



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:20 PM UTC

PDB ID : 4V62 / pdb_00004v62
Title : Crystal Structure of cyanobacterial Photosystem II
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on : 2008-01-17
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

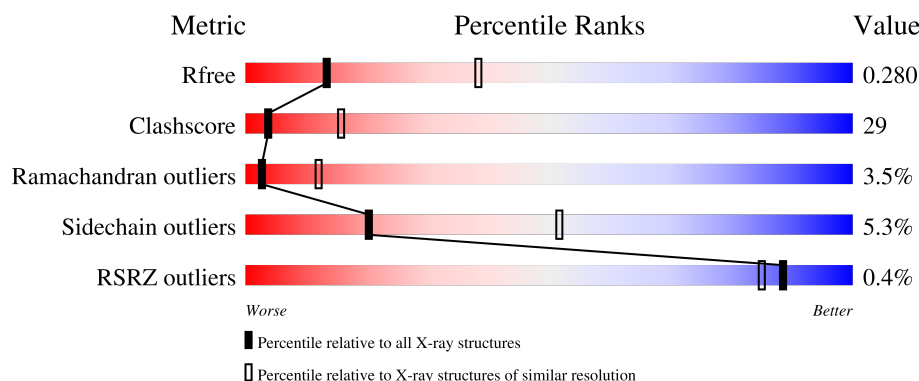
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

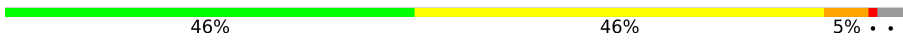
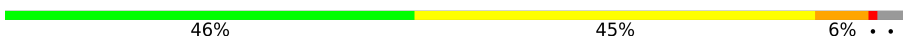
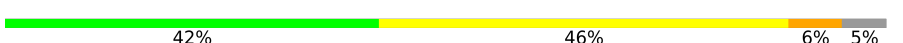
The reported resolution of this entry is 2.90 Å.

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



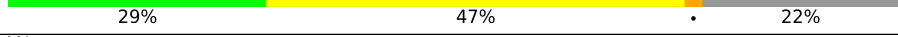
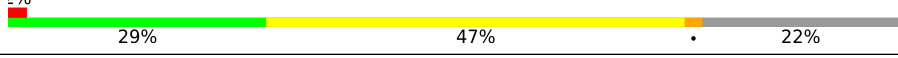
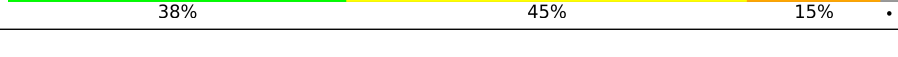
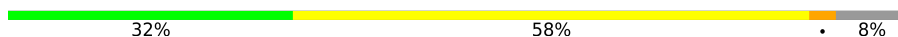
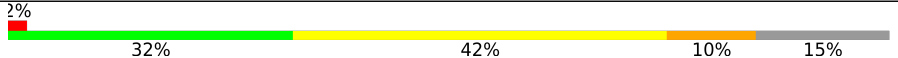
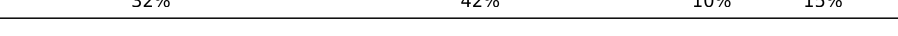
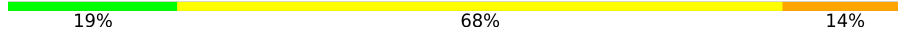
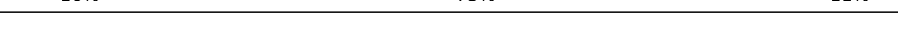
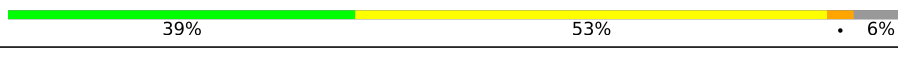
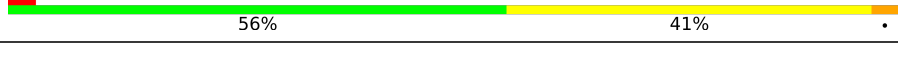
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	473	

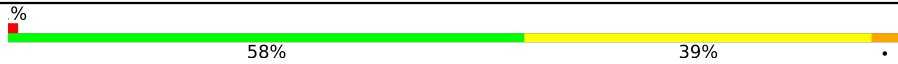
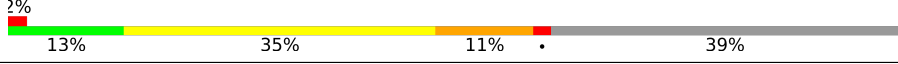
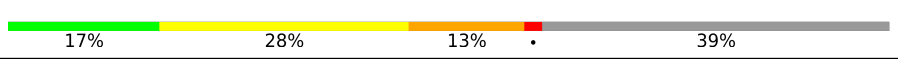
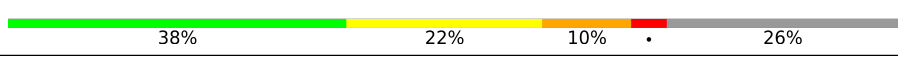
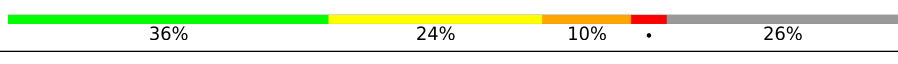
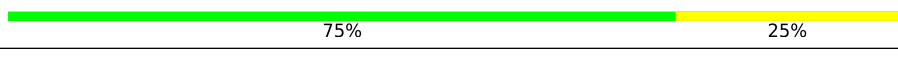
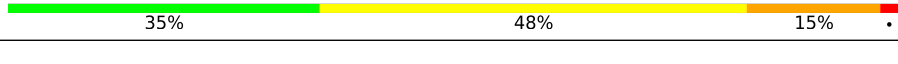
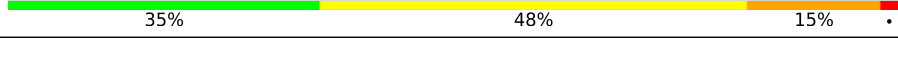
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Mol	Chain	Length	Quality of chain
3	BC	473	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	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	50	
18	BX	50	
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
22	CLA	AA	402	X	-	-	-
22	CLA	AA	403	X	-	-	-
22	CLA	AA	404	X	-	-	-
22	CLA	AA	406	X	-	-	-
22	CLA	AB	601	X	-	-	-
22	CLA	AB	602	X	-	-	-
22	CLA	AB	603	X	-	-	-
22	CLA	AB	604	X	-	-	-
22	CLA	AB	605	X	-	-	-
22	CLA	AB	606	X	-	-	-
22	CLA	AB	607	X	-	-	-
22	CLA	AB	608	X	-	-	-
22	CLA	AB	609	X	-	-	-
22	CLA	AB	610	X	-	-	-
22	CLA	AB	611	X	-	-	-
22	CLA	AB	612	X	-	-	-
22	CLA	AB	613	X	-	-	-
22	CLA	AB	614	X	-	-	-
22	CLA	AB	615	X	-	-	-
22	CLA	AB	616	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	BC	508	X	-	-	-
22	CLA	BC	509	X	-	-	-
22	CLA	BC	510	X	-	-	-
22	CLA	BC	511	X	-	-	-
22	CLA	BC	512	X	-	-	-
22	CLA	BC	513	X	-	-	-
22	CLA	BD	402	X	-	-	-
22	CLA	BD	404	X	-	-	-
27	DGD	AA	410	X	-	-	-
27	DGD	AB	626	X	-	-	-
27	DGD	AC	516	X	-	-	-
27	DGD	AC	517	X	-	-	-
27	DGD	AC	518	X	-	-	-
27	DGD	AD	410	X	-	-	-
27	DGD	AH	102	X	-	-	-
27	DGD	BA	411	X	-	-	-
27	DGD	BB	602	X	-	-	-
27	DGD	BC	516	X	-	-	-
27	DGD	BC	517	X	-	-	-
27	DGD	BC	518	X	-	-	-
27	DGD	BD	410	X	-	-	-
27	DGD	BH	101	X	-	-	-
30	LMG	AA	413	X	-	-	-
30	LMG	AA	416	X	-	-	-
30	LMG	AB	621	X	-	-	-
30	LMG	AB	622	X	-	-	-
30	LMG	AB	623	X	-	-	-
30	LMG	AC	519	X	-	-	-
30	LMG	AC	520	X	-	-	-
30	LMG	AD	407	X	-	-	-
30	LMG	AD	408	X	-	-	-
30	LMG	AE	102	X	-	-	-
30	LMG	AI	101	X	-	-	-
30	LMG	AM	101	X	-	-	-
30	LMG	BA	414	X	-	-	-
30	LMG	BB	623	X	-	-	-
30	LMG	BB	624	X	-	-	-
30	LMG	BC	519	X	-	-	-
30	LMG	BC	520	X	-	-	-
30	LMG	BD	407	X	-	-	-
30	LMG	BD	408	X	-	-	-
30	LMG	BE	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMG	BI	101	X	-	-	-
30	LMG	BM	102	X	-	-	-

2 Entry composition

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

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

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

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

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

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Protein ycf12.

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

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

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

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

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

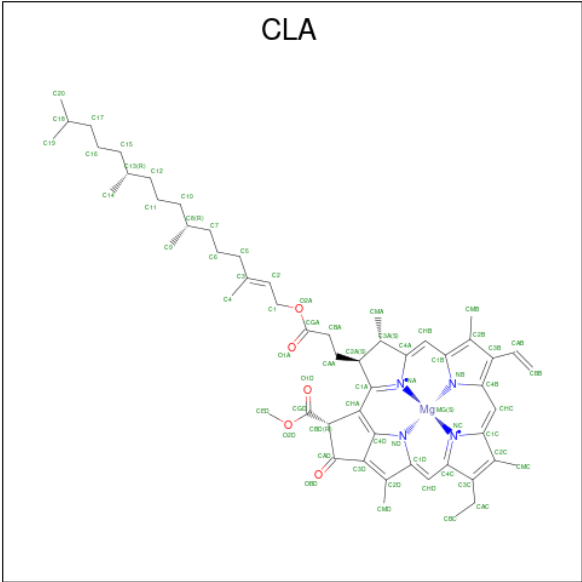
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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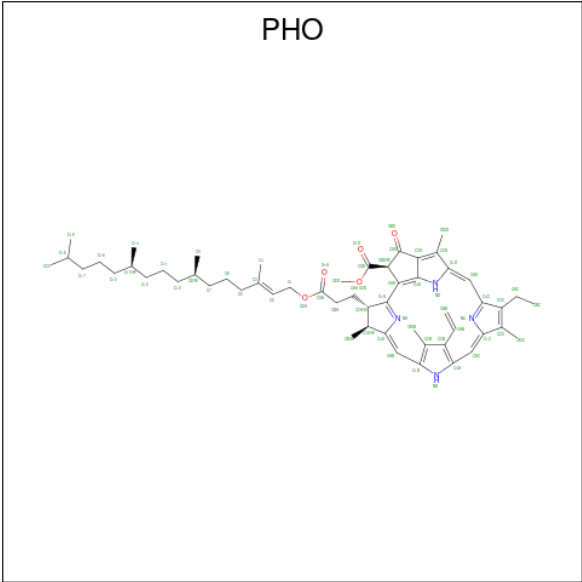
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55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

