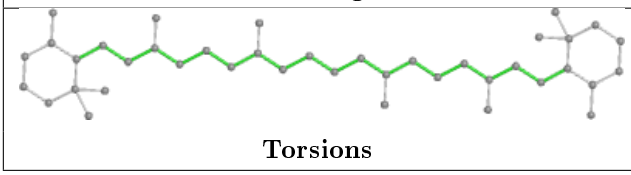
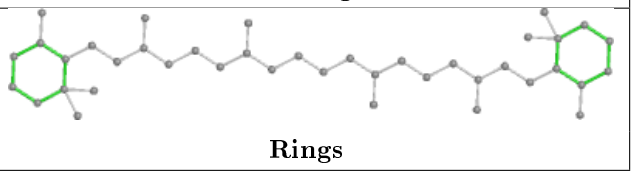


Bond angles

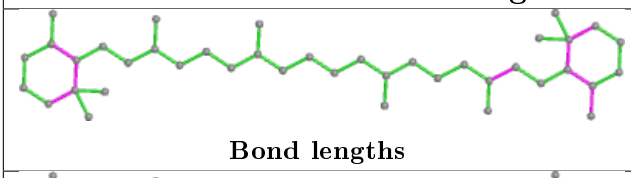


Torsions



Rings

Ligand BCR AB 617



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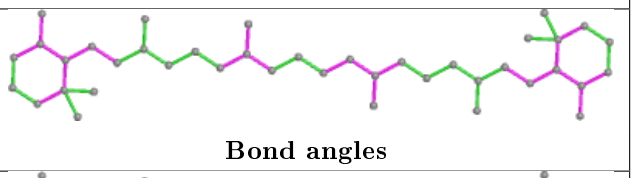
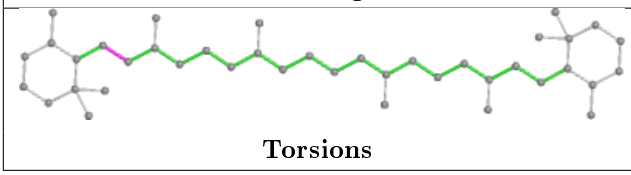


Bond angles



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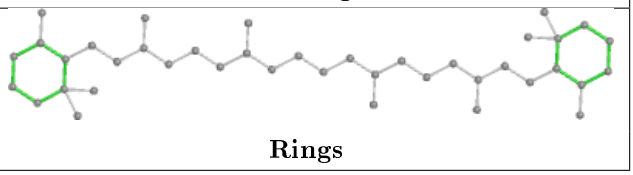
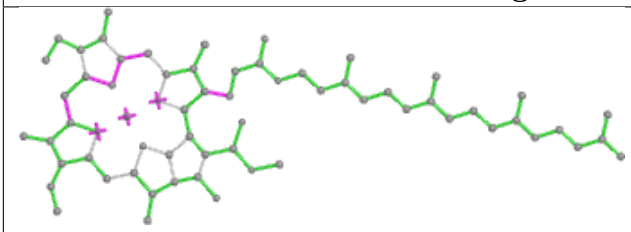


Rings

Ligand CLA BC 501



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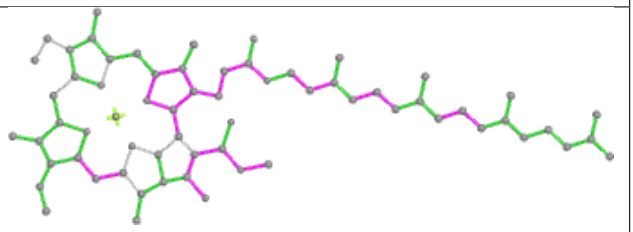
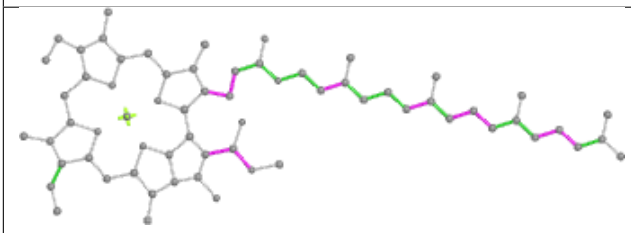


Bond angles



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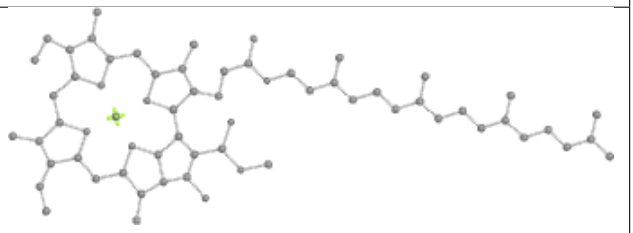
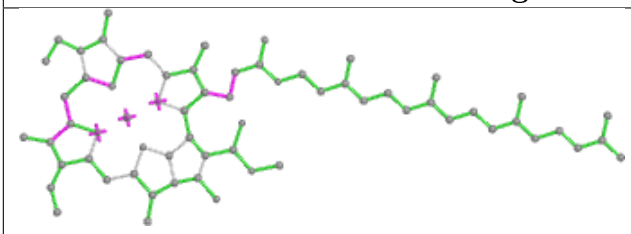


Rings

Ligand CLA AC 510



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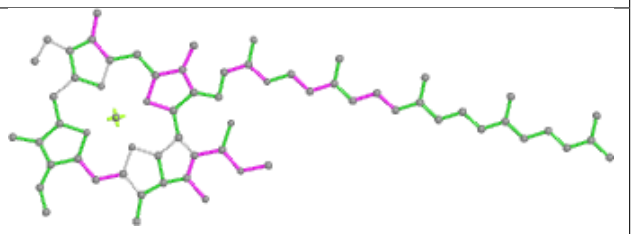
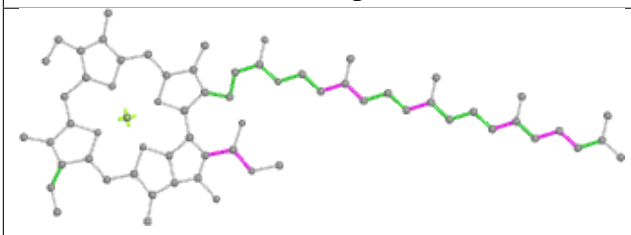


Bond angles



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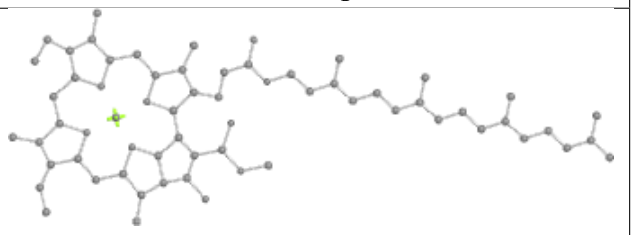
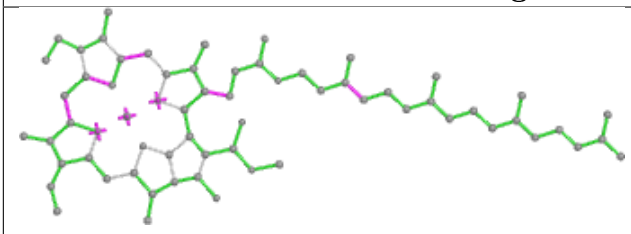


Rings

Ligand CLA AA 403



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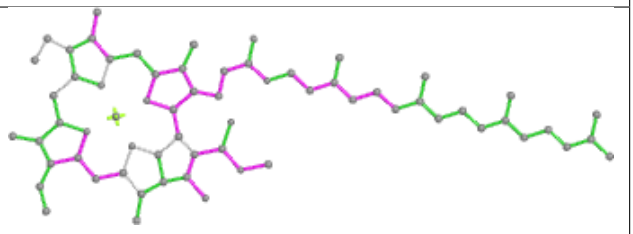
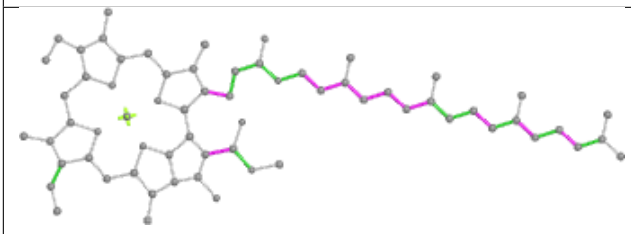
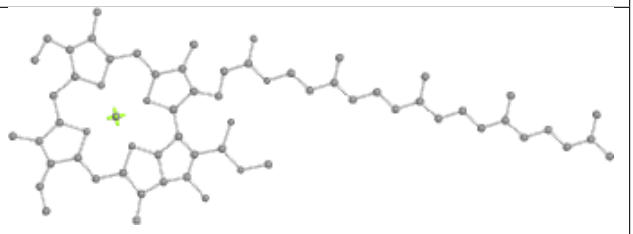


Bond angles

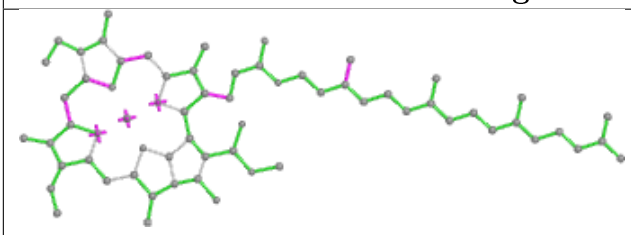


Torsions



Rings

Ligand CLA BB 615



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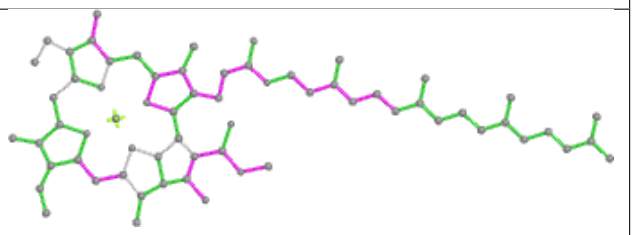
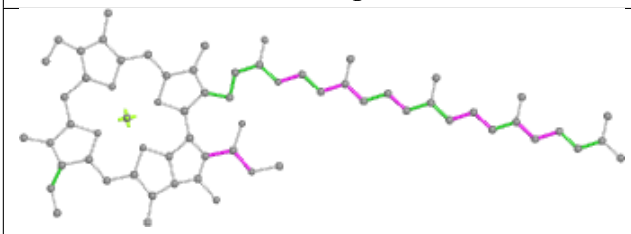


Bond angles



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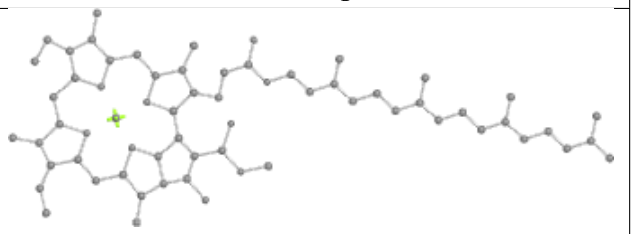

Rings

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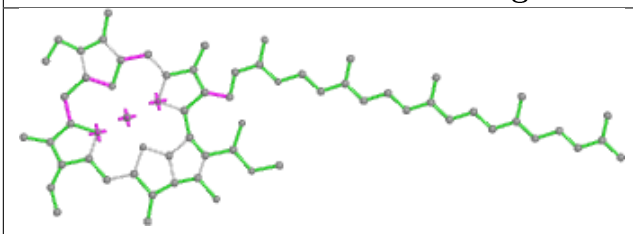

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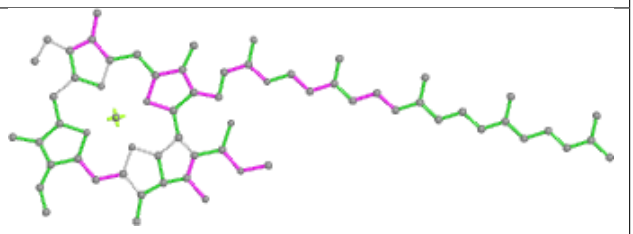
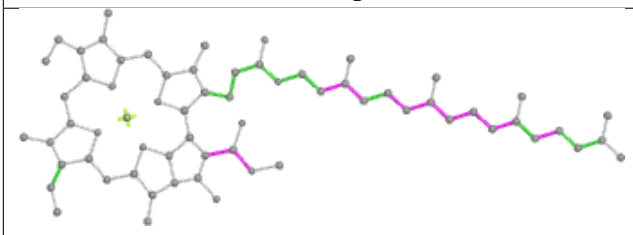
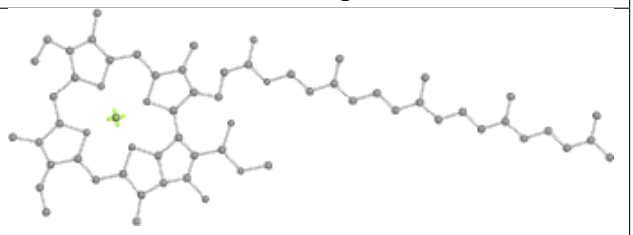


Bond angles

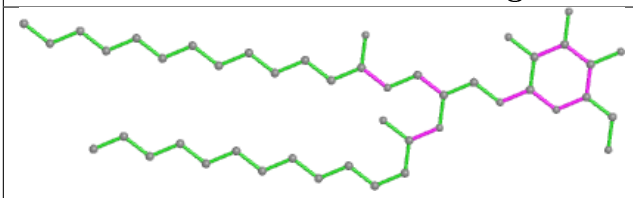


Torsions



Rings

Ligand LMG AC 520



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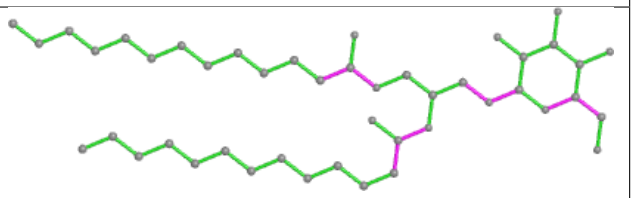
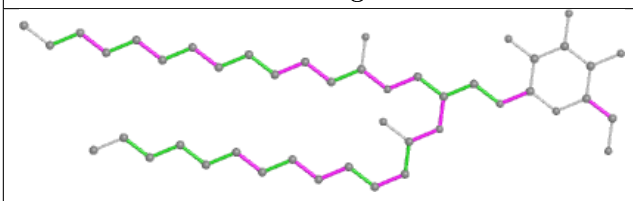


Bond angles



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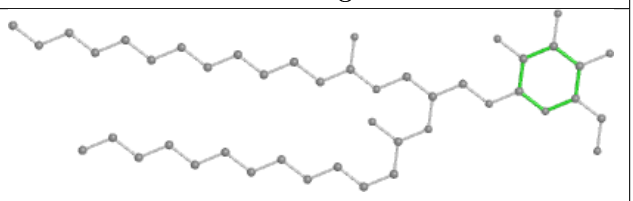
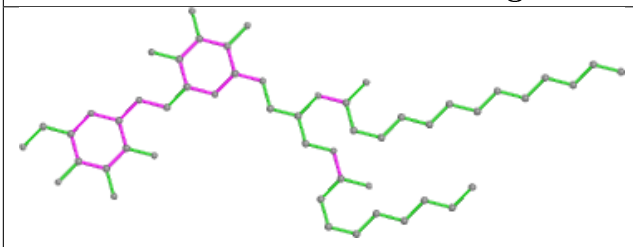
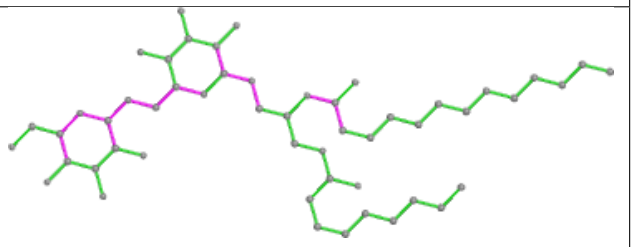


Rings

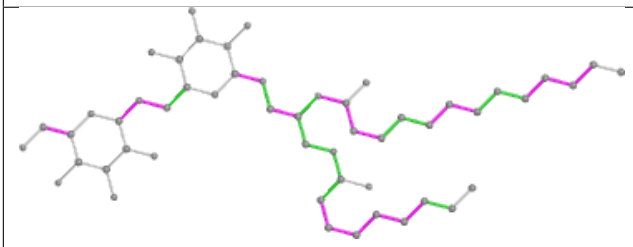
Ligand DGD AB 626



Bond lengths



Bond angles



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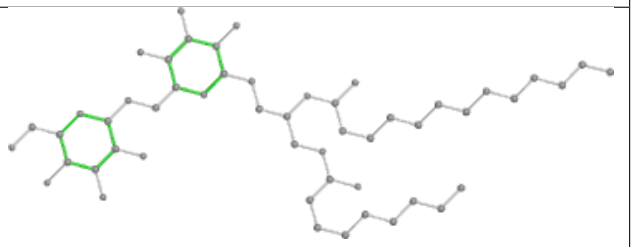
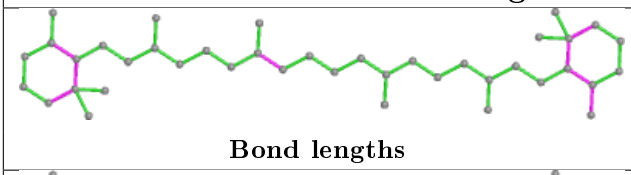
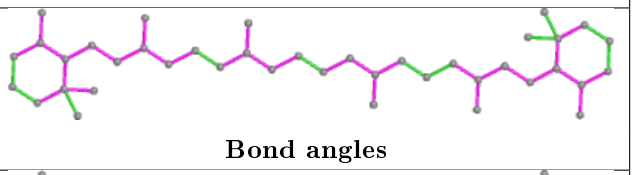


Rings

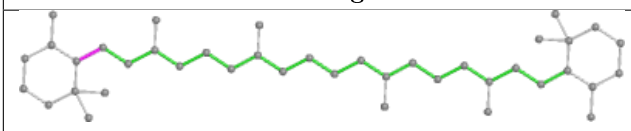
Ligand BCR AH 101



Bond lengths



Bond angles



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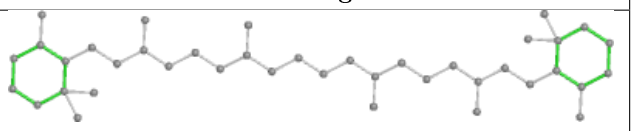
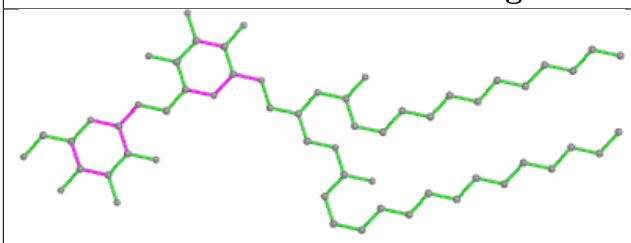
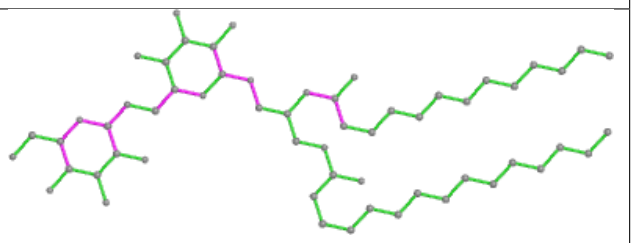


Rings

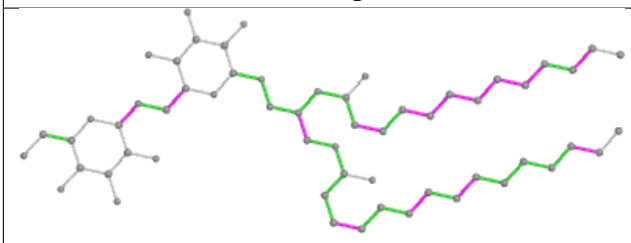
Ligand DGD AH 102



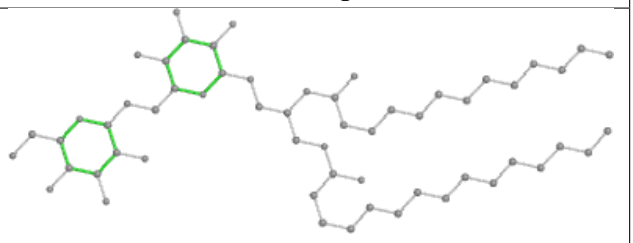
Bond lengths



Bond angles

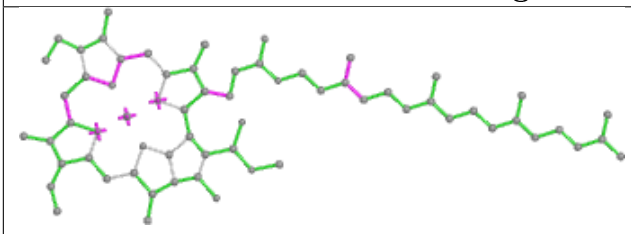


Torsions

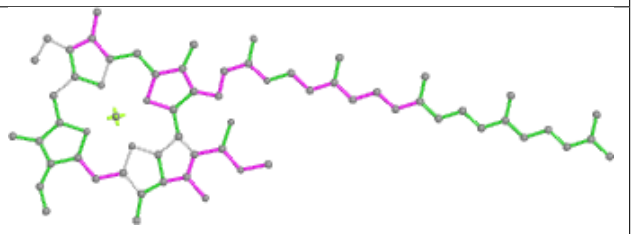


Rings

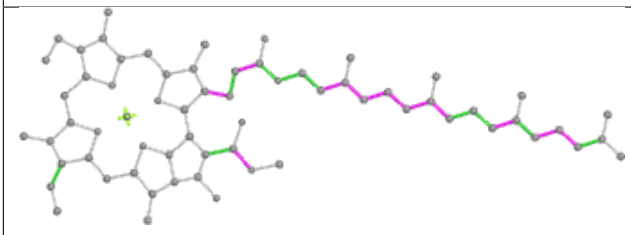
Ligand CLA BB 611



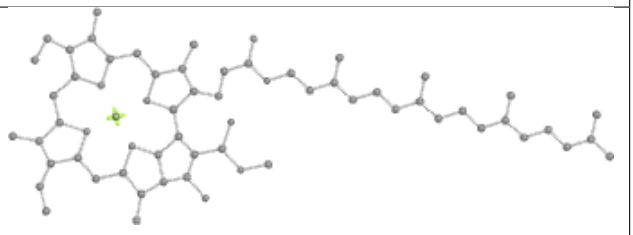
Bond lengths



Bond angles

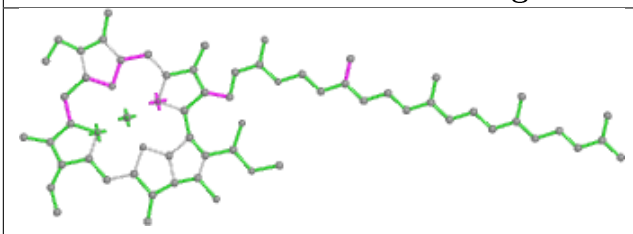


Torsions

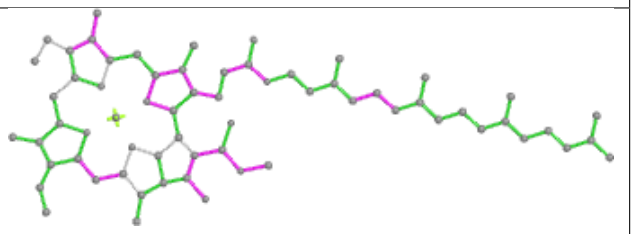


Rings

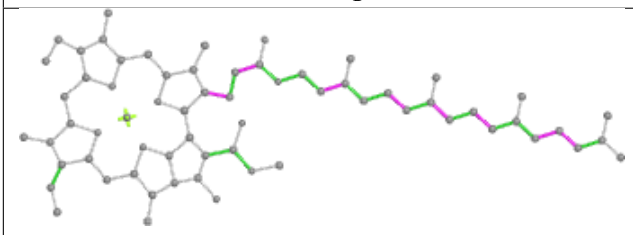
Ligand CLA BA 407



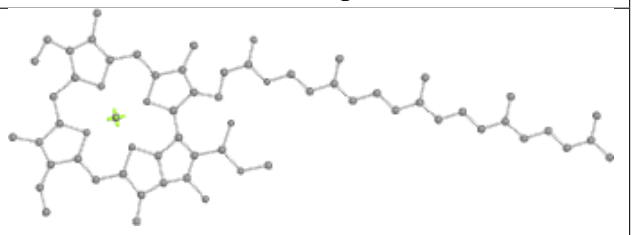
Bond lengths



Bond angles

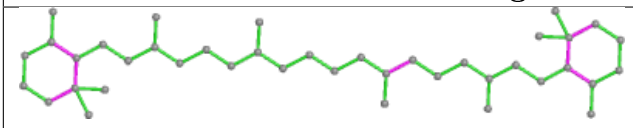


Torsions

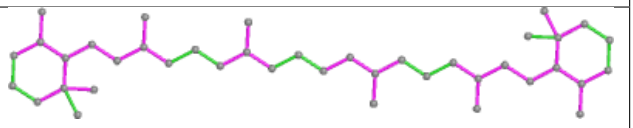


Rings

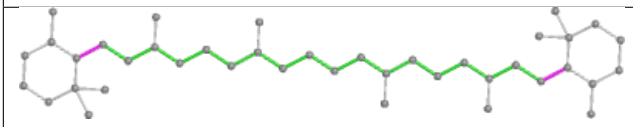
Ligand BCR BA 410



Bond lengths



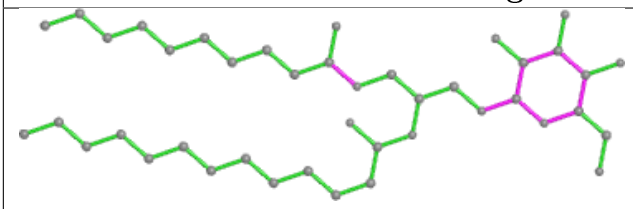
Bond angles



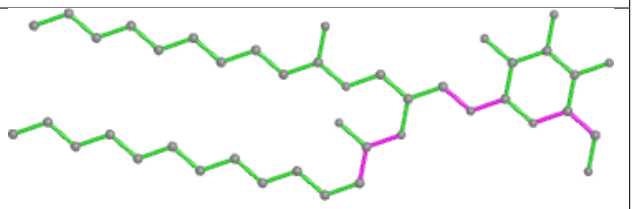
Torsions

Rings

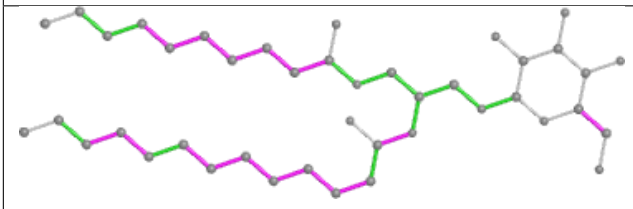
Ligand LMG AB 623



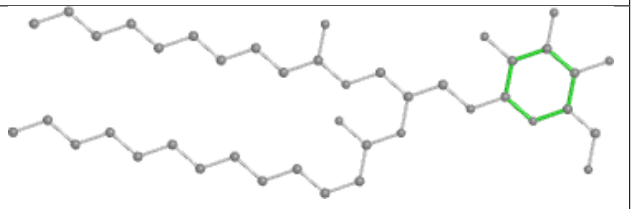
Bond lengths



Bond angles

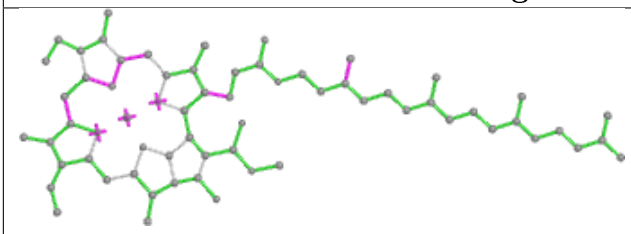


Torsions

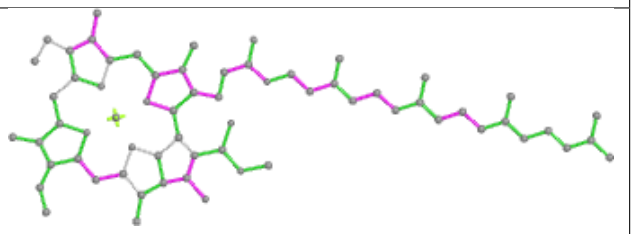


Rings

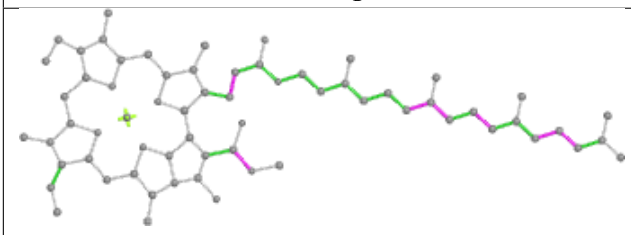
Ligand CLA BC 504



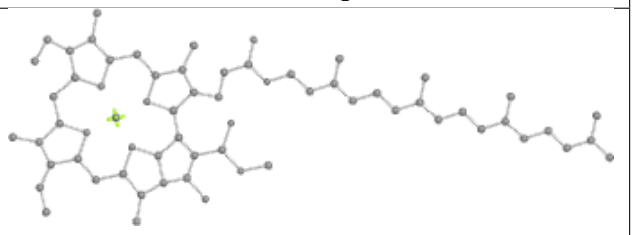
Bond lengths



Bond angles

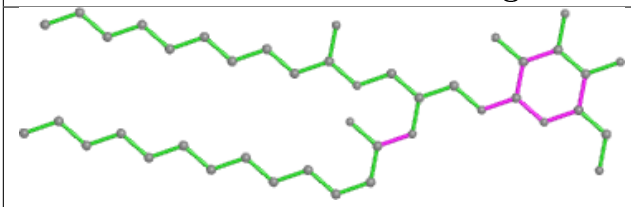


Torsions

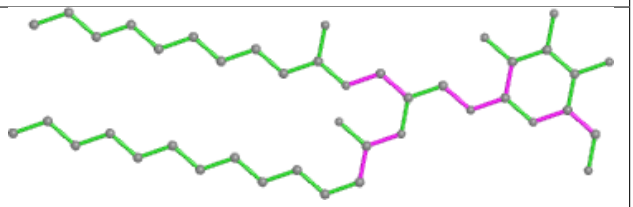


Rings

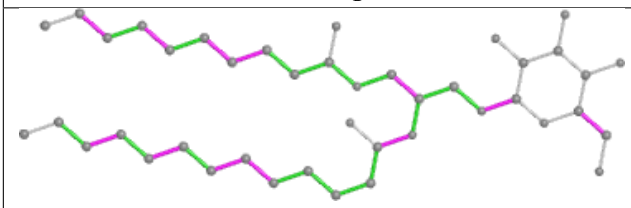
Ligand LMG AM 101



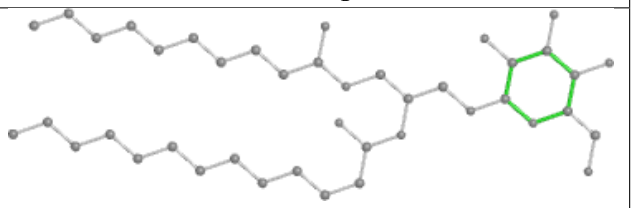
Bond lengths



Bond angles

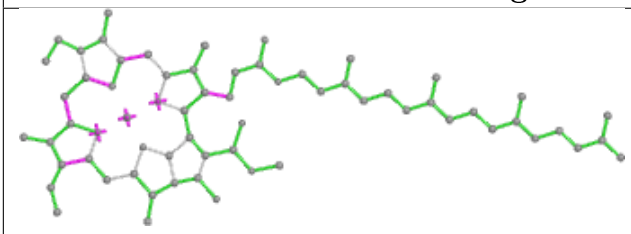


Torsions

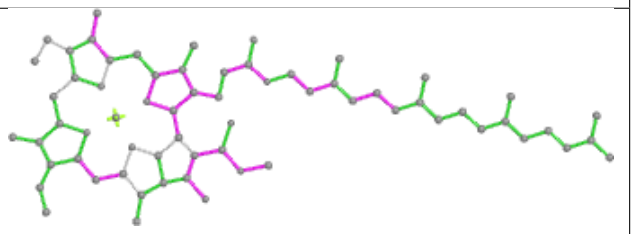


Rings

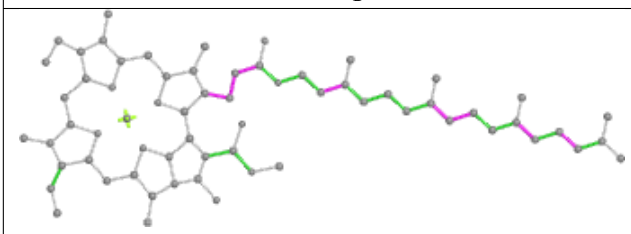
Ligand CLA AD 404



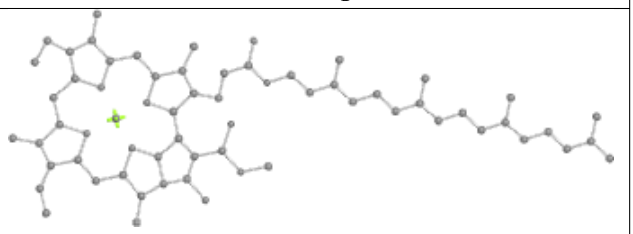
Bond lengths



Bond angles

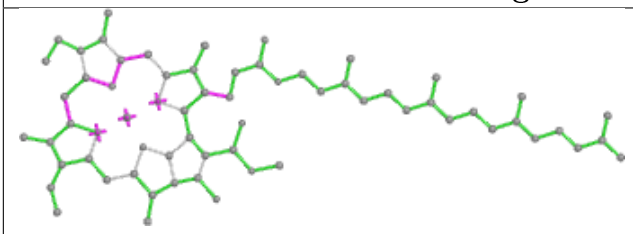


Torsions

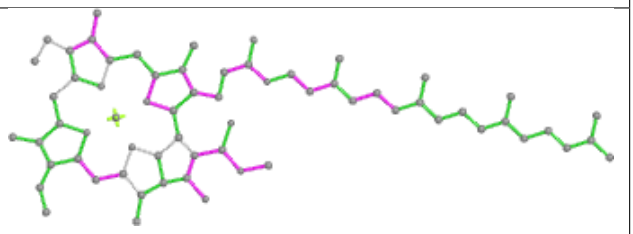


Rings

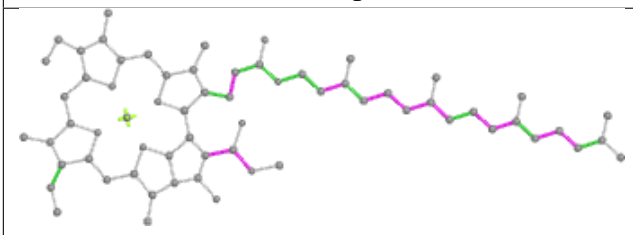
Ligand CLA BB 608



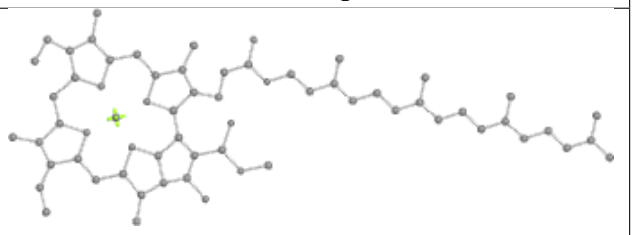
Bond lengths



Bond angles

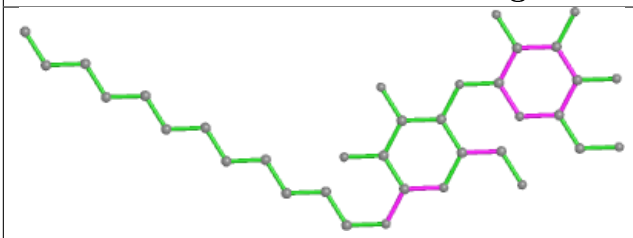


Torsions

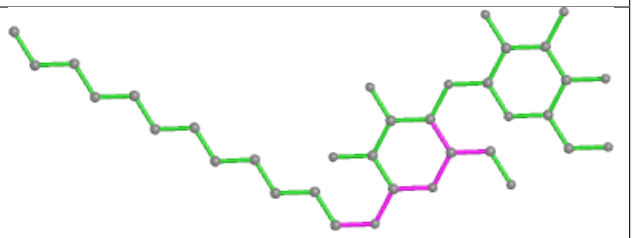


Rings

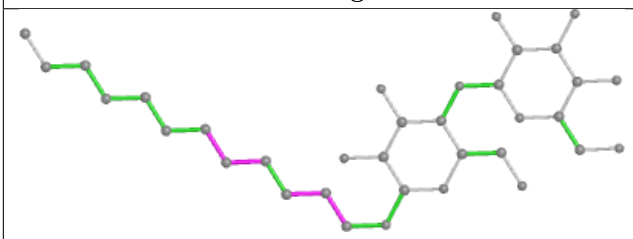
Ligand LMT BB 625



Bond lengths



Bond angles



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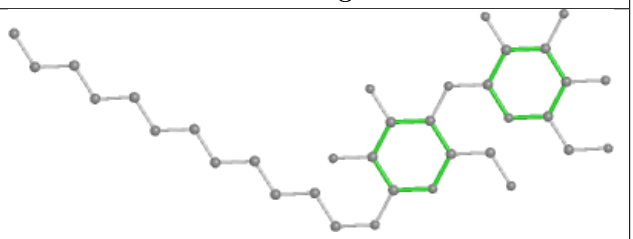
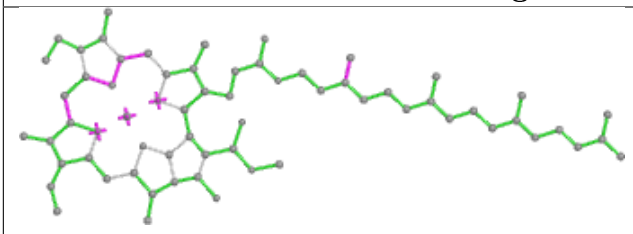


Rings

Ligand CLA BC 512



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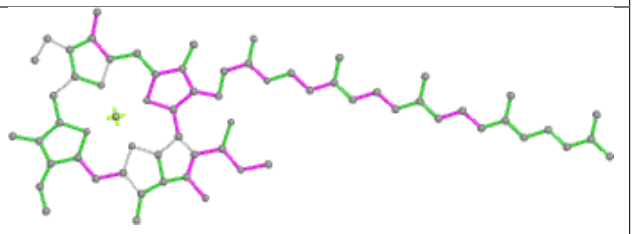
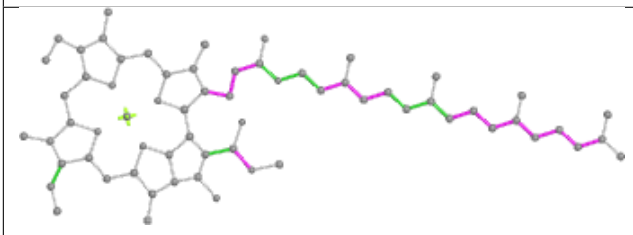


Bond angles



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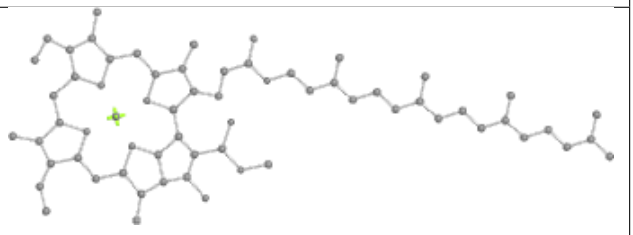
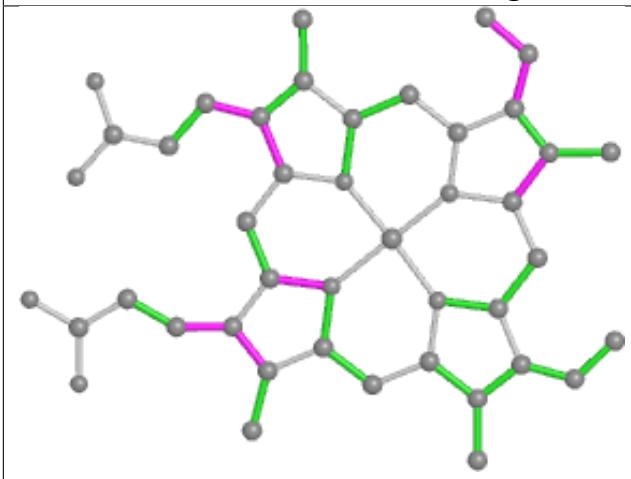
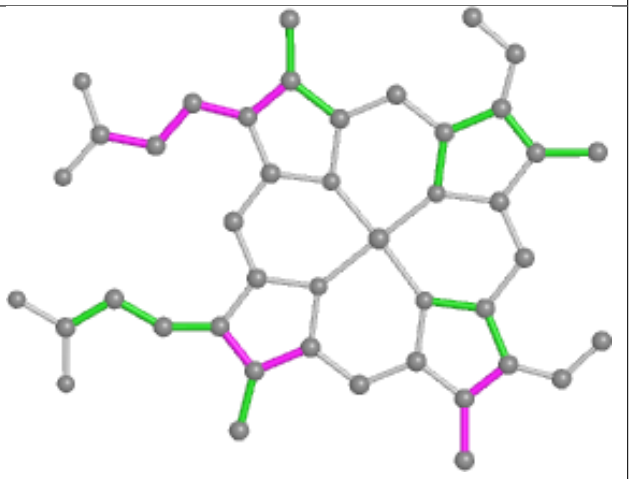


Rings

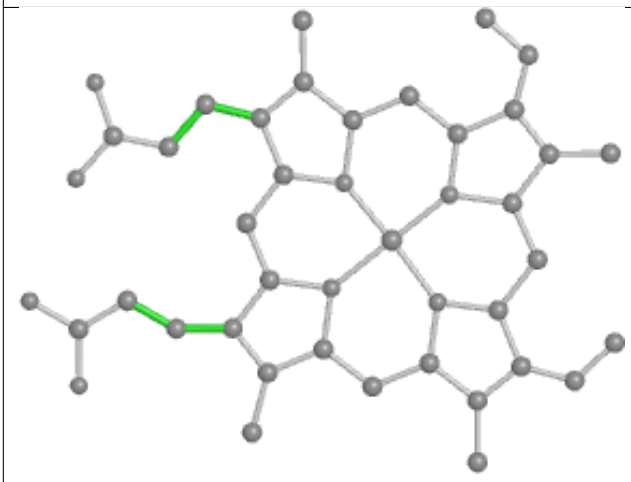
Ligand HEM BV 201



Bond lengths



Bond angles



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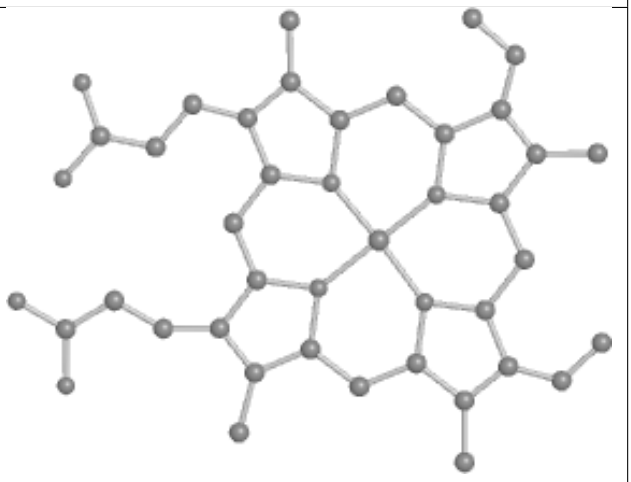
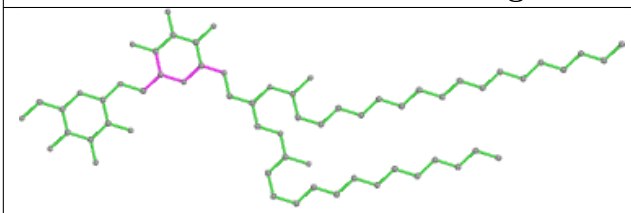
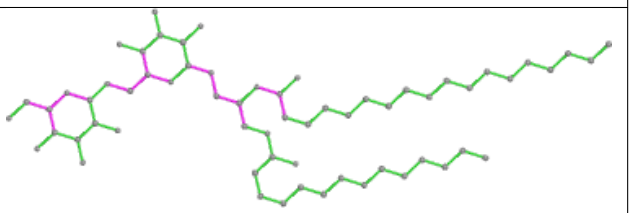


Rings

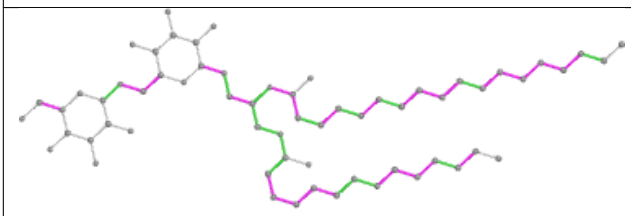
Ligand DGD AC 517



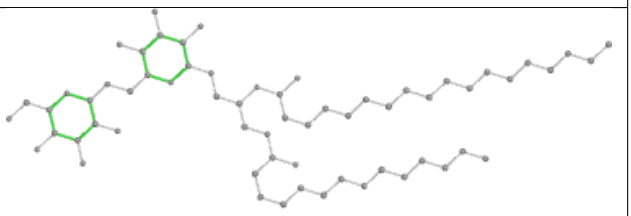
Bond lengths



Bond angles

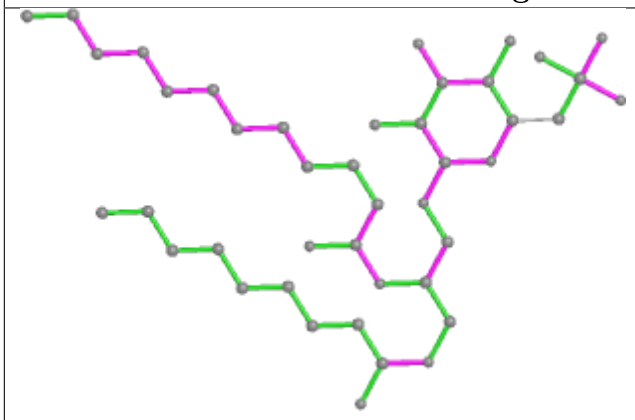


Torsions

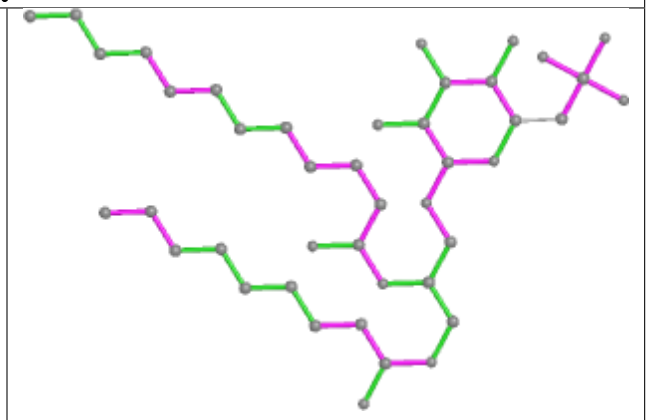


Rings

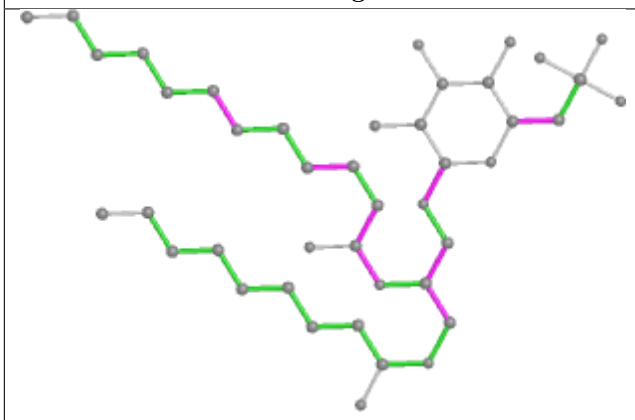
Ligand SQD BD 409



Bond lengths



Bond angles



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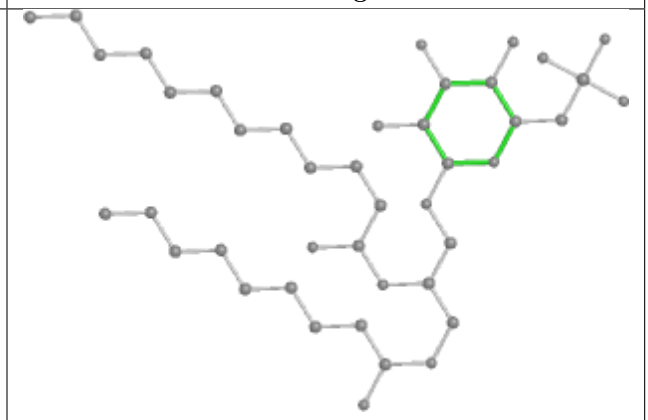
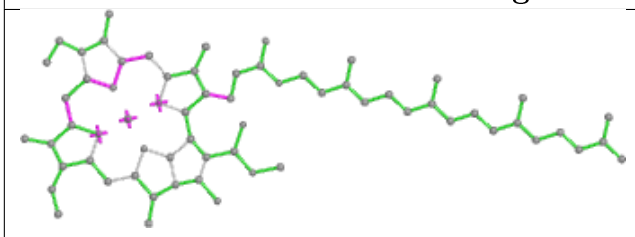
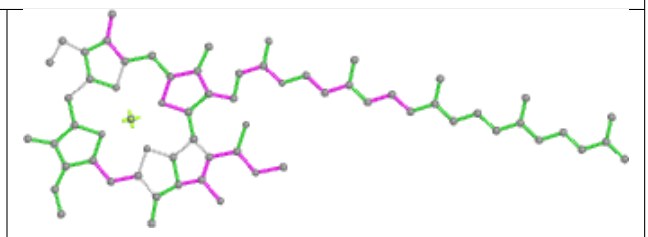


Rings

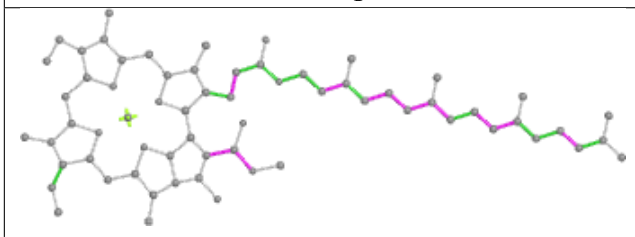
Ligand CLA AB 605



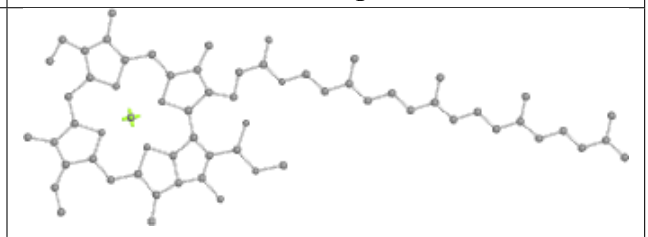
Bond lengths



Bond angles

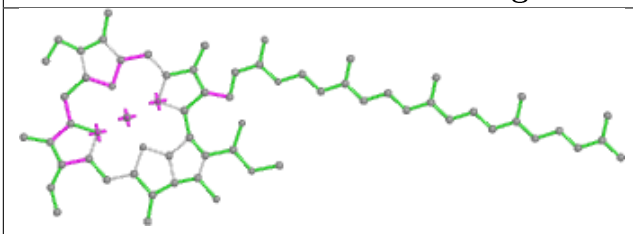


Torsions

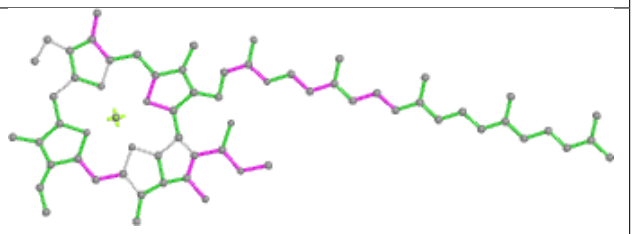


Rings

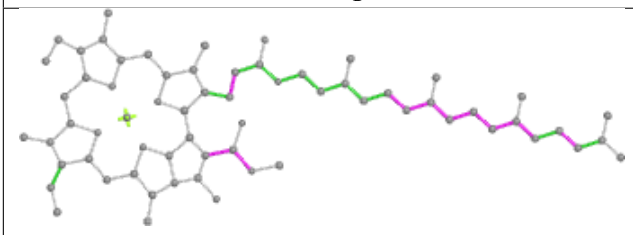
Ligand CLA AC 503



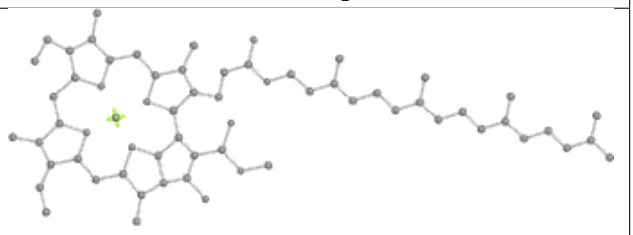
Bond lengths



Bond angles

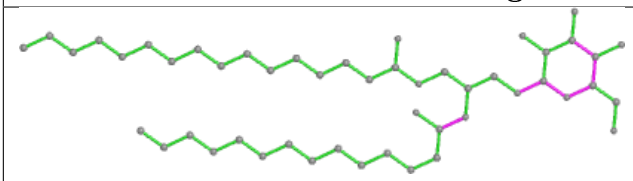


Torsions

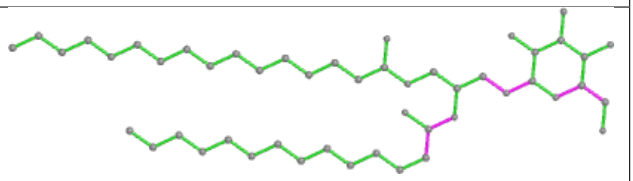


Rings

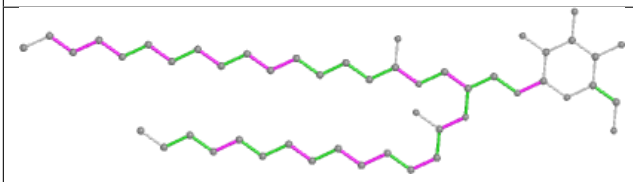
Ligand LMG AB 622



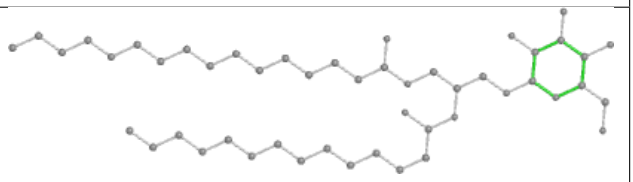
Bond lengths



Bond angles

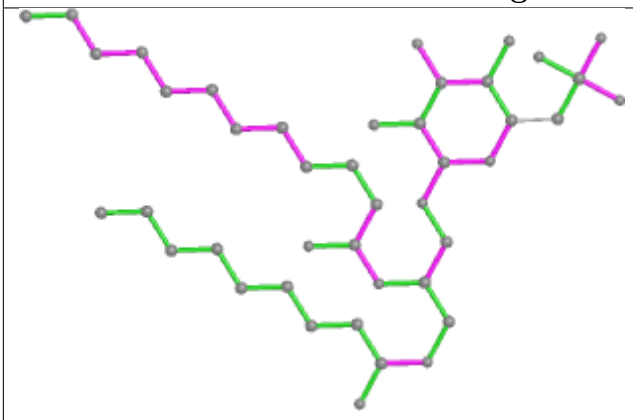


Torsions



Rings

Ligand SQD AD 409



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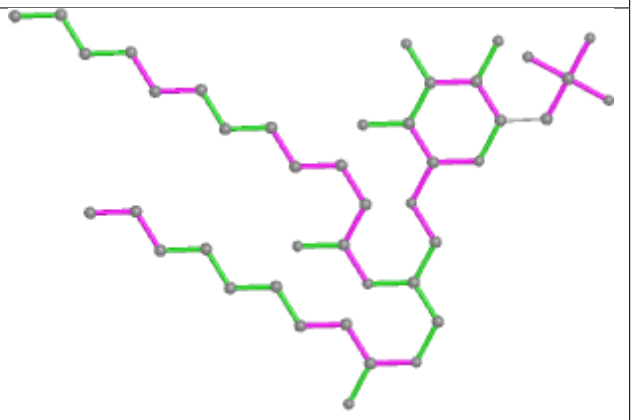
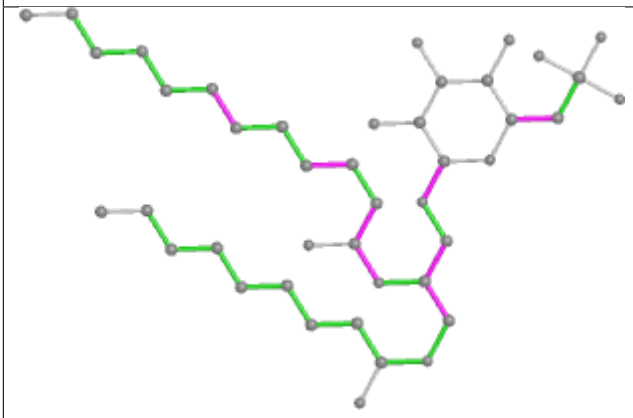
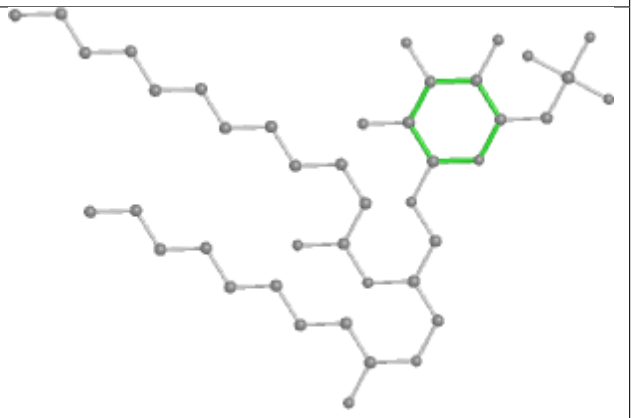


Bond angles

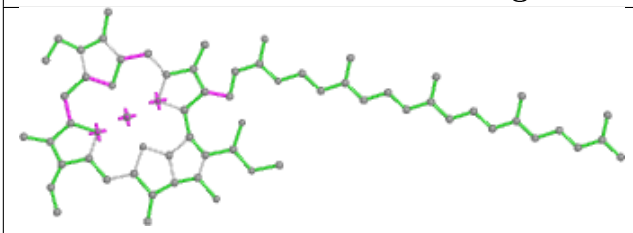


Torsions

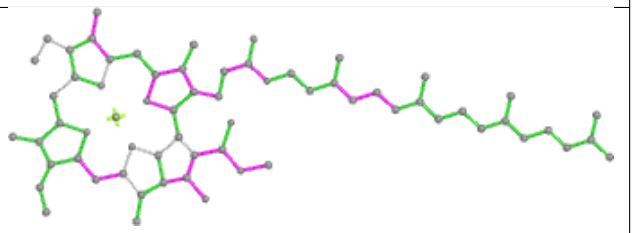


Rings

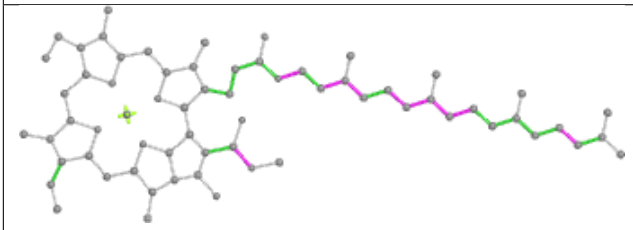
Ligand CLA AB 611



Bond lengths



Bond angles



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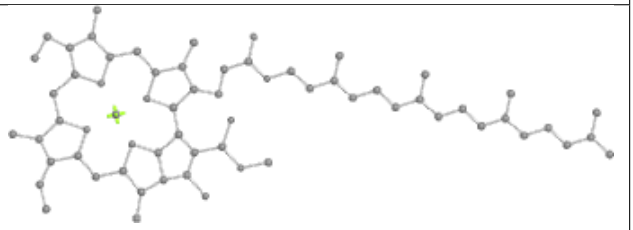
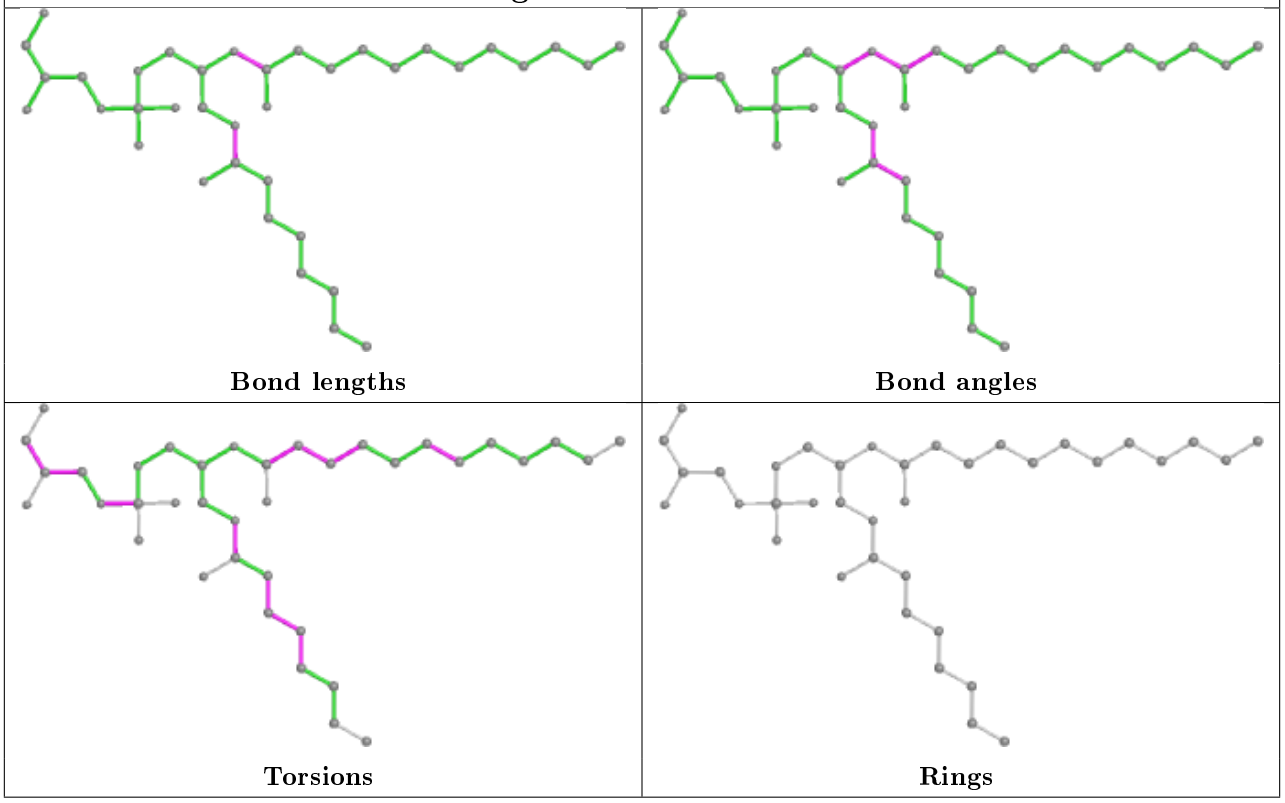
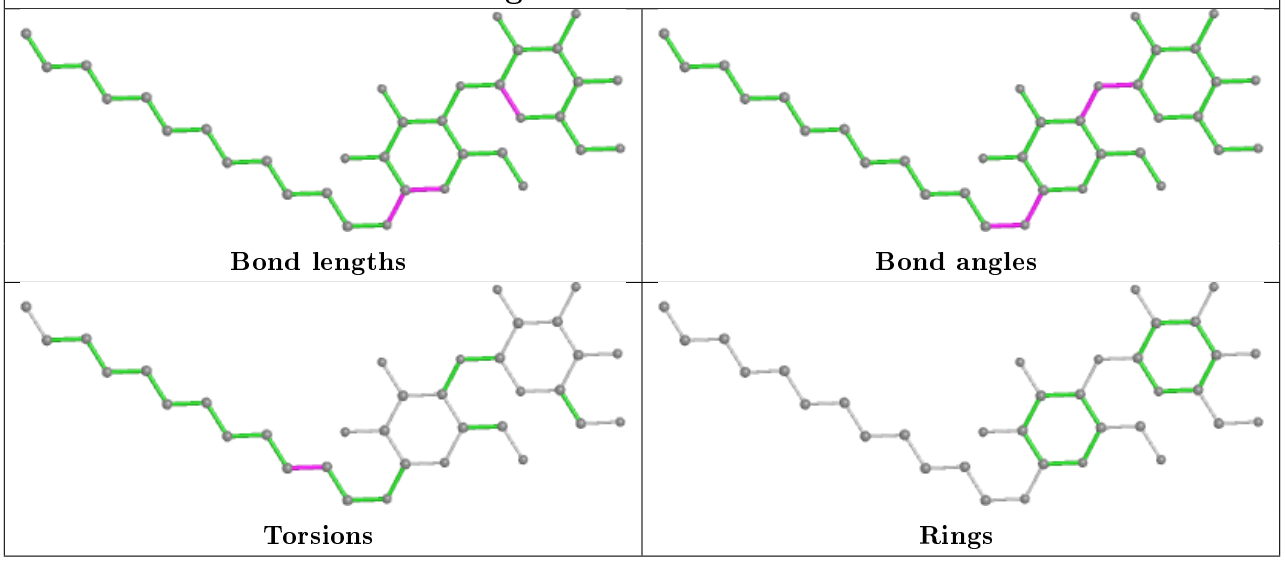


Rings

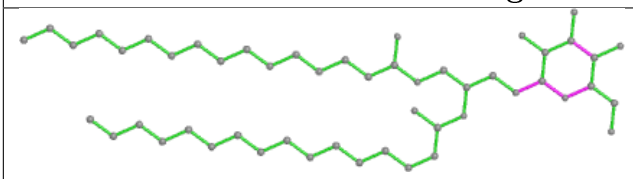
Ligand LHG BC 521

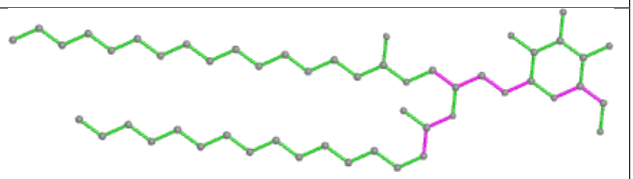


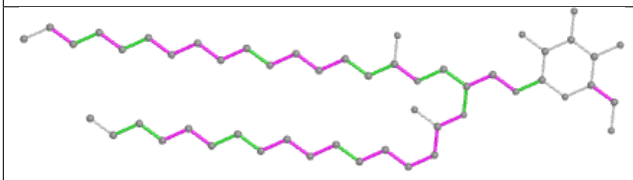
Ligand LMT BM 101

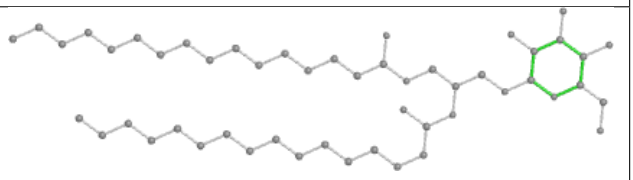


Ligand LMG BA 414

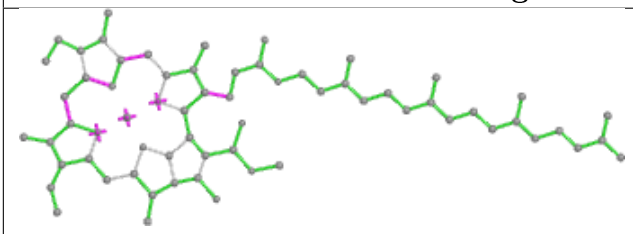

Bond lengths

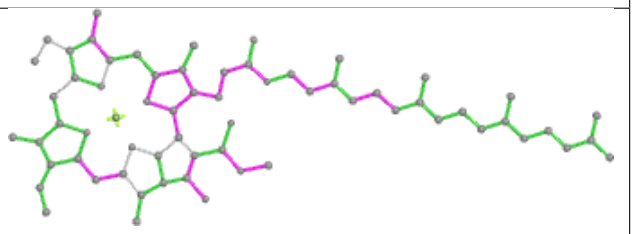

Bond angles

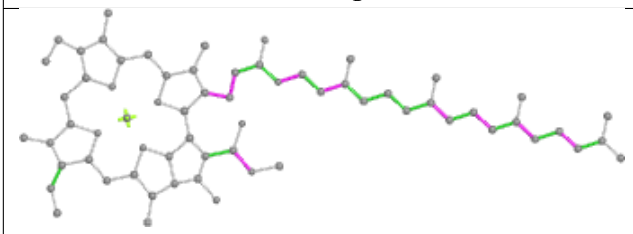

Torsions

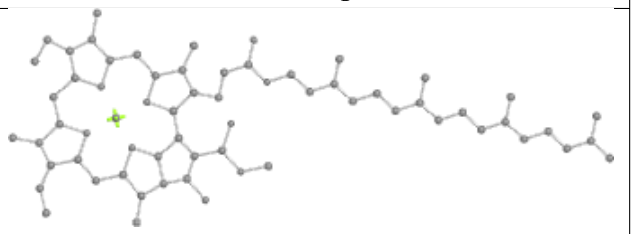

Rings

Ligand CLA AB 606

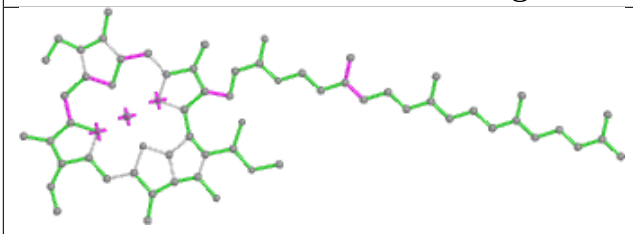

Bond lengths

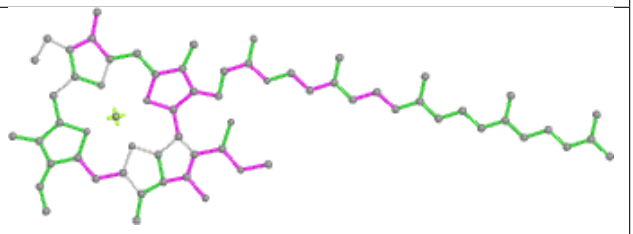

Bond angles

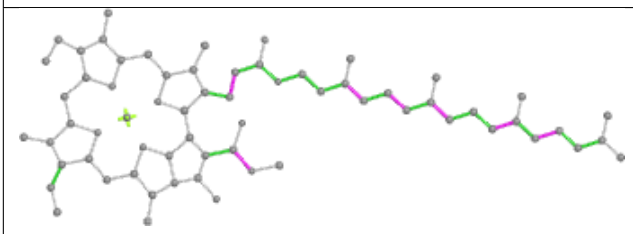

Torsions

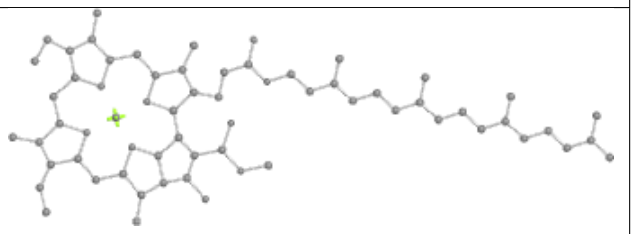

Rings

Ligand CLA AB 603

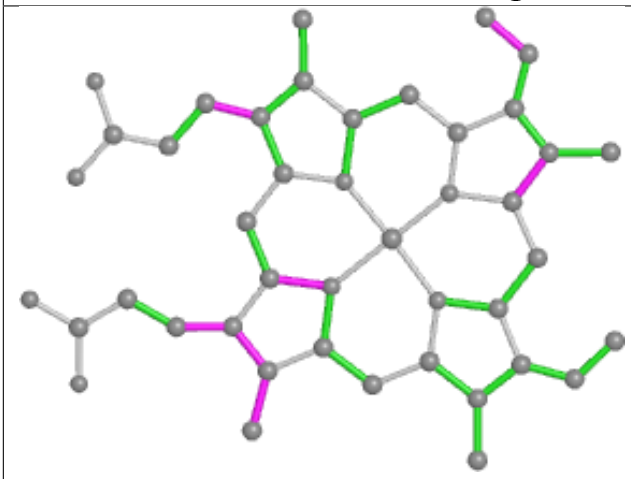

Bond lengths


Bond angles

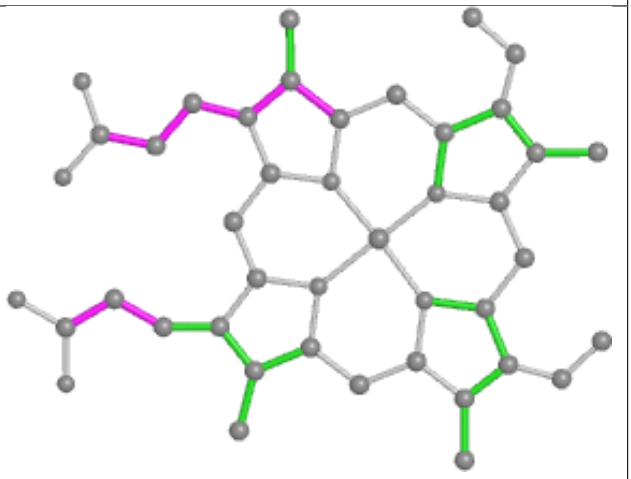

Torsions


Rings

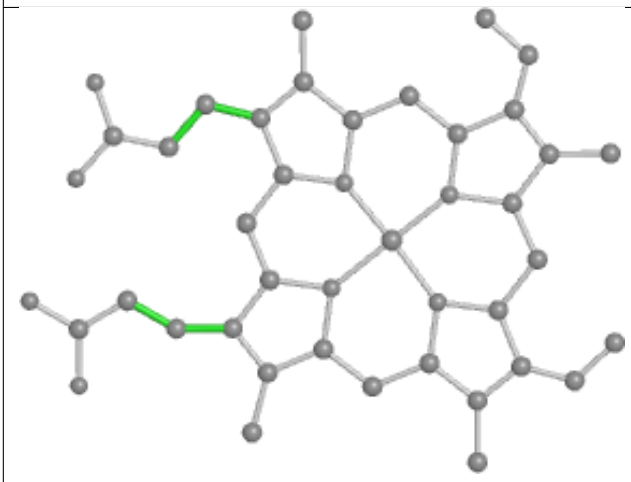
Ligand HEM BE 101



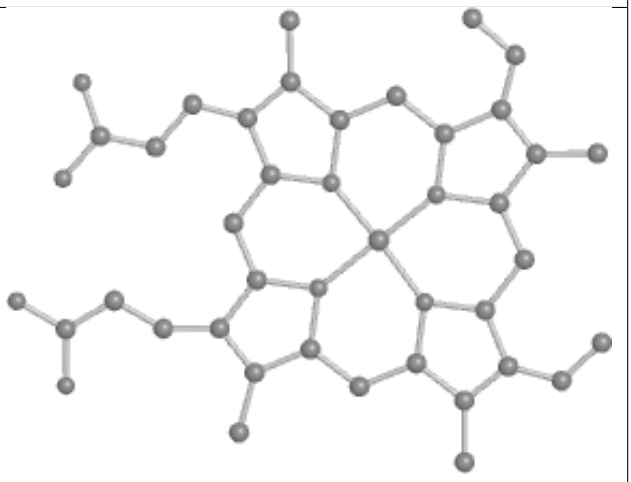
Bond lengths



Bond angles

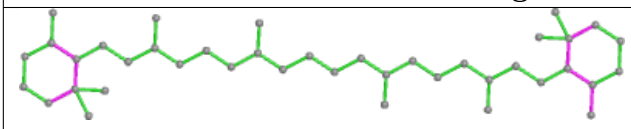


Torsions



Rings

Ligand BCR AZ 101



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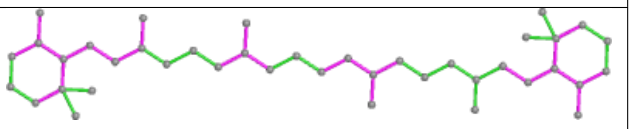
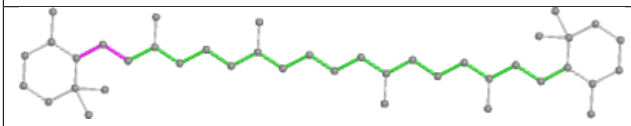
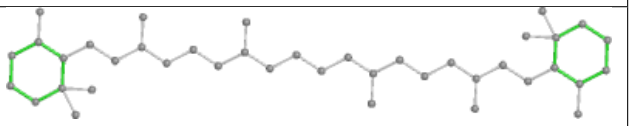


