



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 09:33 PM EDT

PDB ID : 4V82
Title : Crystal structure of cyanobacterial Photosystem II in complex with terbutryn
Authors : Gabdulkhakov, A.; Broser, M.; Guskov, A.; Kern, J.; Glockner, C.; Muh, F.;
Saenger, W.; Zouni, A.
Deposited on : 2010-11-30
Resolution : 3.20 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

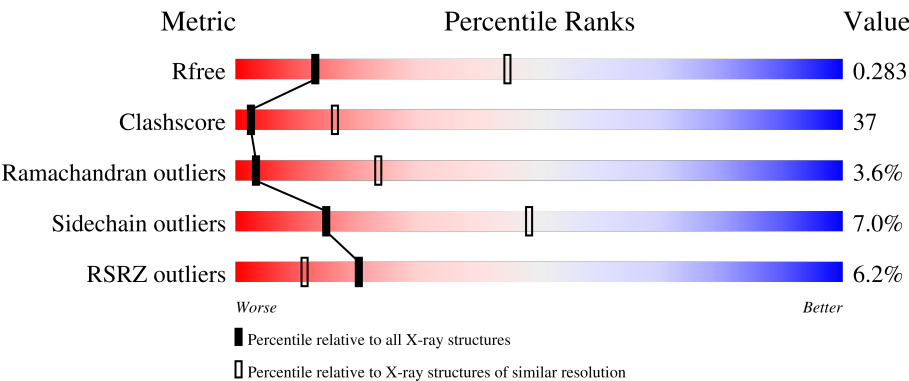
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	BA	344	
2	AB	510	
2	BB	510	
3	AC	461	



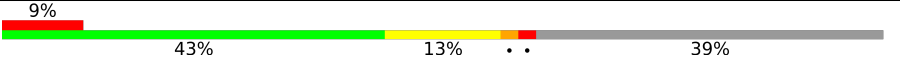
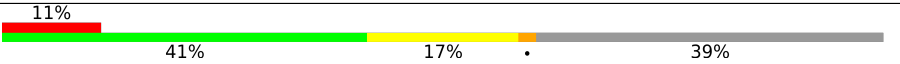
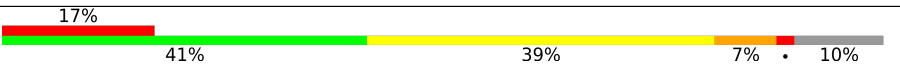
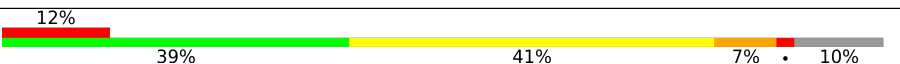
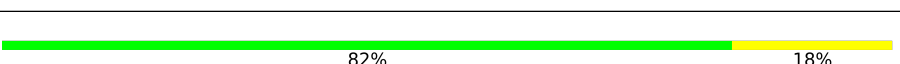
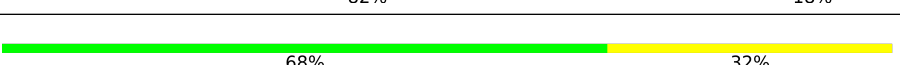
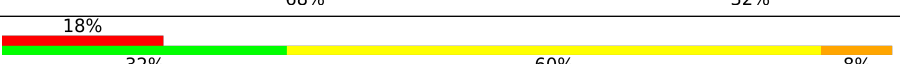
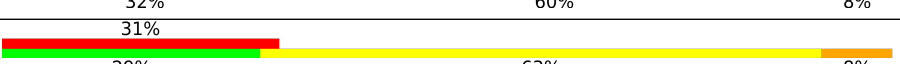
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Mol	Chain	Length	Quality of chain
3	BC	461	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	

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Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	41	
18	BX	41	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AA	404	X	-	-	-
24	CLA	AA	405	X	-	-	-
24	CLA	AA	406	X	-	-	-
24	CLA	AA	407	X	-	-	-
24	CLA	AB	601	X	-	-	X
24	CLA	AB	602	X	-	-	-
24	CLA	AB	603	X	-	-	-
24	CLA	AB	604	X	-	-	-
24	CLA	AB	605	X	-	-	-
24	CLA	AB	606	X	-	-	-
24	CLA	AB	607	X	-	-	-
24	CLA	AB	608	X	-	-	-
24	CLA	AB	609	X	-	-	-
24	CLA	AB	610	X	-	-	-
24	CLA	AB	611	X	-	-	-
24	CLA	AB	612	X	-	-	-
24	CLA	AB	613	X	-	-	-
24	CLA	AB	614	X	-	-	-
24	CLA	AB	615	X	-	-	-
24	CLA	AB	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AC	501	X	-	-	-
24	CLA	AC	502	X	-	-	-
24	CLA	AC	503	X	-	-	-
24	CLA	AC	504	X	-	-	-
24	CLA	AC	505	X	-	-	-
24	CLA	AC	506	X	-	-	-
24	CLA	AC	507	X	-	-	-
24	CLA	AC	508	X	-	-	-
24	CLA	AC	509	X	-	-	-
24	CLA	AC	510	X	-	-	-
24	CLA	AC	511	X	-	X	-
24	CLA	AC	512	X	-	-	X
24	CLA	AC	513	X	-	-	X
24	CLA	AD	401	X	-	-	-
24	CLA	AD	404	X	-	-	-
24	CLA	BA	5405	X	-	-	-
24	CLA	BA	5406	X	-	X	-
24	CLA	BA	5407	X	-	-	-
24	CLA	BA	5408	X	-	-	-
24	CLA	BB	5605	X	-	-	X
24	CLA	BB	5606	X	-	-	-
24	CLA	BB	5607	X	-	-	-
24	CLA	BB	5608	X	-	-	-
24	CLA	BB	5609	X	-	-	-
24	CLA	BB	5610	X	-	-	-
24	CLA	BB	5611	X	-	-	-
24	CLA	BB	5612	X	-	-	-
24	CLA	BB	5613	X	-	-	-
24	CLA	BB	5614	X	-	-	-
24	CLA	BB	5615	X	-	-	-
24	CLA	BB	5616	X	-	-	-
24	CLA	BB	5617	X	-	-	-
24	CLA	BB	5618	X	-	-	-
24	CLA	BB	5619	X	-	-	-
24	CLA	BB	5620	X	-	-	-
24	CLA	BC	5501	X	-	-	-
24	CLA	BC	5502	X	-	-	-
24	CLA	BC	5503	X	-	-	-
24	CLA	BC	5504	X	-	-	-
24	CLA	BC	5505	X	-	-	-
24	CLA	BC	5506	X	-	-	-
24	CLA	BC	5507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	BC	5508	X	-	-	-
24	CLA	BC	5509	X	-	-	-
24	CLA	BC	5510	X	-	-	-
24	CLA	BC	5511	X	-	X	-
24	CLA	BC	5512	X	-	-	-
24	CLA	BC	5513	X	-	-	X
24	CLA	BD	5402	X	-	-	-
24	CLA	BD	5405	X	-	-	-
25	MST	AA	408	-	-	X	-
25	MST	BA	5409	-	-	X	-
27	BCR	AC	515	-	-	-	X
27	BCR	AC	516	-	-	-	X
27	BCR	AJ	101	-	-	-	X
27	BCR	AX	101	-	-	-	X
27	BCR	BC	5515	-	-	-	X
27	BCR	BC	5516	-	-	-	X
27	BCR	BJ	5101	-	-	-	X
27	BCR	BX	5101	-	-	-	X
28	DGD	AA	411	-	-	-	X
28	DGD	AB	628	-	-	-	X
28	DGD	AC	518	X	-	-	X
28	DGD	AC	519	X	-	X	-
28	DGD	AE	101	-	-	-	X
28	DGD	BA	5412	-	-	-	X
28	DGD	BB	5602	-	-	-	X
28	DGD	BC	5518	X	-	-	X
28	DGD	BC	5519	X	-	X	-
28	DGD	BE	5102	-	-	-	X
29	LHG	BA	5415	-	-	-	X
30	SQD	AB	622	-	-	-	X
30	SQD	AF	102	-	-	-	X
30	SQD	BA	5401	-	-	-	X
30	SQD	BB	5625	-	-	-	X
30	SQD	BF	5102	-	-	-	X
31	LMG	AA	414	-	-	-	X
31	LMG	AA	417	-	-	-	X
31	LMG	AB	620	-	-	-	X
31	LMG	AB	621	-	-	-	X
31	LMG	AC	520	-	-	-	X
31	LMG	AC	521	-	-	-	X
31	LMG	AD	407	-	-	-	X
31	LMG	AD	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	LMG	AI	101	-	-	-	X
31	LMG	AJ	102	-	-	-	X
31	LMG	AM	101	-	-	-	X
31	LMG	BA	5402	-	-	-	X
31	LMG	BC	5520	-	-	-	X
31	LMG	BC	5521	-	-	-	X
31	LMG	BD	5408	-	-	-	X
31	LMG	BD	5409	-	-	-	X
31	LMG	BD	5410	-	-	-	X
31	LMG	BE	5101	-	-	-	X
31	LMG	BI	5101	-	-	-	X
31	LMG	BL	5101	-	-	-	X
31	LMG	BM	5102	-	-	-	X
32	LMT	AB	623	-	-	-	X
32	LMT	AB	624	-	-	-	X
32	LMT	AB	629	-	-	-	X
32	LMT	AB	630	-	-	-	X
32	LMT	AD	409	-	-	-	X
32	LMT	AI	102	-	-	-	X
32	LMT	AI	103	-	-	-	X
32	LMT	AM	102	-	-	-	X
32	LMT	BB	5603	-	-	-	X
32	LMT	BB	5604	-	-	-	X
32	LMT	BB	5626	-	-	-	X
32	LMT	BB	5627	-	-	-	X
32	LMT	BC	5522	-	-	-	X
32	LMT	BD	5411	-	-	-	X
32	LMT	BI	5102	-	-	-	X
34	PHO	AD	402	X	-	-	-
34	PHO	AD	403	X	-	-	-
34	PHO	BD	5403	X	-	-	-
34	PHO	BD	5404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			
4	BD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	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	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			
9	BJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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 Photosystem II reaction center 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 reaction center X 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 PSBX PROTEIN.

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				

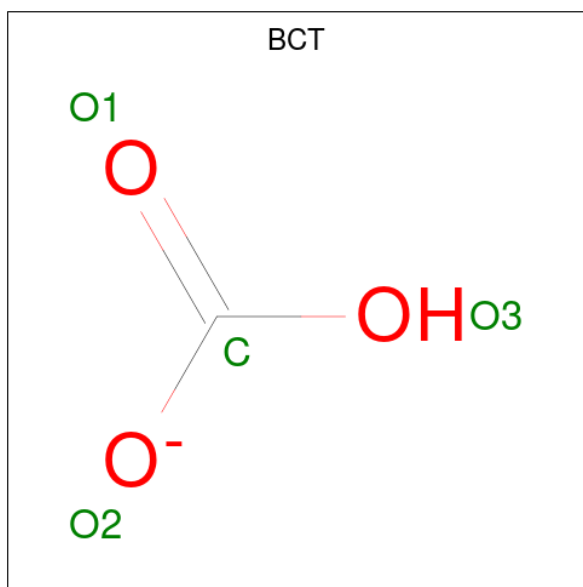
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	BD	1	Total	Fe	0	0
			1	1		

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

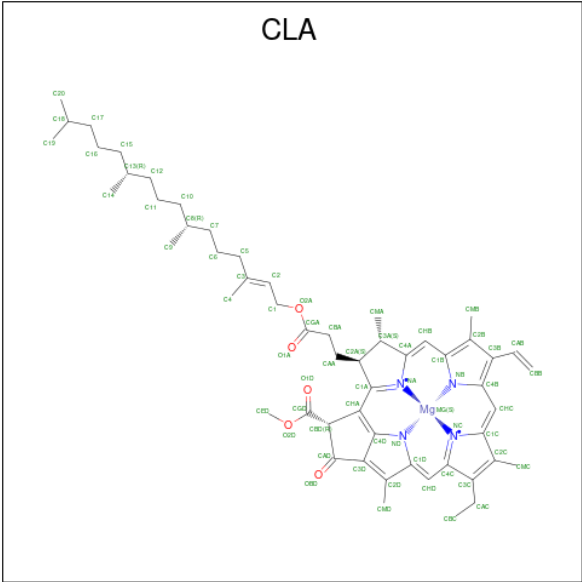


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	AA	1	Total	Cl	0	1
			2	2		
23	BA	1	Total	Cl	0	1
			2	2		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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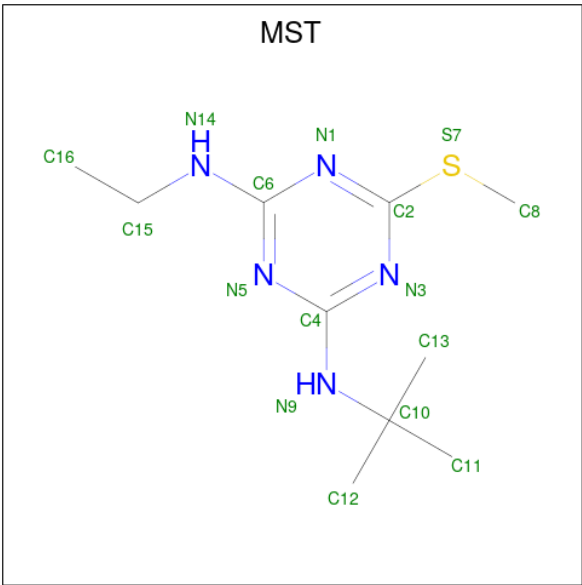
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1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

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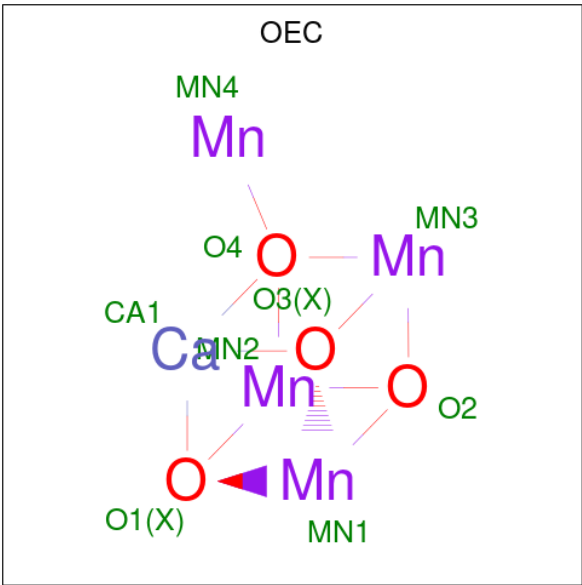
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55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

- Molecule 25 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (three-letter code: MST) (formula: C₁₀H₁₉N₅S).



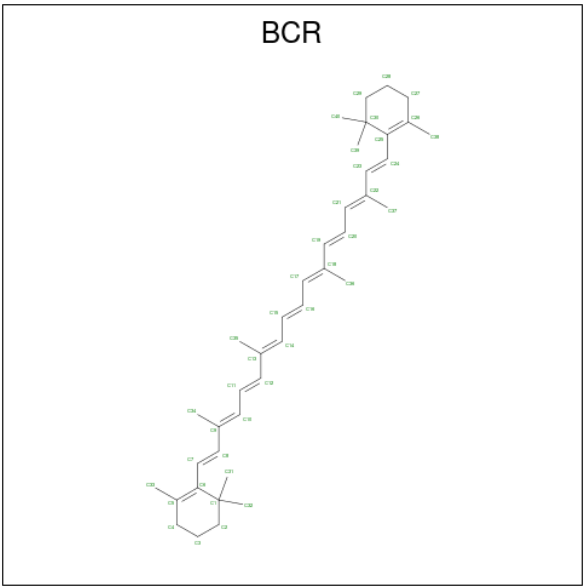
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

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



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



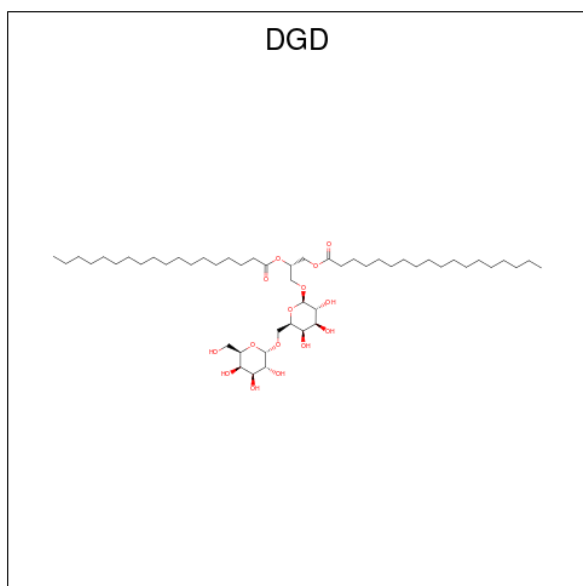
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
27	AT	1	Total C 40 40	0	0
27	AX	1	Total C 40 40	0	0
27	BA	1	Total C 40 40	0	0

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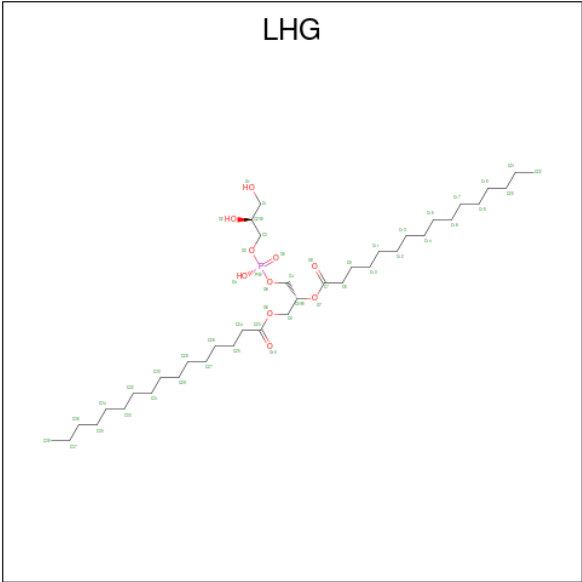
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

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



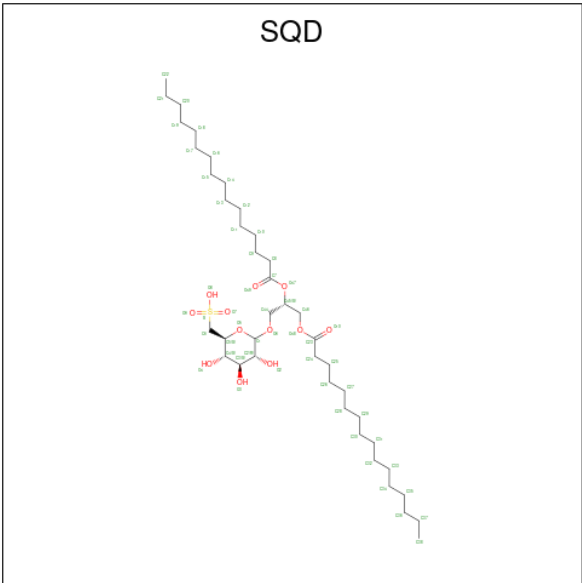
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA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

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



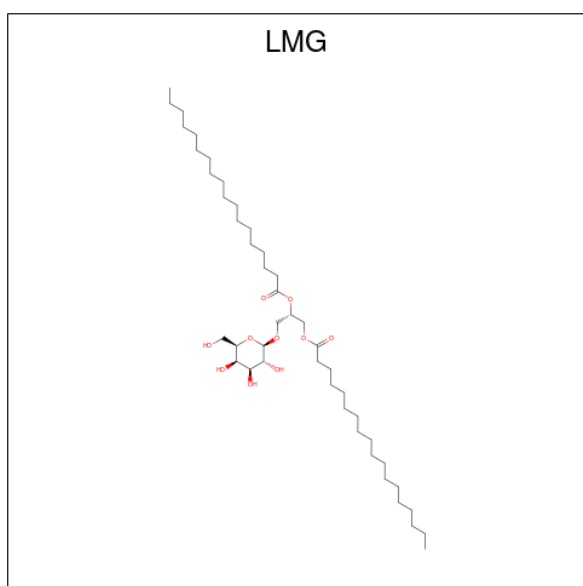
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	AA	1	Total	C	O	S	0	0
			51	38	12	1		
30	AA	1	Total	C	O	S	0	0
			54	41	12	1		
30	AB	1	Total	C	O	S	0	0
			43	30	12	1		
30	AB	1	Total	C	O	S	0	0
			47	34	12	1		
30	AF	1	Total	C	O	S	0	0
			45	32	12	1		
30	BA	1	Total	C	O	S	0	0
			54	41	12	1		
30	BA	1	Total	C	O	S	0	0
			51	38	12	1		
30	BB	1	Total	C	O	S	0	0
			47	34	12	1		
30	BB	1	Total	C	O	S	0	0
			43	30	12	1		
30	BF	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



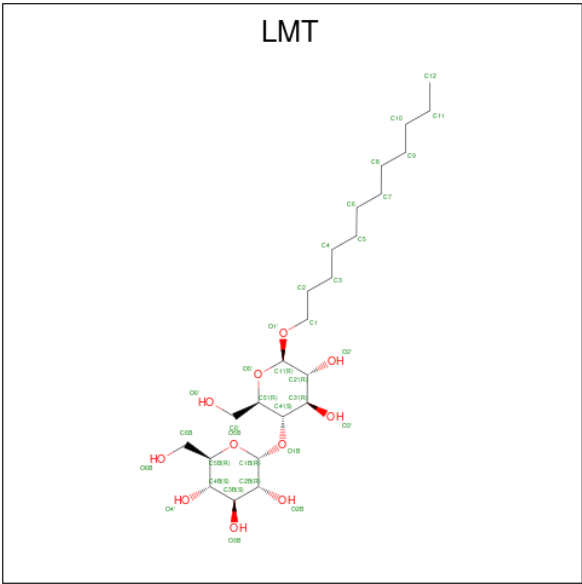
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			42	32	10		
31	AB	1	Total	C	O	0	0
			51	41	10		
31	AB	1	Total	C	O	0	0
			49	39	10		
31	AC	1	Total	C	O	0	0
			48	38	10		
31	AC	1	Total	C	O	0	0
			45	35	10		
31	AD	1	Total	C	O	0	0
			49	39	10		
31	AD	1	Total	C	O	0	0
			48	38	10		
31	AI	1	Total	C	O	0	0
			43	33	10		
31	AJ	1	Total	C	O	0	0
			46	36	10		
31	AM	1	Total	C	O	0	0
			42	32	10		
31	BA	1	Total	C	O	0	0
			42	32	10		
31	BB	1	Total	C	O	0	0
			49	39	10		
31	BC	1	Total	C	O	0	0
			48	38	10		
31	BC	1	Total	C	O	0	0
			45	35	10		
31	BD	1	Total	C	O	0	0
			46	36	10		
31	BD	1	Total	C	O	0	0
			49	39	10		
31	BD	1	Total	C	O	0	0
			48	38	10		
31	BE	1	Total	C	O	0	0
			44	34	10		
31	BI	1	Total	C	O	0	0
			43	33	10		
31	BL	1	Total	C	O	0	0
			51	41	10		
31	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



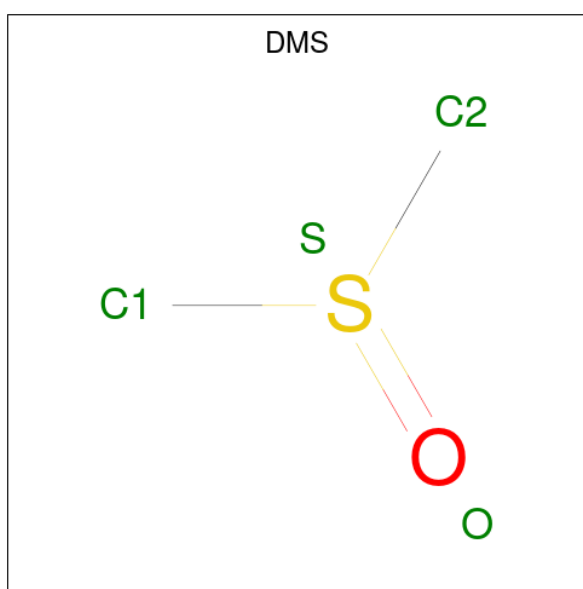
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	BC	1	Total	C	O	0	0
			35	24	11		
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



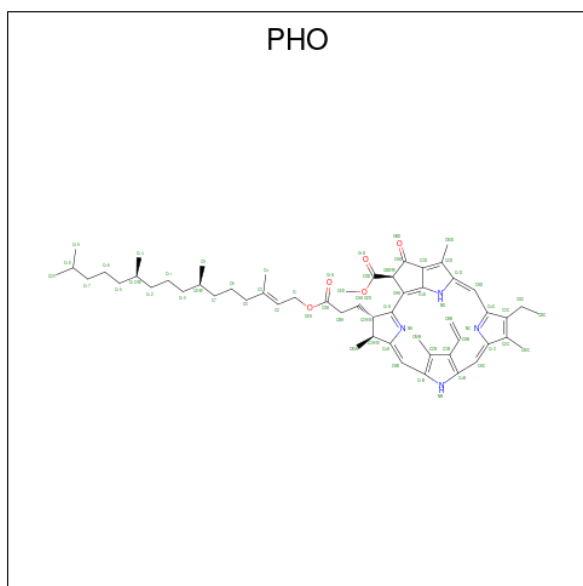
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

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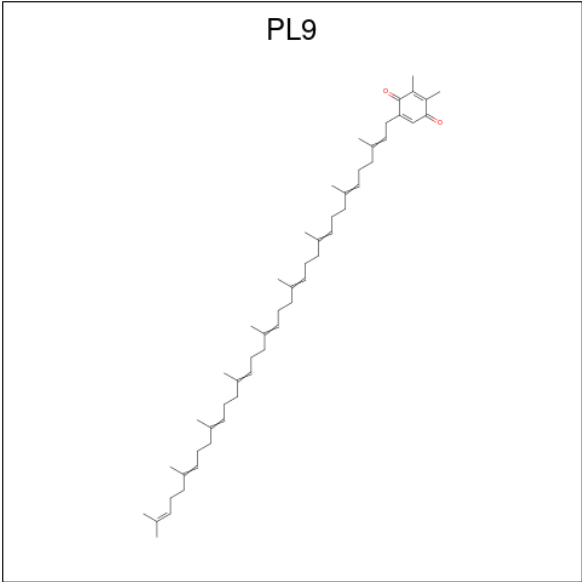
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



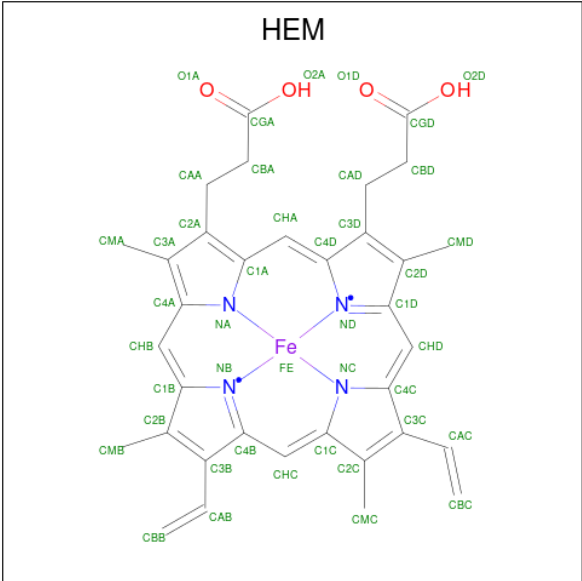
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 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
35	AD	1	Total	C	O	0	0
			55	53	2		
35	BD	1	Total	C	O	0	0
			55	53	2		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

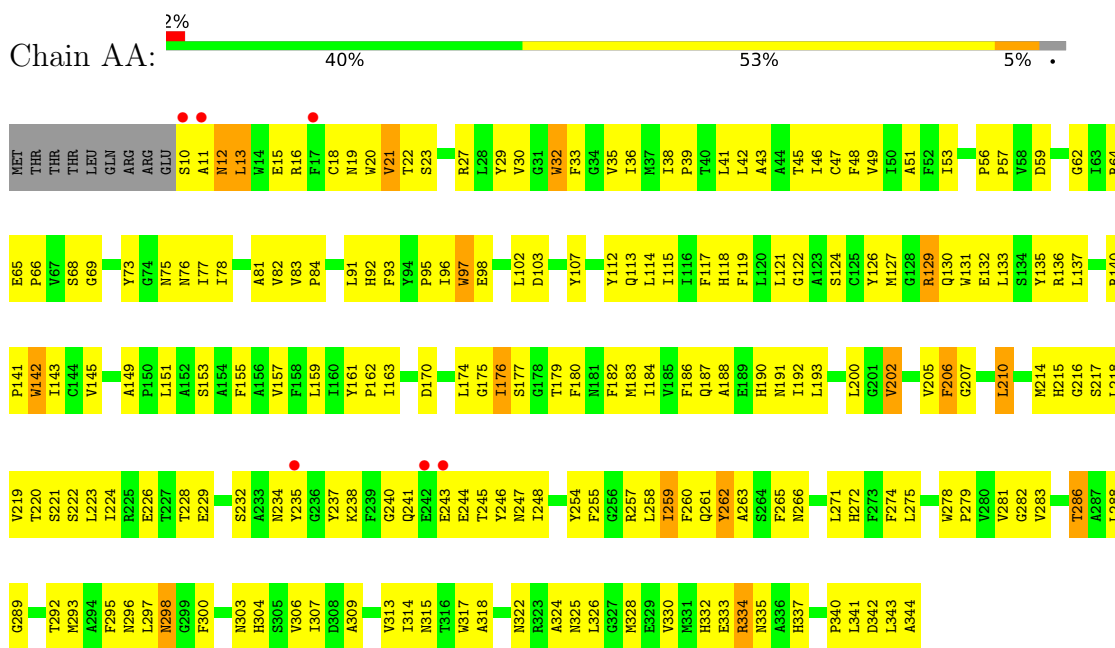
- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	AF	1	Total 1	Ca 1	0	0
37	AK	1	Total 1	Ca 1	0	0
37	AO	1	Total 1	Ca 1	0	0
37	BF	1	Total 1	Ca 1	0	0
37	BK	1	Total 1	Ca 1	0	0
37	BO	1	Total 1	Ca 1	0	0

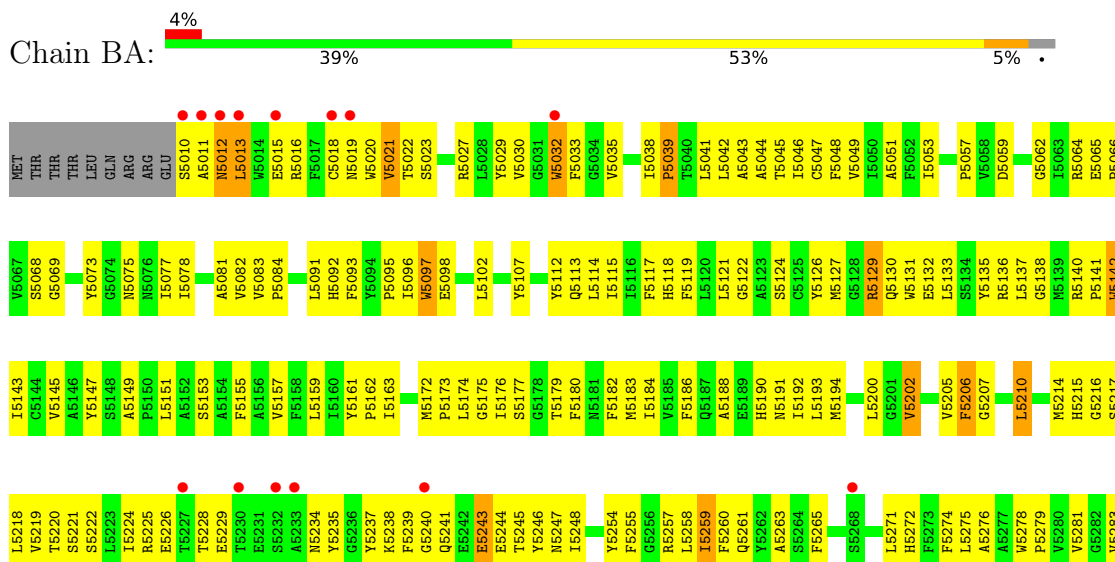
3 Residue-property plots

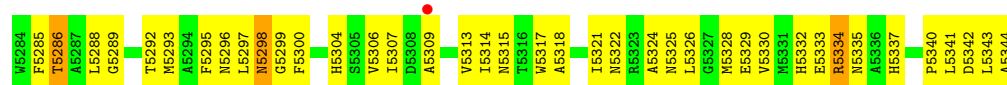
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photosystem Q(B) protein 1

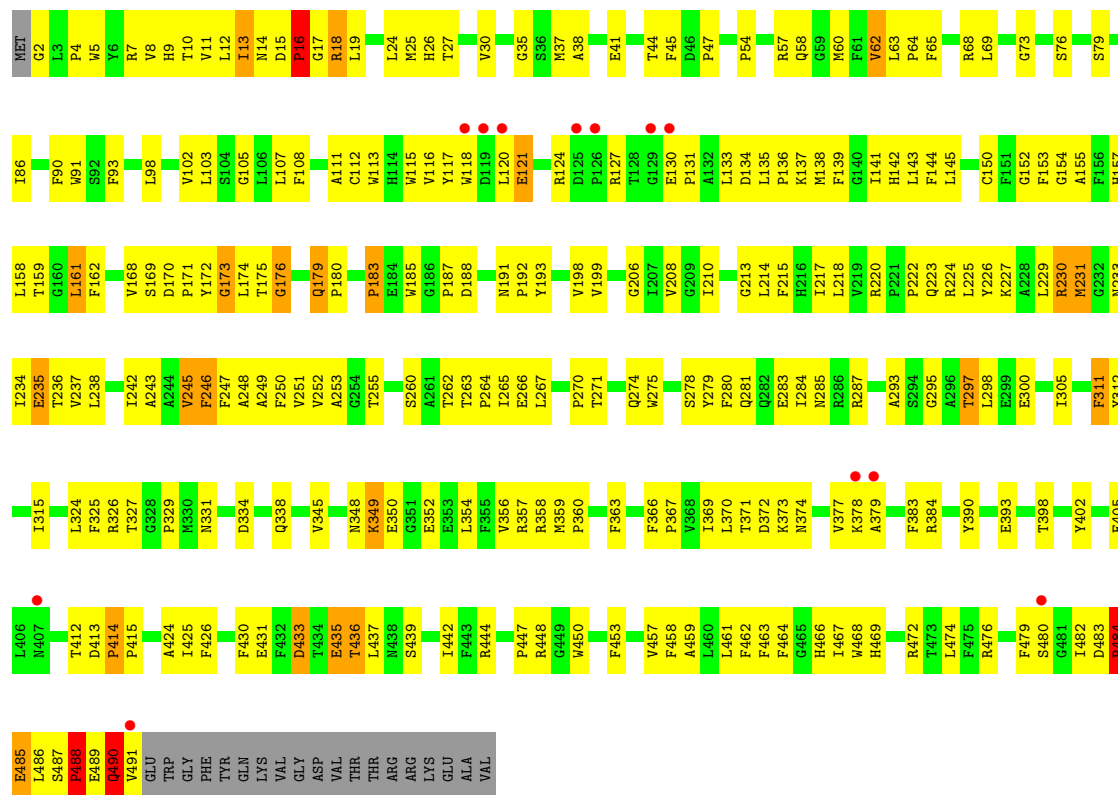


• Molecule 1: Photosystem Q(B) protein 1

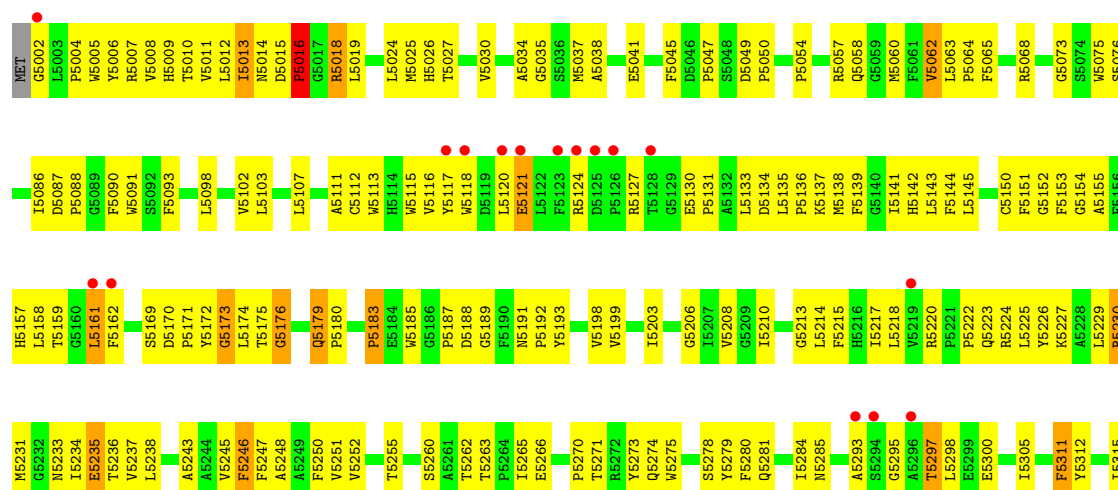


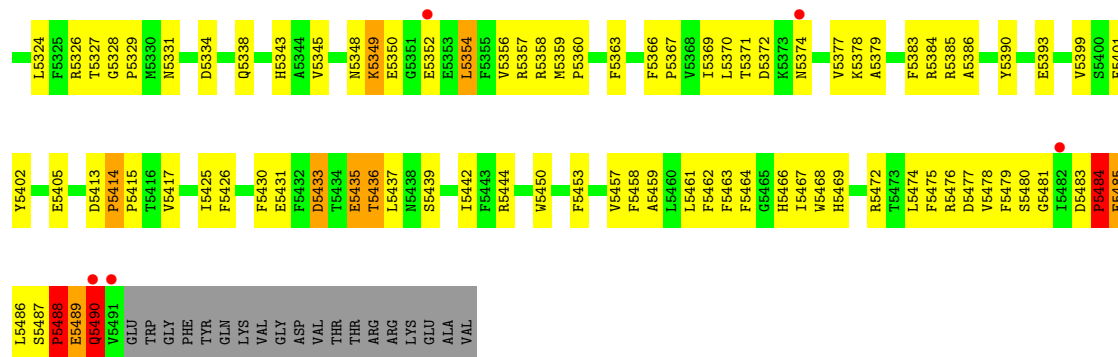


• Molecule 2: Photosystem II core light harvesting protein

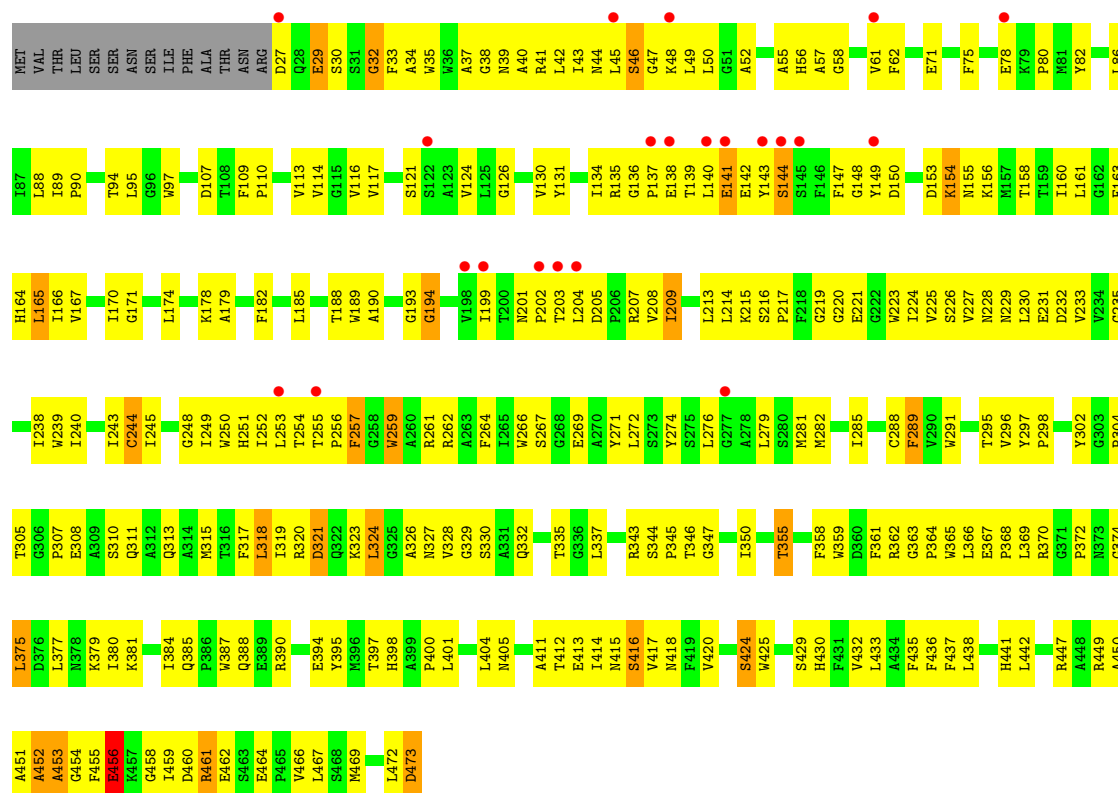


• Molecule 2: Photosystem II core light harvesting protein

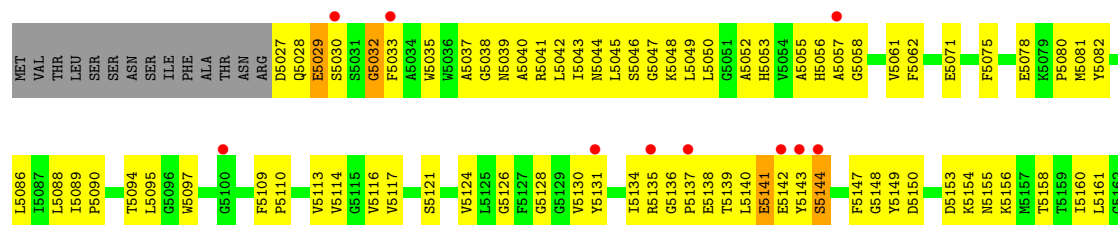
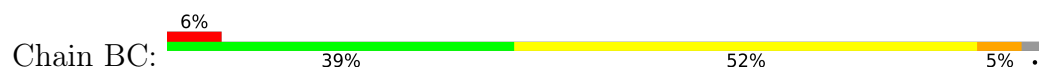


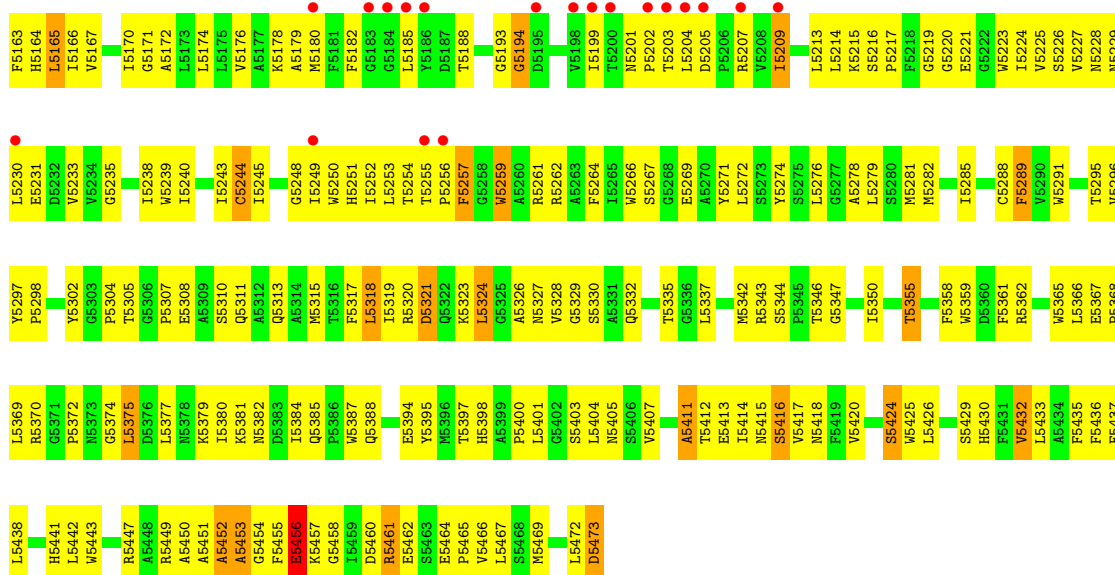


• Molecule 3: Photosystem II CP43 protein

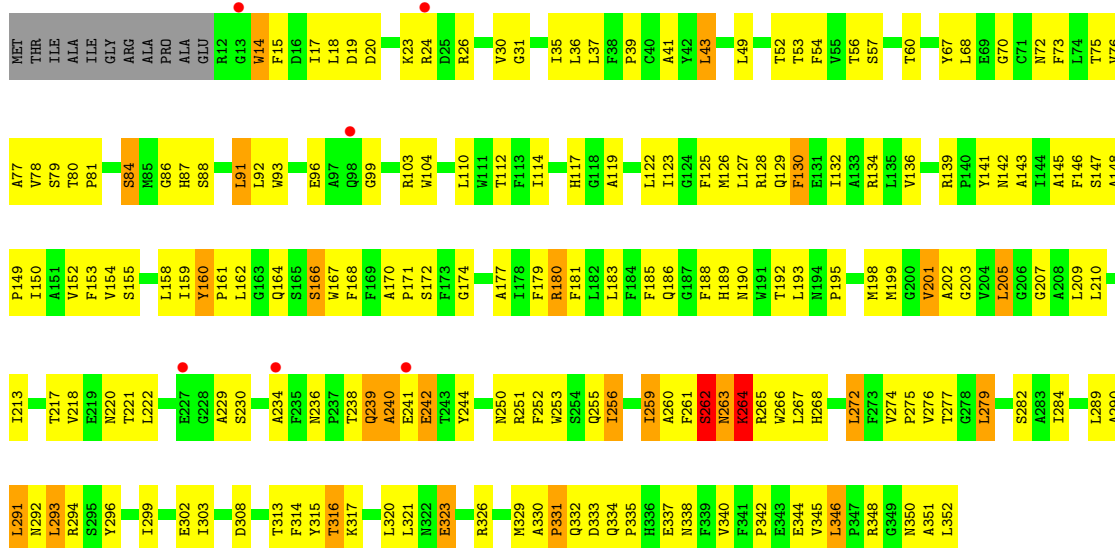
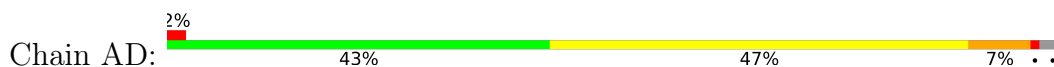


• Molecule 3: Photosystem II CP43 protein

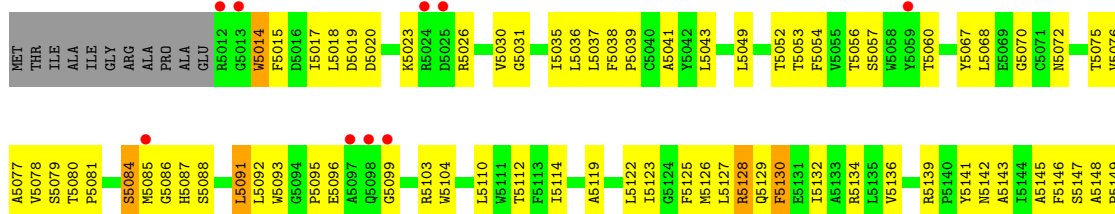
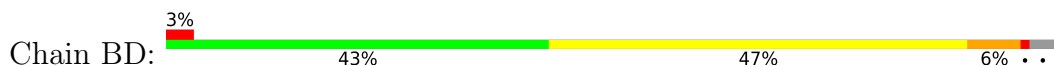


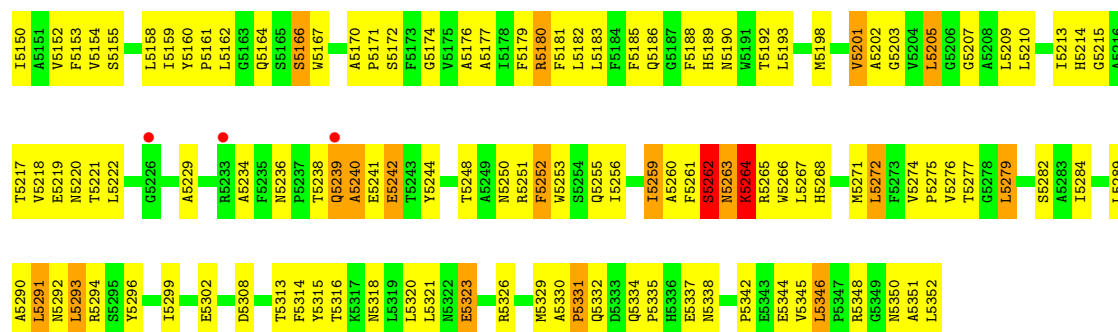


• Molecule 4: Photosystem II D2 protein

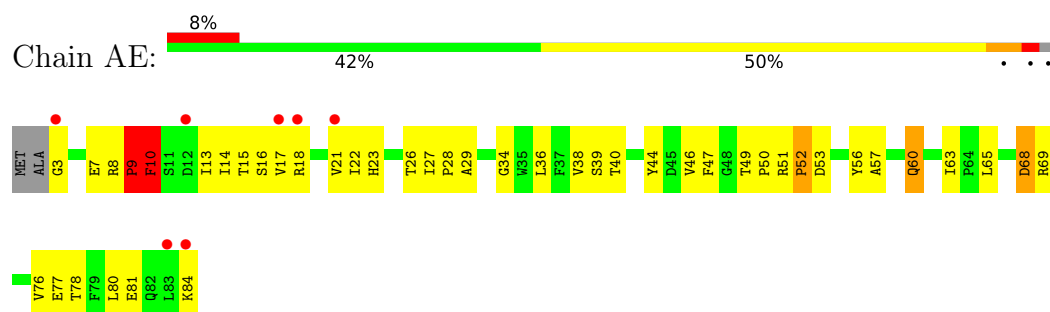


• Molecule 4: Photosystem II D2 protein

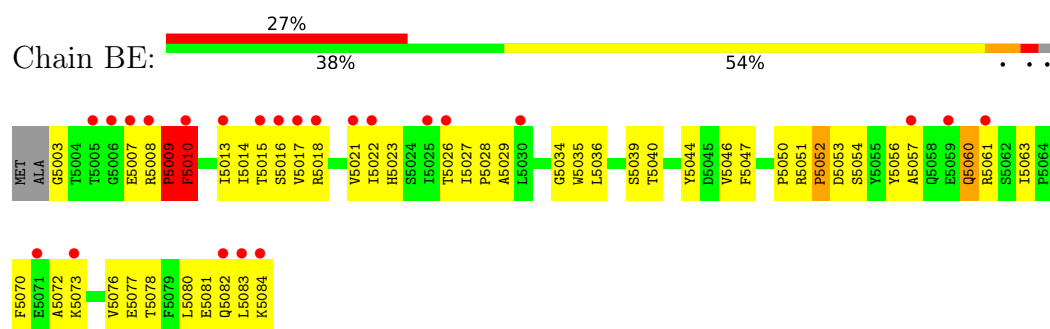




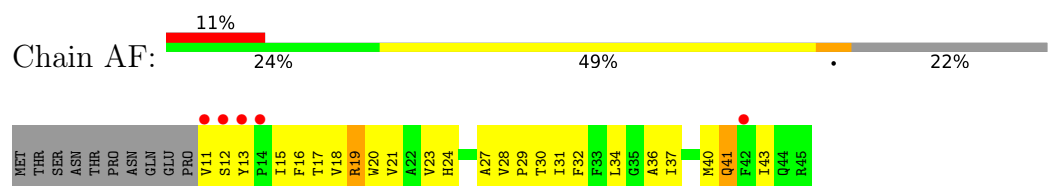
• Molecule 5: Cytochrome b559 subunit alpha



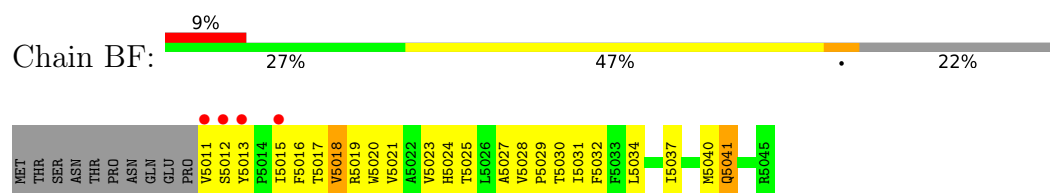
• Molecule 5: Cytochrome b559 subunit alpha



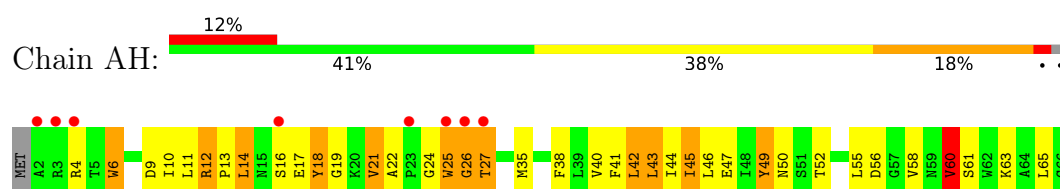
• Molecule 6: Cytochrome b559 subunit beta



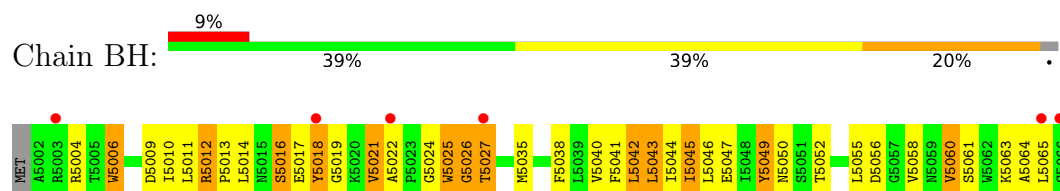
• Molecule 6: Cytochrome b559 subunit beta



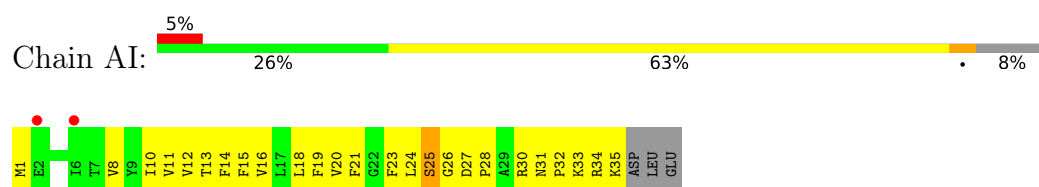
• Molecule 7: Photosystem II reaction center protein H



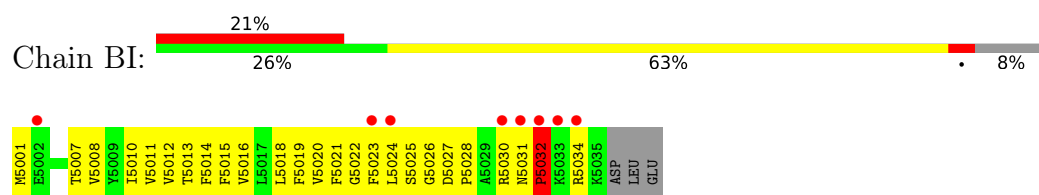
• Molecule 7: Photosystem II reaction center protein H



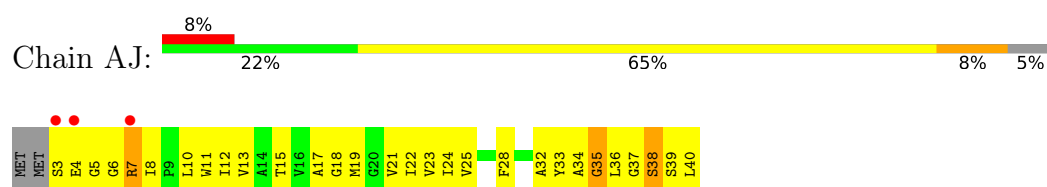
• Molecule 8: Photosystem II reaction center protein I



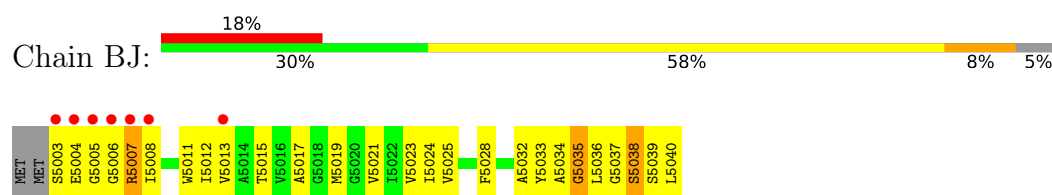
• Molecule 8: Photosystem II reaction center protein I



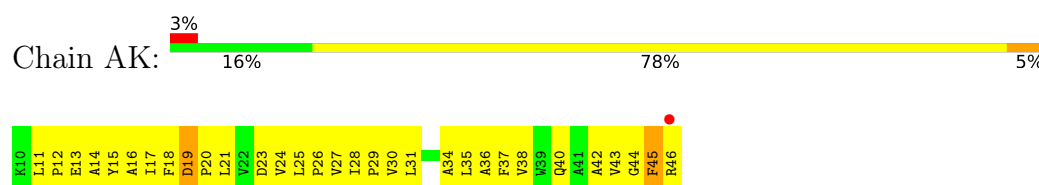
• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K



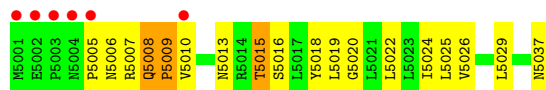
- Molecule 10: Photosystem II reaction center protein K



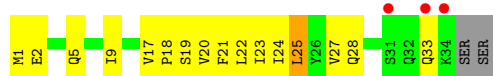
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



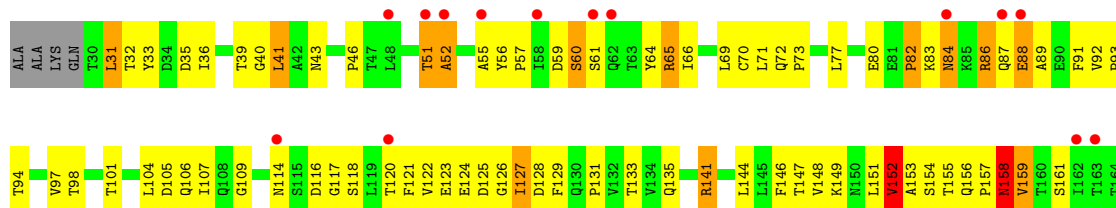
- Molecule 12: Photosystem II reaction center protein M

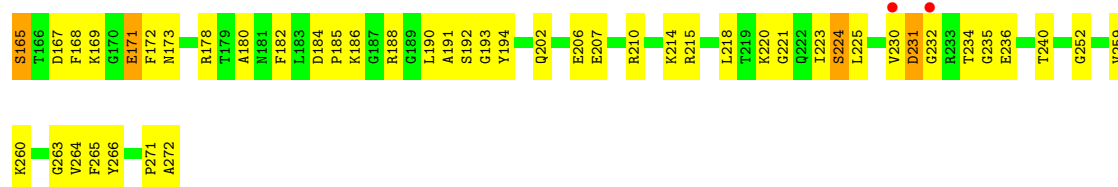


- Molecule 12: Photosystem II reaction center protein M

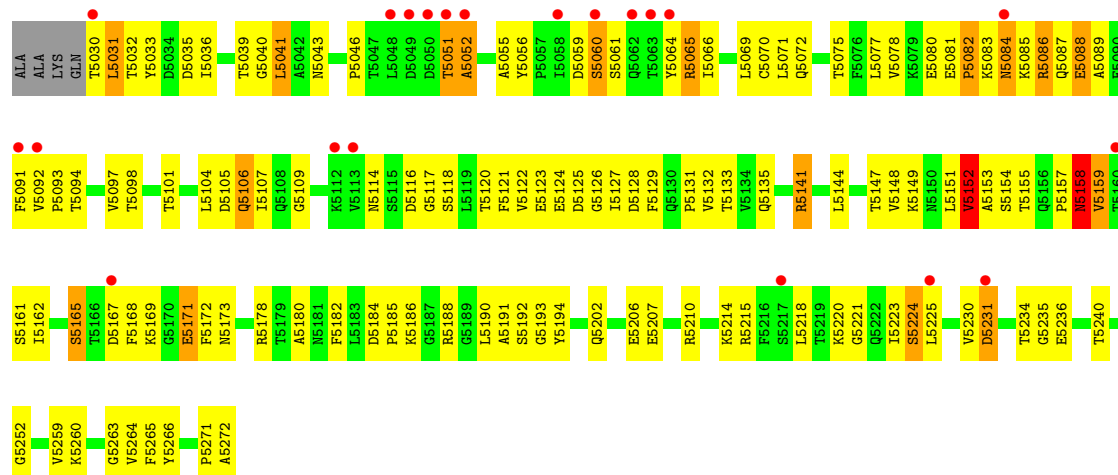


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

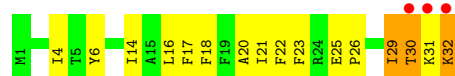




• Molecule 13: Photosystem II manganese-stabilizing polypeptide



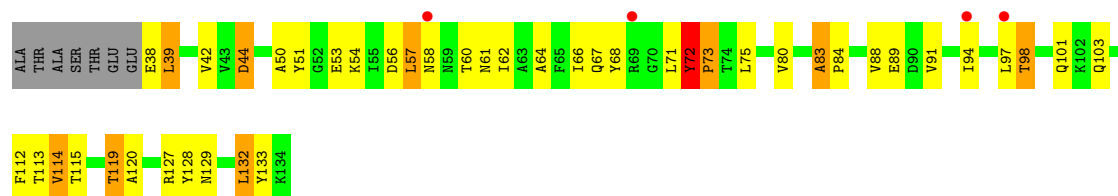
• Molecule 14: Photosystem II reaction center protein T



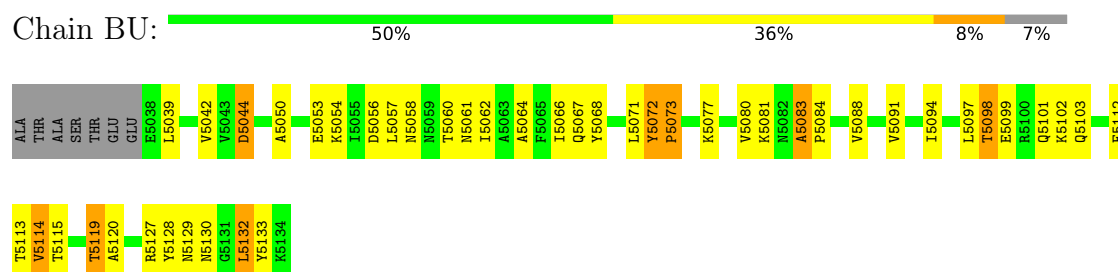
• Molecule 14: Photosystem II reaction center protein T



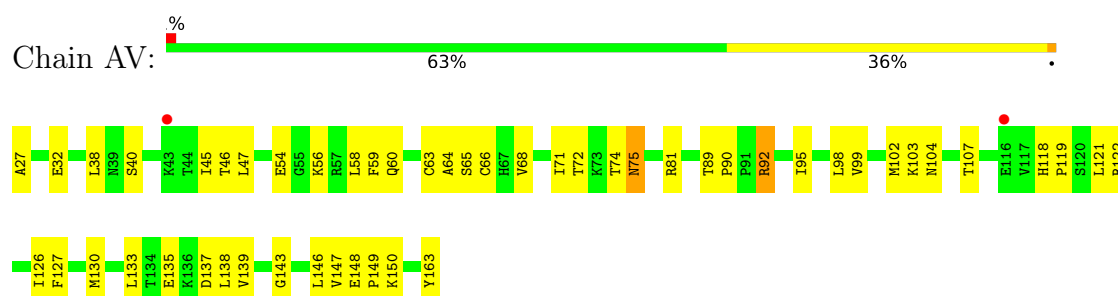
• Molecule 15: Photosystem II 12 kDa extrinsic protein



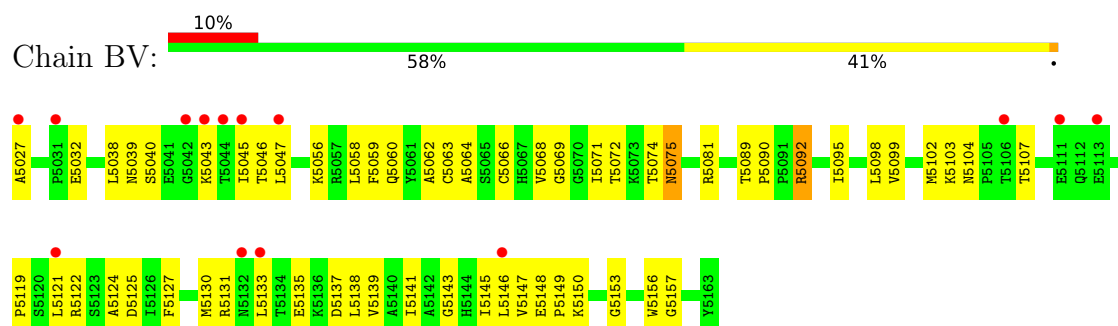
- Molecule 15: Photosystem II 12 kDa extrinsic protein



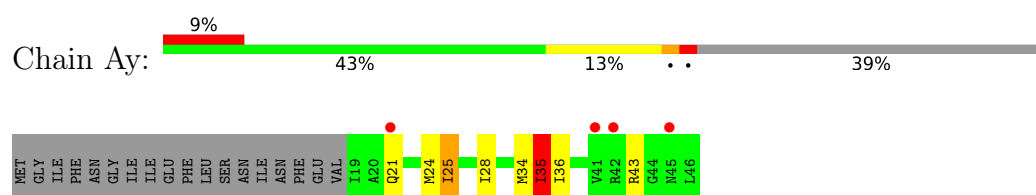
- Molecule 16: Cytochrome c-550



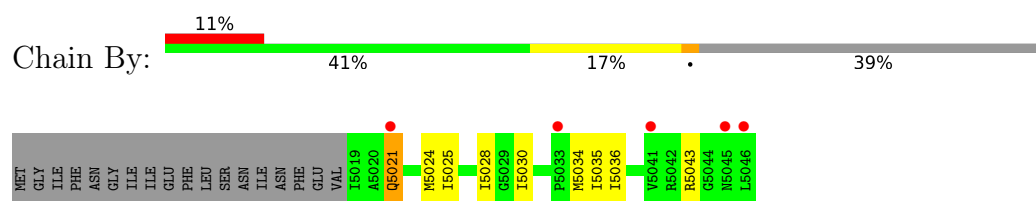
- Molecule 16: Cytochrome c-550



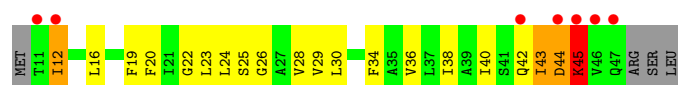
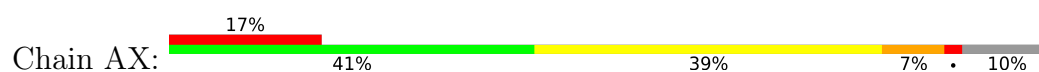
- Molecule 17: Photosystem II reaction center protein ycf12



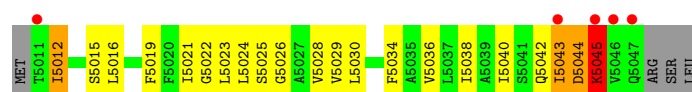
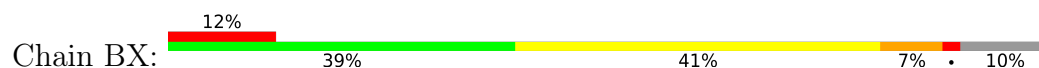
- Molecule 17: Photosystem II reaction center protein ycf12



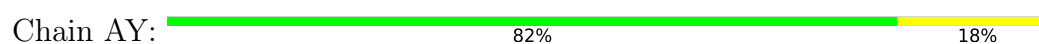
- Molecule 18: Photosystem II reaction center X protein



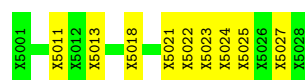
- Molecule 18: Photosystem II reaction center X protein



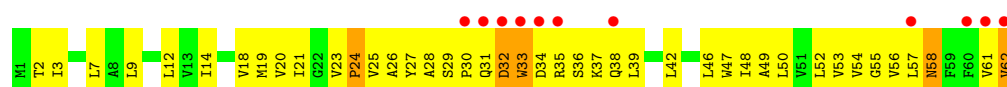
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN



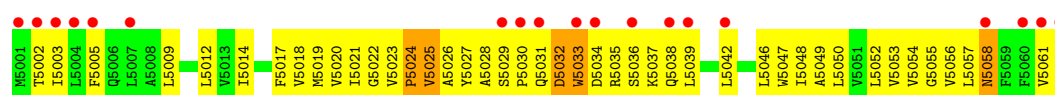
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.08Å 225.37Å 305.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 39.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.20) 99.1 (39.38-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.299 0.262 , 0.283	Depositor DCC
R_{free} test set	3179 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50266	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, CA, DGD, BCR, DMS, LHG, LMG, SQD, OEC, BCT, HEM, FE2, CL, CLA, LMT, PHO, MST

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	0.50	0/2713	0.72	0/3700
1	BA	0.52	0/2713	0.72	0/3700
2	AB	0.51	0/3986	0.73	0/5433
2	BB	0.52	0/3986	0.73	3/5433 (0.1%)
3	AC	0.46	0/3556	0.71	1/4842 (0.0%)
3	BC	0.47	0/3556	0.71	1/4842 (0.0%)
4	AD	0.53	0/2806	0.73	0/3825
4	BD	0.55	0/2806	0.73	0/3825
5	AE	0.51	0/685	0.76	0/933
5	BE	0.54	0/685	0.77	0/933
6	AF	0.75	0/291	0.78	0/397
6	BF	0.71	0/291	0.74	0/397
7	AH	0.47	0/520	0.78	0/709
7	BH	0.49	0/520	0.79	0/709
8	AI	0.58	0/293	0.77	0/395
8	BI	0.64	0/293	0.81	0/395
9	AJ	0.55	0/277	0.86	0/375
9	BJ	0.67	0/277	0.88	0/375
10	AK	0.54	0/303	0.73	0/416
10	BK	0.62	0/303	0.73	0/416
11	AL	0.58	0/311	0.78	1/422 (0.2%)
11	BL	0.57	0/311	0.81	0/422
12	AM	0.65	0/270	0.87	0/367
12	BM	0.66	0/270	0.85	0/367
13	AO	0.49	0/1876	0.76	0/2548
13	BO	0.48	0/1876	0.76	1/2548 (0.0%)
14	AT	0.80	1/284 (0.4%)	0.82	0/381
14	BT	0.81	1/284 (0.4%)	0.87	2/381 (0.5%)
15	AU	0.54	0/785	0.84	2/1064 (0.2%)
15	BU	0.52	0/785	0.83	0/1064
16	AV	0.46	0/1081	0.70	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BV	0.46	0/1081	0.70	0/1468
17	Ay	1.12	1/202 (0.5%)	1.24	1/272 (0.4%)
17	By	1.03	1/202 (0.5%)	1.22	1/272 (0.4%)
18	AX	0.57	0/273	0.76	0/370
18	BX	0.63	0/273	0.69	0/370
20	AZ	0.53	0/490	0.75	1/669 (0.1%)
20	BZ	0.60	0/490	0.80	0/669
All	All	0.53	4/42004 (0.0%)	0.75	14/57172 (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
2	BB	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	By	5030	ILE	CA-CB	-5.67	1.41	1.54
14	BT	5032	LYS	C-OXT	5.50	1.33	1.23
17	Ay	35	ILE	CA-CB	-5.35	1.42	1.54
14	AT	32	LYS	CA-CB	5.19	1.65	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BO	5030	THR	N-CA-CB	-5.76	99.35	110.30
2	BB	5488	PRO	N-CA-C	5.72	126.97	112.10
2	BB	5489	GLU	N-CA-C	5.65	126.27	111.00
14	BT	5004	ILE	CB-CA-C	-5.65	100.31	111.60
3	AC	32	GLY	N-CA-C	-5.56	99.19	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	262	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	BB	5273	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	300	0
1	BA	2628	0	2524	309	0
2	AB	3850	0	3718	344	0
2	BB	3850	0	3718	351	0
3	AC	3444	0	3365	350	0
3	BC	3444	0	3365	358	0
4	AD	2711	0	2610	245	0
4	BD	2711	0	2610	255	0
5	AE	666	0	651	68	0
5	BE	666	0	651	76	0
6	AF	282	0	291	36	0
6	BF	282	0	291	32	0
7	AH	507	0	521	65	0
7	BH	507	0	521	69	0
8	AI	286	0	308	34	0
8	BI	286	0	305	37	0
9	AJ	271	0	276	36	0
9	BJ	271	0	276	38	0
10	AK	293	0	305	48	0
10	BK	293	0	305	45	0
11	AL	304	0	316	34	0
11	BL	304	0	313	35	0
12	AM	267	0	289	26	0
12	BM	267	0	286	26	0
13	AO	1845	0	1801	137	0
13	BO	1845	0	1801	142	0
14	AT	275	0	288	28	0
14	BT	275	0	285	27	0
15	AU	774	0	773	52	0
15	BU	774	0	773	51	0
16	AV	1060	0	1068	48	0
16	BV	1060	0	1068	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	33	0
18	BX	270	0	299	27	0
19	AY	140	0	32	3	0
19	BY	140	0	32	7	0
20	AZ	479	0	516	53	0
20	BZ	479	0	513	55	0
21	AA	1	0	0	0	0
21	BD	1	0	0	0	0
22	AA	4	0	0	0	0
22	BA	4	0	0	0	0
23	AA	2	0	0	1	0
23	BA	2	0	0	0	0
24	AA	260	0	288	41	0
24	AB	1040	0	1152	133	0
24	AC	845	0	936	91	0
24	AD	130	0	144	17	0
24	BA	260	0	288	44	0
24	BB	1040	0	1152	142	0
24	BC	845	0	936	94	0
24	BD	130	0	144	18	0
25	AA	16	0	19	9	0
25	BA	16	0	19	9	0
26	AA	5	0	0	0	0
26	BA	5	0	0	0	0
27	AA	40	0	56	4	0
27	AB	120	0	168	8	0
27	AC	120	0	168	24	0
27	AD	40	0	56	2	0
27	AJ	40	0	56	4	0
27	AK	40	0	56	5	0
27	AT	40	0	56	10	0
27	AX	40	0	56	8	0
27	BA	40	0	56	3	0
27	BB	120	0	168	8	0
27	BC	120	0	168	25	0
27	BD	40	0	56	2	0
27	BJ	40	0	56	3	0
27	BK	40	0	56	5	0
27	BT	40	0	56	6	0
27	BX	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AA	56	0	70	9	0
28	AB	52	0	62	0	0
28	AC	181	0	243	63	0
28	AE	63	0	87	1	0
28	AH	58	0	74	9	0
28	BA	56	0	70	9	0
28	BB	52	0	62	5	0
28	BC	181	0	243	64	0
28	BE	63	0	87	1	0
28	BH	58	0	74	8	0
29	AA	76	0	95	7	0
29	BA	76	0	95	9	0
30	AA	105	0	145	2	0
30	AB	90	0	109	9	0
30	AF	45	0	53	1	0
30	BA	105	0	145	3	0
30	BB	90	0	109	11	0
30	BF	45	0	53	1	0
31	AA	86	0	111	17	0
31	AB	100	0	139	21	0
31	AC	93	0	125	11	0
31	AD	97	0	134	15	0
31	AI	43	0	56	3	0
31	AJ	46	0	61	2	0
31	AM	42	0	54	6	0
31	BA	42	0	53	3	0
31	BB	49	0	68	4	0
31	BC	93	0	125	10	0
31	BD	143	0	195	15	0
31	BE	44	0	58	4	0
31	BI	43	0	56	4	0
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0
32	AB	140	0	184	15	0
32	AD	31	0	35	0	0
32	AI	70	0	92	9	0
32	AM	35	0	46	1	0
32	BB	140	0	184	16	0
32	BC	35	0	46	3	0
32	BD	31	0	35	1	0
32	BI	35	0	46	5	0
32	BM	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AB	8	0	12	0	0
33	AU	4	0	6	0	0
33	AV	4	0	6	0	0
33	BB	8	0	12	0	0
33	BV	8	0	12	0	0
34	AD	128	0	148	14	0
34	BD	128	0	148	15	0
35	AD	55	0	80	15	0
35	BD	55	0	80	16	0
36	AF	43	0	30	8	0
36	AV	43	0	30	4	0
36	BF	43	0	30	7	0
36	BV	43	0	30	6	0
37	AF	1	0	0	0	0
37	AK	1	0	0	0	0
37	AO	1	0	0	0	0
37	BF	1	0	0	0	0
37	BK	1	0	0	0	0
37	BO	1	0	0	0	0
All	All	50266	0	51335	3700	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 37.

The worst 5 of 3700 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)
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG2	1.69	1.27
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG2	1.78	1.17
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.25	1.15
24:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.29	1.14
24:BB:5612:CLA:H42	4:BD:5127:LEU:HD11	1.29	1.14

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	333/344 (97%)	284 (85%)	42 (13%)	7 (2%)	7	37
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	7	37
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	4	25
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	4	26
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	3	23
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	3	22
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	5	30
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	6	34
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	3	22
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	3	22
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	4	28
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	4	28
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	6
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	1	10
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1	12
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	1	12
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	1	5
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	1	5
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	14
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	14
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%)	24 (75%)	8 (25%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	198 (82%)	31 (13%)	12 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	2	18
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	4	25
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	25
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	2	15
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	20
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	22	61
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	22	61
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	0	2
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	0	2
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	0	2
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	16
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	16
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	3	23

5 of 183 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 ⓘ

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%)	250 (92%)	21 (8%)	13	44
1	BA	271/280 (97%)	253 (93%)	18 (7%)	16	51
2	AB	390/407 (96%)	372 (95%)	18 (5%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BB	390/407 (96%)	374 (96%)	16 (4%)	30	66
3	AC	347/362 (96%)	326 (94%)	21 (6%)	18	54
3	BC	347/362 (96%)	325 (94%)	22 (6%)	18	52
4	AD	275/283 (97%)	249 (90%)	26 (10%)	8	32
4	BD	275/283 (97%)	249 (90%)	26 (10%)	8	32
5	AE	72/73 (99%)	66 (92%)	6 (8%)	11	40
5	BE	72/73 (99%)	66 (92%)	6 (8%)	11	40
6	AF	29/39 (74%)	27 (93%)	2 (7%)	15	49
6	BF	29/39 (74%)	28 (97%)	1 (3%)	37	70
7	AH	53/55 (96%)	42 (79%)	11 (21%)	1	6
7	BH	53/55 (96%)	43 (81%)	10 (19%)	1	8
8	AI	32/35 (91%)	32 (100%)	0	100	100
8	BI	32/35 (91%)	31 (97%)	1 (3%)	40	72
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	31	66
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	31	66
10	AK	30/30 (100%)	29 (97%)	1 (3%)	38	71
10	BK	30/30 (100%)	29 (97%)	1 (3%)	38	71
11	AL	35/35 (100%)	33 (94%)	2 (6%)	20	56
11	BL	35/35 (100%)	32 (91%)	3 (9%)	10	38
12	AM	31/33 (94%)	30 (97%)	1 (3%)	39	71
12	BM	31/33 (94%)	29 (94%)	2 (6%)	17	51
13	AO	202/208 (97%)	187 (93%)	15 (7%)	13	46
13	BO	202/208 (97%)	187 (93%)	15 (7%)	13	46
14	AT	29/29 (100%)	28 (97%)	1 (3%)	37	70
14	BT	29/29 (100%)	27 (93%)	2 (7%)	15	49
15	AU	84/89 (94%)	76 (90%)	8 (10%)	8	32
15	BU	84/89 (94%)	76 (90%)	8 (10%)	8	32
16	AV	116/117 (99%)	111 (96%)	5 (4%)	29	64
16	BV	116/117 (99%)	110 (95%)	6 (5%)	23	59
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	0	2
17	By	20/37 (54%)	15 (75%)	5 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AX	30/34 (88%)	29 (97%)	1 (3%)	38	71
18	BX	30/34 (88%)	29 (97%)	1 (3%)	38	71
20	AZ	52/52 (100%)	49 (94%)	3 (6%)	20	55
20	BZ	52/52 (100%)	48 (92%)	4 (8%)	13	44
All	All	4246/4452 (95%)	3950 (93%)	296 (7%)	15	48

5 of 296 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BE	5010	PHE
17	By	5021	GLN
7	BH	5021	VAL
13	BO	5086	ARG
7	AH	25	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	5199	GLN
18	BX	5047	GLN
2	BB	5281	GLN
18	BX	5042	GLN
13	BO	5087	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 196 ligands modelled in this entry, 12 are monoatomic - leaving 184 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	CLA	BA	5408	-	65,73,73	2.56	20 (30%)	76,113,113	2.19	14 (18%)
24	CLA	AC	510	-	65,73,73	2.49	18 (27%)	76,113,113	2.11	12 (15%)
27	BCR	AB	617	-	41,41,41	1.58	7 (17%)	56,56,56	2.12	20 (35%)
28	DGD	BC	5519	-	67,67,67	1.53	12 (17%)	81,81,81	3.36	30 (37%)
24	CLA	AB	614	-	65,73,73	3.12	19 (29%)	76,113,113	2.19	15 (19%)
27	BCR	BD	5407	-	41,41,41	1.83	9 (21%)	56,56,56	2.33	24 (42%)
32	LMT	AI	102	-	36,36,36	1.62	7 (19%)	47,47,47	1.01	2 (4%)
30	SQD	BA	5401	-	53,54,54	2.46	28 (52%)	62,65,65	2.78	21 (33%)
34	PHO	AD	402	-	51,69,69	2.43	11 (21%)	47,99,99	1.88	9 (19%)
24	CLA	AB	601	-	65,73,73	2.96	22 (33%)	76,113,113	2.27	10 (13%)
27	BCR	AB	619	-	41,41,41	1.86	8 (19%)	56,56,56	1.96	19 (33%)
27	BCR	BC	5514	-	41,41,41	1.83	6 (14%)	56,56,56	2.10	24 (42%)
22	BCT	AA	402	21	2,3,3	0.31	0	2,3,3	0.14	0
32	LMT	AM	102	-	36,36,36	1.75	10 (27%)	47,47,47	0.90	1 (2%)
28	DGD	AH	101	-	59,59,67	1.33	9 (15%)	73,73,81	2.10	18 (24%)
34	PHO	BD	5403	-	51,69,69	2.56	11 (21%)	47,99,99	1.92	9 (19%)
24	CLA	AB	602	-	65,73,73	2.45	18 (27%)	76,113,113	2.11	14 (18%)
24	CLA	BC	5501	-	65,73,73	2.67	19 (29%)	76,113,113	2.35	13 (17%)
27	BCR	BT	5101	-	41,41,41	1.78	7 (17%)	56,56,56	2.24	23 (41%)
31	LMG	BA	5402	-	42,42,55	1.08	4 (9%)	50,50,63	2.33	11 (22%)
24	CLA	AB	609	-	65,73,73	2.63	20 (30%)	76,113,113	2.07	14 (18%)
27	BCR	AK	102	-	41,41,41	1.78	7 (17%)	56,56,56	2.47	25 (44%)
27	BCR	AJ	101	-	41,41,41	2.48	13 (31%)	56,56,56	3.23	23 (41%)
24	CLA	BD	5405	-	65,73,73	2.61	18 (27%)	76,113,113	2.23	14 (18%)
30	SQD	AA	413	-	50,51,54	2.41	25 (50%)	59,62,65	2.82	20 (33%)
31	LMG	BM	5102	-	42,42,55	1.01	3 (7%)	50,50,63	1.64	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	AD	409	-	32,32,36	1.75	7 (21%)	43,43,47	1.25	3 (6%)
36	HEM	BV	5201	16	41,50,50	2.96	18 (43%)	45,82,82	2.88	18 (40%)
24	CLA	BB	5612	-	65,73,73	2.61	21 (32%)	76,113,113	2.36	15 (19%)
24	CLA	BB	5618	-	65,73,73	3.05	18 (27%)	76,113,113	2.17	14 (18%)
24	CLA	AC	505	-	65,73,73	2.82	21 (32%)	76,113,113	2.28	13 (17%)
24	CLA	BC	5503	-	65,73,73	2.61	18 (27%)	76,113,113	2.28	16 (21%)
30	SQD	AF	102	-	44,45,54	2.52	20 (45%)	53,56,65	2.95	17 (32%)
31	LMG	BL	5101	-	51,51,55	1.38	3 (5%)	59,59,63	2.00	12 (20%)
29	LHG	AA	412	-	38,38,48	2.02	5 (13%)	41,44,54	1.47	5 (12%)
31	LMG	BB	5624	-	49,49,55	0.80	1 (2%)	57,57,63	1.93	15 (26%)
31	LMG	BC	5520	-	48,48,55	1.09	3 (6%)	56,56,63	1.89	17 (30%)
24	CLA	BB	5615	-	65,73,73	2.52	18 (27%)	76,113,113	2.26	20 (26%)
27	BCR	AC	515	-	41,41,41	1.76	7 (17%)	56,56,56	2.24	20 (35%)
31	LMG	AA	414	-	44,44,55	1.10	2 (4%)	52,52,63	1.51	6 (11%)
27	BCR	BB	5622	-	41,41,41	1.89	8 (19%)	56,56,56	2.06	16 (28%)
24	CLA	AC	506	-	65,73,73	2.72	22 (33%)	76,113,113	2.15	13 (17%)
24	CLA	AB	605	-	65,73,73	2.70	21 (32%)	76,113,113	2.14	16 (21%)
24	CLA	BB	5616	-	65,73,73	2.75	21 (32%)	76,113,113	2.07	13 (17%)
31	LMG	AM	101	-	42,42,55	0.95	2 (4%)	50,50,63	1.64	8 (16%)
32	LMT	AB	629	-	36,36,36	1.59	7 (19%)	47,47,47	1.40	7 (14%)
24	CLA	BC	5507	-	65,73,73	2.48	19 (29%)	76,113,113	2.16	14 (18%)
24	CLA	BA	5406	-	65,73,73	2.59	21 (32%)	76,113,113	2.41	20 (26%)
30	SQD	BB	5625	-	42,43,54	2.60	20 (47%)	51,54,65	2.86	15 (29%)
24	CLA	AB	606	-	65,73,73	2.58	20 (30%)	76,113,113	2.15	15 (19%)
33	DMS	AB	626	-	3,3,3	0.68	0	3,3,3	1.07	0
24	CLA	AB	616	-	65,73,73	2.56	17 (26%)	76,113,113	2.12	11 (14%)
29	LHG	BA	5415	-	36,36,48	1.08	2 (5%)	39,42,54	1.12	3 (7%)
33	DMS	BV	5202	-	3,3,3	0.86	0	3,3,3	1.00	0
31	LMG	BC	5521	-	45,45,55	1.04	2 (4%)	53,53,63	1.91	13 (24%)
24	CLA	BA	5407	-	65,73,73	2.66	20 (30%)	76,113,113	2.27	12 (15%)
36	HEM	BF	5101	5,6	41,50,50	3.06	17 (41%)	45,82,82	3.09	20 (44%)
30	SQD	AA	416	-	53,54,54	2.43	28 (52%)	62,65,65	2.79	21 (33%)
24	CLA	AA	406	-	65,73,73	2.52	20 (30%)	76,113,113	2.23	15 (19%)
24	CLA	AD	404	-	65,73,73	2.60	20 (30%)	76,113,113	2.24	14 (18%)
24	CLA	BB	5617	-	65,73,73	2.34	20 (30%)	76,113,113	2.01	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BB	5613	-	65,73,73	2.65	22 (33%)	76,113,113	2.09	15 (19%)
28	DGD	BH	5101	-	59,59,67	1.31	9 (15%)	73,73,81	2.11	17 (23%)
36	HEM	AV	201	16	41,50,50	2.83	14 (34%)	45,82,82	2.90	18 (40%)
28	DGD	AC	518	-	63,63,67	1.23	6 (9%)	77,77,81	2.80	23 (29%)
32	LMT	AB	630	-	36,36,36	1.74	9 (25%)	47,47,47	1.01	1 (2%)
24	CLA	BC	5506	-	65,73,73	2.72	22 (33%)	76,113,113	2.16	14 (18%)
31	LMG	AB	621	-	49,49,55	0.78	1 (2%)	57,57,63	1.93	14 (24%)
24	CLA	BC	5513	-	65,73,73	3.16	21 (32%)	76,113,113	1.99	13 (17%)
31	LMG	BD	5408	-	46,46,55	0.97	3 (6%)	54,54,63	2.58	16 (29%)
27	BCR	AD	406	-	41,41,41	1.66	7 (17%)	56,56,56	2.35	23 (41%)
24	CLA	AB	610	-	65,73,73	2.46	16 (24%)	76,113,113	2.10	13 (17%)
27	BCR	BX	5101	-	41,41,41	1.89	8 (19%)	56,56,56	2.24	22 (39%)
29	LHG	AA	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.12	3 (7%)
24	CLA	BB	5606	-	65,73,73	2.46	18 (27%)	76,113,113	2.14	14 (18%)
28	DGD	AC	519	-	67,67,67	1.49	13 (19%)	81,81,81	3.36	30 (37%)
24	CLA	AB	613	-	65,73,73	2.32	17 (26%)	76,113,113	2.01	12 (15%)
24	CLA	AB	604	-	65,73,73	2.53	19 (29%)	76,113,113	2.08	13 (17%)
34	PHO	BD	5404	-	51,69,69	2.49	9 (17%)	47,99,99	2.01	12 (25%)
28	DGD	BA	5412	-	57,57,67	1.83	13 (22%)	71,71,81	3.63	23 (32%)
24	CLA	AC	513	-	65,73,73	3.04	18 (27%)	76,113,113	1.98	13 (17%)
24	CLA	BC	5509	-	65,73,73	2.96	18 (27%)	76,113,113	2.14	10 (13%)
28	DGD	AA	411	-	57,57,67	1.80	13 (22%)	71,71,81	3.62	24 (33%)
35	PL9	AD	405	-	55,55,55	3.85	18 (32%)	68,69,69	2.76	24 (35%)
27	BCR	BB	5623	-	41,41,41	1.73	8 (19%)	56,56,56	1.94	17 (30%)
24	CLA	AC	508	-	65,73,73	2.48	17 (26%)	76,113,113	2.24	16 (21%)
24	CLA	BB	5611	-	65,73,73	2.47	21 (32%)	76,113,113	2.29	17 (22%)
27	BCR	AT	101	-	41,41,41	1.65	7 (17%)	56,56,56	2.24	23 (41%)
24	CLA	BC	5511	3	65,73,73	3.16	21 (32%)	76,113,113	2.16	16 (21%)
24	CLA	AC	502	-	65,73,73	2.56	20 (30%)	76,113,113	2.13	12 (15%)
24	CLA	AC	512	-	65,73,73	2.64	19 (29%)	76,113,113	2.22	11 (14%)
31	LMG	BI	5101	-	43,43,55	1.02	3 (6%)	51,51,63	1.68	7 (13%)
24	CLA	BB	5619	-	65,73,73	2.50	17 (26%)	76,113,113	2.26	12 (15%)
36	HEM	AF	101	5,6	41,50,50	2.96	16 (39%)	45,82,82	3.07	20 (44%)
24	CLA	BC	5504	-	65,73,73	2.60	20 (30%)	76,113,113	2.18	12 (15%)
27	BCR	BC	5516	-	41,41,41	1.79	7 (17%)	56,56,56	2.21	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BC	5512	-	65,73,73	2.74	19 (29%)	76,113,113	2.22	10 (13%)
24	CLA	AB	603	-	65,73,73	2.70	20 (30%)	76,113,113	2.20	20 (26%)
24	CLA	BC	5502	-	65,73,73	2.64	20 (30%)	76,113,113	2.24	13 (17%)
31	LMG	AA	417	-	42,42,55	1.07	5 (11%)	50,50,63	2.33	12 (24%)
24	CLA	BB	5610	-	65,73,73	2.64	19 (29%)	76,113,113	2.17	17 (22%)
31	LMG	AC	520	-	48,48,55	1.05	5 (10%)	56,56,63	1.92	19 (33%)
31	LMG	BE	5101	-	44,44,55	1.09	3 (6%)	52,52,63	1.52	6 (11%)
32	LMT	BB	5603	-	36,36,36	1.59	7 (19%)	47,47,47	1.40	7 (14%)
24	CLA	AB	615	-	65,73,73	2.50	17 (26%)	76,113,113	2.22	10 (13%)
31	LMG	AD	408	-	48,48,55	0.96	4 (8%)	56,56,63	2.08	11 (19%)
33	DMS	BV	5203	-	3,3,3	0.83	0	3,3,3	1.21	0
32	LMT	BB	5604	-	36,36,36	1.71	10 (27%)	47,47,47	1.00	1 (2%)
27	BCR	AC	514	-	41,41,41	1.64	7 (17%)	56,56,56	2.14	22 (39%)
24	CLA	BB	5608	-	65,73,73	2.49	20 (30%)	76,113,113	2.13	14 (18%)
24	CLA	BB	5607	-	65,73,73	2.70	19 (29%)	76,113,113	2.19	20 (26%)
24	CLA	BC	5508	-	65,73,73	2.57	18 (27%)	76,113,113	2.32	15 (19%)
28	DGD	AE	101	-	64,64,67	1.55	13 (20%)	78,78,81	1.45	12 (15%)
24	CLA	AC	511	3	65,73,73	3.02	19 (29%)	76,113,113	2.14	17 (22%)
24	CLA	BD	5402	-	65,73,73	2.52	18 (27%)	76,113,113	2.17	16 (21%)
27	BCR	AB	618	-	41,41,41	1.93	7 (17%)	56,56,56	2.07	16 (28%)
24	CLA	AB	611	-	65,73,73	2.48	19 (29%)	76,113,113	2.26	20 (26%)
28	DGD	BC	5518	-	63,63,67	1.26	6 (9%)	77,77,81	2.78	22 (28%)
30	SQD	BB	5601	-	46,47,54	2.47	22 (47%)	55,58,65	2.71	16 (29%)
24	CLA	BC	5505	-	65,73,73	2.85	22 (33%)	76,113,113	2.29	14 (18%)
31	LMG	AC	521	-	45,45,55	1.09	2 (4%)	53,53,63	1.92	14 (26%)
32	LMT	AB	624	-	36,36,36	1.66	8 (22%)	47,47,47	0.93	2 (4%)
27	BCR	AA	410	-	41,41,41	1.63	7 (17%)	56,56,56	2.06	21 (37%)
32	LMT	BB	5626	-	36,36,36	1.78	9 (25%)	47,47,47	1.00	2 (4%)
33	DMS	BB	5628	-	3,3,3	0.71	0	3,3,3	1.16	0
24	CLA	AA	404	-	65,73,73	2.45	16 (24%)	76,113,113	1.97	14 (18%)
24	CLA	AC	503	-	65,73,73	2.54	19 (29%)	76,113,113	2.36	17 (22%)
31	LMG	BD	5410	-	48,48,55	0.94	3 (6%)	56,56,63	2.09	11 (19%)
28	DGD	BC	5517	-	54,54,67	1.44	8 (14%)	68,68,81	2.74	22 (32%)
31	LMG	AI	101	-	43,43,55	1.03	3 (6%)	51,51,63	1.69	8 (15%)
27	BCR	AX	101	-	41,41,41	1.86	8 (19%)	56,56,56	2.21	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	BA	5413	-	38,38,48	2.01	5 (13%)	41,44,54	1.44	5 (12%)
27	BCR	BJ	5101	-	41,41,41	2.42	14 (34%)	56,56,56	3.21	23 (41%)
27	BCR	BC	5515	-	41,41,41	1.90	8 (19%)	56,56,56	2.24	20 (35%)
33	DMS	BB	5629	-	3,3,3	0.68	0	3,3,3	1.24	0
35	PL9	BD	5406	-	55,55,55	3.95	18 (32%)	68,69,69	2.76	23 (33%)
27	BCR	AC	516	-	41,41,41	1.66	8 (19%)	56,56,56	2.25	20 (35%)
28	DGD	AC	517	-	54,54,67	1.35	7 (12%)	68,68,81	2.74	22 (32%)
32	LMT	BM	5101	-	36,36,36	1.76	9 (25%)	47,47,47	0.89	1 (2%)
24	CLA	BB	5620	-	65,73,73	2.56	18 (27%)	76,113,113	2.13	10 (13%)
32	LMT	BD	5411	-	32,32,36	1.74	8 (25%)	43,43,47	1.26	2 (4%)
33	DMS	AB	625	-	3,3,3	0.73	0	3,3,3	1.48	1 (33%)
24	CLA	AD	401	-	65,73,73	2.42	17 (26%)	76,113,113	2.15	16 (21%)
30	SQD	AB	622	-	42,43,54	2.58	19 (45%)	51,54,65	2.84	15 (29%)
32	LMT	BI	5102	-	36,36,36	1.66	8 (22%)	47,47,47	1.00	2 (4%)
28	DGD	BB	5602	-	53,53,67	1.50	7 (13%)	67,67,81	2.08	13 (19%)
30	SQD	BA	5414	-	50,51,54	2.49	26 (52%)	59,62,65	2.79	20 (33%)
32	LMT	BB	5627	-	36,36,36	1.63	8 (22%)	47,47,47	0.92	1 (2%)
33	DMS	AU	201	-	3,3,3	0.92	0	3,3,3	1.14	0
24	CLA	BB	5614	-	65,73,73	2.47	17 (26%)	76,113,113	2.10	13 (17%)
30	SQD	BF	5102	-	44,45,54	2.52	19 (43%)	53,56,65	2.96	19 (35%)
24	CLA	BB	5609	-	65,73,73	2.62	20 (30%)	76,113,113	2.14	17 (22%)
24	CLA	AC	504	-	65,73,73	2.48	20 (30%)	76,113,113	2.18	15 (19%)
24	CLA	BB	5605	-	65,73,73	2.96	20 (30%)	76,113,113	2.22	10 (13%)
27	BCR	BB	5621	-	41,41,41	1.51	7 (17%)	56,56,56	2.10	21 (37%)
33	DMS	AV	202	-	3,3,3	0.76	0	3,3,3	1.08	0
24	CLA	AC	501	-	65,73,73	2.54	20 (30%)	76,113,113	2.32	13 (17%)
31	LMG	AB	620	-	51,51,55	1.33	3 (5%)	59,59,63	2.01	12 (20%)
24	CLA	AB	608	-	65,73,73	2.62	21 (32%)	76,113,113	2.36	15 (19%)
27	BCR	BA	5411	-	41,41,41	1.69	7 (17%)	56,56,56	2.08	22 (39%)
32	LMT	AI	103	-	36,36,36	1.45	6 (16%)	47,47,47	1.77	10 (21%)
24	CLA	AB	607	-	65,73,73	2.46	19 (29%)	76,113,113	2.25	16 (21%)
24	CLA	AA	405	-	65,73,73	2.45	21 (32%)	76,113,113	2.37	20 (26%)
24	CLA	AA	407	-	65,73,73	2.49	18 (27%)	76,113,113	2.22	15 (19%)
24	CLA	AC	507	-	65,73,73	2.37	19 (29%)	76,113,113	2.16	11 (14%)
32	LMT	AB	623	-	36,36,36	1.78	8 (22%)	47,47,47	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	AB	628	-	53,53,67	1.45	7 (13%)	67,67,81	2.05	14 (20%)
30	SQD	AB	627	-	46,47,54	2.48	22 (47%)	55,58,65	2.71	15 (27%)
27	BCR	BK	5102	-	41,41,41	1.91	9 (21%)	56,56,56	2.43	25 (44%)
31	LMG	AJ	102	-	46,46,55	0.97	3 (6%)	54,54,63	2.58	17 (31%)
32	LMT	BC	5522	-	36,36,36	1.52	7 (19%)	47,47,47	1.77	8 (17%)
24	CLA	AC	509	-	65,73,73	2.75	15 (23%)	76,113,113	2.15	12 (15%)
34	PHO	AD	403	-	51,69,69	2.40	9 (17%)	47,99,99	1.98	11 (23%)
31	LMG	BD	5409	-	49,49,55	0.71	0	57,57,63	2.73	20 (35%)
24	CLA	BA	5405	-	65,73,73	2.44	16 (24%)	76,113,113	1.98	15 (19%)
24	CLA	BC	5510	-	65,73,73	2.55	16 (24%)	76,113,113	2.11	11 (14%)
28	DGD	BE	5102	-	64,64,67	1.52	14 (21%)	78,78,81	1.43	11 (14%)
25	MST	AA	408	-	16,16,16	0.50	0	22,22,22	4.16	9 (40%)
22	BCT	BA	5403	21	2,3,3	0.35	0	2,3,3	0.38	0
25	MST	BA	5409	-	16,16,16	0.46	0	22,22,22	4.08	9 (40%)
24	CLA	AB	612	-	65,73,73	2.71	19 (29%)	76,113,113	2.01	13 (17%)
31	LMG	AD	407	-	49,49,55	0.74	1 (2%)	57,57,63	2.72	19 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BA	5408	-	2/2/15/20	12/37/115/115	-
24	CLA	AC	510	-	2/2/15/20	10/37/115/115	-
28	DGD	BC	5519	-	1/1/13/13	7/55/95/95	0/2/2/2
27	BCR	AB	617	-	-	1/29/63/63	0/2/2/2
24	CLA	AB	614	-	2/2/15/20	12/37/115/115	-
27	BCR	BD	5407	-	-	5/29/63/63	0/2/2/2
32	LMT	AI	102	-	-	3/21/61/61	0/2/2/2
34	PHO	AD	402	-	1/1/17/22	11/37/103/103	0/5/6/6
30	SQD	BA	5401	-	-	23/49/69/69	0/1/1/1
24	CLA	AB	601	-	2/2/15/20	12/37/115/115	-
27	BCR	AB	619	-	-	4/29/63/63	0/2/2/2
27	BCR	BC	5514	-	-	5/29/63/63	0/2/2/2
32	LMT	AM	102	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	AH	101	-	-	3/47/87/95	0/2/2/2
34	PHO	BD	5403	-	1/1/17/22	11/37/103/103	0/5/6/6
24	CLA	AB	602	-	2/2/15/20	7/37/115/115	-
24	CLA	BC	5501	-	2/2/15/20	12/37/115/115	-
27	BCR	BT	5101	-	-	4/29/63/63	0/2/2/2
31	LMG	BA	5402	-	-	3/37/57/70	0/1/1/1
24	CLA	AB	609	-	2/2/15/20	7/37/115/115	-
27	BCR	AK	102	-	-	2/29/63/63	0/2/2/2
27	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
24	CLA	BD	5405	-	2/2/15/20	10/37/115/115	-
30	SQD	AA	413	-	-	23/46/66/69	0/1/1/1
31	LMG	BM	5102	-	-	3/37/57/70	0/1/1/1
32	LMT	AD	409	-	-	1/17/57/61	0/2/2/2
36	HEM	BV	5201	16	-	4/12/54/54	-
24	CLA	BB	5612	-	2/2/15/20	10/37/115/115	-
24	CLA	BB	5618	-	2/2/15/20	12/37/115/115	-
24	CLA	AC	505	-	2/2/15/20	8/37/115/115	-
24	CLA	BC	5503	-	2/2/15/20	14/37/115/115	-
30	SQD	AF	102	-	-	22/40/60/69	0/1/1/1
31	LMG	BL	5101	-	-	5/46/66/70	0/1/1/1
29	LHG	AA	412	-	-	19/43/43/53	-
31	LMG	BB	5624	-	-	4/44/64/70	0/1/1/1
31	LMG	BC	5520	-	-	5/43/63/70	0/1/1/1
24	CLA	BB	5615	-	2/2/15/20	10/37/115/115	-
27	BCR	AC	515	-	-	3/29/63/63	0/2/2/2
31	LMG	AA	414	-	-	5/39/59/70	0/1/1/1
27	BCR	BB	5622	-	-	1/29/63/63	0/2/2/2
24	CLA	AC	506	-	2/2/15/20	5/37/115/115	-
24	CLA	AB	605	-	2/2/15/20	7/37/115/115	-
24	CLA	BB	5616	-	2/2/15/20	10/37/115/115	-
31	LMG	AM	101	-	-	3/37/57/70	0/1/1/1
32	LMT	AB	629	-	-	3/21/61/61	0/2/2/2
24	CLA	BC	5507	-	2/2/15/20	6/37/115/115	-
24	CLA	BA	5406	-	2/2/15/20	15/37/115/115	-
30	SQD	BB	5625	-	-	18/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	606	-	2/2/15/20	12/37/115/115	-
24	CLA	AB	616	-	2/2/15/20	11/37/115/115	-
29	LHG	BA	5415	-	-	23/41/41/53	-
31	LMG	BC	5521	-	-	6/40/60/70	0/1/1/1
24	CLA	BA	5407	-	2/2/15/20	3/37/115/115	-
36	HEM	BF	5101	5,6	-	6/12/54/54	-
30	SQD	AA	416	-	-	21/49/69/69	0/1/1/1
24	CLA	AA	406	-	2/2/15/20	3/37/115/115	-
24	CLA	AD	404	-	2/2/15/20	10/37/115/115	-
24	CLA	BB	5617	-	2/2/15/20	9/37/115/115	-
24	CLA	BB	5613	-	2/2/15/20	7/37/115/115	-
28	DGD	BH	5101	-	-	3/47/87/95	0/2/2/2
36	HEM	AV	201	16	-	4/12/54/54	-
28	DGD	AC	518	-	1/1/13/13	8/51/91/95	0/2/2/2
32	LMT	AB	630	-	-	3/21/61/61	0/2/2/2
24	CLA	BC	5506	-	2/2/15/20	5/37/115/115	-
31	LMG	AB	621	-	-	4/44/64/70	0/1/1/1
24	CLA	BC	5513	-	2/2/15/20	10/37/115/115	-
31	LMG	BD	5408	-	-	5/41/61/70	0/1/1/1
27	BCR	AD	406	-	-	5/29/63/63	0/2/2/2
24	CLA	AB	610	-	2/2/15/20	8/37/115/115	-
27	BCR	BX	5101	-	-	1/29/63/63	0/2/2/2
29	LHG	AA	415	-	-	24/41/41/53	-
24	CLA	BB	5606	-	2/2/15/20	7/37/115/115	-
28	DGD	AC	519	-	1/1/13/13	9/55/95/95	0/2/2/2
24	CLA	AB	613	-	2/2/15/20	8/37/115/115	-
24	CLA	AB	604	-	2/2/15/20	9/37/115/115	-
34	PHO	BD	5404	-	1/1/17/22	12/37/103/103	0/5/6/6
28	DGD	BA	5412	-	-	7/45/85/95	0/2/2/2
24	CLA	AC	513	-	2/2/15/20	10/37/115/115	-
24	CLA	BC	5509	-	2/2/15/20	4/37/115/115	-
28	DGD	AA	411	-	-	7/45/85/95	0/2/2/2
35	PL9	AD	405	-	-	16/53/73/73	0/1/1/1
27	BCR	BB	5623	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AC	508	-	2/2/15/20	7/37/115/115	-
24	CLA	BB	5611	-	2/2/15/20	5/37/115/115	-
27	BCR	AT	101	-	-	4/29/63/63	0/2/2/2
24	CLA	BC	5511	3	2/2/15/20	14/37/115/115	-
24	CLA	AC	502	-	2/2/15/20	9/37/115/115	-
24	CLA	AC	512	-	2/2/15/20	12/37/115/115	-
31	LMG	BI	5101	-	-	2/38/58/70	0/1/1/1
24	CLA	BB	5619	-	2/2/15/20	5/37/115/115	-
36	HEM	AF	101	5,6	-	6/12/54/54	-
24	CLA	BC	5504	-	2/2/15/20	9/37/115/115	-
27	BCR	BC	5516	-	-	4/29/63/63	0/2/2/2
24	CLA	BC	5512	-	2/2/15/20	12/37/115/115	-
24	CLA	AB	603	-	2/2/15/20	11/37/115/115	-
24	CLA	BC	5502	-	2/2/15/20	9/37/115/115	-
31	LMG	AA	417	-	-	3/37/57/70	0/1/1/1
24	CLA	BB	5610	-	2/2/15/20	11/37/115/115	-
31	LMG	AC	520	-	-	5/43/63/70	0/1/1/1
31	LMG	BE	5101	-	-	5/39/59/70	0/1/1/1
32	LMT	BB	5603	-	-	3/21/61/61	0/2/2/2
24	CLA	AB	615	-	2/2/15/20	5/37/115/115	-
31	LMG	AD	408	-	-	5/43/63/70	0/1/1/1
32	LMT	BB	5604	-	-	3/21/61/61	0/2/2/2
27	BCR	AC	514	-	-	5/29/63/63	0/2/2/2
24	CLA	BB	5608	-	2/2/15/20	9/37/115/115	-
24	CLA	BB	5607	-	2/2/15/20	11/37/115/115	-
24	CLA	BC	5508	-	2/2/15/20	8/37/115/115	-
28	DGD	AE	101	-	-	5/52/92/95	0/2/2/2
24	CLA	AC	511	3	2/2/15/20	15/37/115/115	-
24	CLA	BD	5402	-	2/2/15/20	11/37/115/115	-
27	BCR	AB	618	-	-	1/29/63/63	0/2/2/2
24	CLA	AB	611	-	2/2/15/20	10/37/115/115	-
28	DGD	BC	5518	-	1/1/13/13	8/51/91/95	0/2/2/2
30	SQD	BB	5601	-	-	24/42/62/69	0/1/1/1
24	CLA	BC	5505	-	2/2/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	AC	521	-	-	6/40/60/70	0/1/1/1
32	LMT	AB	624	-	-	3/21/61/61	0/2/2/2
27	BCR	AA	410	-	-	5/29/63/63	0/2/2/2
32	LMT	BB	5626	-	-	1/21/61/61	0/2/2/2
24	CLA	AA	404	-	2/2/15/20	13/37/115/115	-
24	CLA	AC	503	-	2/2/15/20	13/37/115/115	-
31	LMG	BD	5410	-	-	5/43/63/70	0/1/1/1
28	DGD	BC	5517	-	-	4/42/82/95	0/2/2/2
31	LMG	AI	101	-	-	2/38/58/70	0/1/1/1
27	BCR	AX	101	-	-	2/29/63/63	0/2/2/2
27	BCR	BJ	5101	-	-	1/29/63/63	0/2/2/2
27	BCR	BC	5515	-	-	3/29/63/63	0/2/2/2
35	PL9	BD	5406	-	-	17/53/73/73	0/1/1/1
27	BCR	AC	516	-	-	5/29/63/63	0/2/2/2
28	DGD	AC	517	-	-	4/42/82/95	0/2/2/2
32	LMT	BM	5101	-	-	3/21/61/61	0/2/2/2
24	CLA	BB	5620	-	2/2/15/20	10/37/115/115	-
32	LMT	BD	5411	-	-	1/17/57/61	0/2/2/2
24	CLA	AD	401	-	2/2/15/20	11/37/115/115	-
30	SQD	AB	622	-	-	20/38/58/69	0/1/1/1
32	LMT	BI	5102	-	-	3/21/61/61	0/2/2/2
28	DGD	BB	5602	-	-	6/41/81/95	0/2/2/2
30	SQD	BA	5414	-	-	23/46/66/69	0/1/1/1
32	LMT	BB	5627	-	-	3/21/61/61	0/2/2/2
24	CLA	BB	5614	-	2/2/15/20	9/37/115/115	-
30	SQD	BF	5102	-	-	23/40/60/69	0/1/1/1
24	CLA	BB	5609	-	2/2/15/20	8/37/115/115	-
24	CLA	AC	504	-	2/2/15/20	9/37/115/115	-
24	CLA	BB	5605	-	2/2/15/20	12/37/115/115	-
27	BCR	BB	5621	-	-	1/29/63/63	0/2/2/2
24	CLA	AC	501	-	2/2/15/20	12/37/115/115	-
31	LMG	AB	620	-	-	5/46/66/70	0/1/1/1
24	CLA	AB	608	-	2/2/15/20	10/37/115/115	-
27	BCR	BA	5411	-	-	5/29/63/63	0/2/2/2
32	LMT	AI	103	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	607	-	2/2/15/20	5/37/115/115	-
24	CLA	AA	405	-	2/2/15/20	15/37/115/115	-
24	CLA	AA	407	-	2/2/15/20	13/37/115/115	-
24	CLA	AC	507	-	2/2/15/20	5/37/115/115	-
32	LMT	AB	623	-	-	1/21/61/61	0/2/2/2
28	DGD	AB	628	-	-	7/41/81/95	0/2/2/2
30	SQD	AB	627	-	-	24/42/62/69	0/1/1/1
27	BCR	BK	5102	-	-	2/29/63/63	0/2/2/2
31	LMG	AJ	102	-	-	5/41/61/70	0/1/1/1
34	PHO	AD	403	-	1/1/17/22	10/37/103/103	0/5/6/6
24	CLA	AC	509	-	2/2/15/20	4/37/115/115	-
32	LMT	BC	5522	-	-	2/21/61/61	0/2/2/2
31	LMG	BD	5409	-	-	7/44/64/70	0/1/1/1
24	CLA	BA	5405	-	2/2/15/20	14/37/115/115	-
24	CLA	BC	5510	-	2/2/15/20	11/37/115/115	-
28	DGD	BE	5102	-	-	6/52/92/95	0/2/2/2
25	MST	AA	408	-	-	2/10/10/10	0/1/1/1
29	LHG	BA	5413	-	-	19/43/43/53	-
25	MST	BA	5409	-	-	2/10/10/10	0/1/1/1
24	CLA	AB	612	-	2/2/15/20	10/37/115/115	-
31	LMG	AD	407	-	-	7/44/64/70	0/1/1/1