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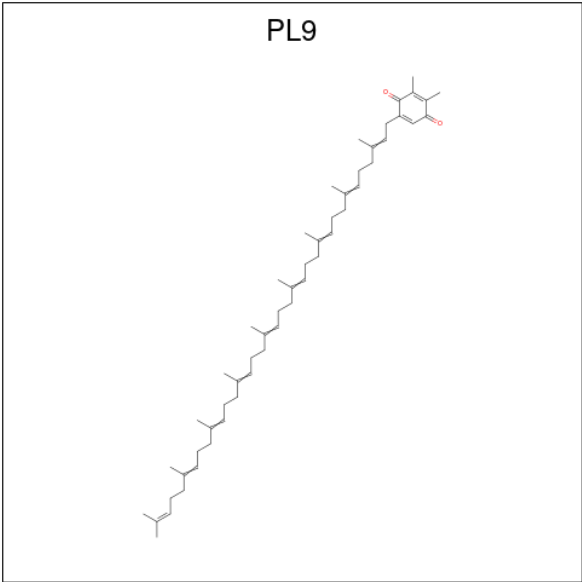
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55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

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



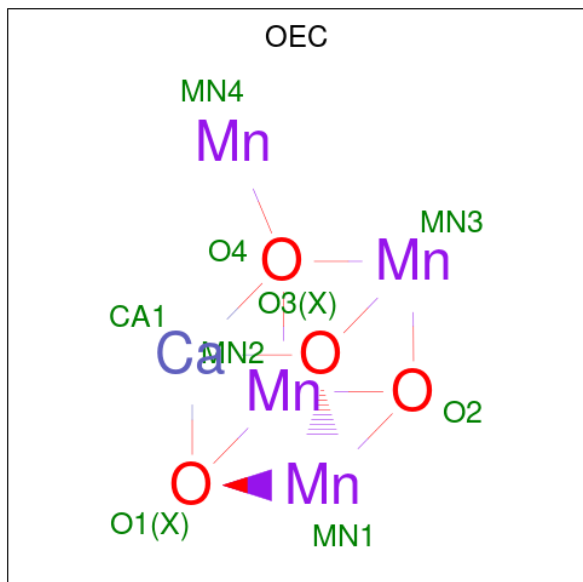
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	AA	1	Total	C	N	O	0	0
			64	55	4	5		
23	AD	1	Total	C	N	O	0	0
			64	55	4	5		
23	BA	1	Total	C	N	O	0	0
			64	55	4	5		
23	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



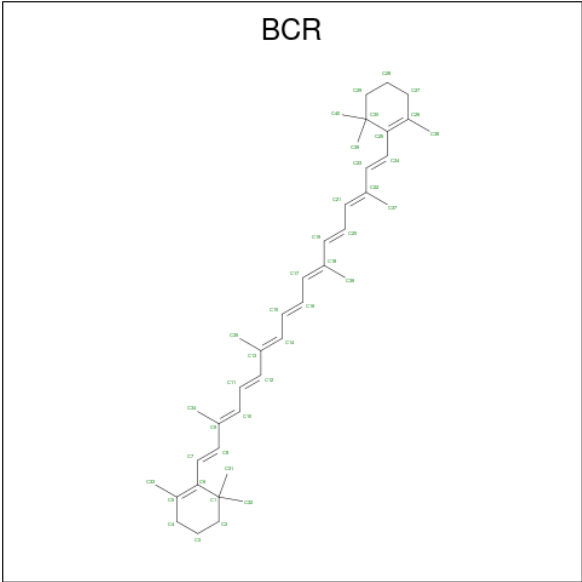
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	AA	1	Total	C	O	0	0
			45	43	2		
24	AD	1	Total	C	O	0	0
			55	53	2		
24	AJ	1	Total	C	O	0	0
			35	33	2		
24	BA	1	Total	C	O	0	0
			45	43	2		
24	BD	1	Total	C	O	0	0
			55	53	2		
24	BJ	1	Total	C	O	0	0
			35	33	2		

- Molecule 25 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



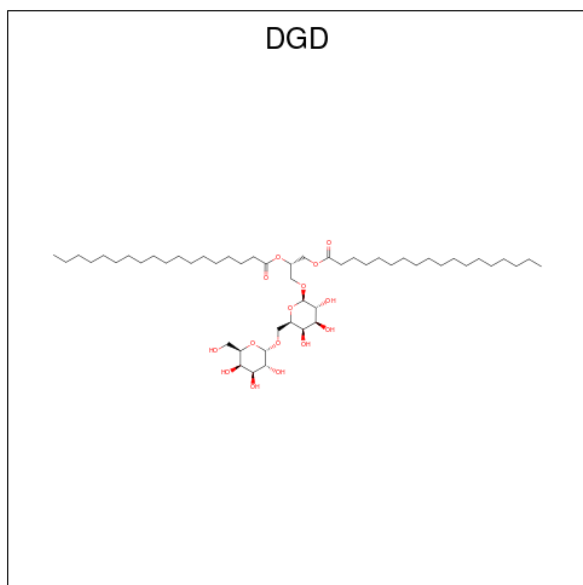
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AA	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AD	1	Total C 40 40	0	0
26	AH	1	Total C 40 40	0	0
26	AJ	1	Total C 40 40	0	0
26	AK	1	Total C 40 40	0	0
26	AT	1	Total C 40 40	0	0
26	AZ	1	Total C 40 40	0	0
26	BA	1	Total C 40 40	0	0

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

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



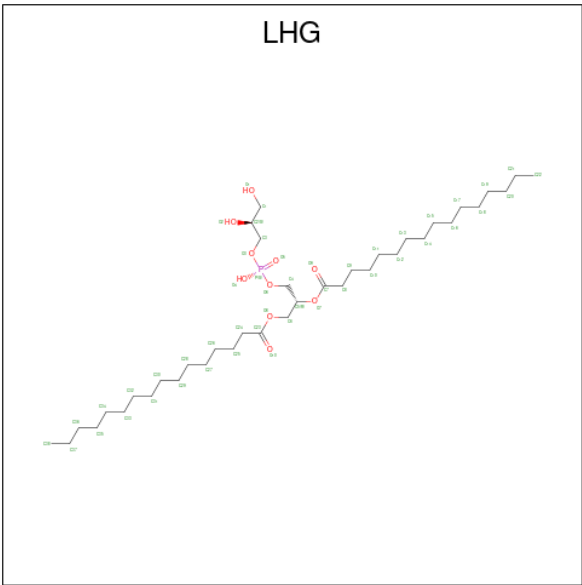
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C O 56 41 15	0	0

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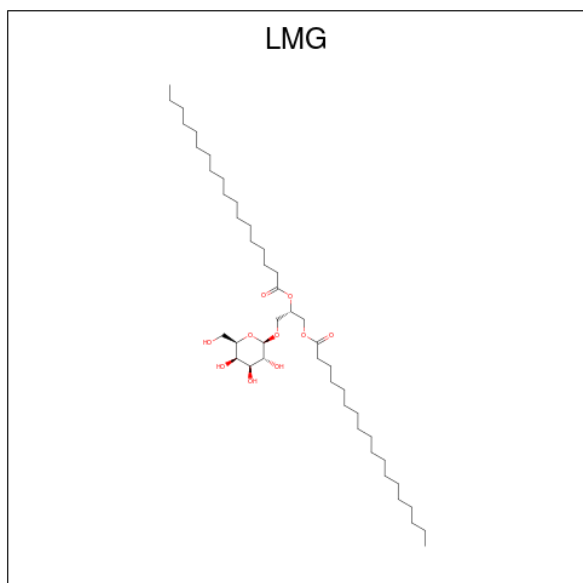
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	AB	1	Total	C	O	0	0
			52	37	15		
27	AC	1	Total	C	O	0	0
			53	38	15		
27	AC	1	Total	C	O	0	0
			62	47	15		
27	AC	1	Total	C	O	0	0
			66	51	15		
27	AD	1	Total	C	O	0	0
			63	48	15		
27	AH	1	Total	C	O	0	0
			58	43	15		
27	BA	1	Total	C	O	0	0
			56	41	15		
27	BB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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	AA	1	Total	C	O	0	0
			51	41	10		

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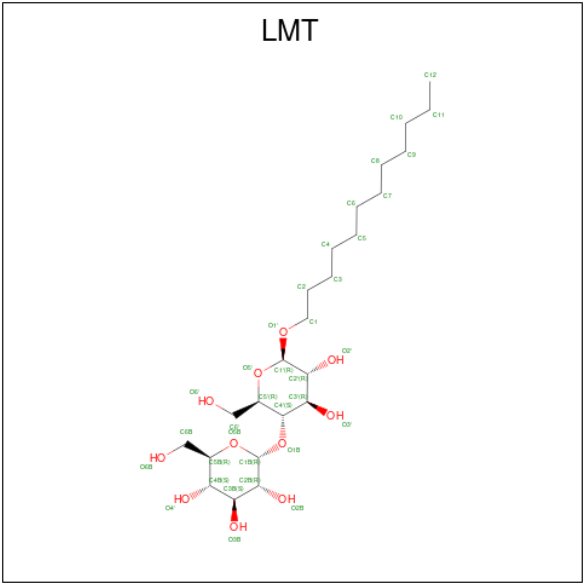
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	AA	1	Total	C	O	0	0
			42	32	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			42	32	10		
30	AC	1	Total	C	O	0	0
			48	38	10		
30	AC	1	Total	C	O	0	0
		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

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



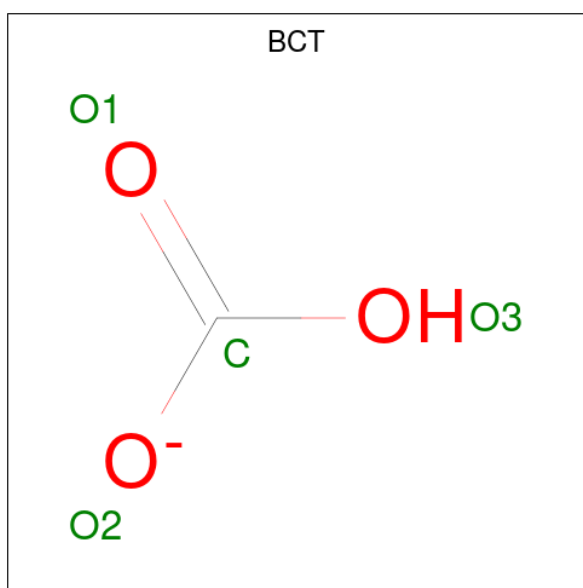
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM	1	Total	C	O	0	0
			35	24	11		
32	AT	1	Total	C	O	0	0
			35	24	11		
32	BB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

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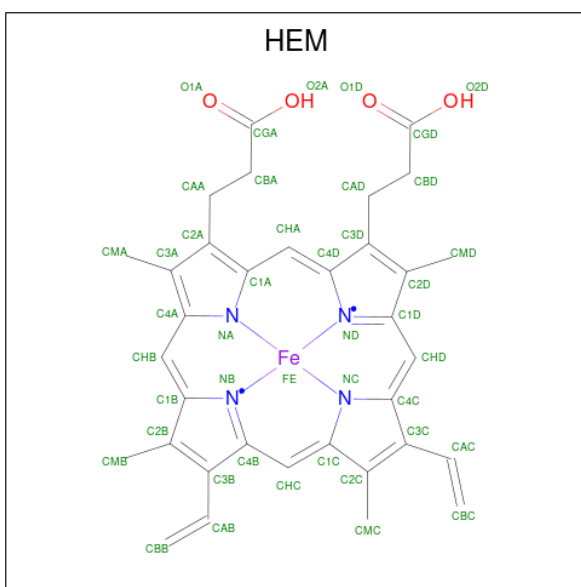
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		
32	BT	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	AD	1	Total	C	O	0	0
			4	1	3		
33	BD	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