Bond angles

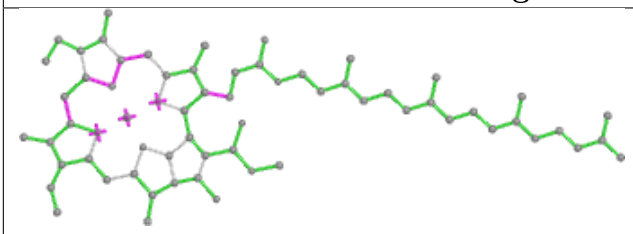


Torsions

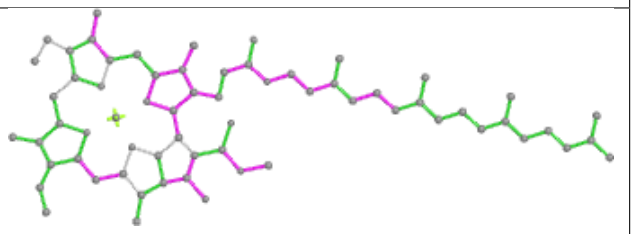


Rings

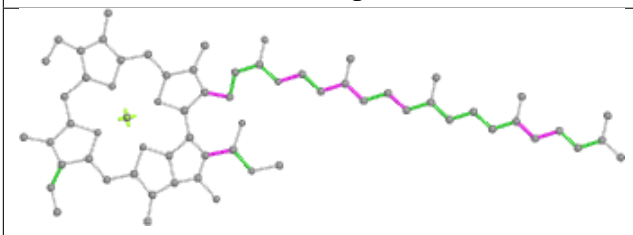
Ligand CLA BB 612



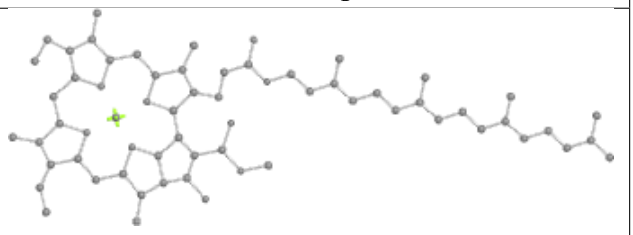
Bond lengths



Bond angles

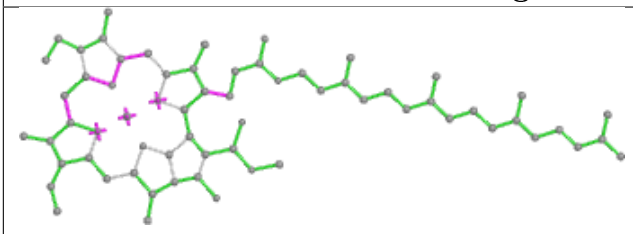


Torsions

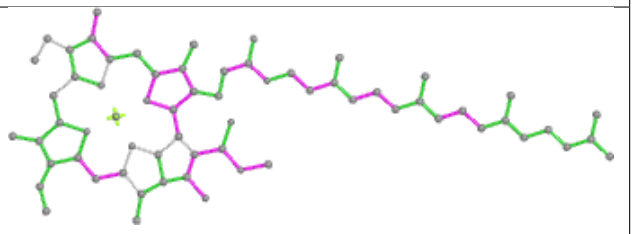


Rings

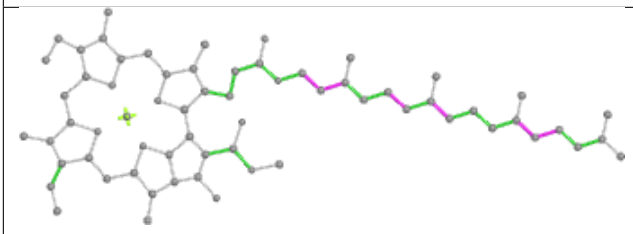
Ligand CLA BB 618



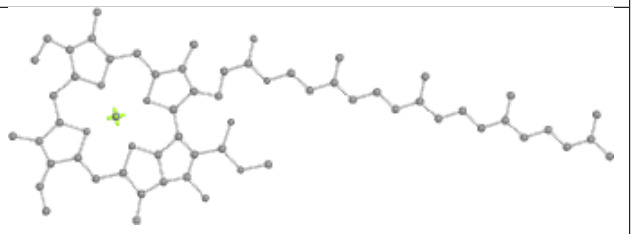
Bond lengths



Bond angles

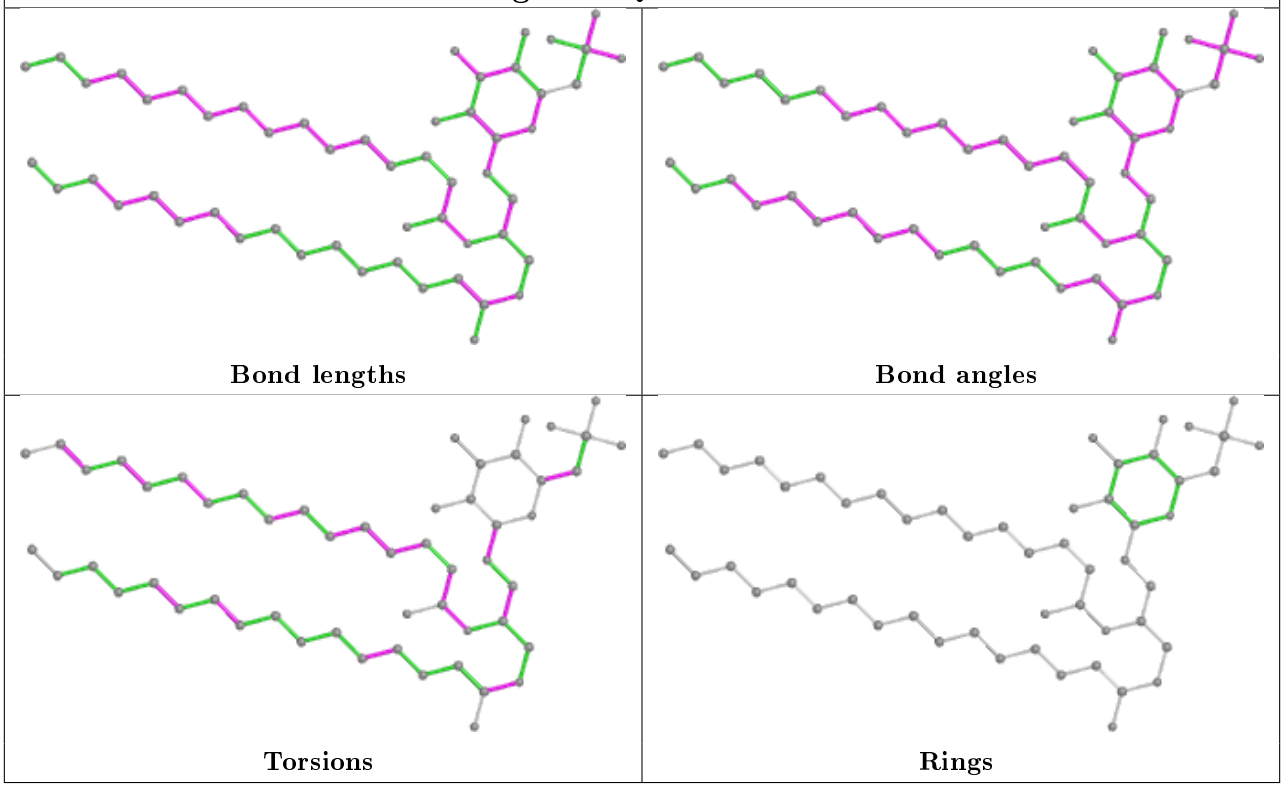


Torsions

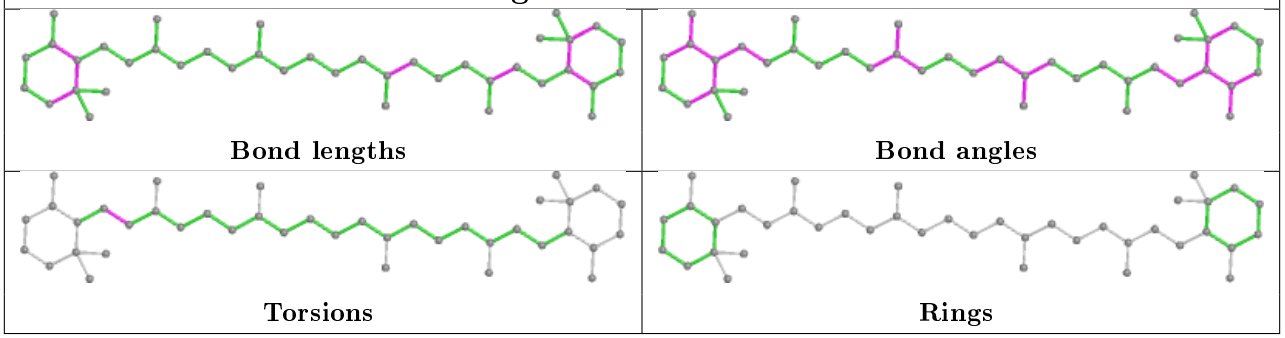


Rings

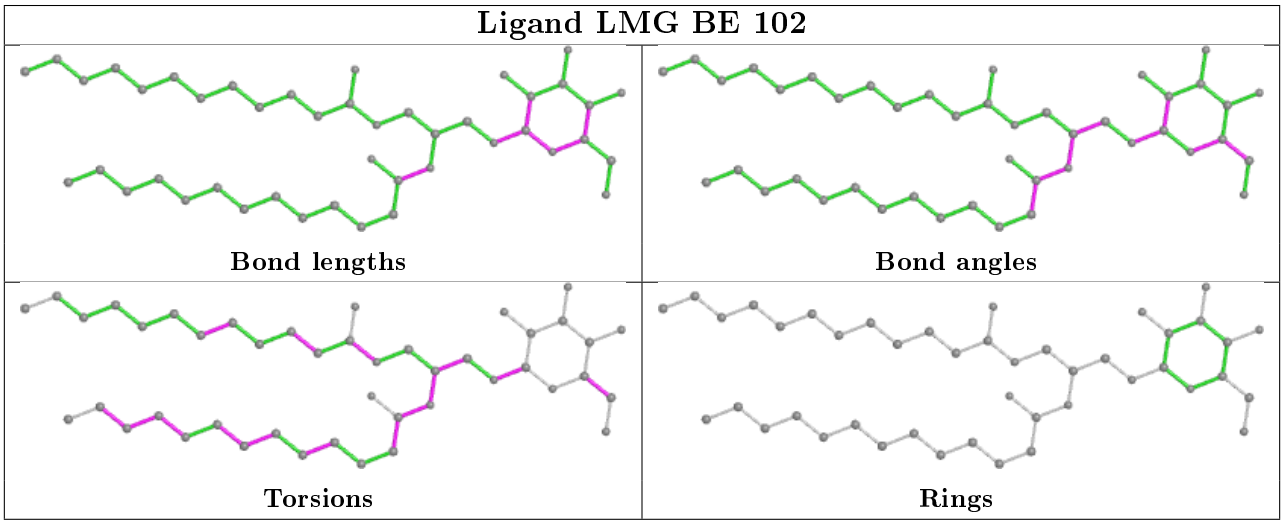
Ligand SQD BA 401



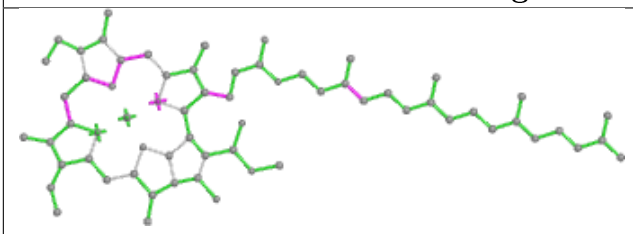
Ligand BCR BB 620



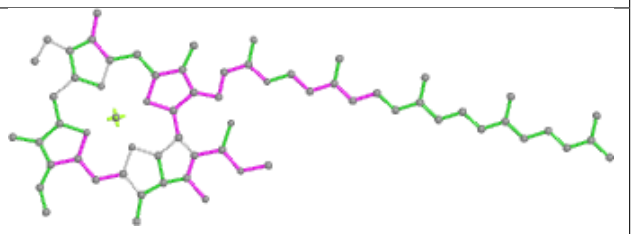
Ligand LMG BE 102



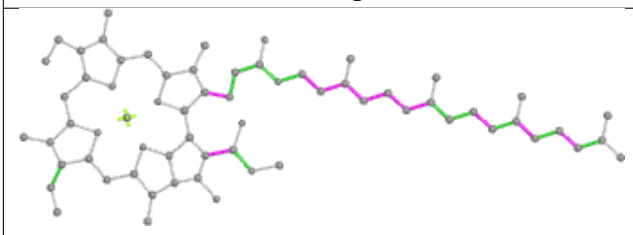
Ligand CLA BA 404



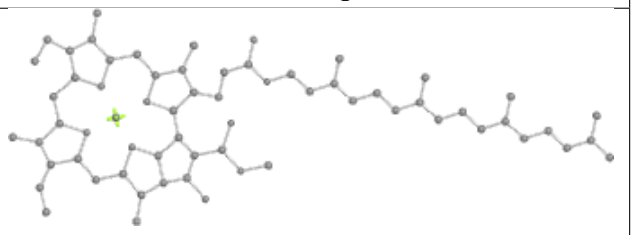
Bond lengths



Bond angles

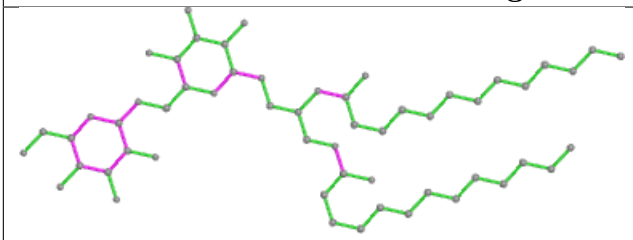


Torsions

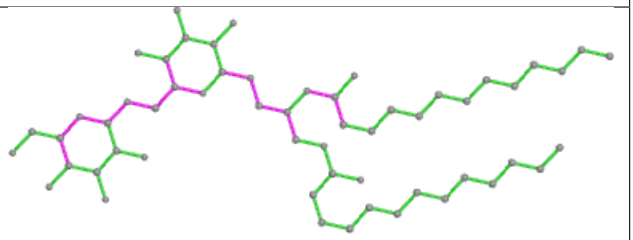


Rings

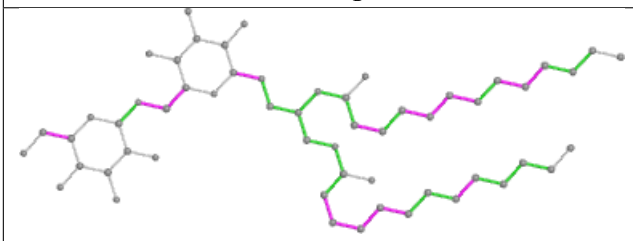
Ligand DGD AA 410



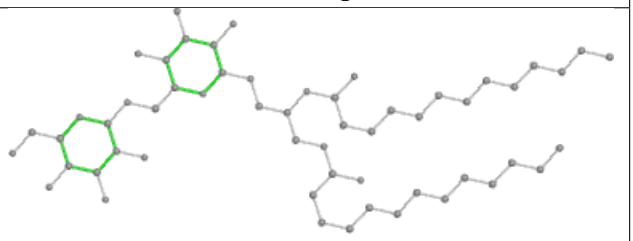
Bond lengths



Bond angles

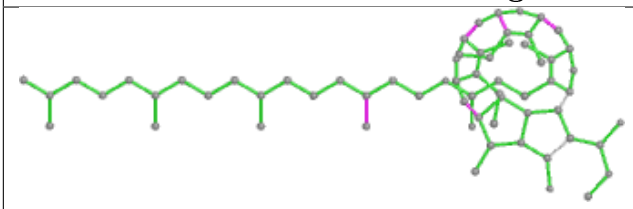


Torsions

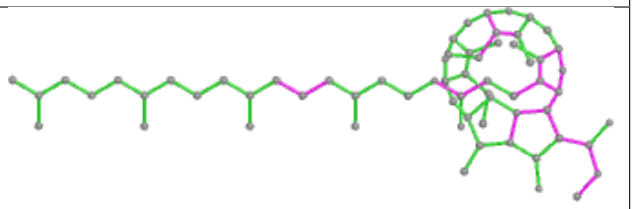


Rings

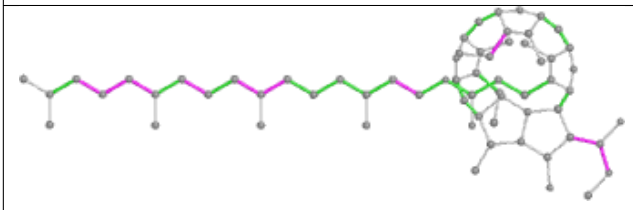
Ligand PHO AD 403



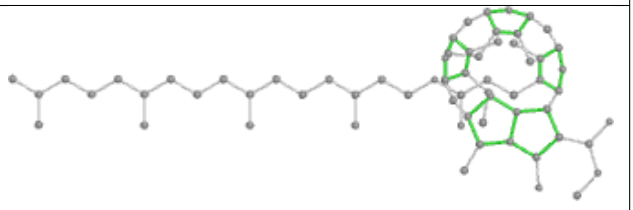
Bond lengths



Bond angles

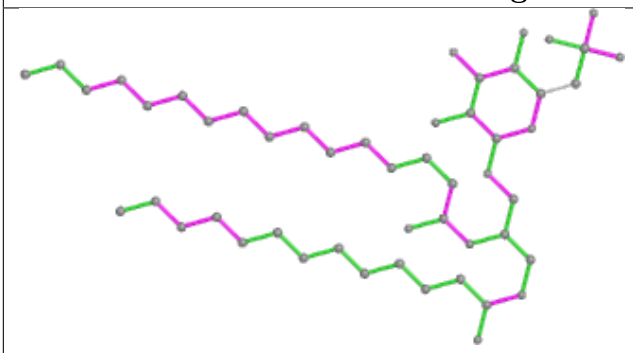


Torsions

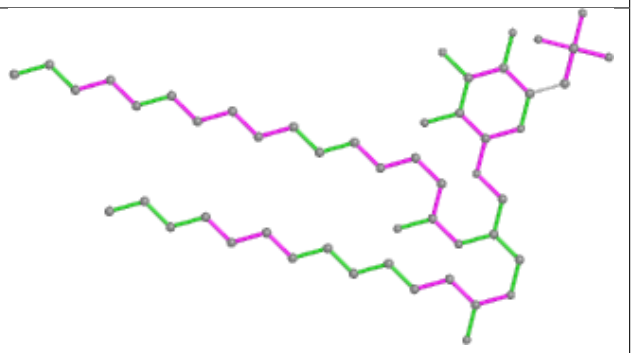


Rings

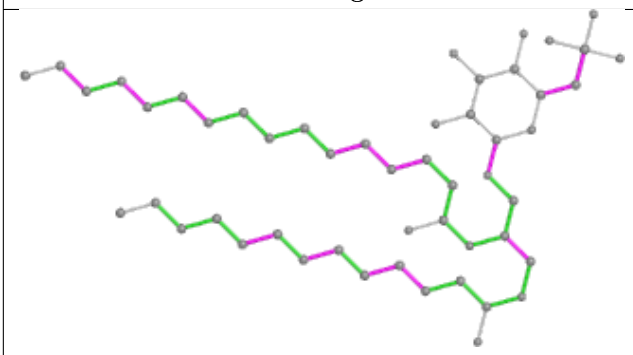
Ligand SQD AA 412



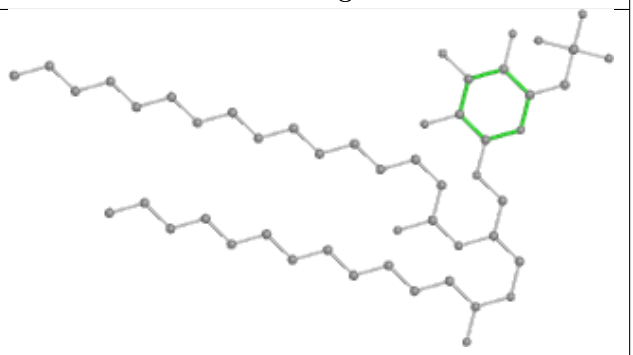
Bond lengths



Bond angles

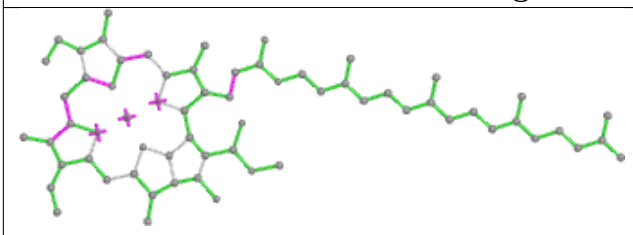


Torsions

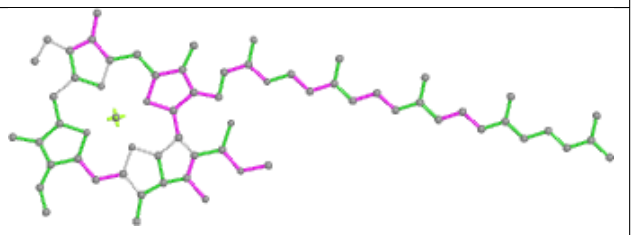


Rings

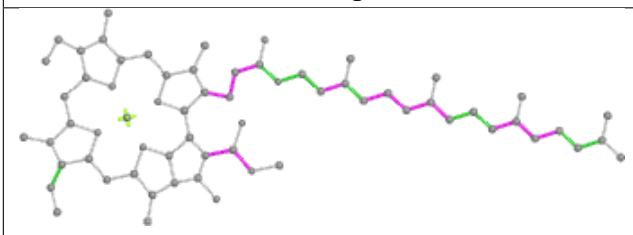
Ligand CLA BB 605



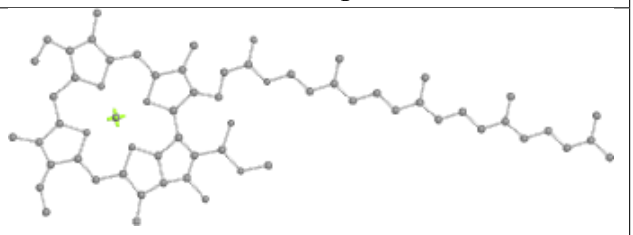
Bond lengths



Bond angles

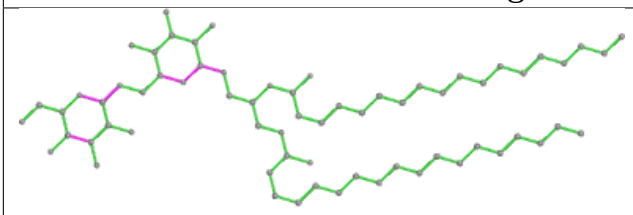


Torsions

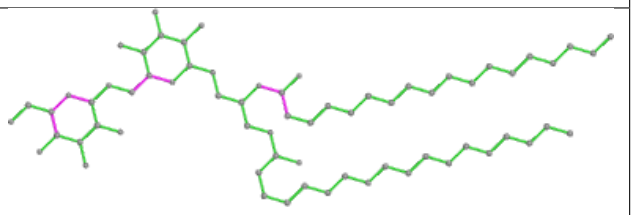


Rings

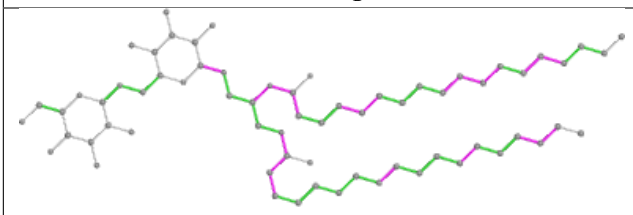
Ligand DGD AC 518



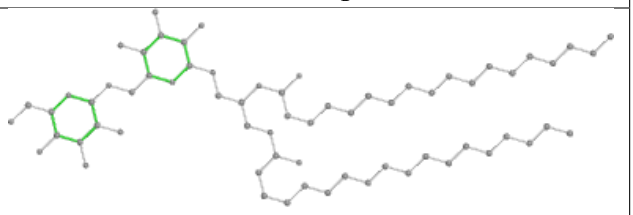
Bond lengths



Bond angles

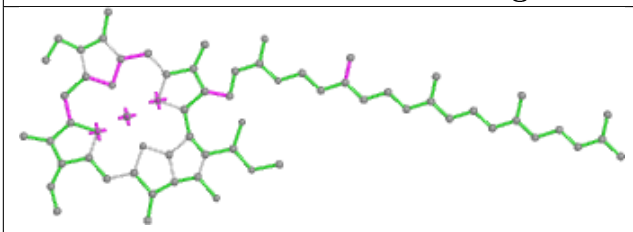


Torsions

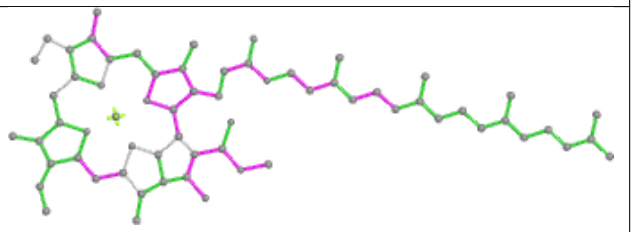


Rings

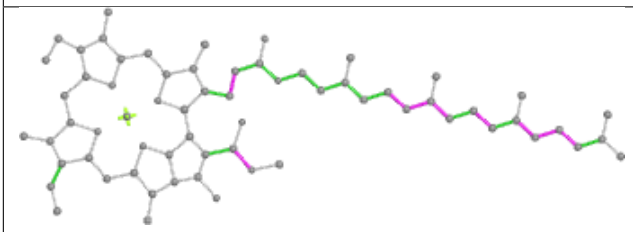
Ligand CLA BC 508



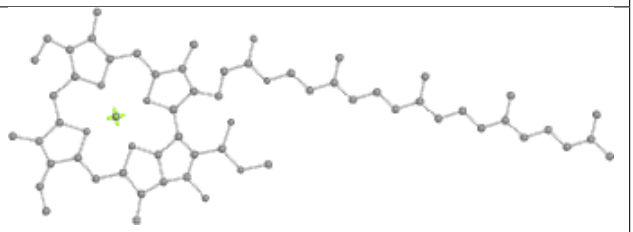
Bond lengths



Bond angles

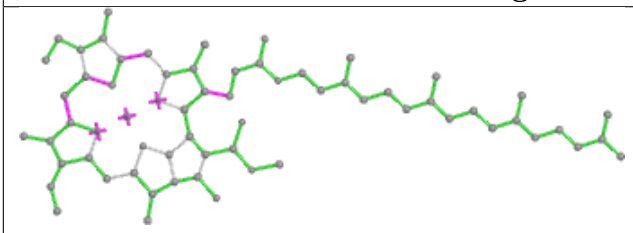


Torsions

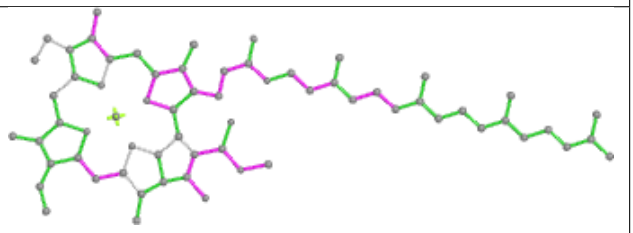


Rings

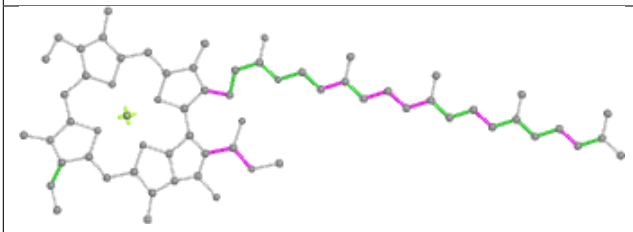
Ligand CLA BA 405



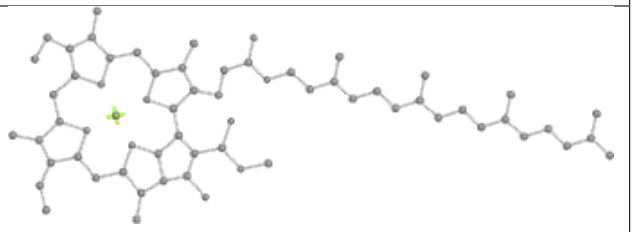
Bond lengths



Bond angles

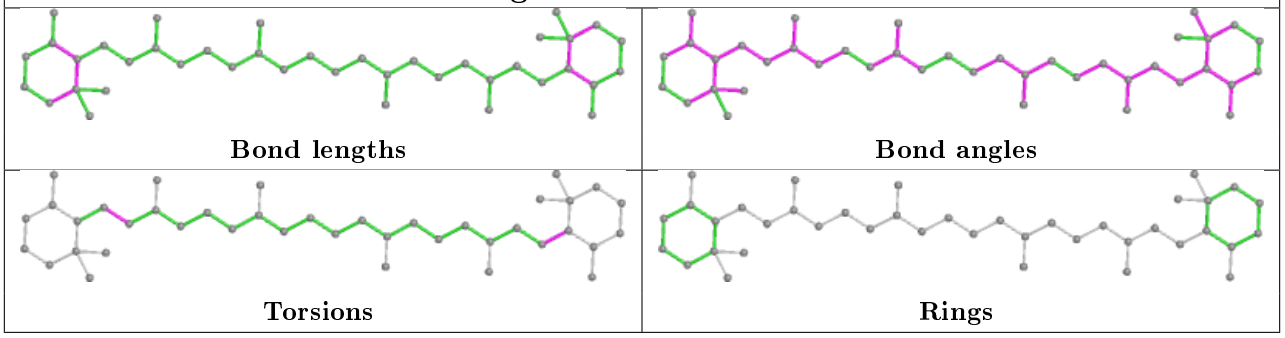


Torsions

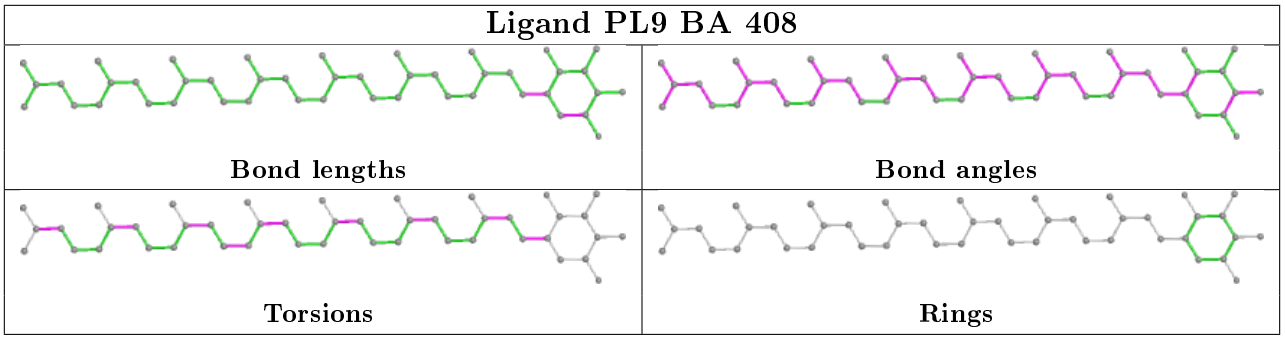


Rings

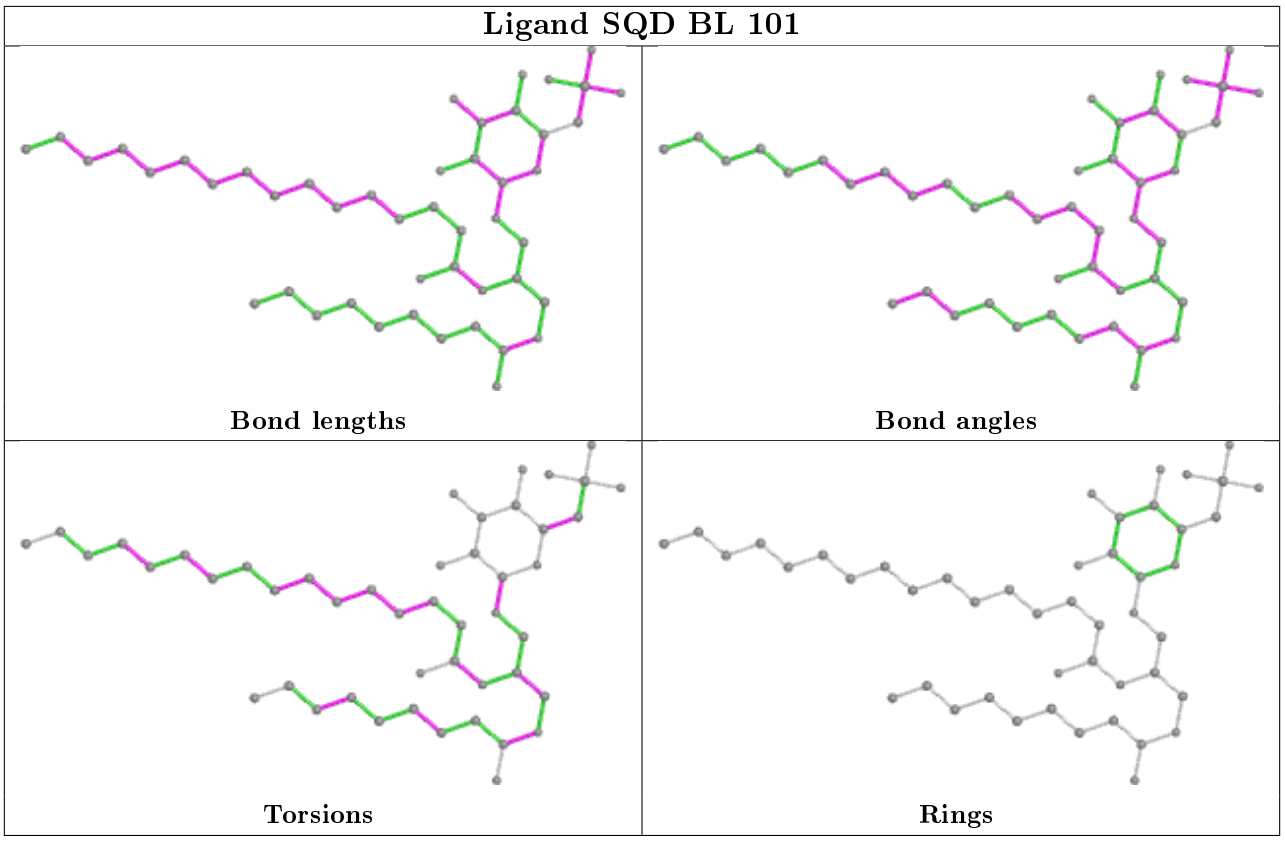
Ligand BCR AB 618



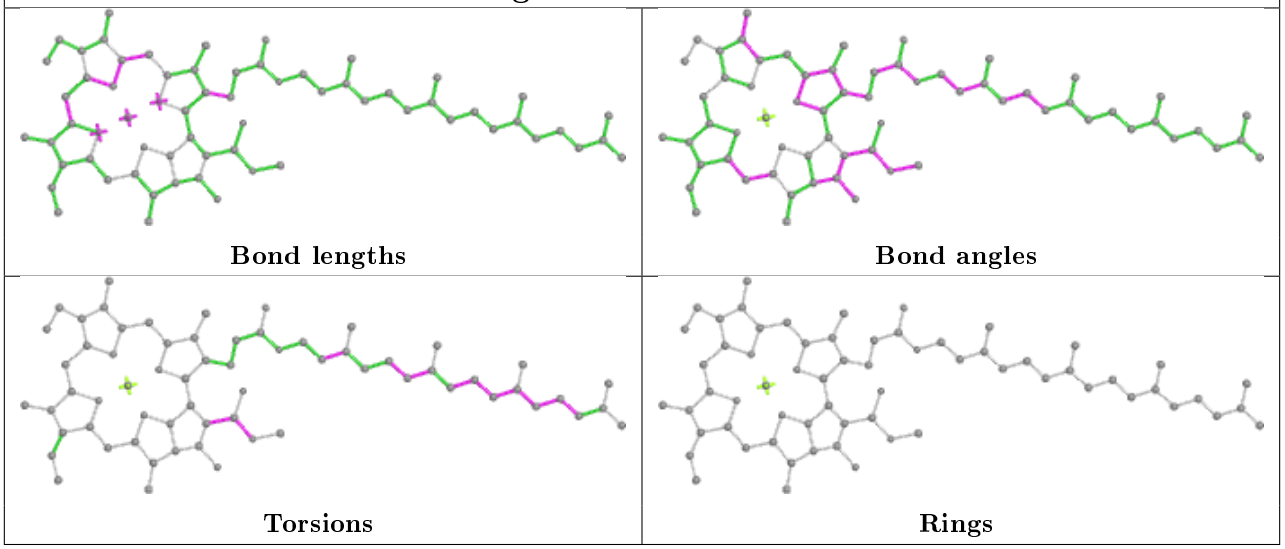
Ligand PL9 BA 408



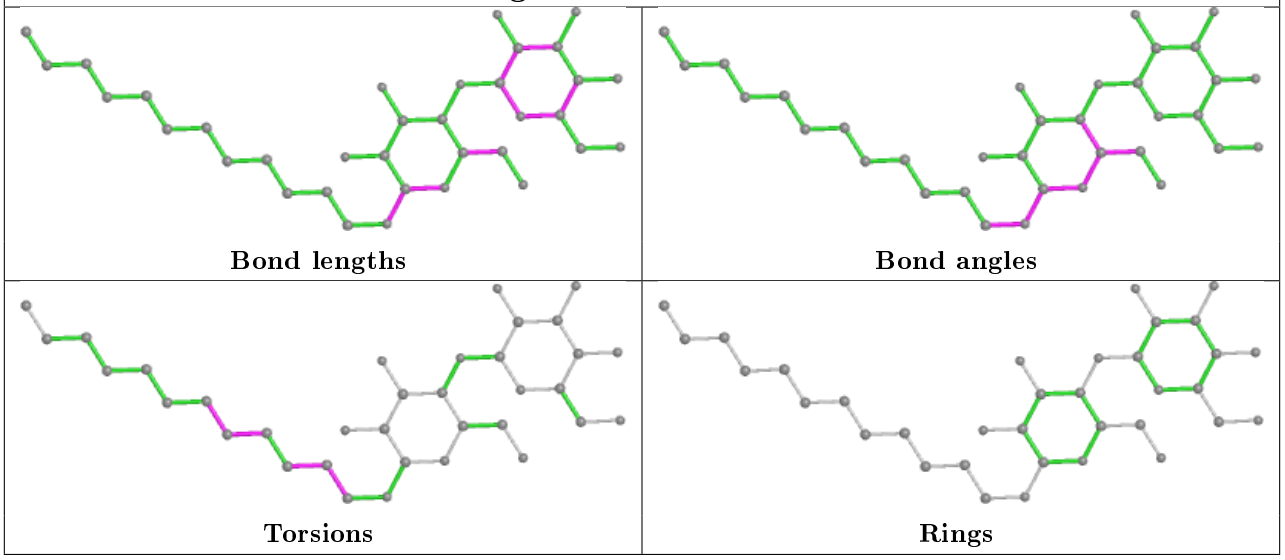
Ligand SQD BL 101



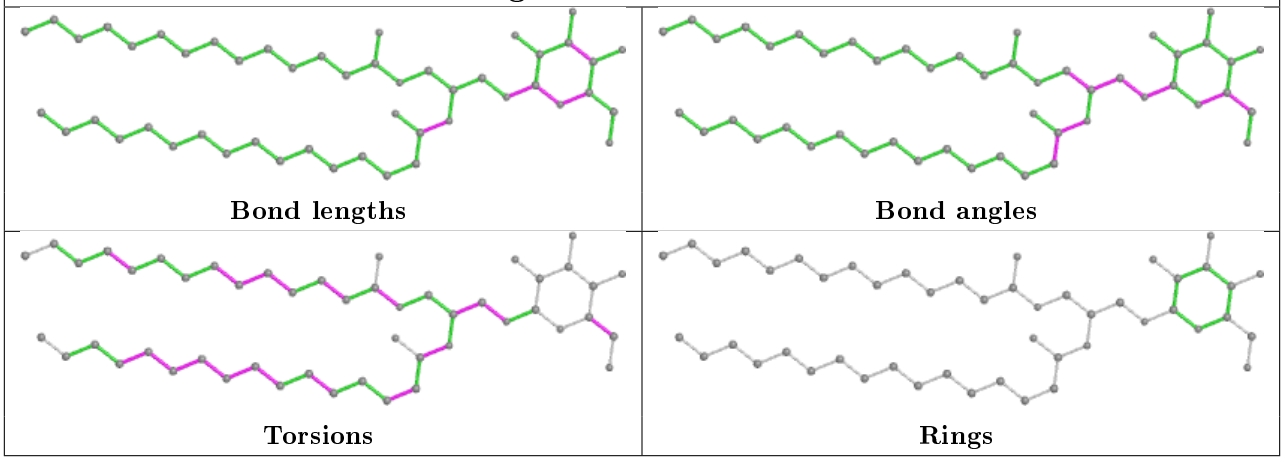
Ligand CLA AC 506



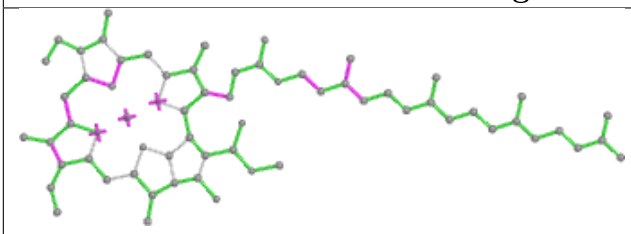
Ligand LMT AB 624



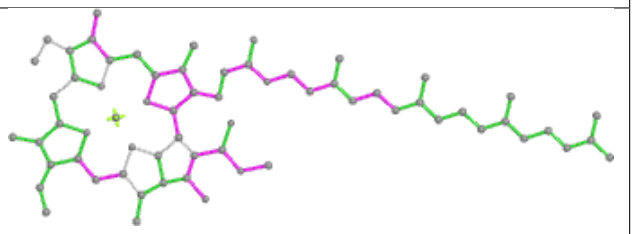
Ligand LMG BB 623



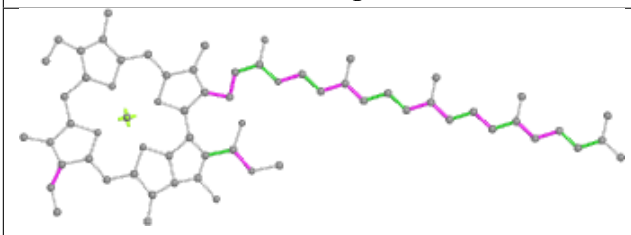
Ligand CLA BB 604



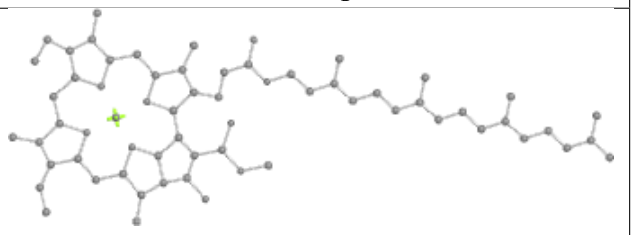
Bond lengths



Bond angles

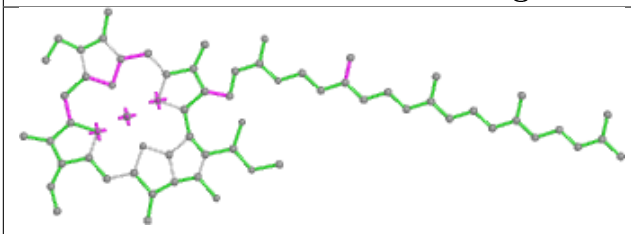


Torsions

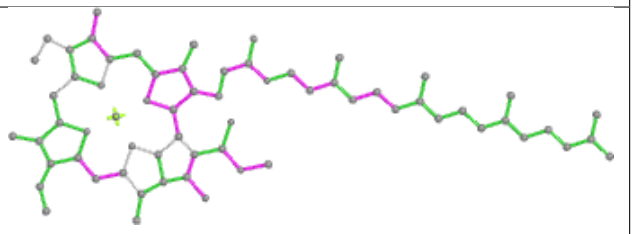


Rings

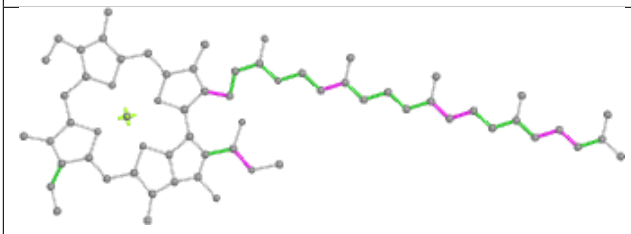
Ligand CLA BB 607



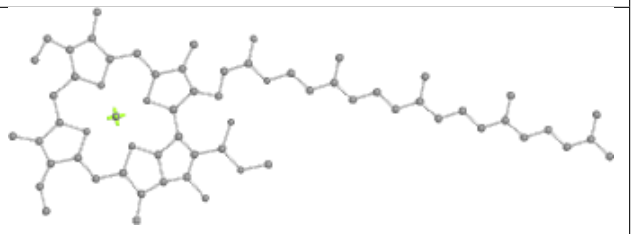
Bond lengths



Bond angles

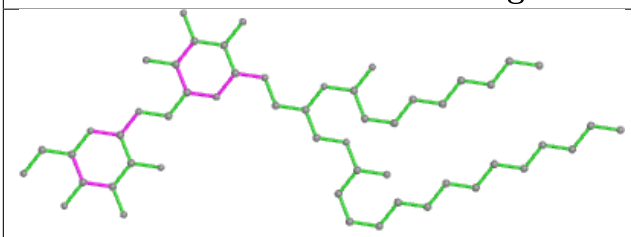


Torsions

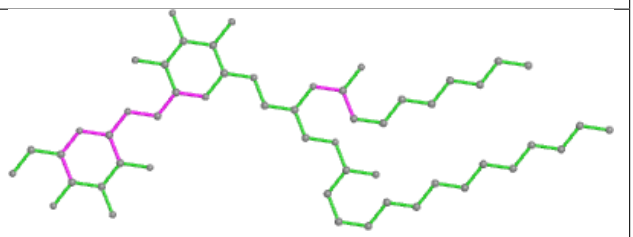


Rings

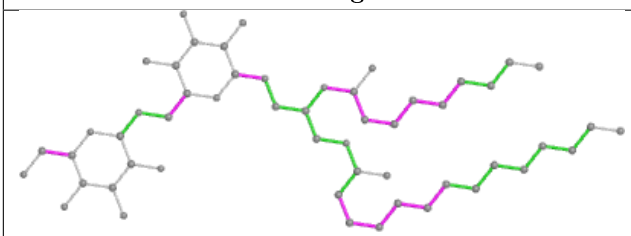
Ligand DGD BC 516



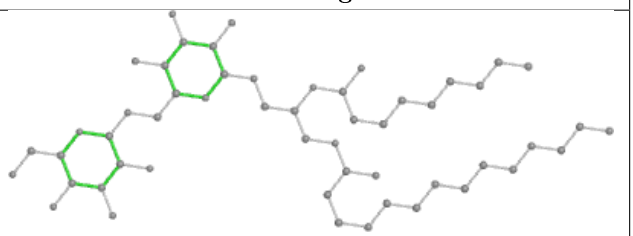
Bond lengths



Bond angles

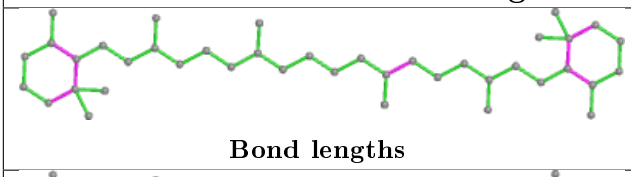


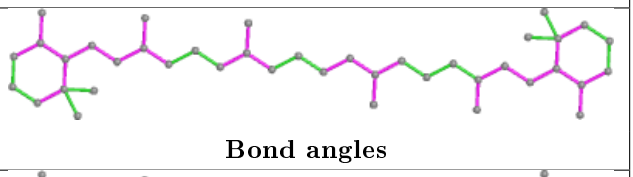
Torsions

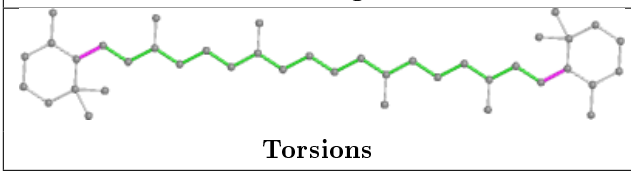


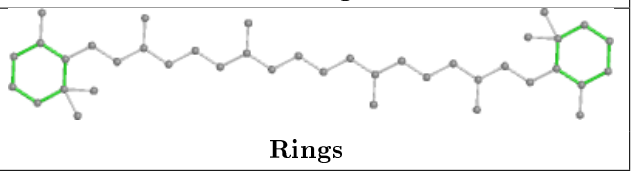
Rings

Ligand BCR AA 409

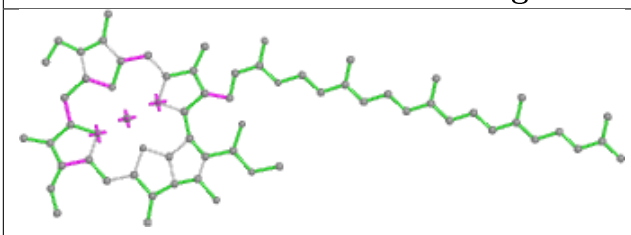

Bond lengths

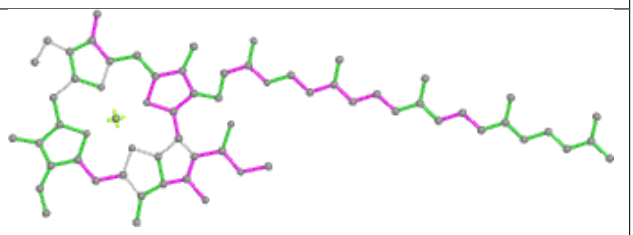

Bond angles

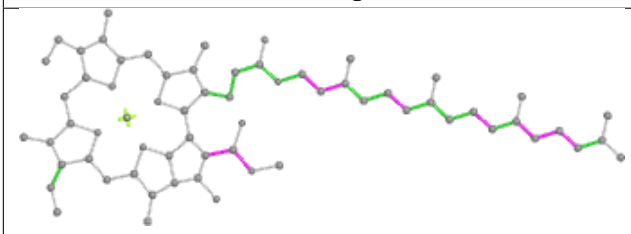

Torsions

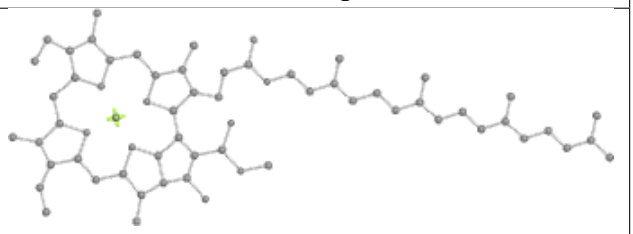

Rings

Ligand CLA AC 509

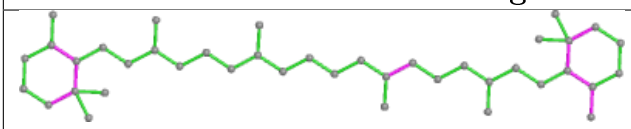

Bond lengths

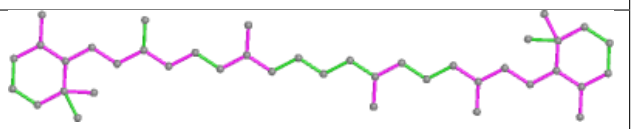

Bond angles

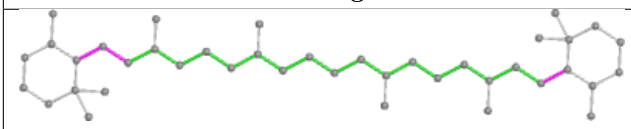

Torsions

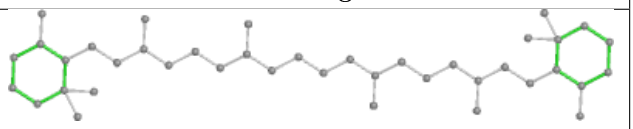

Rings

Ligand BCR AC 514

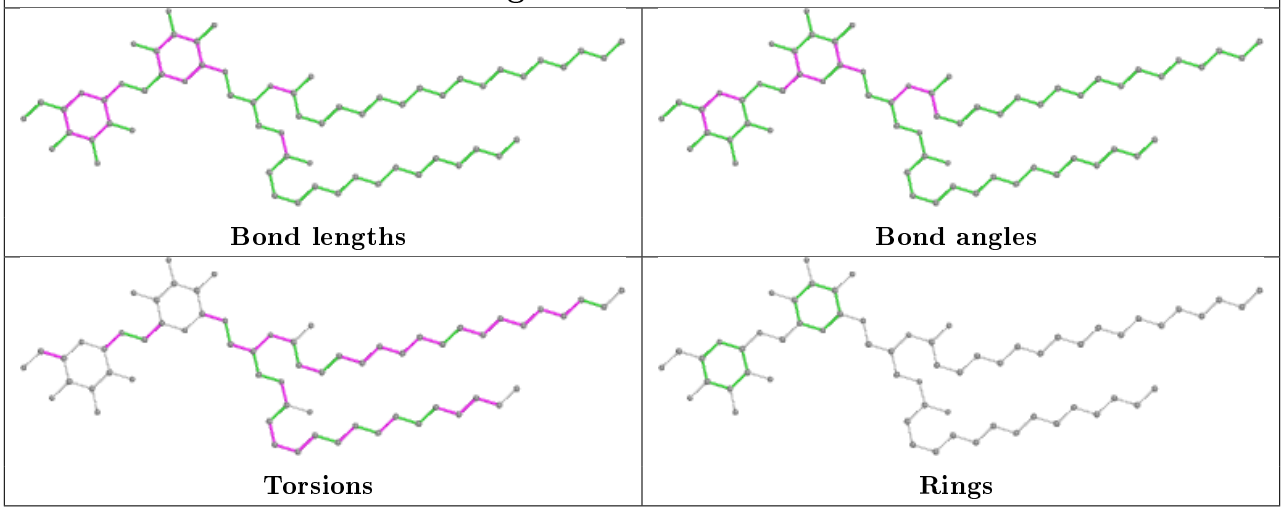

Bond lengths


Bond angles

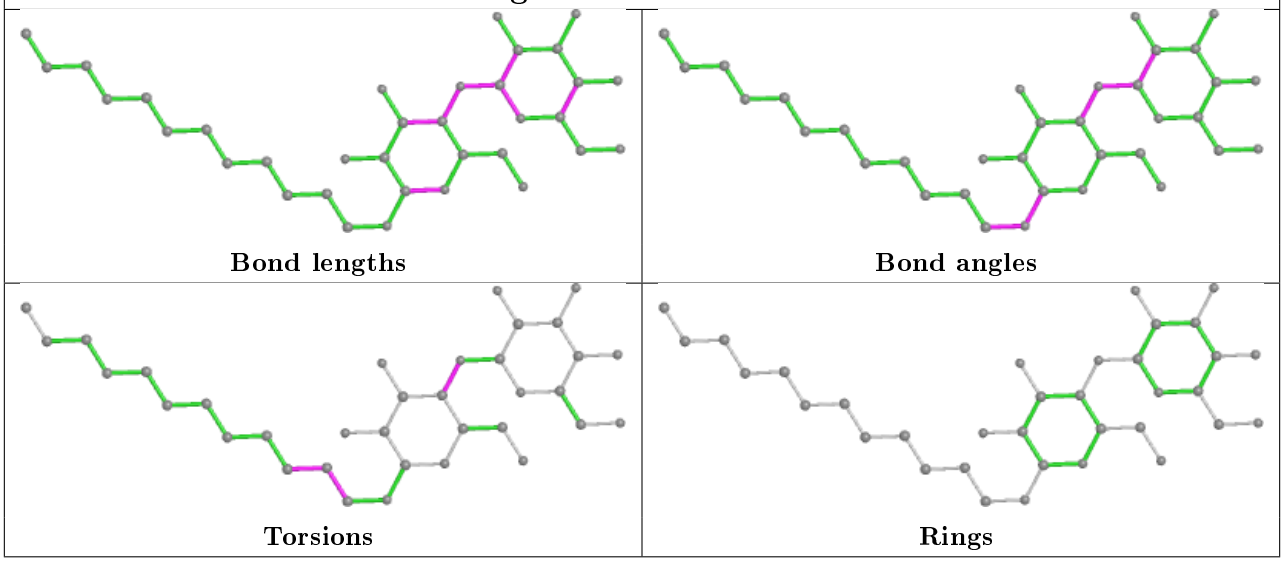

Torsions


Rings

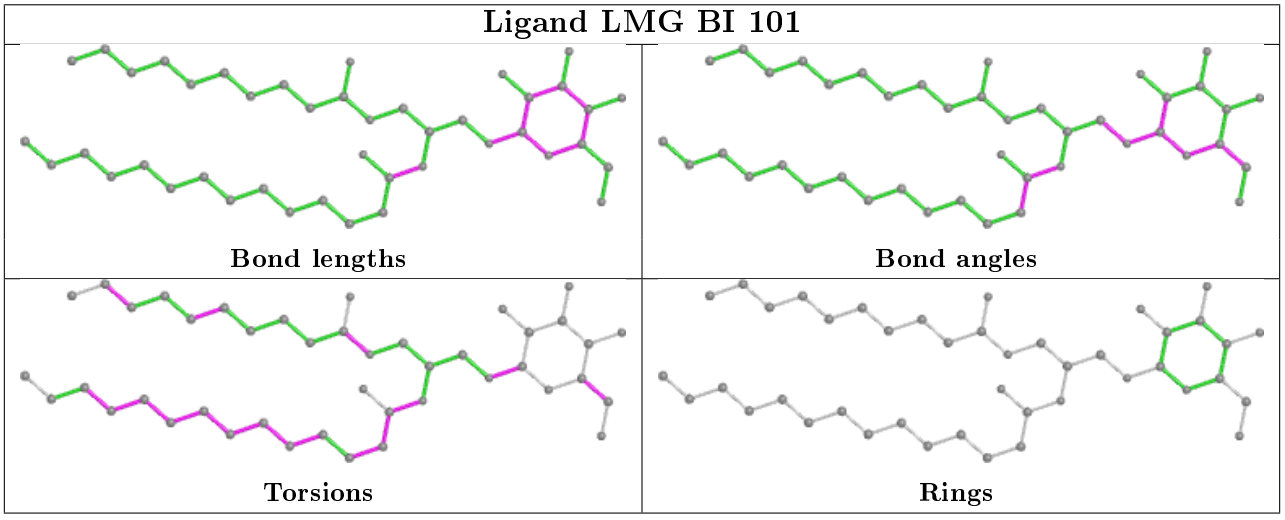
Ligand DGD BD 410



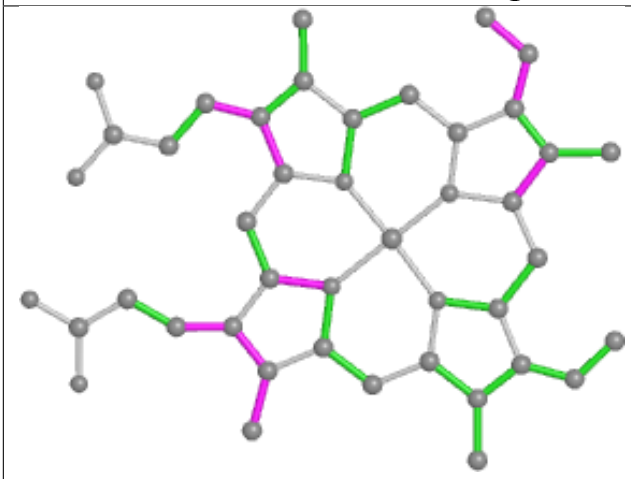
Ligand LMT BB 603



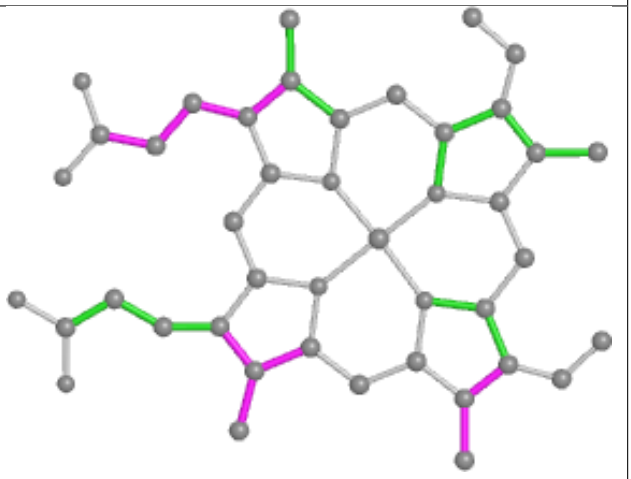
Ligand LMG BI 101



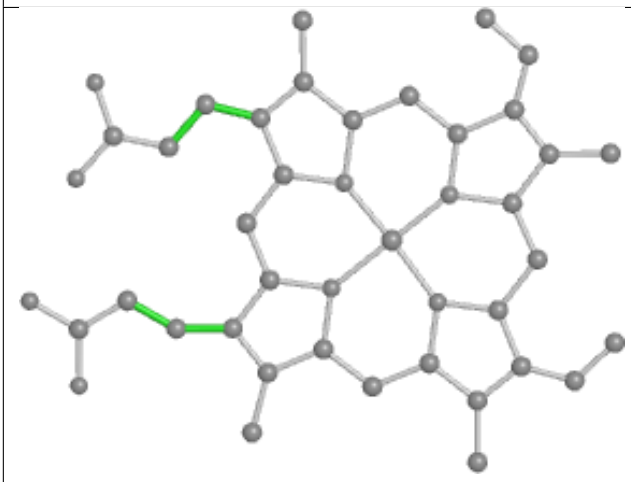
Ligand HEM AV 201



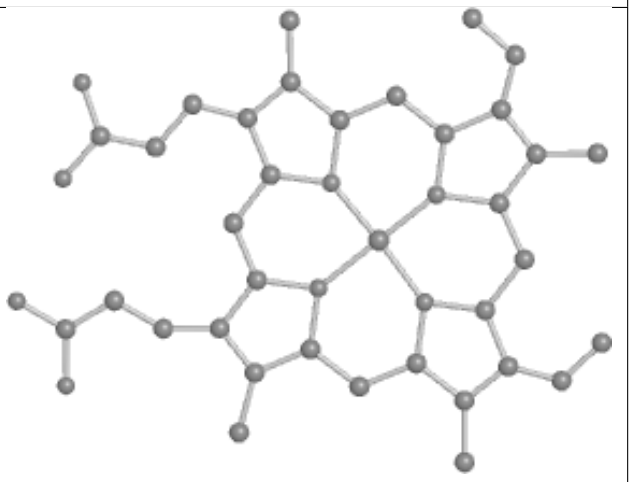
Bond lengths



Bond angles

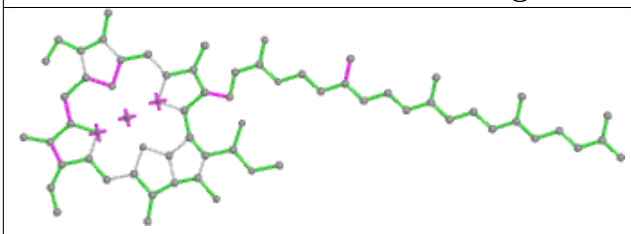


Torsions

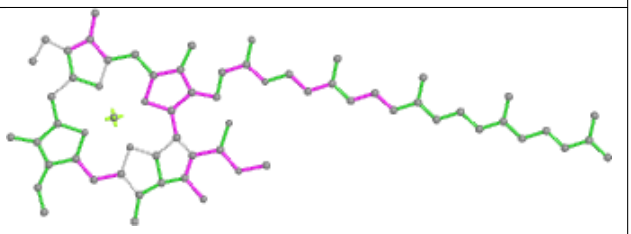


Rings

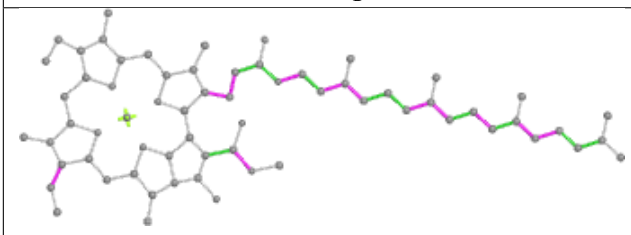
Ligand CLA AB 601



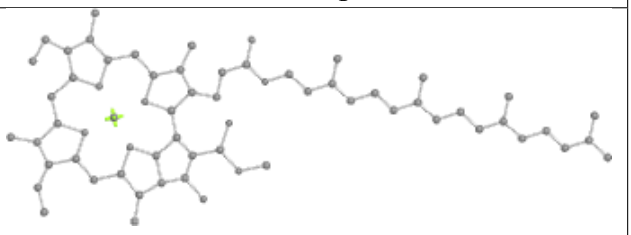
Bond lengths



Bond angles

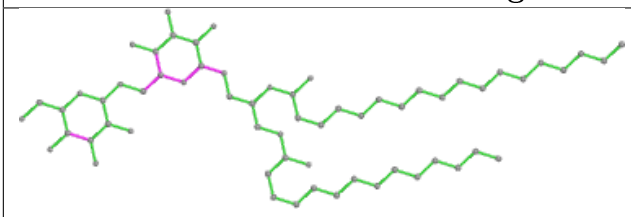


Torsions



Rings

Ligand DGD BC 517



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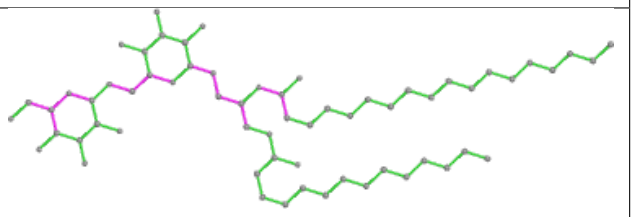
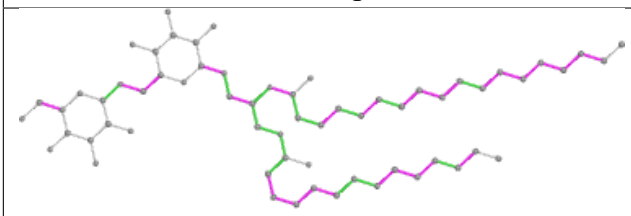
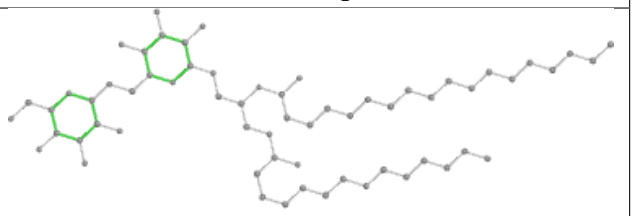


Bond angles

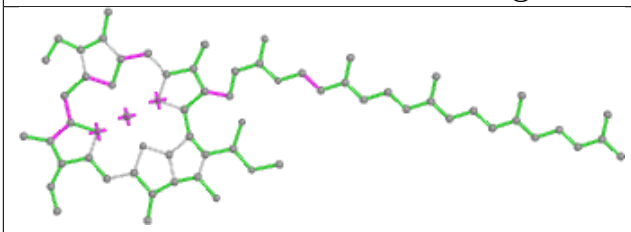


Torsions

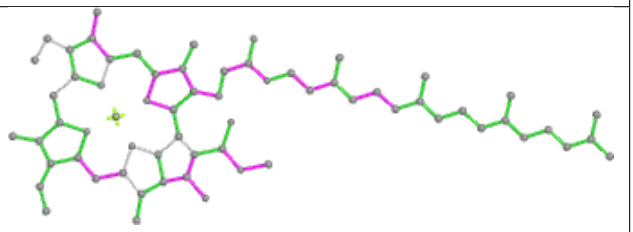


Rings

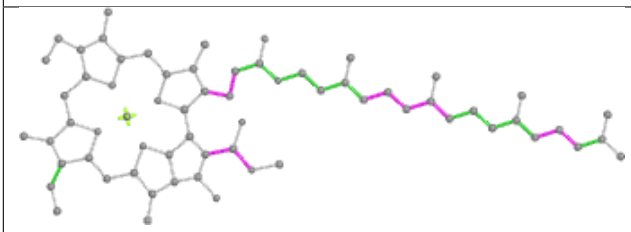
Ligand CLA BB 610



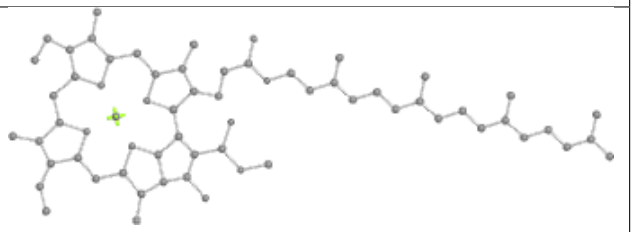
Bond lengths



Bond angles

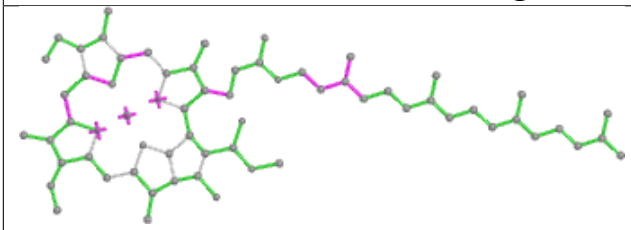


Torsions

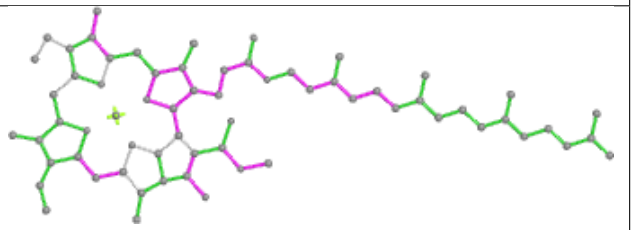


Rings

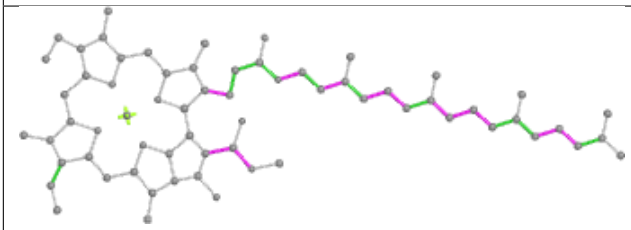
Ligand CLA AB 616



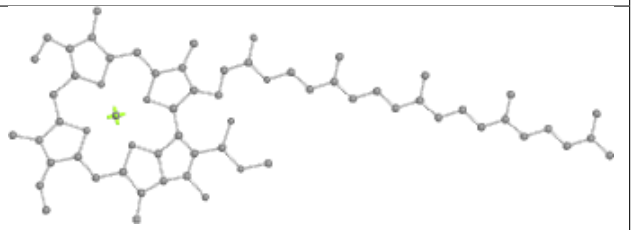
Bond lengths



Bond angles

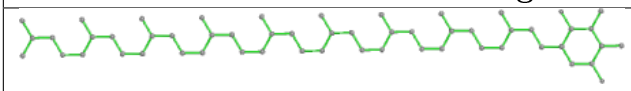


Torsions

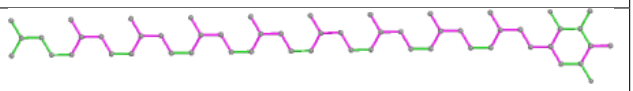


Rings

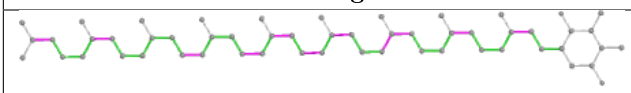
Ligand PL9 BD 405



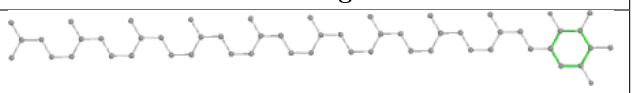
Bond lengths



Bond angles

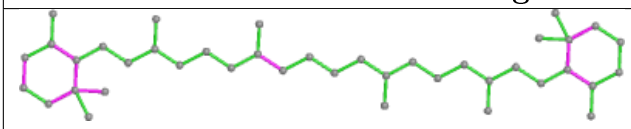


Torsions



Rings

Ligand BCR AJ 102



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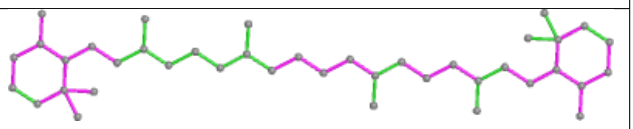
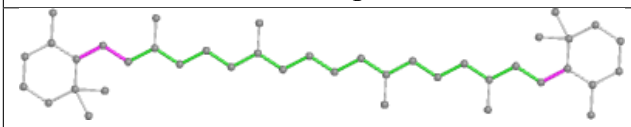
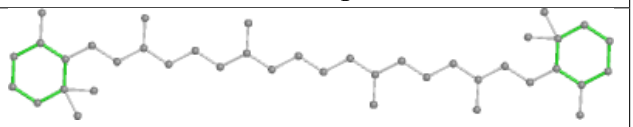


Bond angles

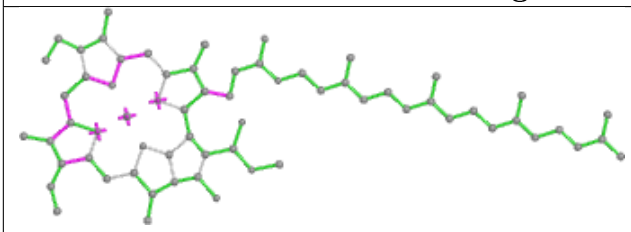


Torsions



Rings

Ligand CLA BC 505



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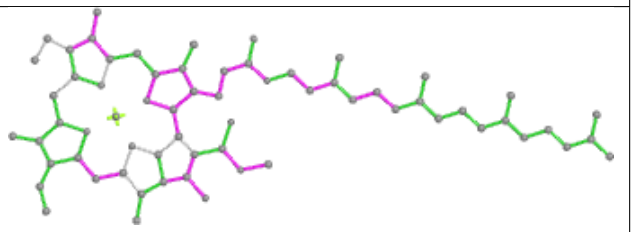
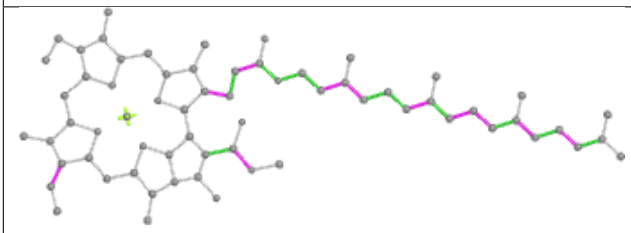
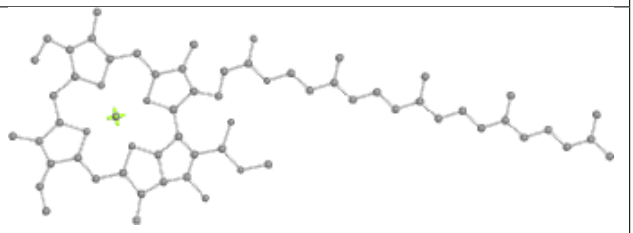