The worst 5 of 2237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	614	CLA	MG-NA	12.11	2.35	2.06
24	BC	5513	CLA	MG-NA	12.03	2.34	2.06
24	BC	5511	CLA	MG-NA	11.84	2.34	2.06
24	AC	513	CLA	MG-NA	11.69	2.34	2.06
24	AC	511	CLA	MG-NA	11.67	2.34	2.06

The worst 5 of 2489 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	601	CLA	C4A-NA-C1A	14.32	113.14	106.71
24	BB	5605	CLA	C4A-NA-C1A	13.87	112.94	106.71
24	AC	512	CLA	C4A-NA-C1A	13.52	112.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5512	CLA	C4A-NA-C1A	13.51	112.78	106.71
24	BB	5619	CLA	C4A-NA-C1A	13.42	112.74	106.71

5 of 148 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	AA	404	CLA	ND
24	AA	404	CLA	C8
24	AA	405	CLA	ND
24	AA	405	CLA	C8
24	AA	406	CLA	ND

5 of 1365 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AA	405	CLA	CHA-CBD-CGD-O1D
24	AA	405	CLA	CHA-CBD-CGD-O2D
24	AA	405	CLA	C6-C7-C8-C9
24	AB	601	CLA	C2A-CAA-CBA-CGA
24	AB	606	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

167 monomers are involved in 1068 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	BA	5408	CLA	11	0
24	AC	510	CLA	6	0
27	AB	617	BCR	3	0
28	BC	5519	DGD	45	0
24	AB	614	CLA	10	0
27	BD	5407	BCR	2	0
32	AI	102	LMT	5	0
30	BA	5401	SQD	3	0
34	AD	402	PHO	11	0
24	AB	601	CLA	5	0
27	AB	619	BCR	3	0
27	BC	5514	BCR	6	0
32	AM	102	LMT	1	0
28	AH	101	DGD	9	0
34	BD	5403	PHO	12	0
24	AB	602	CLA	7	0
24	BC	5501	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BT	5101	BCR	6	0
31	BA	5402	LMG	3	0
24	AB	609	CLA	7	0
27	AK	102	BCR	5	0
27	AJ	101	BCR	4	0
24	BD	5405	CLA	8	0
31	BM	5102	LMG	4	0
36	BV	5201	HEM	6	0
24	BB	5612	CLA	14	0
24	BB	5618	CLA	14	0
24	AC	505	CLA	9	0
24	BC	5503	CLA	5	0
30	AF	102	SQD	1	0
31	BL	5101	LMG	18	0
29	AA	412	LHG	5	0
31	BB	5624	LMG	4	0
31	BC	5520	LMG	3	0
24	BB	5615	CLA	19	0
27	AC	515	BCR	6	0
31	AA	414	LMG	11	0
27	BB	5622	BCR	1	0
24	AC	506	CLA	5	0
24	AB	605	CLA	10	0
24	BB	5616	CLA	12	0
31	AM	101	LMG	6	0
32	AB	629	LMT	4	0
24	BC	5507	CLA	7	0
24	BA	5406	CLA	22	0
30	BB	5625	SQD	6	0
24	AB	606	CLA	9	0
24	AB	616	CLA	4	0
29	BA	5415	LHG	3	0
31	BC	5521	LMG	7	0
24	BA	5407	CLA	1	0
36	BF	5101	HEM	7	0
30	AA	416	SQD	2	0
24	AA	406	CLA	1	0
24	AD	404	CLA	8	0
24	BB	5617	CLA	8	0
24	BB	5613	CLA	7	0
28	BH	5101	DGD	8	0
36	AV	201	HEM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	AC	518	DGD	12	0
32	AB	630	LMT	2	0
24	BC	5506	CLA	4	0
31	AB	621	LMG	4	0
24	BC	5513	CLA	5	0
31	BD	5408	LMG	1	0
27	AD	406	BCR	2	0
24	AB	610	CLA	8	0
27	BX	5101	BCR	4	0
29	AA	415	LHG	2	0
24	BB	5606	CLA	7	0
28	AC	519	DGD	42	0
24	AB	613	CLA	9	0
24	AB	604	CLA	12	0
34	BD	5404	PHO	3	0
28	BA	5412	DGD	9	0
24	AC	513	CLA	3	0
24	BC	5509	CLA	8	0
28	AA	411	DGD	9	0
35	AD	405	PL9	15	0
27	BB	5623	BCR	4	0
24	AC	508	CLA	10	0
24	BB	5611	CLA	10	0
27	AT	101	BCR	10	0
24	BC	5511	CLA	23	0
24	AC	502	CLA	6	0
24	AC	512	CLA	4	0
31	BI	5101	LMG	4	0
24	BB	5619	CLA	8	0
36	AF	101	HEM	8	0
24	BC	5504	CLA	8	0
27	BC	5516	BCR	13	0
24	BC	5512	CLA	5	0
24	AB	603	CLA	15	0
24	BC	5502	CLA	6	0
31	AA	417	LMG	6	0
24	BB	5610	CLA	9	0
31	AC	520	LMG	4	0
31	BE	5101	LMG	4	0
32	BB	5603	LMT	2	0
24	AB	615	CLA	8	0
31	AD	408	LMG	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	BB	5604	LMT	2	0
27	AC	514	BCR	6	0
24	BB	5608	CLA	12	0
24	BB	5607	CLA	15	0
24	BC	5508	CLA	9	0
28	AE	101	DGD	1	0
24	AC	511	CLA	22	0
24	BD	5402	CLA	10	0
27	AB	618	BCR	2	0
24	AB	611	CLA	15	0
28	BC	5518	DGD	10	0
30	BB	5601	SQD	5	0
24	BC	5505	CLA	9	0
31	AC	521	LMG	7	0
32	AB	624	LMT	9	0
27	AA	410	BCR	4	0
32	BB	5626	LMT	2	0
24	AA	404	CLA	12	0
24	AC	503	CLA	6	0
31	BD	5410	LMG	10	0
28	BC	5517	DGD	10	0
31	AI	101	LMG	3	0
27	AX	101	BCR	8	0
29	BA	5413	LHG	6	0
27	BJ	5101	BCR	3	0
27	BC	5515	BCR	6	0
35	BD	5406	PL9	16	0
27	AC	516	BCR	12	0
28	AC	517	DGD	10	0
32	BM	5101	LMT	2	0
24	BB	5620	CLA	4	0
32	BD	5411	LMT	1	0
24	AD	401	CLA	9	0
30	AB	622	SQD	6	0
32	BI	5102	LMT	5	0
28	BB	5602	DGD	5	0
32	BB	5627	LMT	10	0
24	BB	5614	CLA	9	0
30	BF	5102	SQD	1	0
24	BB	5609	CLA	12	0
24	AC	504	CLA	10	0
24	BB	5605	CLA	5	0

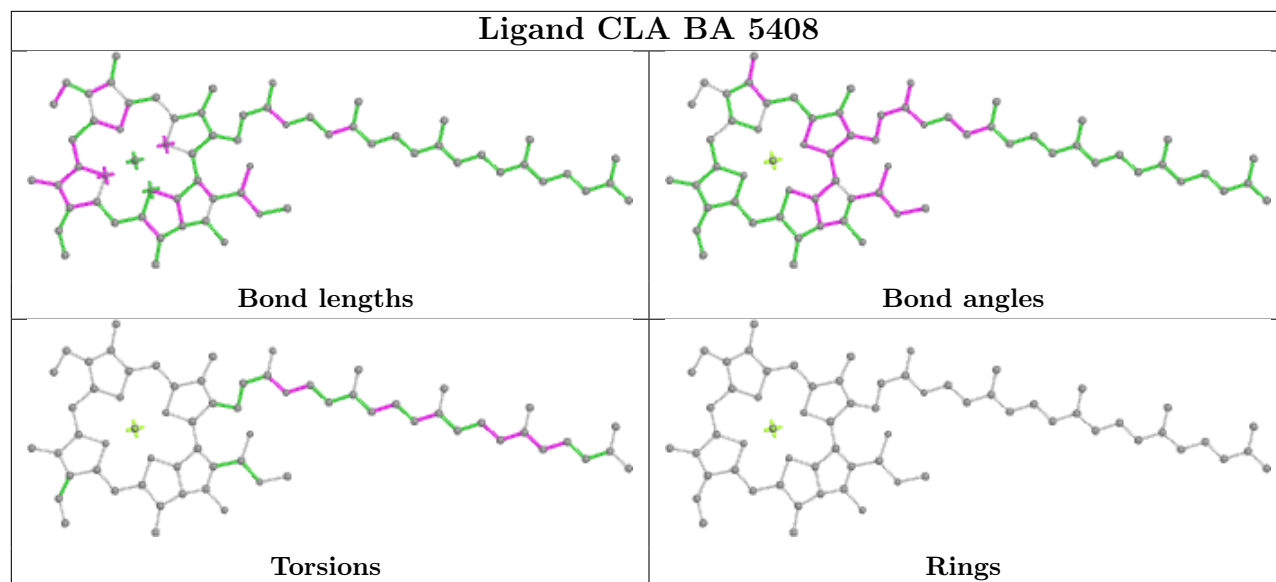
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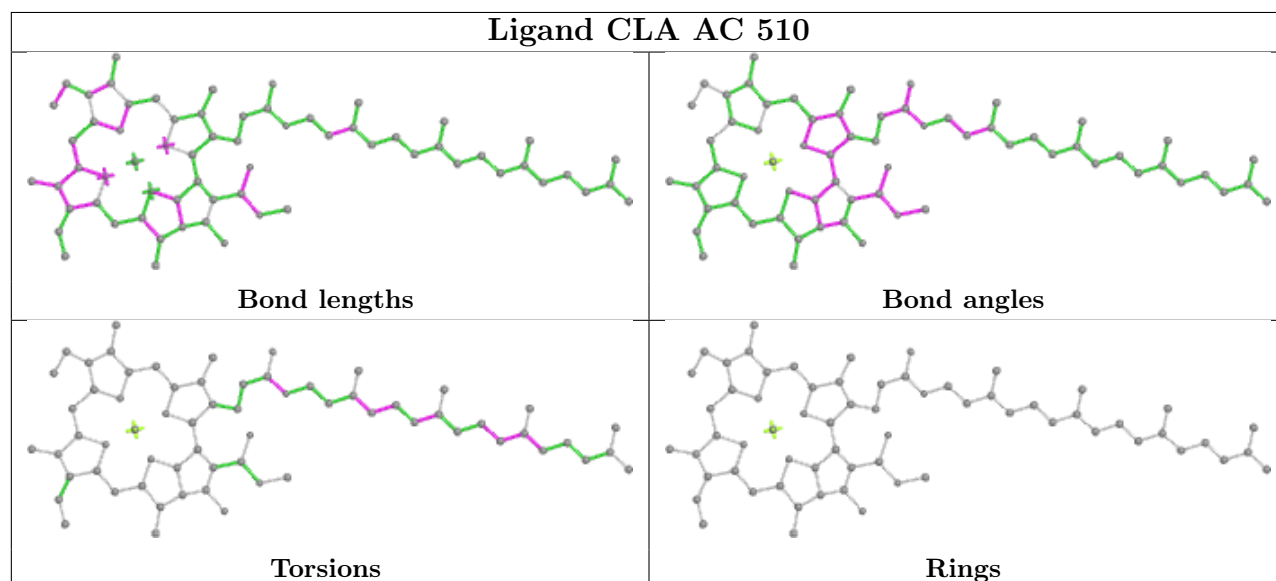
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31	AB	620	LMG	17	0
24	AB	608	CLA	15	0
27	BA	5411	BCR	3	0
32	AI	103	LMT	4	0
24	AB	607	CLA	10	0
24	AA	405	CLA	20	0
24	AA	407	CLA	9	0
24	AC	507	CLA	5	0
30	AB	627	SQD	3	0
27	BK	5102	BCR	5	0
31	AJ	102	LMG	2	0
32	BC	5522	LMT	3	0
24	AC	509	CLA	6	0
34	AD	403	PHO	3	0
31	BD	5409	LMG	4	0
24	BA	5405	CLA	11	0
24	BC	5510	CLA	6	0
28	BE	5102	DGD	1	0
25	AA	408	MST	9	0
25	BA	5409	MST	9	0
24	AB	612	CLA	12	0
31	AD	407	LMG	4	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 than 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.

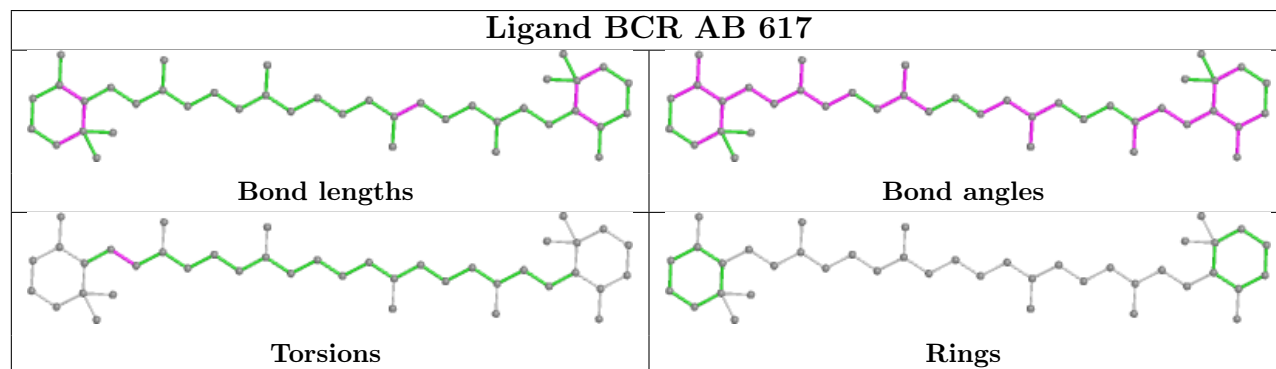
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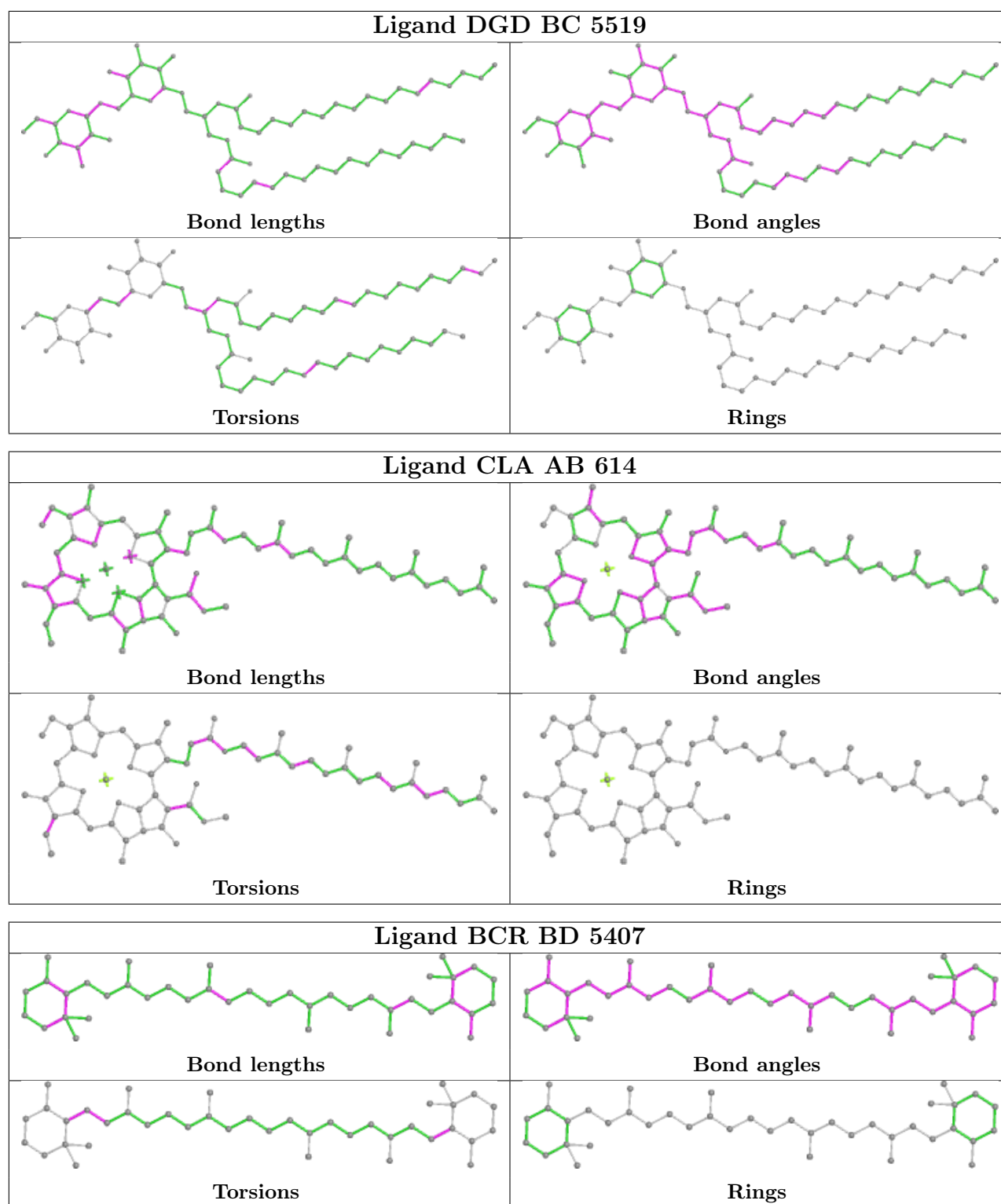


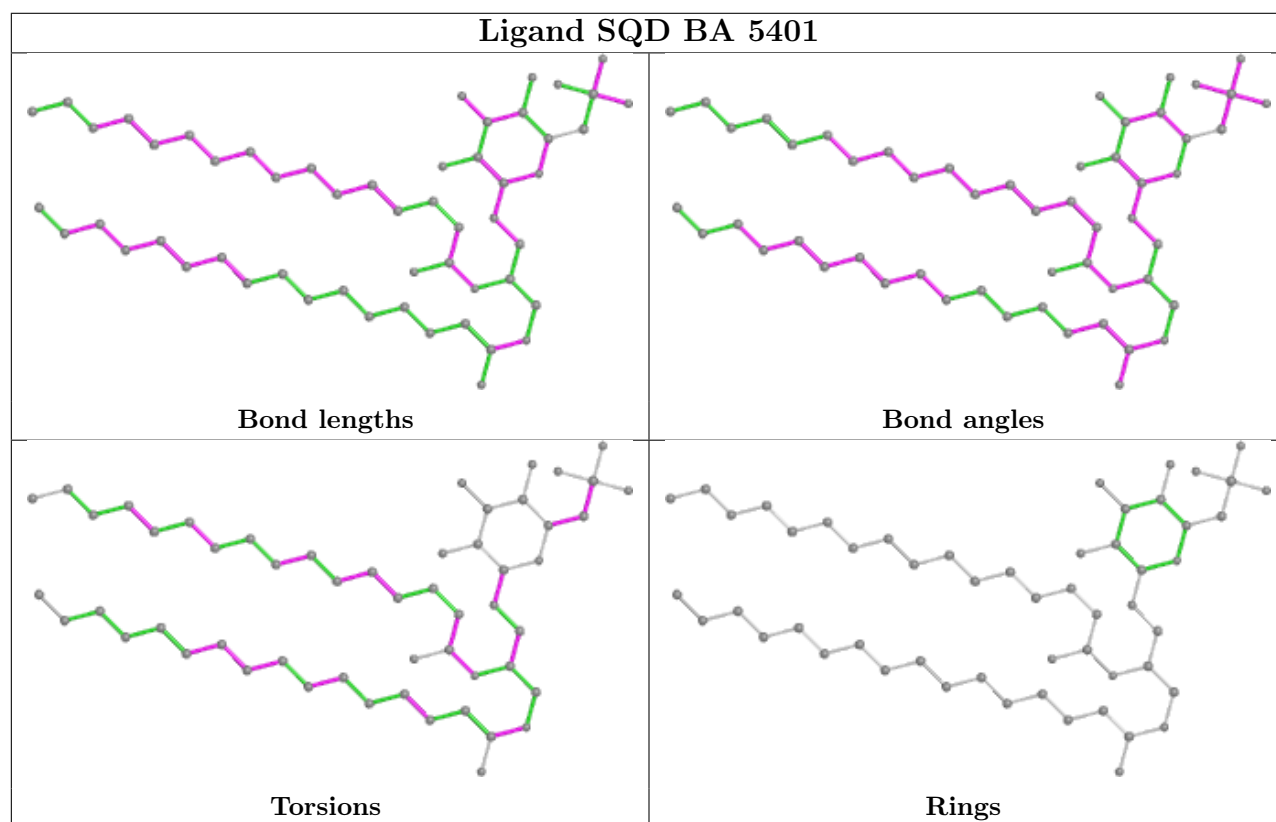
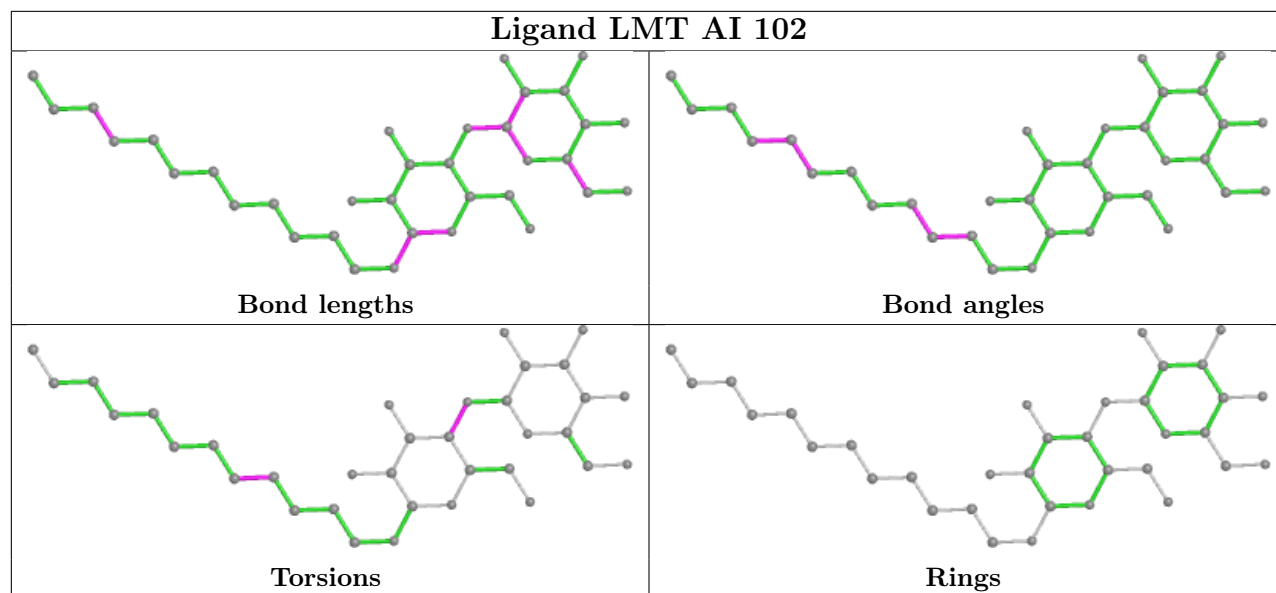
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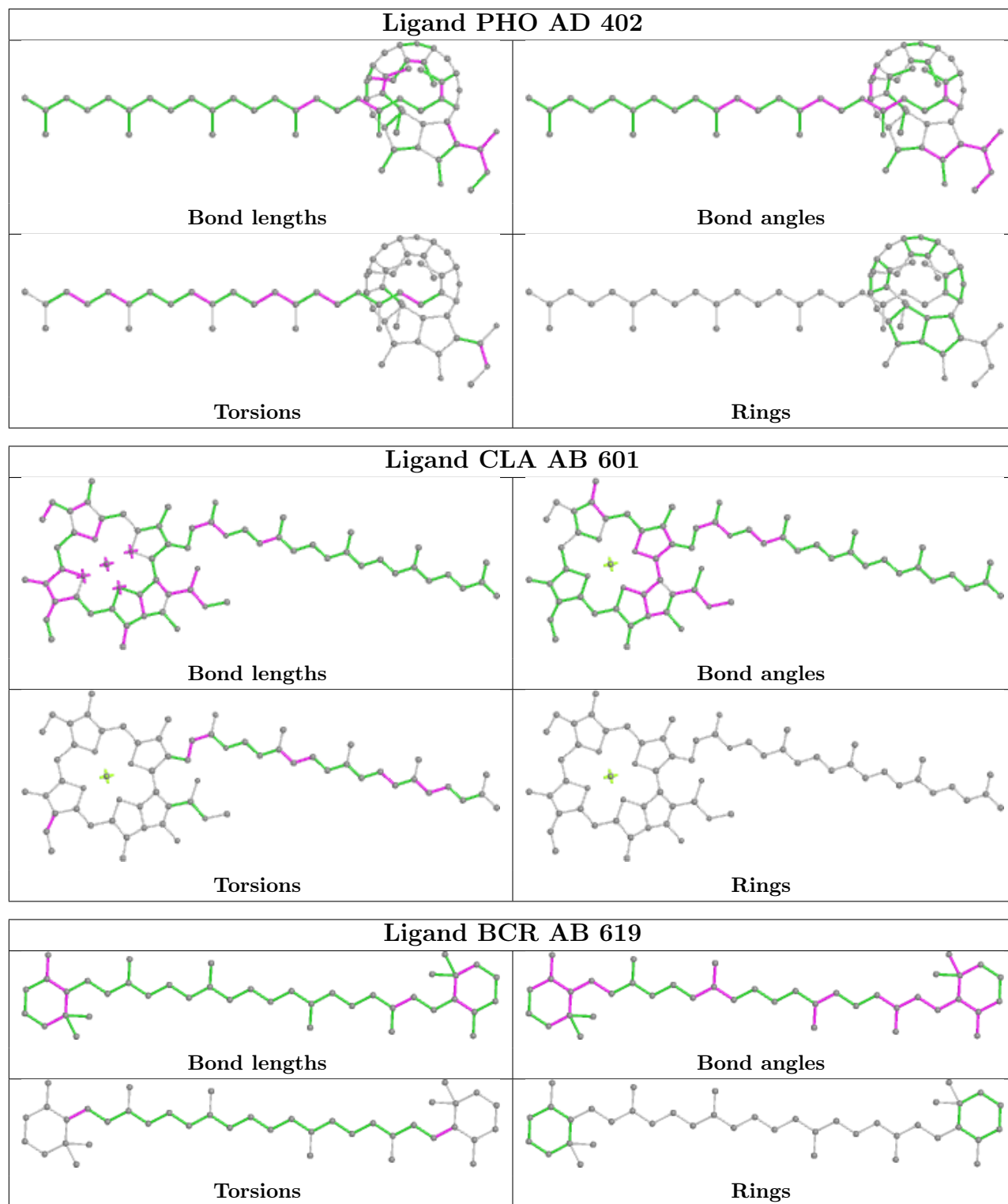


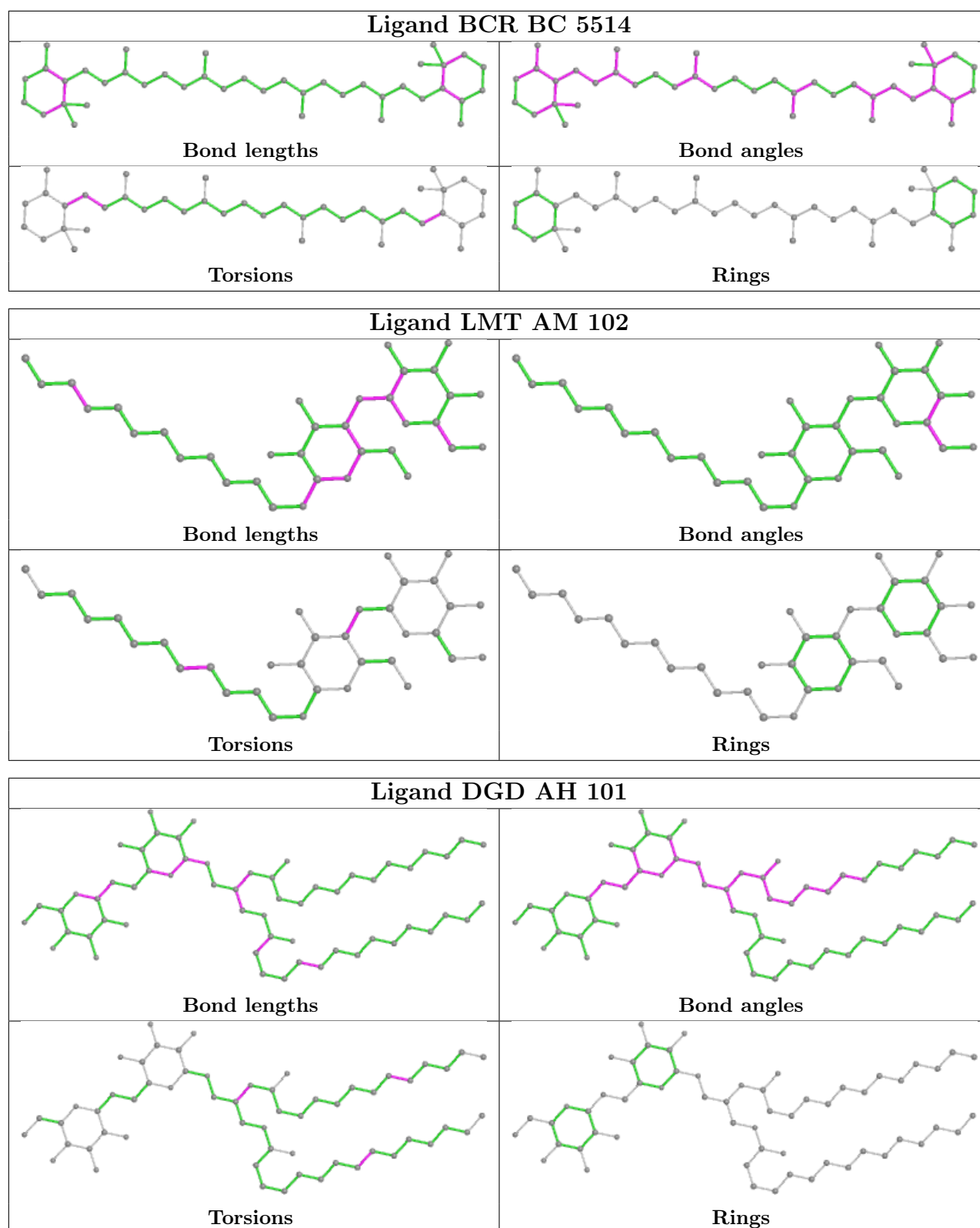
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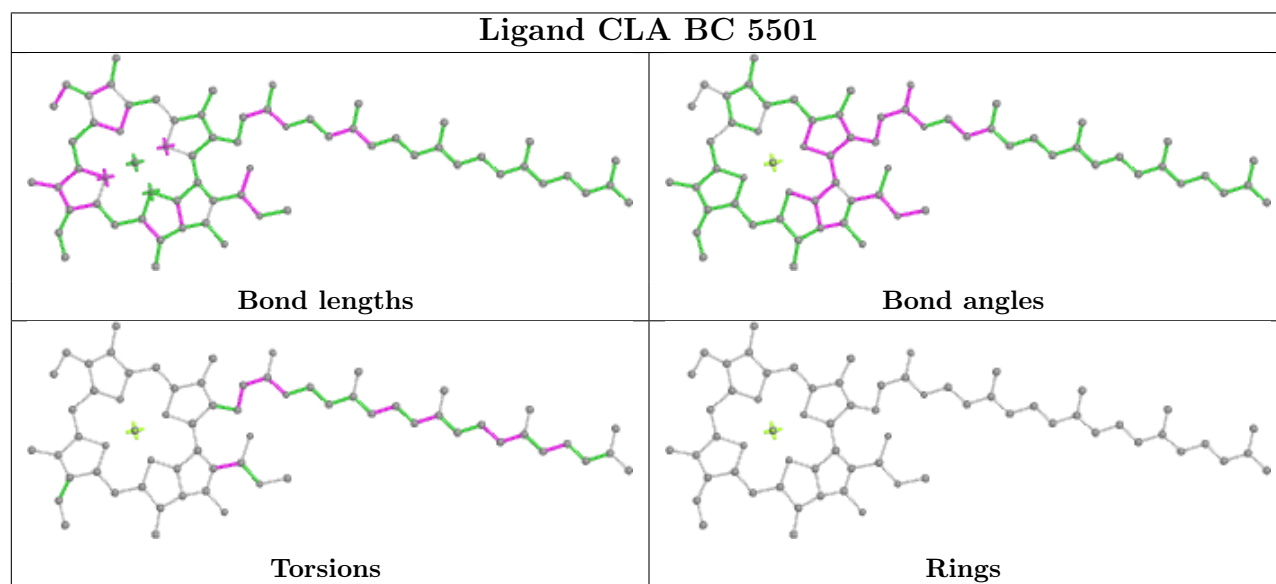
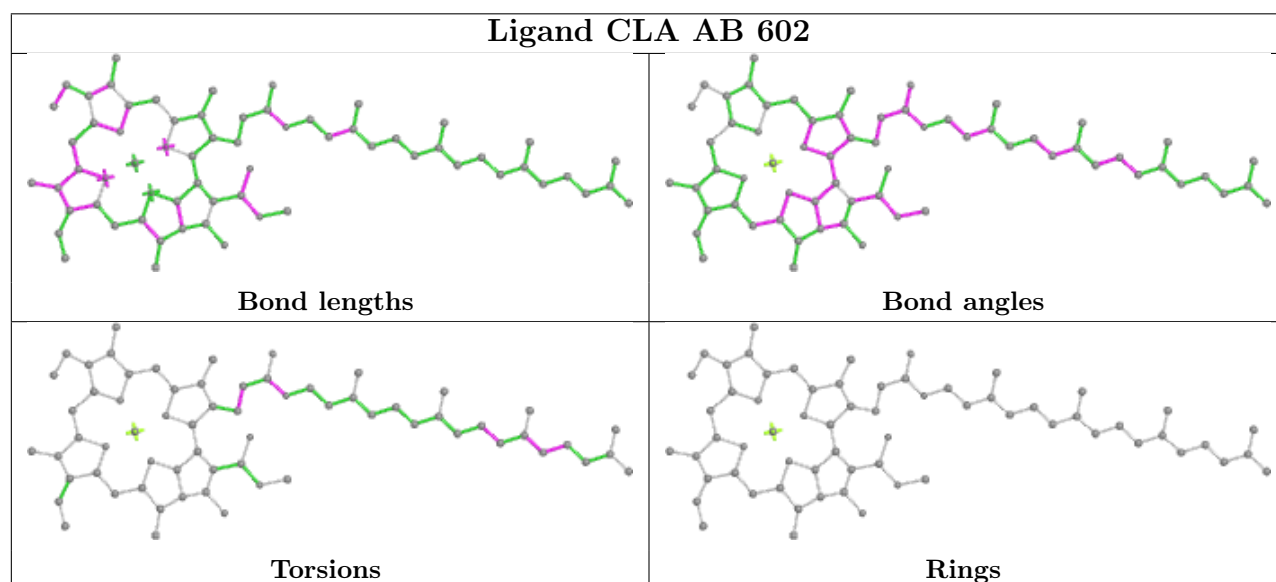
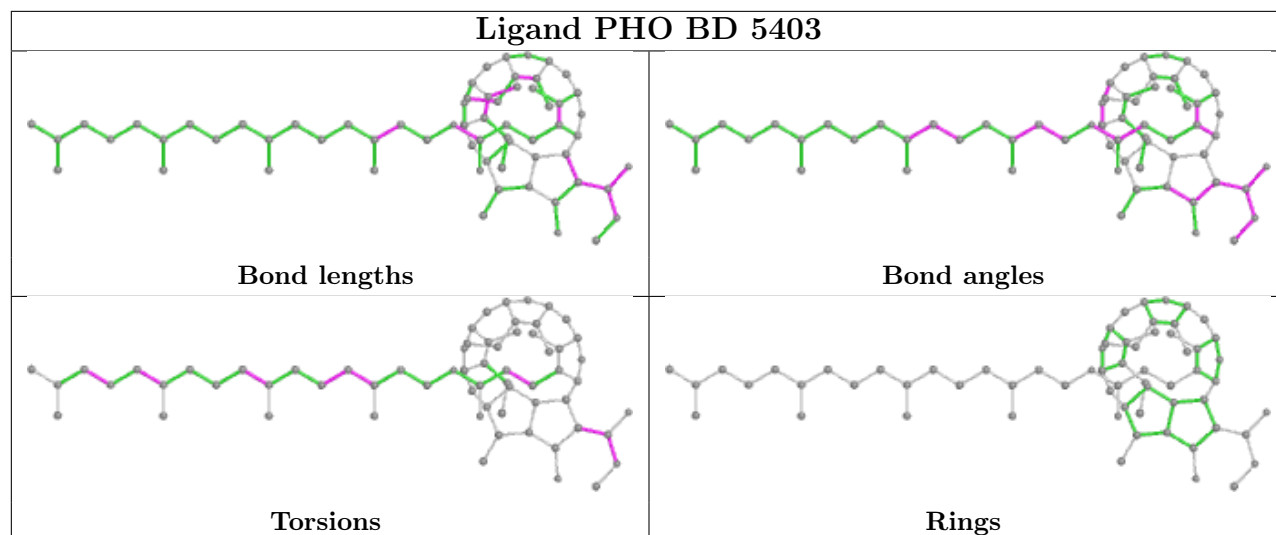


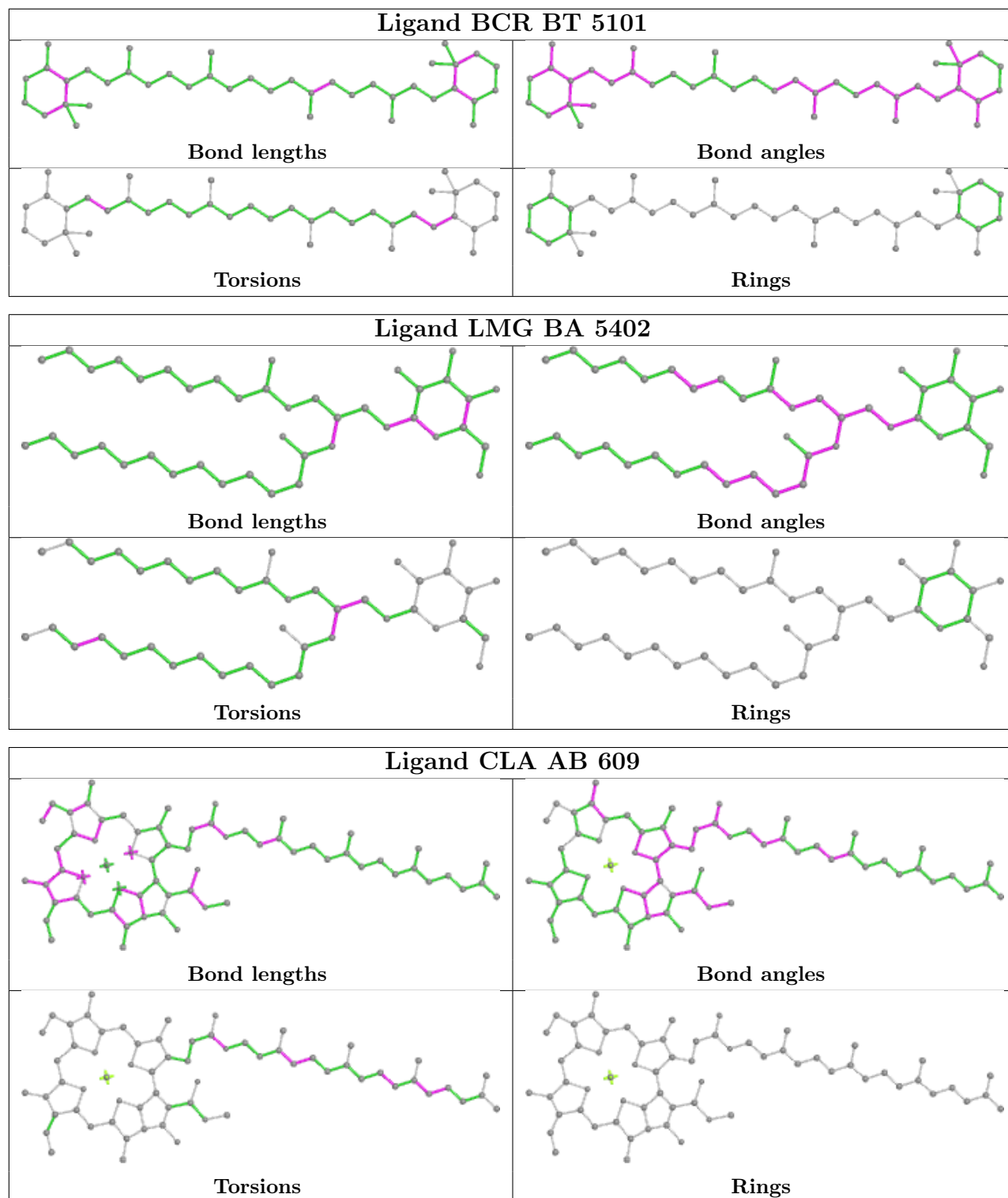


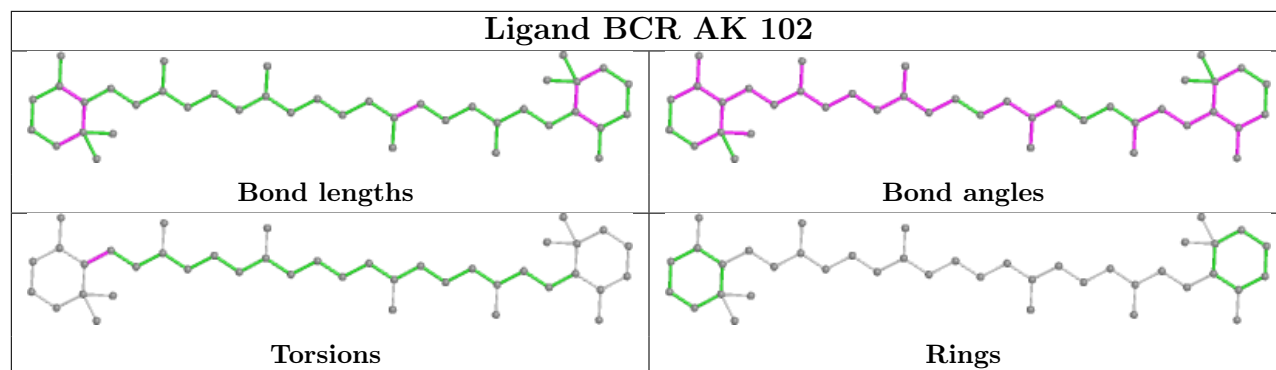
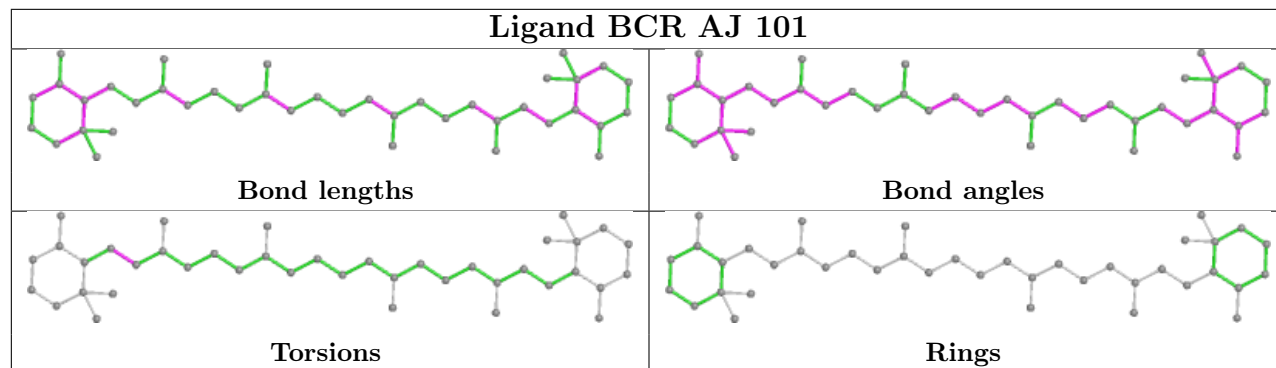
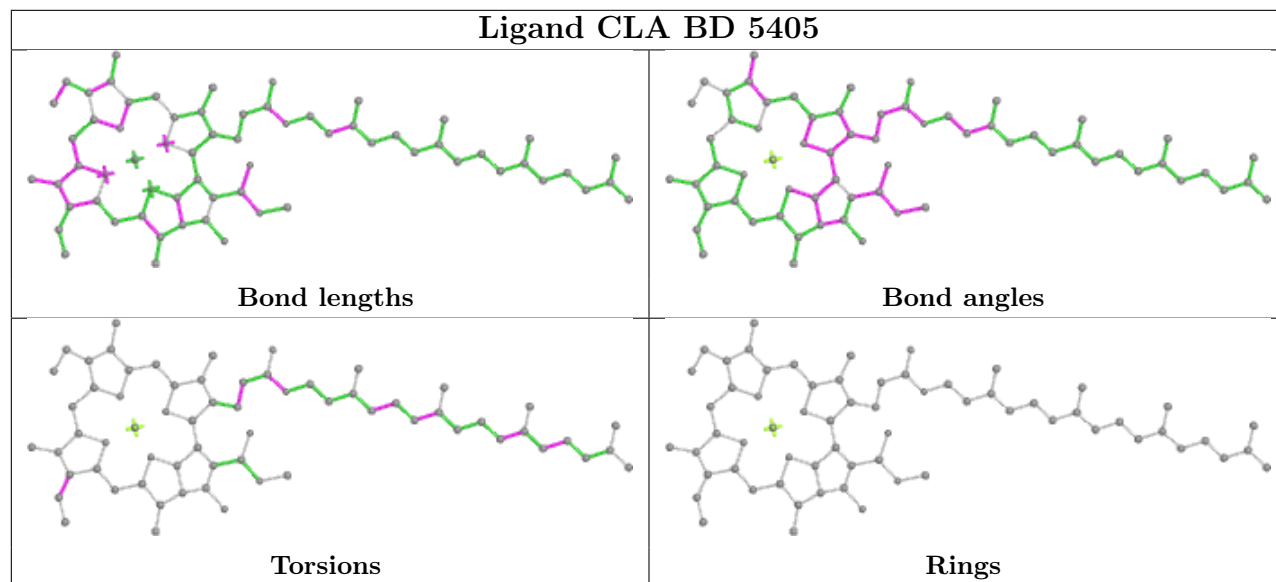


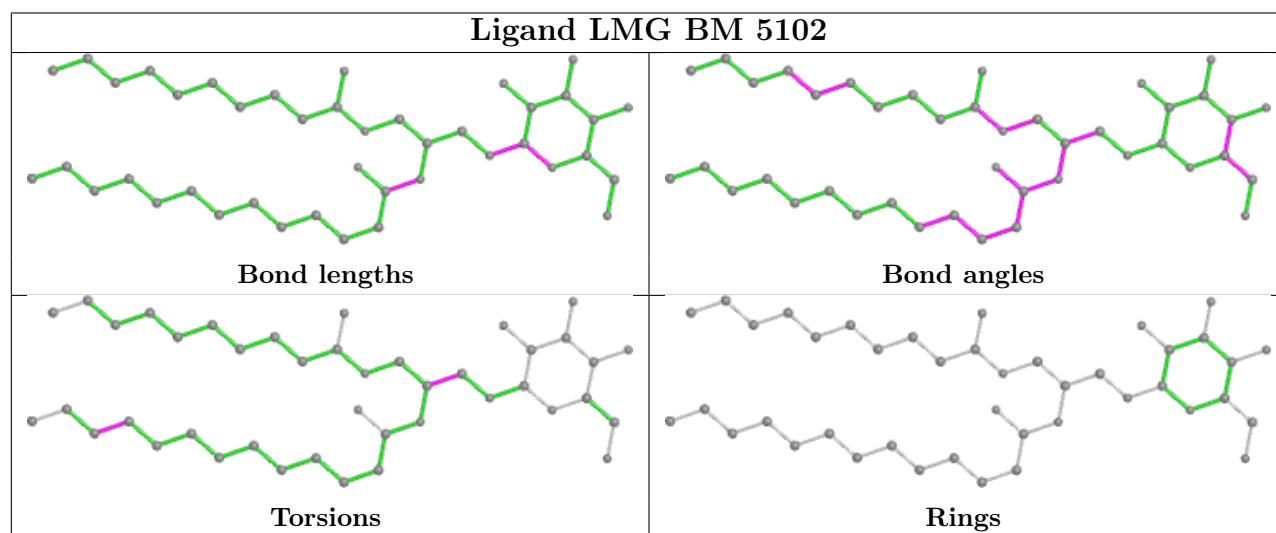
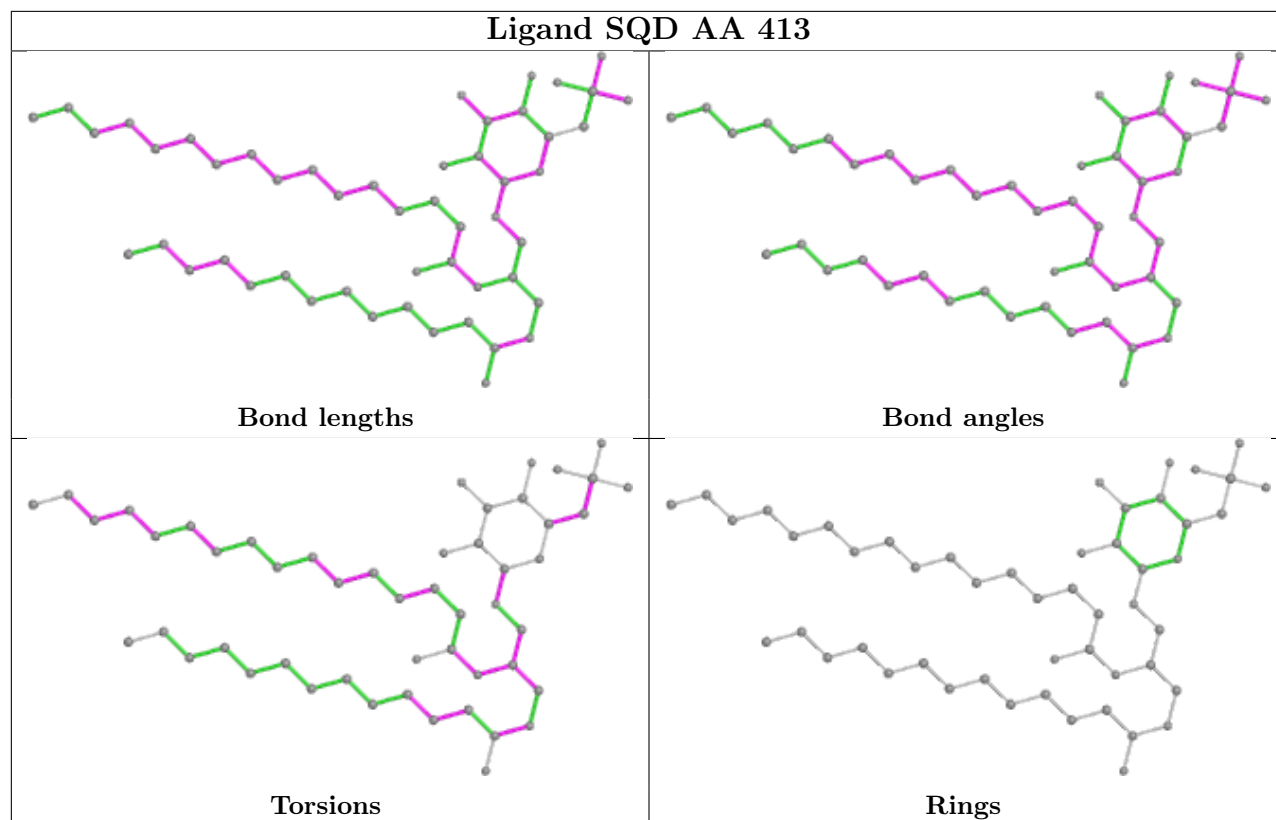




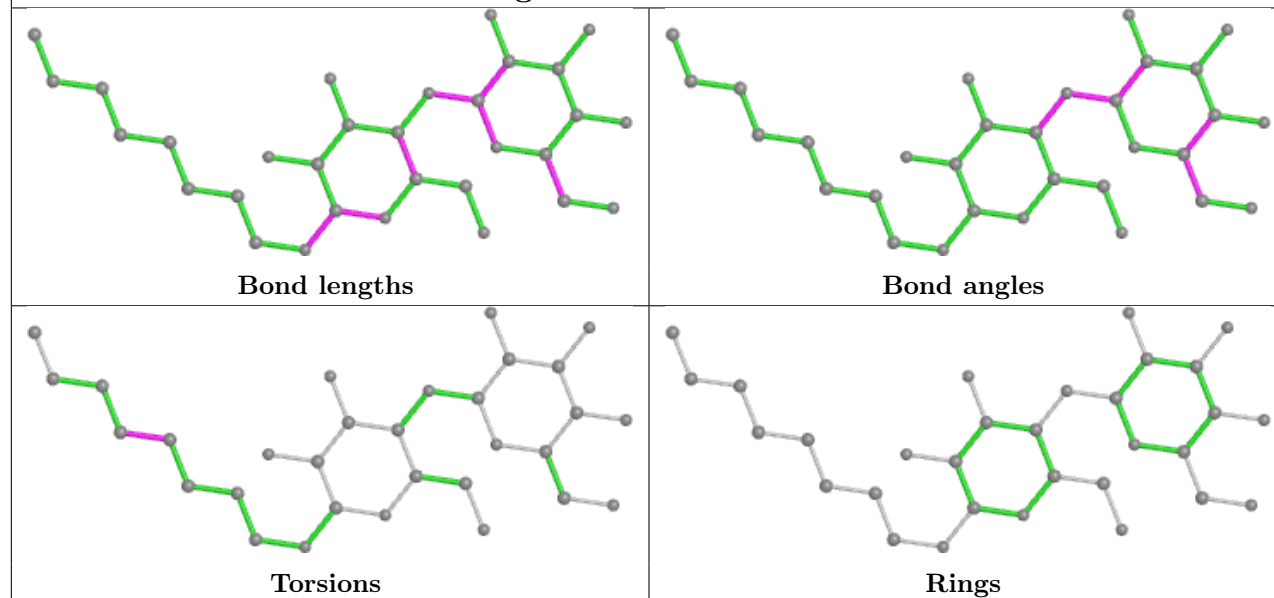




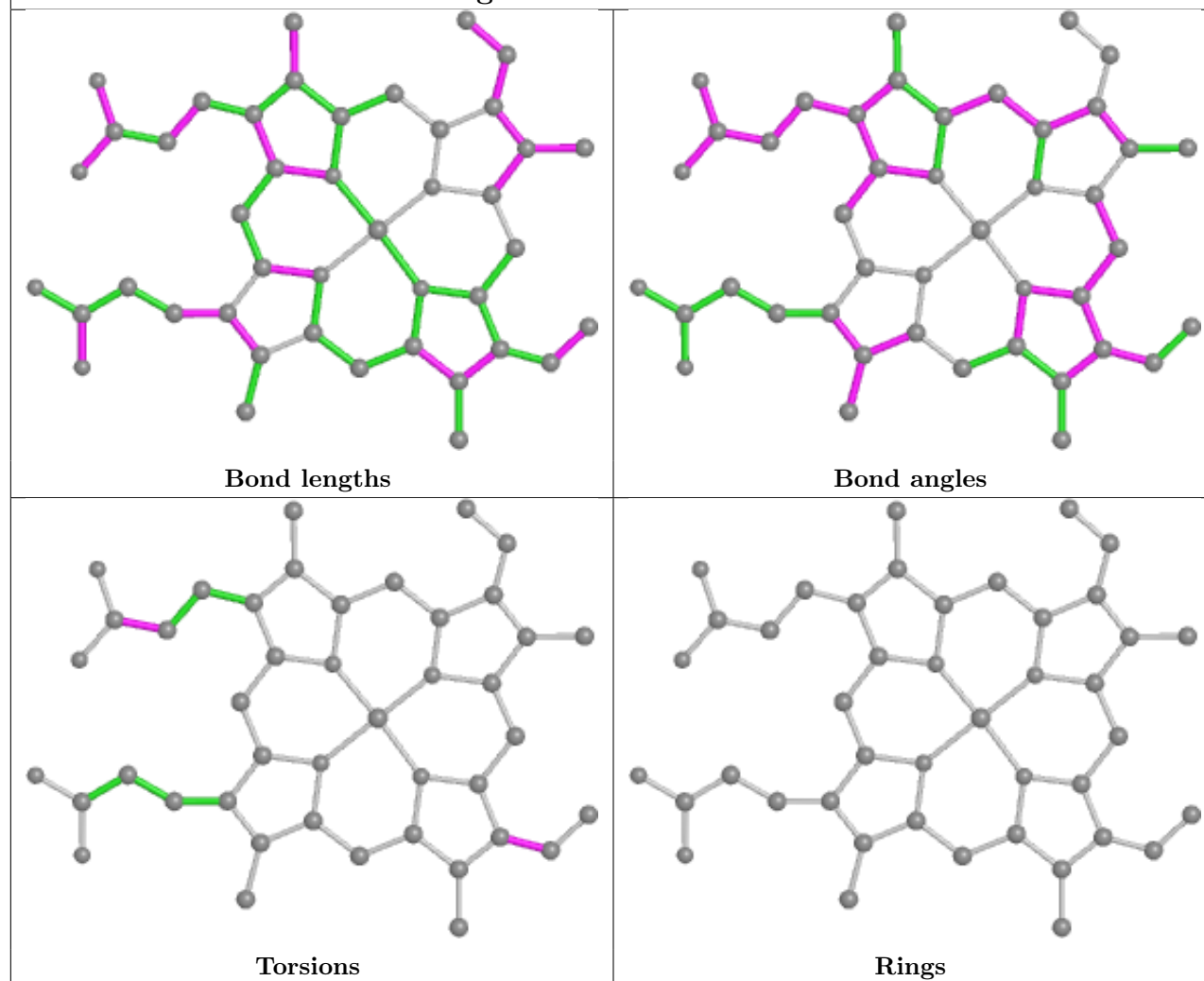
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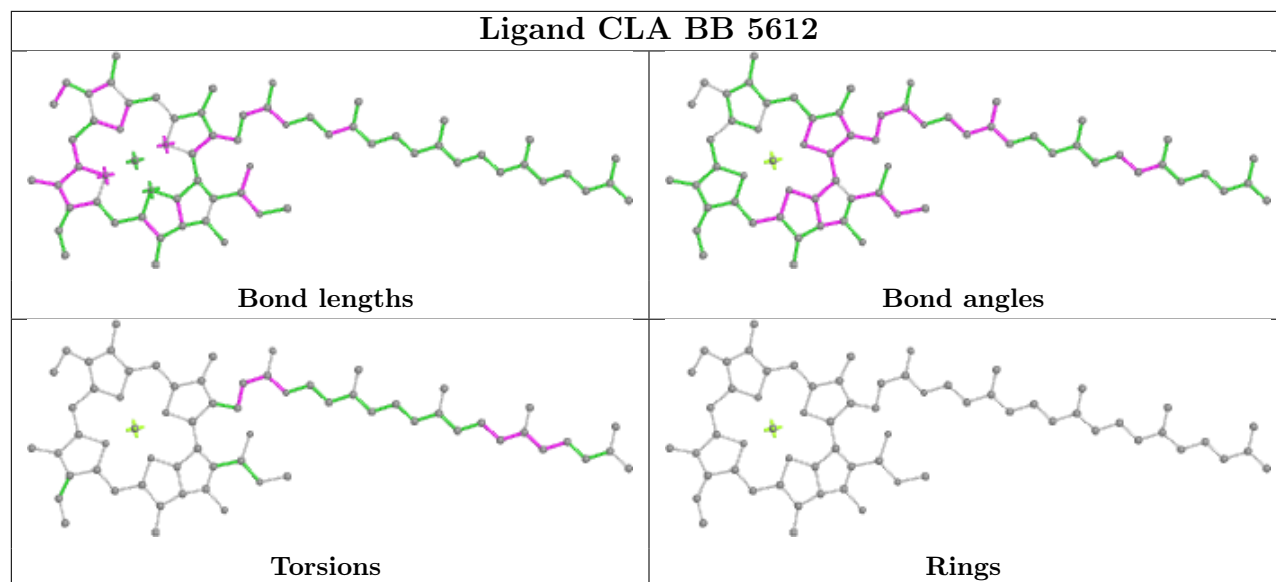
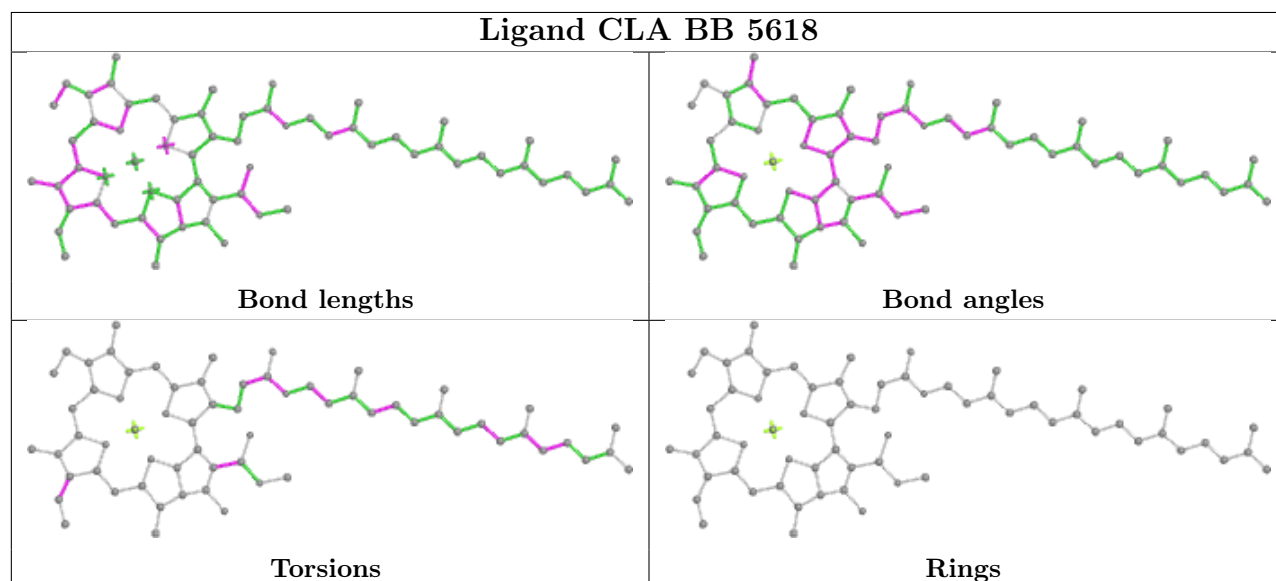
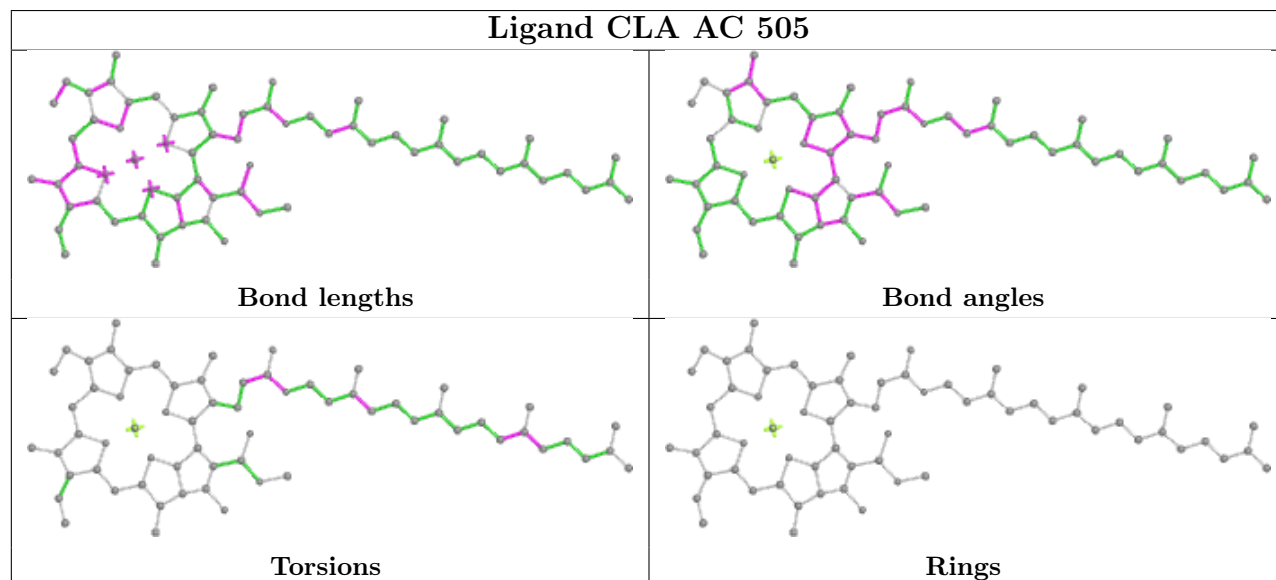


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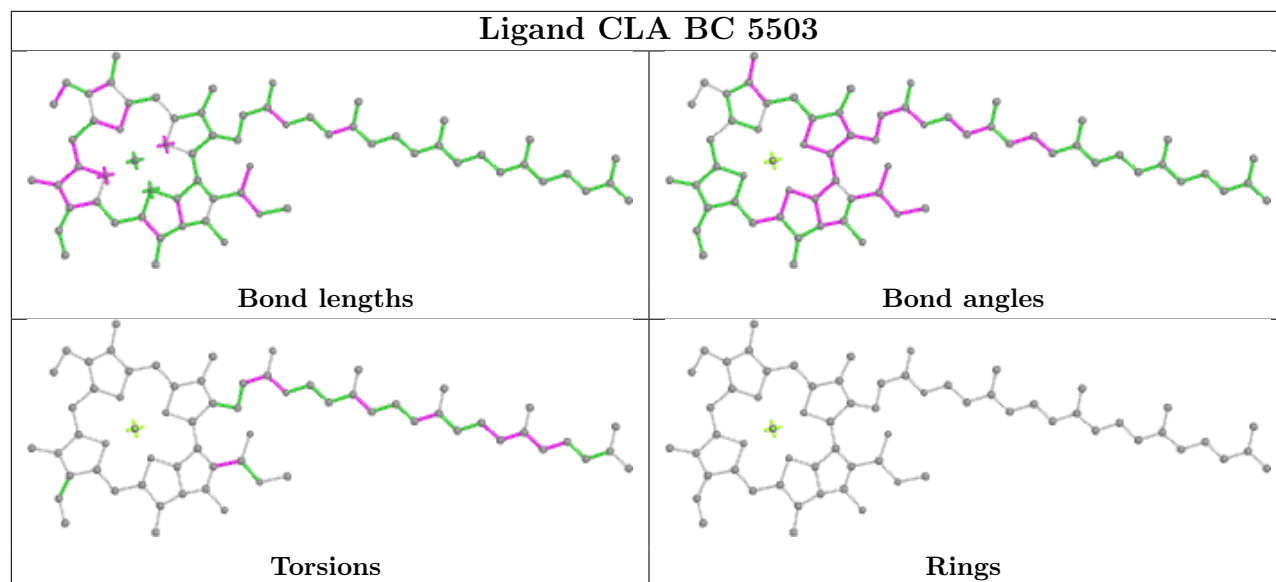


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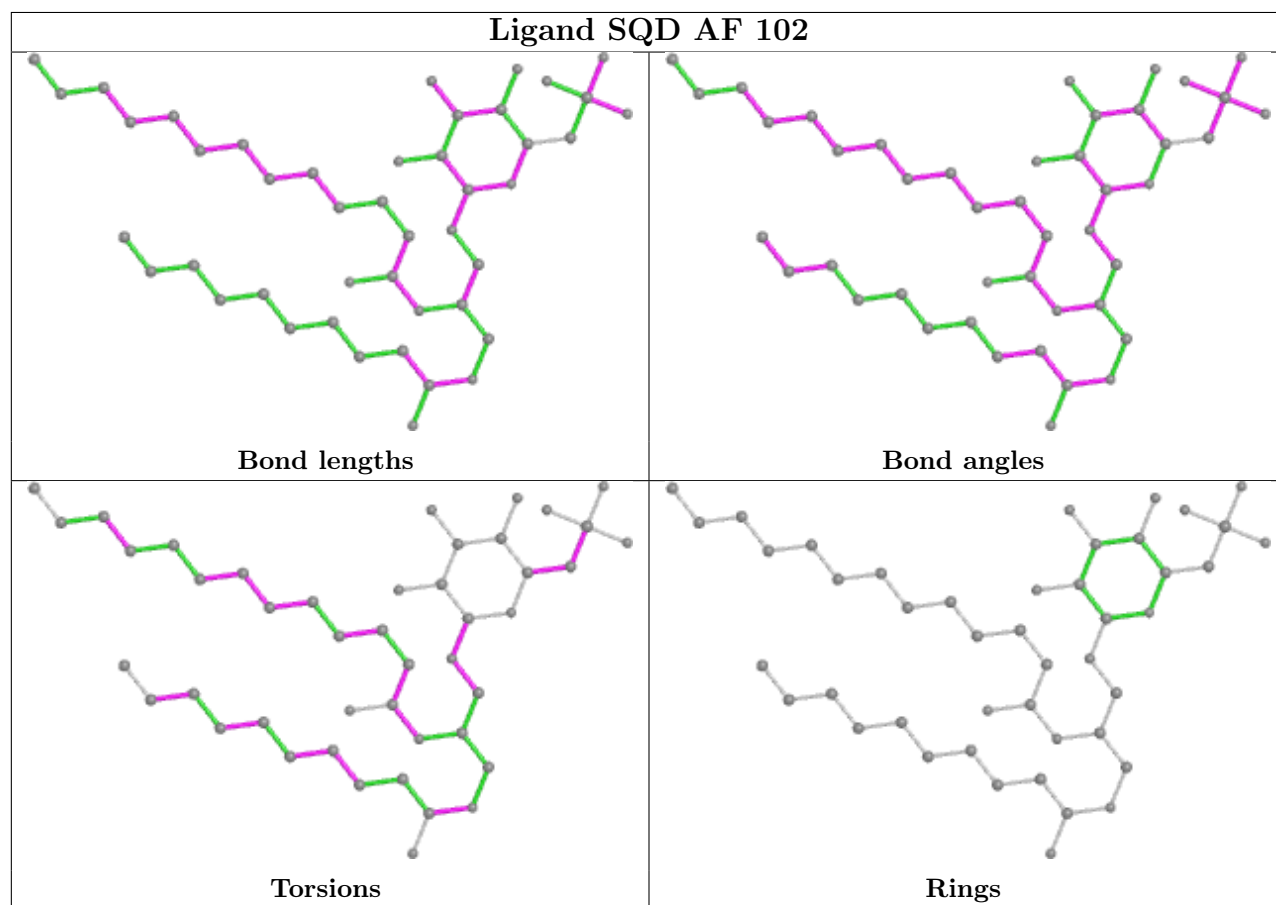


Ligand CLA BB 5612**Ligand CLA BB 5618****Ligand CLA AC 505**

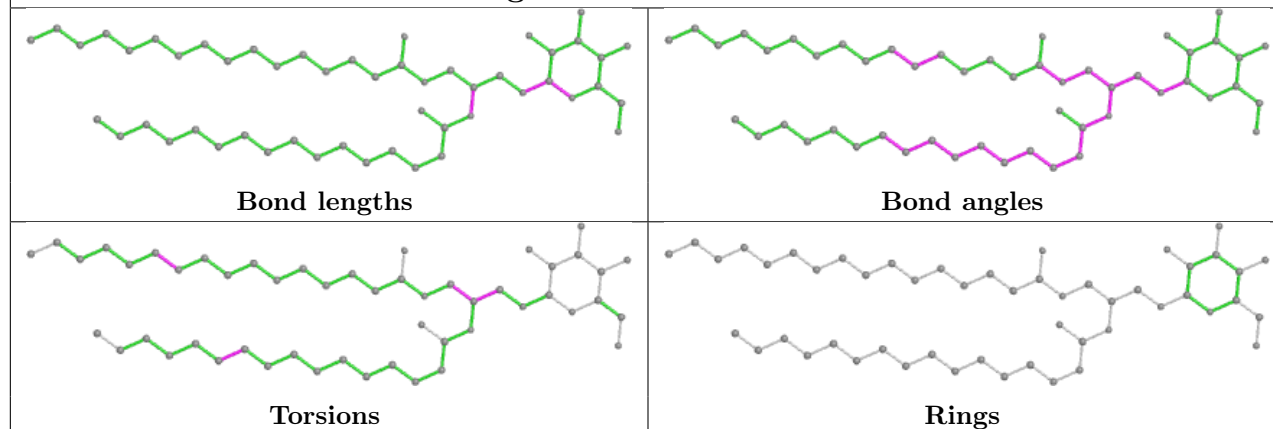
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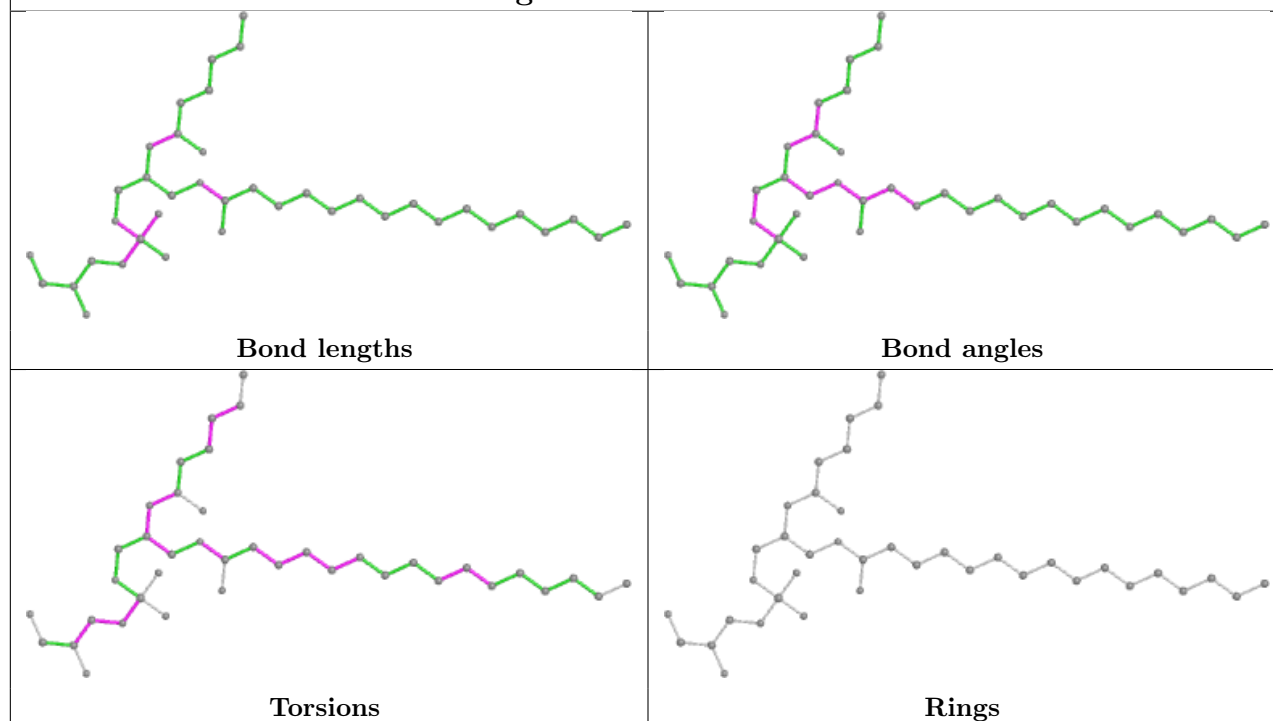
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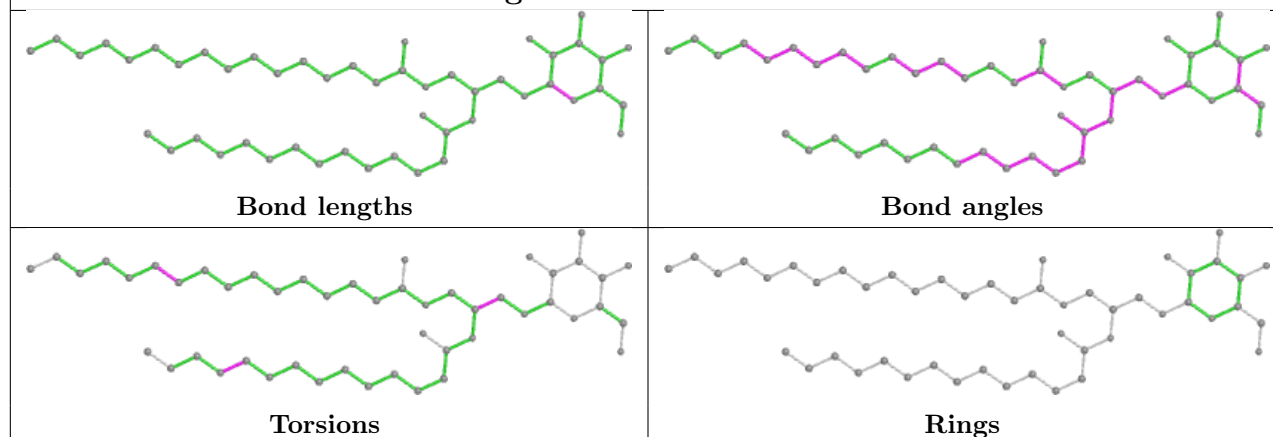
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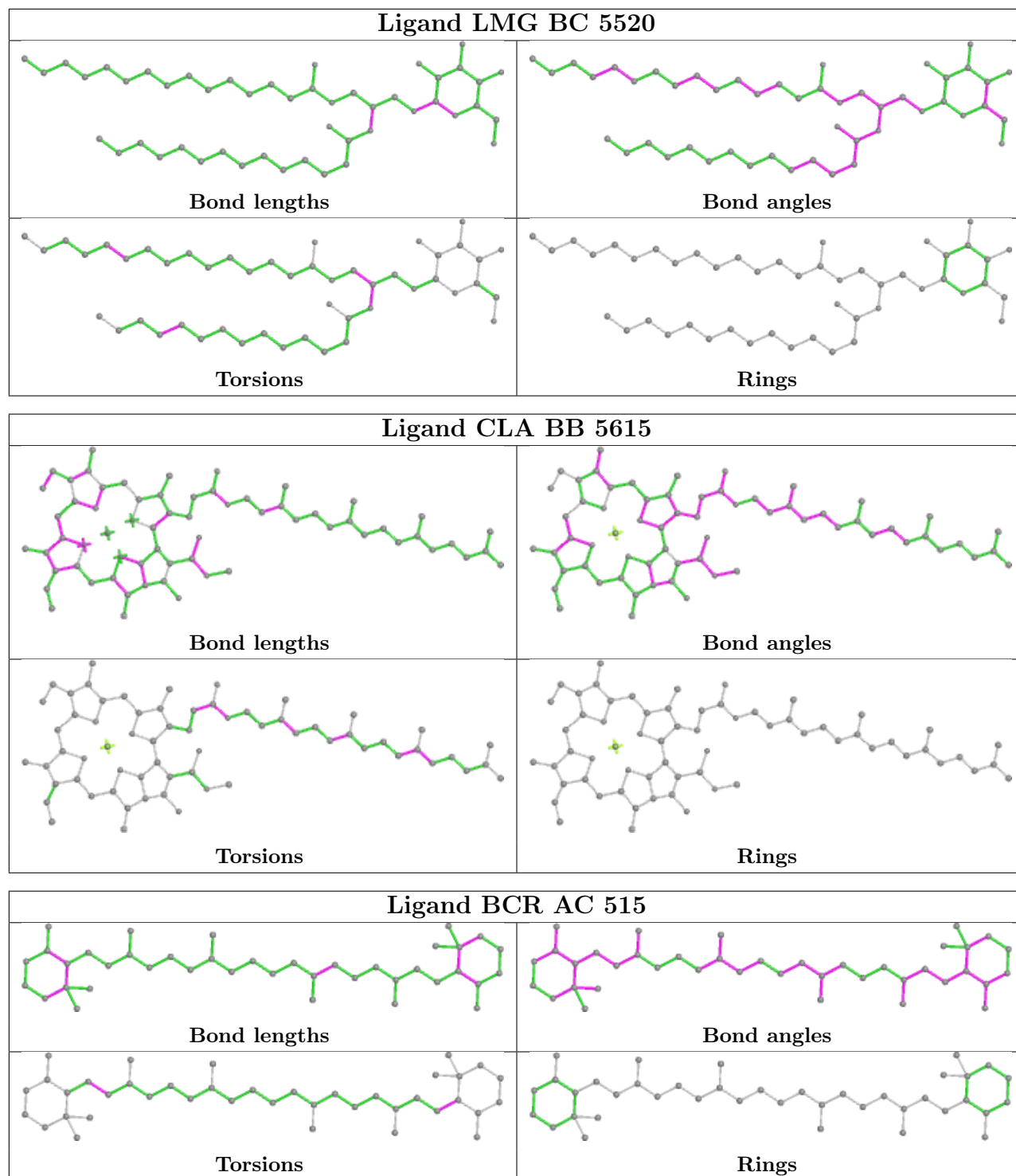


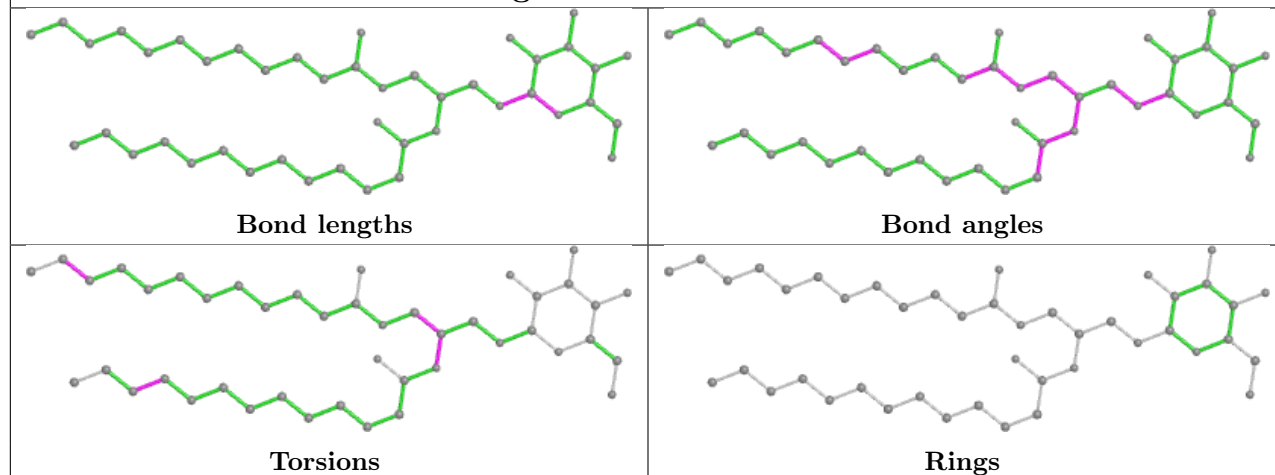
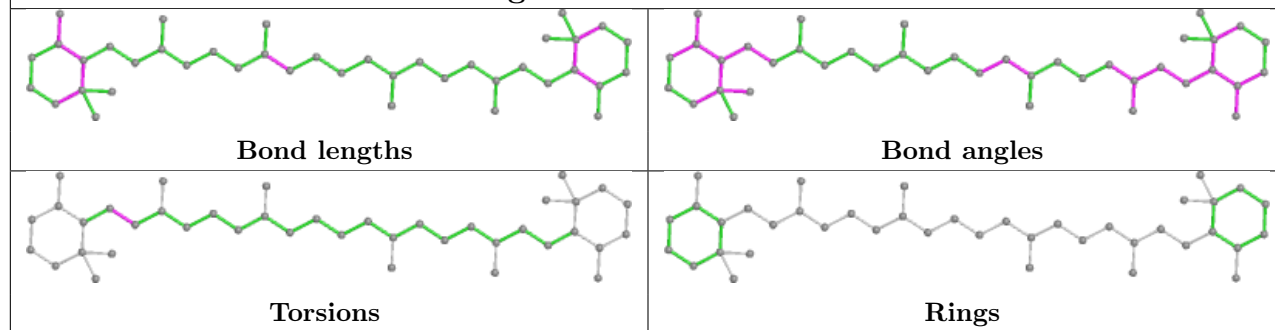
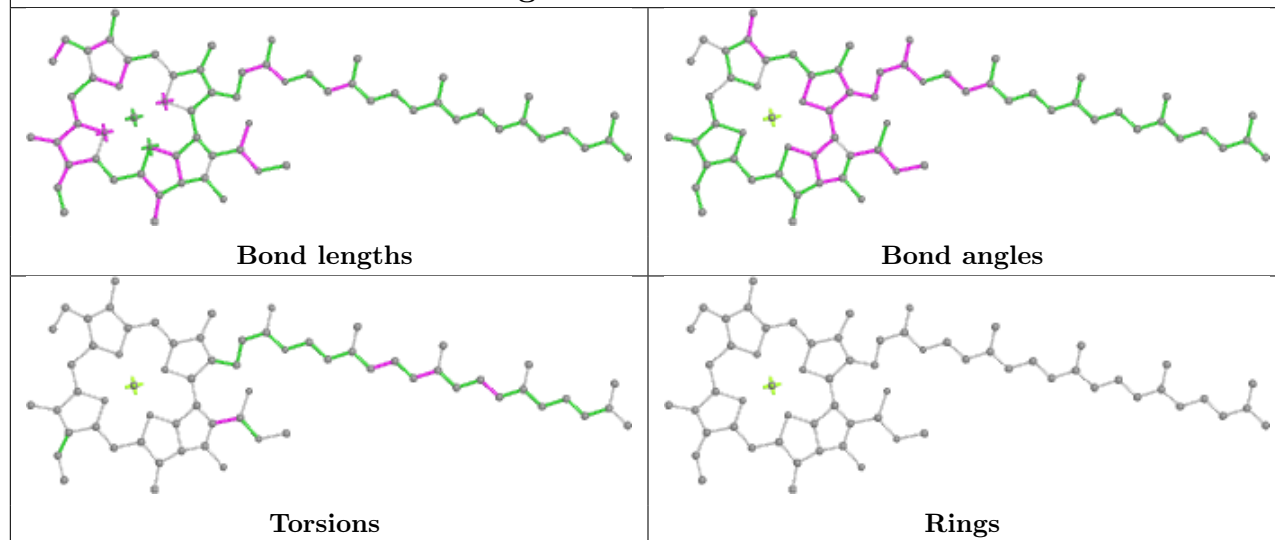
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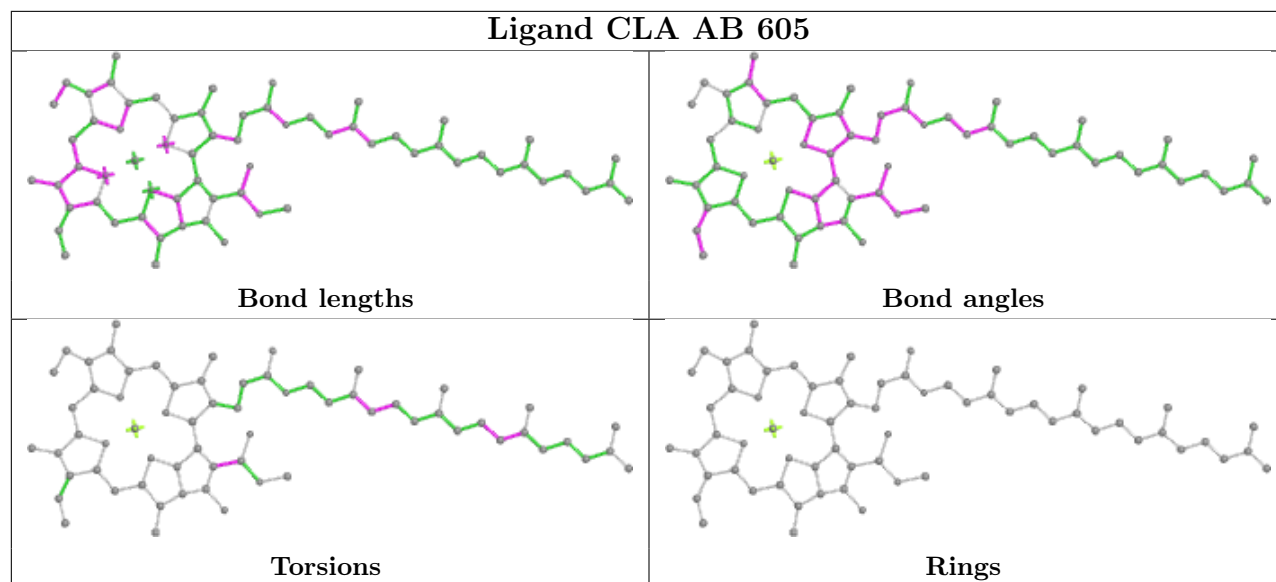
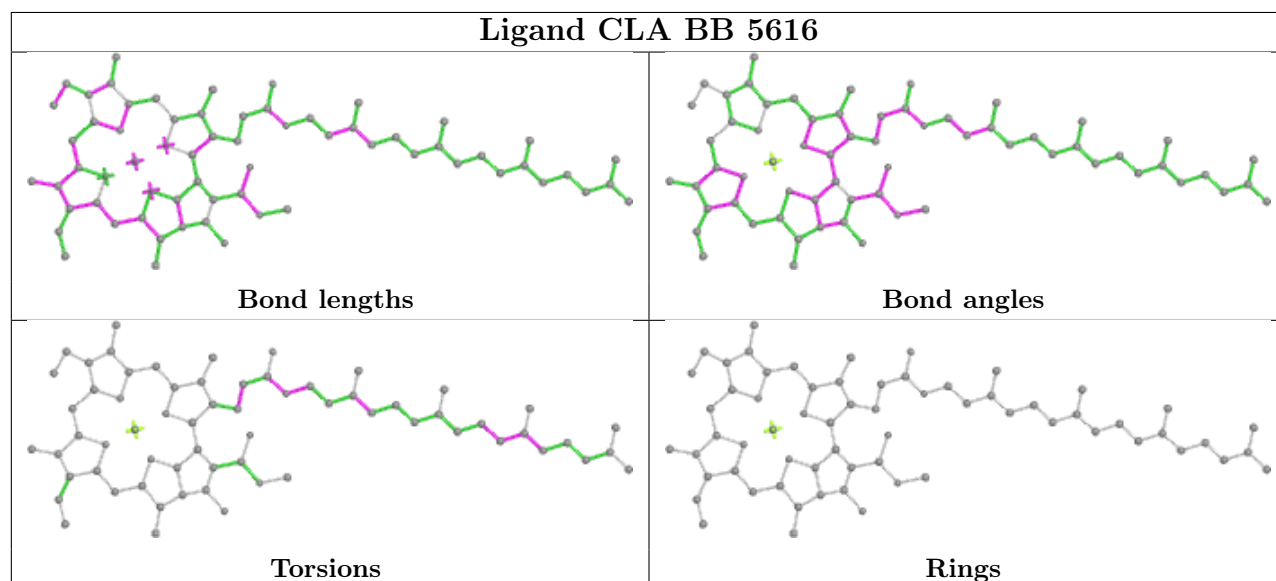
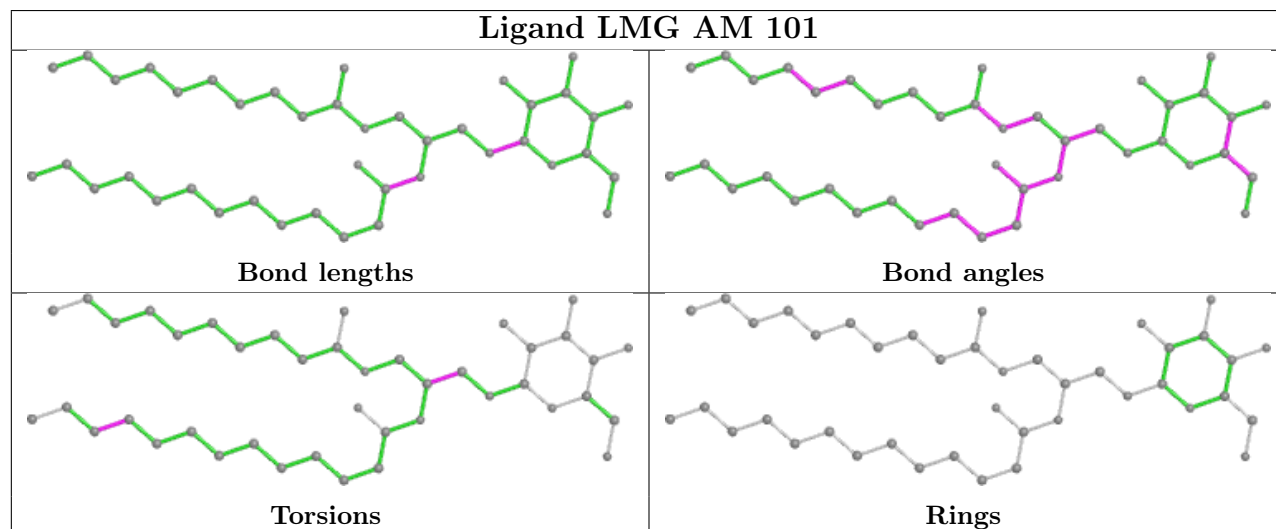