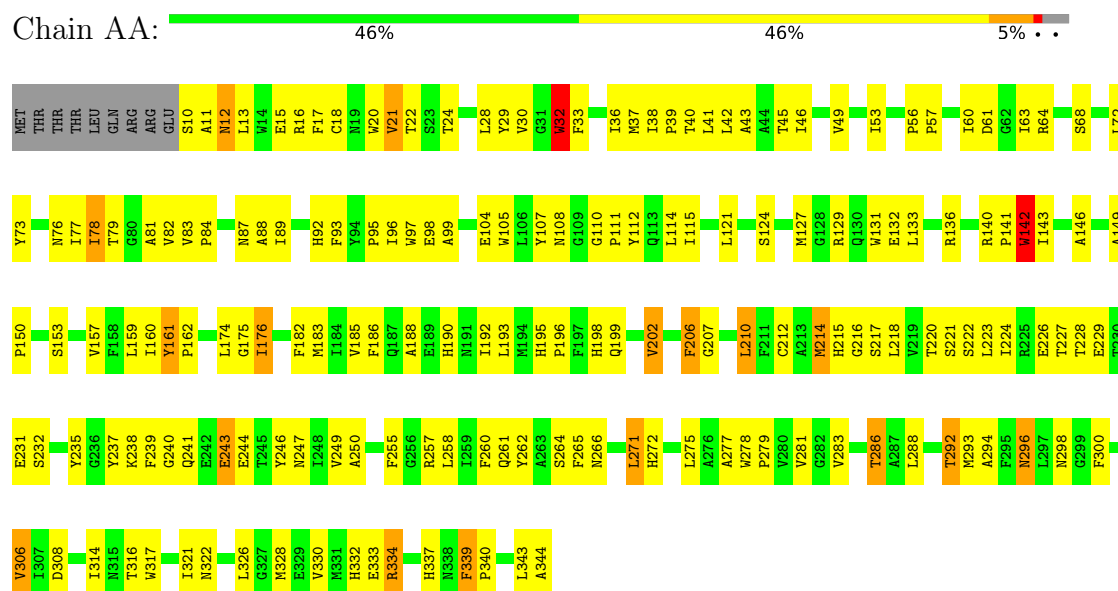
- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

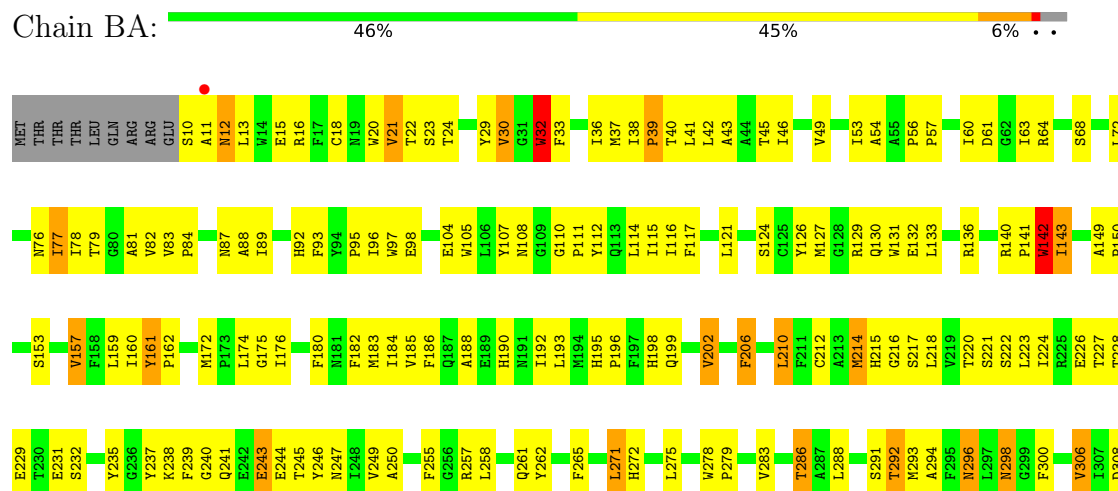
3 Residue-property plots

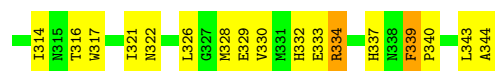
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



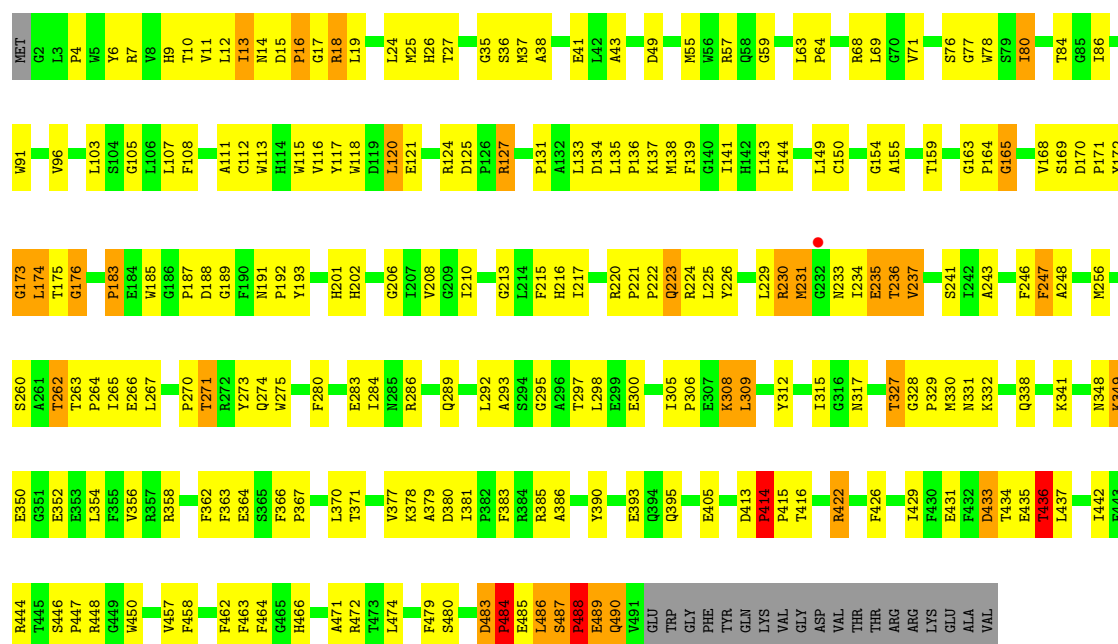
• Molecule 1: Photosystem Q(B) protein





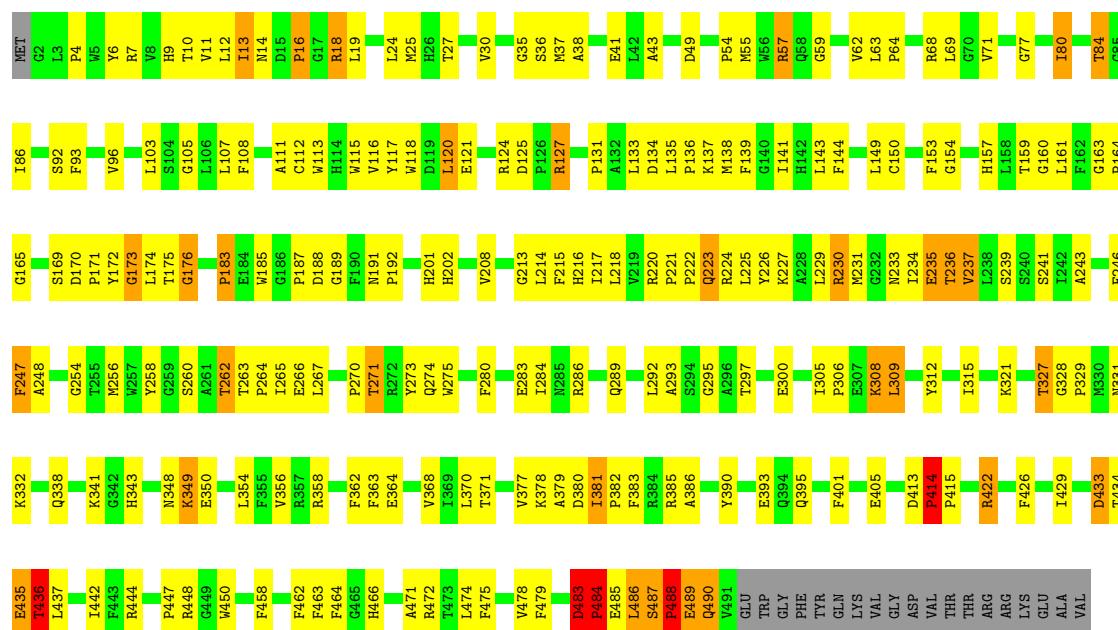
• Molecule 2: Photosystem II core light harvesting protein

Chain AB: 52% 37% 6% . .



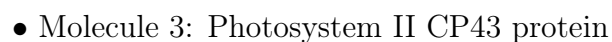
• Molecule 2: Photosystem II core light harvesting protein

Chain BB: 52% 37% 6% . .



• Molecule 3: Photosystem II CP43 protein

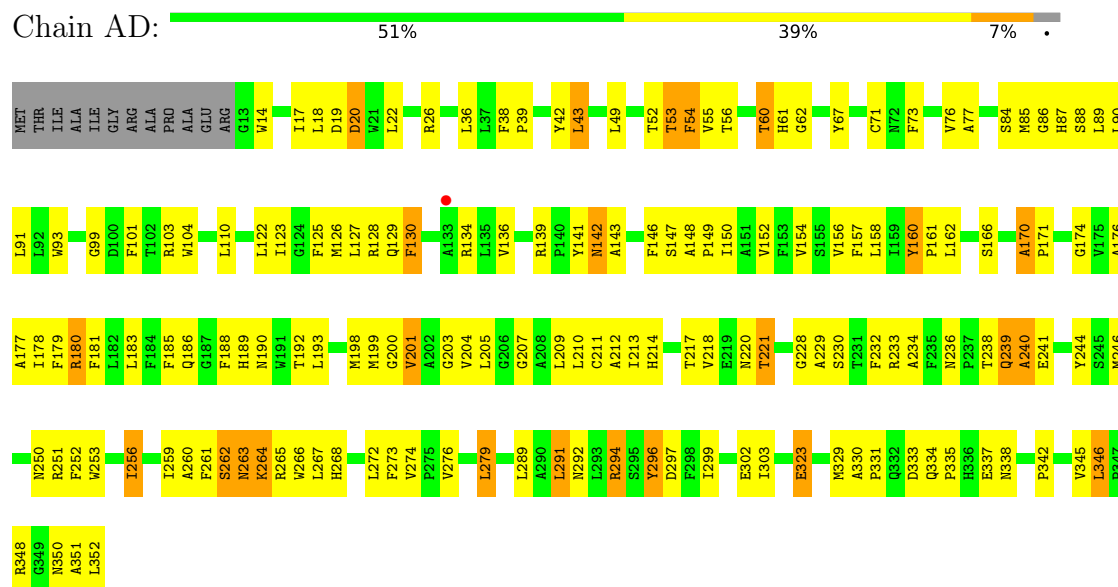
Frequency	Percentage
Daily	42%
Often	46%
Sometimes	6%
Never	5%