Bond angles

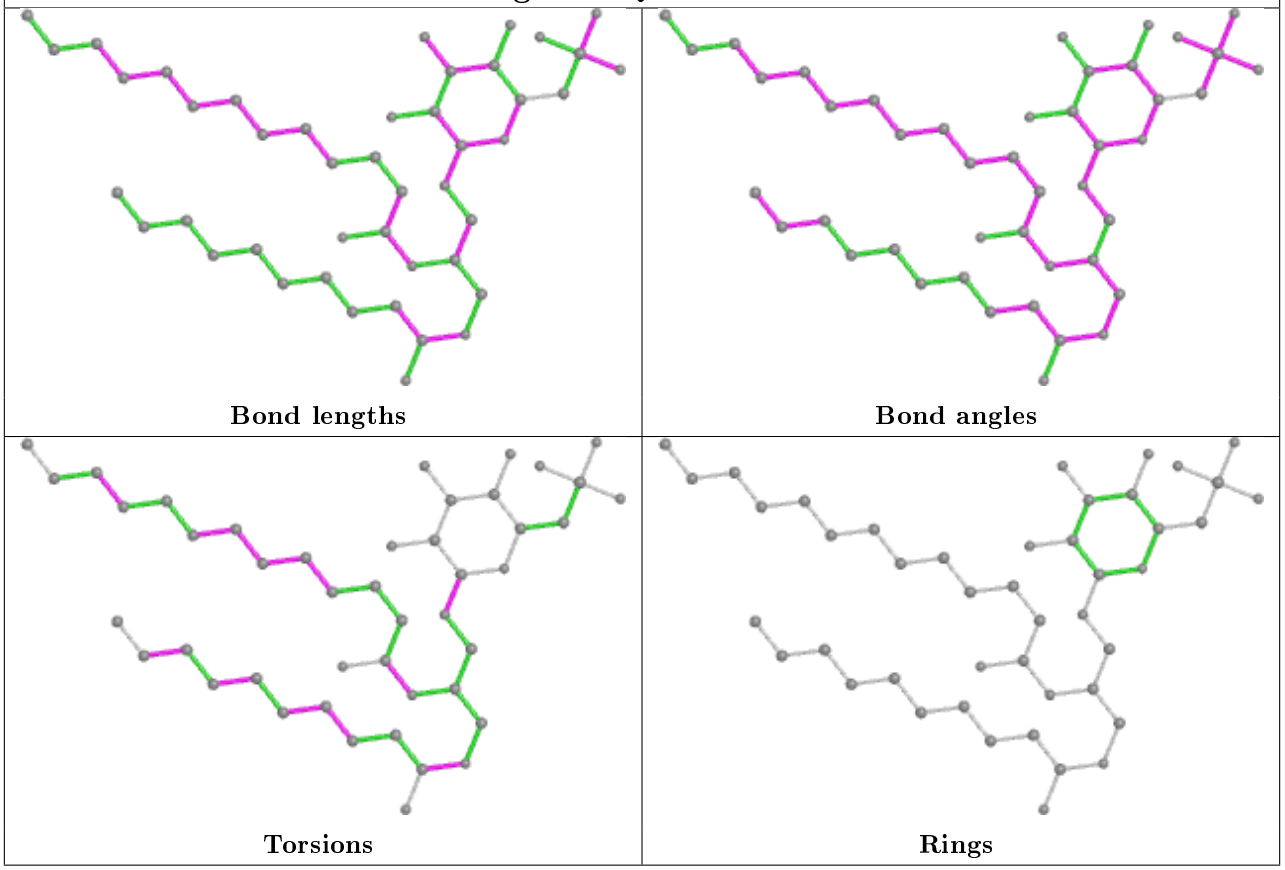


Torsions

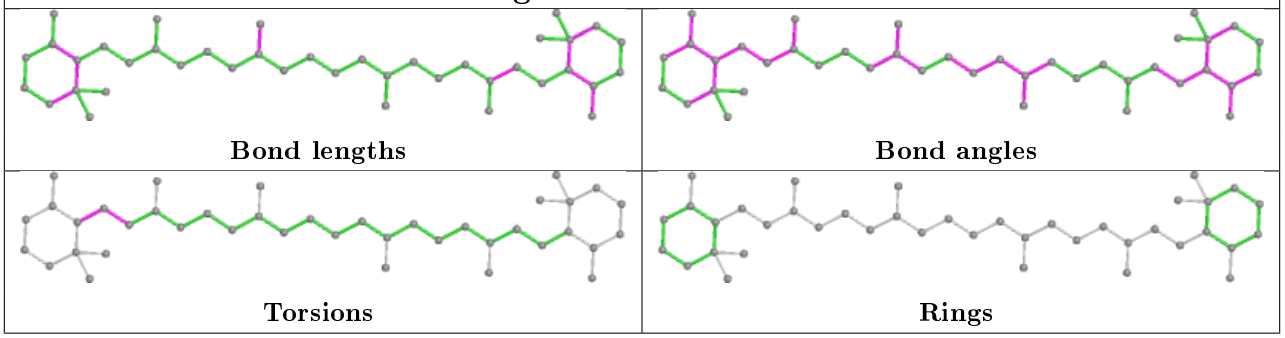


Rings

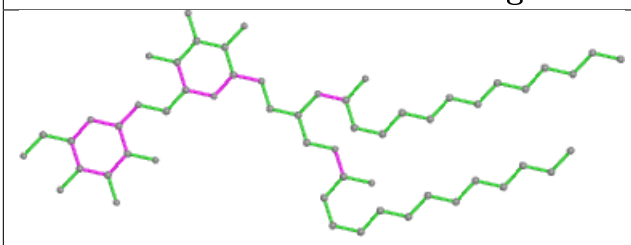
Ligand SQD AF 101



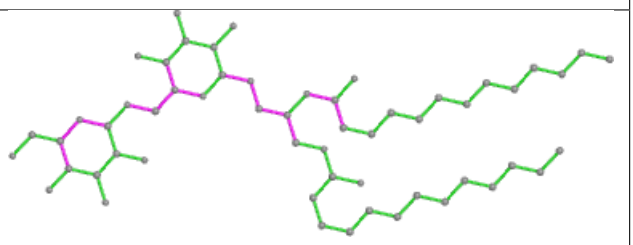
Ligand BCR BZ 101



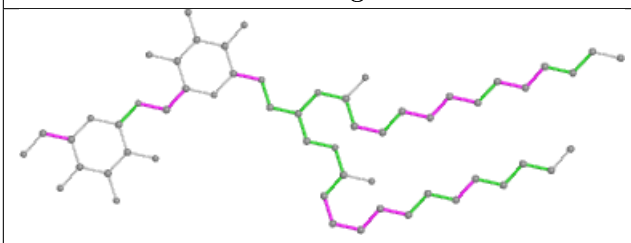
Ligand DGD BA 411



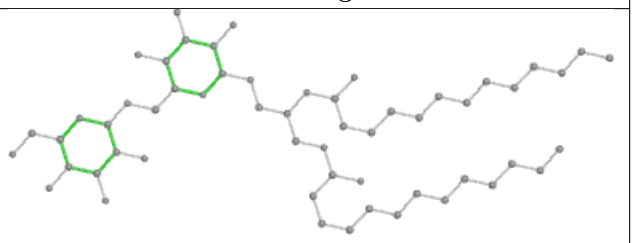
Bond lengths



Bond angles

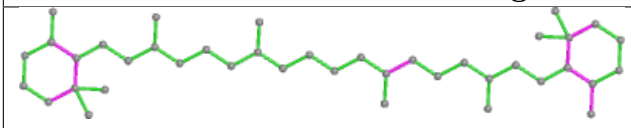


Torsions

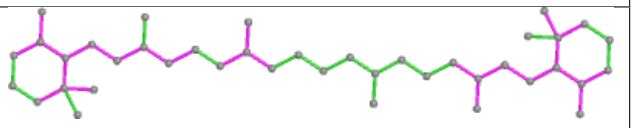


Rings

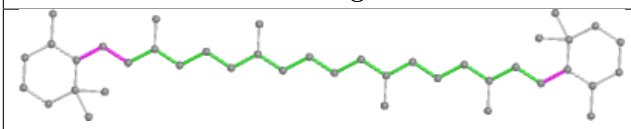
Ligand BCR BC 514



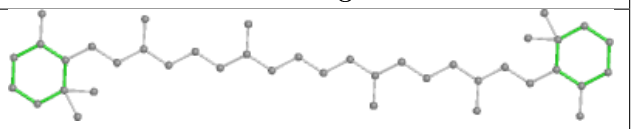
Bond lengths



Bond angles

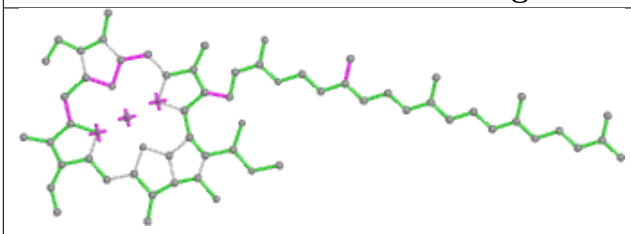


Torsions

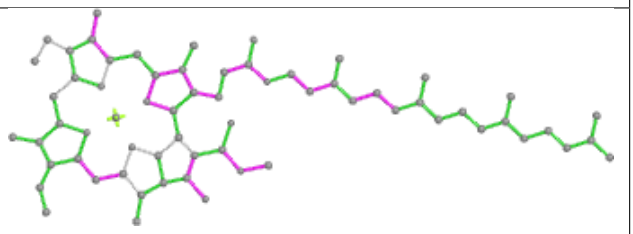


Rings

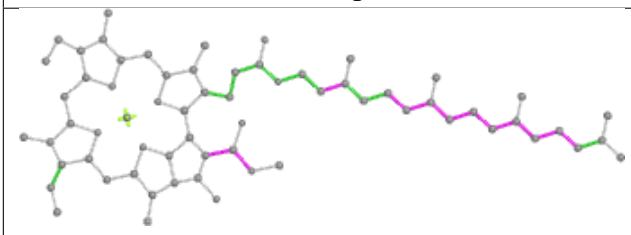
Ligand CLA BC 506



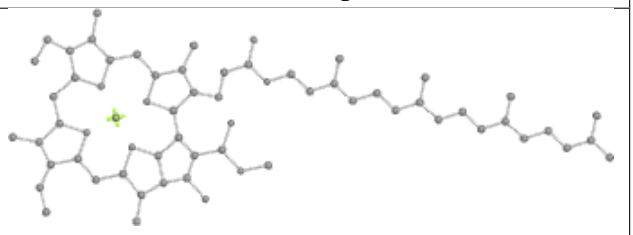
Bond lengths



Bond angles

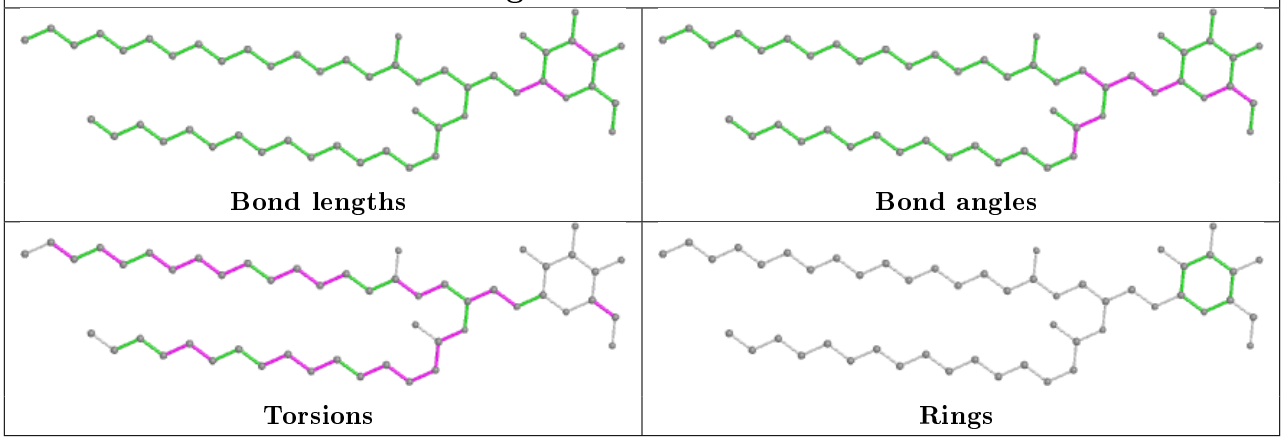


Torsions

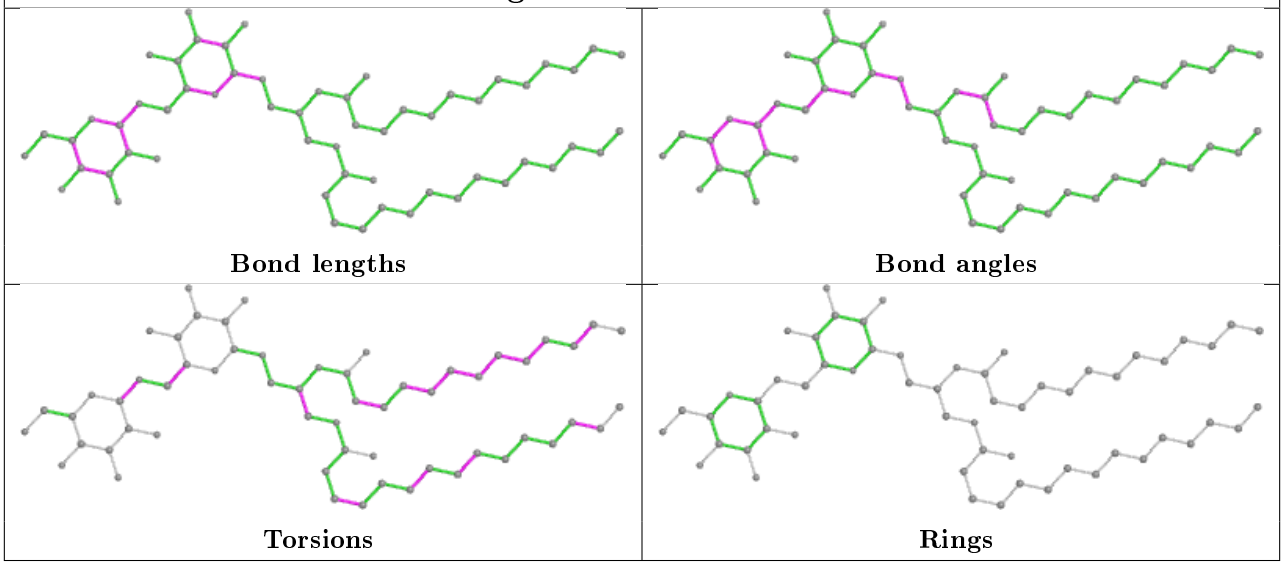


Rings

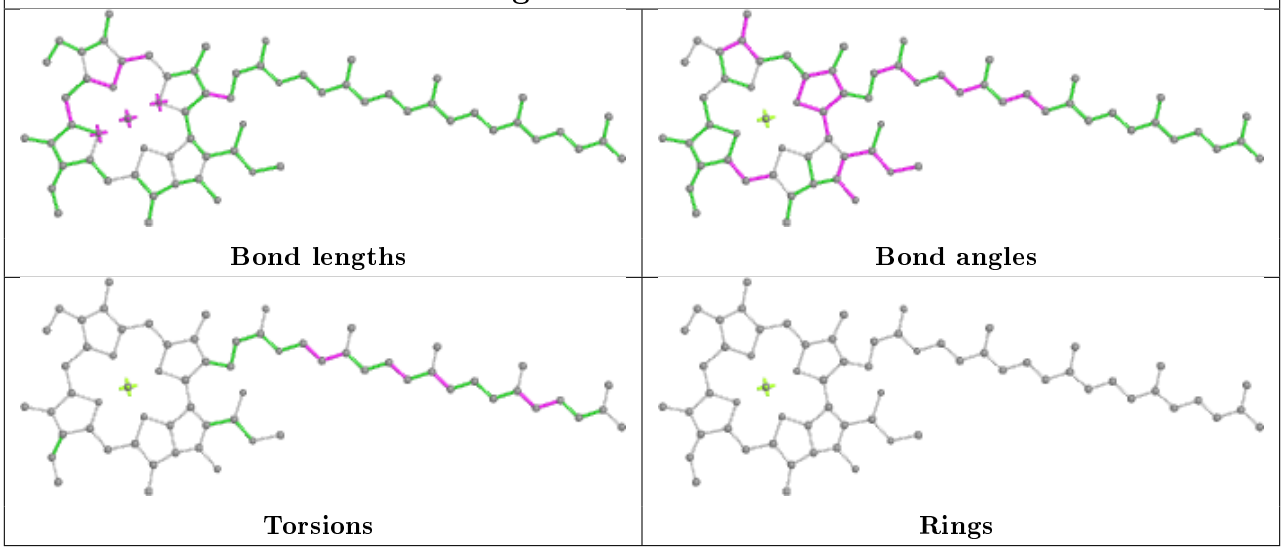
Ligand LMG AA 413



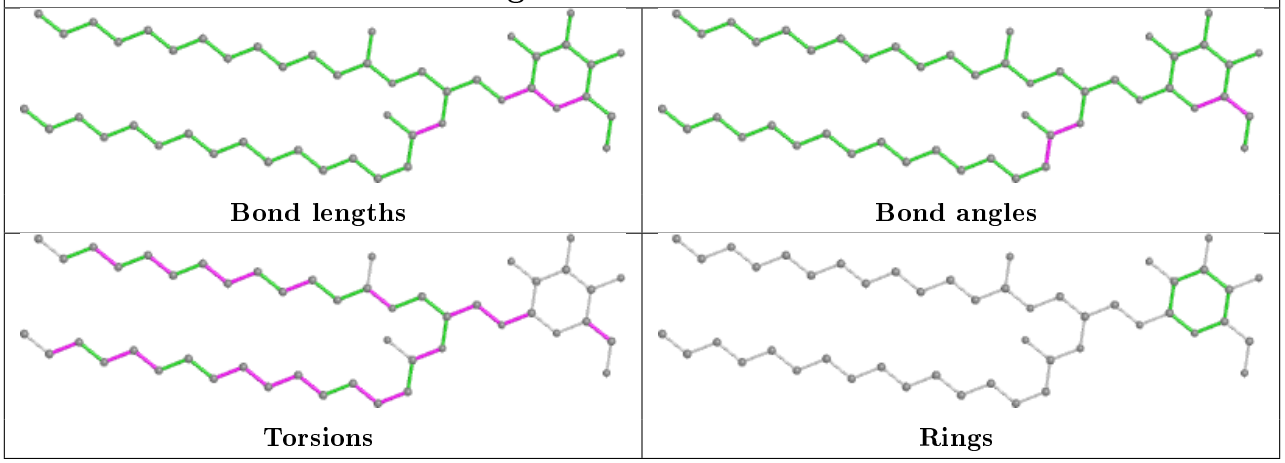
Ligand DGD BH 101



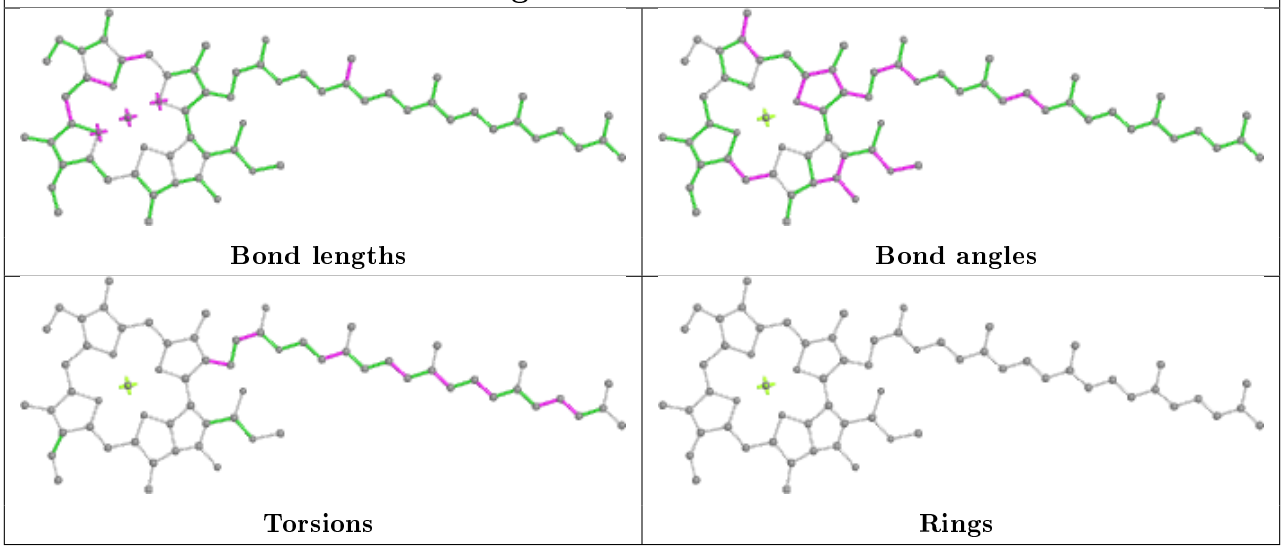
Ligand CLA AB 615



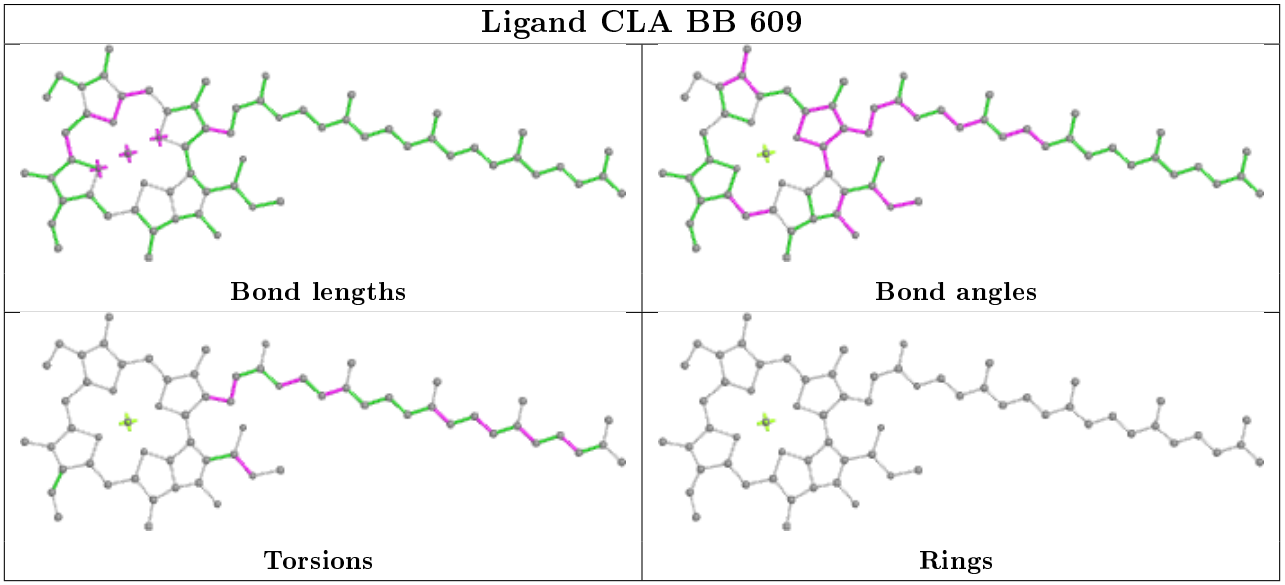
Ligand LMG BD 408



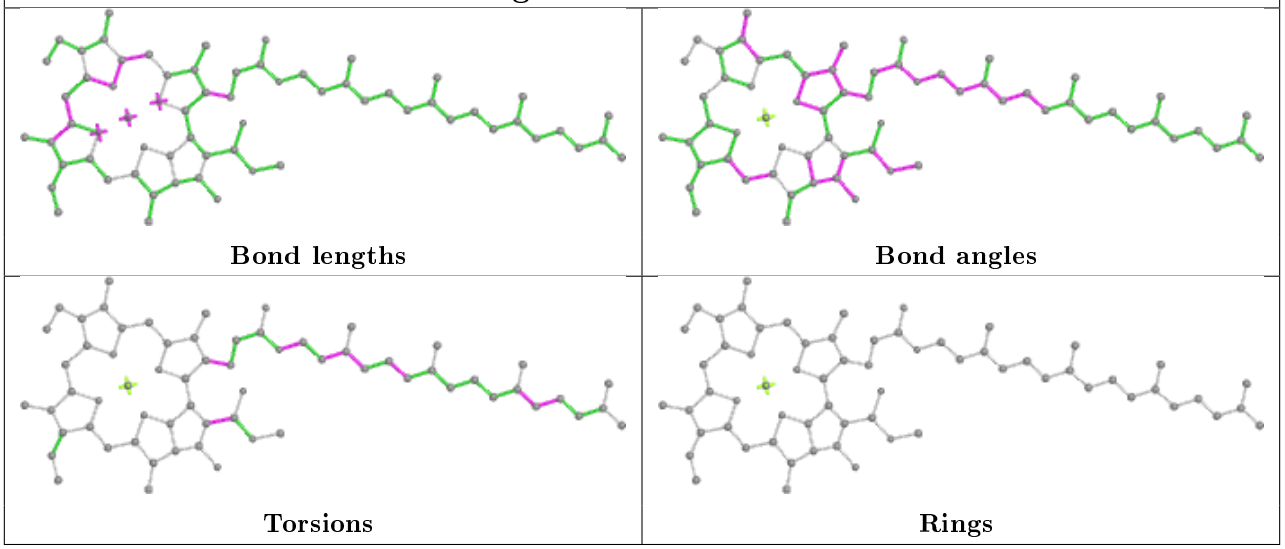
Ligand CLA AA 406



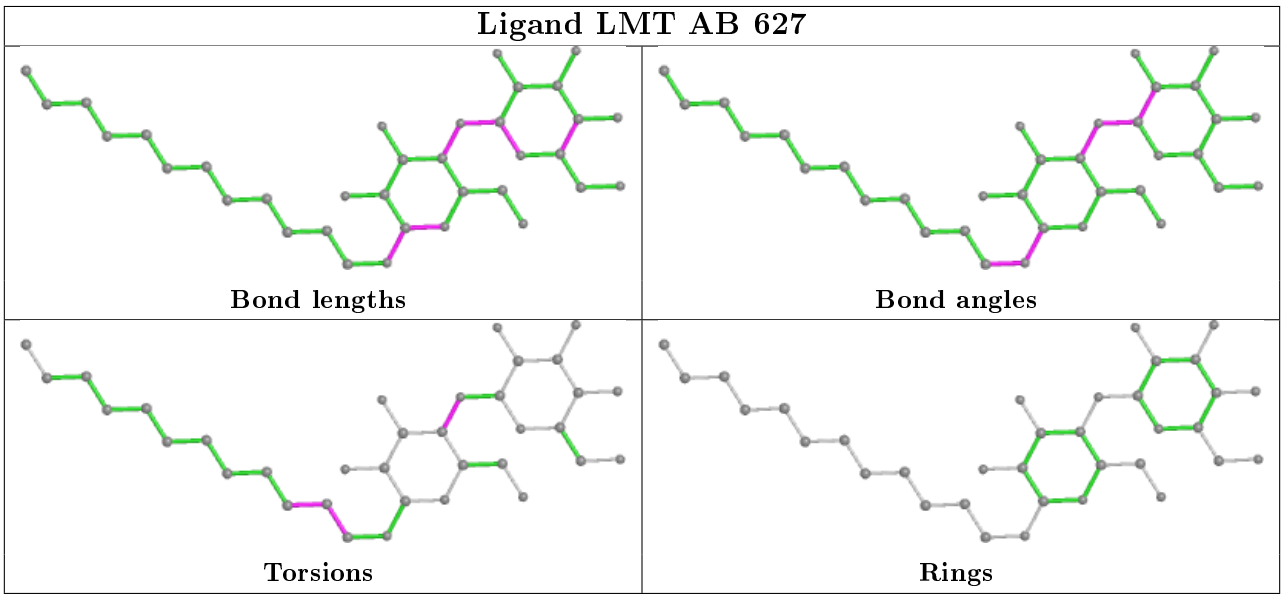
Ligand CLA BB 609



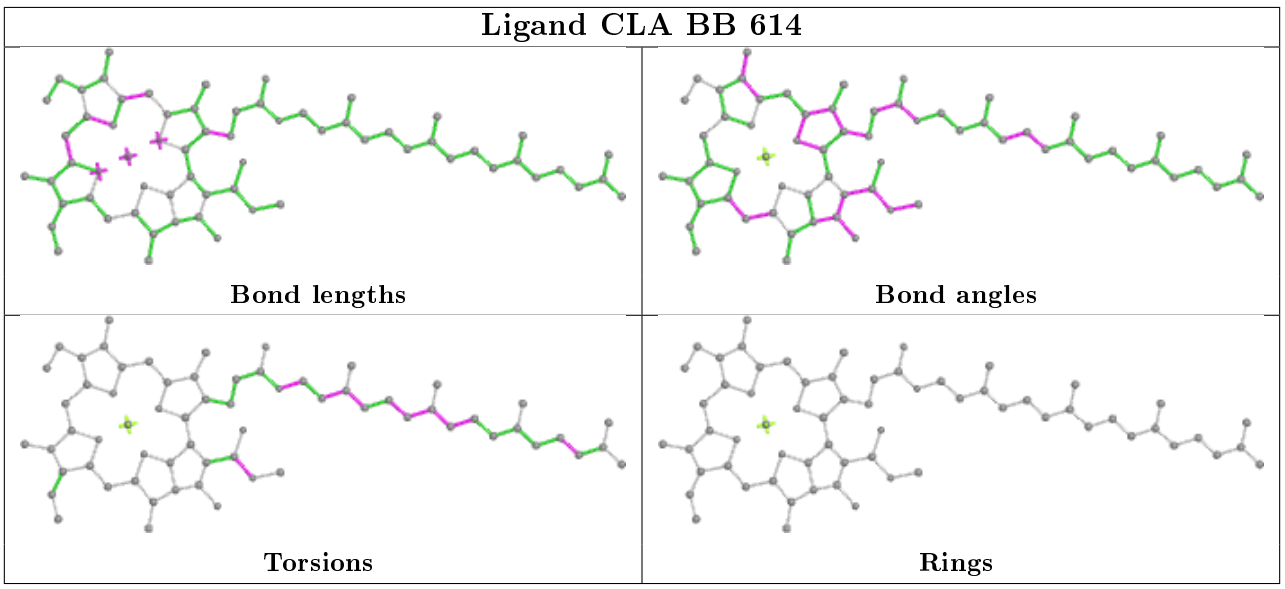
Ligand CLA AB 609



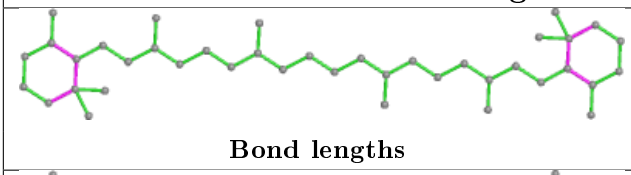
Ligand LMT AB 627



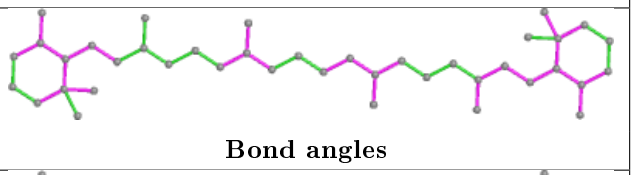
Ligand CLA BB 614



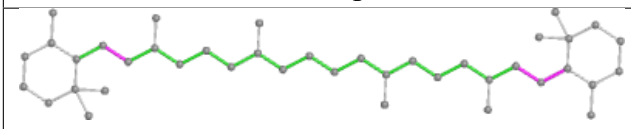
Ligand BCR AC 515



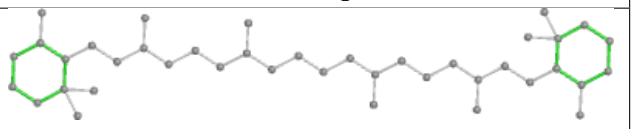
Bond lengths



Bond angles

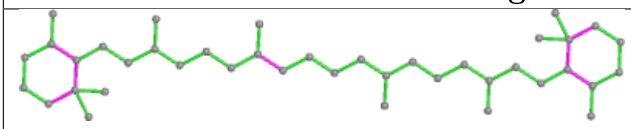


Torsions

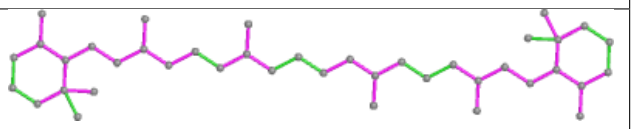


Rings

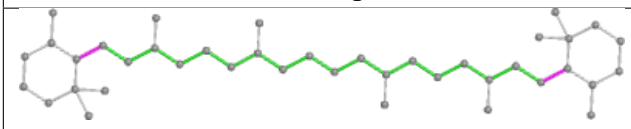
Ligand BCR BK 102



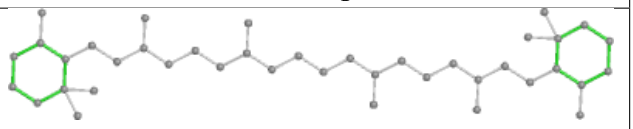
Bond lengths



Bond angles

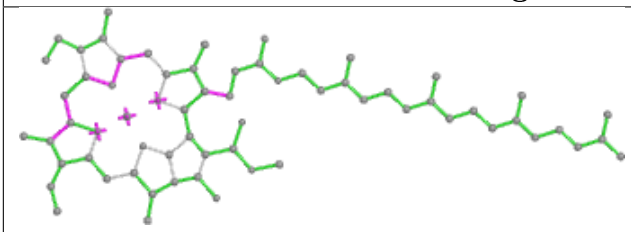


Torsions

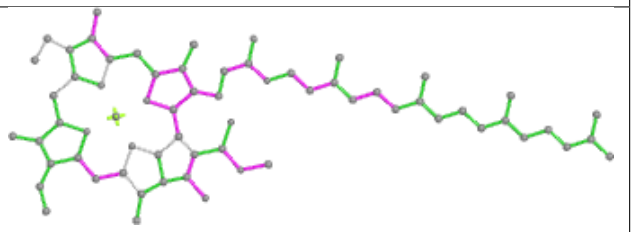


Rings

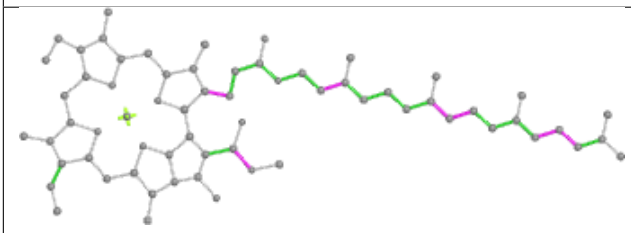
Ligand CLA AB 604



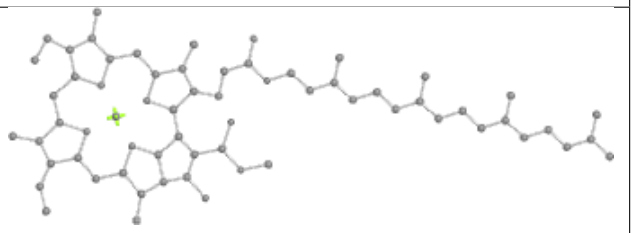
Bond lengths



Bond angles

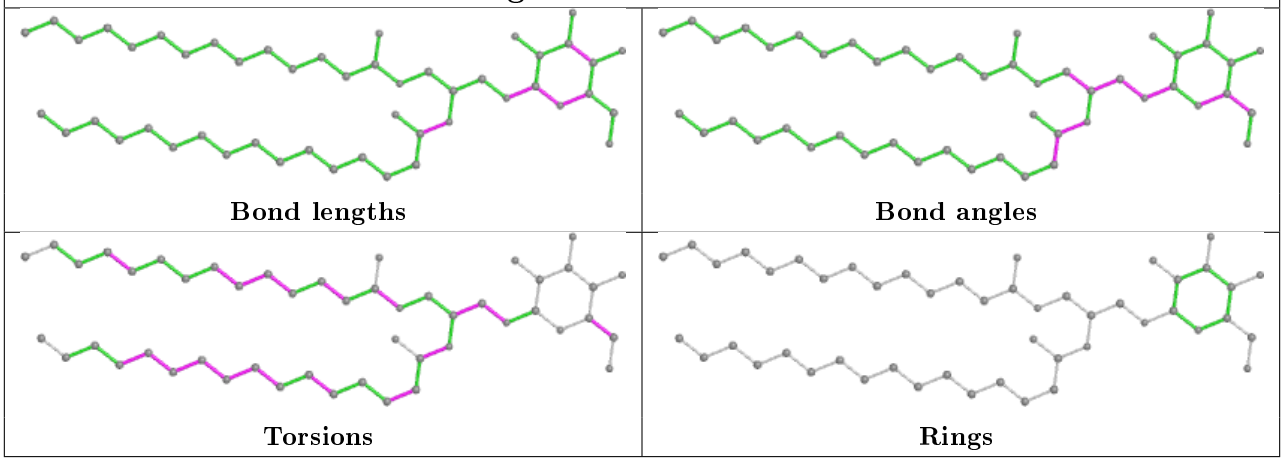


Torsions

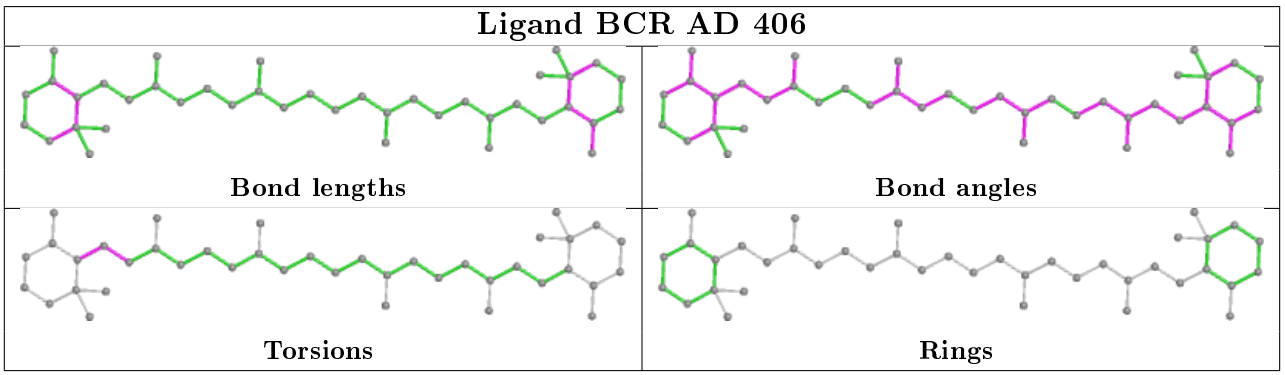


Rings

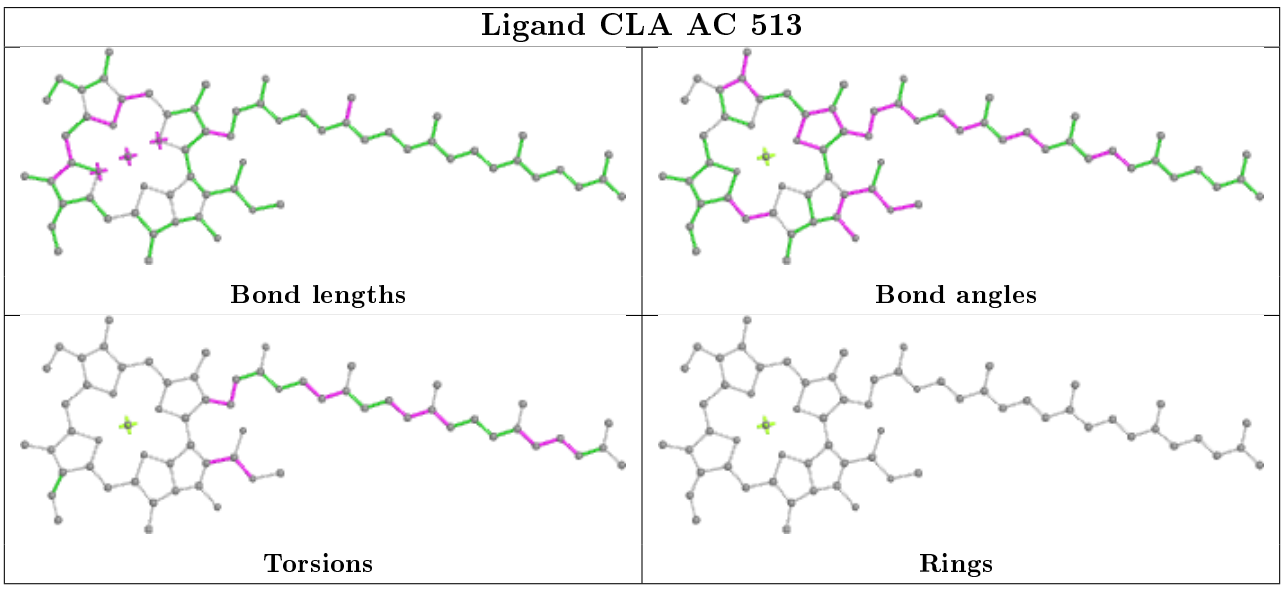
Ligand LMG AB 621



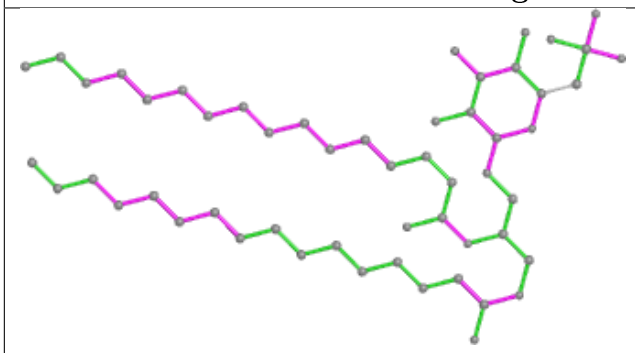
Ligand BCR AD 406



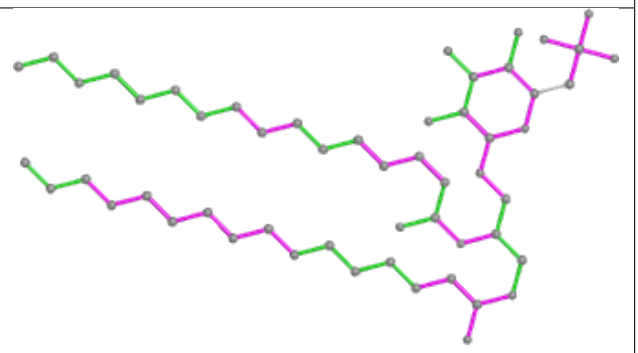
Ligand CLA AC 513



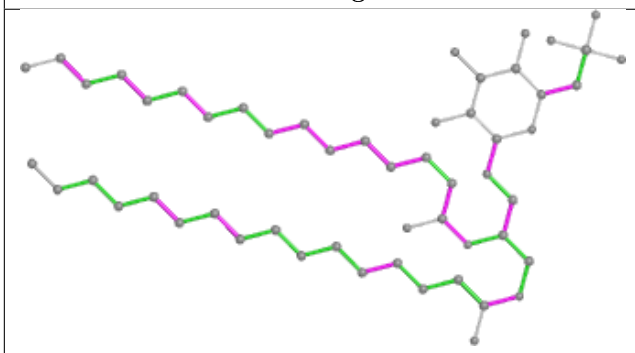
Ligand SQD AA 415



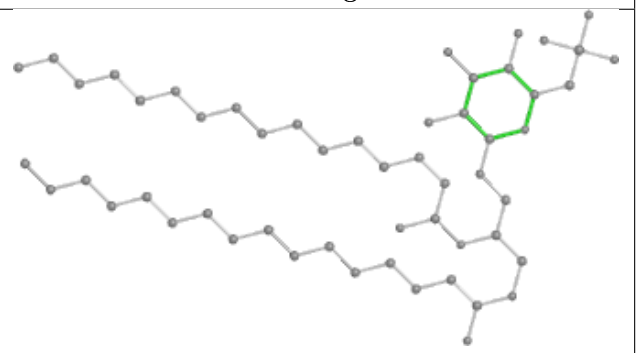
Bond lengths



Bond angles

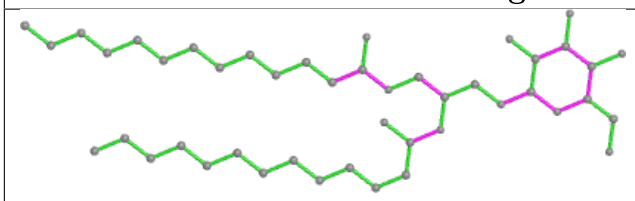


Torsions

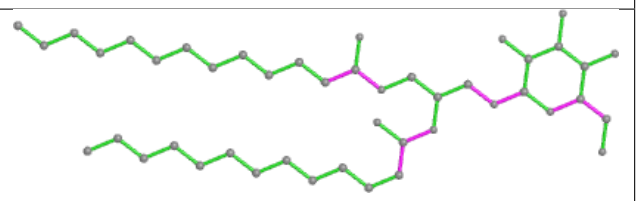


Rings

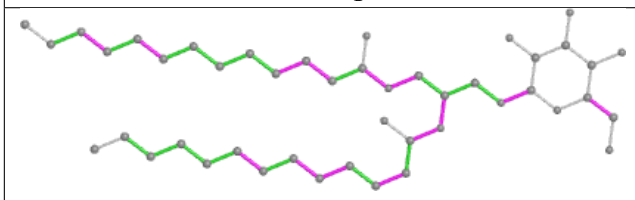
Ligand LMG BC 520



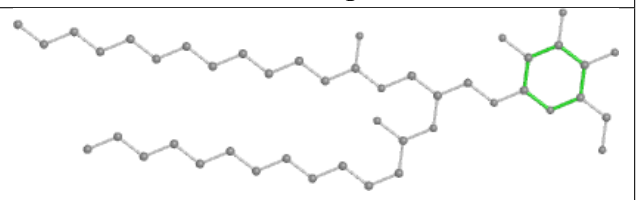
Bond lengths



Bond angles

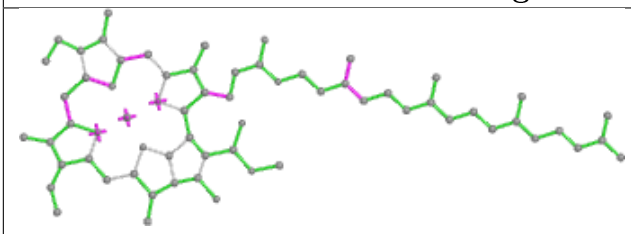


Torsions

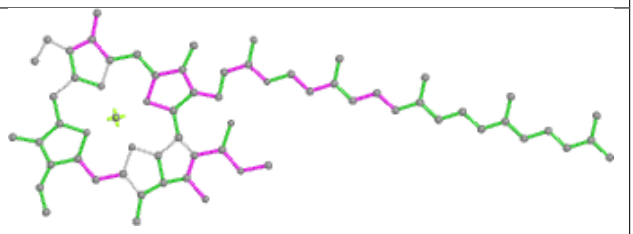


Rings

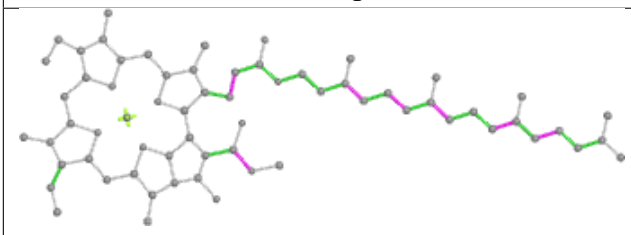
Ligand CLA BB 606



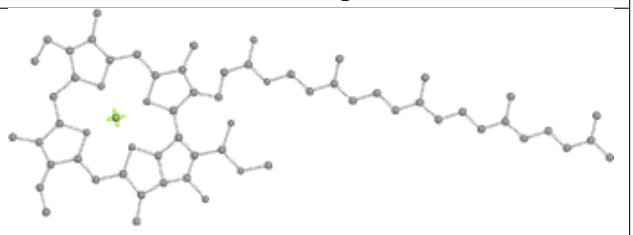
Bond lengths



Bond angles

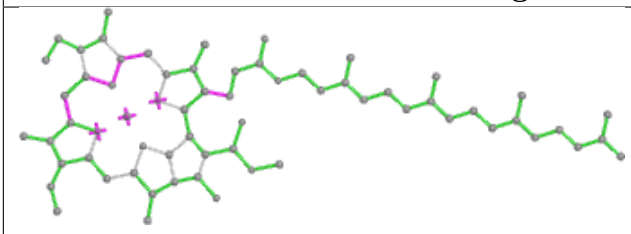


Torsions

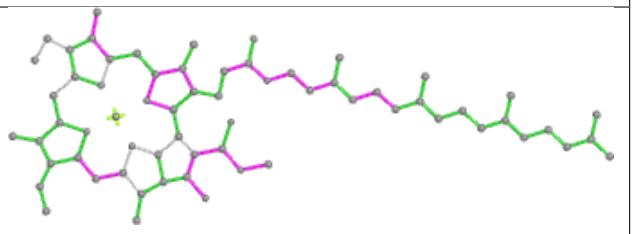


Rings

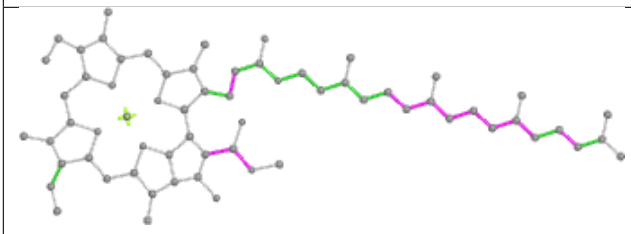
Ligand CLA BC 503



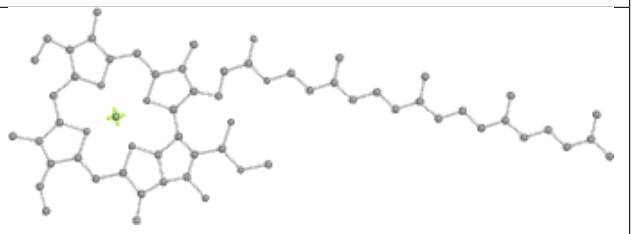
Bond lengths



Bond angles

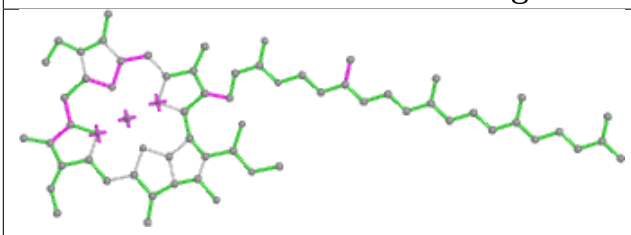


Torsions

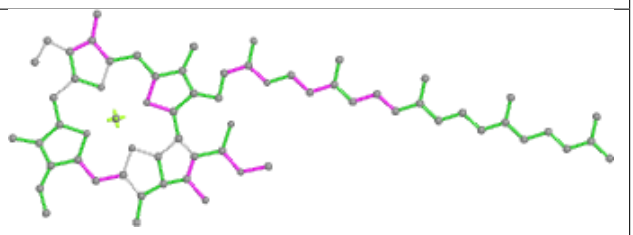


Rings

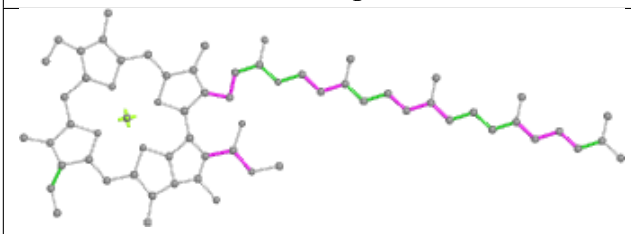
Ligand CLA BC 513



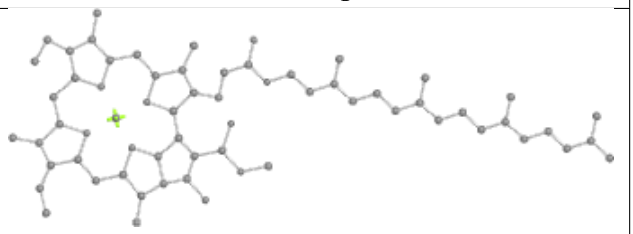
Bond lengths



Bond angles

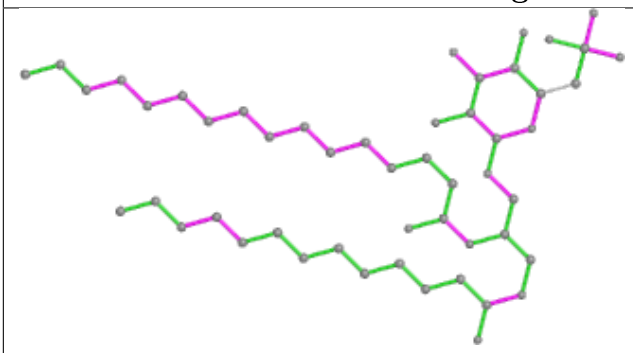


Torsions

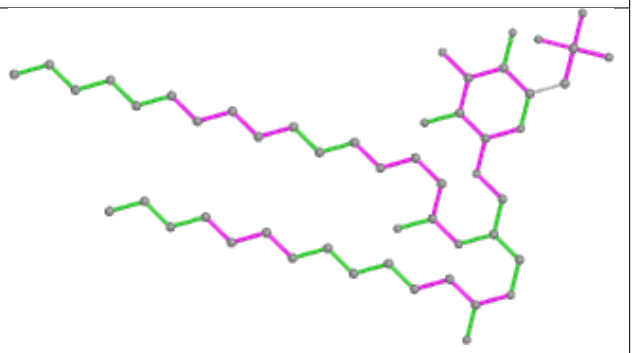


Rings

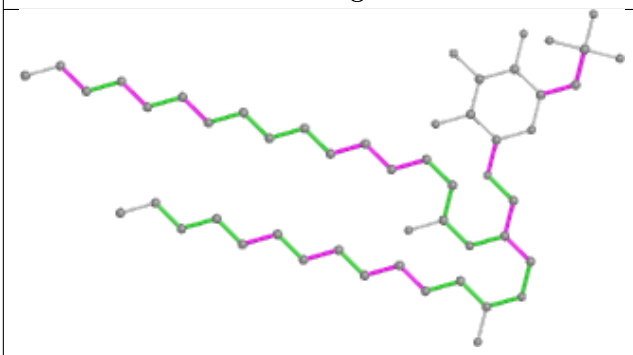
Ligand SQD BA 413



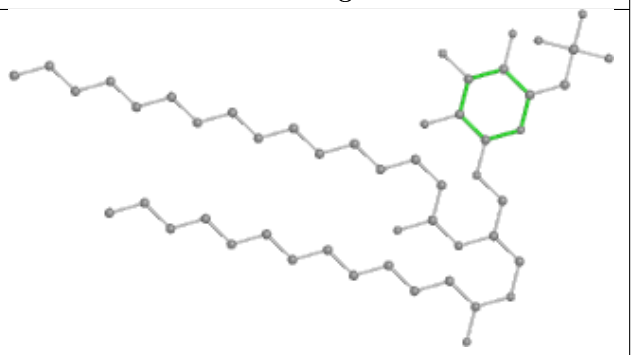
Bond lengths



Bond angles

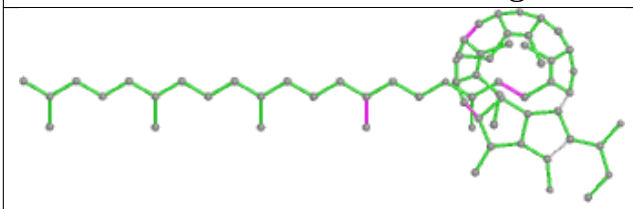


Torsions

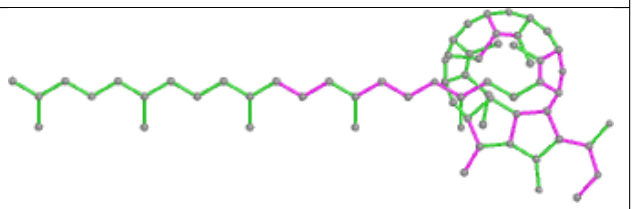


Rings

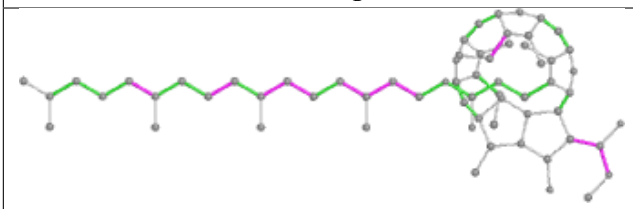
Ligand PHO BA 406



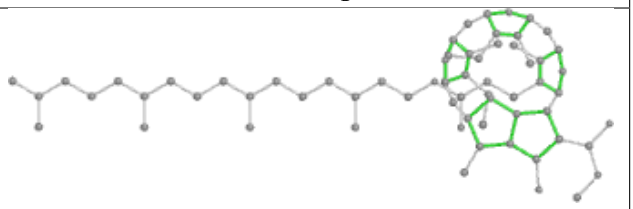
Bond lengths



Bond angles

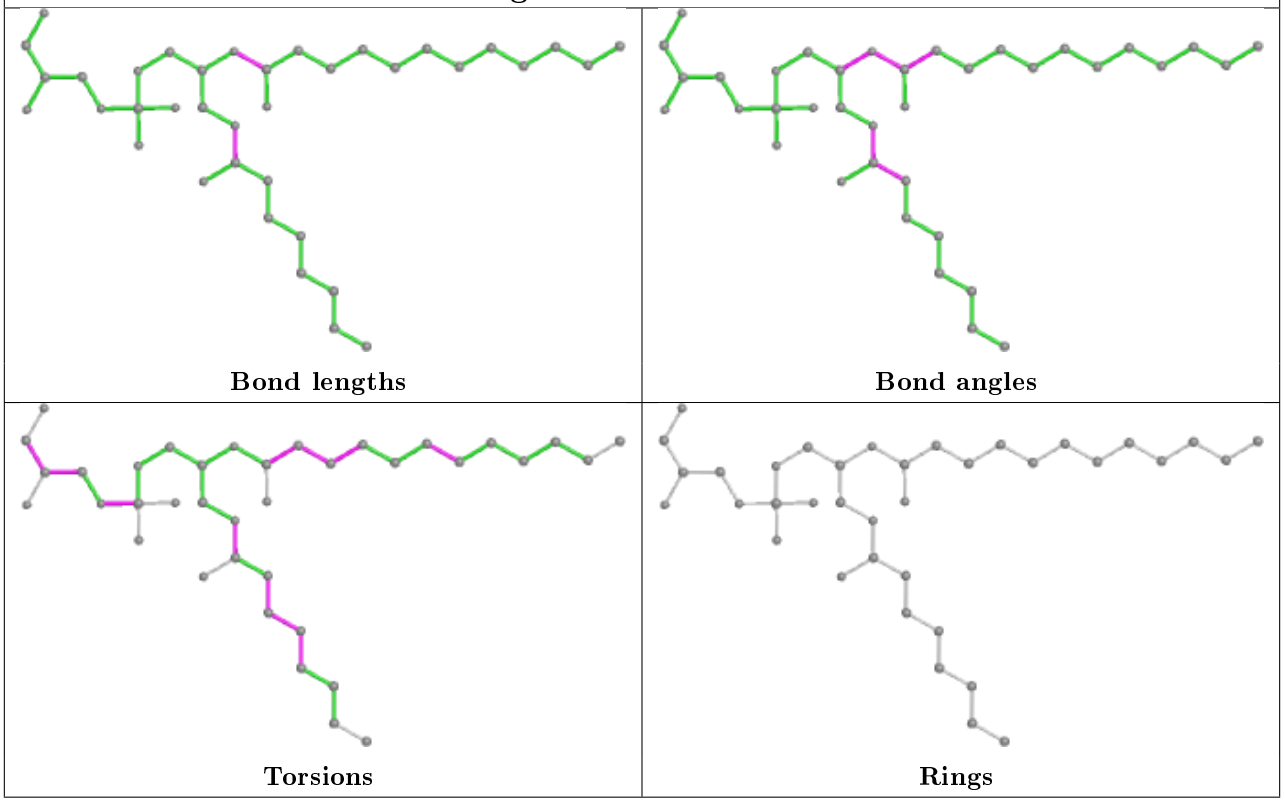


Torsions

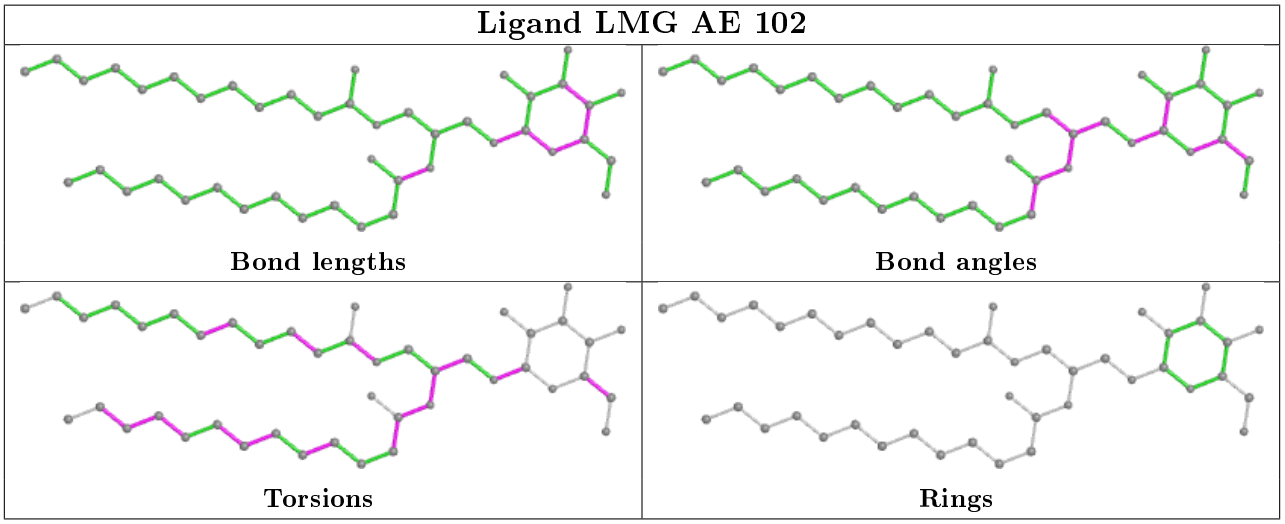


Rings

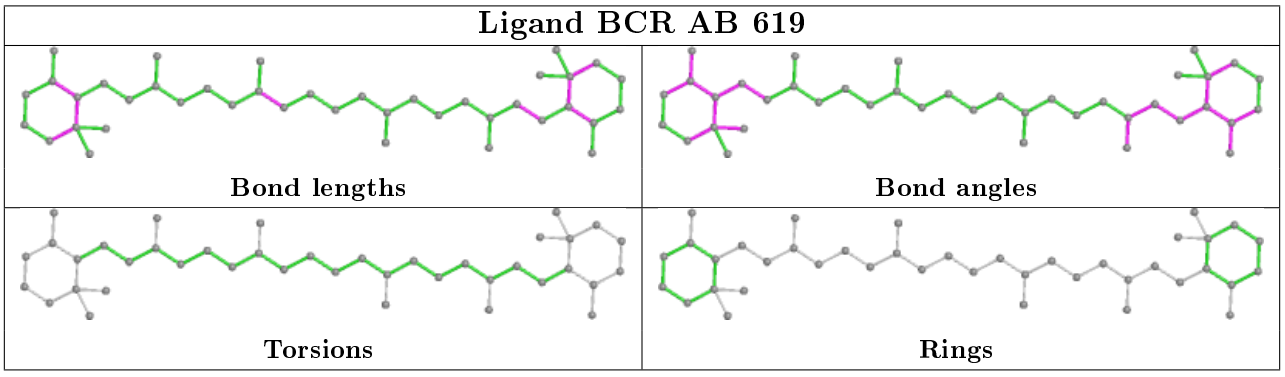
Ligand LHG AC 521



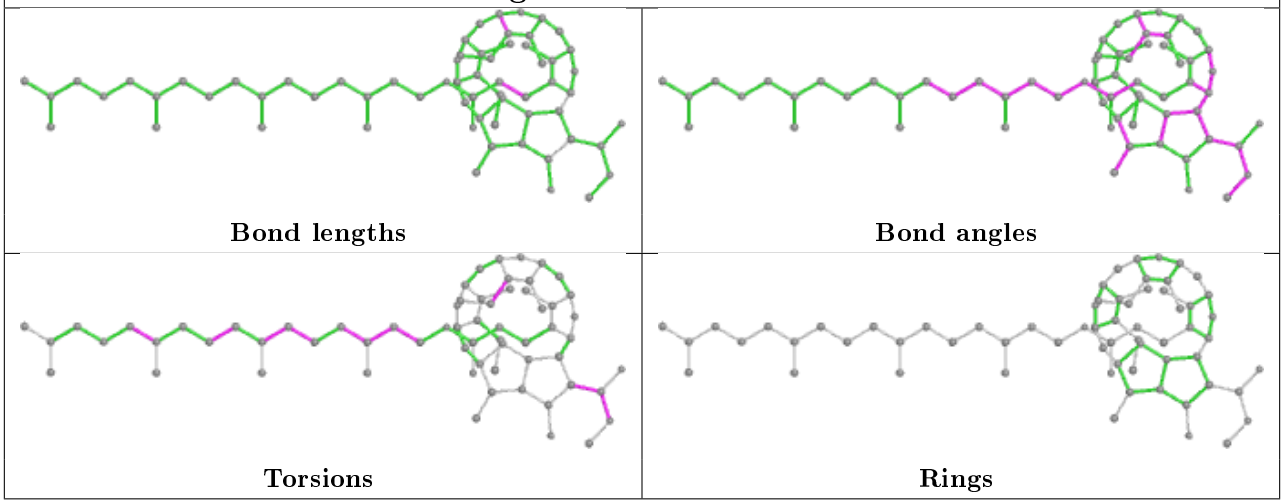
Ligand LMG AE 102



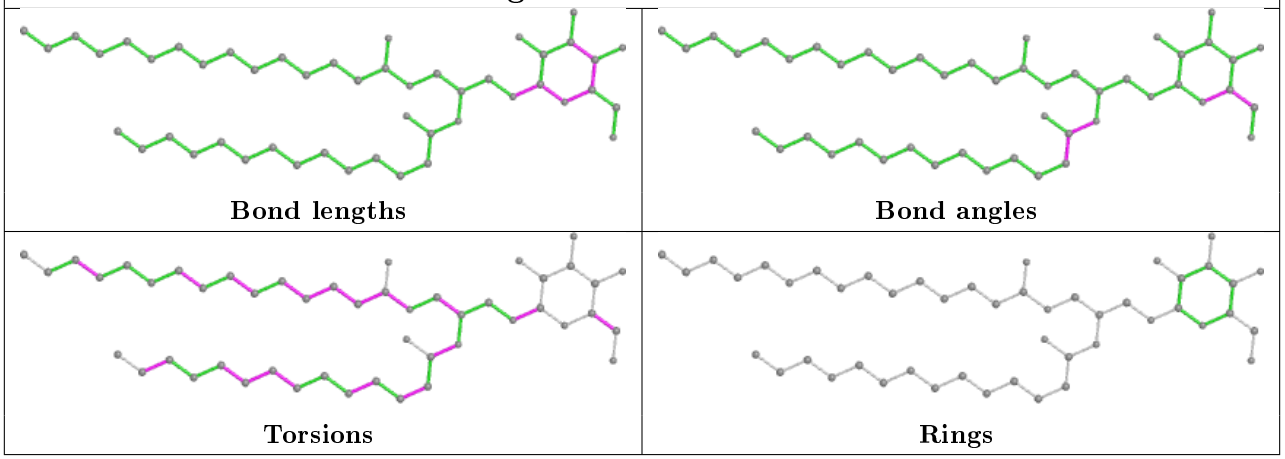
Ligand BCR AB 619



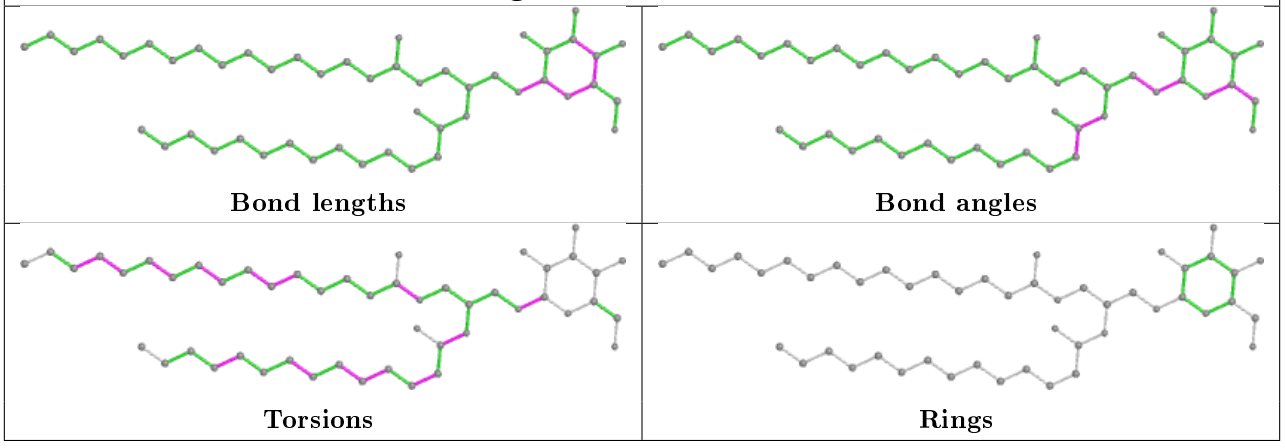
Ligand PHO AA 405



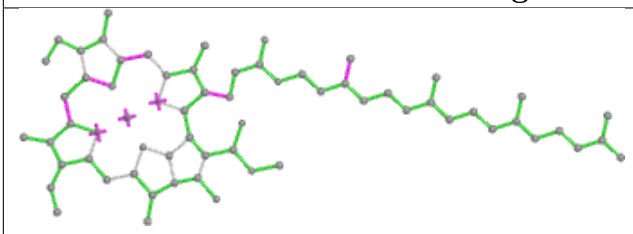
Ligand LMG AC 519

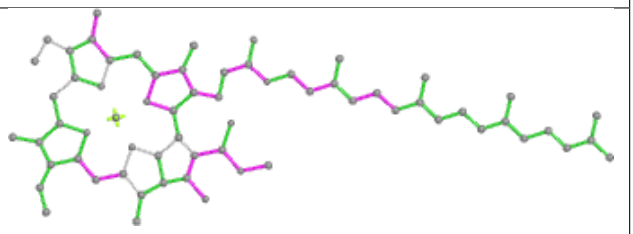


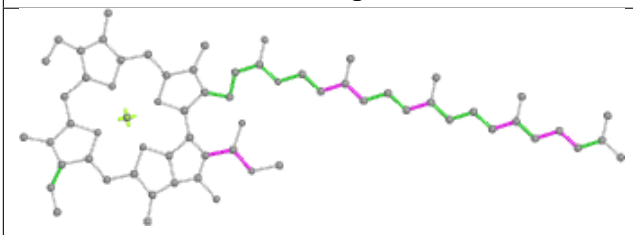
Ligand LMG BB 624

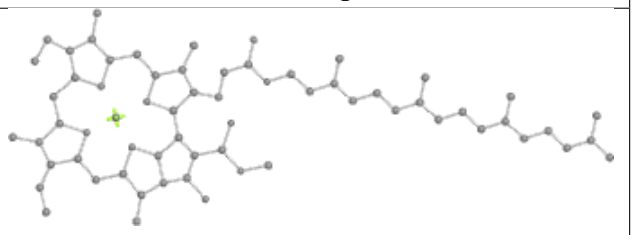


Ligand CLA BC 510

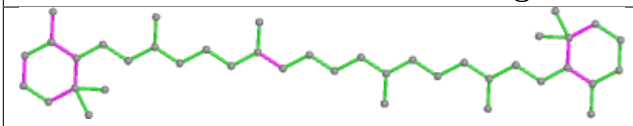

Bond lengths

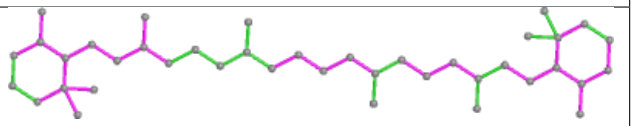

Bond angles

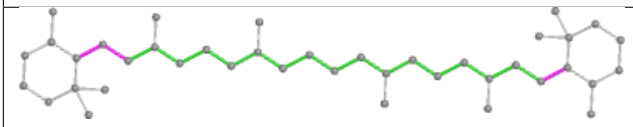

Torsions


Rings

Ligand BCR BJ 102

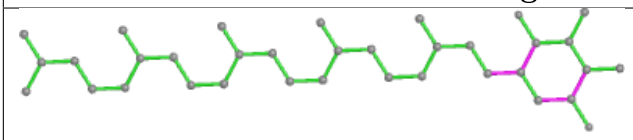

Bond lengths

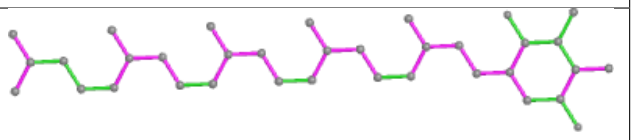

Bond angles

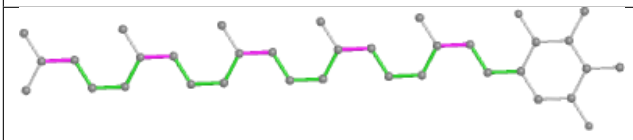

Torsions

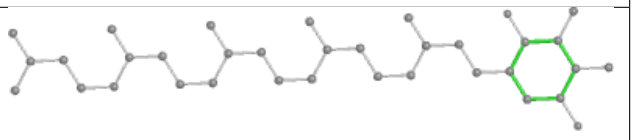

Rings

Ligand PL9 AJ 101

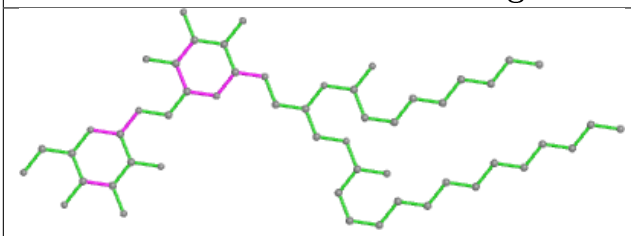

Bond lengths


Bond angles

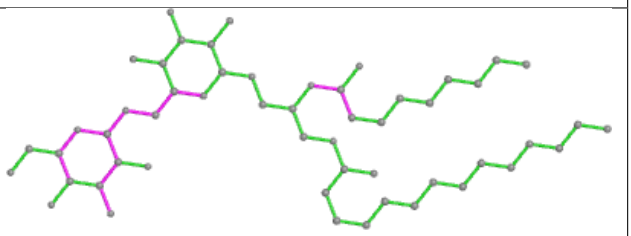

Torsions


Rings

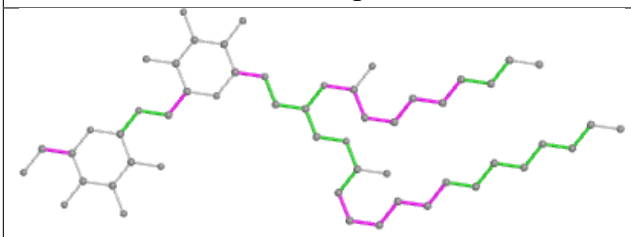
Ligand DGD AC 516



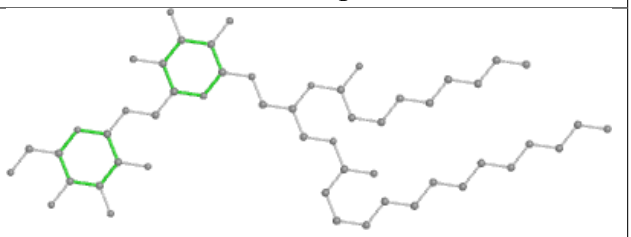
Bond lengths



Bond angles

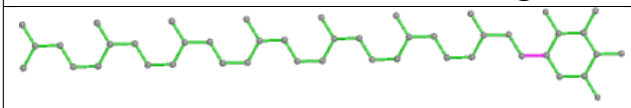


Torsions

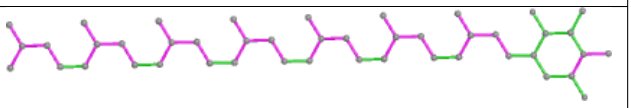


Rings

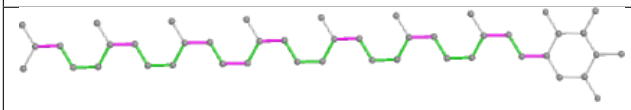
Ligand PL9 AA 407



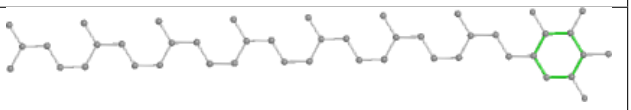
Bond lengths



Bond angles

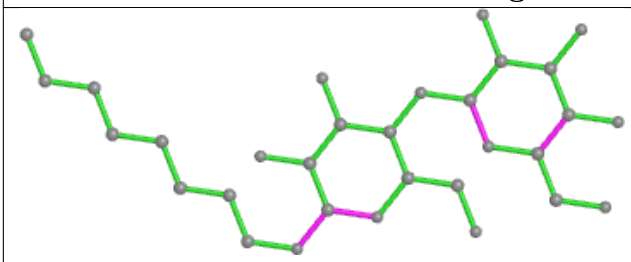


Torsions

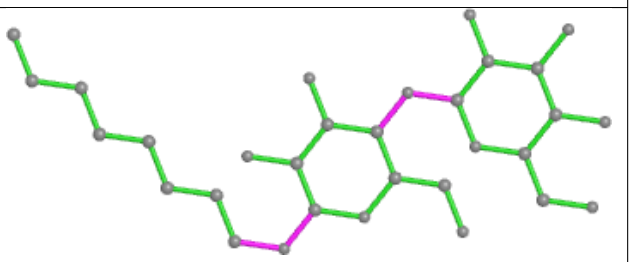


Rings

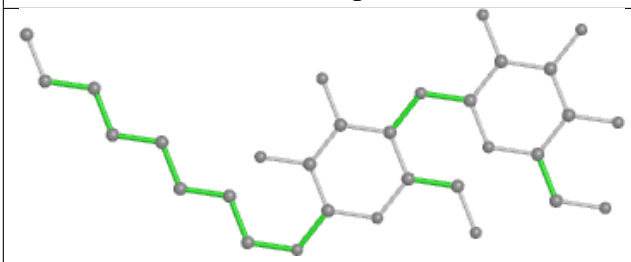
Ligand LMT BD 411



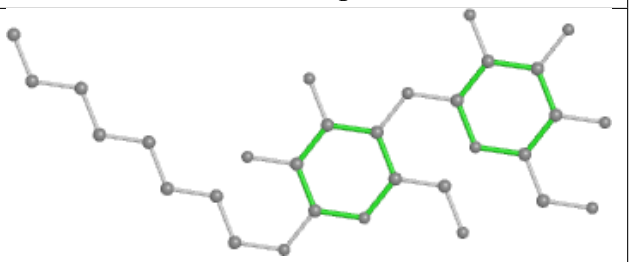
Bond lengths



Bond angles

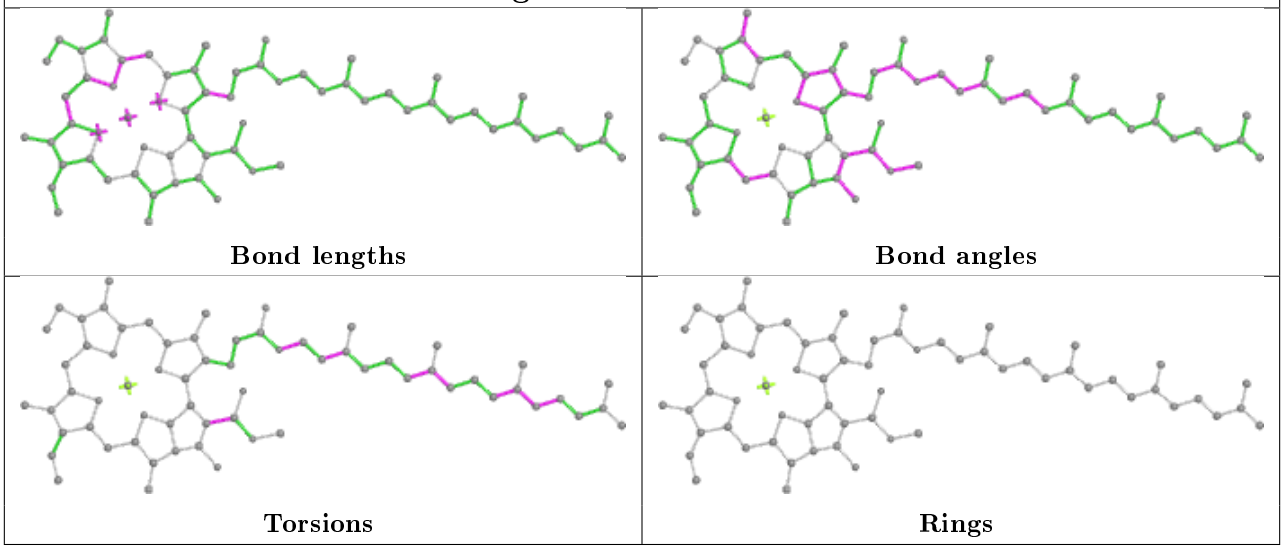


Torsions

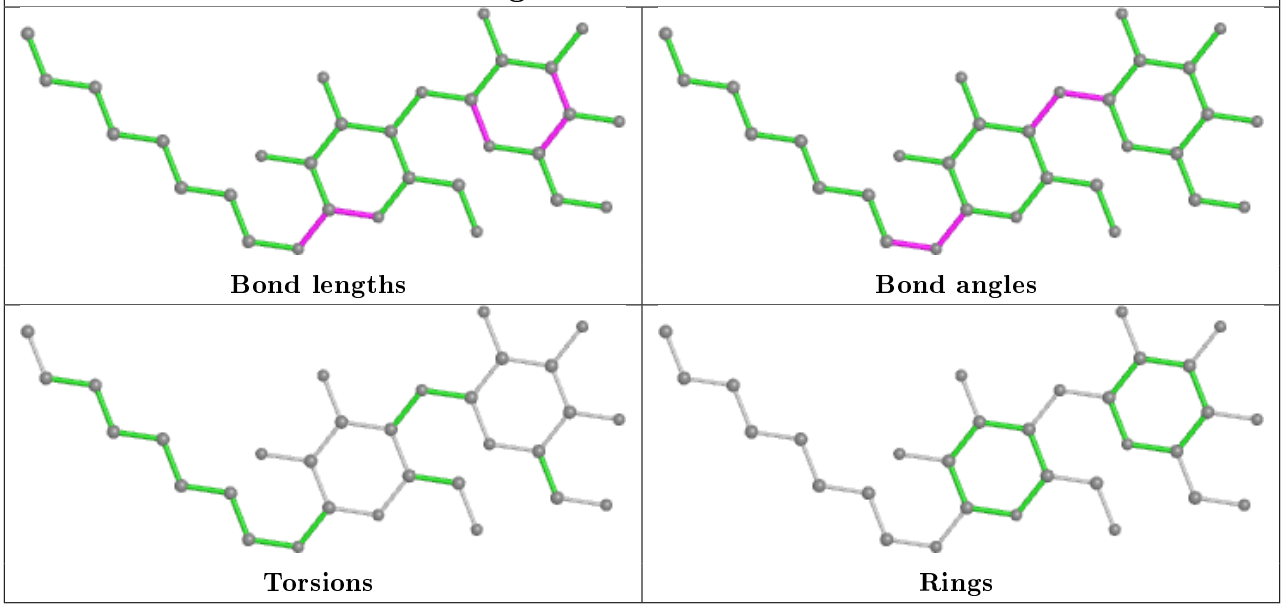


Rings

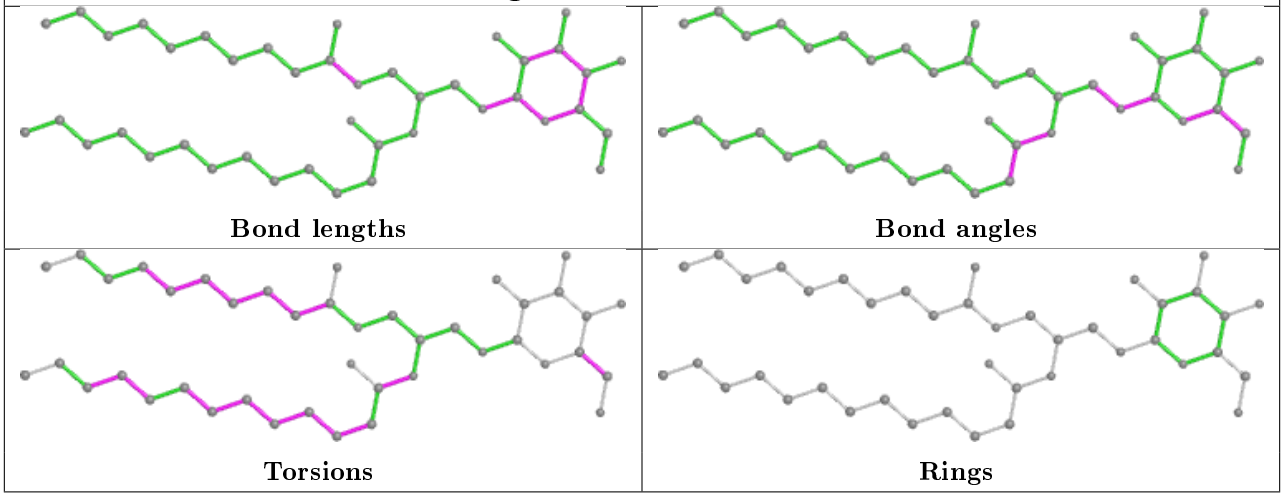
Ligand CLA BC 502



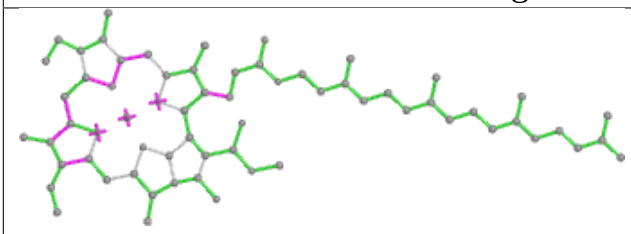
Ligand LMT AD 411



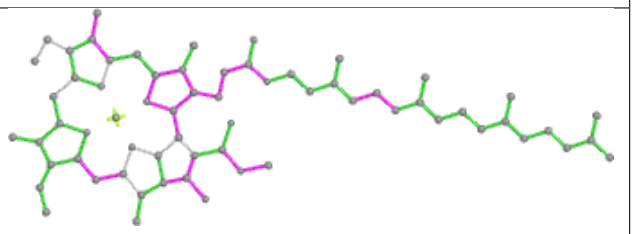
Ligand LMG AA 416



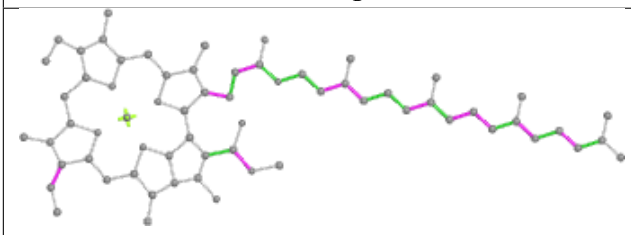
Ligand CLA AC 505



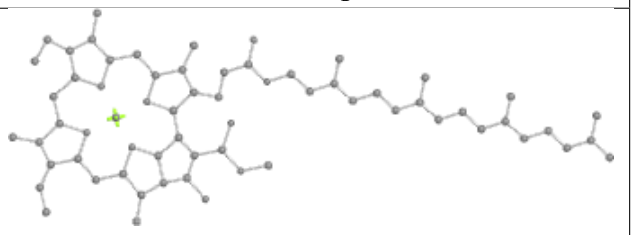
Bond lengths



Bond angles

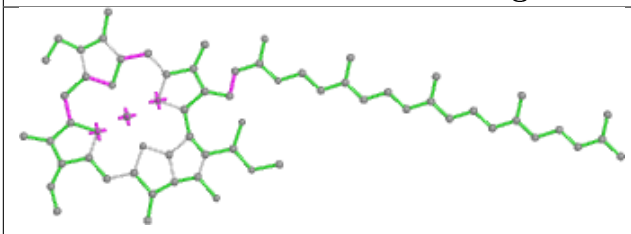


Torsions

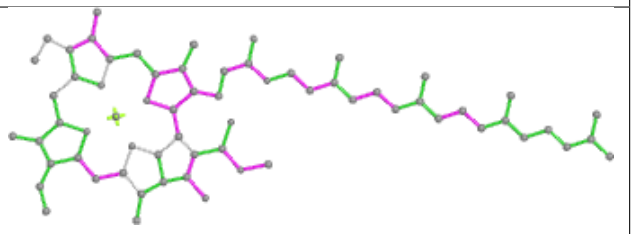


Rings

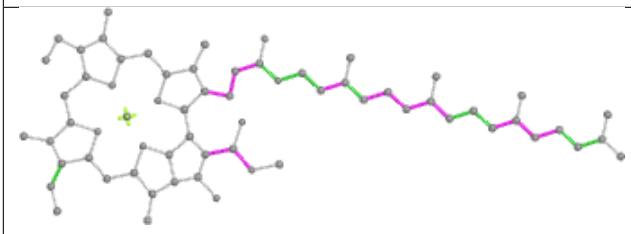
Ligand CLA AB 602



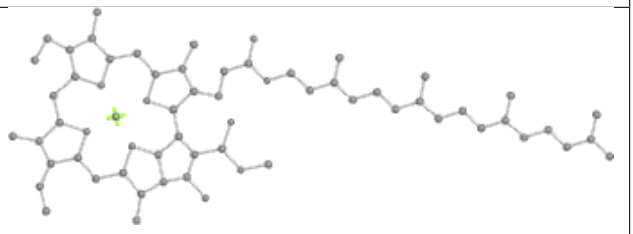
Bond lengths



Bond angles

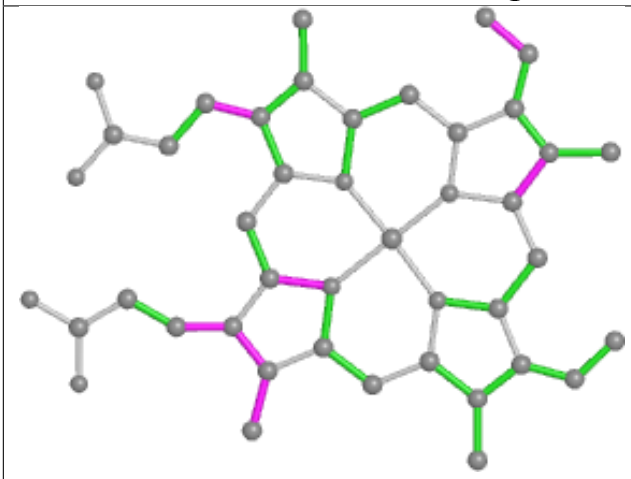


Torsions

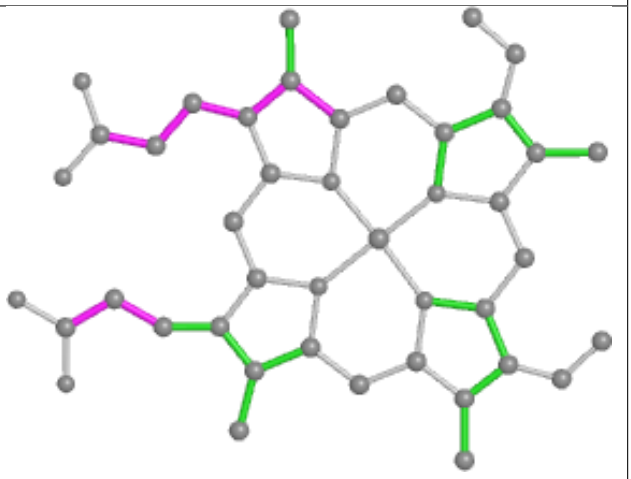


Rings

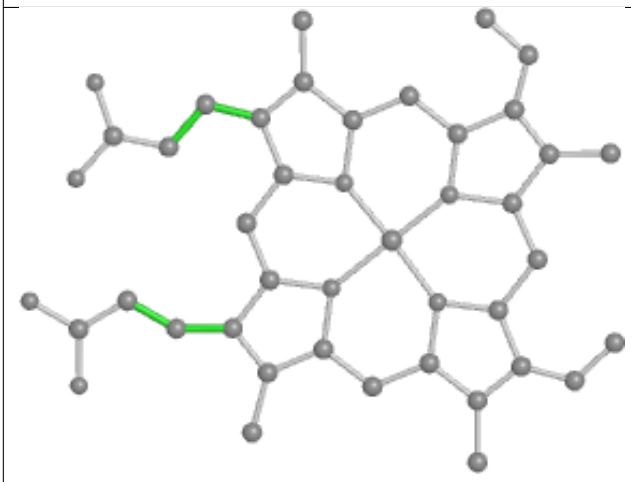
Ligand HEM AE 101



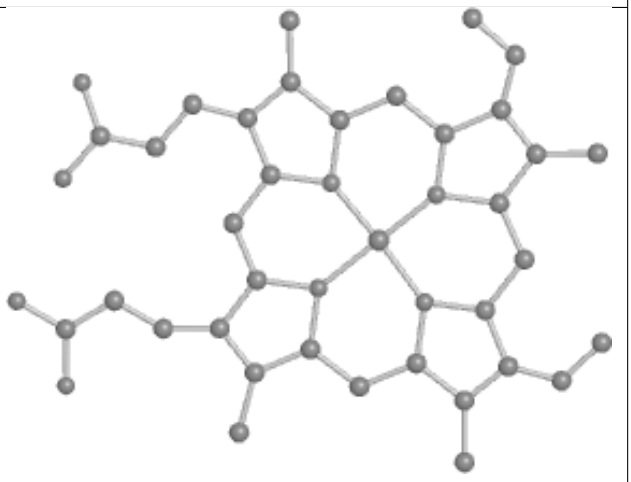
Bond lengths



Bond angles

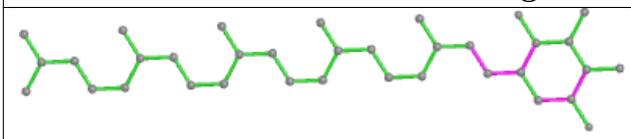


Torsions

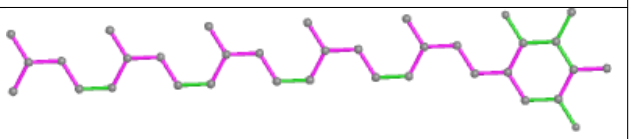


Rings

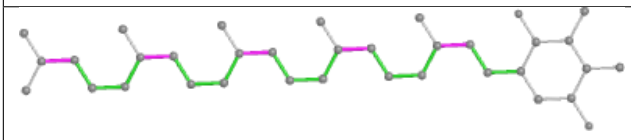
Ligand PL9 BJ 101



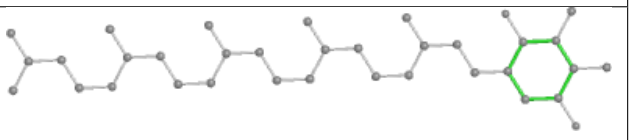
Bond lengths



Bond angles

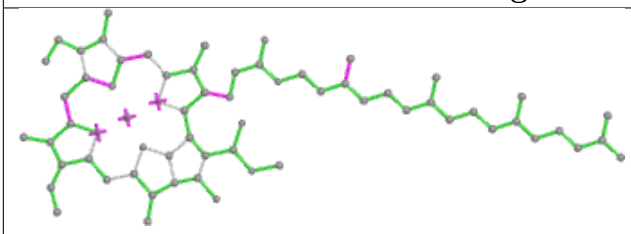


Torsions

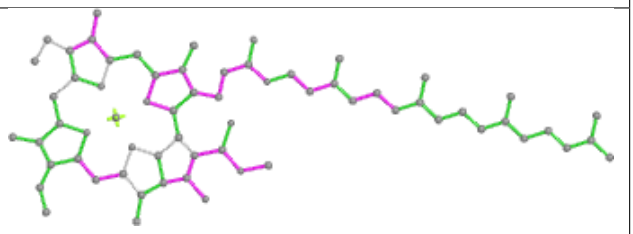


Rings

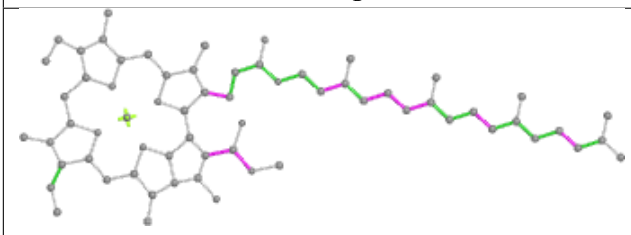
Ligand CLA AA 404



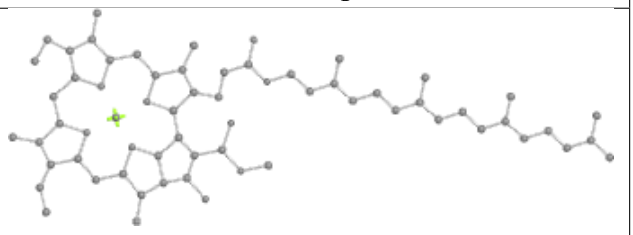
Bond lengths



Bond angles

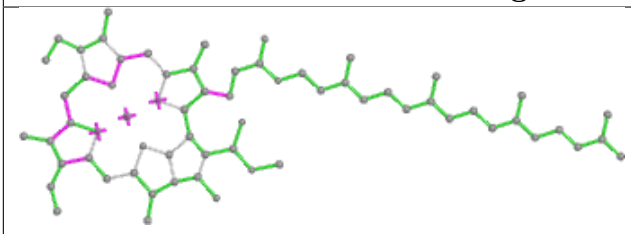


Torsions

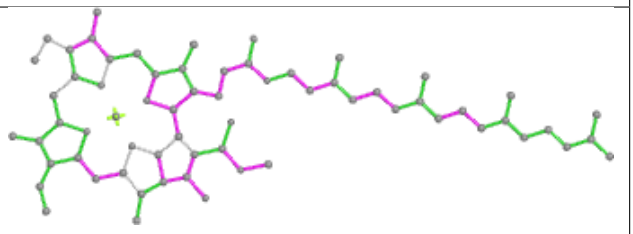


Rings

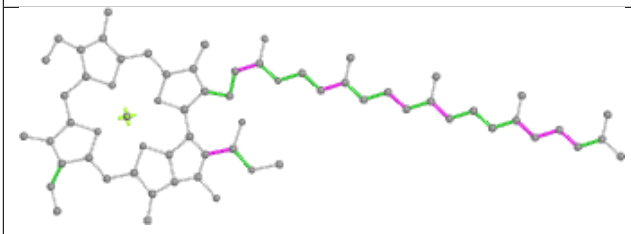
Ligand CLA AD 402



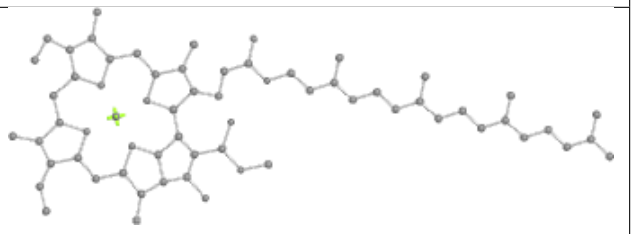
Bond lengths



Bond angles

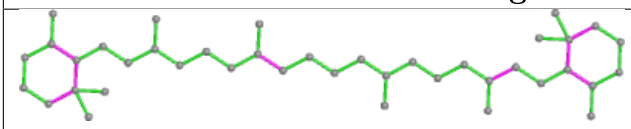


Torsions

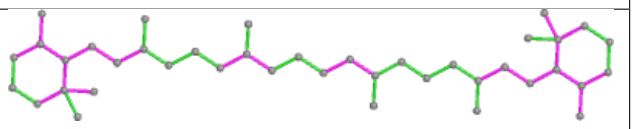


Rings

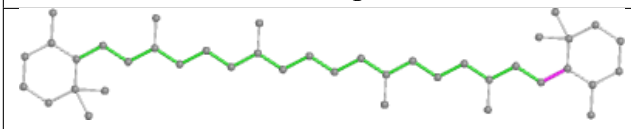
Ligand BCR AB 620



Bond lengths



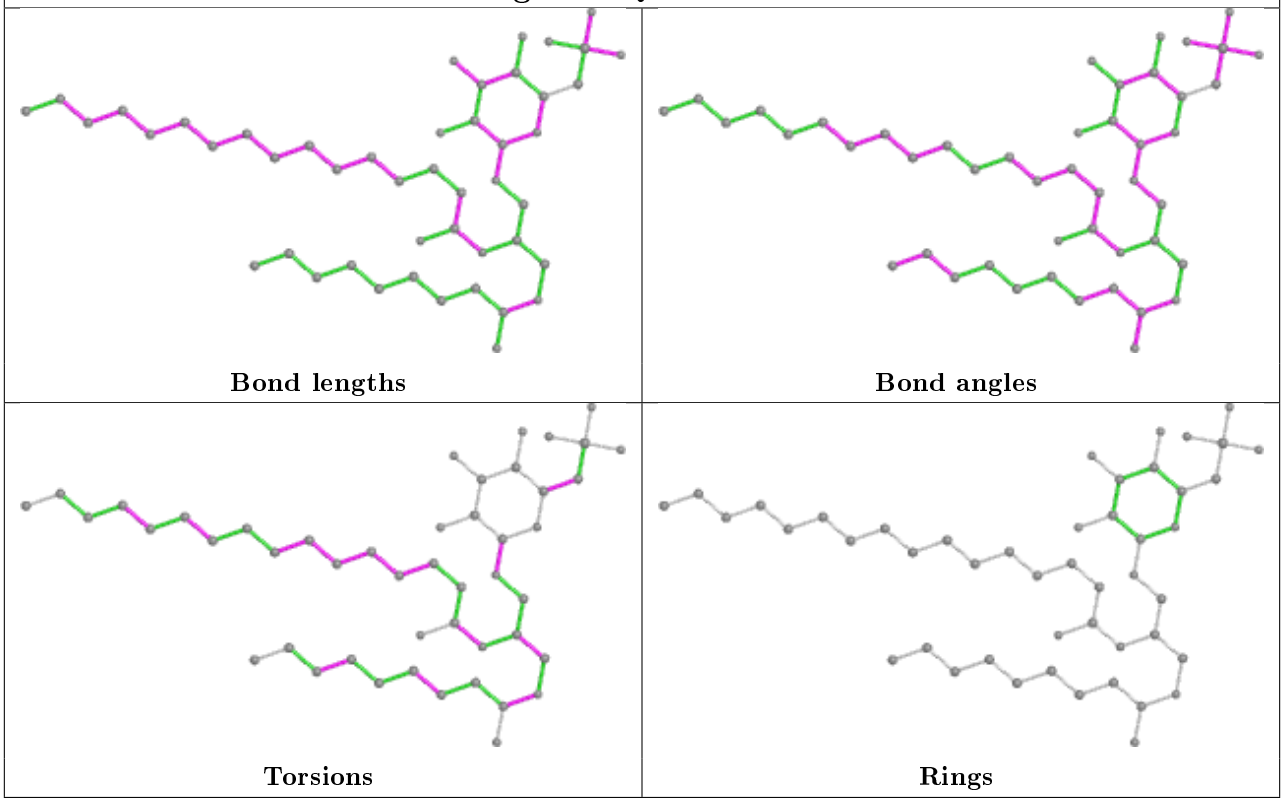
Bond angles



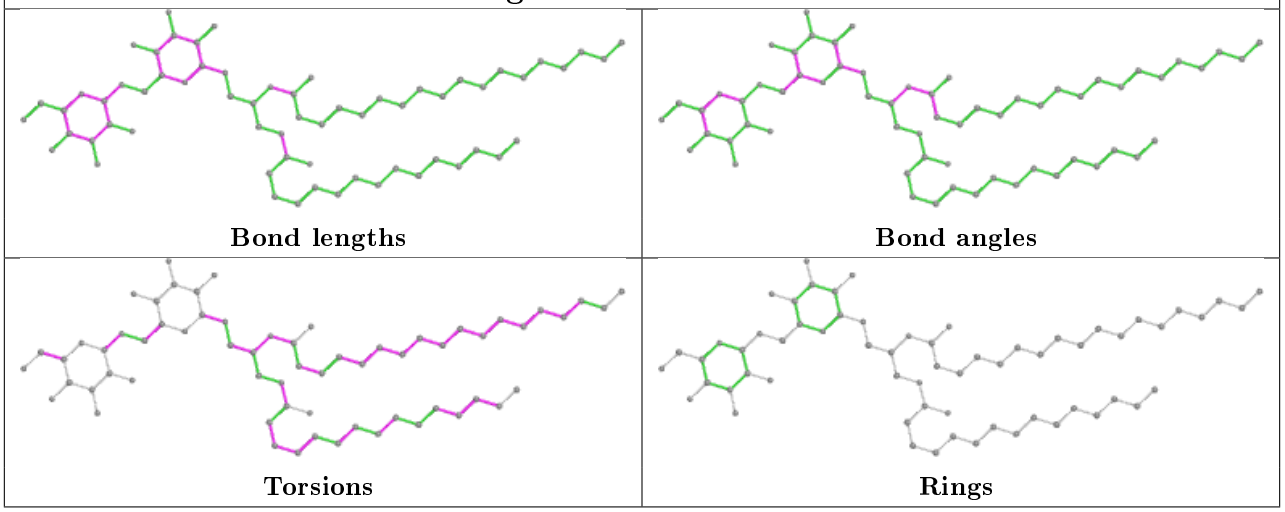
Torsions

Rings

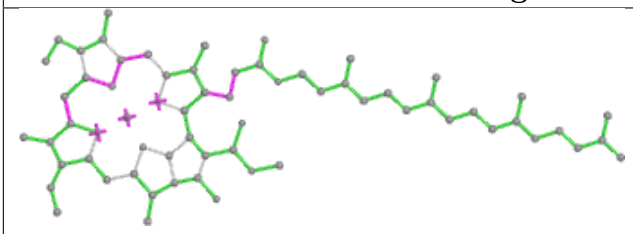
Ligand SQD BB 601



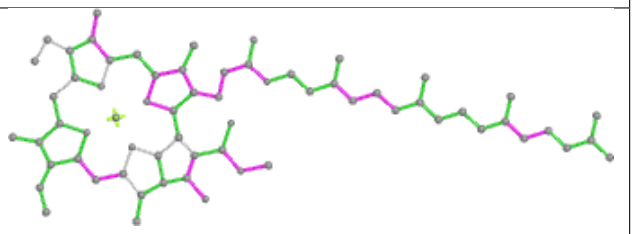
Ligand DGD AD 410



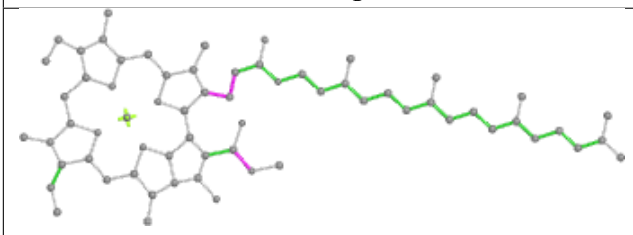
Ligand CLA AA 402



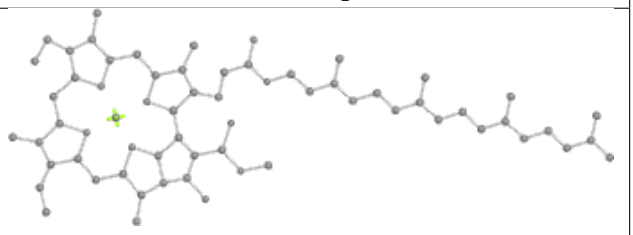
Bond lengths



Bond angles

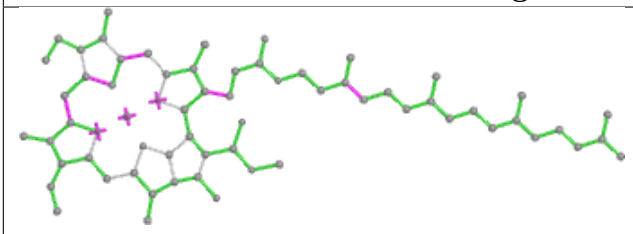


Torsions

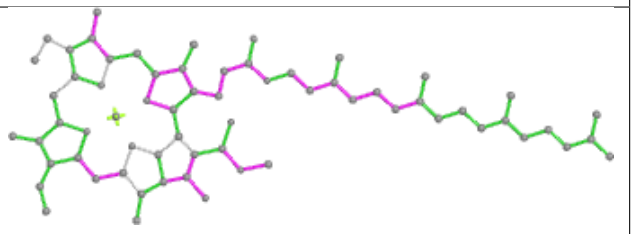


Rings

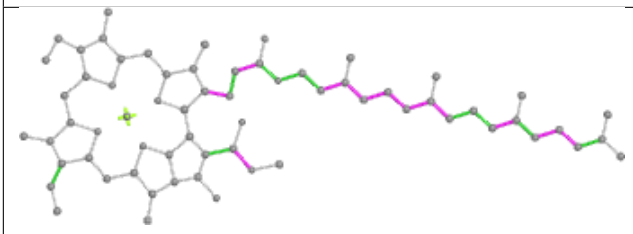
Ligand CLA AB 608



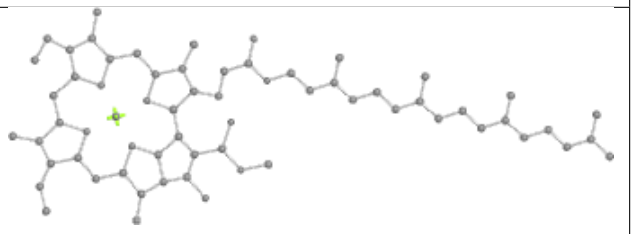
Bond lengths



Bond angles

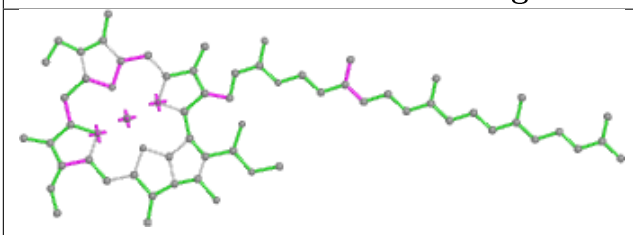


Torsions

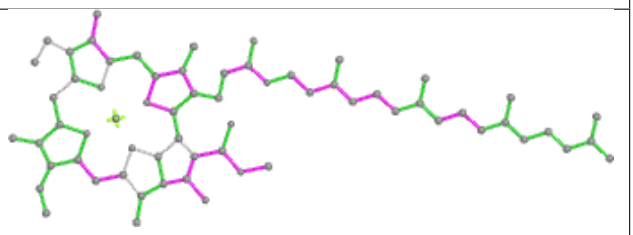


Rings

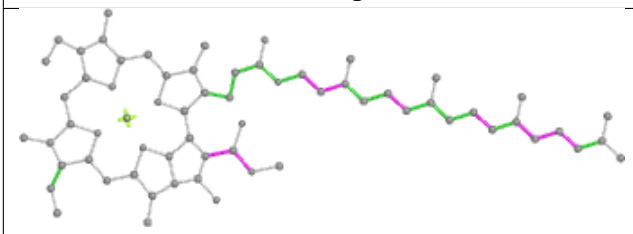
Ligand CLA BC 509



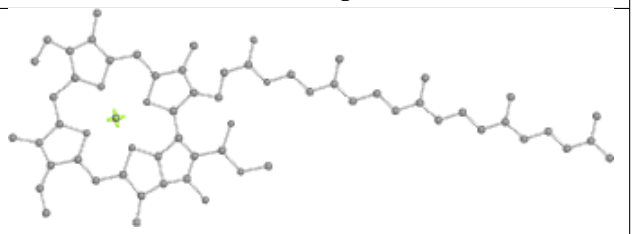
Bond lengths



Bond angles

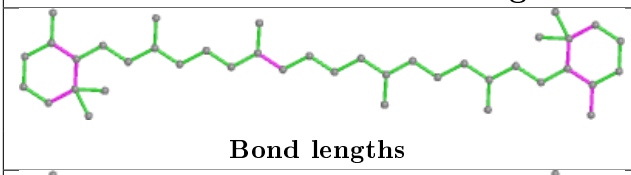


Torsions

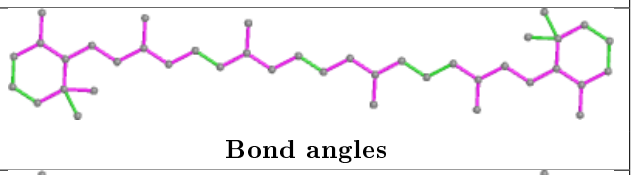


Rings

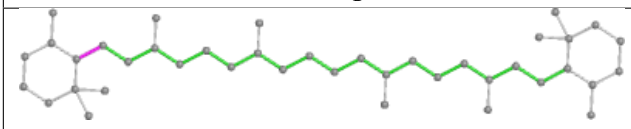
Ligand BCR BX 101



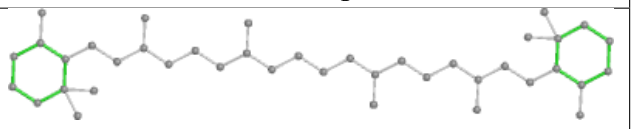
Bond lengths



Bond angles

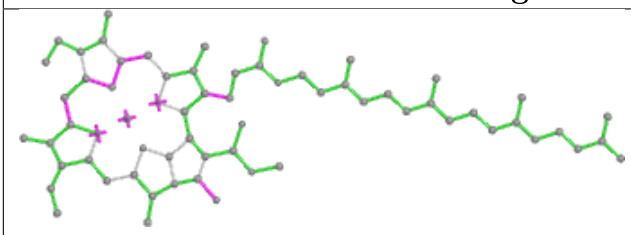


Torsions

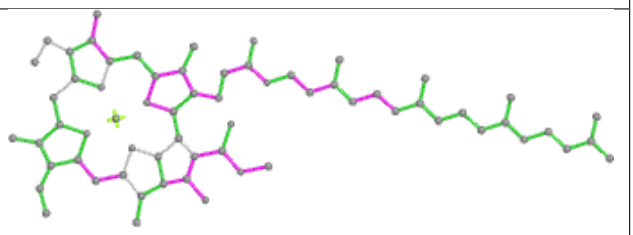


Rings

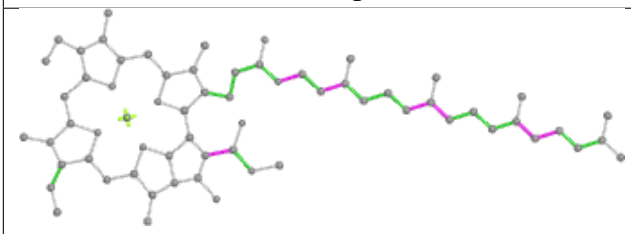
Ligand CLA AC 502



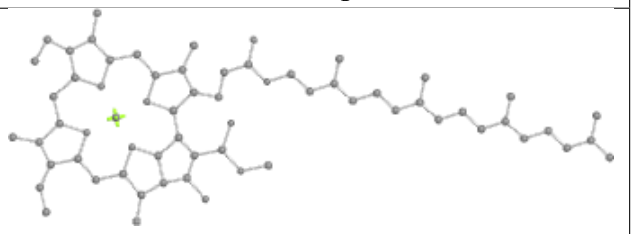
Bond lengths



Bond angles

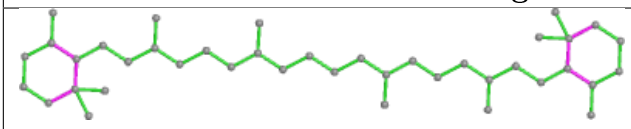


Torsions

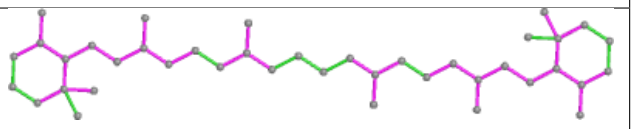


Rings

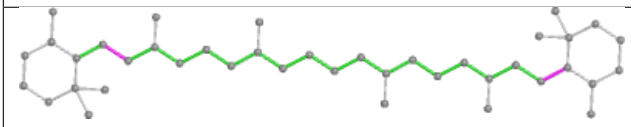
Ligand BCR AT 102



Bond lengths



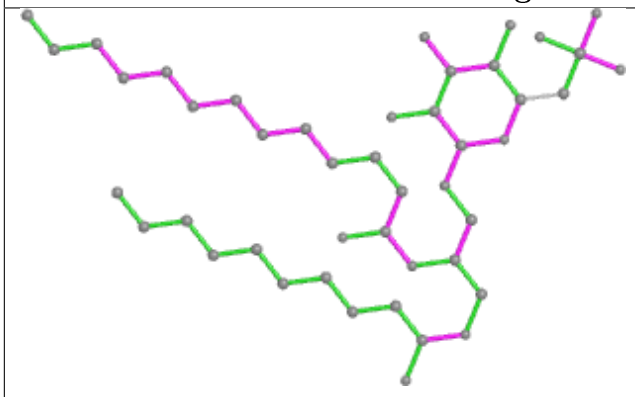
Bond angles



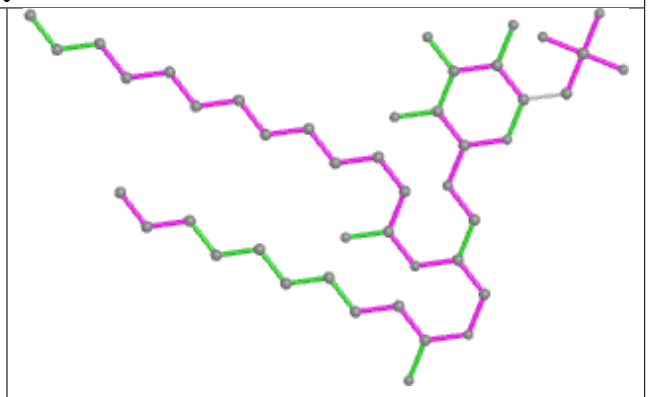
Torsions

Rings

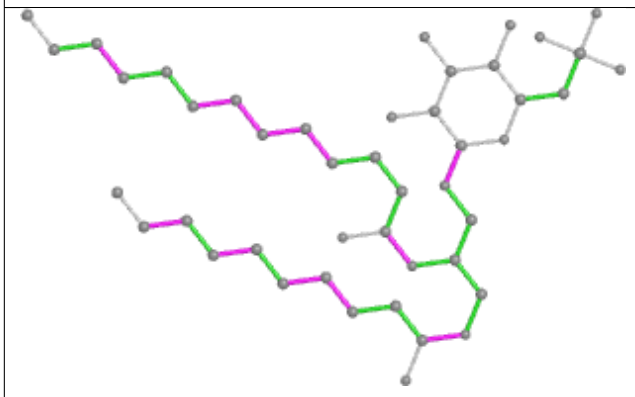
Ligand SQD BF 101



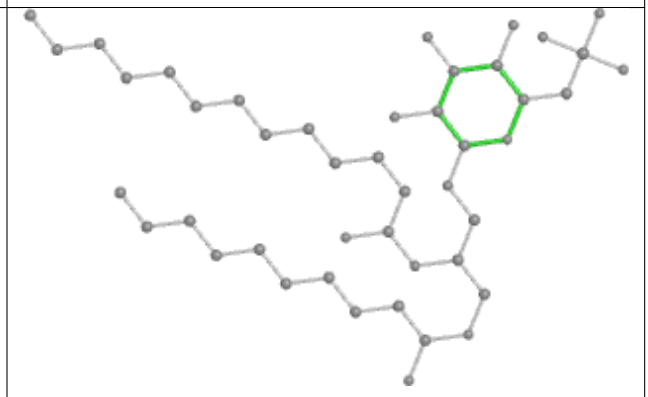
Bond lengths



Bond angles

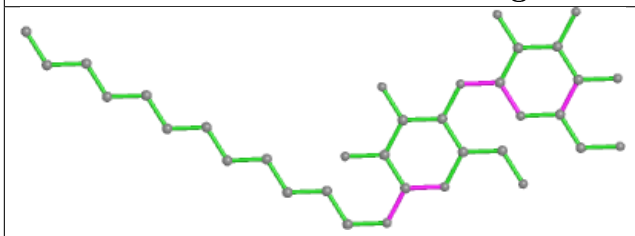


Torsions

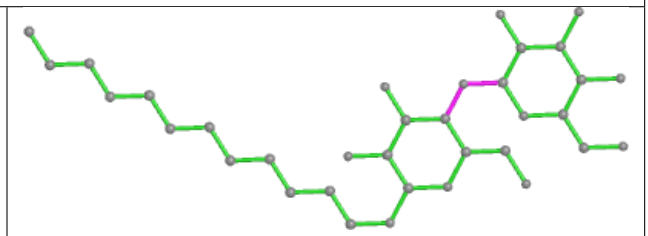


Rings

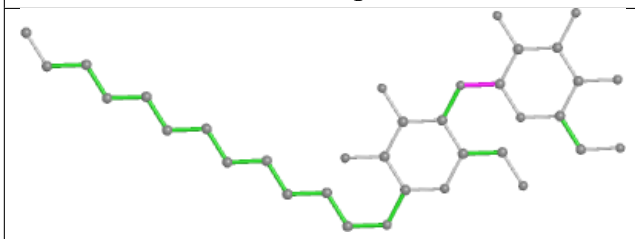
Ligand LMT BB 626



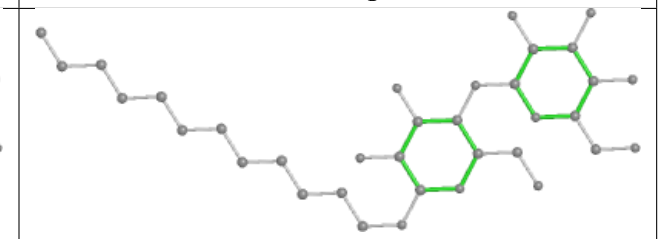
Bond lengths



Bond angles

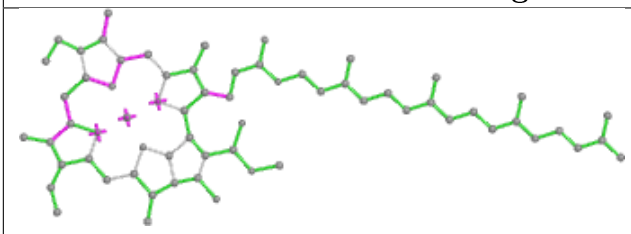


Torsions



Rings

Ligand CLA AC 512



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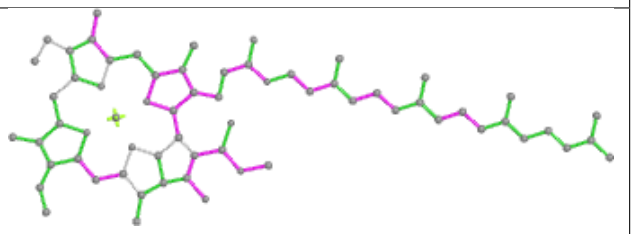
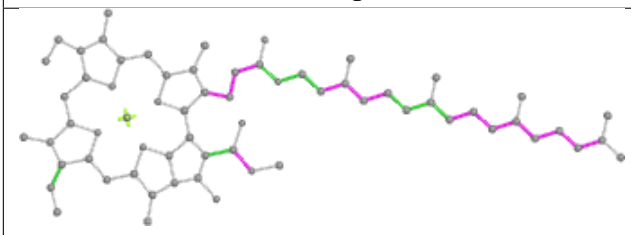
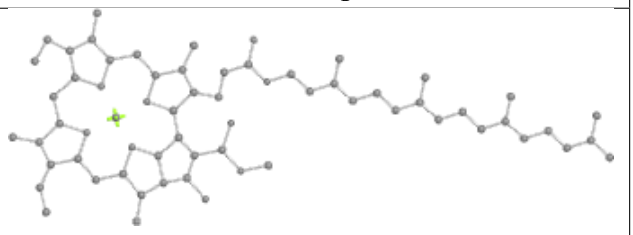


Bond angles

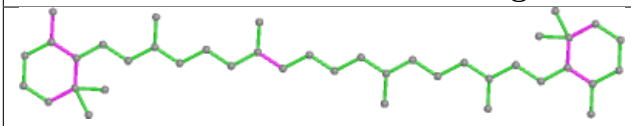


Torsions

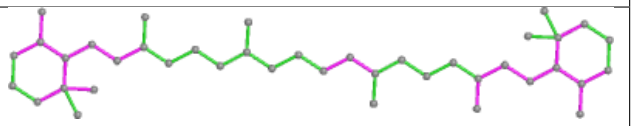


Rings

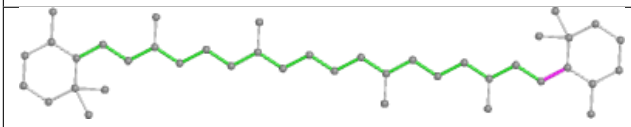
Ligand BCR BB 622



Bond lengths



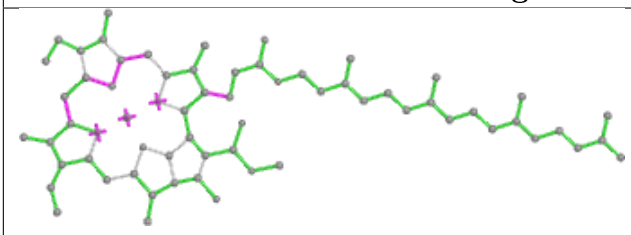
Bond angles



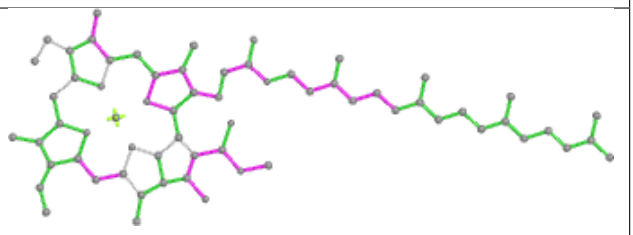
Torsions

Rings

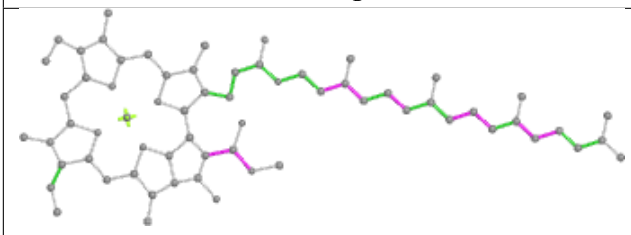
Ligand CLA AB 612



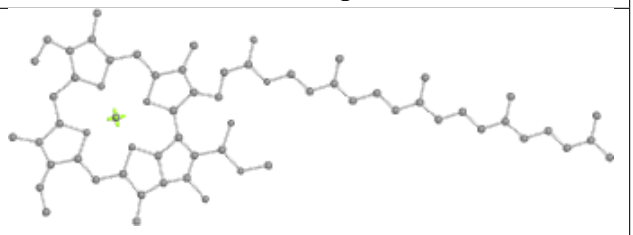
Bond lengths



Bond angles

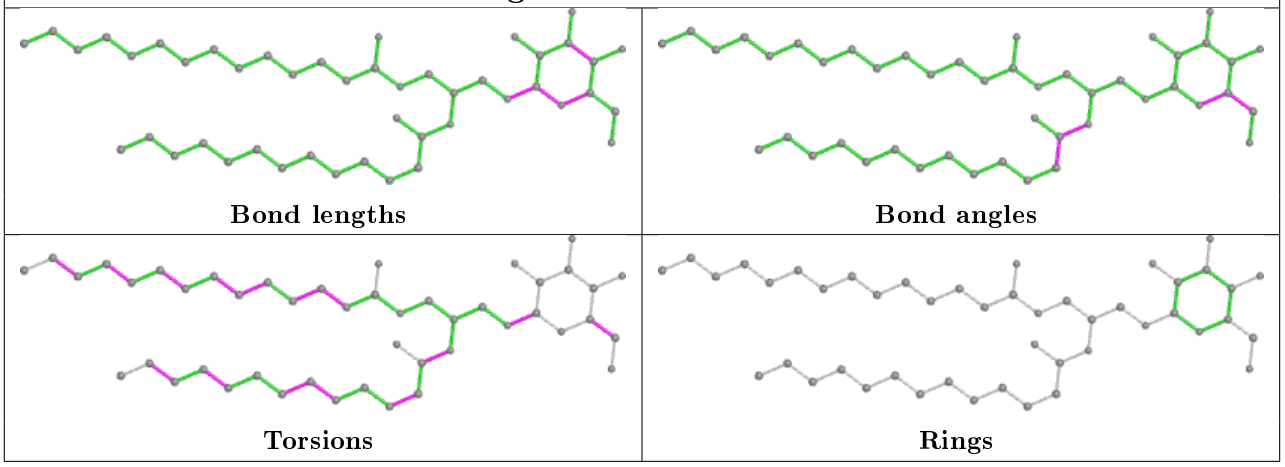


Torsions

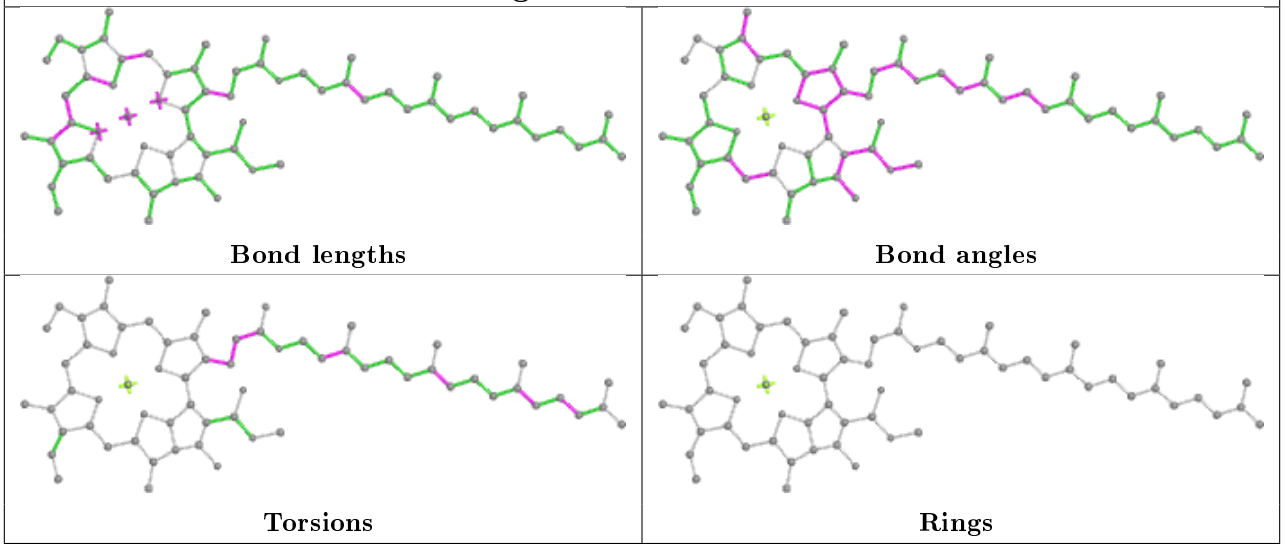


Rings

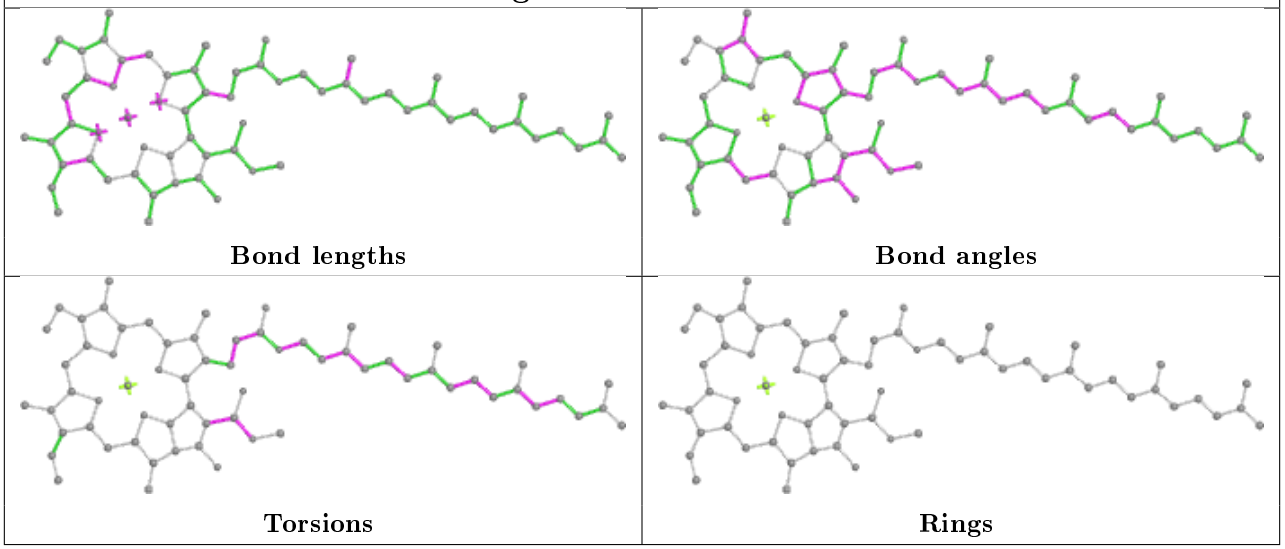
Ligand LMG BD 407



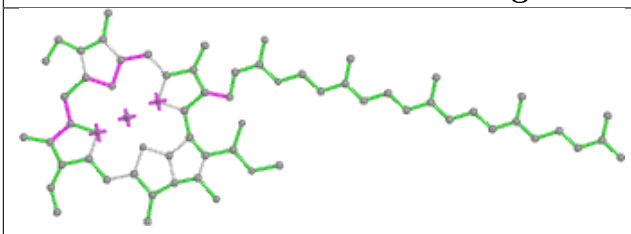
Ligand CLA BD 404



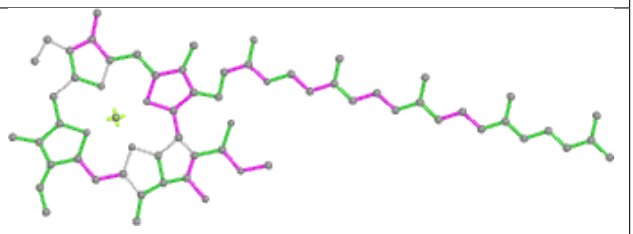
Ligand CLA AB 610



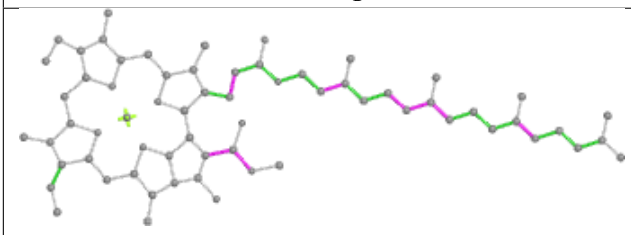
Ligand CLA BC 511



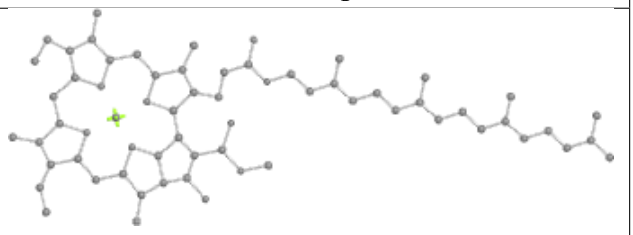
Bond lengths



Bond angles

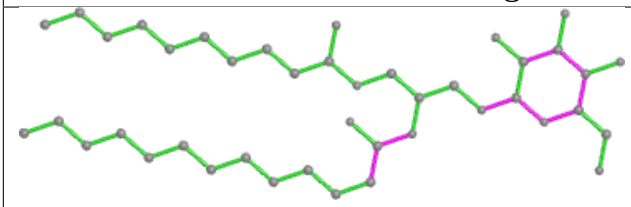


Torsions

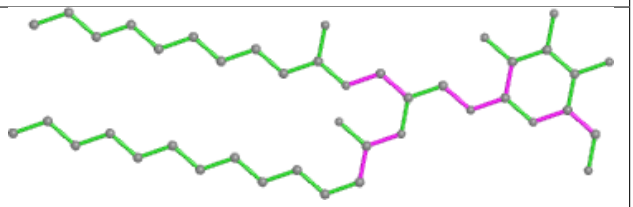


Rings

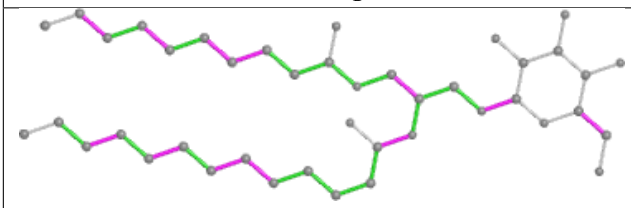
Ligand LMG BM 102



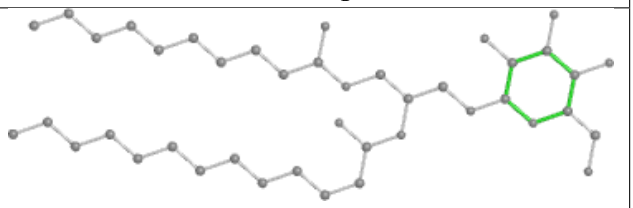
Bond lengths



Bond angles

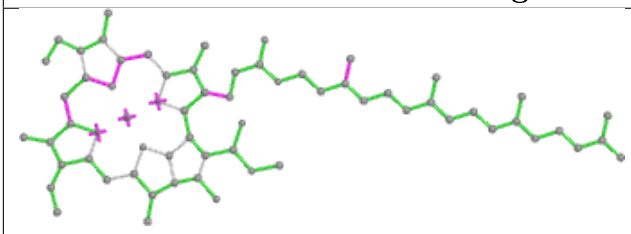


Torsions

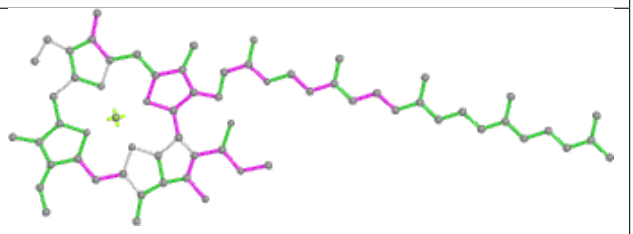


Rings

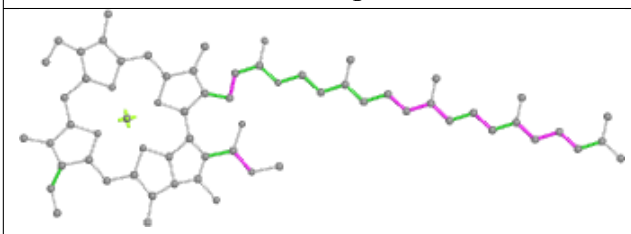
Ligand CLA AC 508



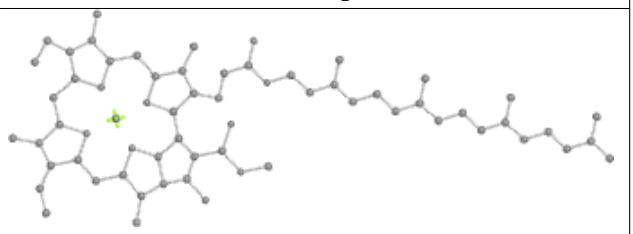
Bond lengths



Bond angles

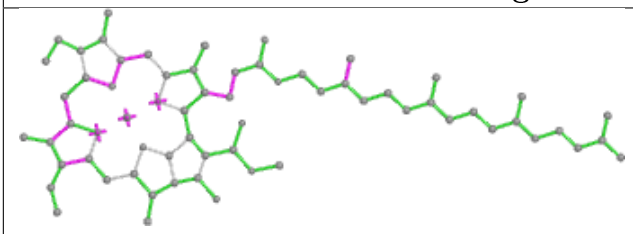


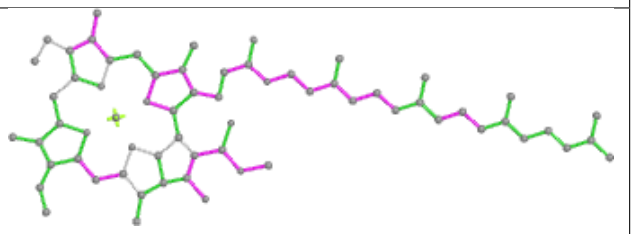
Torsions

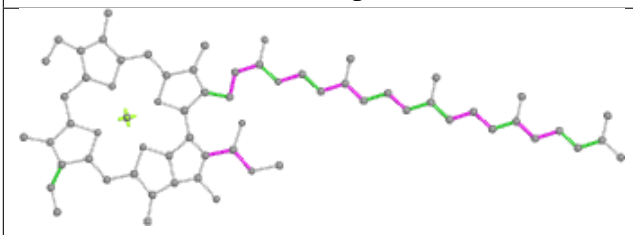


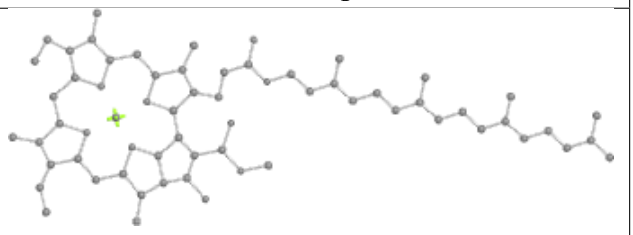
Rings

Ligand CLA BB 613

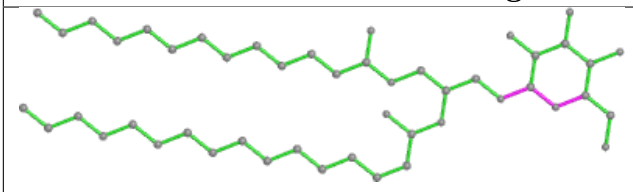

Bond lengths

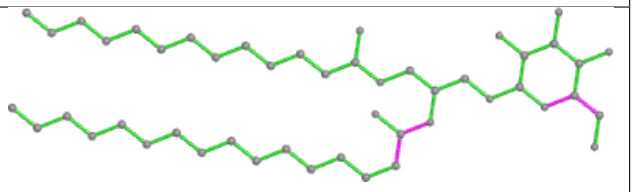

Bond angles

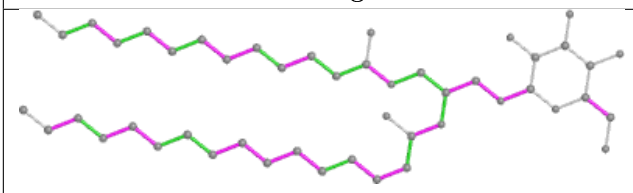

Torsions

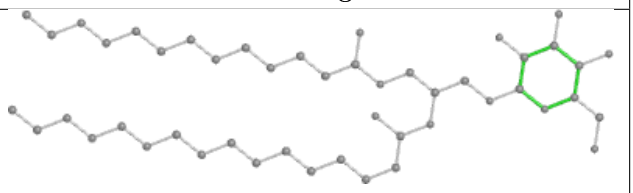

Rings

Ligand LMG AD 408

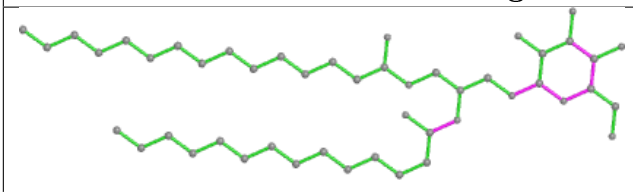

Bond lengths

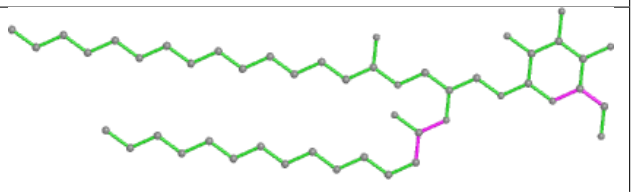

Bond angles

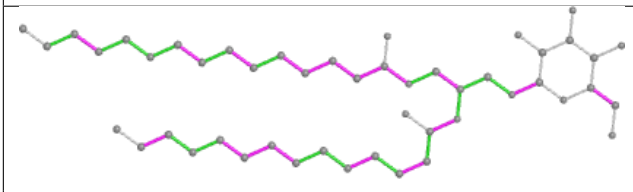

Torsions

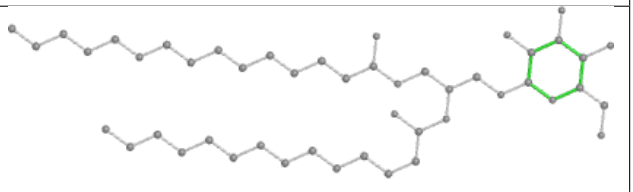

Rings

Ligand LMG BC 519

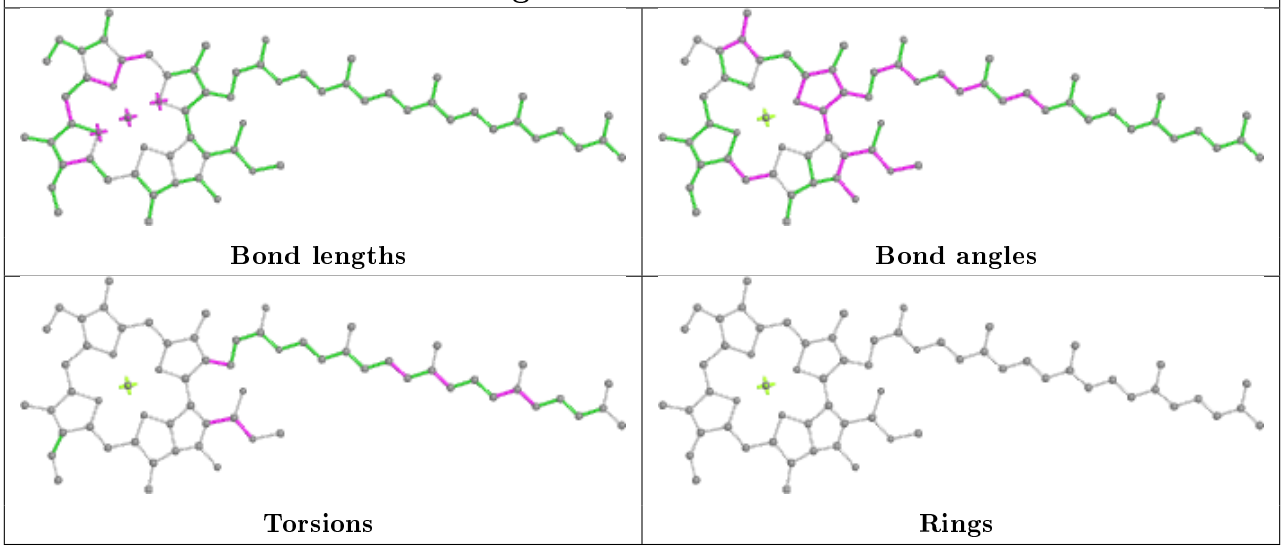

Bond lengths


Bond angles

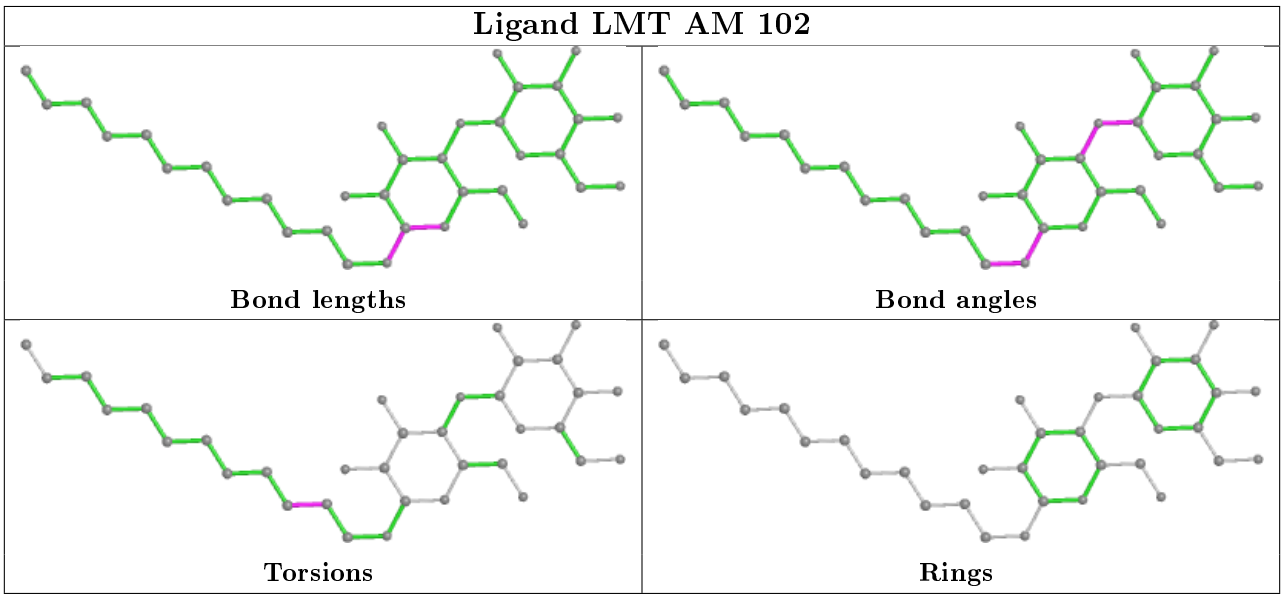

Torsions


Rings

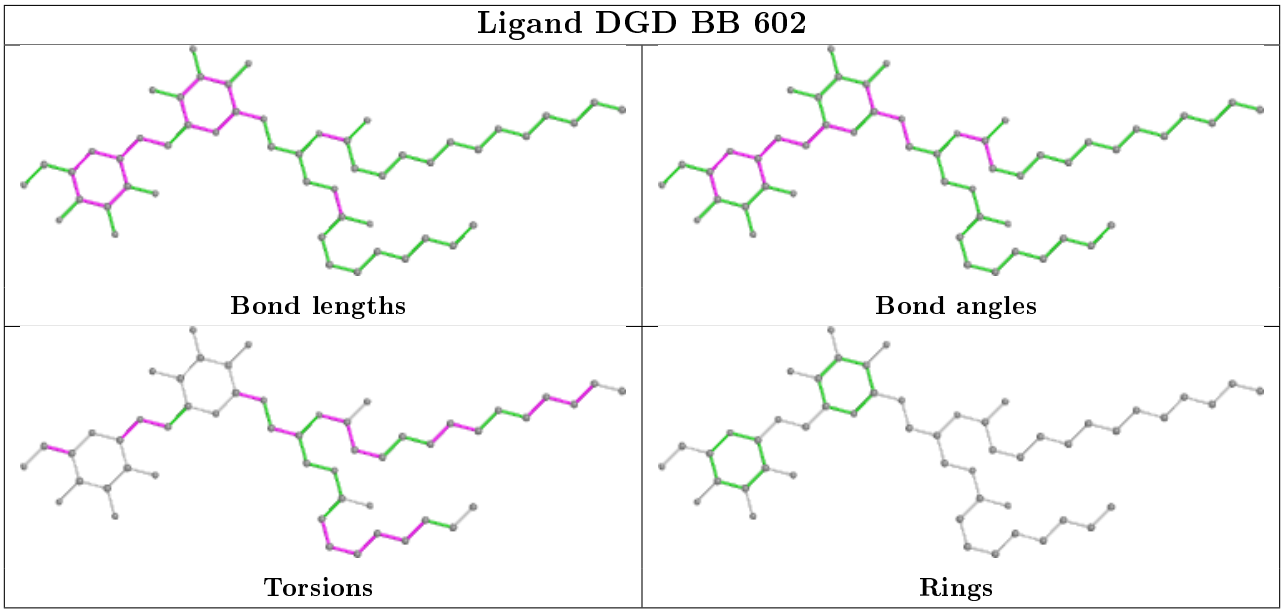
Ligand CLA BC 507



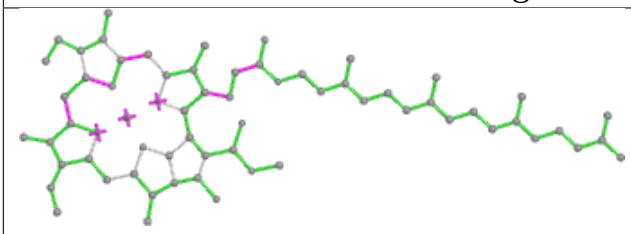
Ligand LMT AM 102



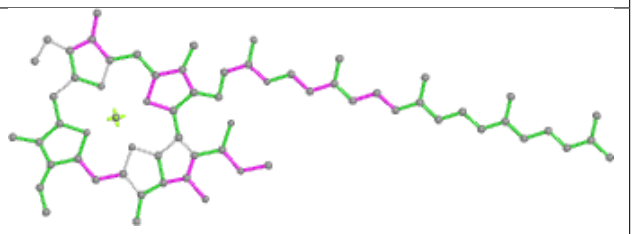
Ligand DGD BB 602



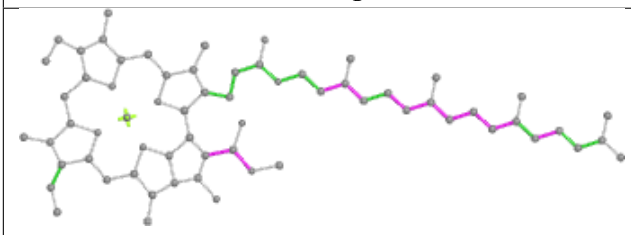
Ligand CLA BB 616



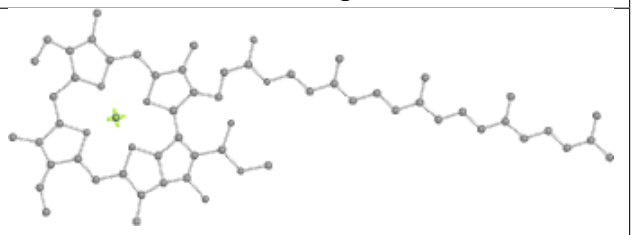
Bond lengths



Bond angles

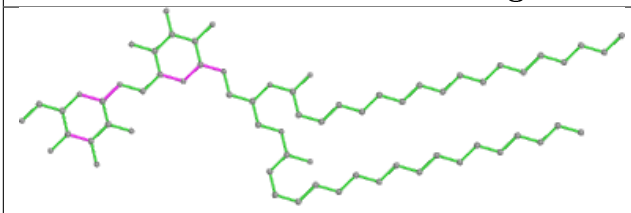


Torsions

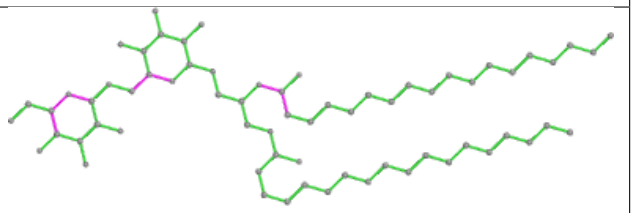


Rings

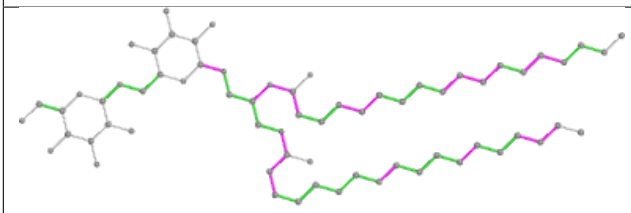
Ligand DGD BC 518



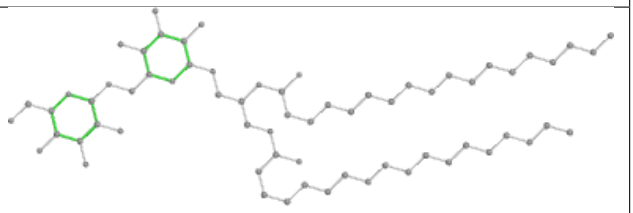
Bond lengths



Bond angles

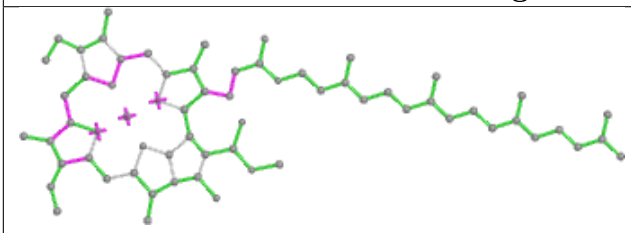


Torsions

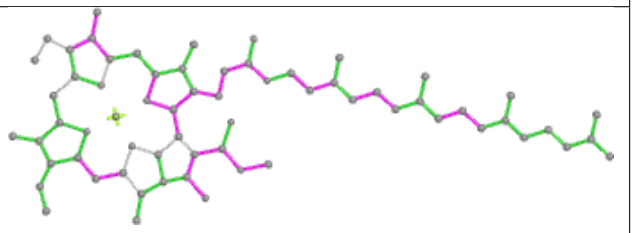


Rings

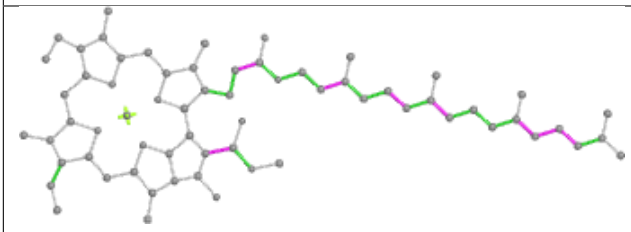
Ligand CLA BD 402



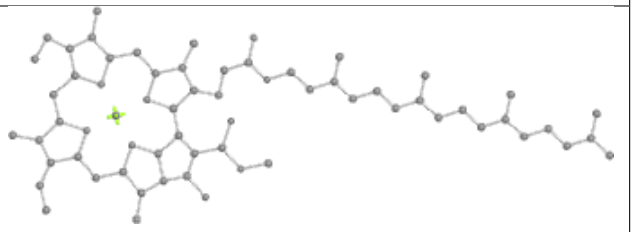
Bond lengths



Bond angles

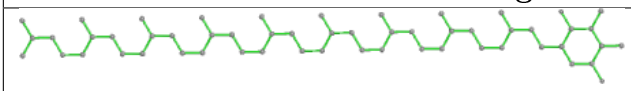


Torsions

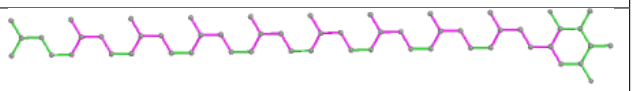


Rings

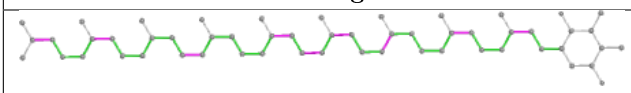
Ligand PL9 AD 405



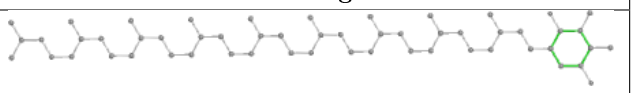
Bond lengths



Bond angles

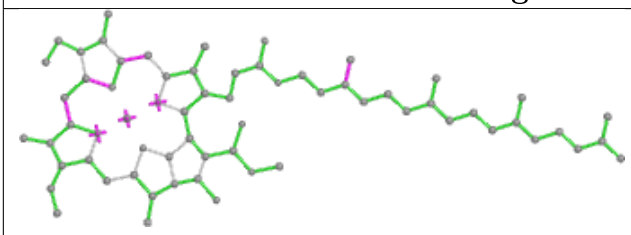


Torsions

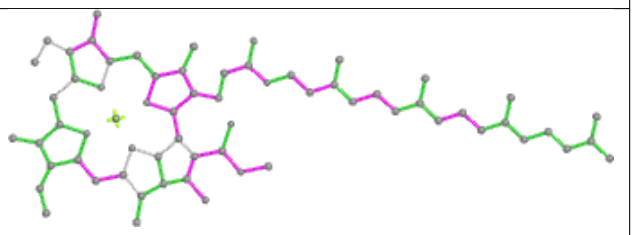


Rings

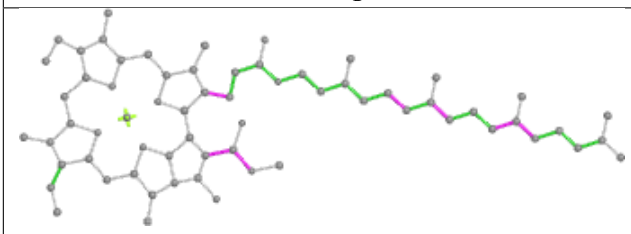
Ligand CLA AC 507



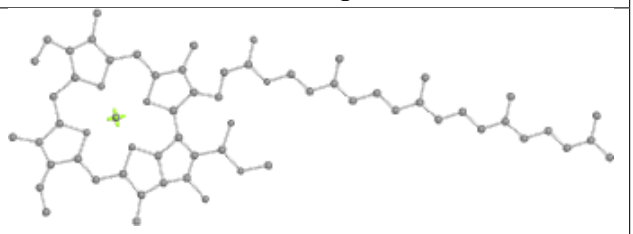
Bond lengths



Bond angles

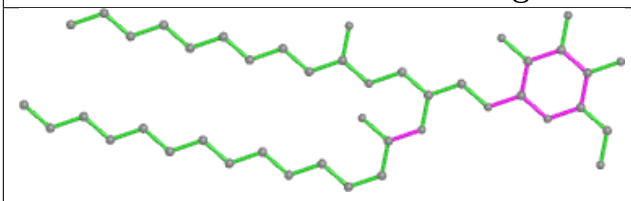


Torsions

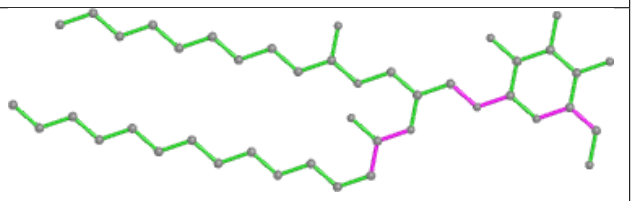


Rings

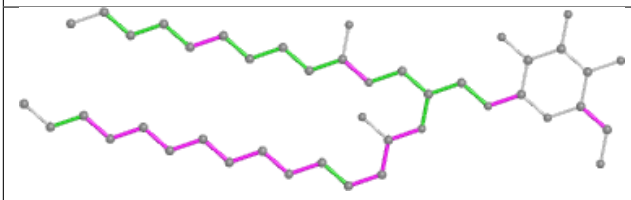
Ligand LMG AI 101



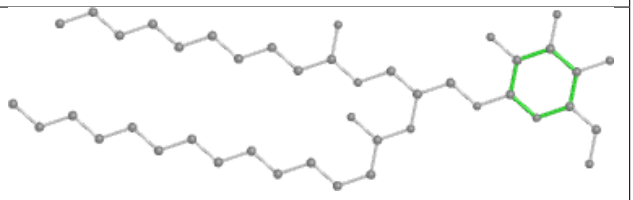
Bond lengths



Bond angles

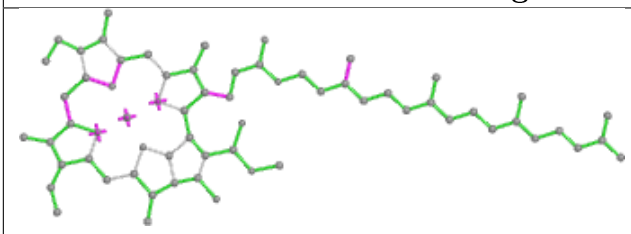


Torsions

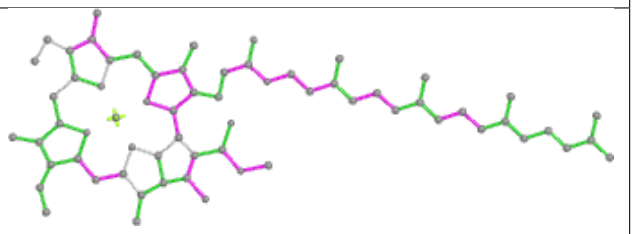


Rings

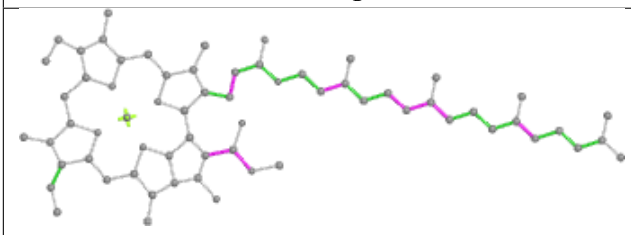
Ligand CLA AC 511



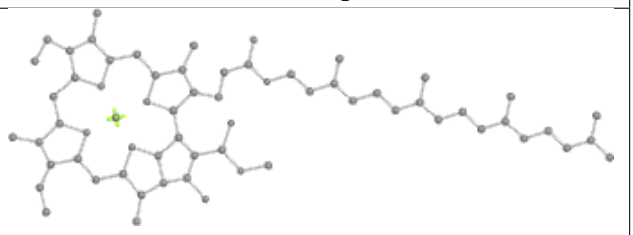
Bond lengths



Bond angles

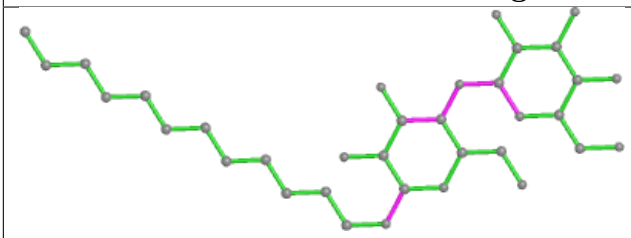


Torsions

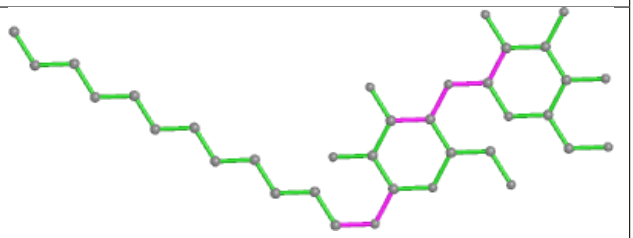


Rings

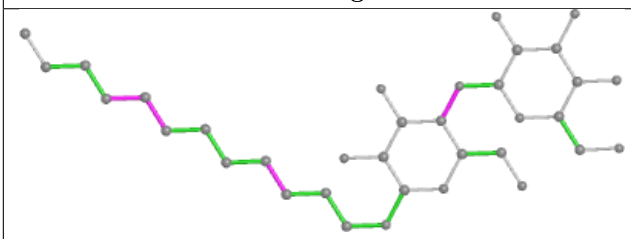
Ligand LMT AT 101



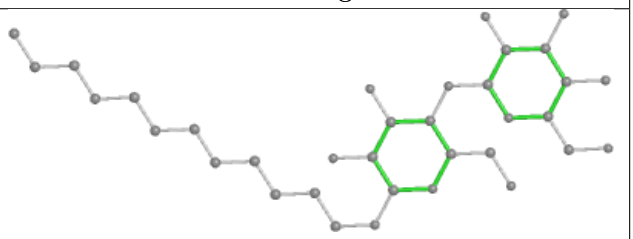
Bond lengths



Bond angles

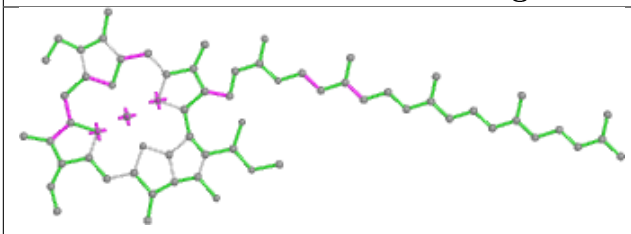


Torsions

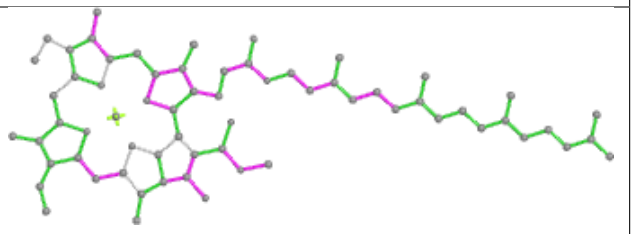


Rings

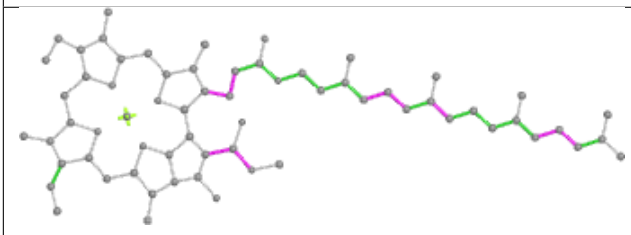
Ligand CLA AB 607



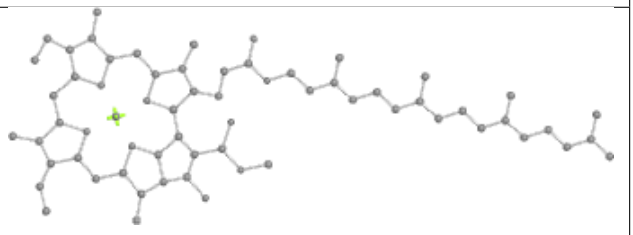
Bond lengths



Bond angles

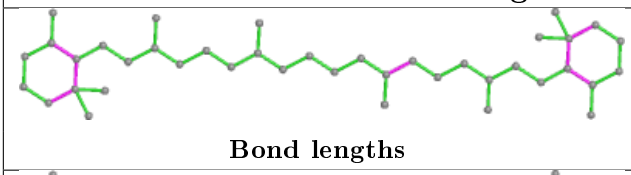


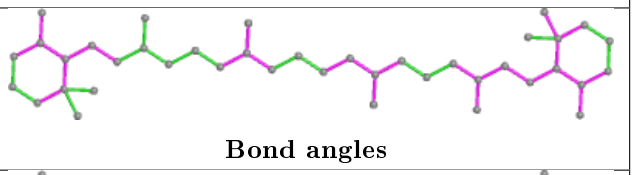
Torsions

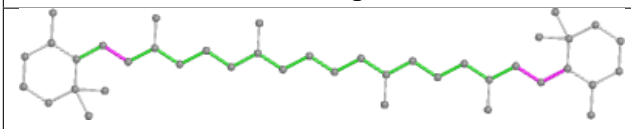


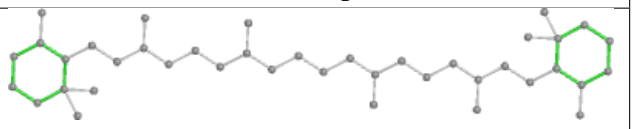
Rings

Ligand BCR BC 515

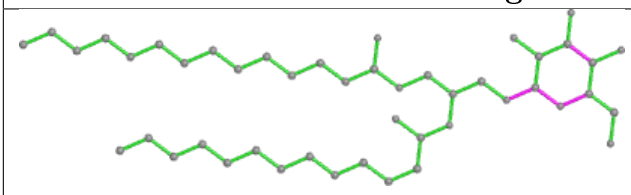

Bond lengths

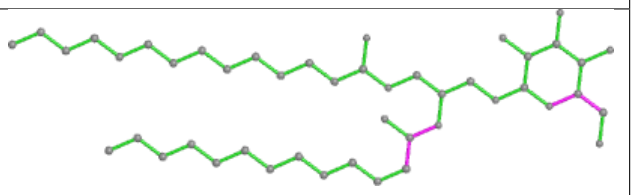

Bond angles

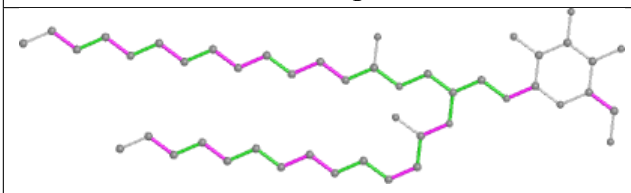

Torsions

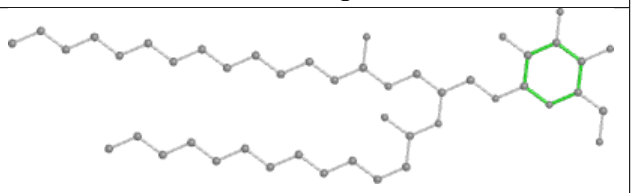

Rings

Ligand LMG AD 407

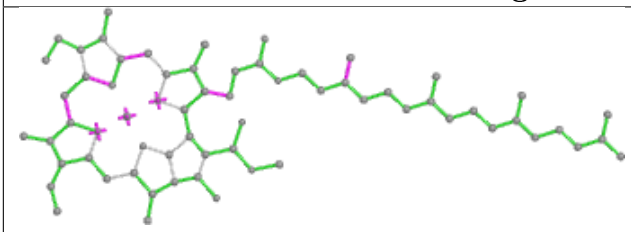

Bond lengths

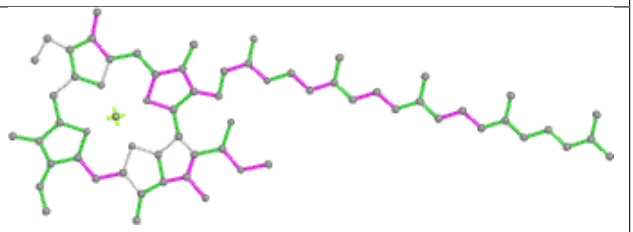

Bond angles

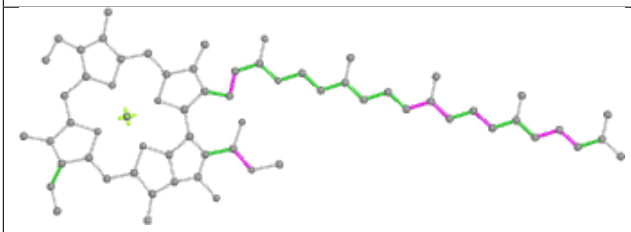

Torsions

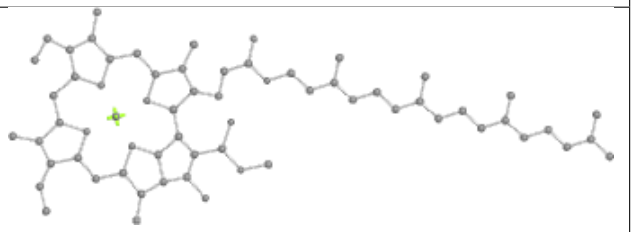

Rings

Ligand CLA AC 504


Bond lengths


Bond angles


Torsions


Rings

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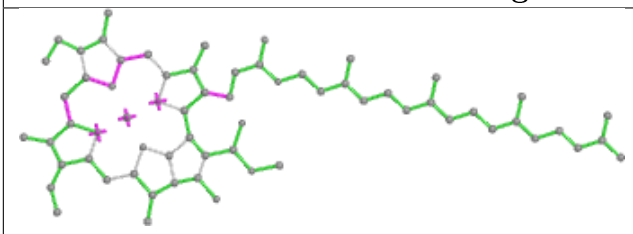
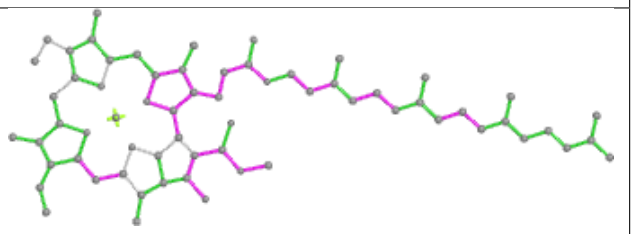
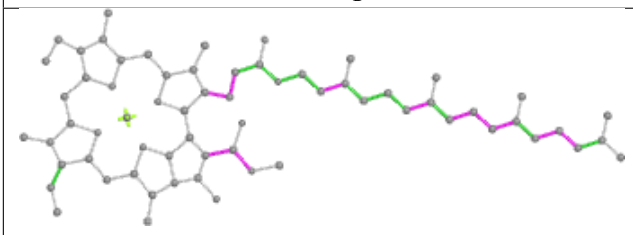