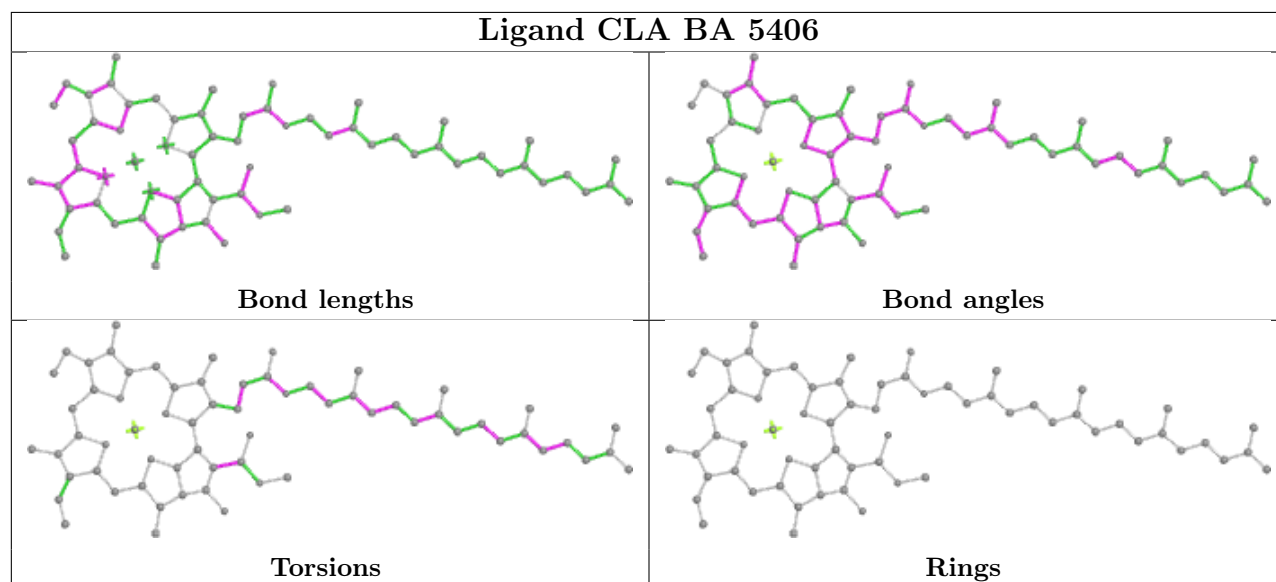
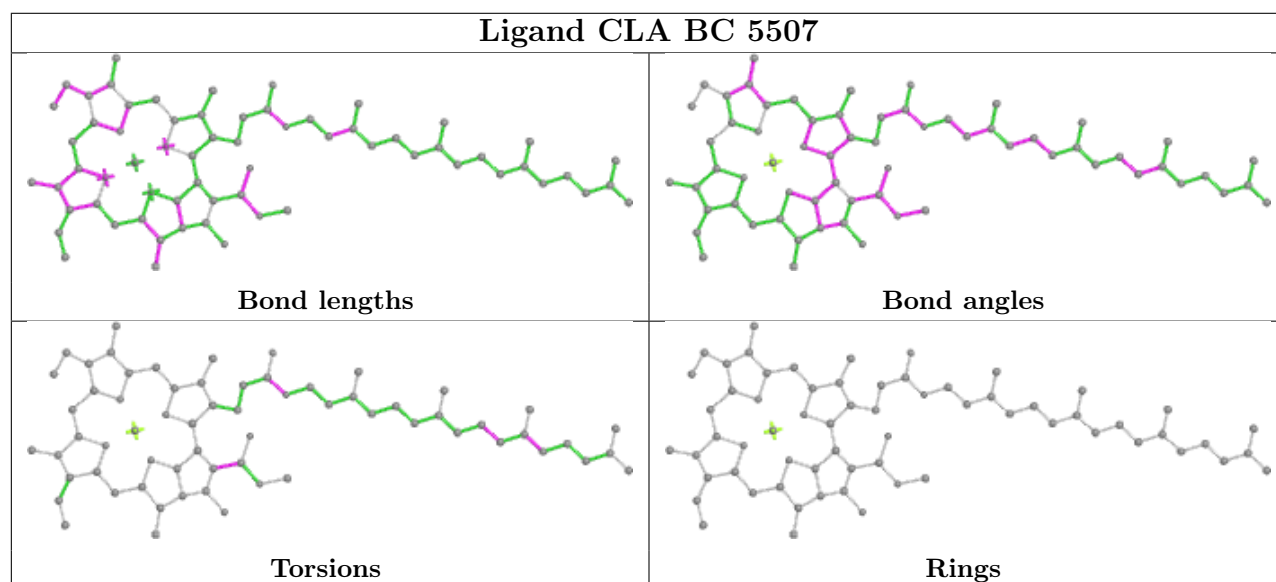
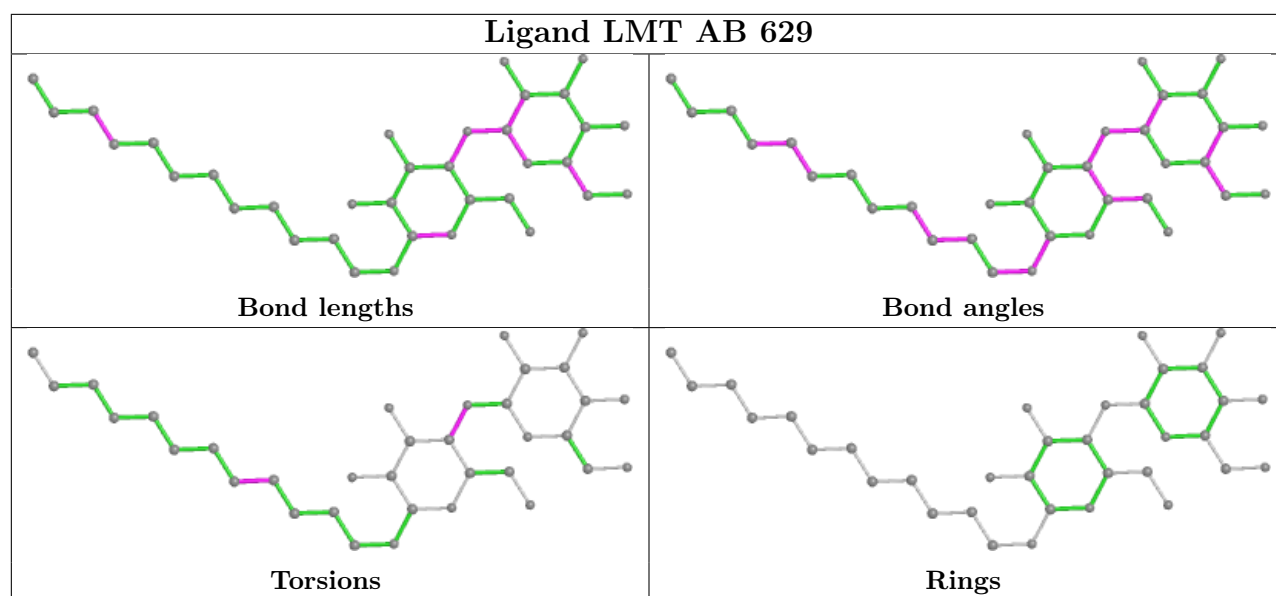
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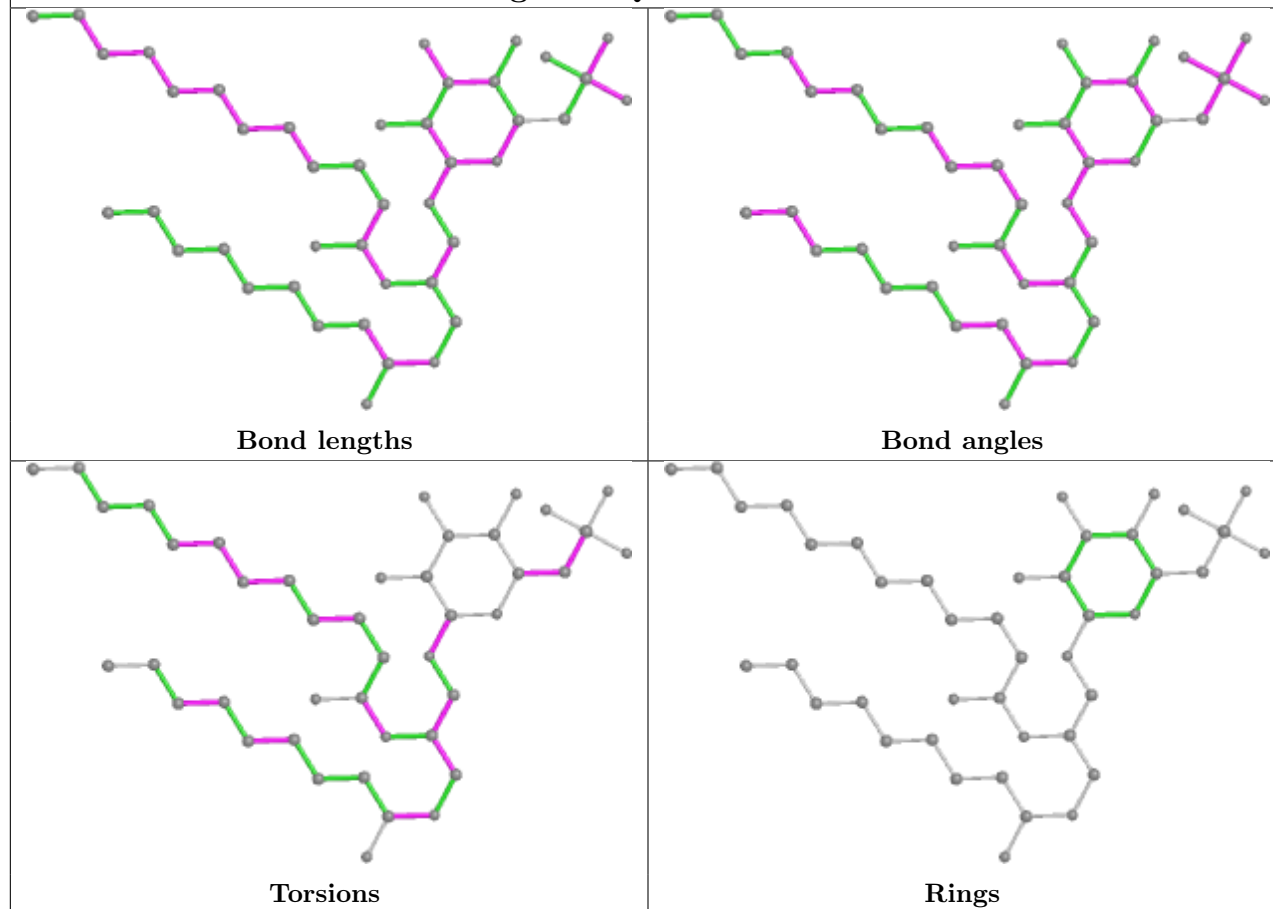


Ligand LMG AA 414**Ligand BCR BB 5622****Ligand CLA AC 506**

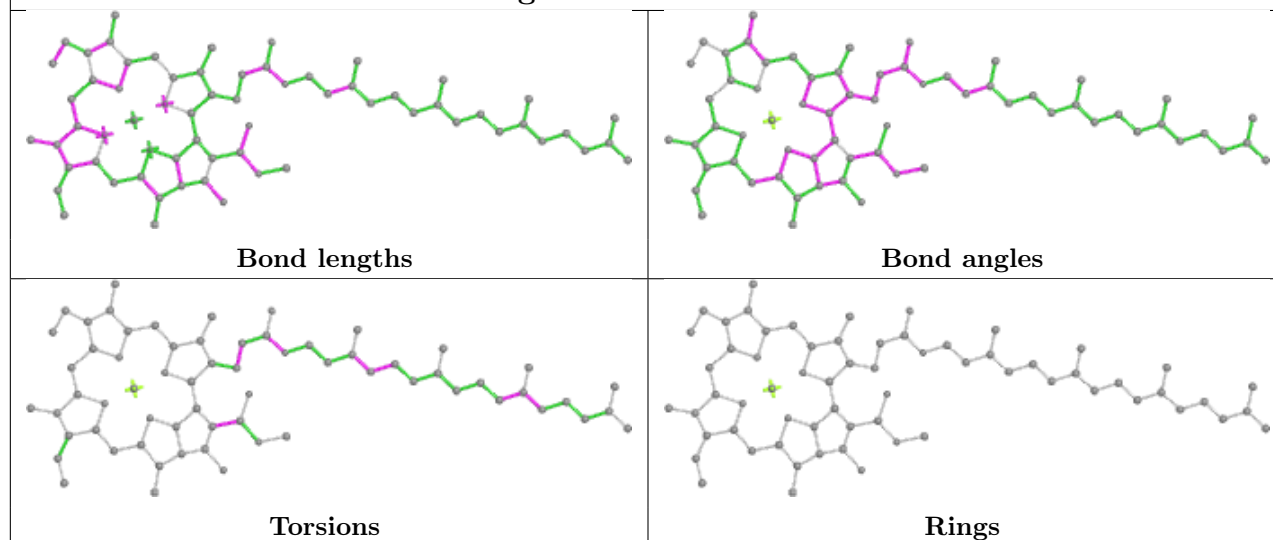
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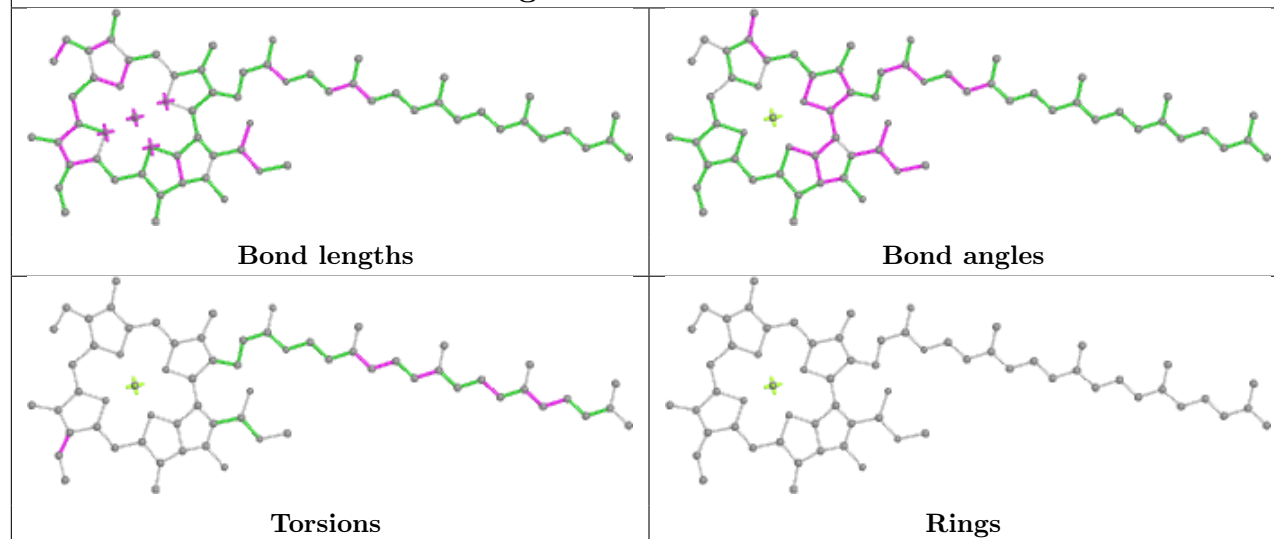
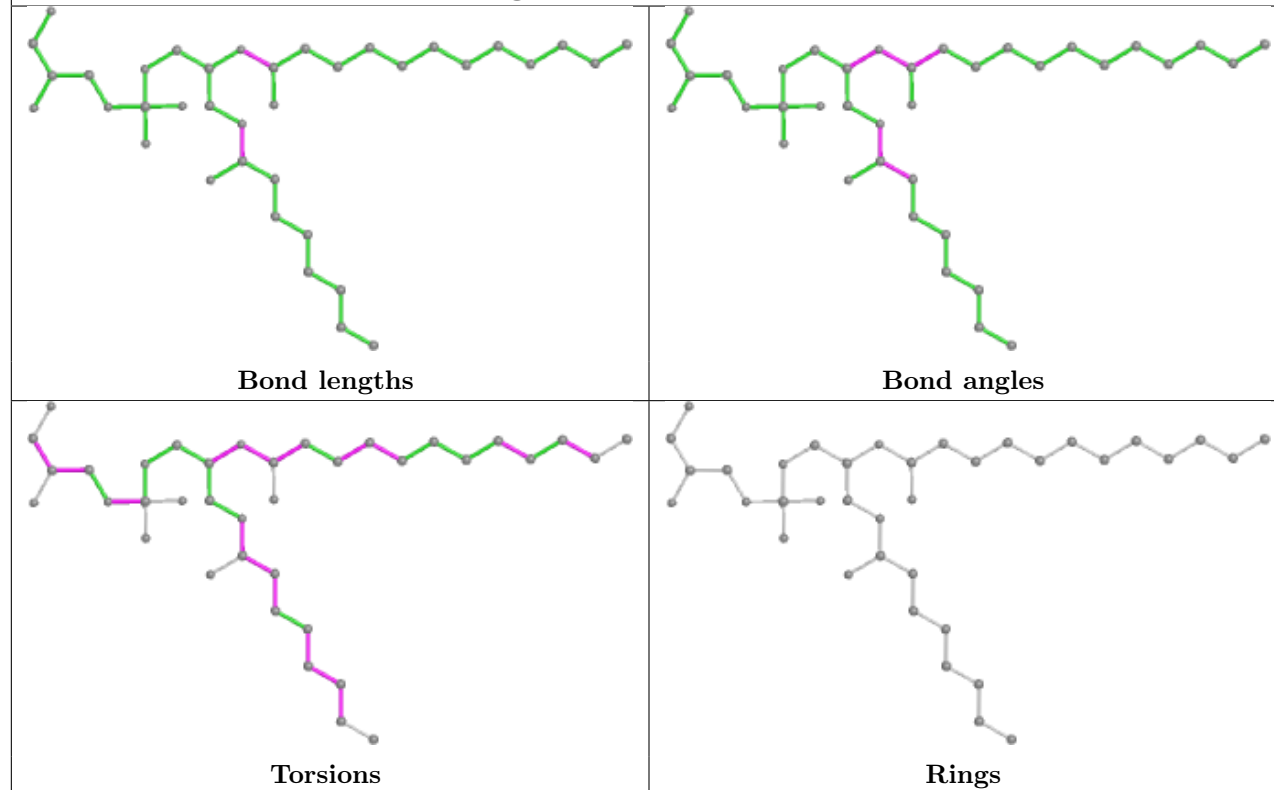


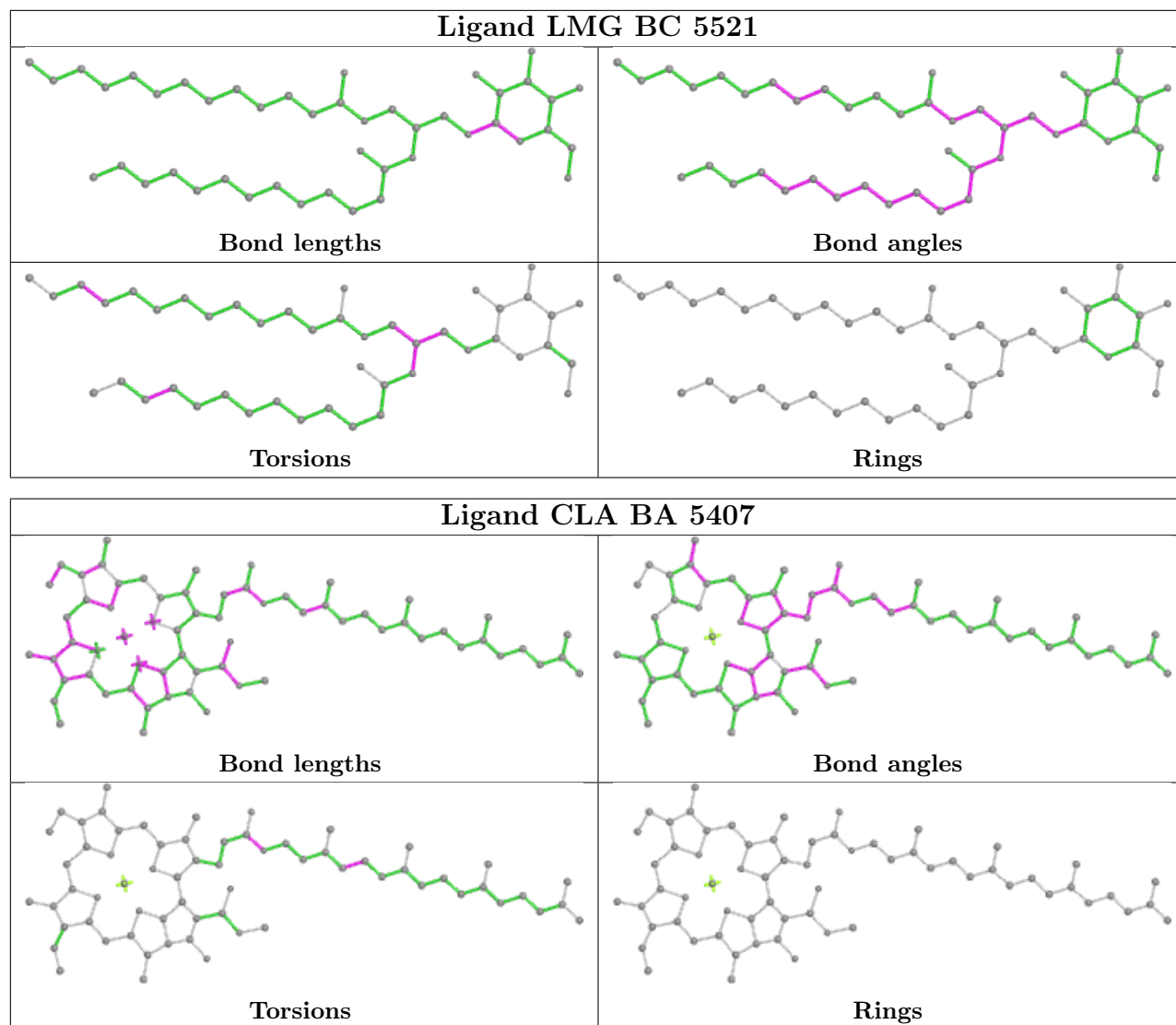
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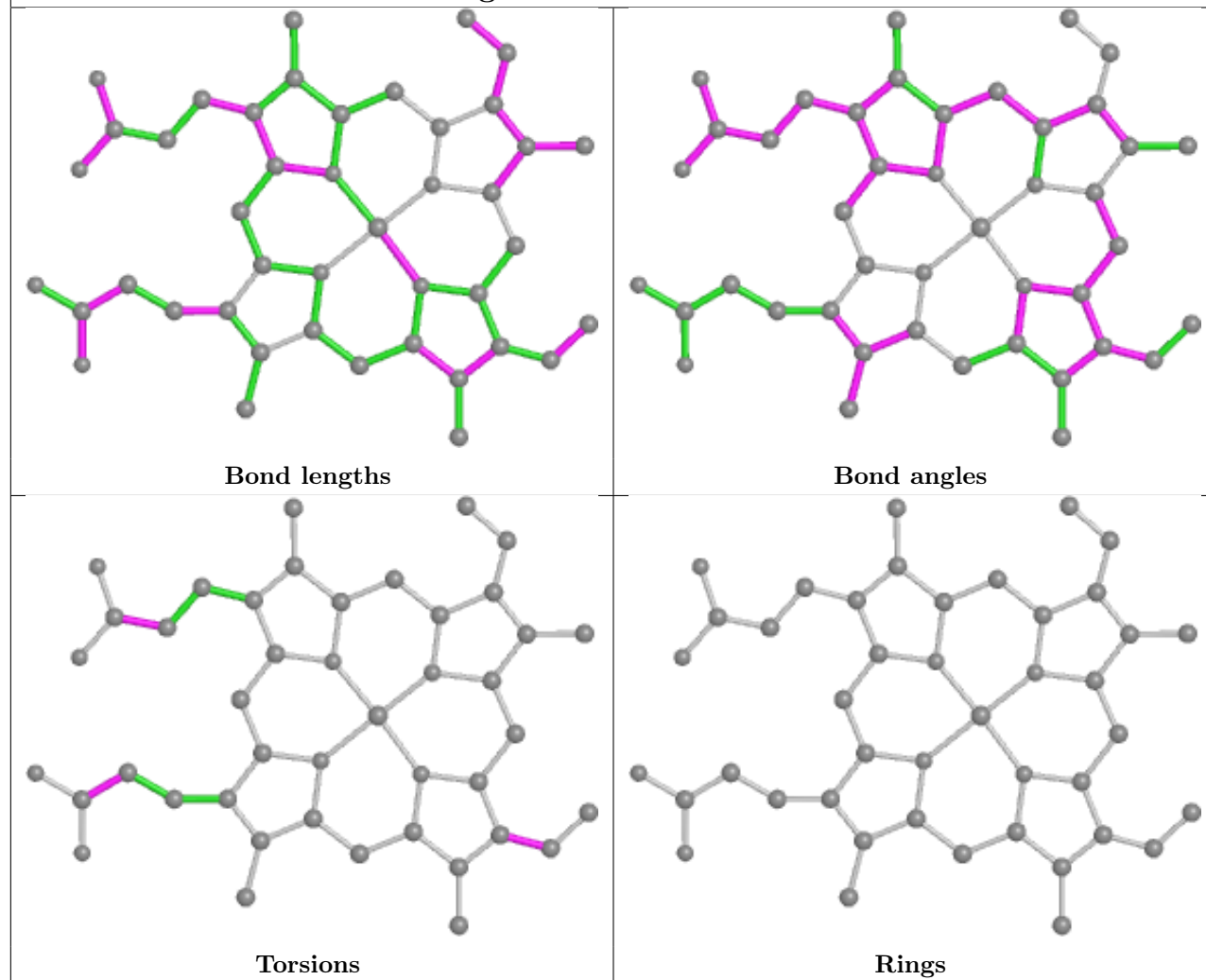
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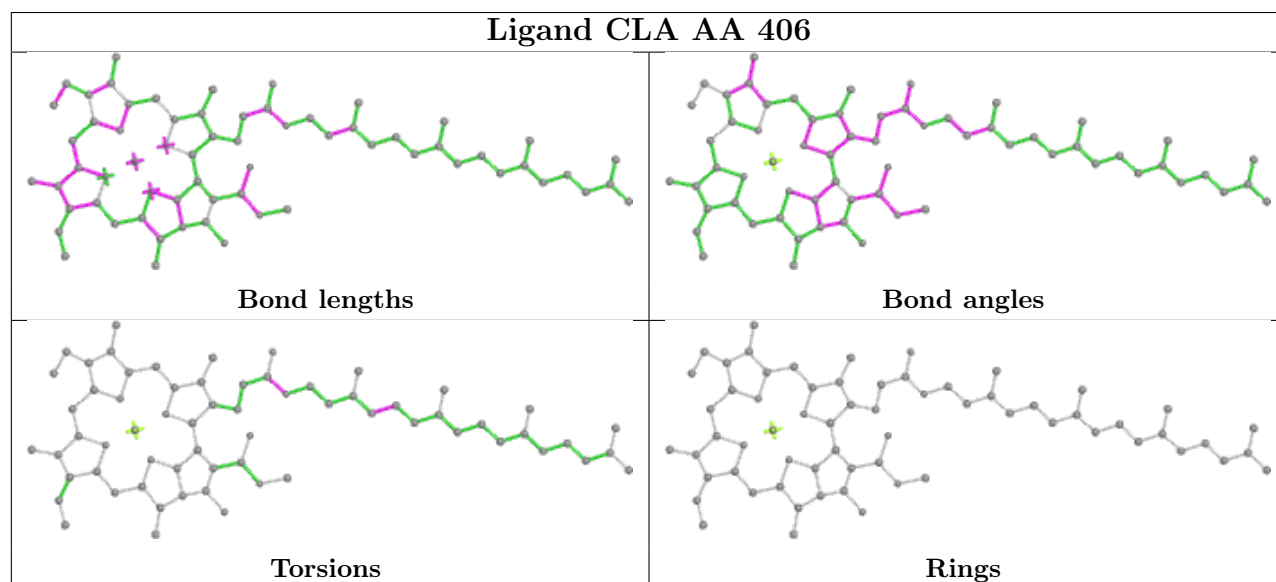
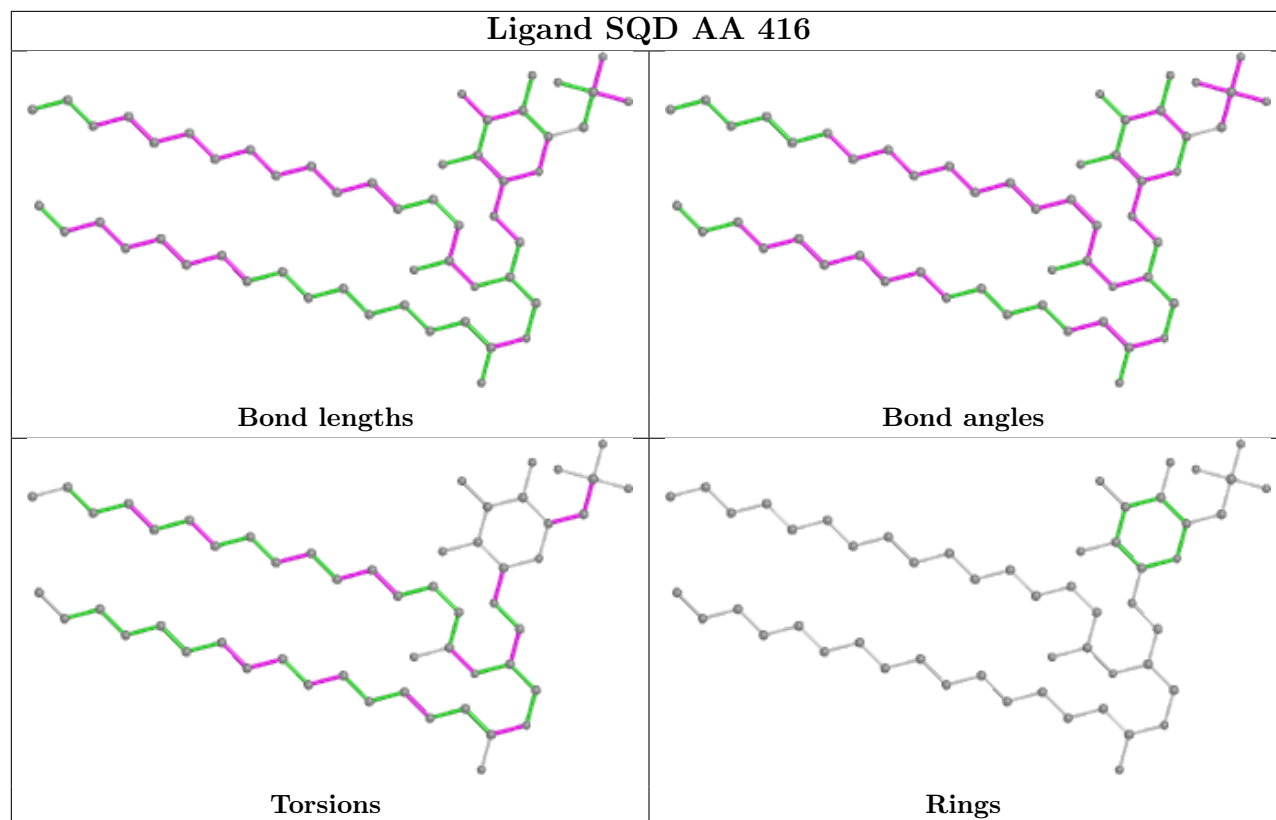


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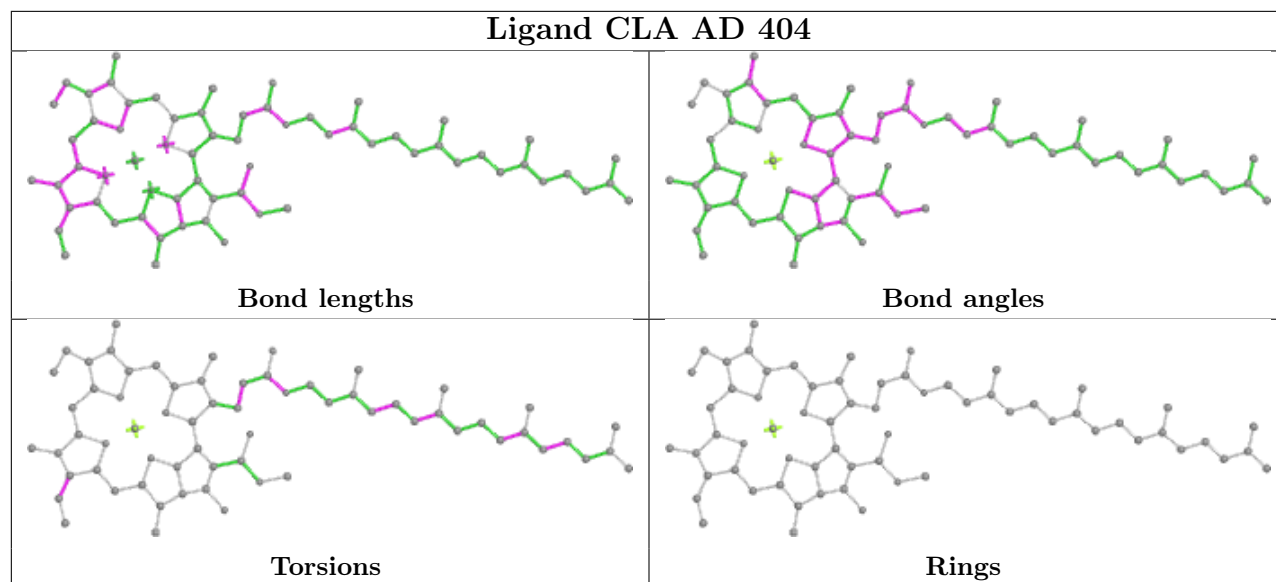


Ligand HEM BF 5101

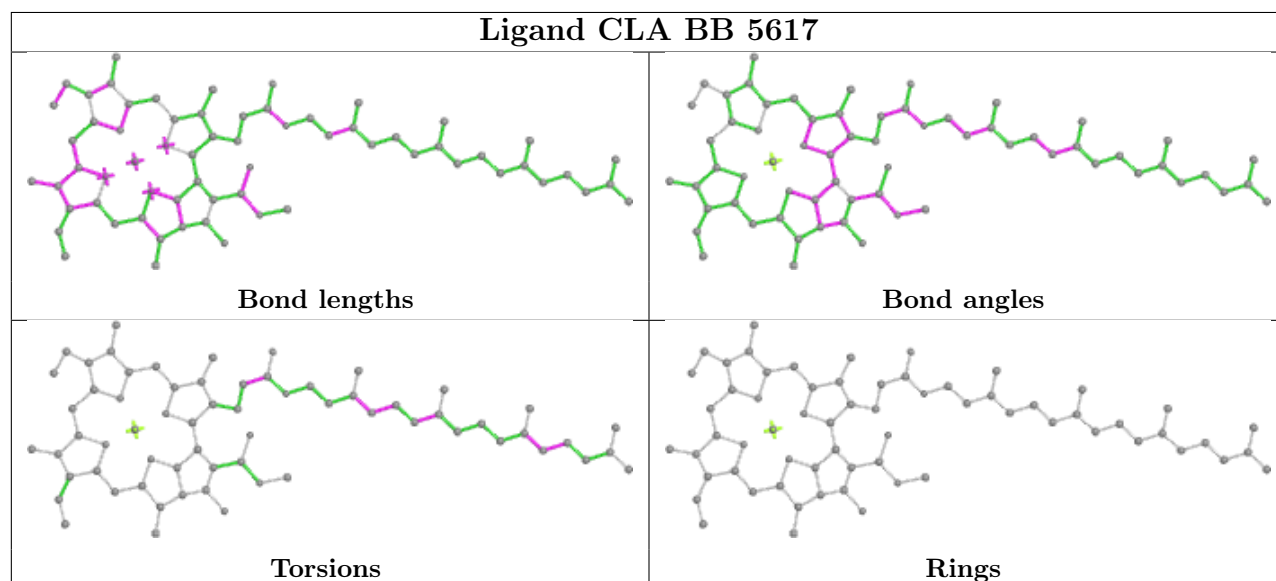




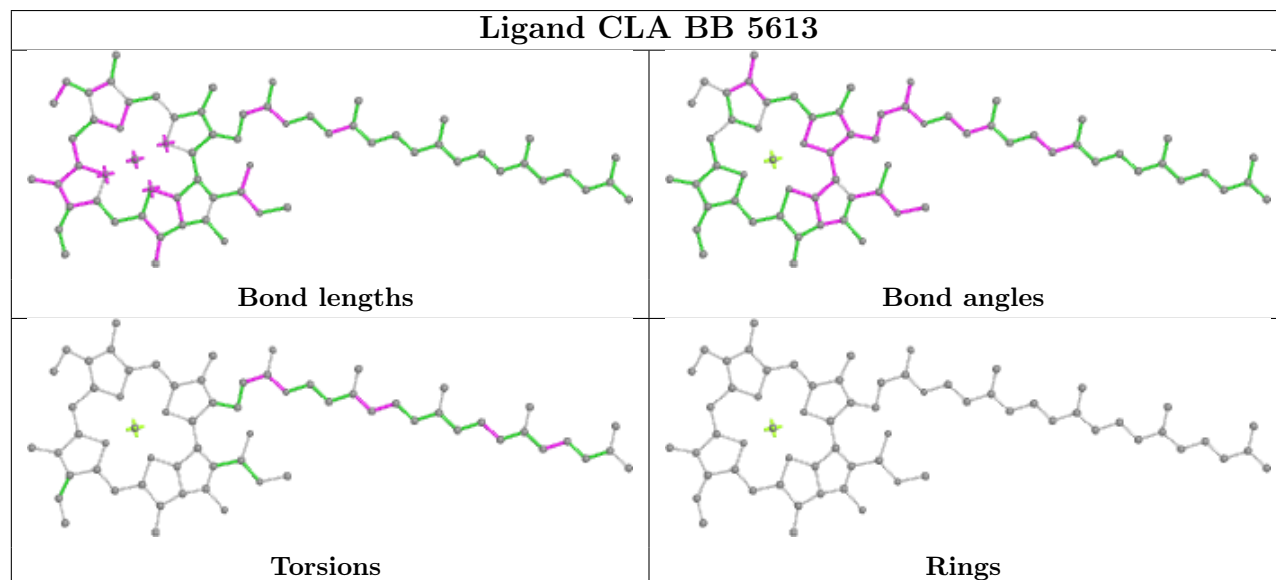
Ligand CLA AD 404



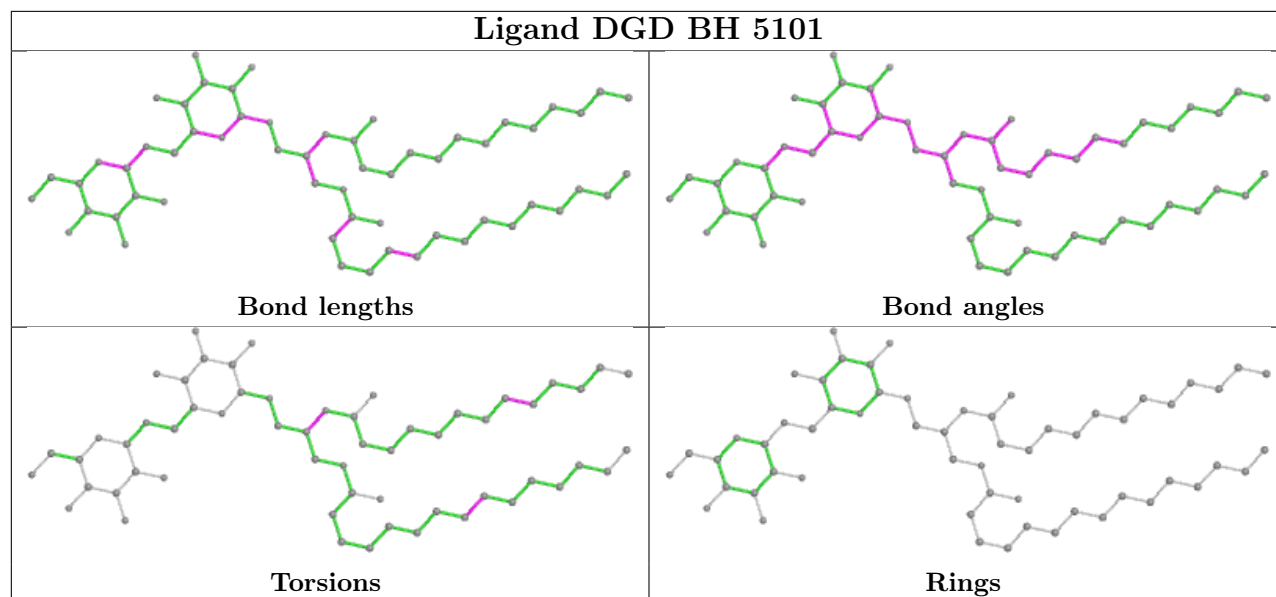
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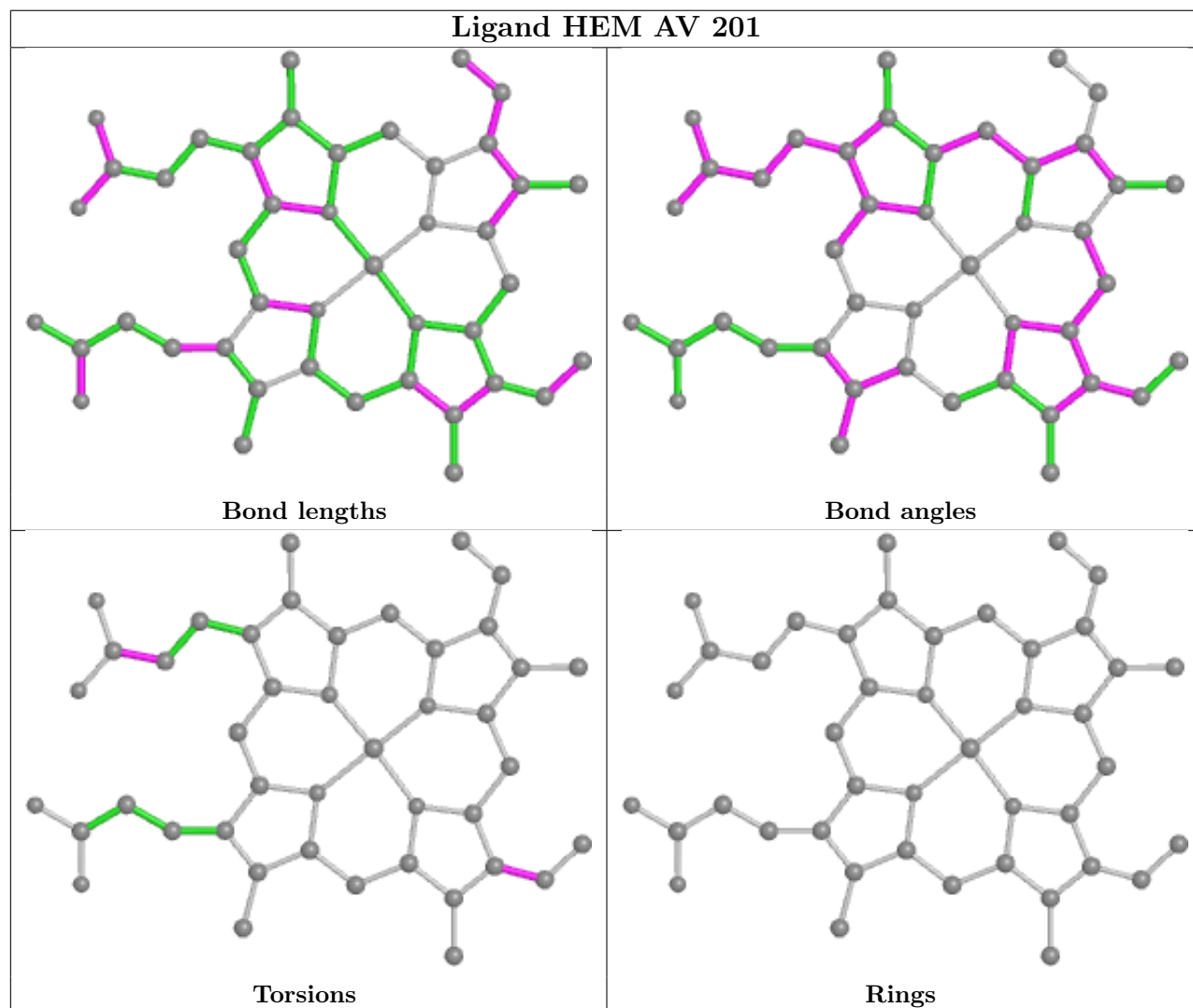
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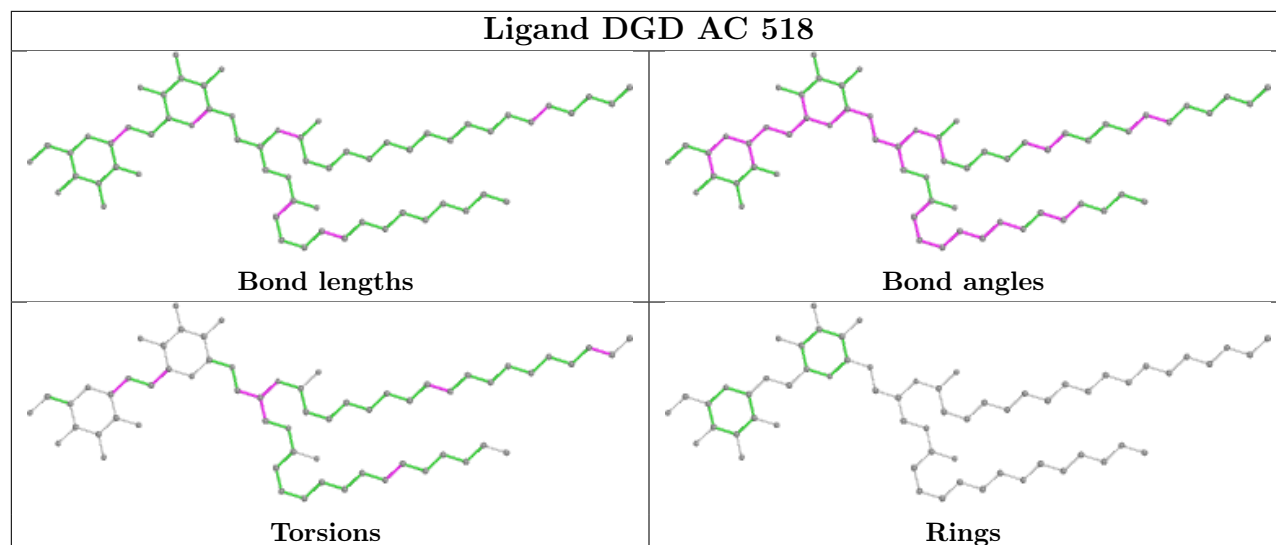
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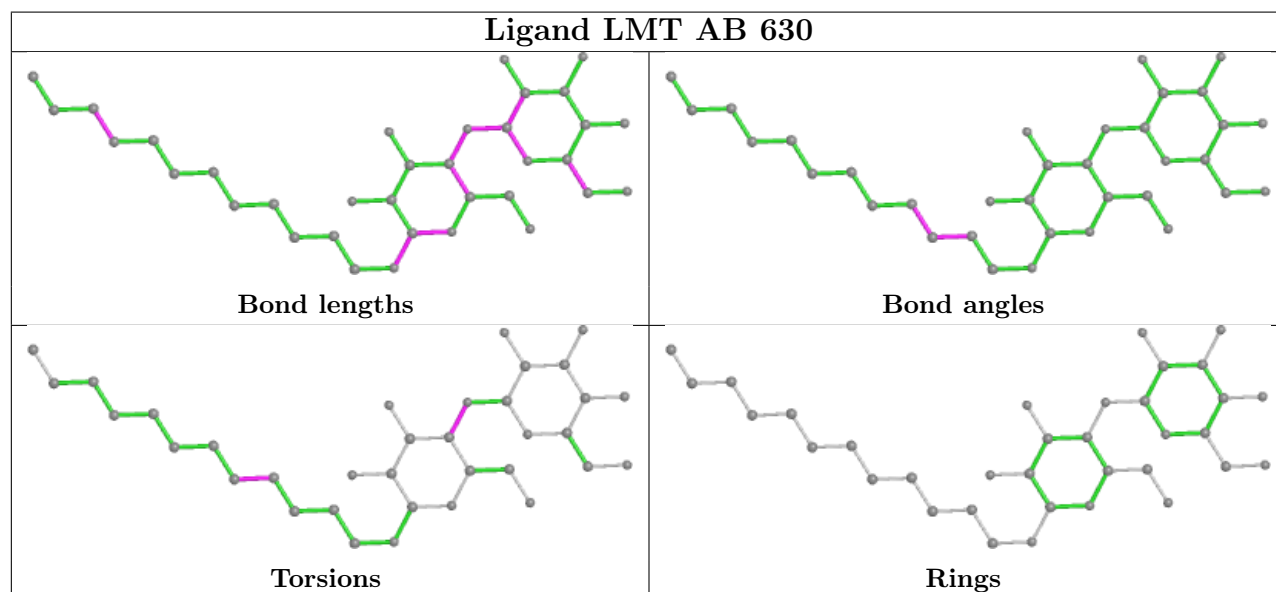
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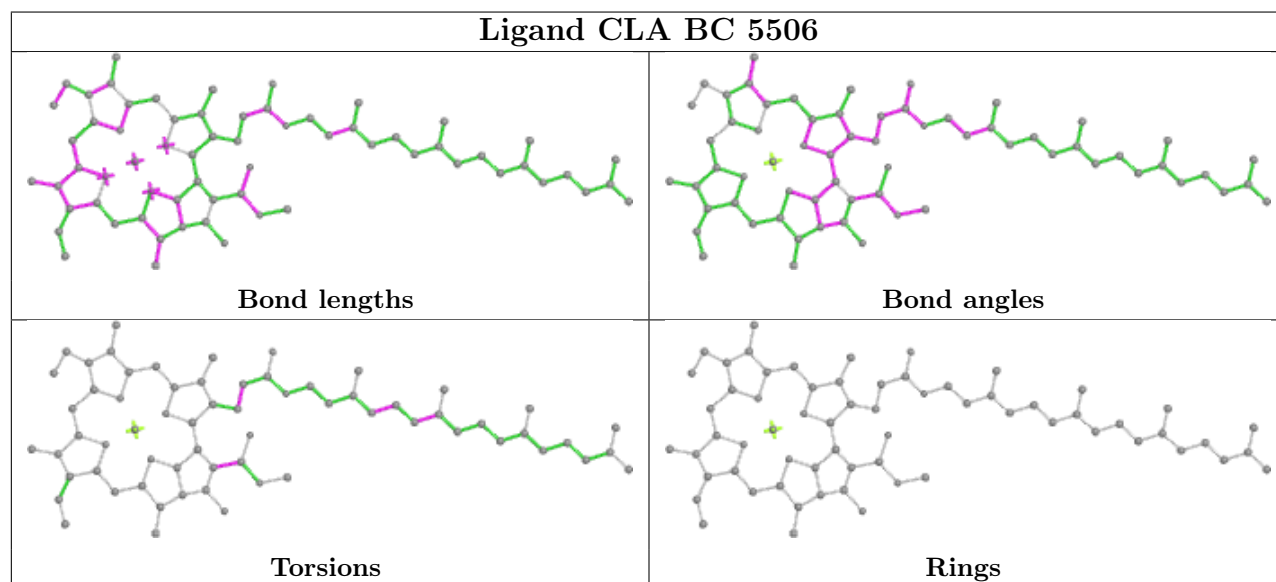
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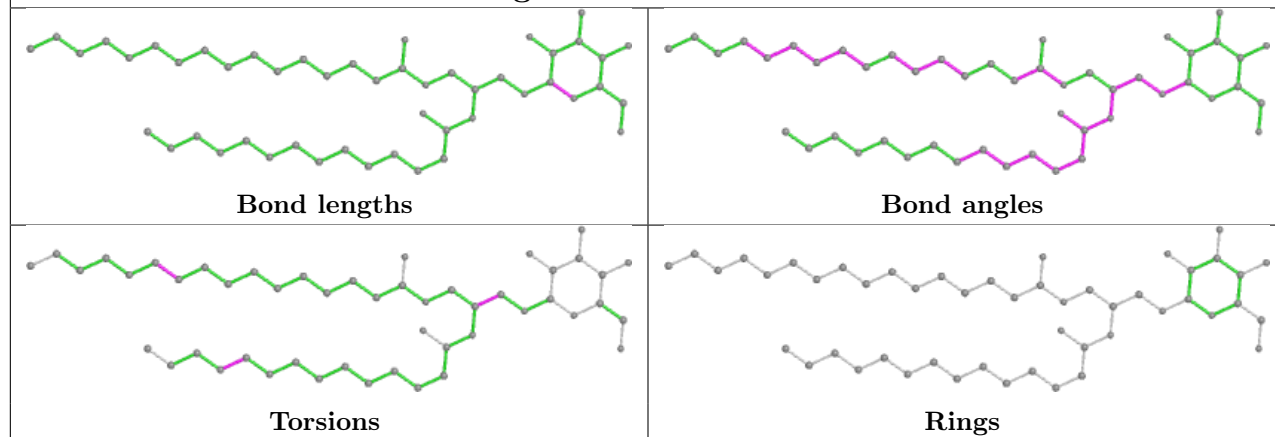
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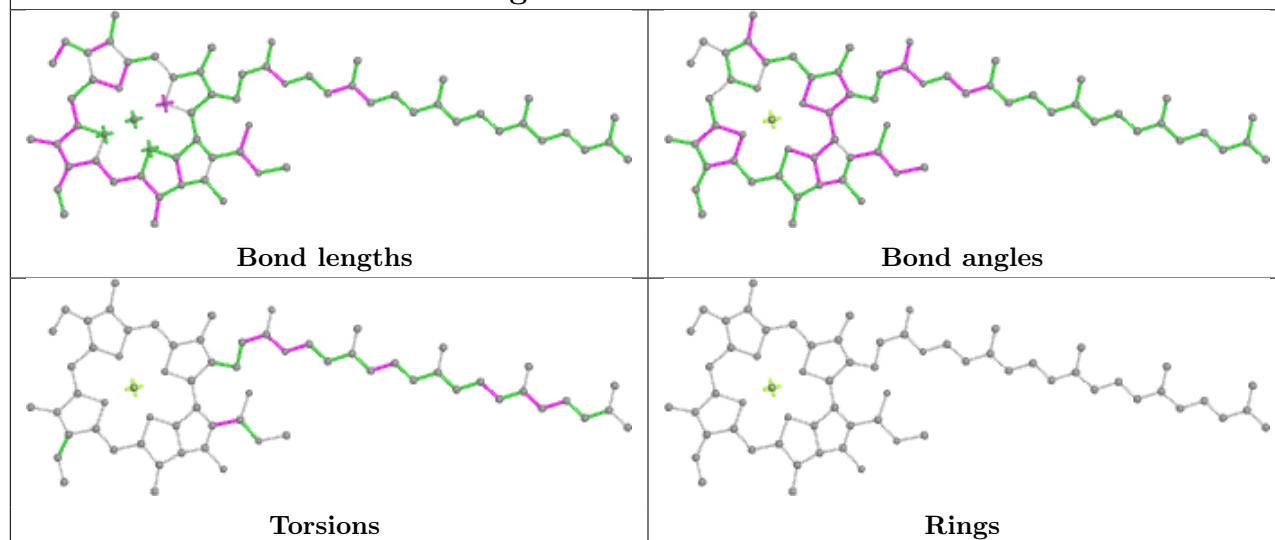
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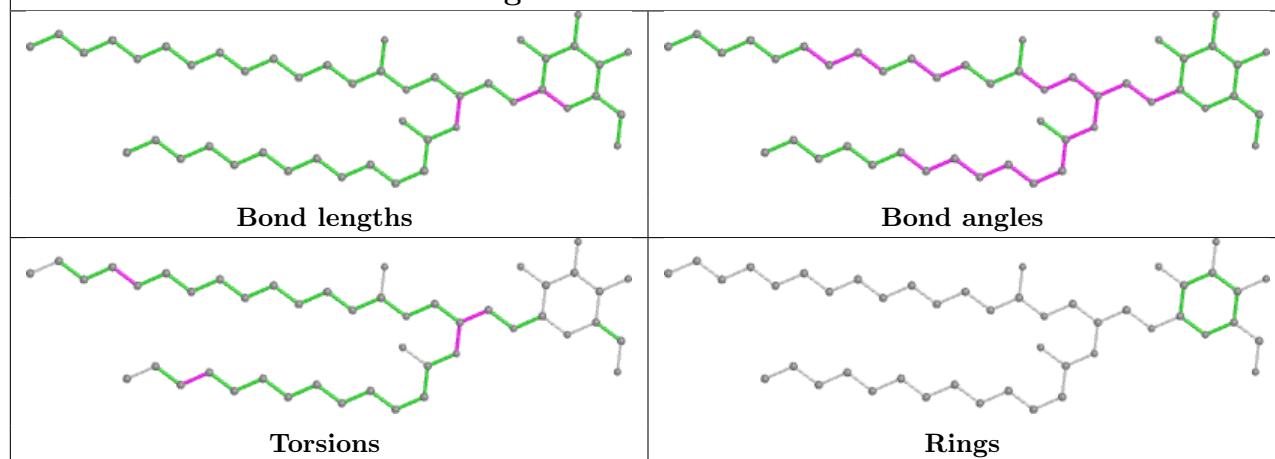
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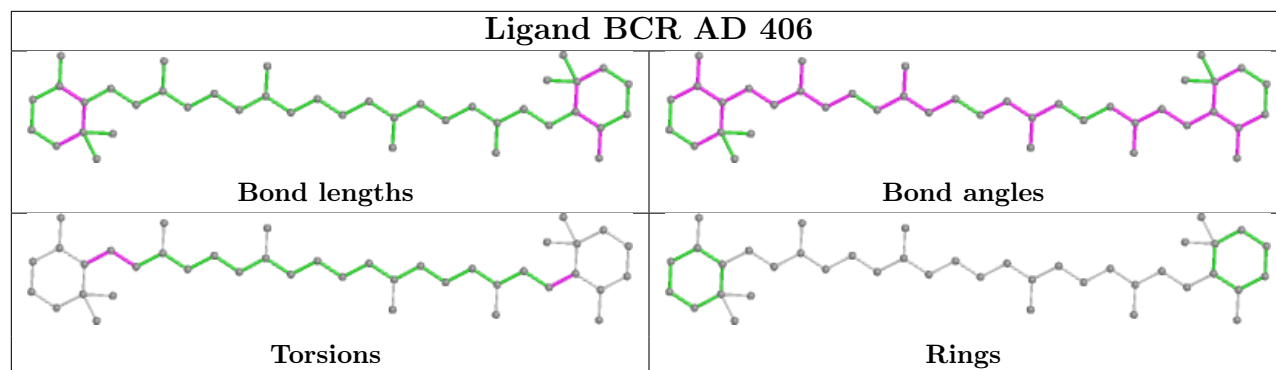
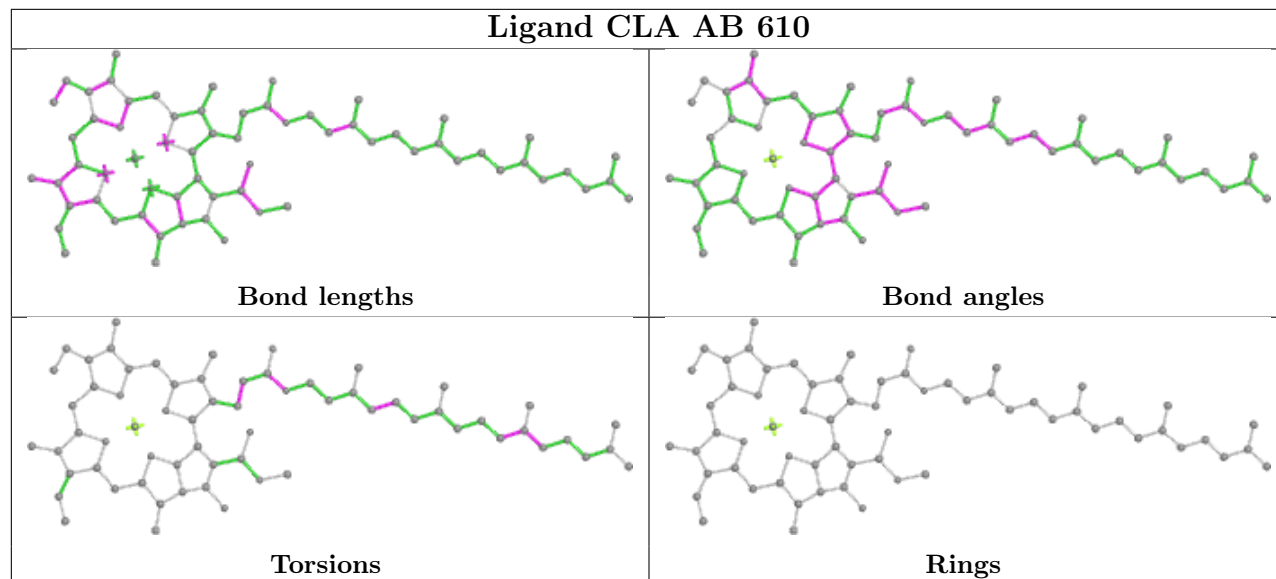
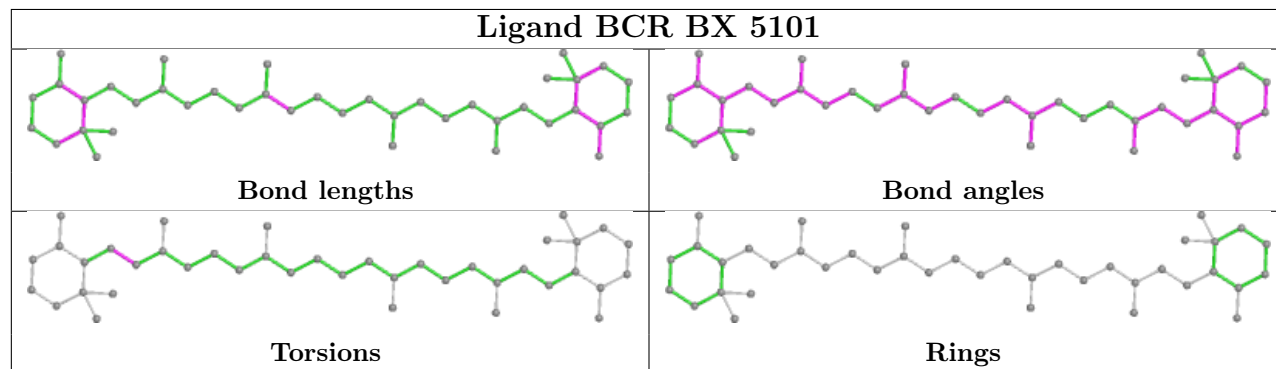


Ligand CLA BC 5513

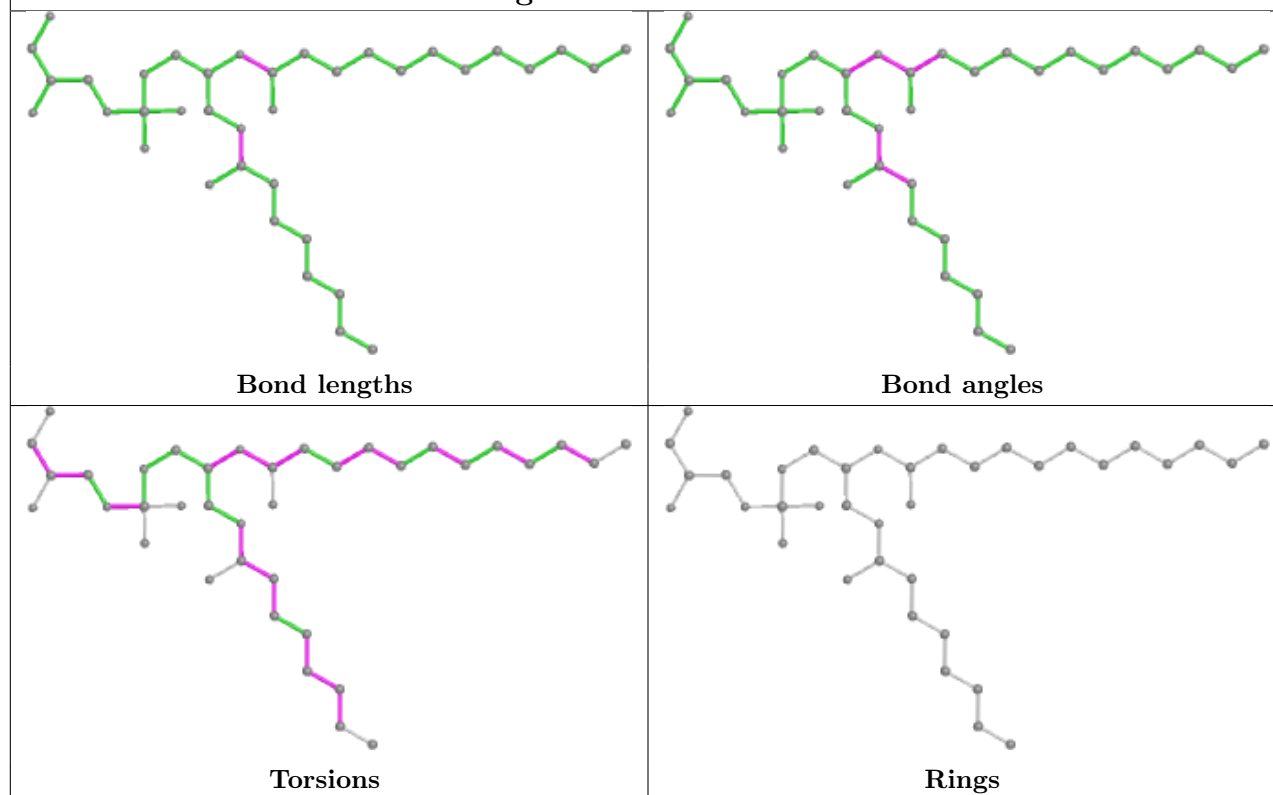


Ligand LMG BD 5408

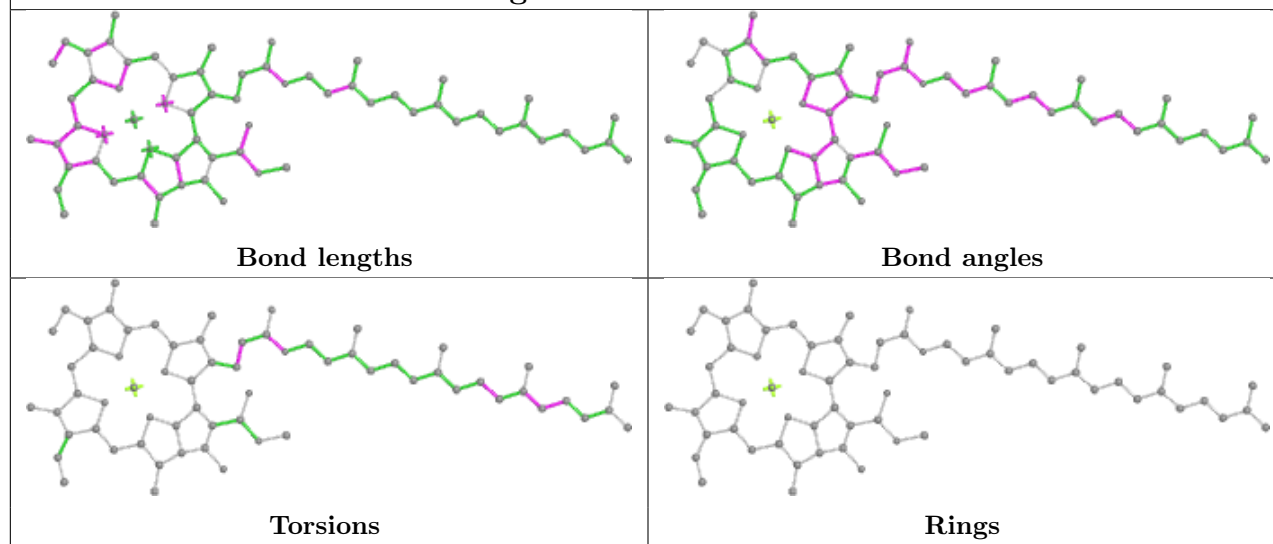


Ligand BCR AD 406**Ligand CLA AB 610****Ligand BCR BX 5101**

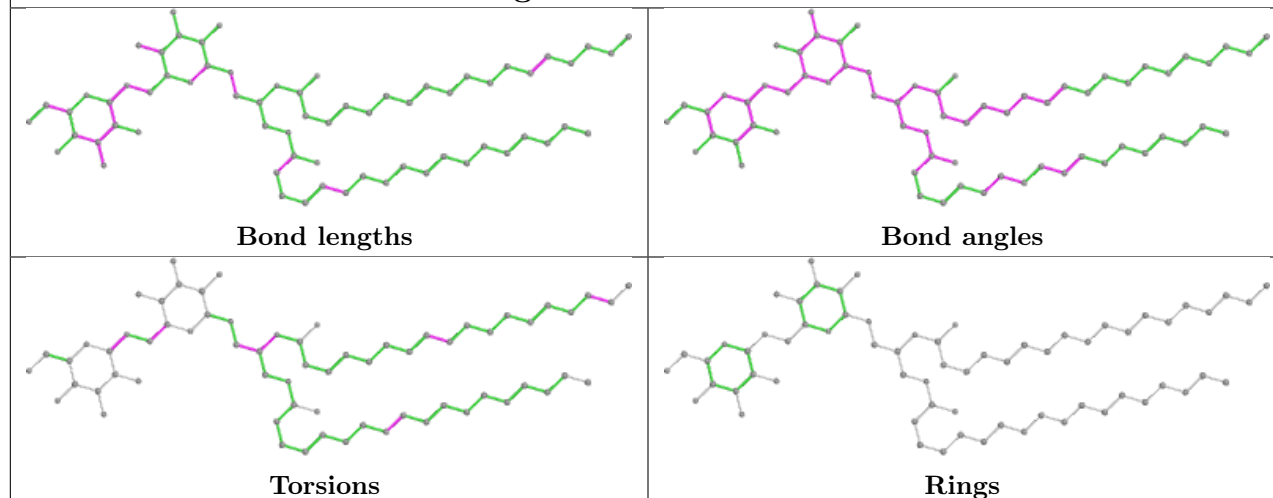
Ligand LHG AA 415



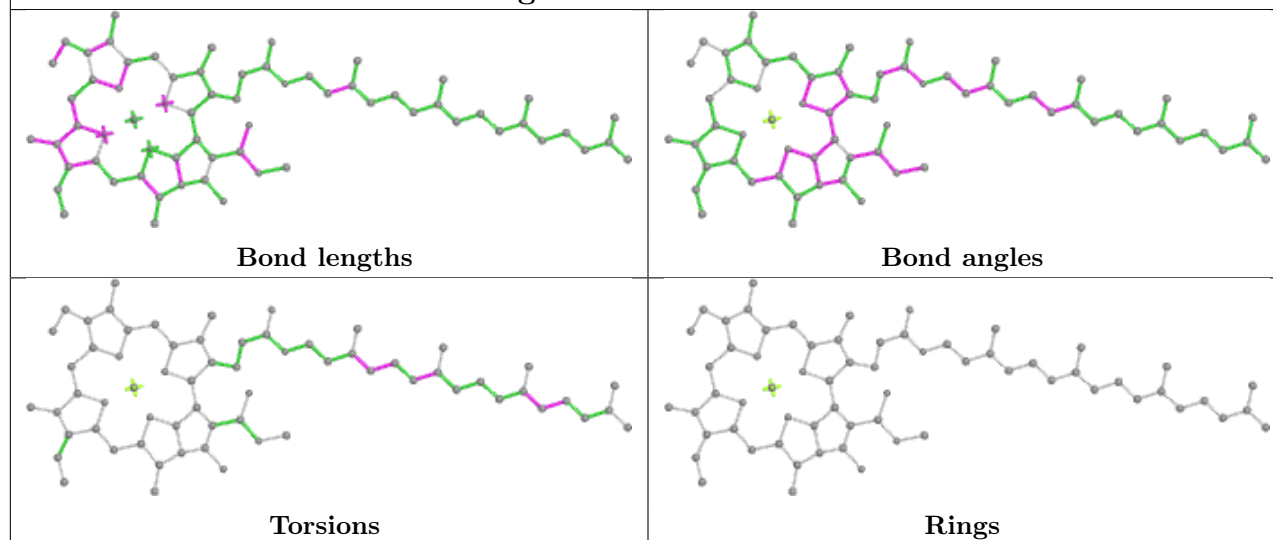
Ligand CLA BB 5606



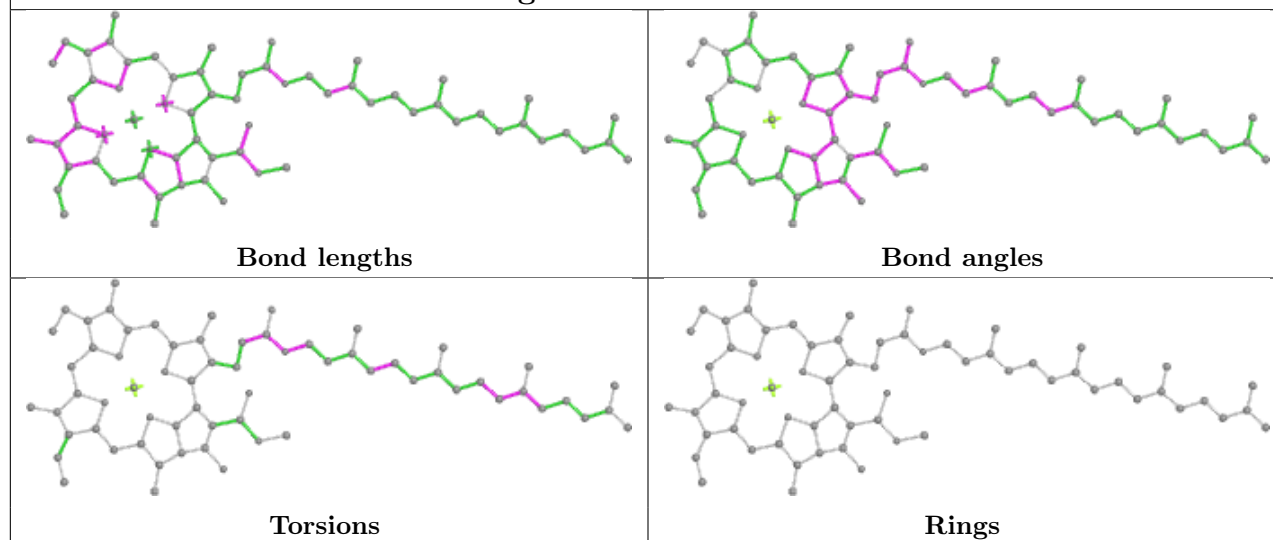
Ligand DGD AC 519

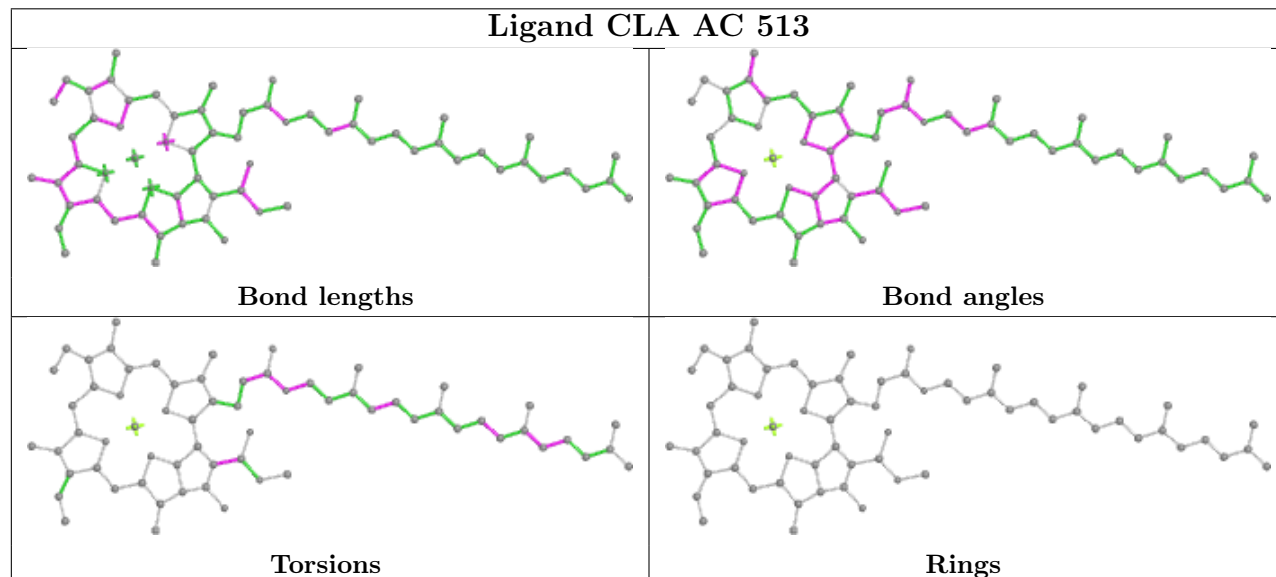
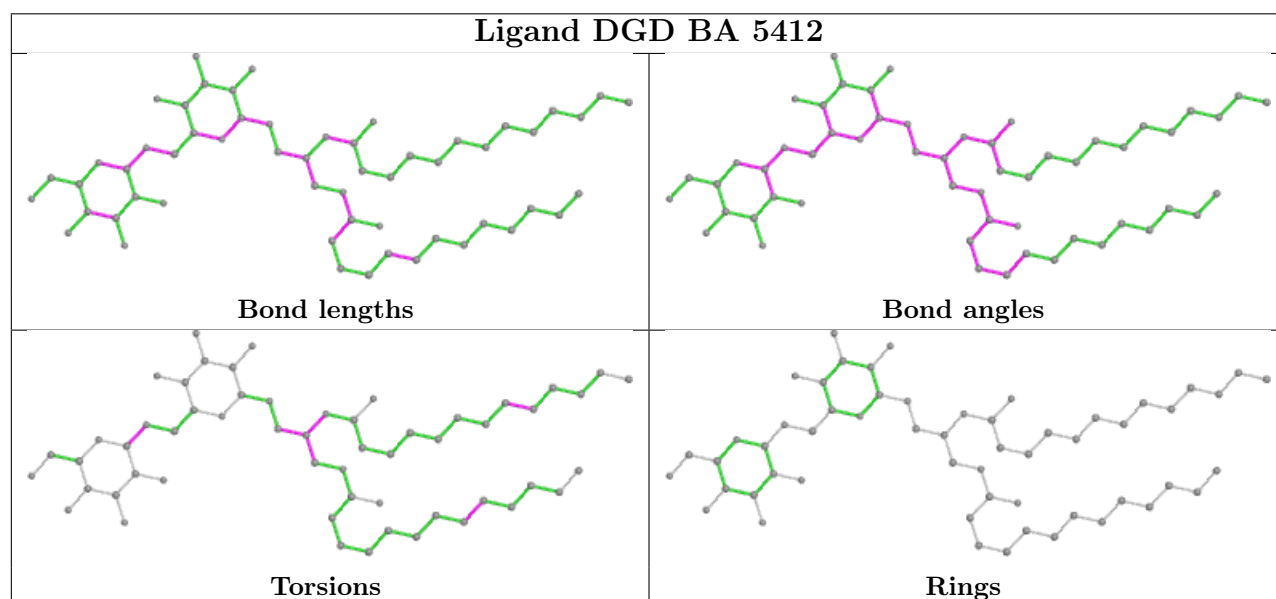
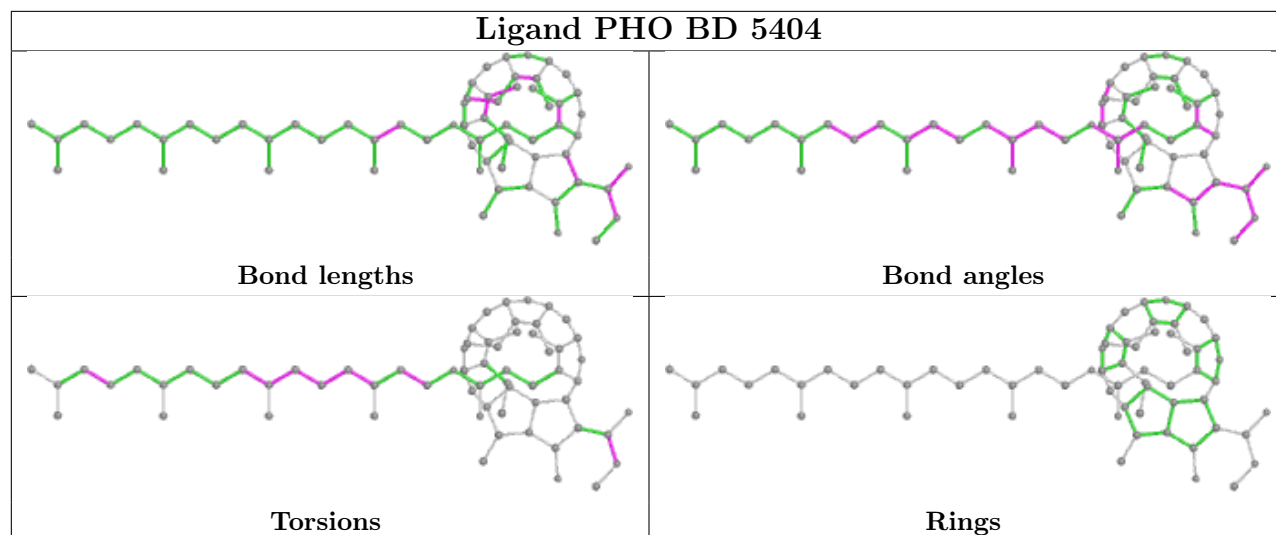


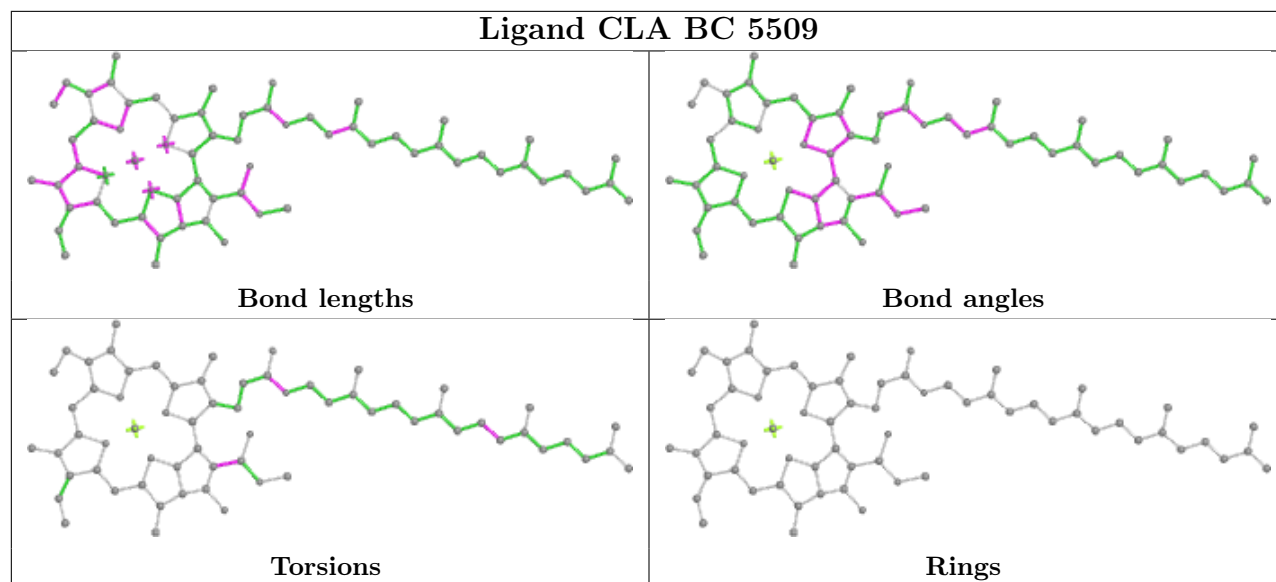
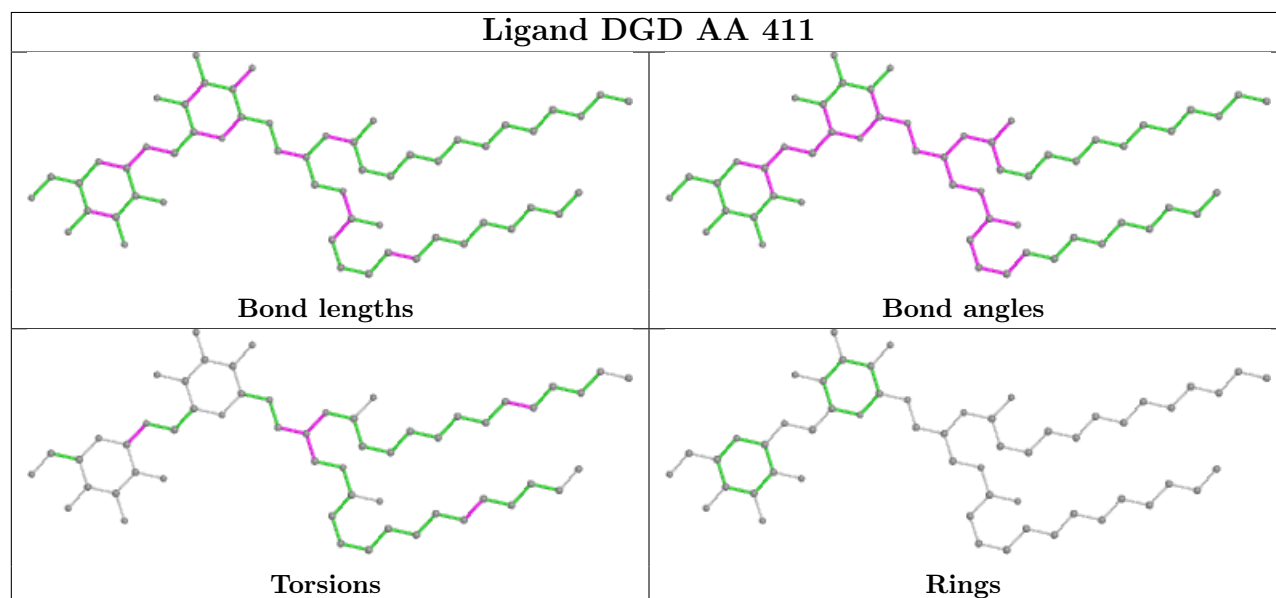
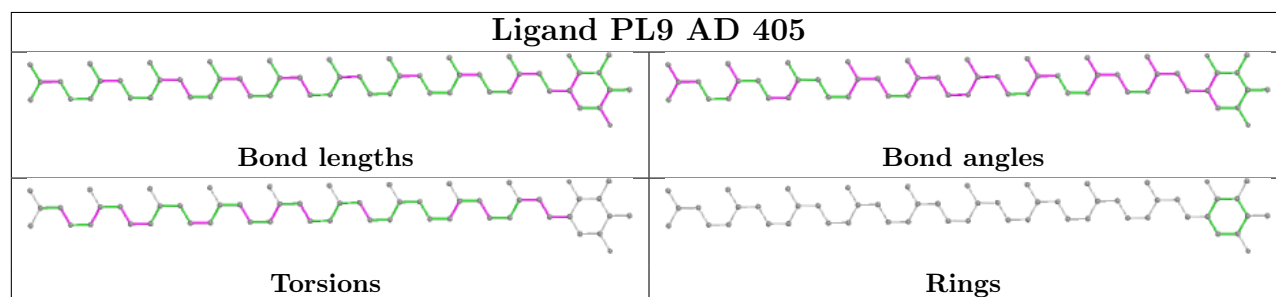
Ligand CLA AB 613

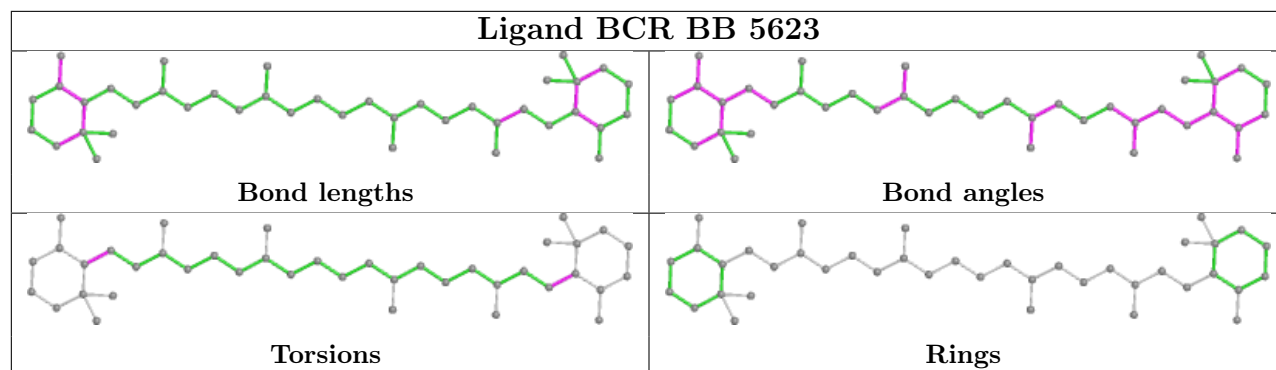
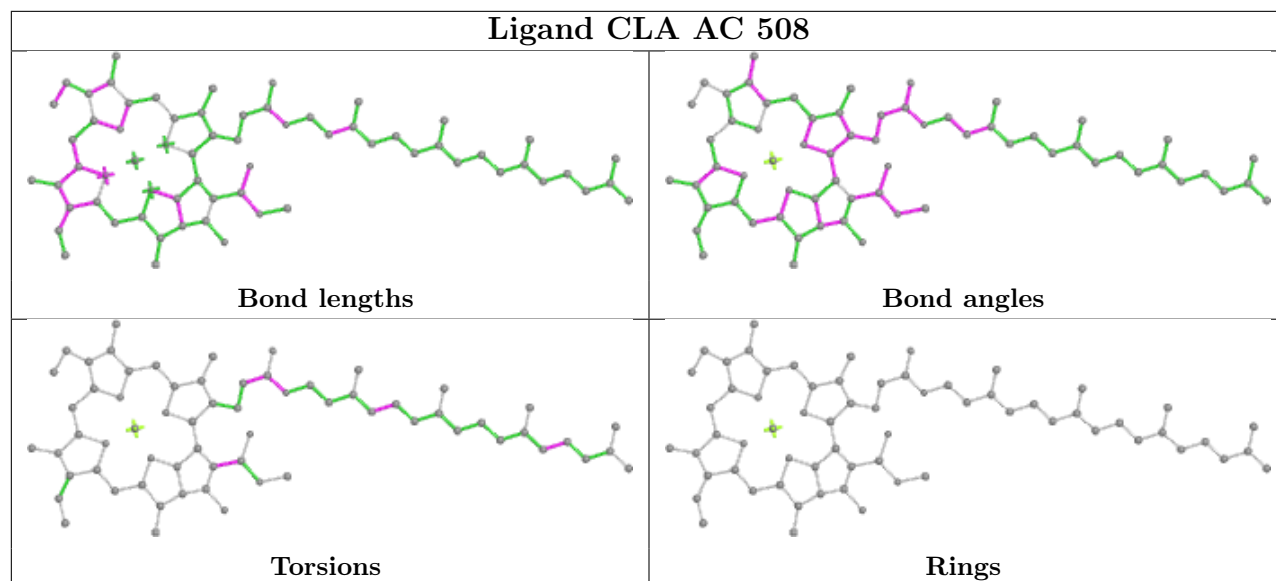
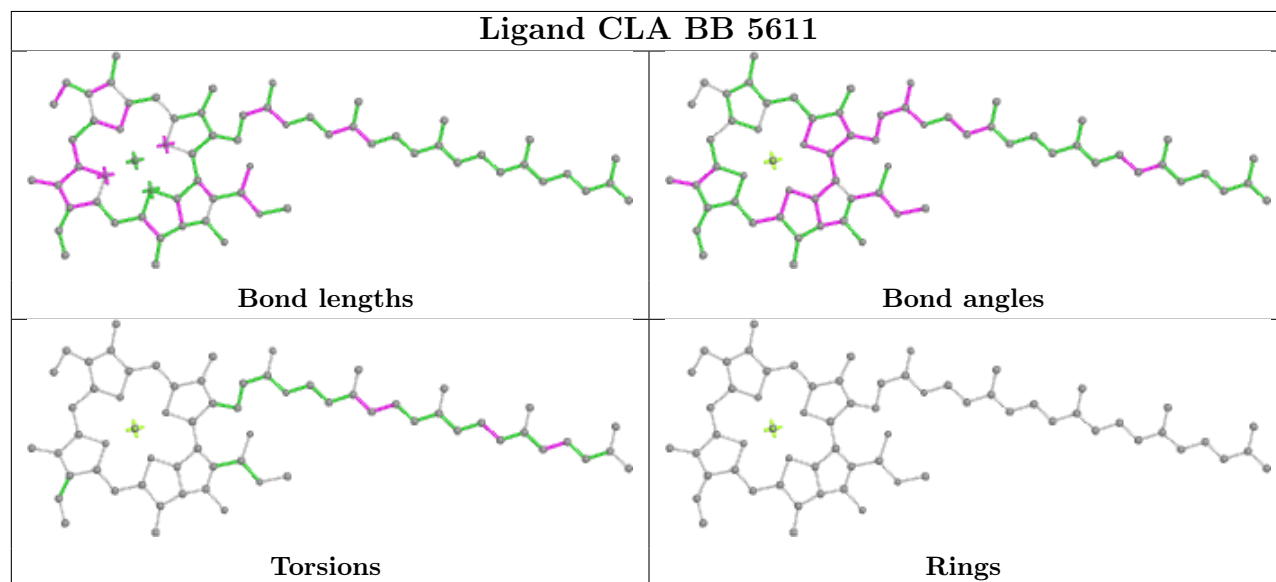