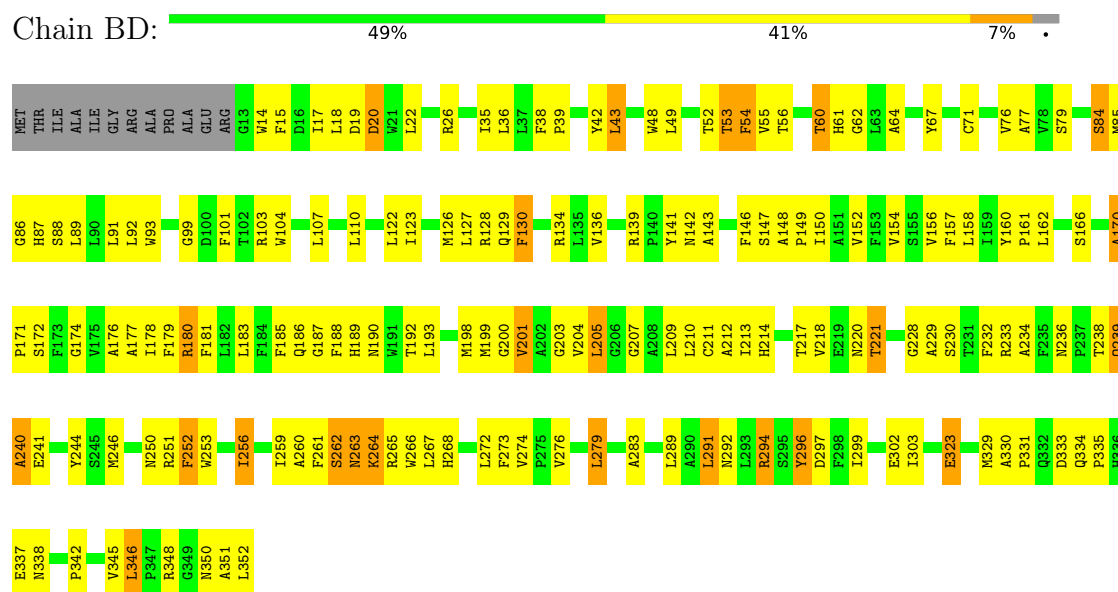
Frequency	Percentage
Daily	42%
Often	46%
Sometimes	7%
Never	5%



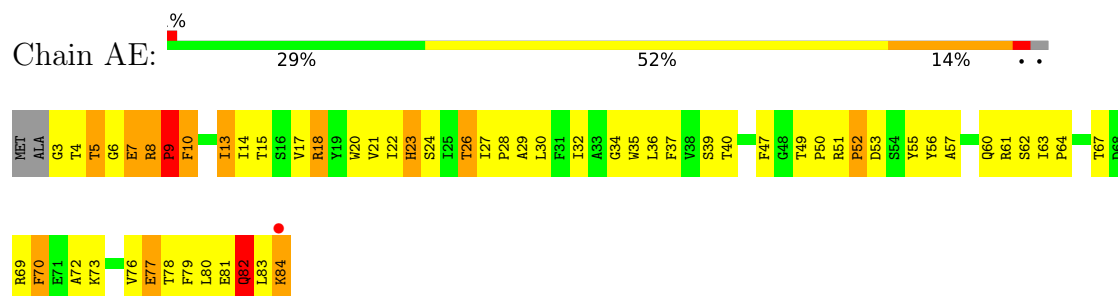
- Molecule 4: Photosystem II reaction center D2 protein



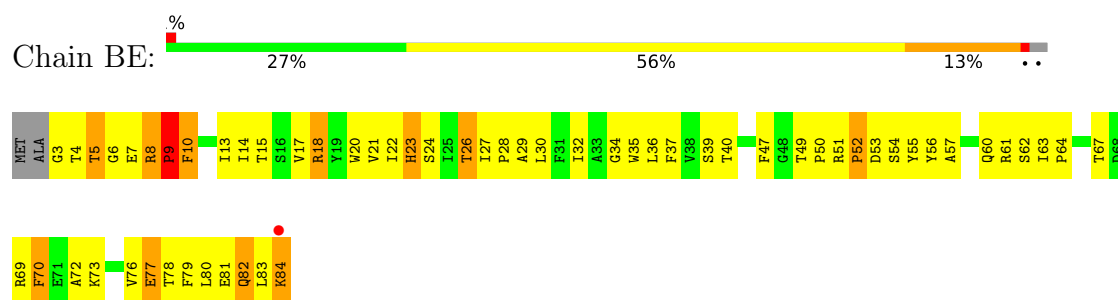
- Molecule 4: Photosystem II reaction center D2 protein



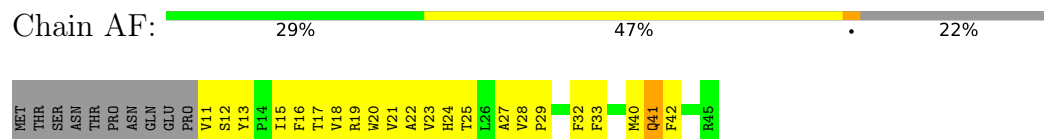
- Molecule 5: Cytochrome b559 subunit alpha



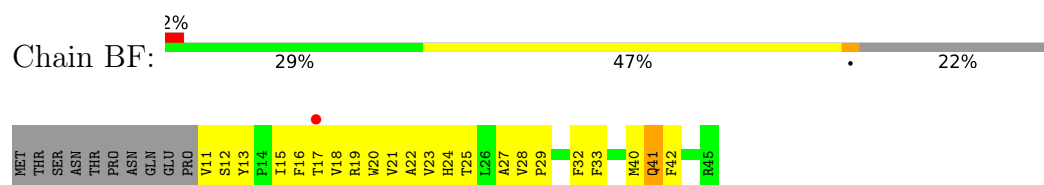
- Molecule 5: Cytochrome b559 subunit alpha



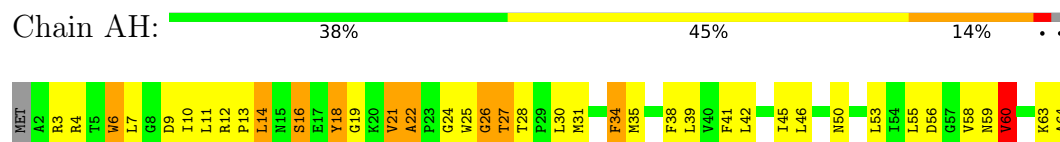
• Molecule 6: Cytochrome b559 subunit beta



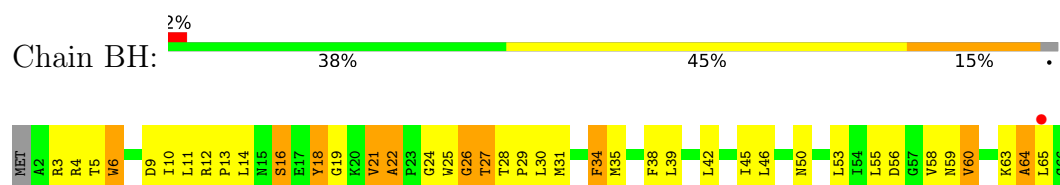
• Molecule 6: Cytochrome b559 subunit beta



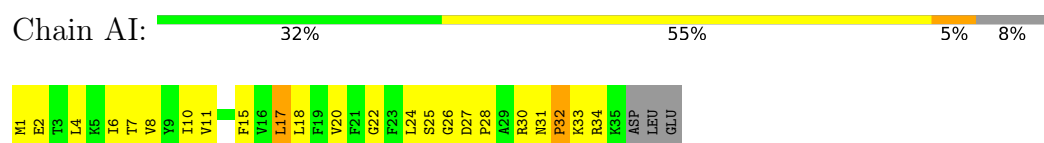
• Molecule 7: Photosystem II reaction center protein H



• Molecule 7: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein I



• Molecule 8: Photosystem II reaction center protein I

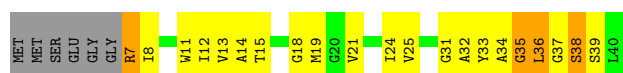




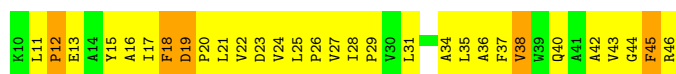
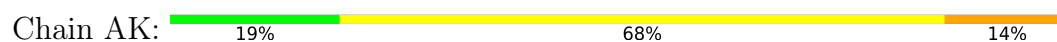
- Molecule 9: Photosystem II reaction center protein J



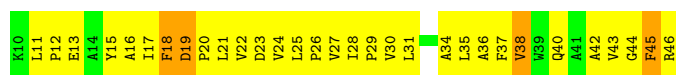
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

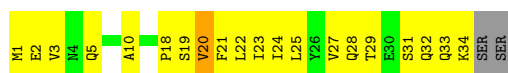


- Molecule 11: Photosystem II reaction center protein L



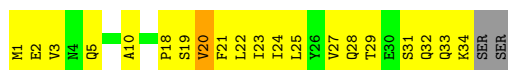
- Molecule 12: Photosystem II reaction center protein M





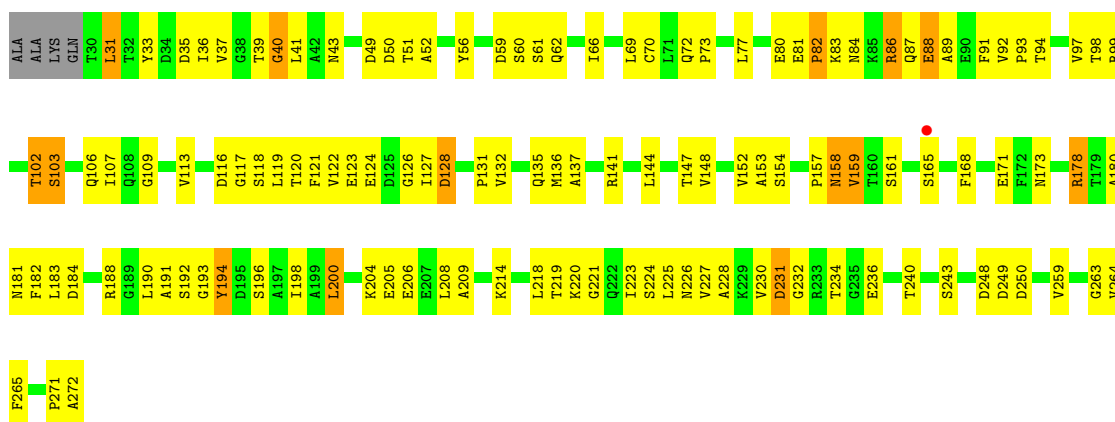
- Molecule 12: Photosystem II reaction center protein M

Chain BM: 39% 53% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO: 48% 45% 6%



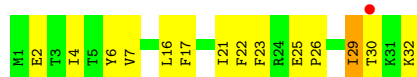
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain BO: 47% 45% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain AT: 3% 56% 41%



- Molecule 14: Photosystem II reaction center protein T

Chain BT: 56% 41% .



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain AU: 49% 37% 7% 7% .



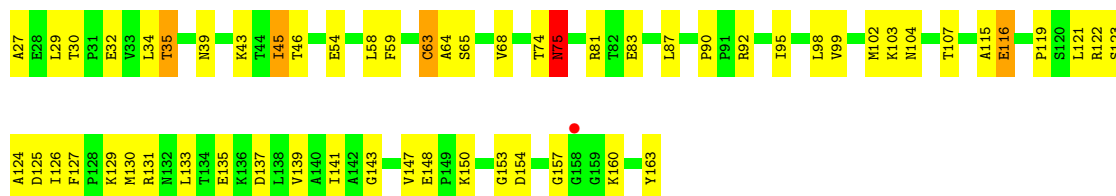
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain BU: 51% 36% 6% 7% .



- Molecule 16: Cytochrome c-550

Chain AV: 58% 39% . .



- Molecule 16: Cytochrome c-550

Chain BV: 57% 39% .