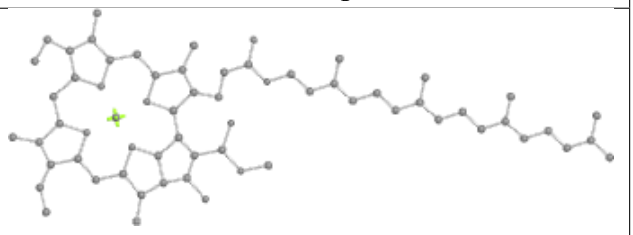
Bond lengths



Bond angles

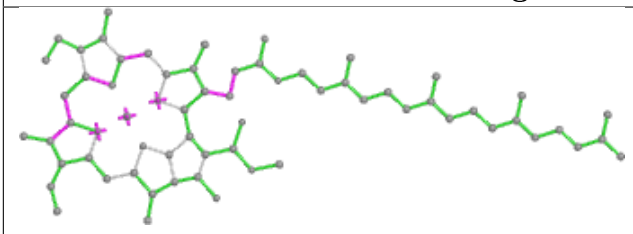


Torsions

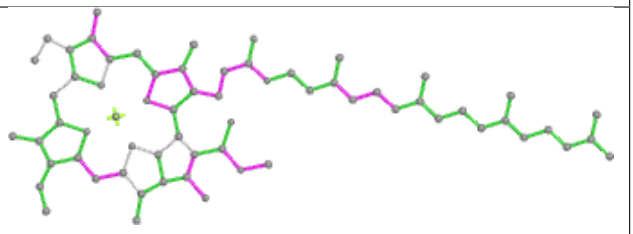


Rings

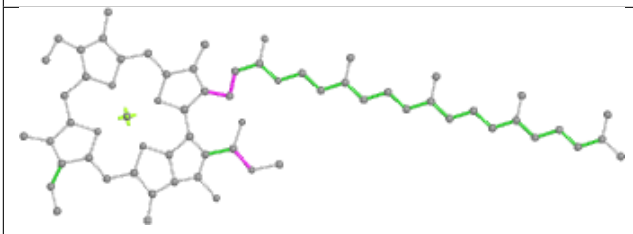
Ligand CLA BA 403



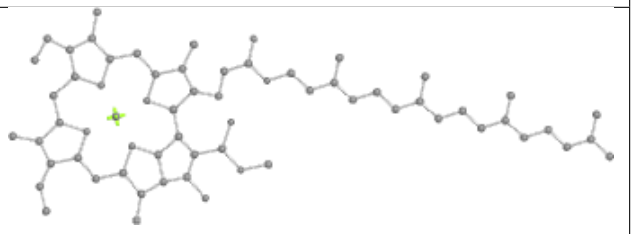
Bond lengths



Bond angles

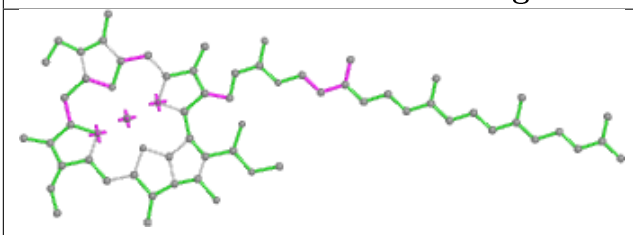


Torsions

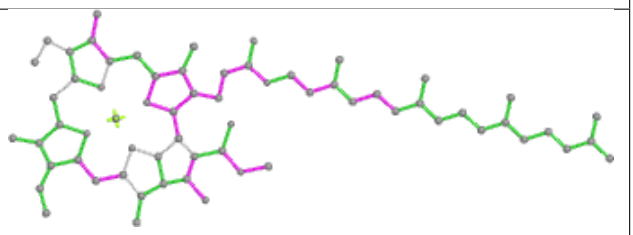


Rings

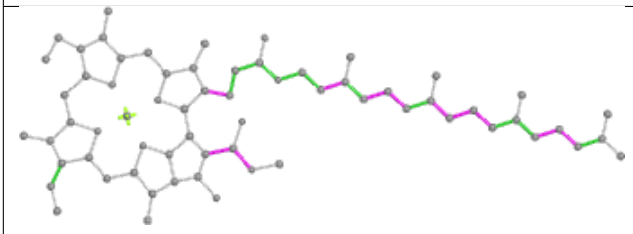
Ligand CLA BB 619



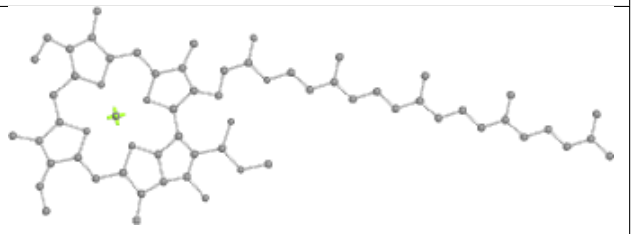
Bond lengths



Bond angles

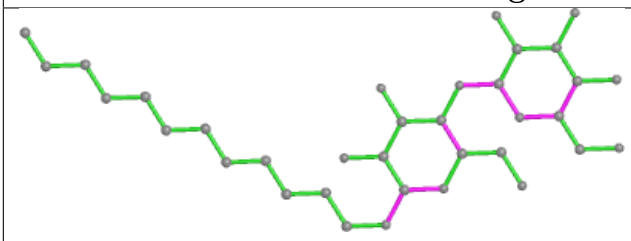


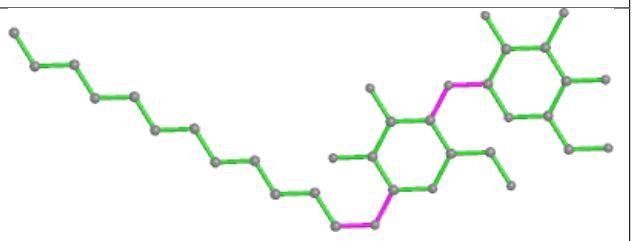
Torsions

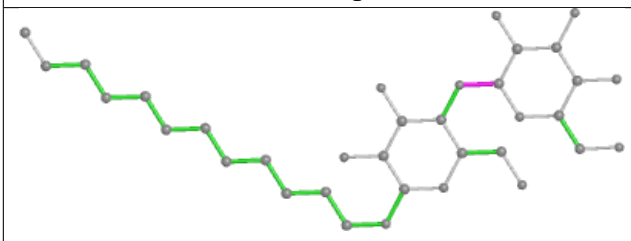


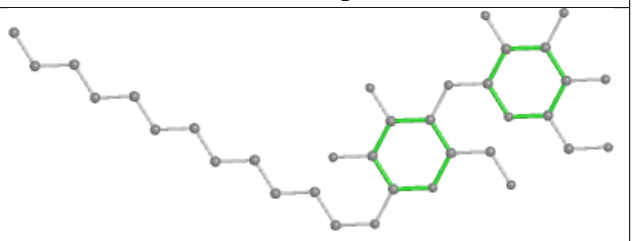
Rings

Ligand LMT AB 625

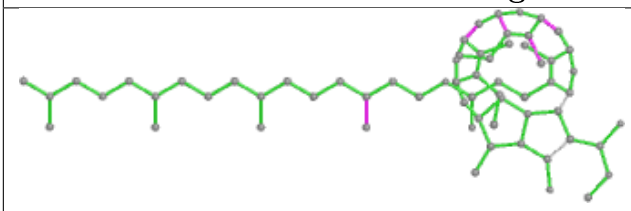

Bond lengths


Bond angles


Torsions


Rings

Ligand PHO BD 403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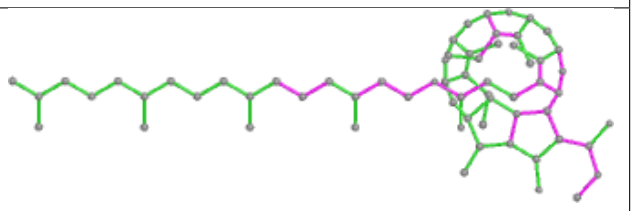
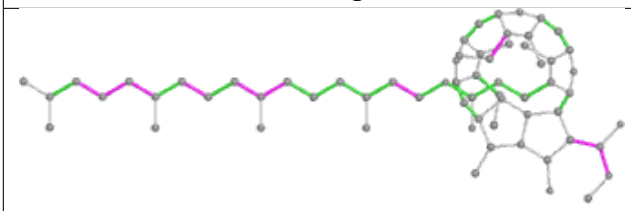
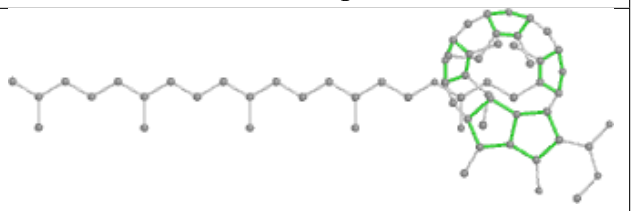
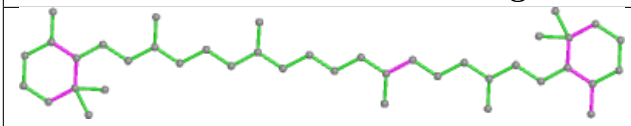
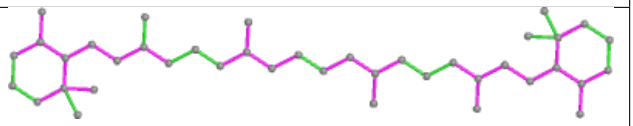

Bond angles

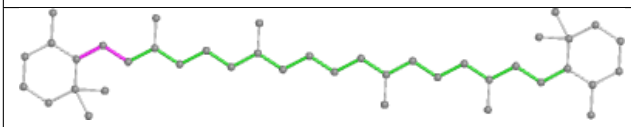

Torsions

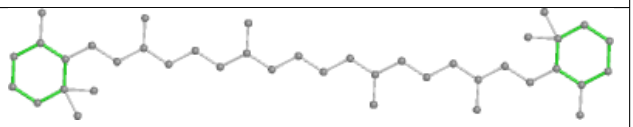

Rings

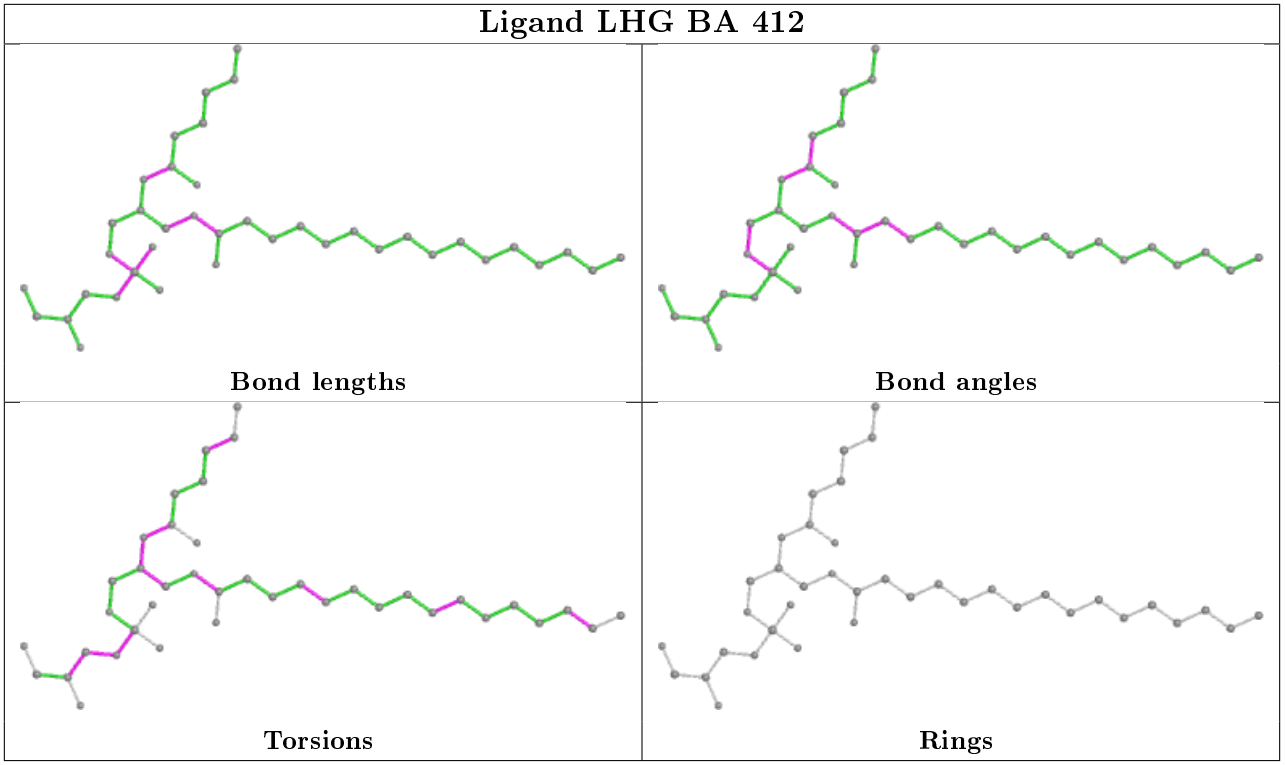
Ligand BCR BD 406

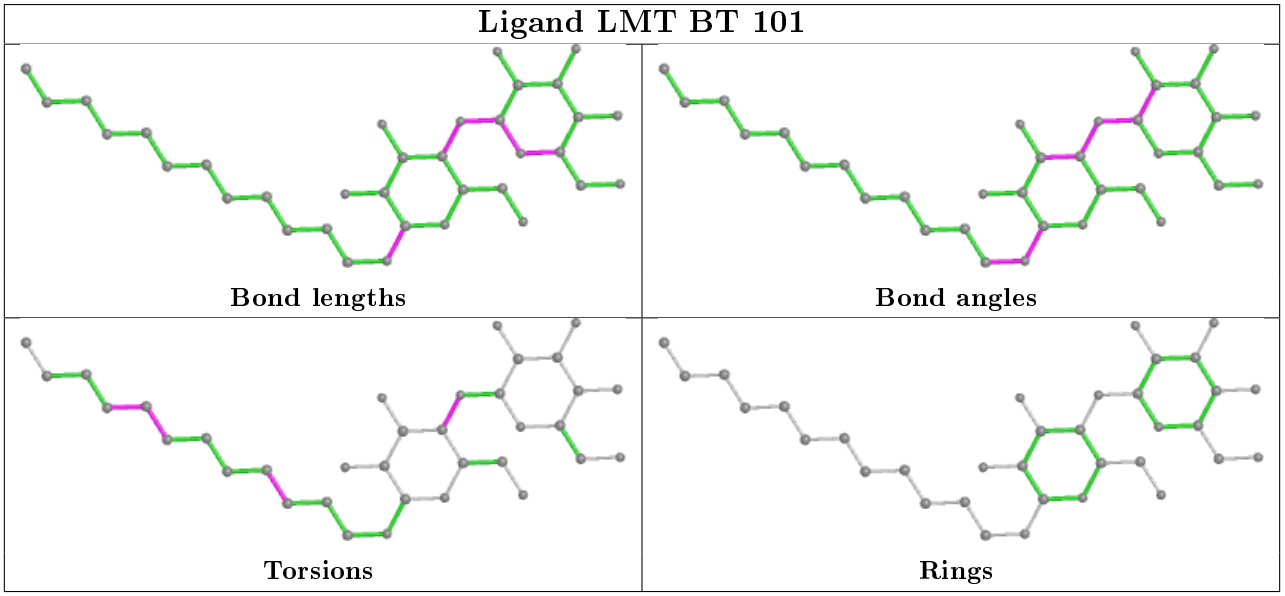

Bond lengths


Bond angles


Torsions


Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	335/344 (97%)	-0.44	7 (2%) 63 61	23, 59, 88, 103	0
1	BA	335/344 (97%)	-0.25	6 (1%) 68 67	47, 70, 89, 103	0
2	AB	490/510 (96%)	-0.24	7 (1%) 75 75	37, 63, 86, 99	0
2	BB	490/510 (96%)	-0.25	10 (2%) 65 63	41, 64, 87, 103	0
3	AC	447/473 (94%)	-0.19	11 (2%) 57 55	43, 72, 87, 102	0
3	BC	447/473 (94%)	0.05	19 (4%) 35 31	54, 83, 95, 101	0
4	AD	340/352 (96%)	-0.42	3 (0%) 84 84	29, 59, 84, 95	0
4	BD	340/352 (96%)	-0.32	5 (1%) 73 73	40, 69, 91, 101	0
5	AE	82/84 (97%)	0.10	6 (7%) 15 11	54, 75, 93, 99	0
5	BE	82/84 (97%)	0.50	8 (9%) 7 5	71, 85, 98, 104	0
6	AF	35/45 (77%)	-0.14	2 (5%) 23 19	56, 73, 94, 97	0
6	BF	35/45 (77%)	0.35	5 (14%) 2 2	75, 82, 97, 99	0
7	AH	65/66 (98%)	0.15	3 (4%) 32 29	57, 76, 92, 97	0
7	BH	65/66 (98%)	0.29	8 (12%) 4 3	62, 80, 91, 103	0
8	AI	35/38 (92%)	-0.08	3 (8%) 10 8	57, 70, 87, 94	0
8	BI	35/38 (92%)	-0.05	0 100 100	69, 80, 92, 95	0
9	AJ	34/40 (85%)	-0.41	0 100 100	65, 74, 83, 89	0
9	BJ	34/40 (85%)	-0.19	1 (2%) 51 47	73, 81, 93, 98	0
10	AK	37/37 (100%)	-0.36	1 (2%) 54 50	67, 75, 87, 93	0
10	BK	37/37 (100%)	0.01	2 (5%) 25 22	84, 90, 96, 101	0
11	AL	37/37 (100%)	0.19	6 (16%) 1 1	45, 60, 98, 107	0
11	BL	37/37 (100%)	0.25	5 (13%) 3 2	46, 62, 94, 102	0
12	AM	34/36 (94%)	-0.05	2 (5%) 22 18	51, 65, 94, 100	0
12	BM	34/36 (94%)	-0.17	2 (5%) 22 18	55, 61, 76, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AO	243/247 (98%)	0.08	13 (5%) 26 22	39, 70, 93, 107	0
13	BO	243/247 (98%)	0.21	17 (6%) 16 12	48, 76, 97, 107	0
14	AT	32/32 (100%)	0.11	3 (9%) 8 6	53, 63, 102, 104	0
14	BT	32/32 (100%)	-0.13	2 (6%) 20 16	57, 67, 93, 103	0
15	AU	97/104 (93%)	-0.06	1 (1%) 82 82	43, 63, 78, 86	0
15	BU	97/104 (93%)	-0.22	1 (1%) 82 82	55, 67, 77, 87	0
16	AV	137/137 (100%)	-0.22	1 (0%) 87 87	49, 66, 76, 79	0
16	BV	137/137 (100%)	0.13	8 (5%) 23 19	64, 79, 95, 102	0
17	Ay	28/46 (60%)	0.37	4 (14%) 2 2	79, 91, 97, 99	0
17	By	28/46 (60%)	0.42	3 (10%) 6 4	89, 98, 102, 106	0
18	AX	37/50 (74%)	-0.19	2 (5%) 25 22	70, 79, 93, 95	0
18	BX	37/50 (74%)	0.34	6 (16%) 1 1	75, 82, 91, 94	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.31	10 (16%) 1 1	76, 85, 103, 110	0
20	BZ	62/62 (100%)	0.66	12 (19%) 1 0	86, 96, 105, 110	0
All	All	5214/5536 (94%)	-0.12	205 (3%) 39 35	23, 71, 94, 110	0

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BH	65	LEU	8.6
12	AM	33	GLN	6.7
11	BL	1	MET	6.3
3	BC	473	ASP	6.2
14	AT	30	THR	6.0

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 carbohydrates 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
32	LMT	AB	627	35/35	0.47	0.54	73,103,106,107	0
32	LMT	AB	624	35/35	0.50	0.63	71,100,106,107	0
24	PL9	AJ	101	35/55	0.60	0.56	93,101,107,109	0
32	LMT	BI	102	35/35	0.62	0.56	90,104,106,106	0
30	LMG	AI	101	43/55	0.62	0.47	83,92,97,98	0
27	DGD	AD	410	63/66	0.63	0.54	91,97,107,108	0
27	DGD	BD	410	63/66	0.64	0.52	84,100,105,105	0
30	LMG	AC	520	45/55	0.65	0.42	75,92,97,98	0
29	SQD	BF	101	45/54	0.65	0.38	95,98,103,104	0
32	LMT	BD	411	31/35	0.65	0.50	67,91,99,100	0
32	LMT	BB	603	35/35	0.66	0.36	68,86,95,96	0
26	BCR	BJ	102	40/40	0.68	0.50	93,98,101,102	0
28	LHG	BC	521	37/49	0.68	0.49	90,100,113,114	0
28	LHG	AC	521	37/49	0.69	0.45	78,99,109,109	0
32	LMT	AT	101	35/35	0.69	0.34	72,91,97,98	0
25	OEC	BA	409	5/9	0.71	0.14	30,74,79,92	0
30	LMG	AB	623	42/55	0.71	0.36	70,89,92,93	0
26	BCR	AJ	102	40/40	0.71	0.41	85,91,101,102	0
27	DGD	BB	602	52/66	0.71	0.32	71,85,104,105	0
22	CLA	BB	604	65/65	0.71	0.35	86,98,107,109	0
24	PL9	BJ	101	35/55	0.71	0.44	78,99,111,112	0
32	LMT	BB	625	35/35	0.72	0.43	66,103,111,111	0
30	LMG	BC	520	45/55	0.72	0.48	86,93,101,102	0
29	SQD	AF	101	45/54	0.72	0.36	82,97,102,103	0
30	LMG	AA	416	42/55	0.73	0.37	67,92,96,99	0
30	LMG	BI	101	43/55	0.73	0.38	84,90,99,100	0
22	CLA	BB	619	65/65	0.74	0.29	75,81,93,95	0
22	CLA	AB	601	65/65	0.75	0.39	88,97,102,105	0
22	CLA	BA	407	65/65	0.75	0.35	72,76,103,104	0
32	LMT	AD	411	31/35	0.75	0.47	52,96,104,104	0
32	LMT	AB	625	35/35	0.75	0.43	82,98,100,101	0
29	SQD	BA	401	54/54	0.76	0.34	82,91,107,108	0
35	CA	BO	301	1/1	0.76	0.33	100,100,100,100	0
27	DGD	AA	410	56/66	0.76	0.32	78,86,91,92	0
27	DGD	BA	411	56/66	0.76	0.35	76,85,103,104	0
32	LMT	AI	102	35/35	0.77	0.49	74,92,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CA	AK	101	1/1	0.77	0.09	95,95,95,95	0
32	LMT	BB	626	35/35	0.77	0.31	76,93,101,102	0
22	CLA	AC	513	65/65	0.77	0.35	92,98,104,106	0
30	LMG	AE	102	44/55	0.78	0.34	81,91,96,96	0
26	BCR	AH	101	40/40	0.78	0.32	76,88,95,95	0
32	LMT	BT	101	35/35	0.78	0.34	77,91,94,95	0
30	LMG	AC	519	48/55	0.79	0.31	75,84,89,90	0
26	BCR	AZ	101	40/40	0.79	0.32	75,82,90,91	0
27	DGD	AB	626	52/66	0.79	0.30	79,94,105,107	0
26	BCR	BC	515	40/40	0.79	0.31	74,80,91,92	0
22	CLA	AA	406	65/65	0.79	0.31	54,60,89,90	0
32	LMT	BM	101	35/35	0.79	0.30	70,88,97,101	0
30	LMG	BM	102	42/55	0.79	0.31	72,90,95,98	0
22	CLA	AC	512	65/65	0.80	0.32	91,95,106,106	0
26	BCR	BX	101	40/40	0.80	0.30	76,79,89,90	0
30	LMG	AM	101	42/55	0.80	0.29	68,86,93,95	0
22	CLA	AB	616	65/65	0.80	0.27	73,85,105,106	0
29	SQD	BD	409	43/54	0.80	0.25	73,88,110,111	0
29	SQD	BA	413	51/54	0.81	0.25	73,90,103,104	0
26	BCR	BZ	101	40/40	0.81	0.28	81,90,93,94	0
30	LMG	BE	102	44/55	0.81	0.38	75,92,98,99	0
22	CLA	BC	512	65/65	0.81	0.31	95,99,109,110	0
22	CLA	AD	404	65/65	0.82	0.32	80,83,102,103	0
29	SQD	AD	409	43/54	0.82	0.24	68,92,108,111	0
22	CLA	BC	513	65/65	0.82	0.34	96,99,106,107	0
32	LMT	AM	102	35/35	0.83	0.30	67,89,93,96	0
22	CLA	BD	404	65/65	0.83	0.27	89,92,101,102	0
22	CLA	BB	609	65/65	0.83	0.26	72,80,96,96	0
22	CLA	AB	606	65/65	0.84	0.26	73,87,96,96	0
29	SQD	AA	415	54/54	0.84	0.27	71,87,105,105	0
29	SQD	AA	412	51/54	0.84	0.23	73,83,98,99	0
29	SQD	BL	101	47/54	0.84	0.25	75,91,115,116	0
26	BCR	BK	102	40/40	0.84	0.35	76,81,85,85	0
26	BCR	AK	102	40/40	0.85	0.30	73,77,81,81	0
35	CA	BK	101	1/1	0.85	0.13	90,90,90,90	0
24	PL9	AA	407	45/55	0.85	0.32	83,87,94,95	0
30	LMG	BD	408	48/55	0.86	0.25	68,75,85,87	0
22	CLA	AC	506	65/65	0.86	0.22	83,87,101,102	0
24	PL9	BA	408	45/55	0.86	0.30	82,88,90,92	0
27	DGD	BC	518	66/66	0.86	0.25	71,78,89,90	0
30	LMG	BC	519	48/55	0.86	0.31	83,90,94,95	0
27	DGD	BC	517	62/66	0.86	0.22	78,82,100,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	BC	506	65/65	0.86	0.24	81,85,97,99	0
30	LMG	AB	621	49/55	0.87	0.23	62,75,80,83	0
30	LMG	BD	407	46/55	0.87	0.24	70,80,92,94	0
22	CLA	AC	507	65/65	0.87	0.27	83,90,95,97	0
22	CLA	BB	612	65/65	0.88	0.28	82,89,92,95	0
30	LMG	BB	623	49/55	0.88	0.23	70,78,88,91	0
26	BCR	AB	620	40/40	0.88	0.24	75,77,83,84	0
29	SQD	BB	601	47/54	0.88	0.23	74,87,109,111	0
26	BCR	BD	406	40/40	0.88	0.23	66,78,92,92	0
30	LMG	AA	413	51/55	0.88	0.24	70,74,77,79	0
26	BCR	AC	515	40/40	0.89	0.22	69,75,80,81	0
27	DGD	AC	516	53/66	0.89	0.23	57,72,91,92	0
27	DGD	AC	517	62/66	0.89	0.22	70,78,91,92	0
22	CLA	AC	511	65/65	0.89	0.25	77,85,89,90	0
22	CLA	BC	511	65/65	0.89	0.25	91,99,104,105	0
22	CLA	AB	604	65/65	0.89	0.25	67,73,91,91	0
22	CLA	AB	609	65/65	0.89	0.26	76,87,91,92	0
22	CLA	BC	507	65/65	0.89	0.24	84,92,96,97	0
27	DGD	AC	518	66/66	0.89	0.22	62,68,84,86	0
22	CLA	BC	508	65/65	0.89	0.24	92,97,101,106	0
27	DGD	BC	516	53/66	0.90	0.23	69,77,96,97	0
30	LMG	AD	408	48/55	0.90	0.23	63,68,74,80	0
30	LMG	BA	414	51/55	0.90	0.20	62,71,78,80	0
26	BCR	AB	618	40/40	0.90	0.20	75,78,82,83	0
22	CLA	AC	504	65/65	0.90	0.23	78,86,107,107	0
26	BCR	BC	514	40/40	0.90	0.24	81,83,87,87	0
28	LHG	AA	411	39/49	0.90	0.22	63,68,76,78	0
30	LMG	AB	622	49/55	0.90	0.19	64,73,80,83	0
22	CLA	BC	505	65/65	0.90	0.22	88,93,94,95	0
22	CLA	AB	614	65/65	0.91	0.23	78,85,98,99	0
30	LMG	BB	624	49/55	0.91	0.18	68,72,78,79	0
22	CLA	AB	610	65/65	0.91	0.21	60,67,79,80	0
22	CLA	BC	503	65/65	0.91	0.20	82,97,100,101	0
22	CLA	BB	618	65/65	0.91	0.21	69,84,87,88	0
22	CLA	AC	508	65/65	0.91	0.21	80,86,99,101	0
27	DGD	BH	101	58/66	0.91	0.19	66,73,80,81	0
22	CLA	BC	502	65/65	0.91	0.21	81,85,101,103	0
35	CA	AO	301	1/1	0.91	0.23	87,87,87,87	0
26	BCR	AC	514	40/40	0.91	0.22	56,66,73,74	0
28	LHG	BA	412	39/49	0.91	0.23	72,77,80,81	0
26	BCR	AB	619	40/40	0.91	0.18	62,70,82,83	0
34	HEM	BE	101	43/43	0.92	0.28	93,95,104,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	BB	613	65/65	0.92	0.22	69,77,82,84	0
22	CLA	AB	615	65/65	0.92	0.21	83,93,97,99	0
26	BCR	BB	622	40/40	0.92	0.25	67,71,79,80	0
22	CLA	BC	504	65/65	0.92	0.19	87,92,102,102	0
26	BCR	BA	410	40/40	0.92	0.20	61,74,82,83	0
22	CLA	BB	617	65/65	0.92	0.22	75,79,99,100	0
22	CLA	BC	510	65/65	0.92	0.22	79,83,92,92	0
30	LMG	AD	407	46/55	0.92	0.20	63,71,90,92	0
27	DGD	AH	102	58/66	0.92	0.19	57,72,85,86	0
26	BCR	BB	621	40/40	0.92	0.19	57,69,82,83	0
26	BCR	AA	409	40/40	0.92	0.20	59,67,70,71	0
22	CLA	BC	509	65/65	0.92	0.22	73,83,93,94	0
26	BCR	BB	620	40/40	0.92	0.20	66,69,72,73	0
26	BCR	AT	102	40/40	0.92	0.21	72,79,91,91	0
24	PL9	AD	405	55/55	0.93	0.21	52,67,71,73	0
22	CLA	AB	608	65/65	0.93	0.19	72,79,87,91	0
22	CLA	BC	501	65/65	0.93	0.20	76,80,87,88	0
31	CL	BA	415	1/1	0.93	0.30	81,81,81,81	0
24	PL9	BD	405	55/55	0.93	0.21	63,70,76,78	0
22	CLA	AC	505	65/65	0.93	0.20	69,73,77,79	0
34	HEM	AE	101	43/43	0.93	0.28	85,92,103,106	0
26	BCR	AB	617	40/40	0.93	0.17	56,67,75,76	0
22	CLA	AA	404	65/65	0.93	0.21	63,72,97,99	0
25	OEC	AA	408	5/9	0.93	0.14	56,62,67,75	0
23	PHO	BD	403	64/64	0.93	0.23	77,88,92,93	0
22	CLA	BB	607	65/65	0.93	0.19	53,64,86,87	0
22	CLA	AB	612	65/65	0.93	0.21	63,75,81,83	0
22	CLA	BB	606	65/65	0.93	0.19	58,61,74,76	0
26	BCR	AD	406	40/40	0.94	0.16	64,72,85,85	0
22	CLA	AC	503	65/65	0.94	0.22	78,86,92,95	0
22	CLA	AB	602	65/65	0.94	0.23	81,85,88,90	0
22	CLA	AB	611	65/65	0.94	0.19	62,68,71,73	0
22	CLA	BA	405	65/65	0.94	0.20	72,76,104,105	0
23	PHO	AD	403	64/64	0.94	0.18	39,56,70,72	0
22	CLA	AB	603	65/65	0.94	0.17	54,60,72,74	0
22	CLA	AD	402	65/65	0.94	0.21	47,58,69,71	0
31	CL	AA	414	1/1	0.94	0.63	73,73,73,73	0
22	CLA	BB	605	65/65	0.94	0.20	77,82,86,89	0
22	CLA	BB	615	65/65	0.94	0.18	60,72,77,81	0
22	CLA	AB	605	65/65	0.94	0.21	68,76,84,85	0
23	PHO	AA	405	64/64	0.95	0.16	40,64,67,69	0
22	CLA	AB	613	65/65	0.95	0.18	65,69,84,87	0

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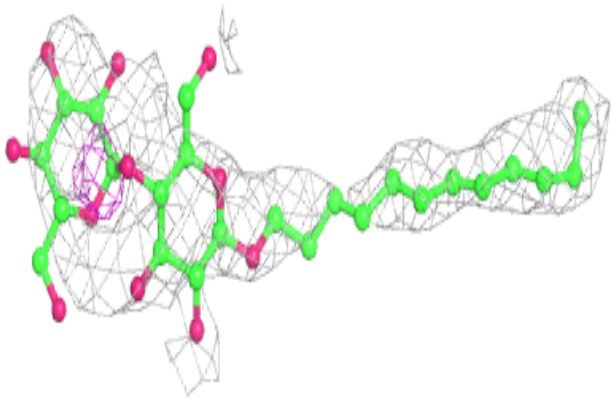
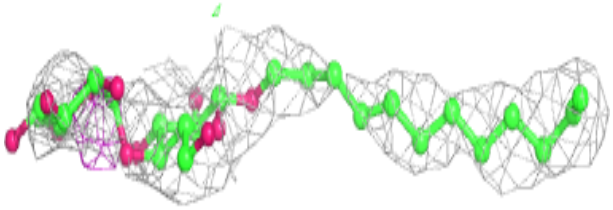
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	BB	614	65/65	0.95	0.16	59,68,75,77	0
22	CLA	AC	502	65/65	0.95	0.16	50,58,81,84	0
22	CLA	AB	607	65/65	0.95	0.14	50,55,74,74	0
22	CLA	BB	608	65/65	0.95	0.19	45,53,76,78	0
33	BCT	BD	401	4/4	0.95	0.20	84,86,87,88	0
22	CLA	BA	404	65/65	0.95	0.16	55,60,68,70	0
22	CLA	AC	501	65/65	0.95	0.20	78,83,85,86	0
22	CLA	BA	403	65/65	0.95	0.17	57,64,71,75	0
22	CLA	AC	509	65/65	0.95	0.20	59,74,86,89	0
23	PHO	BA	406	64/64	0.95	0.17	54,61,70,74	0
22	CLA	BB	611	65/65	0.95	0.17	67,74,81,85	0
22	CLA	BB	616	65/65	0.95	0.15	49,54,79,82	0
22	CLA	AA	403	65/65	0.95	0.16	41,48,56,60	0
22	CLA	BB	610	65/65	0.95	0.17	60,70,77,81	0
34	HEM	BV	201	43/43	0.96	0.19	58,67,76,79	0
22	CLA	AA	402	65/65	0.96	0.17	51,58,66,69	0
22	CLA	BD	402	65/65	0.96	0.17	50,57,79,83	0
22	CLA	AC	510	65/65	0.96	0.14	48,56,70,72	0
34	HEM	AV	201	43/43	0.96	0.20	60,63,66,67	0
33	BCT	AD	401	4/4	0.97	0.18	90,91,91,92	0
21	FE2	AA	401	1/1	0.98	0.12	69,69,69,69	0
21	FE2	BA	402	1/1	0.98	0.12	81,81,81,81	0

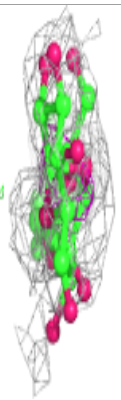
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT AB 627:

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

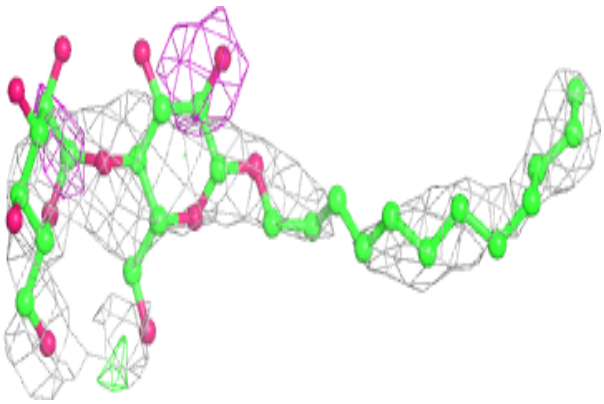


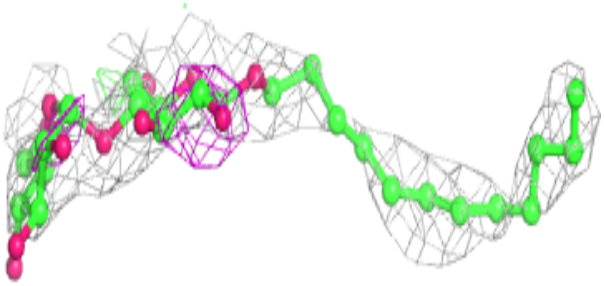


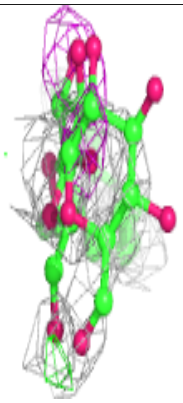


Electron density around LMT AB 624:

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

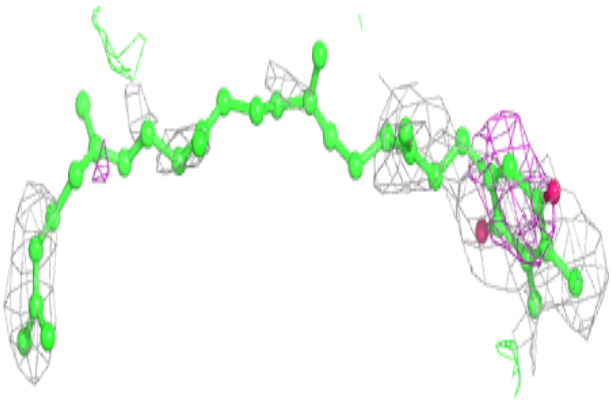


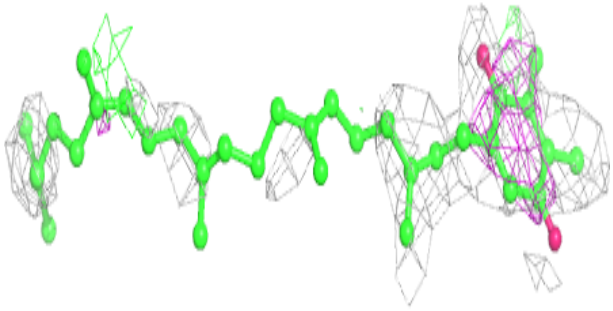


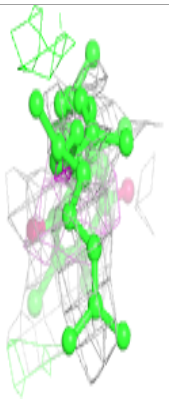


Electron density around PL9 AJ 101:

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

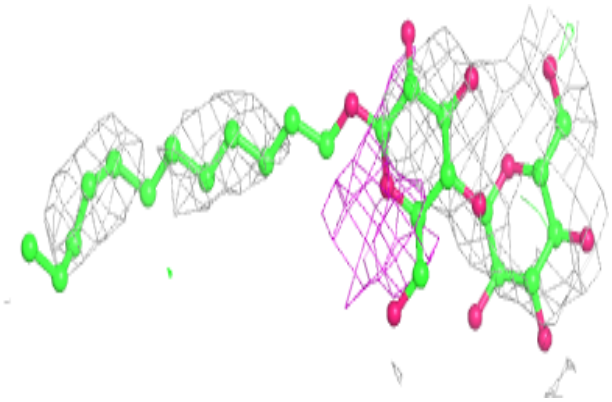


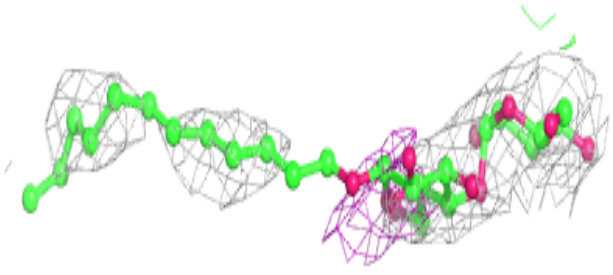


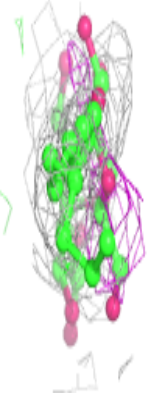


Electron density around LMT BI 102:

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

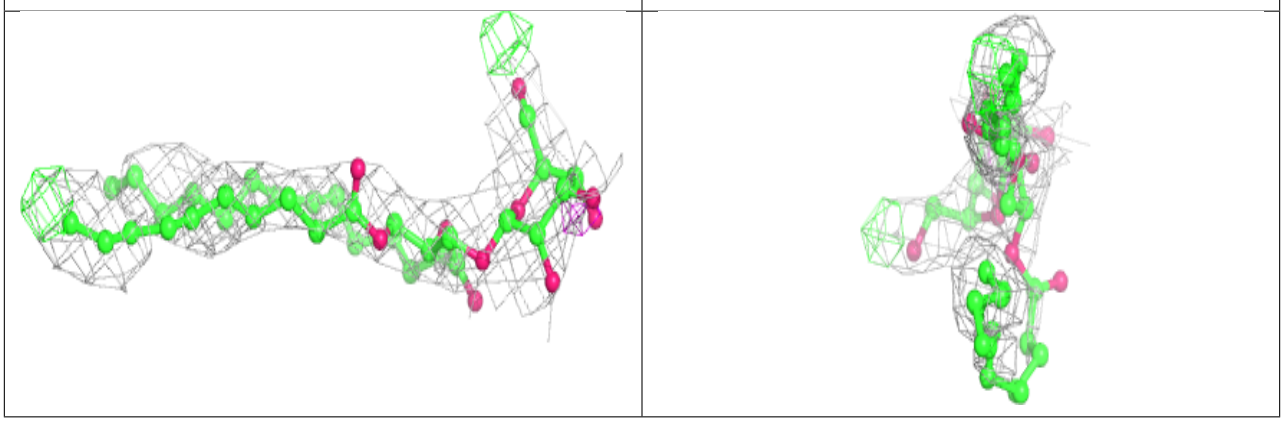






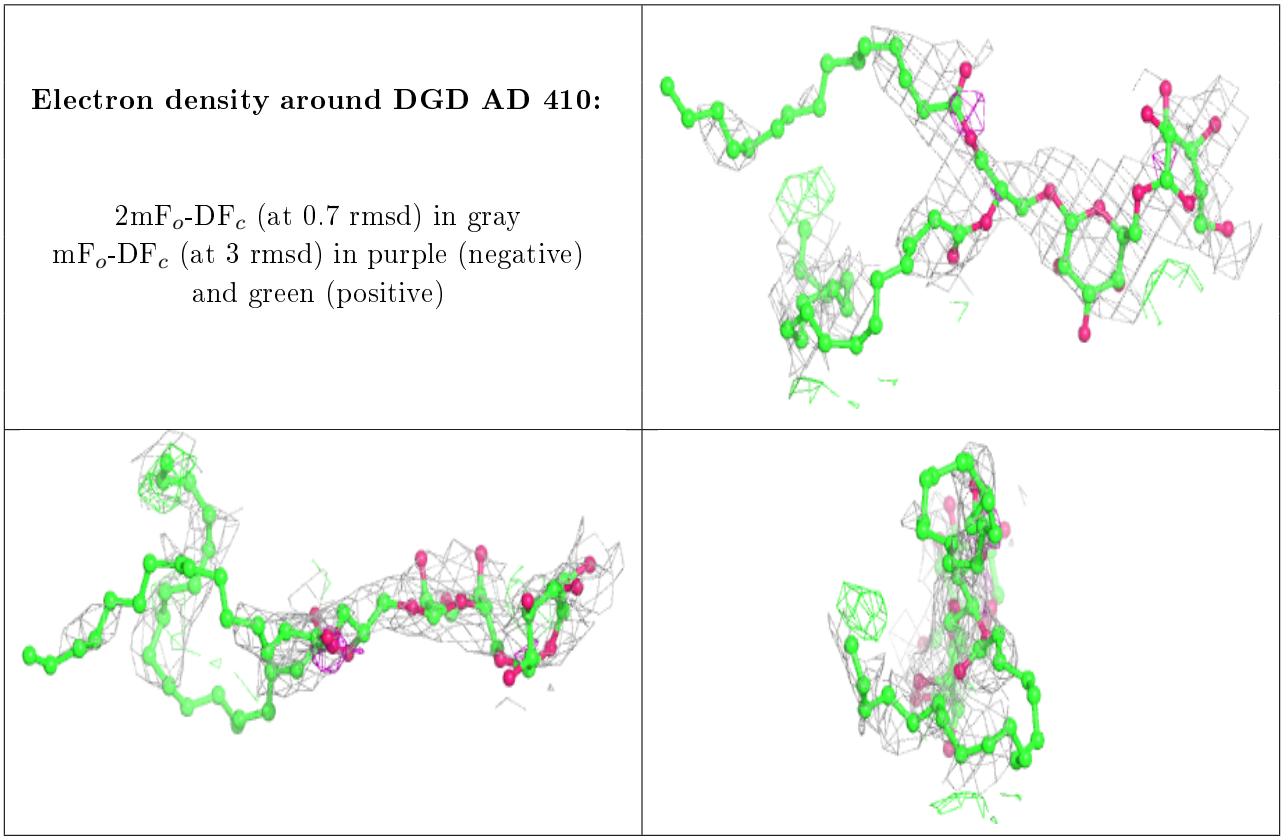
Electron density around LMG AI 101:

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



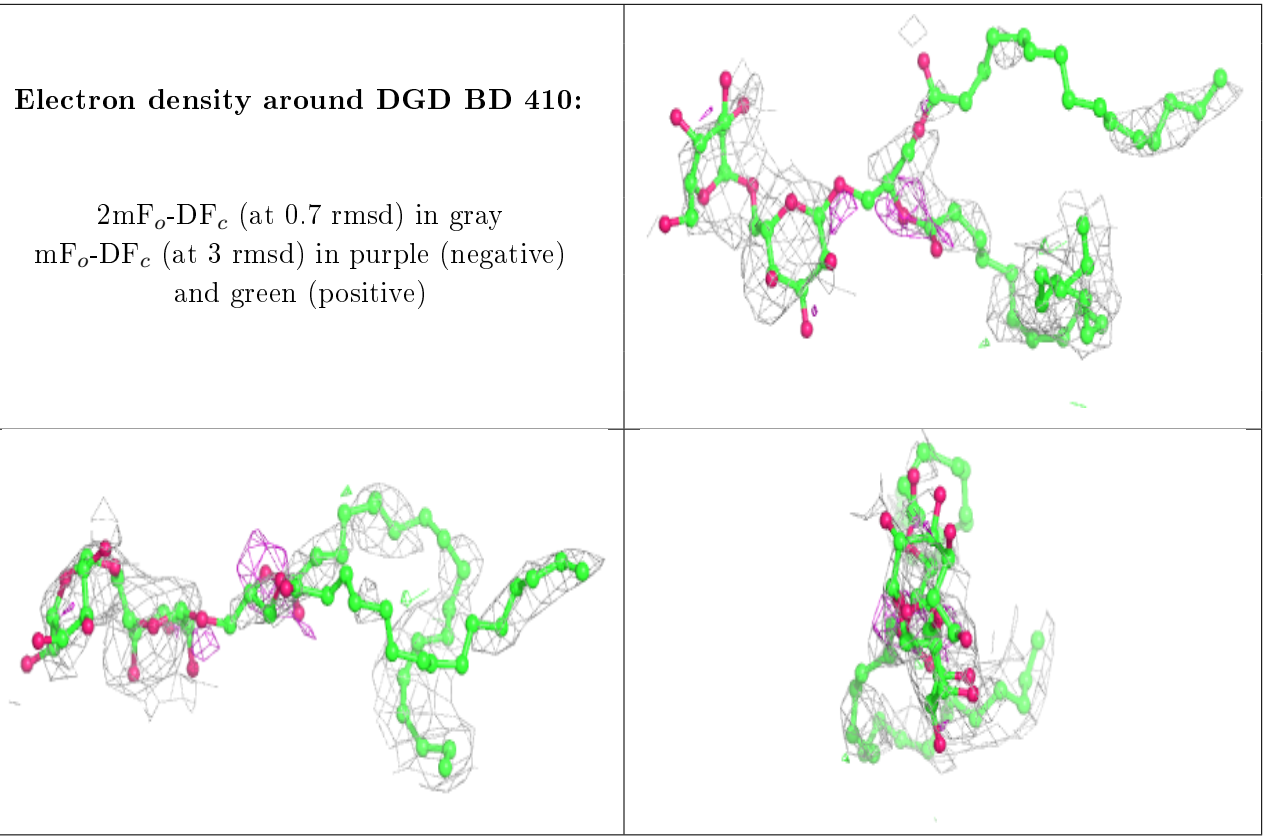
Electron density around DGD AD 410:

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



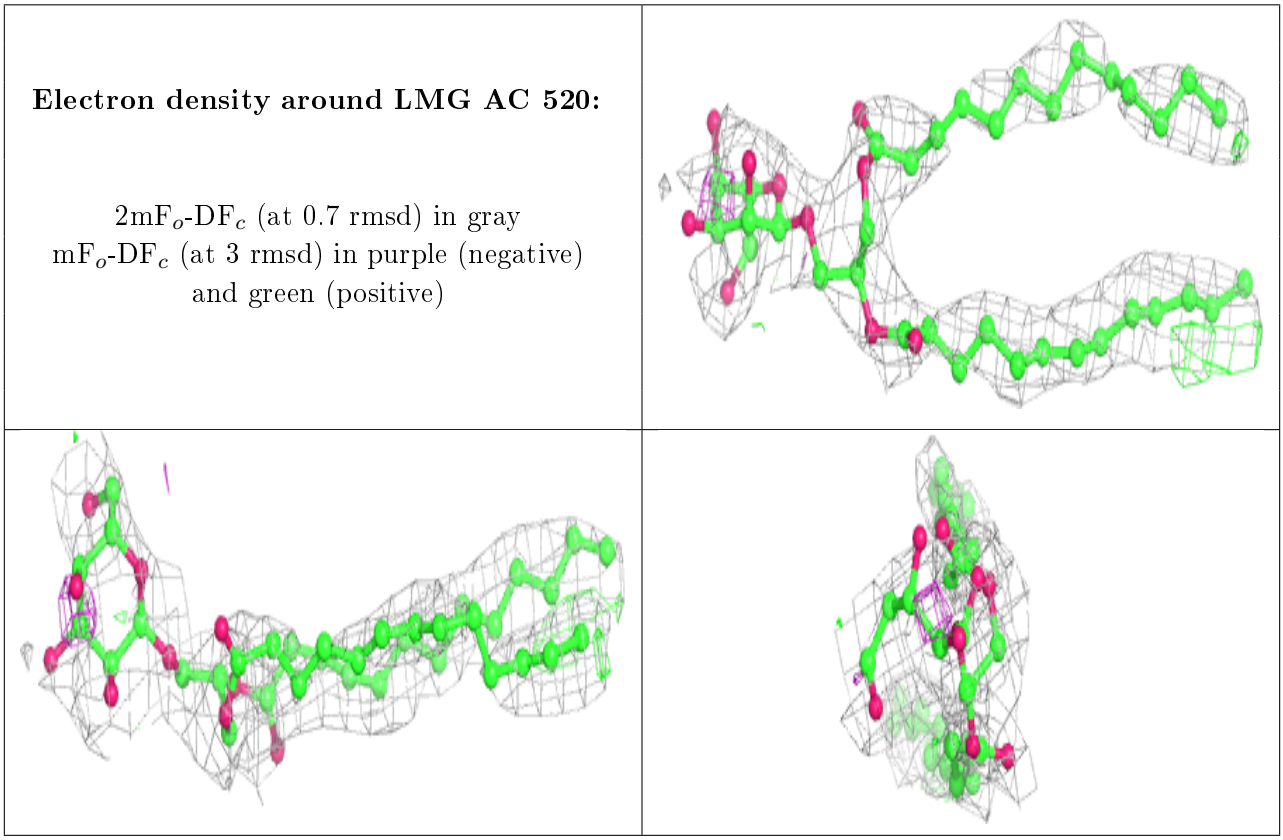
Electron density around DGD BD 410:

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



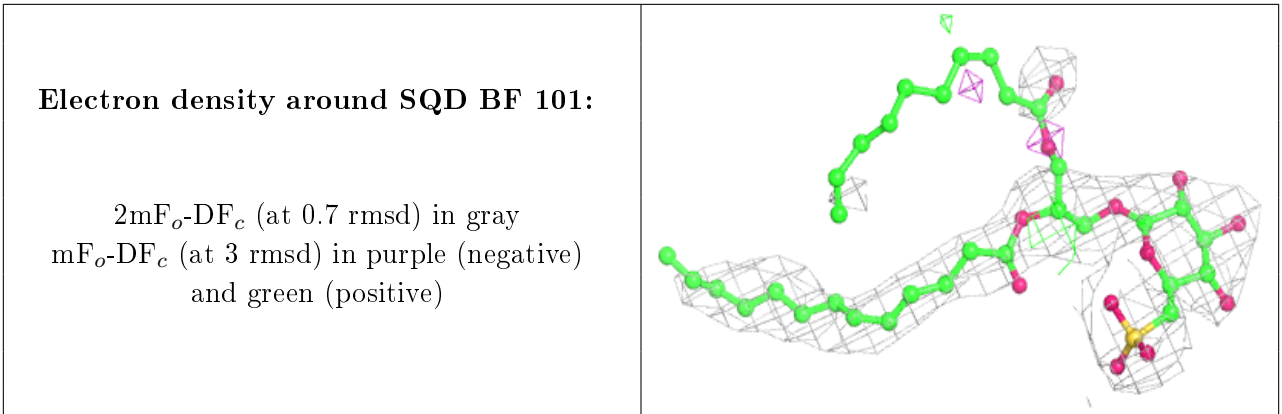
Electron density around LMG AC 520:

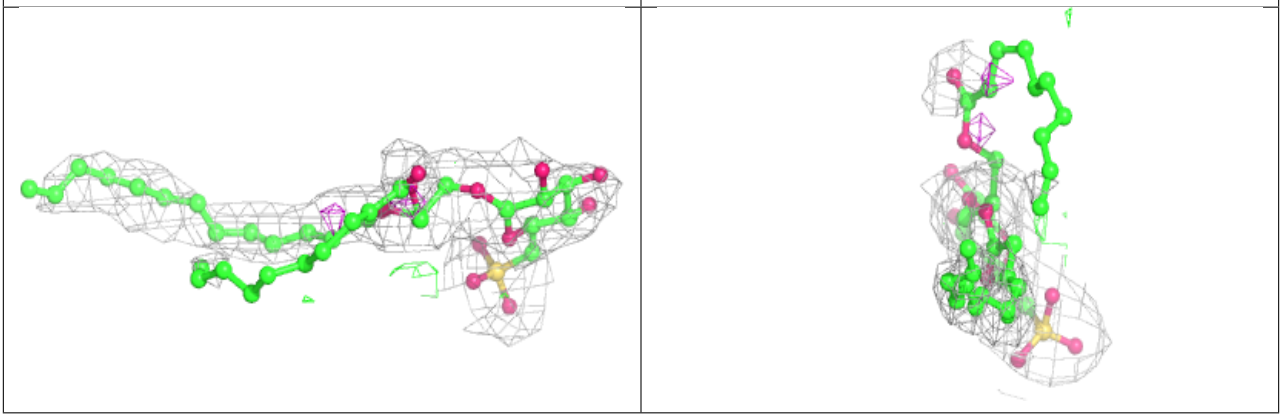
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD BF 101:

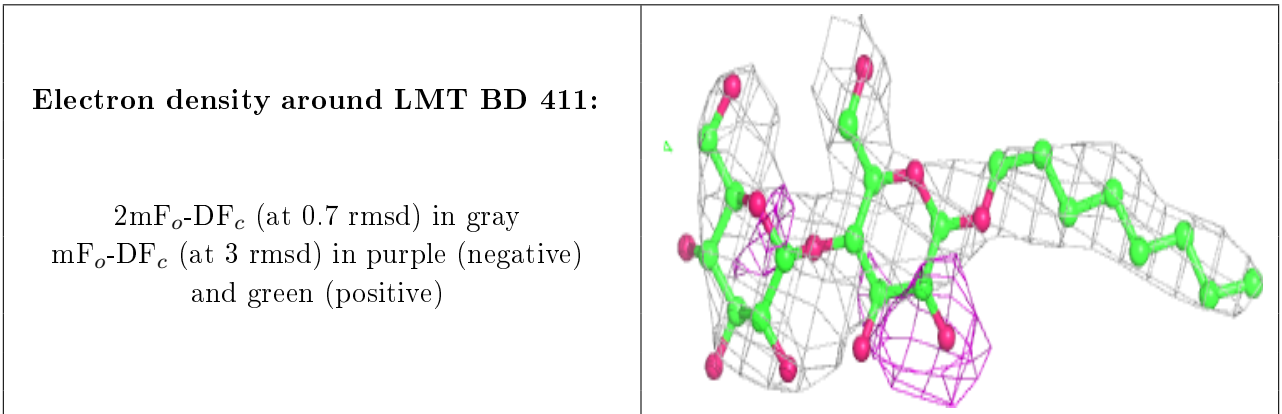
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

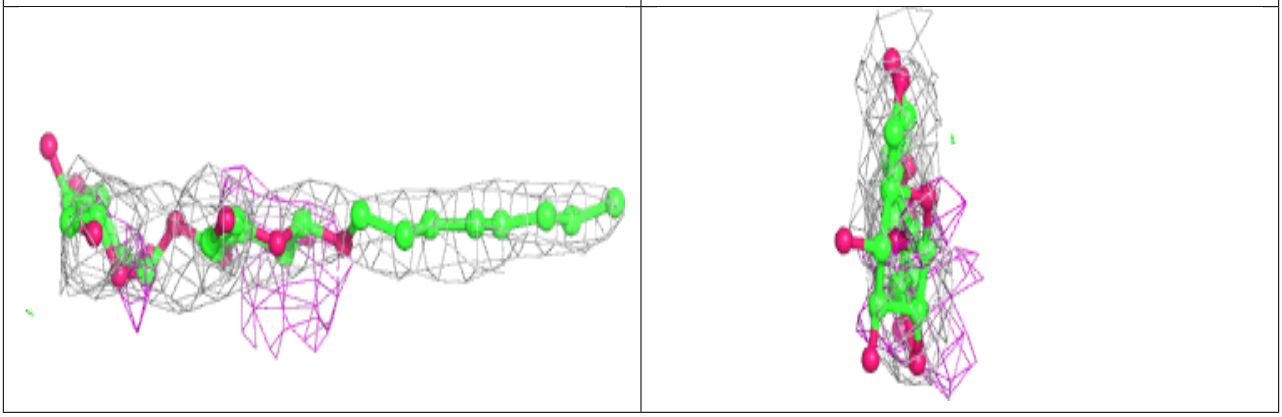




Electron density around LMT BD 411:

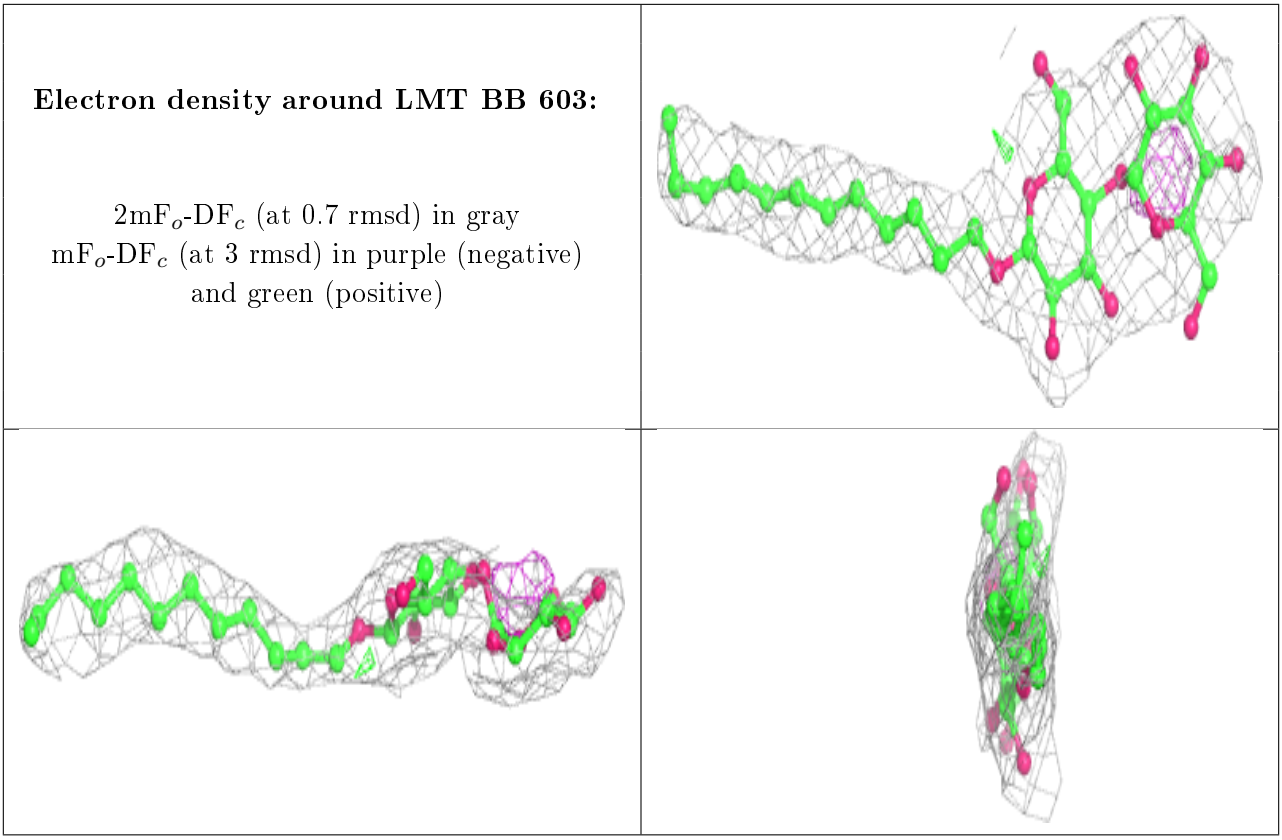
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





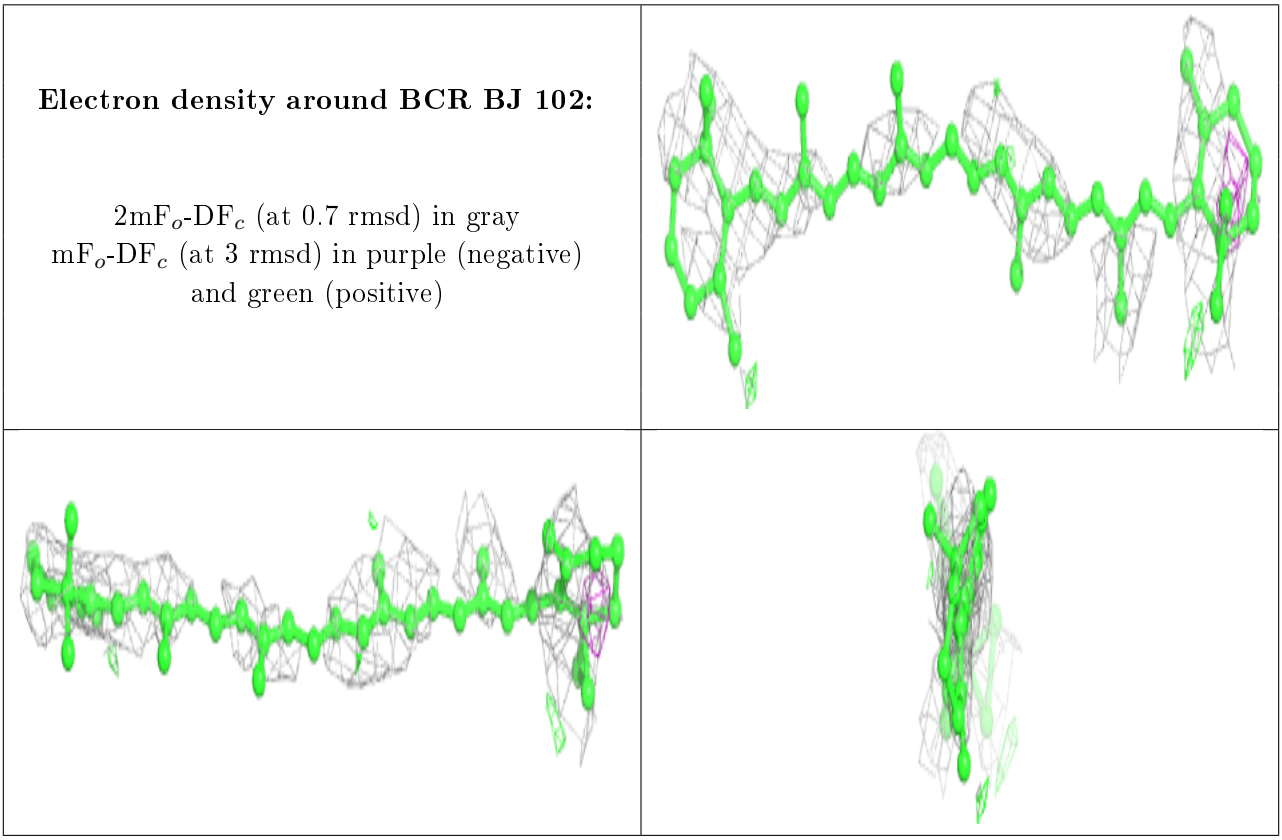
Electron density around LMT BB 603:

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



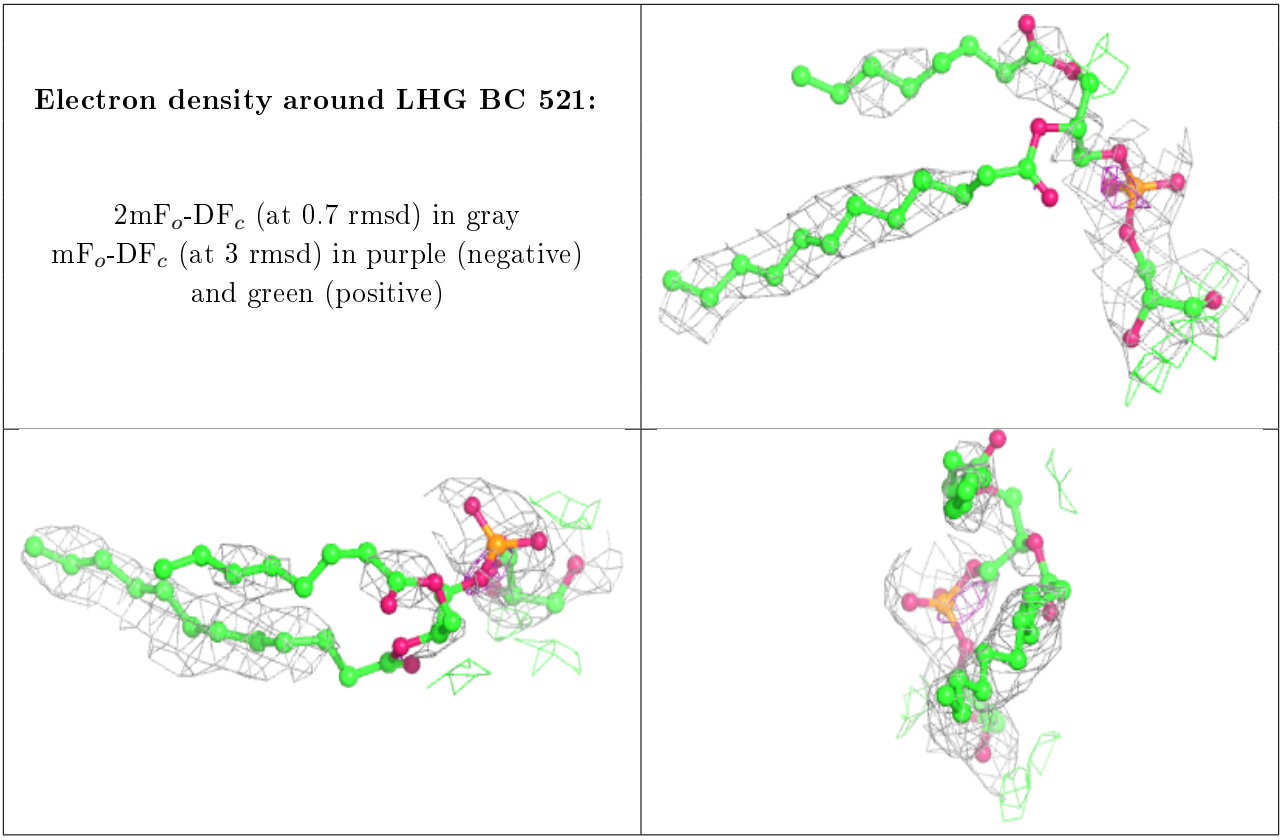
Electron density around BCR BJ 102:

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



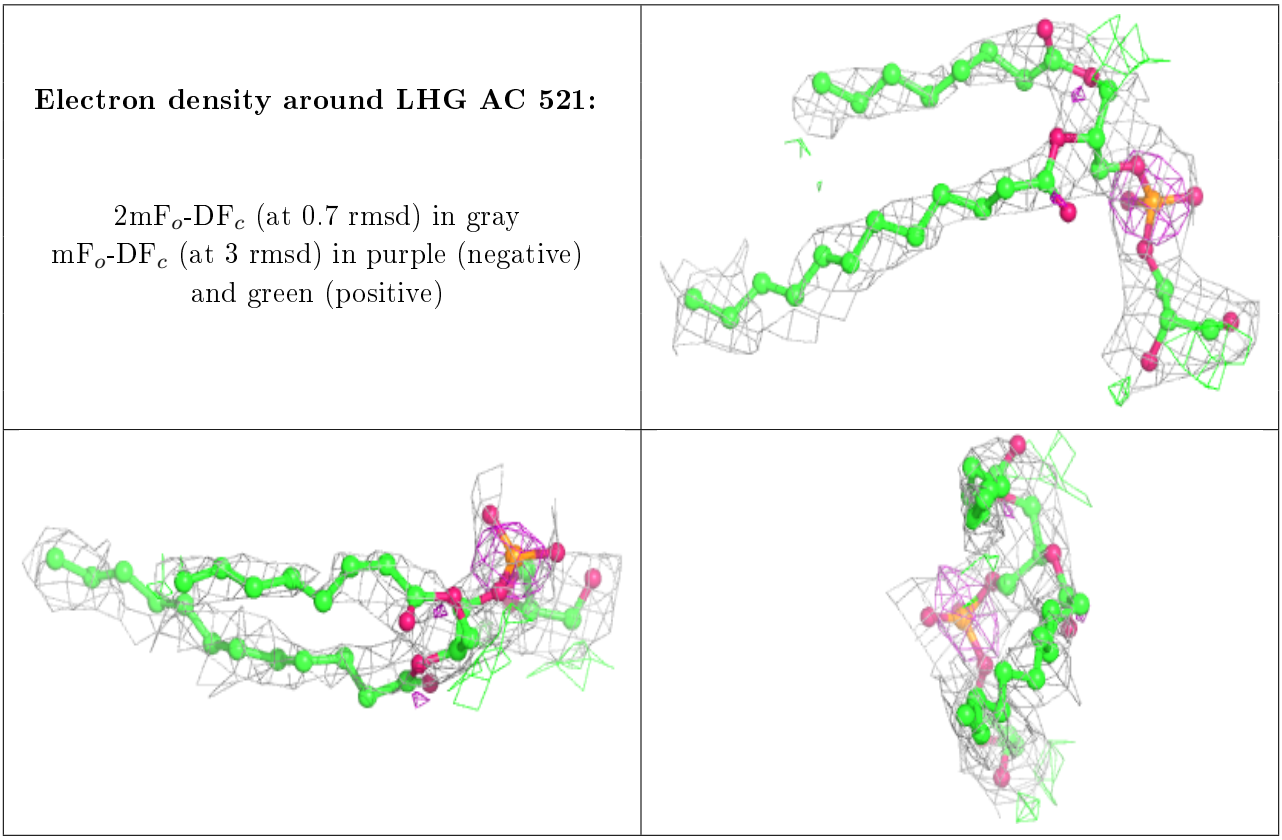
Electron density around LHG BC 521:

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



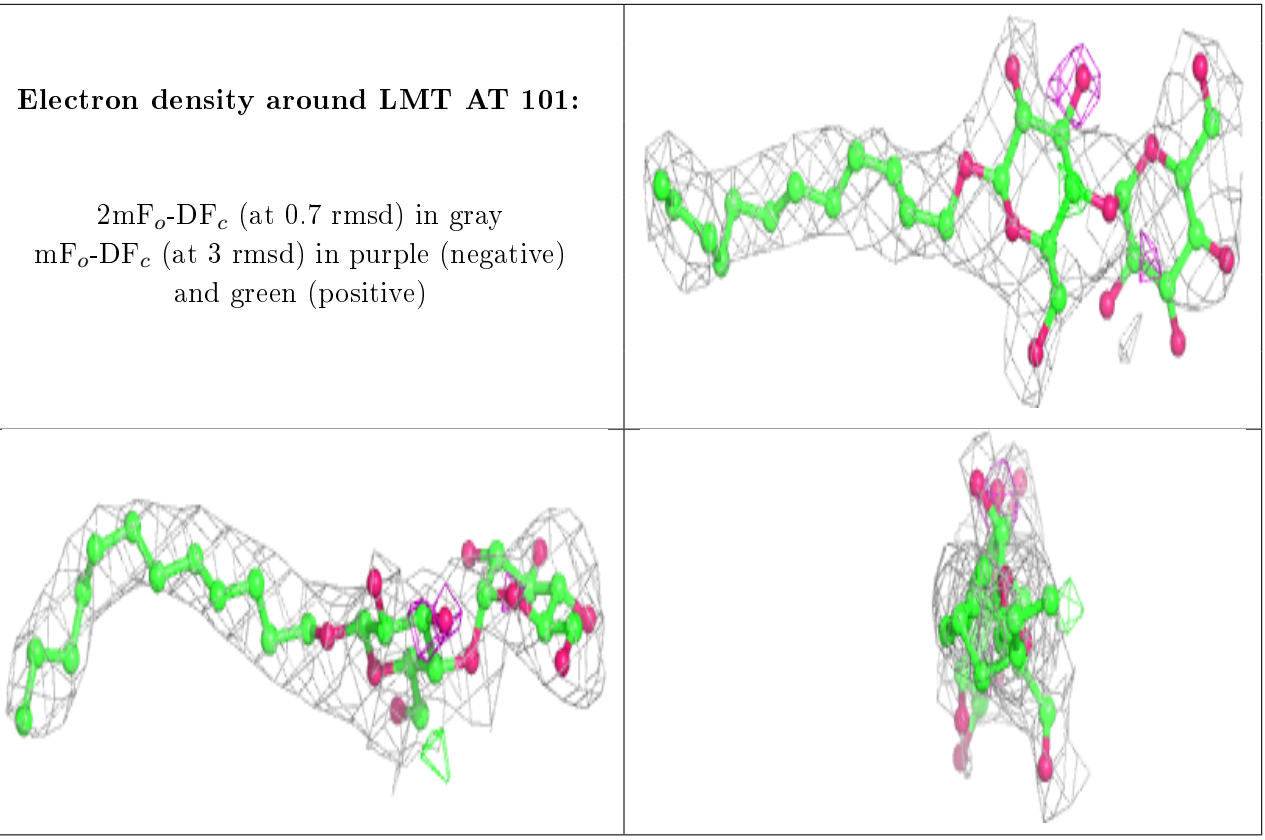
Electron density around LHG AC 521:

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



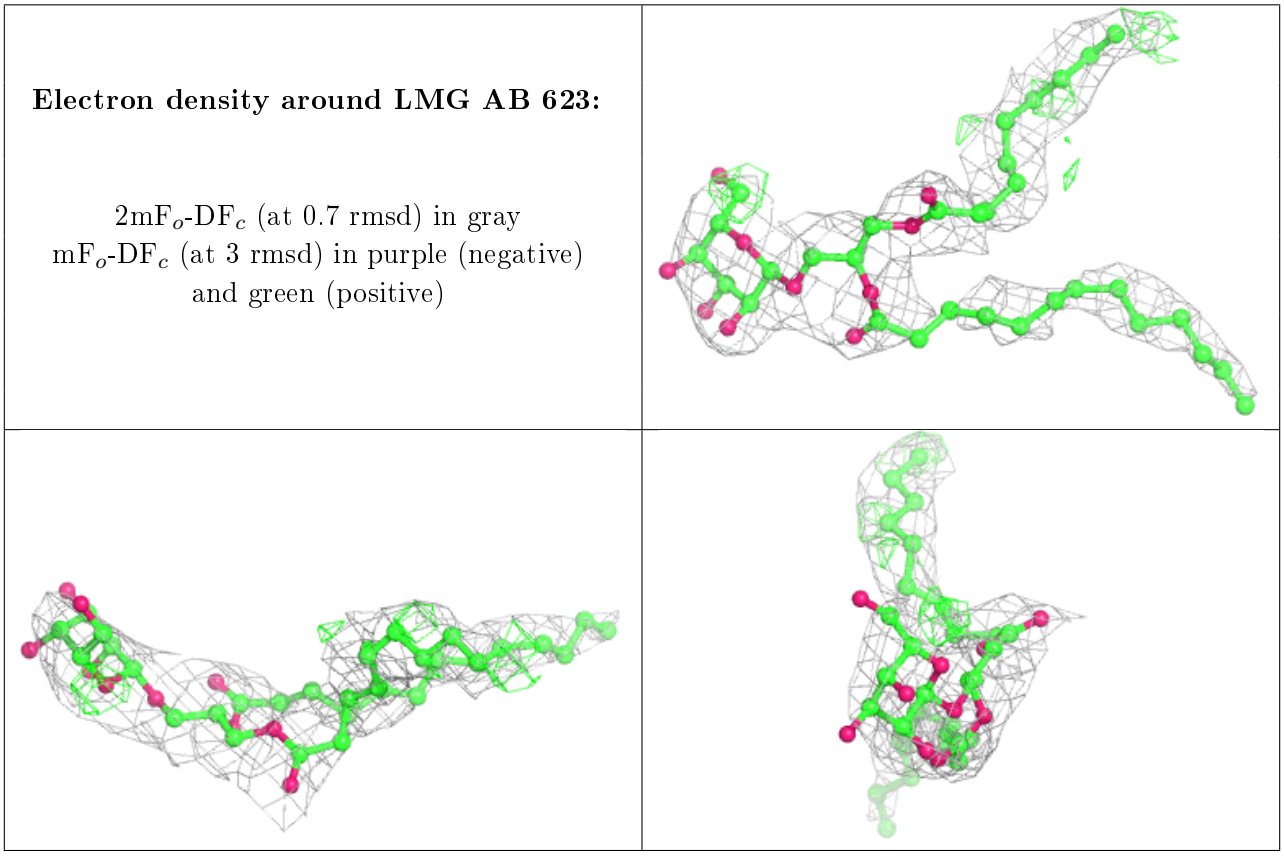
Electron density around LMT AT 101:

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



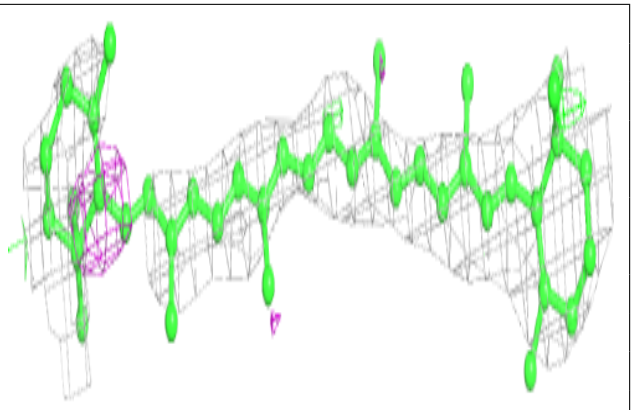
Electron density around LMG AB 623:

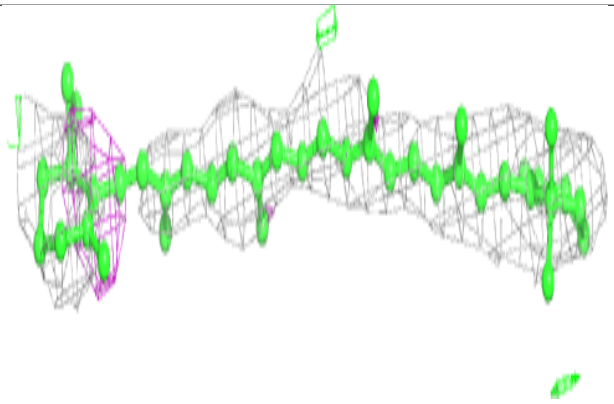
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

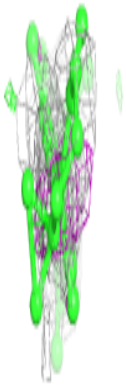


Electron density around BCR AJ 102:

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

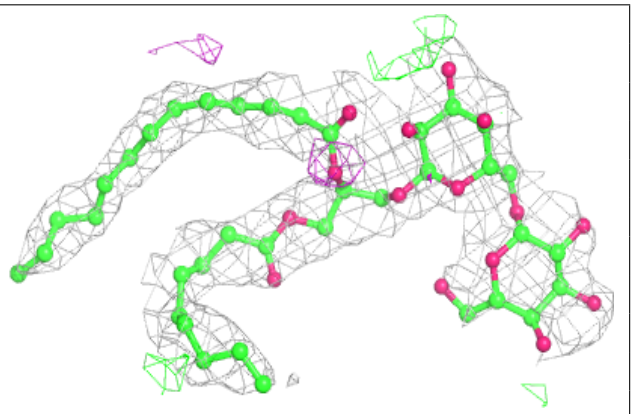


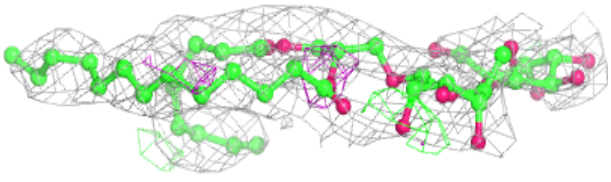


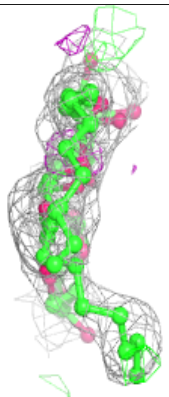


Electron density around DGD BB 602:

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

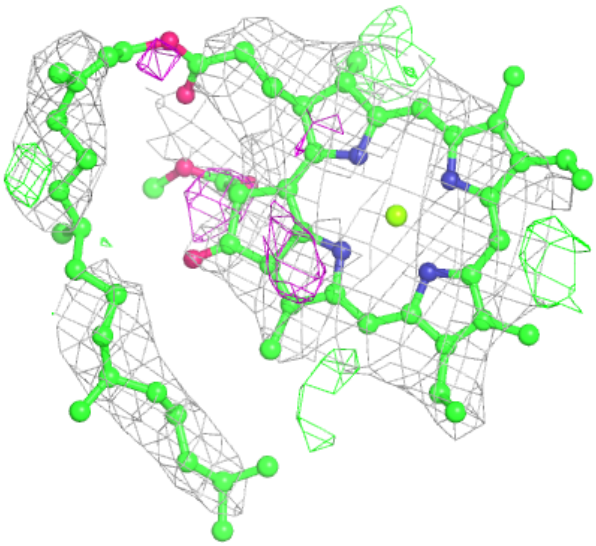


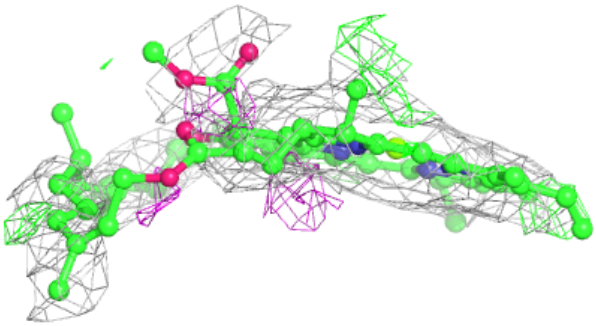


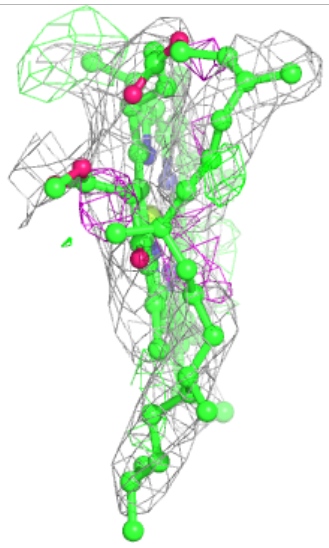


Electron density around CLA BB 604:

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

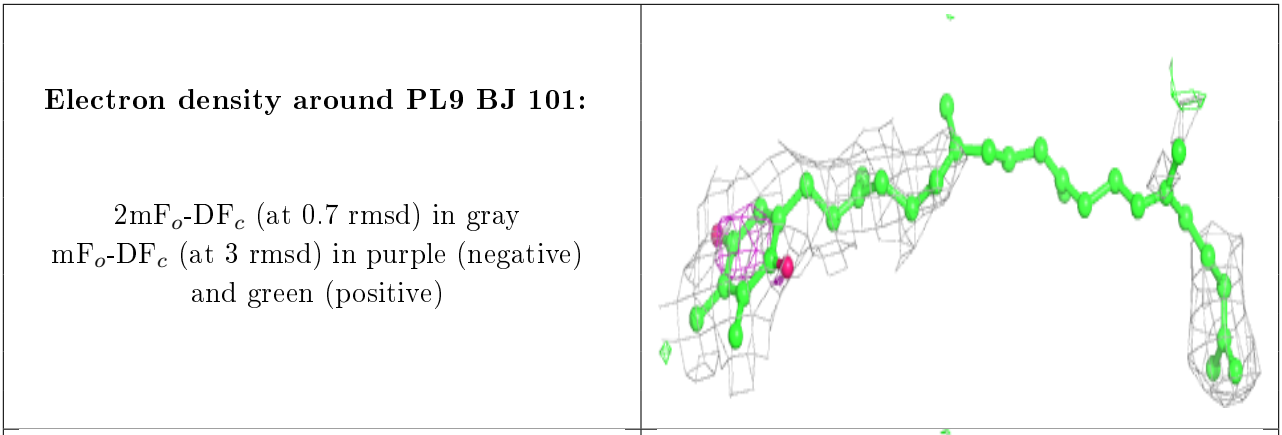






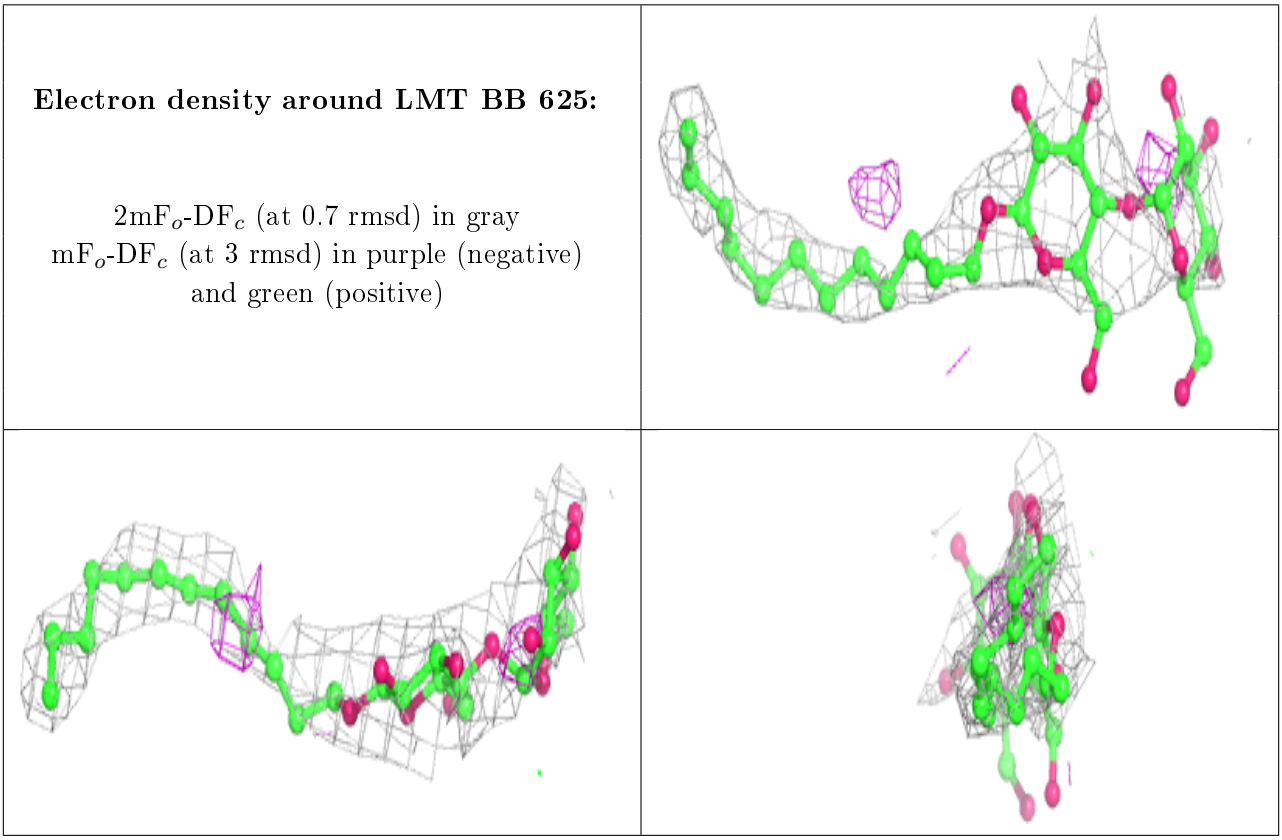
Electron density around PL9 BJ 101:

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



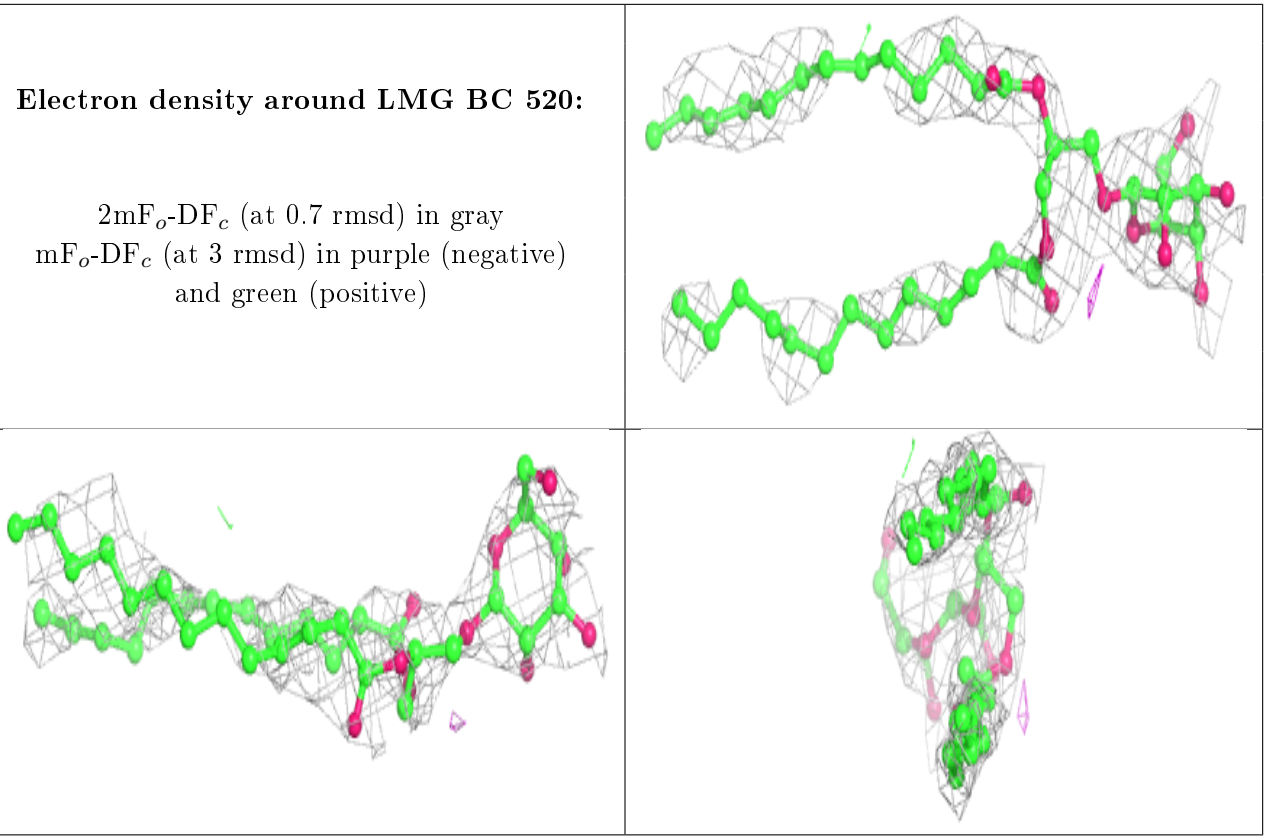
Electron density around LMT BB 625:

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



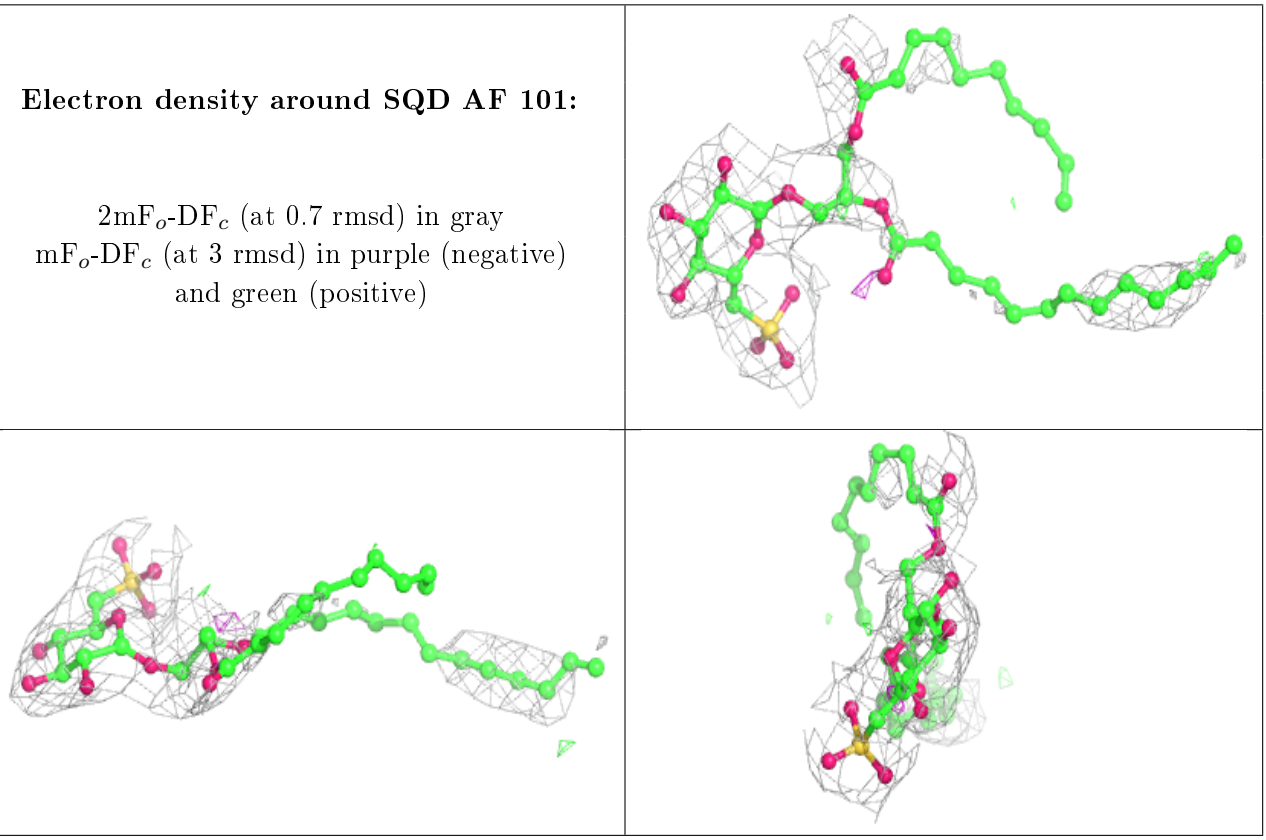
Electron density around LMG BC 520:

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



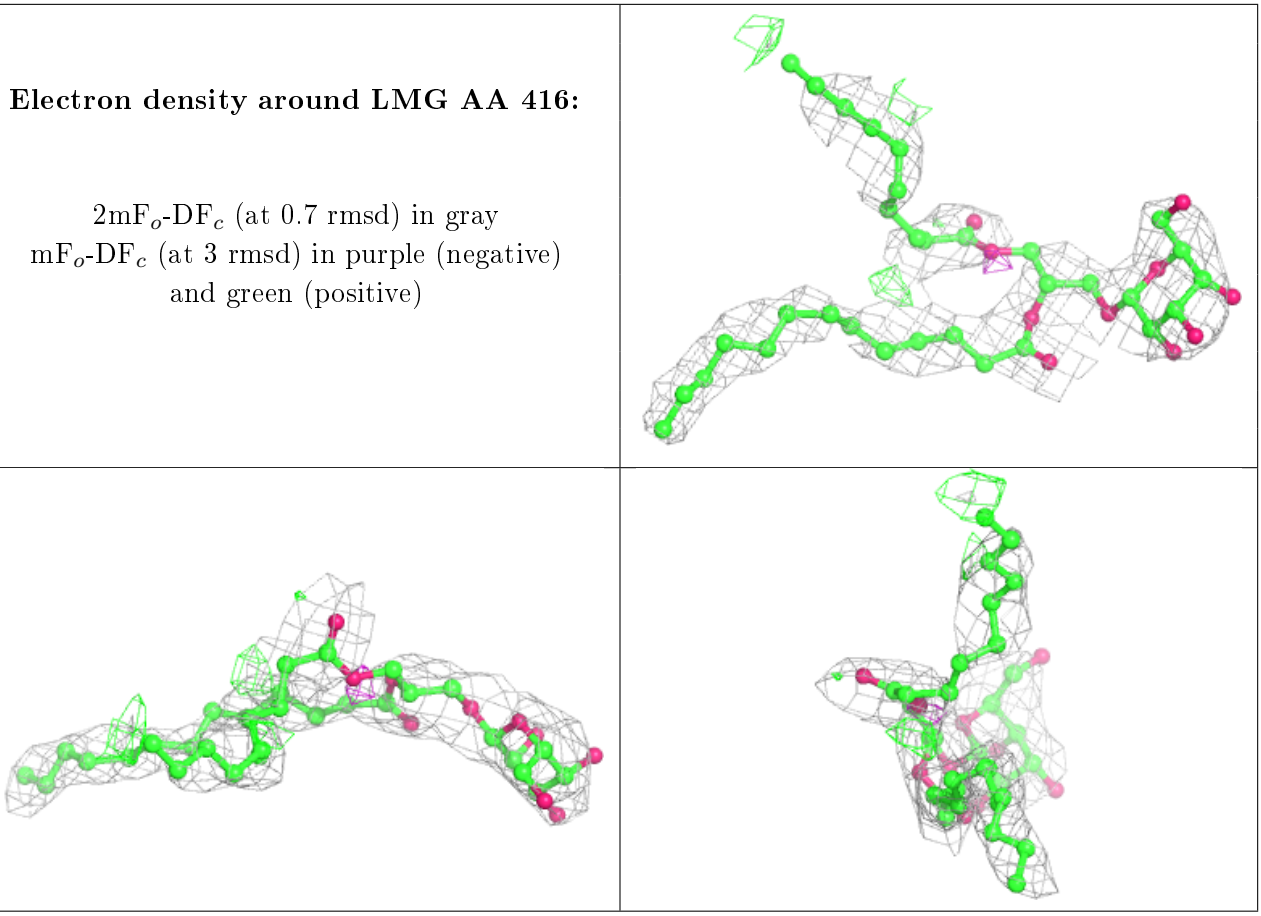
Electron density around SQD AF 101:

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



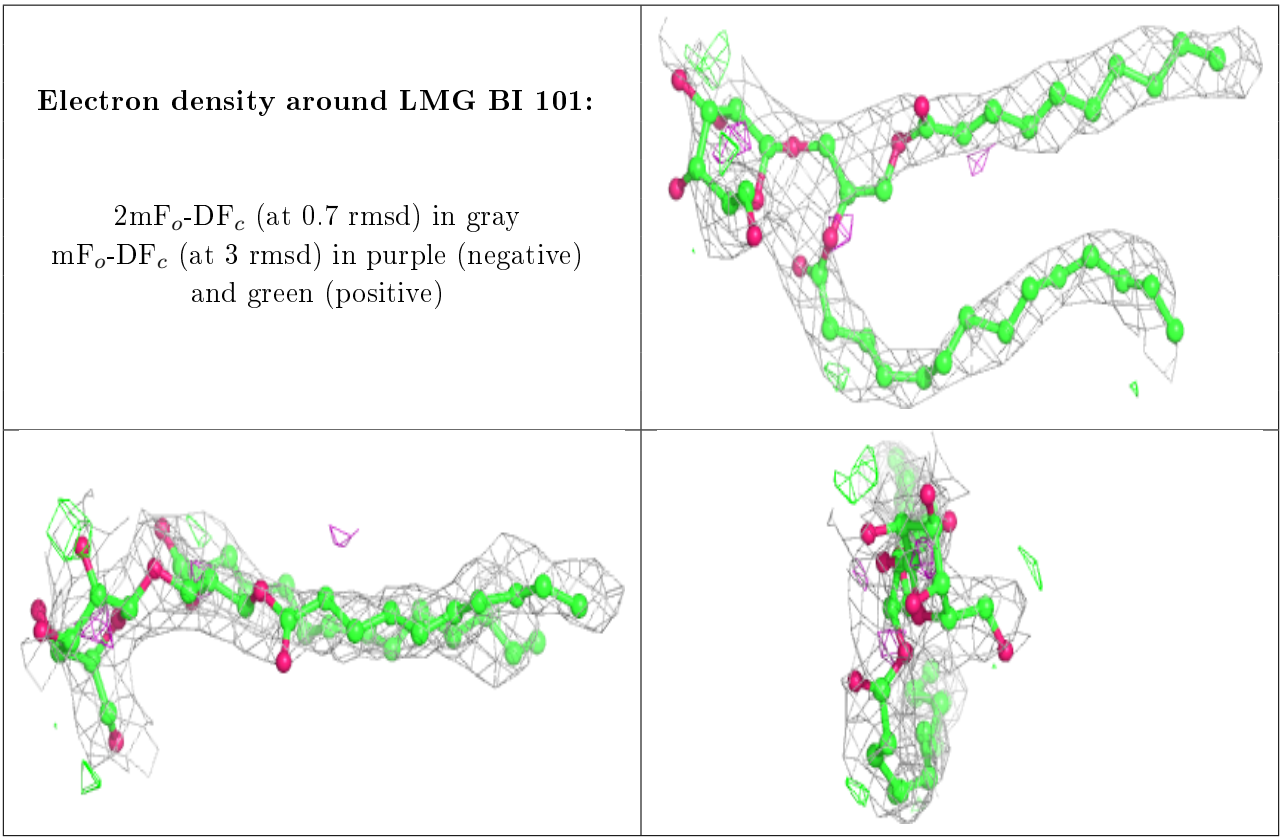
Electron density around LMG AA 416:

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



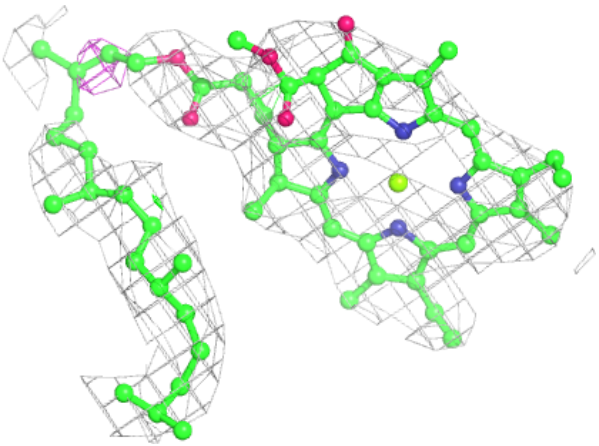
Electron density around LMG BI 101:

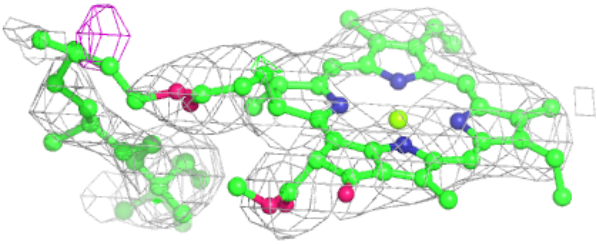
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

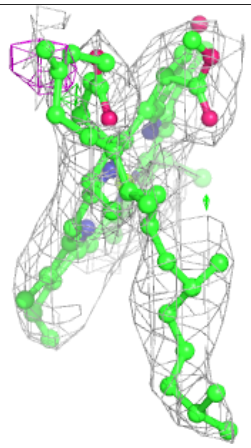


Electron density around CLA BB 619:

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

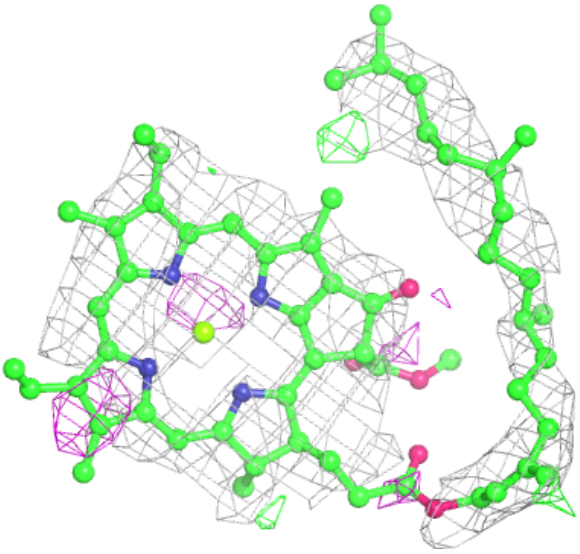


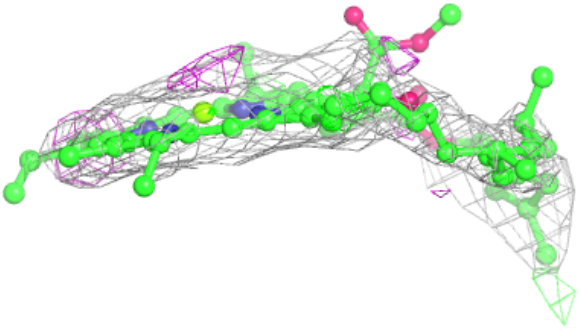


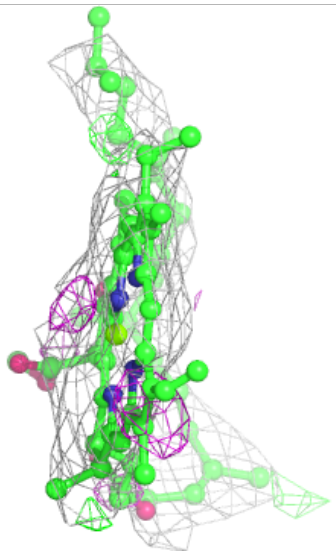


Electron density around CLA AB 601:

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

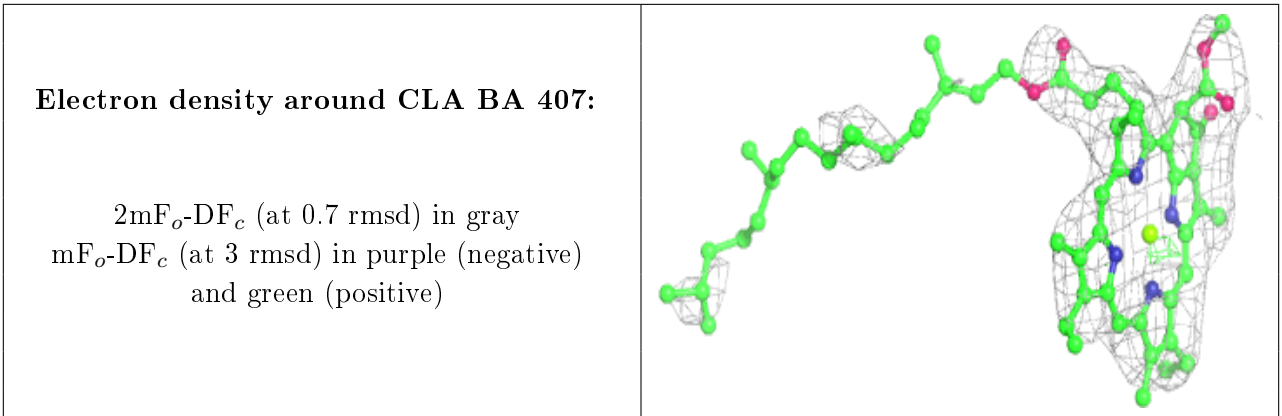






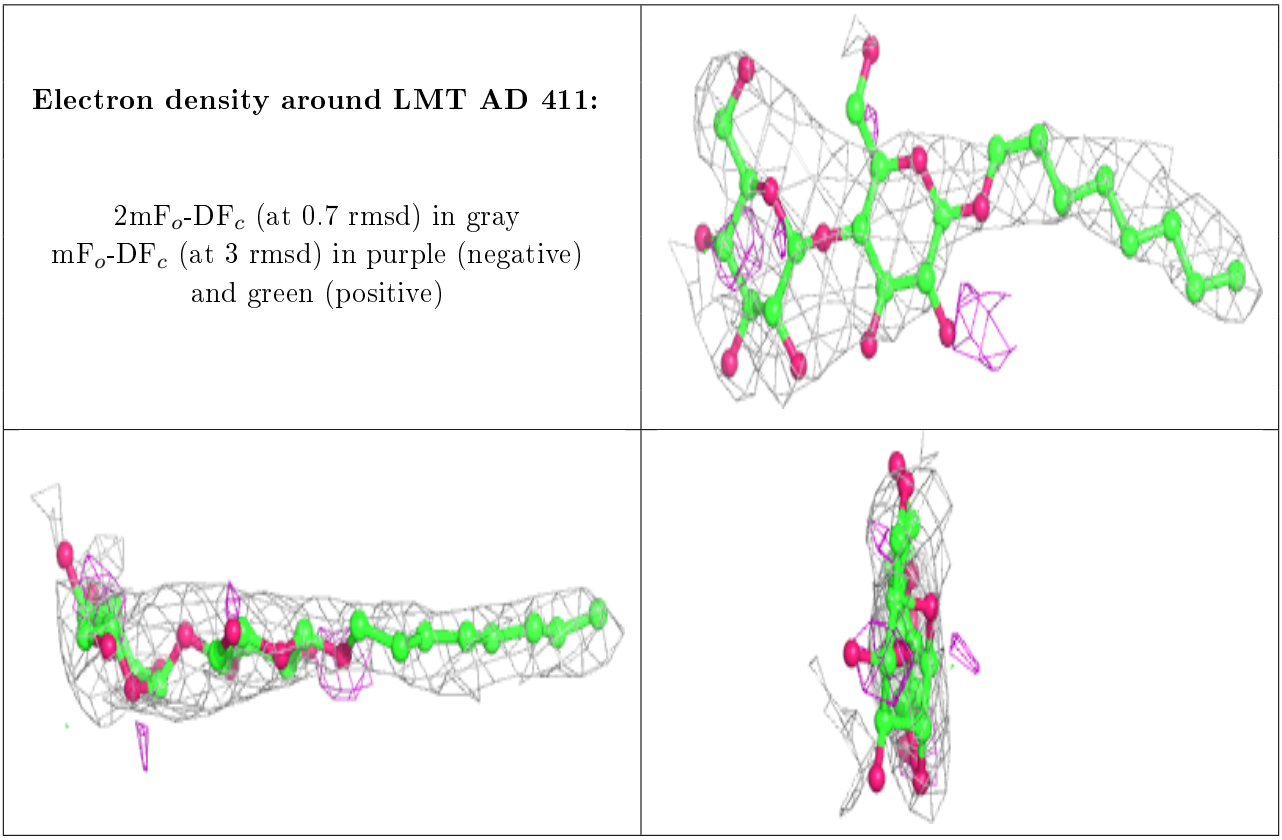
Electron density around CLA BA 407:

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



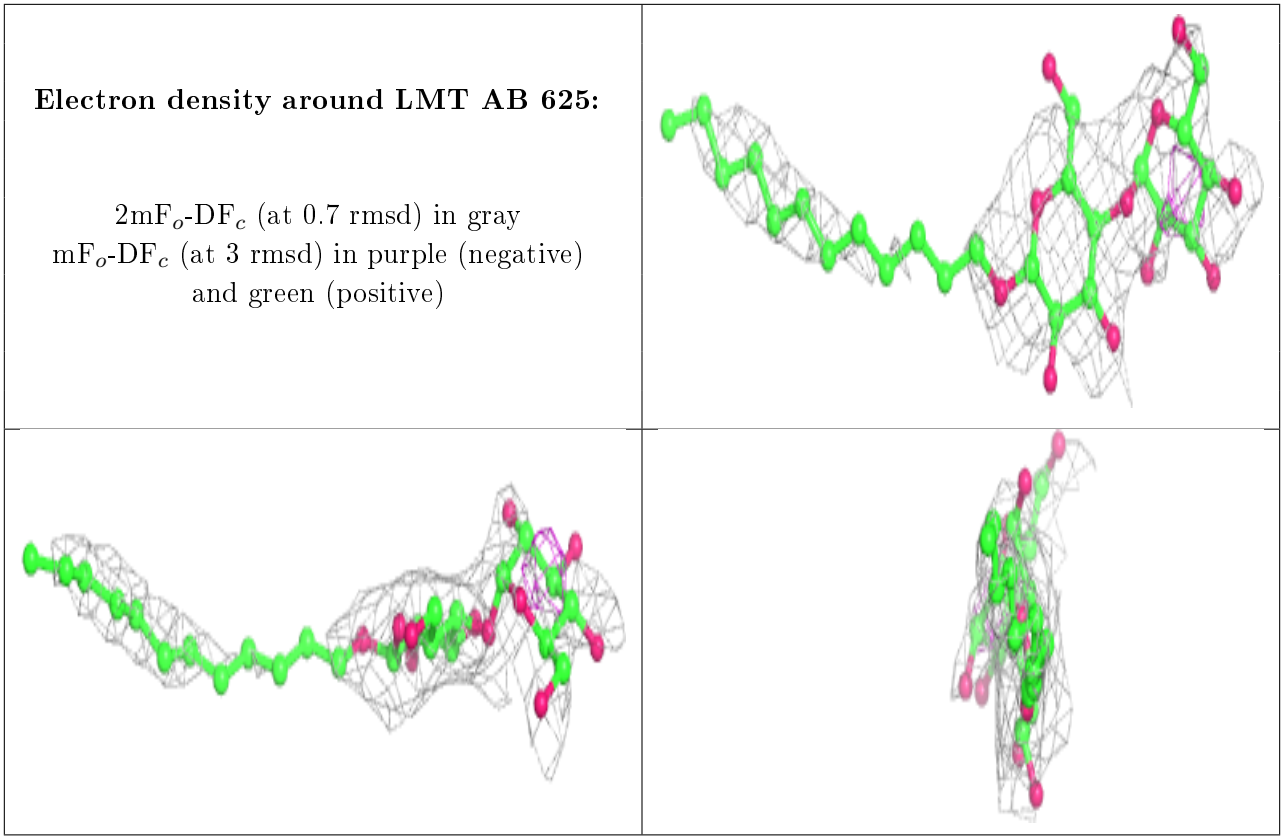
Electron density around LMT AD 411:

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



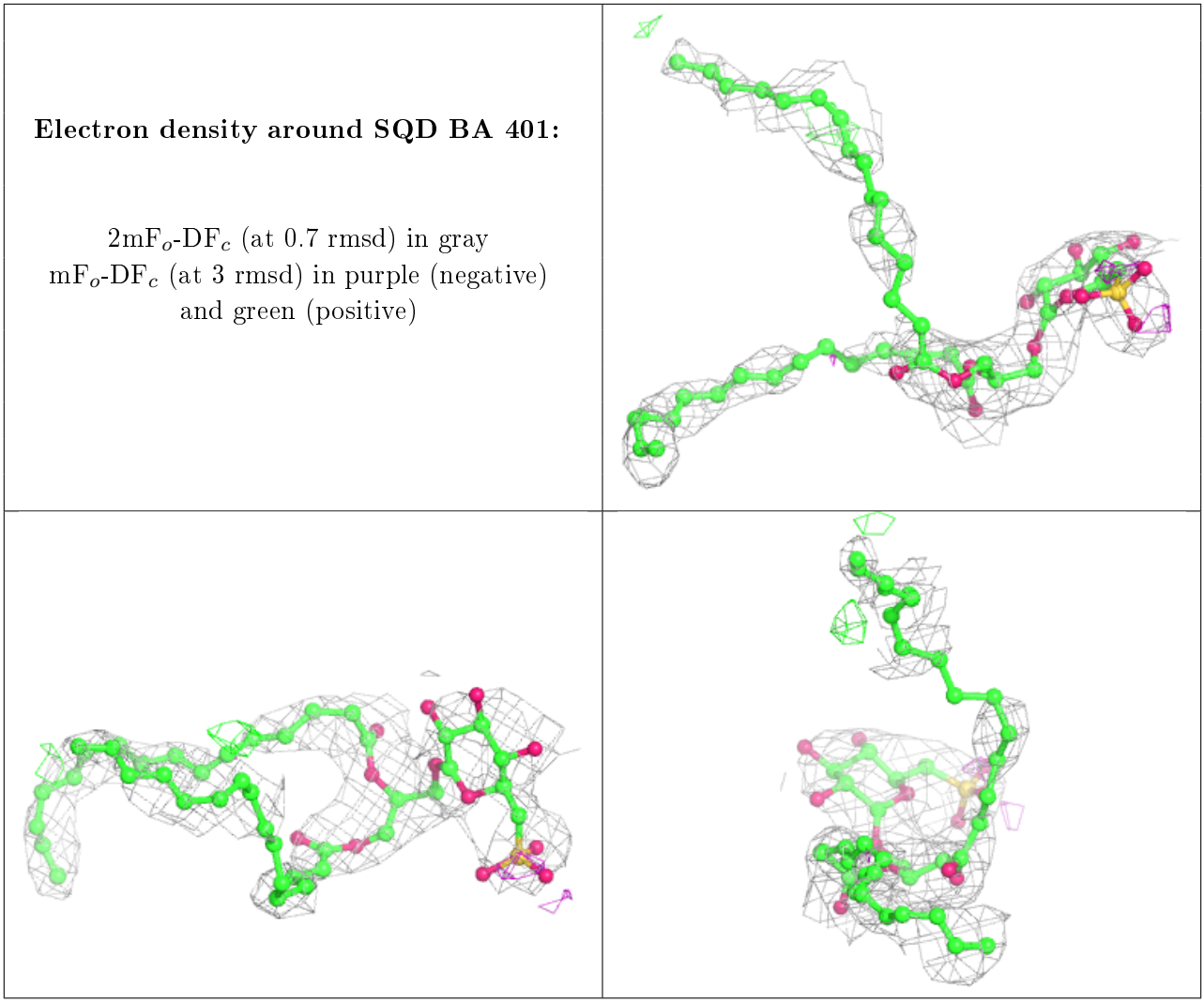
Electron density around LMT AB 625:

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



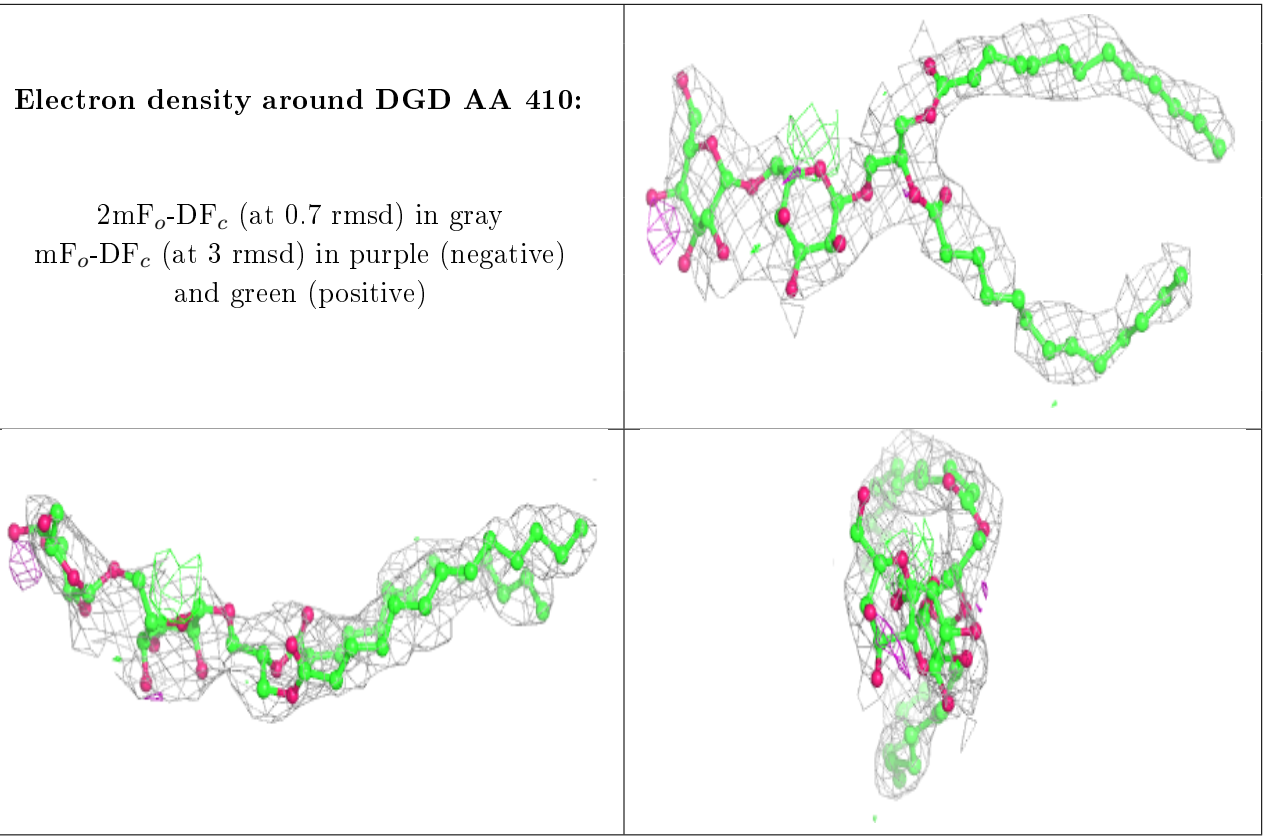
Electron density around SQD BA 401:

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



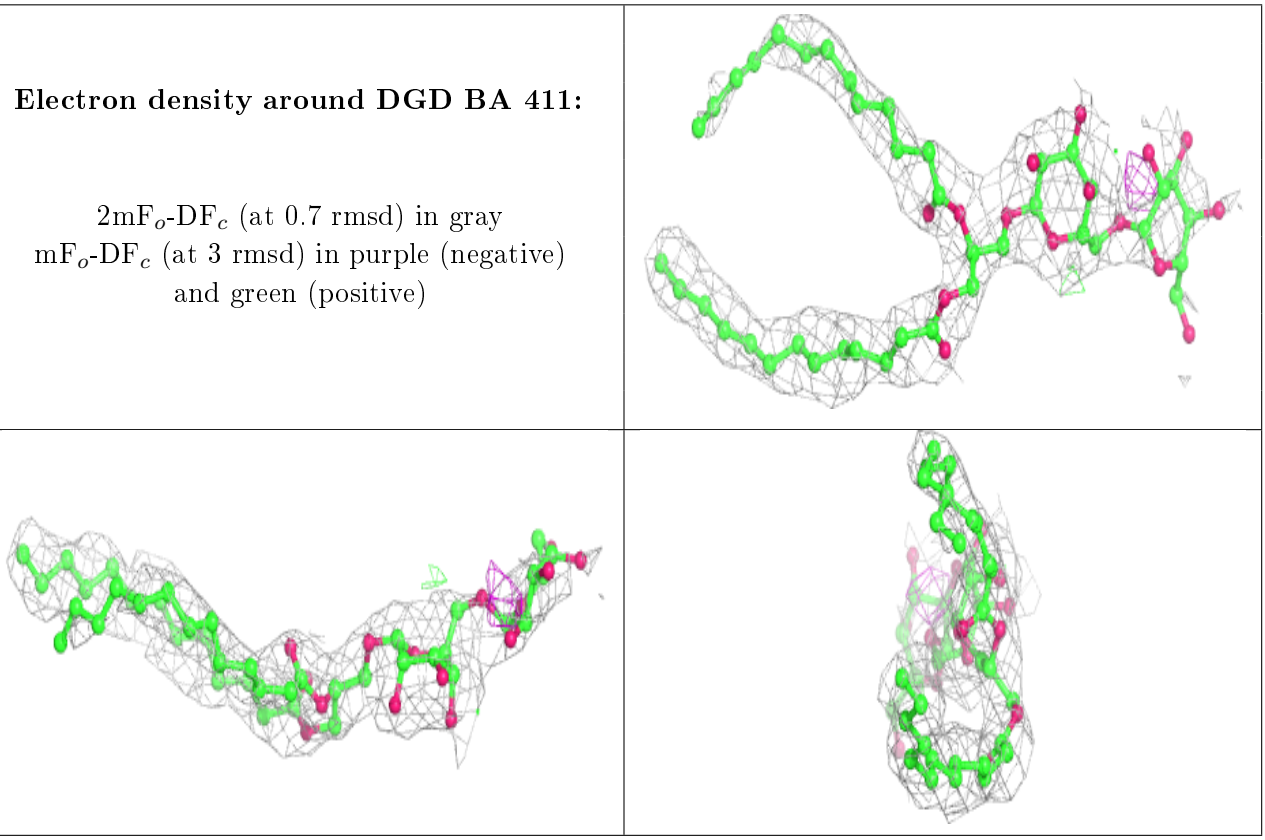
Electron density around DGD AA 410:

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



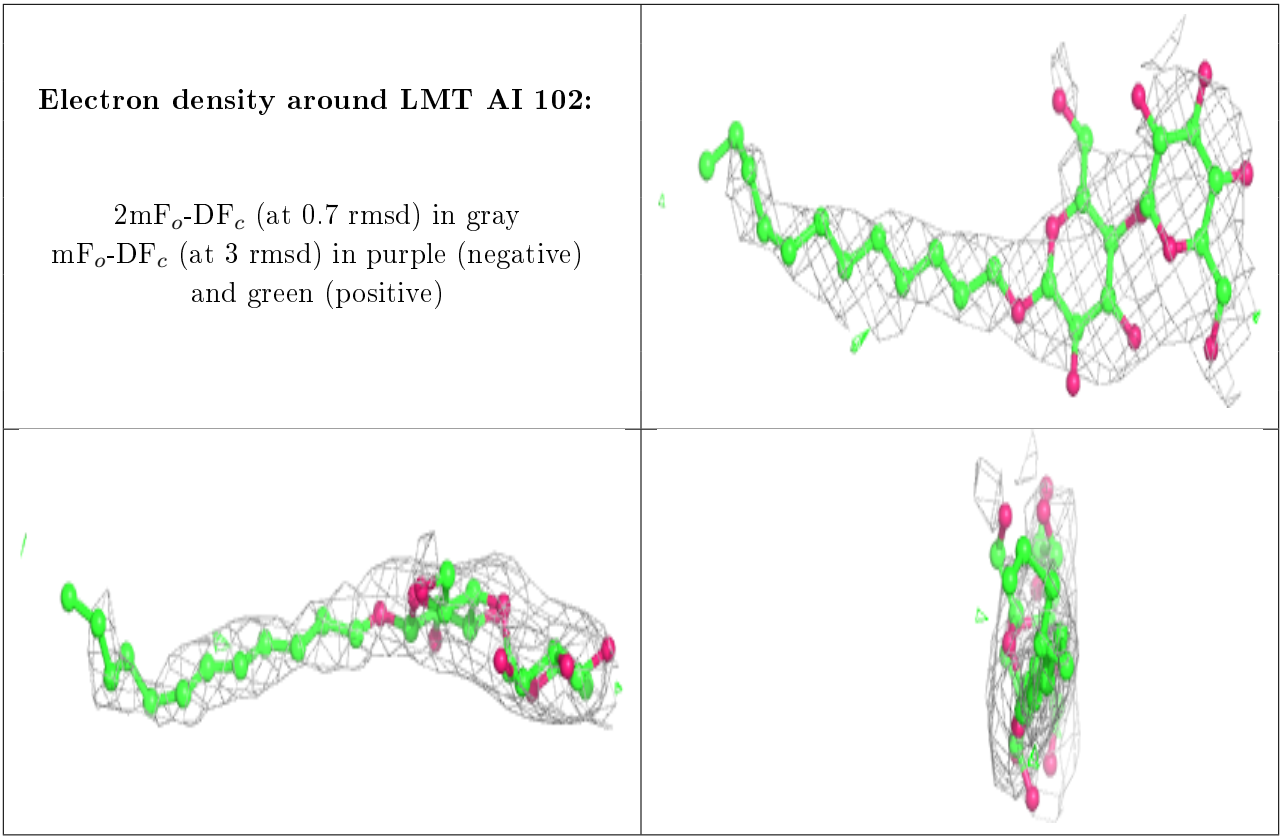
Electron density around DGD BA 411:

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



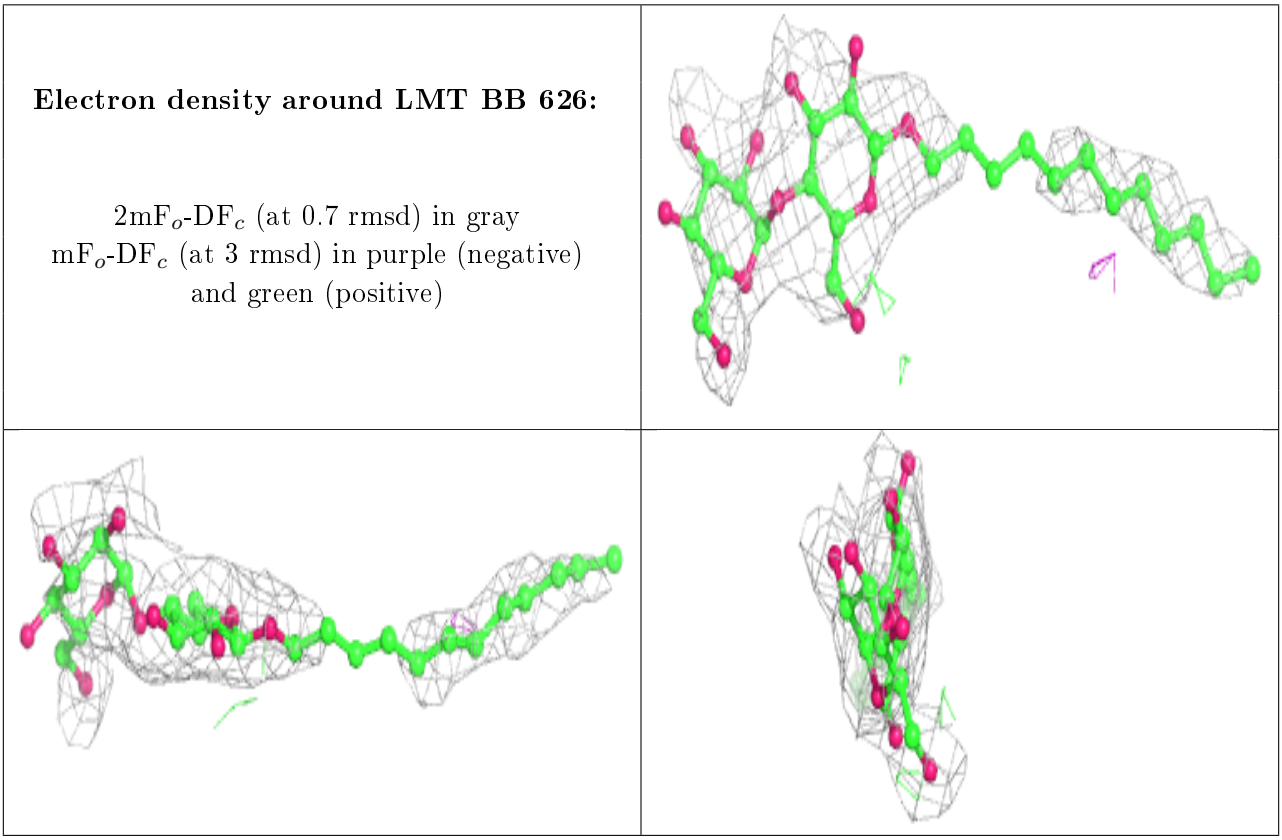
Electron density around LMT AI 102:

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



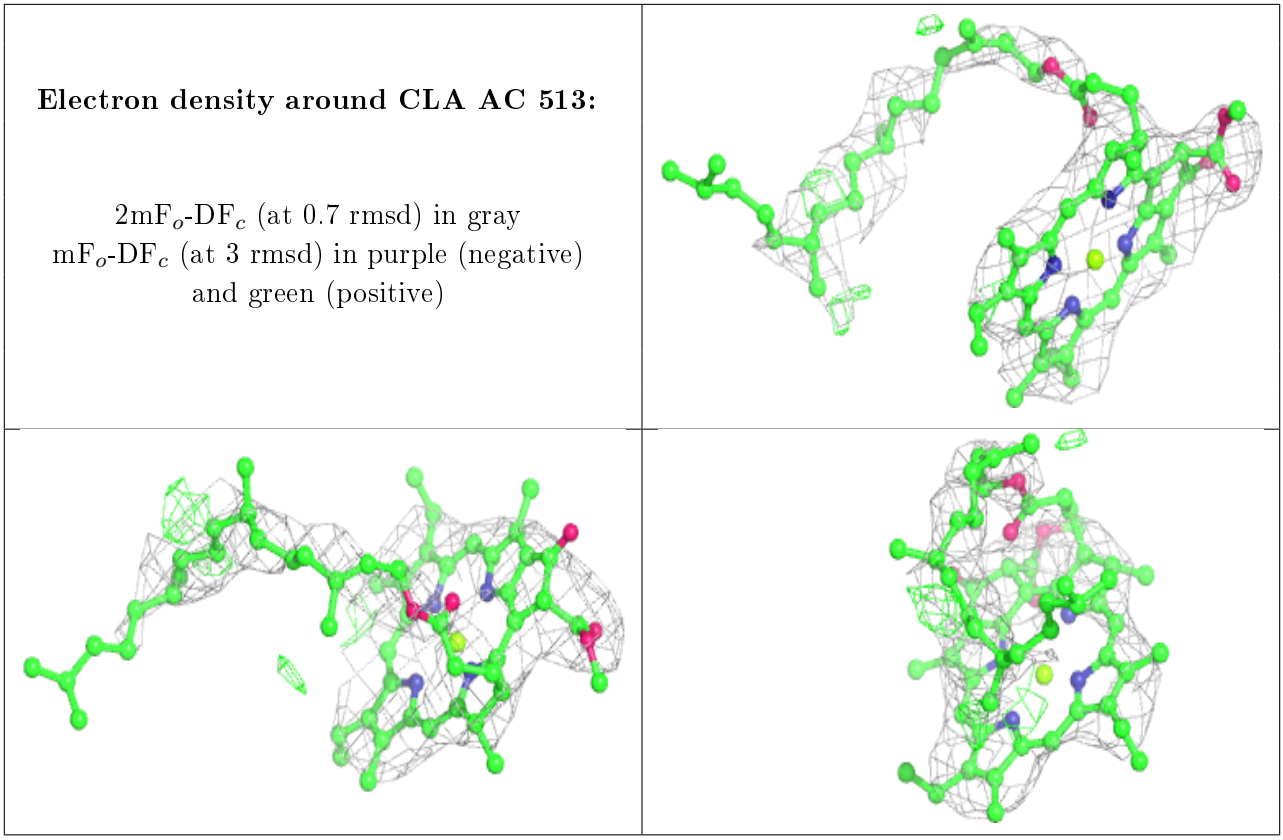
Electron density around LMT BB 626:

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



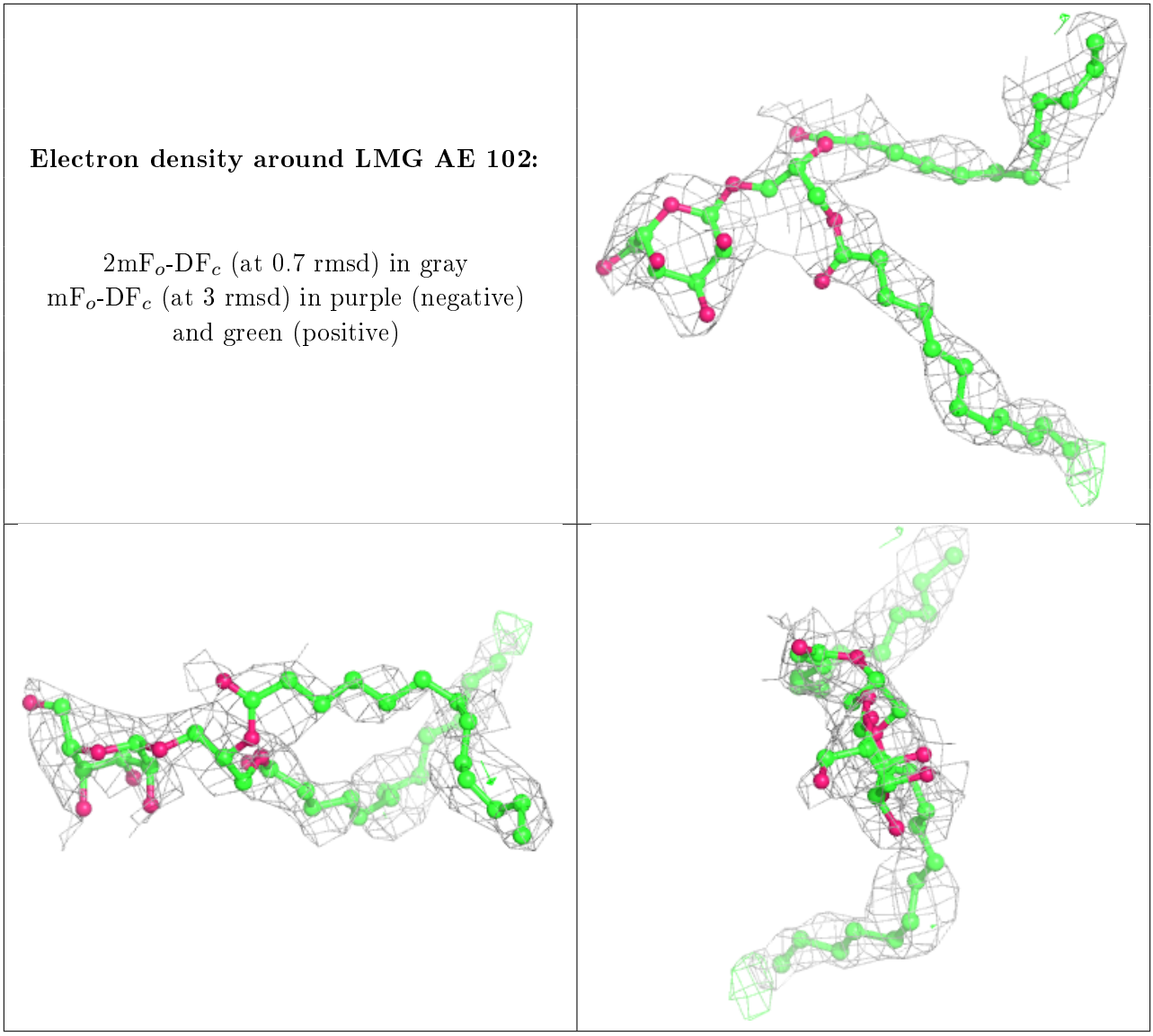
Electron density around CLA AC 513:

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



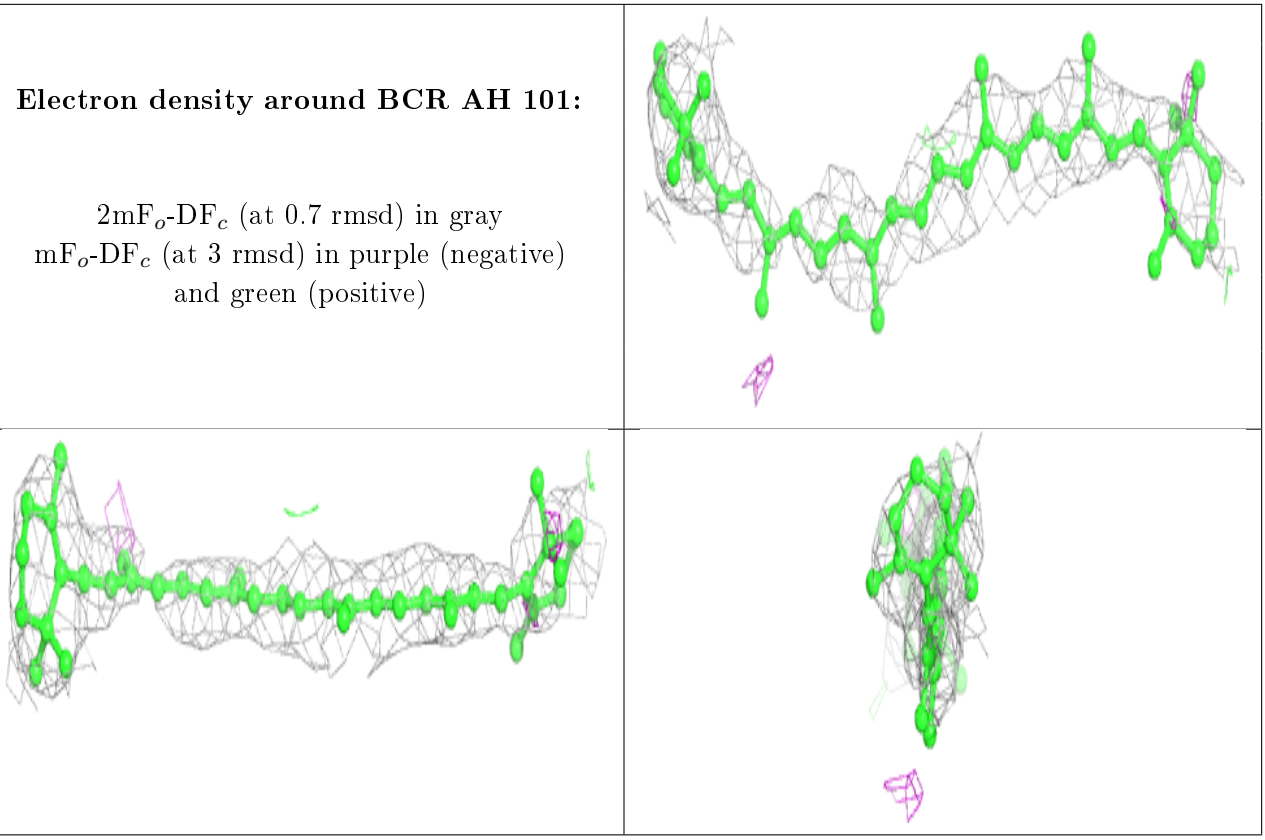
Electron density around LMG AE 102:

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



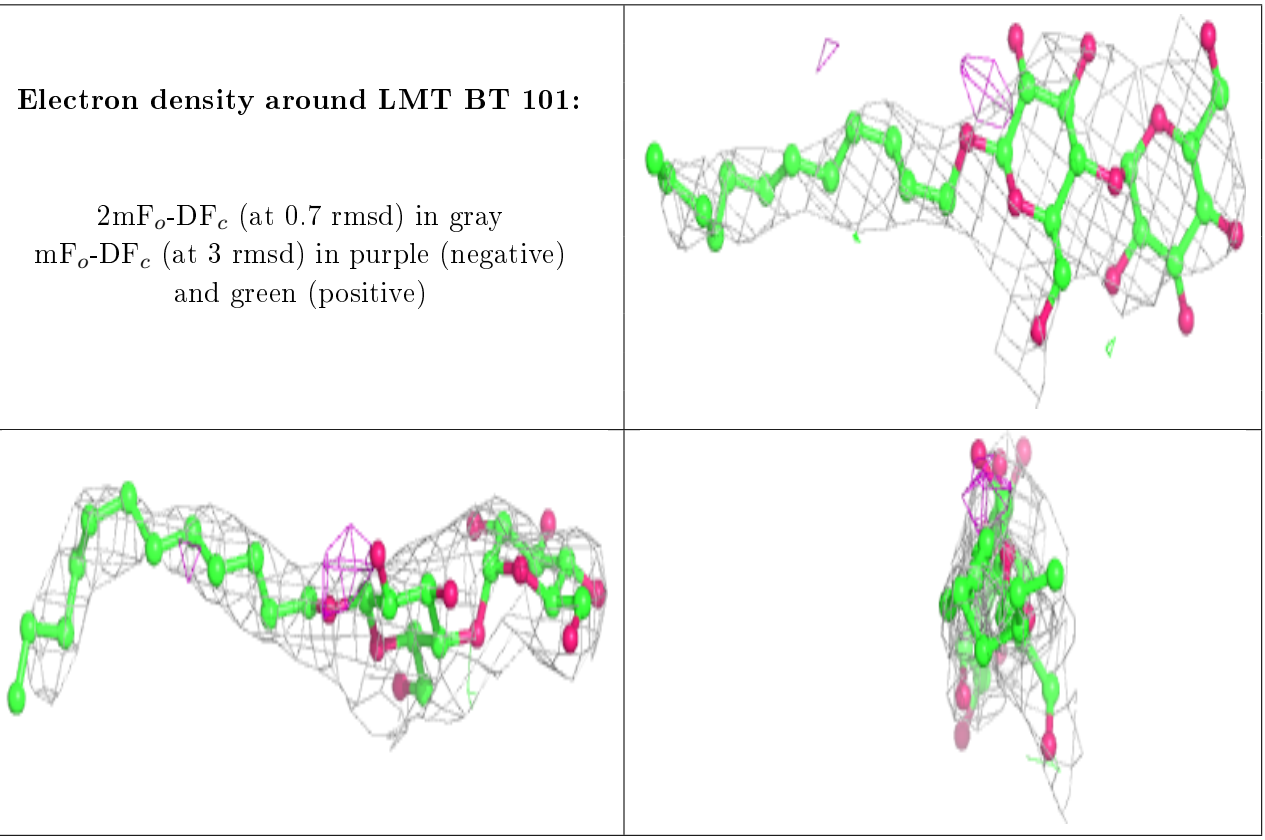
Electron density around BCR AH 101:

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



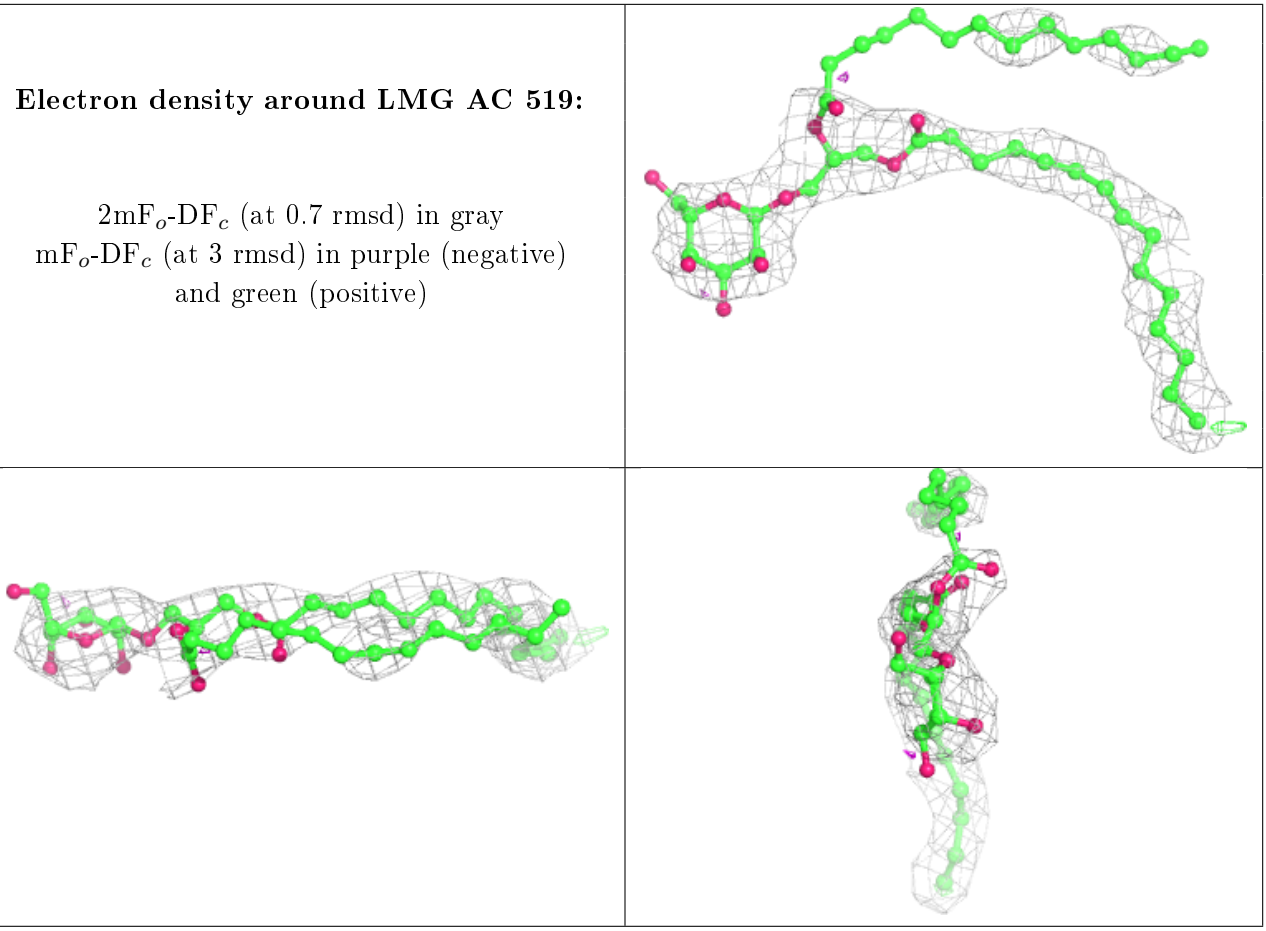
Electron density around LMT BT 101:

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



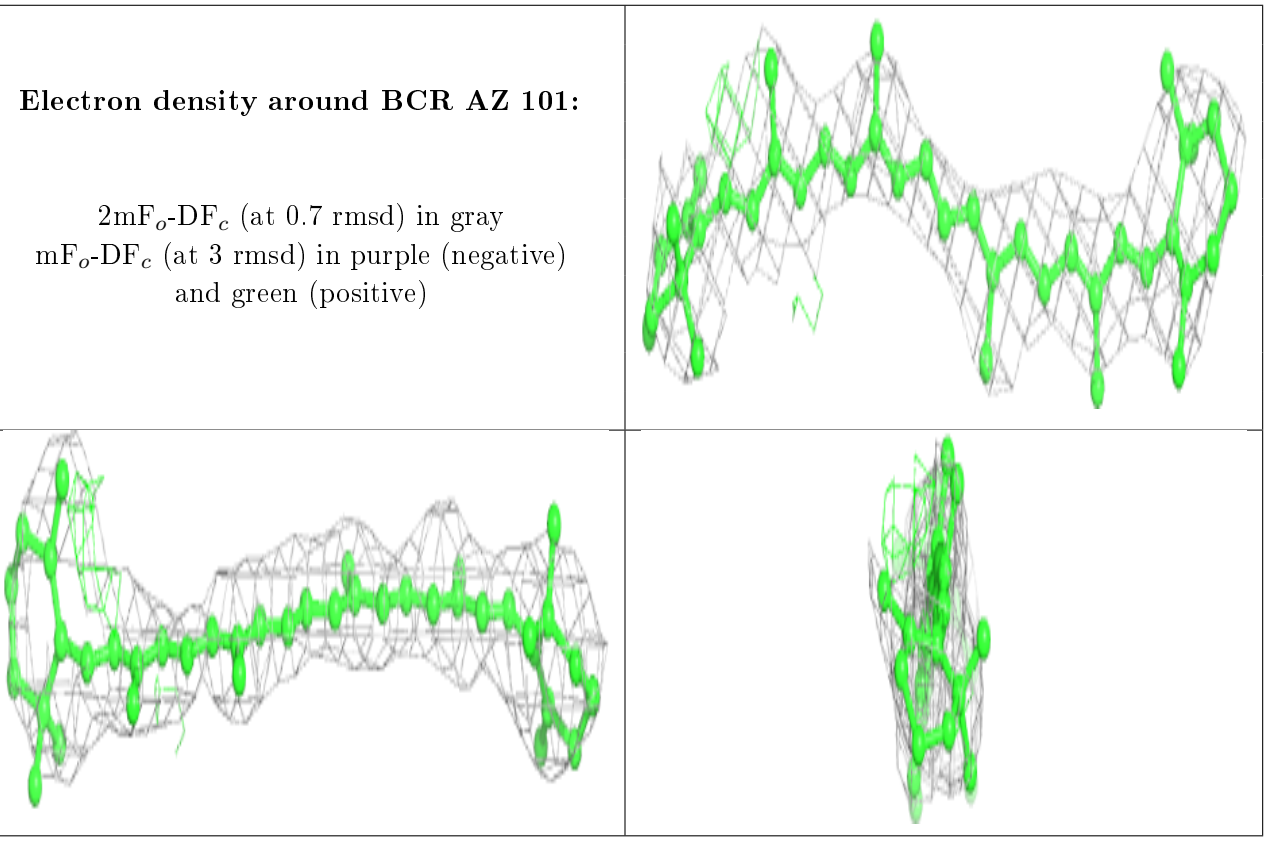
Electron density around LMG AC 519:

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



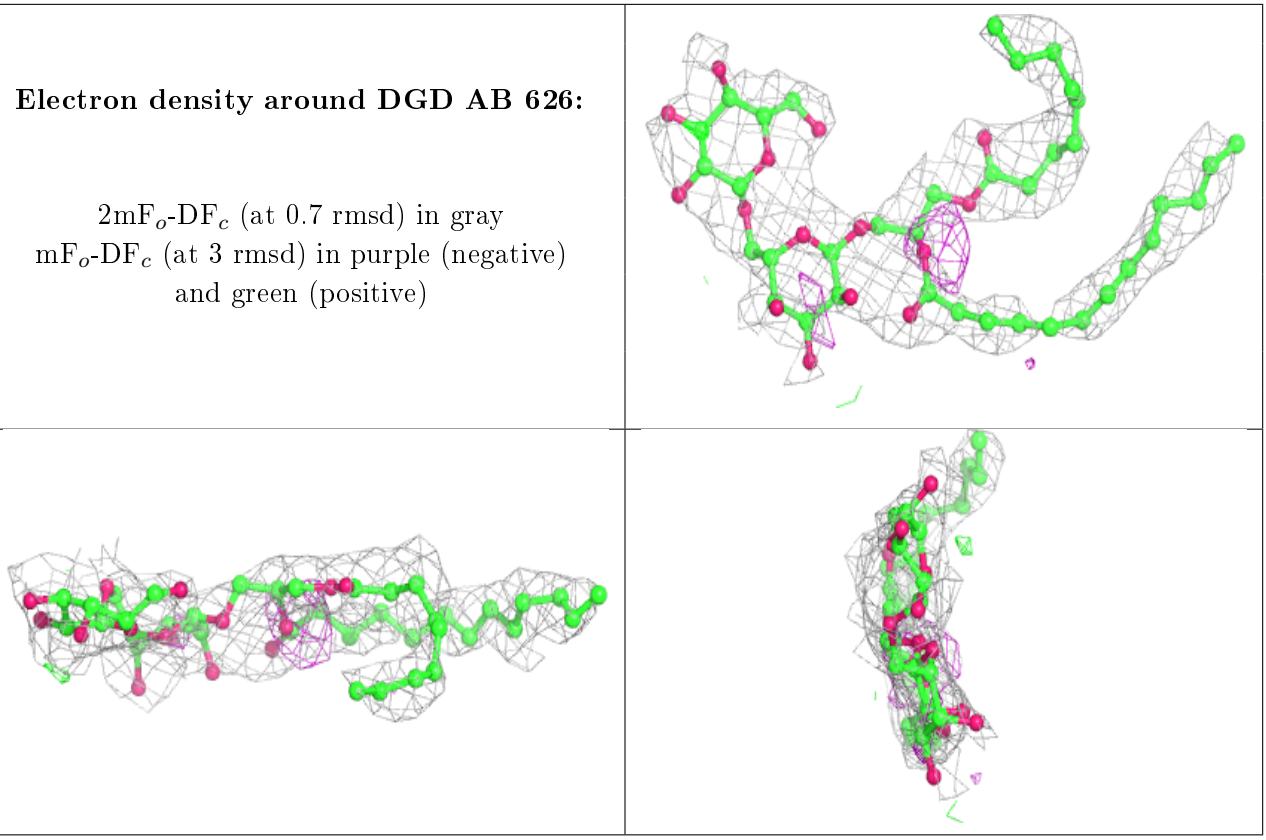
Electron density around BCR AZ 101:

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



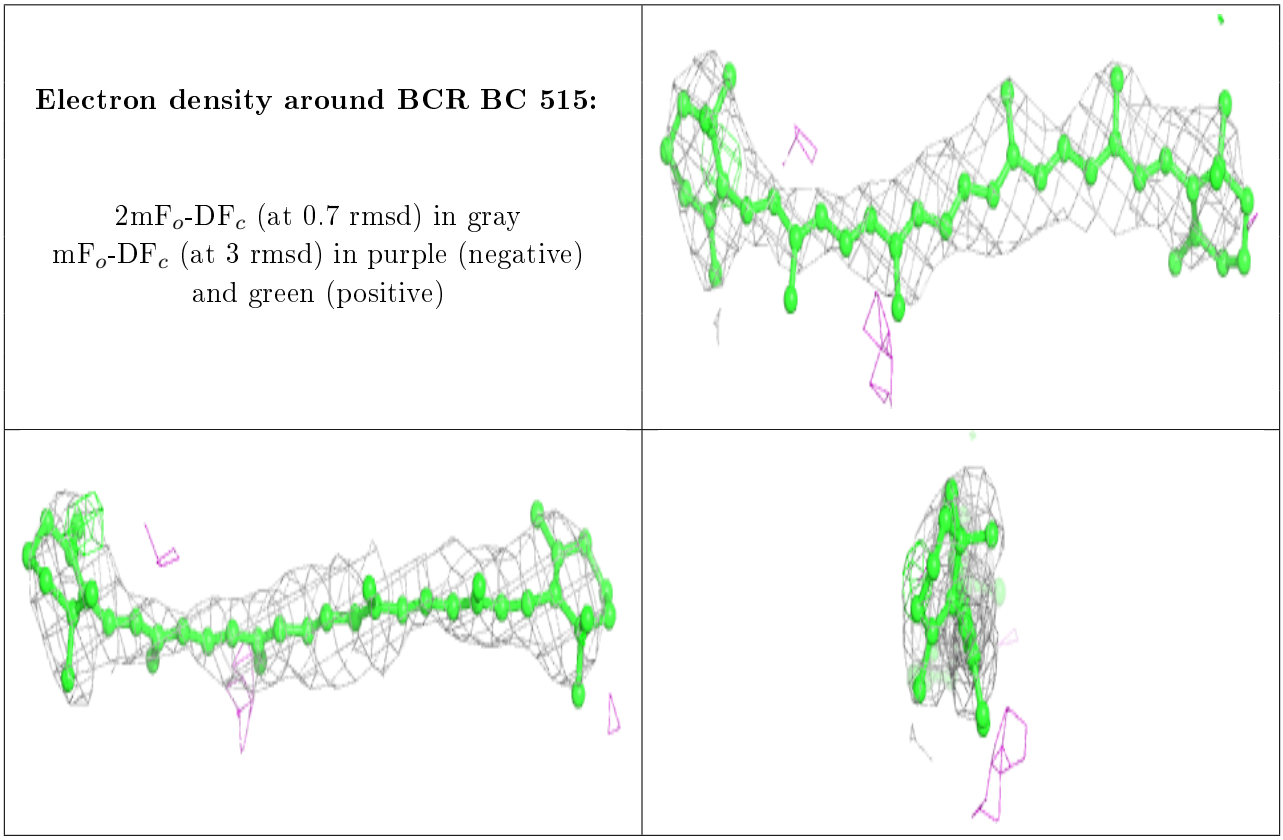
Electron density around DGD AB 626:

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



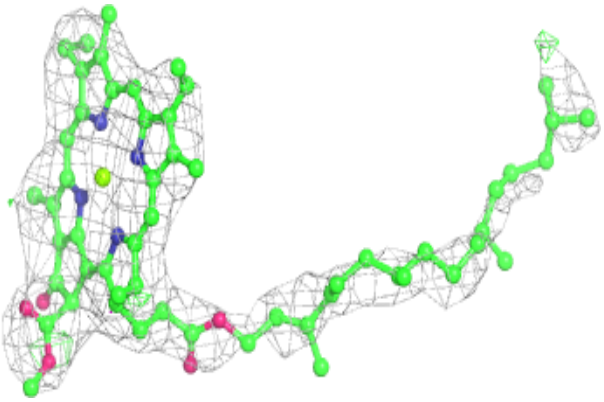
Electron density around BCR BC 515:

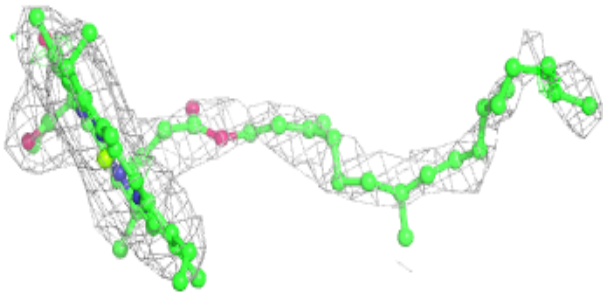
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

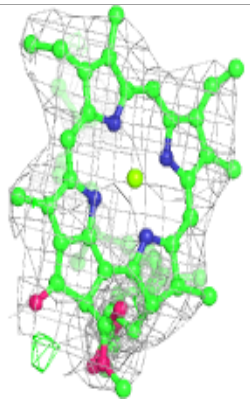


Electron density around CLA AA 406:

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

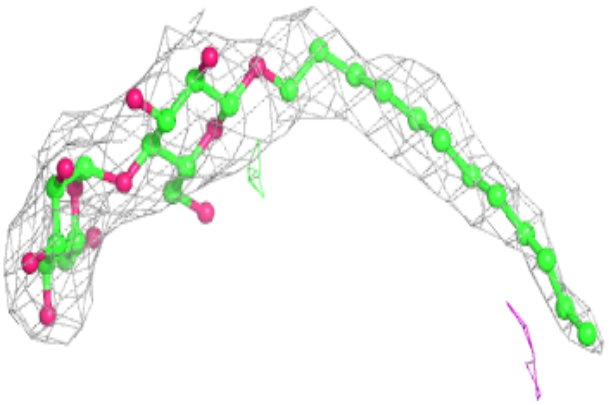


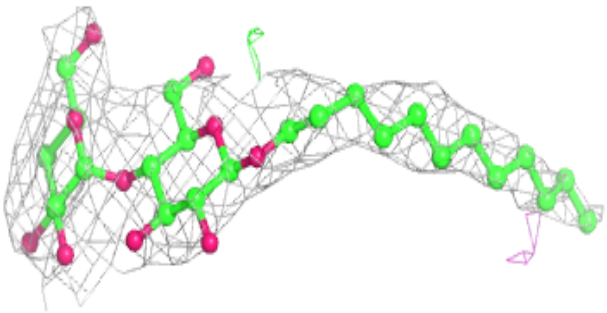


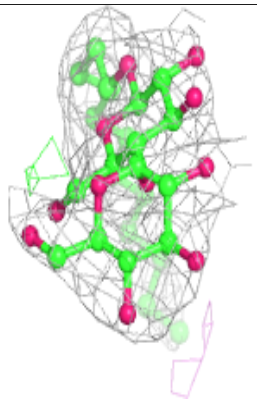


Electron density around LMT BM 101:

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

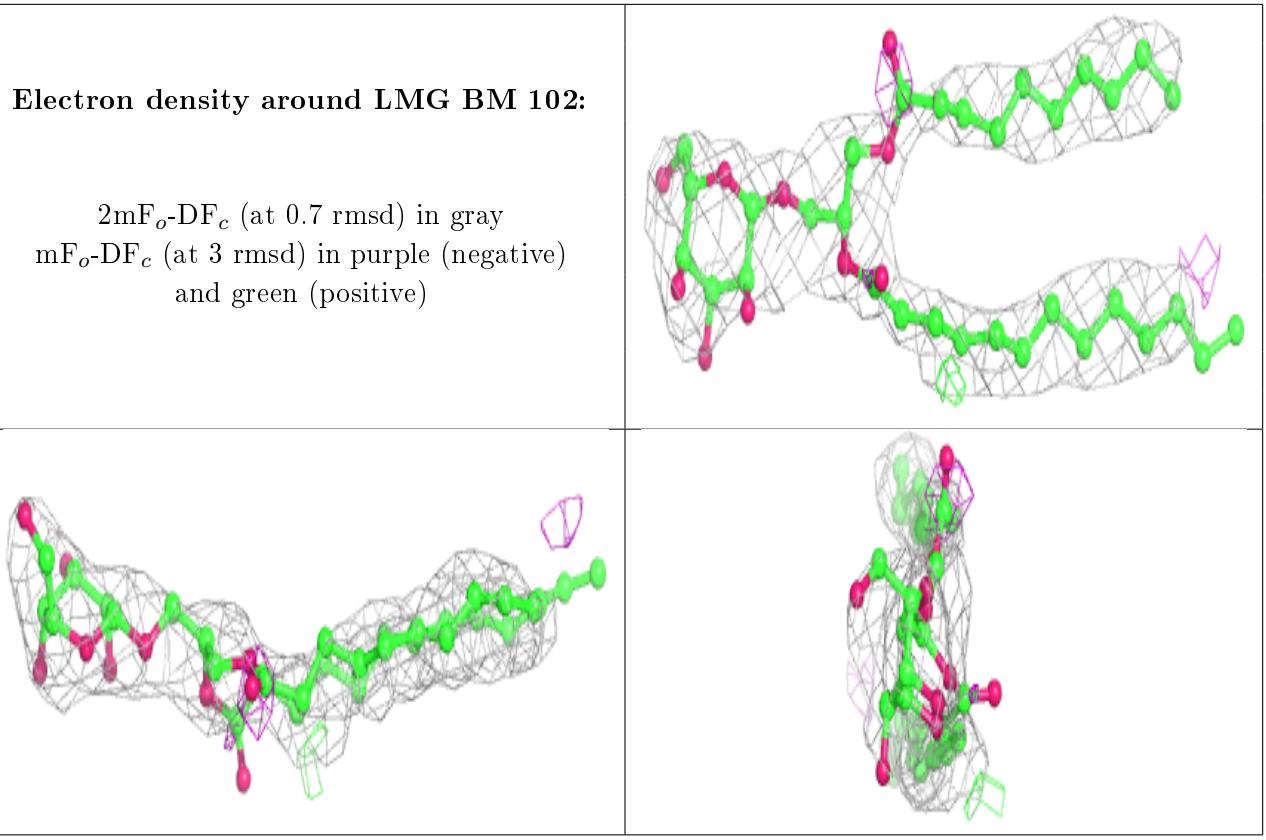






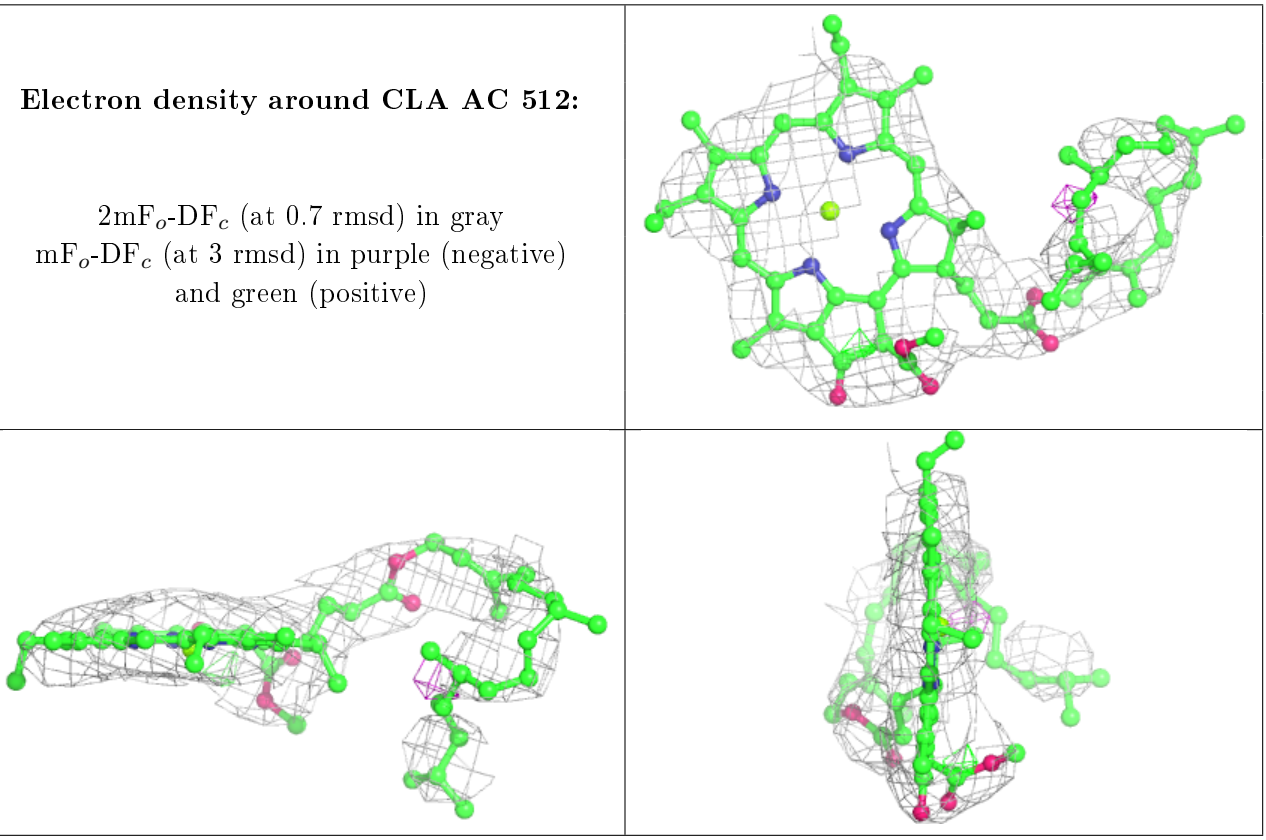
Electron density around LMG BM 102:

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



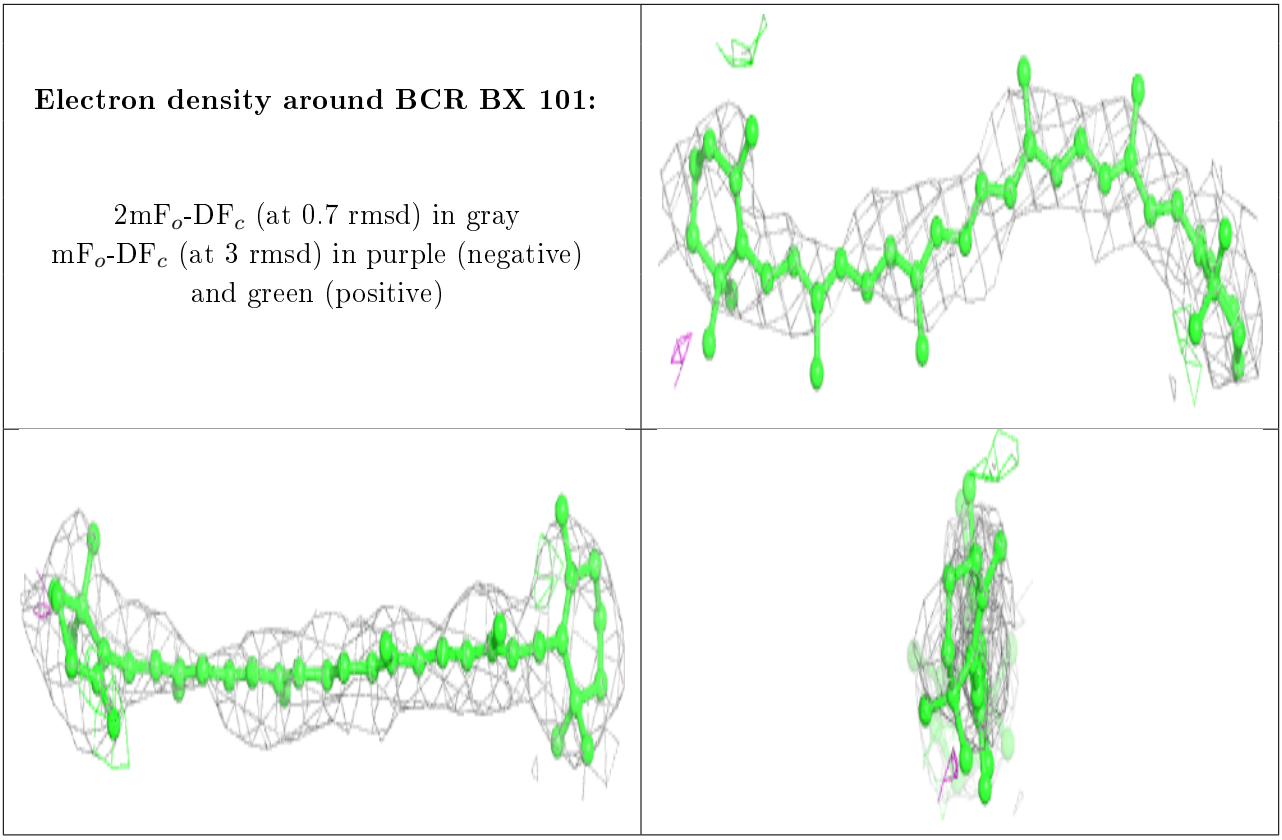
Electron density around CLA AC 512:

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



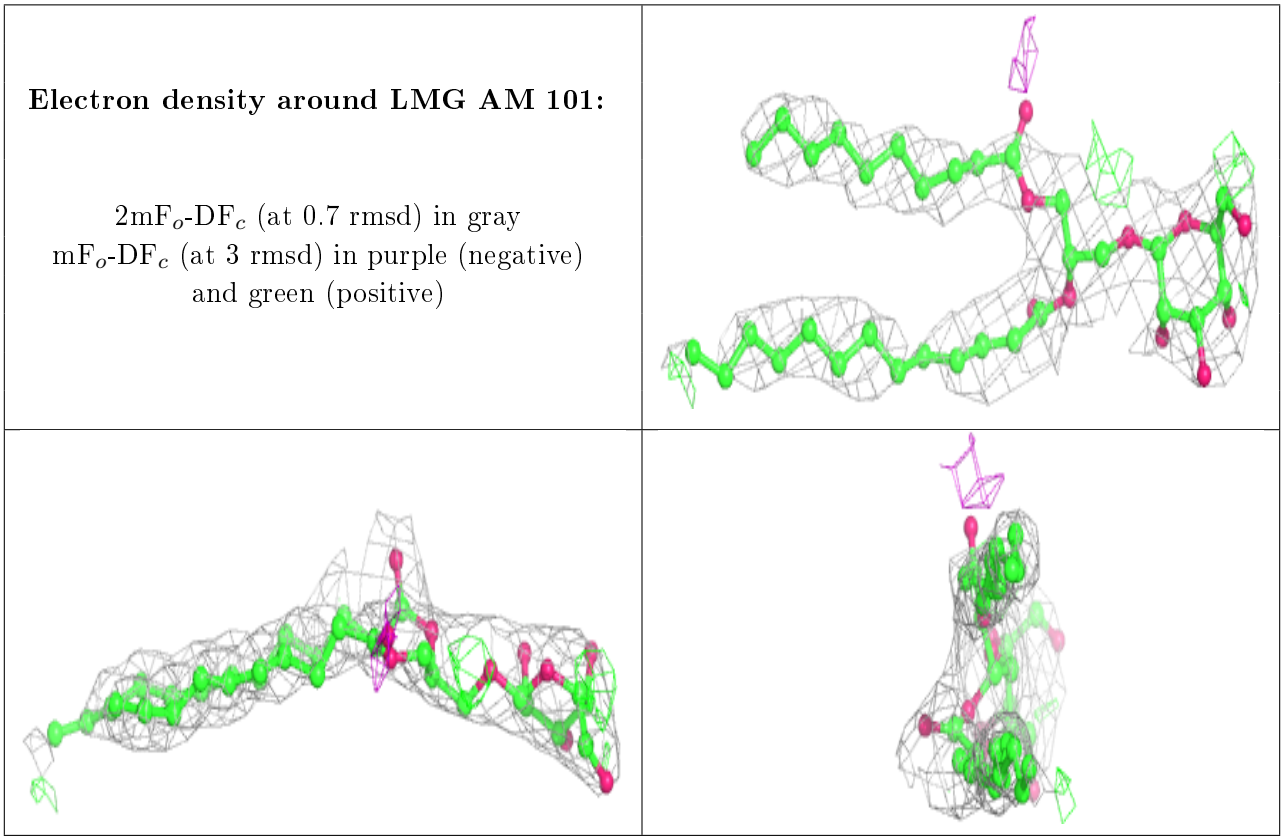
Electron density around BCR BX 101:

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



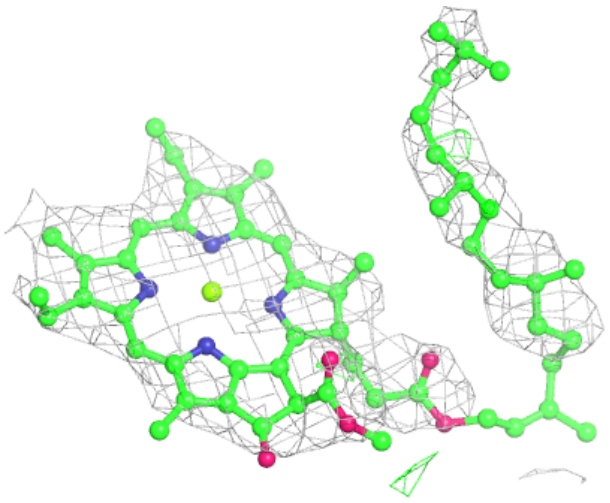
Electron density around LMG AM 101:

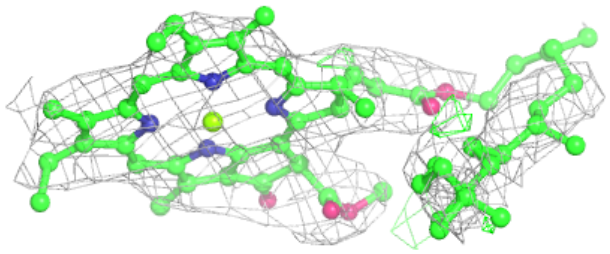
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

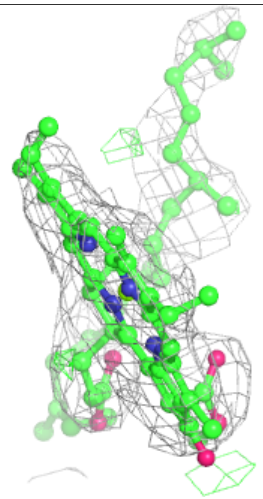


Electron density around CLA AB 616:

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

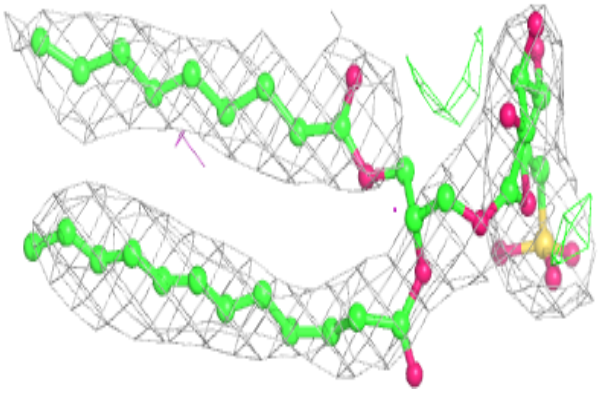


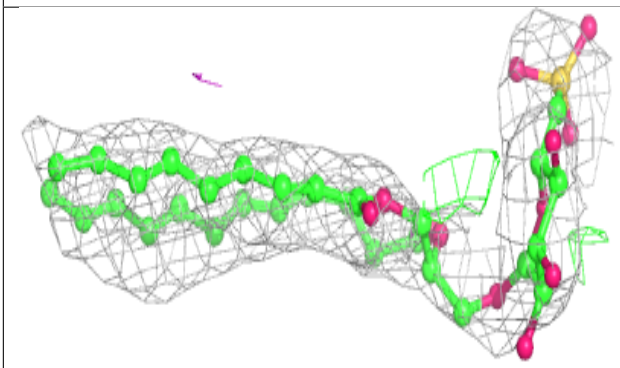


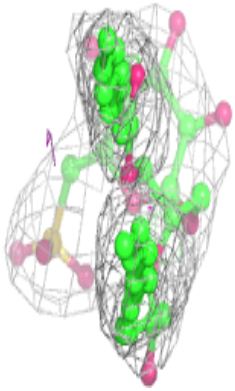


Electron density around SQD BD 409:

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

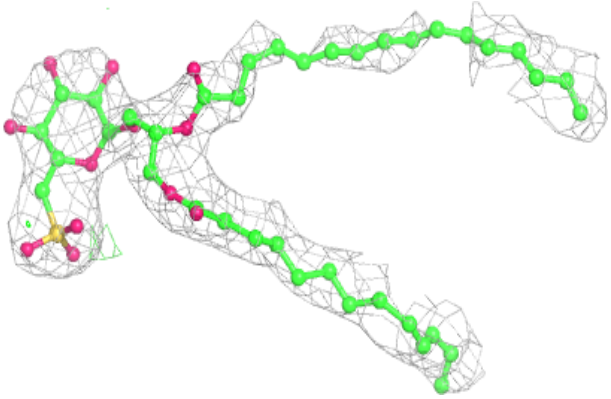


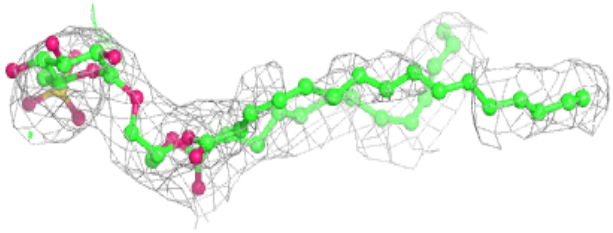


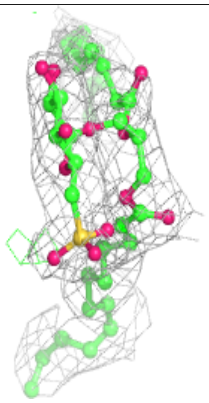


Electron density around SQD BA 413:

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

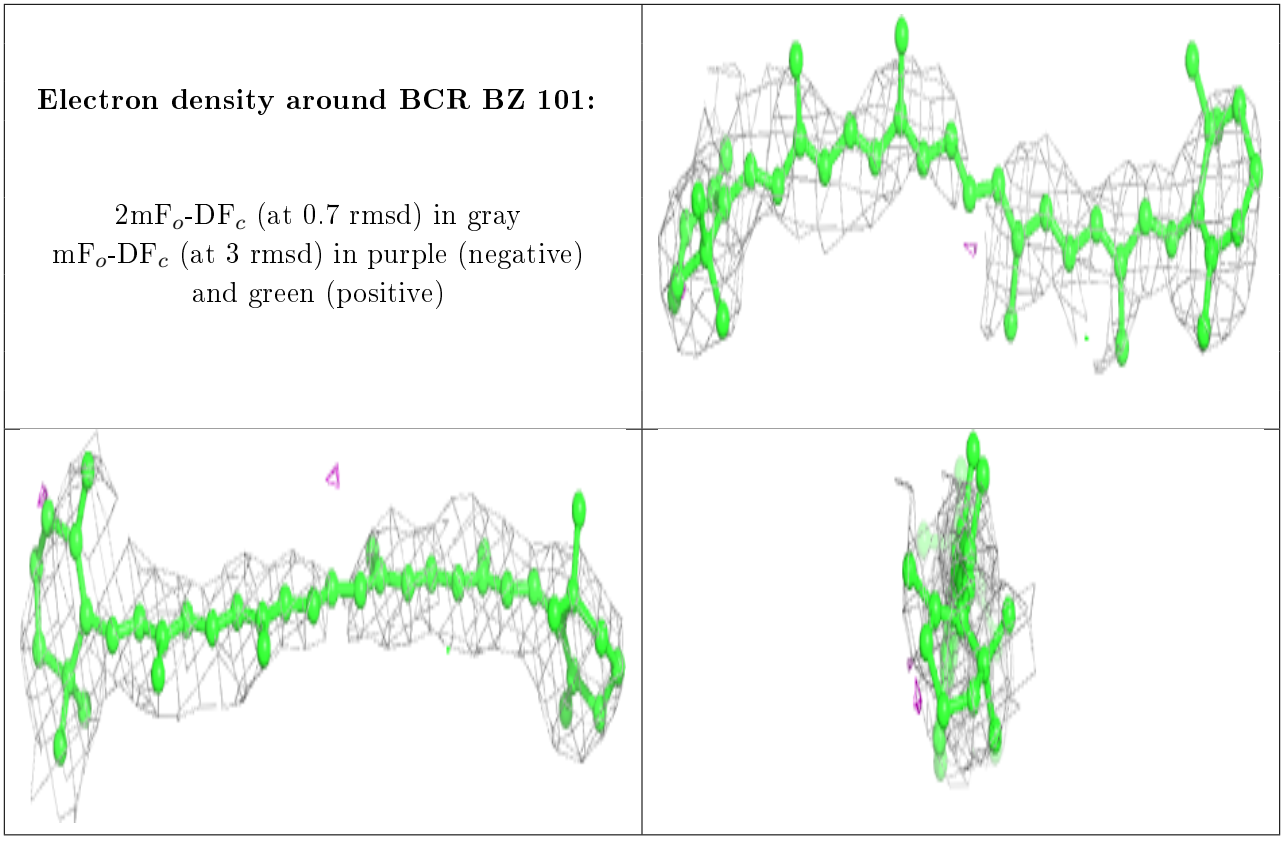






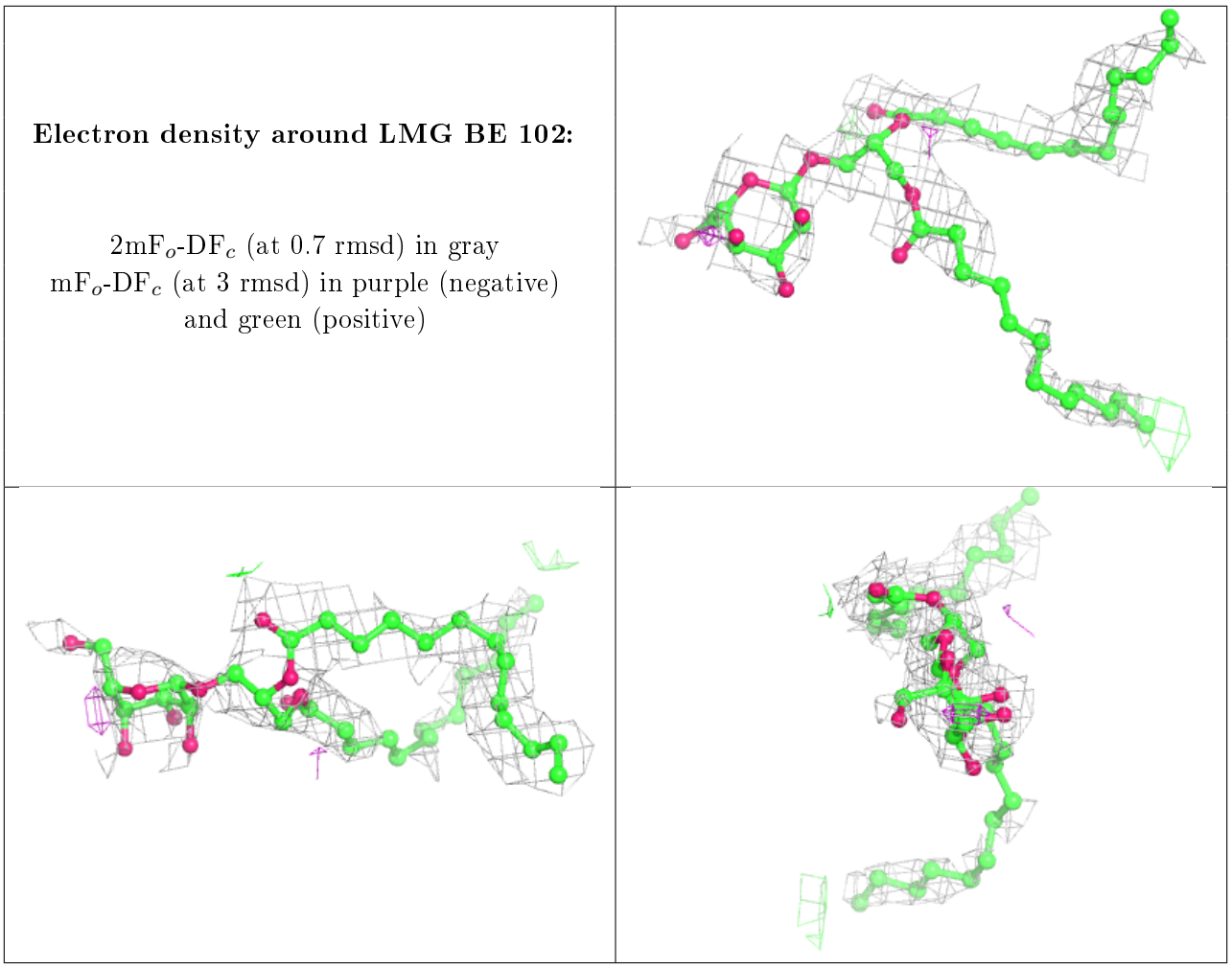
Electron density around BCR BZ 101:

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



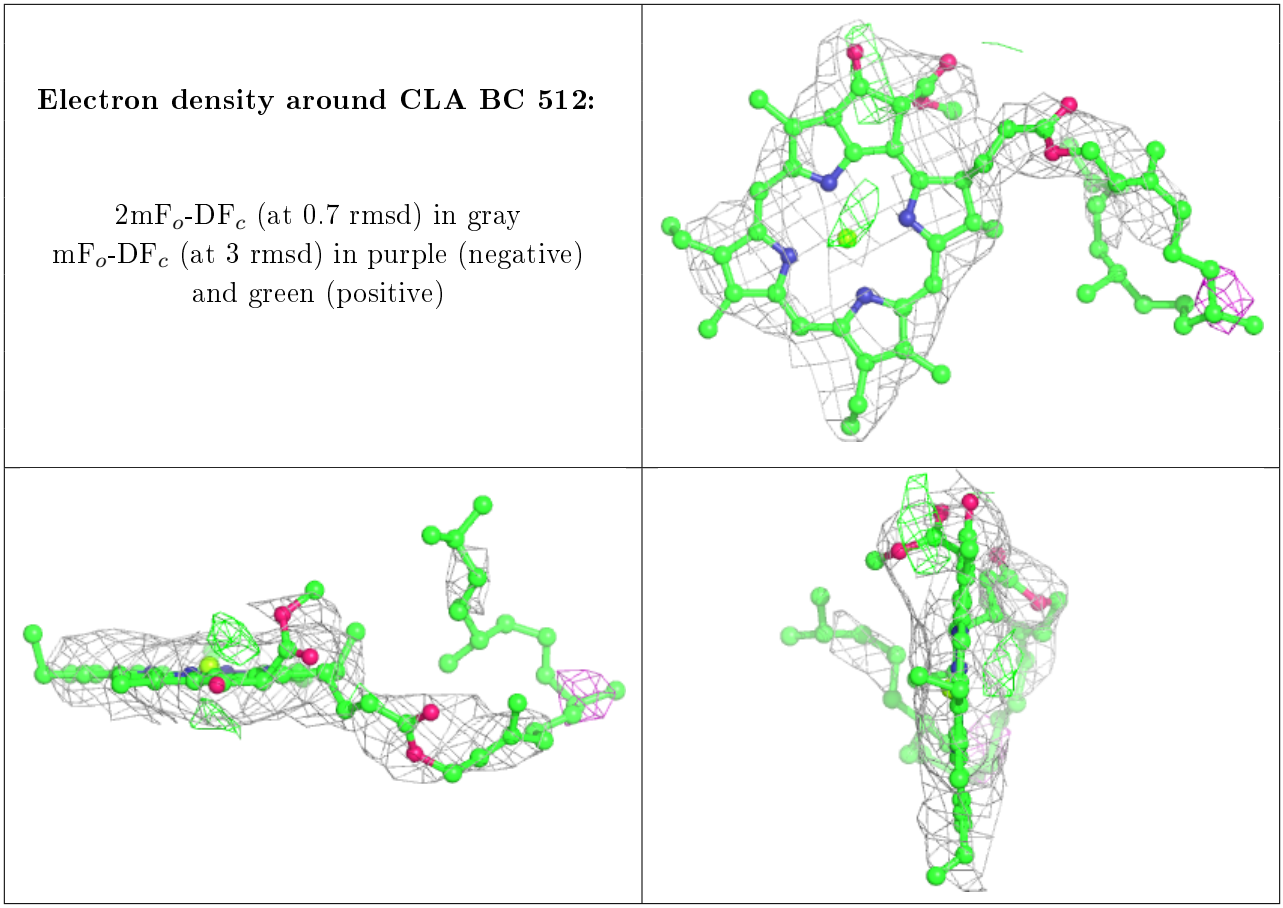
Electron density around LMG BE 102:

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



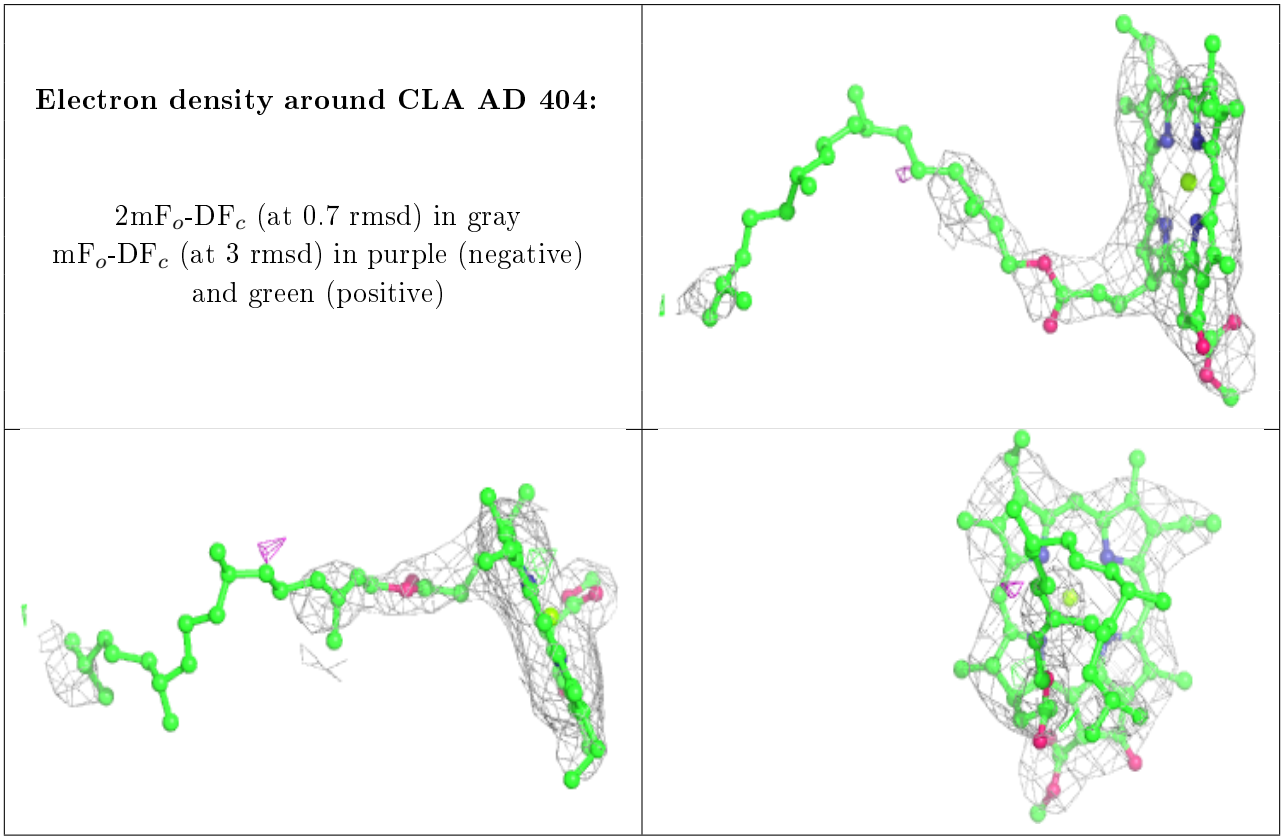
Electron density around CLA BC 512:

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



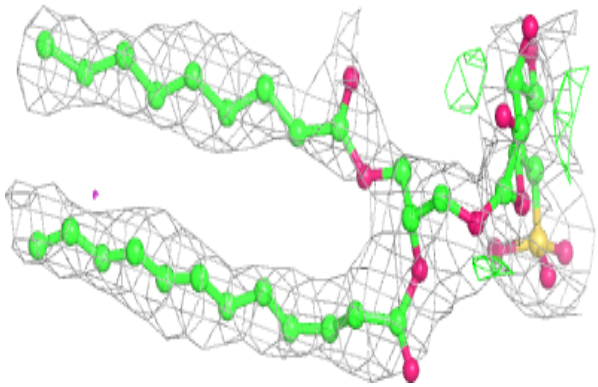
Electron density around CLA AD 404:

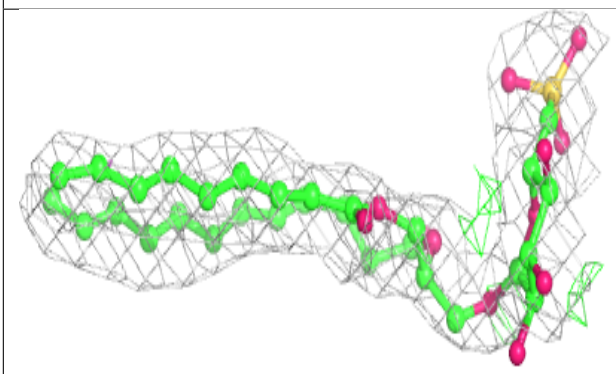
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

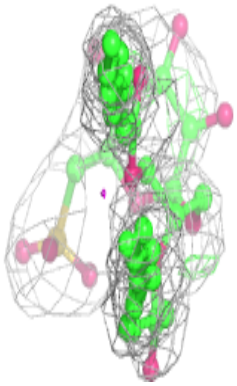


Electron density around SQD AD 409:

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

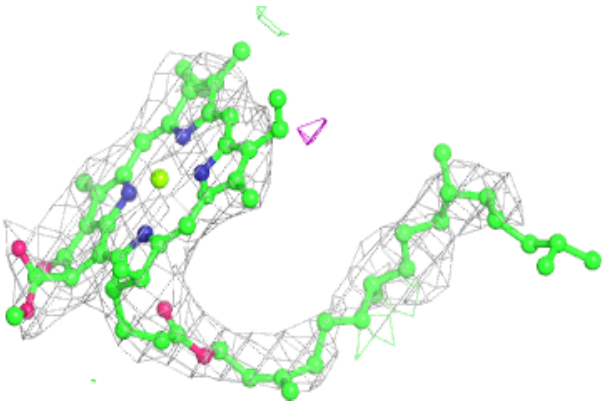


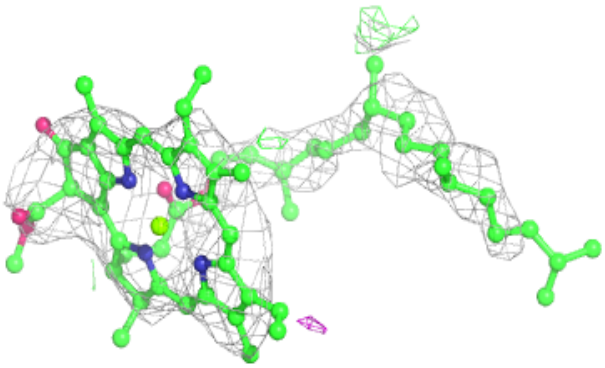


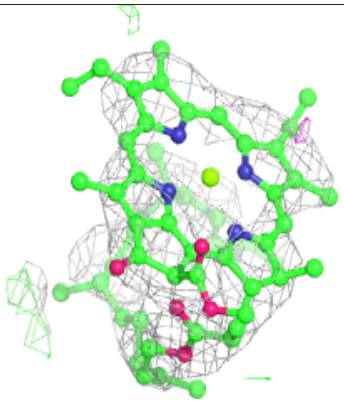


Electron density around CLA BC 513:

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

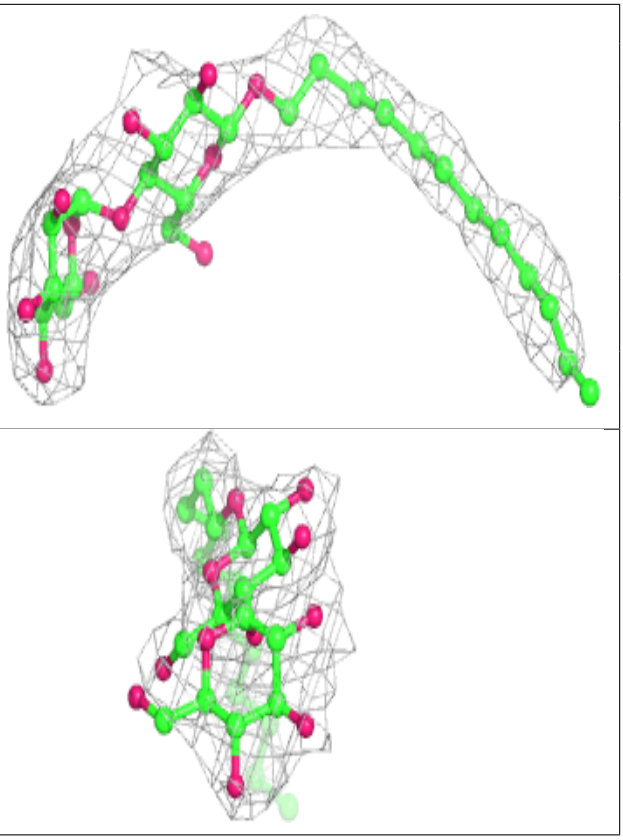






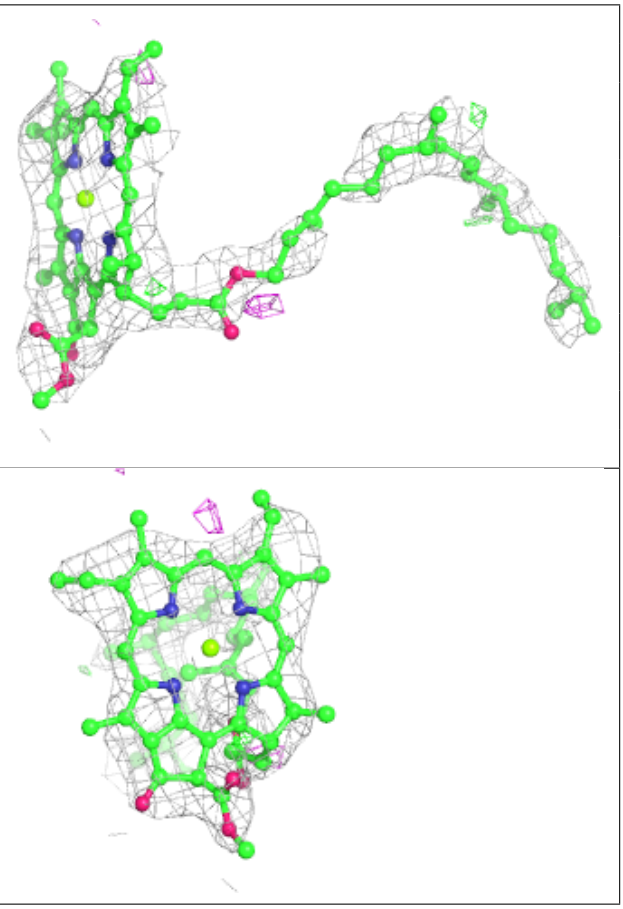
Electron density around LMT AM 102:

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



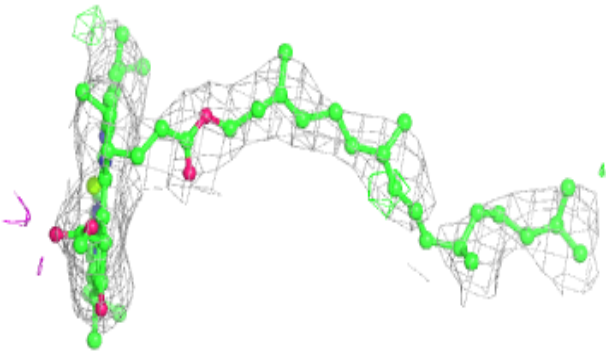
Electron density around CLA BD 404:

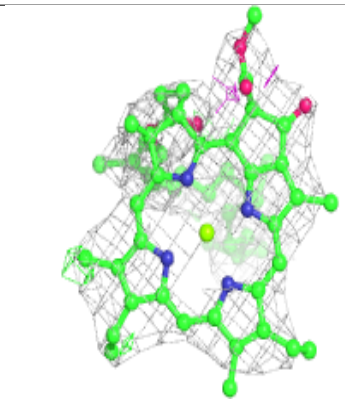
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

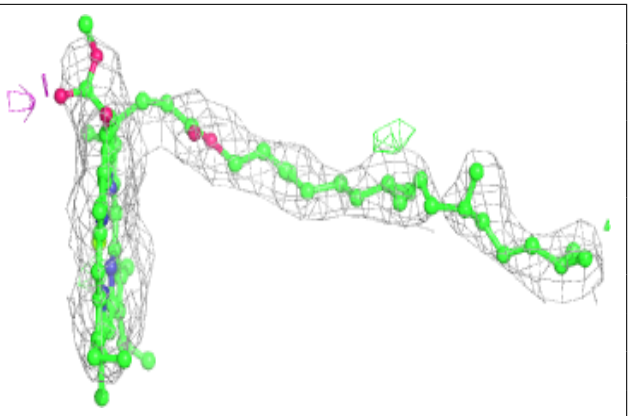


Electron density around CLA BB 609:

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

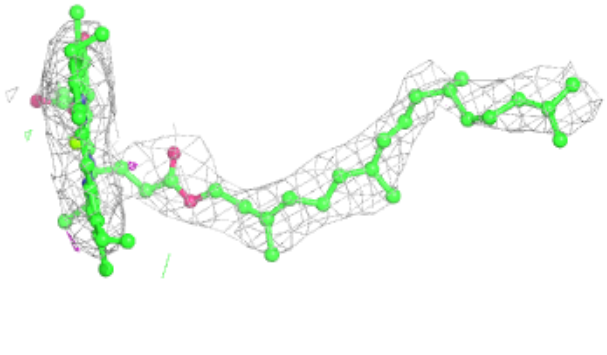


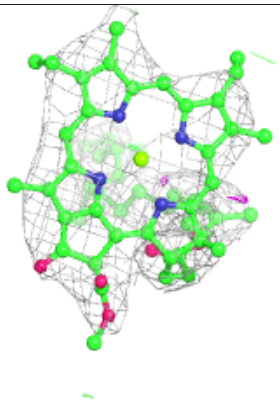


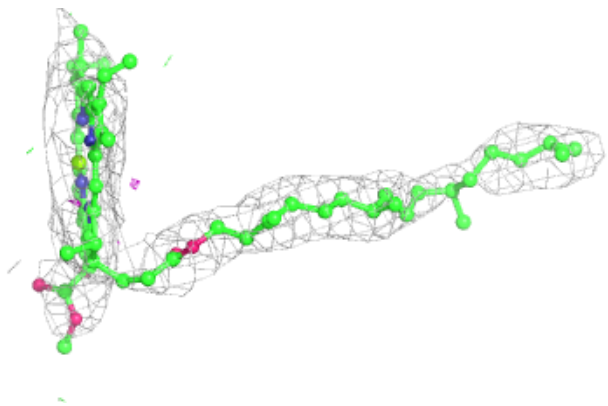


Electron density around CLA AB 606:

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

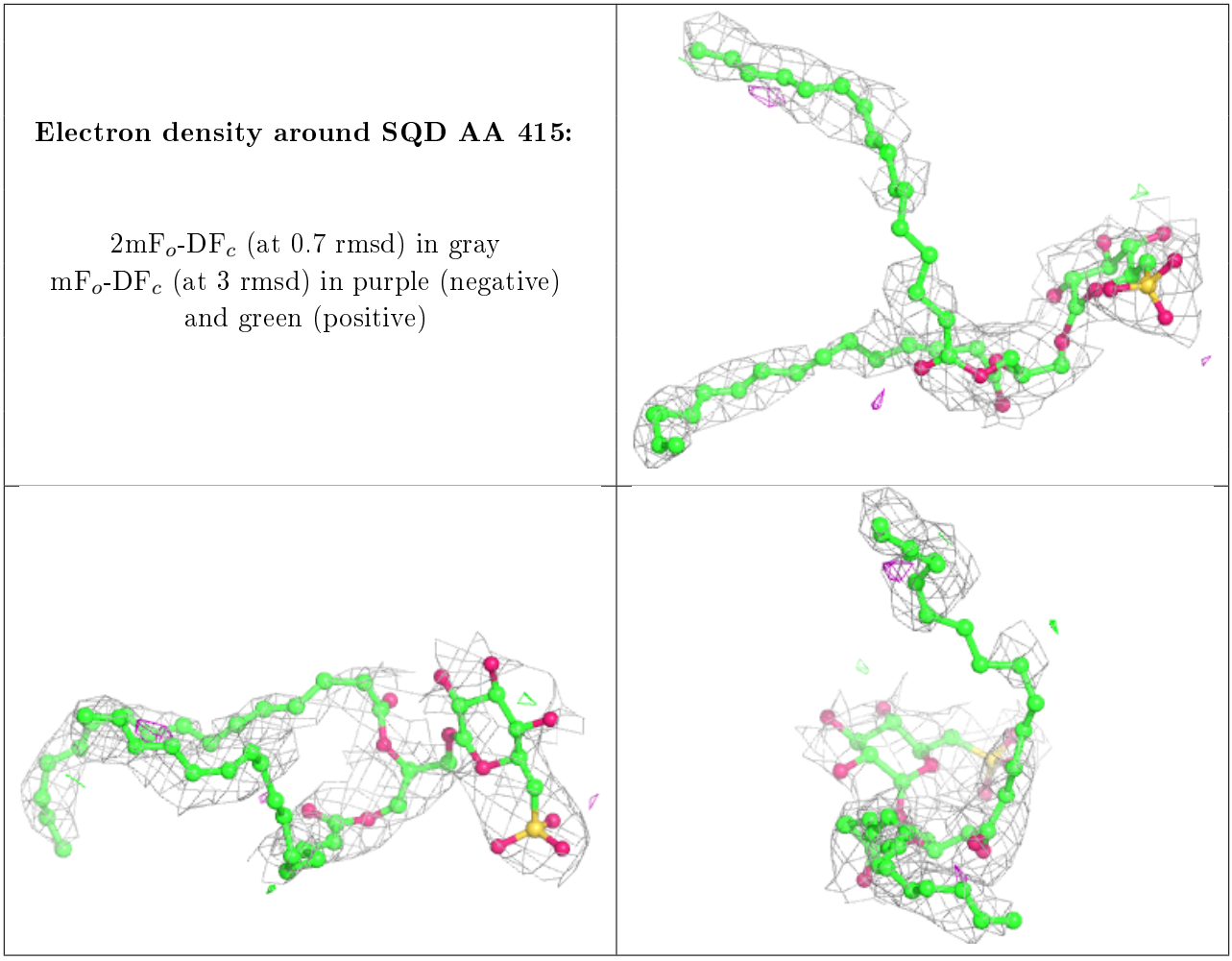






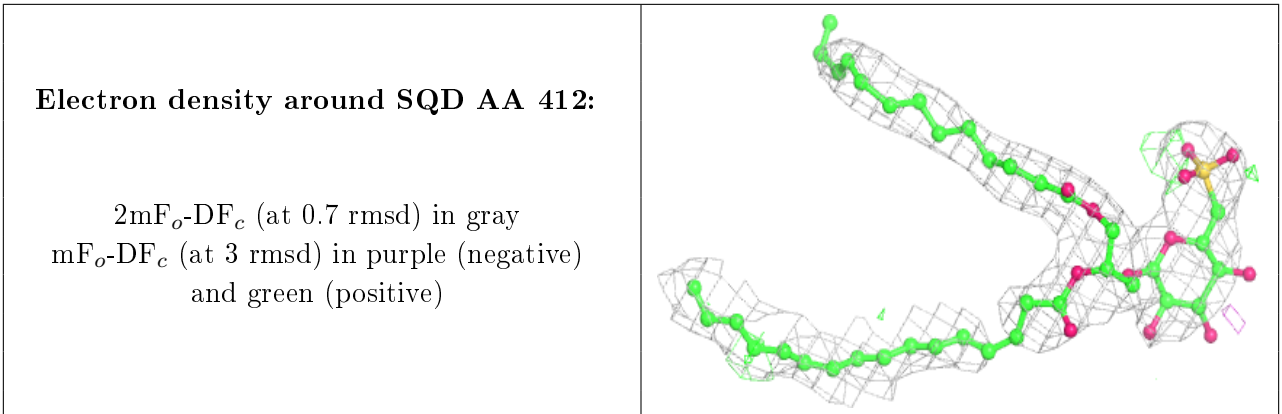
Electron density around SQD AA 415:

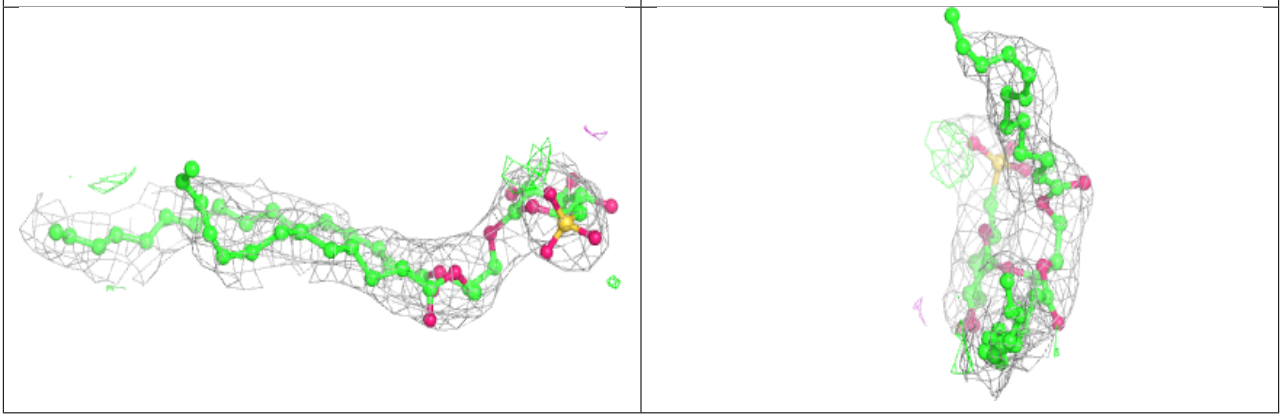
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD AA 412:

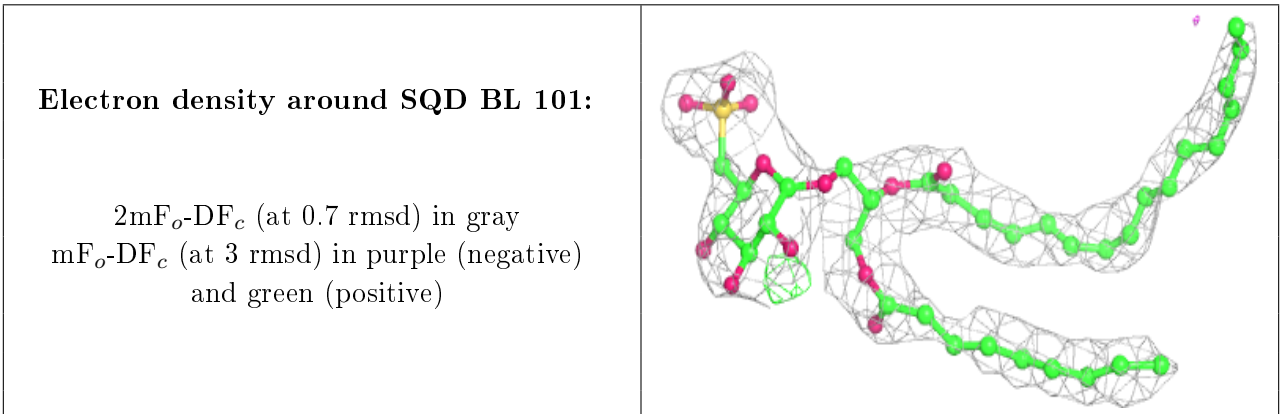
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

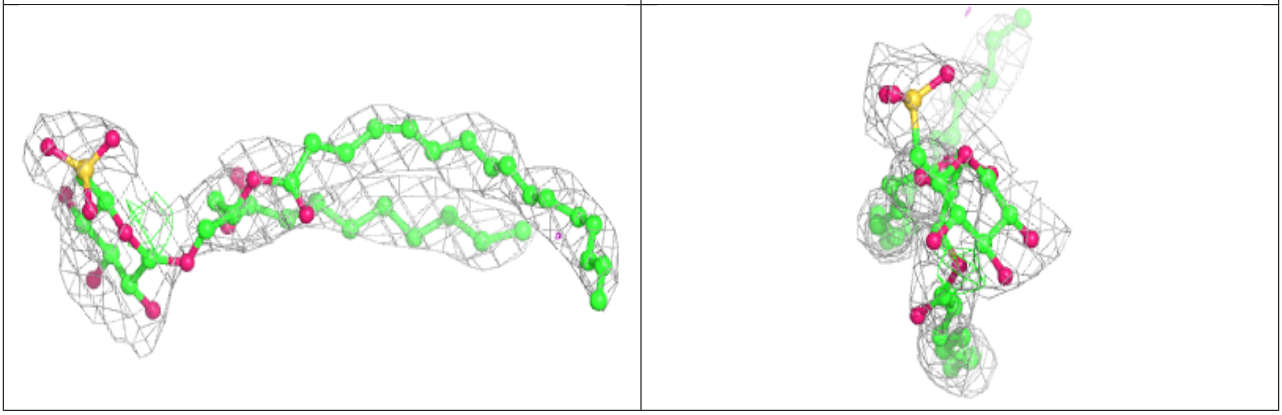




Electron density around SQD BL 101:

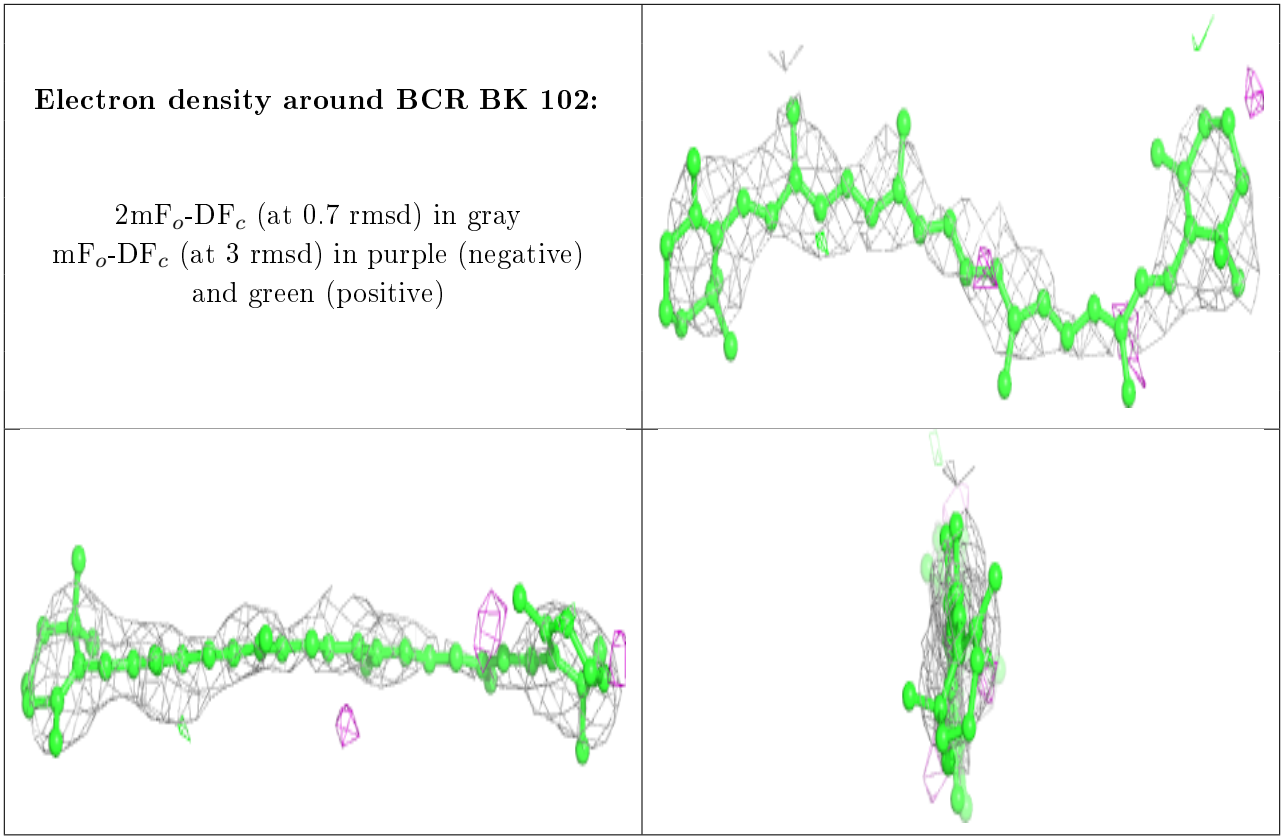
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





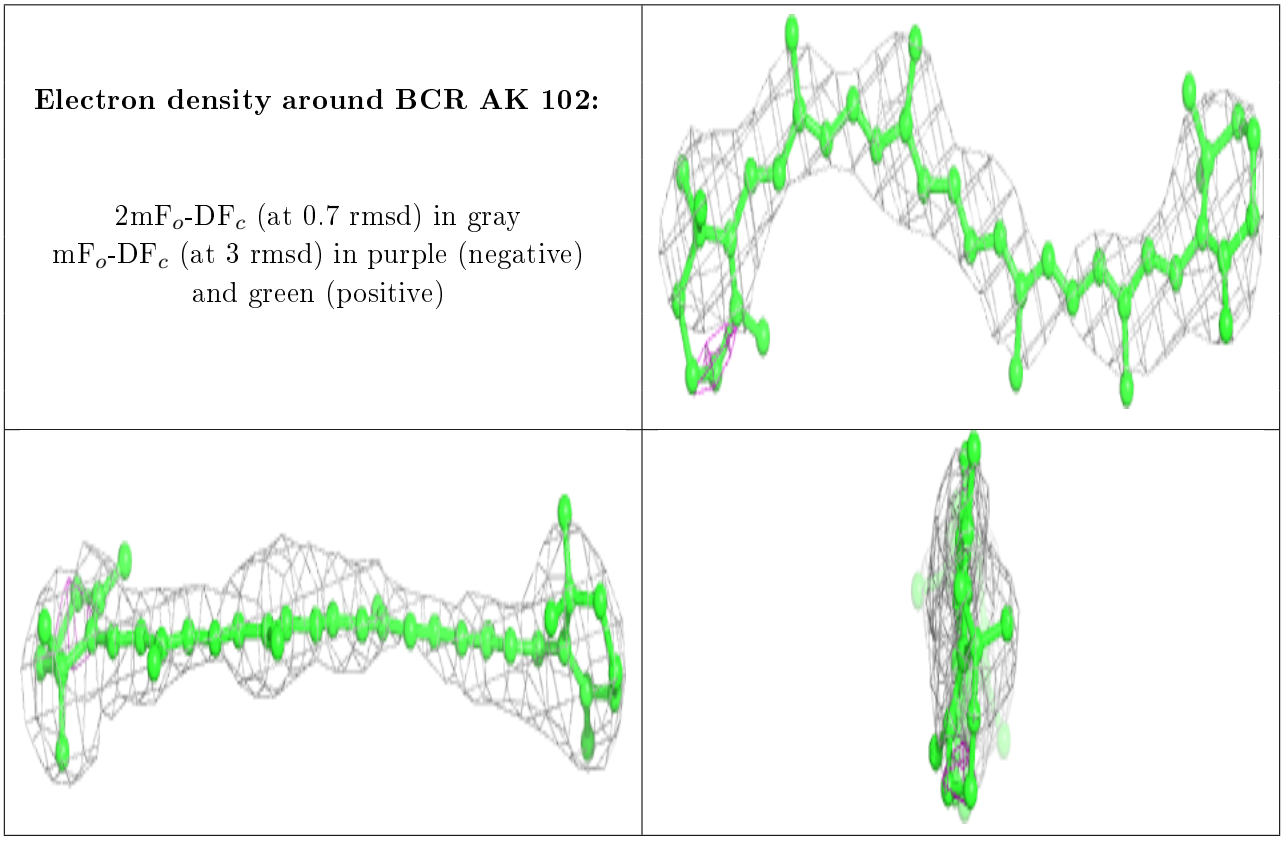
Electron density around BCR BK 102:

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



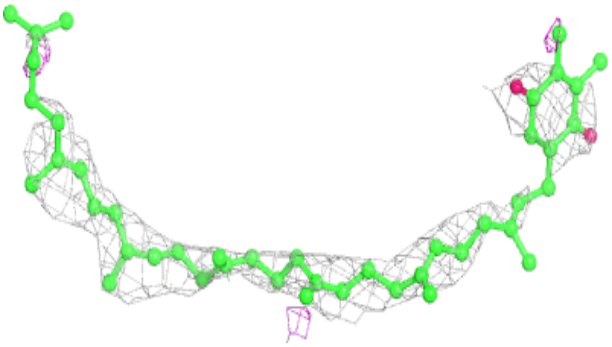
Electron density around BCR AK 102:

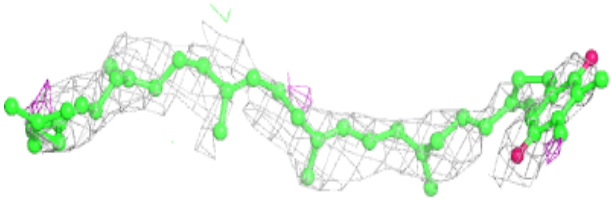
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

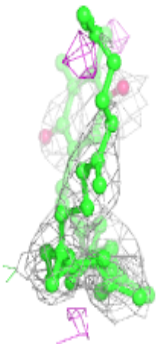


Electron density around PL9 AA 407:

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

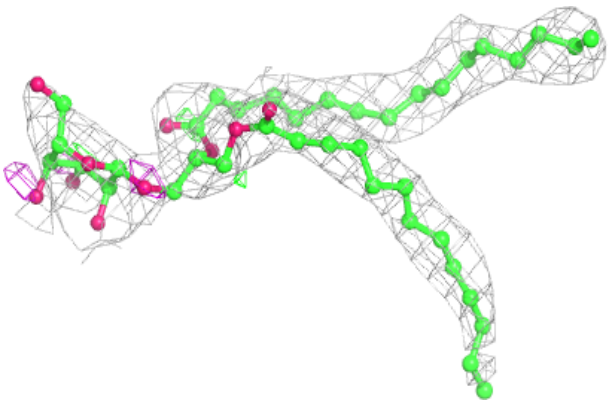


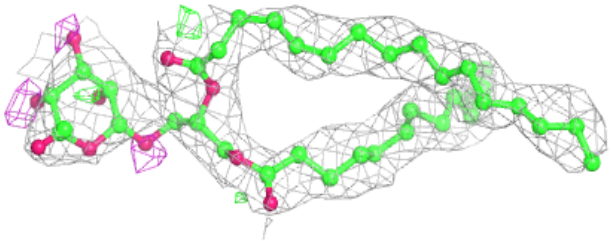




Electron density around LMG BD 408:

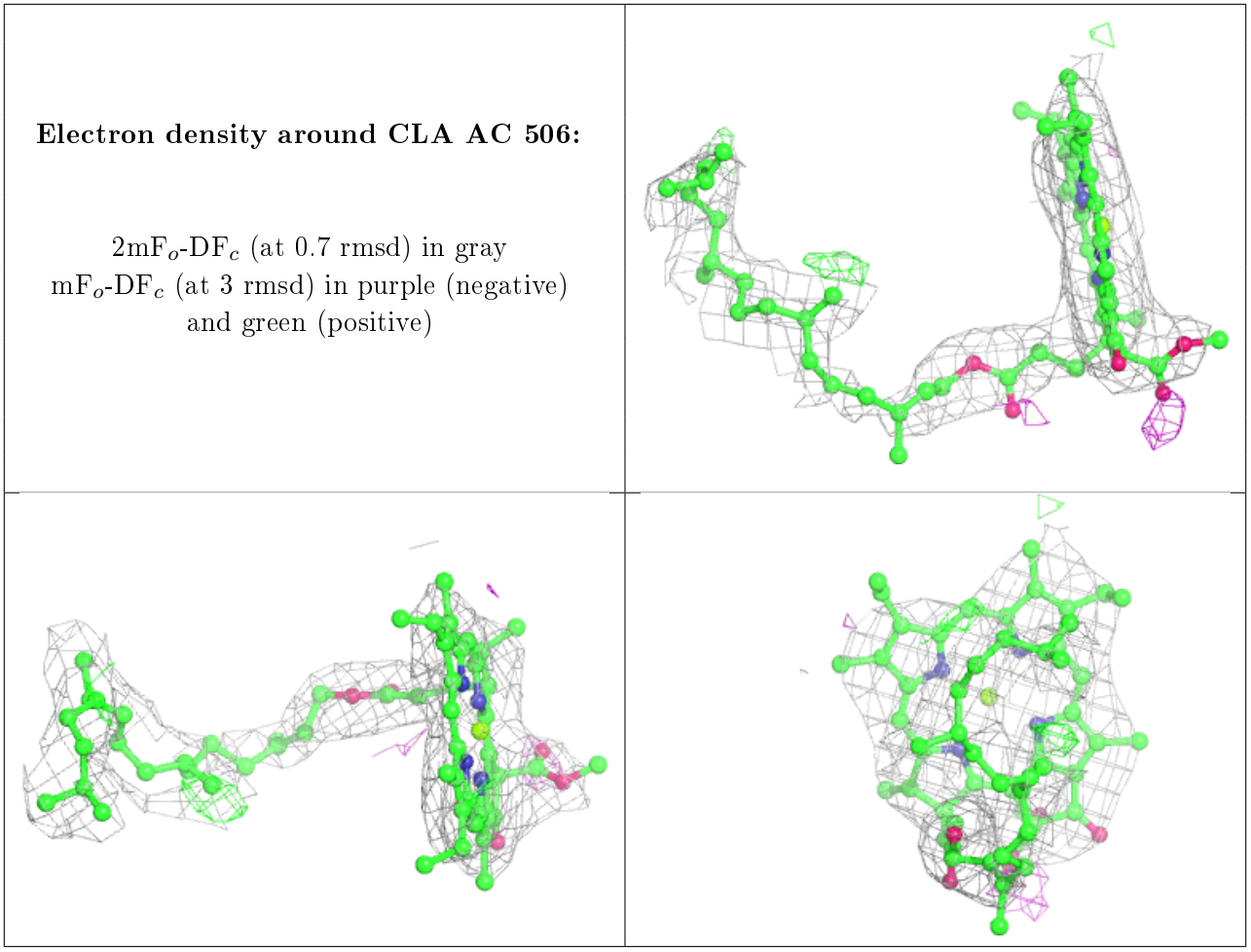
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





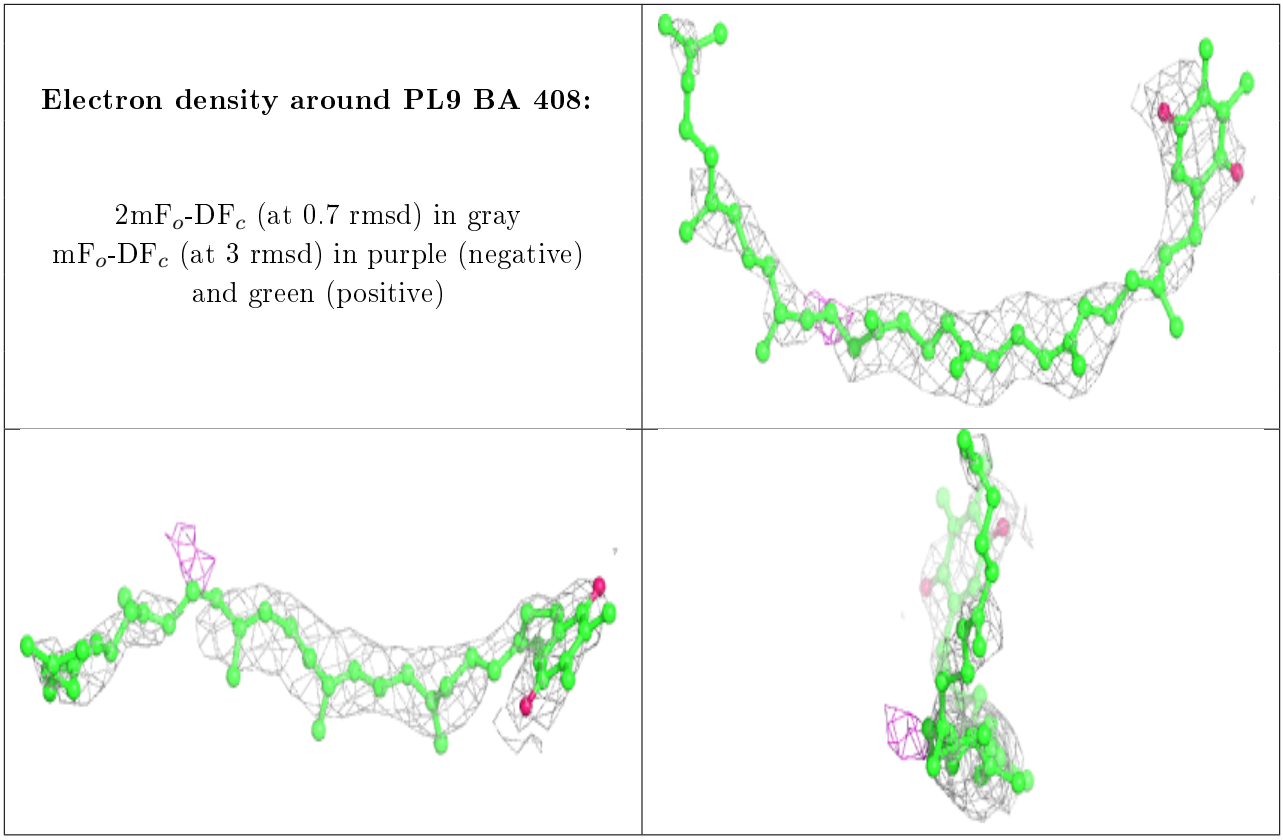
Electron density around CLA AC 506:

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



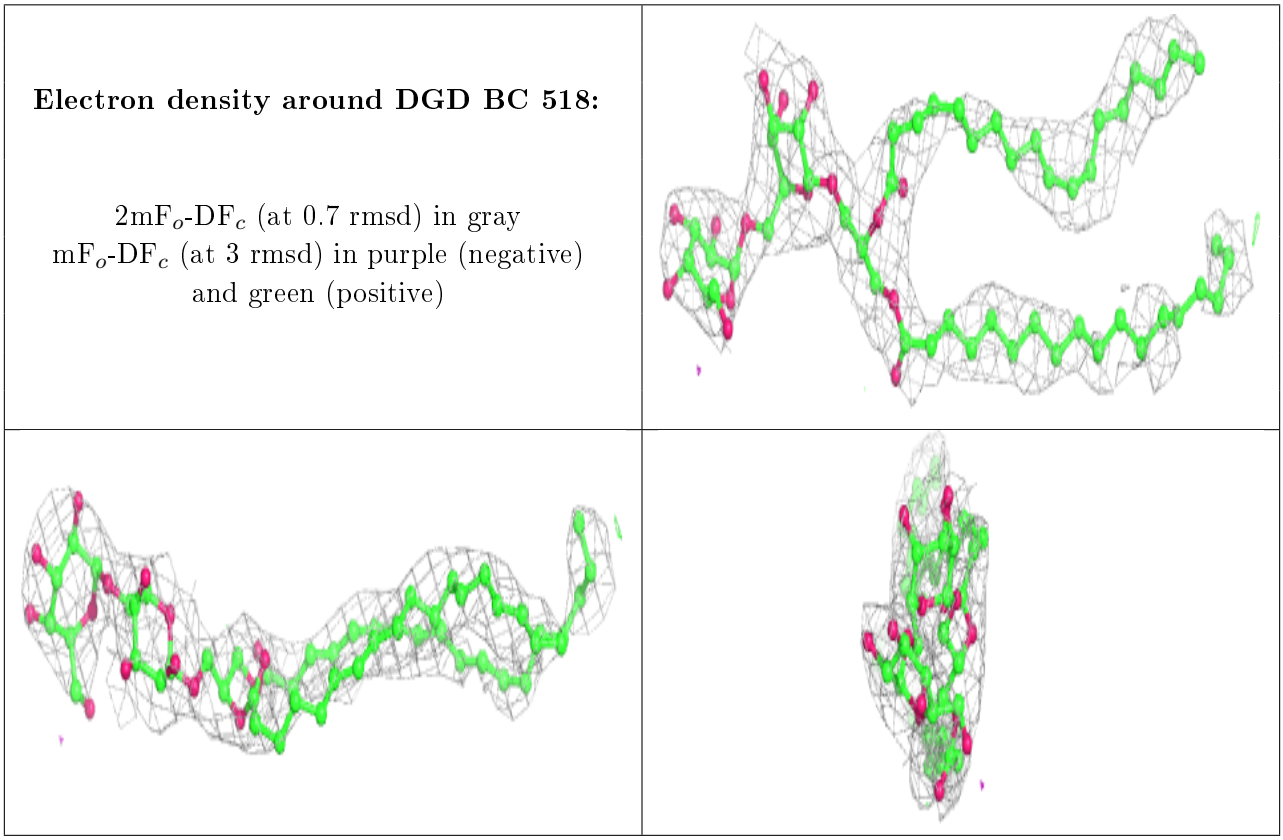
Electron density around PL9 BA 408:

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



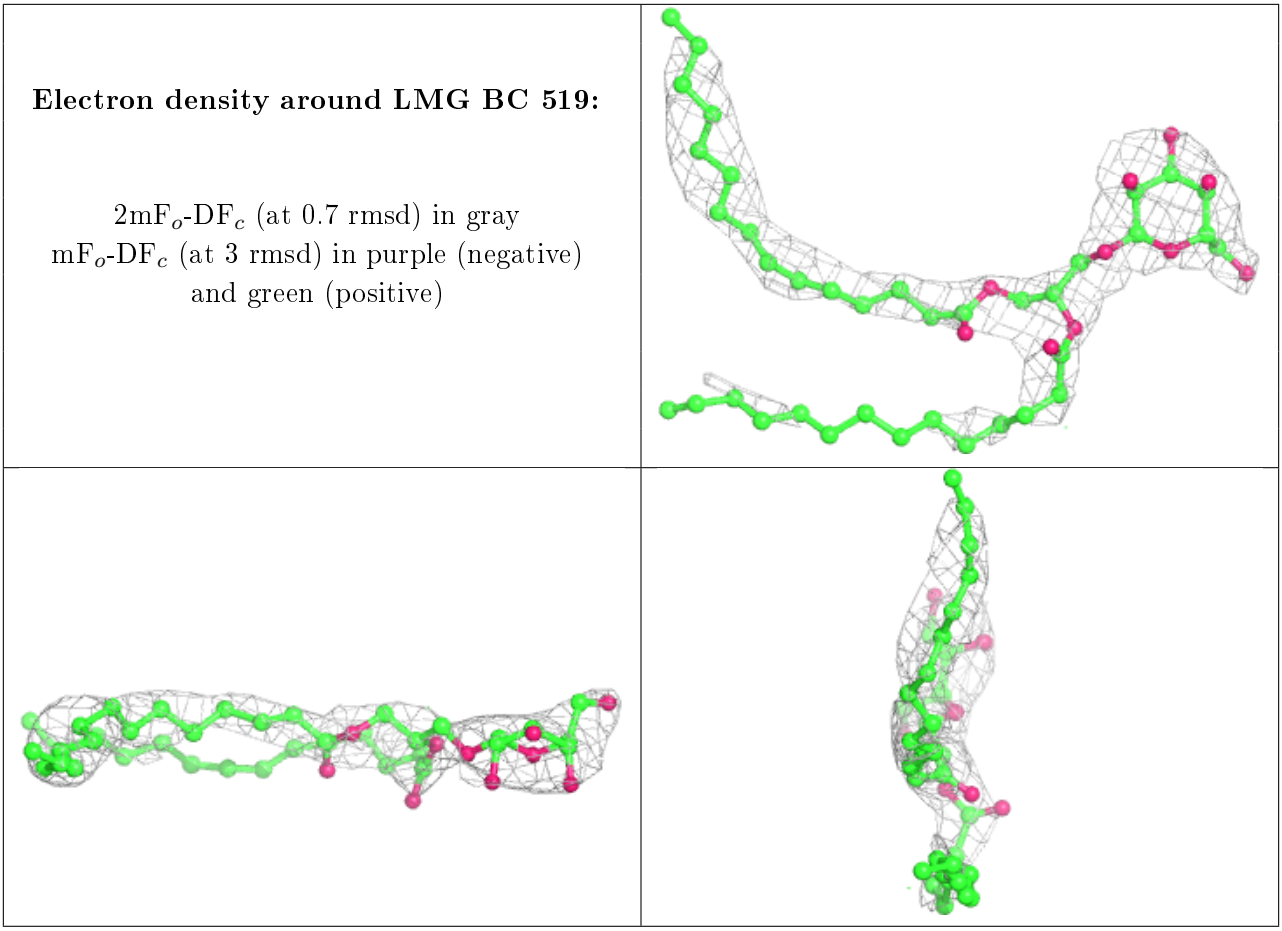
Electron density around DGD BC 518:

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



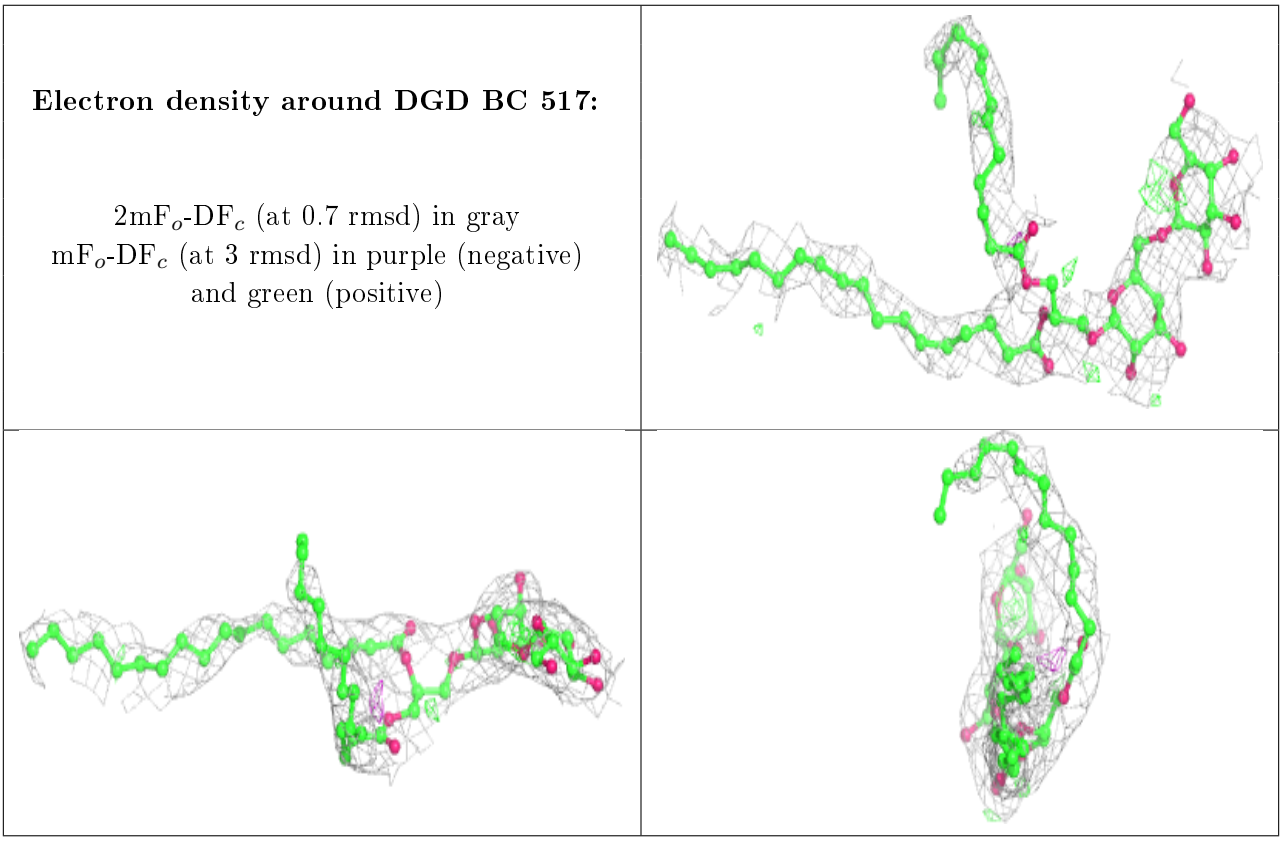
Electron density around LMG BC 519:

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



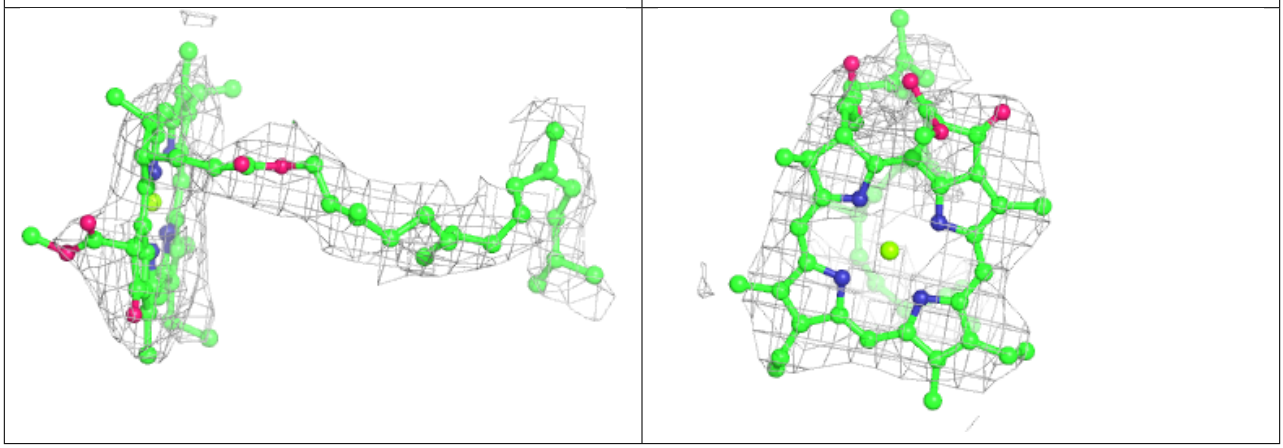
Electron density around DGD BC 517:

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



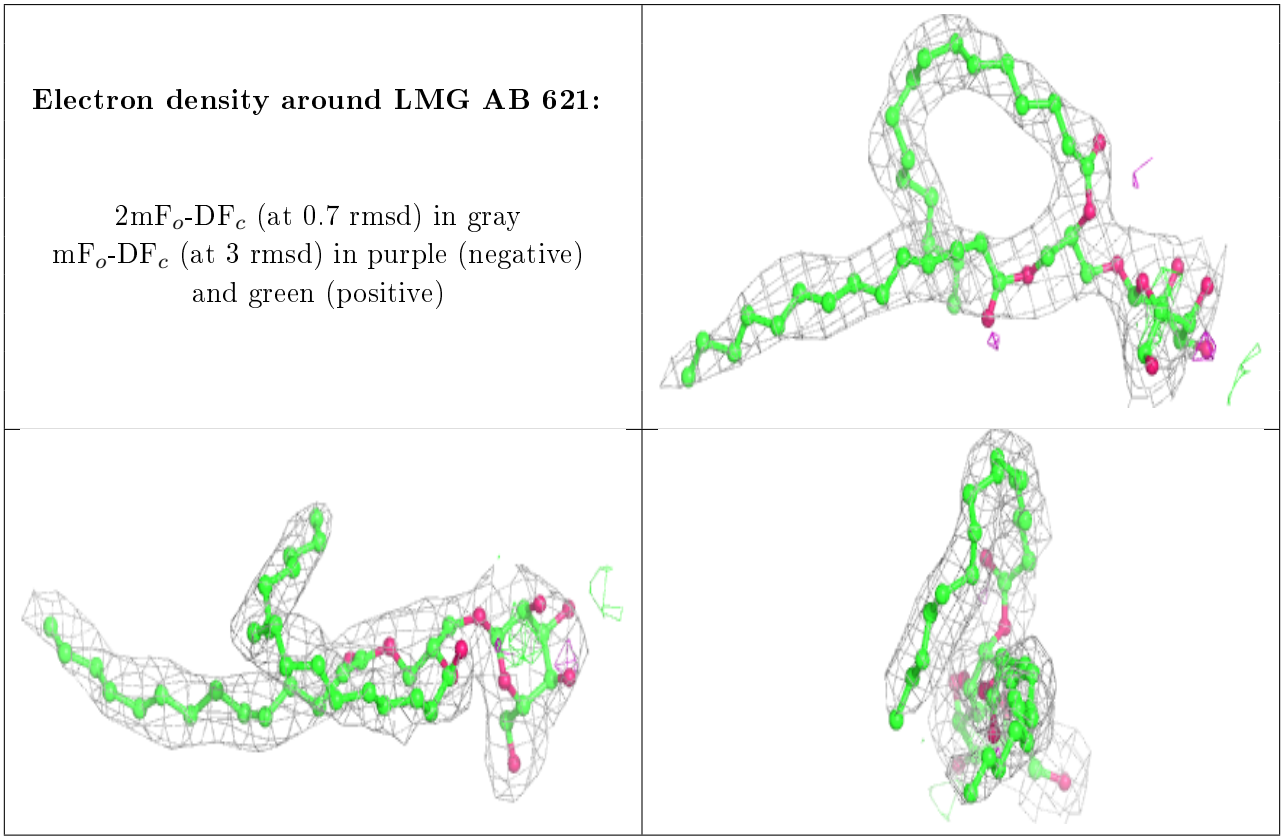
Electron density around CLA BC 506:

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



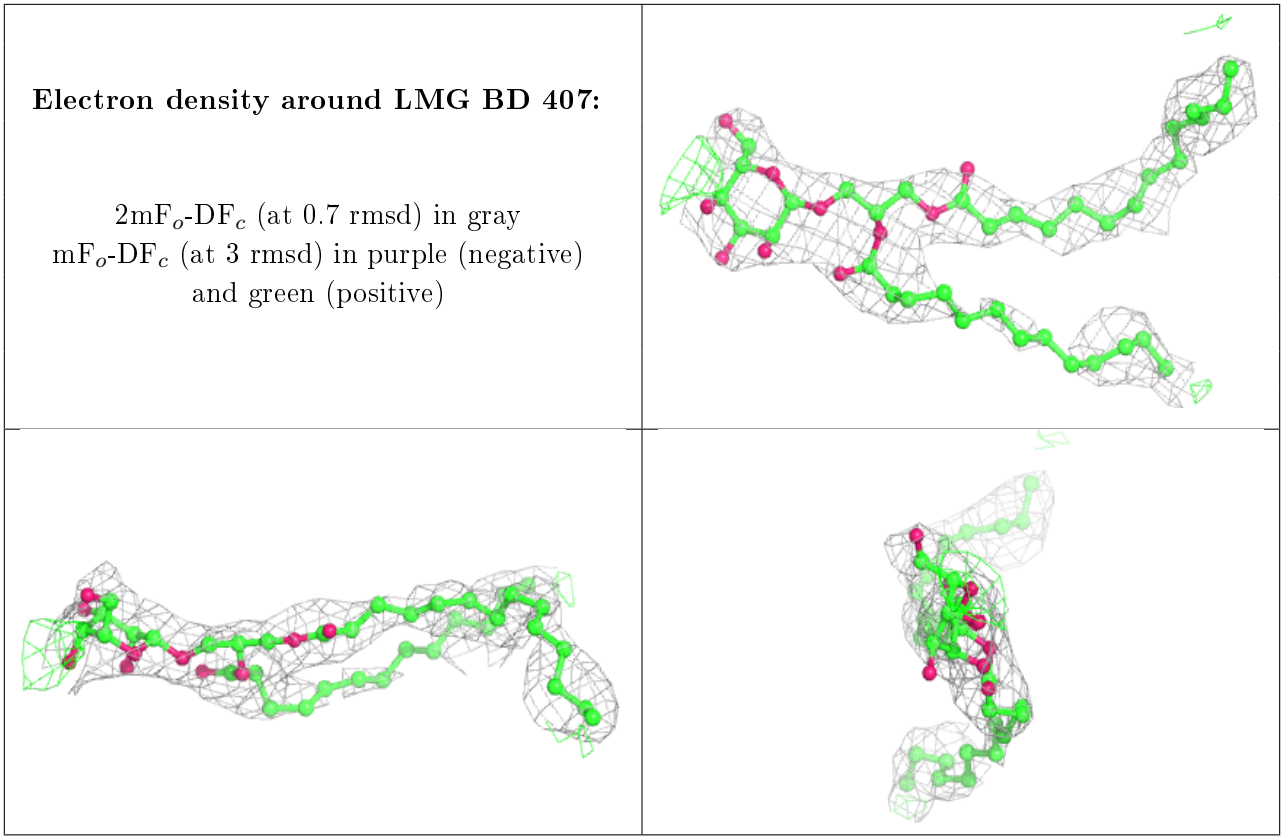
Electron density around LMG AB 621:

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



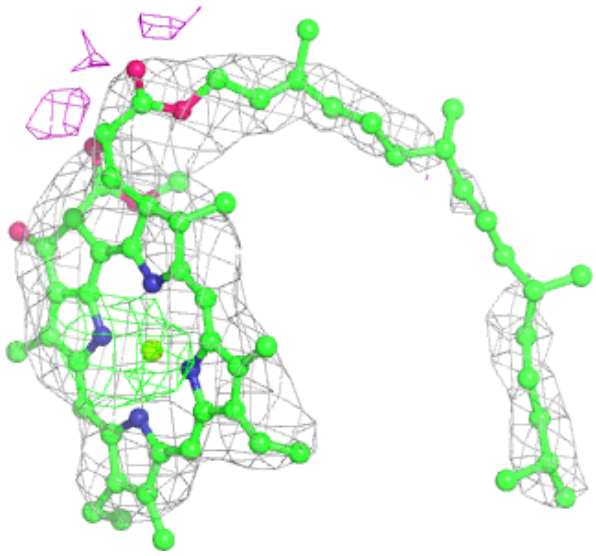
Electron density around LMG BD 407:

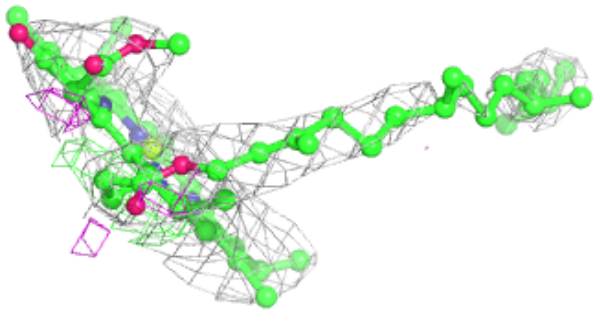
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

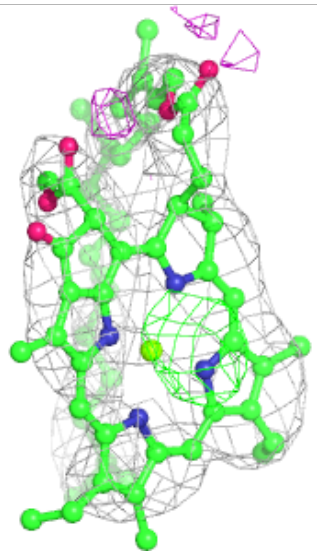


Electron density around CLA AC 507:

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

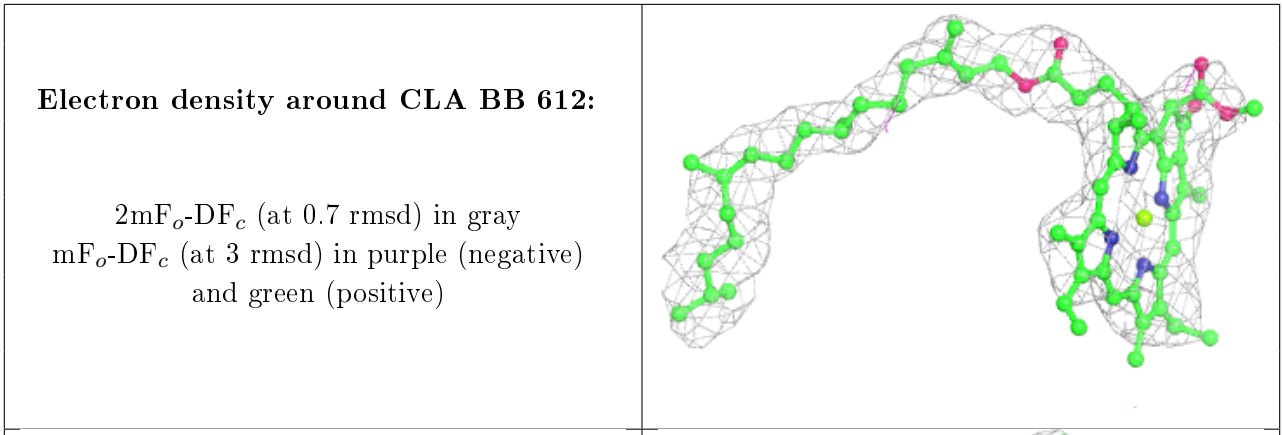






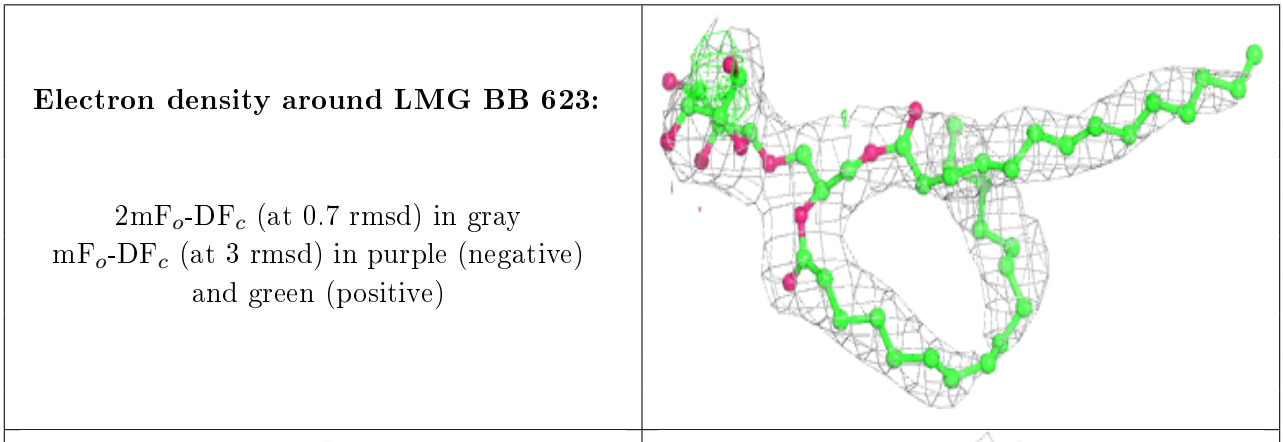
Electron density around CLA BB 612:

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



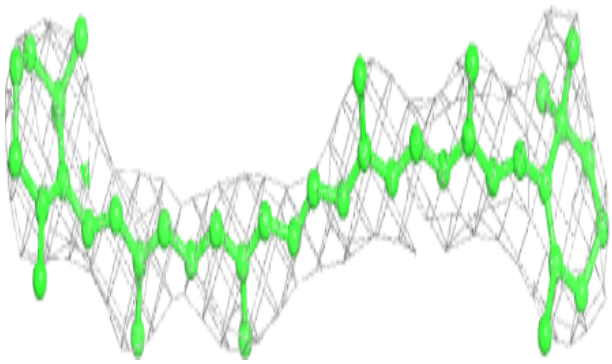
Electron density around LMG BB 623:

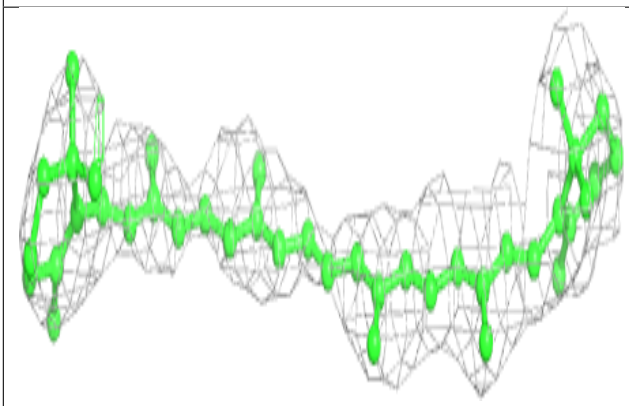
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

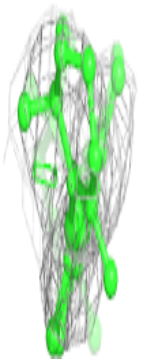


Electron density around BCR AB 620:

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

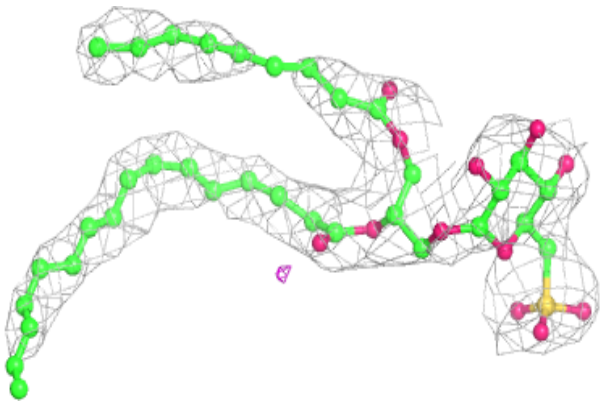


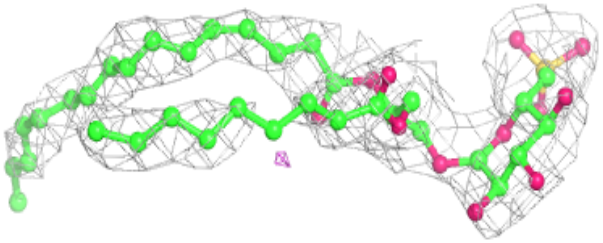


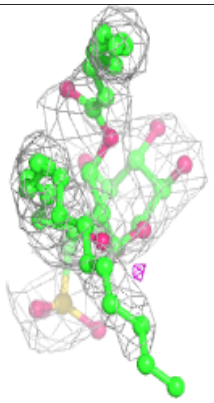


Electron density around SQD BB 601:

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

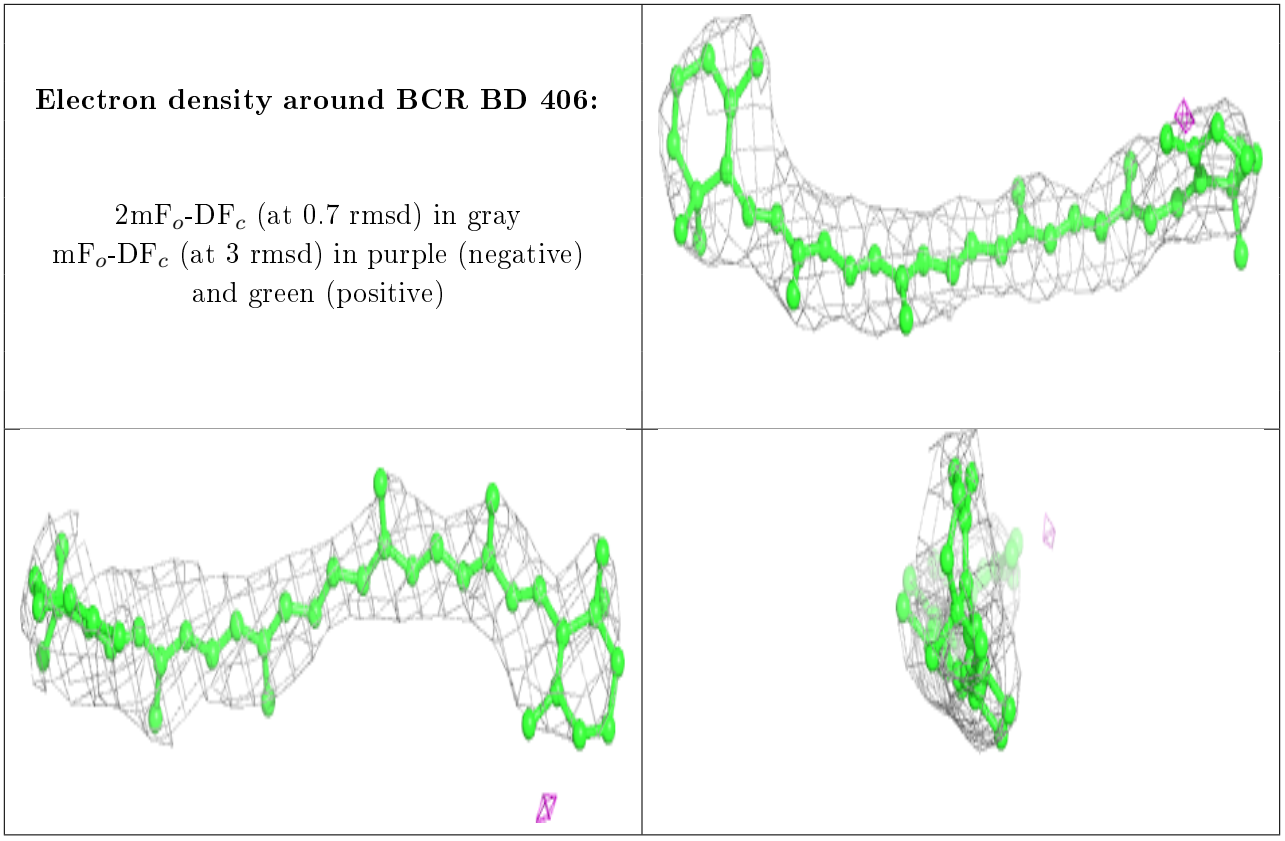






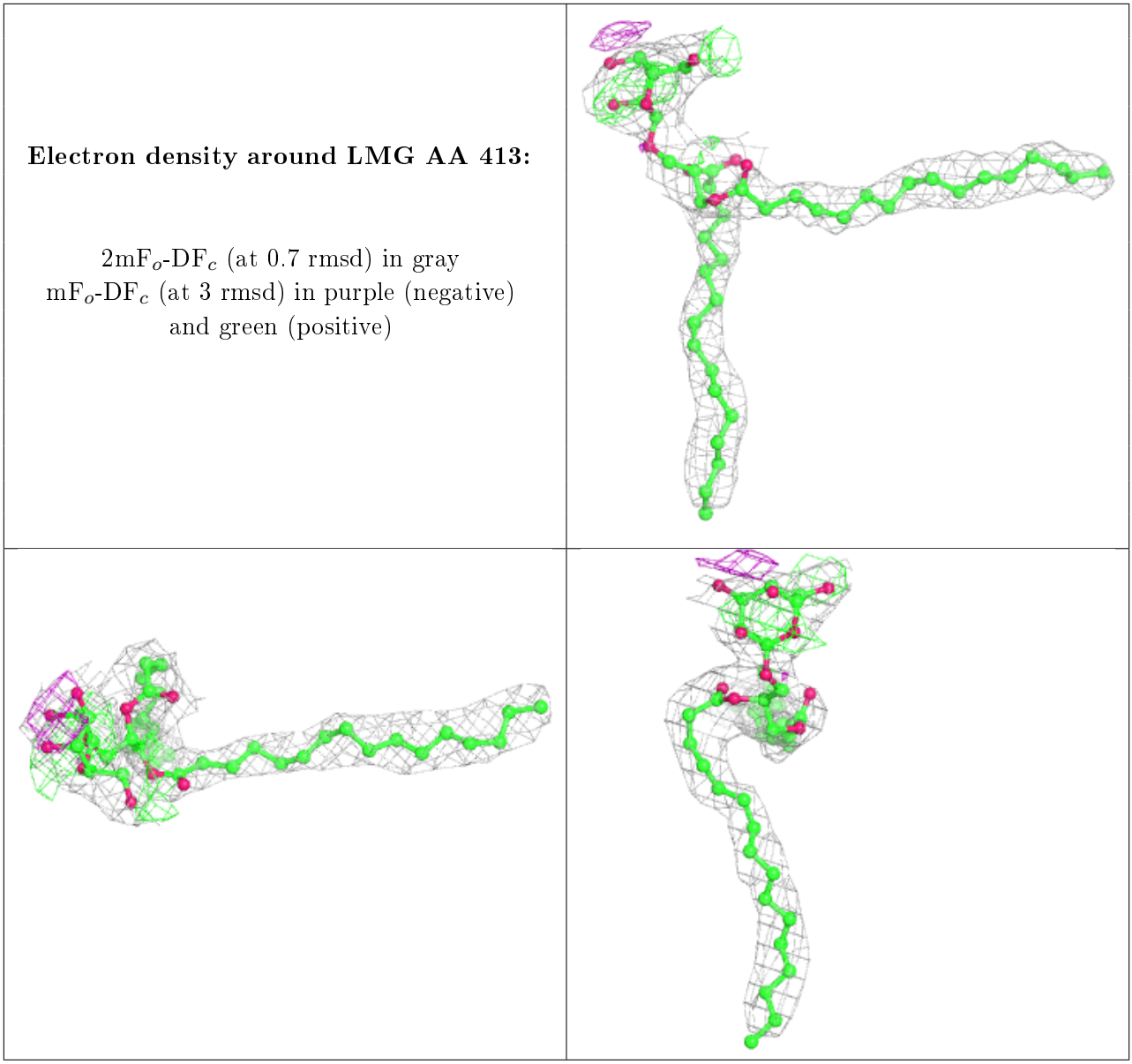
Electron density around BCR BD 406:

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



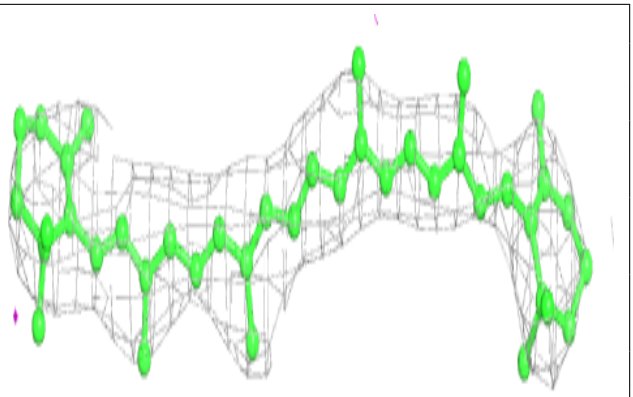
Electron density around LMG AA 413:

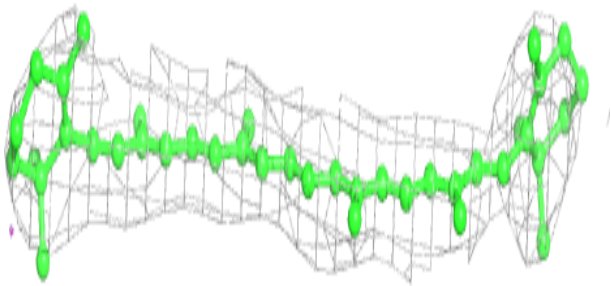
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

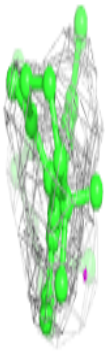


Electron density around BCR AC 515:

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

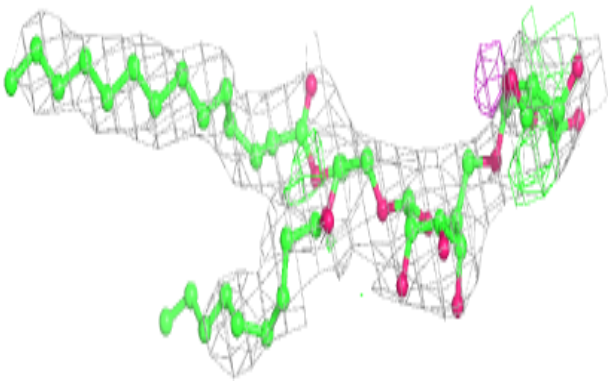


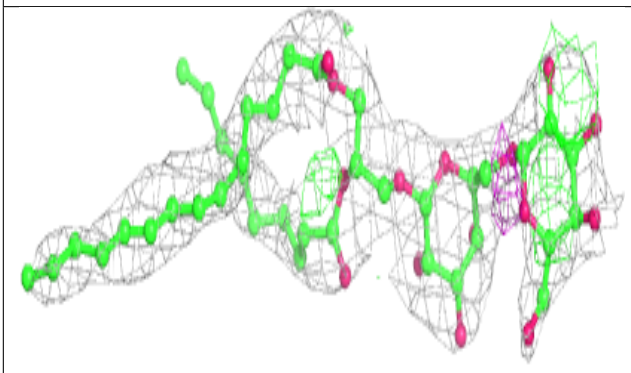


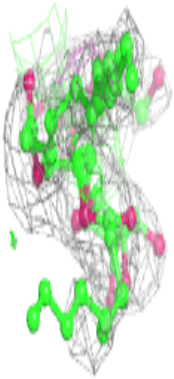


Electron density around DGD AC 516:

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

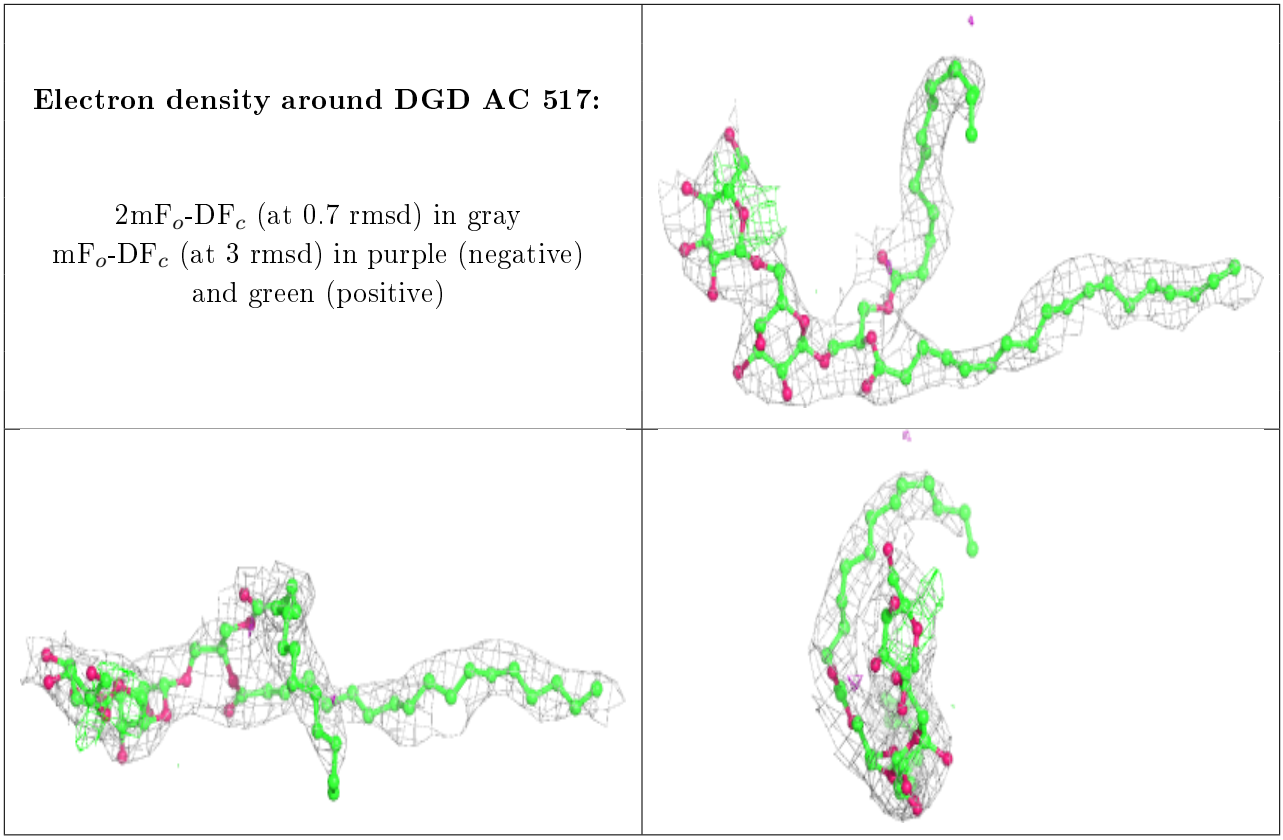






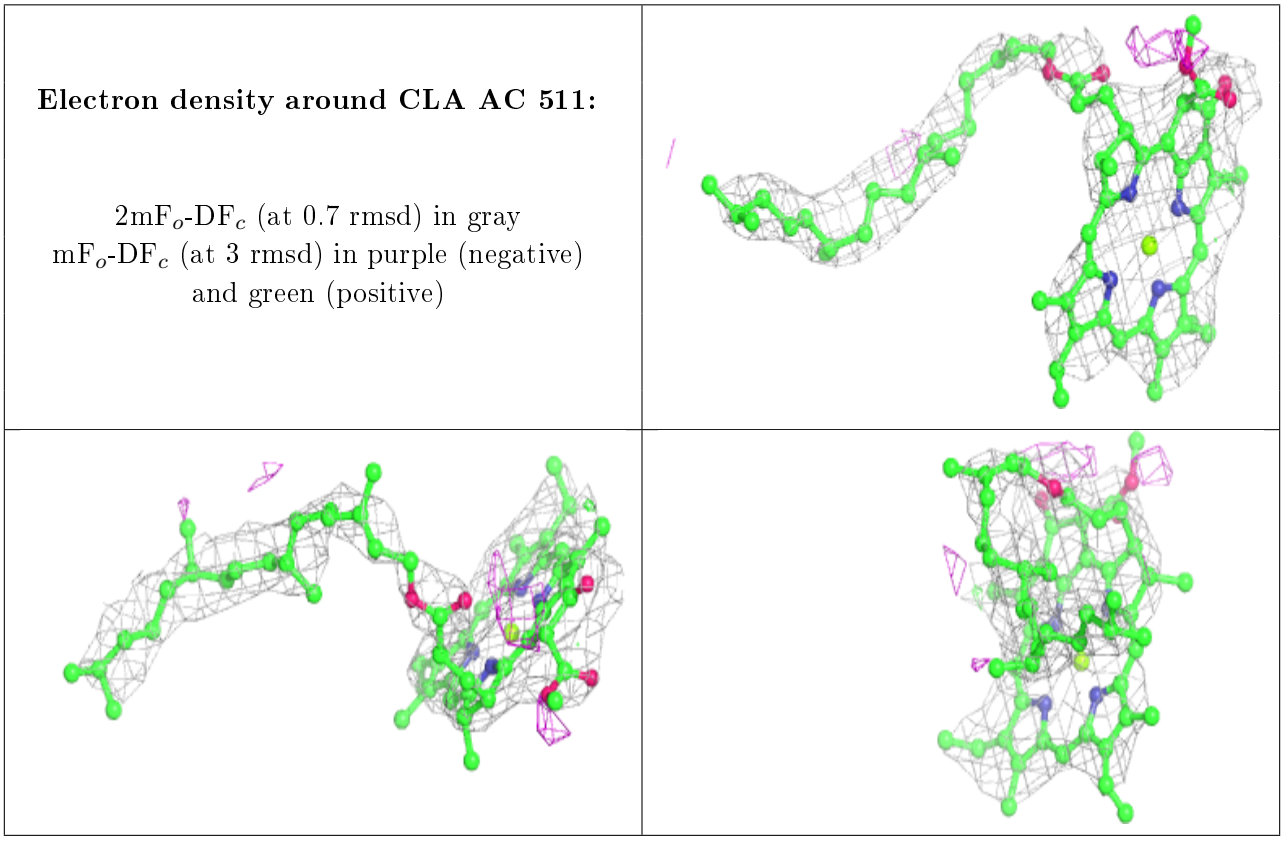
Electron density around DGD AC 517:

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



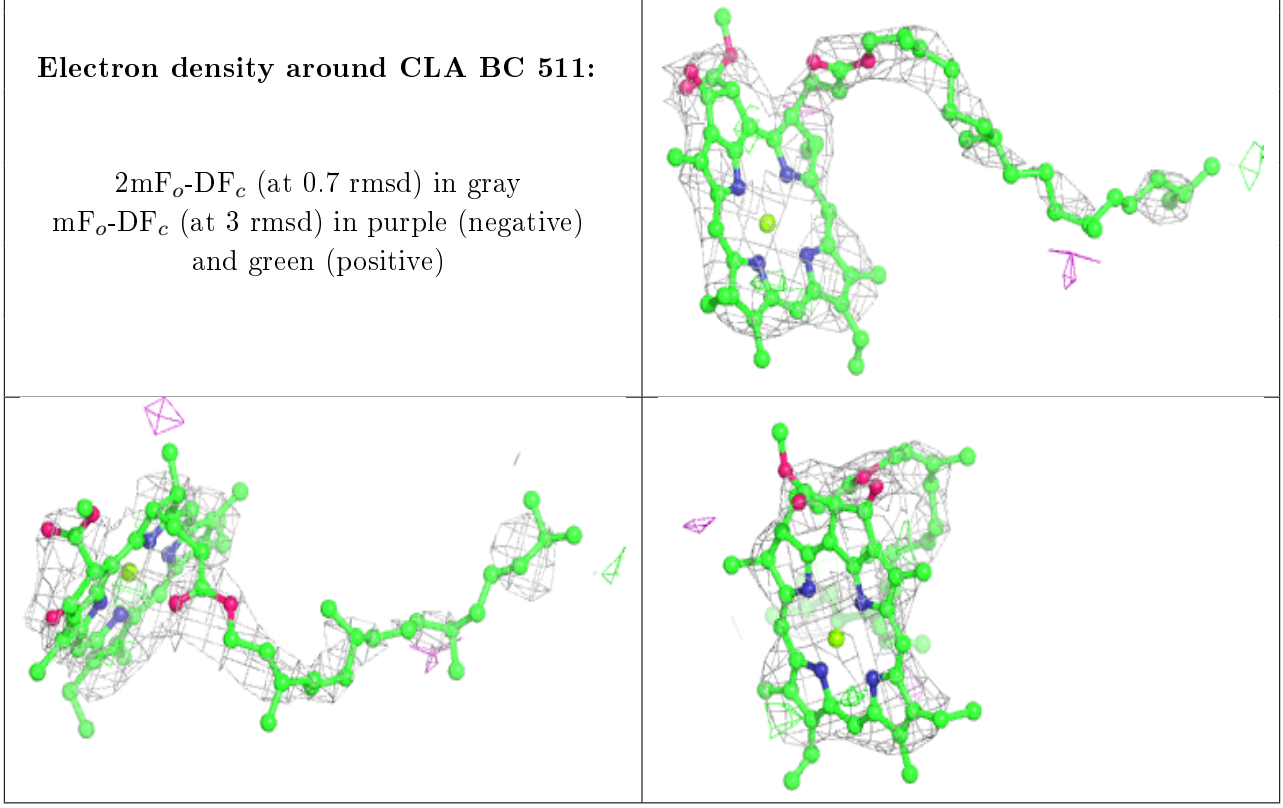
Electron density around CLA AC 511:

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



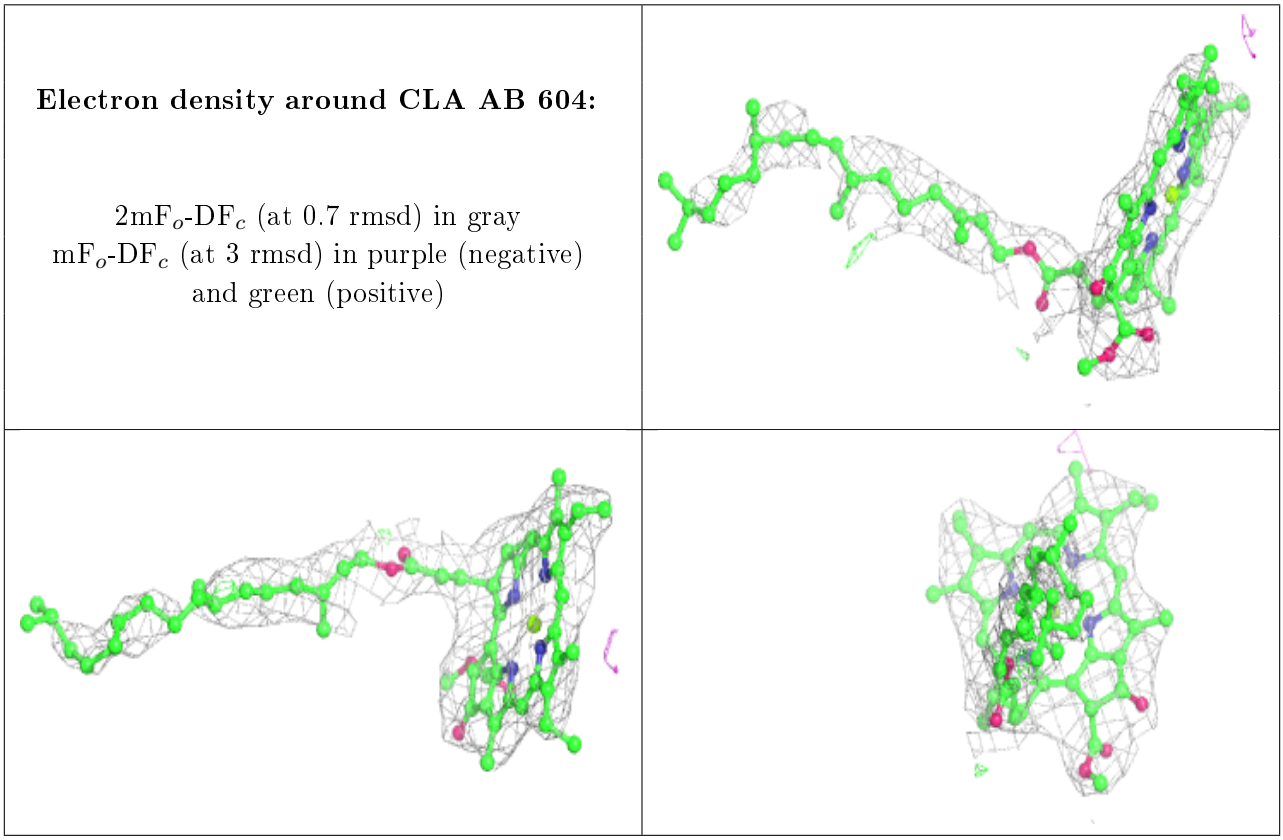
Electron density around CLA BC 511:

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



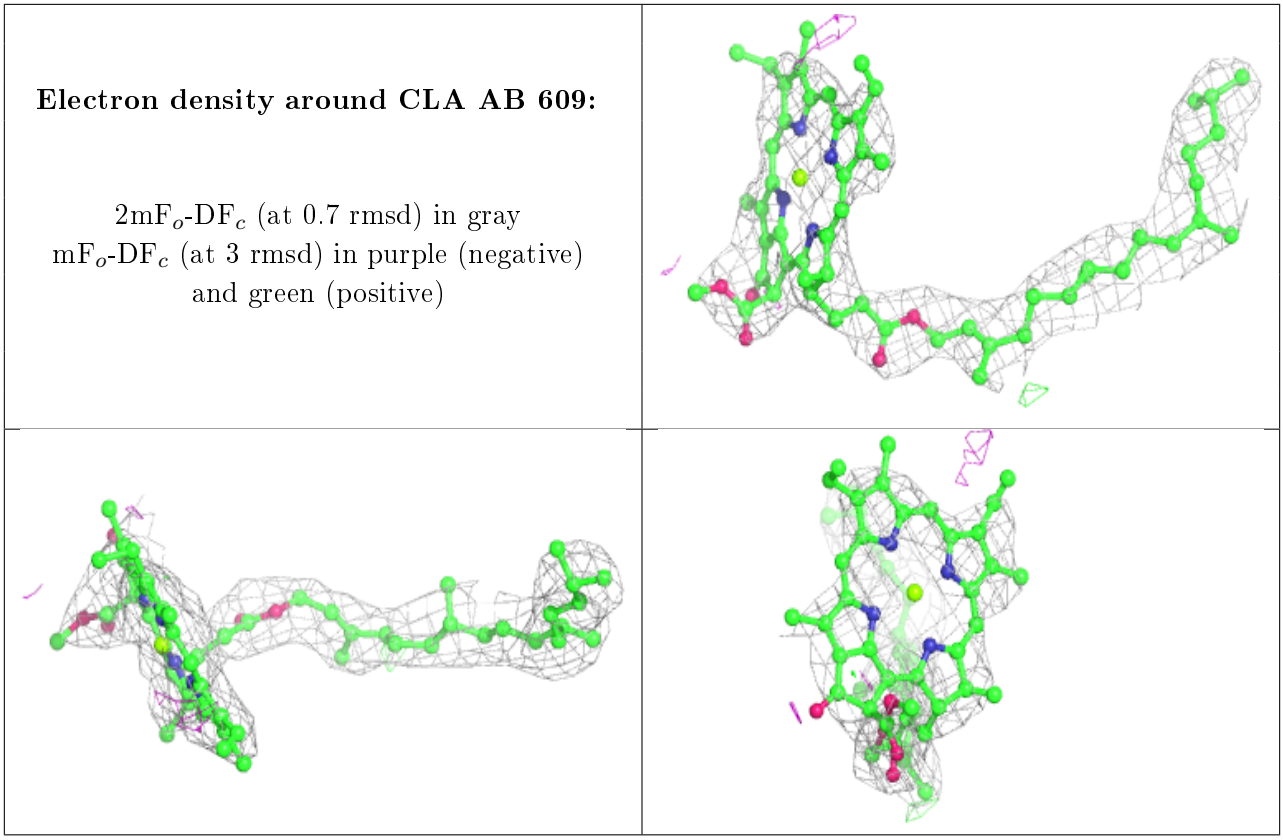
Electron density around CLA AB 604:

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



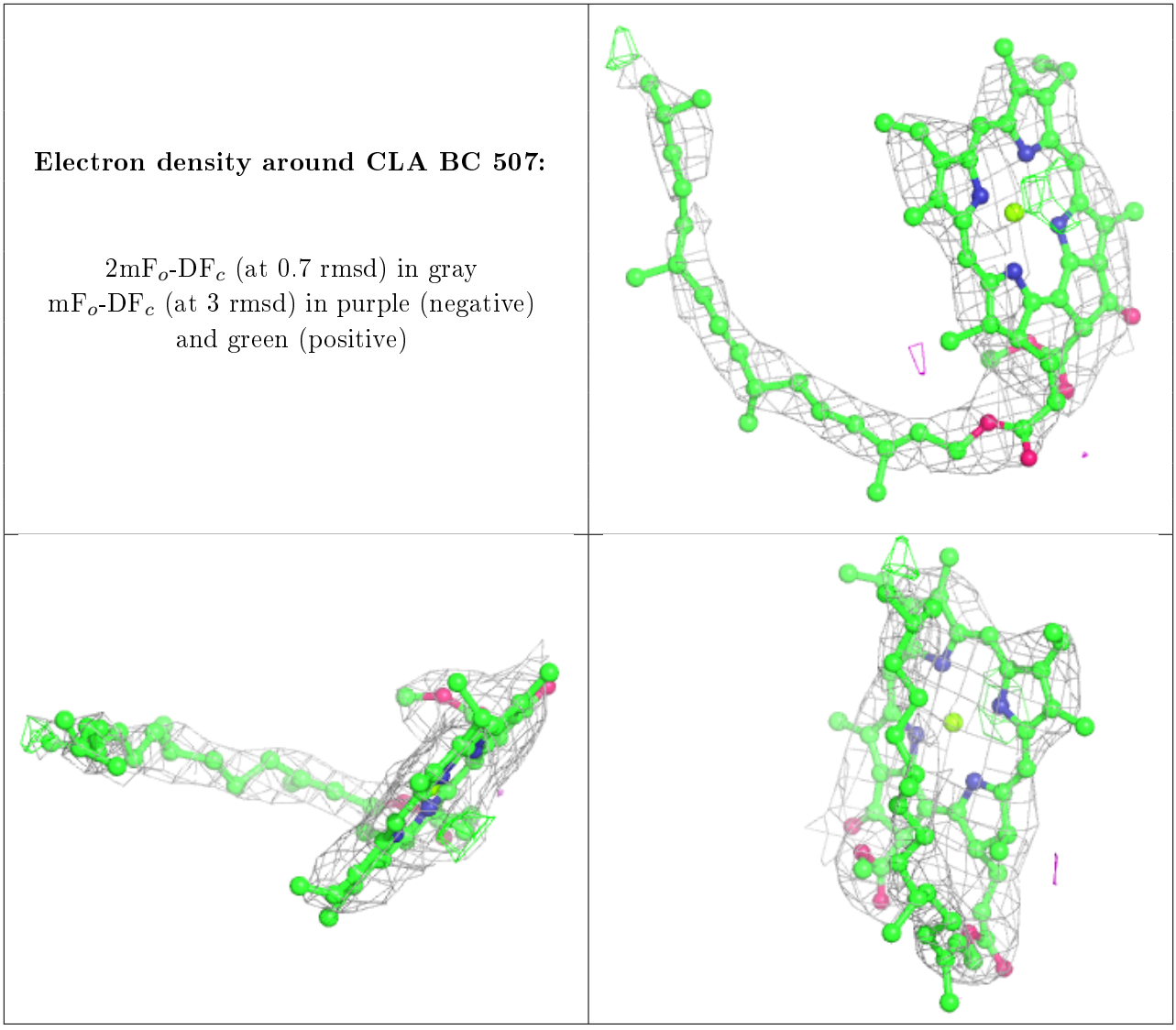
Electron density around CLA AB 609:

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



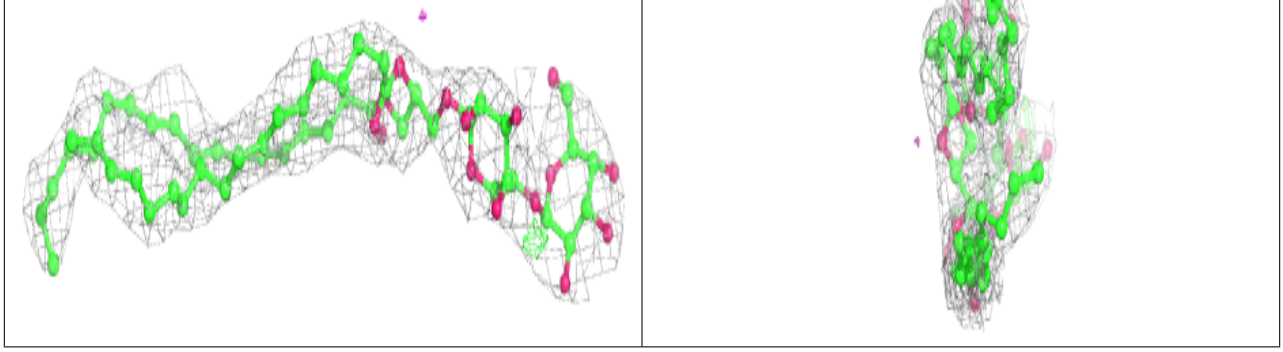
Electron density around CLA BC 507:

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



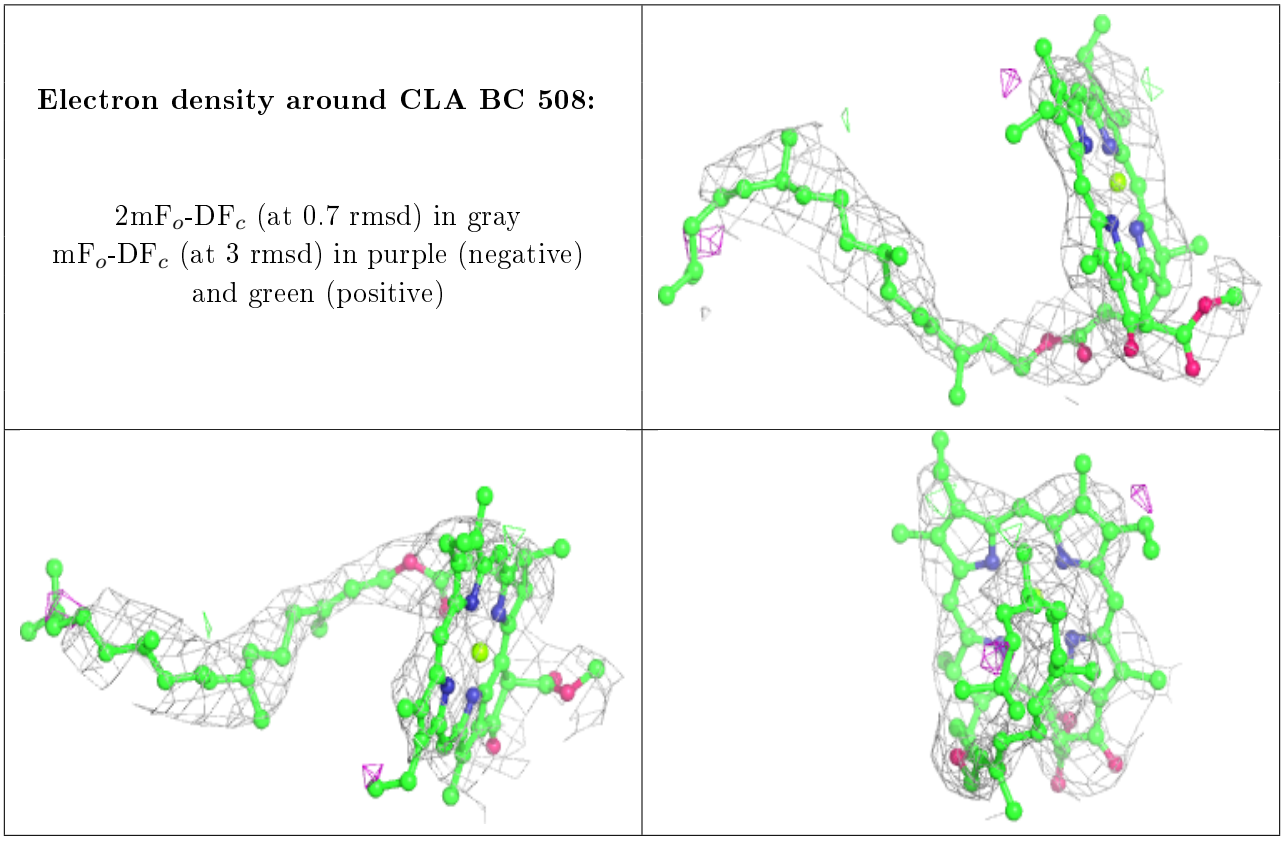
Electron density around DGD AC 518:

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



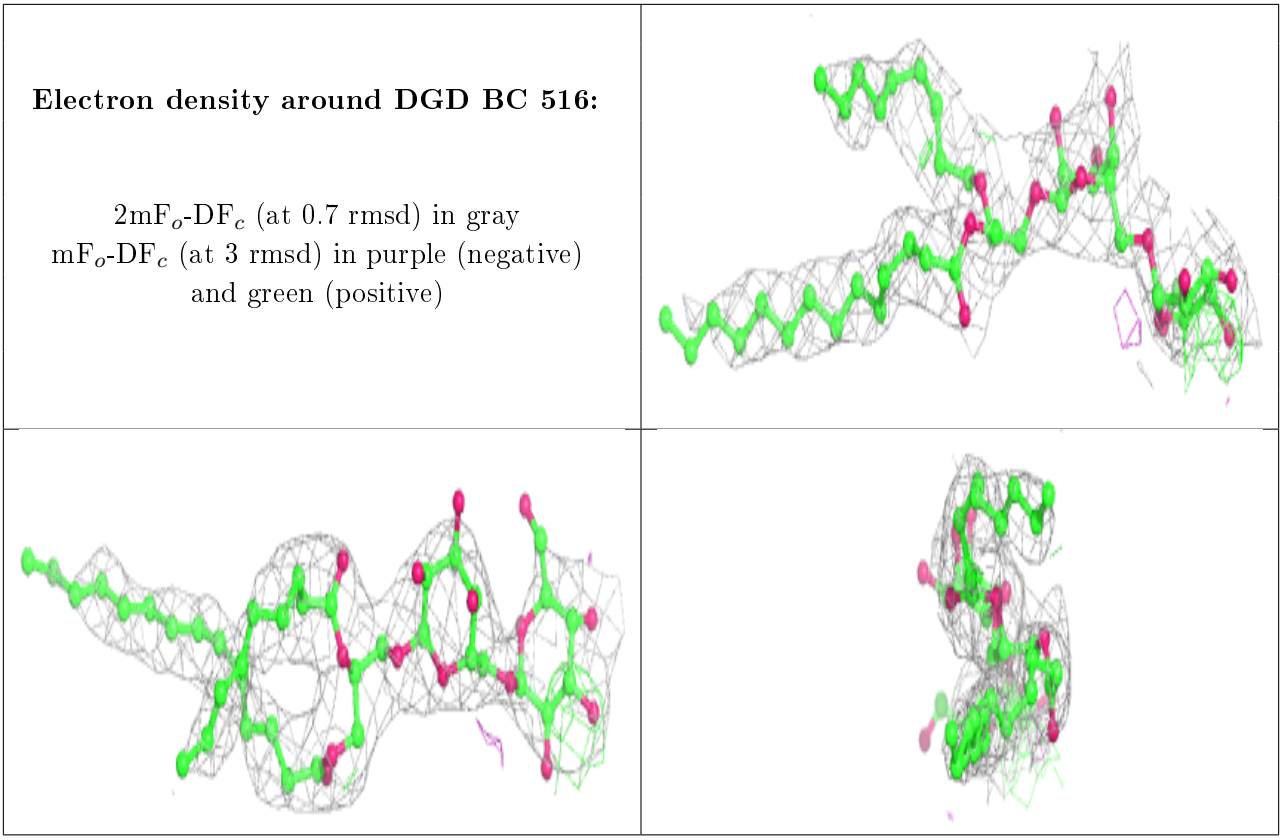
Electron density around CLA BC 508:

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



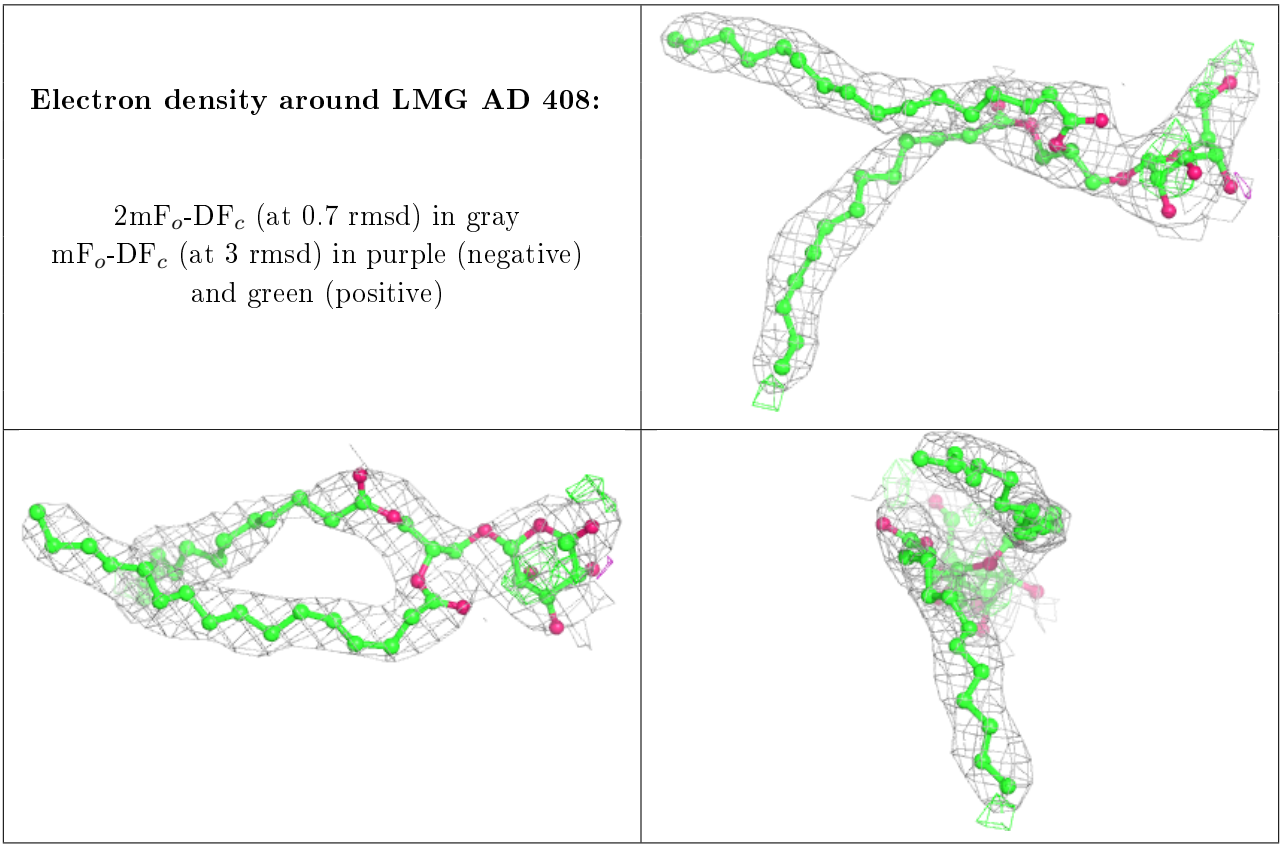
Electron density around DGD BC 516:

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



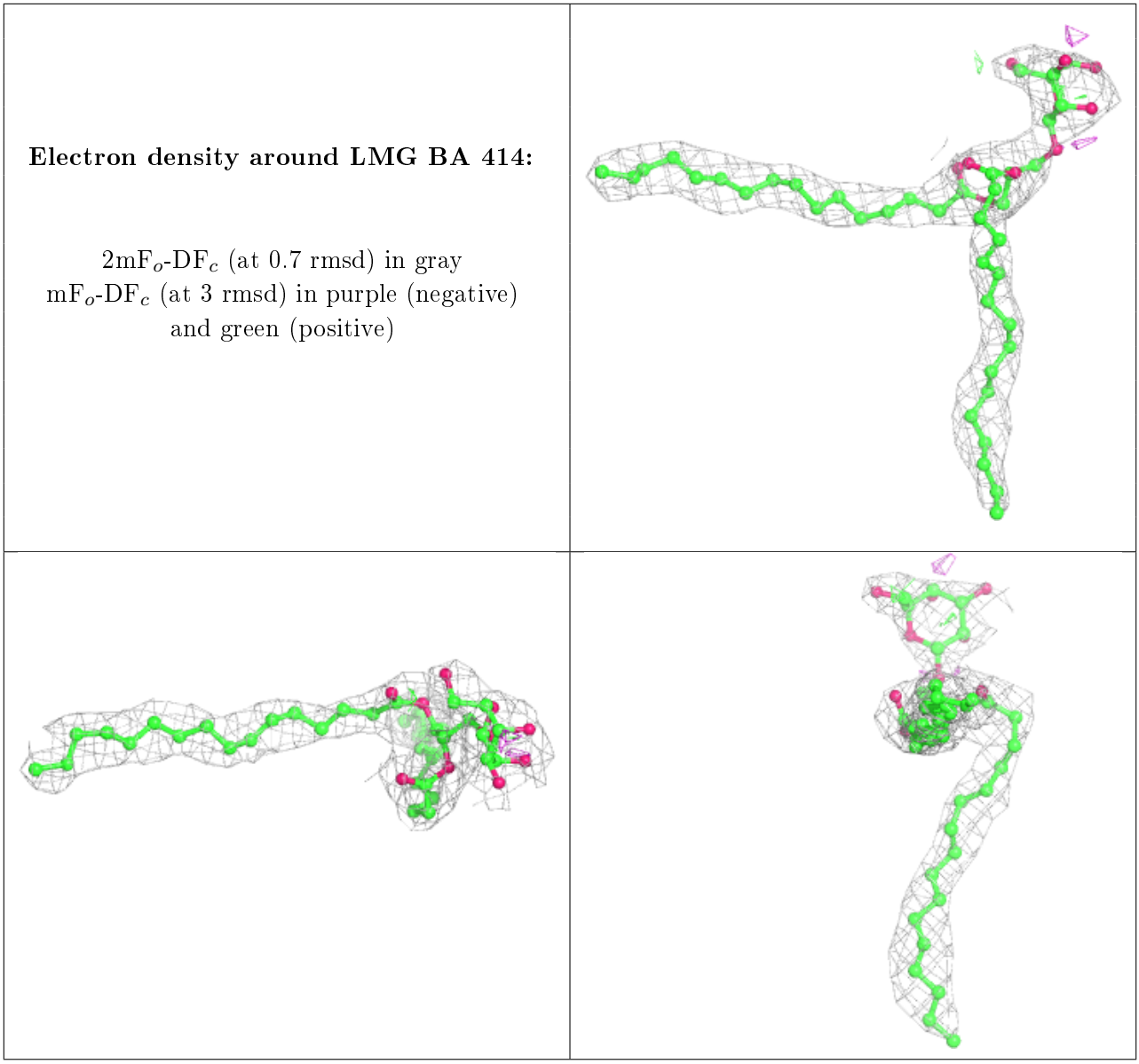
Electron density around LMG AD 408:

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



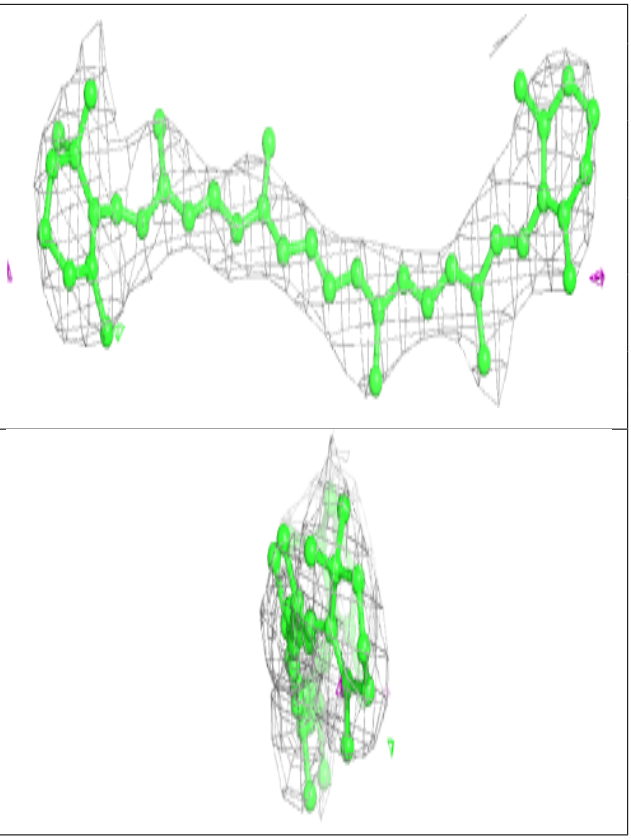
Electron density around LMG BA 414:

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



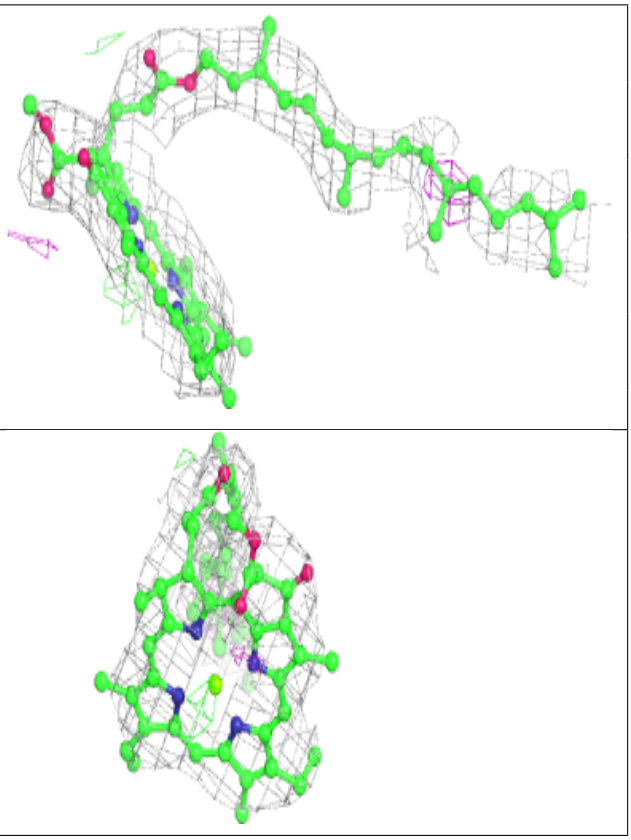
Electron density around BCR AB 618:

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



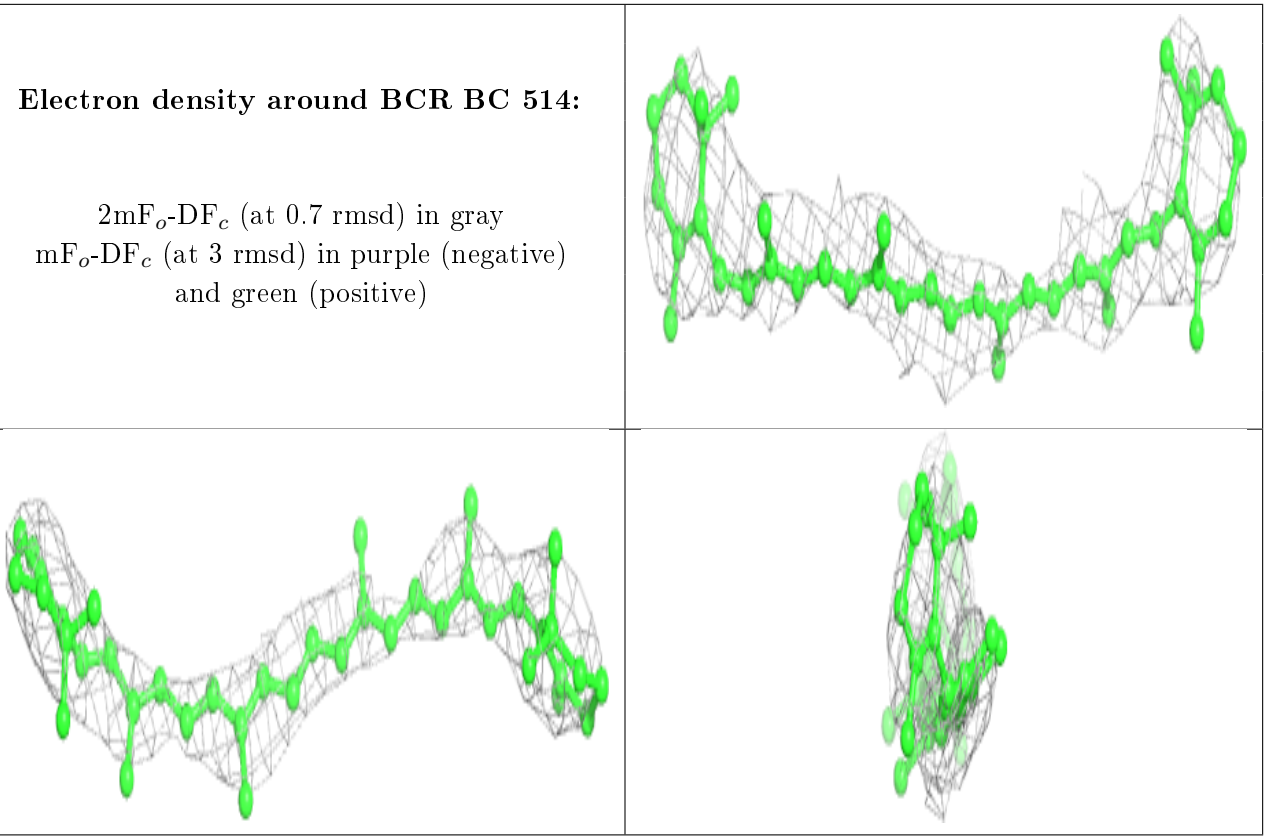
Electron density around CLA AC 504:

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



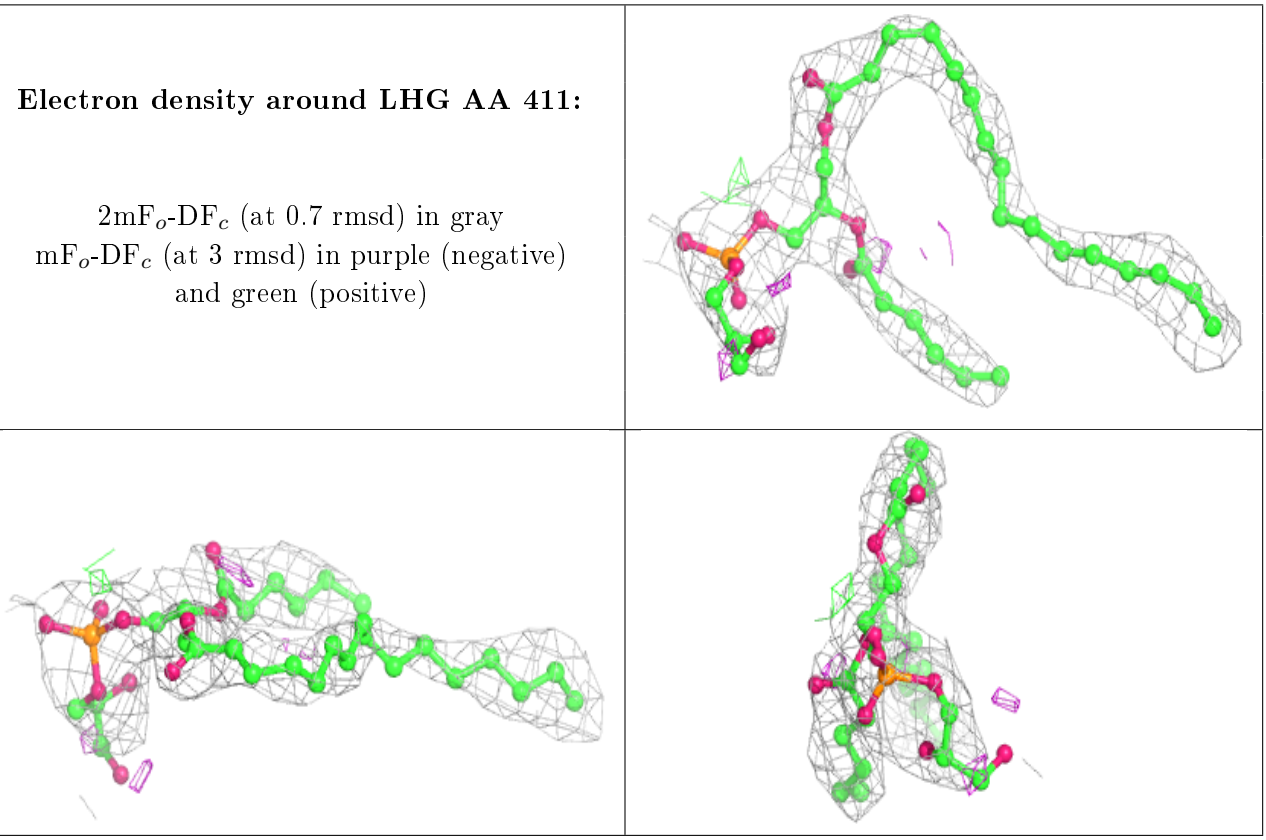
Electron density around BCR BC 514:

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



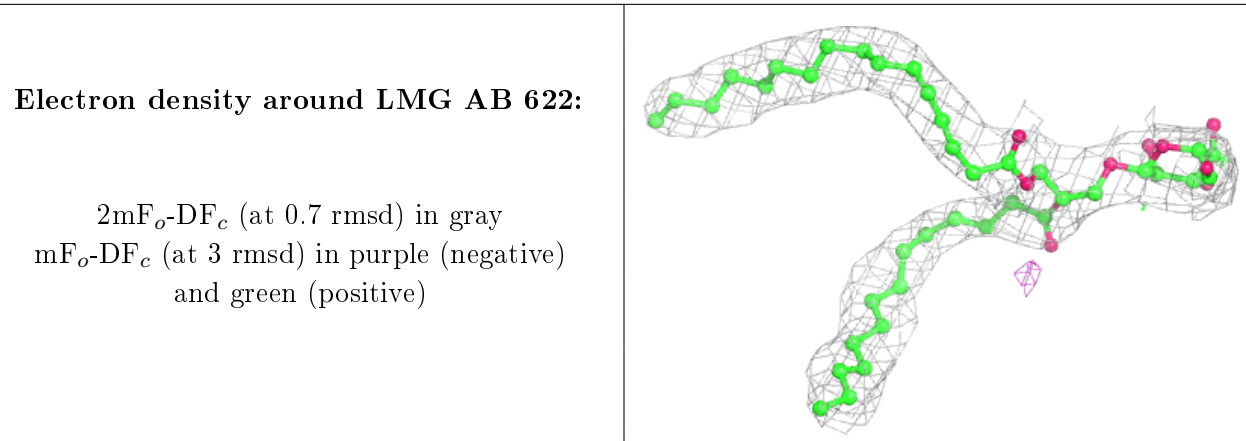
Electron density around LHG AA 411:

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



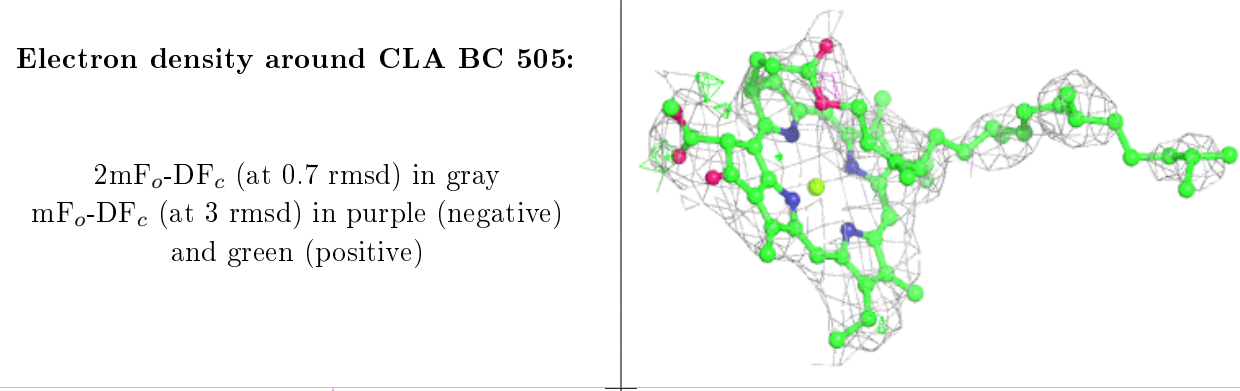
Electron density around LMG AB 622:

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



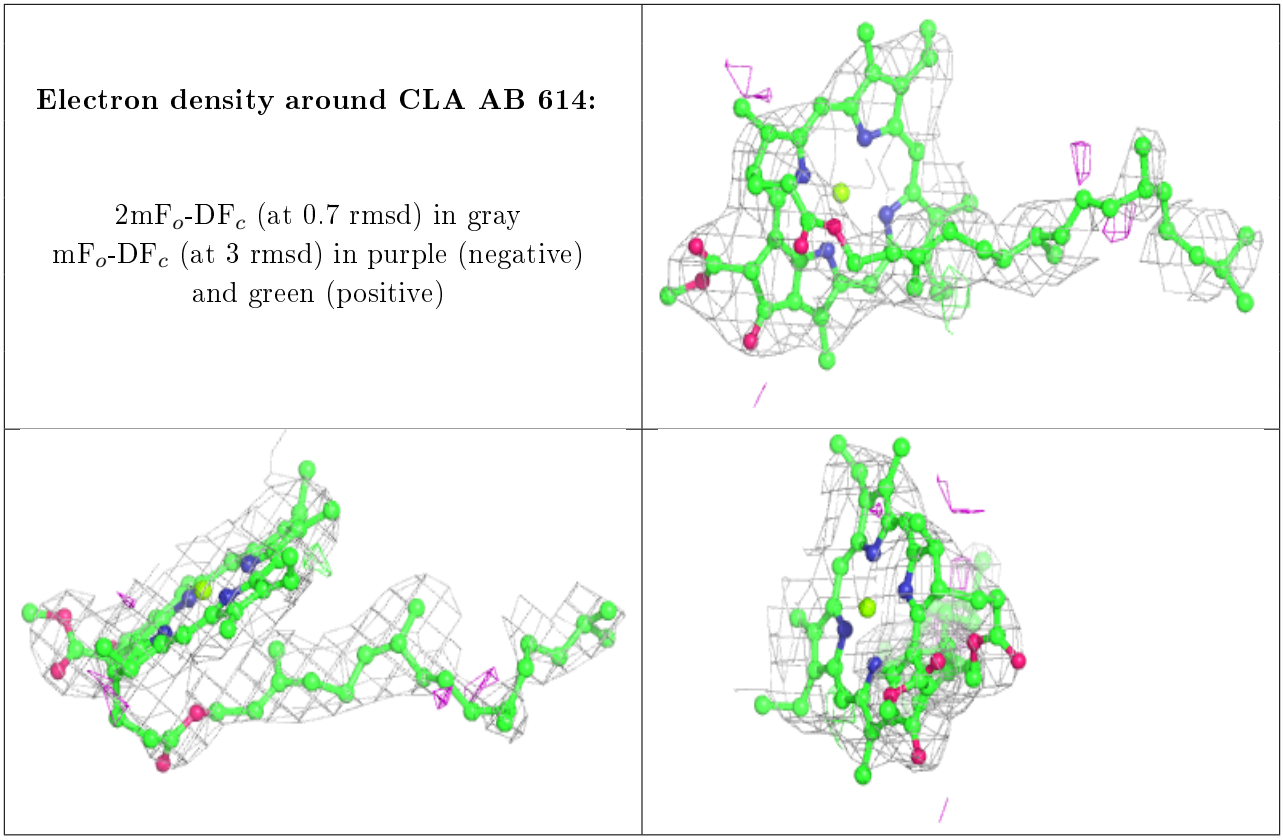
Electron density around CLA BC 505:

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



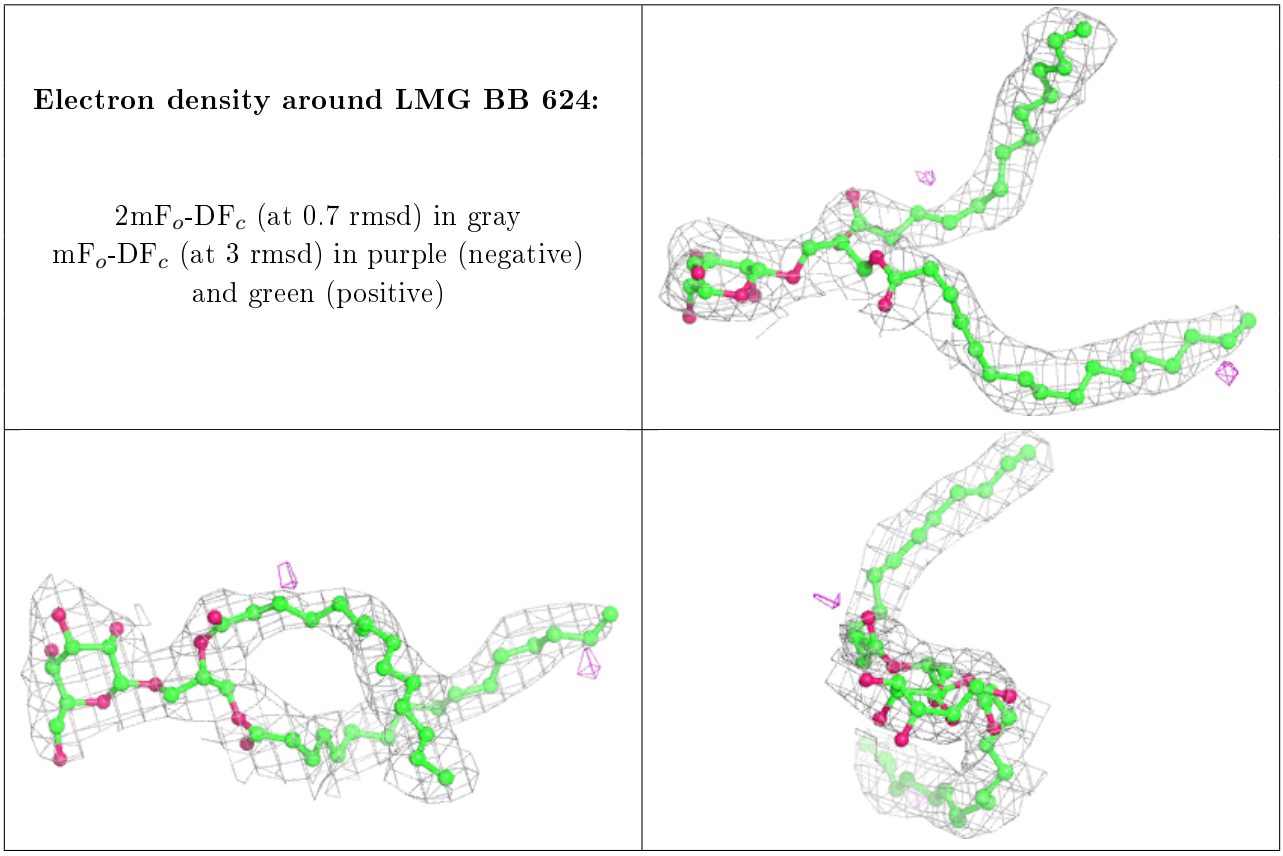
Electron density around CLA AB 614:

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



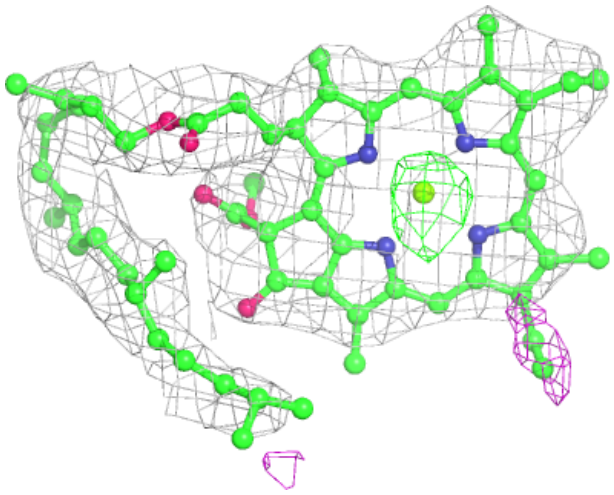
Electron density around LMG BB 624:

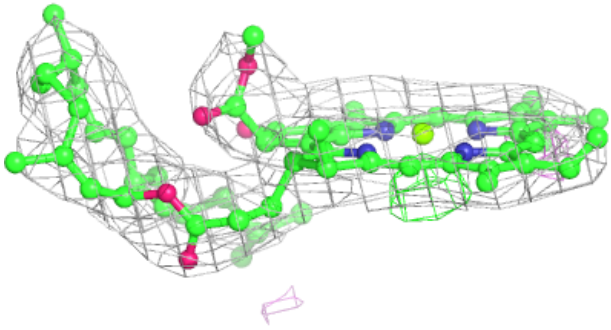
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

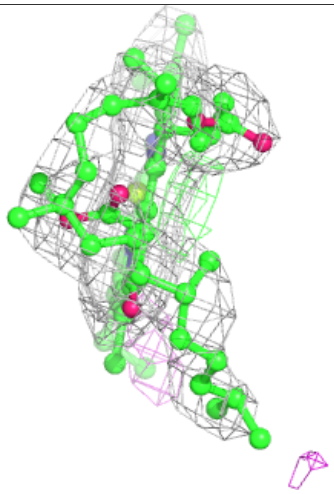


Electron density around CLA AB 610:

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

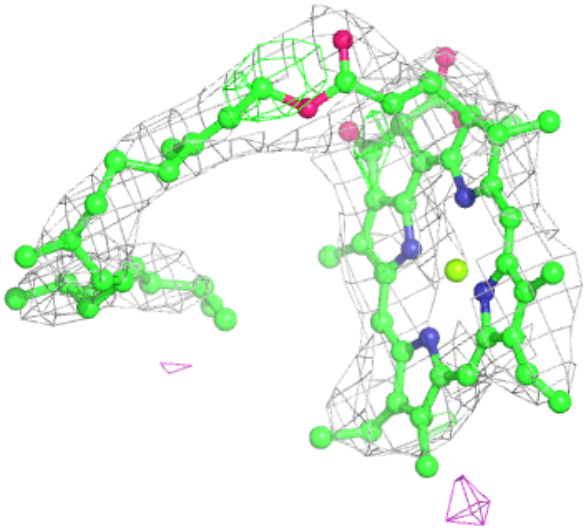


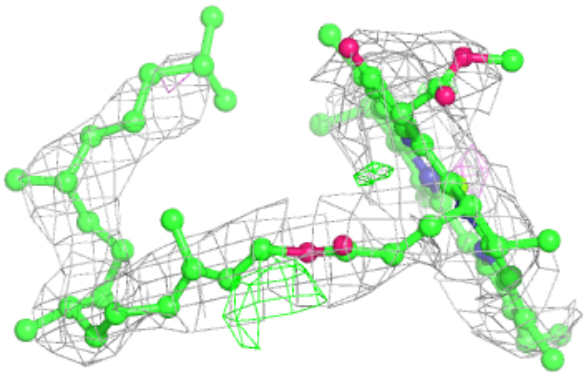


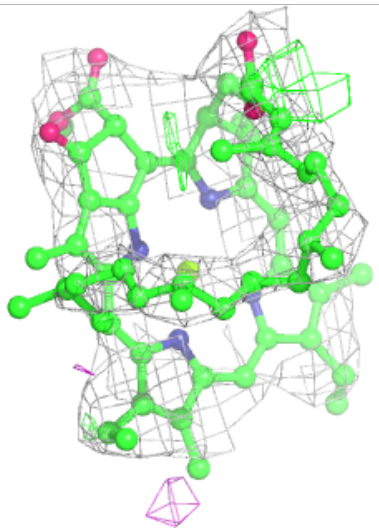


Electron density around CLA BC 503:

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

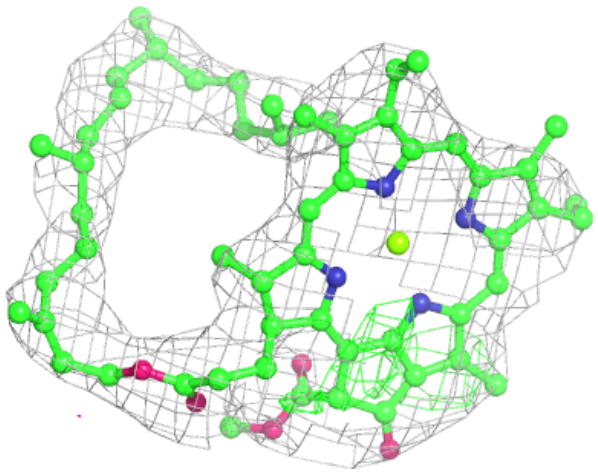


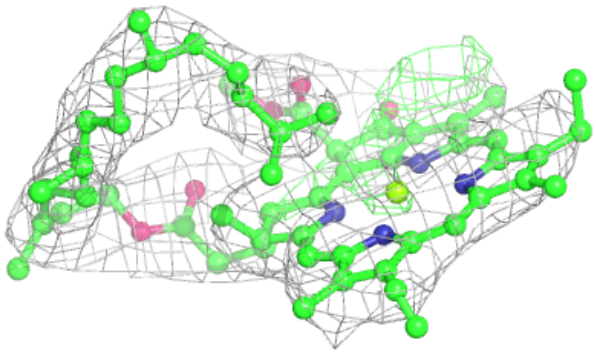


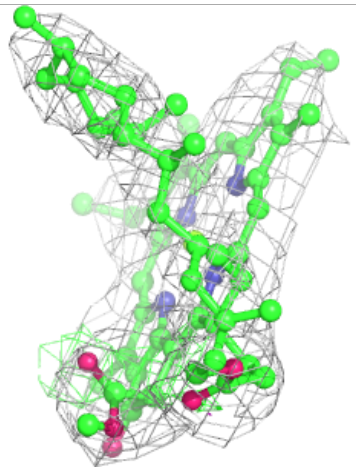


Electron density around CLA BB 618:

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

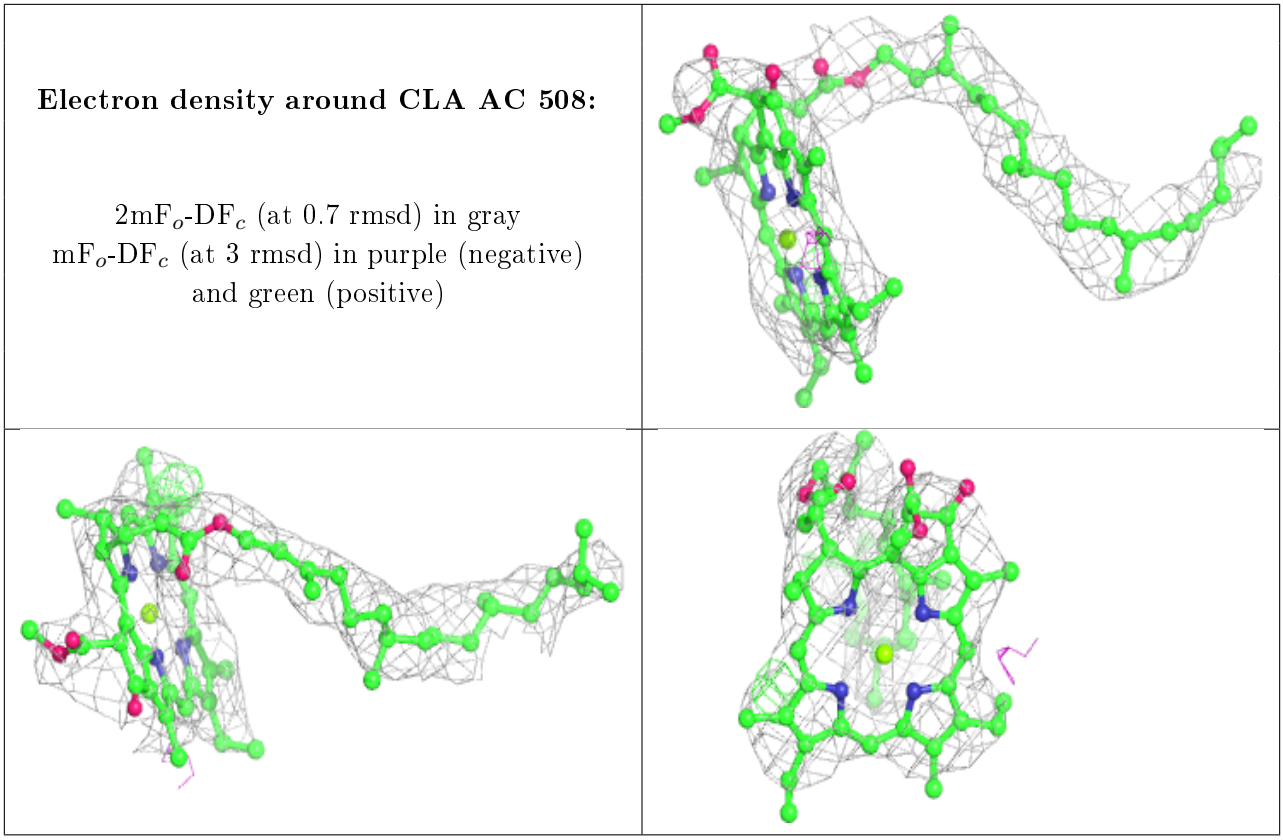






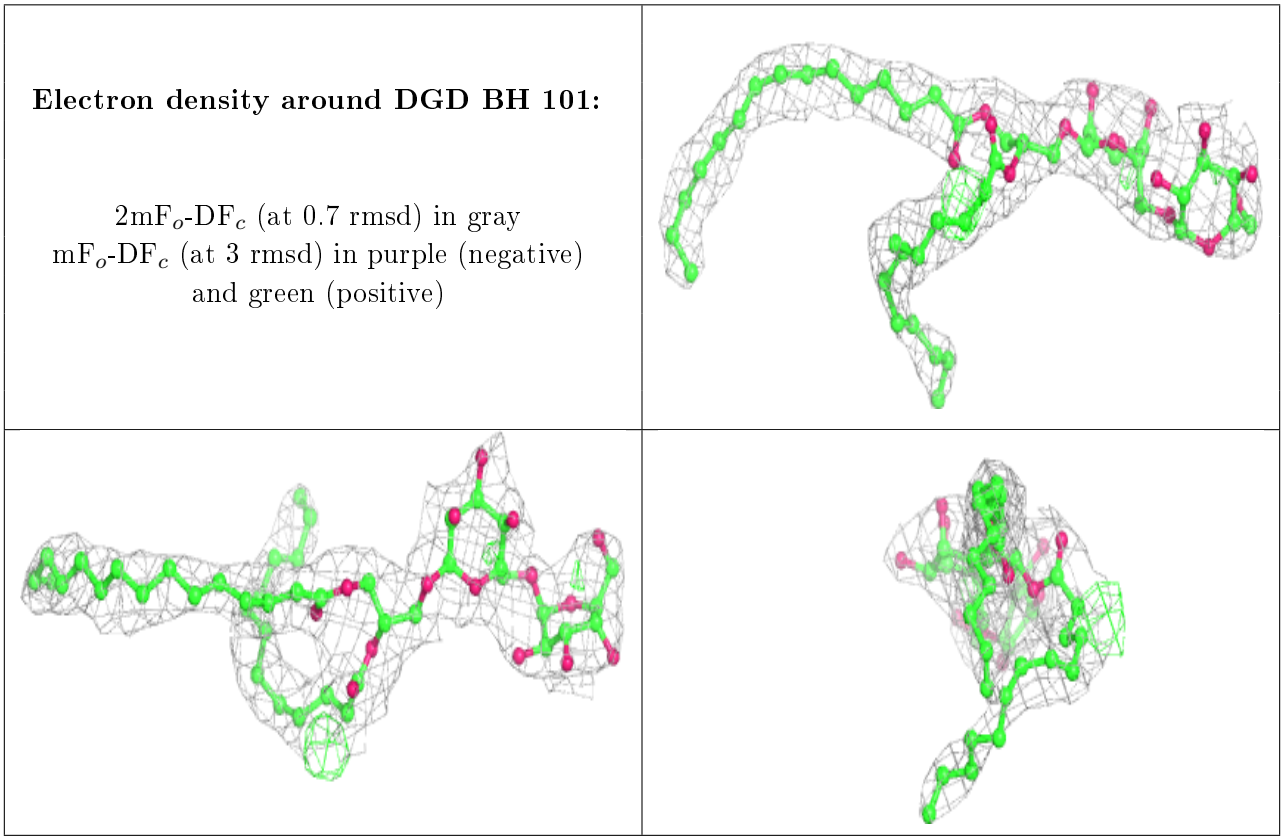
Electron density around CLA AC 508:

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



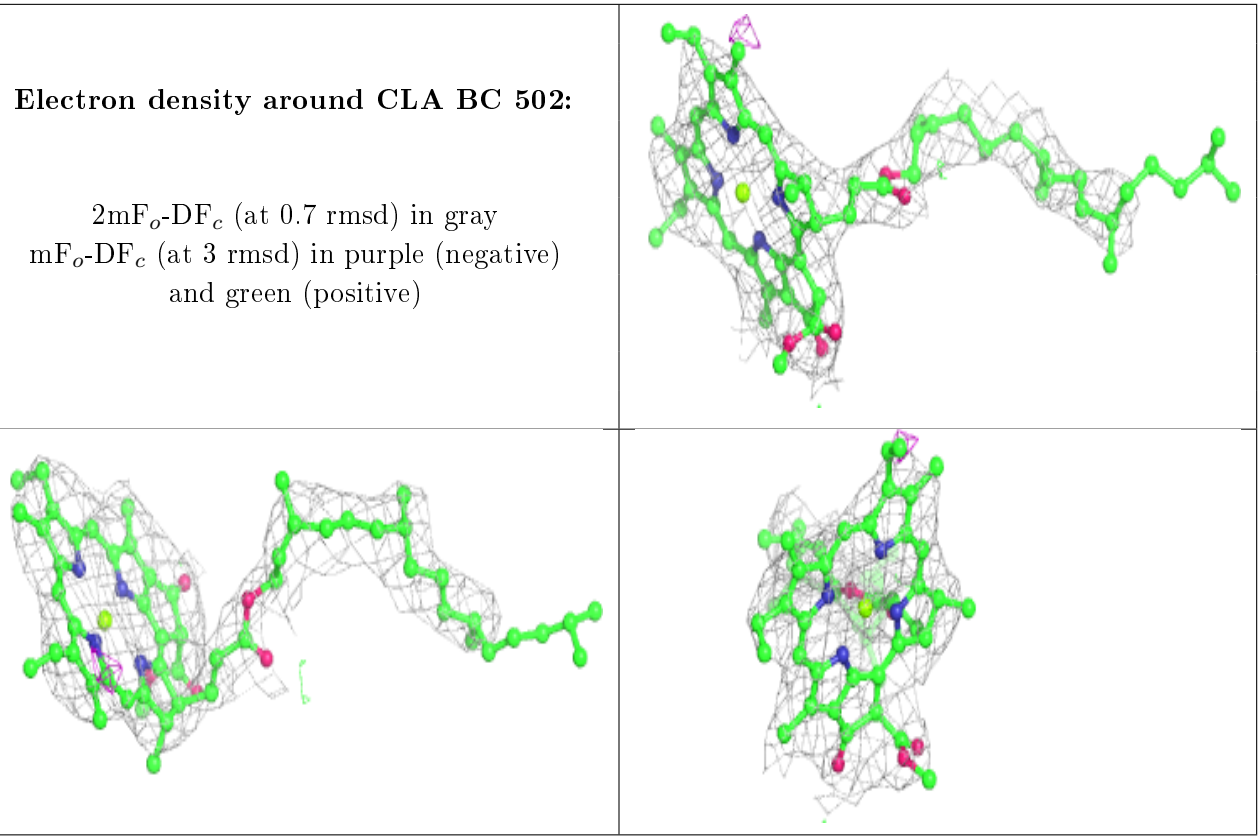
Electron density around DGD BH 101:

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



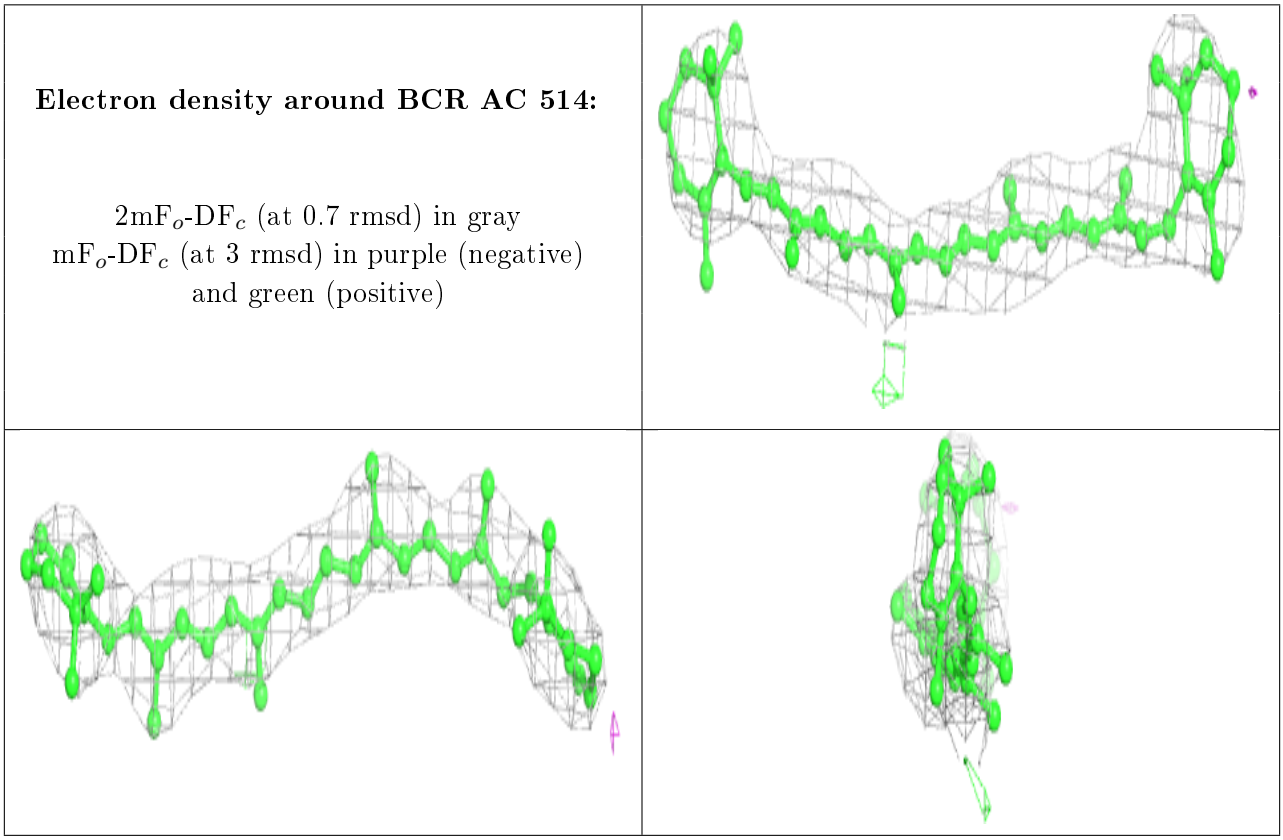
Electron density around CLA BC 502:

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



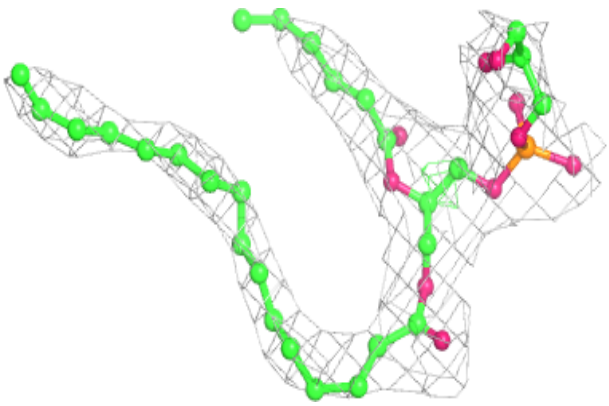
Electron density around BCR AC 514:

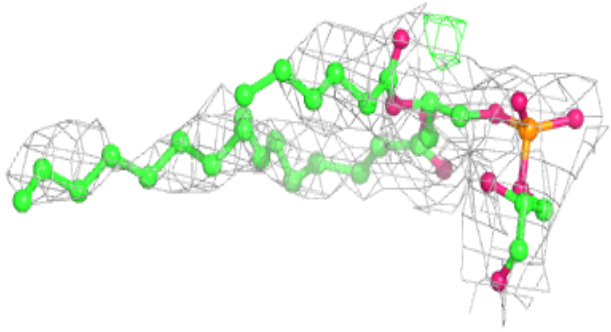
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

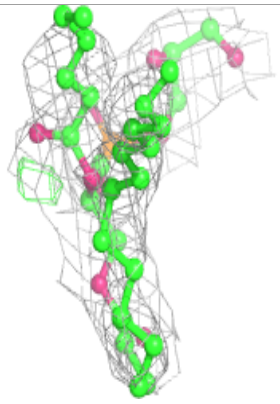


Electron density around LHG BA 412:

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

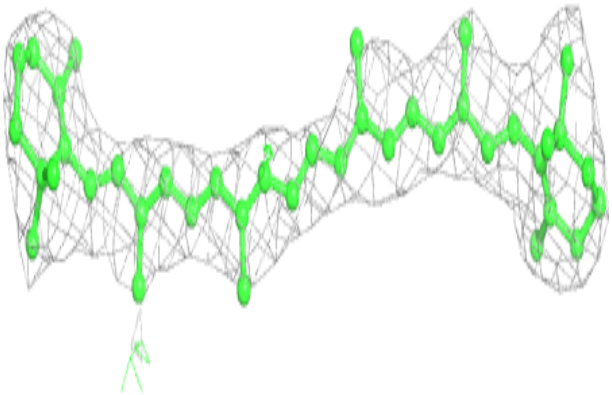


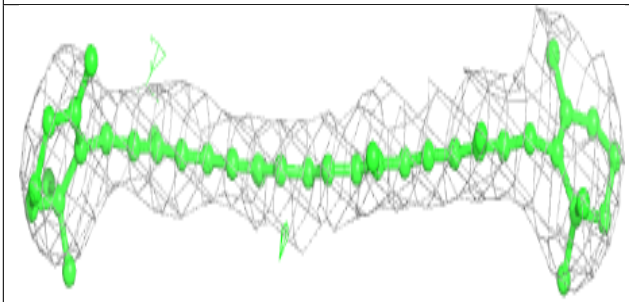




Electron density around BCR AB 619:

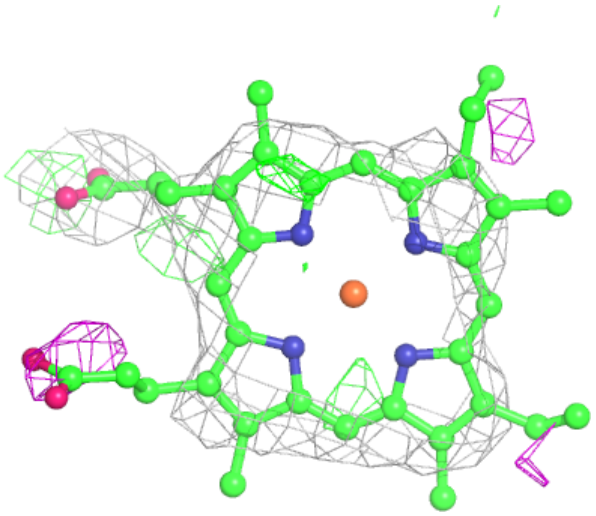
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

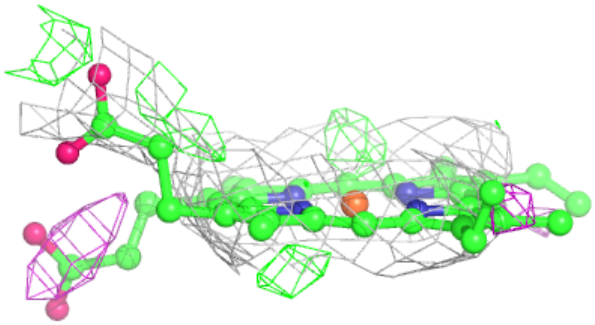


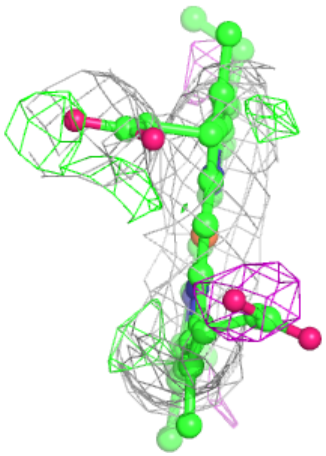


Electron density around HEM BE 101:

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

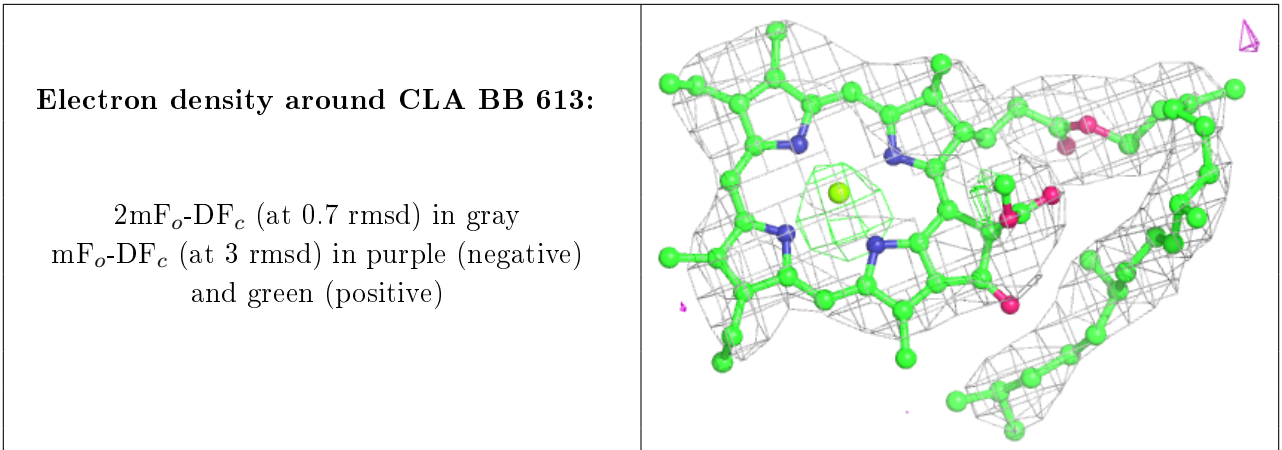






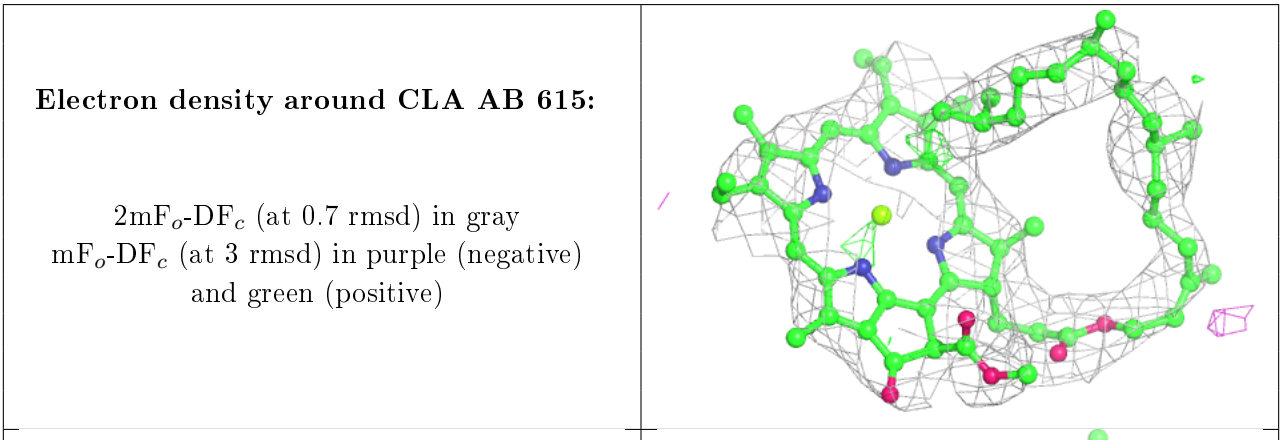
Electron density around CLA BB 613:

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



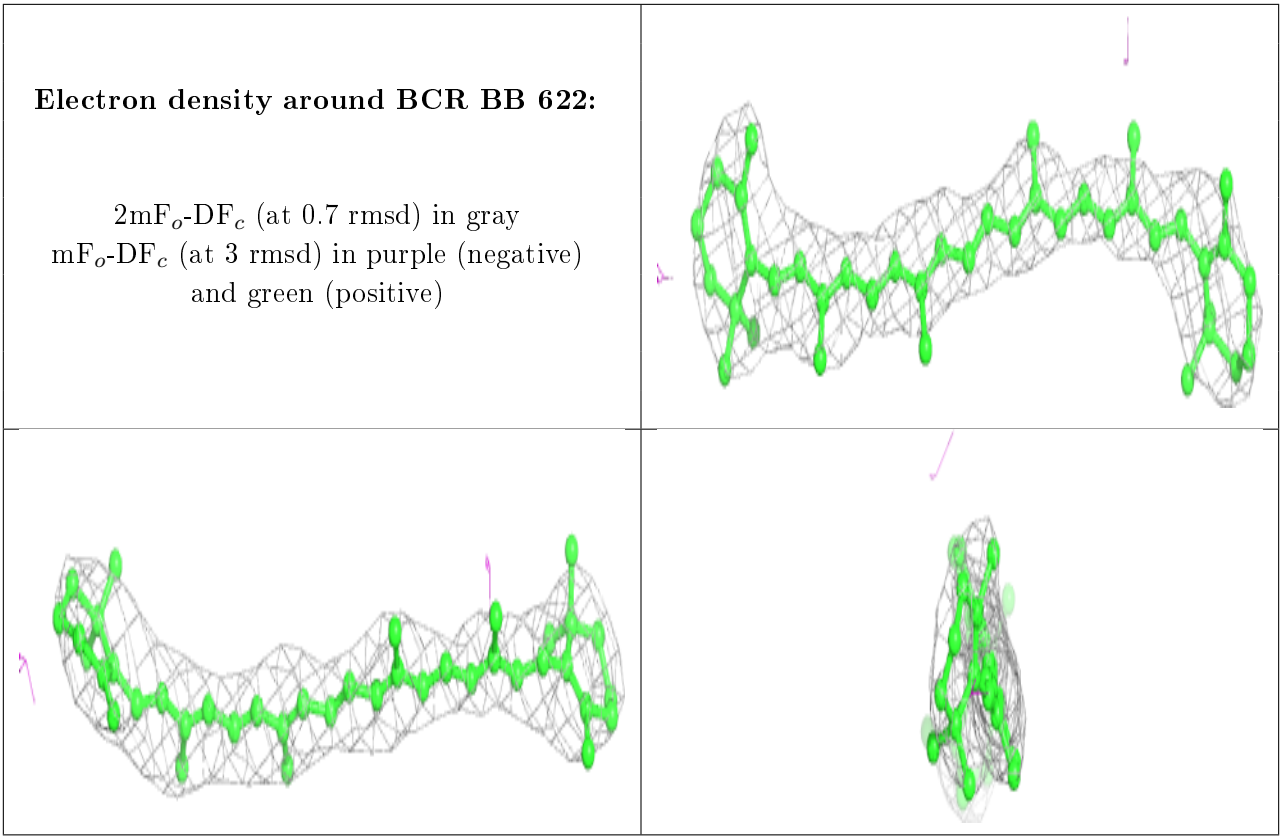
Electron density around CLA AB 615:

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



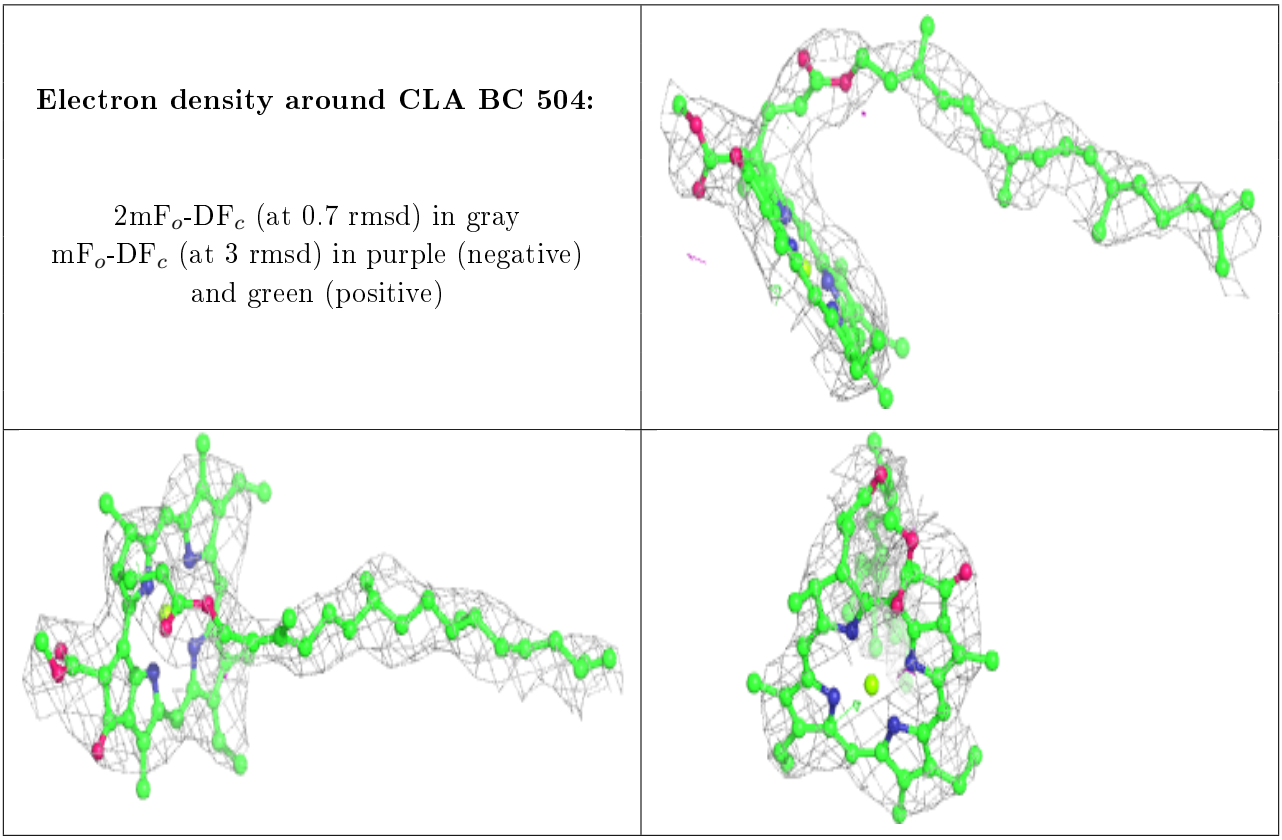
Electron density around BCR BB 622:

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



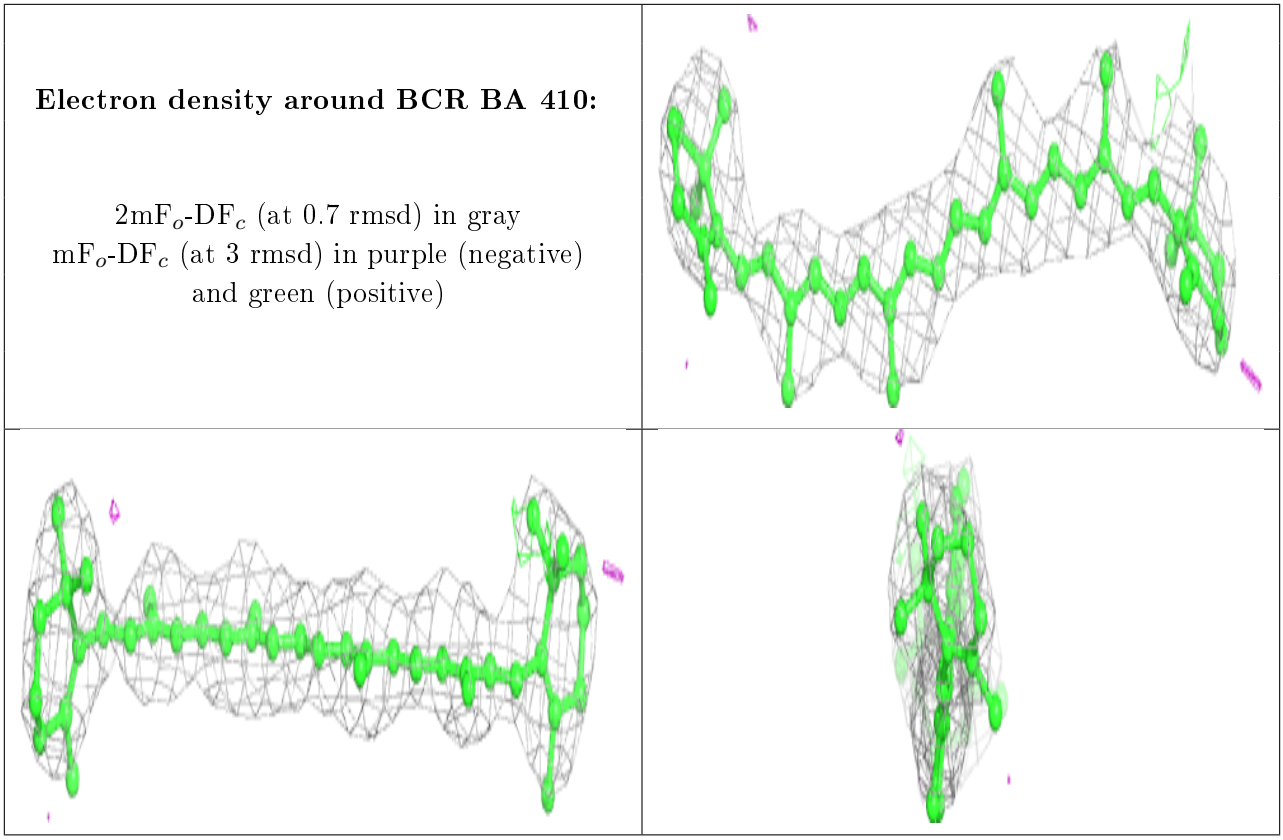
Electron density around CLA BC 504:

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



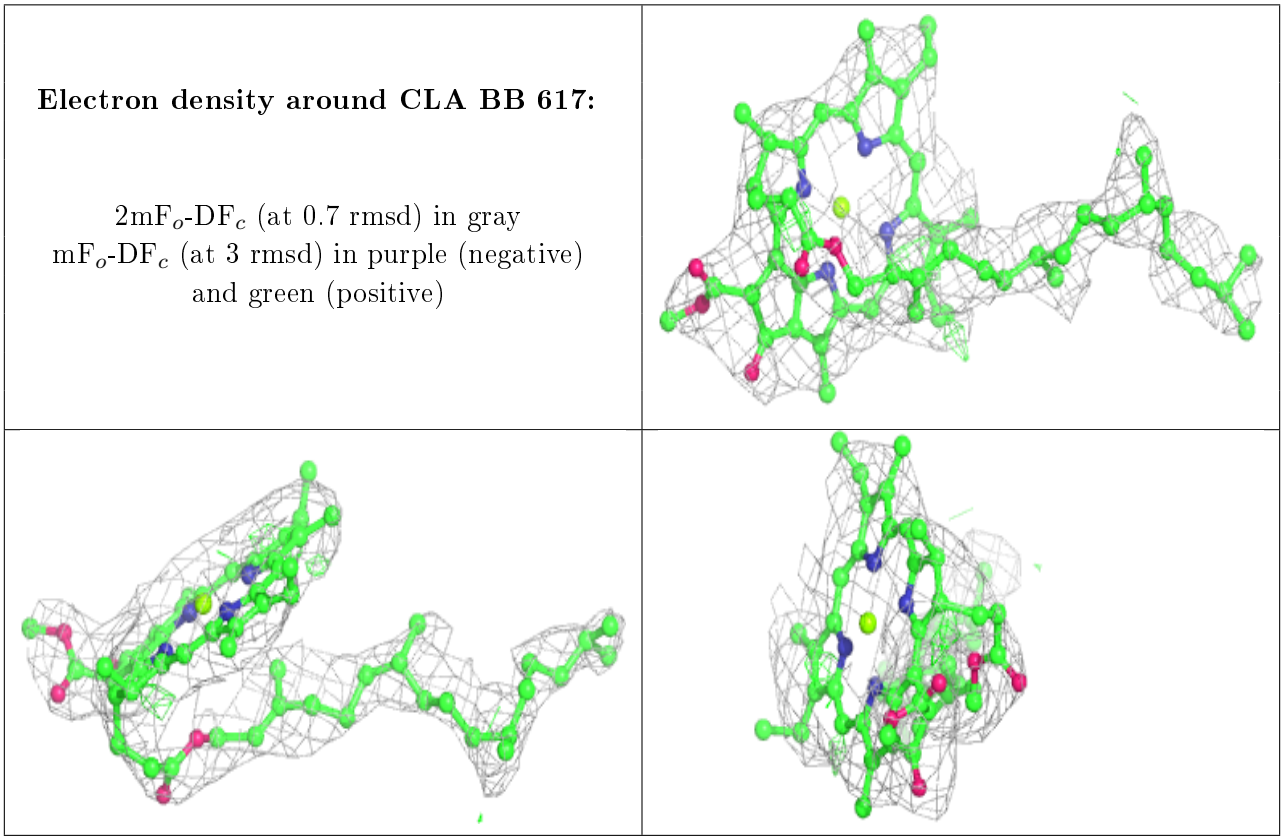
Electron density around BCR BA 410:

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



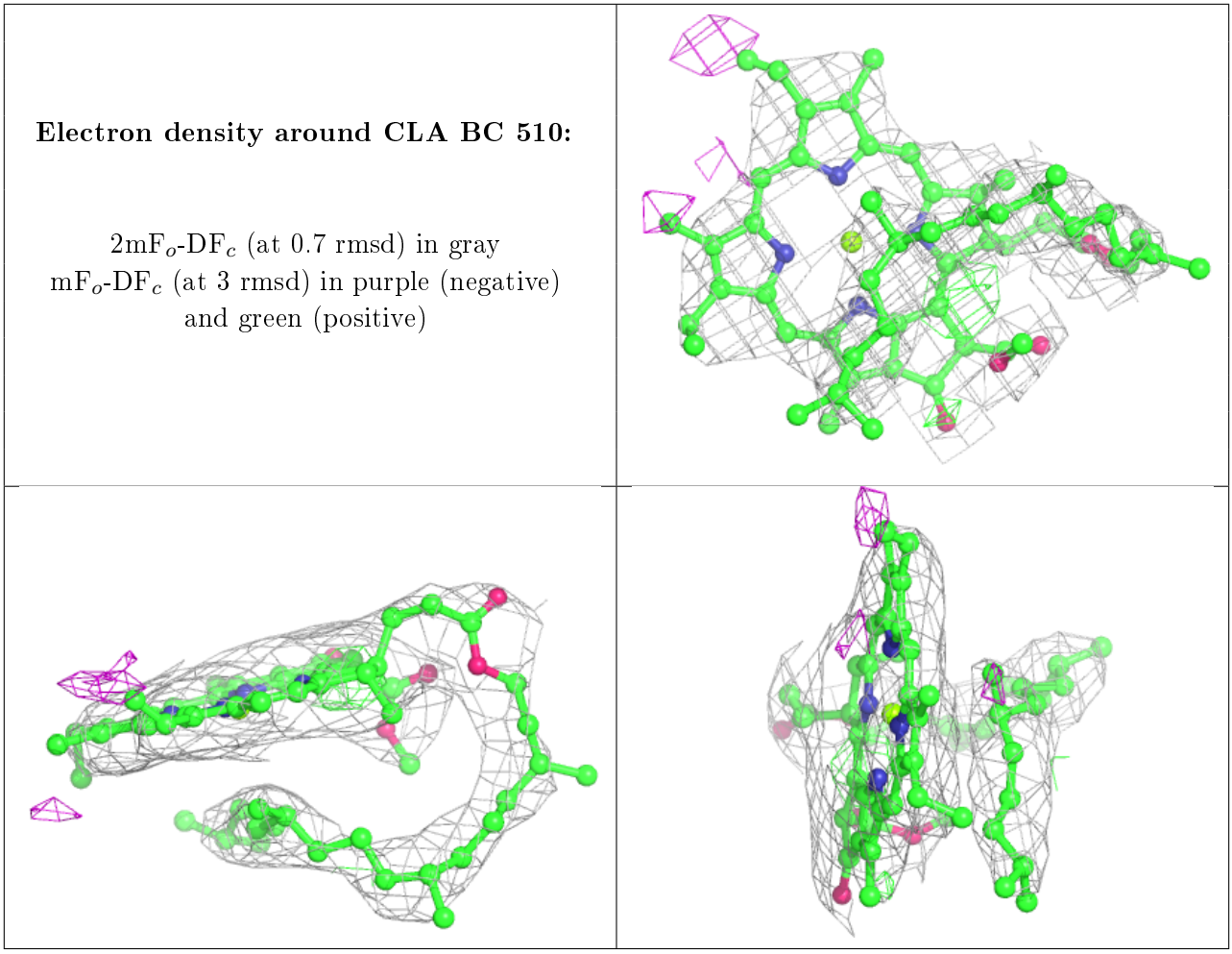
Electron density around CLA BB 617:

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



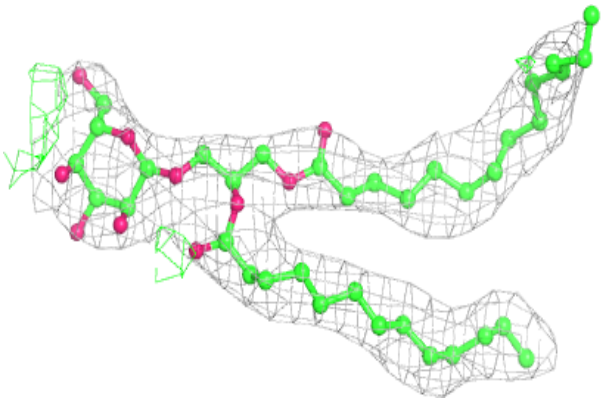
Electron density around CLA BC 510:

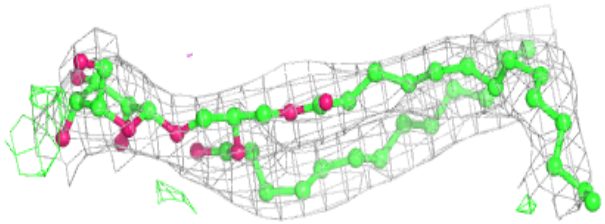
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

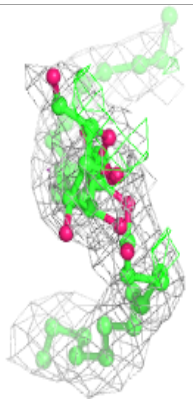


Electron density around LMG AD 407:

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

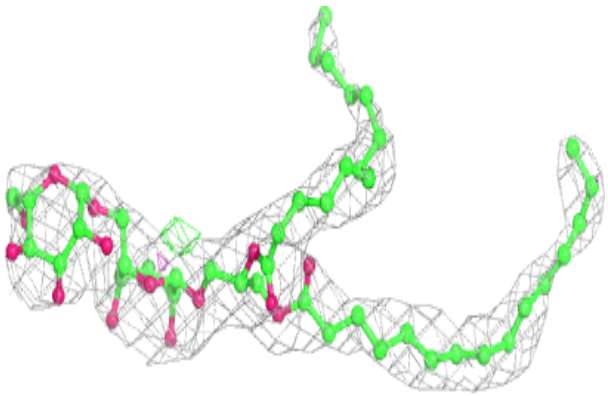


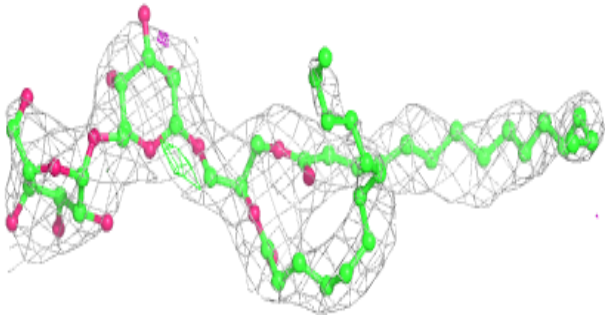


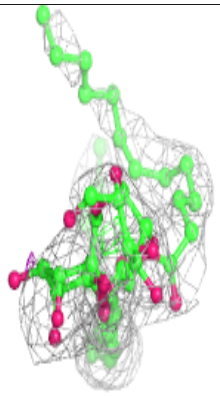


Electron density around DGD AH 102:

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

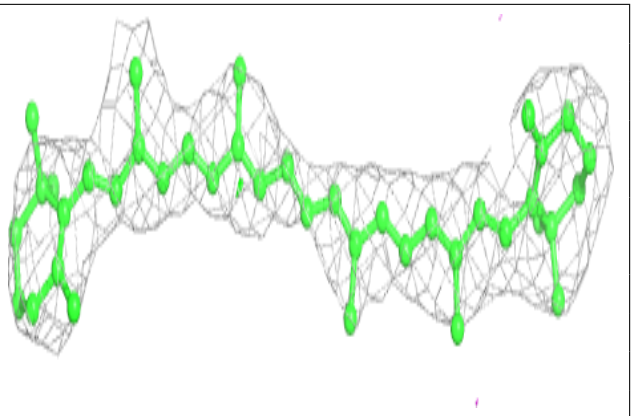


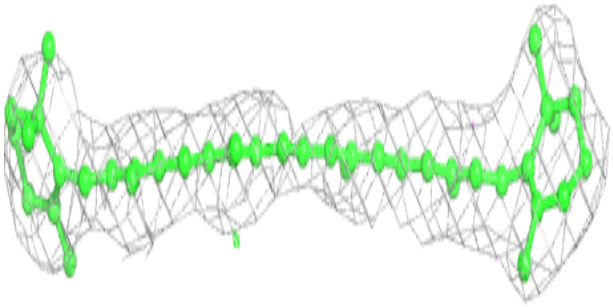




Electron density around BCR BB 621:

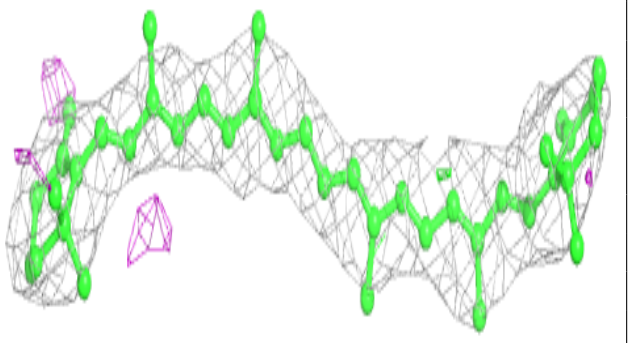
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

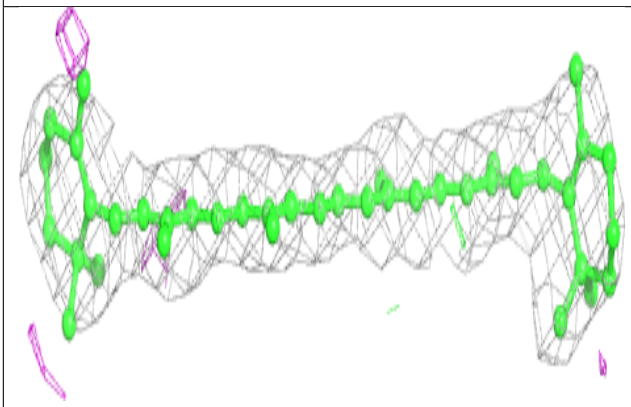




Electron density around BCR AA 409:

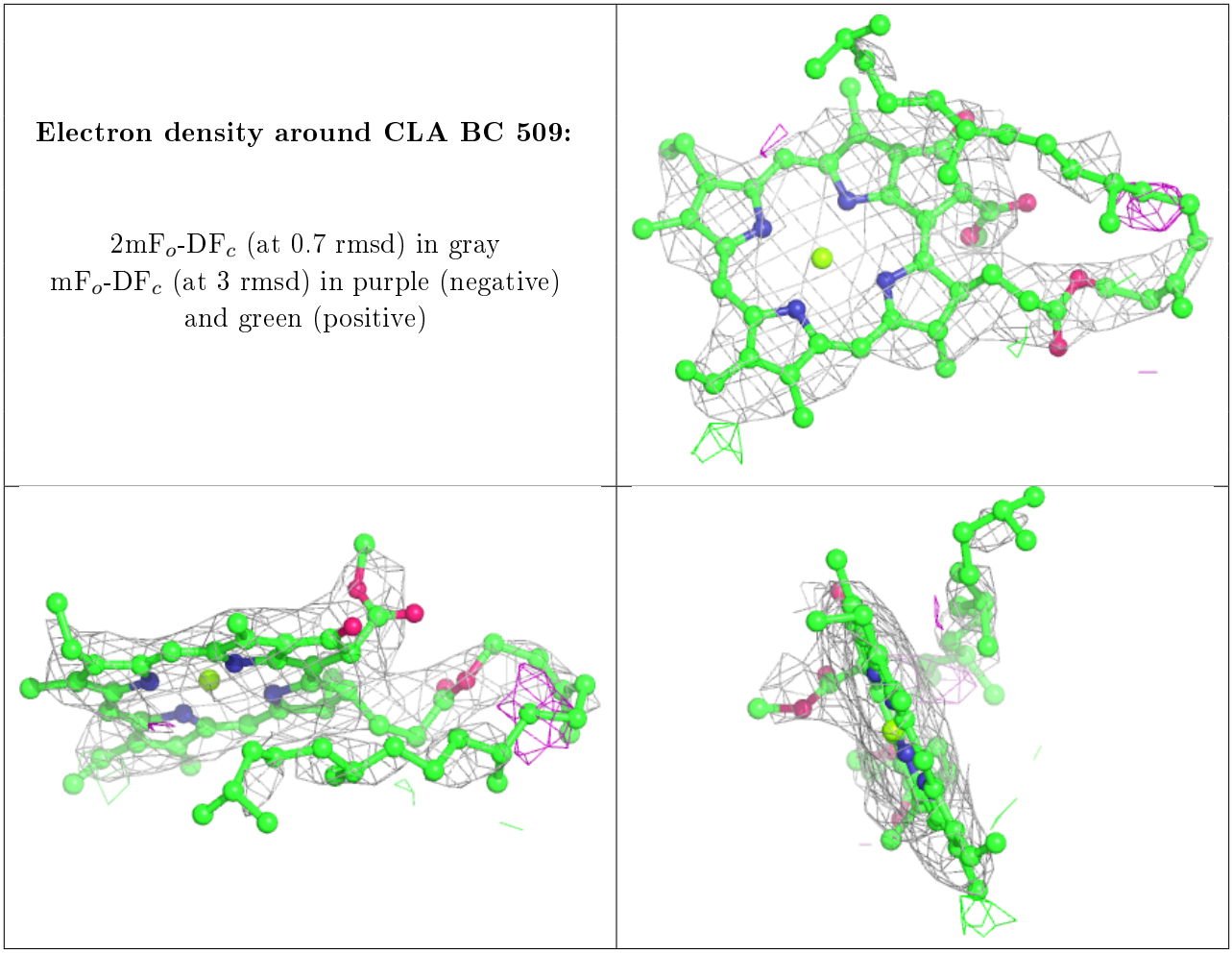
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





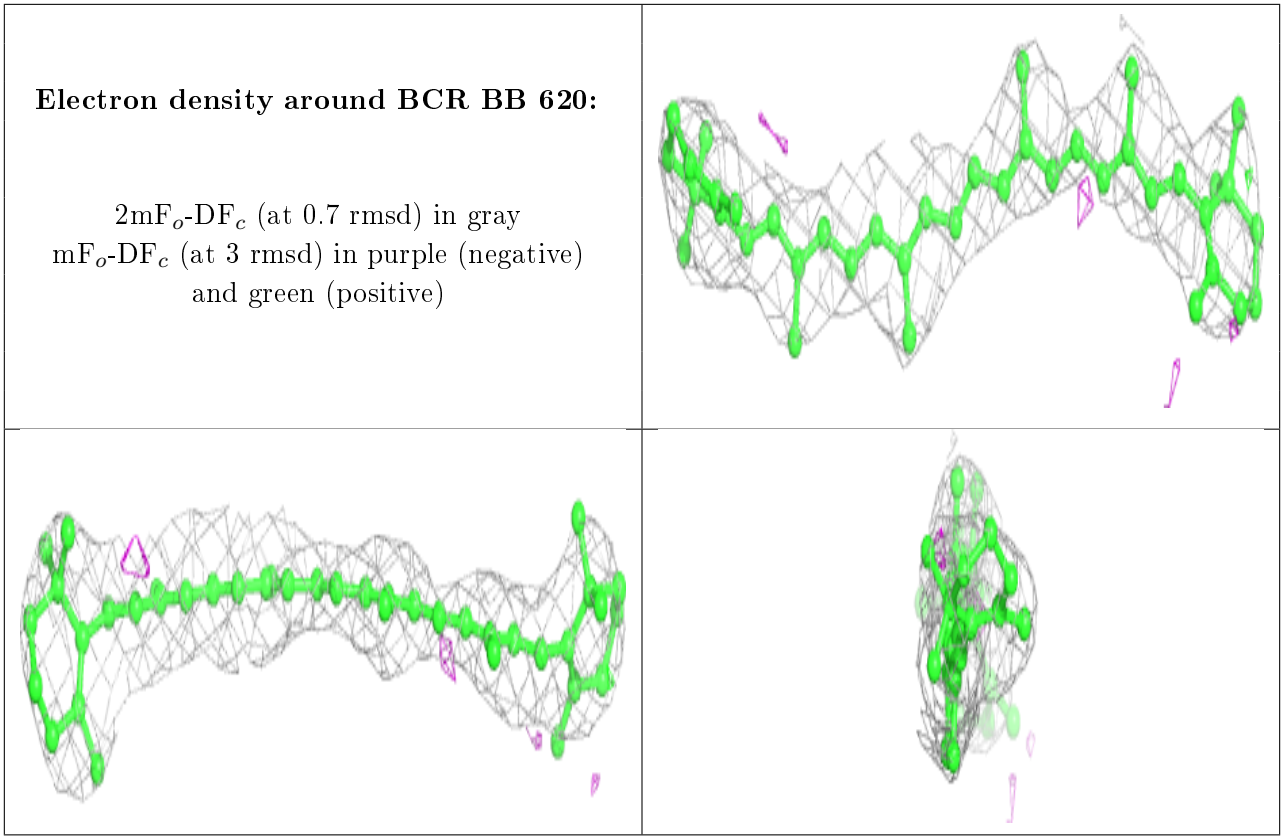
Electron density around CLA BC 509:

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



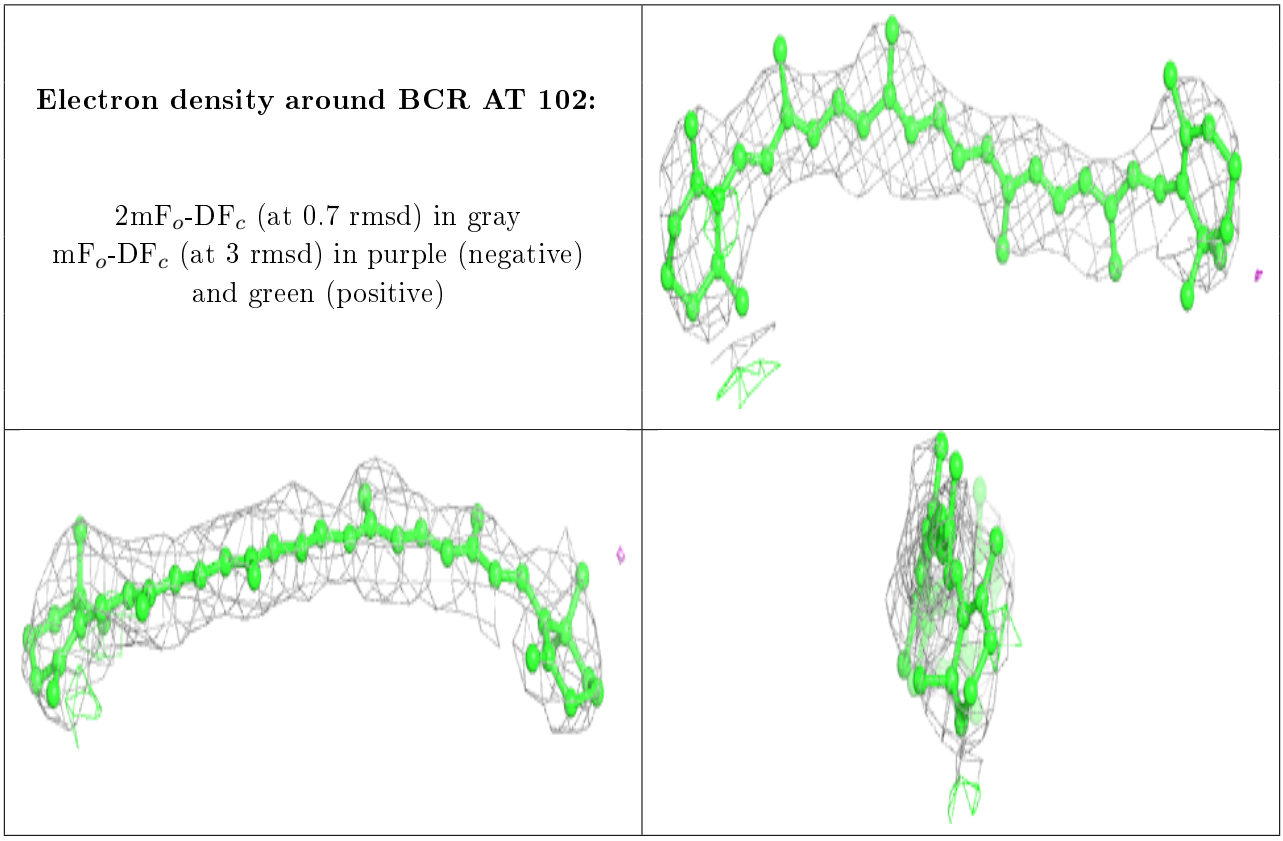
Electron density around BCR BB 620:

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



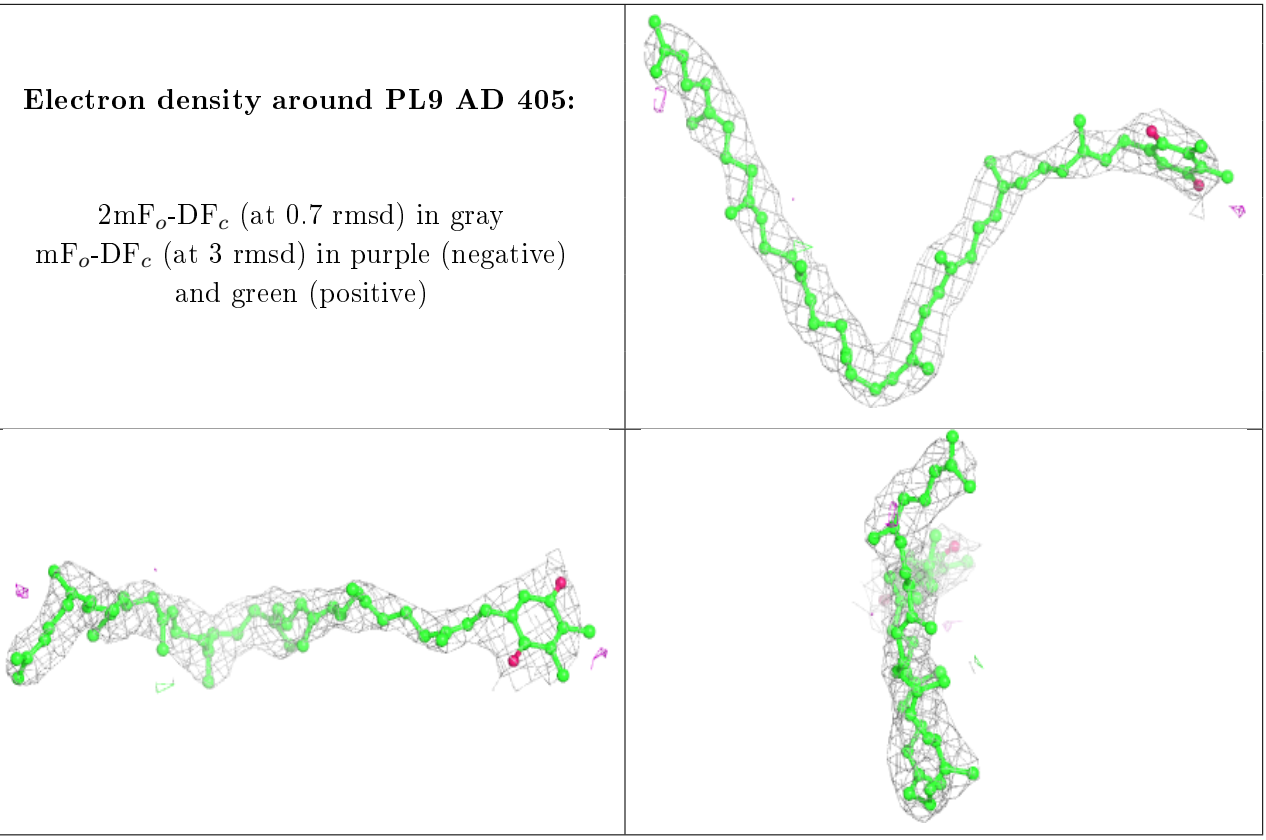
Electron density around BCR AT 102:

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



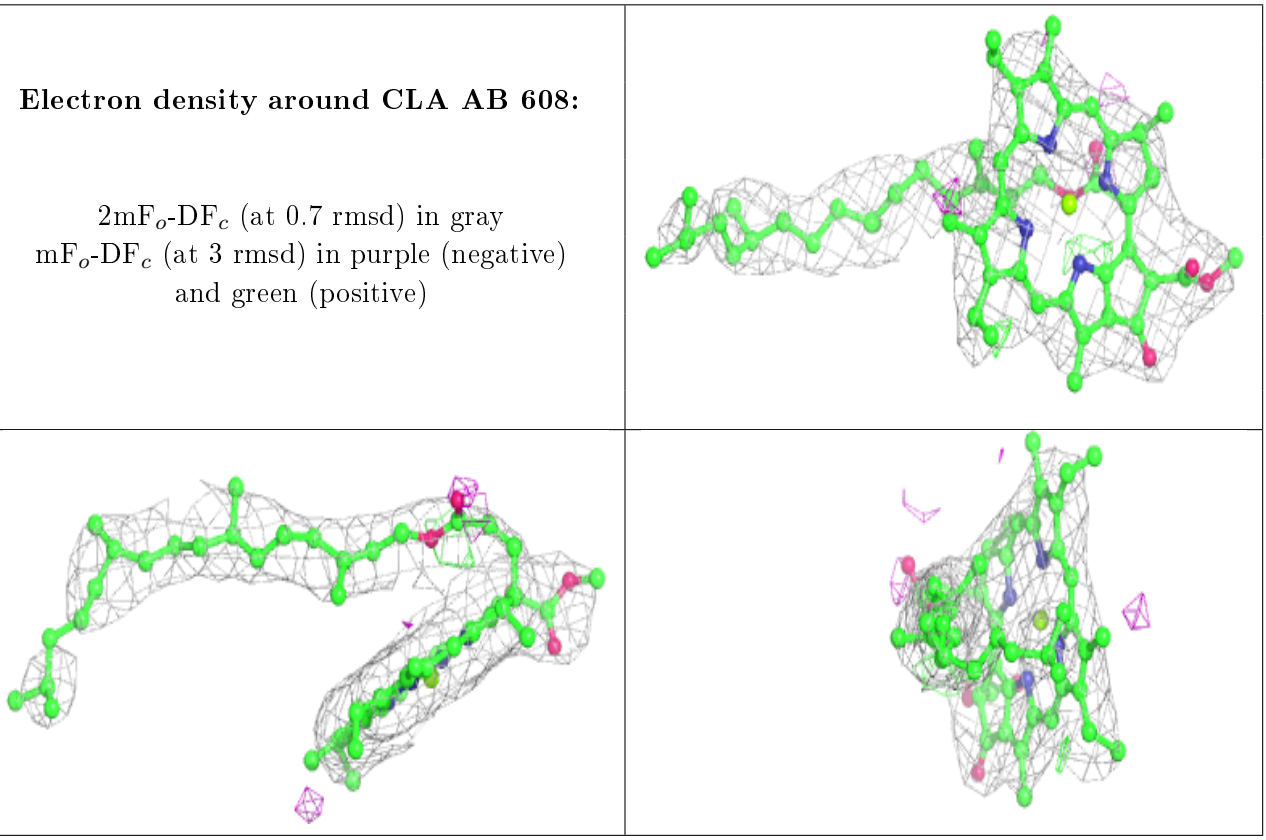
Electron density around PL9 AD 405:

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



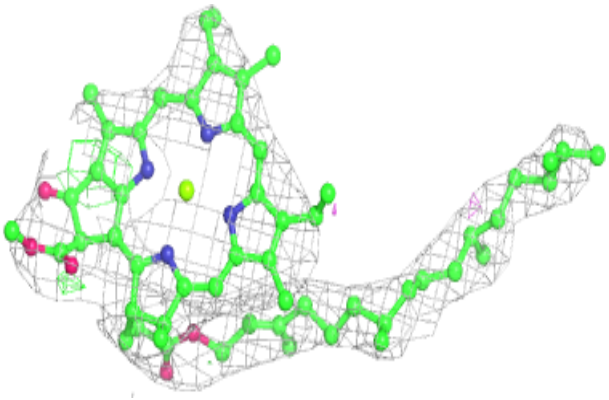
Electron density around CLA AB 608:

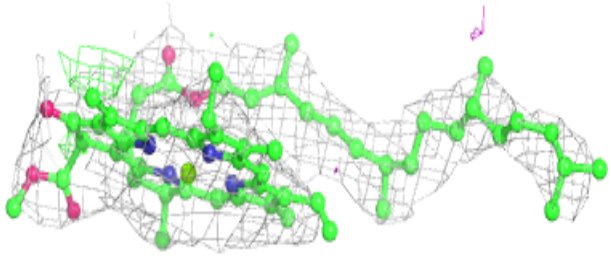
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

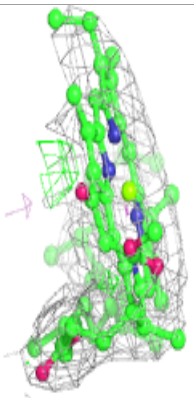


Electron density around CLA BC 501:

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

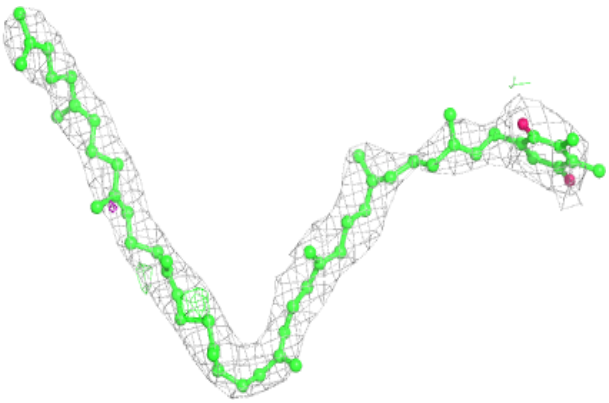


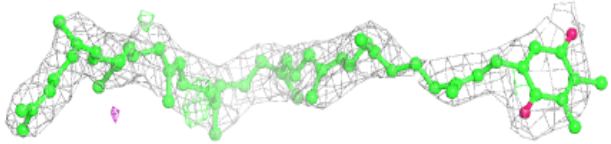


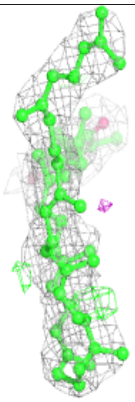


Electron density around PL9 BD 405:

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

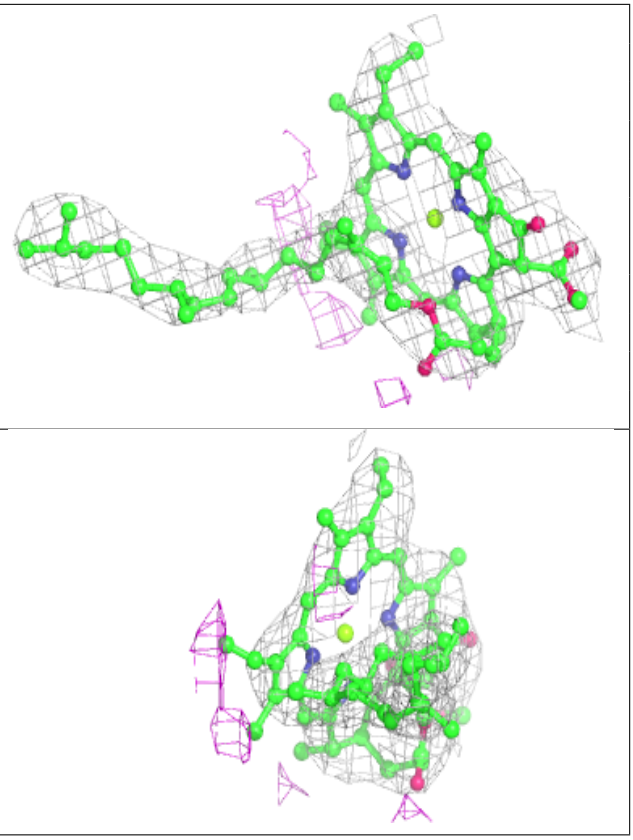


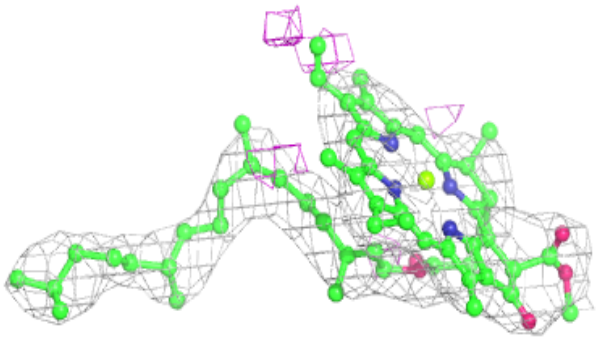




Electron density around CLA AC 505:

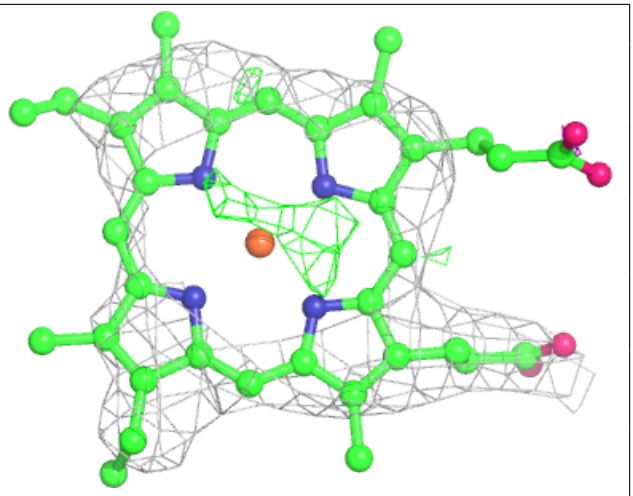
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

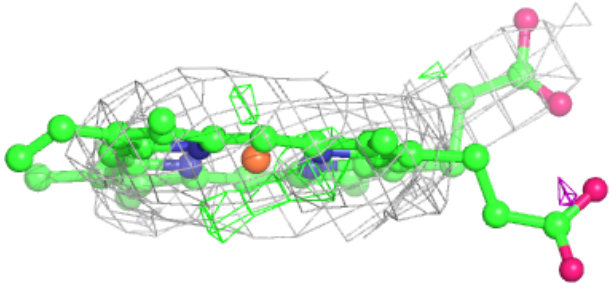


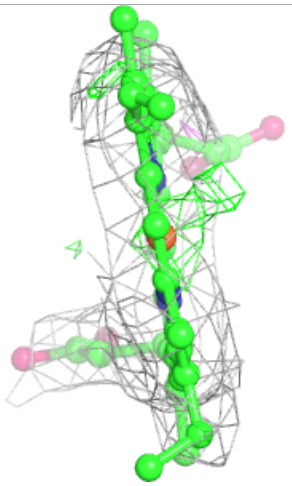


Electron density around HEM AE 101:

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

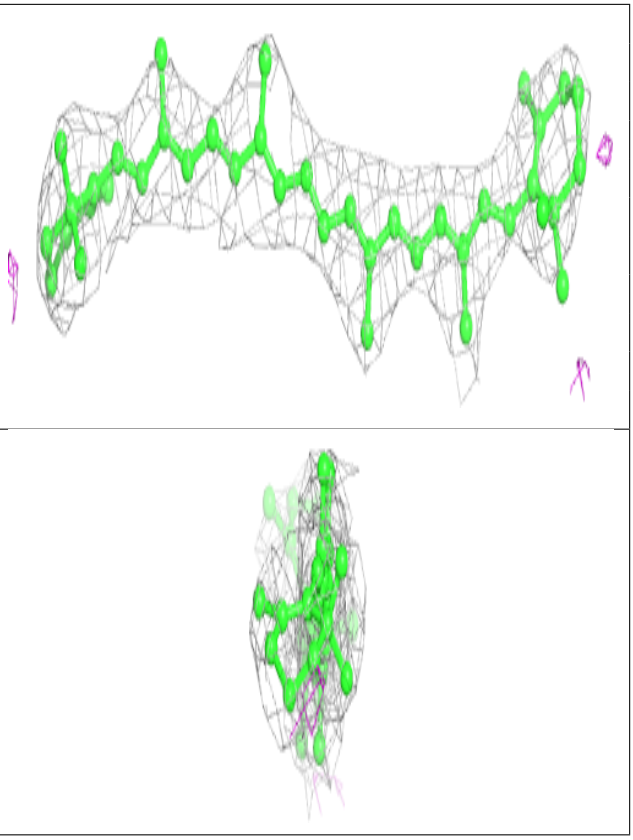






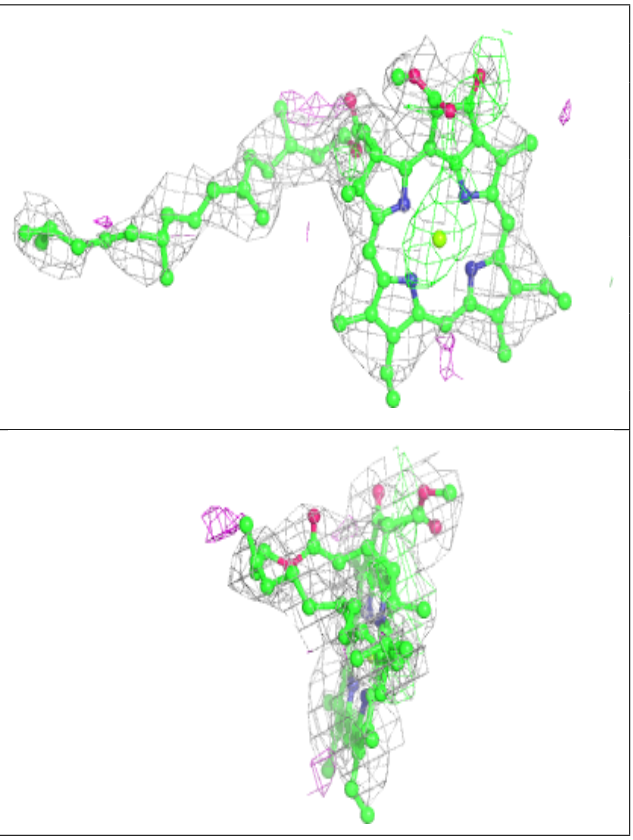
Electron density around BCR AB 617:

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



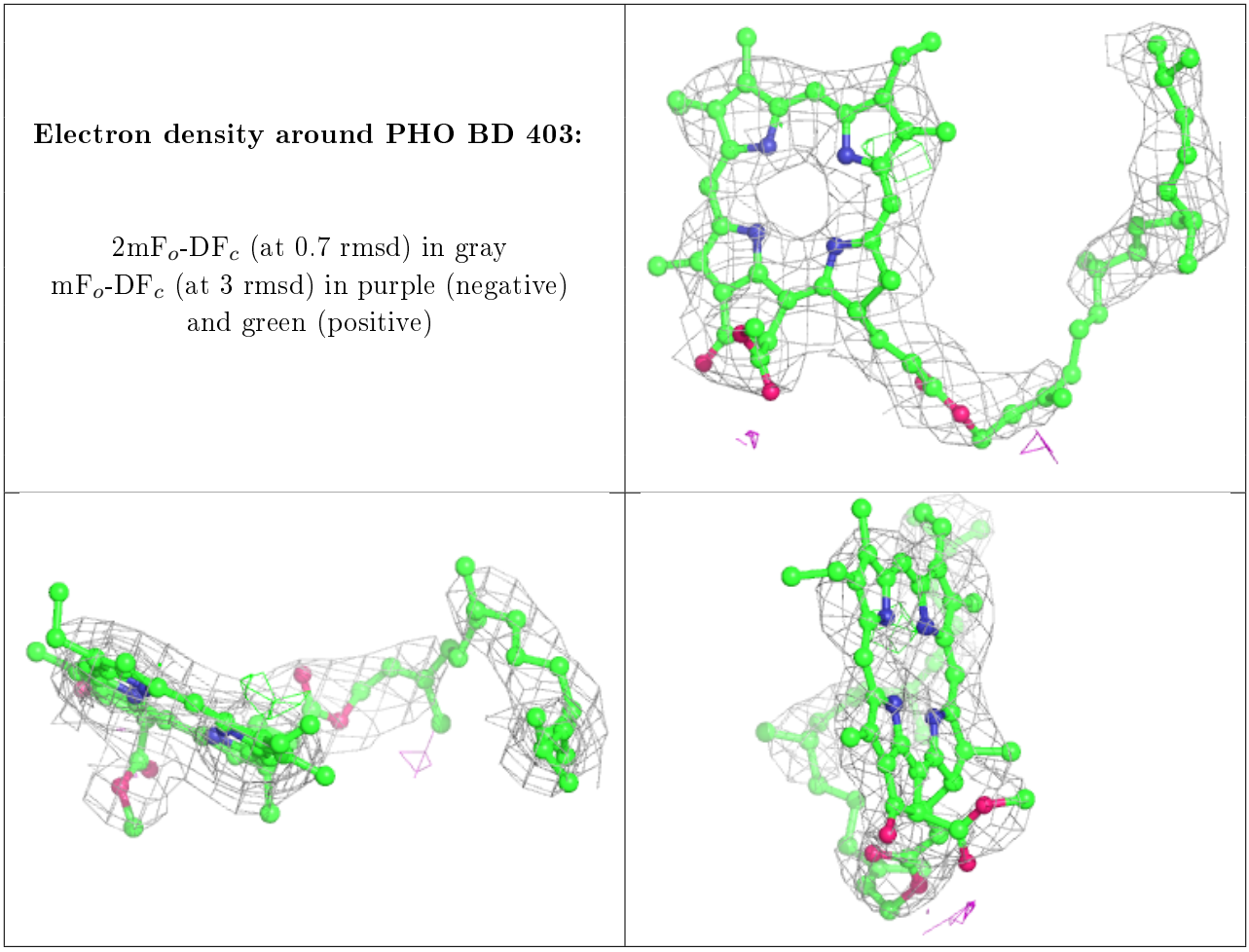
Electron density around CLA AA 404:

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



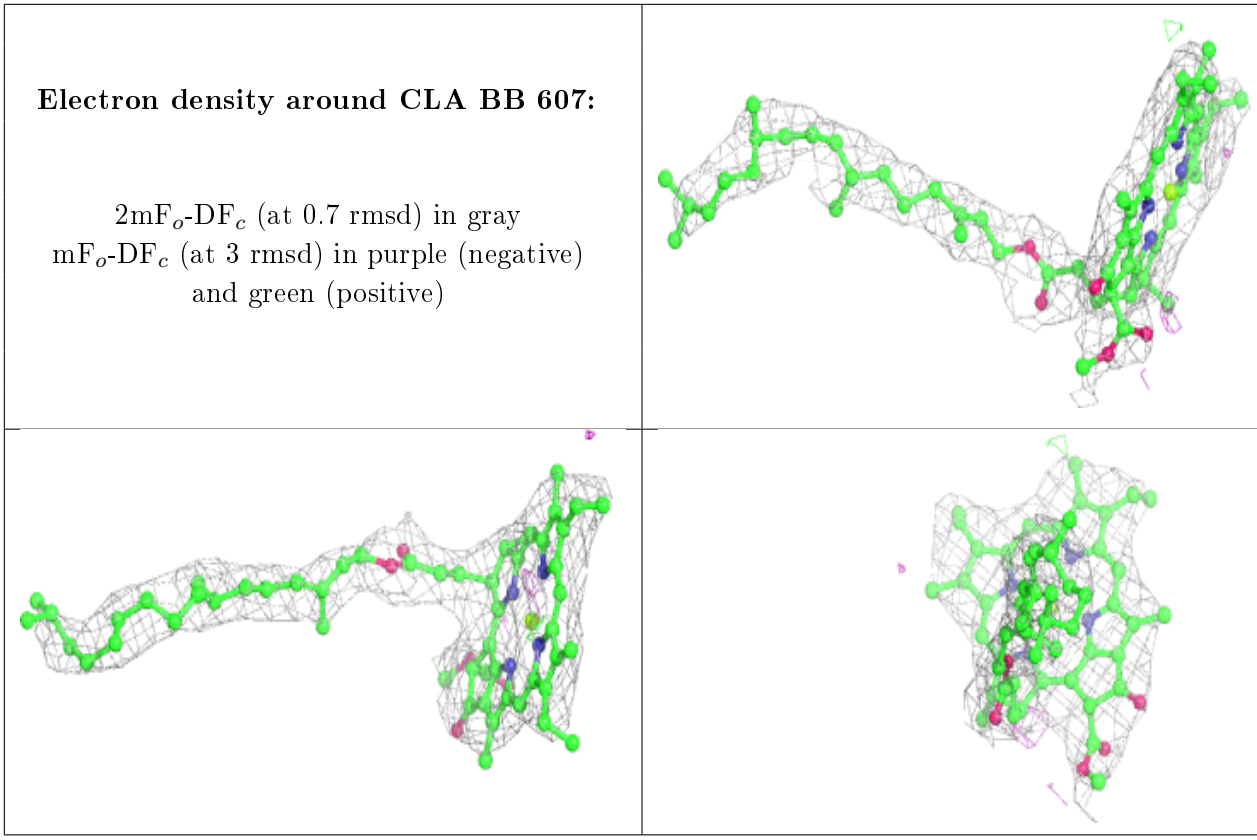
Electron density around PHO BD 403:

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



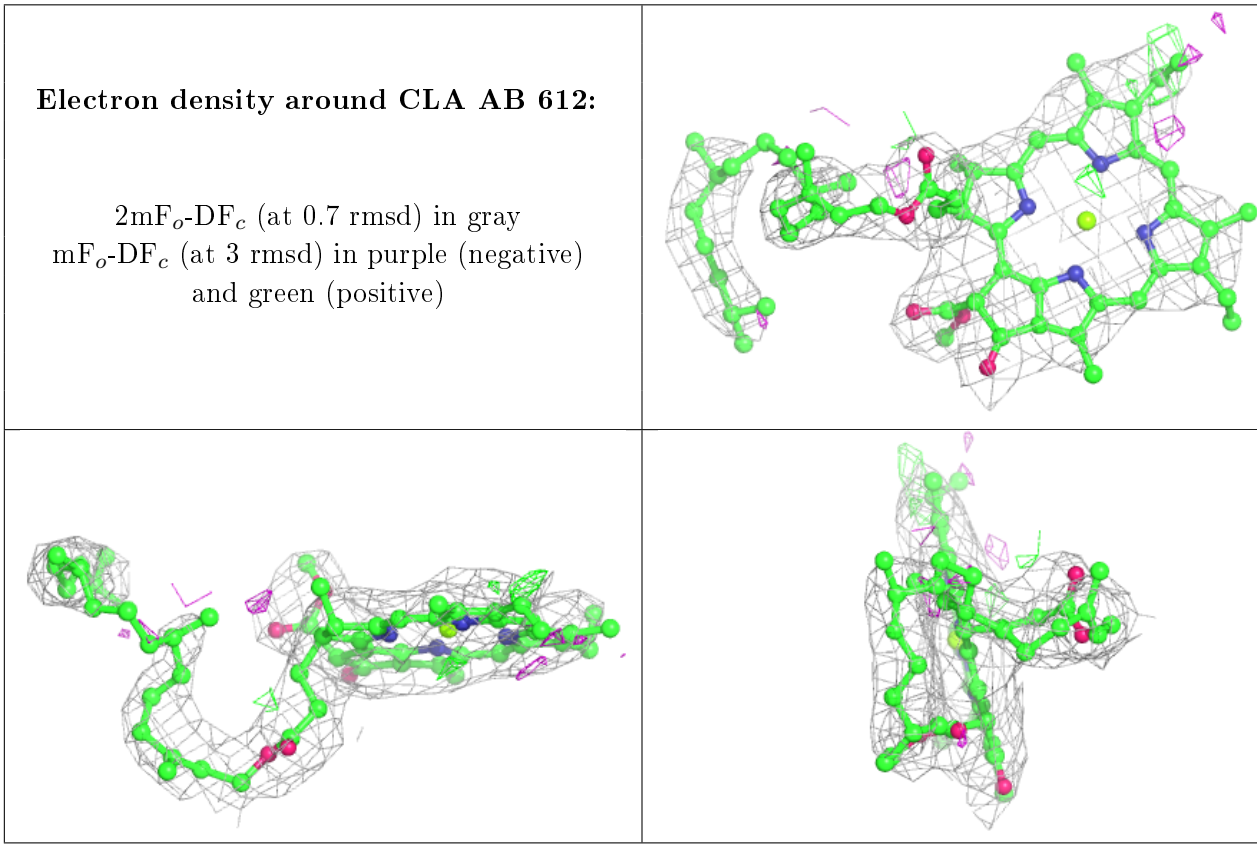
Electron density around CLA BB 607:

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



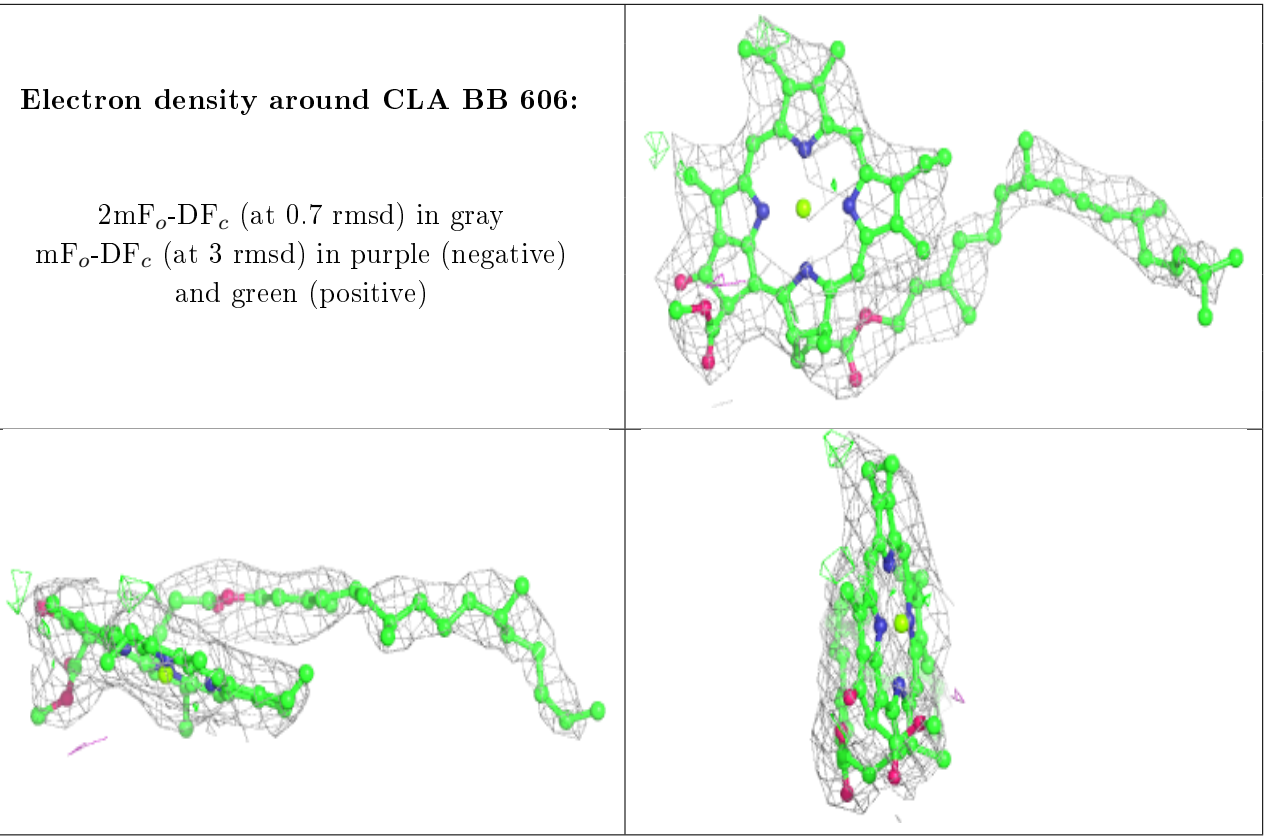
Electron density around CLA AB 612:

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



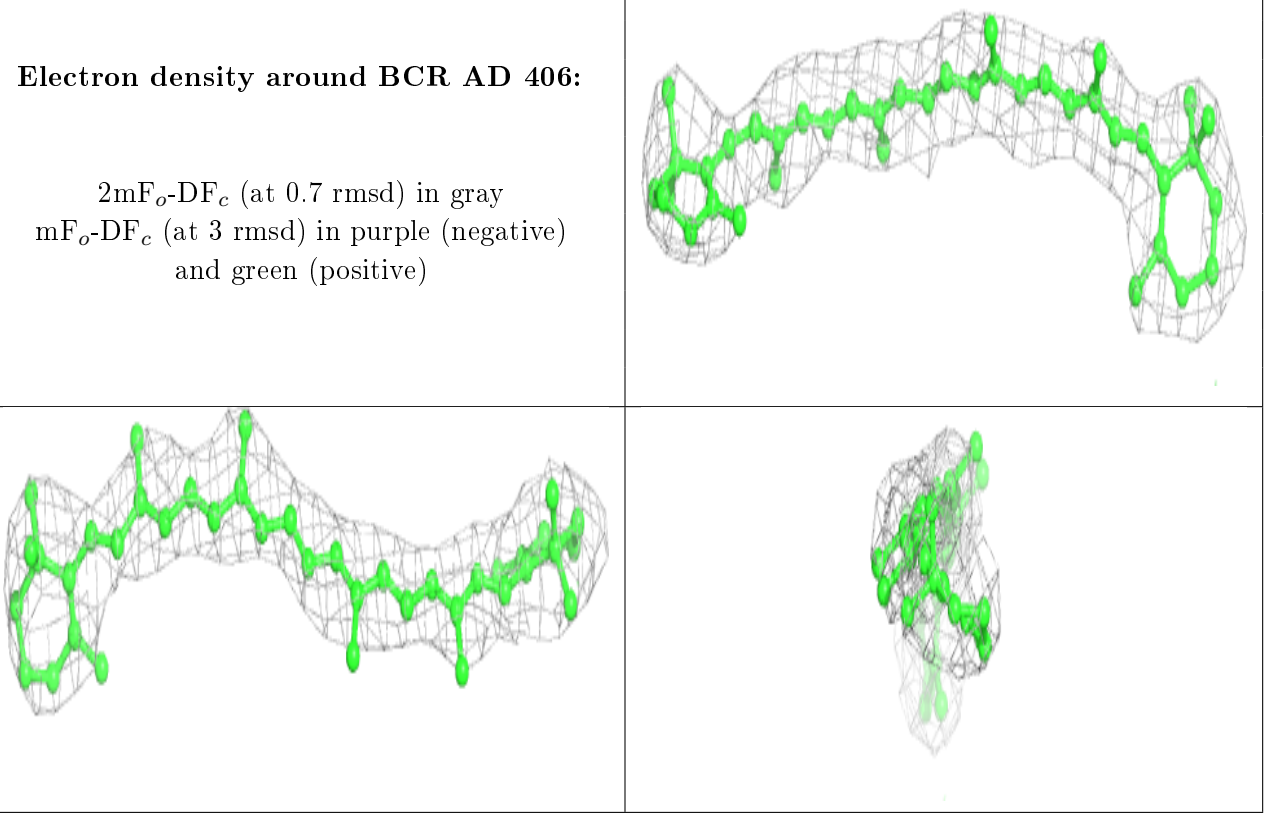
Electron density around CLA BB 606:

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



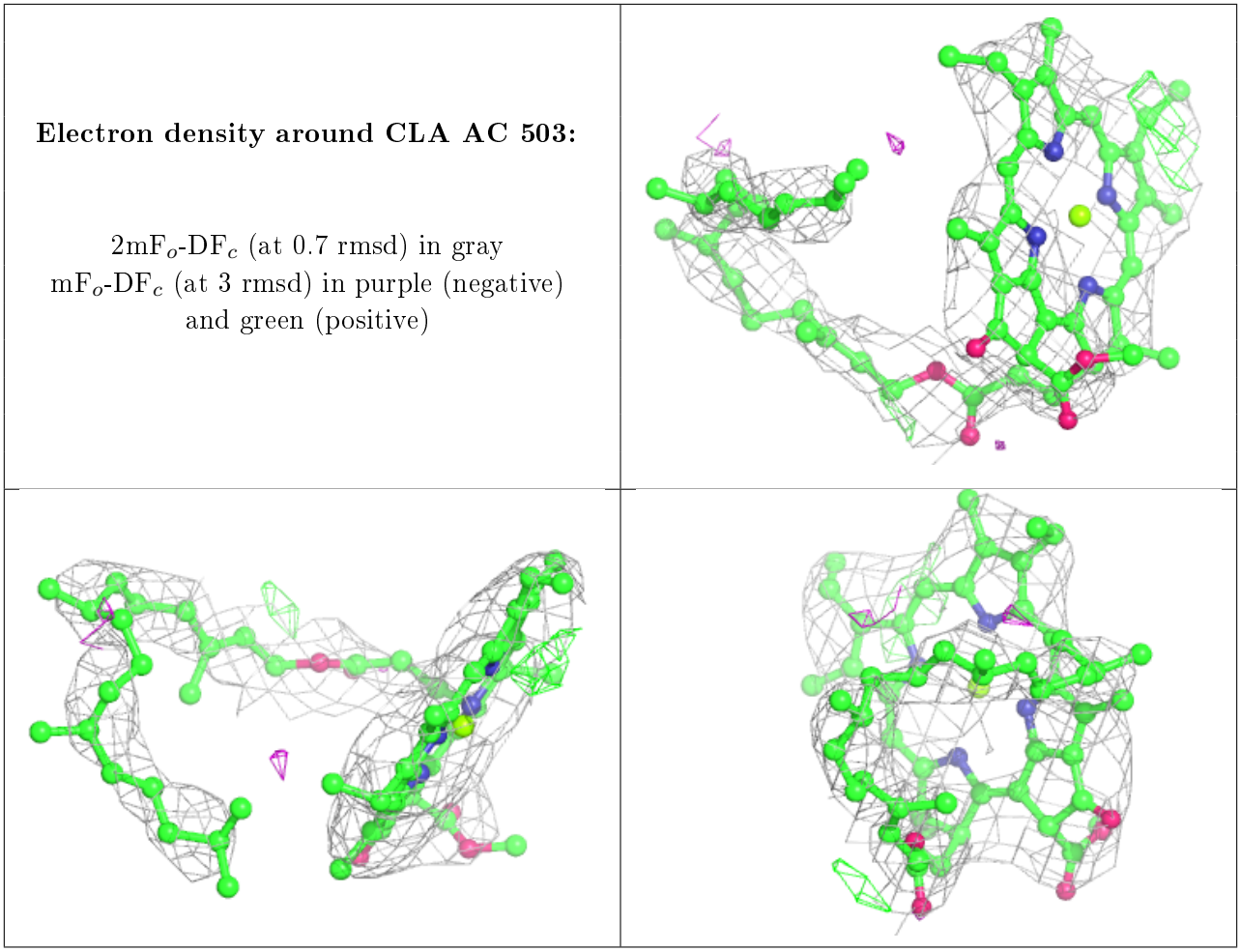
Electron density around BCR AD 406:

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



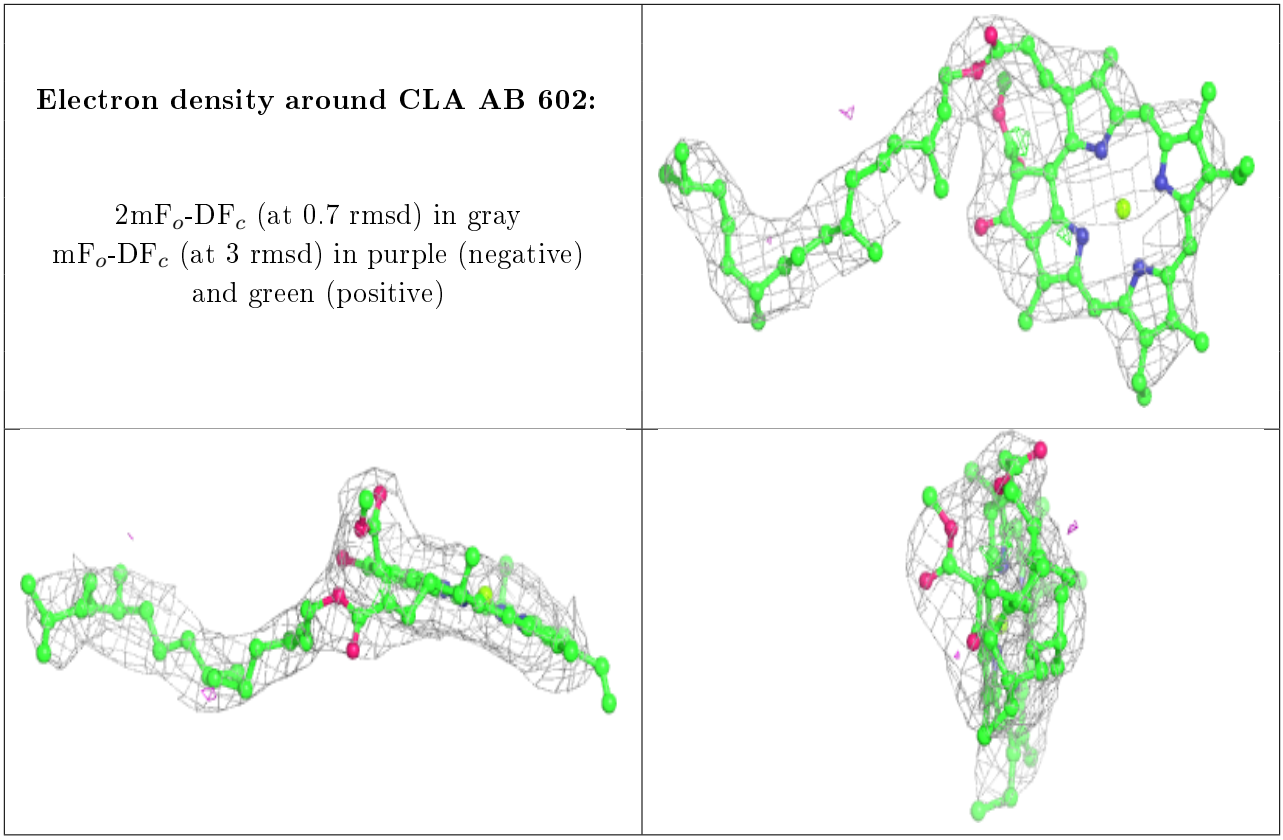
Electron density around CLA AC 503:

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



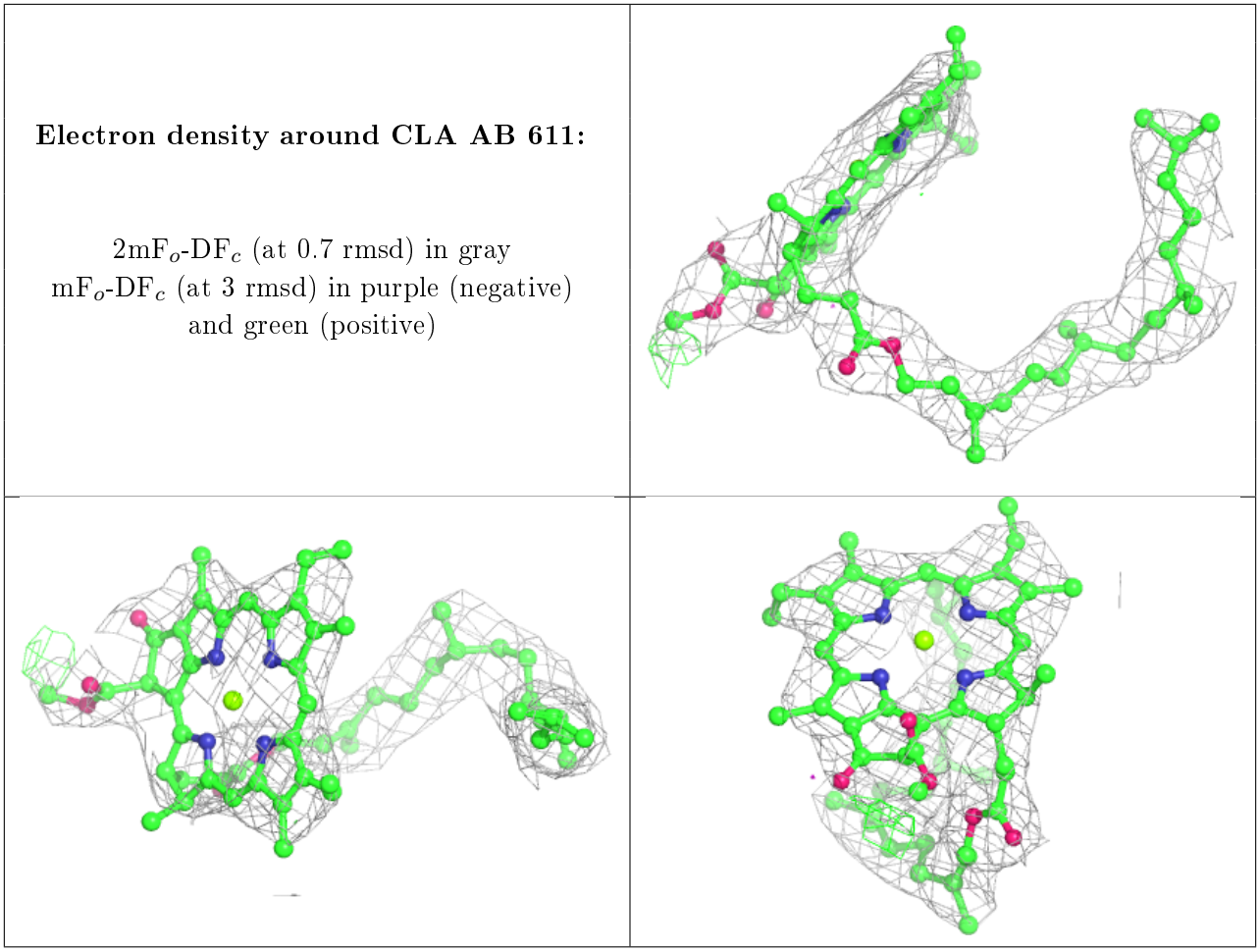
Electron density around CLA AB 602:

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



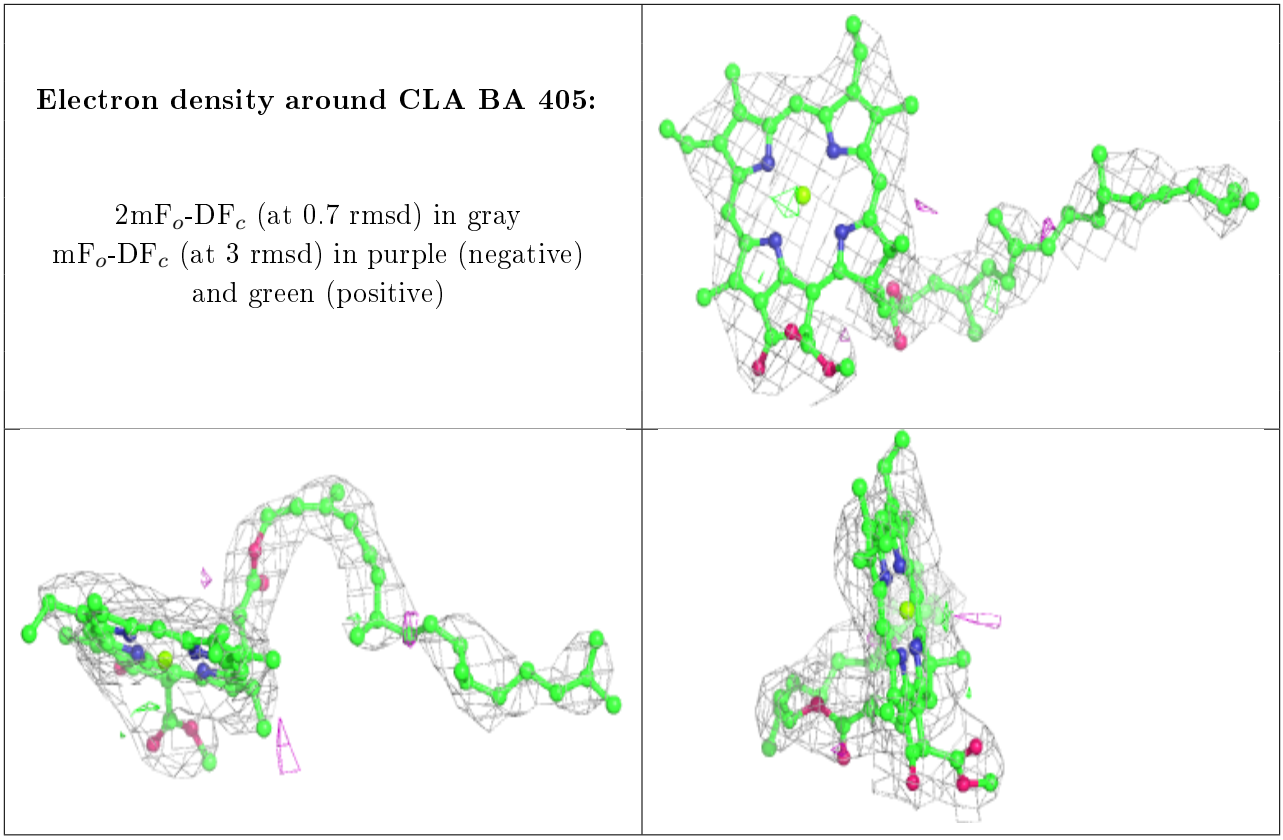
Electron density around CLA AB 611:

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



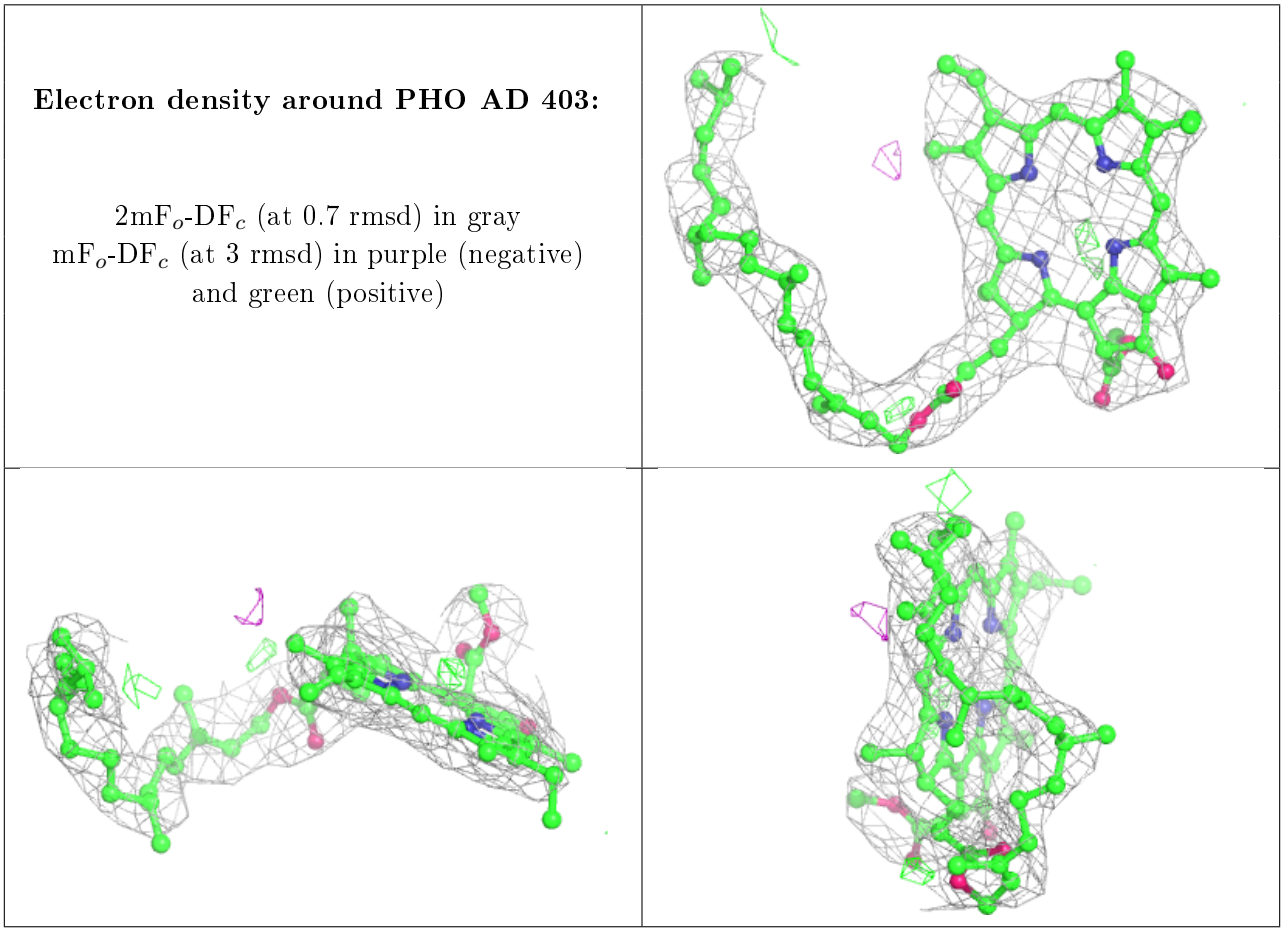
Electron density around CLA BA 405:

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



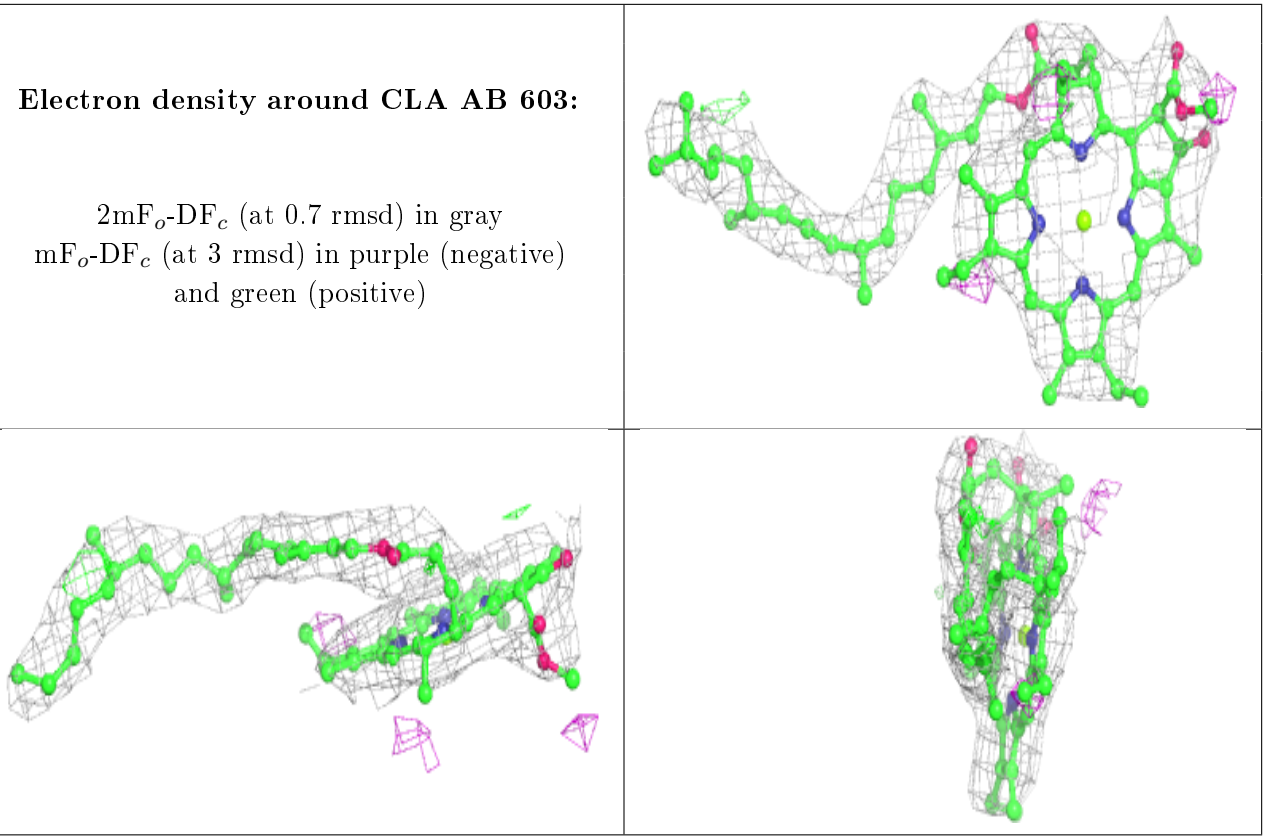
Electron density around PHO AD 403:

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



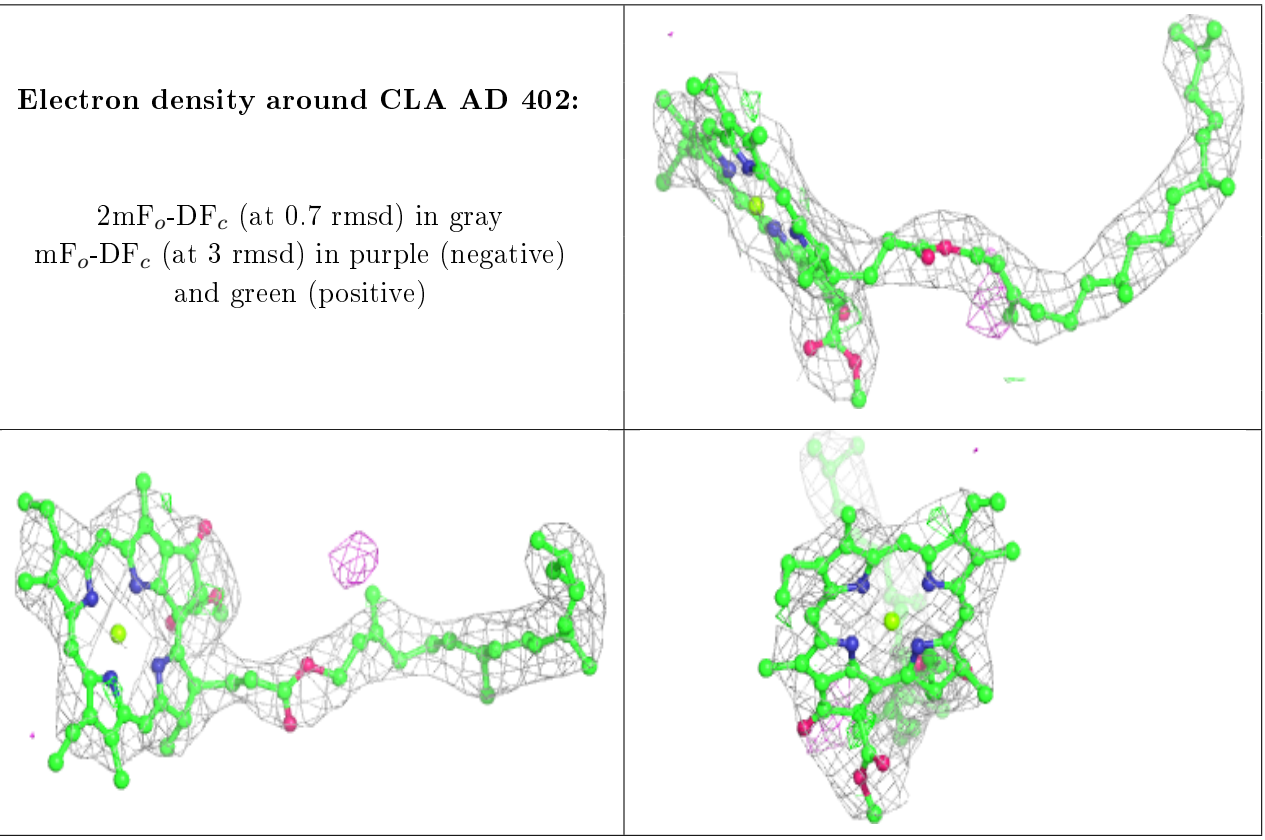
Electron density around CLA AB 603:

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



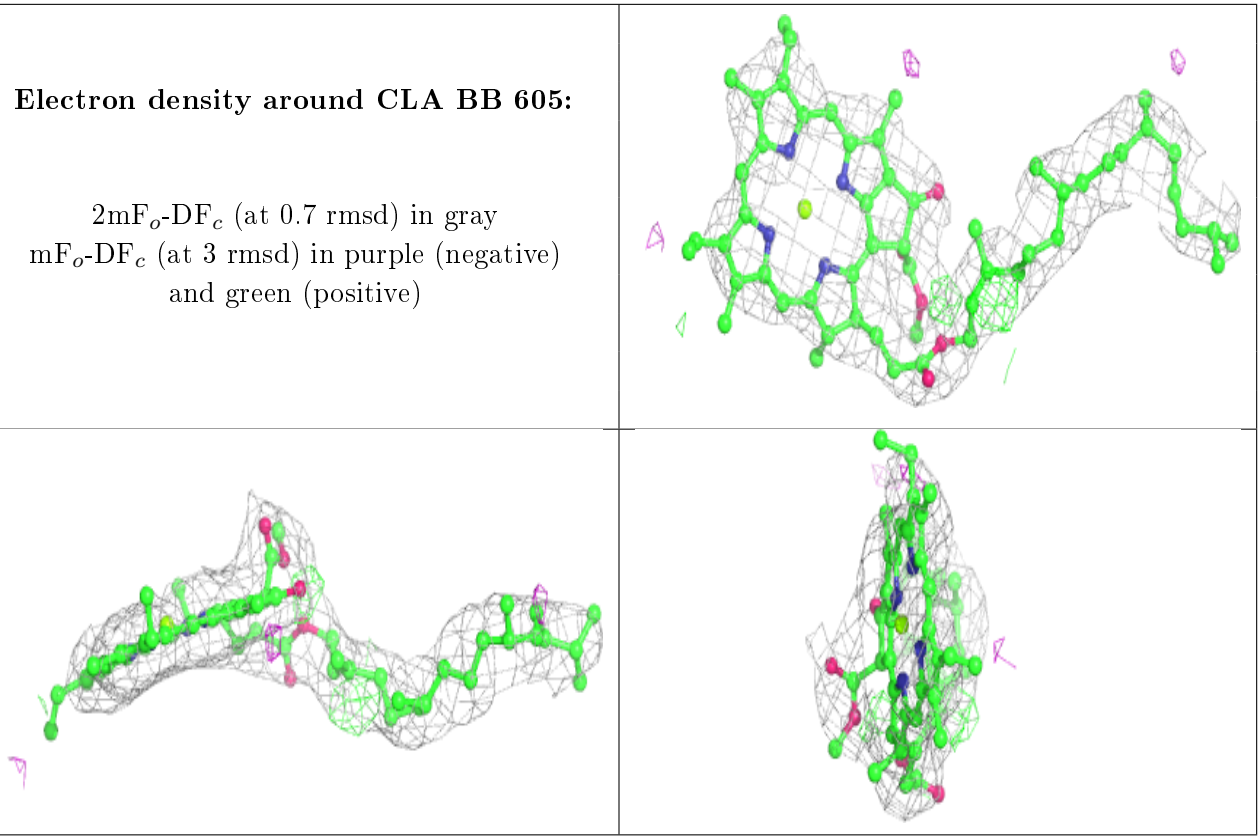
Electron density around CLA AD 402:

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



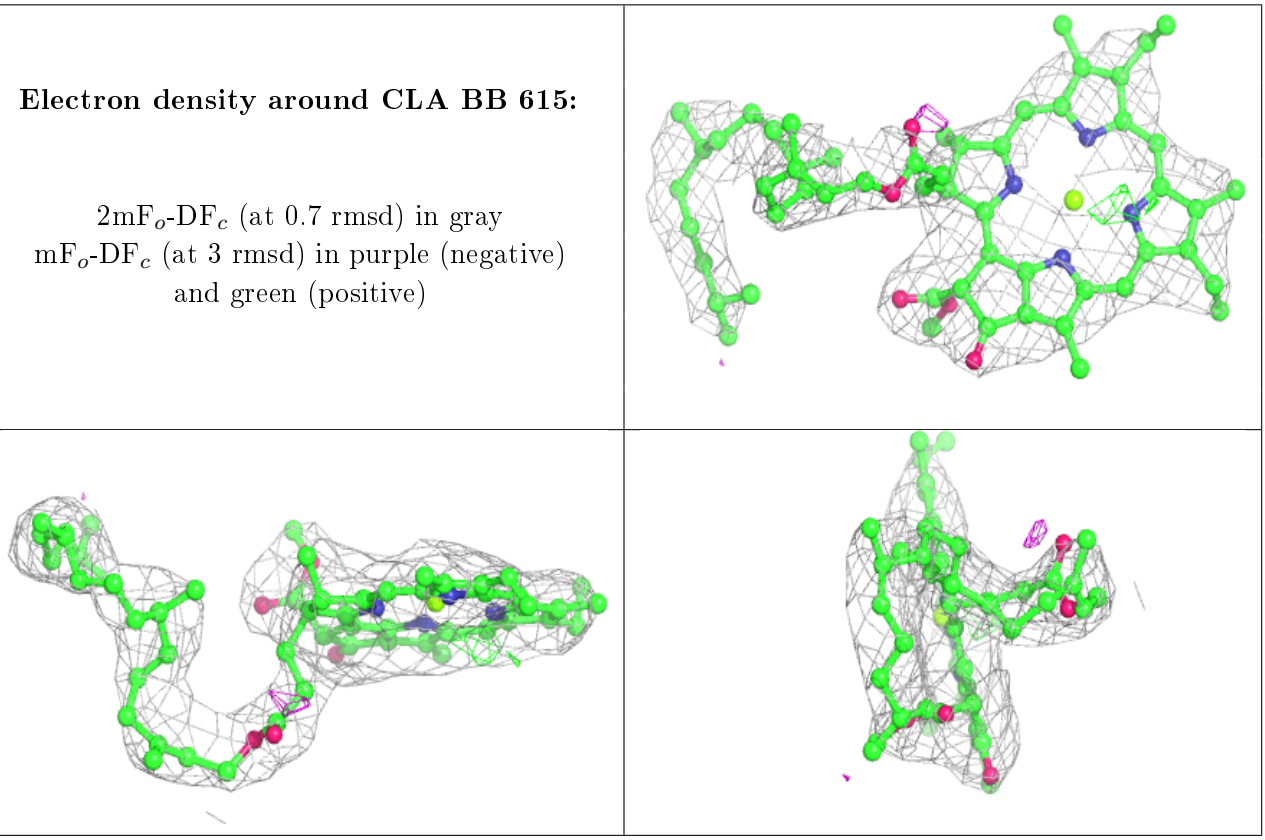
Electron density around CLA BB 605:

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



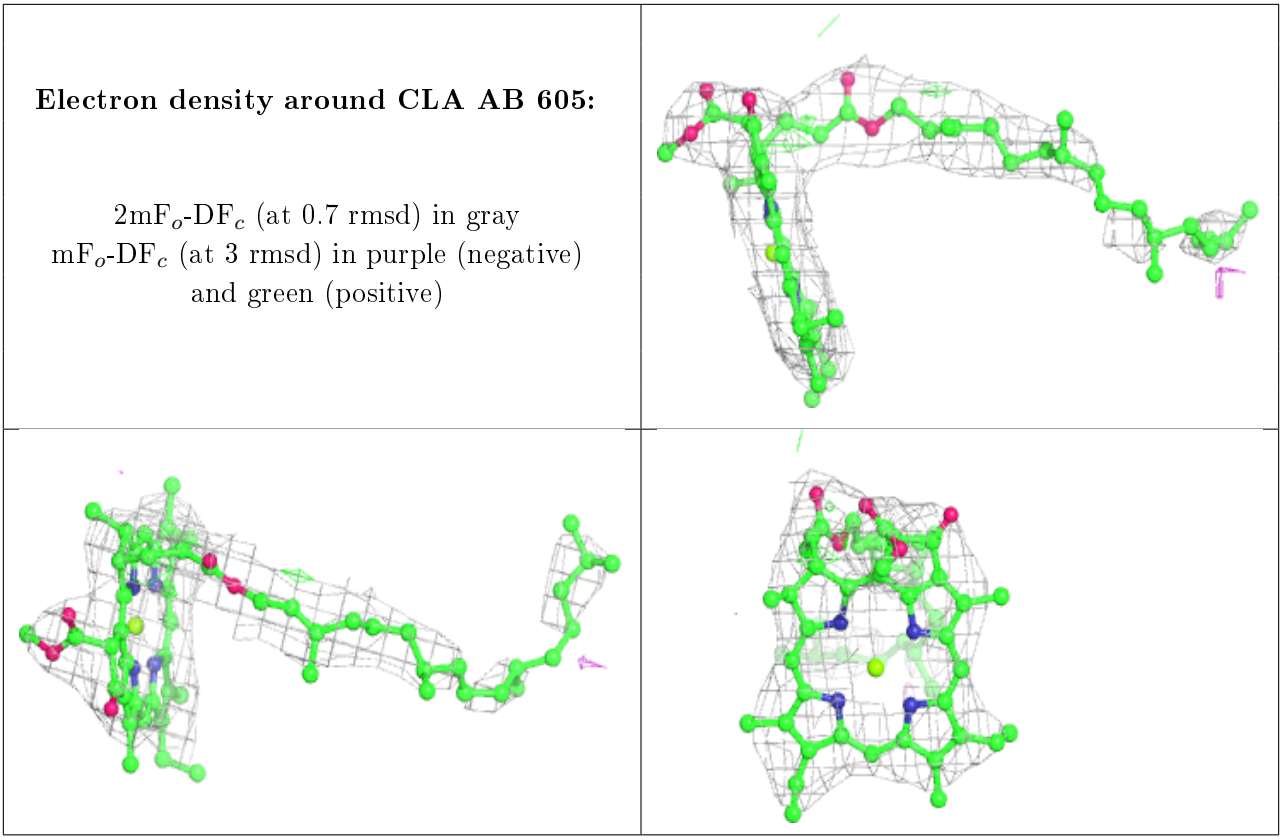
Electron density around CLA BB 615:

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



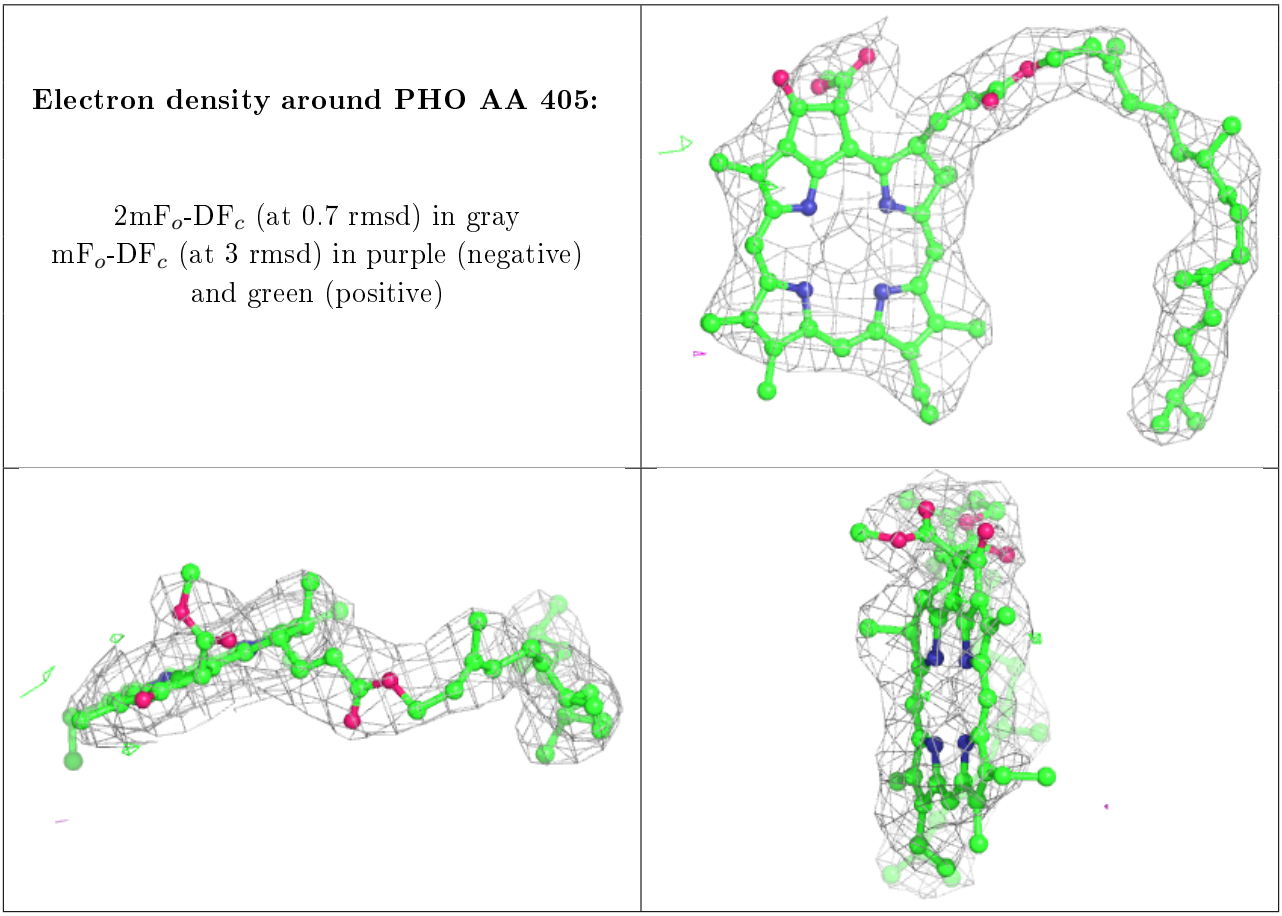
Electron density around CLA AB 605:

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



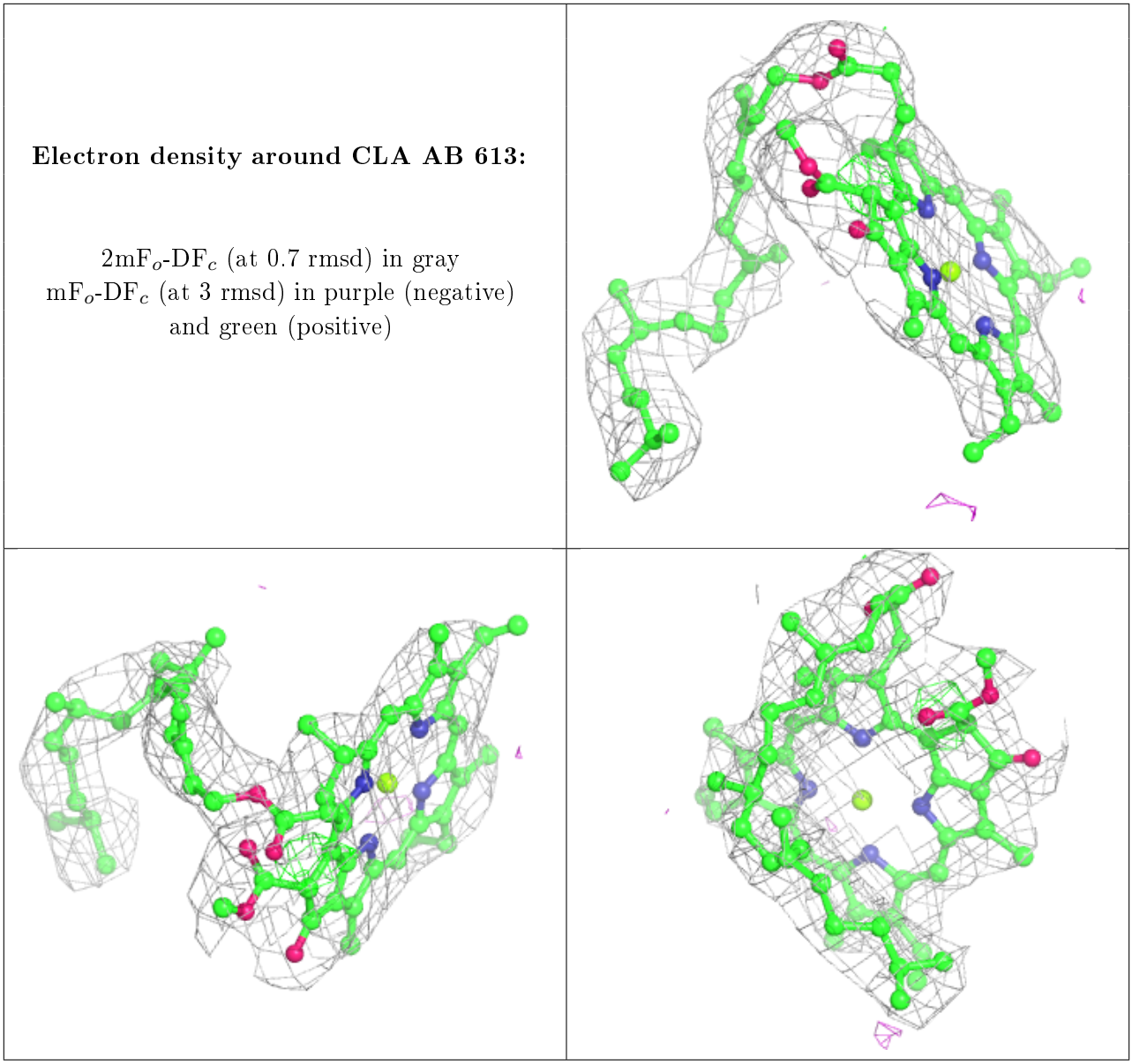
Electron density around PHO AA 405:

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



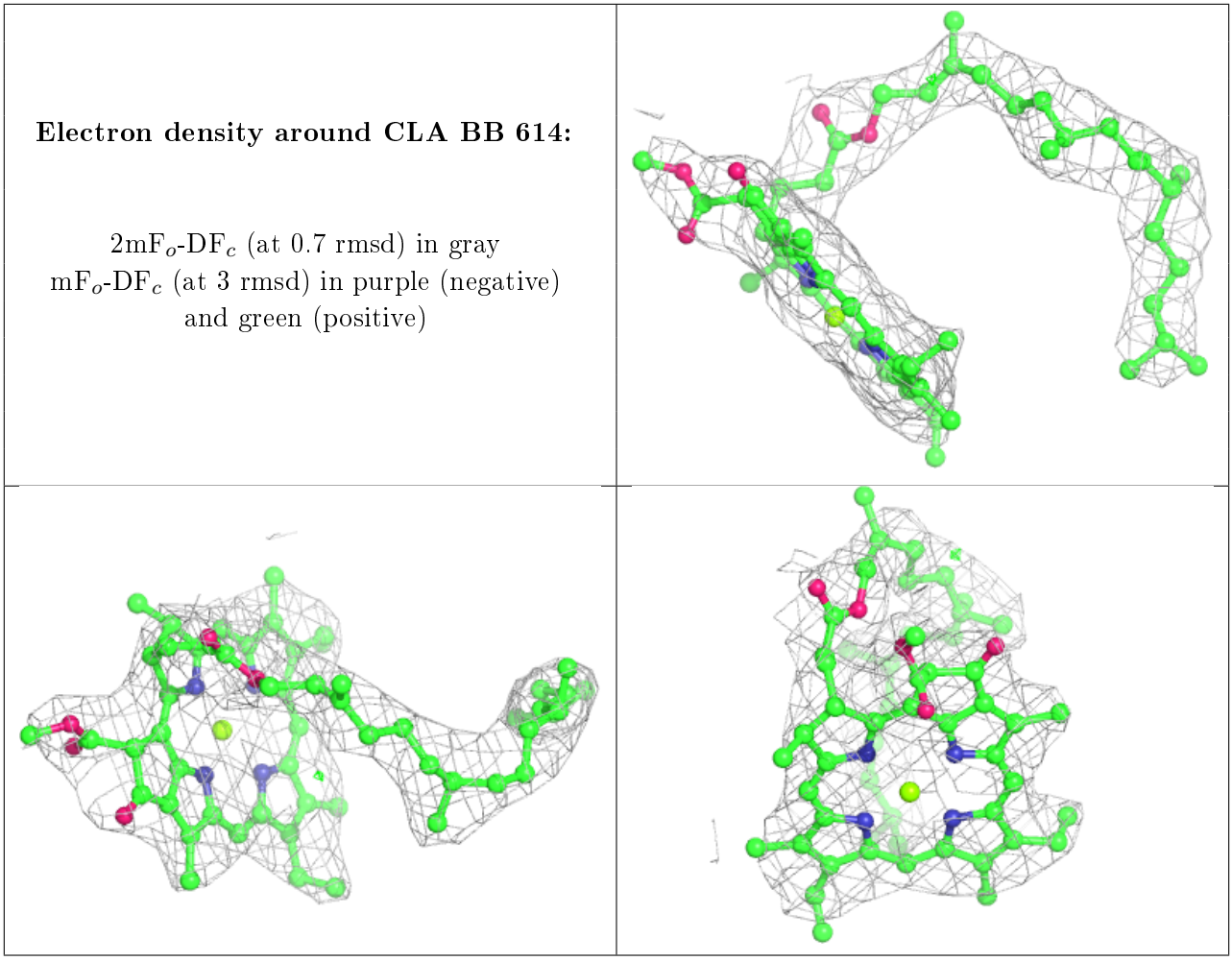
Electron density around CLA AB 613:

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



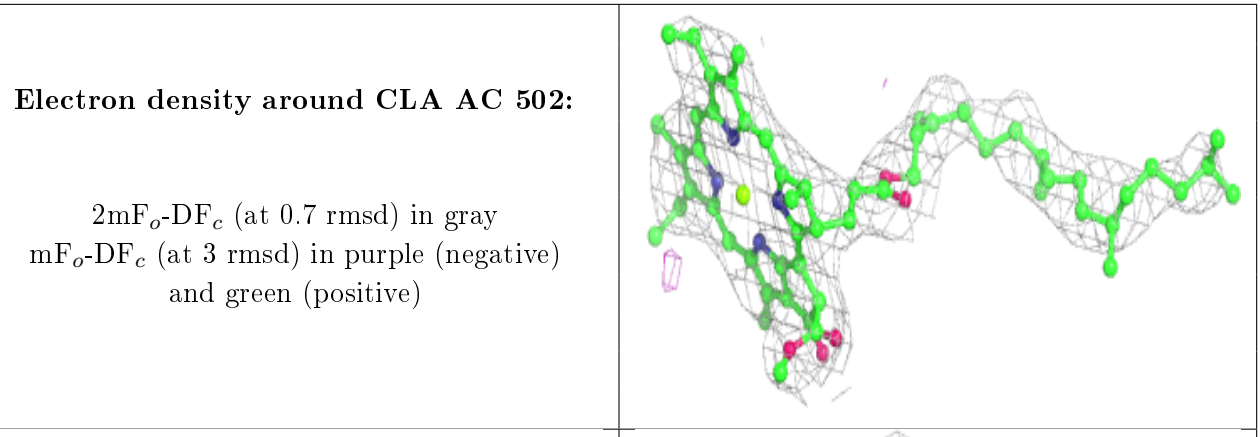
Electron density around CLA BB 614:

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



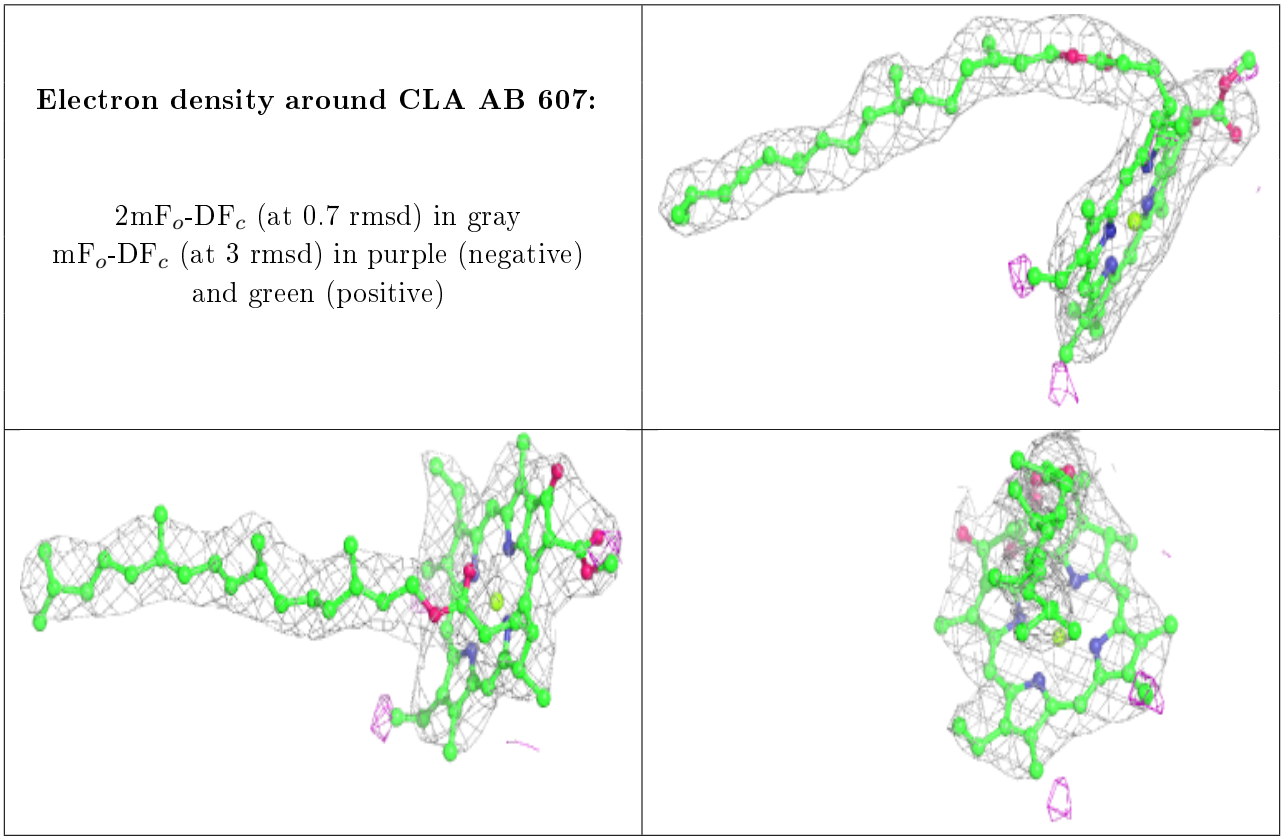
Electron density around CLA AC 502:

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



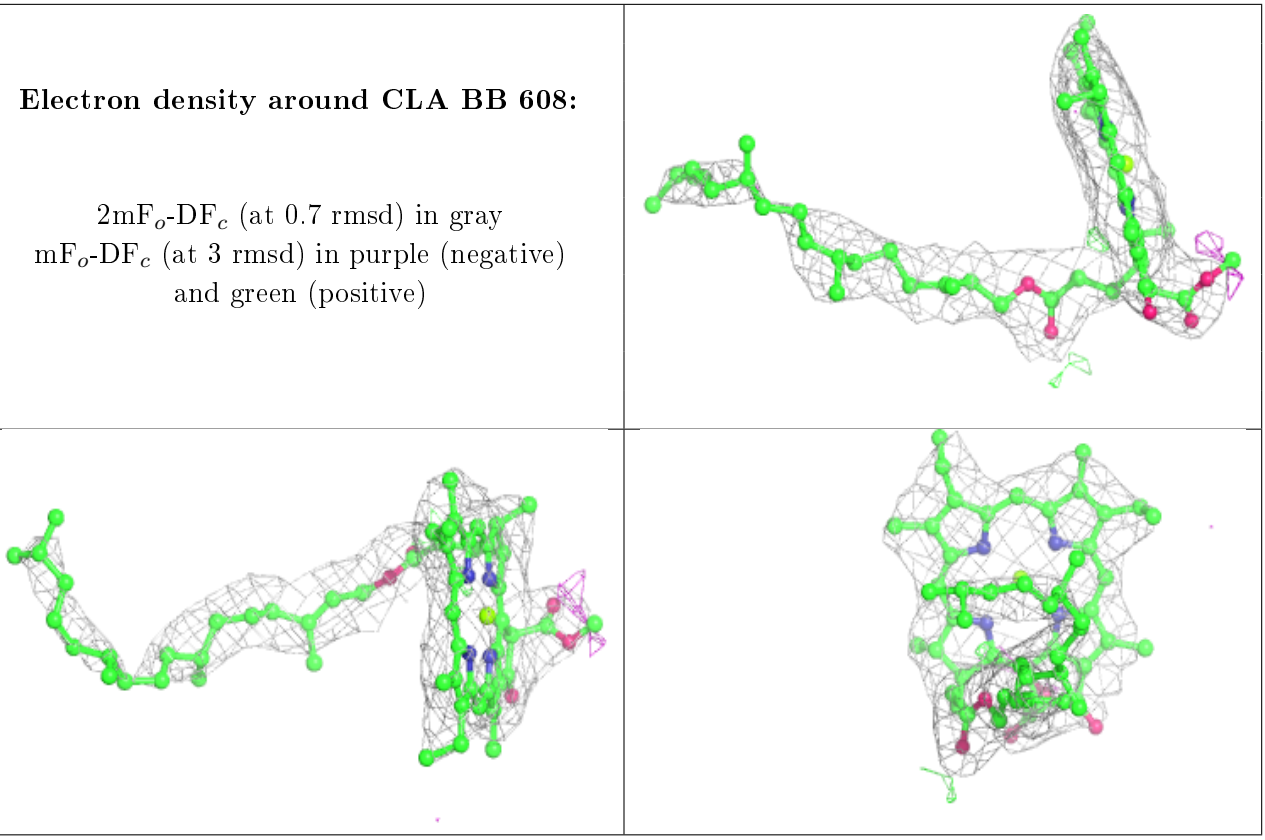
Electron density around CLA AB 607:

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



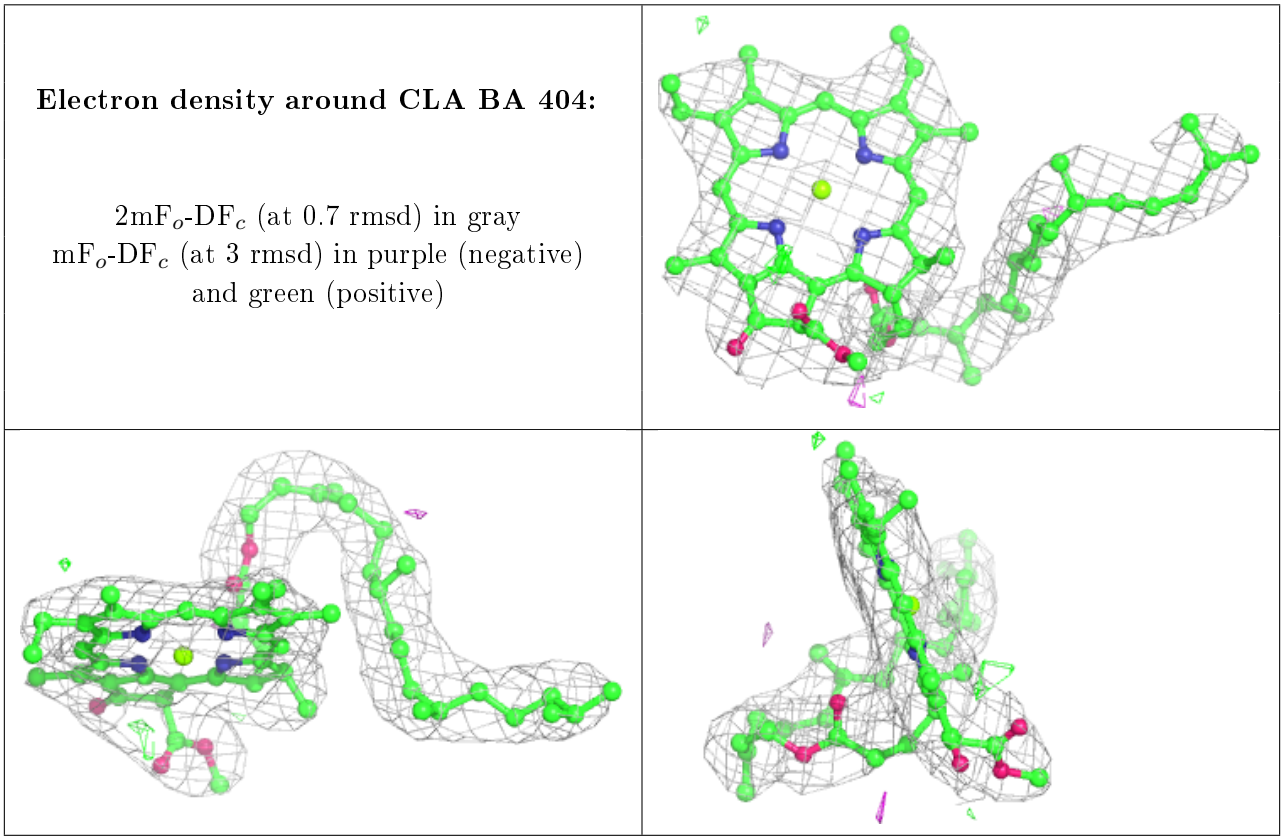
Electron density around CLA BB 608:

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



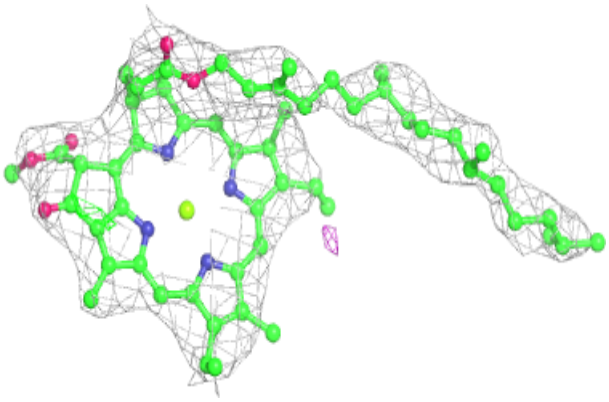
Electron density around CLA BA 404:

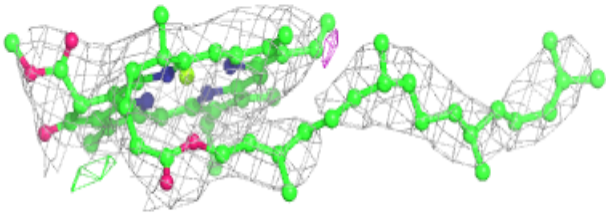
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

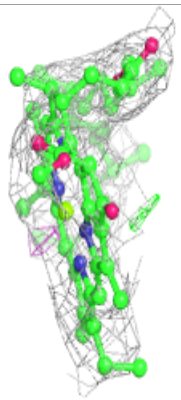


Electron density around CLA AC 501:

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

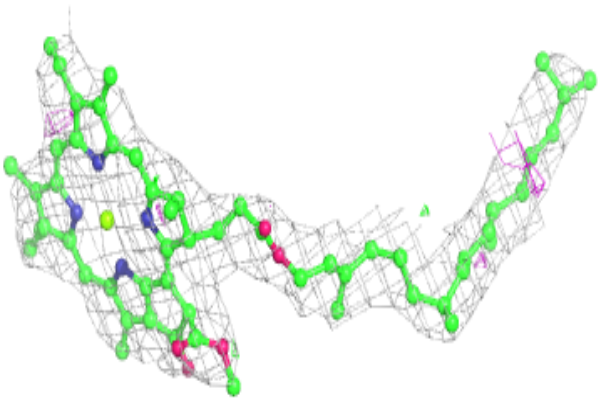


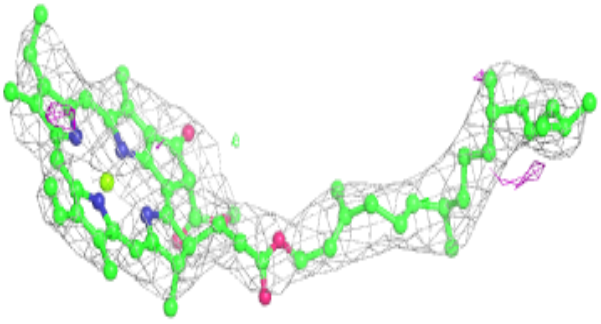


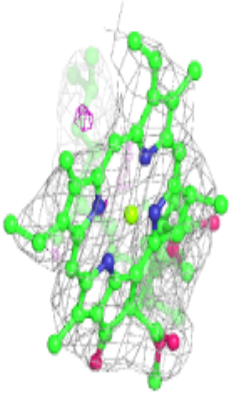


Electron density around CLA BA 403:

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

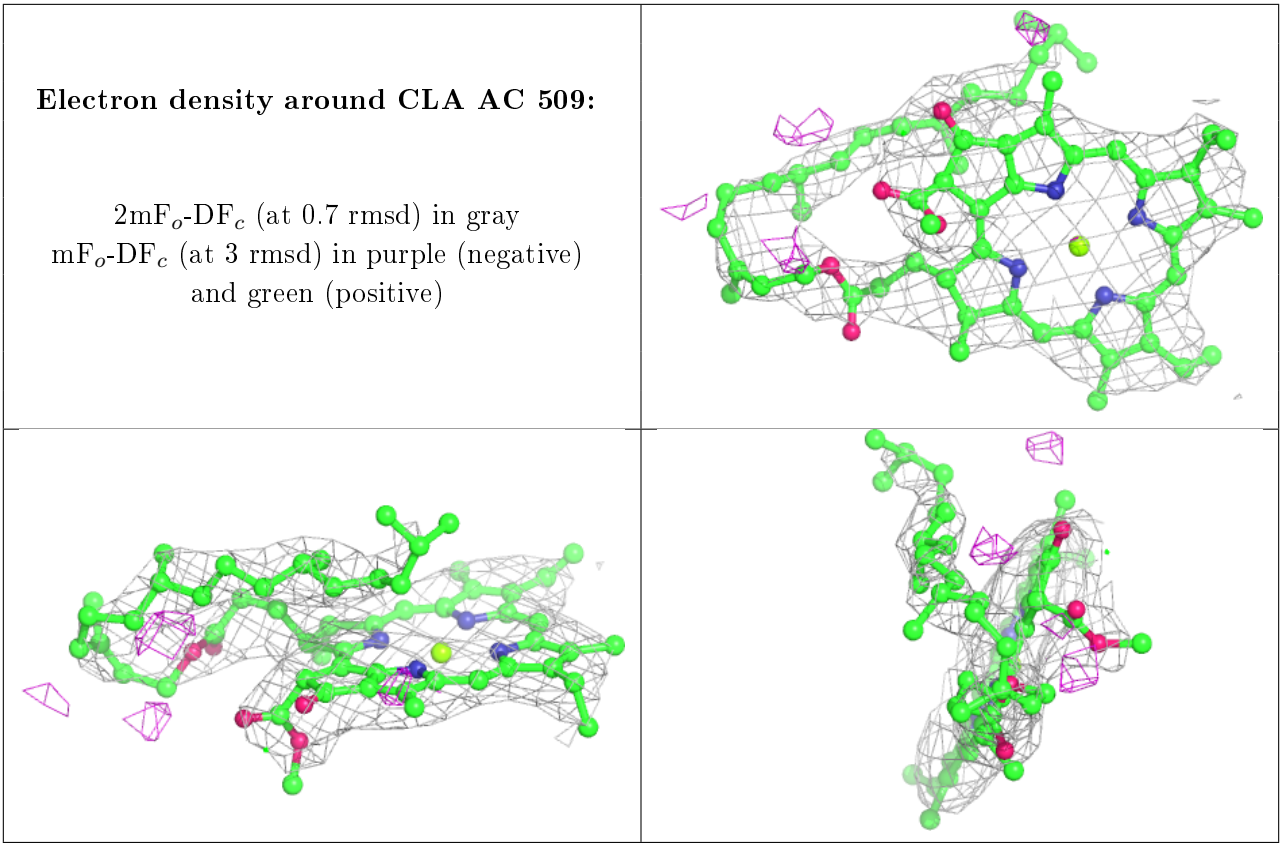






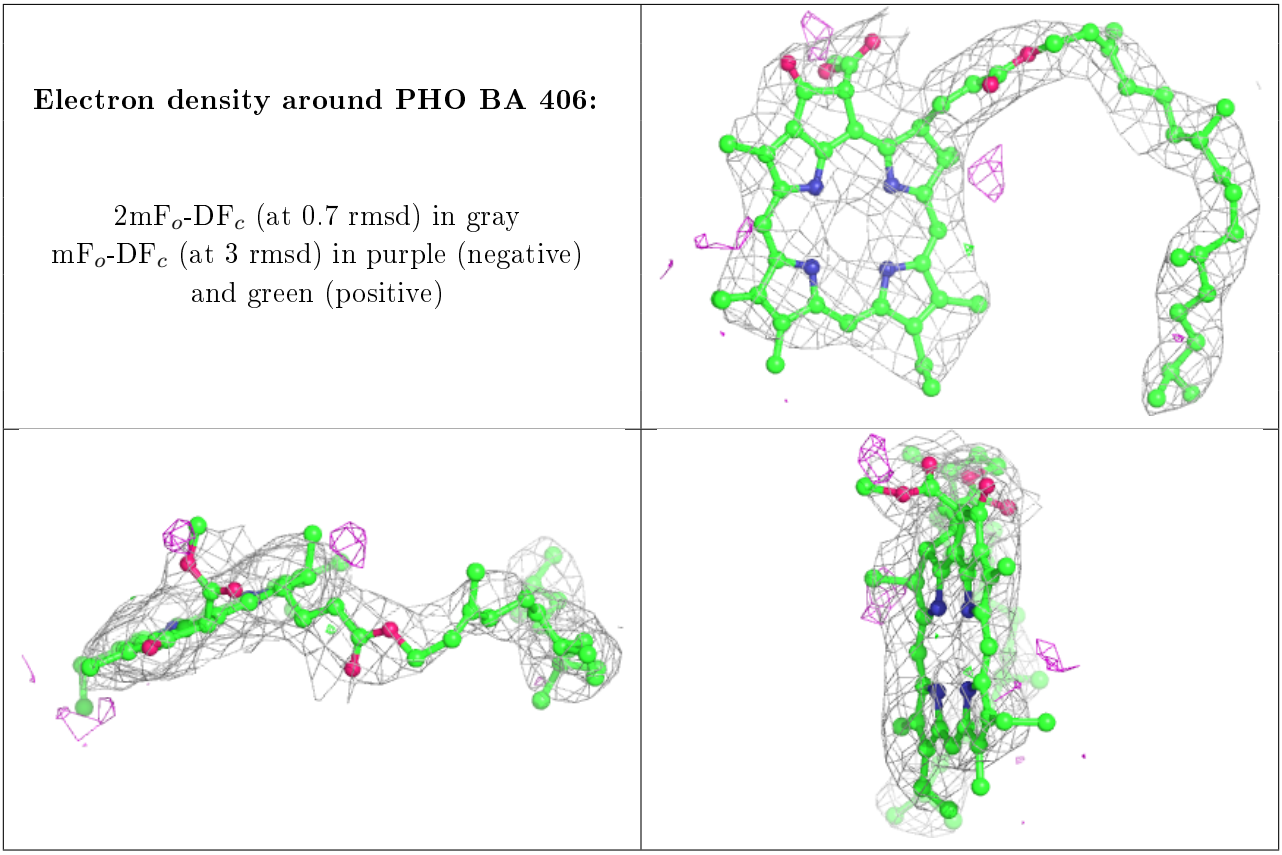
Electron density around CLA AC 509:

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



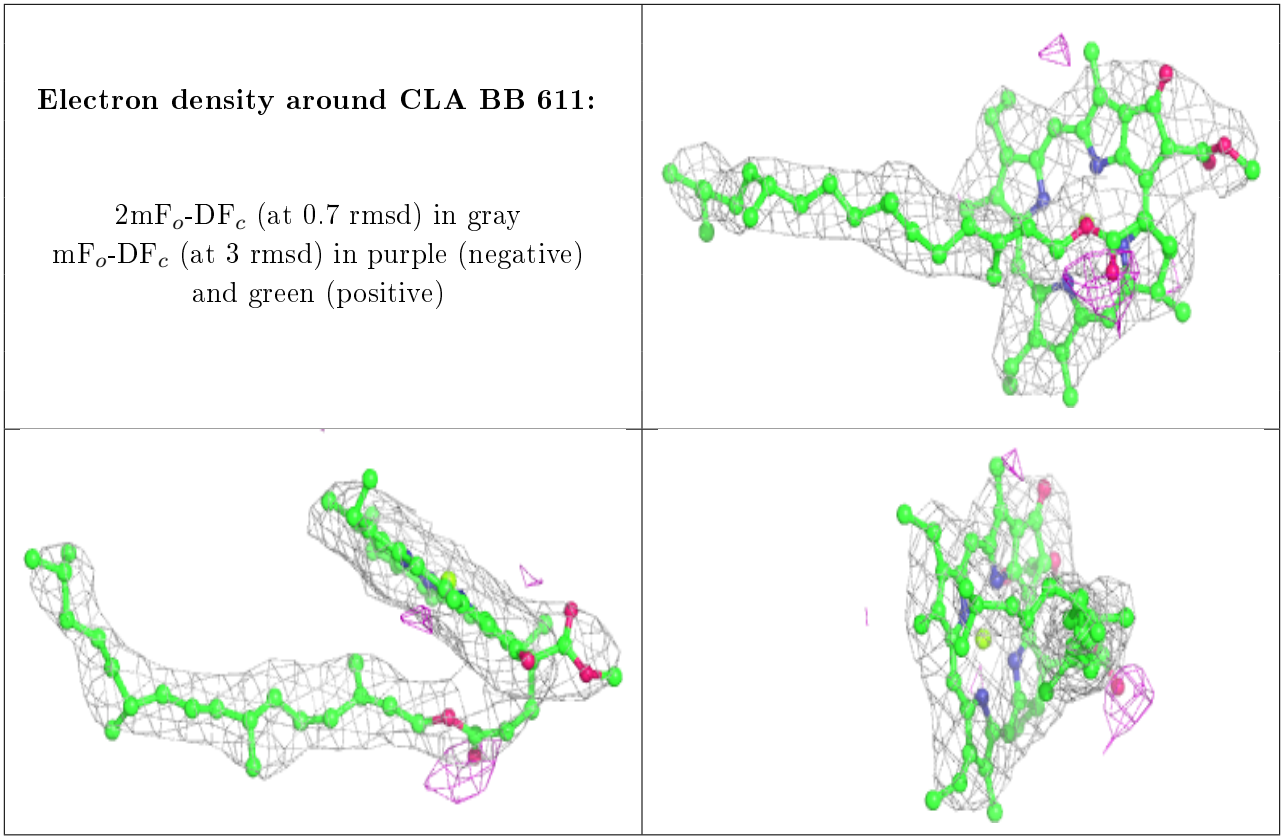
Electron density around PHO BA 406:

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



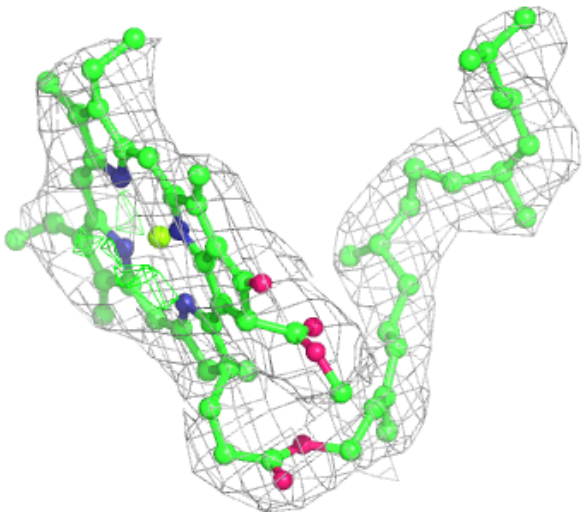
Electron density around CLA BB 611:

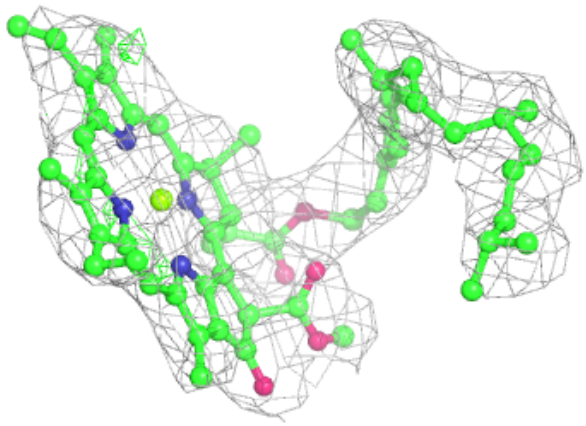
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

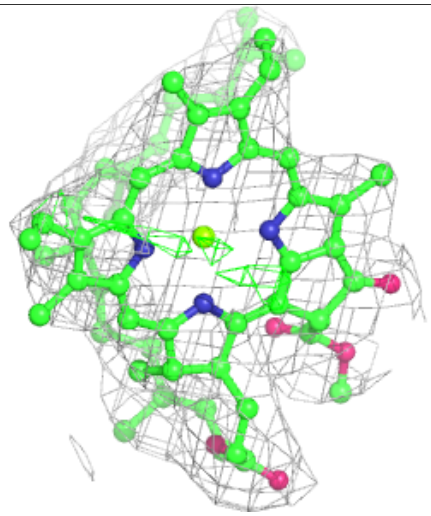


Electron density around CLA BB 616:

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

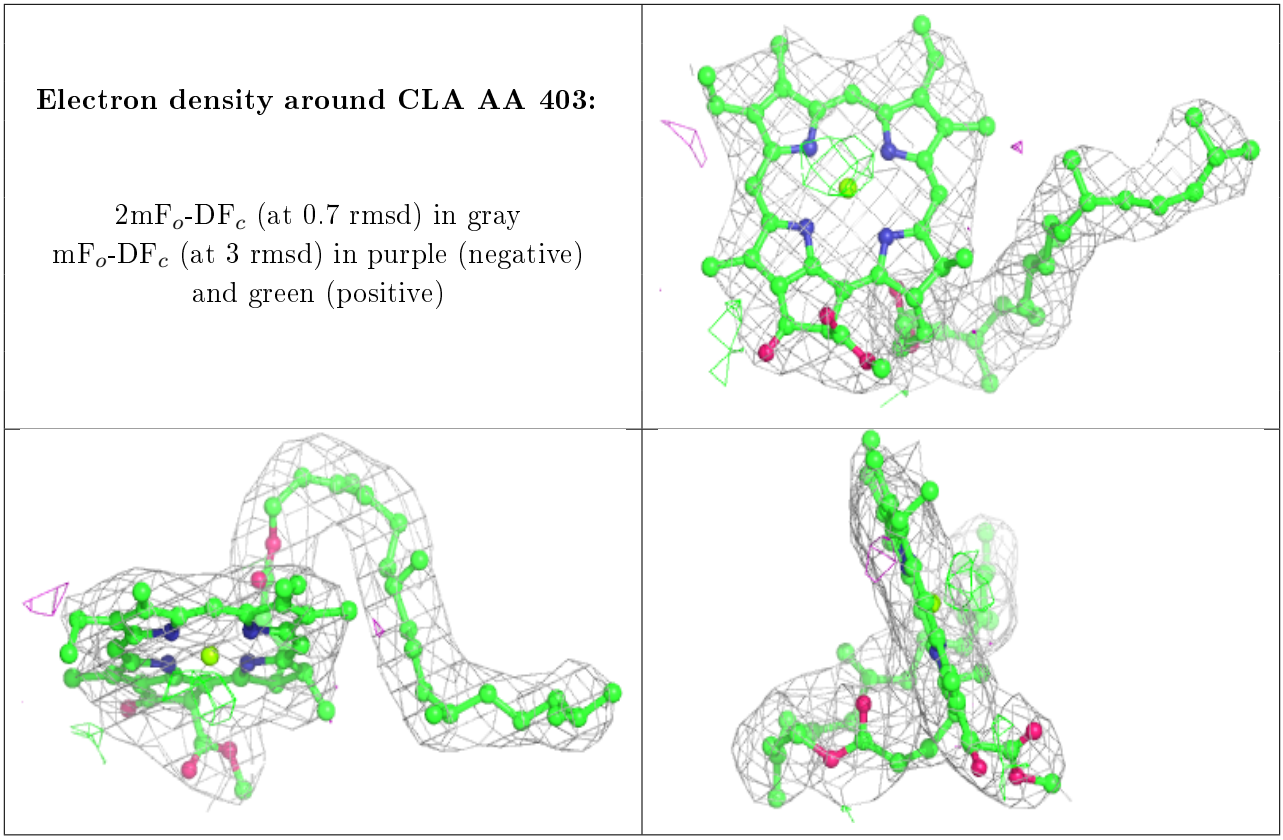






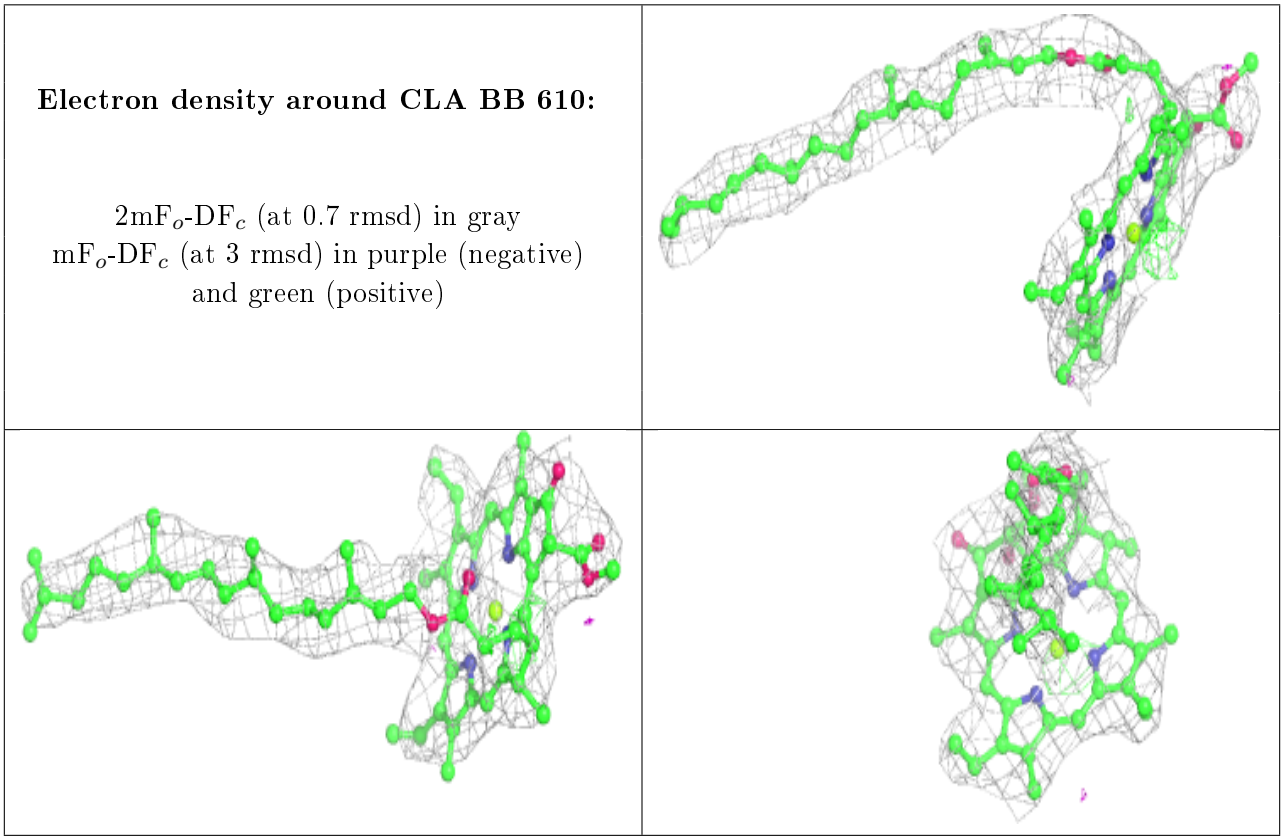
Electron density around CLA AA 403:

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



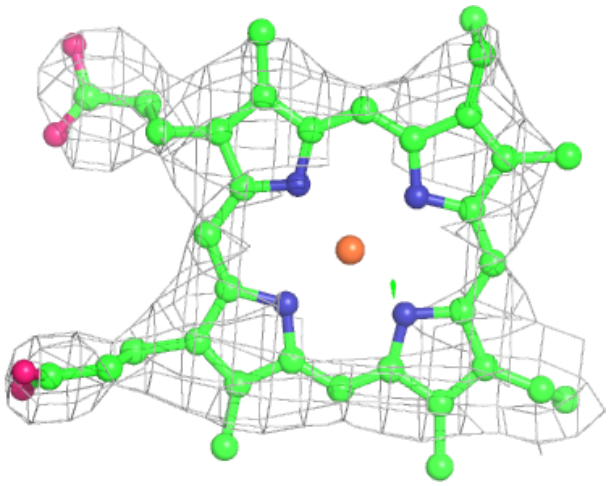
Electron density around CLA BB 610:

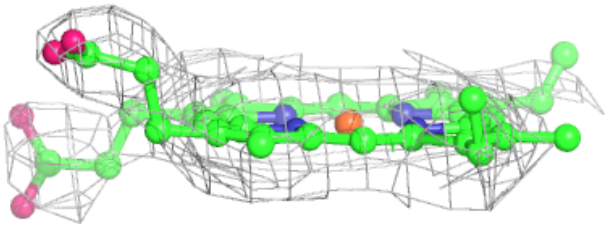
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

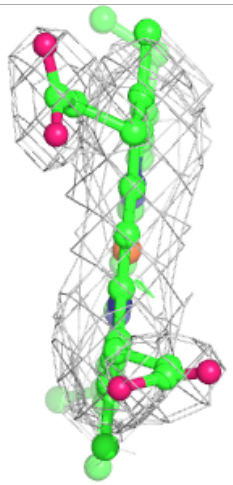


Electron density around HEM BV 201:

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

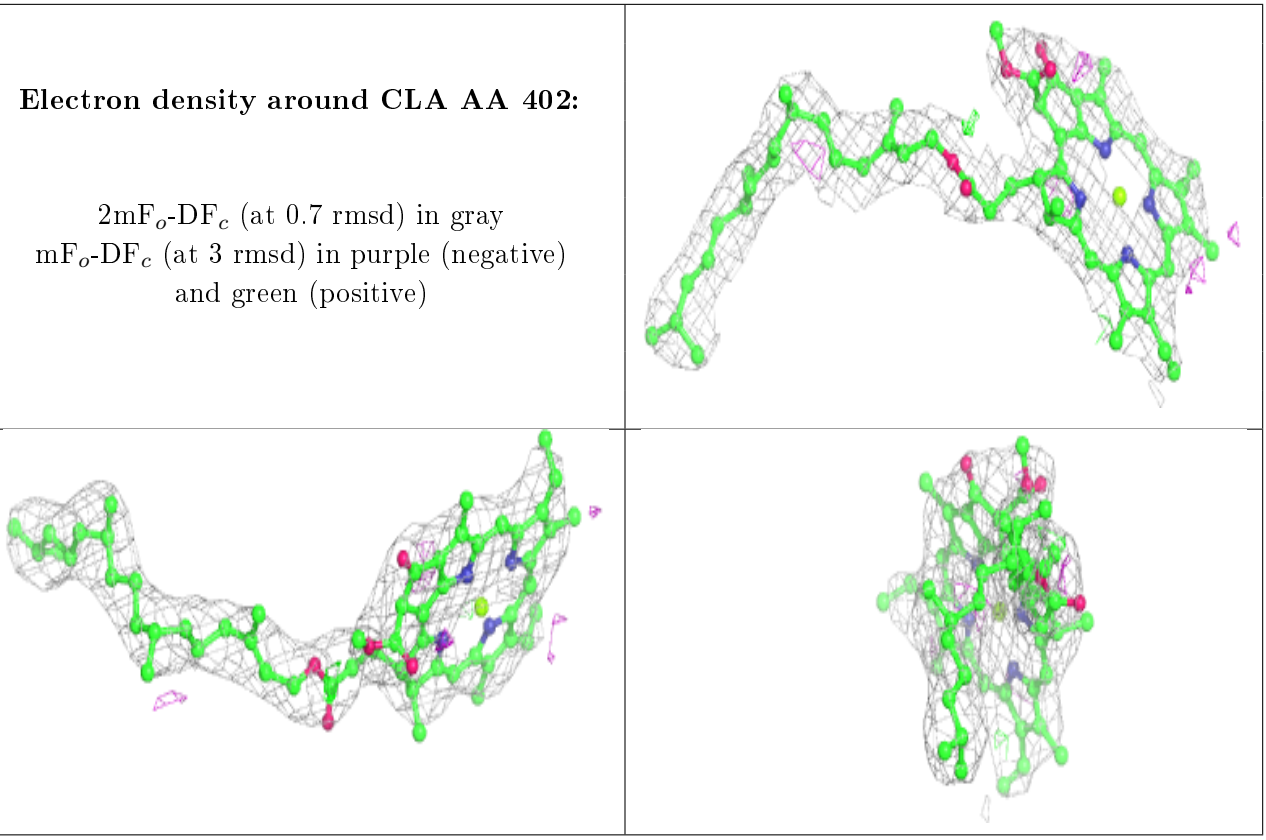






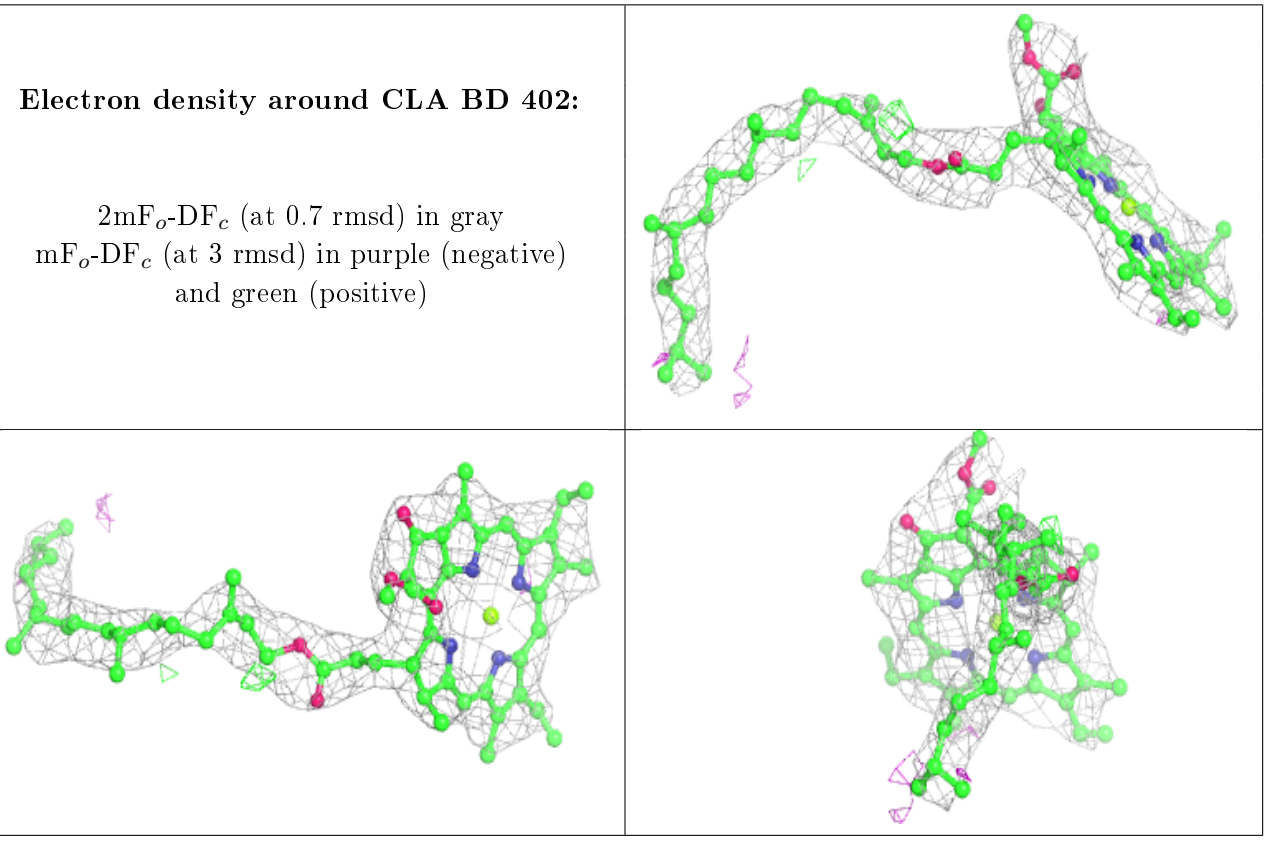
Electron density around CLA AA 402:

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



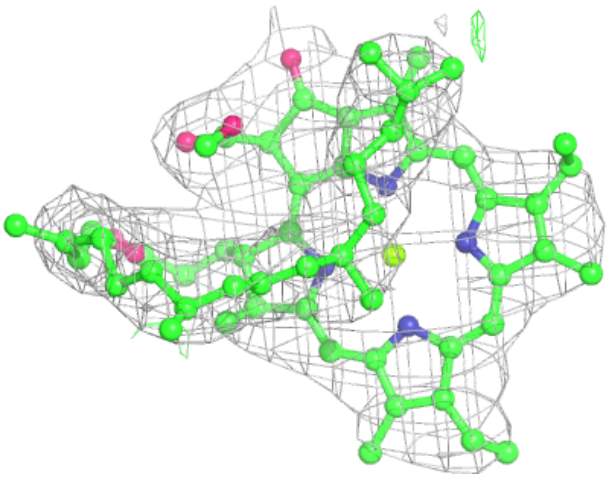
Electron density around CLA BD 402:

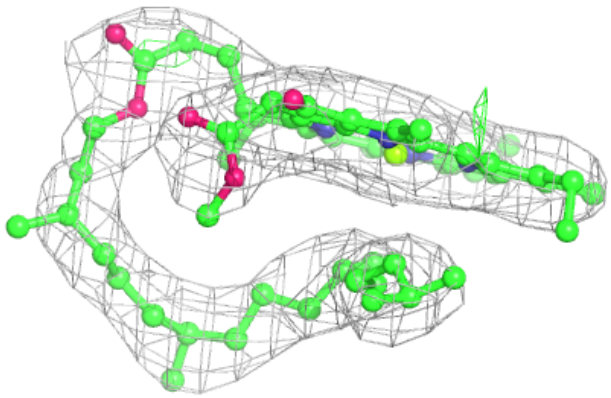
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

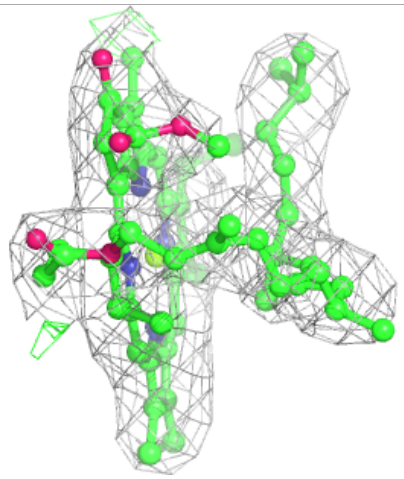


Electron density around CLA AC 510:

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

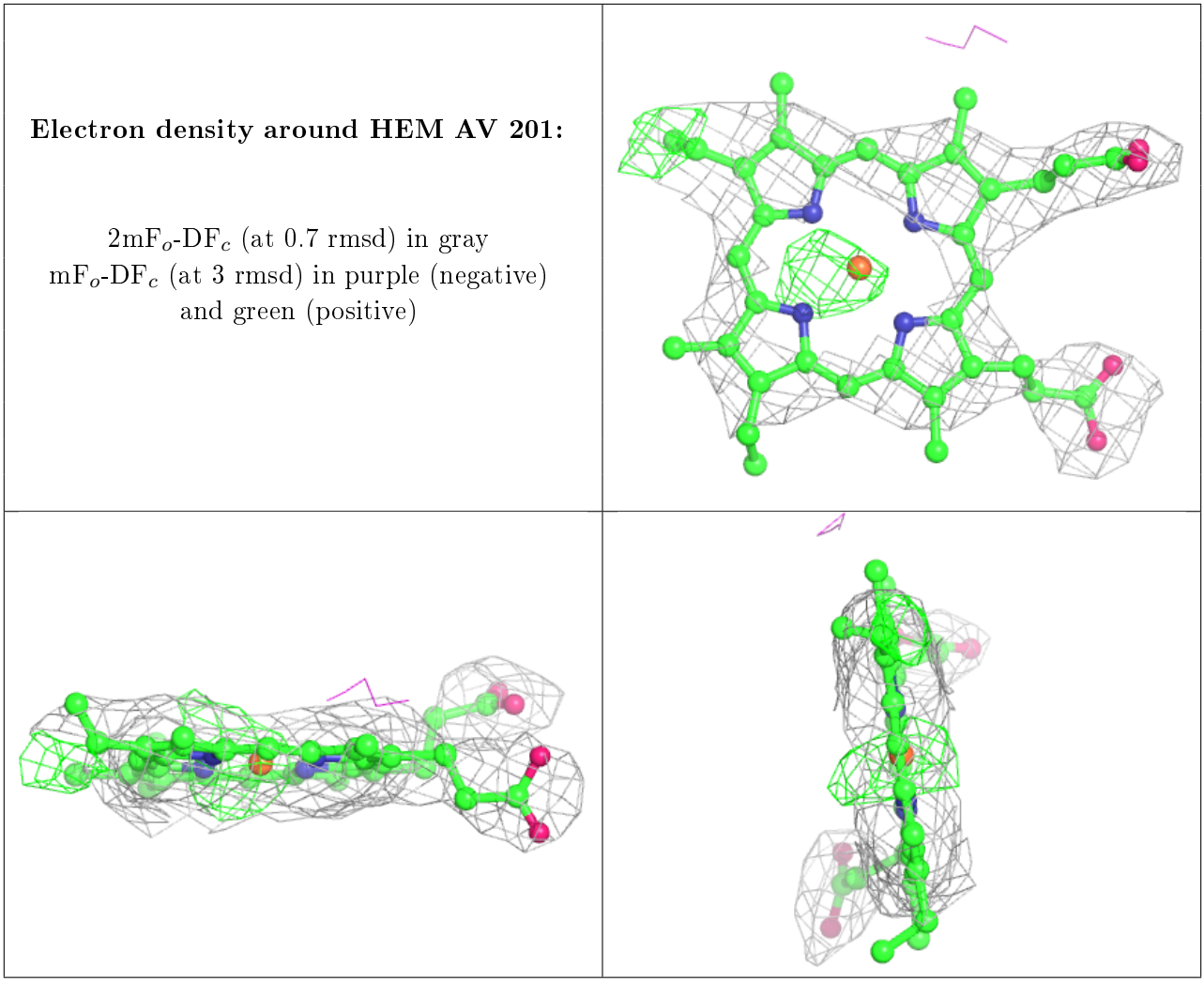






Electron density around HEM AV 201:

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



6.5 Other polymers

There are no such residues in this entry.