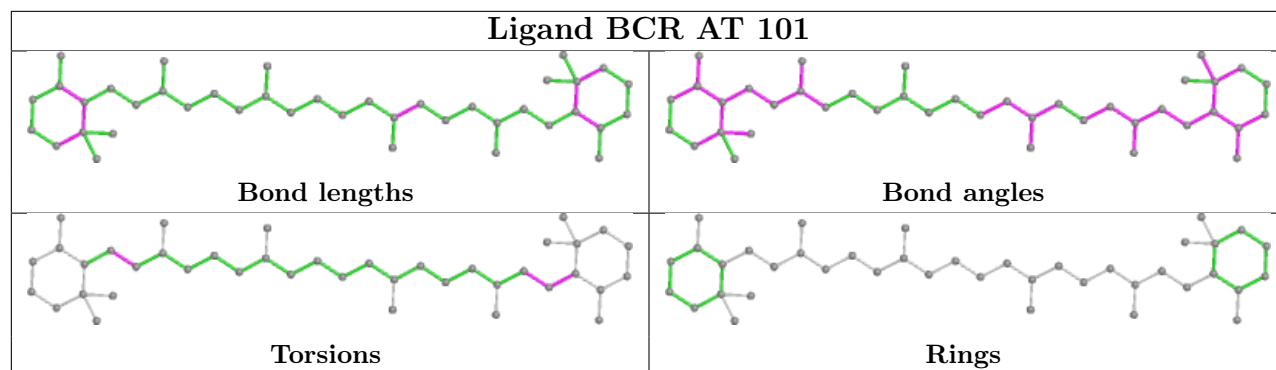
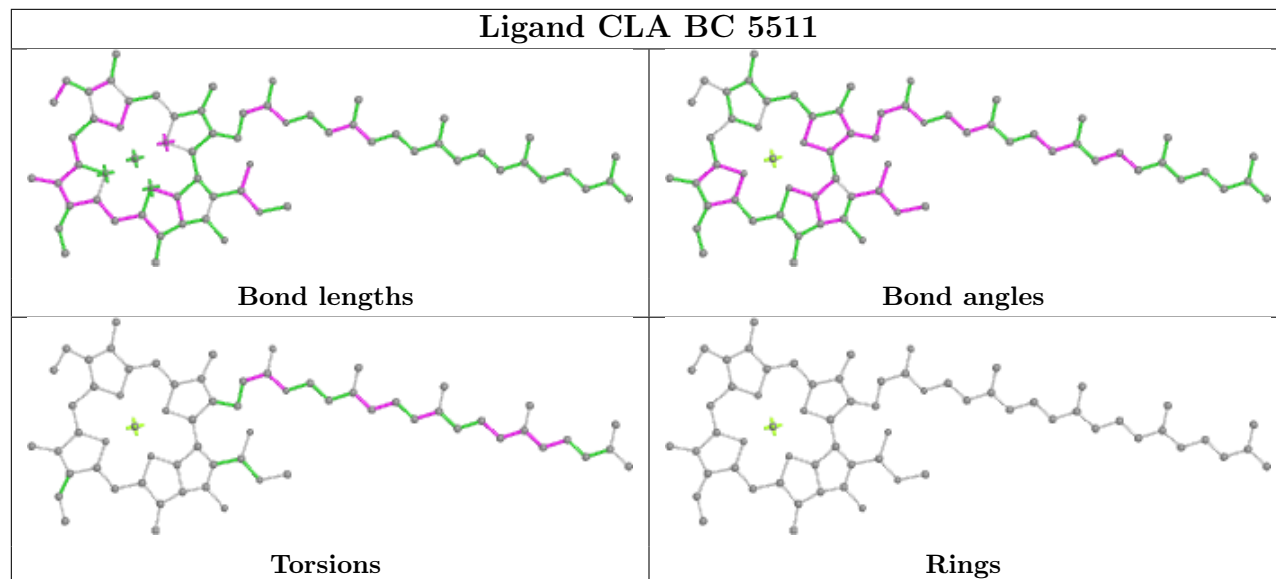
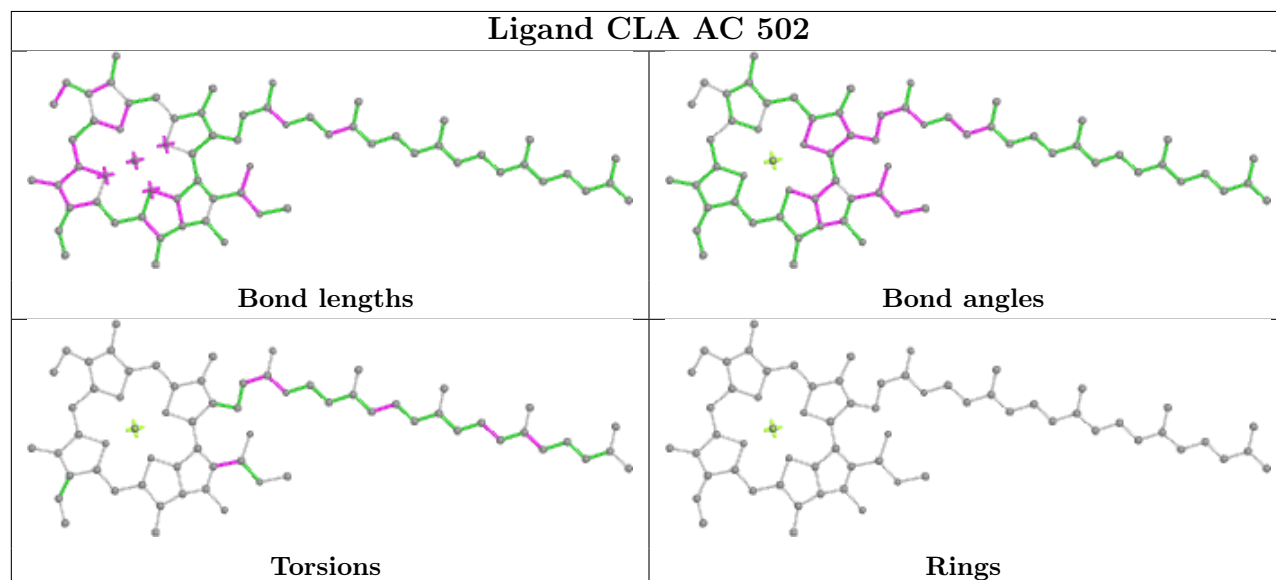
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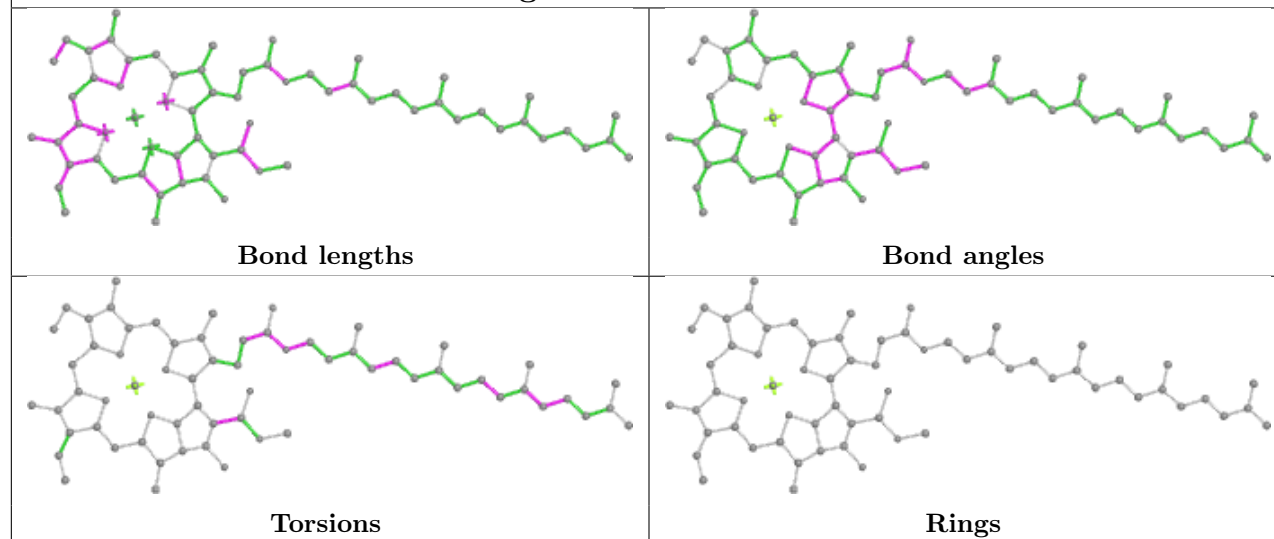
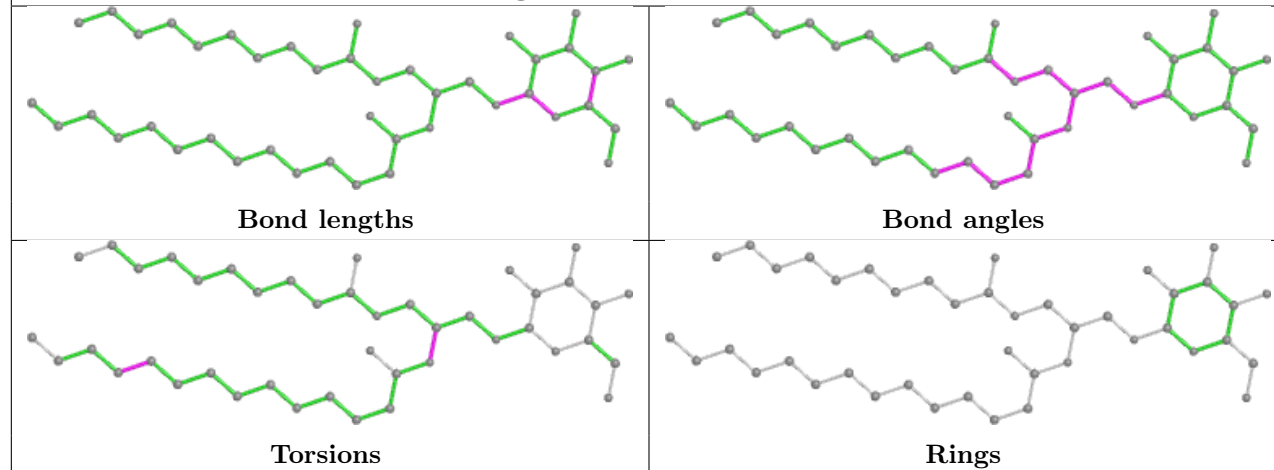
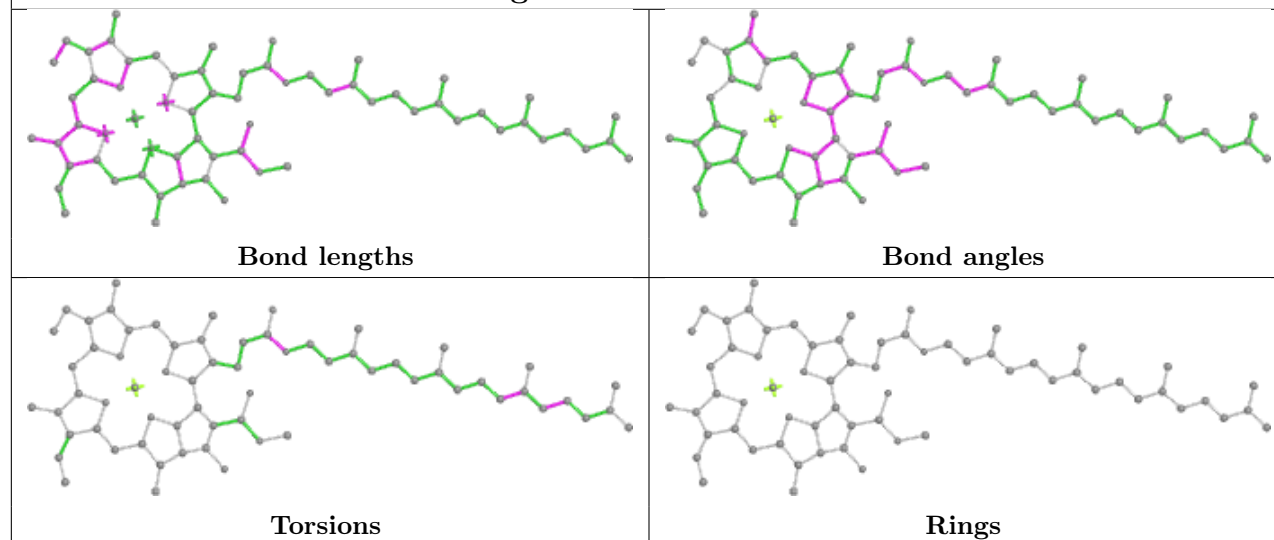




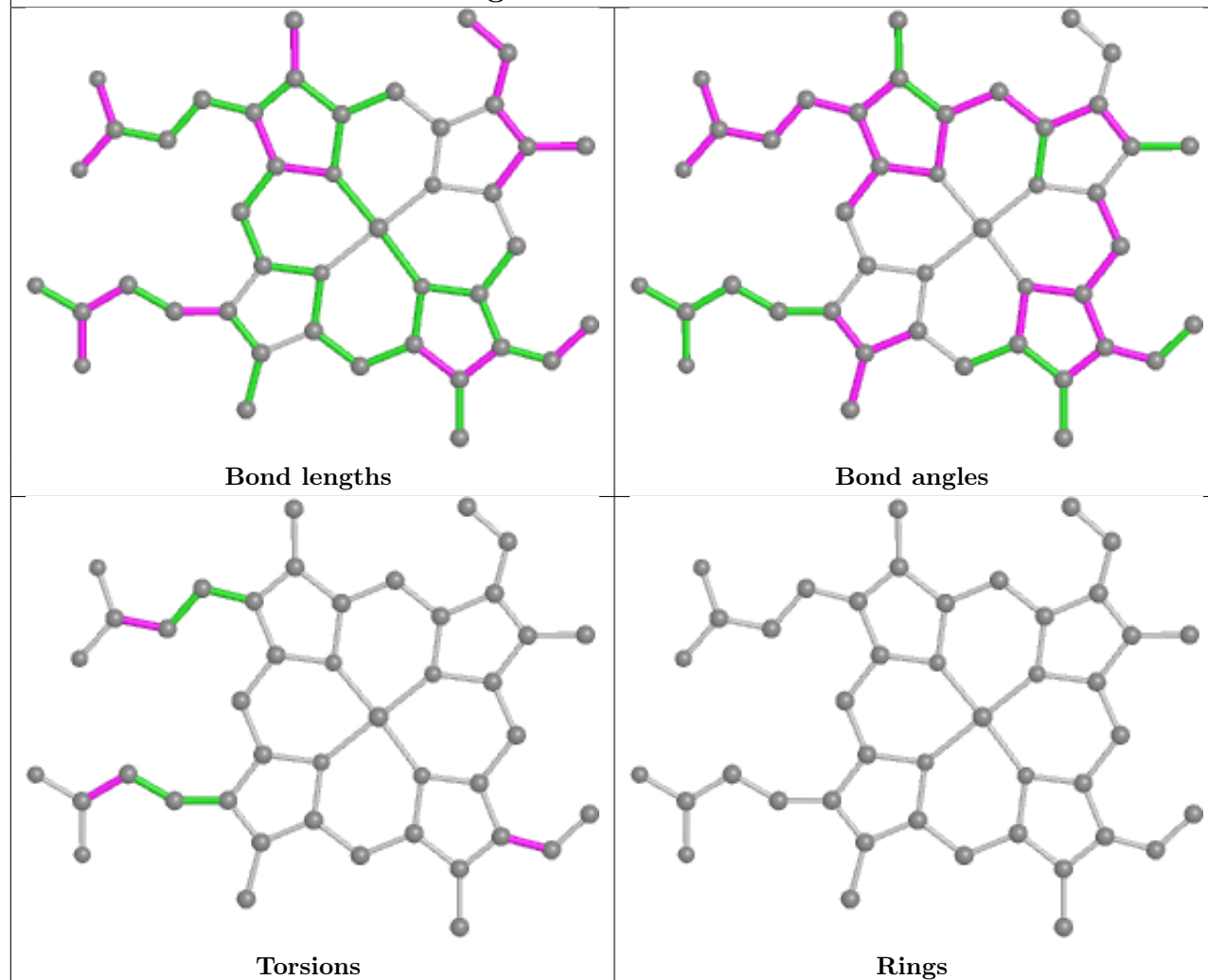
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Ligand BCR BB 5623**Ligand CLA AC 508****Ligand CLA BB 5611**

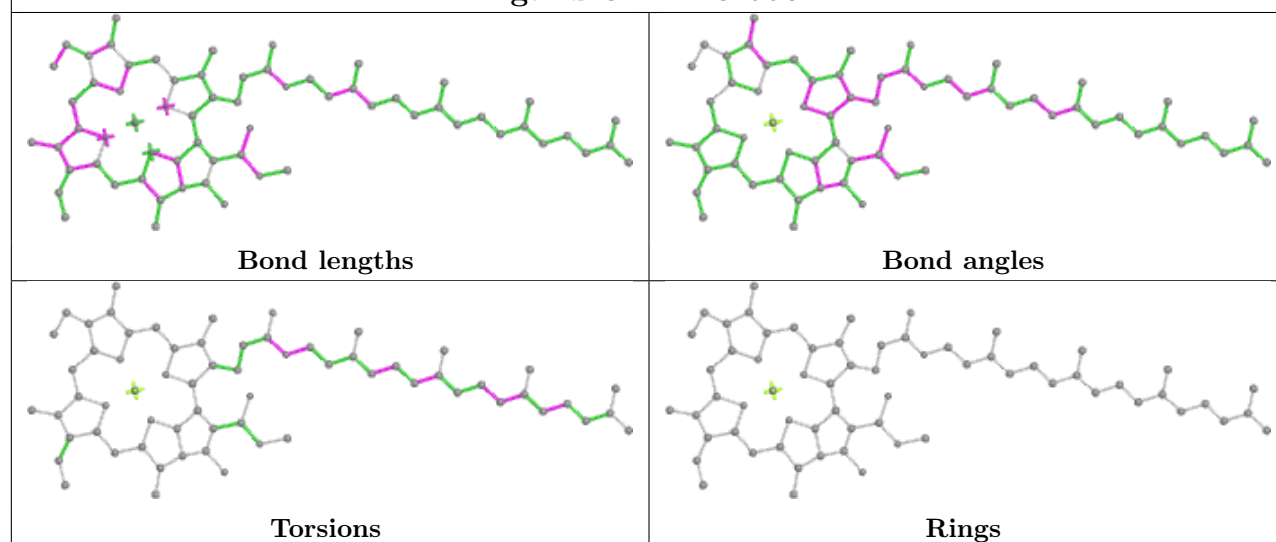
Ligand BCR AT 101**Ligand CLA BC 5511****Ligand CLA AC 502**

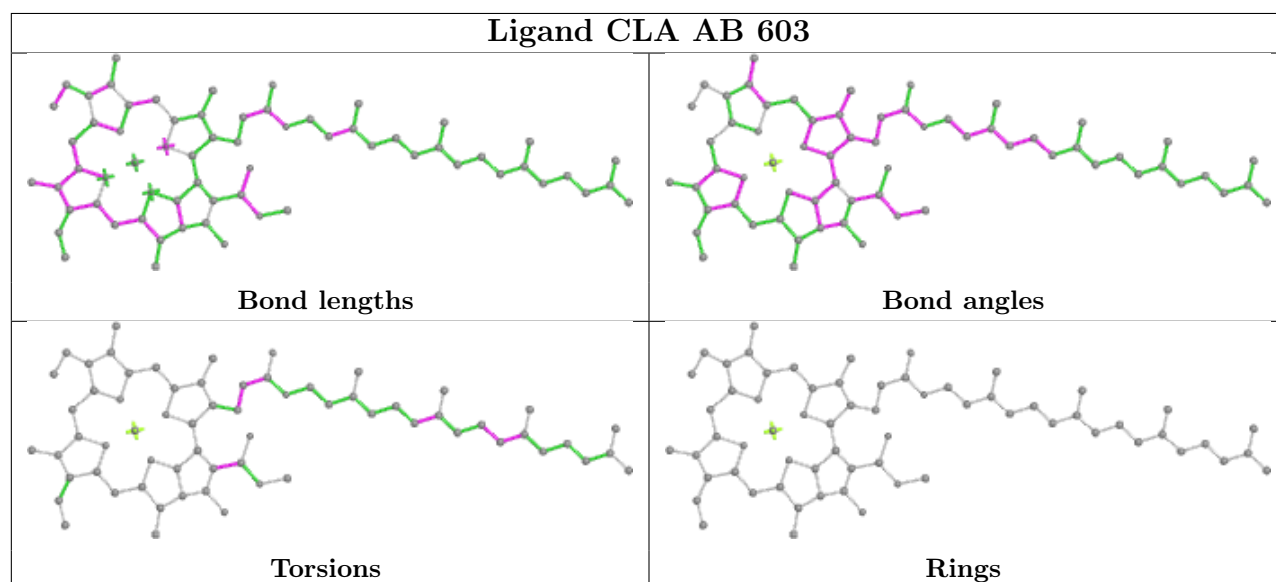
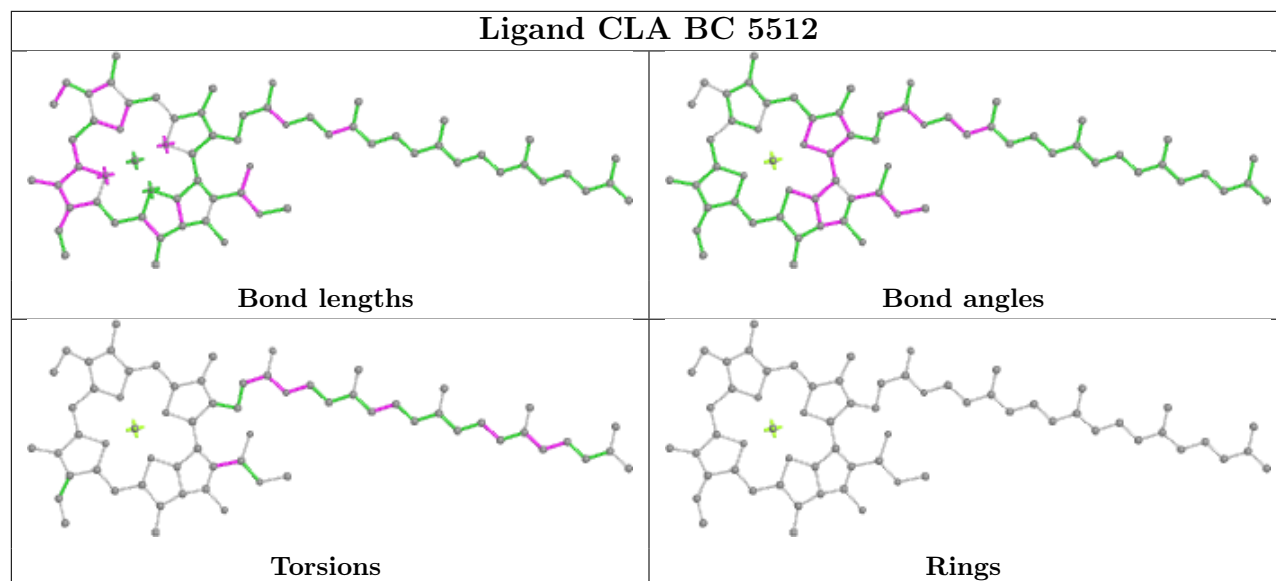
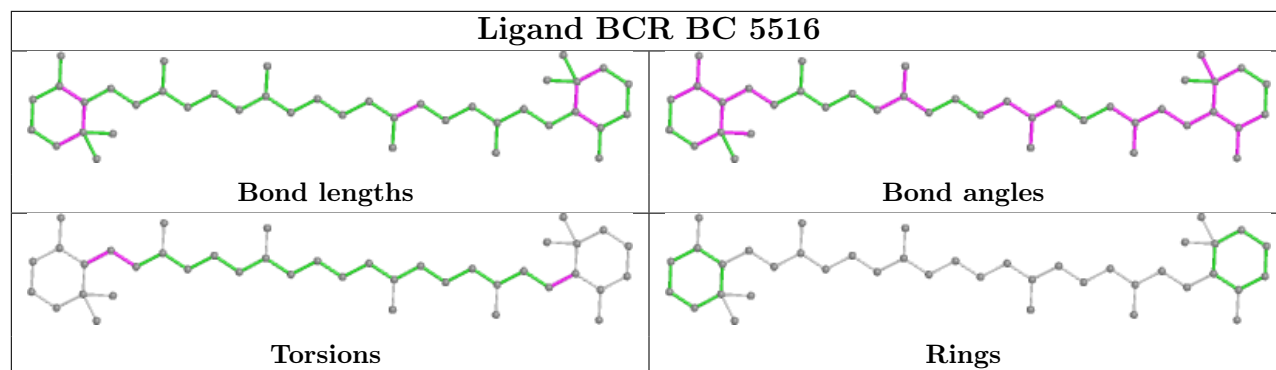
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Ligand HEM AF 101

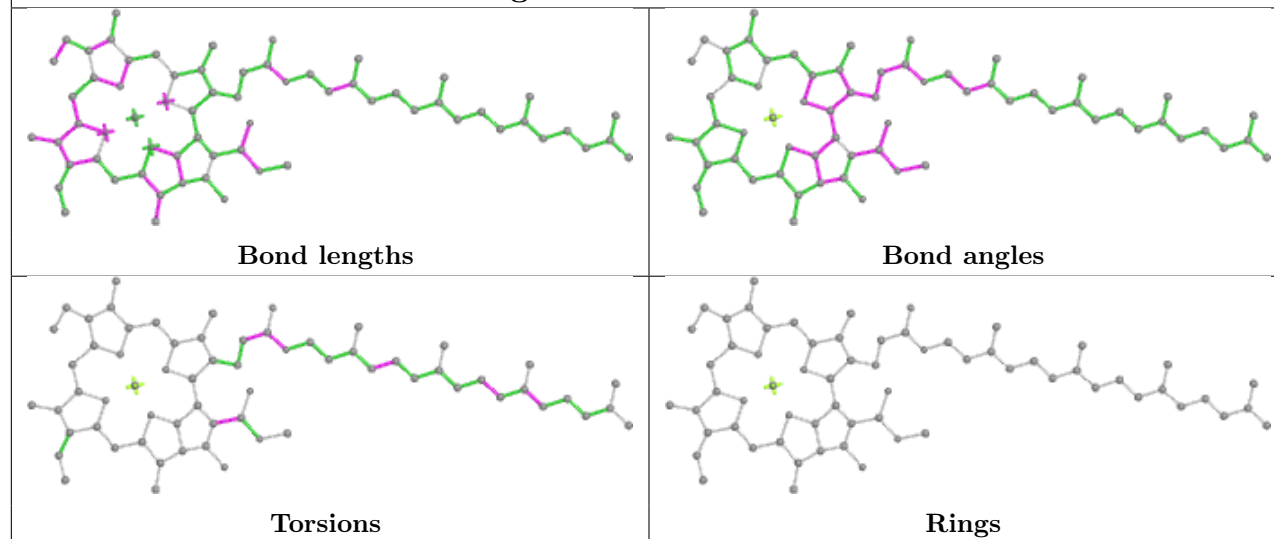


Ligand CLA BC 5504

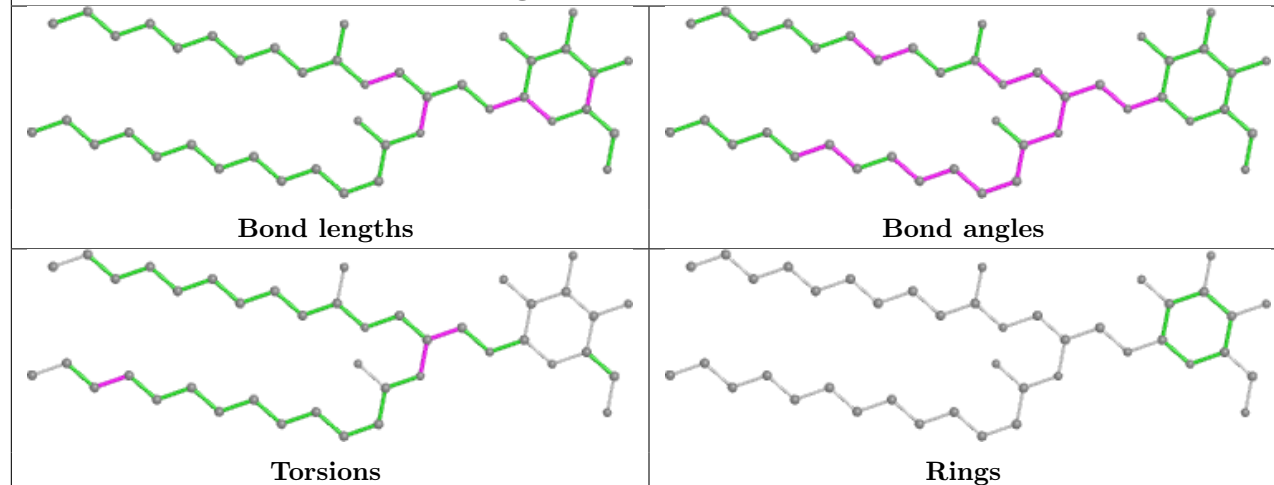




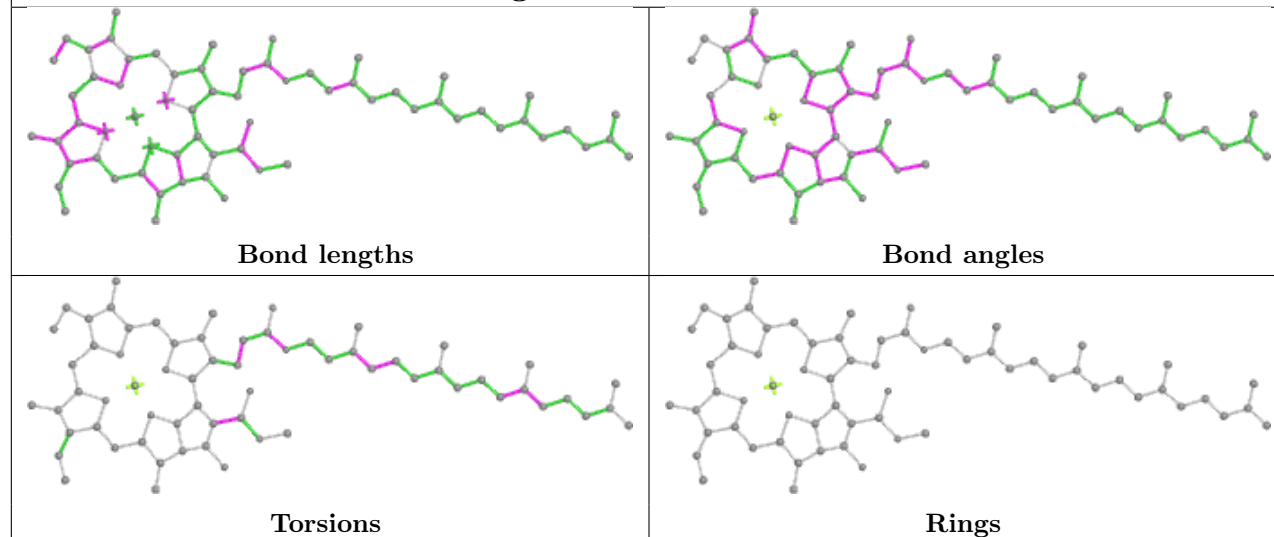
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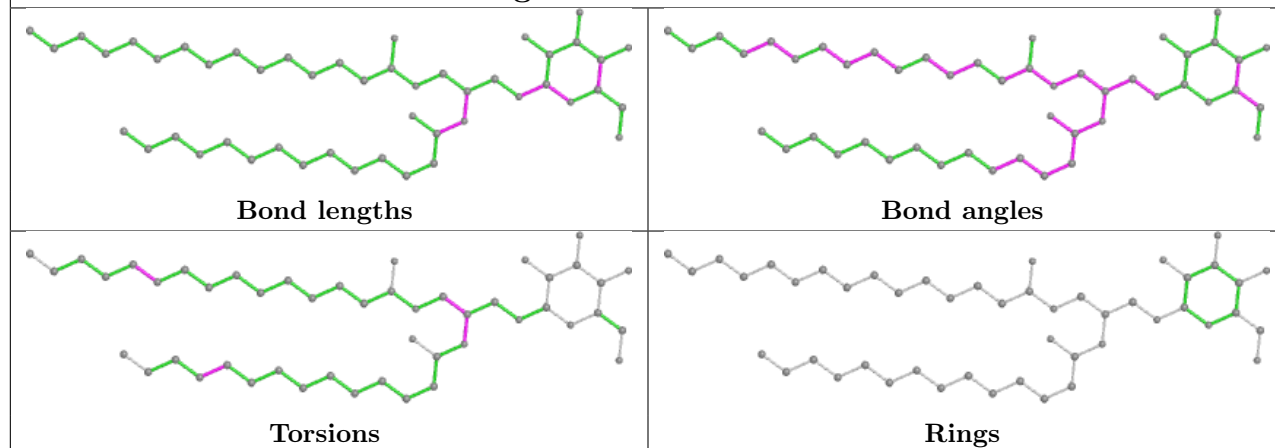
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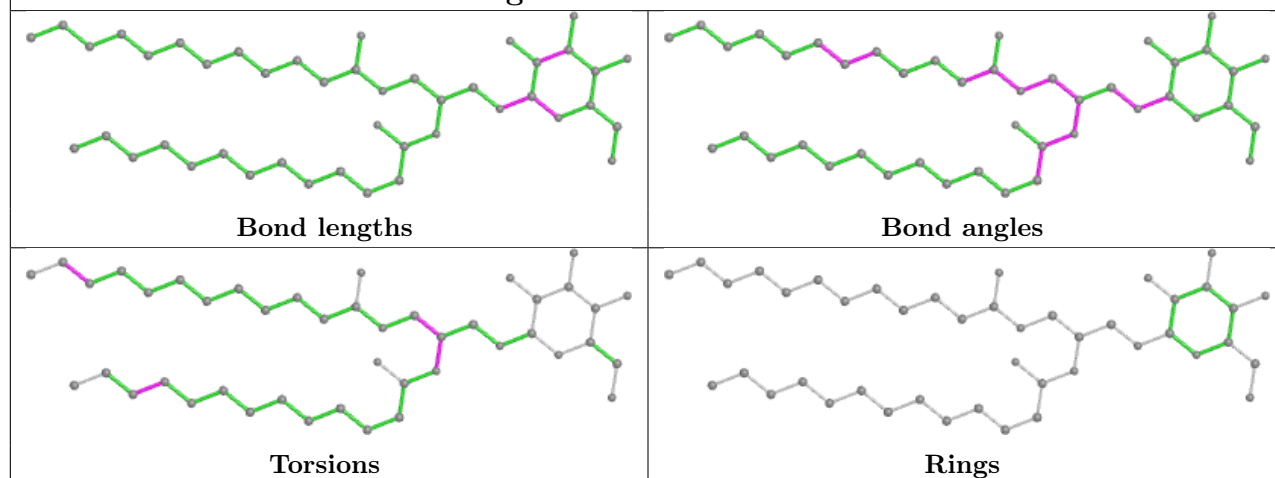
Ligand CLA BB 5610



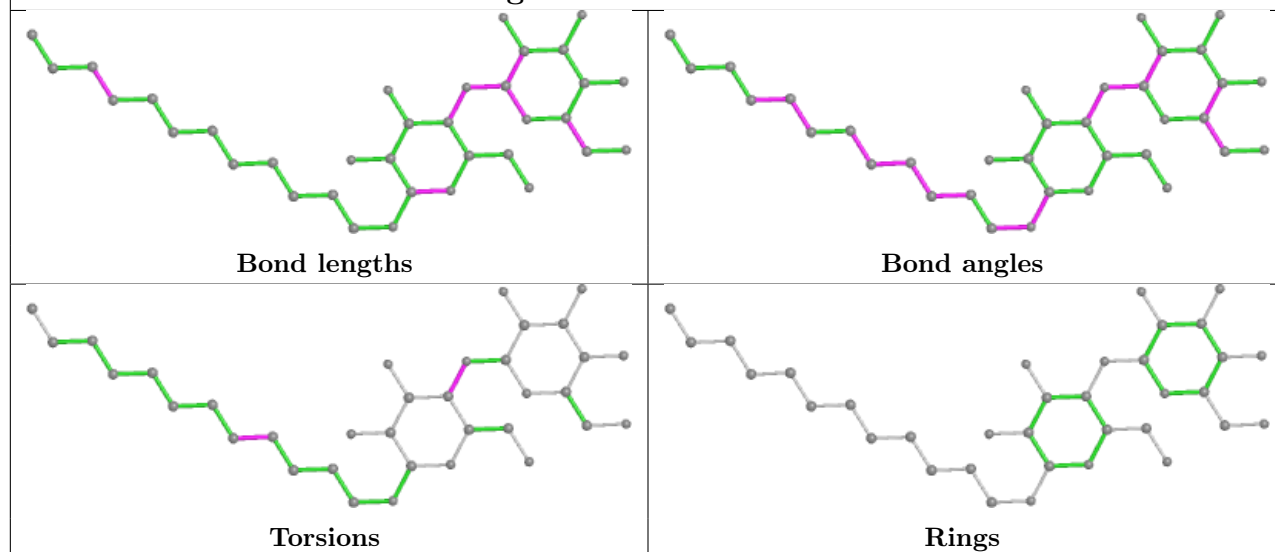
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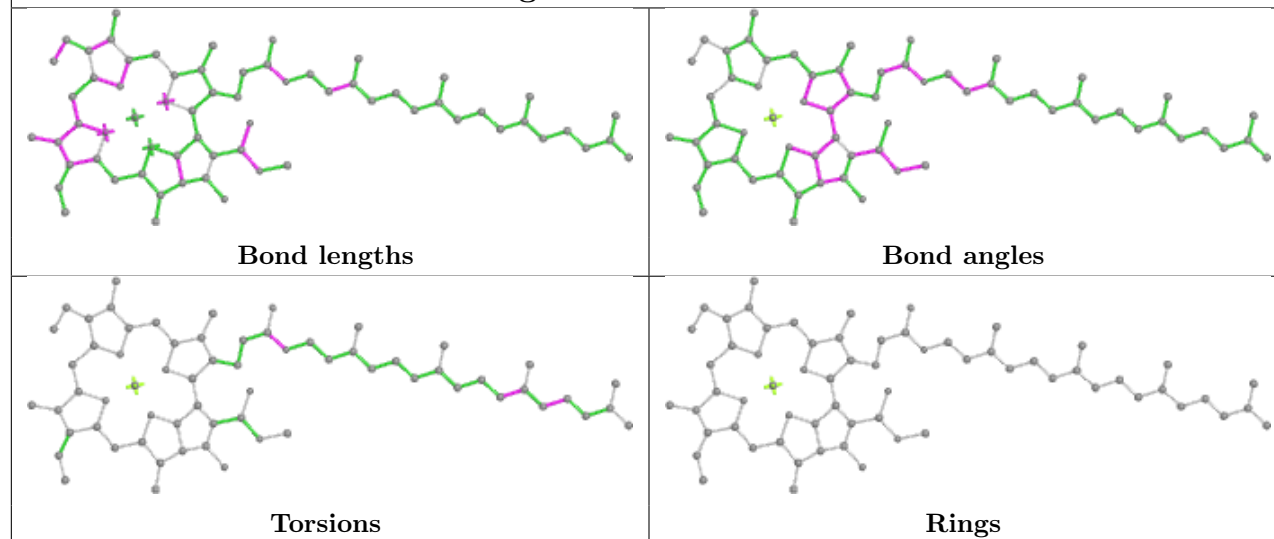
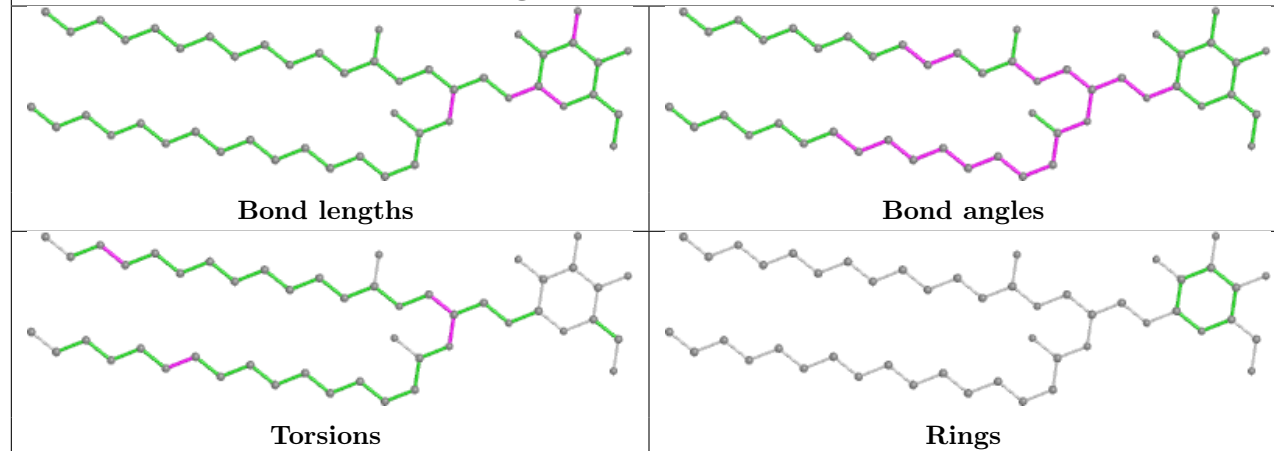
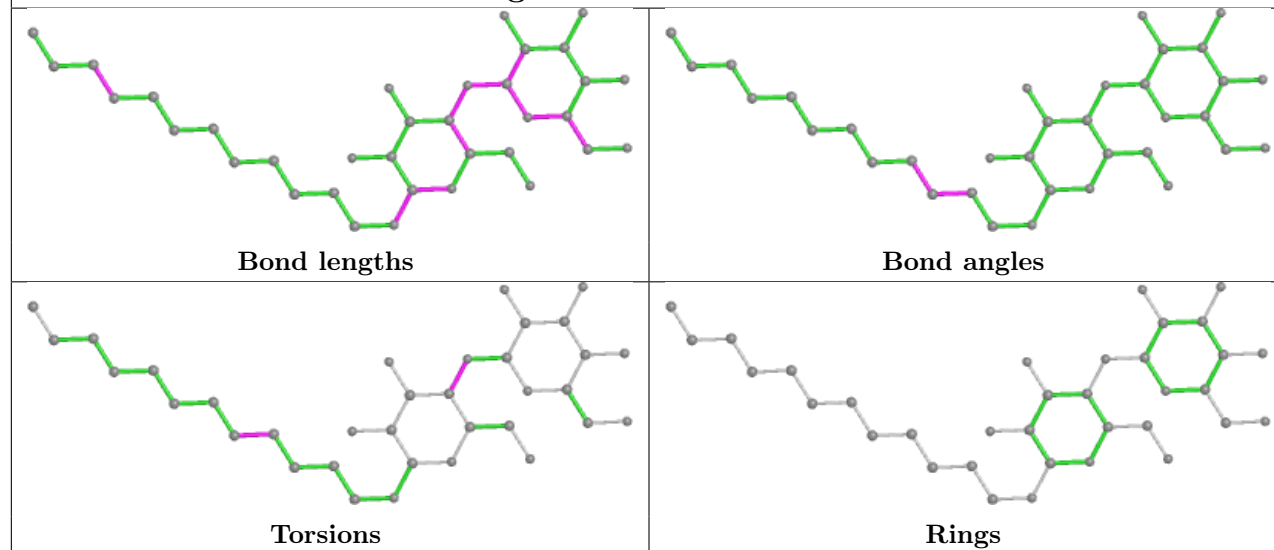


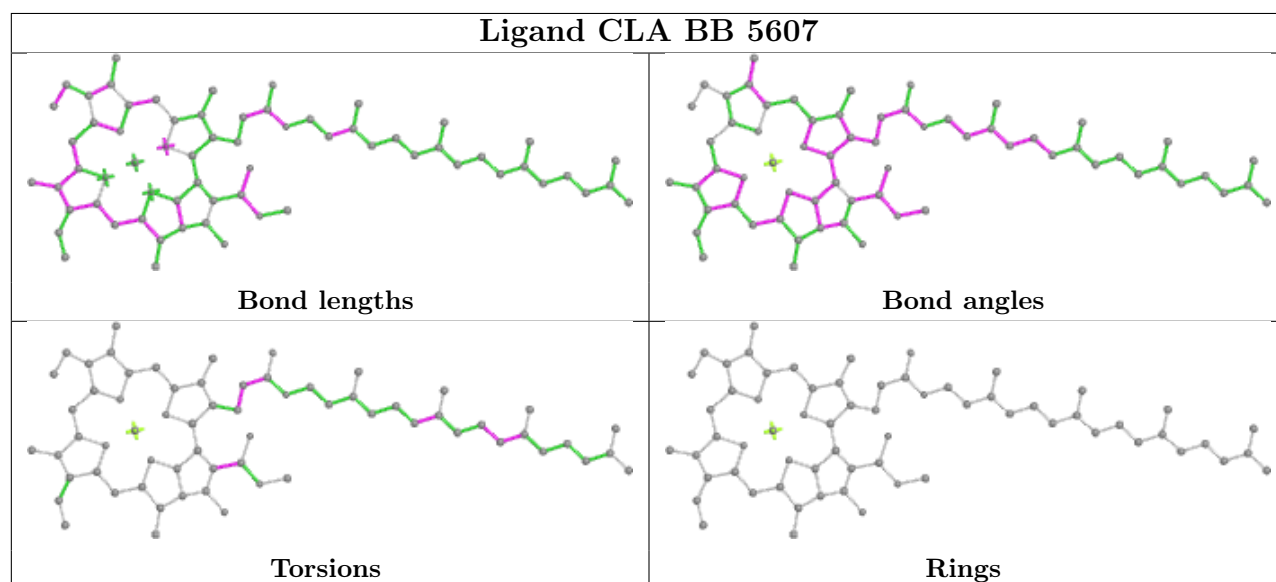
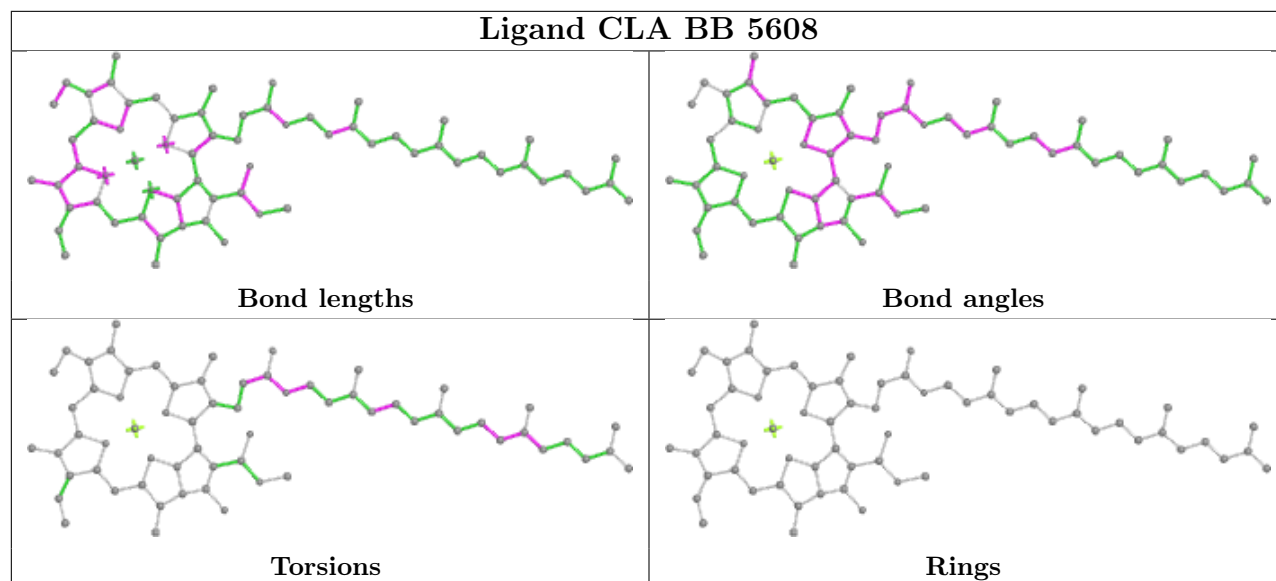
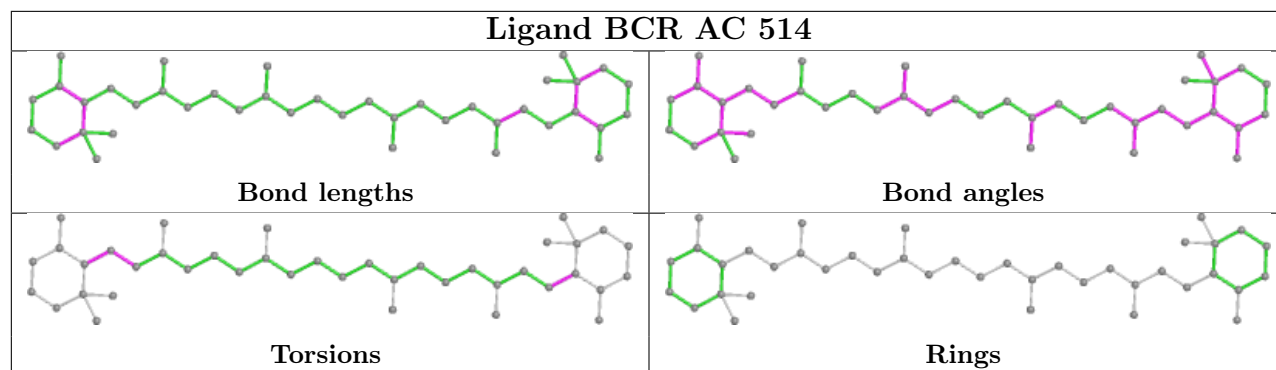
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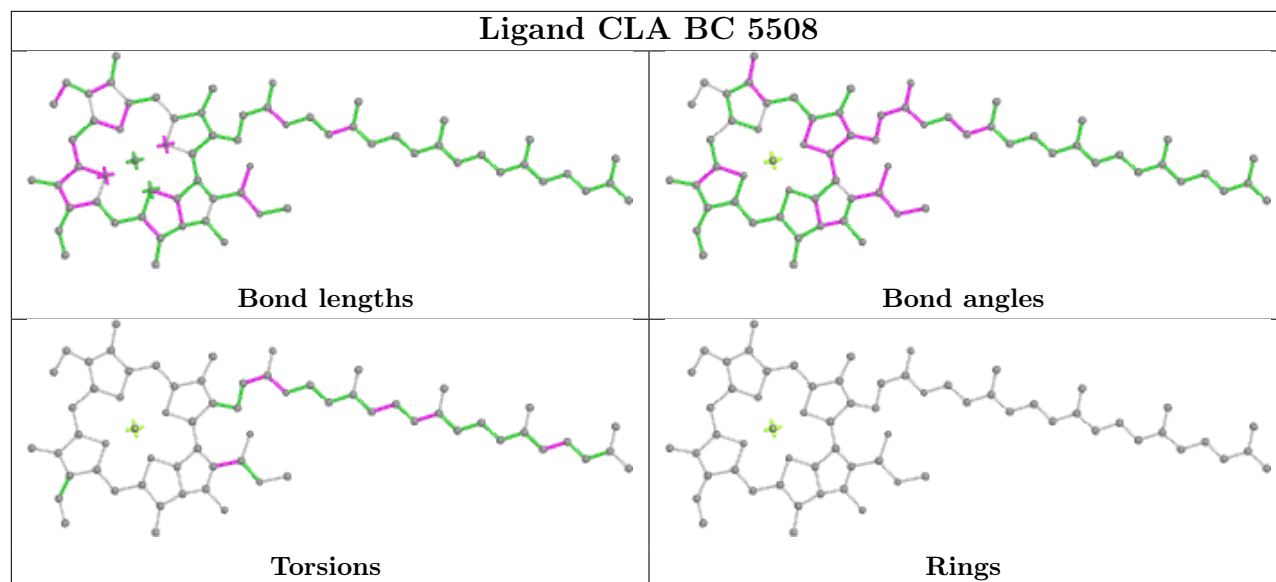
Ligand LMT BB 5603



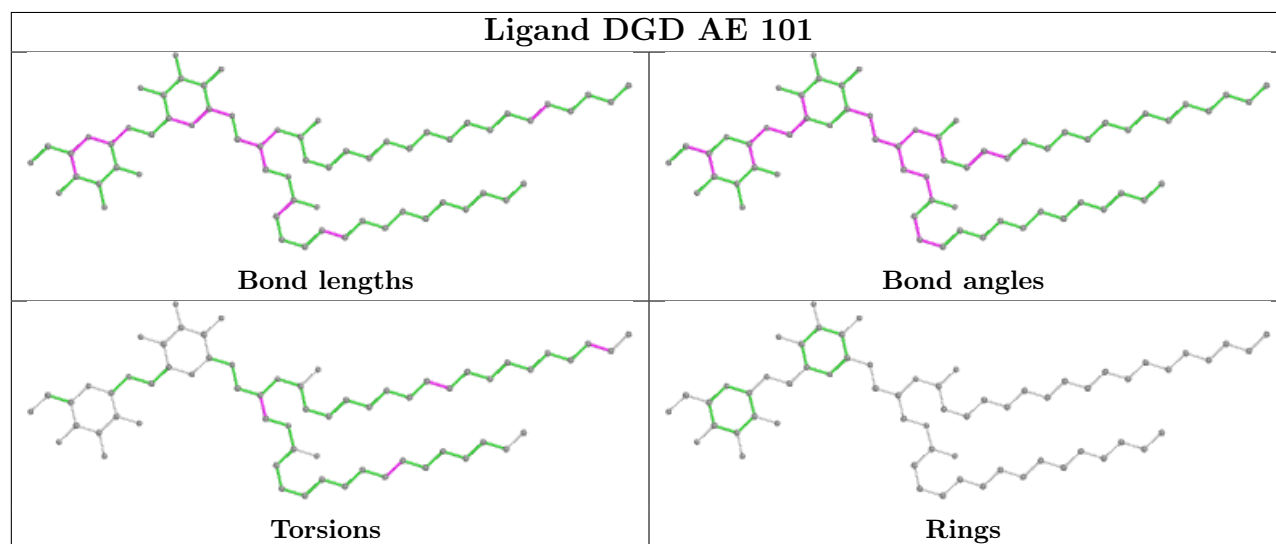
Ligand CLA AB 615**Ligand LMG AD 408****Ligand LMT BB 5604**



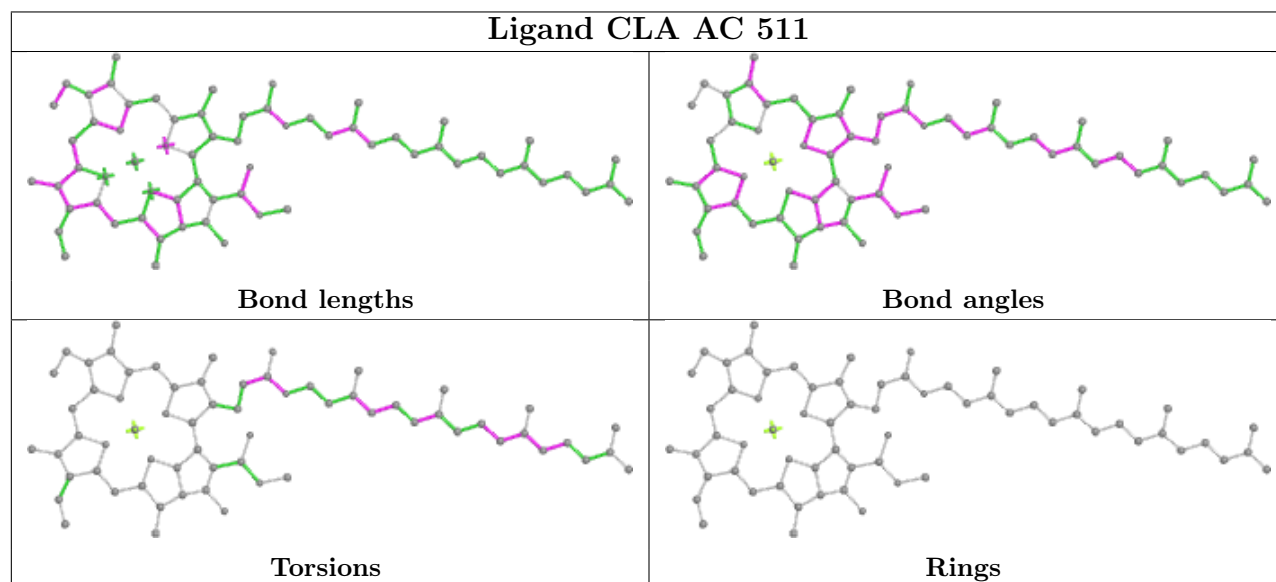
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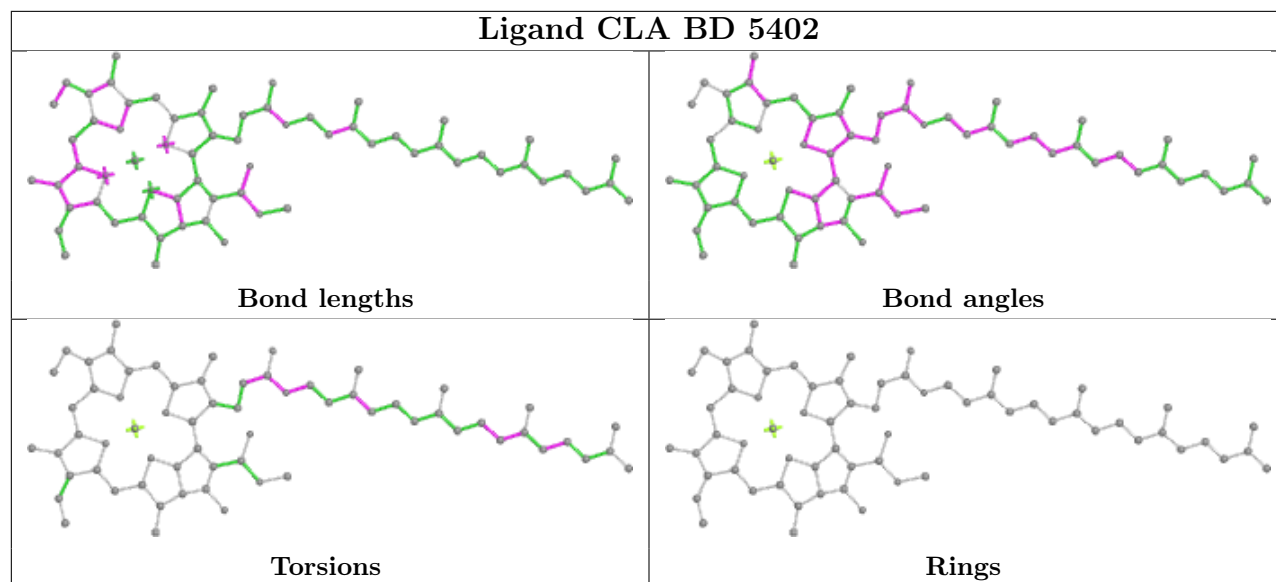
Ligand DGD AE 101



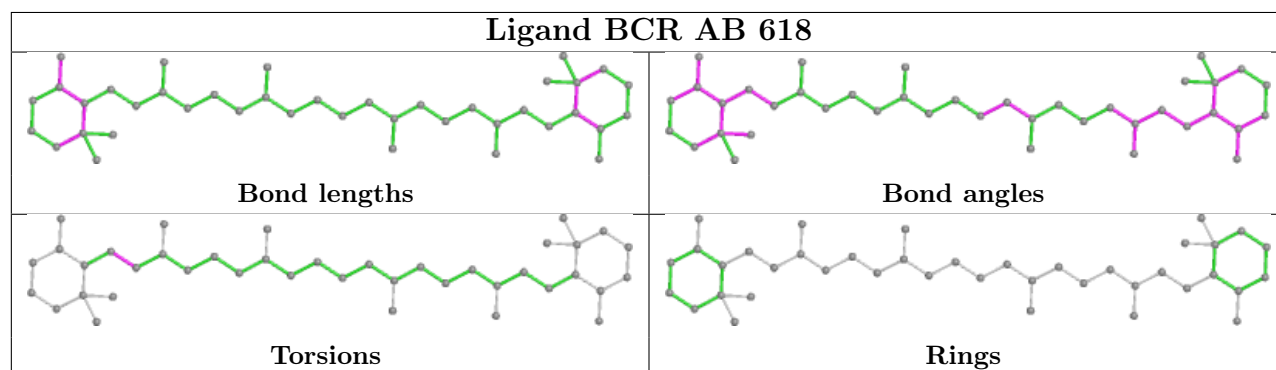
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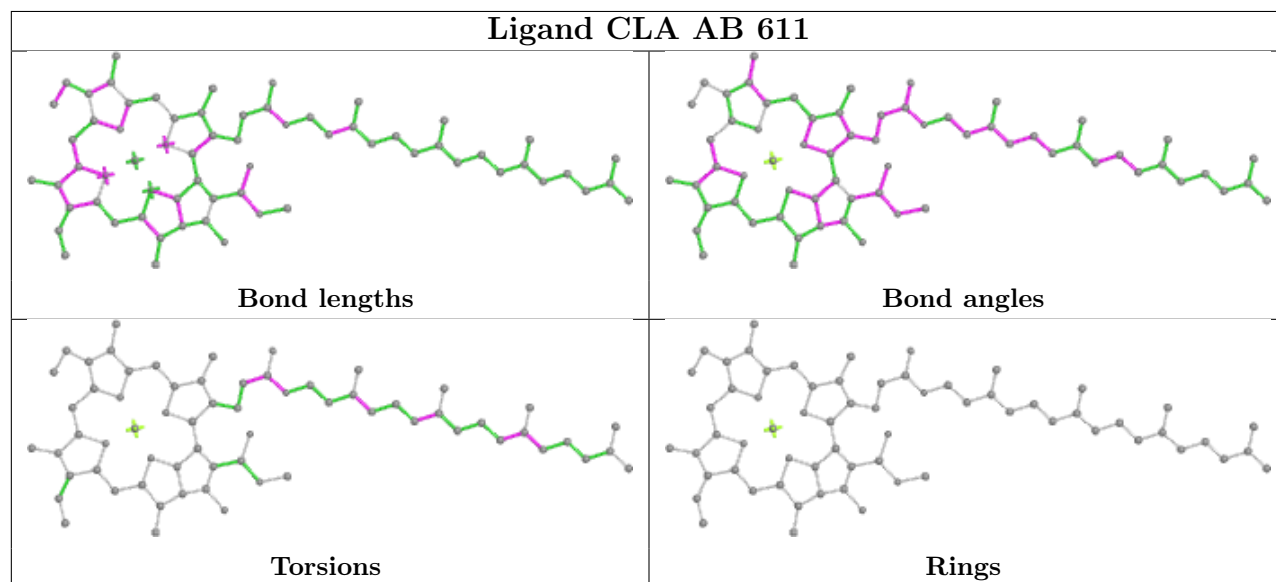
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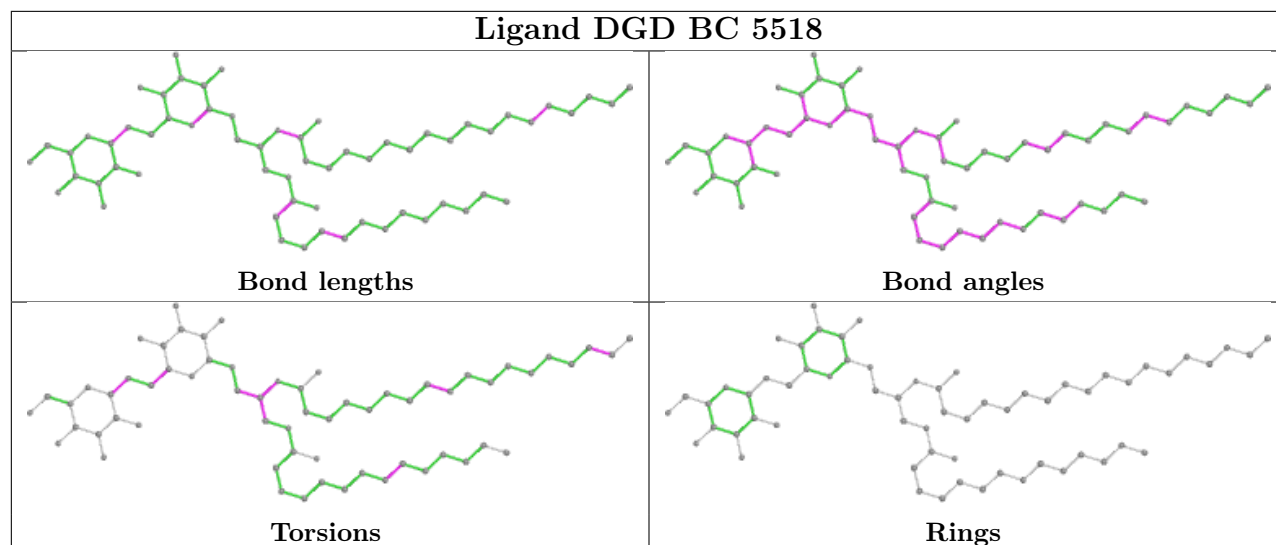
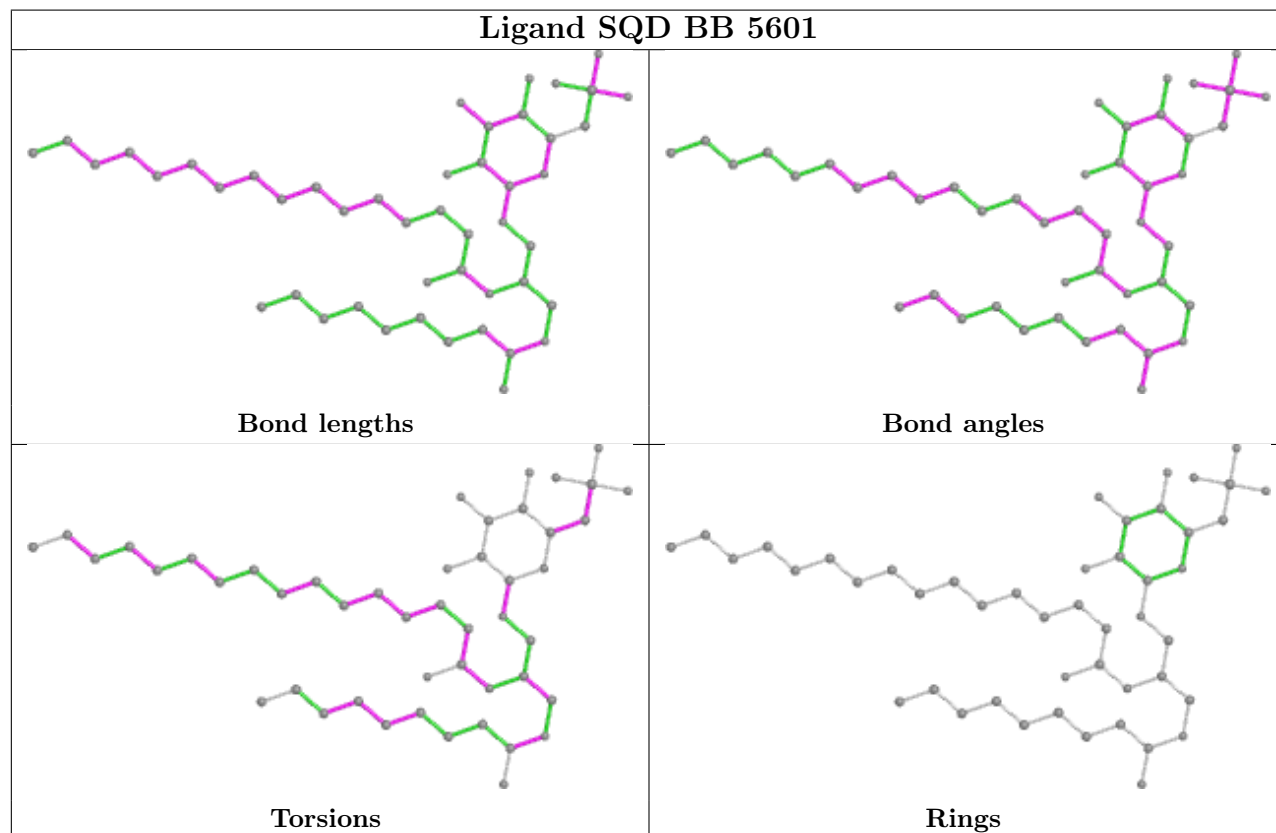


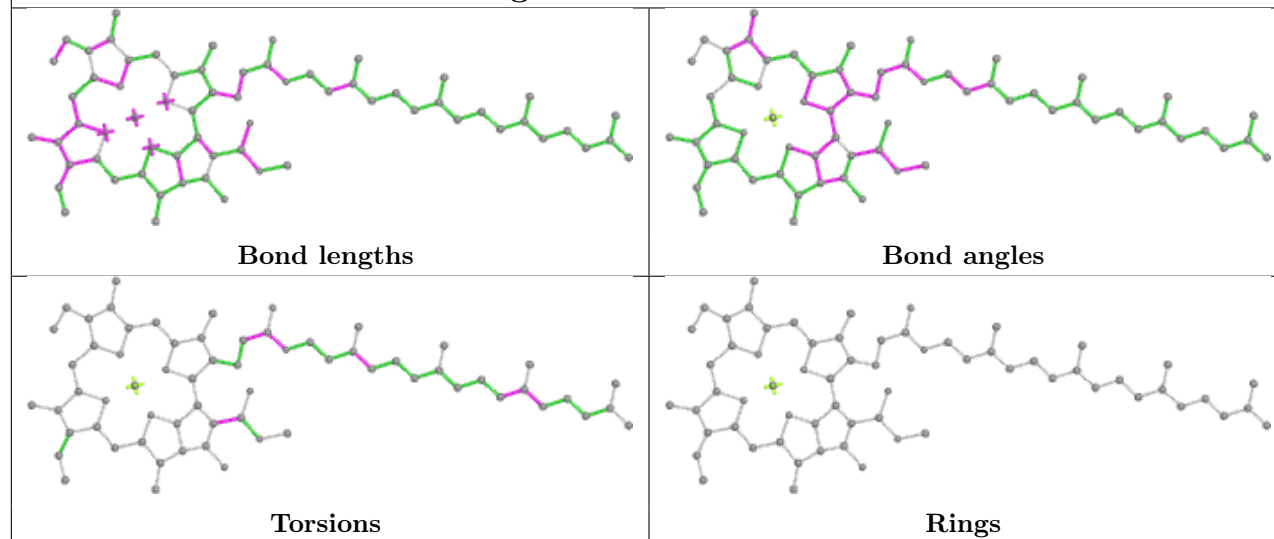
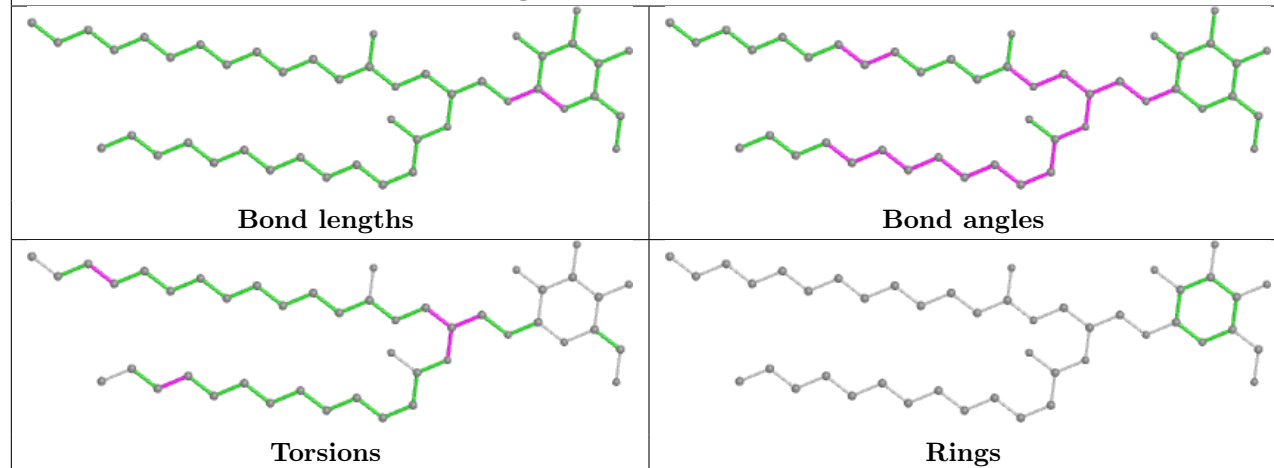
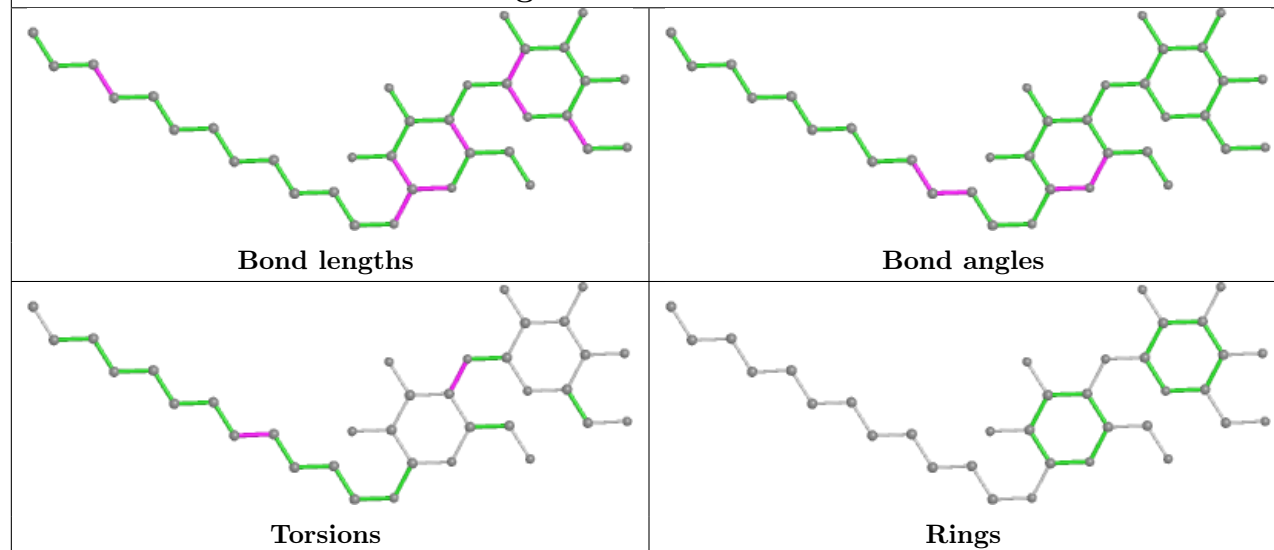
Ligand BCR AB 618



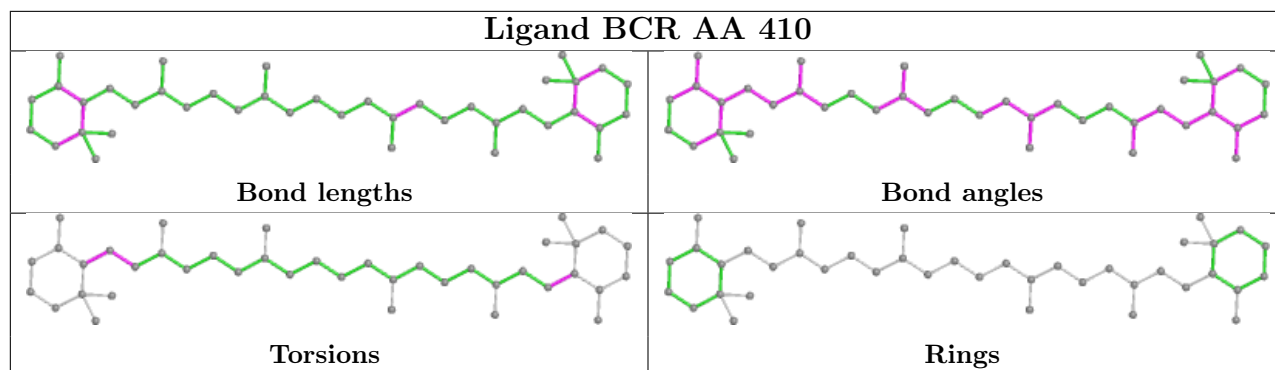
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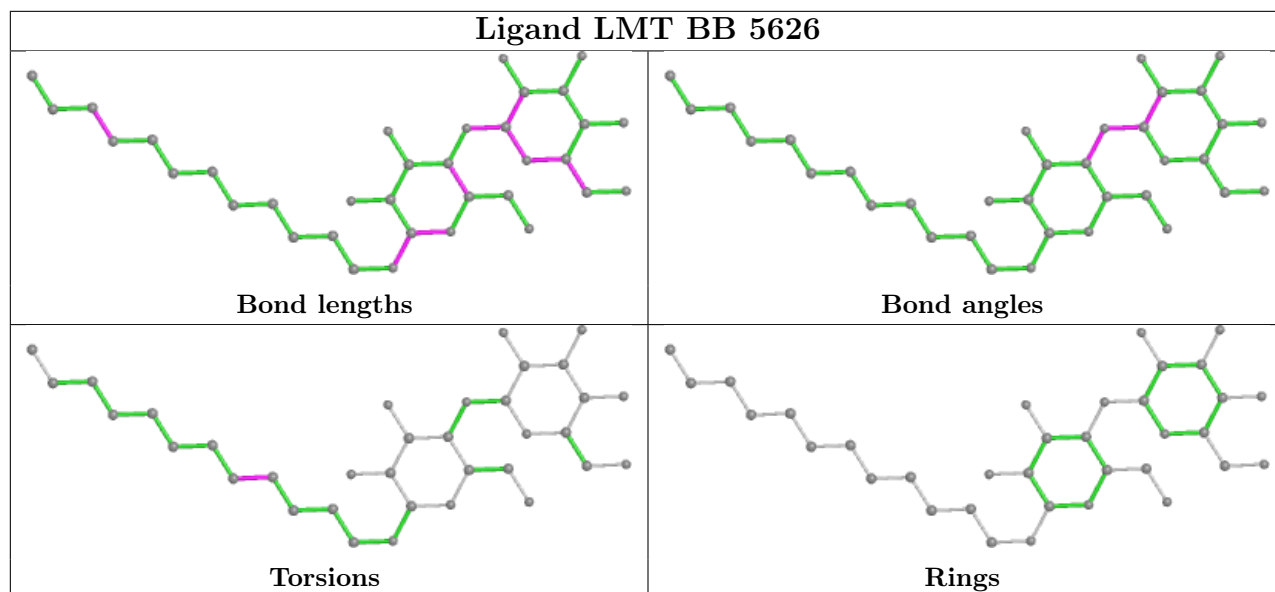
Ligand DGD BC 5518**Ligand SQD BB 5601**

Ligand CLA BC 5505**Ligand LMG AC 521****Ligand LMT AB 624**

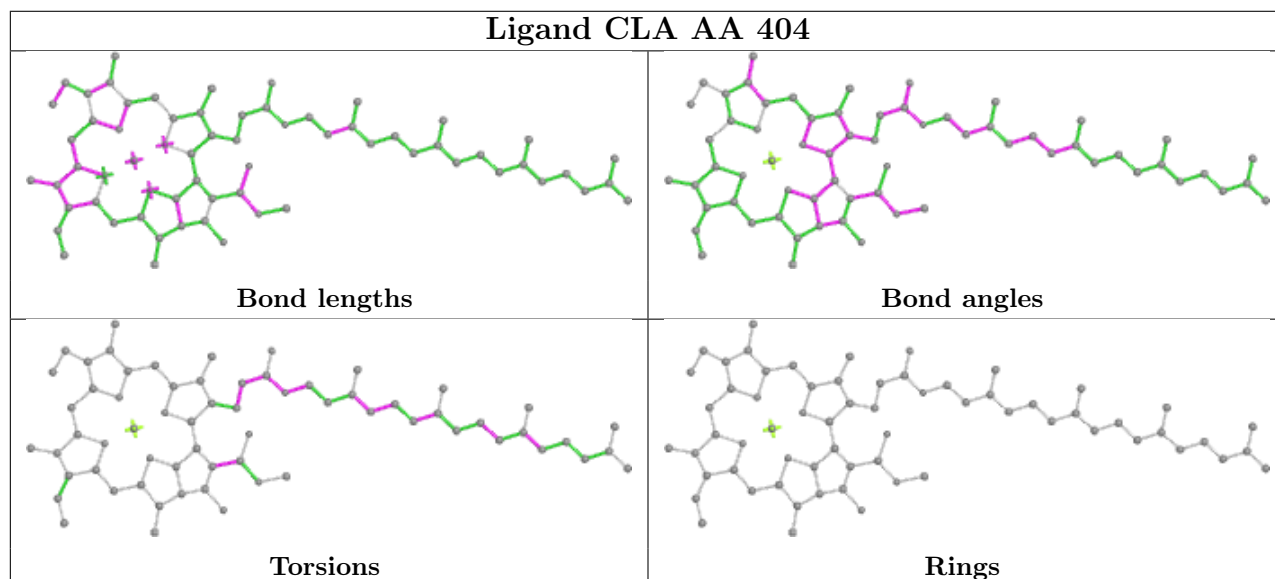
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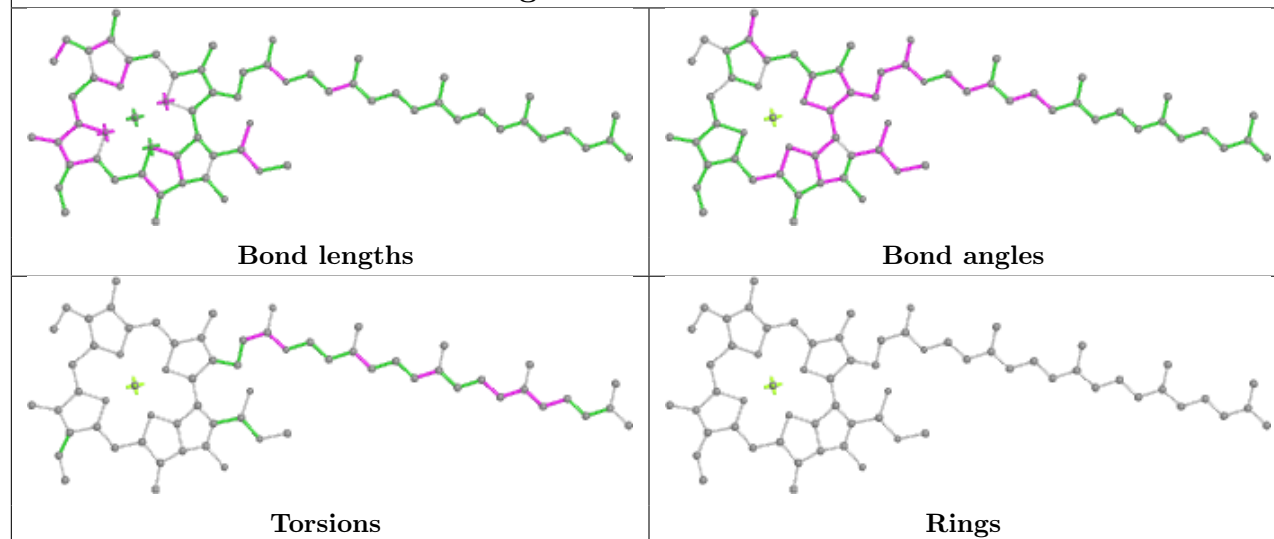
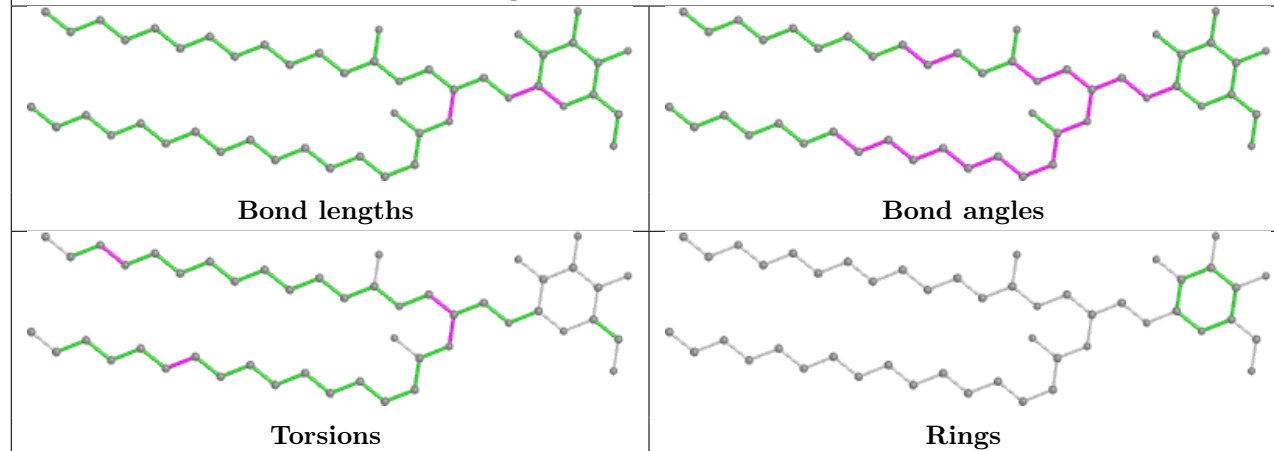
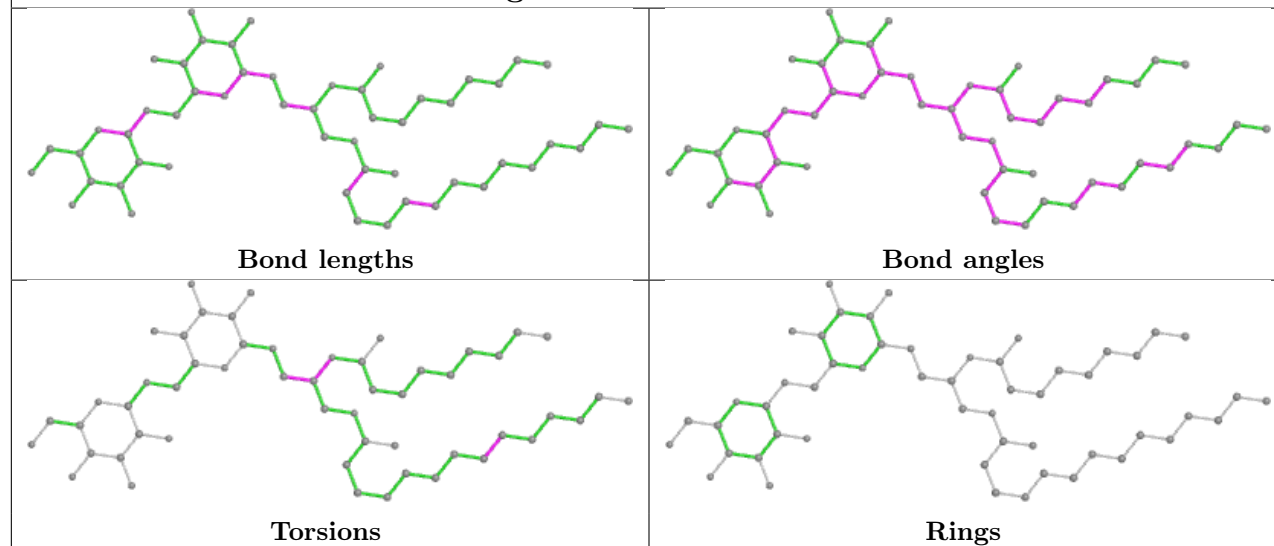


Ligand LMT BB 5626

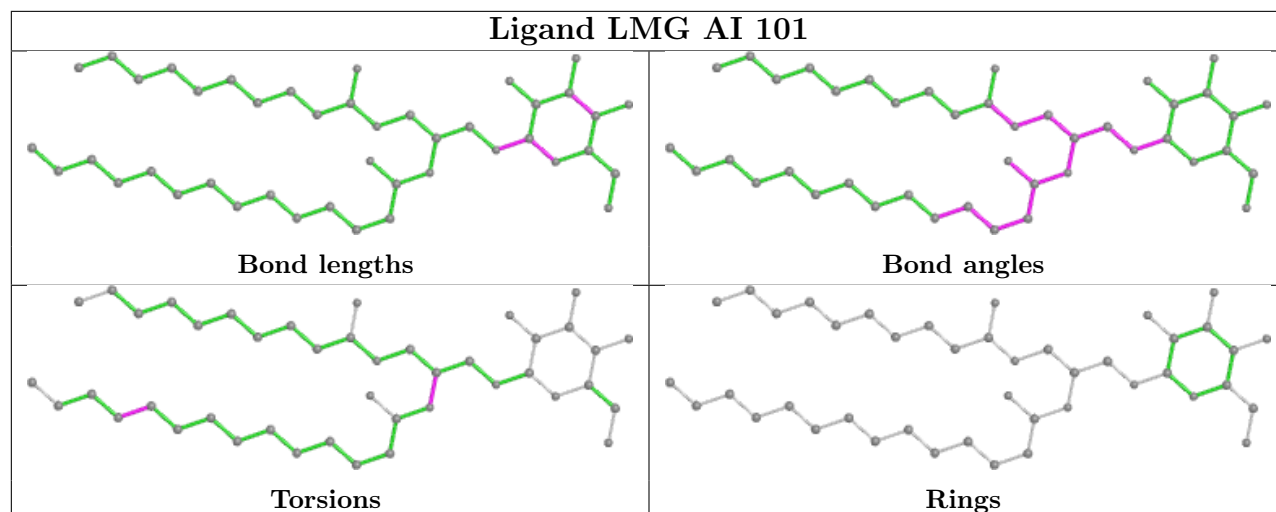


Ligand CLA AA 404

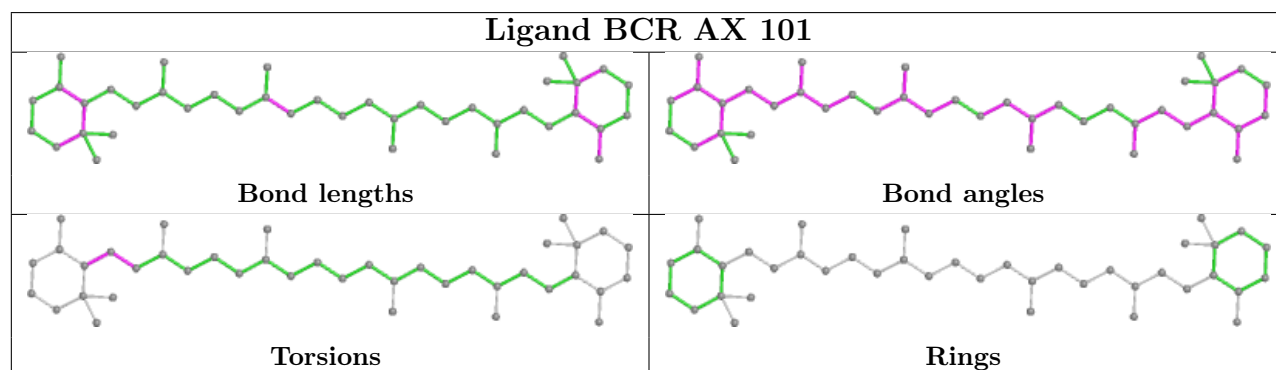


Ligand CLA AC 503**Ligand LMG BD 5410****Ligand DGD BC 5517**

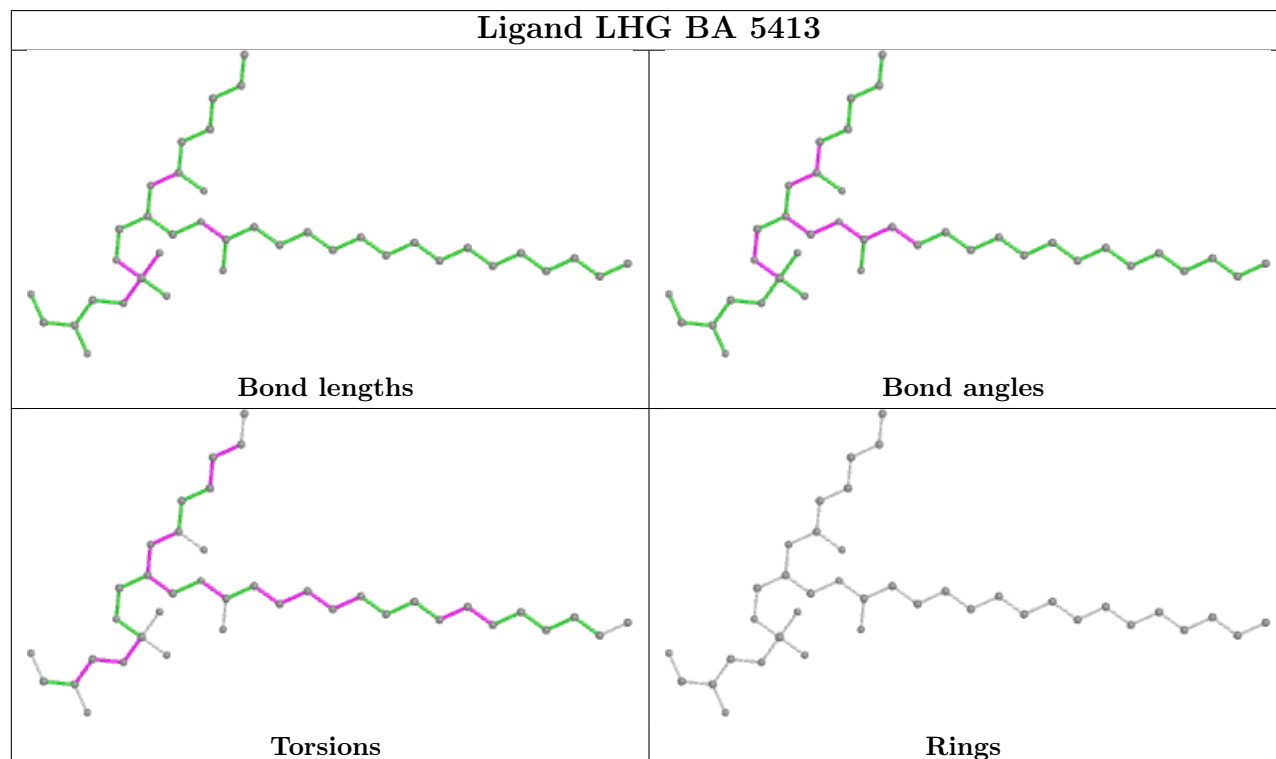
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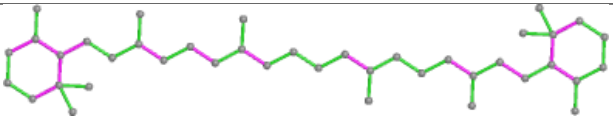
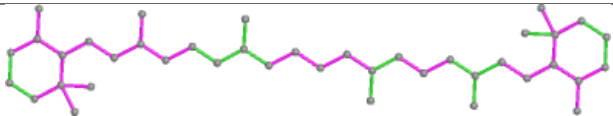
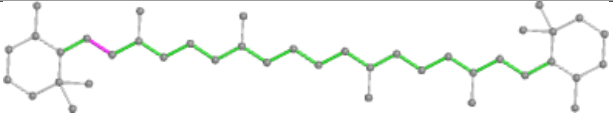
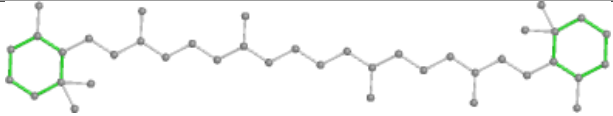


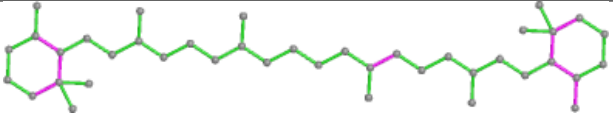
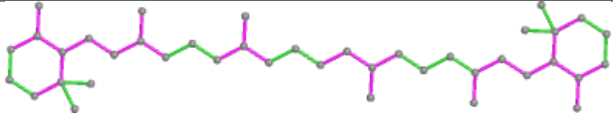
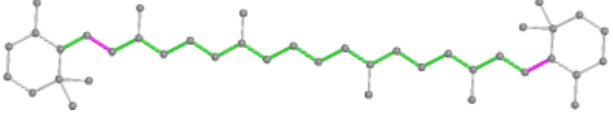
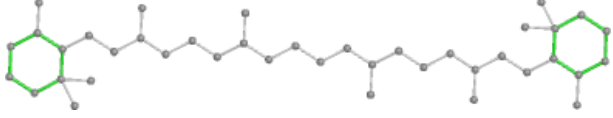
Ligand BCR AX 101

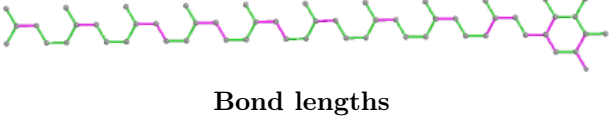
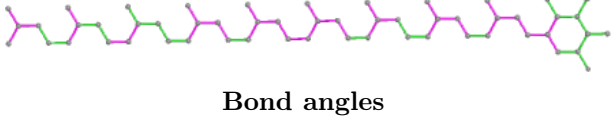
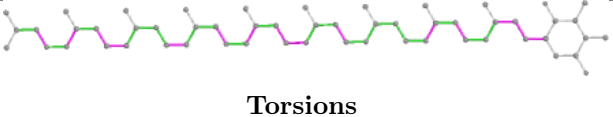
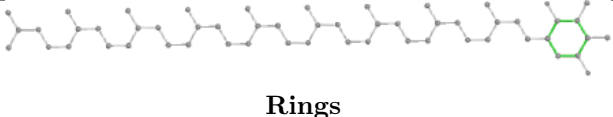


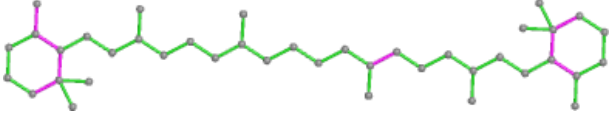
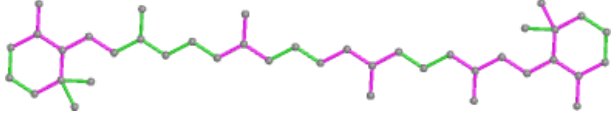
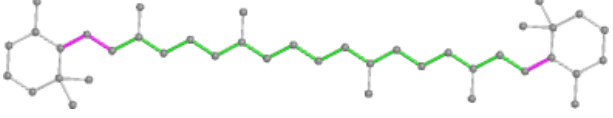
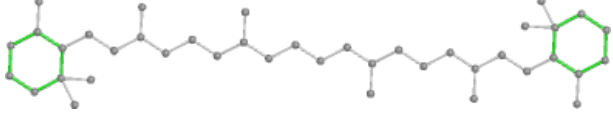
Ligand LHG BA 5413

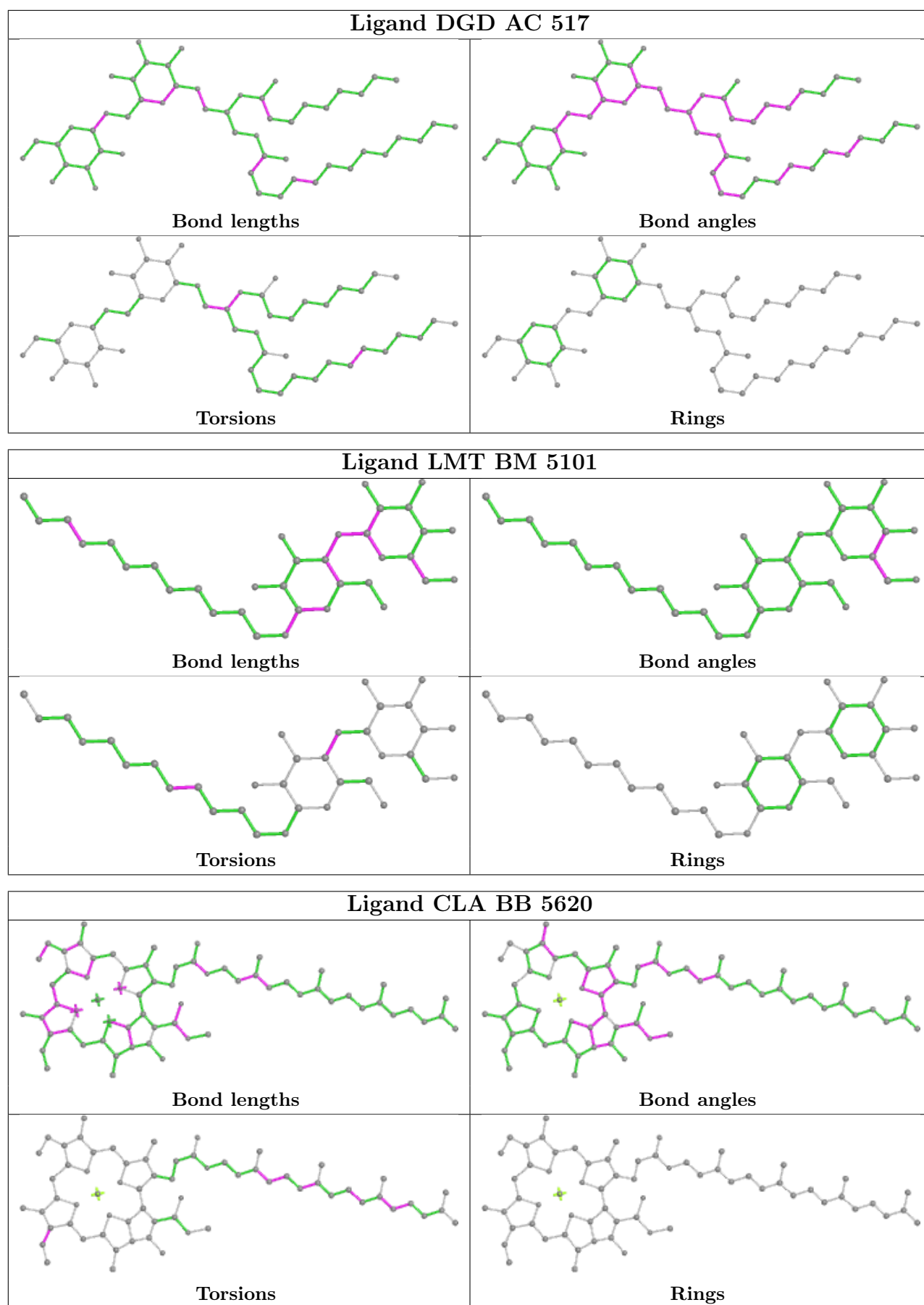


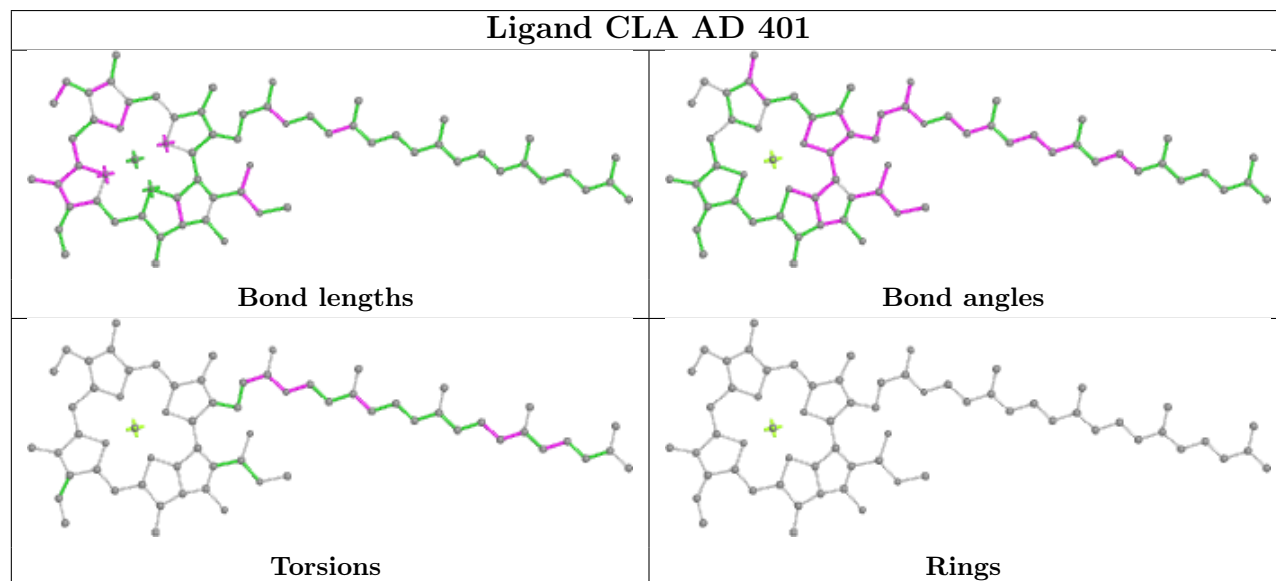
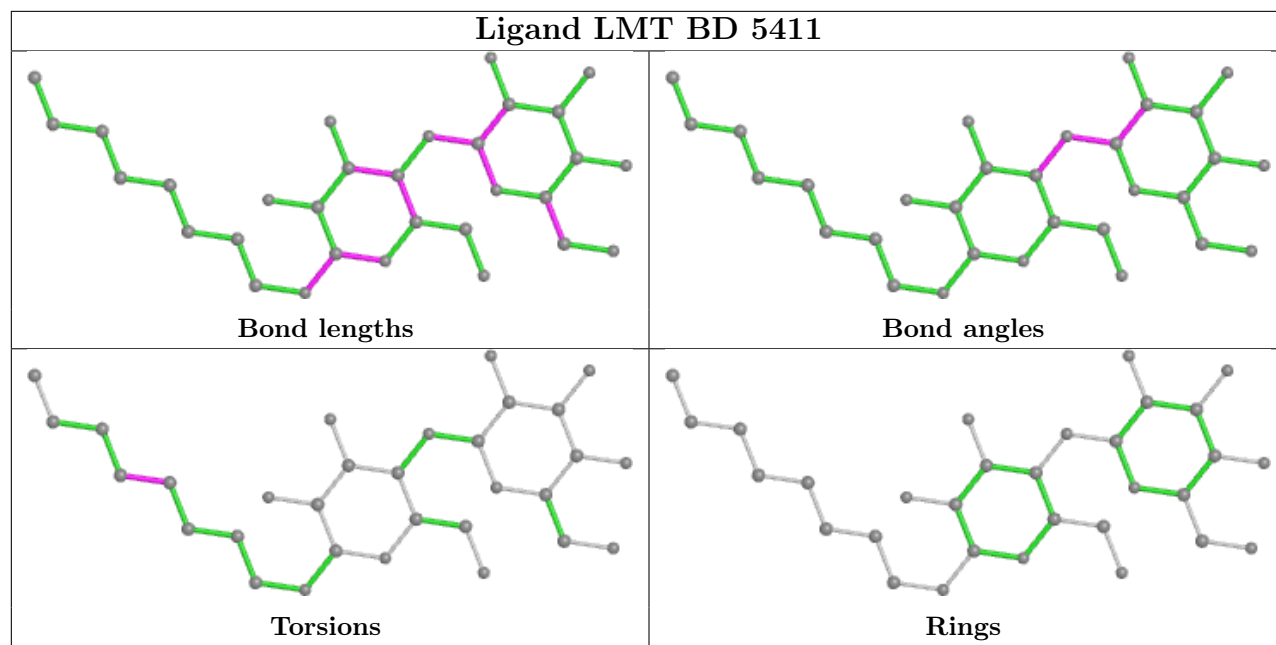
Ligand BCR BJ 5101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BC 5515	
	