- Molecule 17: Protein ycf12



- Molecule 17: Protein ycf12



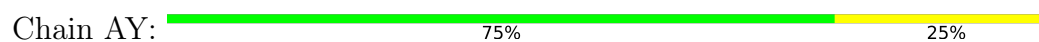
- Molecule 18: Photosystem II PsbX protein



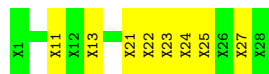
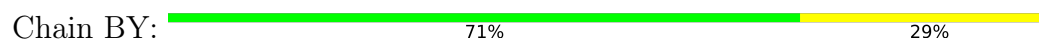
- Molecule 18: Photosystem II PsbX protein



- Molecule 19: Photosystem II protein Y



- Molecule 19: Photosystem II protein Y



- 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	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.90) 96.8 (10.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292 0.243 , 0.280	Depositor DCC
R_{free} test set	3869 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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: OEC, BCT, SQD, HEM, CL, LMG, CLA, LHG, LMT, FE2, CA, BCR, DGD, PL9, PHO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.55	0/2713	1.06	19/3700 (0.5%)
1	BA	0.53	0/2713	1.05	20/3700 (0.5%)
2	AB	0.55	0/3986	1.04	30/5433 (0.6%)
2	BB	0.54	0/3986	1.02	29/5433 (0.5%)
3	AC	0.50	0/3556	1.01	13/4842 (0.3%)
3	BC	0.47	0/3556	0.99	17/4842 (0.4%)
4	AD	0.58	0/2801	1.01	12/3818 (0.3%)
4	BD	0.52	0/2801	1.00	13/3818 (0.3%)
5	AE	0.52	0/685	1.20	11/933 (1.2%)
5	BE	0.49	0/685	1.18	9/933 (1.0%)
6	AF	0.53	0/291	0.85	0/397
6	BF	0.53	0/291	0.84	0/397
7	AH	0.50	0/520	1.01	3/709 (0.4%)
7	BH	0.49	0/520	0.99	3/709 (0.4%)
8	AI	0.54	0/293	1.08	2/395 (0.5%)
8	BI	0.53	0/293	1.05	2/395 (0.5%)
9	AJ	0.50	0/255	1.17	2/346 (0.6%)
9	BJ	0.53	0/255	1.12	2/346 (0.6%)
10	AK	0.52	0/303	0.96	1/416 (0.2%)
10	BK	0.51	0/303	0.93	1/416 (0.2%)
11	AL	0.52	0/311	1.02	1/422 (0.2%)
11	BL	0.52	0/311	1.00	0/422
12	AM	0.54	0/270	0.91	0/367
12	BM	0.56	0/270	0.88	0/367
13	AO	0.53	0/1876	1.03	11/2548 (0.4%)
13	BO	0.51	0/1876	1.02	12/2548 (0.5%)
14	AT	0.60	0/284	0.96	0/381
14	BT	0.59	0/284	1.00	1/381 (0.3%)
15	AU	0.55	0/785	1.11	6/1064 (0.6%)
15	BU	0.51	0/785	1.10	6/1064 (0.6%)
16	AV	0.50	0/1081	0.95	4/1468 (0.3%)
16	BV	0.46	0/1081	0.94	3/1468 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ay	0.66	0/202	1.23	1/272 (0.4%)
17	By	0.57	0/202	1.26	1/272 (0.4%)
18	AX	0.51	0/273	1.00	1/370 (0.3%)
18	BX	0.49	0/273	1.01	2/370 (0.5%)
20	AZ	0.48	0/490	1.12	4/669 (0.6%)
20	BZ	0.49	0/490	1.14	4/669 (0.6%)
All	All	0.52	0/41950	1.03	246/57100 (0.4%)

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

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

There are no bond length outliers.

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AZ	34	ASP	N-CA-C	-9.30	101.71	113.43
20	BZ	34	ASP	N-CA-C	-9.13	101.92	113.43
17	Ay	22	LEU	N-CA-C	-9.06	101.48	112.54
17	By	22	LEU	N-CA-C	-8.92	101.66	112.54
3	AC	182	PHE	N-CA-C	8.81	123.86	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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	195	0
1	BA	2628	0	2524	192	0
2	AB	3850	0	3718	235	0
2	BB	3850	0	3718	238	0
3	AC	3444	0	3365	277	0
3	BC	3444	0	3365	277	0
4	AD	2706	0	2608	184	0
4	BD	2706	0	2608	192	0
5	AE	666	0	651	69	0
5	BE	666	0	651	74	0
6	AF	282	0	291	30	0
6	BF	282	0	291	31	0
7	AH	507	0	521	57	0
7	BH	507	0	521	55	0
8	AI	286	0	308	22	0
8	BI	286	0	308	21	0
9	AJ	249	0	262	30	0
9	BJ	249	0	262	28	0
10	AK	293	0	305	50	0
10	BK	293	0	305	52	0
11	AL	304	0	316	19	0
11	BL	304	0	316	21	0
12	AM	267	0	289	28	0
12	BM	267	0	289	27	0
13	AO	1845	0	1801	125	0
13	BO	1845	0	1801	127	0
14	AT	275	0	288	22	0
14	BT	275	0	288	21	0
15	AU	774	0	773	48	0
15	BU	774	0	773	48	0
16	AV	1060	0	1068	45	0
16	BV	1060	0	1068	45	0
17	Ay	201	0	226	36	0
17	By	201	0	226	36	0
18	AX	270	0	299	29	0
18	BX	270	0	299	27	0
19	AY	140	0	32	4	0
19	BY	140	0	32	6	0
20	AZ	479	0	516	60	0
20	BZ	479	0	516	61	0
21	AA	1	0	0	0	0
21	BA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AA	260	0	288	19	0
22	AB	1040	0	1152	71	0
22	AC	845	0	936	50	0
22	AD	130	0	144	10	0
22	BA	260	0	288	20	0
22	BB	1040	0	1152	76	0
22	BC	845	0	936	50	0
22	BD	130	0	144	11	0
23	AA	64	0	74	5	0
23	AD	64	0	74	3	0
23	BA	64	0	74	5	0
23	BD	64	0	74	6	0
24	AA	45	0	61	5	0
24	AD	55	0	80	9	0
24	AJ	35	0	45	0	0
24	BA	45	0	61	6	0
24	BD	55	0	80	8	0
24	BJ	35	0	45	0	0
25	AA	5	0	0	0	0
25	BA	5	0	0	0	0
26	AA	40	0	56	6	0
26	AB	160	0	224	9	0
26	AC	80	0	112	13	0
26	AD	40	0	56	3	0
26	AH	40	0	56	2	0
26	AJ	40	0	56	5	0
26	AK	40	0	56	13	0
26	AT	40	0	56	7	0
26	AZ	40	0	56	4	0
26	BA	40	0	56	3	0
26	BB	120	0	168	5	0
26	BC	80	0	112	16	0
26	BD	40	0	56	3	0
26	BJ	40	0	56	5	0
26	BK	40	0	56	13	0
26	BX	40	0	56	4	0
26	BZ	40	0	56	4	0
27	AA	56	0	70	0	0
27	AB	52	0	62	3	0
27	AC	181	0	245	19	0
27	AD	63	0	87	0	0
27	AH	58	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BA	56	0	70	0	0
27	BB	52	0	62	3	0
27	BC	181	0	245	22	0
27	BD	63	0	87	0	0
27	BH	58	0	74	1	0
28	AA	39	0	51	3	0
28	AC	37	0	44	5	0
28	BA	39	0	51	4	0
28	BC	37	0	44	4	0
29	AA	105	0	145	10	0
29	AD	43	0	49	2	0
29	AF	45	0	53	2	0
29	BA	105	0	145	6	0
29	BB	47	0	60	2	0
29	BD	43	0	49	2	0
29	BF	45	0	53	1	0
29	BL	47	0	60	2	0
30	AA	93	0	126	5	0
30	AB	140	0	190	4	0
30	AC	93	0	126	6	0
30	AD	94	0	128	9	0
30	AE	44	0	58	4	0
30	AI	43	0	56	3	0
30	AM	42	0	54	4	0
30	BA	51	0	72	2	0
30	BB	98	0	136	2	0
30	BC	93	0	126	8	0
30	BD	94	0	128	10	0
30	BE	44	0	58	4	0
30	BI	43	0	56	3	0
30	BM	42	0	54	4	0
31	AA	1	0	0	0	0
31	BA	1	0	0	0	0
32	AB	105	0	138	7	0
32	AD	31	0	35	1	0
32	AI	35	0	46	4	0
32	AM	35	0	46	1	0
32	AT	35	0	46	3	0
32	BB	105	0	138	6	0
32	BD	31	0	35	0	0
32	BI	35	0	46	3	0
32	BM	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BT	35	0	46	3	0
33	AD	4	0	0	1	0
33	BD	4	0	0	1	0
34	AE	43	0	30	5	0
34	AV	43	0	30	3	0
34	BE	43	0	30	6	0
34	BV	43	0	30	3	0
35	AK	1	0	0	0	0
35	AO	1	0	0	0	0
35	BK	1	0	0	0	0
35	BO	1	0	0	0	0
All	All	50234	0	51364	2938	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 29.

The worst 5 of 2938 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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%)	285 (86%)	41 (12%)	7 (2%)	5 21

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Ay	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
17	By	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
18	AX	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	0	1
18	BX	35/50 (70%)	27 (77%)	4 (11%)	4 (11%)	0	1
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	6
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	6
All	All	5138/5480 (94%)	4278 (83%)	679 (13%)	181 (4%)	3	12

5 of 181 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	256 (94%)	15 (6%)	19	50
1	BA	271/280 (97%)	257 (95%)	14 (5%)	21	52
2	AB	390/407 (96%)	373 (96%)	17 (4%)	25	59
2	BB	390/407 (96%)	372 (95%)	18 (5%)	24	57
3	AC	347/374 (93%)	334 (96%)	13 (4%)	30	64
3	BC	347/374 (93%)	332 (96%)	15 (4%)	26	60
4	AD	275/283 (97%)	257 (94%)	18 (6%)	15	44
4	BD	275/283 (97%)	256 (93%)	19 (7%)	14	41
5	AE	72/73 (99%)	65 (90%)	7 (10%)	8	25
5	BE	72/73 (99%)	65 (90%)	7 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	29/39 (74%)	29 (100%)	0	100	100
6	BF	29/39 (74%)	29 (100%)	0	100	100
7	AH	53/55 (96%)	50 (94%)	3 (6%)	18	49
7	BH	53/55 (96%)	50 (94%)	3 (6%)	18	49
8	AI	32/35 (91%)	30 (94%)	2 (6%)	16	45
8	BI	32/35 (91%)	30 (94%)	2 (6%)	16	45
9	AJ	24/28 (86%)	23 (96%)	1 (4%)	26	60
9	BJ	24/28 (86%)	23 (96%)	1 (4%)	26	60
10	AK	30/30 (100%)	27 (90%)	3 (10%)	7	24
10	BK	30/30 (100%)	28 (93%)	2 (7%)	15	43
11	AL	35/35 (100%)	32 (91%)	3 (9%)	10	30
11	BL	35/35 (100%)	32 (91%)	3 (9%)	10	30
12	AM	31/33 (94%)	30 (97%)	1 (3%)	34	68
12	BM	31/33 (94%)	29 (94%)	2 (6%)	15	44
13	AO	202/208 (97%)	196 (97%)	6 (3%)	36	70
13	BO	202/208 (97%)	196 (97%)	6 (3%)	36	70
14	AT	29/29 (100%)	28 (97%)	1 (3%)	32	66
14	BT	29/29 (100%)	28 (97%)	1 (3%)	32	66
15	AU	84/89 (94%)	80 (95%)	4 (5%)	23	55
15	BU	84/89 (94%)	80 (95%)	4 (5%)	23	55
16	AV	116/117 (99%)	112 (97%)	4 (3%)	32	66
16	BV	116/117 (99%)	112 (97%)	4 (3%)	32	66
17	Ay	20/37 (54%)	17 (85%)	3 (15%)	3	10
17	By	20/37 (54%)	17 (85%)	3 (15%)	3	10
18	AX	30/42 (71%)	24 (80%)	6 (20%)	1	4
18	BX	30/42 (71%)	24 (80%)	6 (20%)	1	4
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	8	26
20	BZ	52/52 (100%)	47 (90%)	5 (10%)	8	26
All	All	4244/4492 (94%)	4017 (95%)	227 (5%)	20	52

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	202	VAL
18	BX	47	GLN
2	BB	490	GLN
18	BX	42	GLN
13	BO	86	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
4	BD	117	HIS
13	BO	202	GLN
4	BD	239	GLN
12	BM	33	GLN
15	BU	93	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	AB	622	-	49,49,55	1.08	6 (12%)	57,57,63	1.02	3 (5%)
22	CLA	BA	407	1	69,73,73	1.23	6 (8%)	82,113,113	1.66	9 (10%)
26	BCR	AD	406	-	41,41,41	1.88	7 (17%)	56,56,56	2.35	22 (39%)
22	CLA	AB	614	2	69,73,73	1.42	9 (13%)	82,113,113	1.83	13 (15%)
22	CLA	AC	511	3	69,73,73	1.48	6 (8%)	82,113,113	1.84	10 (12%)
32	LMT	AT	101	-	36,36,36	1.36	5 (13%)	47,47,47	1.08	4 (8%)
22	CLA	BB	619	-	69,73,73	1.32	7 (10%)	82,113,113	1.83	11 (13%)
22	CLA	BC	510	-	69,73,73	1.20	8 (11%)	82,113,113	1.70	11 (13%)
27	DGD	AB	626	-	53,53,67	1.87	17 (32%)	67,67,81	1.58	9 (13%)
24	PL9	BD	405	-	55,55,55	0.55	0	68,69,69	1.73	18 (26%)
26	BCR	AH	101	-	41,41,41	1.89	7 (17%)	56,56,56	2.30	22 (39%)
22	CLA	BA	404	-	69,73,73	1.28	6 (8%)	82,113,113	1.85	15 (18%)
22	CLA	BD	404	-	69,73,73	1.41	11 (15%)	82,113,113	1.73	11 (13%)
26	BCR	AB	617	-	41,41,41	1.72	8 (19%)	56,56,56	2.04	15 (26%)
29	SQD	BB	601	-	45,47,54	2.69	23 (51%)	55,58,65	2.58	16 (29%)
26	BCR	AC	515	-	41,41,41	1.72	6 (14%)	56,56,56	2.22	19 (33%)
27	DGD	AD	410	-	64,64,67	1.84	16 (25%)	78,78,81	1.38	7 (8%)
30	LMG	BB	624	-	49,49,55	1.06	5 (10%)	57,57,63	1.01	3 (5%)
22	CLA	BC	511	3	69,73,73	1.50	8 (11%)	82,113,113	1.85	10 (12%)
22	CLA	AB	616	-	69,73,73	1.32	8 (11%)	82,113,113	1.77	11 (13%)
22	CLA	BC	502	3	69,73,73	1.31	6 (8%)	82,113,113	1.78	10 (12%)
22	CLA	AC	506	3	69,73,73	1.32	6 (8%)	82,113,113	1.78	10 (12%)
27	DGD	BD	410	-	64,64,67	1.78	17 (26%)	78,78,81	1.38	7 (8%)
24	PL9	AA	407	-	45,45,55	0.94	2 (4%)	56,57,69	1.70	15 (26%)
22	CLA	BC	501	3	69,73,73	1.35	4 (5%)	82,113,113	1.78	12 (14%)
34	HEM	BV	201	16	50,50,50	1.98	16 (32%)	67,82,82	1.94	13 (19%)
27	DGD	AC	516	-	54,54,67	1.24	8 (14%)	68,68,81	1.51	7 (10%)
26	BCR	BX	101	-	41,41,41	1.88	7 (17%)	56,56,56	2.31	23 (41%)
29	SQD	BL	101	-	45,47,54	2.73	23 (51%)	55,58,65	2.58	15 (27%)
30	LMG	AB	621	-	49,49,55	1.04	5 (10%)	57,57,63	1.02	4 (7%)
22	CLA	BC	508	3	69,73,73	1.38	8 (11%)	82,113,113	1.80	11 (13%)
22	CLA	AC	507	-	69,73,73	1.26	5 (7%)	82,113,113	1.81	12 (14%)
22	CLA	BB	608	2	69,73,73	1.25	5 (7%)	82,113,113	1.70	10 (12%)
22	CLA	BB	615	-	69,73,73	1.35	9 (13%)	82,113,113	1.73	11 (13%)
29	SQD	AD	409	-	41,43,54	2.78	19 (46%)	51,54,65	2.82	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	AA	405	-	58,69,69	1.71	8 (13%)	55,99,99	1.97	16 (29%)
22	CLA	BB	612	2	69,73,73	1.40	5 (7%)	82,113,113	1.72	12 (14%)
33	BCT	BD	401	21	3,3,3	0.53	0	2,3,3	0.36	0
26	BCR	BB	620	-	41,41,41	1.59	8 (19%)	56,56,56	2.04	15 (26%)
30	LMG	AI	101	-	43,43,55	1.50	8 (18%)	51,51,63	1.05	3 (5%)
22	CLA	BD	402	4	69,73,73	1.48	8 (11%)	82,113,113	1.81	10 (12%)
22	CLA	AC	512	-	69,73,73	1.43	10 (14%)	82,113,113	1.82	11 (13%)
32	LMT	AD	411	-	32,32,36	1.53	5 (15%)	43,43,47	1.01	2 (4%)
28	LHG	BC	521	-	36,36,48	1.08	2 (5%)	39,42,54	1.14	3 (7%)
27	DGD	AC	518	-	67,67,67	1.05	6 (8%)	81,81,81	1.27	4 (4%)
27	DGD	AC	517	-	63,63,67	1.07	5 (7%)	77,77,81	1.55	10 (12%)
28	LHG	AA	411	-	38,38,48	2.04	5 (13%)	41,44,54	1.40	4 (9%)
32	LMT	BB	626	-	36,36,36	1.37	5 (13%)	47,47,47	0.95	2 (4%)
34	HEM	AE	101	6,5	50,50,50	2.05	17 (34%)	67,82,82	2.08	12 (17%)
22	CLA	AC	508	3	69,73,73	1.39	7 (10%)	82,113,113	1.86	10 (12%)
22	CLA	AA	402	1	69,73,73	1.32	8 (11%)	82,113,113	1.72	9 (10%)
26	BCR	BB	621	-	41,41,41	1.89	6 (14%)	56,56,56	2.17	18 (32%)
22	CLA	AC	501	3	69,73,73	1.33	4 (5%)	82,113,113	1.76	11 (13%)
22	CLA	BB	614	2	69,73,73	1.15	5 (7%)	82,113,113	1.63	10 (12%)
22	CLA	BC	503	3	69,73,73	1.46	7 (10%)	82,113,113	1.81	10 (12%)
23	PHO	BA	406	-	58,69,69	1.59	7 (12%)	55,99,99	2.00	17 (30%)
32	LMT	BD	411	-	32,32,36	1.42	4 (12%)	43,43,47	0.96	2 (4%)
34	HEM	AV	201	16	50,50,50	1.99	16 (32%)	67,82,82	1.93	11 (16%)
22	CLA	BB	605	2	69,73,73	1.25	6 (8%)	82,113,113	1.62	12 (14%)
30	LMG	AB	623	-	42,42,55	1.49	8 (19%)	50,50,63	0.99	3 (6%)
30	LMG	BC	520	-	45,45,55	1.55	10 (22%)	53,53,63	1.03	4 (7%)
22	CLA	BC	512	-	69,73,73	1.43	10 (14%)	82,113,113	1.83	11 (13%)
30	LMG	AA	413	-	51,51,55	0.91	3 (5%)	59,59,63	0.99	4 (6%)
22	CLA	AB	607	-	69,73,73	1.37	11 (15%)	82,113,113	1.76	9 (10%)
26	BCR	AK	102	-	41,41,41	1.87	6 (14%)	56,56,56	2.58	26 (46%)
30	LMG	BC	519	-	48,48,55	1.28	6 (12%)	56,56,63	0.84	2 (3%)
22	CLA	AD	404	-	69,73,73	1.41	8 (11%)	82,113,113	1.76	11 (13%)
32	LMT	AM	102	-	36,36,36	1.21	2 (5%)	47,47,47	0.96	2 (4%)
24	PL9	BJ	101	-	35,35,55	1.44	5 (14%)	44,45,69	1.70	13 (29%)
22	CLA	AB	601	-	69,73,73	1.43	8 (11%)	82,113,113	1.81	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	AM	101	-	42,42,55	1.63	6 (14%)	50,50,63	1.16	5 (10%)
32	LMT	AB	625	-	36,36,36	1.39	7 (19%)	47,47,47	0.97	2 (4%)
27	DGD	AA	410	-	57,57,67	1.50	12 (21%)	71,71,81	1.42	8 (11%)
26	BCR	AB	619	-	41,41,41	1.96	7 (17%)	56,56,56	2.13	17 (30%)
26	BCR	BZ	101	-	41,41,41	2.03	9 (21%)	56,56,56	2.13	20 (35%)
26	BCR	BK	102	-	41,41,41	1.88	7 (17%)	56,56,56	2.58	27 (48%)
27	DGD	BA	411	-	57,57,67	1.63	13 (22%)	71,71,81	1.41	8 (11%)
29	SQD	AF	101	-	43,45,54	2.56	21 (48%)	53,56,65	2.74	20 (37%)
30	LMG	BM	102	-	42,42,55	1.66	8 (19%)	50,50,63	1.11	4 (8%)
23	PHO	AD	403	-	58,69,69	1.68	6 (10%)	55,99,99	1.99	14 (25%)
22	CLA	AB	603	2	69,73,73	1.35	8 (11%)	82,113,113	1.72	11 (13%)
22	CLA	BA	403	1	69,73,73	1.37	8 (11%)	82,113,113	1.70	9 (10%)
22	CLA	AB	608	2	69,73,73	1.32	7 (10%)	82,113,113	1.70	11 (13%)
22	CLA	AA	404	-	69,73,73	1.23	5 (7%)	82,113,113	1.70	10 (12%)
34	HEM	BE	101	6,5	50,50,50	2.10	17 (34%)	67,82,82	2.10	12 (17%)