Bond lengths	Bond angles
	
Torsions	Rings

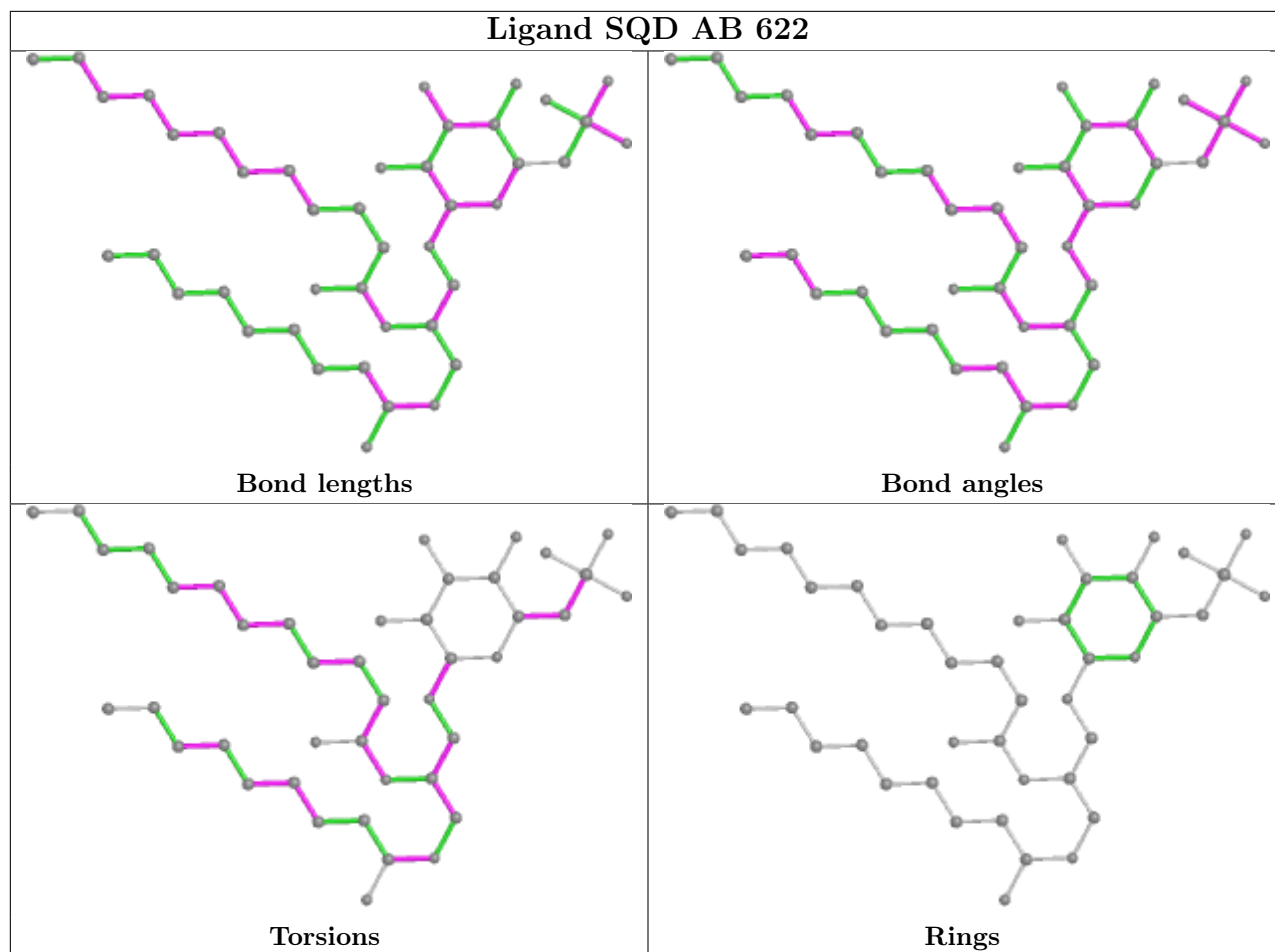
Ligand PL9 BD 5406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR AC 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

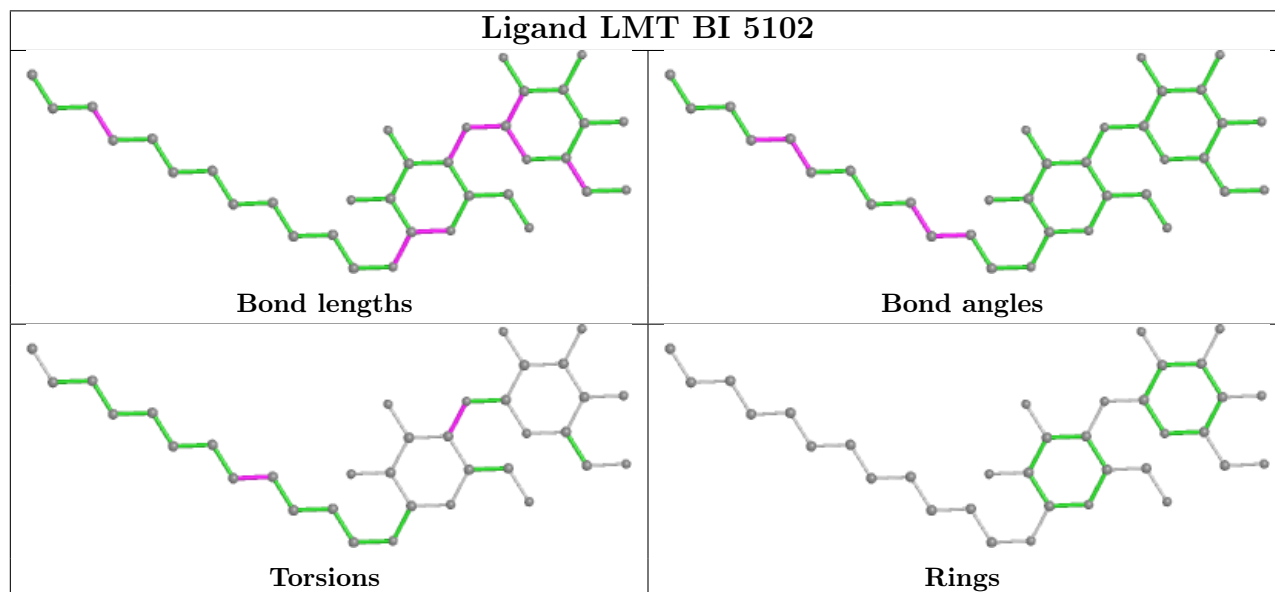




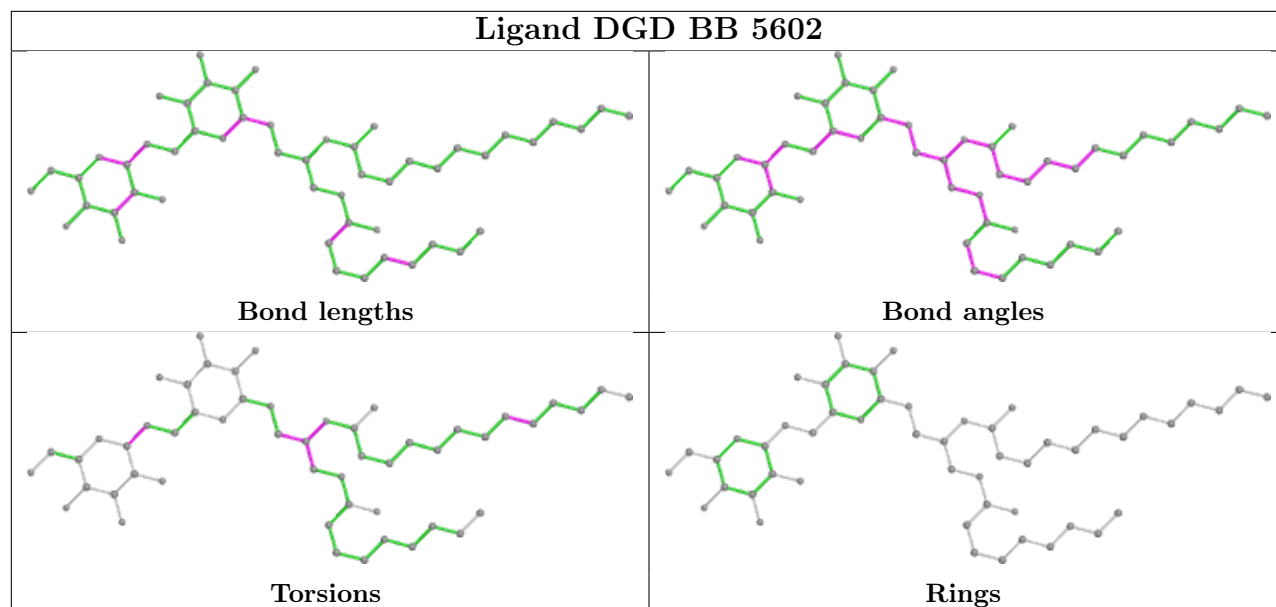
Ligand SQD AB 622



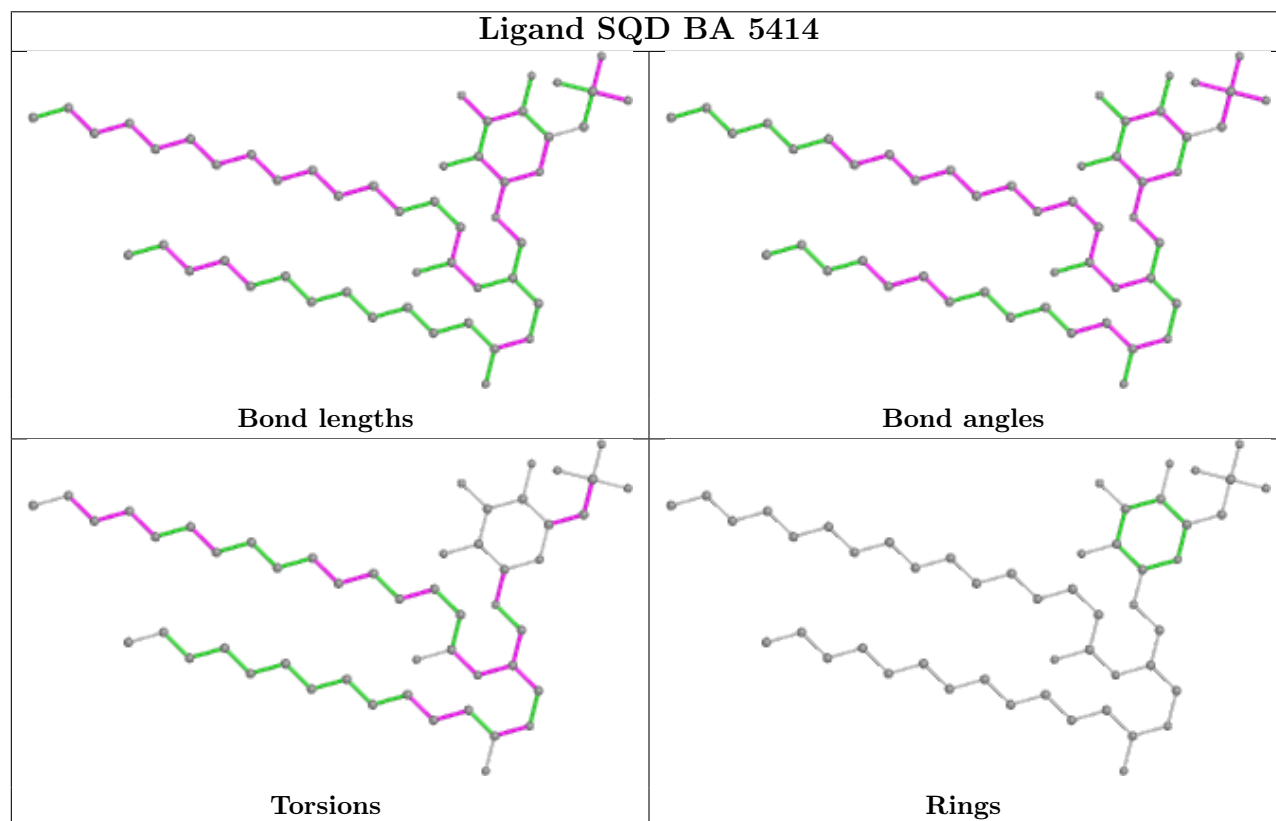
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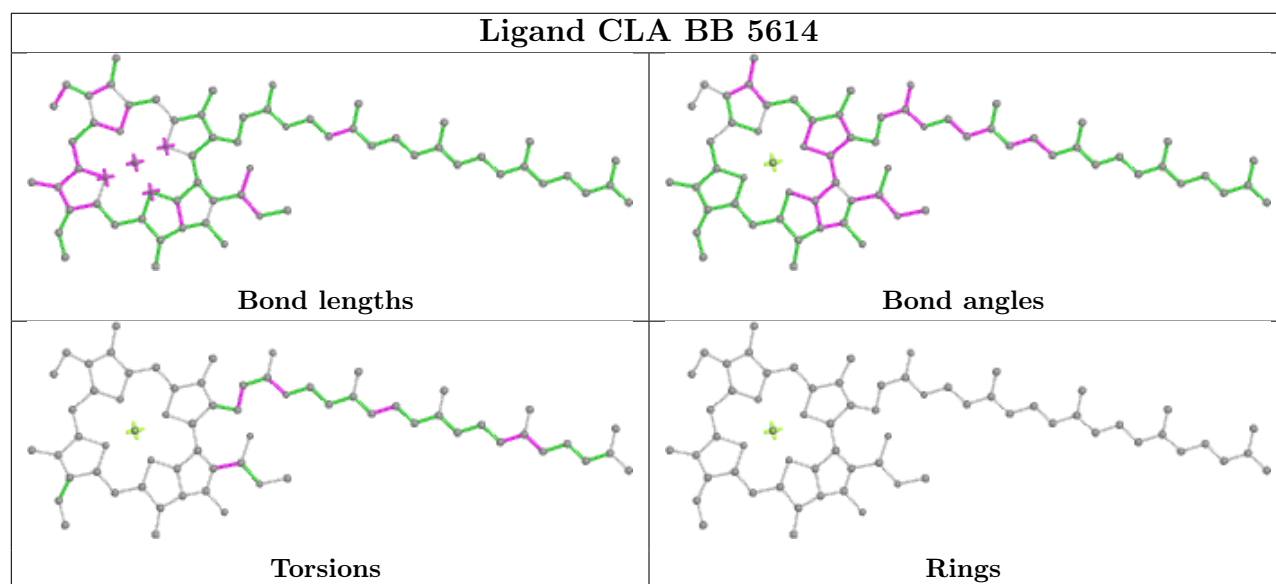
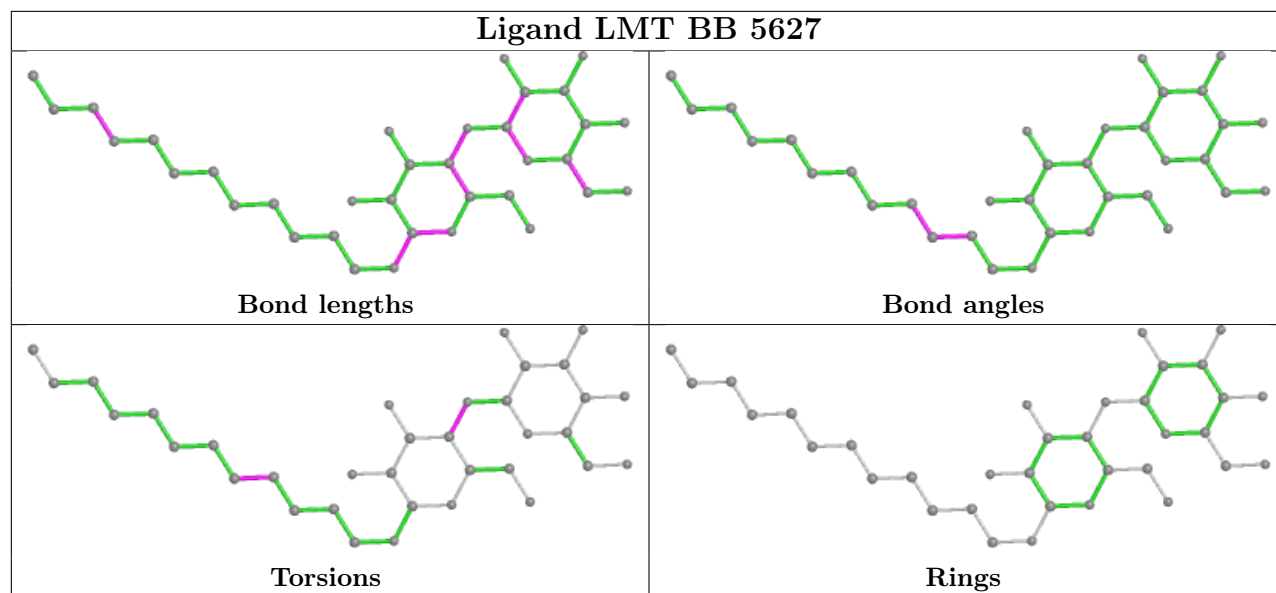


Ligand DGD BB 5602

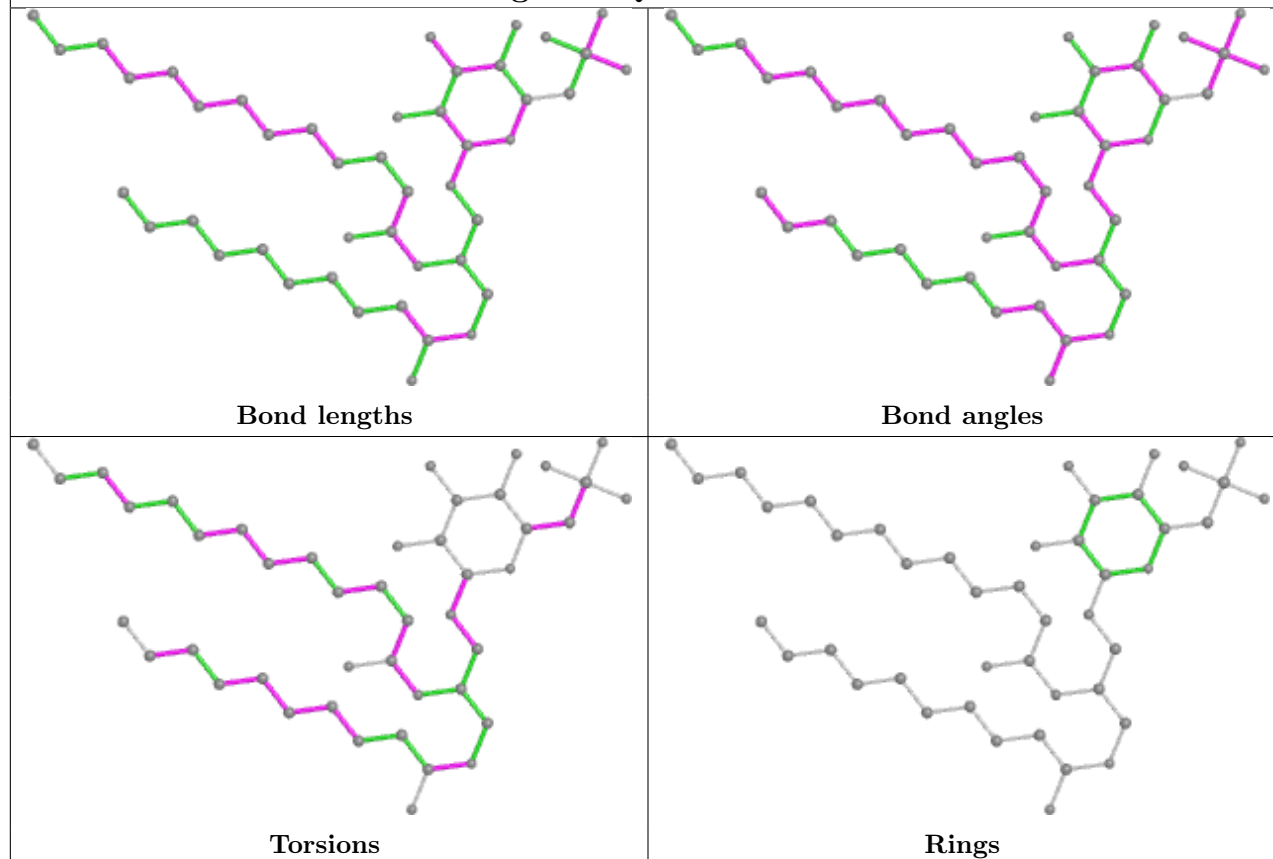


Ligand SQD BA 5414

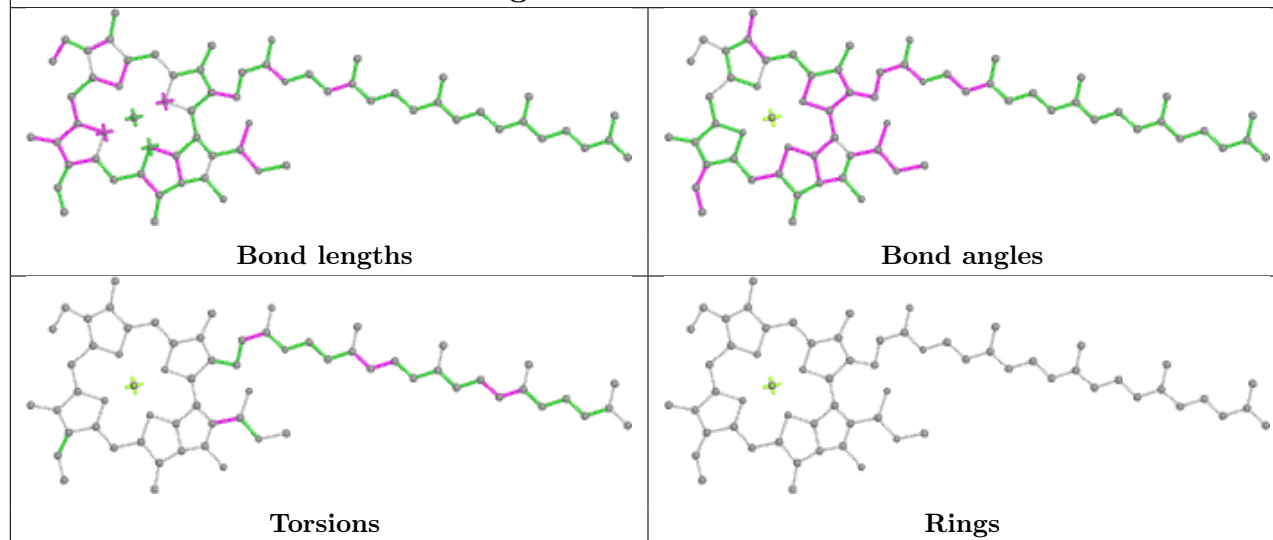


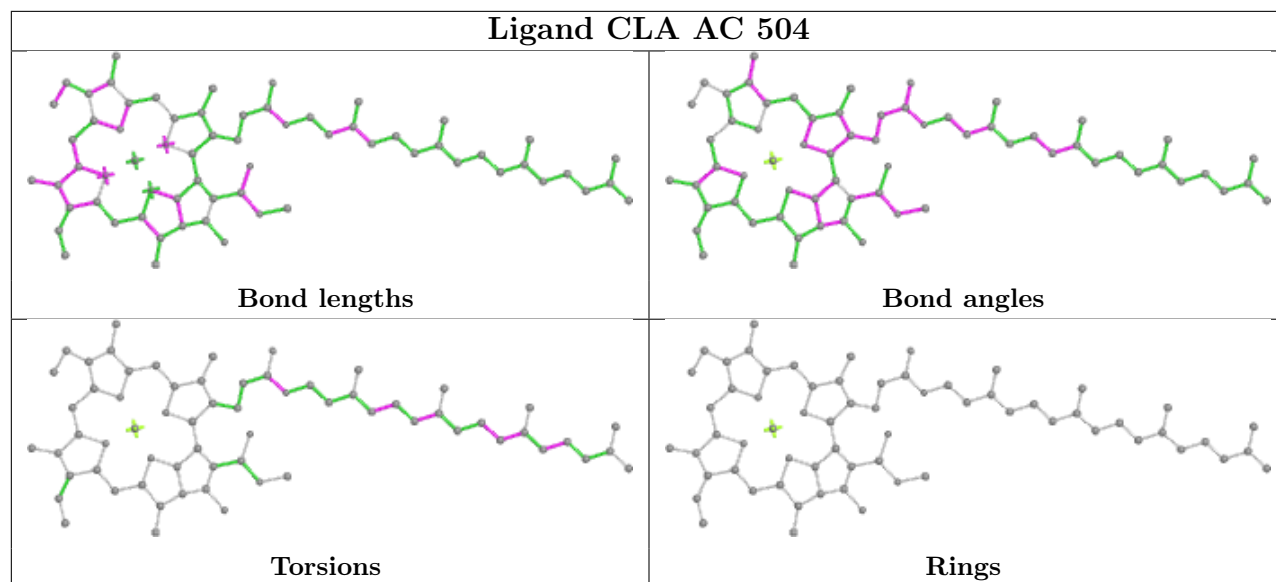
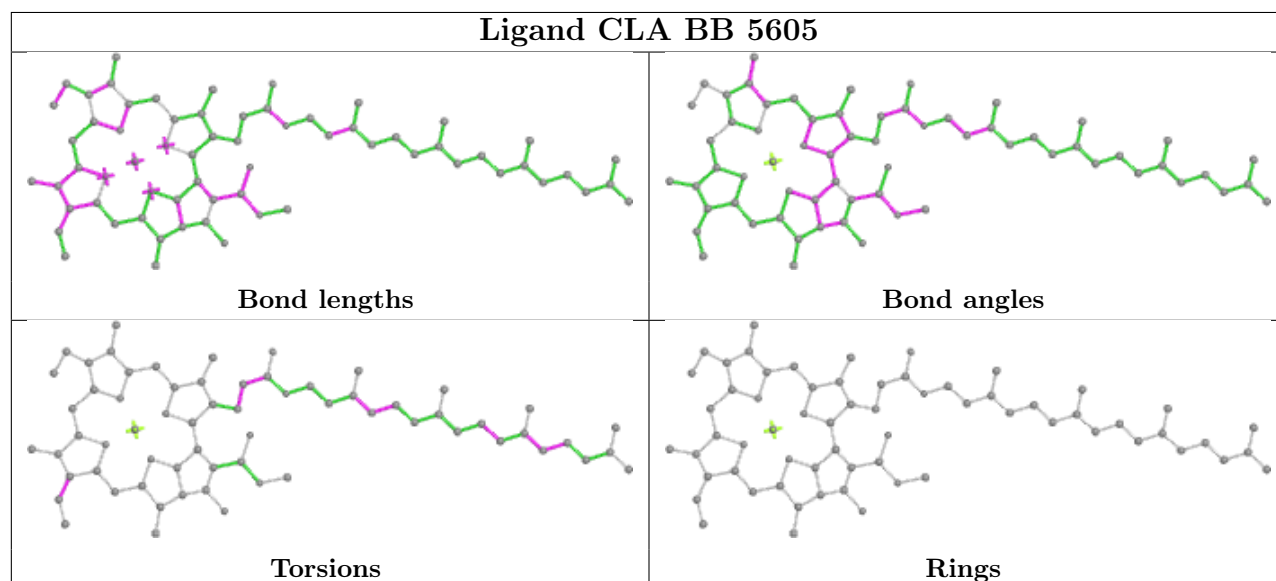
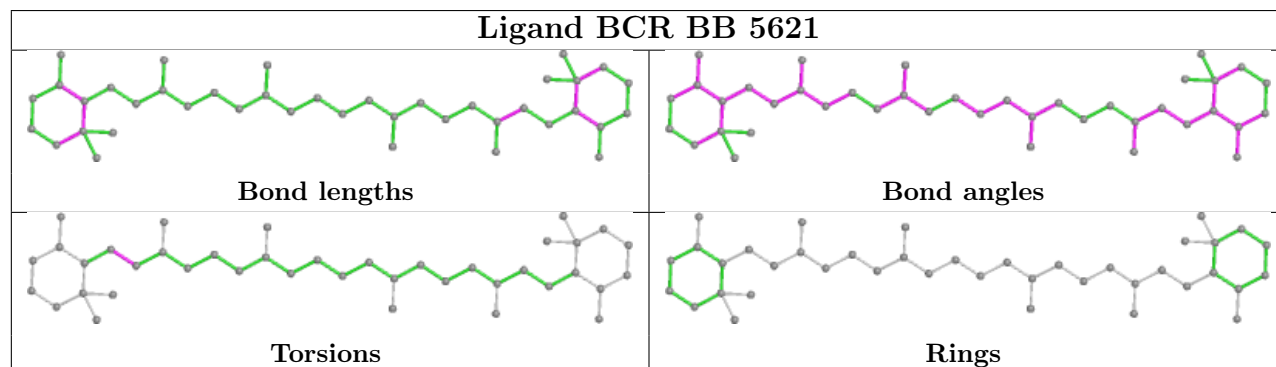


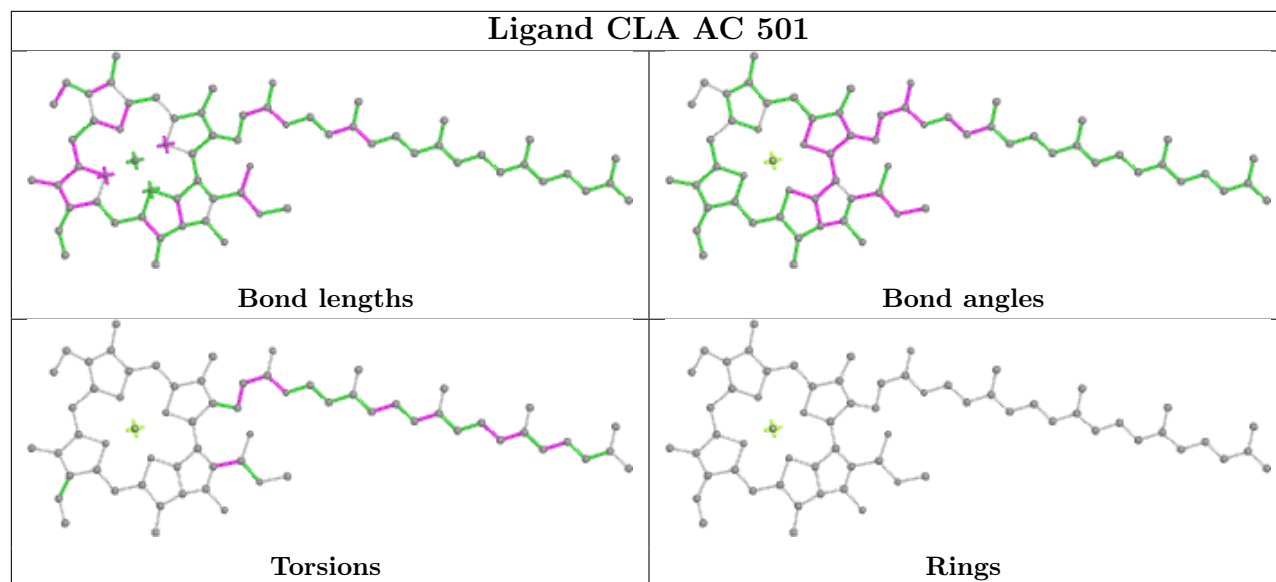
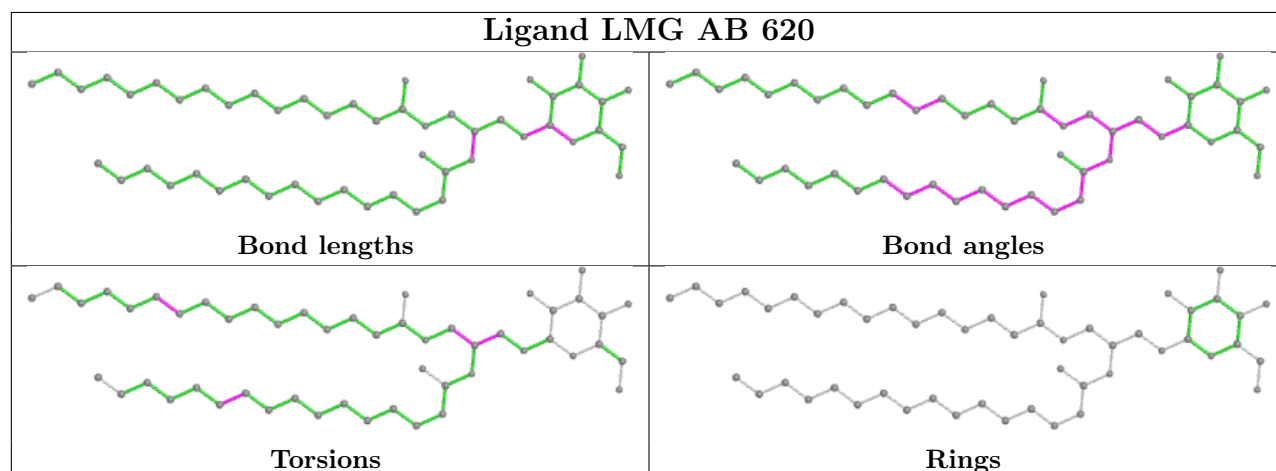
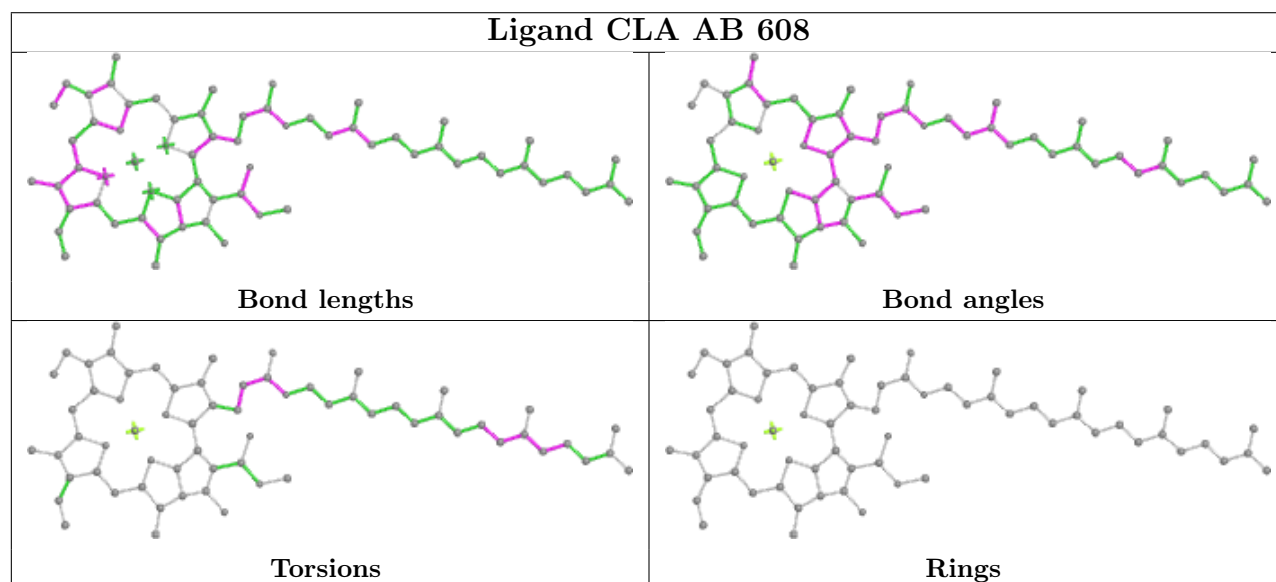
Ligand SQD BF 5102

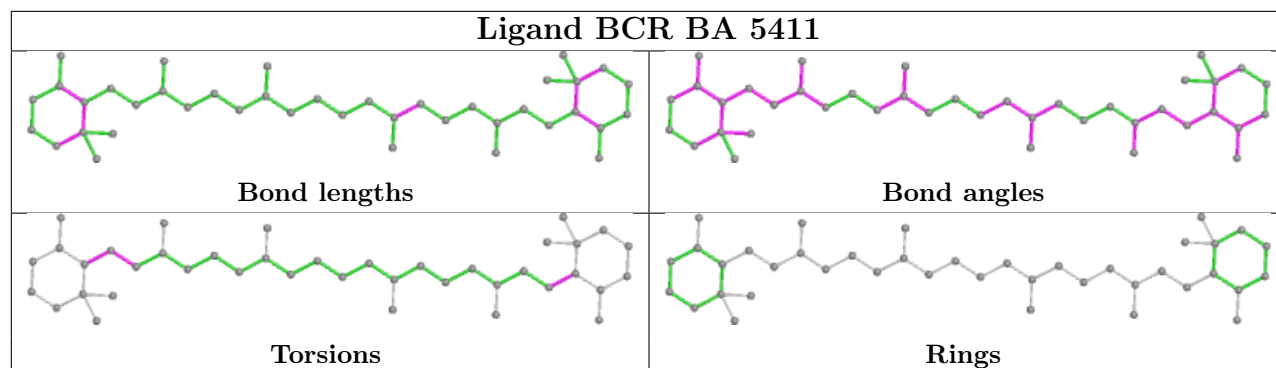
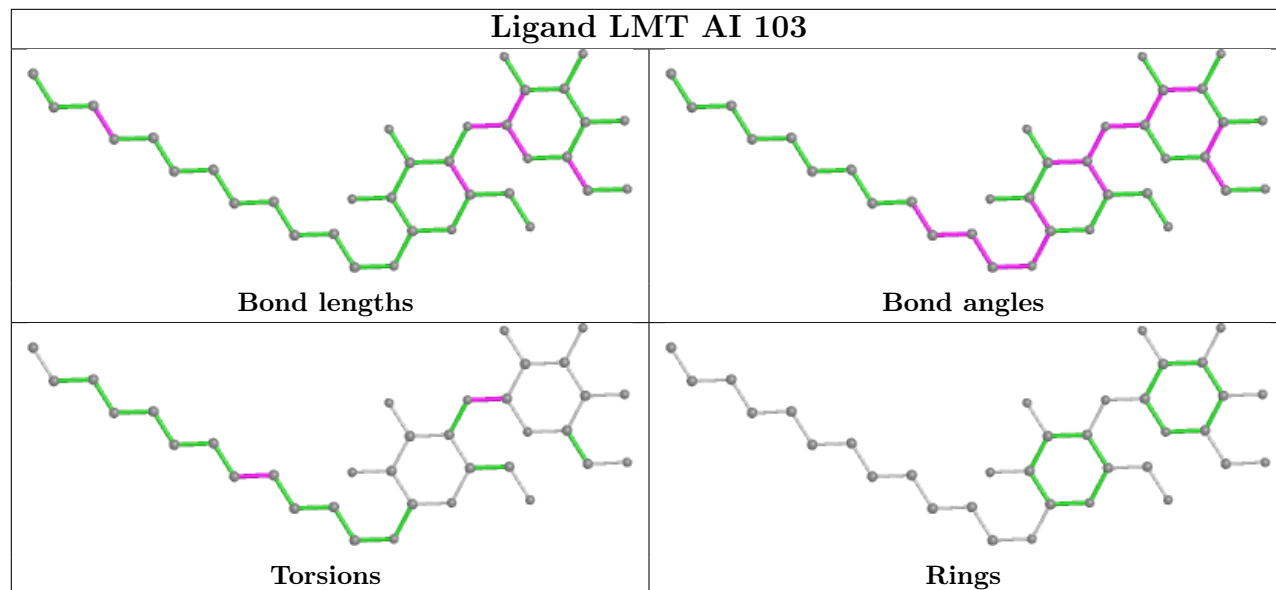
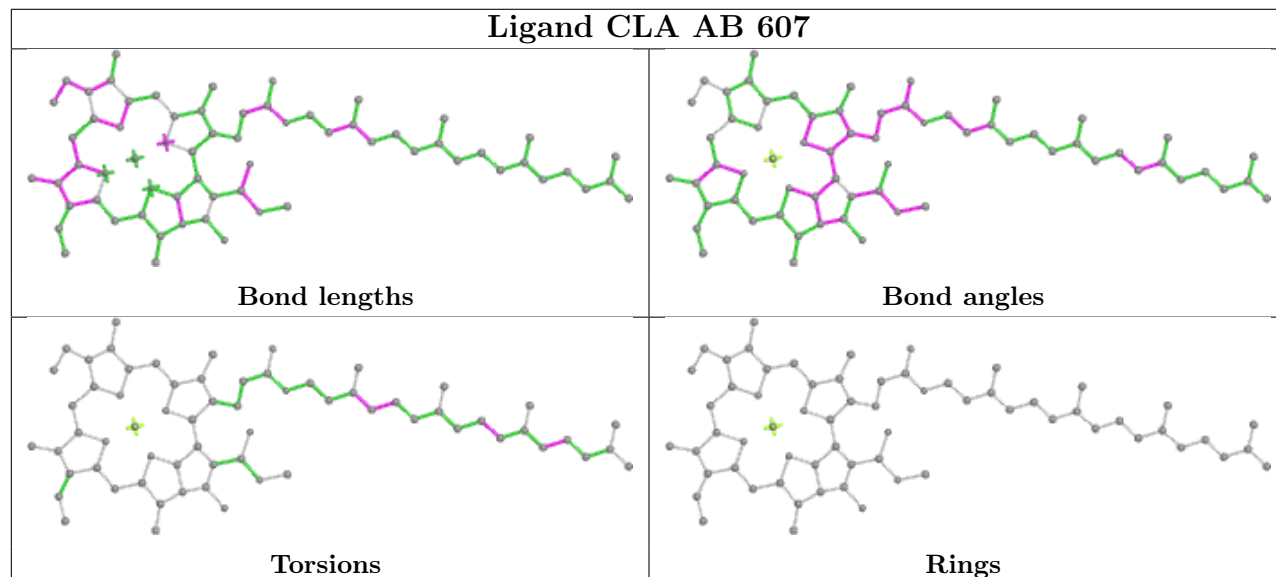


Ligand CLA BB 5609

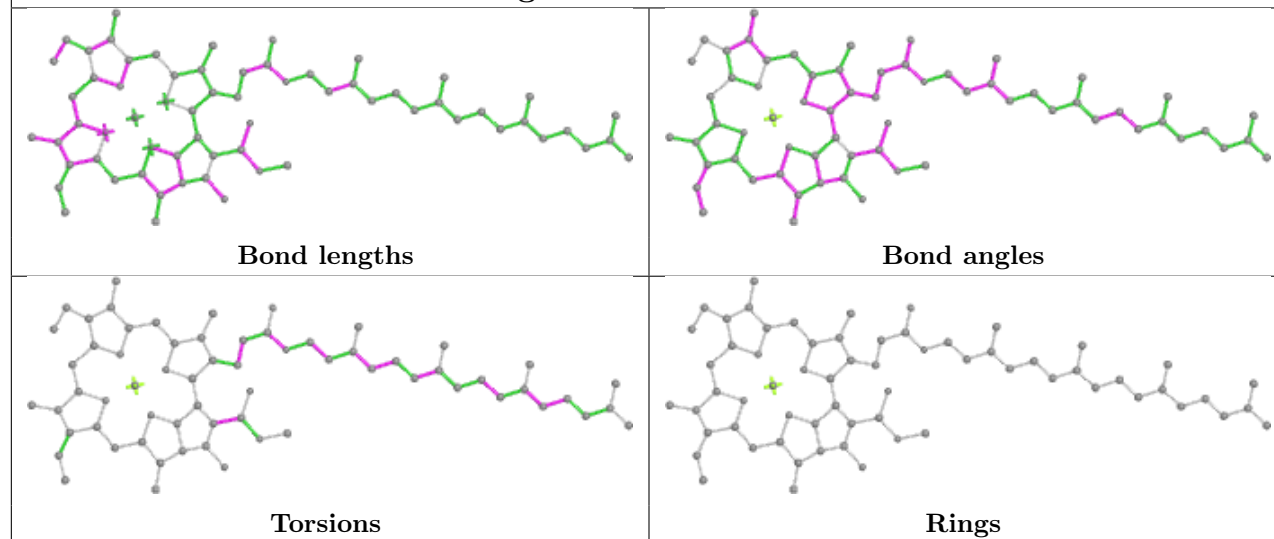


Ligand CLA AC 504**Ligand CLA BB 5605****Ligand BCR BB 5621**

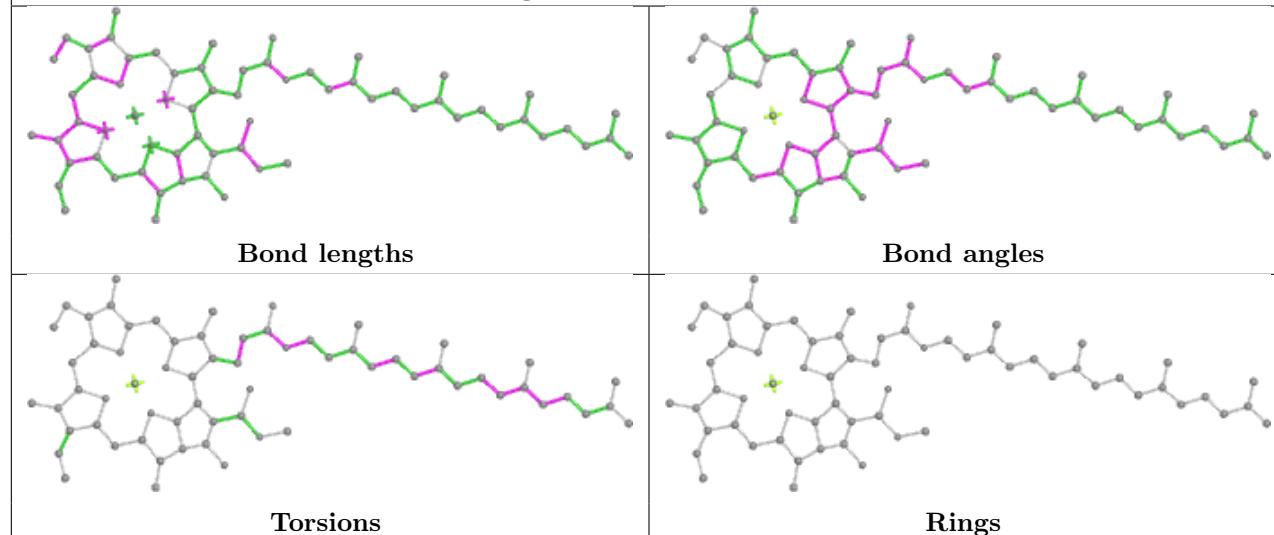
Ligand CLA AC 501**Ligand LMG AB 620****Ligand CLA AB 608**

Ligand BCR BA 5411**Ligand LMT AI 103****Ligand CLA AB 607**

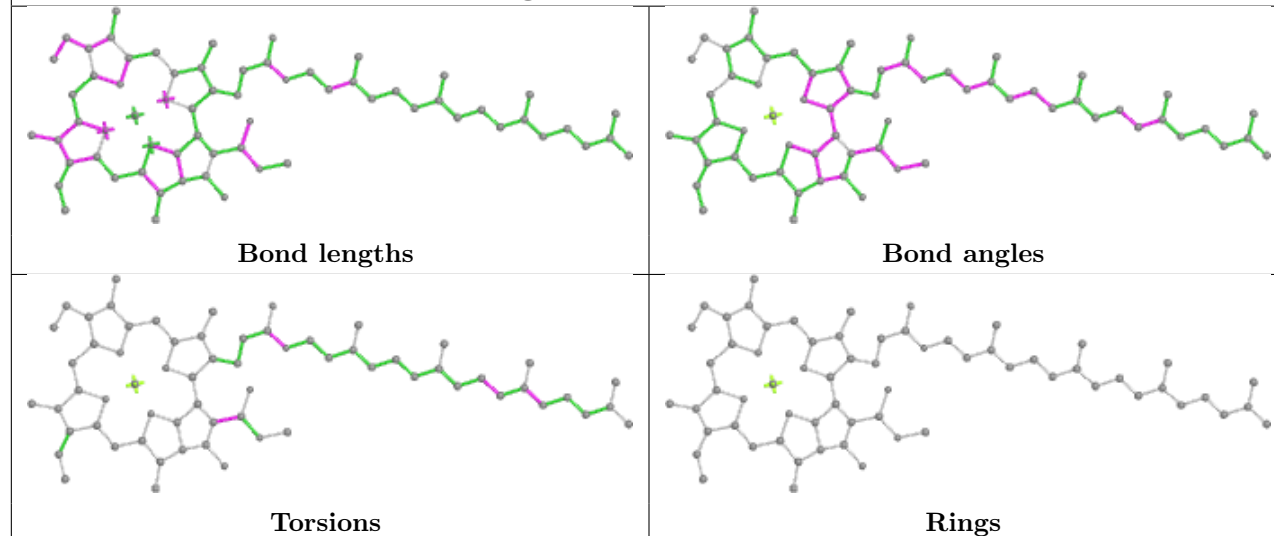
Ligand CLA AA 405

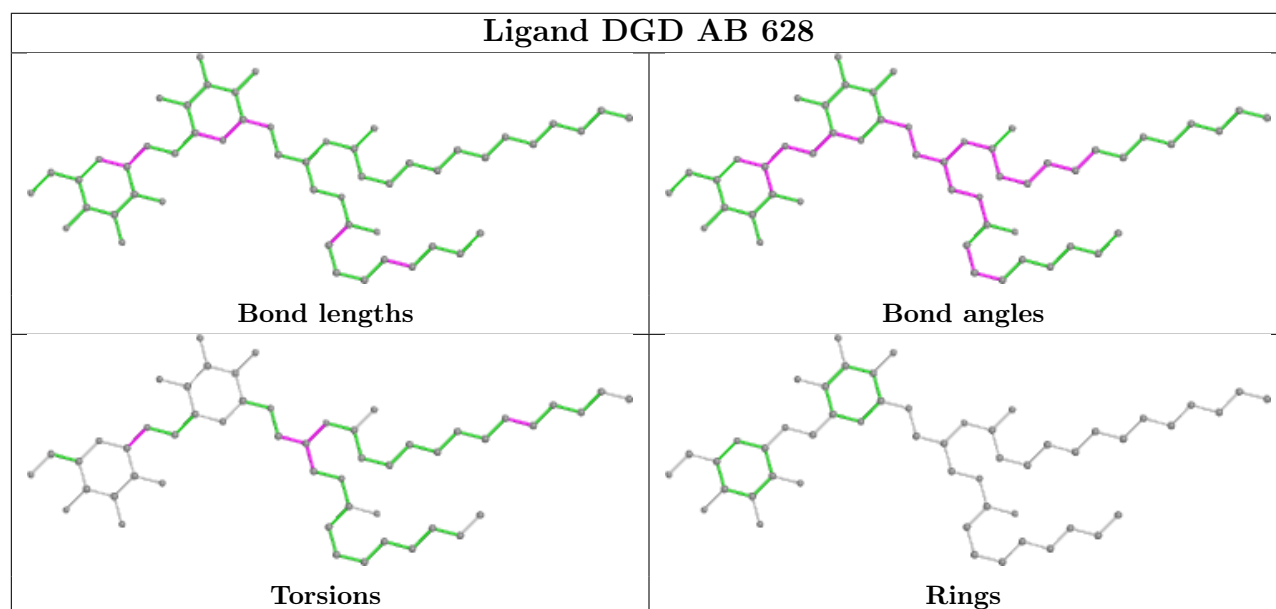
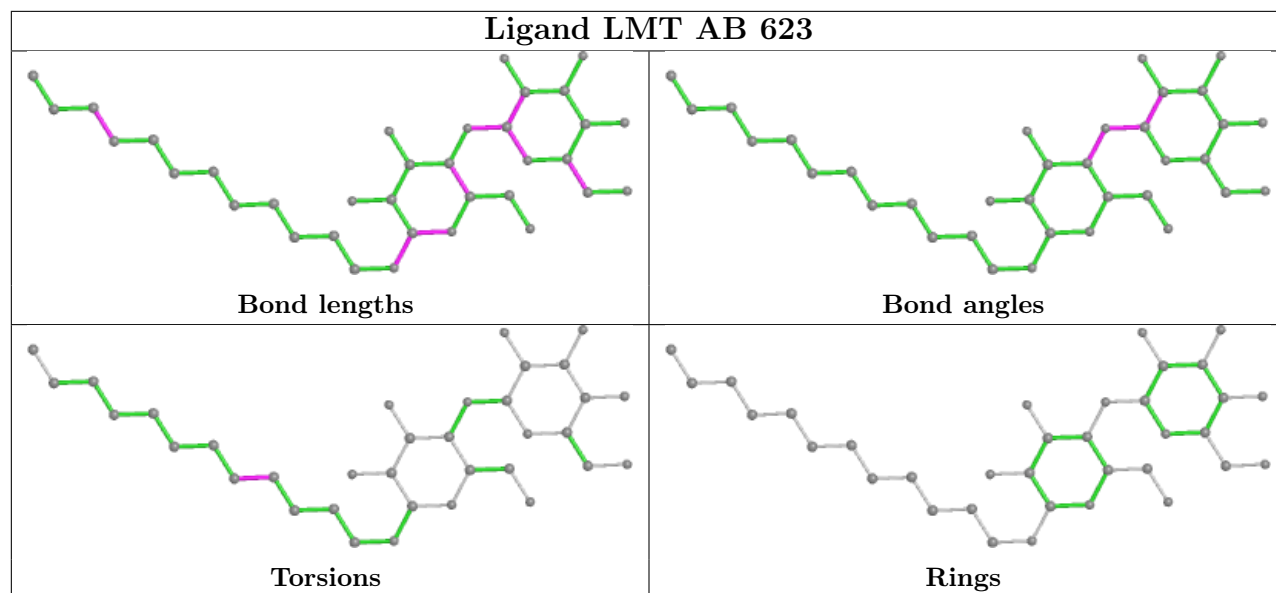


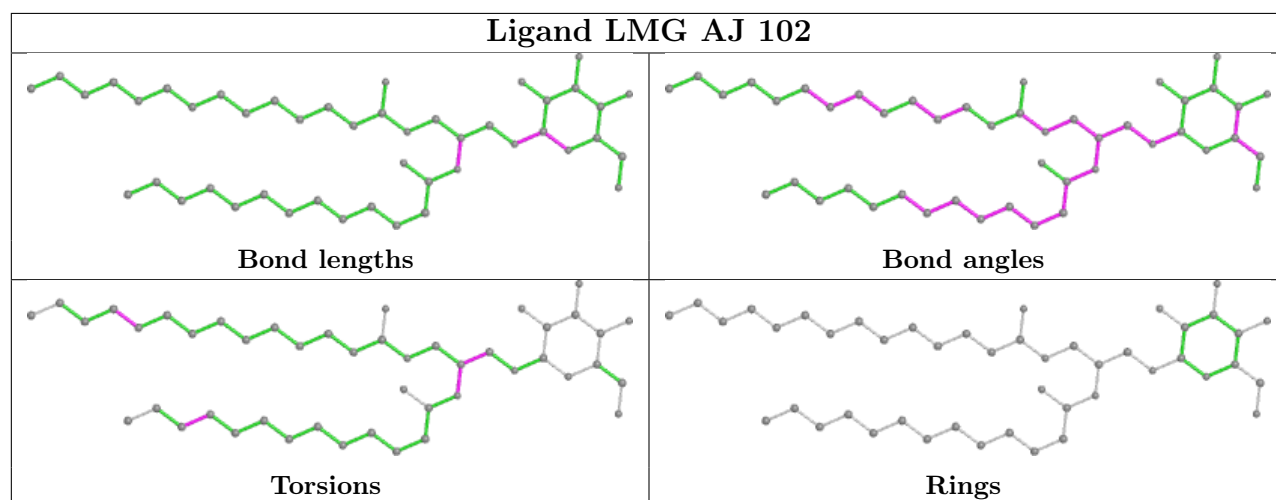
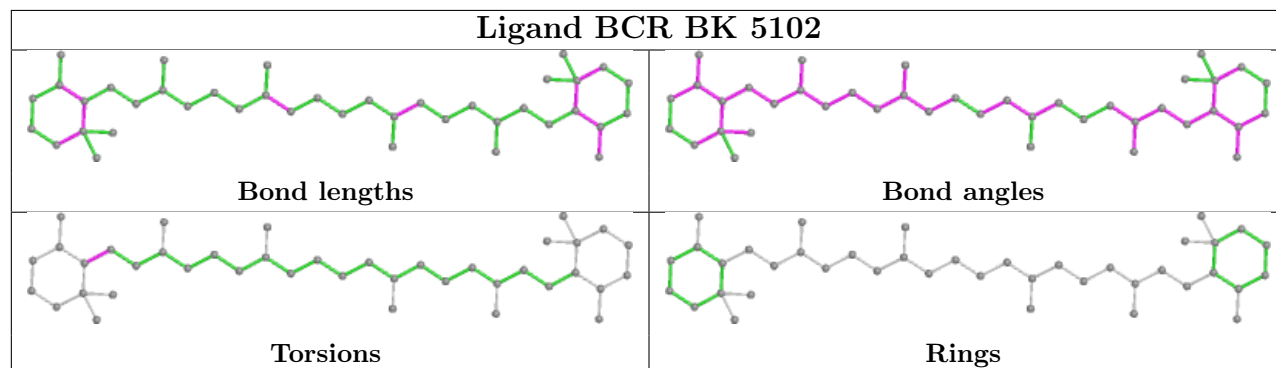
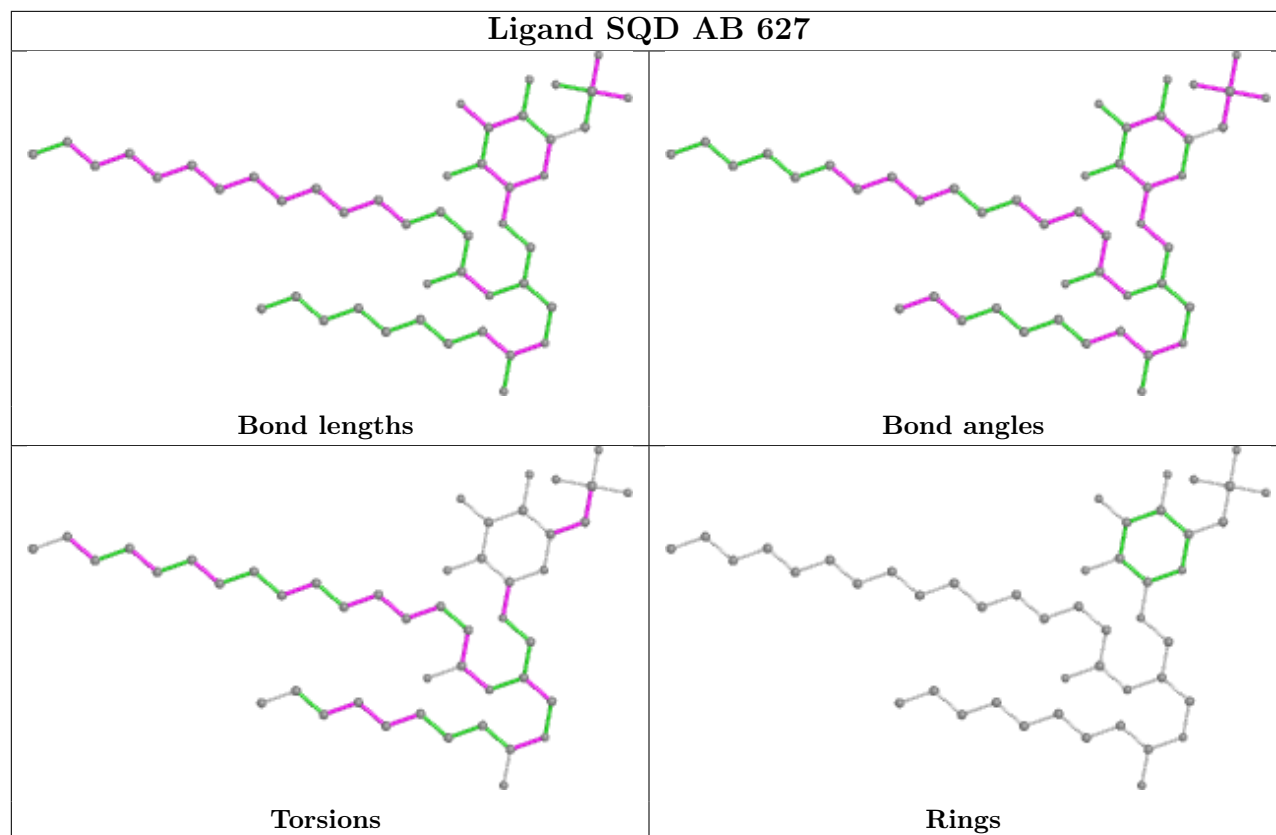
Ligand CLA AA 407

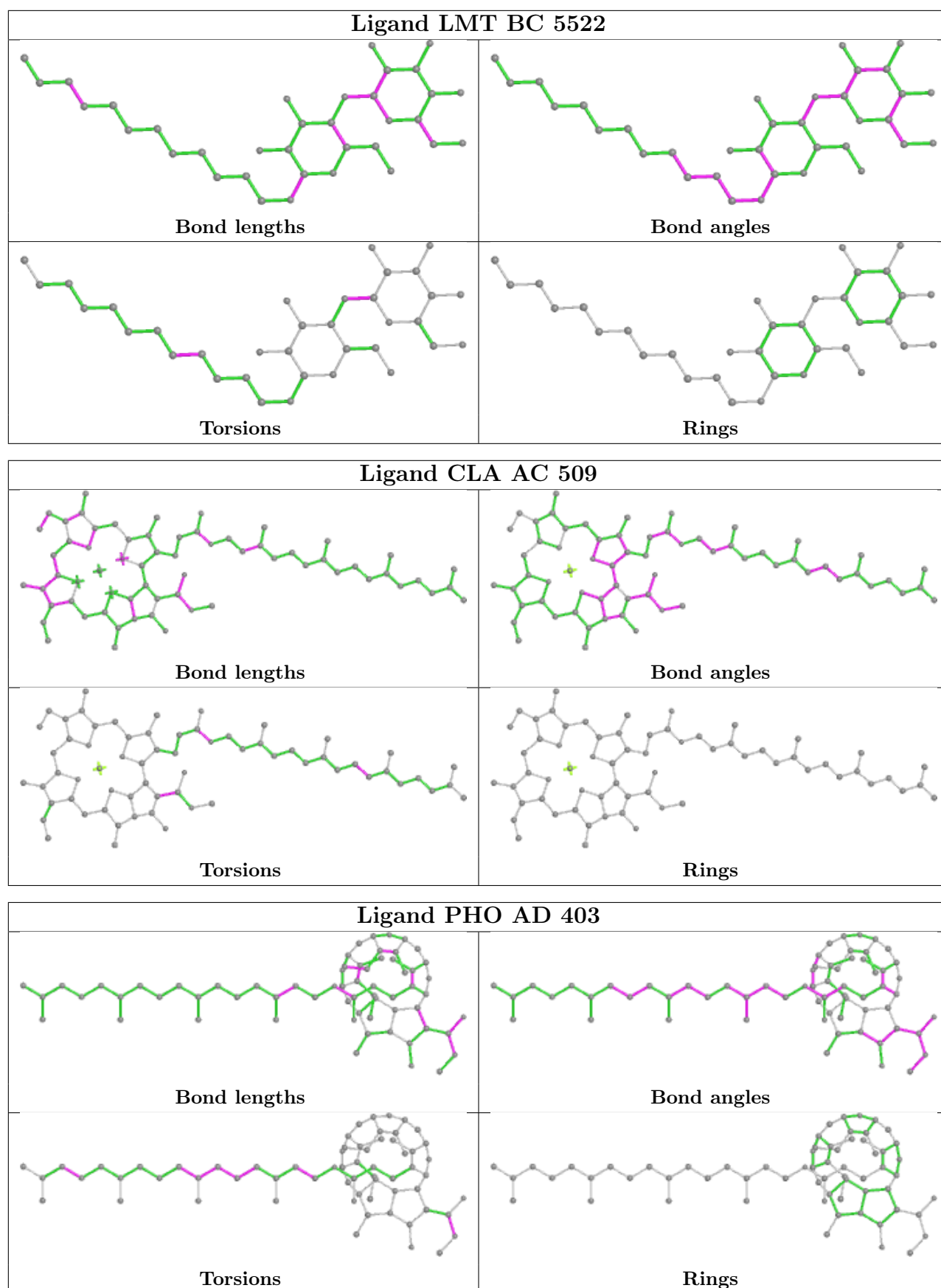


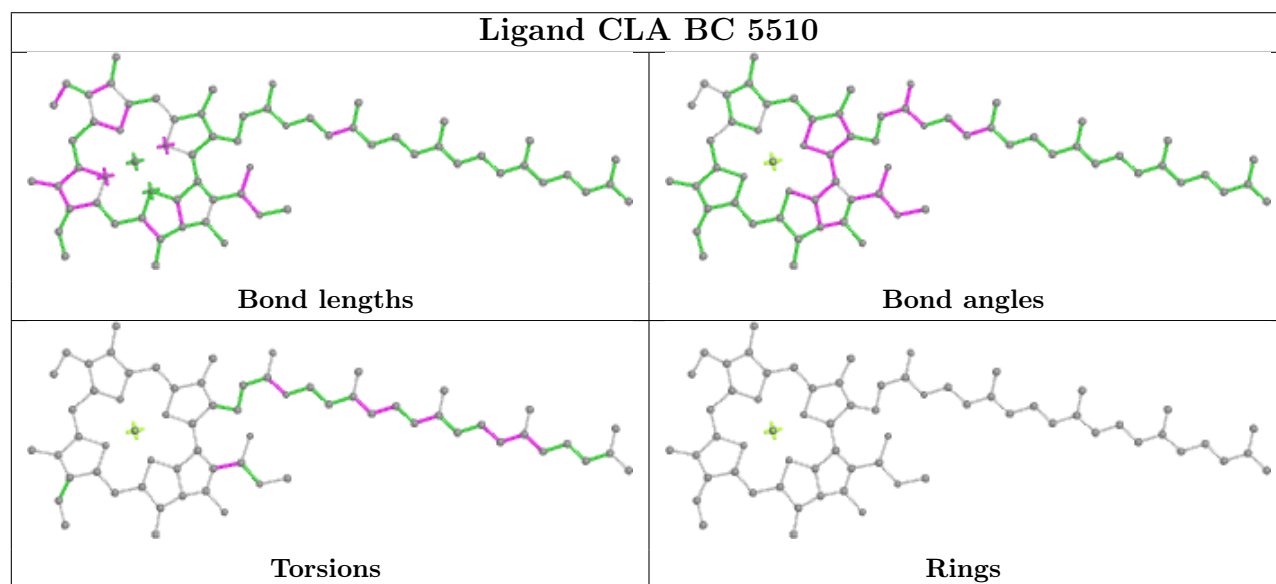
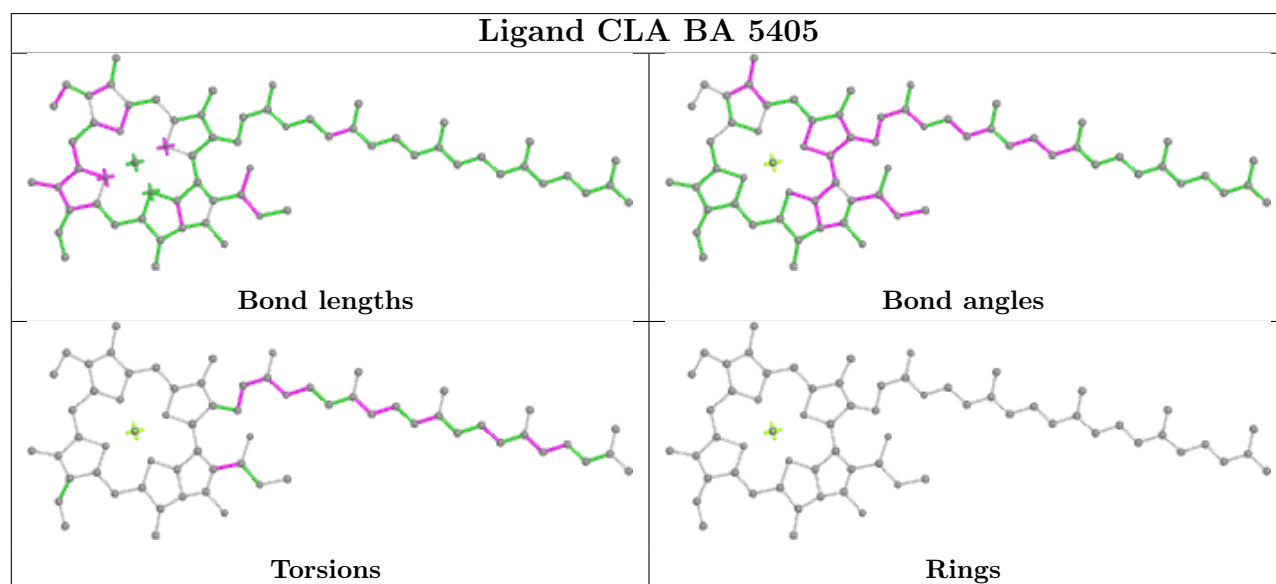
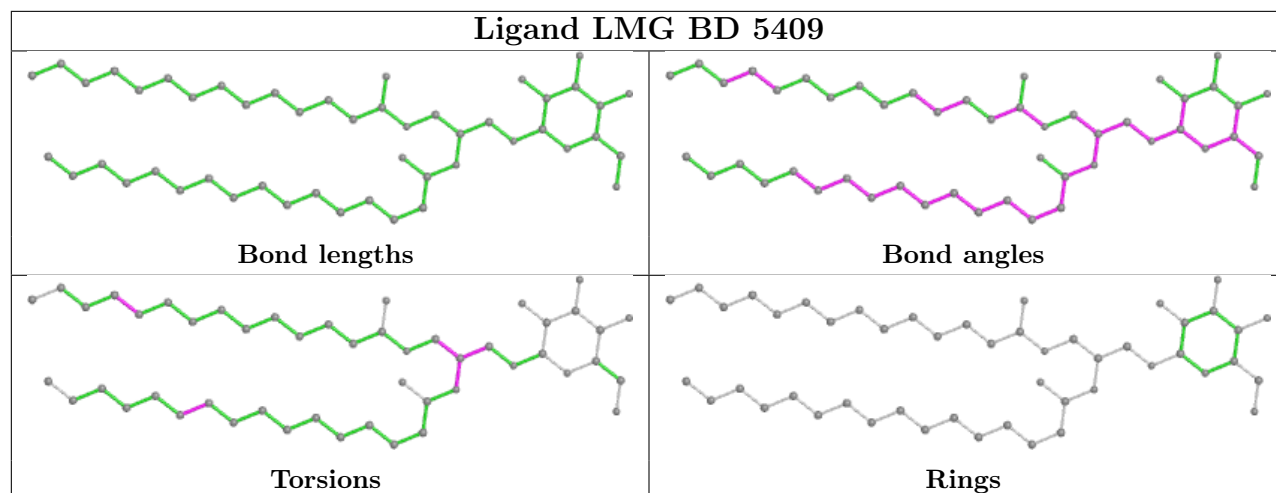
Ligand CLA AC 507

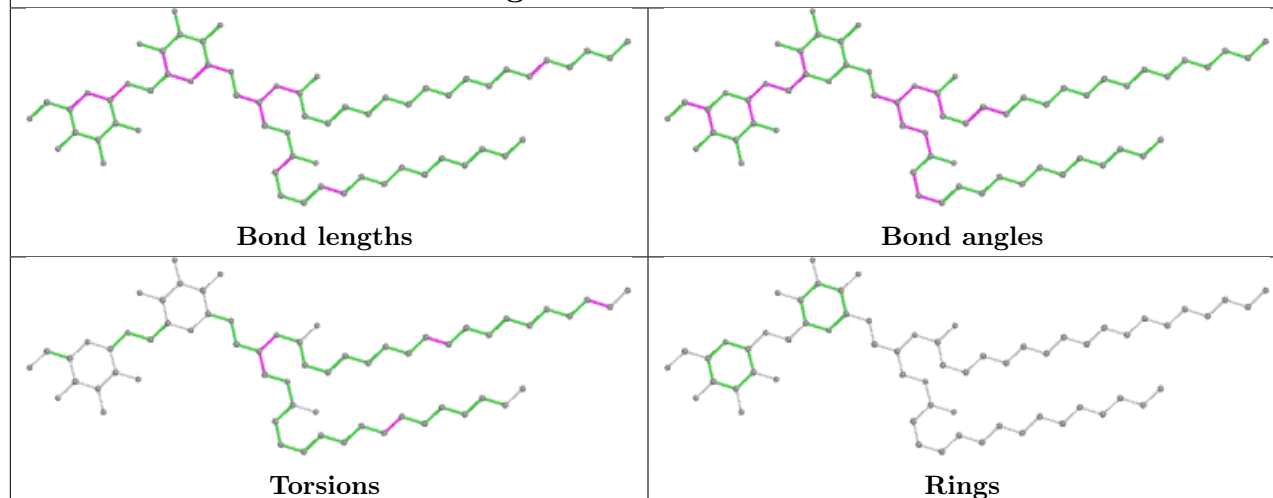
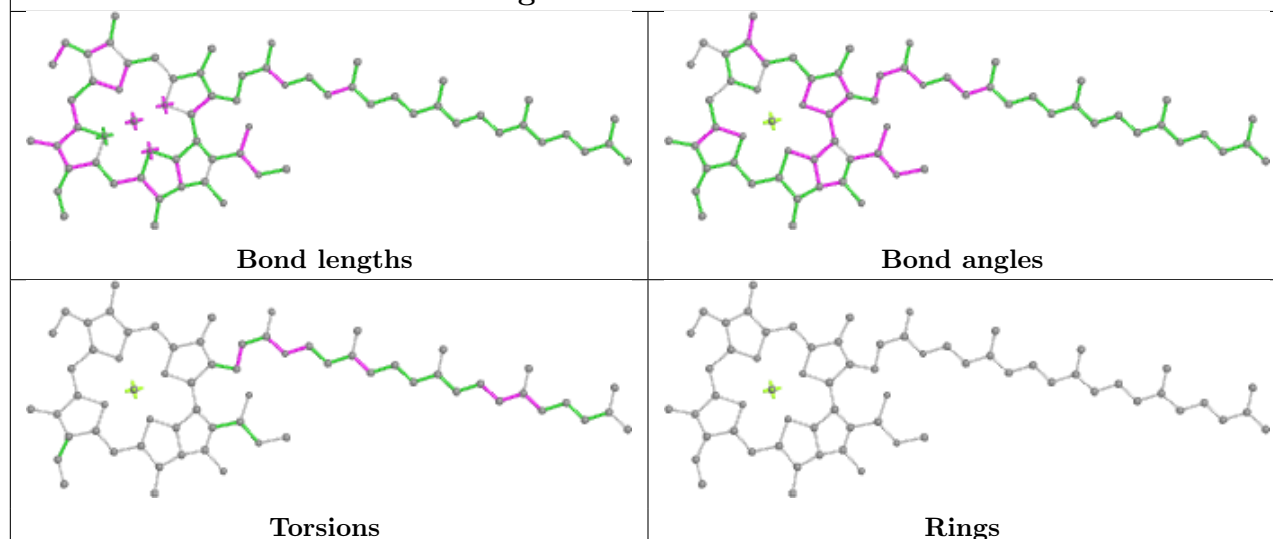
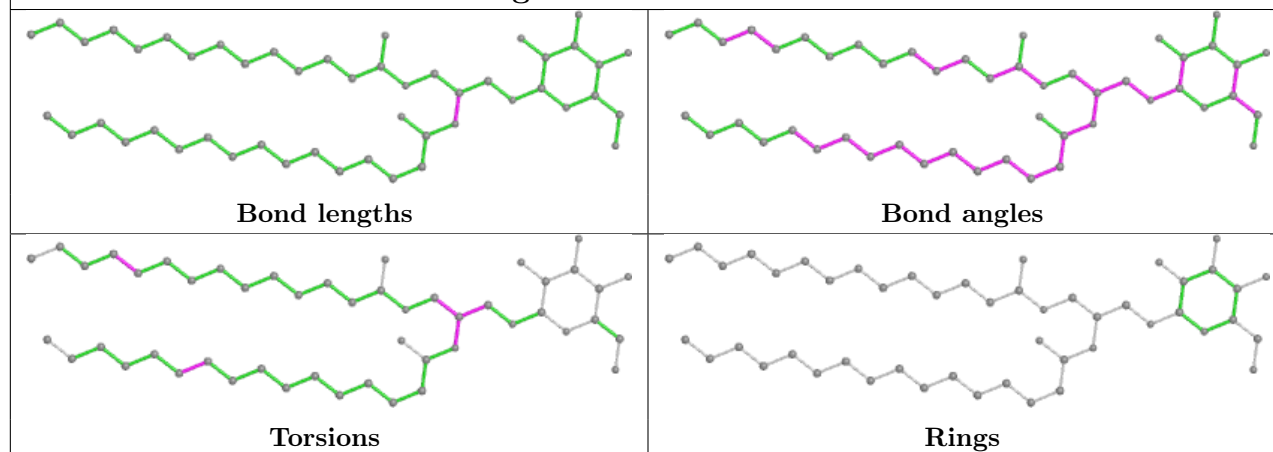










Ligand DGD BE 5102**Ligand CLA AB 612****Ligand LMG AD 407**

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, 95th 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%)	-0.01	6 (1%) 68 55	82, 104, 147, 160	0
1	BA	335/344 (97%)	-0.02	15 (4%) 33 21	86, 106, 148, 160	0
2	AB	490/510 (96%)	-0.02	12 (2%) 59 44	81, 103, 136, 152	0
2	BB	490/510 (96%)	0.09	21 (4%) 35 22	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.29	22 (4%) 29 17	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.24	29 (6%) 18 11	91, 124, 149, 159	0
4	AD	341/352 (96%)	0.00	6 (1%) 68 55	81, 105, 139, 153	0
4	BD	341/352 (96%)	-0.02	12 (3%) 44 28	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.45	7 (8%) 10 6	104, 126, 151, 155	0
5	BE	82/84 (97%)	1.23	23 (28%) 0 0	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.39	5 (14%) 2 1	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.27	4 (11%) 5 3	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.48	8 (12%) 4 2	113, 124, 140, 147	0
7	BH	65/66 (98%)	0.51	6 (9%) 9 5	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.07	2 (5%) 23 13	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.69	8 (22%) 0 0	108, 116, 142, 147	0
9	AJ	38/40 (95%)	0.02	3 (7%) 12 6	109, 122, 157, 159	0
9	BJ	38/40 (95%)	0.46	7 (18%) 1 1	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.08	1 (2%) 54 39	121, 135, 145, 147	0
10	BK	37/37 (100%)	0.13	1 (2%) 54 39	123, 136, 147, 148	0
11	AL	37/37 (100%)	0.26	4 (10%) 5 3	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.46	6 (16%) 1 1	90, 104, 158, 160	0
12	AM	34/36 (94%)	0.24	3 (8%) 10 5	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.12	2 (5%) 22 13	90, 99, 140, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.33	16 (6%) 18 11	83, 116, 148, 160	0
13	BO	243/247 (98%)	0.29	21 (8%) 10 5	85, 117, 147, 160	0
14	AT	32/32 (100%)	0.35	3 (9%) 8 4	92, 106, 158, 160	0
14	BT	32/32 (100%)	0.01	1 (3%) 49 32	93, 106, 158, 160	0
15	AU	97/104 (93%)	0.25	4 (4%) 37 24	93, 105, 116, 125	0
15	BU	97/104 (93%)	0.15	0 100 100	94, 106, 116, 127	0
16	AV	137/137 (100%)	0.11	2 (1%) 73 61	96, 112, 128, 132	0
16	BV	137/137 (100%)	0.46	14 (10%) 6 4	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.62	4 (14%) 2 1	141, 154, 160, 160	0
17	By	28/46 (60%)	0.80	5 (17%) 1 1	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.42	7 (18%) 1 1	121, 129, 147, 150	0
18	BX	37/41 (90%)	0.38	5 (13%) 3 2	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.63	11 (17%) 1 1	134, 148, 160, 160	0
20	BZ	62/62 (100%)	1.40	19 (30%) 0 0	135, 150, 160, 160	0
All	All	5224/5494 (95%)	0.20	325 (6%) 20 11	81, 113, 149, 160	0

The worst 5 of 325 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BZ	5062	VAL	9.2
20	BZ	5061	VAL	7.5
13	BO	5084	ASN	7.4
20	BZ	5001	MET	6.3
7	BH	5066	GLY	6.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	CA	BF	5103	1/1	0.16	0.16	146,146,146,146	0
37	CA	AF	103	1/1	0.35	0.23	150,150,150,150	0
28	DGD	AE	101	63/66	0.36	0.71	146,160,160,160	0
32	LMT	BB	5626	35/35	0.39	0.62	131,160,160,160	0
31	LMG	AI	101	43/55	0.40	0.78	159,160,160,160	0
31	LMG	AC	521	45/55	0.40	0.63	154,160,160,160	0
28	DGD	BE	5102	63/66	0.44	0.70	145,160,160,160	0
29	LHG	BA	5415	37/49	0.48	0.61	151,160,160,160	0
37	CA	AO	301	1/1	0.51	0.23	152,152,152,152	0
28	DGD	BB	5602	52/66	0.51	0.53	152,160,160,160	0
28	DGD	BA	5412	56/66	0.53	0.58	150,160,160,160	0
32	LMT	AB	623	35/35	0.53	0.72	135,160,160,160	0
27	BCR	AJ	101	40/40	0.54	0.66	158,160,160,160	0
28	DGD	AB	628	52/66	0.55	0.60	154,160,160,160	0
28	DGD	AA	411	56/66	0.56	0.54	148,158,160,160	0
31	LMG	BC	5520	48/55	0.57	0.55	138,159,160,160	0
31	LMG	BI	5101	43/55	0.58	0.70	160,160,160,160	0
30	SQD	BB	5625	43/54	0.59	0.47	132,148,160,160	0
31	LMG	AC	520	48/55	0.60	0.57	136,157,160,160	0
27	BCR	AX	101	40/40	0.60	0.49	135,143,158,159	0
31	LMG	BA	5402	42/55	0.61	0.50	144,157,160,160	0
31	LMG	AA	414	44/55	0.61	0.46	140,160,160,160	0
27	BCR	BX	5101	40/40	0.62	0.49	136,143,157,158	0
31	LMG	BC	5521	45/55	0.64	0.55	154,160,160,160	0
27	BCR	BJ	5101	40/40	0.64	0.51	160,160,160,160	0
32	LMT	BI	5102	35/35	0.64	0.84	151,160,160,160	0
37	CA	BK	5101	1/1	0.64	0.22	145,145,145,145	0
30	SQD	BA	5401	54/54	0.65	0.47	136,160,160,160	0
31	LMG	BE	5101	44/55	0.65	0.46	140,160,160,160	0
32	LMT	BB	5603	35/35	0.65	0.46	132,160,160,160	0
30	SQD	AB	622	43/54	0.66	0.42	133,149,160,160	0
31	LMG	BD	5410	48/55	0.66	0.57	126,131,141,141	0
32	LMT	BD	5411	31/35	0.67	0.49	140,152,160,160	0
31	LMG	AM	101	42/55	0.67	0.53	136,158,160,160	0
27	BCR	BC	5516	40/40	0.67	0.45	136,140,145,145	0
32	LMT	AB	629	35/35	0.68	0.48	133,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	LMG	AA	417	42/55	0.68	0.45	145,157,160,160	0
30	SQD	BF	5102	45/54	0.68	0.56	154,160,160,160	0
37	CA	BO	5301	1/1	0.68	0.33	160,160,160,160	0
31	LMG	AB	621	49/55	0.69	0.44	145,150,157,160	0
32	LMT	BB	5604	35/35	0.70	0.52	131,160,160,160	0
32	LMT	AI	102	35/35	0.70	0.59	149,158,160,160	0
28	DGD	BC	5518	62/66	0.70	0.49	147,156,160,160	0
24	CLA	AB	601	65/65	0.71	0.55	146,159,160,160	0
31	LMG	BD	5408	46/55	0.71	0.46	139,145,160,160	0
27	BCR	AC	516	40/40	0.71	0.46	135,138,143,143	0
32	LMT	AD	409	31/35	0.71	0.43	139,154,160,160	0
27	BCR	BC	5515	40/40	0.71	0.43	150,152,155,156	0
24	CLA	BB	5605	65/65	0.72	0.58	146,159,160,160	0
32	LMT	AB	624	35/35	0.72	0.59	156,160,160,160	0
24	CLA	BC	5513	65/65	0.72	0.50	158,160,160,160	0
27	BCR	AC	515	40/40	0.72	0.44	149,152,155,155	0
24	CLA	AC	513	65/65	0.72	0.44	158,160,160,160	0
23	CL	BA	5404[A]	1/1	0.73	0.34	29,29,29,29	1
31	LMG	AB	620	51/55	0.73	0.48	125,139,150,151	0
30	SQD	BA	5414	51/54	0.73	0.36	145,150,160,160	0
32	LMT	BM	5101	35/35	0.73	0.39	126,149,154,155	0
30	SQD	BB	5601	47/54	0.73	0.39	137,156,160,160	0
24	CLA	AB	609	65/65	0.73	0.39	126,136,141,143	0
32	LMT	AI	103	35/35	0.73	0.47	156,158,160,160	0
26	OEC	BA	5410	5/9	0.73	0.22	23,88,99,134	0
23	CL	BA	5404[B]	1/1	0.73	0.34	115,115,115,115	1
31	LMG	BM	5102	42/55	0.74	0.45	136,160,160,160	0
32	LMT	AB	630	35/35	0.74	0.49	132,160,160,160	0
30	SQD	AF	102	45/54	0.74	0.45	154,160,160,160	0
31	LMG	AJ	102	46/55	0.74	0.43	139,144,160,160	0
33	DMS	AU	201	4/4	0.75	0.40	160,160,160,160	0
32	LMT	BB	5627	35/35	0.75	0.45	156,160,160,160	0
24	CLA	AC	506	65/65	0.75	0.37	136,143,160,160	0
30	SQD	AA	416	54/54	0.76	0.34	136,160,160,160	0
24	CLA	BB	5613	65/65	0.76	0.37	127,135,140,142	0
31	LMG	BB	5624	49/55	0.76	0.40	145,150,157,160	0
31	LMG	AD	408	48/55	0.76	0.47	121,130,139,139	0
24	CLA	BC	5506	65/65	0.76	0.39	136,143,160,160	0
28	DGD	AC	518	62/66	0.76	0.41	146,155,160,160	0
27	BCR	BT	5101	40/40	0.77	0.40	124,143,147,147	0
30	SQD	AB	627	47/54	0.77	0.36	138,157,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMT	BC	5522	35/35	0.77	0.67	157,160,160,160	0
29	LHG	AA	415	37/49	0.77	0.35	149,160,160,160	0
31	LMG	AD	407	49/55	0.78	0.46	126,133,143,145	0
32	LMT	AM	102	35/35	0.78	0.43	126,149,154,154	0
31	LMG	BL	5101	51/55	0.79	0.46	122,138,151,152	0
27	BCR	BK	5102	40/40	0.80	0.37	136,140,152,152	0
28	DGD	BC	5519	66/66	0.80	0.36	112,121,158,159	0
31	LMG	BD	5409	49/55	0.80	0.41	128,133,144,146	0
27	BCR	BC	5514	40/40	0.80	0.43	123,126,129,129	0
24	CLA	AC	512	65/65	0.80	0.44	154,158,160,160	0
24	CLA	BC	5512	65/65	0.81	0.35	157,160,160,160	0
24	CLA	BC	5511	65/65	0.81	0.43	154,158,159,160	0
27	BCR	AK	102	40/40	0.81	0.38	133,139,151,152	0
27	BCR	BB	5623	40/40	0.82	0.37	111,116,131,131	0
28	DGD	AC	517	53/66	0.82	0.39	121,128,135,140	0
27	BCR	AT	101	40/40	0.82	0.39	126,140,146,147	0
24	CLA	BC	5505	65/65	0.82	0.36	123,148,152,153	0
24	CLA	BB	5620	65/65	0.83	0.29	143,147,160,160	0
33	DMS	AV	202	4/4	0.83	0.64	148,148,148,149	0
24	CLA	BB	5610	65/65	0.83	0.31	121,132,140,141	0
24	CLA	AB	606	65/65	0.83	0.33	120,133,140,141	0
24	CLA	BD	5405	65/65	0.83	0.34	125,131,148,149	0
28	DGD	BH	5101	58/66	0.83	0.37	107,118,156,160	0
24	CLA	BC	5507	65/65	0.83	0.36	136,150,153,154	0
30	SQD	AA	413	51/54	0.84	0.31	143,150,160,160	0
37	CA	AK	101	1/1	0.84	0.12	146,146,146,146	0
24	CLA	BC	5503	65/65	0.84	0.35	137,147,148,152	0
24	CLA	AB	614	65/65	0.84	0.37	129,133,160,160	0
28	DGD	AC	519	66/66	0.84	0.36	110,120,157,158	0
24	CLA	BC	5508	65/65	0.84	0.33	142,146,157,159	0
33	DMS	BB	5628	4/4	0.85	0.58	156,157,157,157	0
35	PL9	BD	5406	55/55	0.85	0.34	103,110,115,116	0
24	CLA	BB	5606	65/65	0.85	0.30	124,127,130,131	0
27	BCR	AB	619	40/40	0.85	0.29	111,117,131,131	0
24	CLA	AB	616	65/65	0.86	0.39	143,147,160,160	0
24	CLA	AB	602	65/65	0.86	0.33	124,127,129,132	0
28	DGD	AH	101	58/66	0.86	0.30	108,120,155,157	0
24	CLA	BA	5405	65/65	0.87	0.30	90,101,105,109	0
23	CL	AA	403[A]	1/1	0.87	0.31	33,33,33,33	1
23	CL	AA	403[B]	1/1	0.87	0.31	108,108,108,108	1
24	CLA	AA	406	65/65	0.87	0.34	105,112,138,139	0
24	CLA	AD	404	65/65	0.87	0.35	126,130,148,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	BCR	AB	617	40/40	0.87	0.32	112,121,125,125	0
27	BCR	AB	618	40/40	0.87	0.27	109,117,122,122	0
28	DGD	BC	5517	53/66	0.87	0.28	124,130,136,139	0
24	CLA	BB	5618	65/65	0.87	0.32	128,133,160,160	0
29	LHG	BA	5413	39/49	0.88	0.27	113,122,128,129	0
27	BCR	AC	514	40/40	0.88	0.33	120,123,127,128	0
24	CLA	AB	603	65/65	0.88	0.36	107,109,119,121	0
27	BCR	BD	5407	40/40	0.88	0.30	112,127,132,132	0
24	CLA	AC	501	65/65	0.88	0.37	133,136,139,143	0
27	BCR	AD	406	40/40	0.88	0.31	110,126,131,131	0
24	CLA	AC	503	65/65	0.88	0.48	137,144,147,152	0
24	CLA	AC	505	65/65	0.88	0.40	121,146,150,151	0
24	CLA	BA	5407	65/65	0.88	0.29	110,114,138,139	0
24	CLA	AB	615	65/65	0.88	0.33	134,139,155,157	0
24	CLA	AC	507	65/65	0.88	0.38	137,149,152,153	0
24	CLA	AC	511	65/65	0.88	0.33	152,155,157,158	0
24	CLA	BA	5406	65/65	0.89	0.28	89,94,108,112	0
33	DMS	AB	625	4/4	0.89	0.44	156,157,157,157	0
33	DMS	AB	626	4/4	0.89	0.26	129,130,130,130	0
24	CLA	AC	509	65/65	0.89	0.39	115,128,135,137	0
27	BCR	BA	5411	40/40	0.89	0.29	94,122,132,132	0
27	BCR	BB	5621	40/40	0.89	0.32	112,120,124,125	0
34	PHO	BD	5403	64/64	0.89	0.34	102,109,118,118	0
24	CLA	BA	5408	65/65	0.89	0.30	95,103,150,150	0
24	CLA	BC	5509	65/65	0.89	0.30	116,128,138,138	0
24	CLA	AC	504	65/65	0.89	0.34	129,134,160,160	0
24	CLA	BC	5501	65/65	0.89	0.30	134,137,141,144	0
24	CLA	AB	608	65/65	0.89	0.40	123,127,135,140	0
24	CLA	BC	5504	65/65	0.89	0.33	132,135,160,160	0
24	CLA	BB	5607	65/65	0.89	0.28	108,111,120,123	0
34	PHO	BD	5404	64/64	0.90	0.28	123,125,129,130	0
35	PL9	AD	405	55/55	0.90	0.36	99,109,113,113	0
24	CLA	AB	605	65/65	0.90	0.28	105,113,122,124	0
24	CLA	BB	5619	65/65	0.90	0.34	135,137,155,157	0
24	CLA	BB	5611	65/65	0.90	0.28	95,102,132,136	0
24	CLA	AC	508	65/65	0.90	0.35	140,144,157,158	0
24	CLA	BC	5502	65/65	0.90	0.32	108,111,143,144	0
29	LHG	AA	412	39/49	0.90	0.28	110,118,128,132	0
24	CLA	BB	5614	65/65	0.90	0.32	117,123,124,128	0
24	CLA	AB	610	65/65	0.91	0.33	117,121,123,127	0
24	CLA	BB	5612	65/65	0.91	0.39	122,127,136,139	0
24	CLA	BD	5402	65/65	0.91	0.26	97,101,117,119	0

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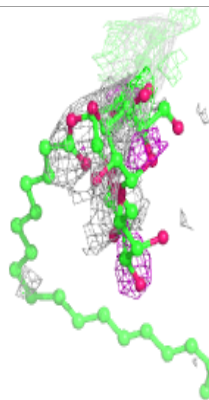
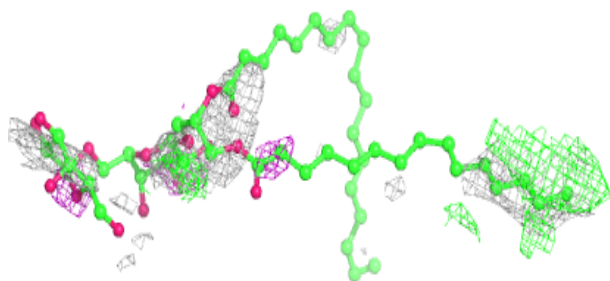
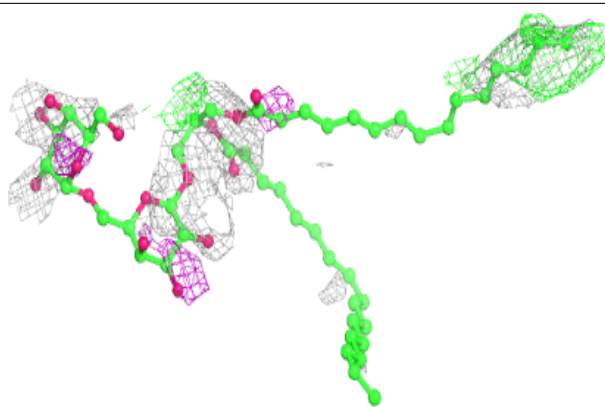
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	AC	502	65/65	0.91	0.36	103,109,142,143	0
36	HEM	BF	5101	43/43	0.91	0.44	148,152,160,160	0
24	CLA	BB	5609	65/65	0.91	0.34	103,110,124,124	0
27	BCR	AA	410	40/40	0.91	0.27	91,122,130,130	0
24	CLA	BB	5616	65/65	0.91	0.31	108,110,120,122	0
24	CLA	BC	5510	65/65	0.91	0.34	113,116,130,131	0
24	CLA	AA	407	65/65	0.91	0.33	93,101,150,151	0
33	DMS	BV	5202	4/4	0.91	0.27	148,149,149,150	0
24	CLA	AA	404	65/65	0.92	0.26	89,99,106,108	0
24	CLA	BB	5615	65/65	0.92	0.26	101,113,117,120	0
25	MST	BA	5409	16/16	0.92	0.23	124,129,131,132	0
24	CLA	AC	510	65/65	0.92	0.33	110,113,129,130	0
34	PHO	AD	402	64/64	0.92	0.30	99,109,116,117	0
24	CLA	BB	5617	65/65	0.92	0.33	98,102,138,141	0
24	CLA	AB	607	65/65	0.92	0.26	94,100,132,135	0
27	BCR	BB	5622	40/40	0.92	0.34	110,117,120,121	0
33	DMS	BB	5629	4/4	0.93	0.29	125,126,127,127	0
24	CLA	AB	613	65/65	0.93	0.26	99,102,136,140	0
36	HEM	BV	5201	43/43	0.93	0.27	97,102,106,109	0
33	DMS	BV	5203	4/4	0.93	0.67	160,160,160,160	0
24	CLA	AB	604	65/65	0.93	0.30	96,104,125,127	0
34	PHO	AD	403	64/64	0.93	0.28	119,123,128,129	0
25	MST	AA	408	16/16	0.93	0.26	123,126,129,130	0
24	CLA	AD	401	65/65	0.93	0.27	93,100,115,119	0
24	CLA	AB	612	65/65	0.93	0.29	107,111,120,121	0
24	CLA	AB	611	65/65	0.94	0.30	99,113,116,122	0
21	FE2	BD	5401	1/1	0.94	0.11	119,119,119,119	0
24	CLA	AA	405	65/65	0.94	0.26	88,93,108,111	0
36	HEM	AF	101	43/43	0.94	0.38	148,152,159,160	0
24	CLA	BB	5608	65/65	0.95	0.32	96,103,124,125	0
26	OEC	AA	409	5/9	0.95	0.28	82,83,90,110	0
36	HEM	AV	201	43/43	0.96	0.27	94,100,102,103	0
22	BCT	BA	5403	4/4	0.97	0.16	135,136,136,137	0
21	FE2	AA	401	1/1	0.98	0.17	115,115,115,115	0
22	BCT	AA	402	4/4	0.99	0.20	135,136,137,137	0