26	BCR	BJ	102	-	41,41,41	2.18	8 (19%)	56,56,56	3.47	23 (41%)
29	SQD	AA	412	-	49,51,54	2.53	25 (51%)	59,62,65	2.66	19 (32%)
22	CLA	AB	610	-	69,73,73	1.28	9 (13%)	82,113,113	1.77	12 (14%)
26	BCR	AB	620	-	41,41,41	1.88	7 (17%)	56,56,56	2.10	19 (33%)
30	LMG	AE	102	-	44,44,55	1.34	6 (13%)	52,52,63	1.08	6 (11%)
23	PHO	BD	403	-	58,69,69	1.67	6 (10%)	55,99,99	2.01	15 (27%)
22	CLA	AC	513	3	69,73,73	1.53	8 (11%)	82,113,113	1.77	10 (12%)
22	CLA	BB	617	2	69,73,73	1.39	8 (11%)	82,113,113	1.80	12 (14%)
24	PL9	AJ	101	-	35,35,55	1.40	4 (11%)	44,45,69	1.75	12 (27%)
33	BCT	AD	401	21	3,3,3	0.53	0	2,3,3	0.37	0
28	LHG	BA	412	-	38,38,48	1.99	6 (15%)	41,44,54	1.39	4 (9%)
30	LMG	AC	520	-	45,45,55	1.53	9 (20%)	53,53,63	1.01	3 (5%)
22	CLA	AC	505	3	69,73,73	1.49	10 (14%)	82,113,113	1.78	9 (10%)
27	DGD	BC	517	-	63,63,67	1.11	6 (9%)	77,77,81	1.56	8 (10%)
24	PL9	BA	408	-	45,45,55	0.97	2 (4%)	56,57,69	1.64	14 (25%)
26	BCR	AJ	102	-	41,41,41	2.07	9 (21%)	56,56,56	3.47	22 (39%)
22	CLA	AC	504	-	69,73,73	1.26	9 (13%)	82,113,113	1.67	11 (13%)
32	LMT	BT	101	-	36,36,36	1.31	5 (13%)	47,47,47	1.05	4 (8%)
26	BCR	AA	409	-	41,41,41	1.69	7 (17%)	56,56,56	2.13	21 (37%)
22	CLA	AB	615	-	69,73,73	1.28	9 (13%)	82,113,113	1.82	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	BC	506	3	69,73,73	1.27	6 (8%)	82,113,113	1.75	9 (10%)
26	BCR	BB	622	-	41,41,41	1.86	7 (17%)	56,56,56	2.09	17 (30%)
32	LMT	BB	625	-	36,36,36	1.55	9 (25%)	47,47,47	1.24	3 (6%)
24	PL9	AD	405	-	55,55,55	0.57	0	68,69,69	1.72	18 (26%)
29	SQD	BA	401	-	52,54,54	2.69	31 (59%)	62,65,65	2.62	22 (35%)
22	CLA	AB	613	-	69,73,73	1.23	5 (7%)	82,113,113	1.72	10 (12%)
22	CLA	BC	513	3	69,73,73	1.47	8 (11%)	82,113,113	1.78	9 (10%)
22	CLA	AA	406	1	69,73,73	1.25	5 (7%)	82,113,113	1.66	10 (12%)
26	BCR	AC	514	-	41,41,41	1.82	8 (19%)	56,56,56	2.17	22 (39%)
22	CLA	AB	602	2	69,73,73	1.27	8 (11%)	82,113,113	1.62	11 (13%)
22	CLA	AB	609	2	69,73,73	1.38	6 (8%)	82,113,113	1.69	11 (13%)
22	CLA	AB	612	-	69,73,73	1.26	6 (8%)	82,113,113	1.71	10 (12%)
30	LMG	BA	414	-	51,51,55	0.93	4 (7%)	59,59,63	1.01	4 (6%)
22	CLA	BB	616	-	69,73,73	1.18	8 (11%)	82,113,113	1.69	9 (10%)
22	CLA	BB	618	-	69,73,73	1.22	8 (11%)	82,113,113	1.80	11 (13%)
28	LHG	AC	521	-	36,36,48	1.09	2 (5%)	39,42,54	1.14	3 (7%)
30	LMG	AD	408	-	48,48,55	1.07	3 (6%)	56,56,63	1.00	2 (3%)
32	LMT	AI	102	-	36,36,36	1.44	4 (11%)	47,47,47	0.95	2 (4%)
26	BCR	AB	618	-	41,41,41	1.74	6 (14%)	56,56,56	2.25	26 (46%)
30	LMG	AA	416	-	42,42,55	1.51	7 (16%)	50,50,63	0.97	3 (6%)
22	CLA	BC	507	-	69,73,73	1.28	6 (8%)	82,113,113	1.81	12 (14%)
22	CLA	AD	402	4	69,73,73	1.49	10 (14%)	82,113,113	1.81	8 (9%)
27	DGD	BH	101	-	59,59,67	1.22	9 (15%)	73,73,81	1.43	6 (8%)
22	CLA	BB	613	-	69,73,73	1.31	7 (10%)	82,113,113	1.77	12 (14%)
30	LMG	BB	623	-	49,49,55	1.09	5 (10%)	57,57,63	1.04	4 (7%)
22	CLA	AB	606	2	69,73,73	1.34	4 (5%)	82,113,113	1.71	9 (10%)
26	BCR	AZ	101	-	41,41,41	1.91	7 (17%)	56,56,56	2.14	19 (33%)
22	CLA	BB	609	2	69,73,73	1.42	6 (8%)	82,113,113	1.74	9 (10%)
26	BCR	BD	406	-	41,41,41	1.97	8 (19%)	56,56,56	2.34	22 (39%)
22	CLA	BC	505	3	69,73,73	1.57	9 (13%)	82,113,113	1.83	10 (12%)
32	LMT	BM	101	-	36,36,36	1.21	3 (8%)	47,47,47	0.97	2 (4%)
22	CLA	AC	509	-	69,73,73	1.35	9 (13%)	82,113,113	1.74	11 (13%)
26	BCR	AT	102	-	41,41,41	1.66	6 (14%)	56,56,56	2.25	26 (46%)
32	LMT	AB	627	-	36,36,36	1.46	6 (16%)	47,47,47	1.04	3 (6%)
29	SQD	BD	409	-	41,43,54	2.76	20 (48%)	51,54,65	2.81	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	BB	611	2	69,73,73	1.34	8 (11%)	82,113,113	1.68	13 (15%)
32	LMT	AB	624	-	36,36,36	1.45	7 (19%)	47,47,47	1.21	3 (6%)
32	LMT	BI	102	-	36,36,36	1.54	4 (11%)	47,47,47	0.97	2 (4%)
27	DGD	BC	516	-	54,54,67	1.36	9 (16%)	68,68,81	1.49	7 (10%)
29	SQD	BF	101	-	43,45,54	2.64	20 (46%)	53,56,65	2.72	19 (35%)
22	CLA	AC	510	-	69,73,73	1.22	10 (14%)	82,113,113	1.66	11 (13%)
22	CLA	BC	504	-	69,73,73	1.29	8 (11%)	82,113,113	1.68	8 (9%)
22	CLA	AC	502	3	69,73,73	1.32	8 (11%)	82,113,113	1.73	9 (10%)
29	SQD	AA	415	-	52,54,54	2.65	30 (57%)	62,65,65	2.60	21 (33%)
30	LMG	BD	408	-	48,48,55	1.16	4 (8%)	56,56,63	1.00	2 (3%)
22	CLA	AA	403	-	69,73,73	1.28	8 (11%)	82,113,113	1.78	14 (17%)
22	CLA	AC	503	3	69,73,73	1.50	8 (11%)	82,113,113	1.85	9 (10%)
27	DGD	AH	102	-	59,59,67	1.27	9 (15%)	73,73,81	1.44	7 (9%)
27	DGD	BB	602	-	53,53,67	1.87	17 (32%)	67,67,81	1.56	8 (11%)
30	LMG	BI	101	-	43,43,55	1.56	8 (18%)	51,51,63	1.07	4 (7%)
22	CLA	AB	604	2	69,73,73	1.45	10 (14%)	82,113,113	1.84	9 (10%)
26	BCR	BA	410	-	41,41,41	1.76	7 (17%)	56,56,56	2.12	24 (42%)
26	BCR	BC	514	-	41,41,41	1.97	8 (19%)	56,56,56	2.16	23 (41%)
22	CLA	BA	405	-	69,73,73	1.25	6 (8%)	82,113,113	1.74	11 (13%)
29	SQD	BA	413	-	49,51,54	2.56	25 (51%)	59,62,65	2.62	19 (32%)
30	LMG	AC	519	-	48,48,55	1.26	5 (10%)	56,56,63	0.84	2 (3%)
22	CLA	AB	611	2	69,73,73	1.21	7 (10%)	82,113,113	1.69	9 (10%)
30	LMG	BD	407	-	46,46,55	1.04	4 (8%)	54,54,63	0.91	2 (3%)
30	LMG	AD	407	-	46,46,55	0.97	4 (8%)	54,54,63	0.90	2 (3%)
27	DGD	BC	518	-	67,67,67	1.18	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	BE	102	-	44,44,55	1.35	6 (13%)	52,52,63	1.08	5 (9%)
22	CLA	AB	605	-	69,73,73	1.32	6 (8%)	82,113,113	1.71	11 (13%)
22	CLA	BB	610	-	69,73,73	1.40	9 (13%)	82,113,113	1.78	10 (12%)
22	CLA	BB	604	-	69,73,73	1.50	11 (15%)	82,113,113	1.83	10 (12%)
26	BCR	BC	515	-	41,41,41	1.87	7 (17%)	56,56,56	2.20	20 (35%)
22	CLA	BC	509	-	69,73,73	1.37	8 (11%)	82,113,113	1.78	11 (13%)
22	CLA	BB	607	2	69,73,73	1.47	9 (13%)	82,113,113	1.81	9 (10%)
22	CLA	BB	606	2	69,73,73	1.28	6 (8%)	82,113,113	1.70	11 (13%)
32	LMT	BB	603	-	36,36,36	1.43	8 (22%)	47,47,47	1.06	3 (6%)