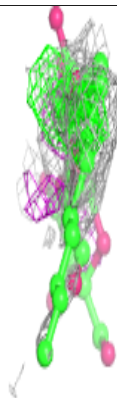
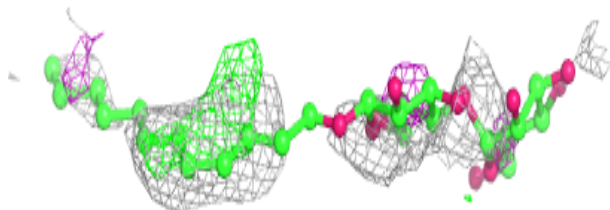
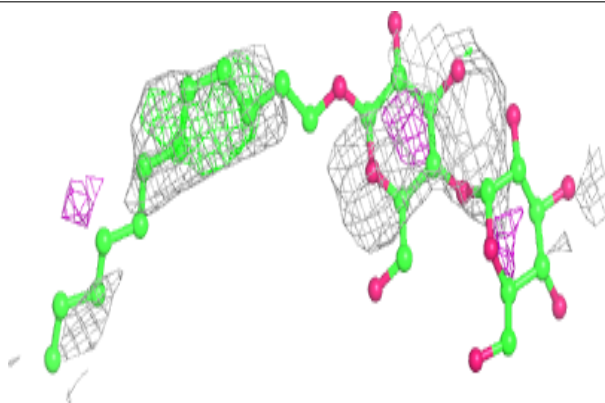
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD 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)

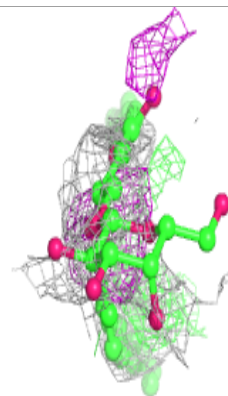
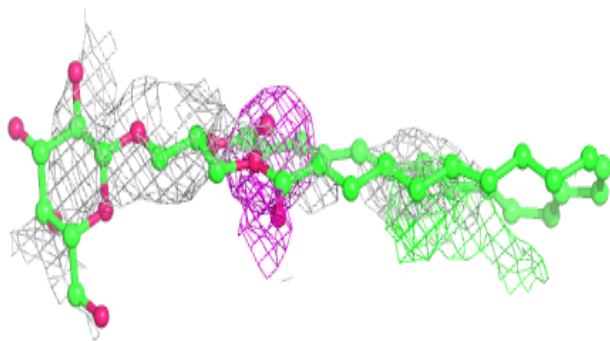
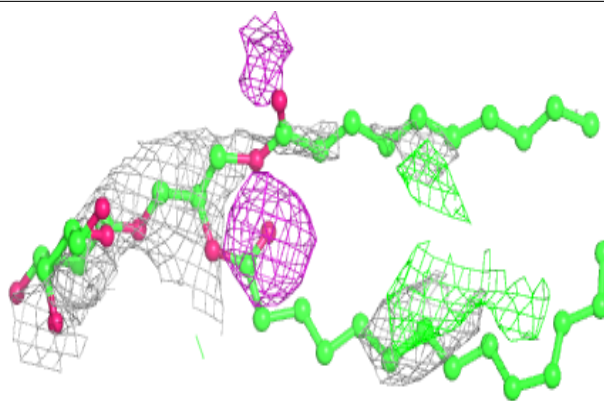
**Electron density around LMT BB 5626:**

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

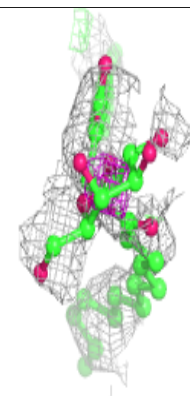
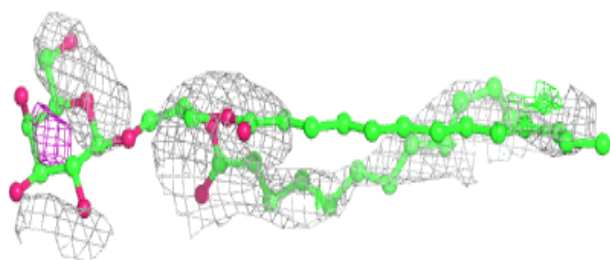
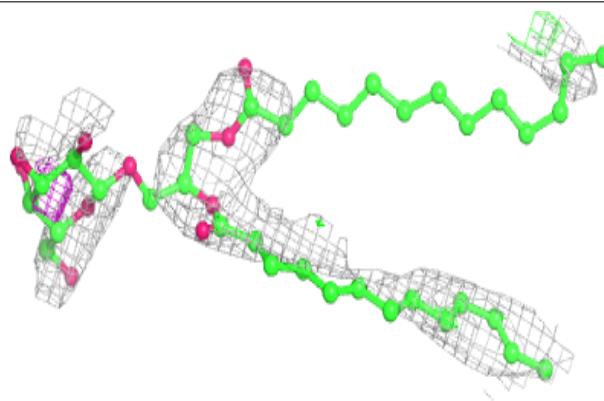


Electron density around LMG AI 101:

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

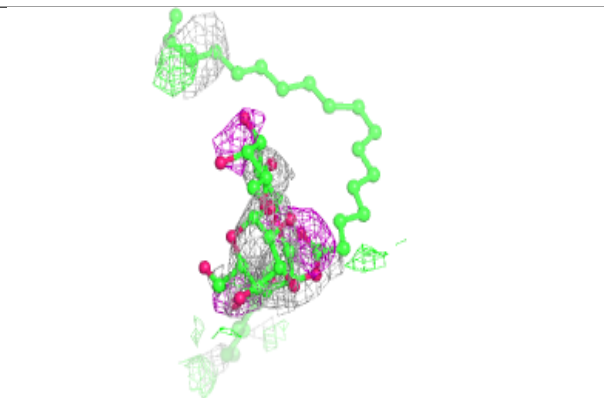
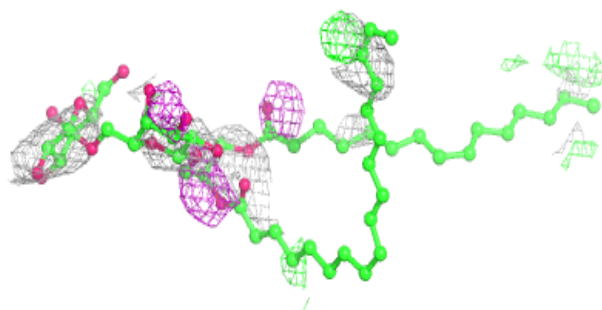
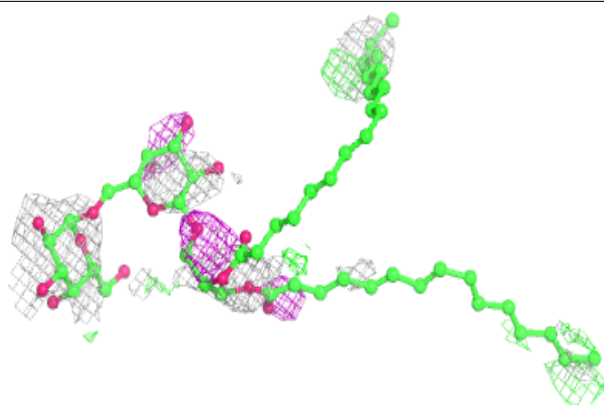
**Electron density around LMG AC 521:**

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

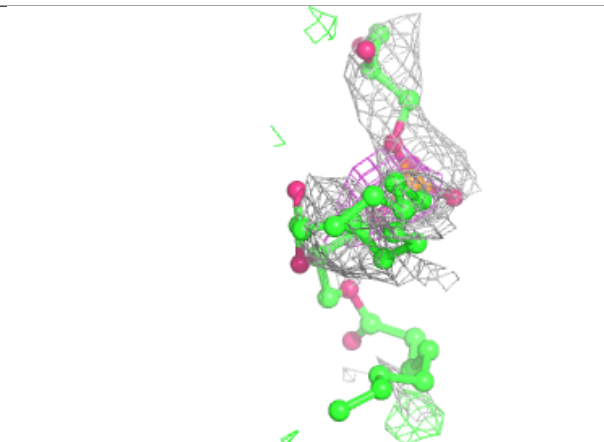
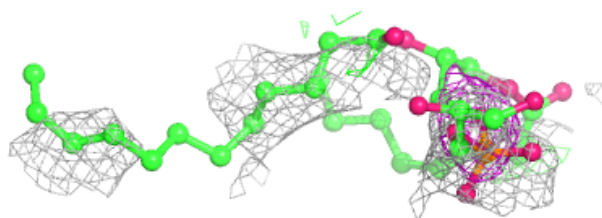
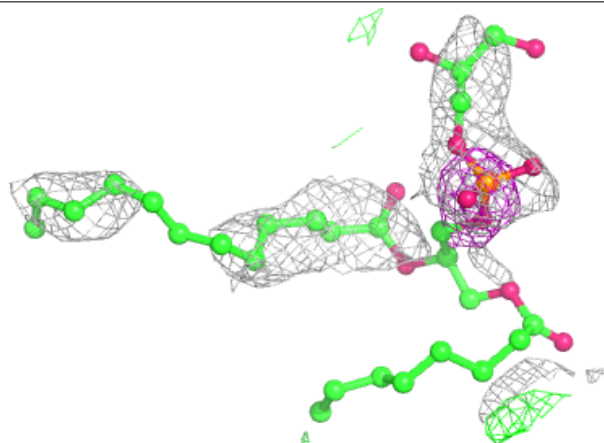


Electron density around DGD BE 5102:

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

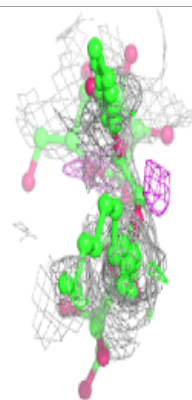
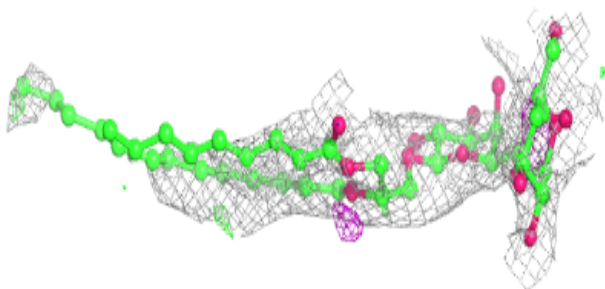
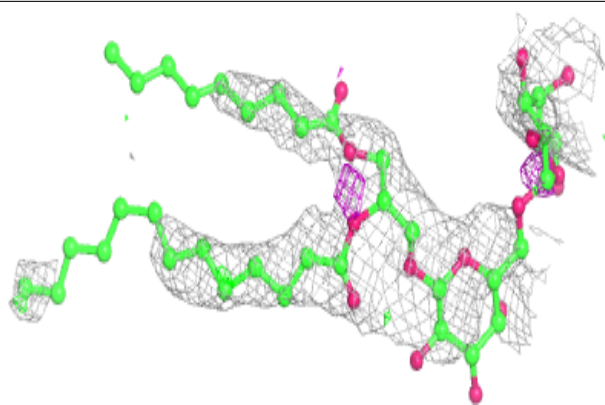
**Electron density around LHG BA 5415:**

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

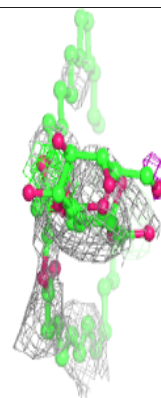
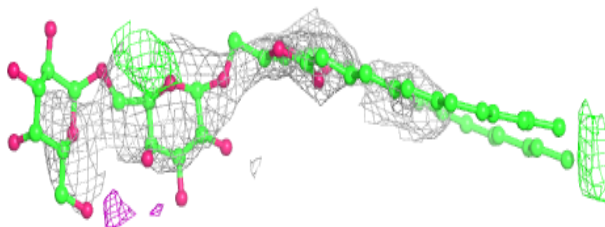
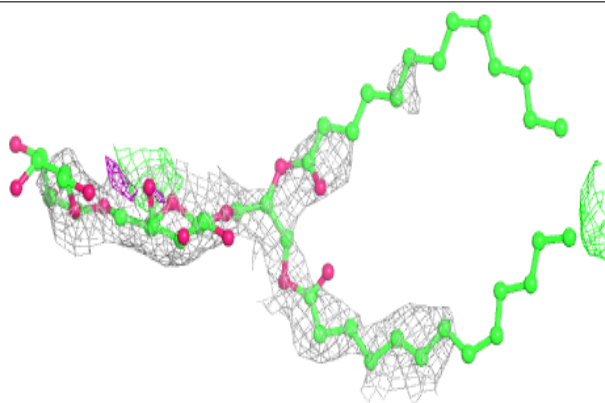


Electron density around DGD BB 5602:

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

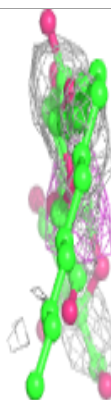
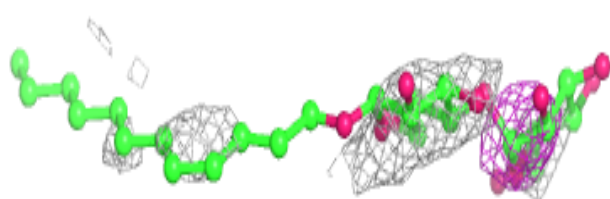
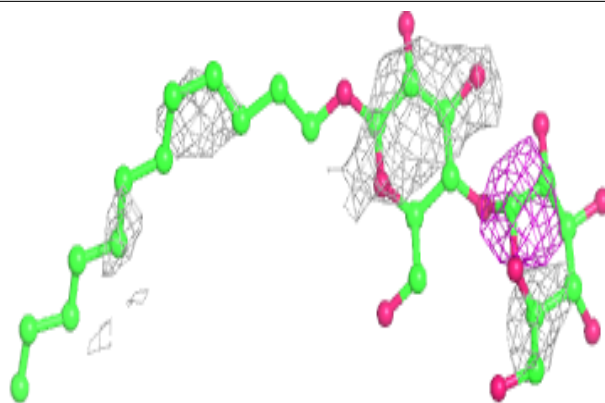
**Electron density around DGD BA 5412:**

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

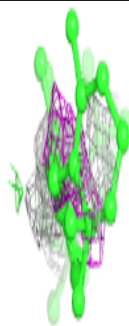
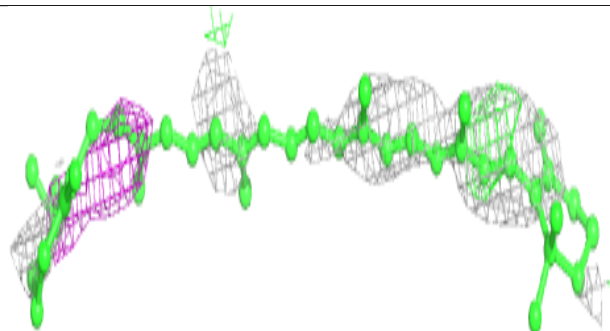
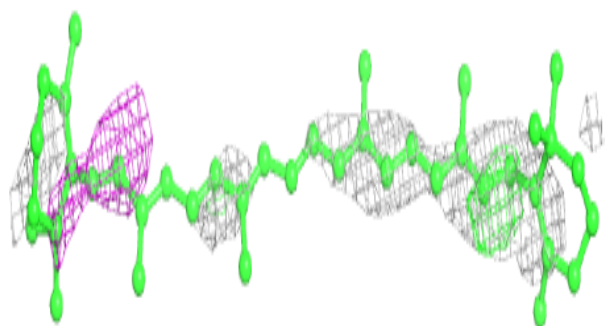


Electron density around LMT AB 623:

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

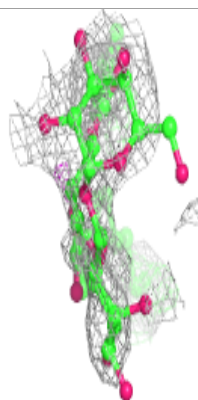
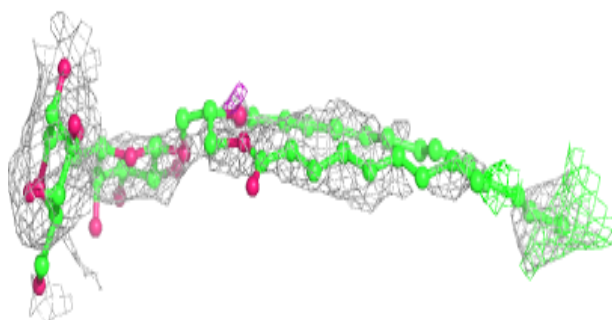
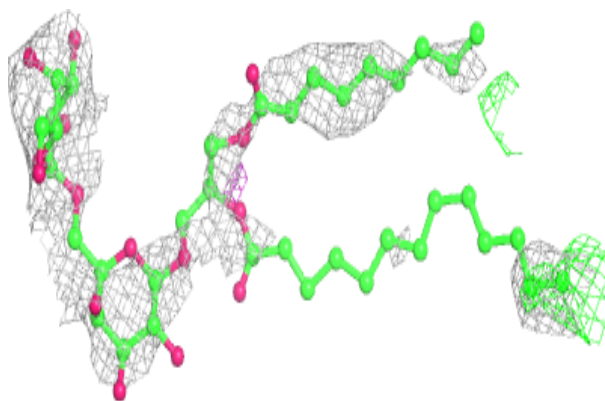
**Electron density around BCR AJ 101:**

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

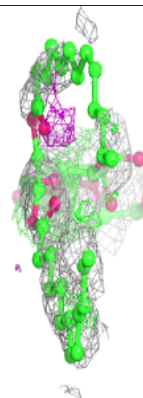
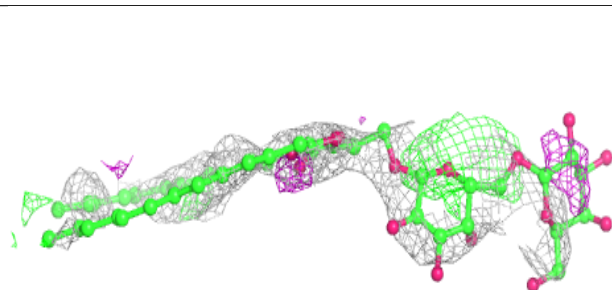
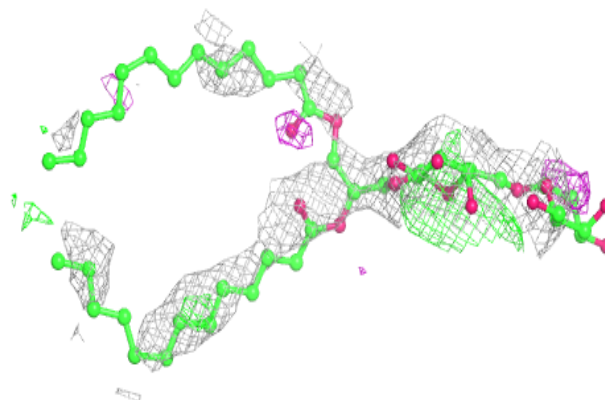


Electron density around DGD AB 628:

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

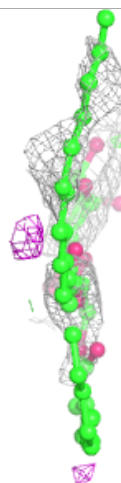
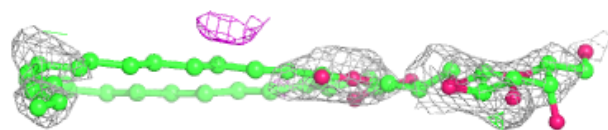
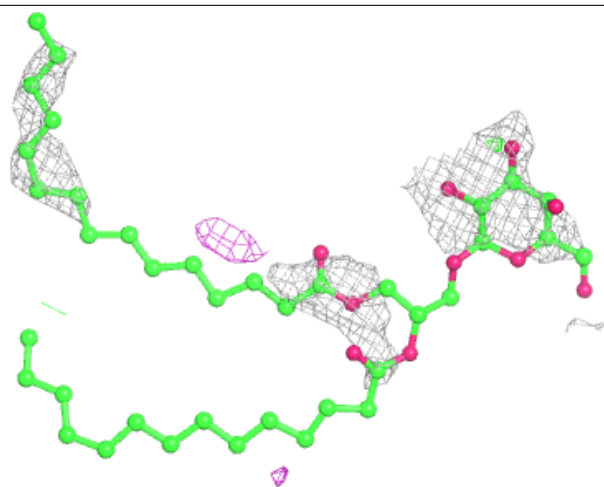
**Electron density around DGD AA 411:**

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



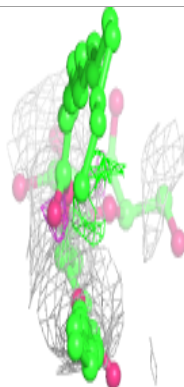
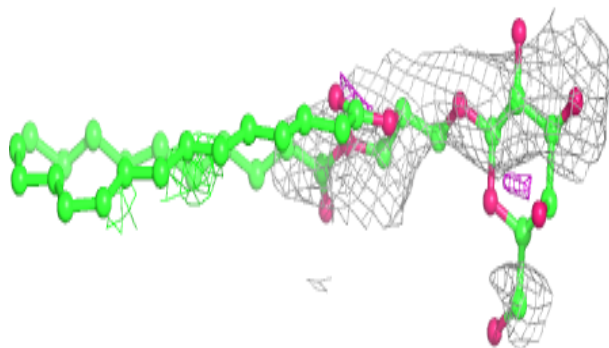
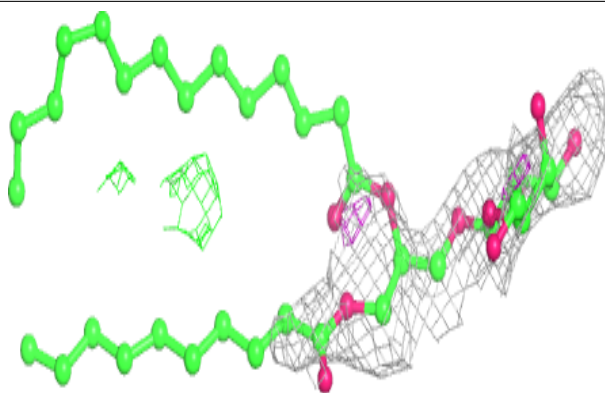
Electron density around LMG BC 5520:

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

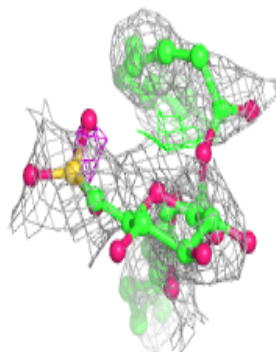
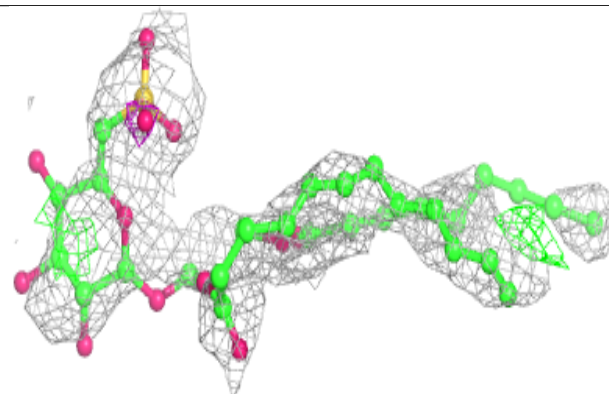
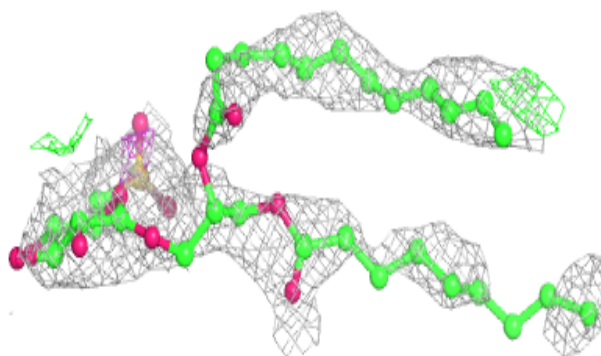


Electron density around LMG BI 5101:

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

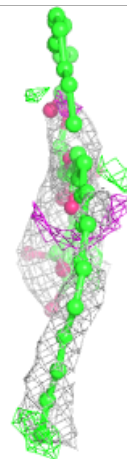
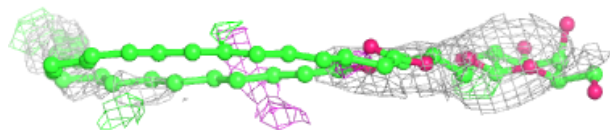
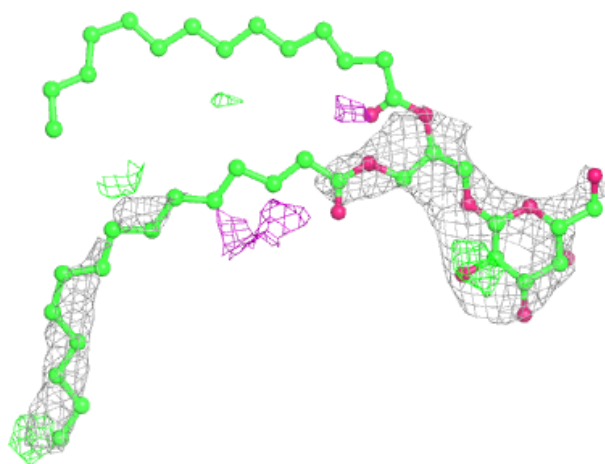
**Electron density around SQD BB 5625:**

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



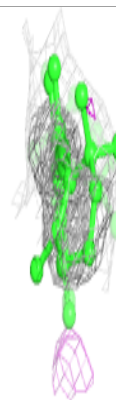
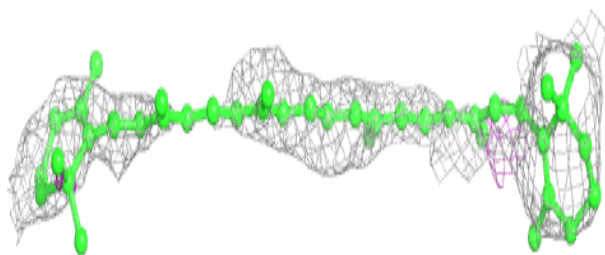
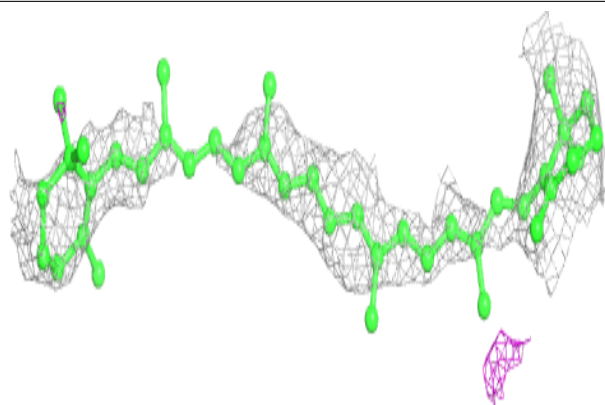
Electron density around LMG AC 520:

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



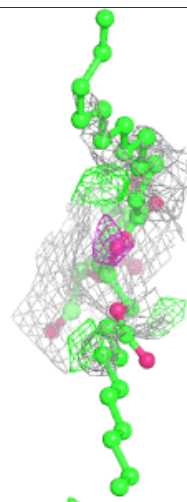
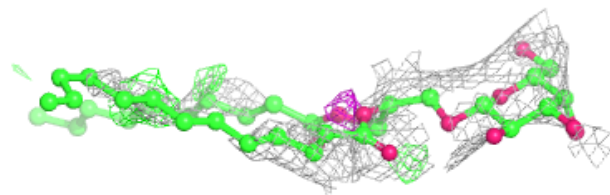
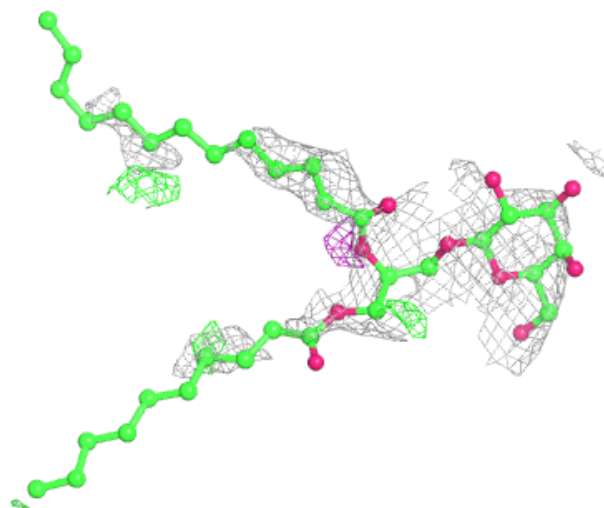
Electron density around BCR AX 101:

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



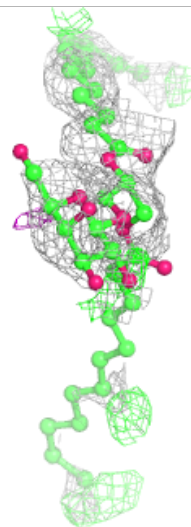
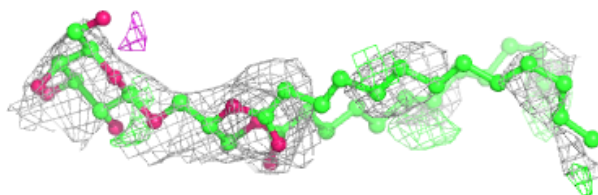
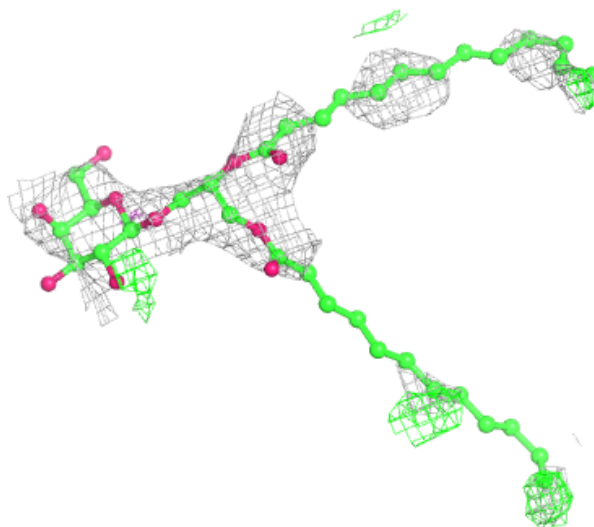
Electron density around LMG BA 5402:

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



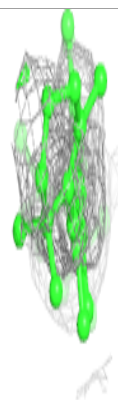
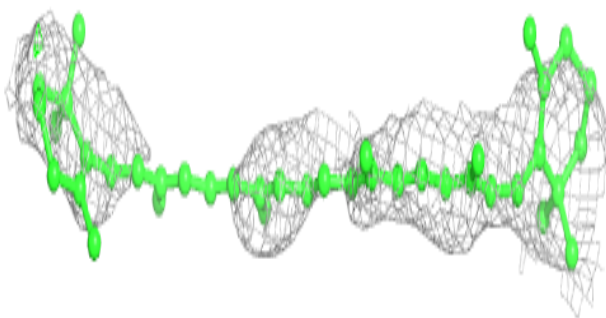
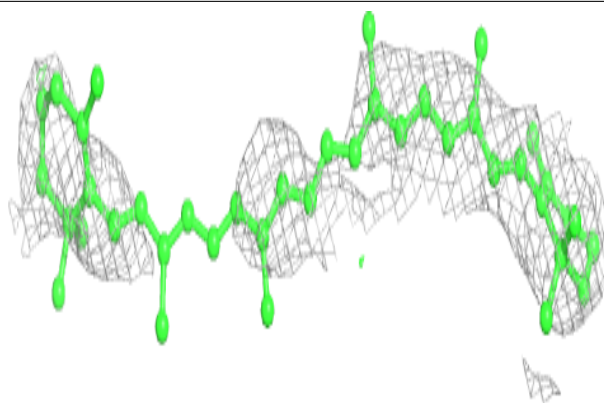
Electron density around LMG AA 414:

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

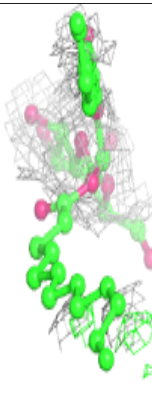
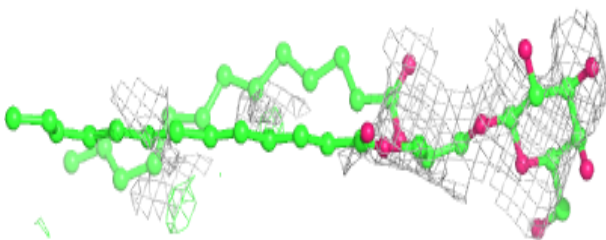
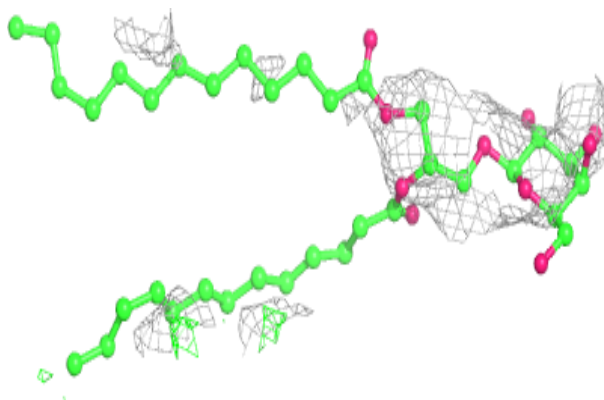


Electron density around BCR BX 5101:

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

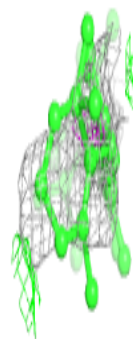
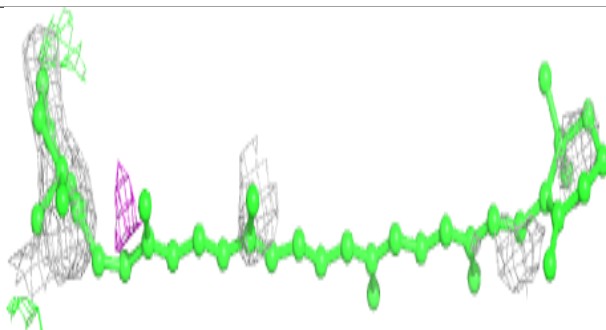
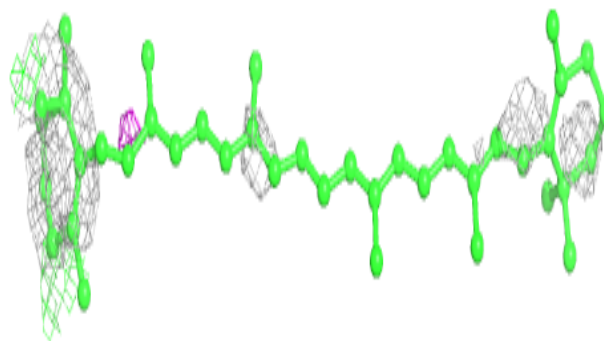
**Electron density around LMG BC 5521:**

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

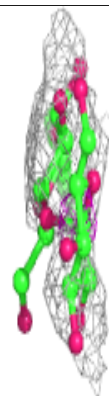
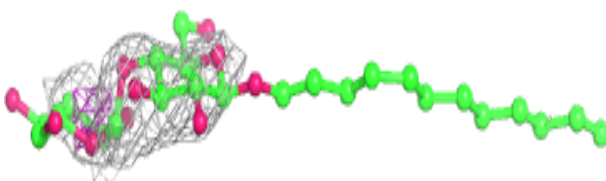
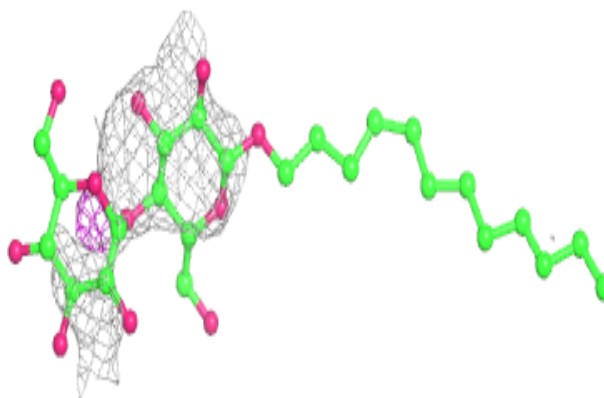


Electron density around BCR BJ 5101:

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

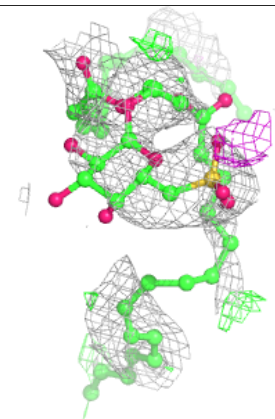
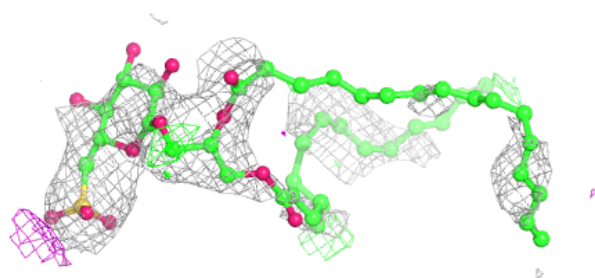
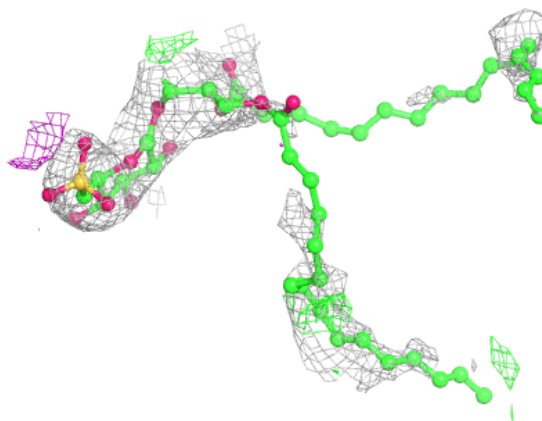
**Electron density around LMT BI 5102:**

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



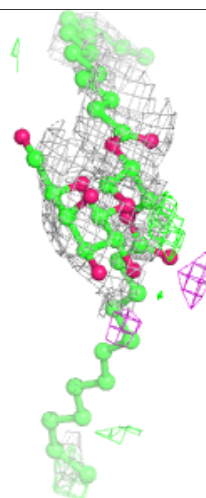
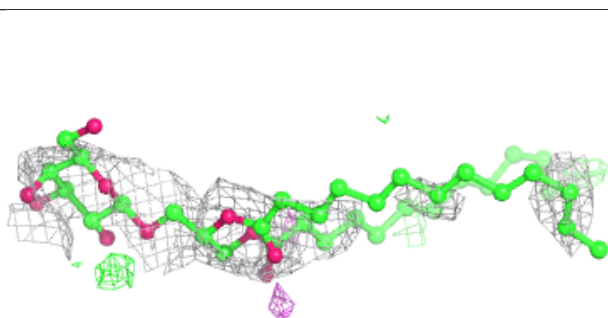
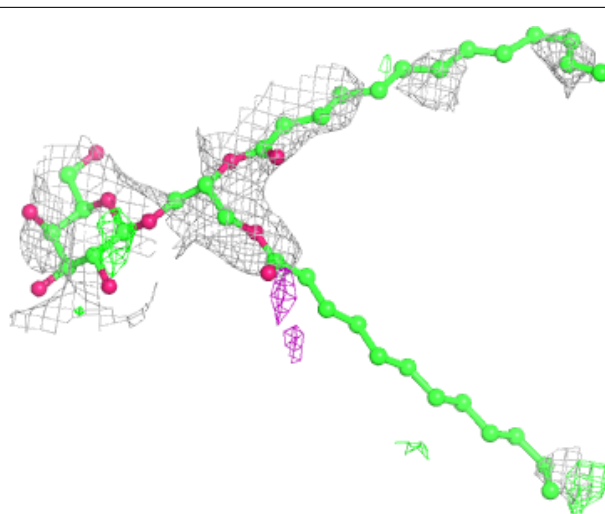
Electron density around SQD BA 5401:

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



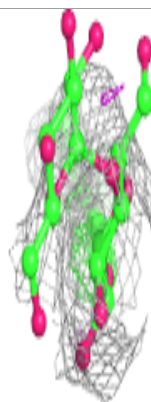
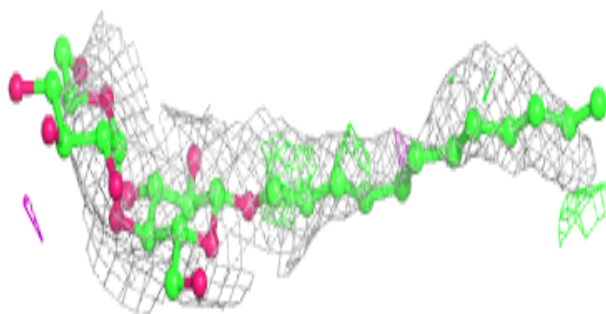
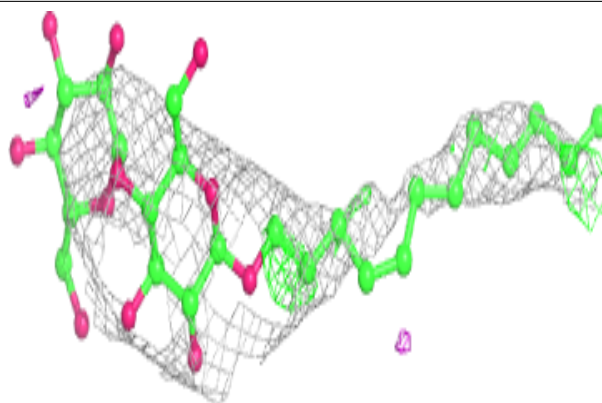
Electron density around LMG BE 5101:

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

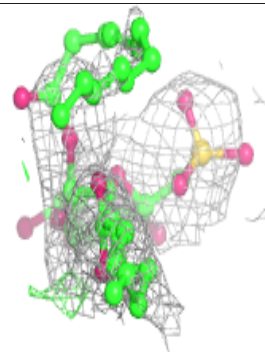
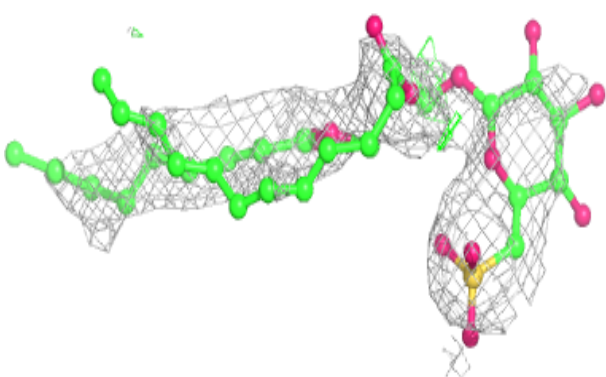
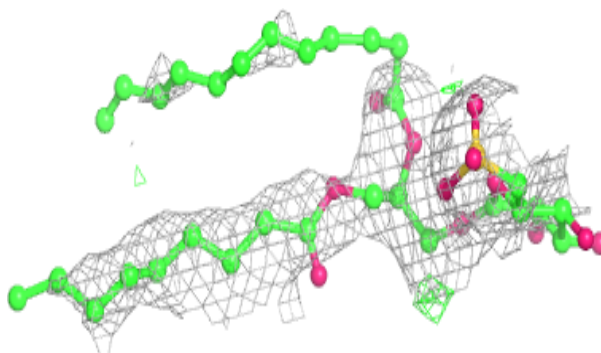


Electron density around LMT BB 5603:

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

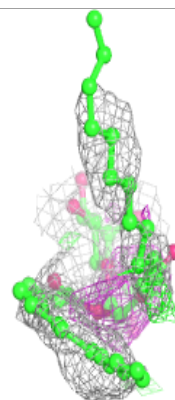
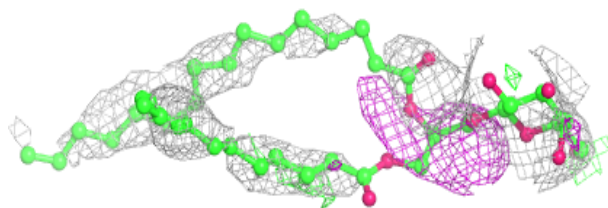
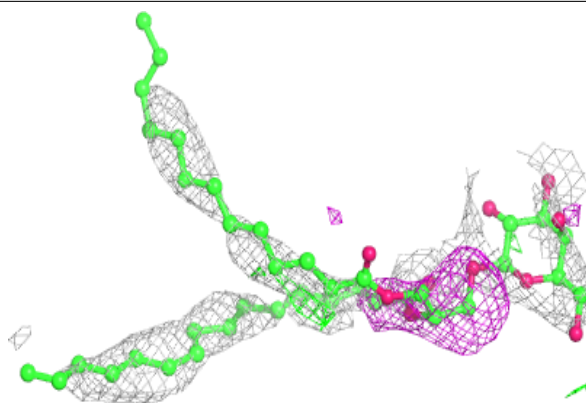
**Electron density around SQD AB 622:**

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

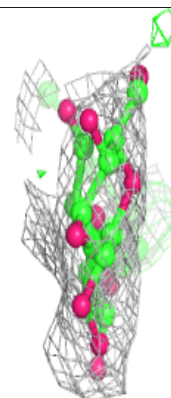
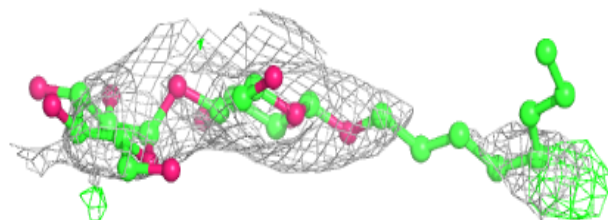
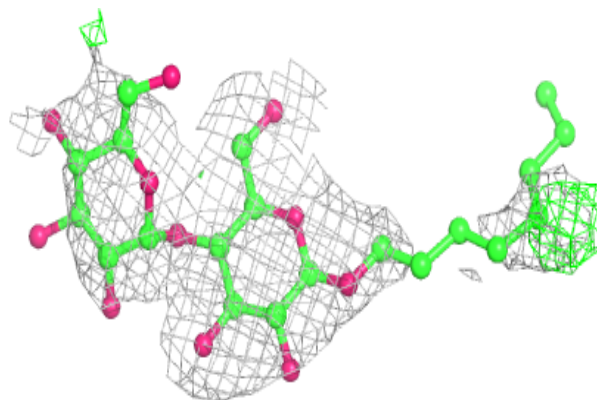


Electron density around LMG BD 5410:

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

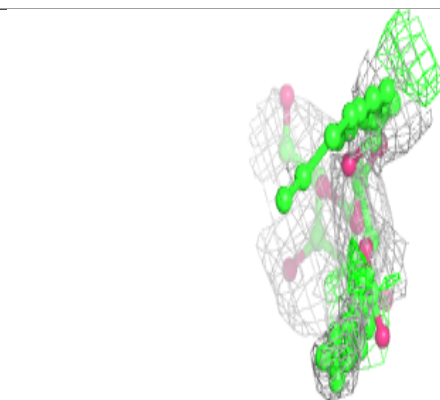
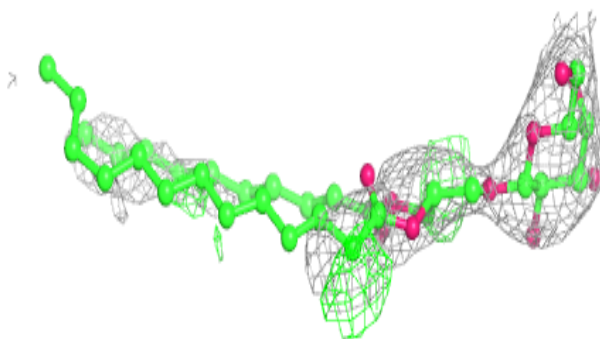
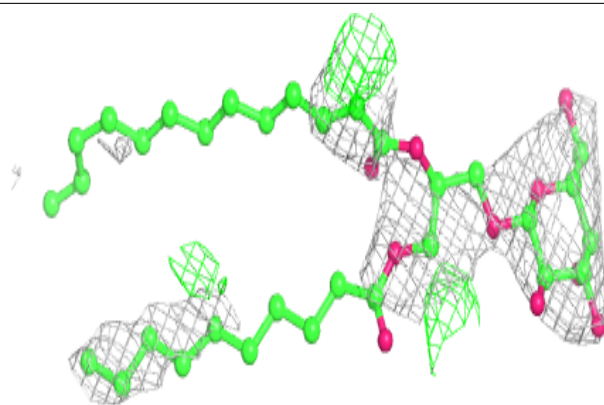
**Electron density around LMT BD 5411:**

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

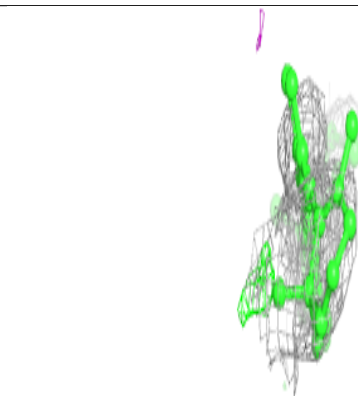
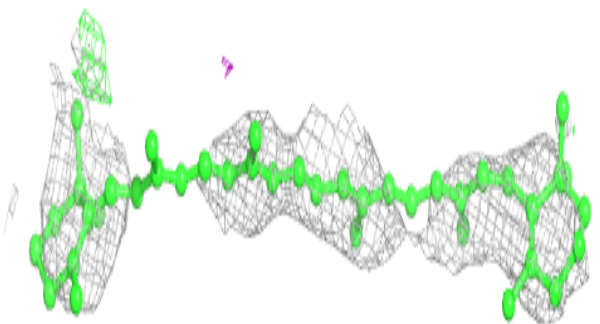
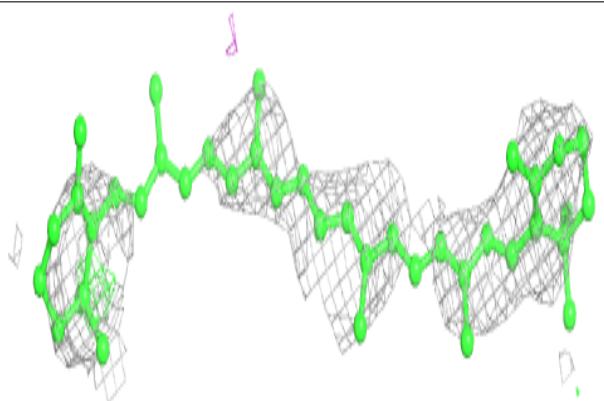


Electron density around LMG AM 101:

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

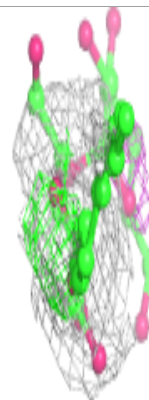
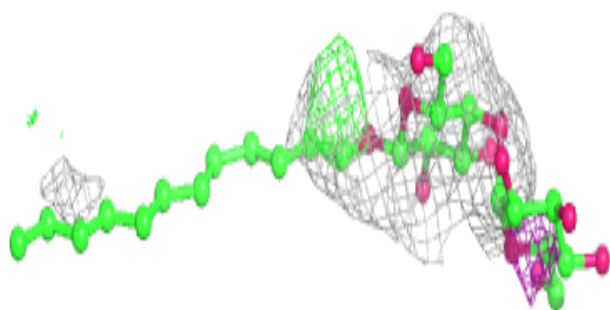
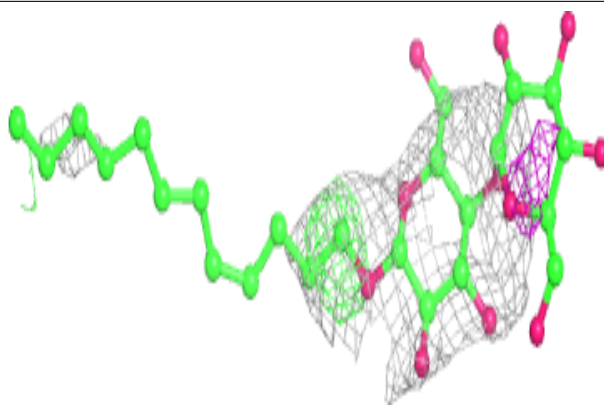
**Electron density around BCR BC 5516:**

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



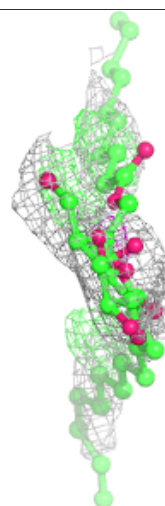
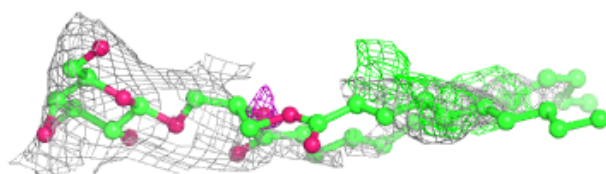
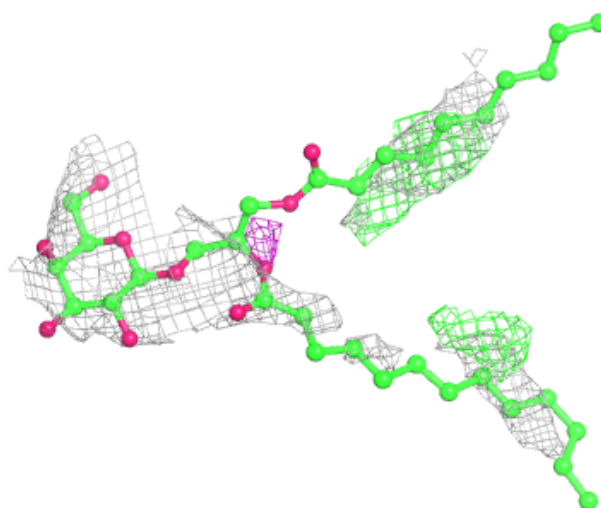
Electron density around LMT AB 629:

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



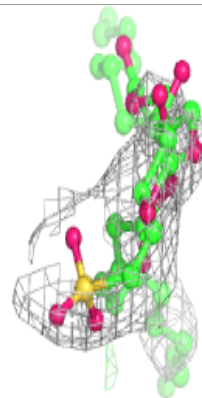
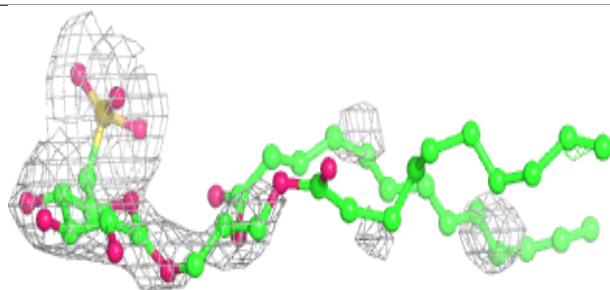
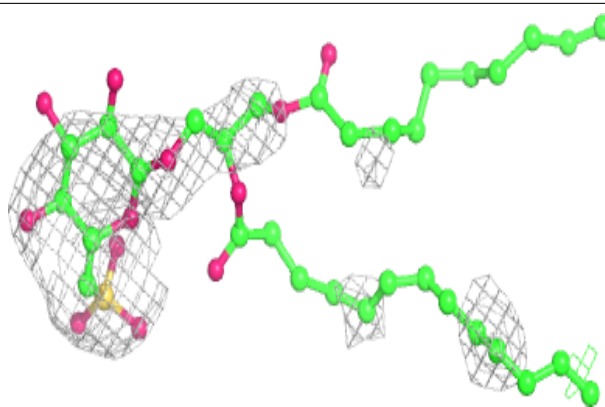
Electron density around LMG AA 417:

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

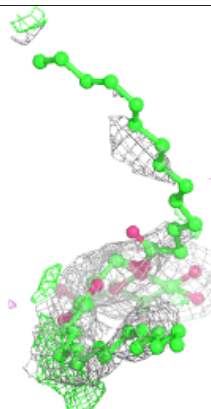
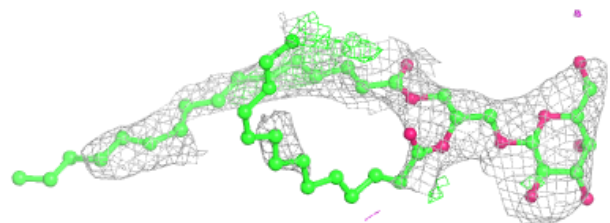
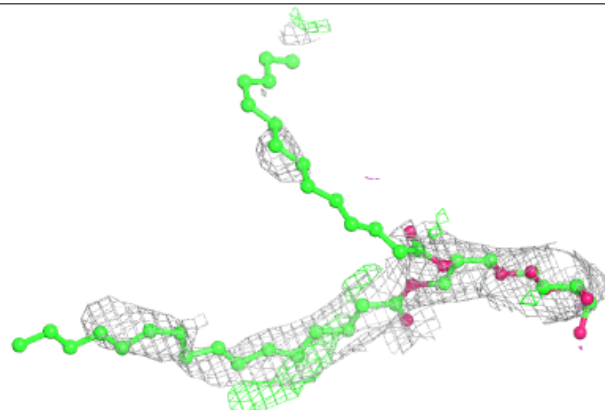


Electron density around SQD BF 5102:

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

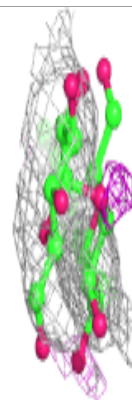
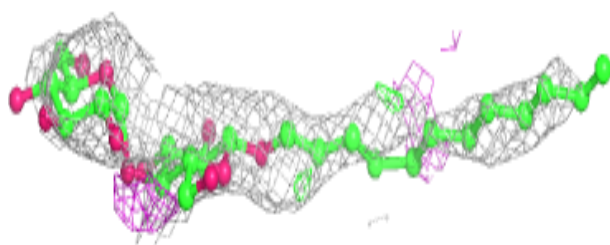
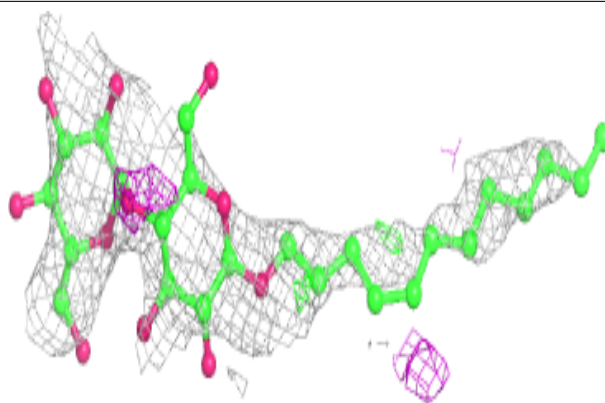
**Electron density around LMG AB 621:**

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

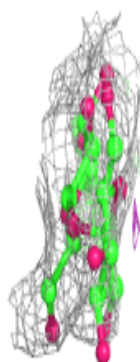
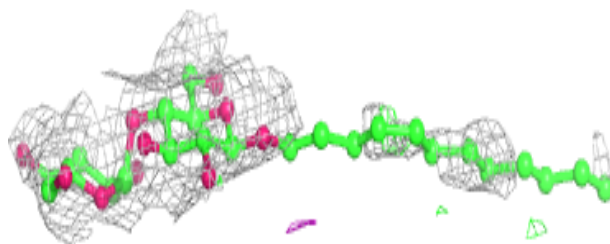
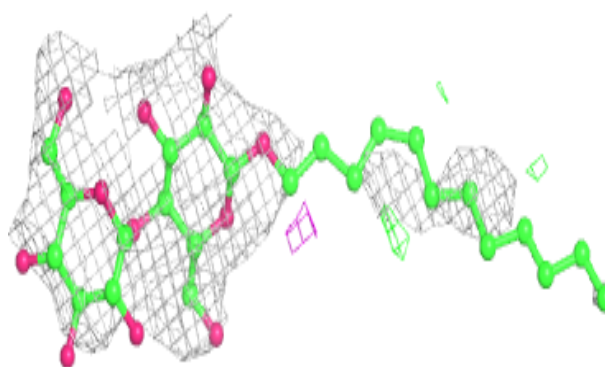


Electron density around LMT BB 5604:

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

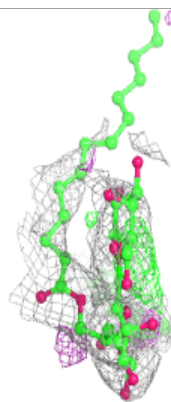
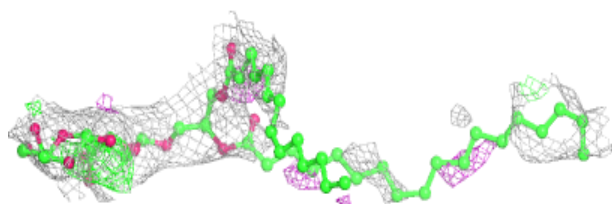
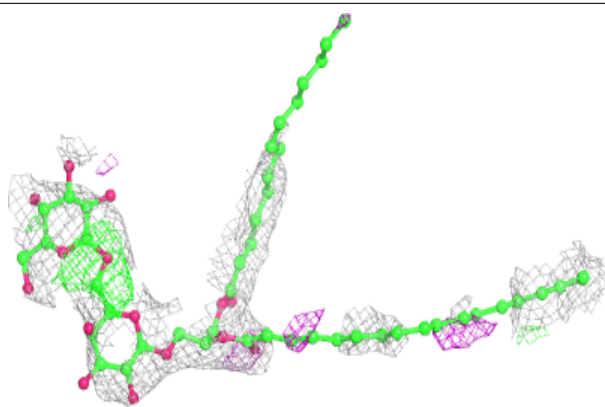
**Electron density around LMT AI 102:**

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



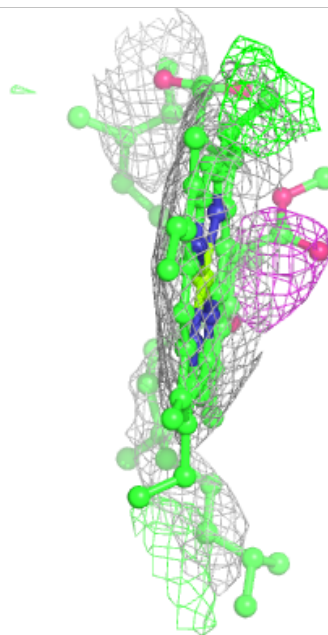
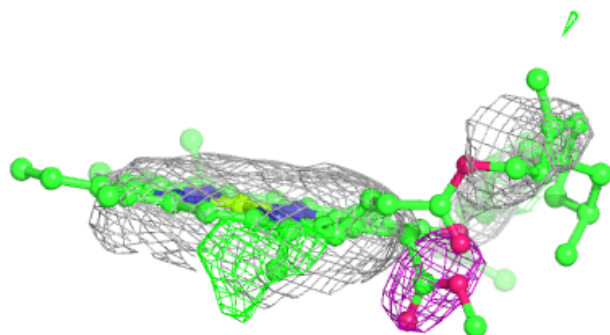
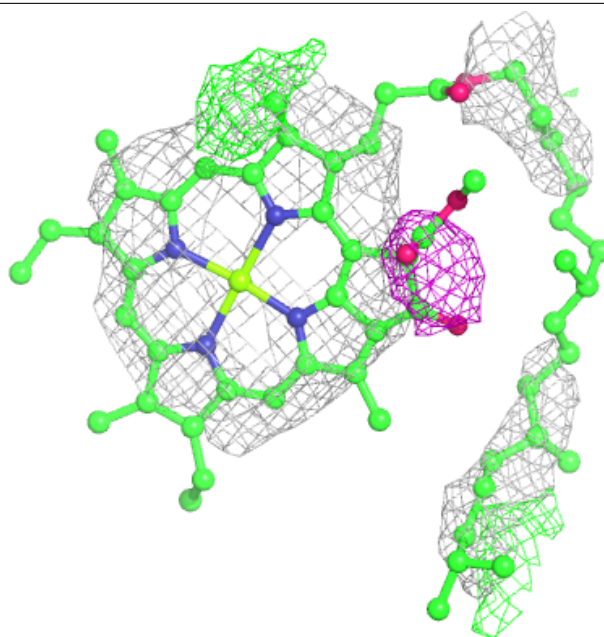
Electron density around DGD BC 5518:

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



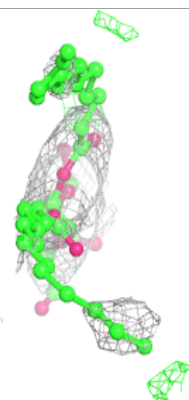
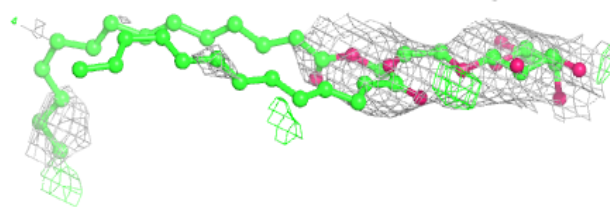
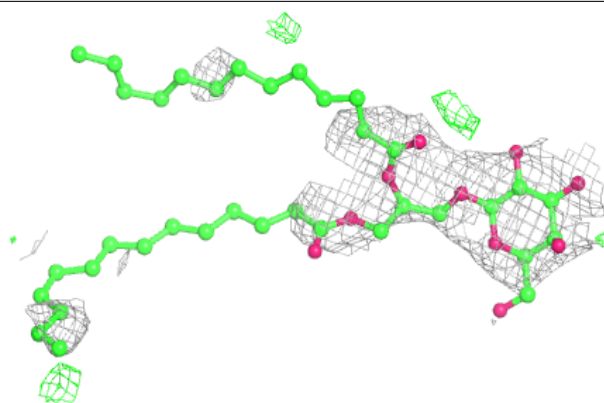
Electron density around CLA AB 601:

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

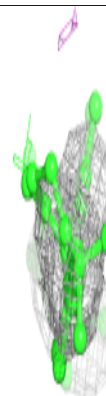
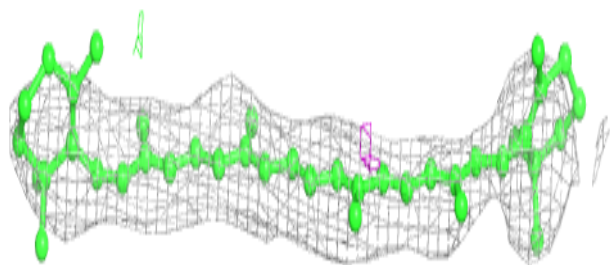
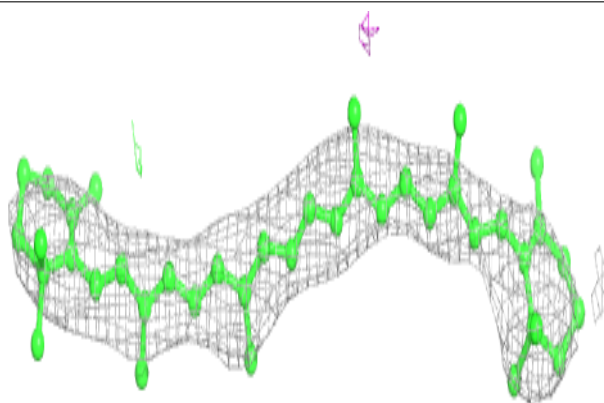


Electron density around LMG BD 5408:

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

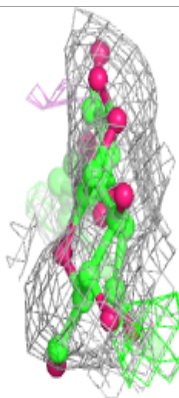
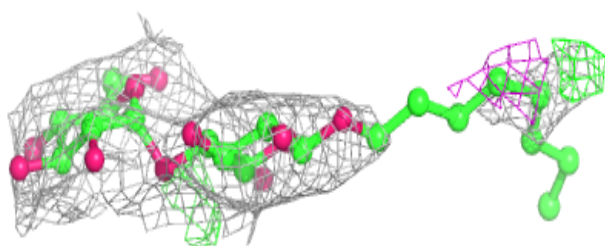
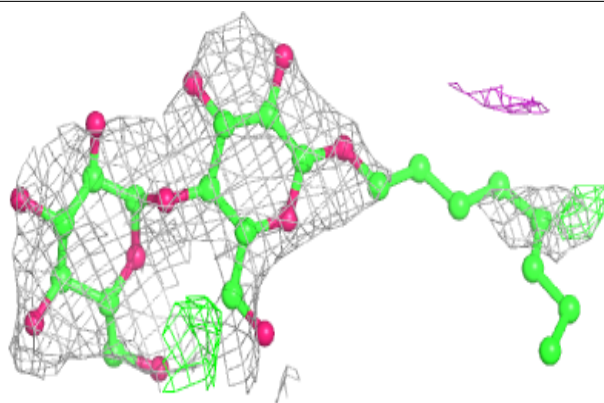
**Electron density around BCR AC 516:**

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

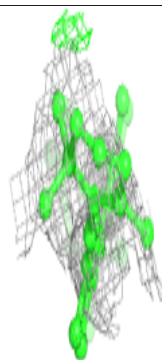
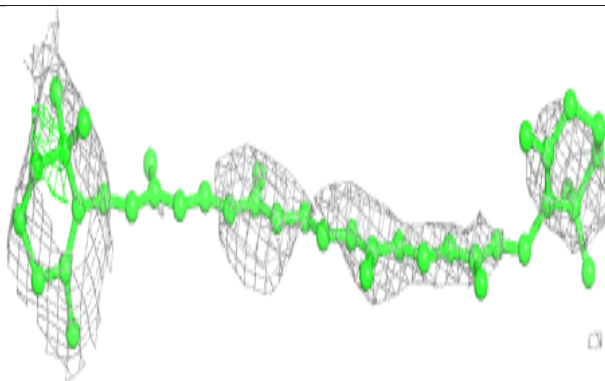
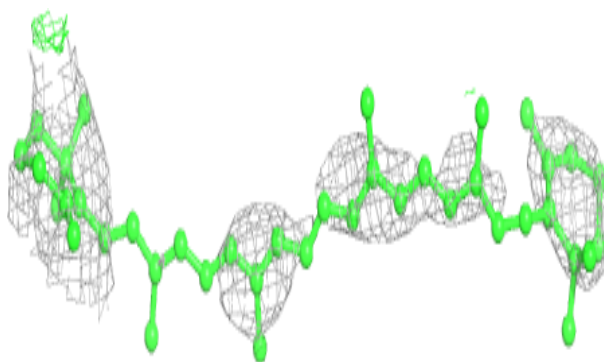


Electron density around LMT AD 409:

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

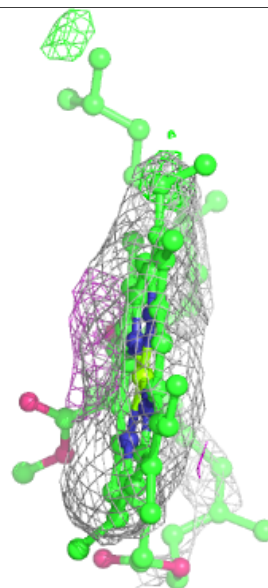
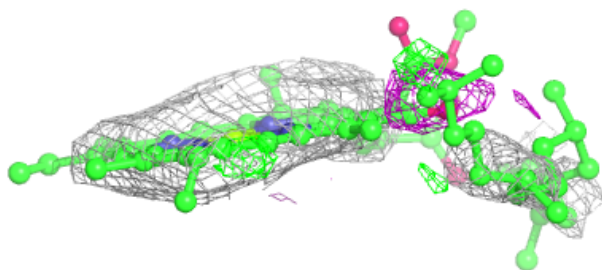
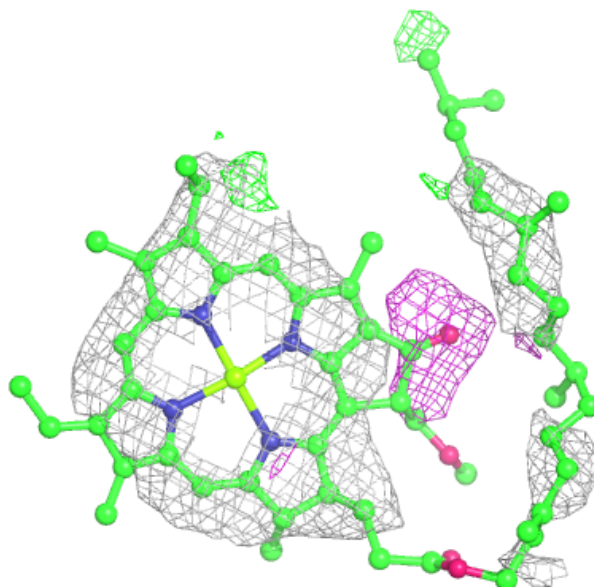
**Electron density around BCR BC 5515:**

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



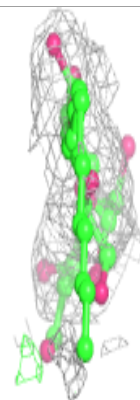
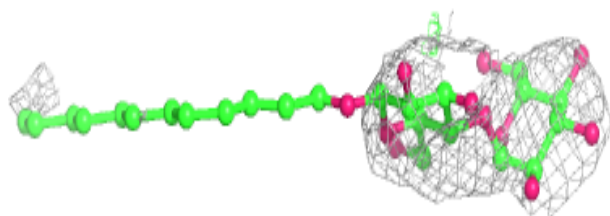
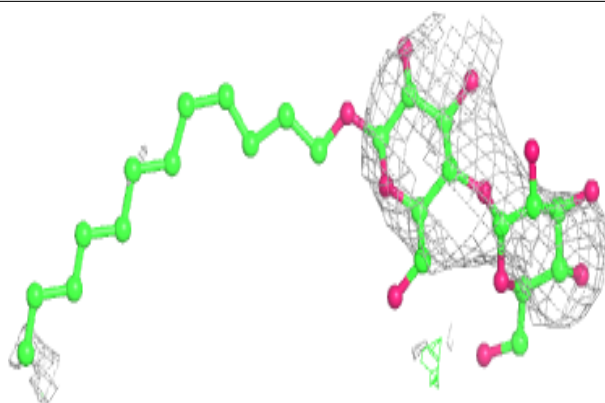
Electron density around CLA BB 5605:

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

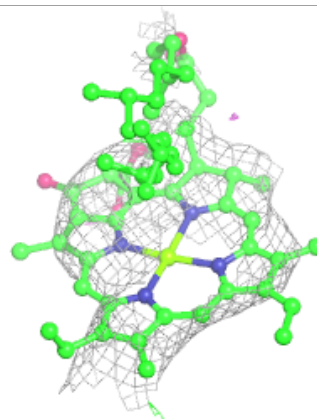
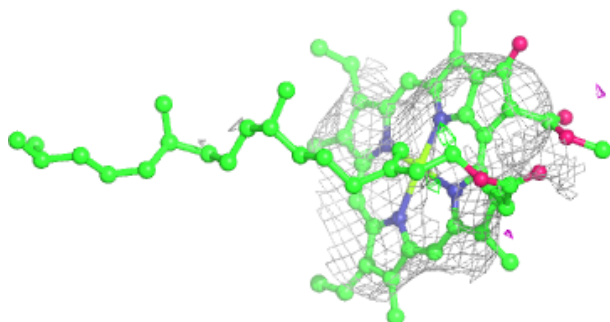
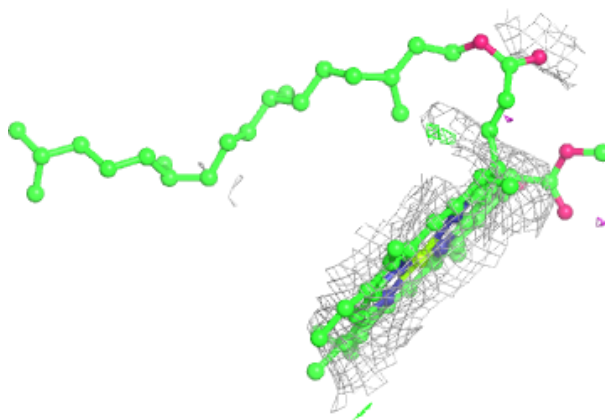


Electron density around LMT AB 624:

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

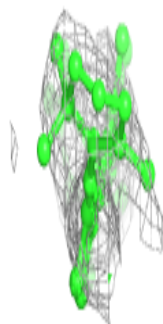
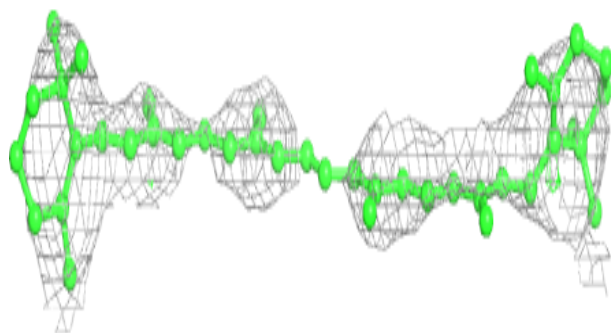
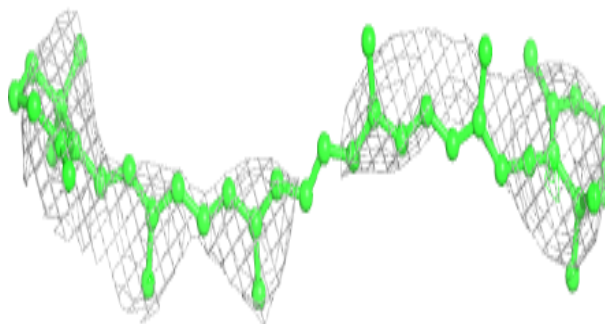
**Electron density around CLA BC 5513:**

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

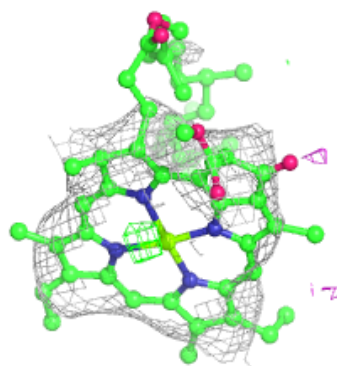
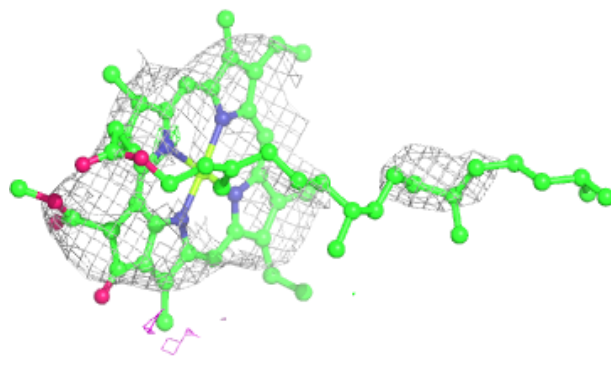
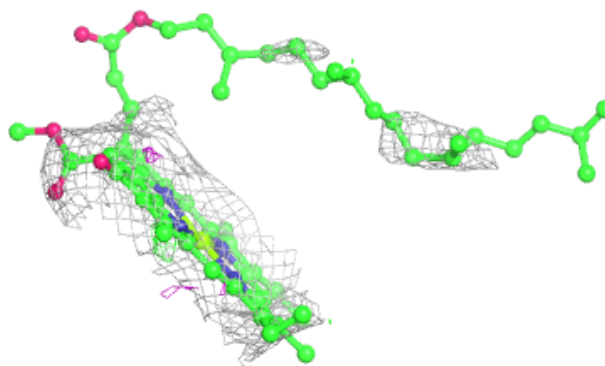


Electron density around BCR AC 515:

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

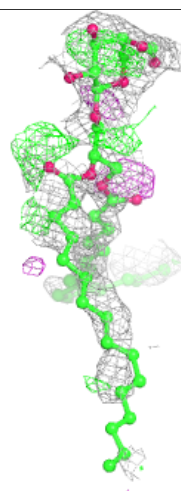
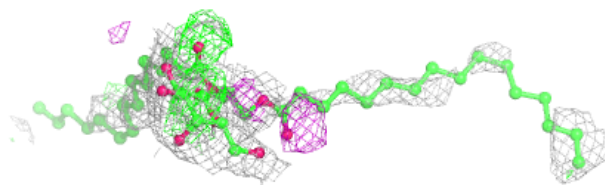
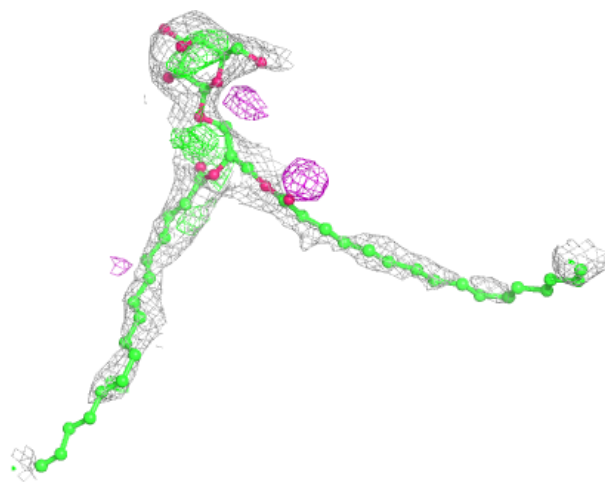
**Electron density around CLA AC 513:**

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



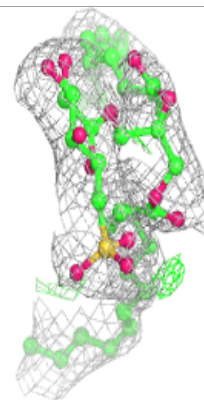
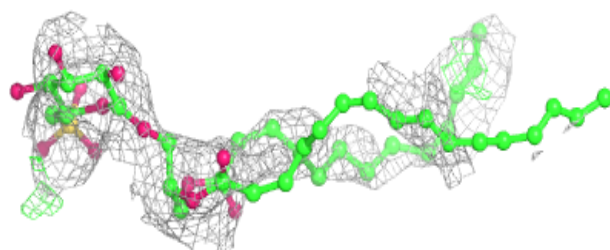
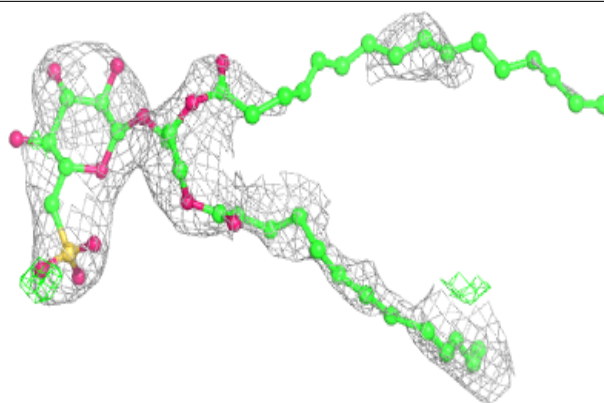
Electron density around LMG AB 620:

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

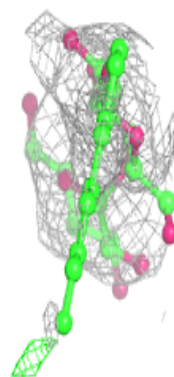
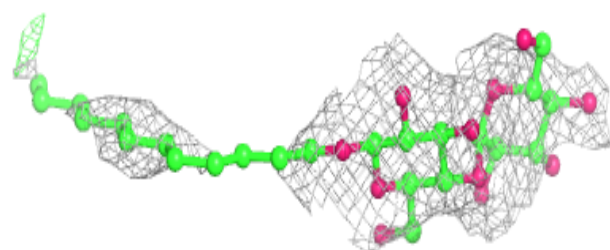
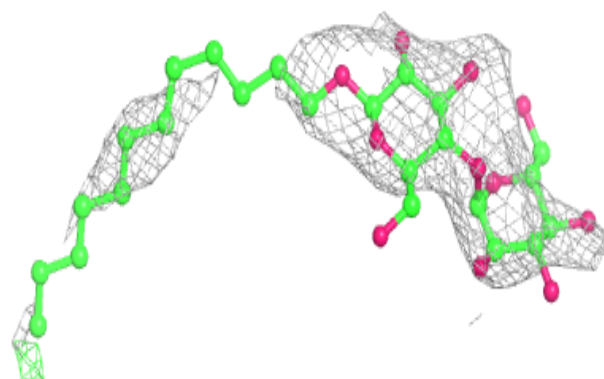


Electron density around SQD BA 5414:

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

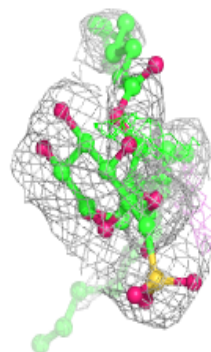
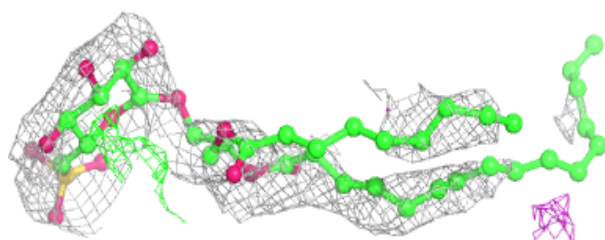
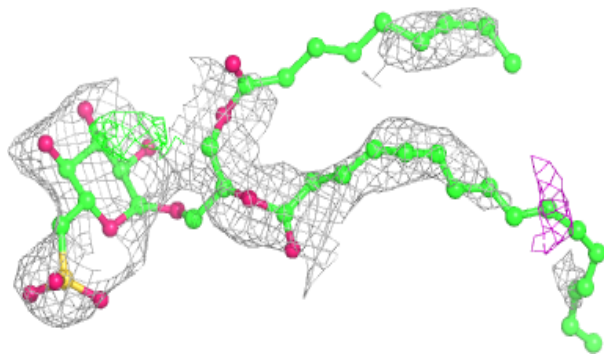
**Electron density around LMT BM 5101:**

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

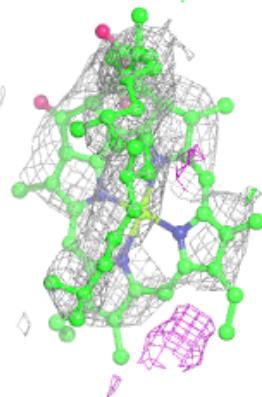
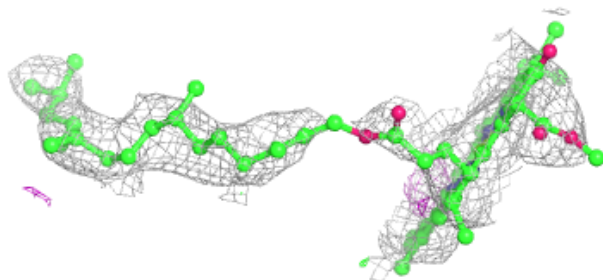
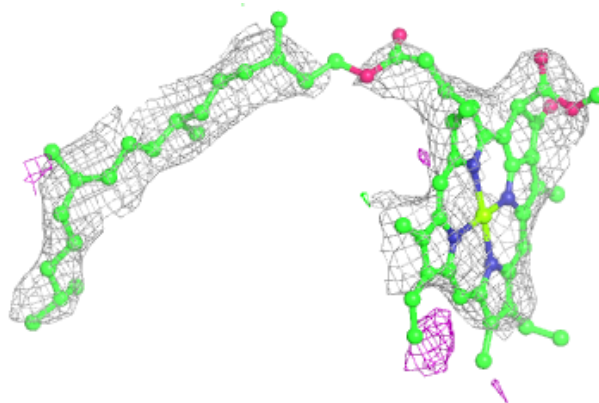


Electron density around SQD BB 5601:

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

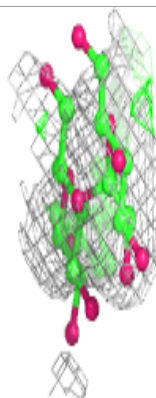
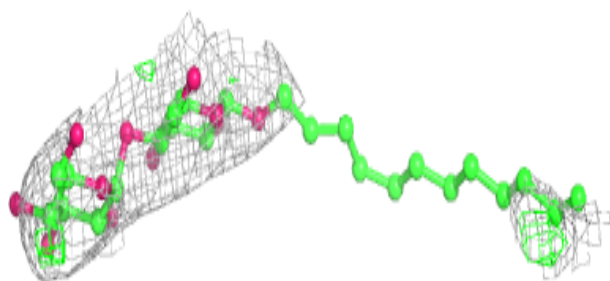
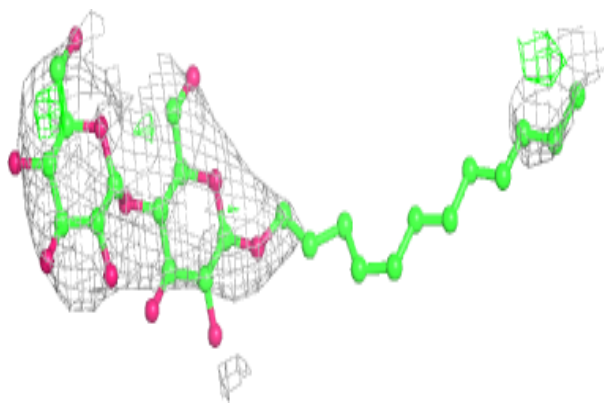
**Electron density around CLA AB 609:**

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

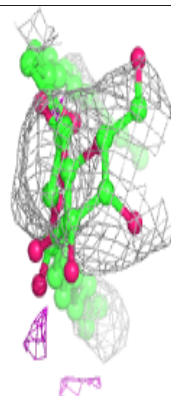
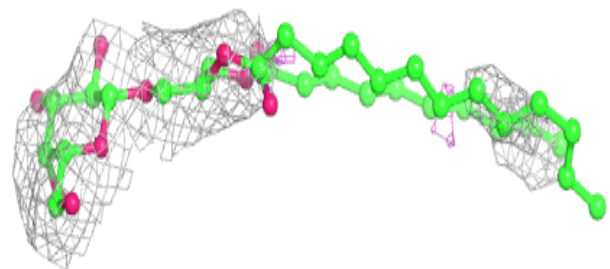
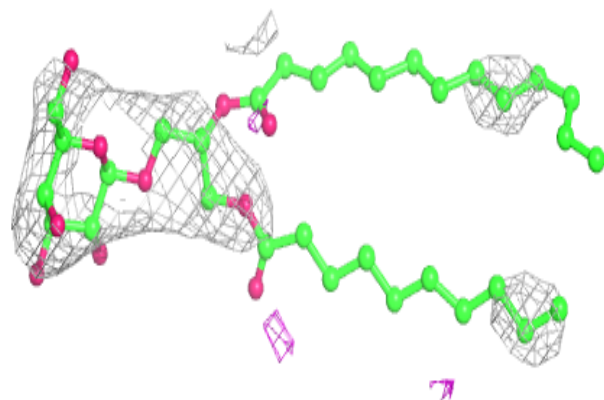


Electron density around LMT AI 103:

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

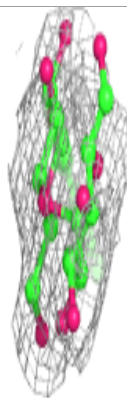
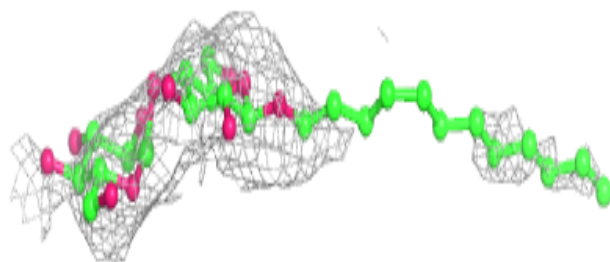
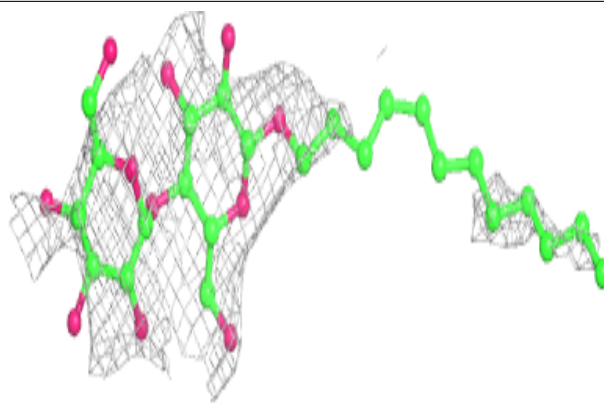
**Electron density around LMG BM 5102:**

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

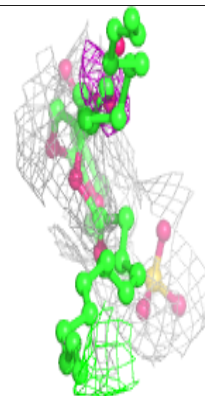
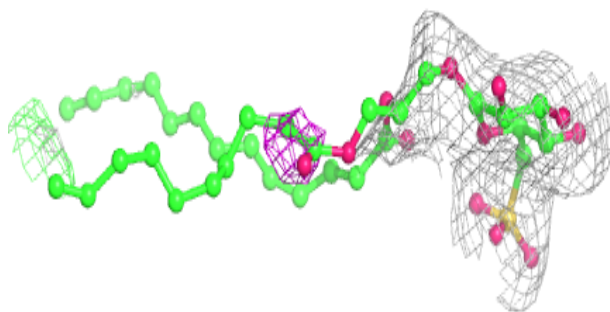
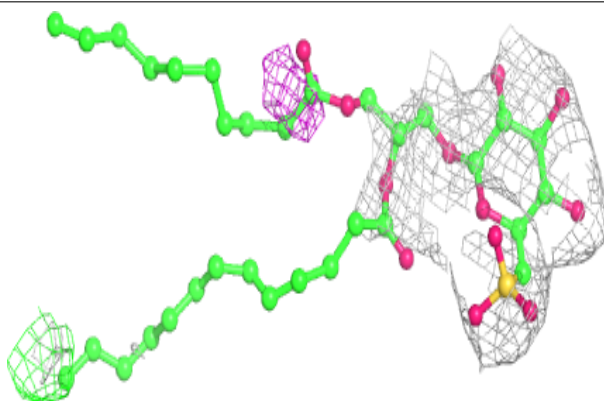


Electron density around LMT AB 630:

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

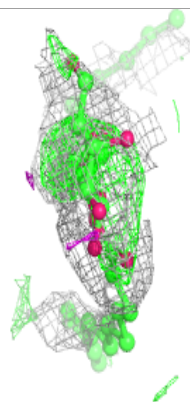
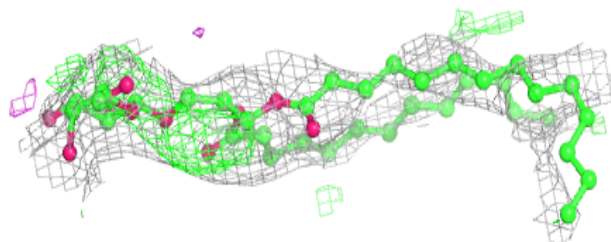
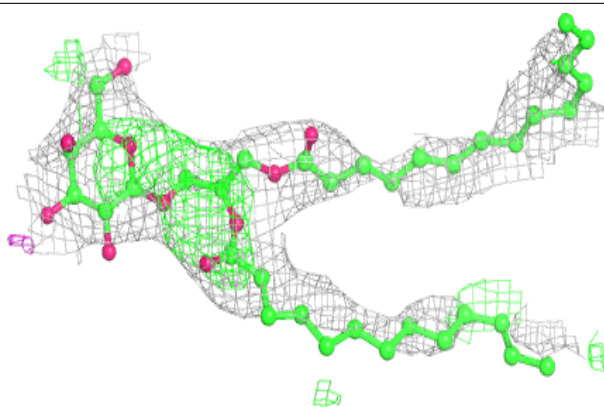
**Electron density around SQD AF 102:**

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

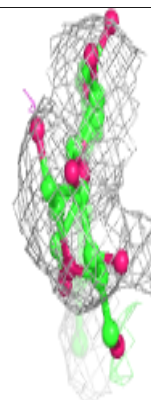
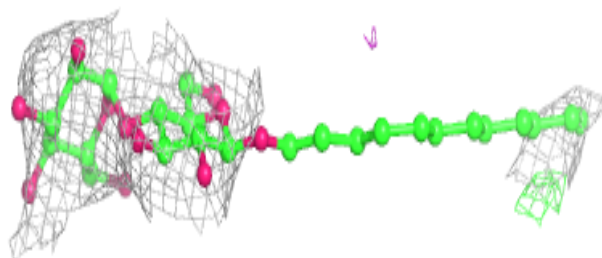
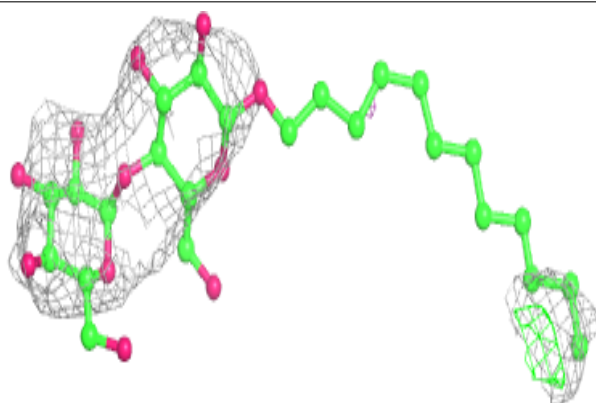


Electron density around LMG AJ 102:

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

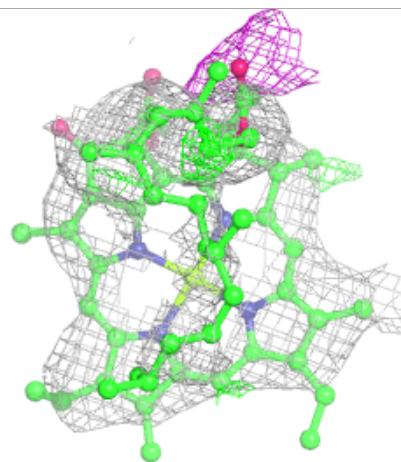
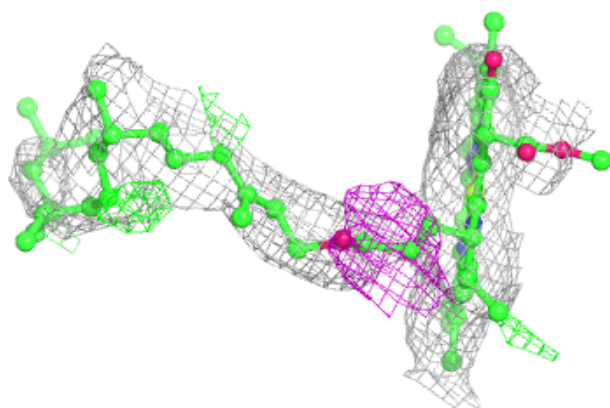
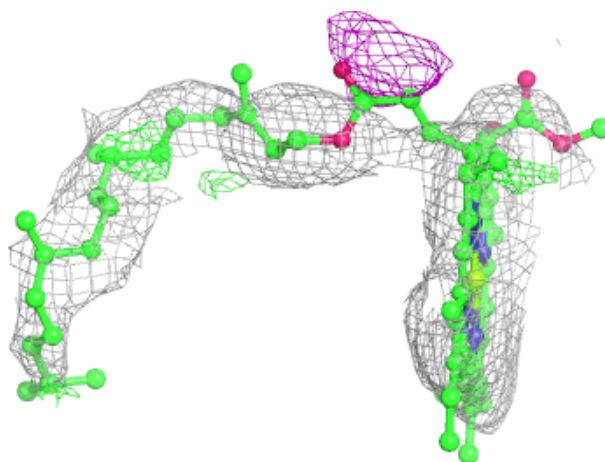
**Electron density around LMT BB 5627:**

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



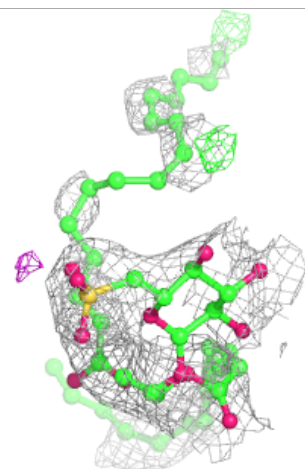
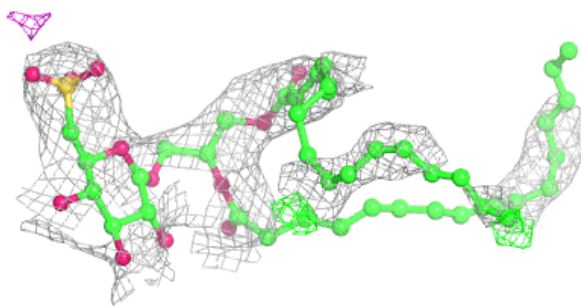
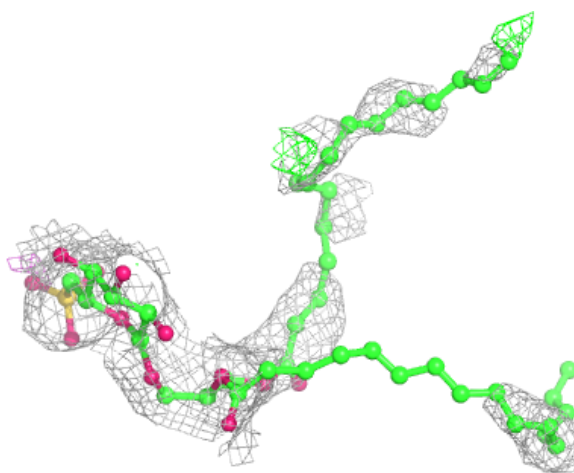
Electron density around CLA AC 506:

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



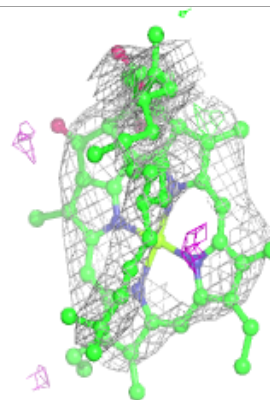
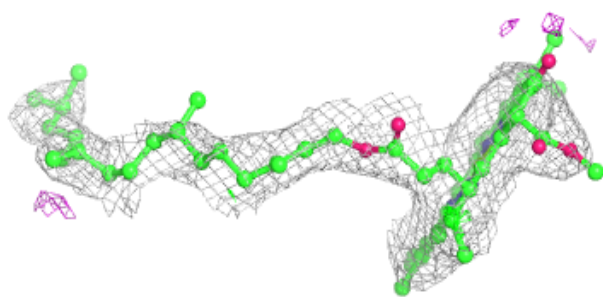
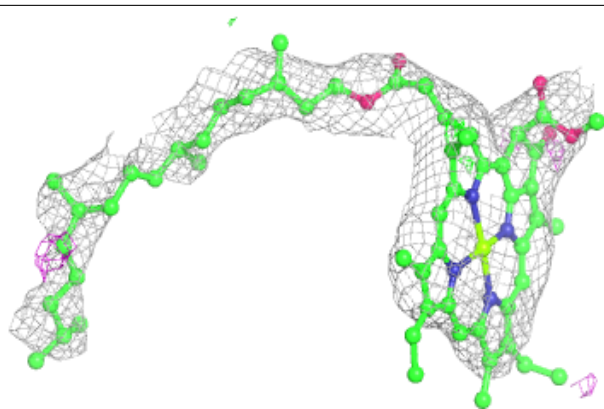
Electron density around SQD AA 416:

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

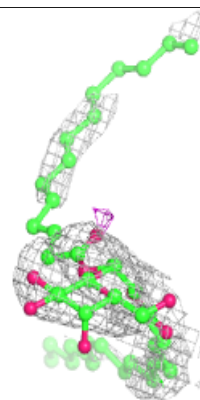
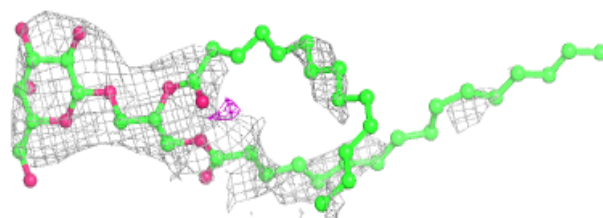
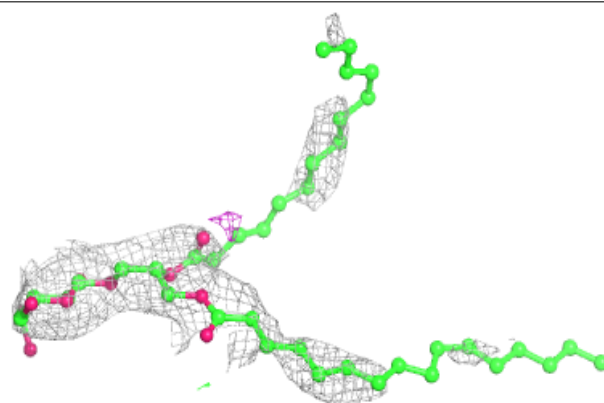


Electron density around CLA BB 5613:

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

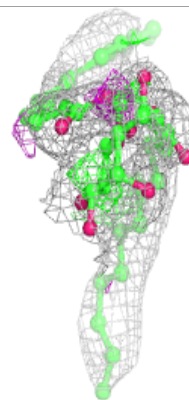
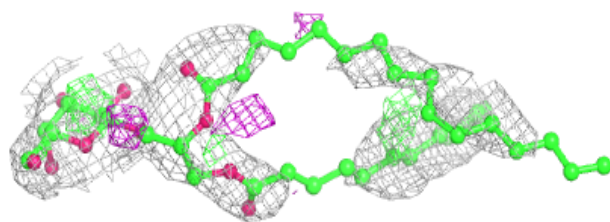
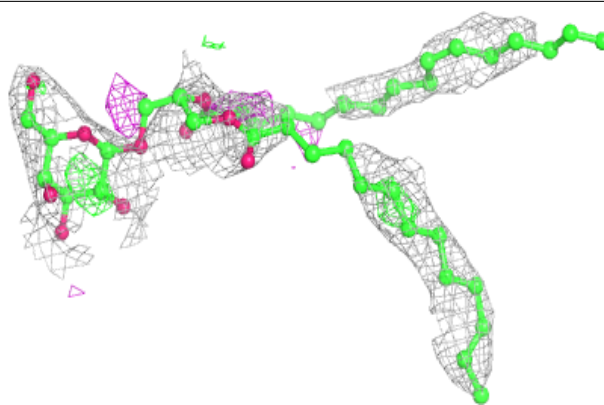
**Electron density around LMG BB 5624:**

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



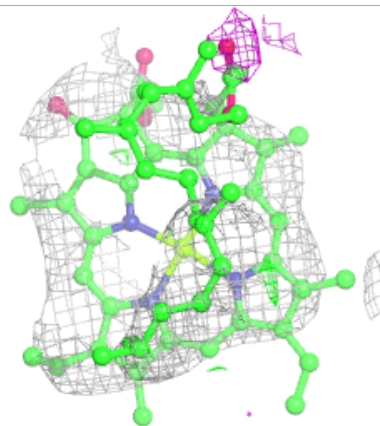
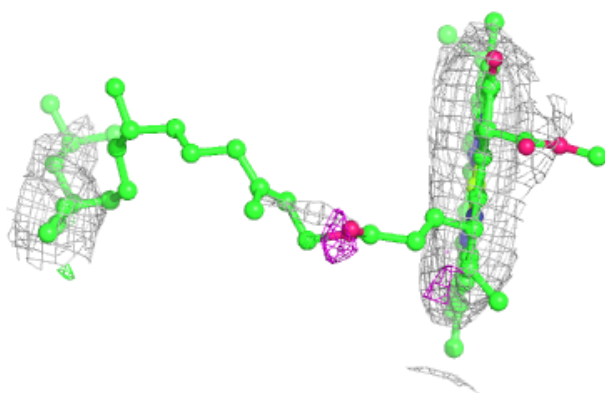
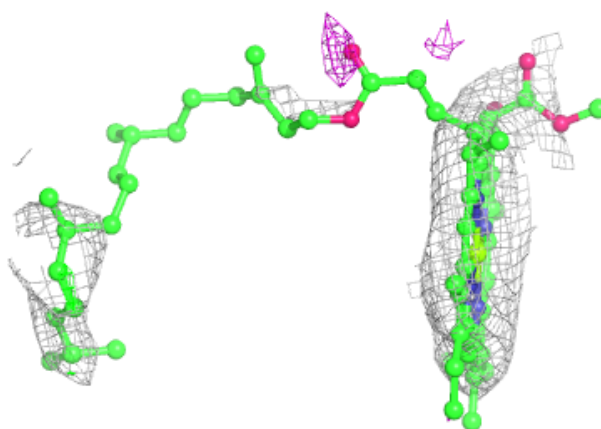
Electron density around LMG AD 408:

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



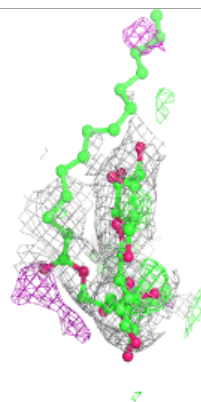
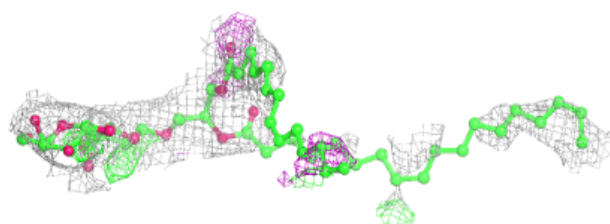
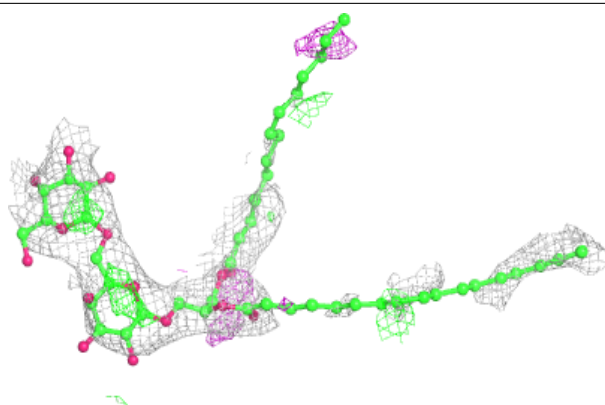
Electron density around CLA BC 5506:

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

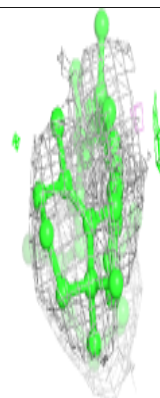
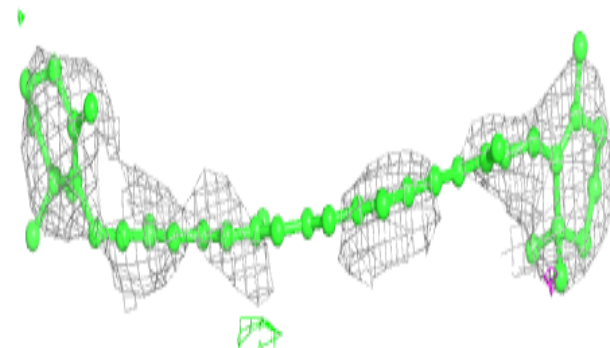
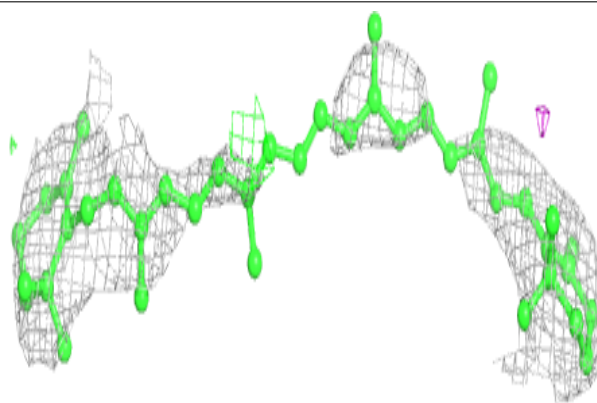


Electron density around DGD AC 518:

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

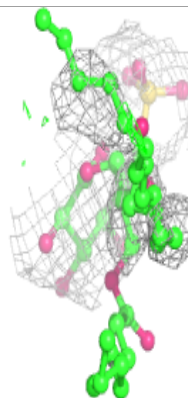
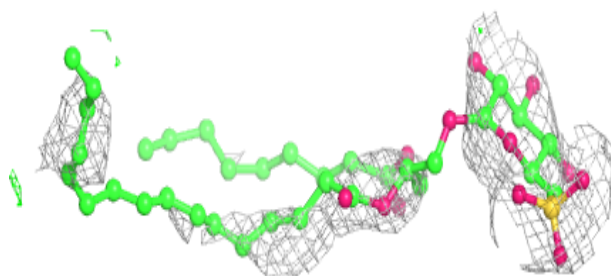
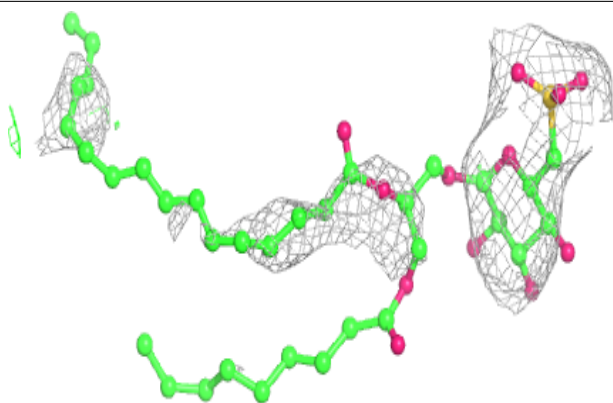
**Electron density around BCR BT 5101:**

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

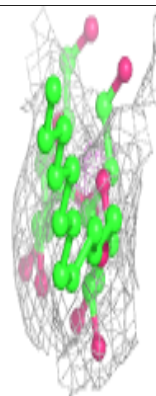
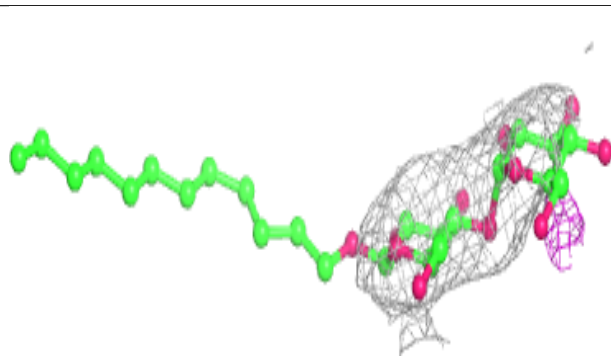
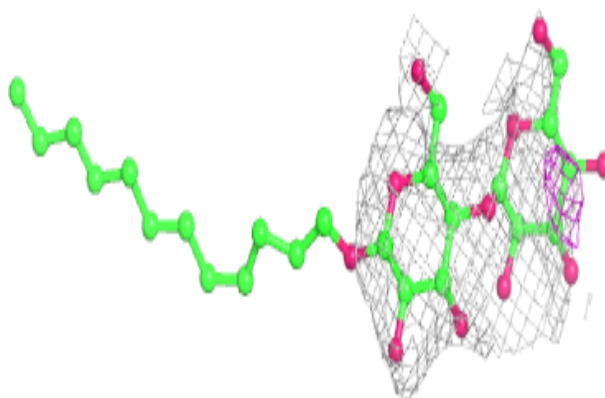


Electron density around SQD AB 627:

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

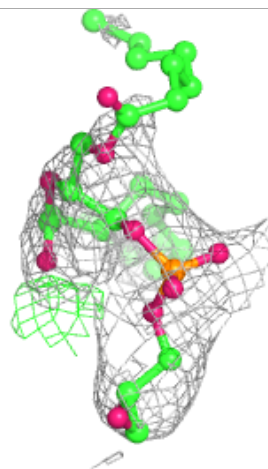
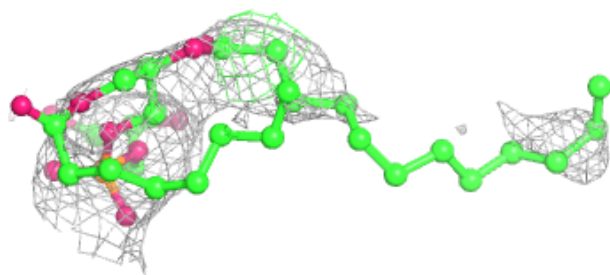
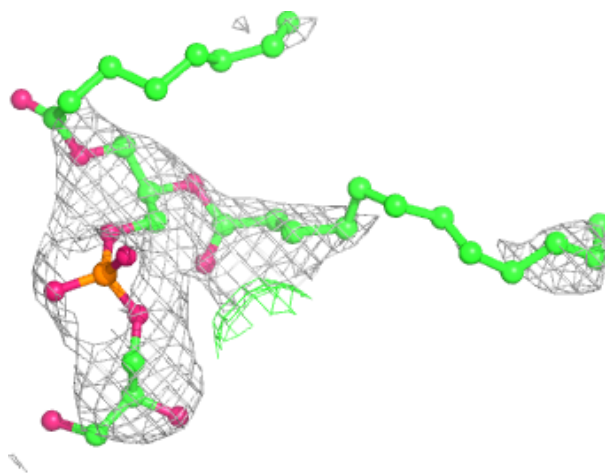
**Electron density around LMT BC 5522:**

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



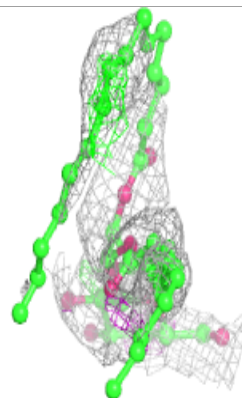
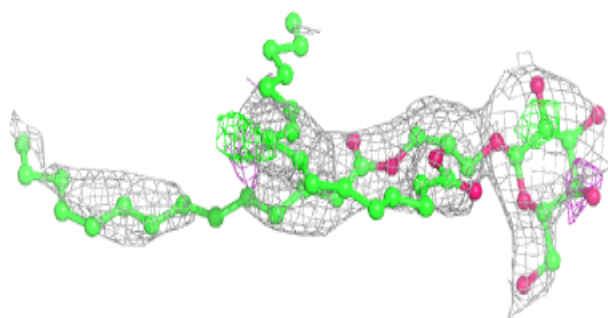
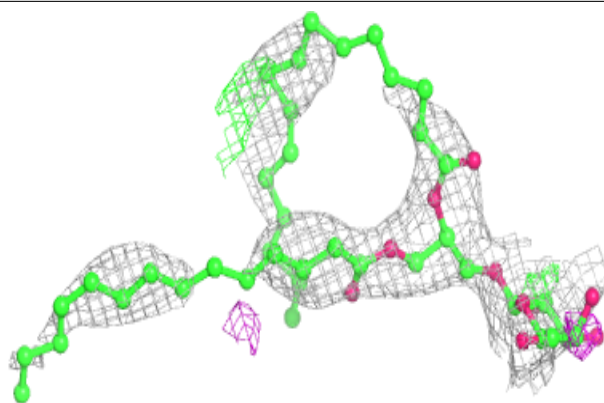
Electron density around LHG AA 415:

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

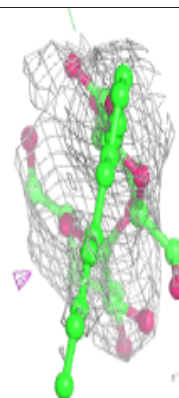
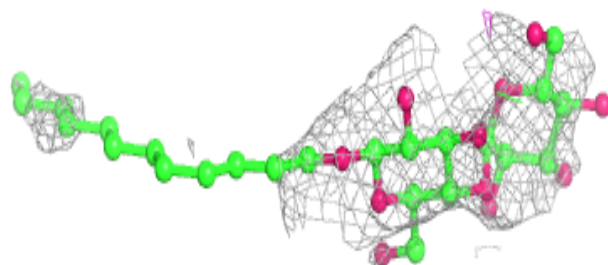
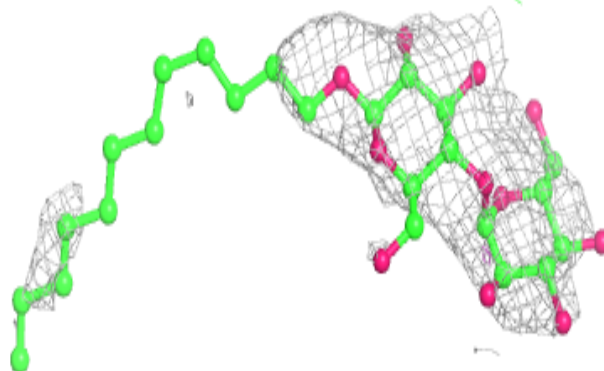


Electron density around LMG AD 407:

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

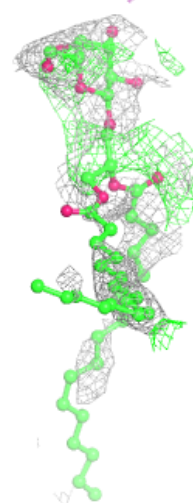
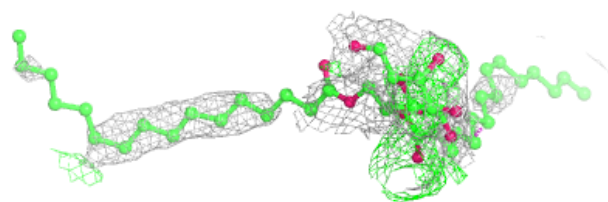
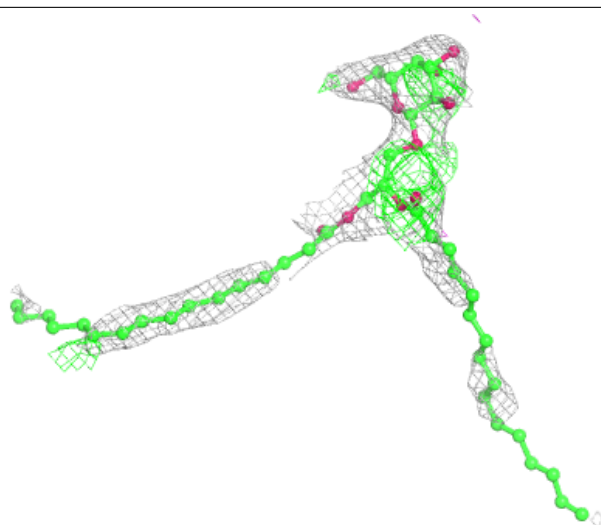
**Electron density around LMT AM 102:**

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



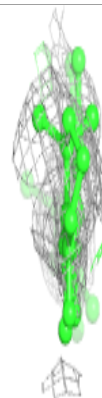
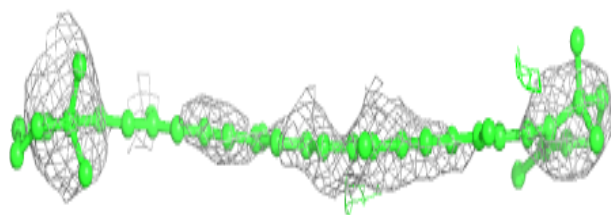
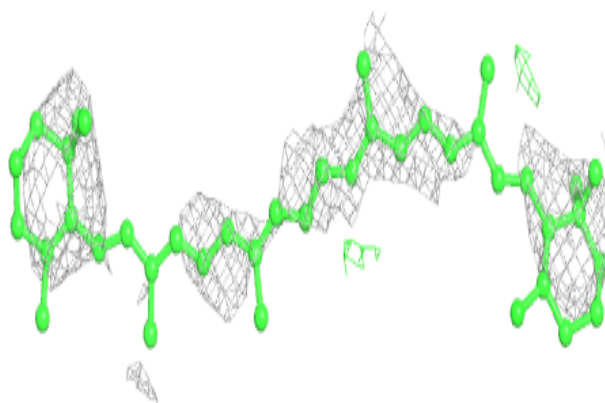
Electron density around LMG BL 5101:

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

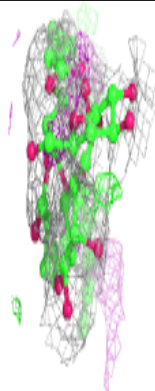
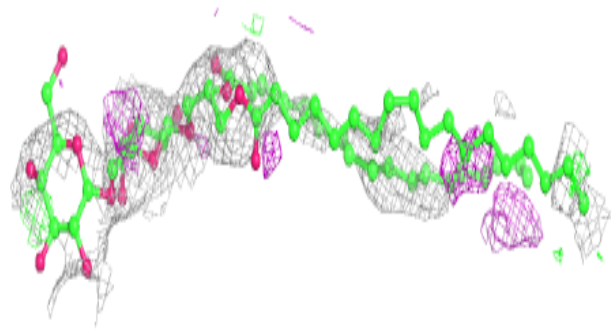
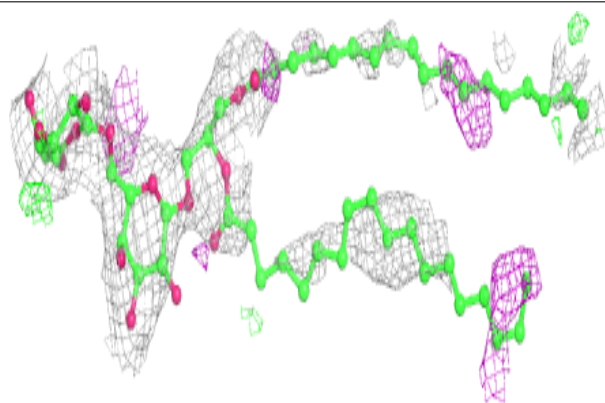


Electron density around BCR BK 5102:

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

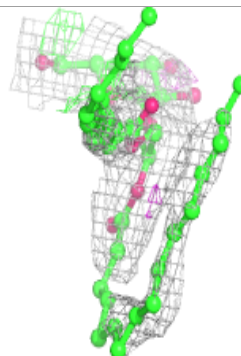
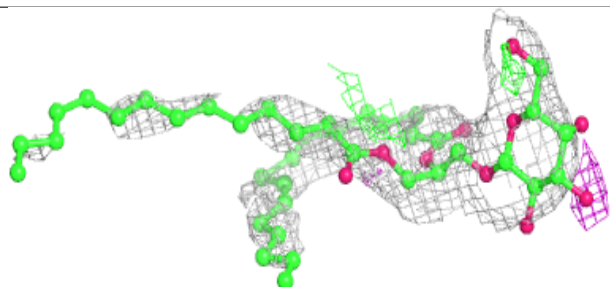
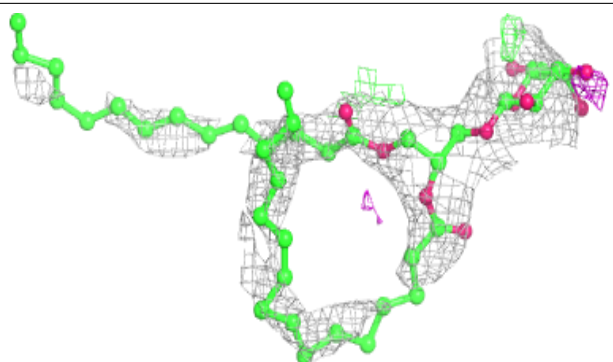
**Electron density around DGD BC 5519:**

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

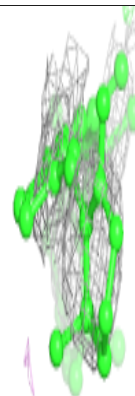
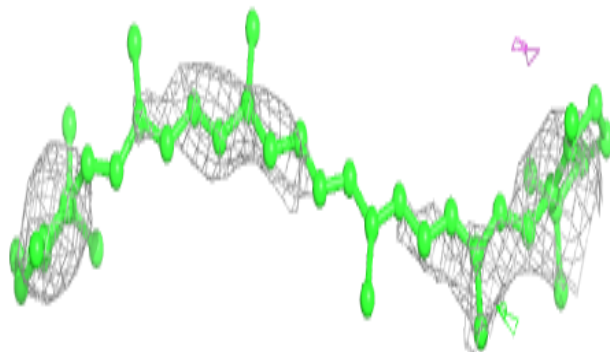
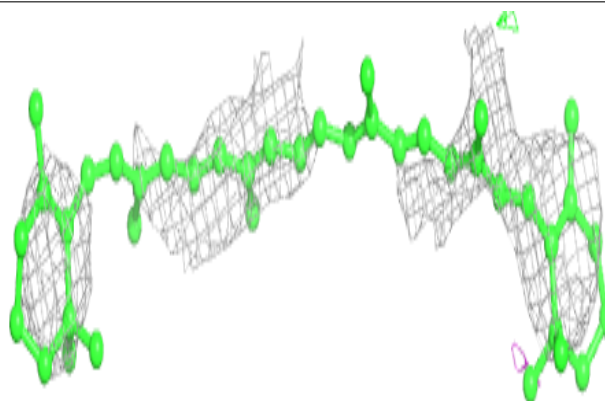


Electron density around LMG BD 5409:

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

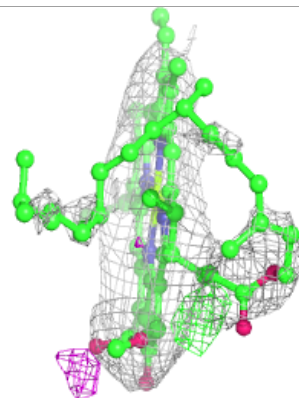
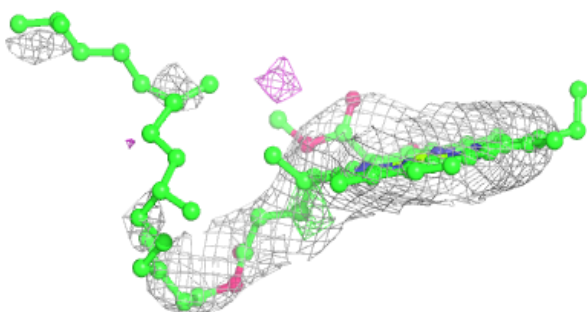
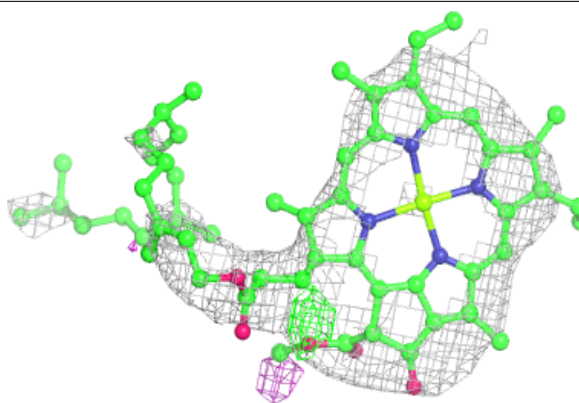
**Electron density around BCR BC 5514:**

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

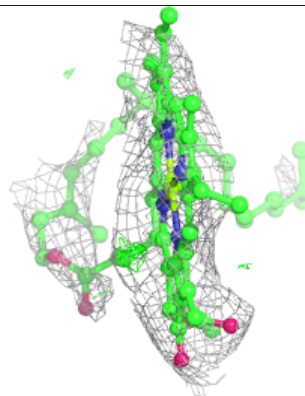
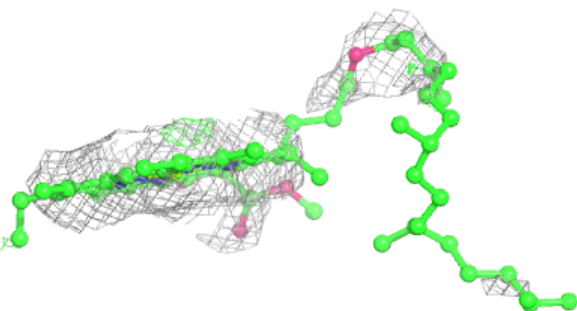
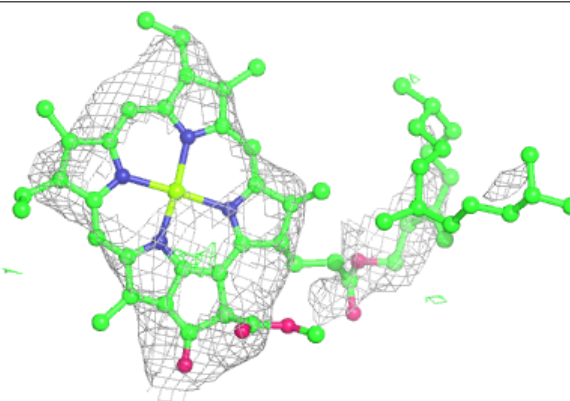


Electron density around CLA AC 512:

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

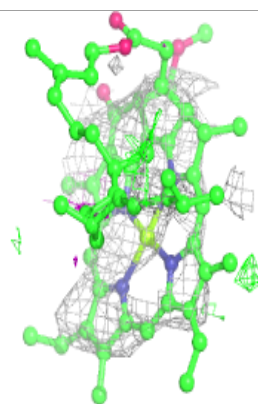
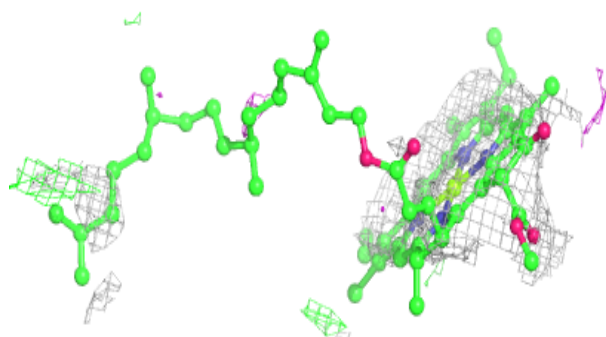
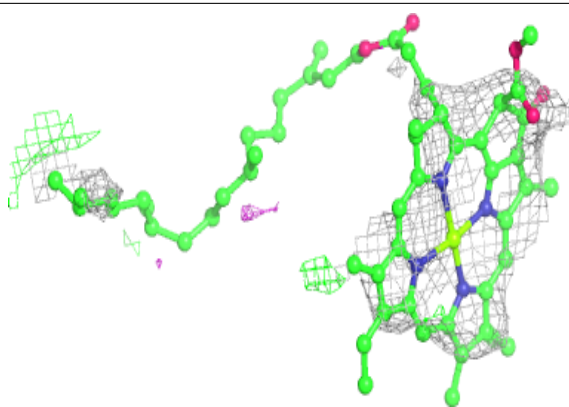
**Electron density around CLA BC 5512:**

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

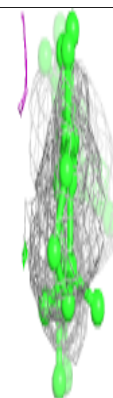
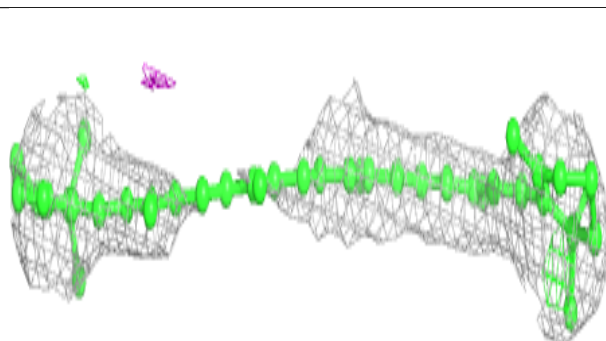
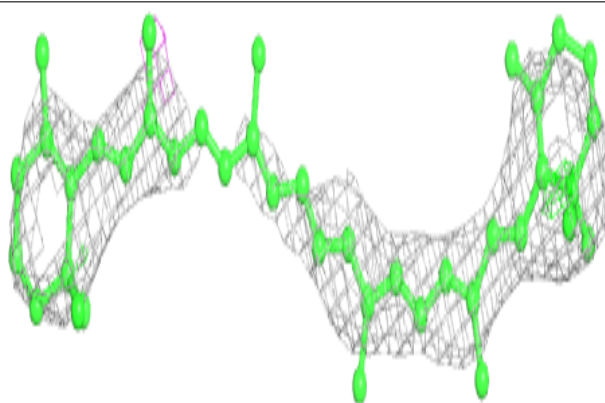


Electron density around CLA BC 5511:

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

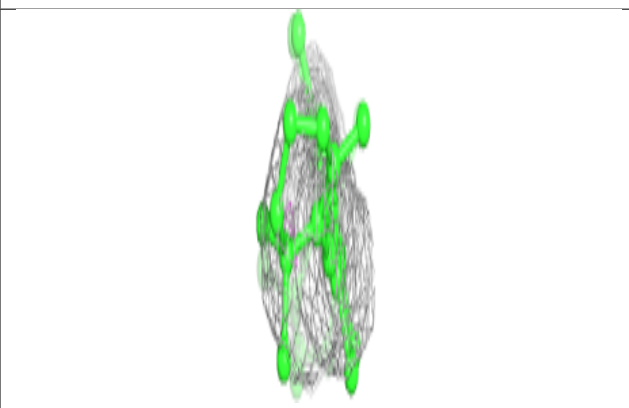
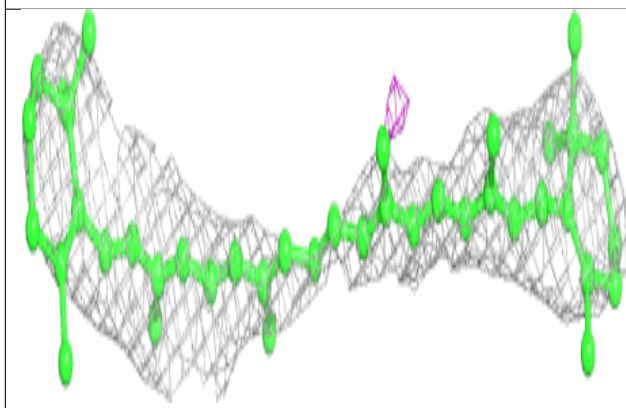
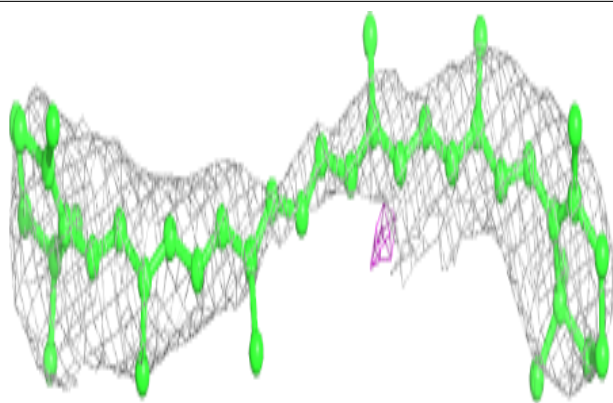
**Electron density around BCR AK 102:**

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

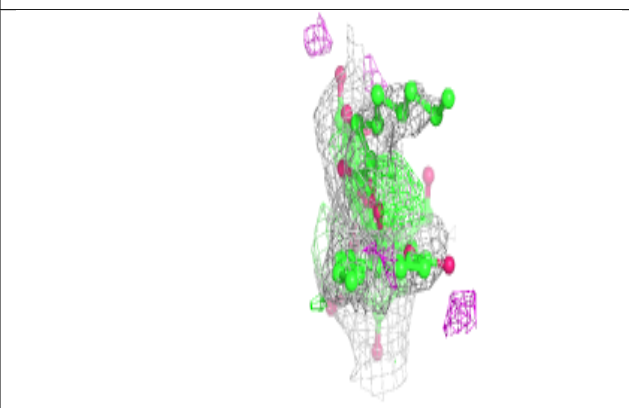
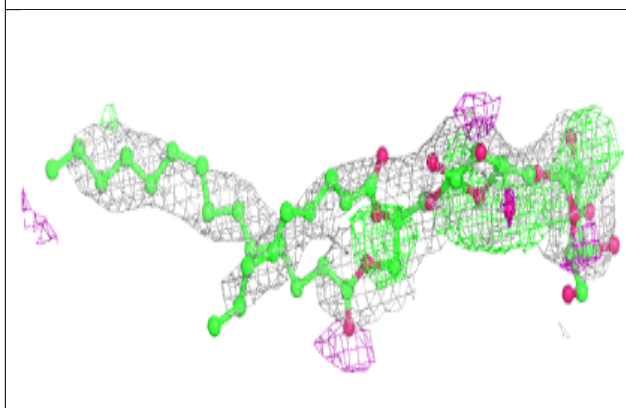
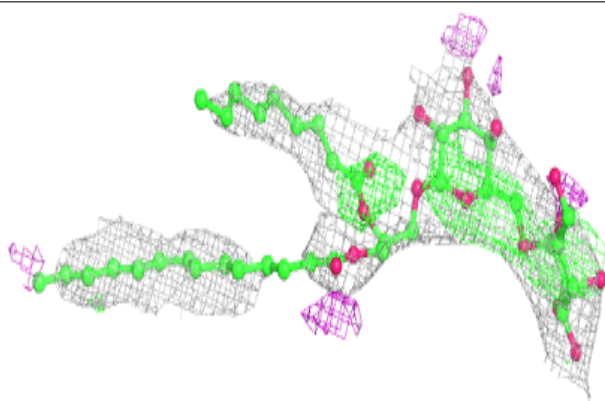


Electron density around BCR BB 5623:

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

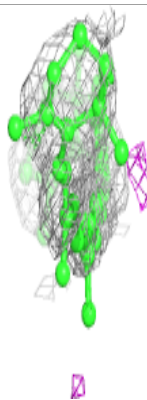
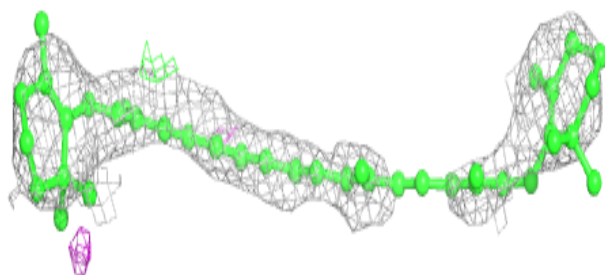
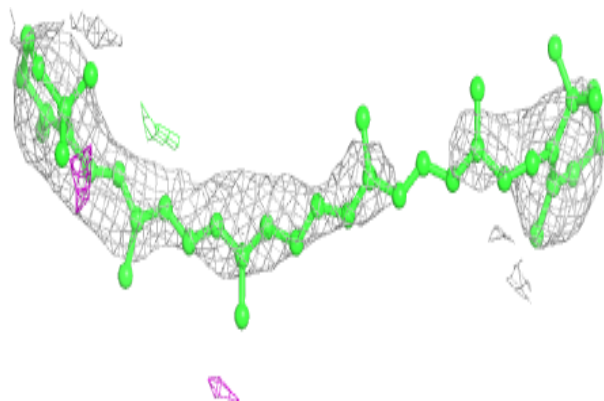
**Electron density around DGD AC 517:**

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

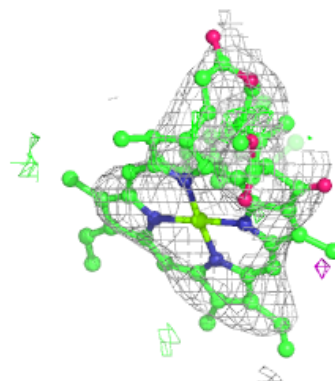
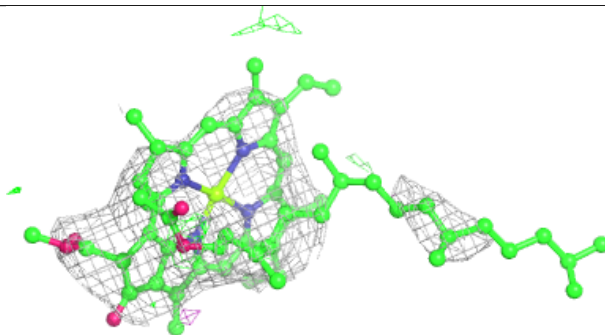
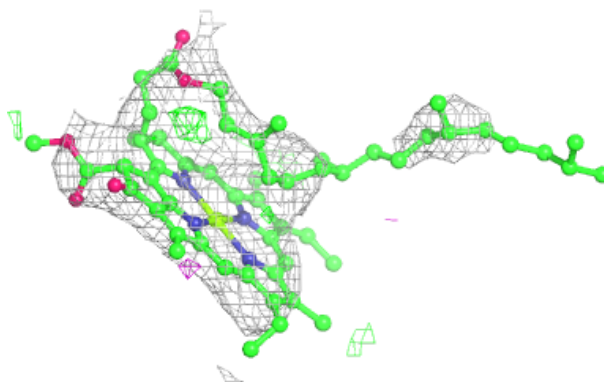


Electron density around BCR AT 101:

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

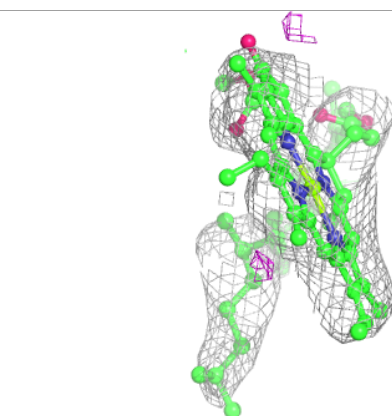
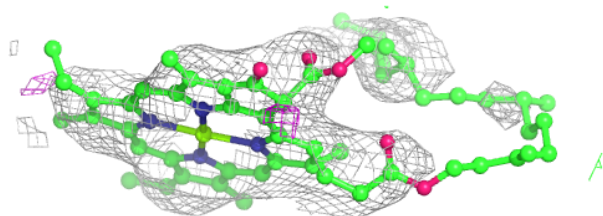
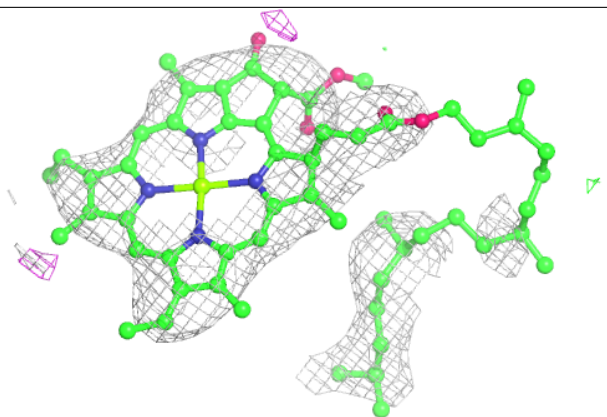
**Electron density around CLA BC 5505:**

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

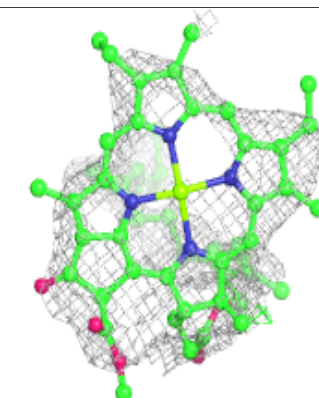
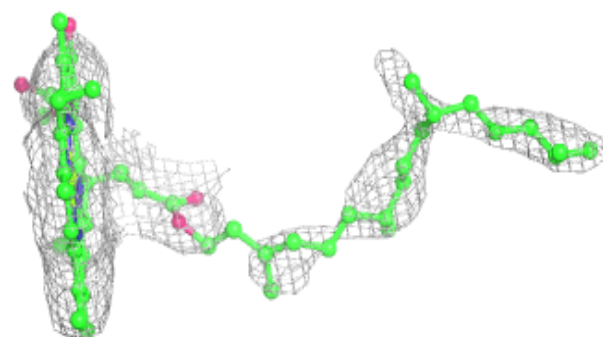
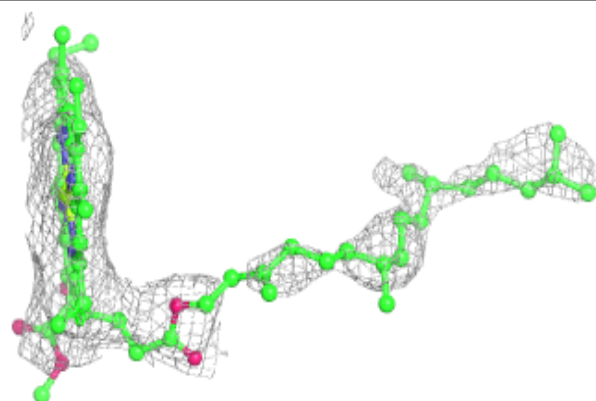


Electron density around CLA BB 5620:

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

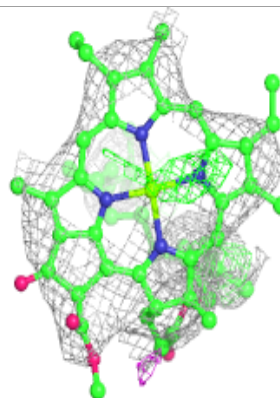
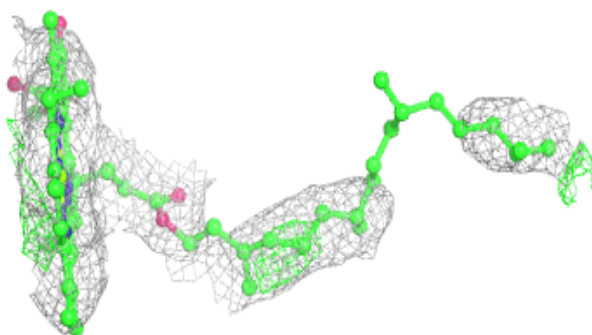
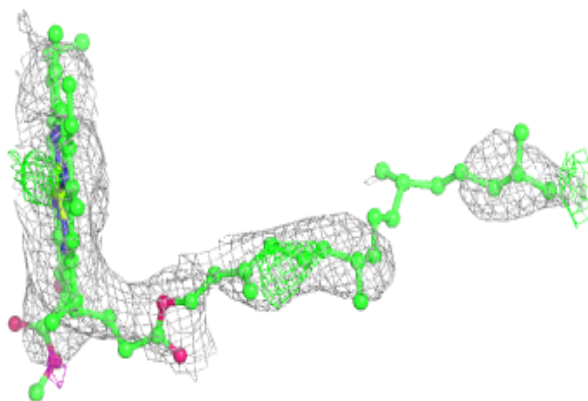
**Electron density around CLA BB 5610:**

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

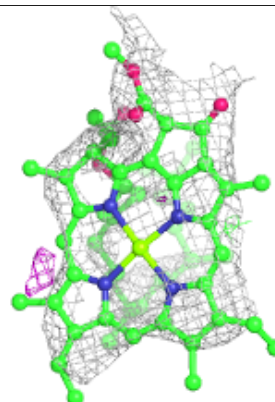
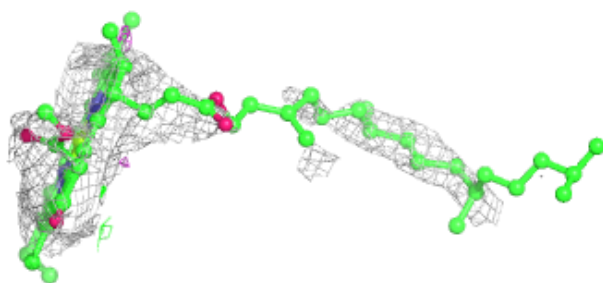
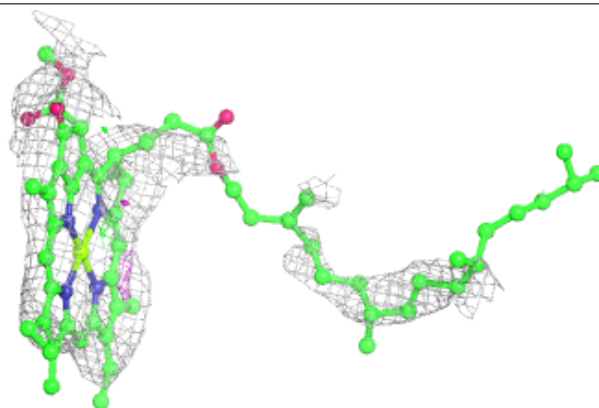


Electron density around CLA AB 606:

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

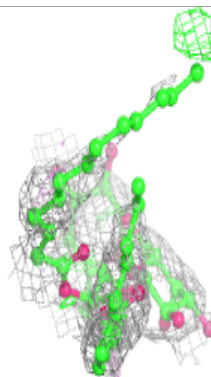
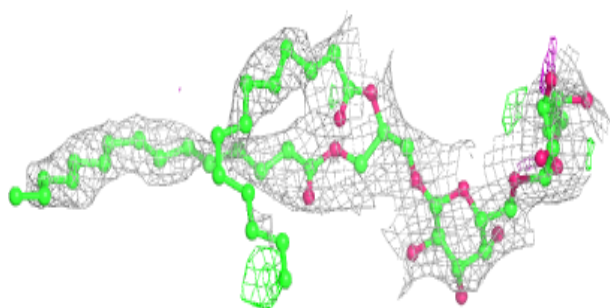
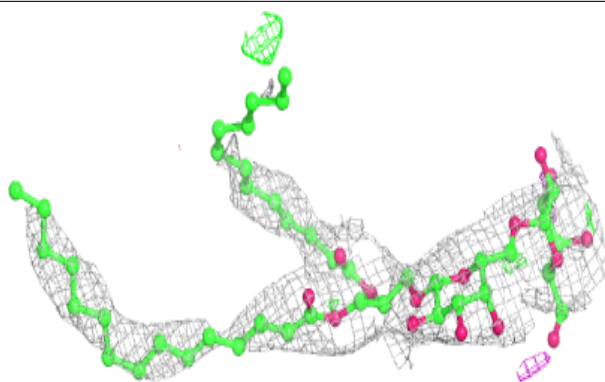
**Electron density around CLA BD 5405:**

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



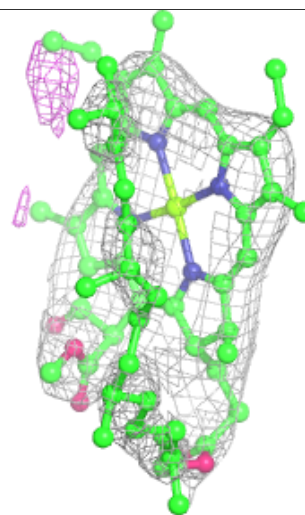
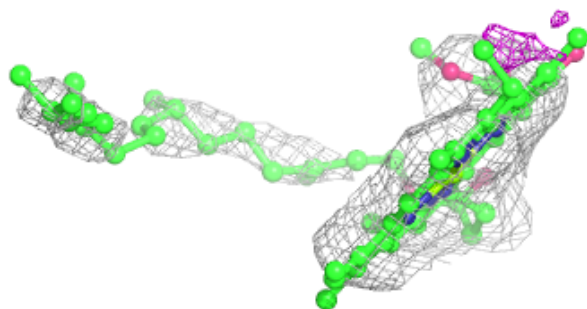
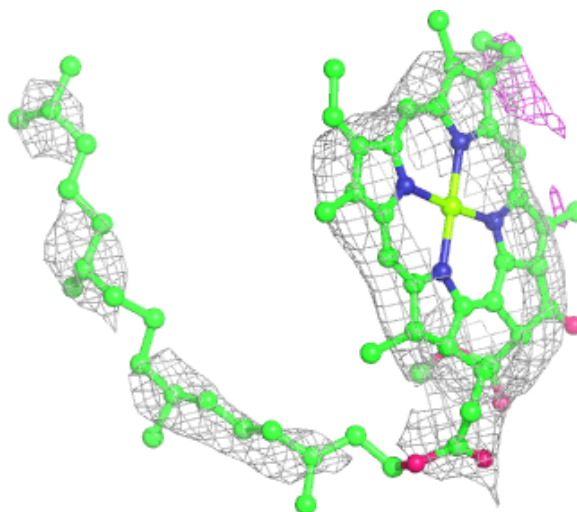
Electron density around DGD BH 5101:

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



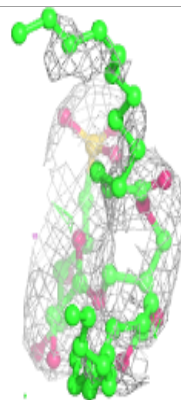
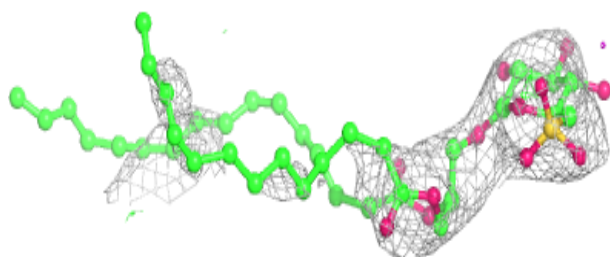
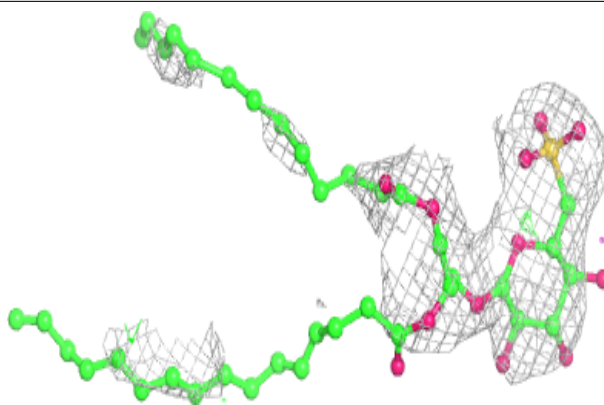
Electron density around CLA BC 5507:

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



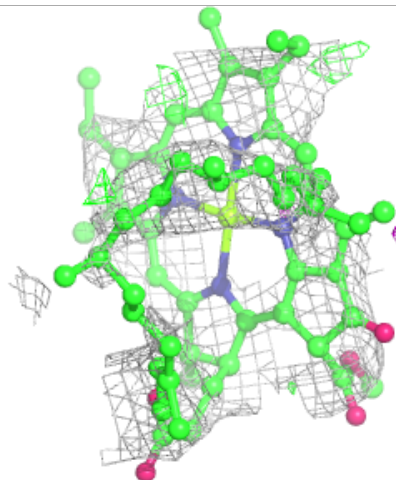
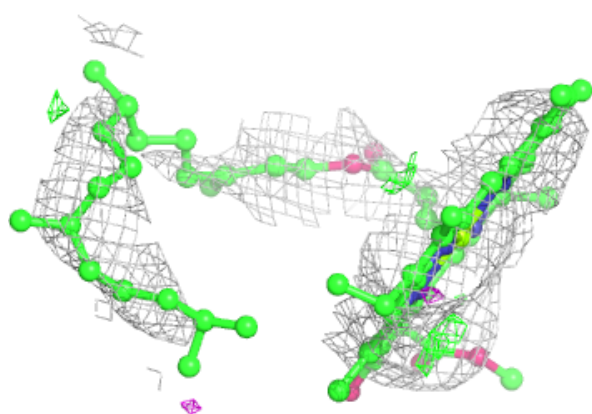
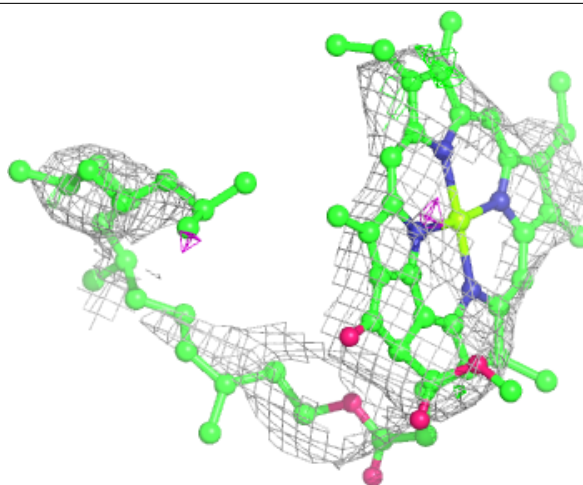
Electron density around SQD AA 413:

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



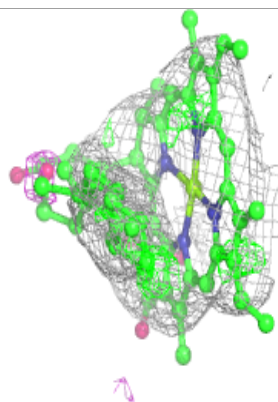
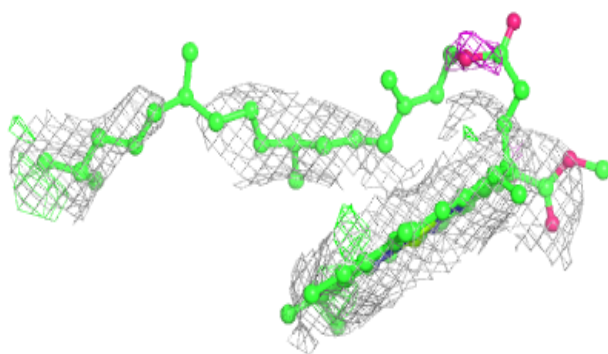
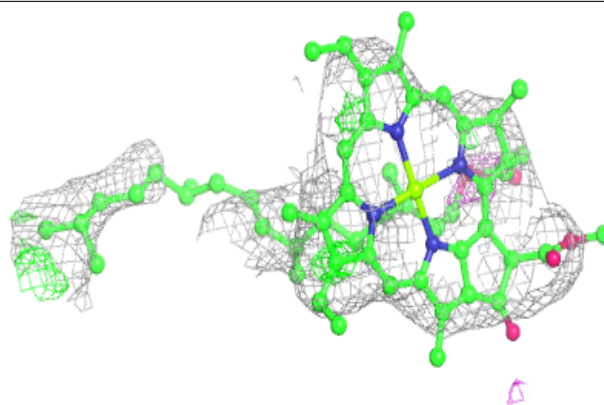
Electron density around CLA BC 5503:

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

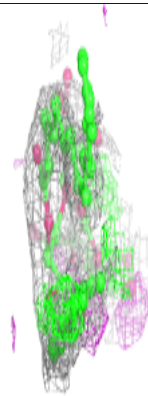
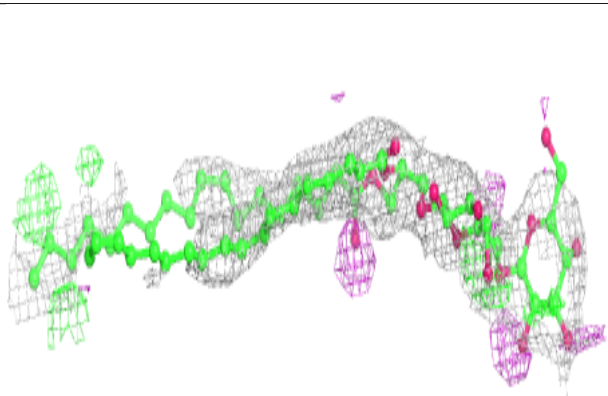
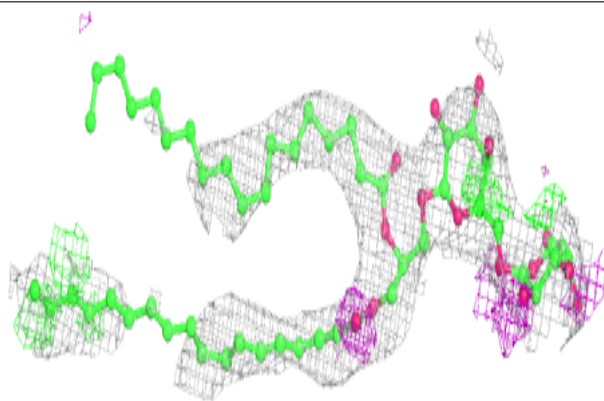


Electron density around CLA AB 614:

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

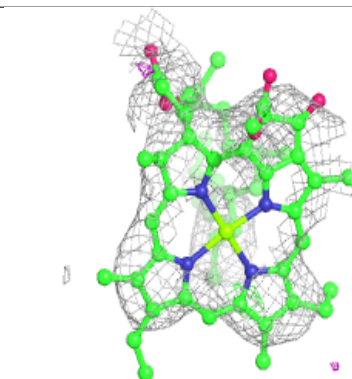
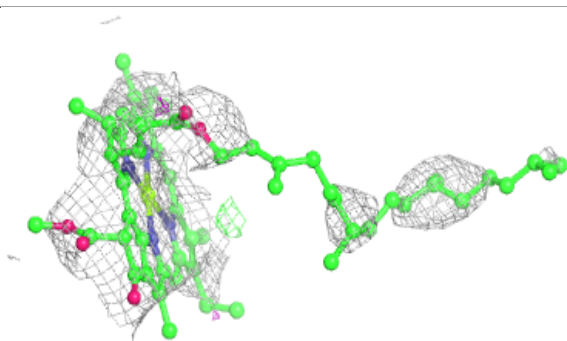
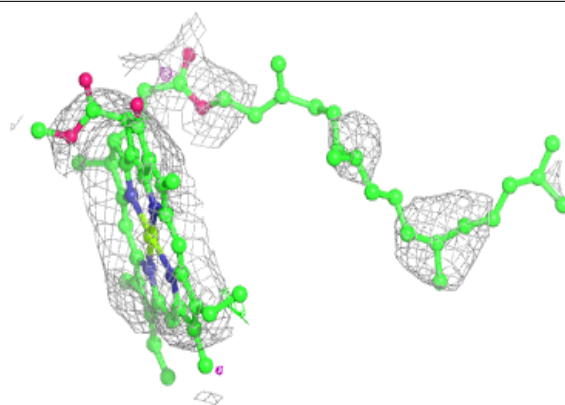
**Electron density around DGD AC 519:**

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

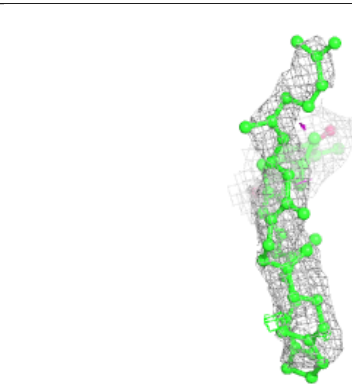
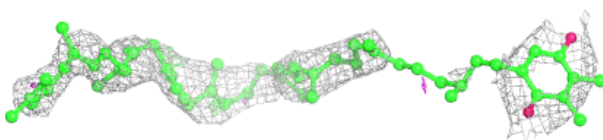
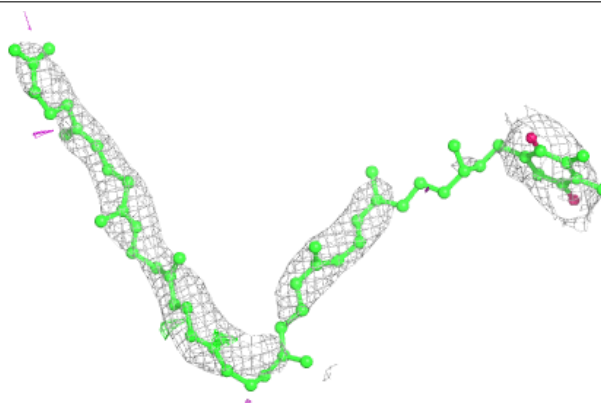


Electron density around CLA BC 5508:

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

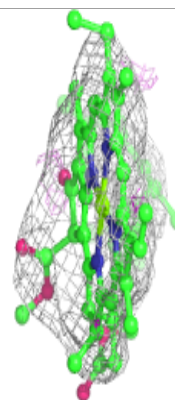
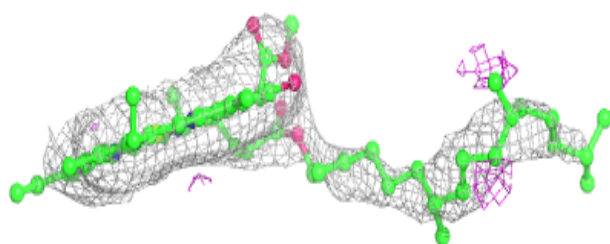
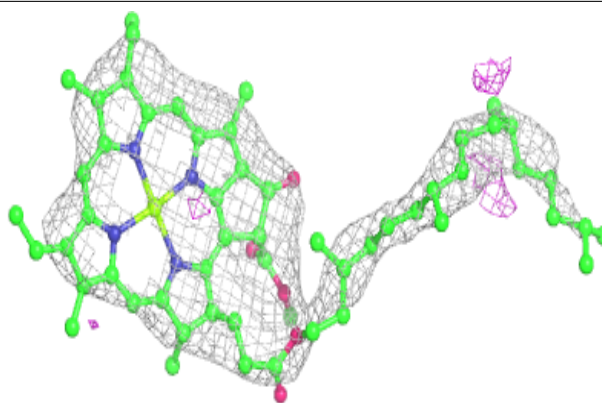
**Electron density around PL9 BD 5406:**

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

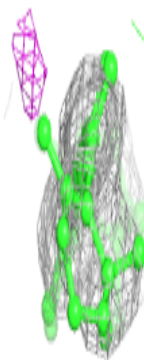
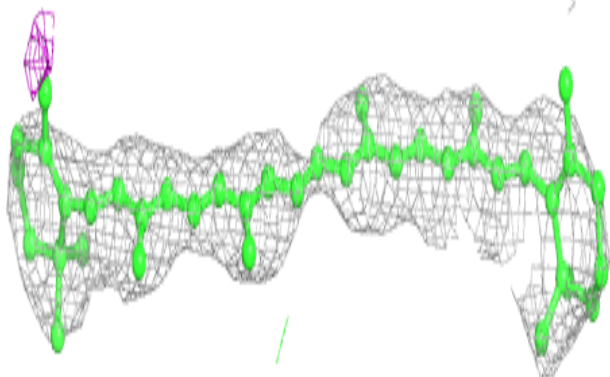
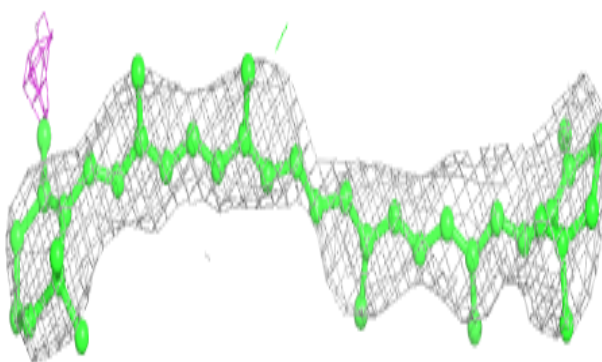


Electron density around CLA BB 5606:

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

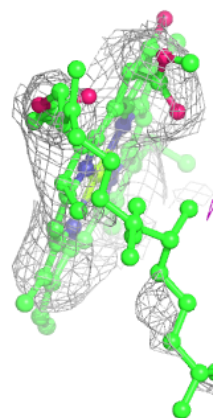
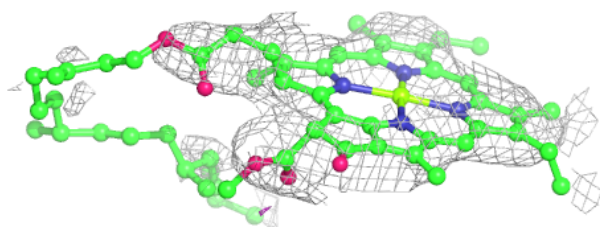
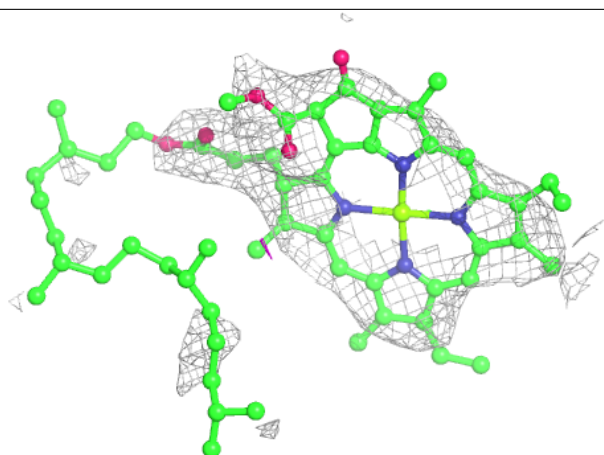
**Electron density around BCR AB 619:**

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

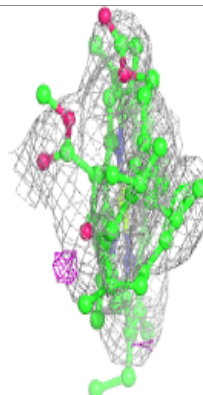
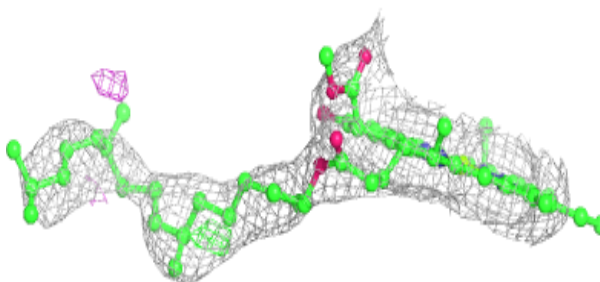
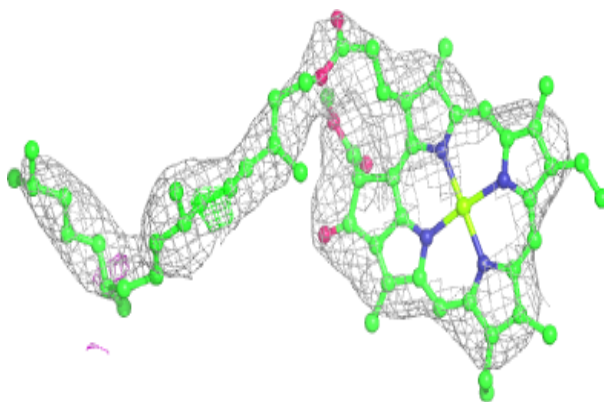


Electron density around CLA AB 616:

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

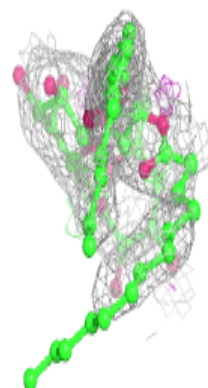
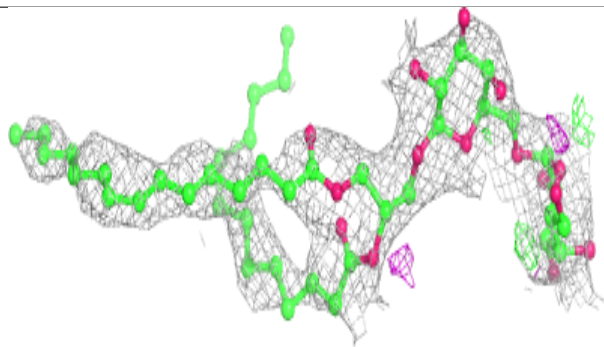
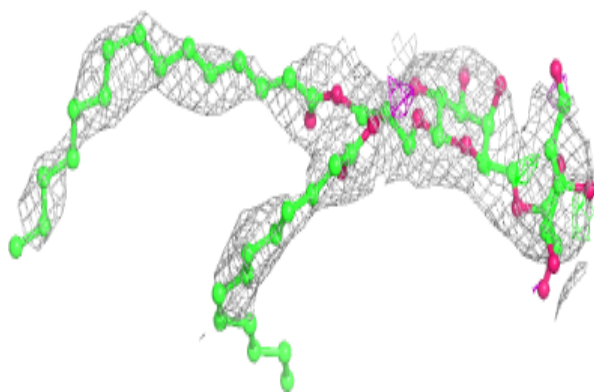
**Electron density around CLA AB 602:**

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

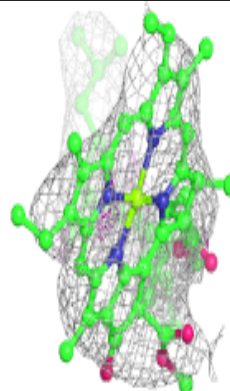
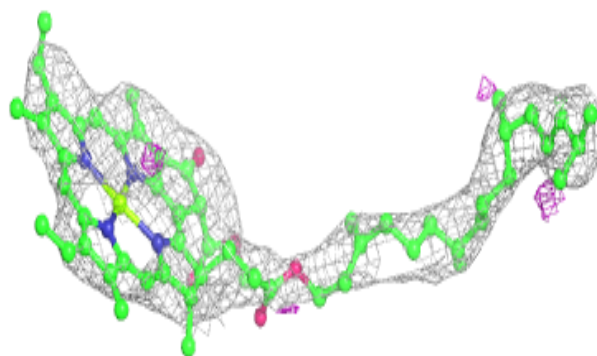
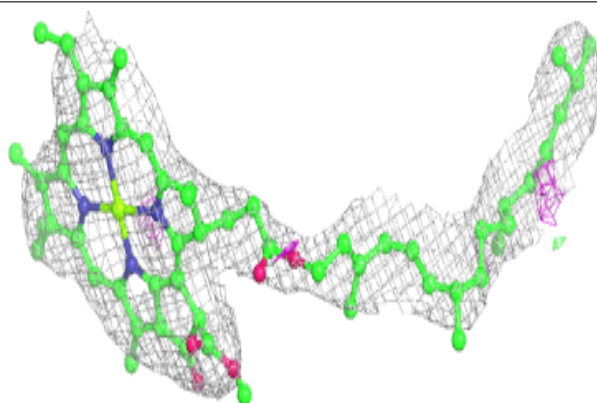


Electron density around DGD AH 101:

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

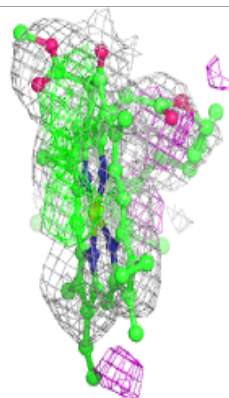
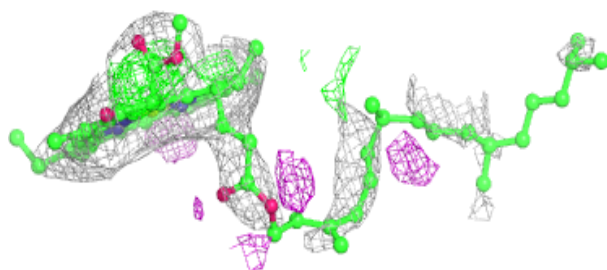
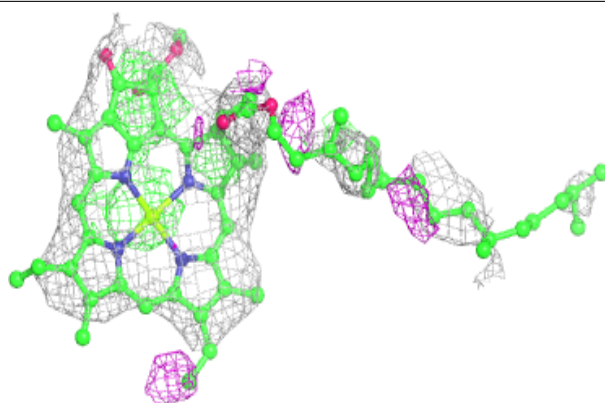
**Electron density around CLA BA 5405:**

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

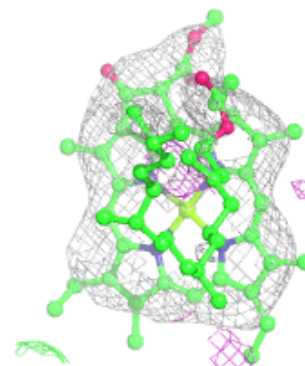
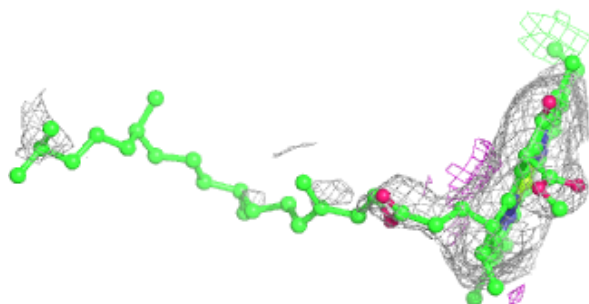
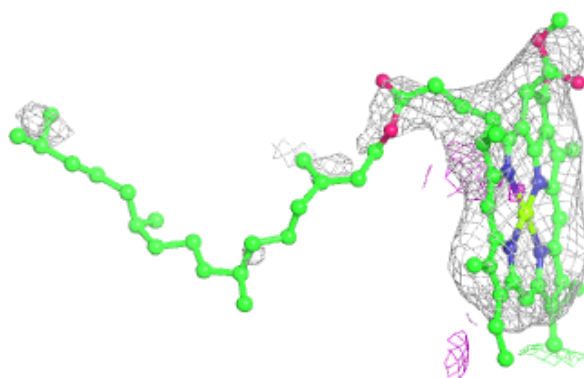


Electron density around CLA AA 406:

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

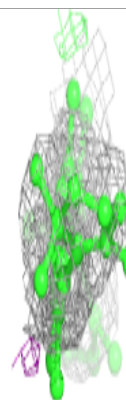
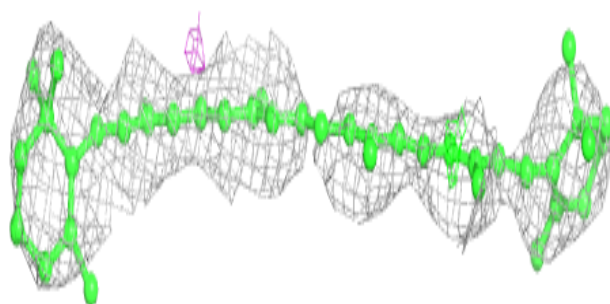
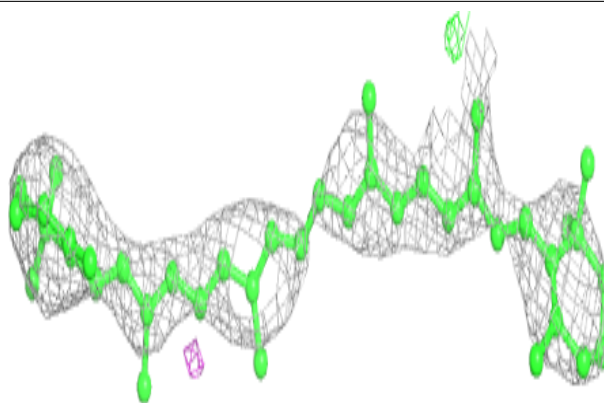
**Electron density around CLA AD 404:**

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

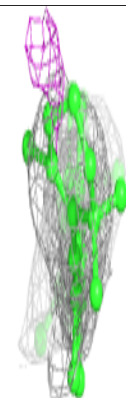
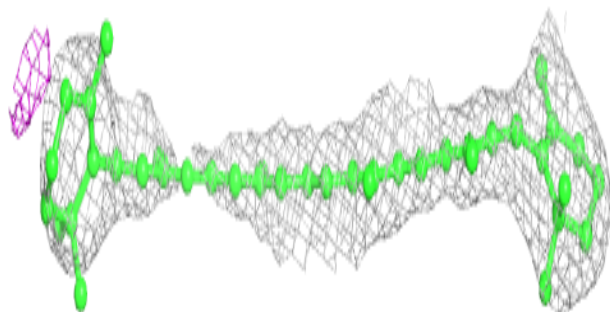
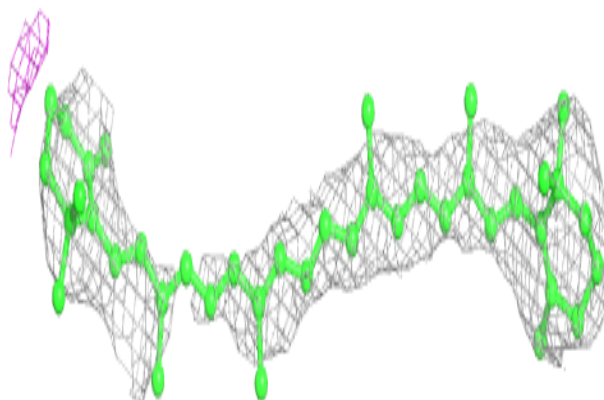


Electron density around BCR AB 617:

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

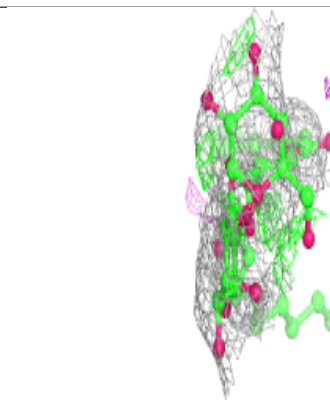
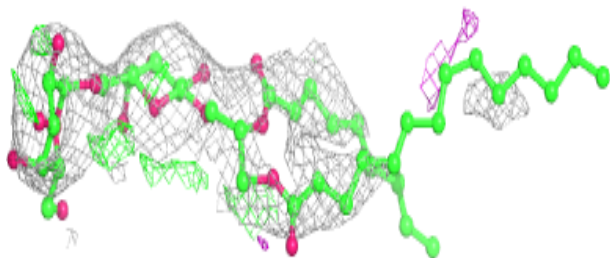
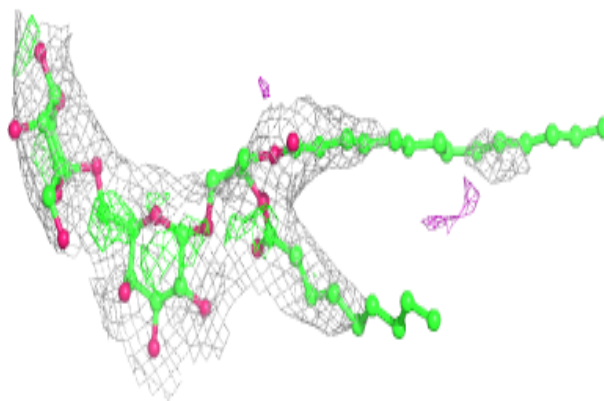
**Electron density around BCR AB 618:**

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

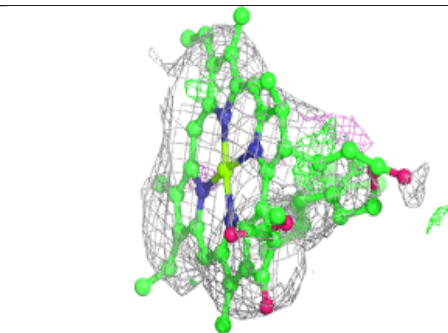
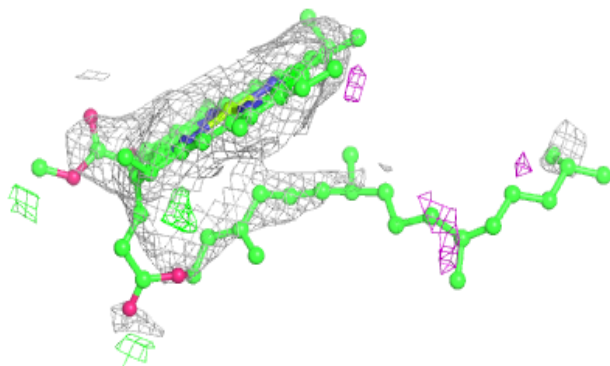
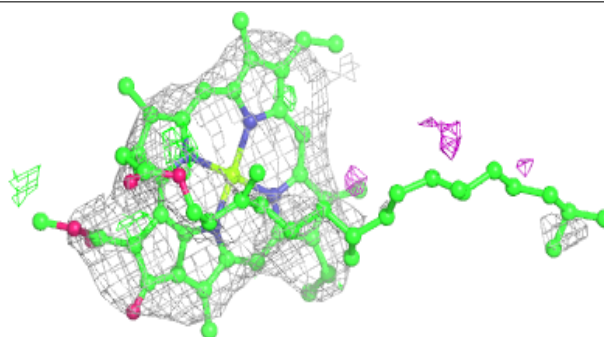


Electron density around DGD BC 5517:

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

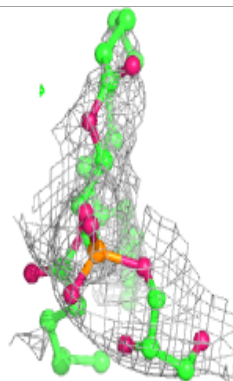
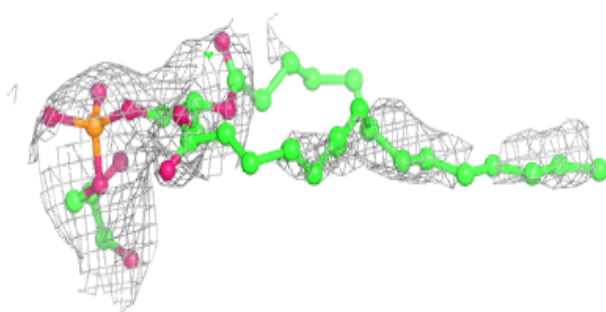
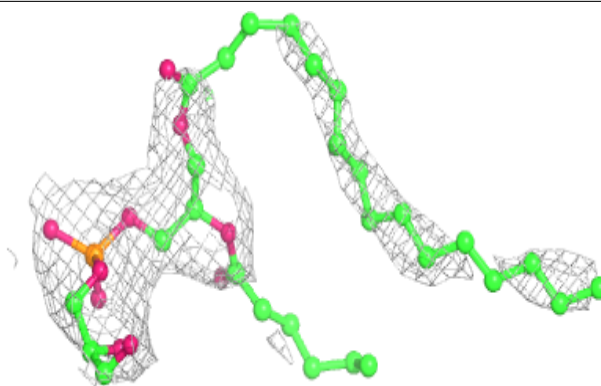
**Electron density around CLA BB 5618:**

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

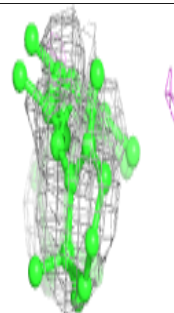
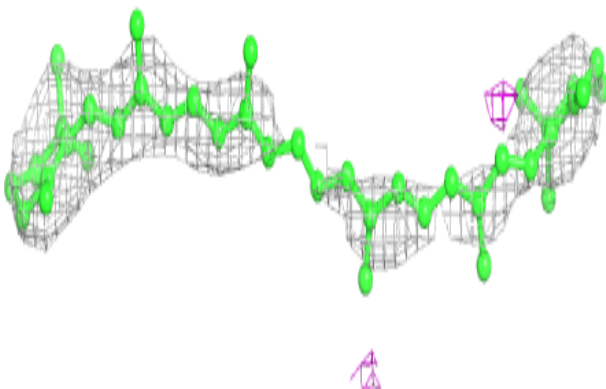
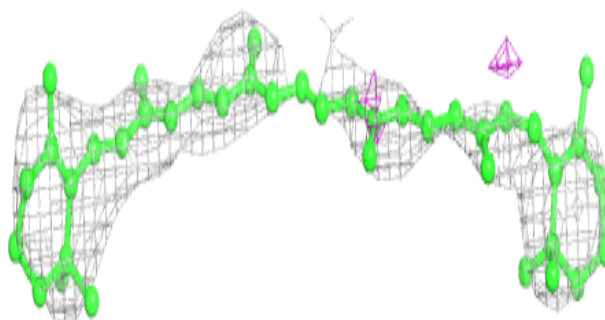


Electron density around LHG BA 5413:

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

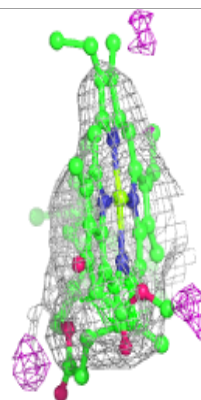
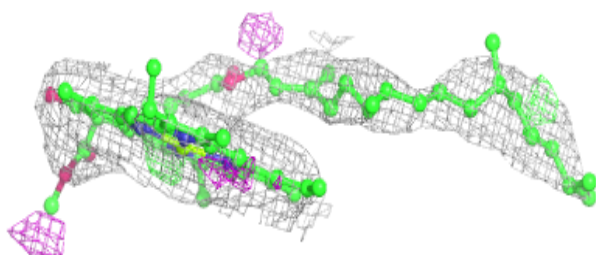
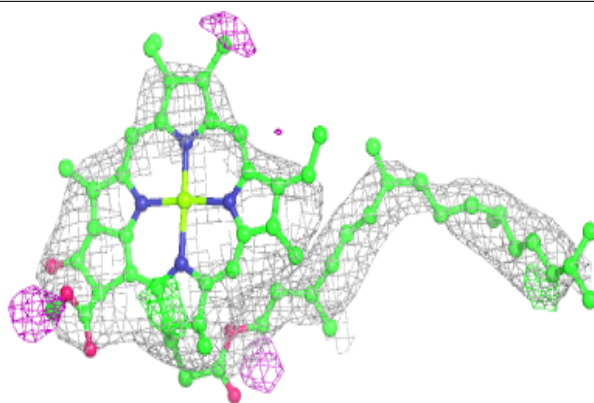
**Electron density around BCR AC 514:**

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

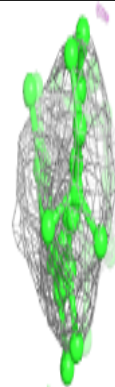
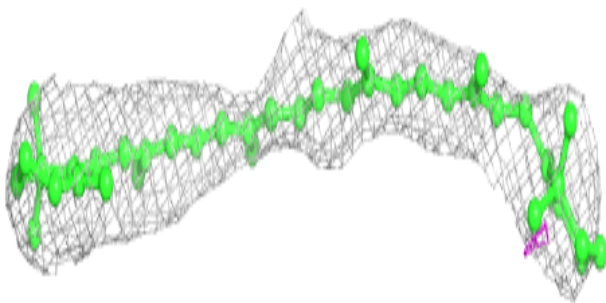
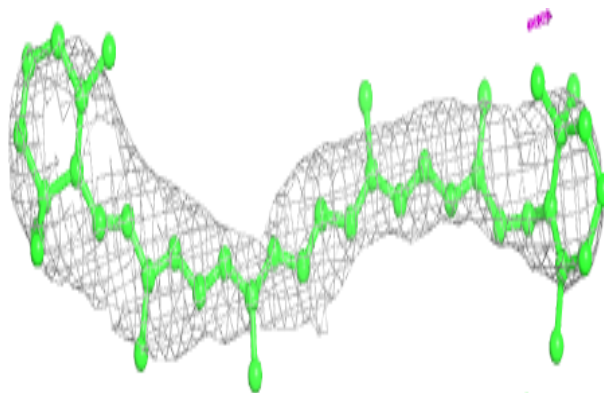


Electron density around CLA AB 603:

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

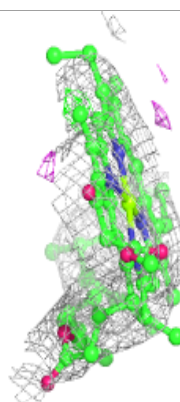
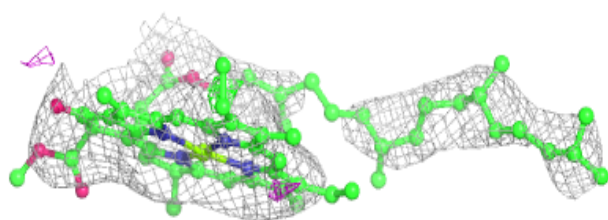
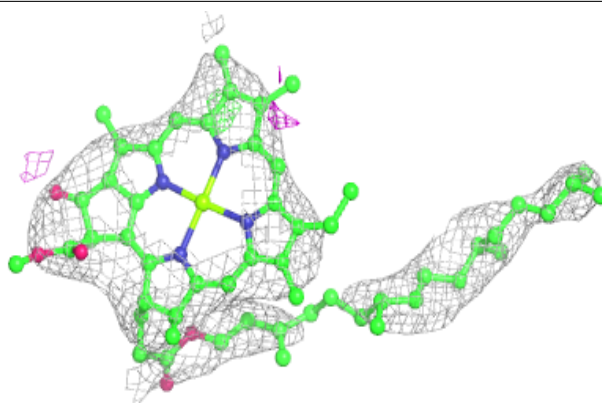
**Electron density around BCR BD 5407:**

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

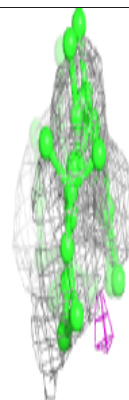
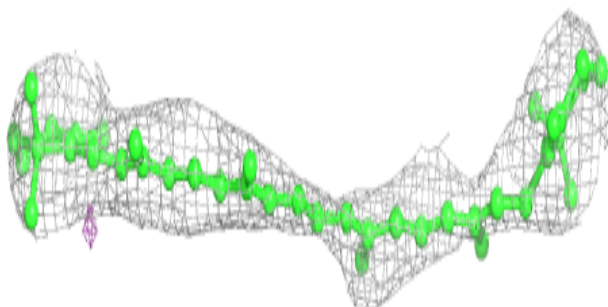
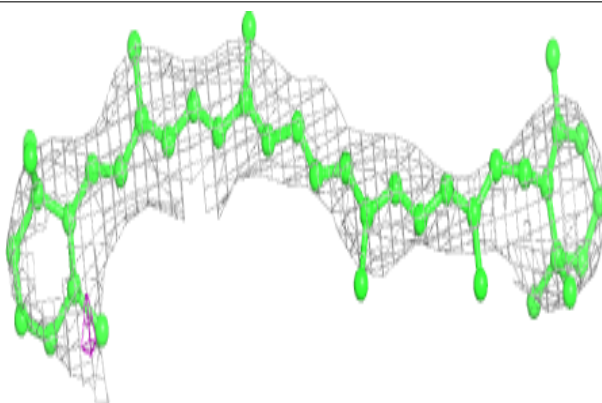


Electron density around CLA AC 501:

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

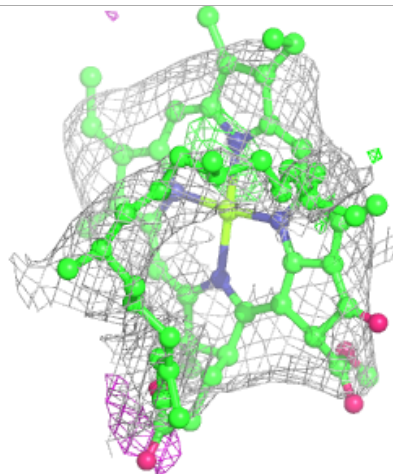
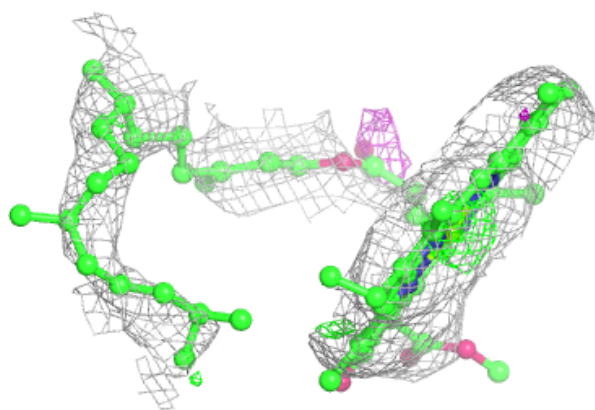
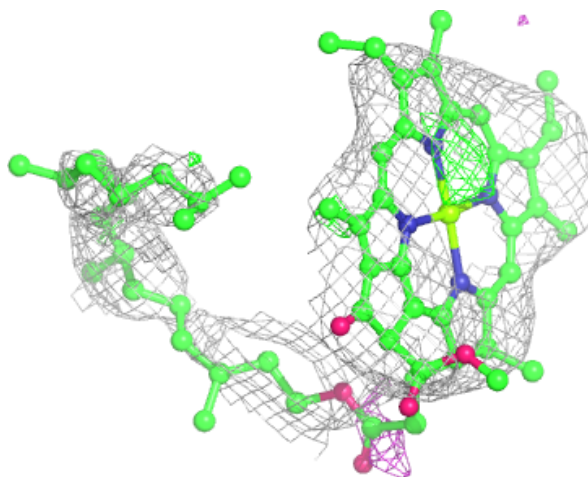
**Electron density around BCR AD 406:**

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



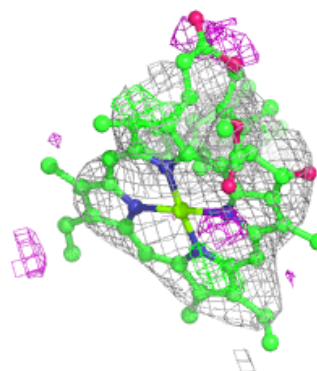
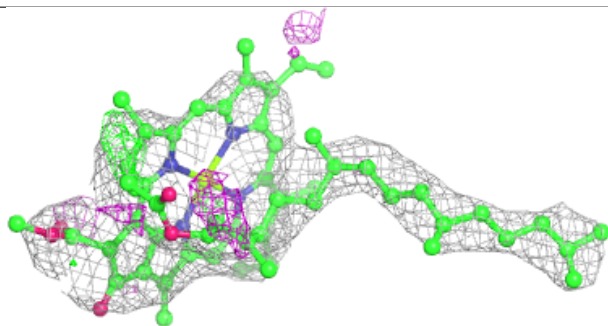
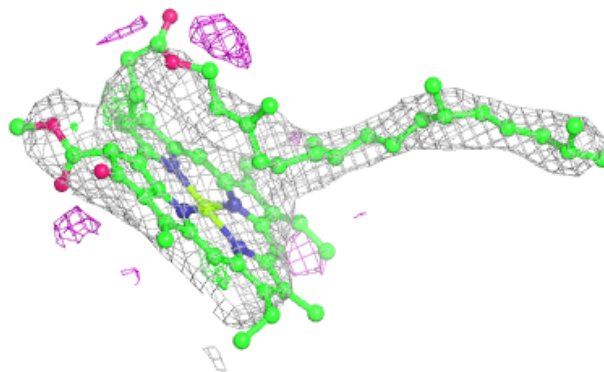
Electron density around CLA AC 503:

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

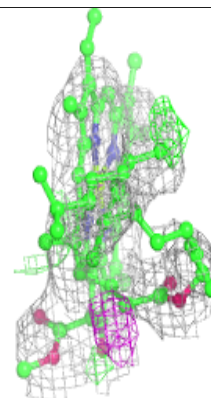
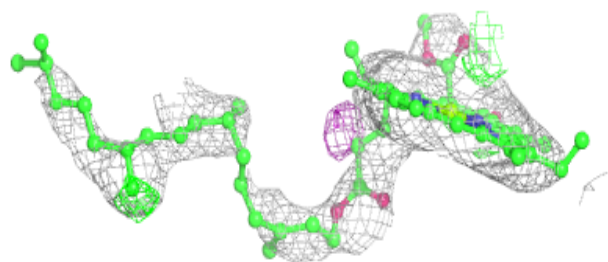
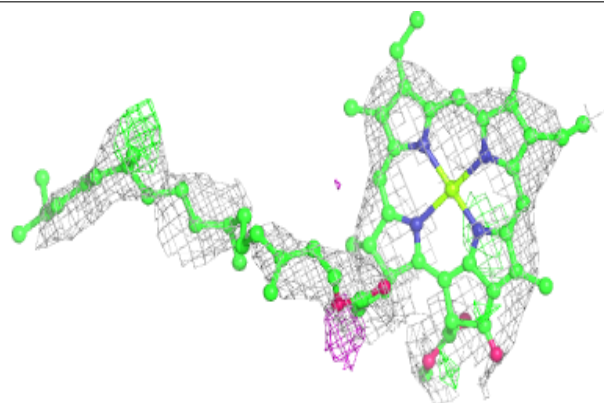


Electron density around CLA AC 505:

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

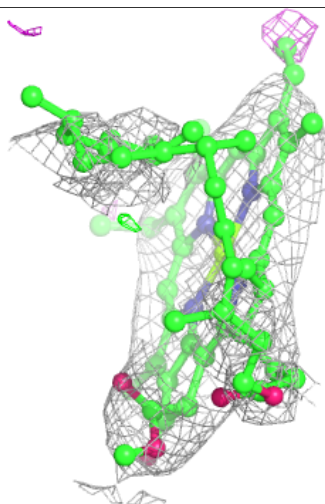
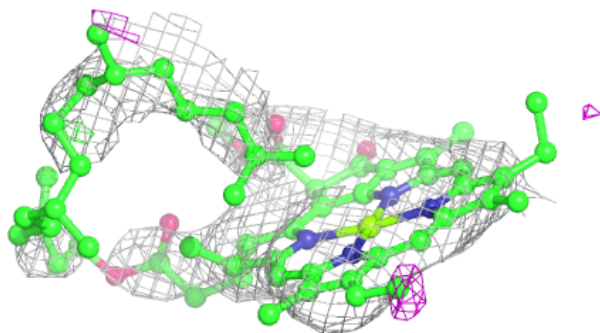
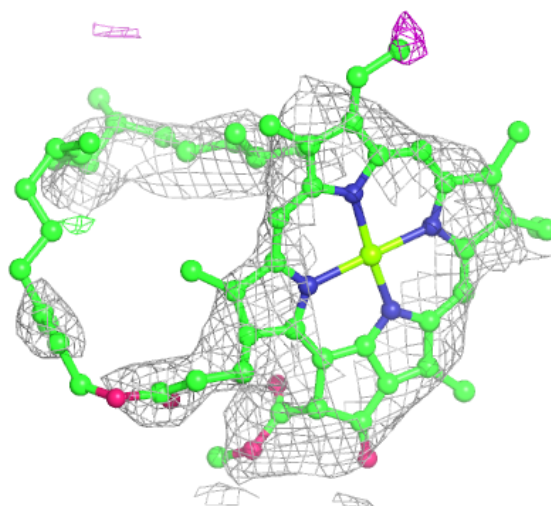
**Electron density around CLA BA 5407:**

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



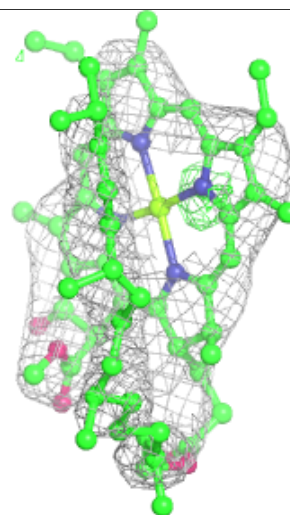
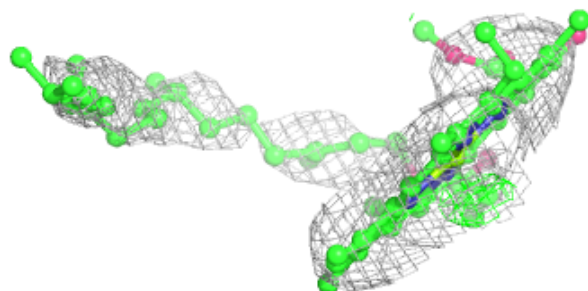
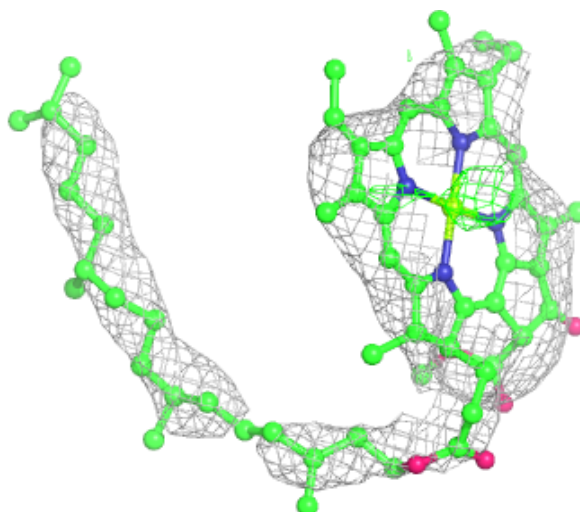
Electron density around CLA AB 615:

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



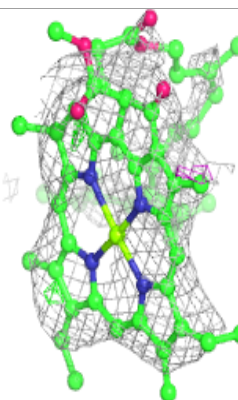
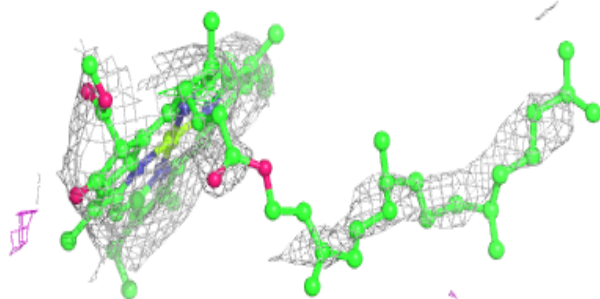
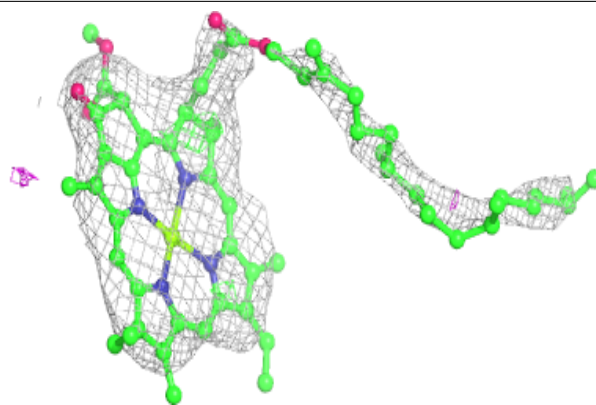
Electron density around CLA AC 507:

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

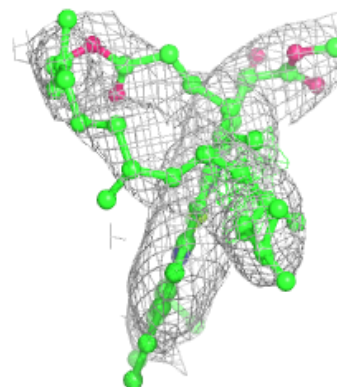
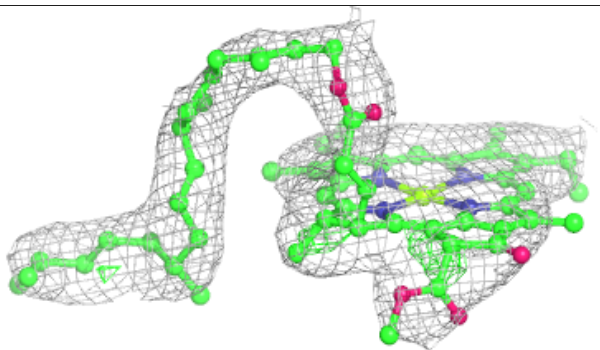
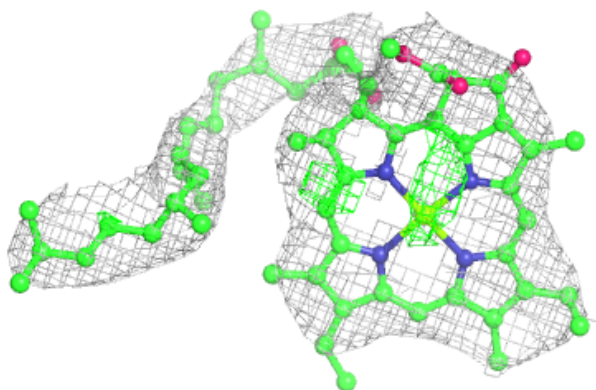


Electron density around CLA AC 511:

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

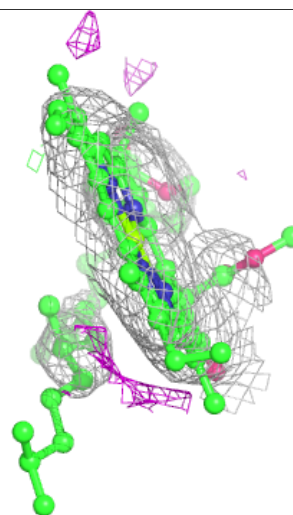
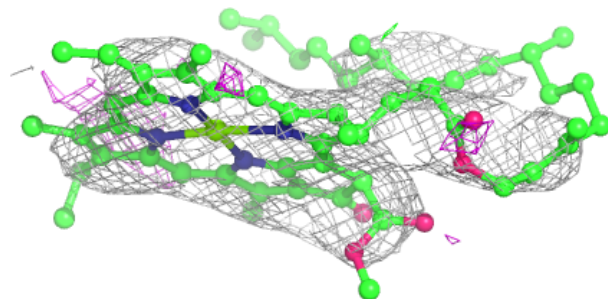
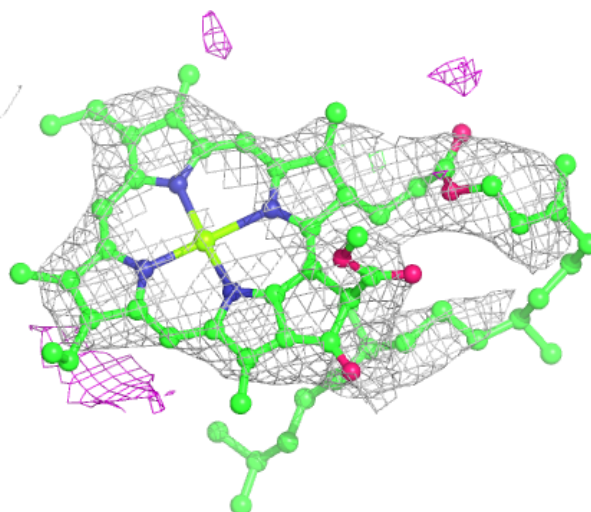
**Electron density around CLA BA 5406:**

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



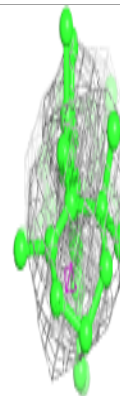
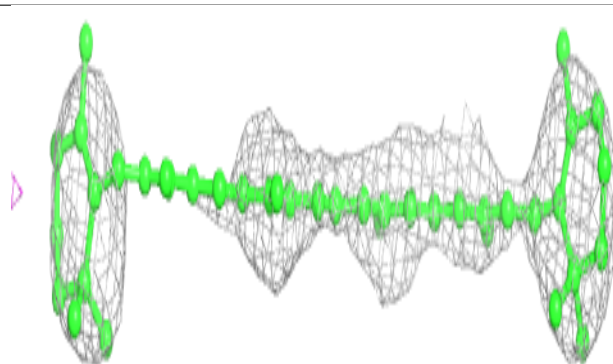
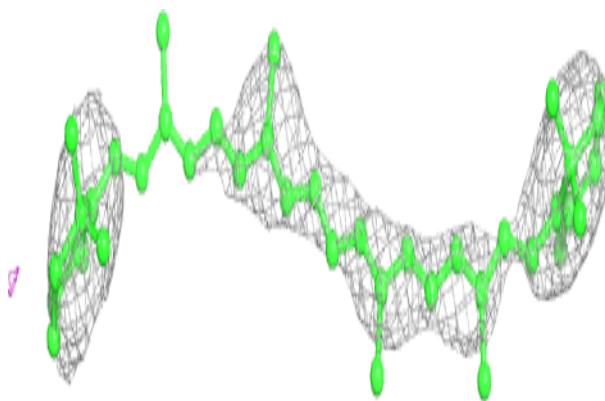
Electron density around CLA AC 509:

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

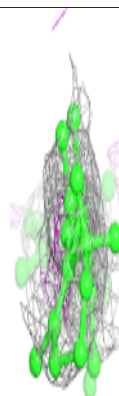
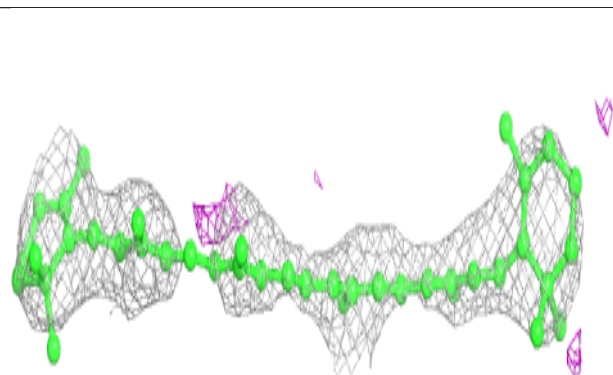
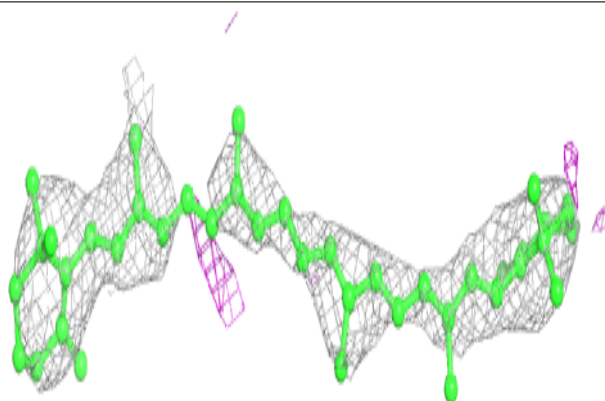


Electron density around BCR BA 5411:

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

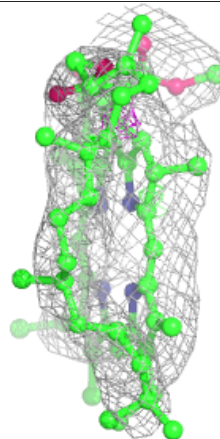
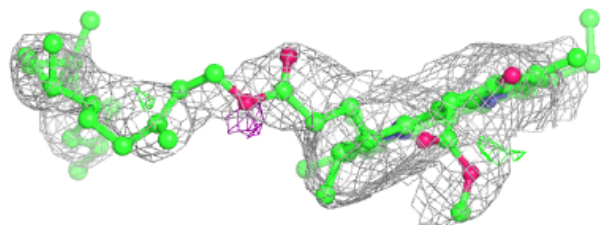
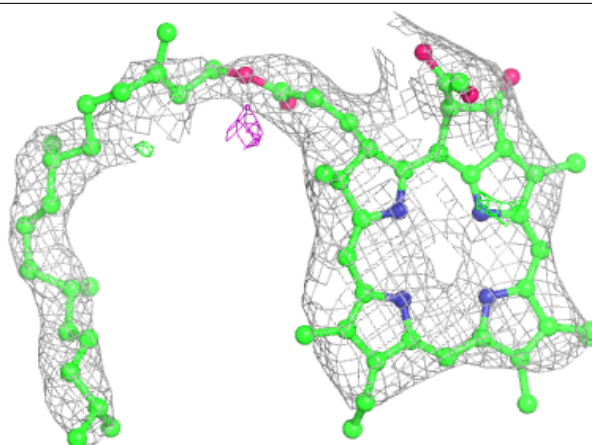
**Electron density around BCR BB 5621:**

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

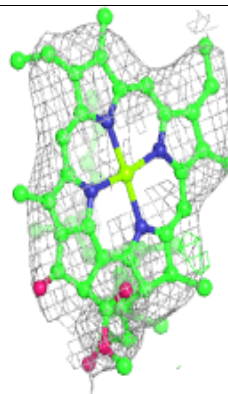
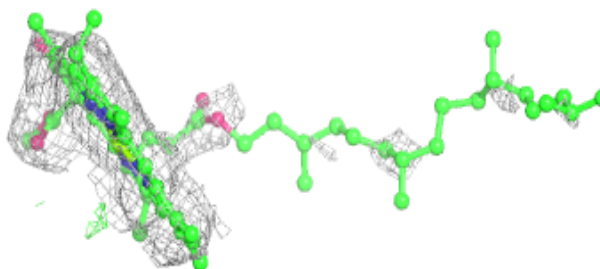
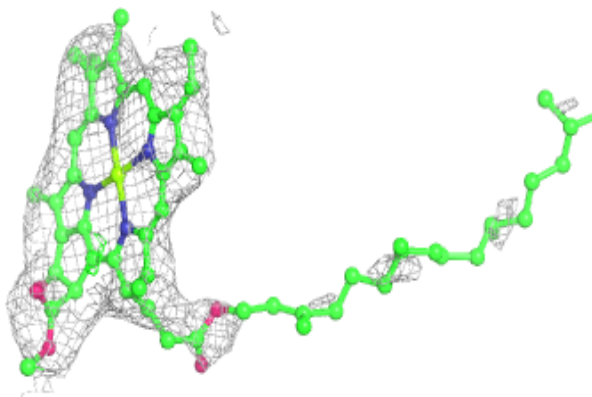


Electron density around PHO BD 5403:

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

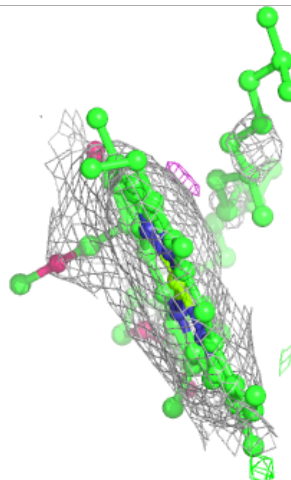
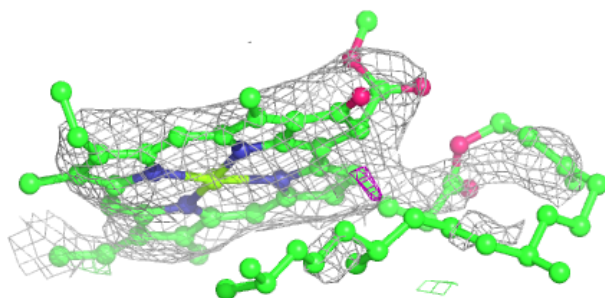
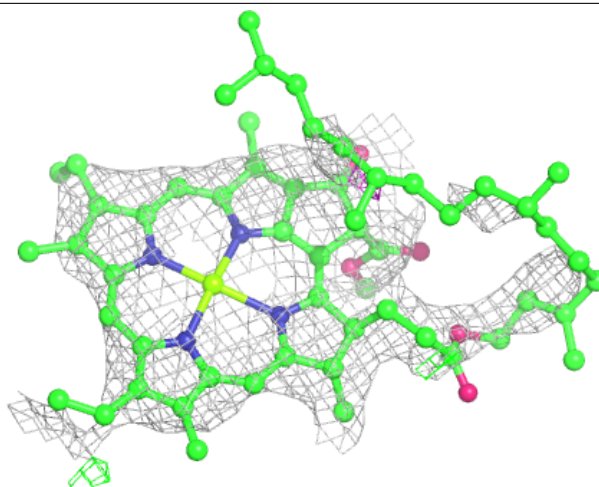
**Electron density around CLA BA 5408:**

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



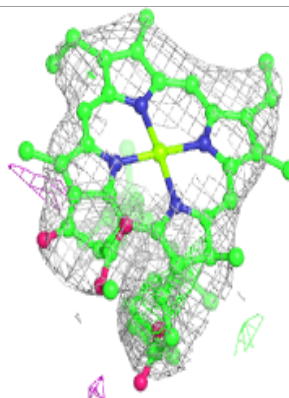
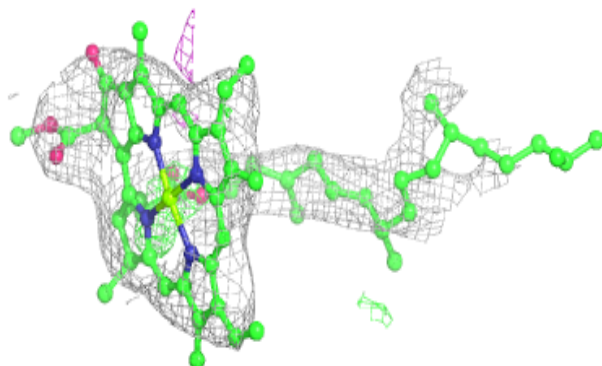
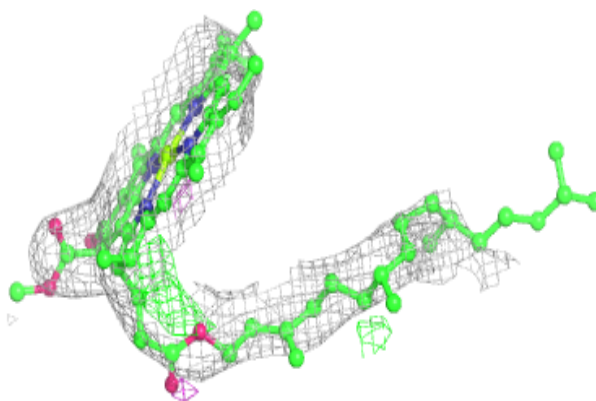
Electron density around CLA BC 5509:

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

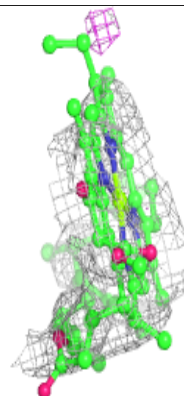
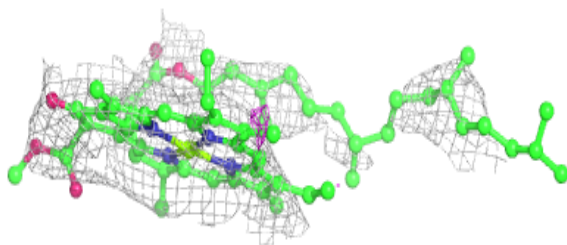
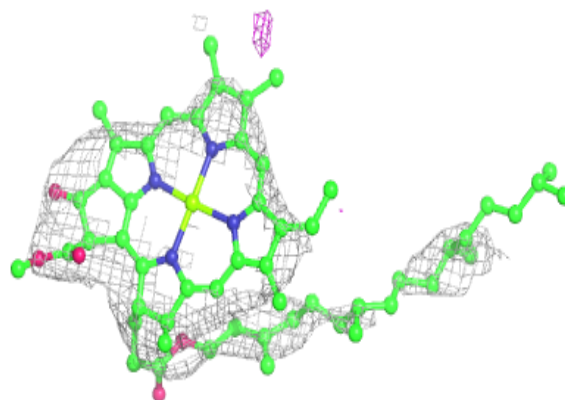


Electron density around CLA AC 504:

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

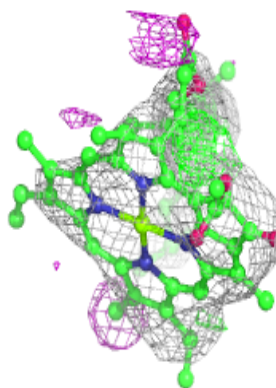
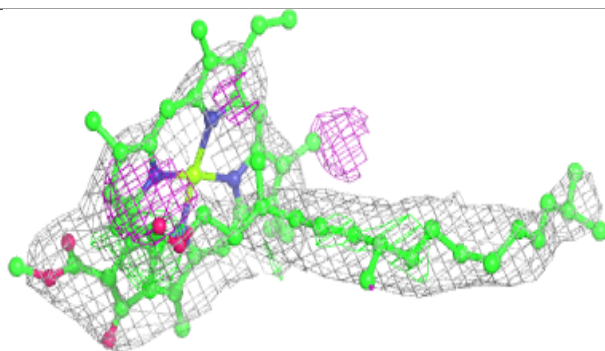
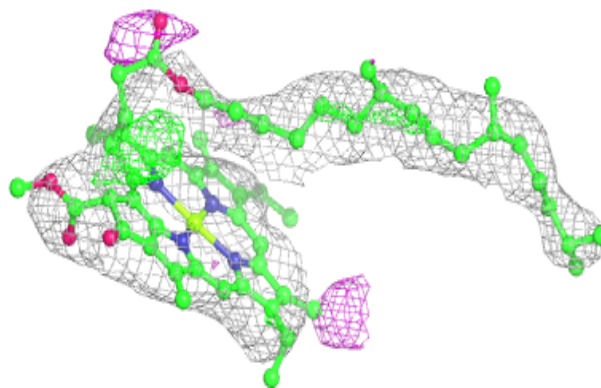
**Electron density around CLA BC 5501:**

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

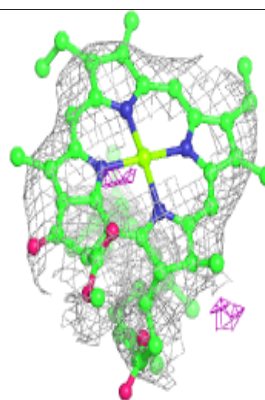
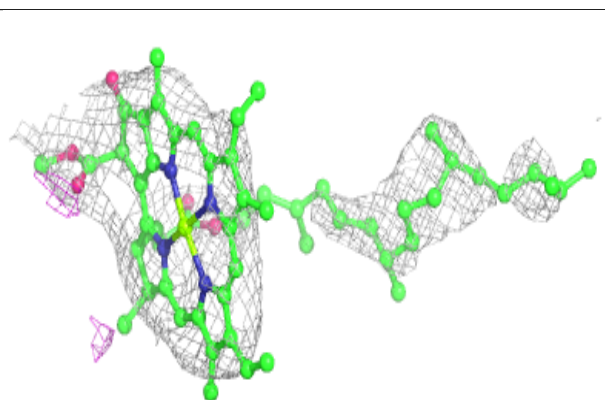
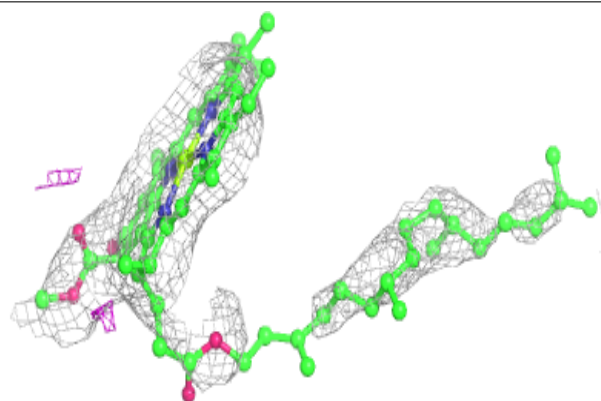


Electron density around CLA AB 608:

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

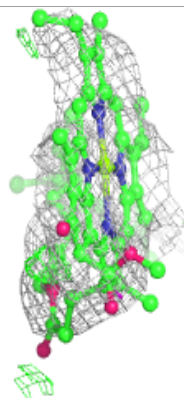
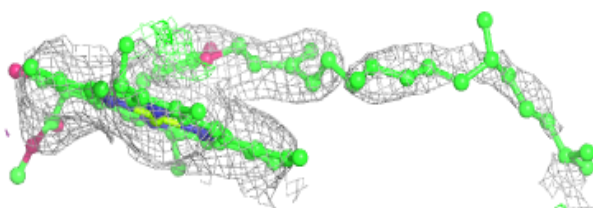
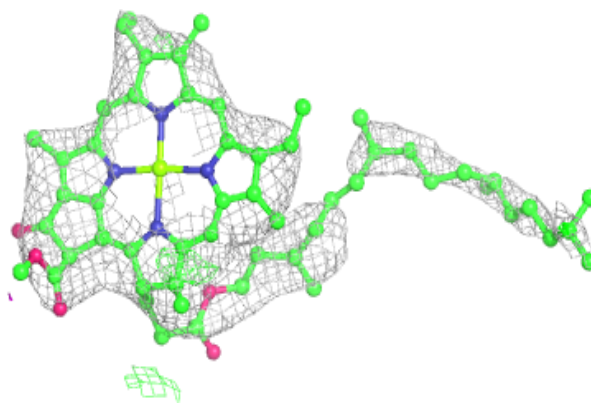
**Electron density around CLA BC 5504:**

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

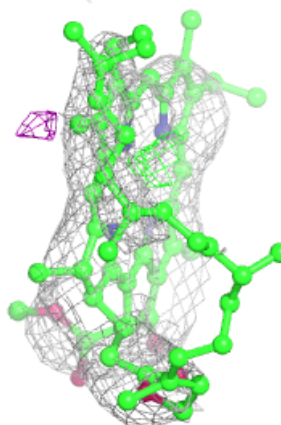
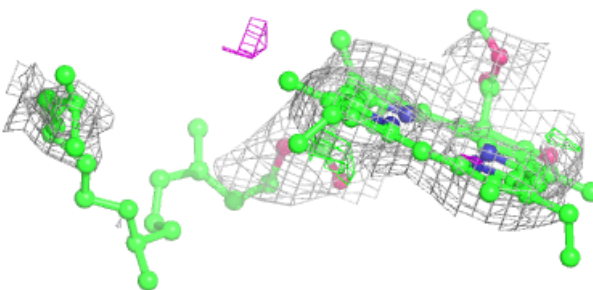
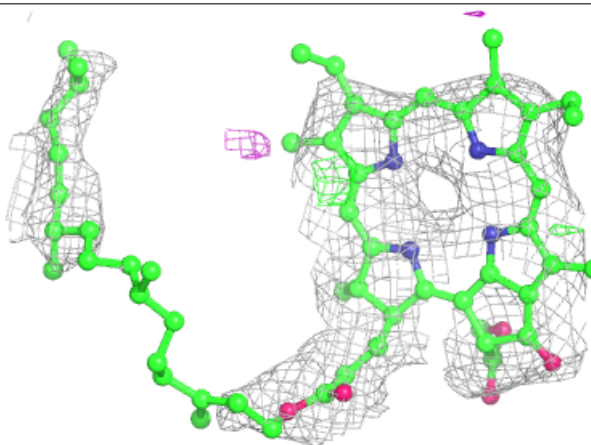


Electron density around CLA BB 5607:

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

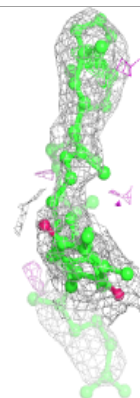
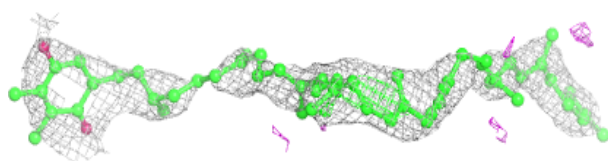
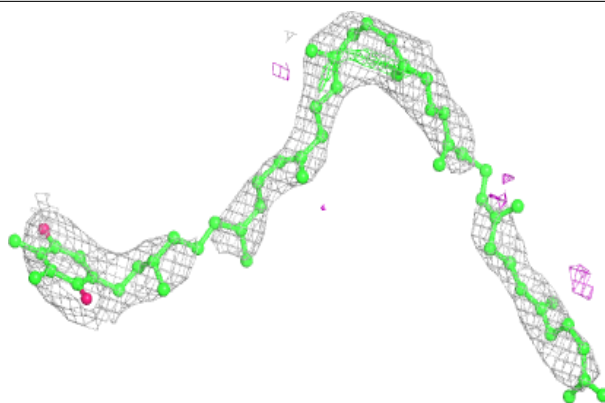
**Electron density around PHO BD 5404:**

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

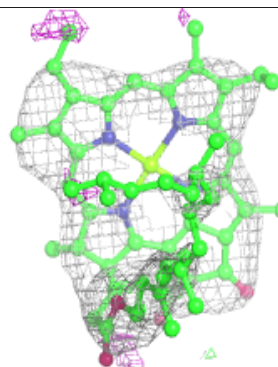
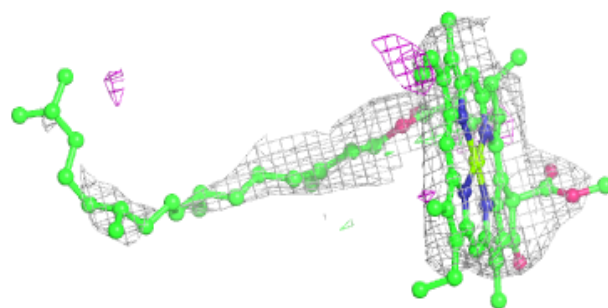
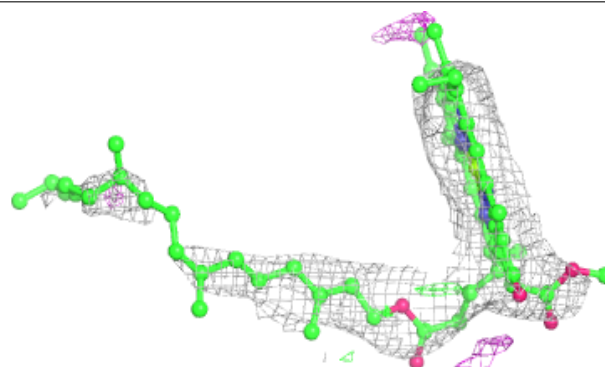


Electron density around PL9 AD 405:

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

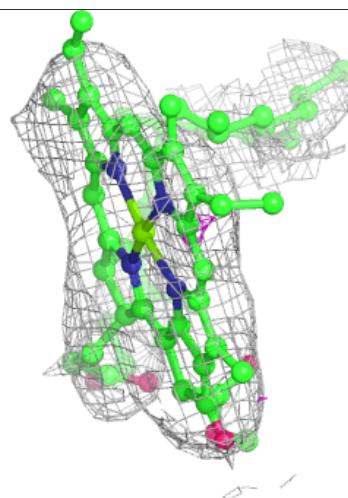
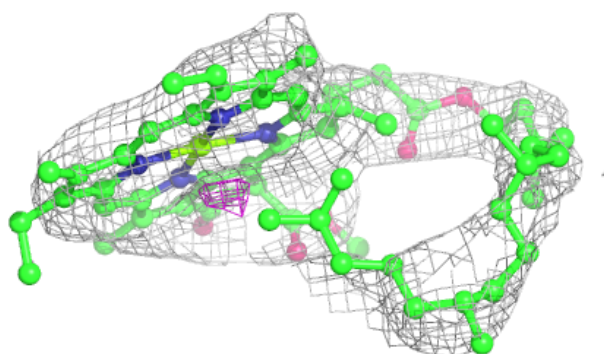
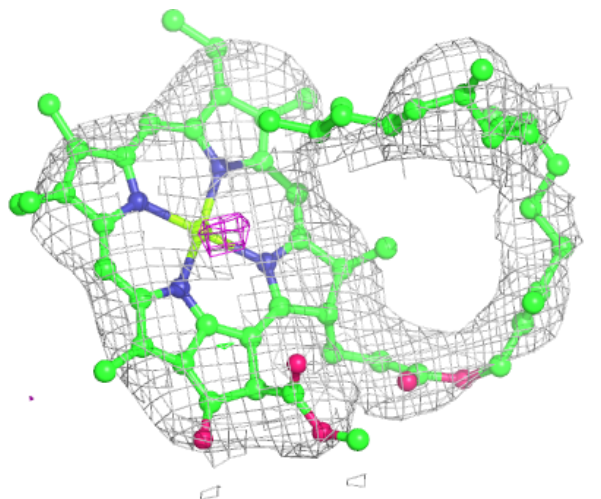
**Electron density around CLA AB 605:**

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



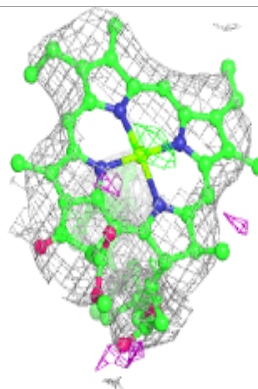
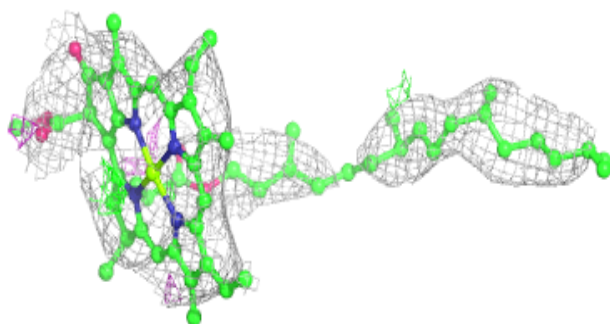
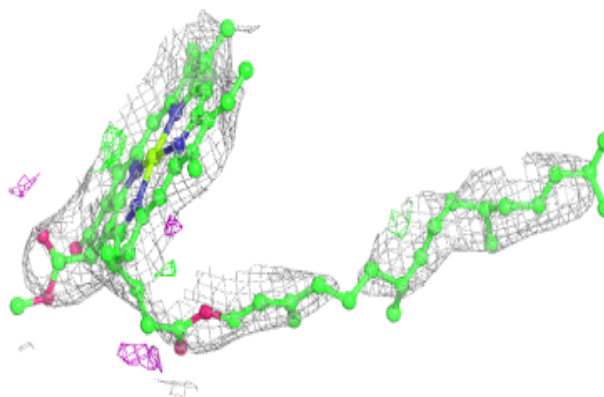
Electron density around CLA BB 5619:

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

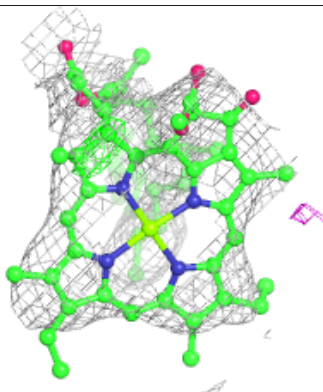
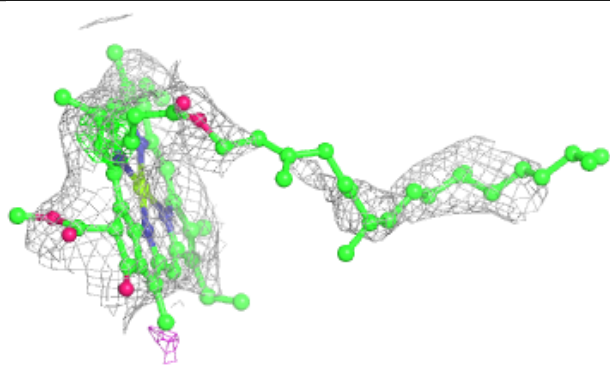
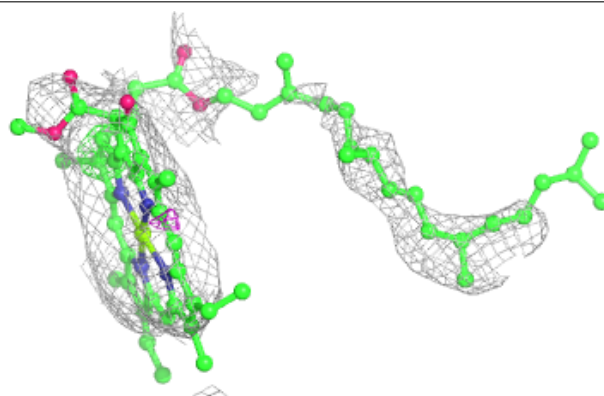


Electron density around CLA BB 5611:

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

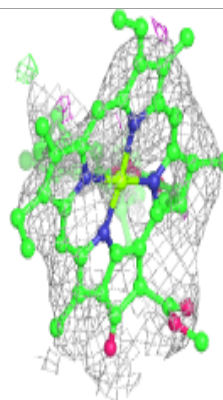
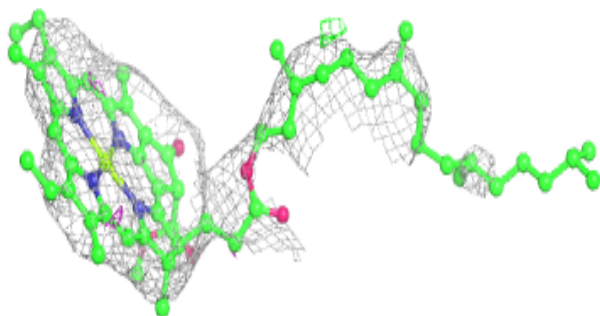
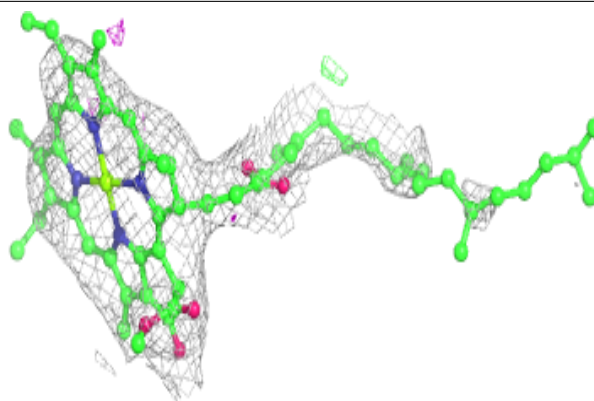
**Electron density around CLA AC 508:**

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

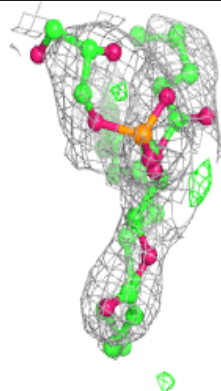
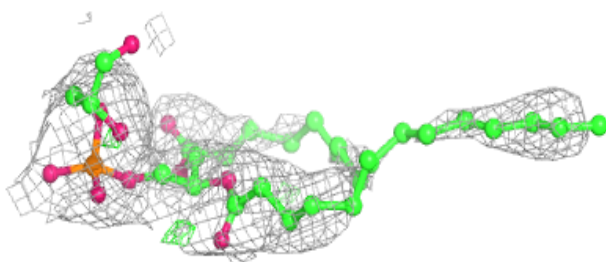
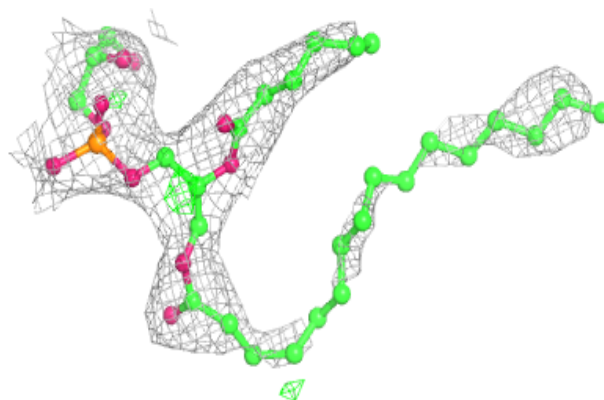


Electron density around CLA BC 5502:

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

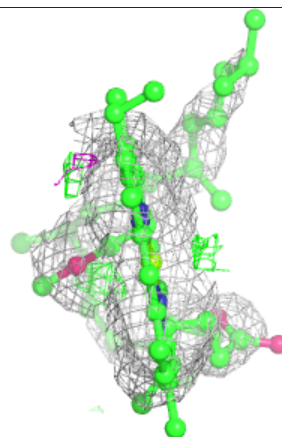
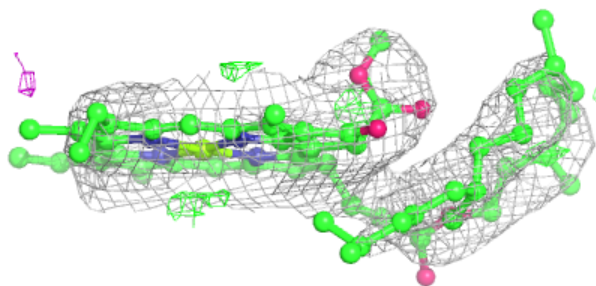
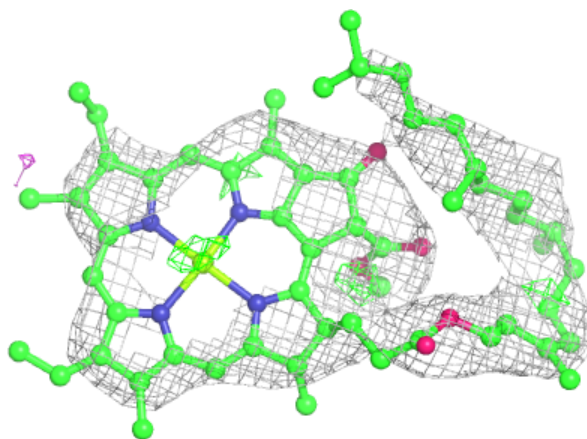
**Electron density around LHG AA 412:**

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



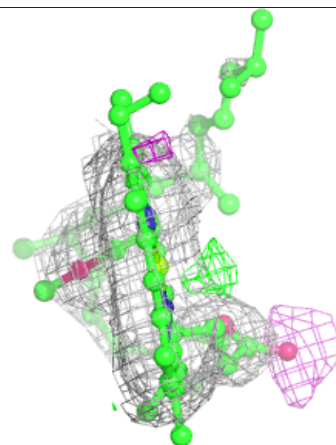
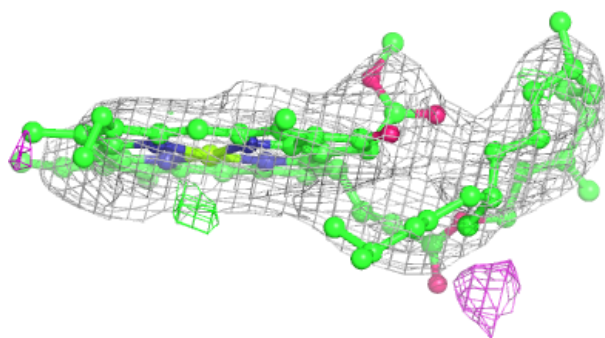
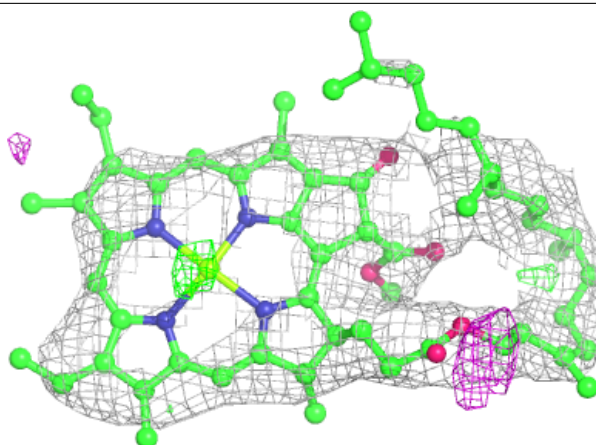
Electron density around CLA BB 5614:

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

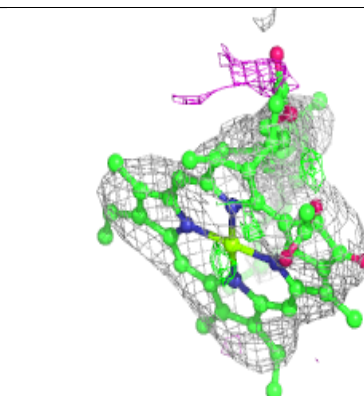
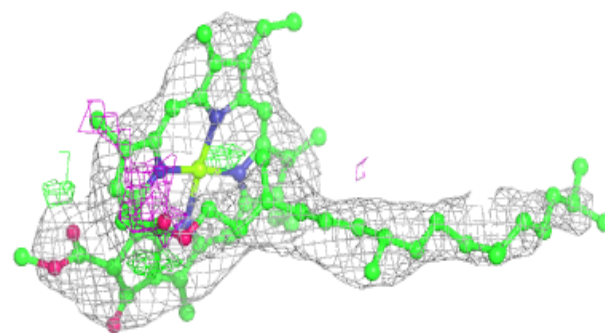
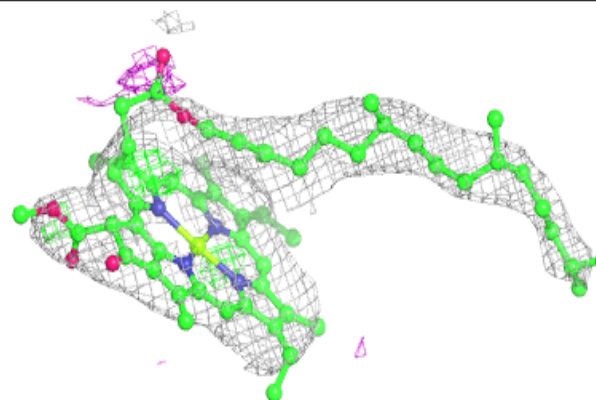


Electron density around CLA AB 610:

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

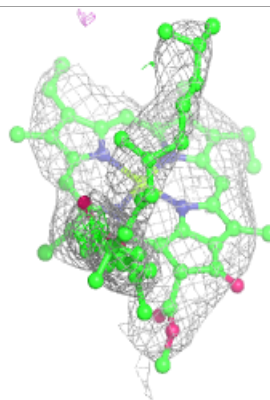
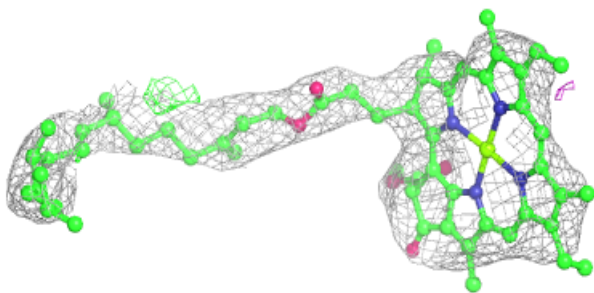
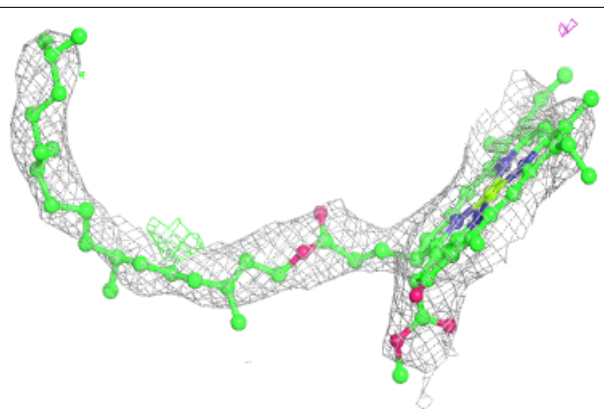
**Electron density around CLA BB 5612:**

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

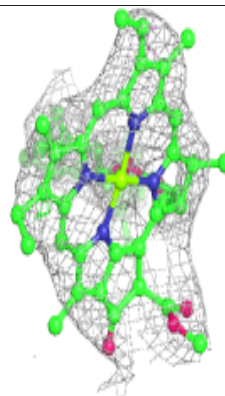
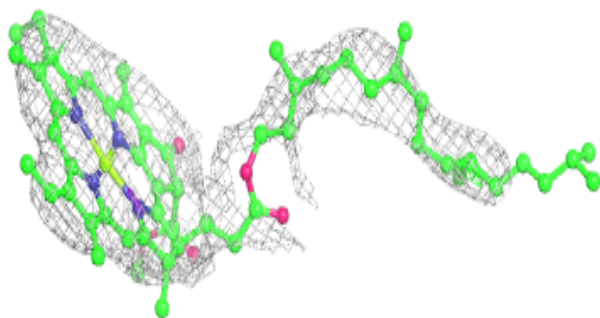
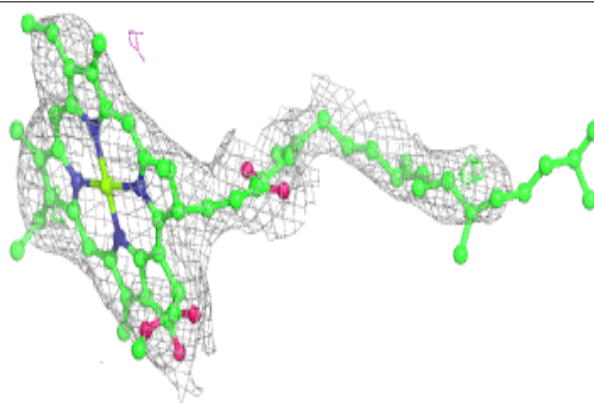


Electron density around CLA BD 5402:

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

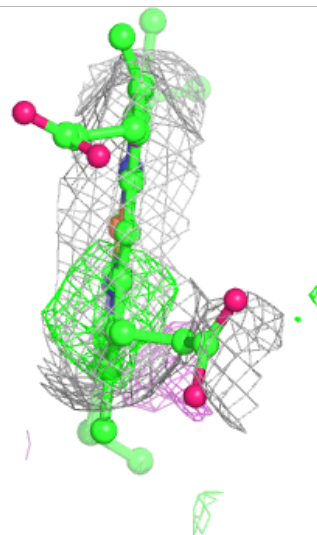
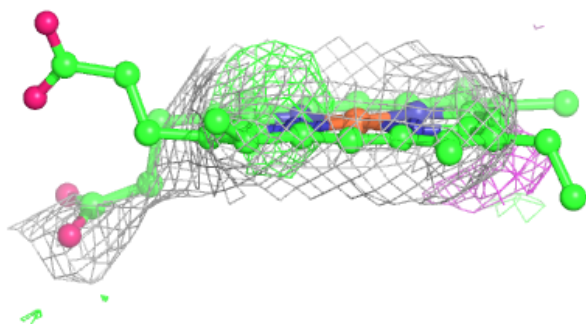
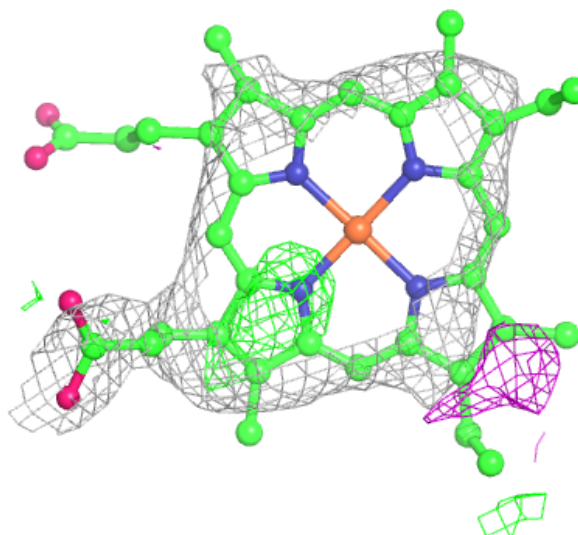
**Electron density around CLA AC 502:**

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



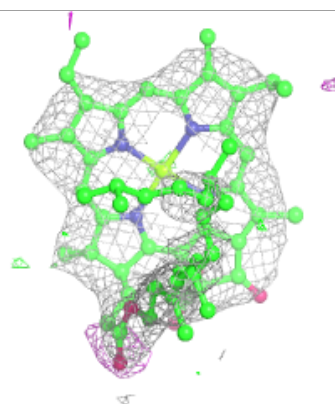
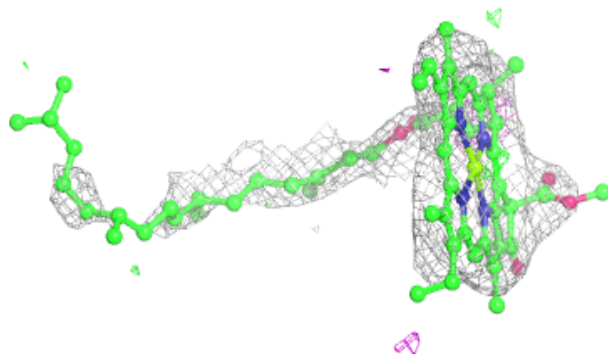
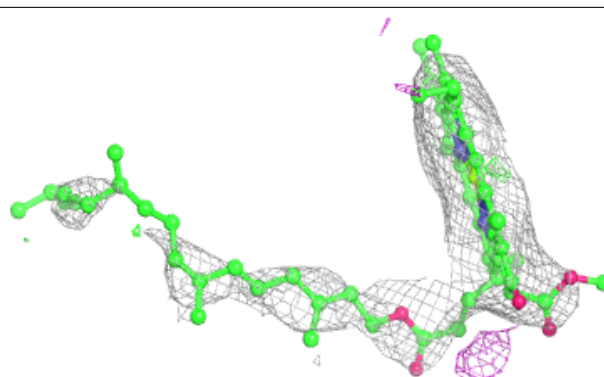
Electron density around HEM BF 5101:

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

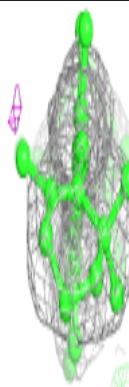
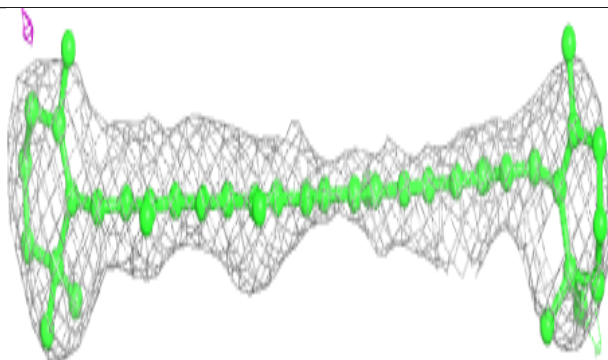
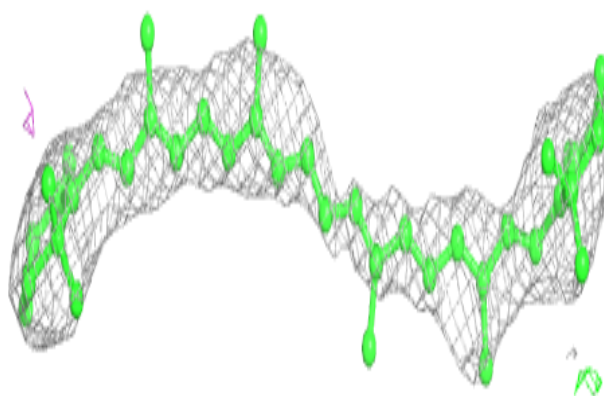


Electron density around CLA BB 5609:

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

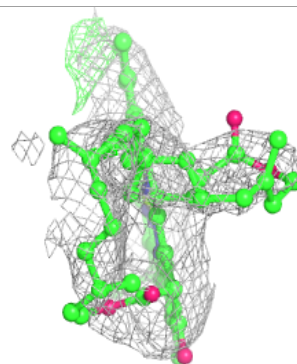
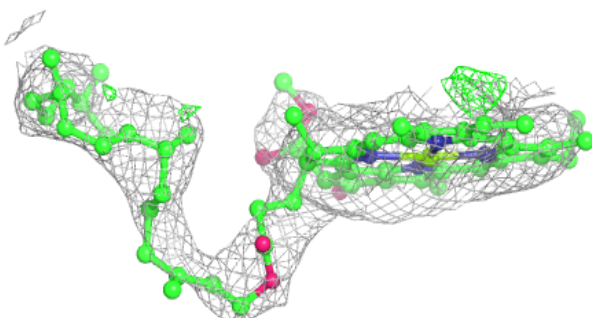
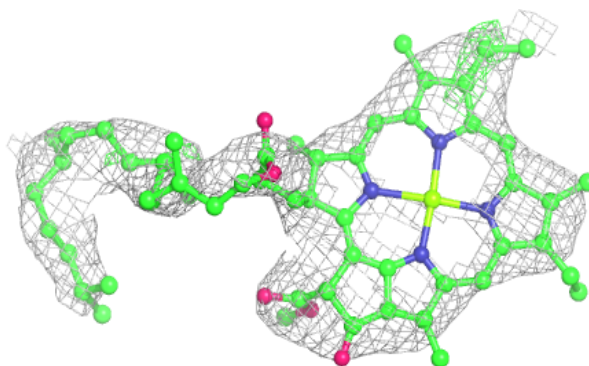
**Electron density around BCR AA 410:**

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

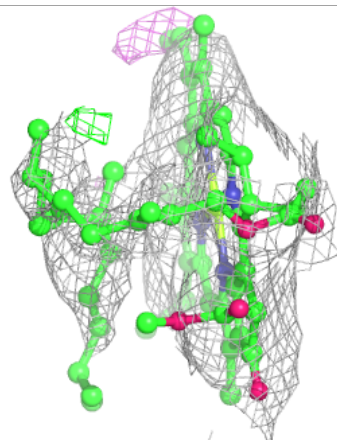
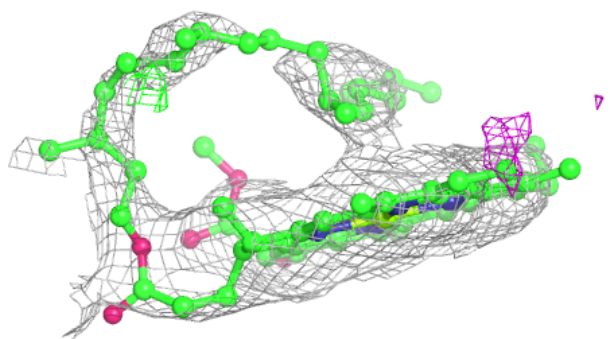
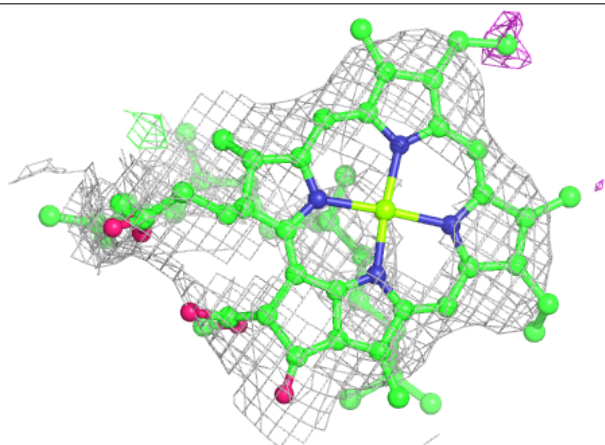


Electron density around CLA BB 5616:

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

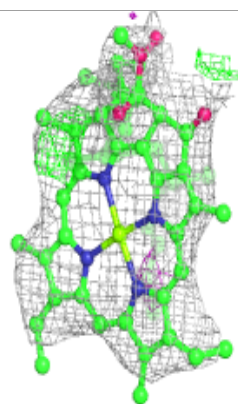
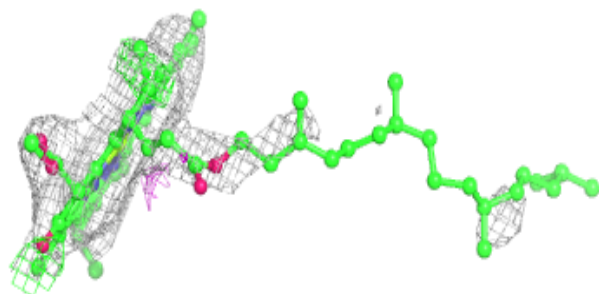
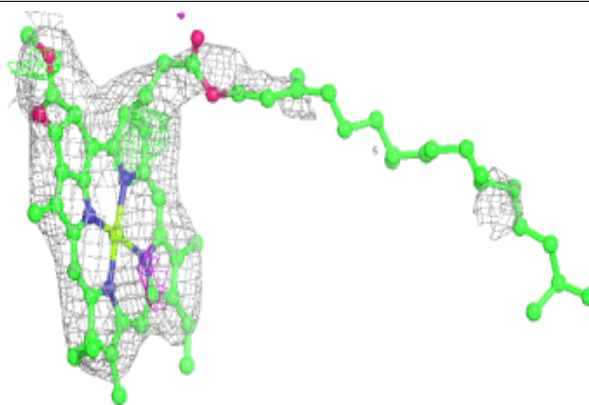
**Electron density around CLA BC 5510:**

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

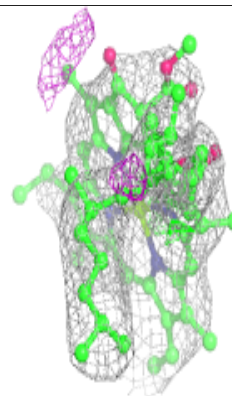
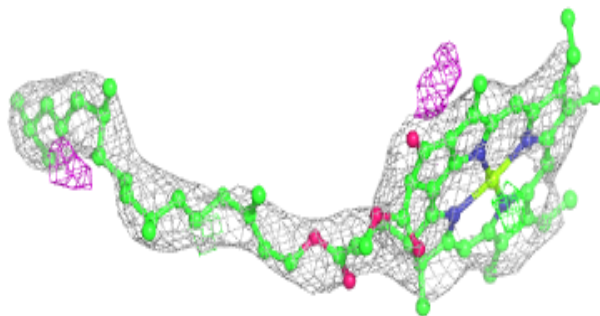
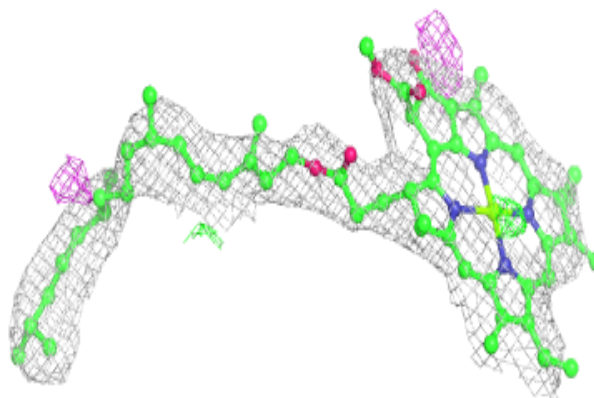


Electron density around CLA AA 407:

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

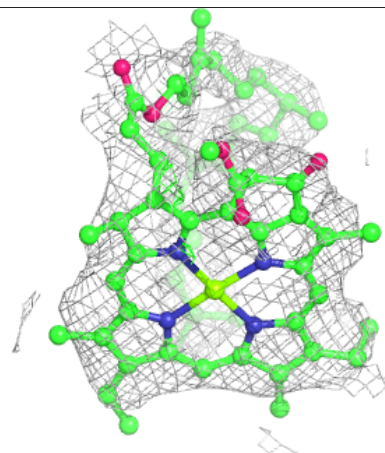
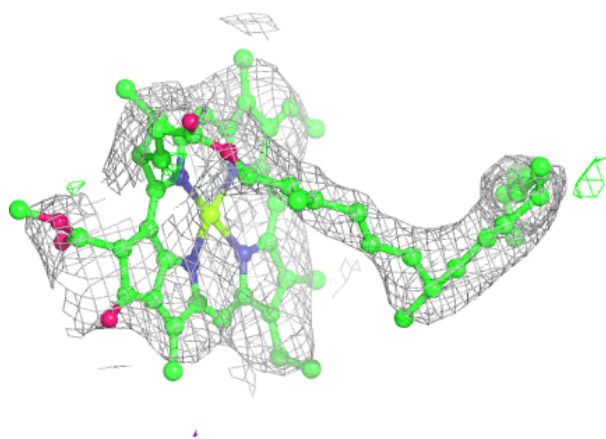
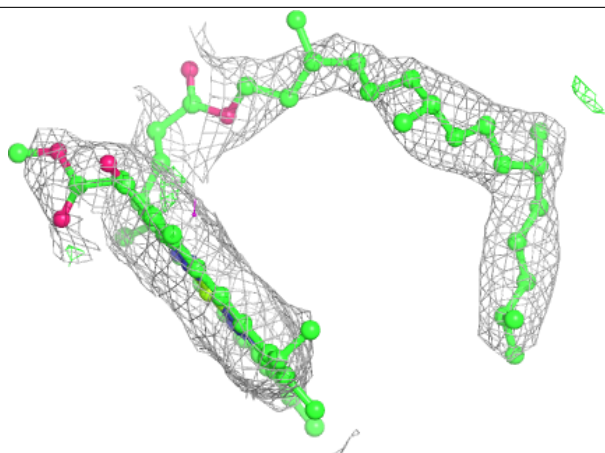
**Electron density around CLA AA 404:**

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



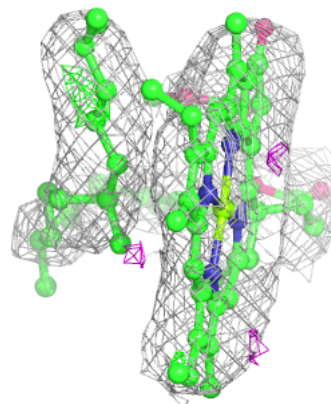
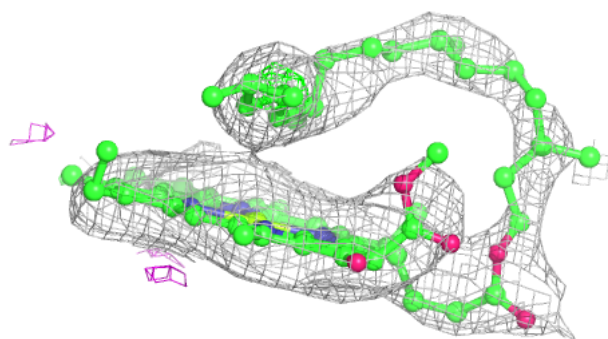
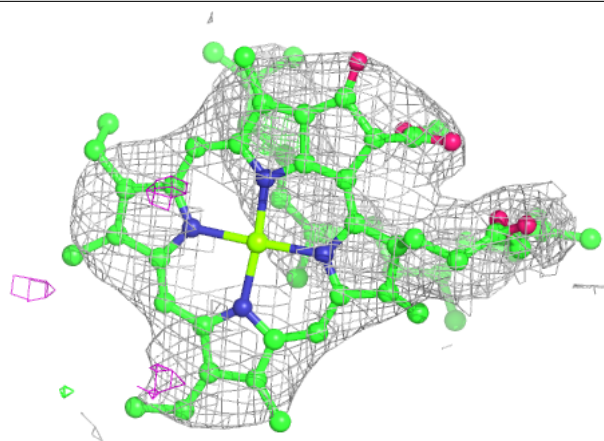
Electron density around CLA BB 5615:

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



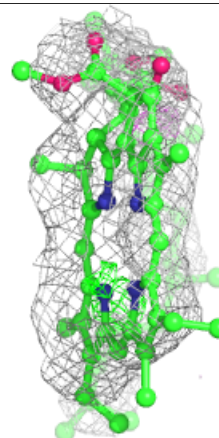
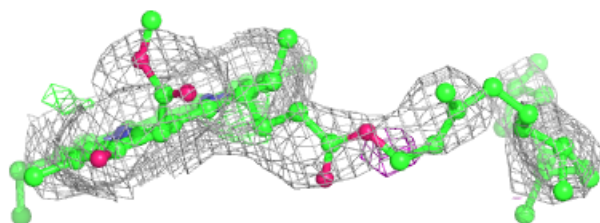
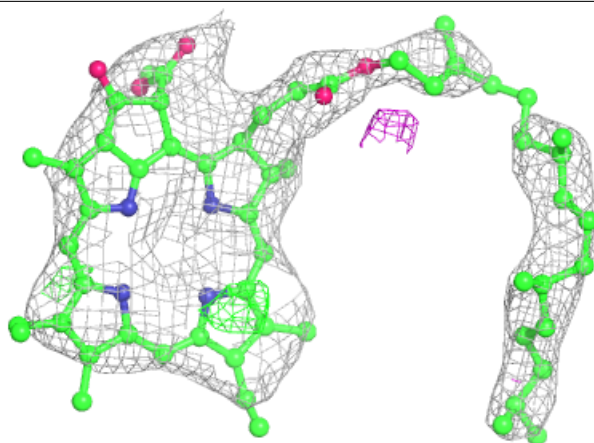
Electron density around CLA AC 510:

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



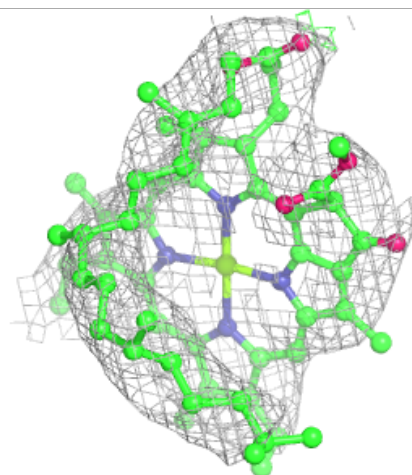
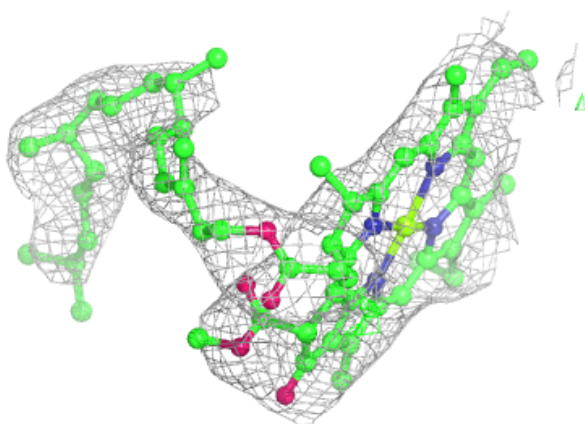
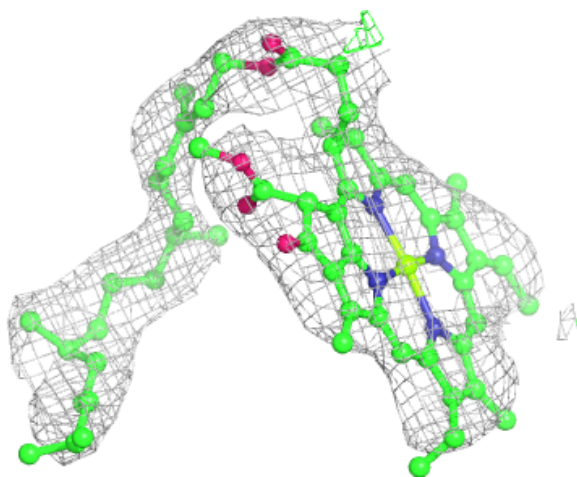
Electron density around PHO AD 402:

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



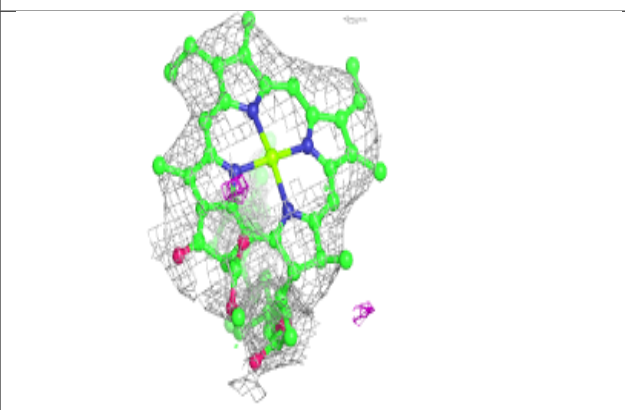
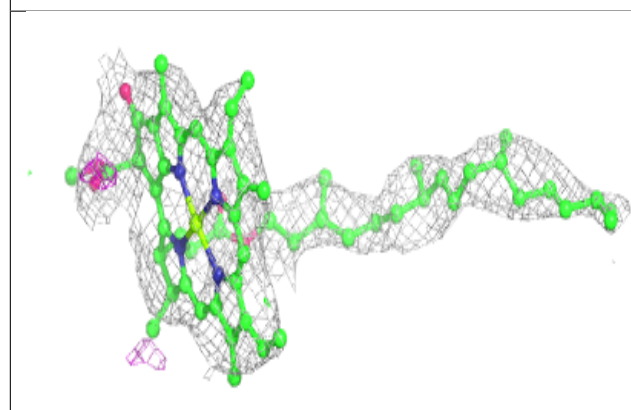
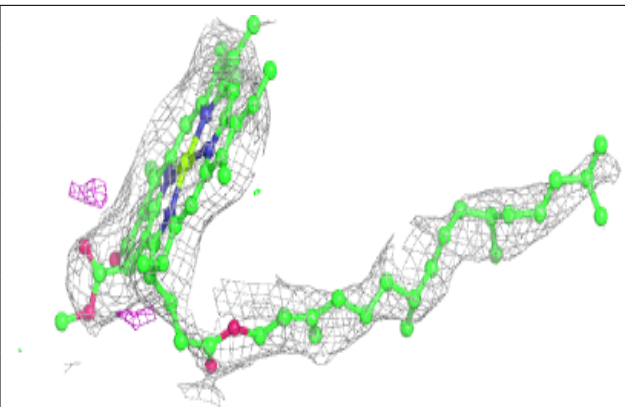
Electron density around CLA BB 5617:

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

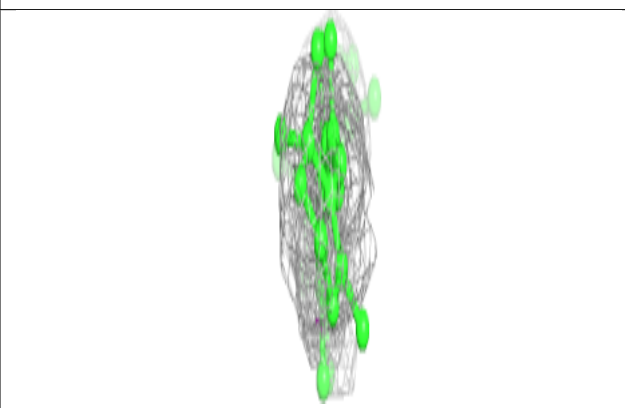
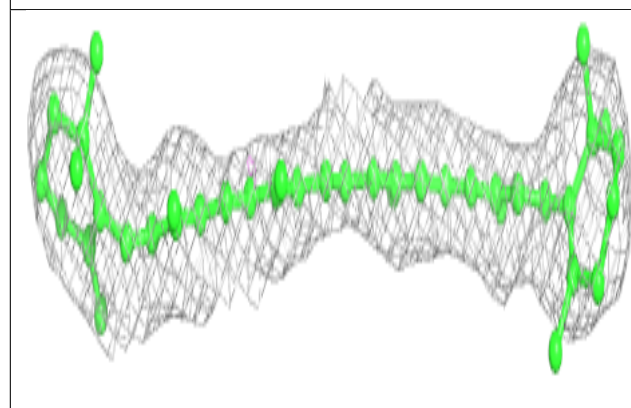
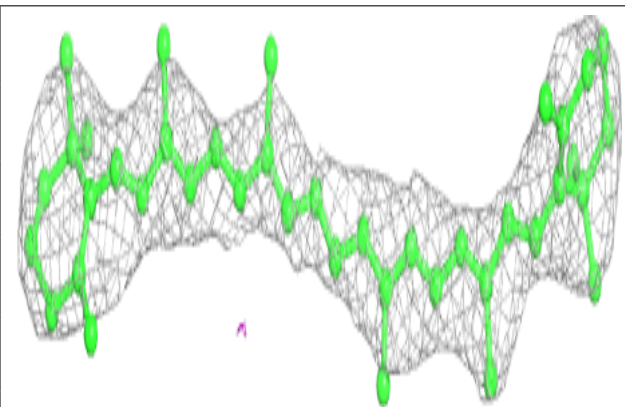


Electron density around CLA AB 607:

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

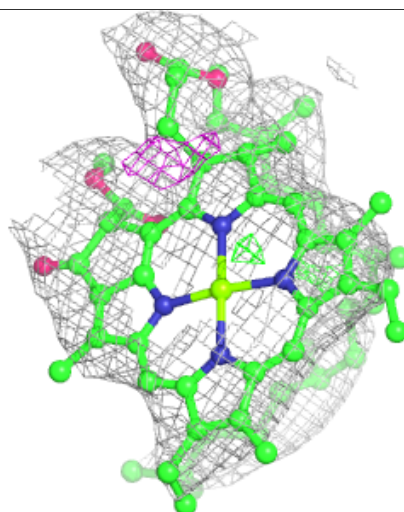
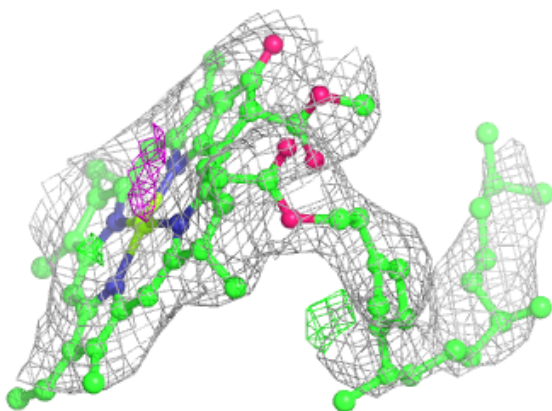
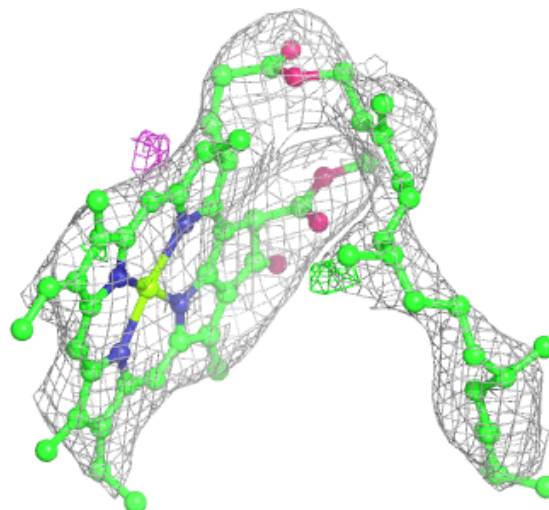
**Electron density around BCR BB 5622:**

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



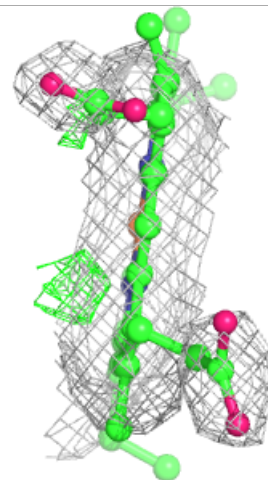
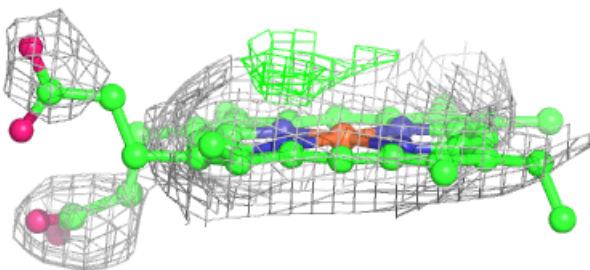
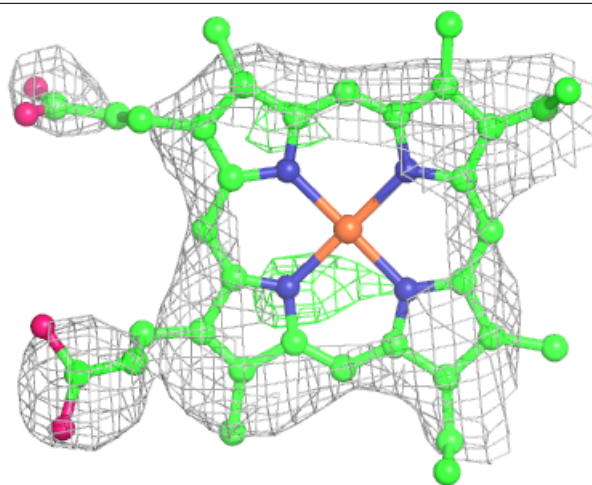
Electron density around CLA AB 613:

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



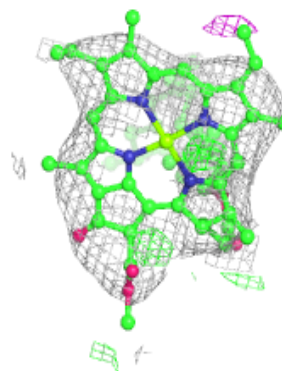
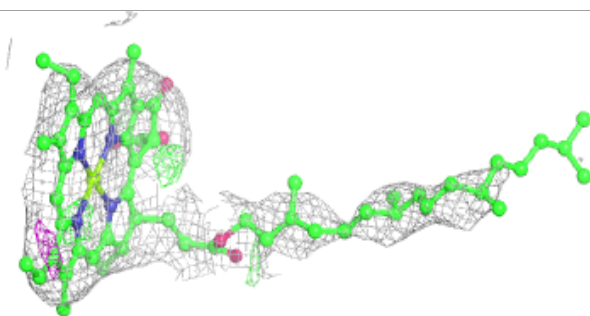
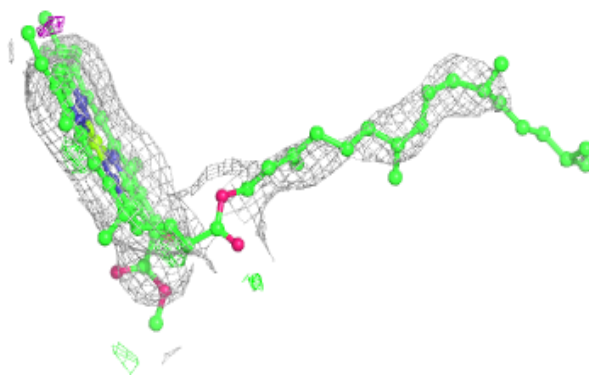
Electron density around HEM BV 5201:

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

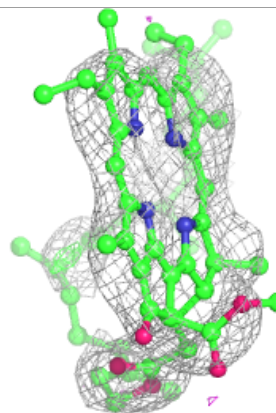
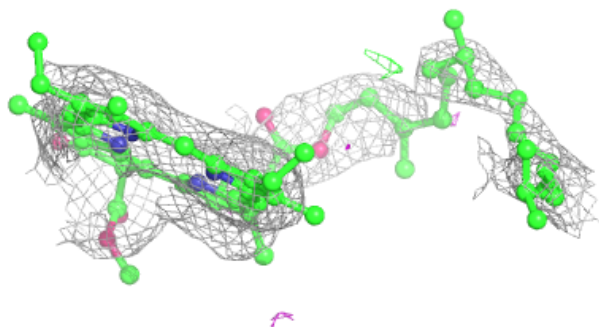
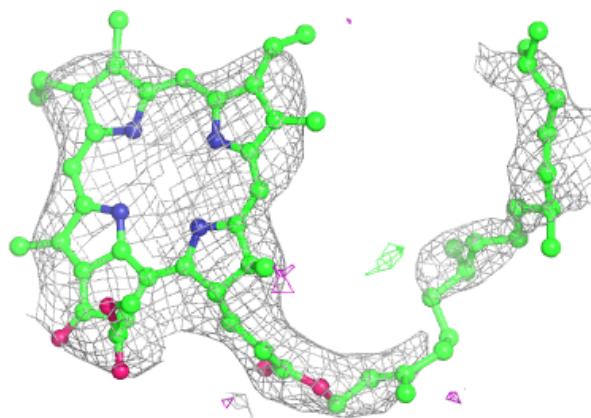


Electron density around CLA AB 604:

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

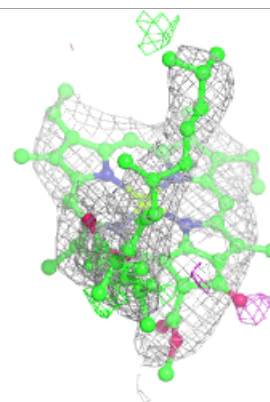
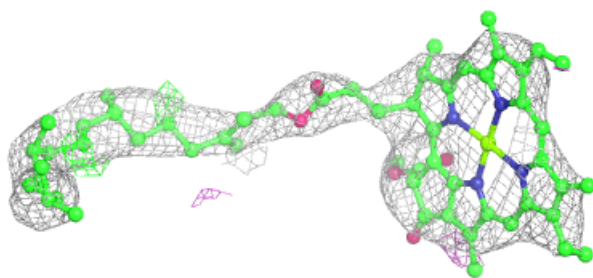
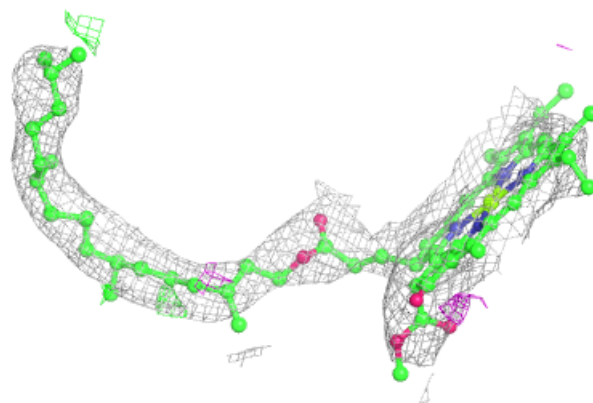
**Electron density around PHO AD 403:**

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

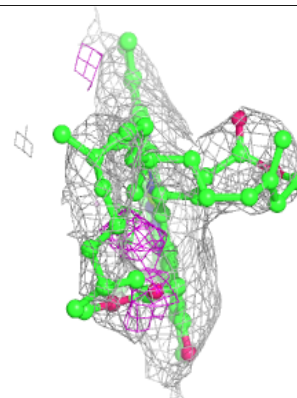
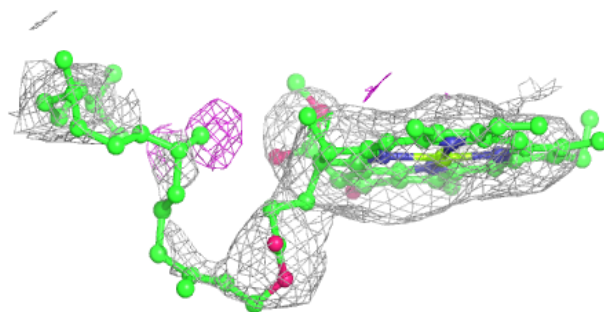
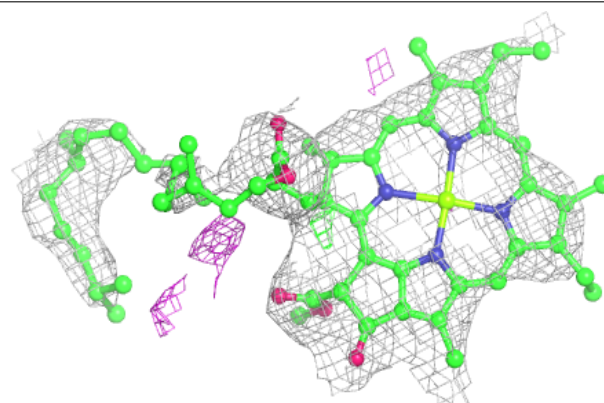


Electron density around CLA AD 401:

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

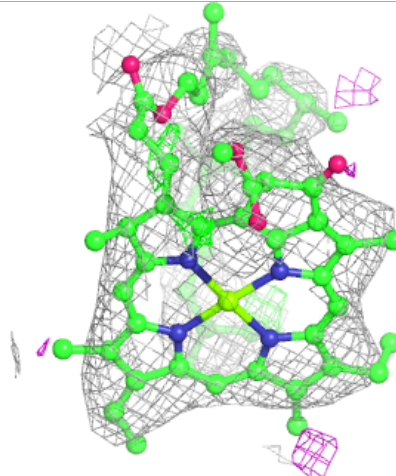
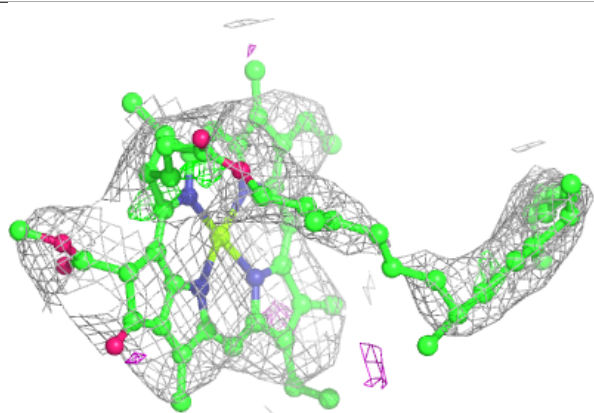
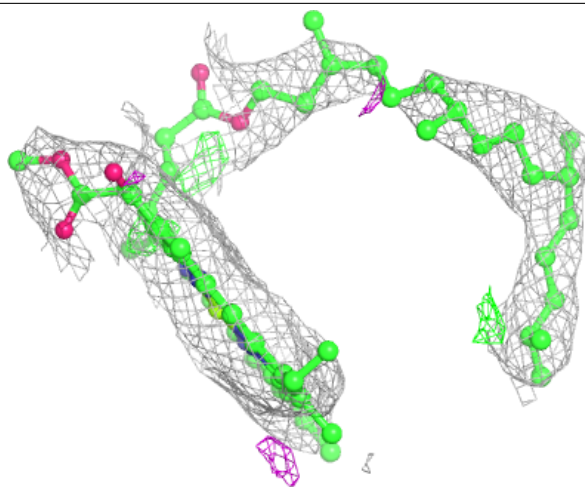
**Electron density around CLA AB 612:**

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



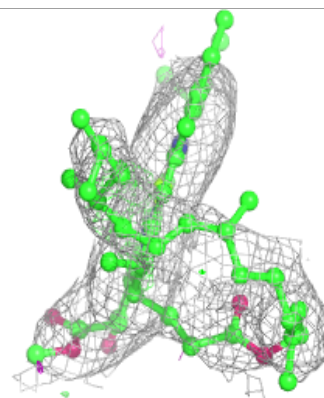
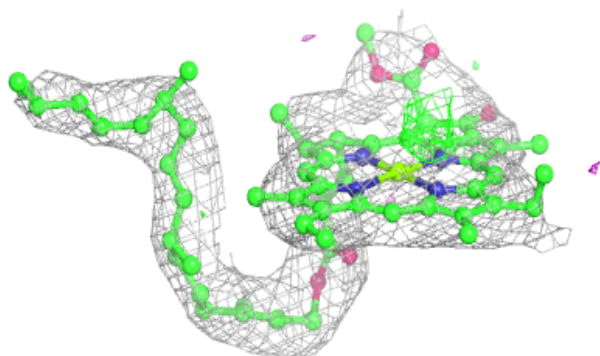
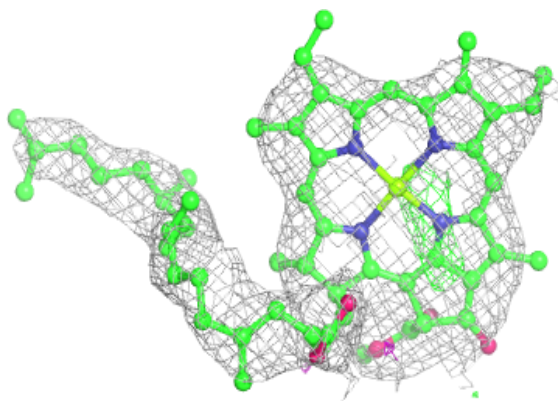
Electron density around CLA AB 611:

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



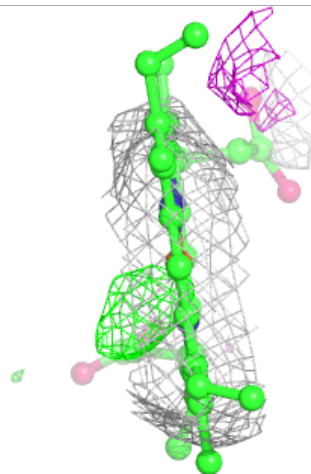
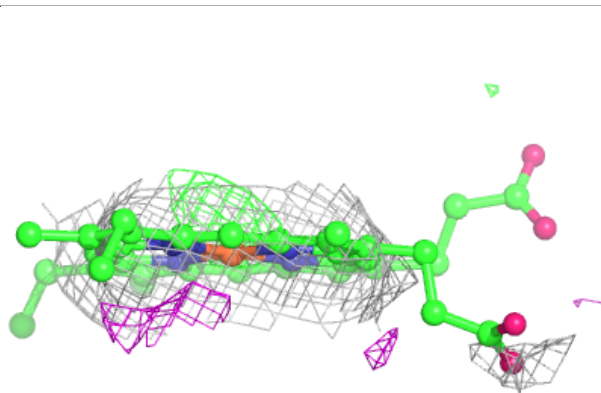
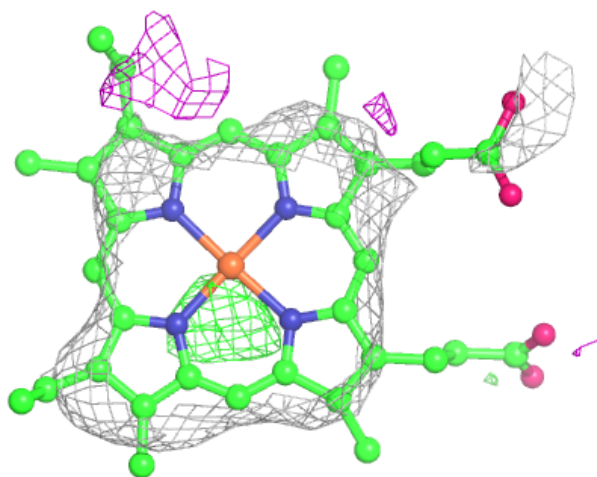
Electron density around CLA AA 405:

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



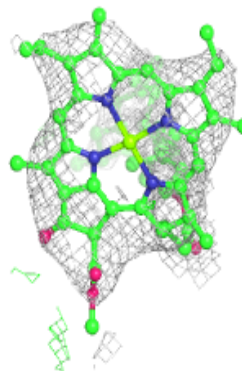
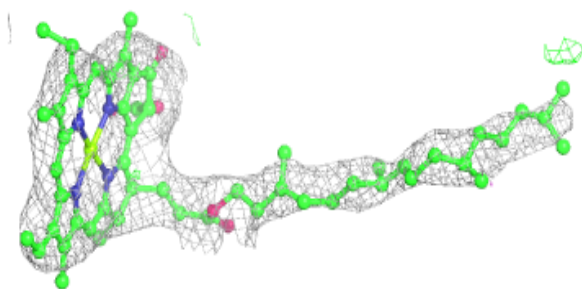
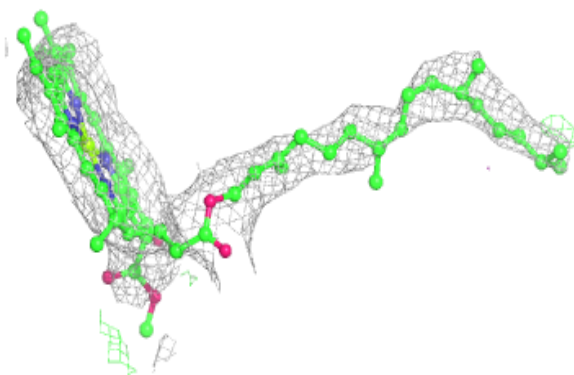
Electron density around HEM AF 101:

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



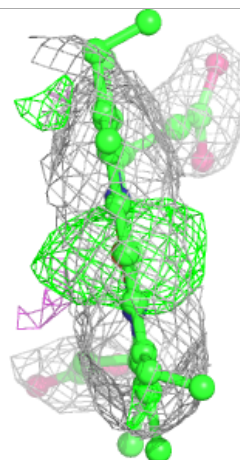
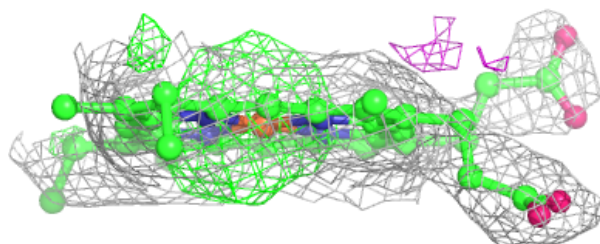
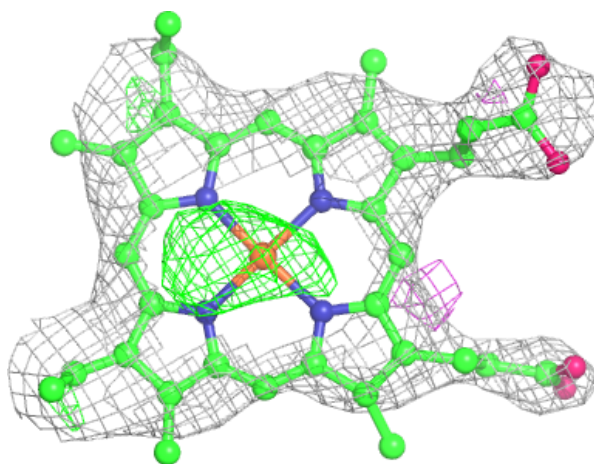
Electron density around CLA BB 5608:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.