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
30	LMG	AB	622	-	2/2/8/8	19/44/64/70	0/1/1/1
22	CLA	BA	407	1	1/1/15/20	11/39/115/115	-
26	BCR	AD	406	-	-	3/29/63/63	0/2/2/2
22	CLA	AB	614	2	1/1/15/20	18/39/115/115	-
22	CLA	AC	511	3	1/1/15/20	14/39/115/115	-
32	LMT	AT	101	-	-	4/21/61/61	0/2/2/2
22	CLA	BB	619	-	1/1/15/20	16/39/115/115	-
22	CLA	BC	510	-	1/1/15/20	13/39/115/115	-
27	DGD	AB	626	-	3/3/13/13	25/41/81/95	0/2/2/2
24	PL9	BD	405	-	-	16/53/73/73	0/1/1/1
26	BCR	AH	101	-	-	2/29/63/63	0/2/2/2
22	CLA	BA	404	-	1/1/15/20	15/39/115/115	-
22	CLA	BD	404	-	1/1/15/20	9/39/115/115	-
26	BCR	AB	617	-	-	1/29/63/63	0/2/2/2
30	LMG	BB	624	-	2/2/8/8	17/44/64/70	0/1/1/1
27	DGD	AD	410	-	3/3/13/13	34/52/92/95	0/2/2/2
26	BCR	AC	515	-	-	4/29/63/63	0/2/2/2
29	SQD	BB	601	-	-	18/42/62/69	0/1/1/1
22	CLA	BC	511	3	1/1/15/20	14/39/115/115	-
22	CLA	AB	616	-	1/1/15/20	17/39/115/115	-
22	CLA	BC	502	3	1/1/15/20	11/39/115/115	-
22	CLA	AC	506	3	1/1/15/20	17/39/115/115	-
27	DGD	BD	410	-	3/3/13/13	34/52/92/95	0/2/2/2
24	PL9	AA	407	-	-	16/41/61/73	0/1/1/1
22	CLA	BC	501	3	1/1/15/20	11/39/115/115	-
34	HEM	BV	201	16	-	8/14/54/54	-
27	DGD	AC	516	-	3/3/13/13	17/42/82/95	0/2/2/2
26	BCR	BX	101	-	-	2/29/63/63	0/2/2/2
29	SQD	BL	101	-	-	18/42/62/69	0/1/1/1
30	LMG	AB	621	-	2/2/8/8	22/44/64/70	0/1/1/1
22	CLA	BC	508	3	1/1/15/20	14/39/115/115	-
22	CLA	AC	507	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BB	608	2	1/1/15/20	18/39/115/115	-
22	CLA	BB	615	-	1/1/15/20	13/39/115/115	-
29	SQD	AD	409	-	-	11/38/58/69	0/1/1/1
23	PHO	AA	405	-	-	12/37/103/103	0/5/6/6
22	CLA	BB	612	2	1/1/15/20	10/39/115/115	-
30	LMG	AI	101	-	2/2/8/8	18/38/58/70	0/1/1/1
26	BCR	BB	620	-	-	1/29/63/63	0/2/2/2
22	CLA	BD	402	4	1/1/15/20	13/39/115/115	-
22	CLA	AC	512	-	1/1/15/20	23/39/115/115	-
32	LMT	AD	411	-	-	0/17/57/61	0/2/2/2
28	LHG	BC	521	-	-	15/41/41/53	-
27	DGD	AC	518	-	3/3/13/13	20/55/95/95	0/2/2/2
27	DGD	AC	517	-	3/3/13/13	29/51/91/95	0/2/2/2
28	LHG	AA	411	-	-	14/43/43/53	-
32	LMT	BB	626	-	-	2/21/61/61	0/2/2/2
34	HEM	AE	101	6,5	-	4/14/54/54	-
22	CLA	AC	508	3	1/1/15/20	14/39/115/115	-
22	CLA	AA	402	1	1/1/15/20	5/39/115/115	-
26	BCR	BB	621	-	-	0/29/63/63	0/2/2/2
22	CLA	AC	501	3	1/1/15/20	11/39/115/115	-
22	CLA	BB	614	2	1/1/15/20	16/39/115/115	-
22	CLA	BC	503	3	1/1/15/20	15/39/115/115	-
23	PHO	BA	406	-	-	12/37/103/103	0/5/6/6
32	LMT	BD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	AV	201	16	-	7/14/54/54	-
22	CLA	BB	605	2	1/1/15/20	21/39/115/115	-
30	LMG	AB	623	-	2/2/8/8	17/37/57/70	0/1/1/1
30	LMG	BC	520	-	2/2/8/8	18/40/60/70	0/1/1/1
22	CLA	BC	512	-	1/1/15/20	23/39/115/115	-
30	LMG	AA	413	-	2/2/8/8	29/46/66/70	0/1/1/1
22	CLA	AB	607	-	1/1/15/20	13/39/115/115	-
26	BCR	AK	102	-	-	4/29/63/63	0/2/2/2
30	LMG	BC	519	-	2/2/8/8	24/43/63/70	0/1/1/1
22	CLA	AD	404	-	1/1/15/20	11/39/115/115	-
32	LMT	AM	102	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PL9	BJ	101	-	-	10/29/49/73	0/1/1/1
22	CLA	AB	601	-	1/1/15/20	20/39/115/115	-
30	LMG	AM	101	-	2/2/8/8	16/37/57/70	0/1/1/1
32	LMT	AB	625	-	-	2/21/61/61	0/2/2/2
27	DGD	AA	410	-	3/3/13/13	18/45/85/95	0/2/2/2
27	DGD	BA	411	-	3/3/13/13	18/45/85/95	0/2/2/2
26	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
26	BCR	BK	102	-	-	4/29/63/63	0/2/2/2
26	BCR	BZ	101	-	-	3/29/63/63	0/2/2/2
29	SQD	AF	101	-	-	14/40/60/69	0/1/1/1
30	LMG	BM	102	-	2/2/8/8	16/37/57/70	0/1/1/1
22	CLA	AB	603	2	1/1/15/20	11/39/115/115	-
22	CLA	BA	403	1	1/1/15/20	5/39/115/115	-
23	PHO	AD	403	-	-	12/37/103/103	0/5/6/6
22	CLA	AB	608	2	1/1/15/20	19/39/115/115	-
22	CLA	AA	404	-	1/1/15/20	13/39/115/115	-
34	HEM	BE	101	6,5	-	4/14/54/54	-
26	BCR	BJ	102	-	-	5/29/63/63	0/2/2/2
29	SQD	AA	412	-	-	17/46/66/69	0/1/1/1
22	CLA	AB	610	-	1/1/15/20	17/39/115/115	-
26	BCR	AB	620	-	-	2/29/63/63	0/2/2/2
30	LMG	AE	102	-	2/2/8/8	19/39/59/70	0/1/1/1
23	PHO	BD	403	-	-	12/37/103/103	0/5/6/6
22	CLA	AC	513	3	1/1/15/20	18/39/115/115	-
22	CLA	BB	617	2	1/1/15/20	17/39/115/115	-
24	PL9	AJ	101	-	-	10/29/49/73	0/1/1/1
28	LHG	BA	412	-	-	14/43/43/53	-
30	LMG	AC	520	-	2/2/8/8	18/40/60/70	0/1/1/1
22	CLA	AC	505	3	1/1/15/20	20/39/115/115	-
27	DGD	BC	517	-	3/3/13/13	30/51/91/95	0/2/2/2
24	PL9	BA	408	-	-	16/41/61/73	0/1/1/1
26	BCR	AJ	102	-	-	3/29/63/63	0/2/2/2
22	CLA	AC	504	-	1/1/15/20	10/39/115/115	-
32	LMT	BT	101	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	AA	409	-	-	5/29/63/63	0/2/2/2
22	CLA	AB	615	-	1/1/15/20	10/39/115/115	-
22	CLA	BC	506	3	1/1/15/20	17/39/115/115	-
26	BCR	BB	622	-	-	2/29/63/63	0/2/2/2
32	LMT	BB	625	-	-	4/21/61/61	0/2/2/2
24	PL9	AD	405	-	-	16/53/73/73	0/1/1/1
29	SQD	BA	401	-	-	21/49/69/69	0/1/1/1
22	CLA	AB	613	-	1/1/15/20	16/39/115/115	-
22	CLA	BC	513	3	1/1/15/20	18/39/115/115	-
22	CLA	AA	406	1	1/1/15/20	12/39/115/115	-
26	BCR	AC	514	-	-	5/29/63/63	0/2/2/2
22	CLA	AB	602	2	1/1/15/20	21/39/115/115	-
22	CLA	AB	609	2	1/1/15/20	9/39/115/115	-
22	CLA	AB	612	-	1/1/15/20	12/39/115/115	-
30	LMG	BA	414	-	2/2/8/8	27/46/66/70	0/1/1/1
22	CLA	BB	616	-	1/1/15/20	15/39/115/115	-
22	CLA	BB	618	-	1/1/15/20	10/39/115/115	-
30	LMG	AD	408	-	2/2/8/8	25/43/63/70	0/1/1/1
28	LHG	AC	521	-	-	16/41/41/53	-
32	LMT	AI	102	-	-	4/21/61/61	0/2/2/2
26	BCR	AB	618	-	-	3/29/63/63	0/2/2/2
30	LMG	AA	416	-	2/2/8/8	17/37/57/70	0/1/1/1
22	CLA	BC	507	-	1/1/15/20	13/39/115/115	-
22	CLA	AD	402	4	1/1/15/20	12/39/115/115	-
27	DGD	BH	101	-	3/3/13/13	18/47/87/95	0/2/2/2
22	CLA	BB	613	-	1/1/15/20	17/39/115/115	-
30	LMG	BB	623	-	2/2/8/8	22/44/64/70	0/1/1/1
22	CLA	AB	606	2	1/1/15/20	16/39/115/115	-
26	BCR	AZ	101	-	-	3/29/63/63	0/2/2/2
22	CLA	BB	609	2	1/1/15/20	16/39/115/115	-
26	BCR	BD	406	-	-	3/29/63/63	0/2/2/2
22	CLA	BC	505	3	1/1/15/20	20/39/115/115	-
32	LMT	BM	101	-	-	1/21/61/61	0/2/2/2
22	CLA	AC	509	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	AT	102	-	-	3/29/63/63	0/2/2/2
32	LMT	AB	627	-	-	4/21/61/61	0/2/2/2
29	SQD	BD	409	-	-	11/38/58/69	0/1/1/1
22	CLA	BB	611	2	1/1/15/20	19/39/115/115	-
32	LMT	AB	624	-	-	4/21/61/61	0/2/2/2
32	LMT	BI	102	-	-	4/21/61/61	0/2/2/2
27	DGD	BC	516	-	3/3/13/13	17/42/82/95	0/2/2/2
29	SQD	BF	101	-	-	14/40/60/69	0/1/1/1
22	CLA	AC	510	-	1/1/15/20	13/39/115/115	-
22	CLA	BC	504	-	1/1/15/20	10/39/115/115	-
22	CLA	AC	502	3	1/1/15/20	11/39/115/115	-
29	SQD	AA	415	-	-	22/49/69/69	0/1/1/1
30	LMG	BD	408	-	2/2/8/8	25/43/63/70	0/1/1/1
22	CLA	AA	403	-	1/1/15/20	15/39/115/115	-
22	CLA	AC	503	3	1/1/15/20	15/39/115/115	-
27	DGD	AH	102	-	3/3/13/13	18/47/87/95	0/2/2/2
27	DGD	BB	602	-	3/3/13/13	25/41/81/95	0/2/2/2
30	LMG	BI	101	-	2/2/8/8	19/38/58/70	0/1/1/1
22	CLA	AB	604	2	1/1/15/20	11/39/115/115	-
26	BCR	BA	410	-	-	5/29/63/63	0/2/2/2
26	BCR	BC	514	-	-	5/29/63/63	0/2/2/2
22	CLA	BA	405	-	1/1/15/20	13/39/115/115	-
29	SQD	BA	413	-	-	18/46/66/69	0/1/1/1
30	LMG	AC	519	-	2/2/8/8	24/43/63/70	0/1/1/1
22	CLA	AB	611	2	1/1/15/20	16/39/115/115	-
30	LMG	BD	407	-	2/2/8/8	16/41/61/70	0/1/1/1
30	LMG	AD	407	-	2/2/8/8	17/41/61/70	0/1/1/1
27	DGD	BC	518	-	3/3/13/13	19/55/95/95	0/2/2/2
30	LMG	BE	102	-	2/2/8/8	19/39/59/70	0/1/1/1
22	CLA	AB	605	-	1/1/15/20	17/39/115/115	-
22	CLA	BB	610	-	1/1/15/20	14/39/115/115	-
22	CLA	BB	604	-	1/1/15/20	21/39/115/115	-
26	BCR	BC	515	-	-	4/29/63/63	0/2/2/2
22	CLA	BC	509	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BB	607	2	1/1/15/20	11/39/115/115	-
22	CLA	BB	606	2	1/1/15/20	11/39/115/115	-
32	LMT	BB	603	-	-	4/21/61/61	0/2/2/2

The worst 5 of 1408 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BC	505	CLA	MG-NA	8.49	2.26	2.06
29	BL	101	SQD	C4-C3	8.41	1.74	1.52
28	AA	411	LHG	P-O5	8.39	1.79	1.50
28	BA	412	LHG	P-O5	8.07	1.78	1.50
22	BC	511	CLA	MG-NA	7.96	2.25	2.06

The worst 5 of 1845 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	604	CLA	C4A-NA-C1A	13.13	112.67	106.68
22	BB	607	CLA	C4A-NA-C1A	12.99	112.61	106.68
22	AC	508	CLA	C4A-NA-C1A	12.89	112.56	106.68
22	BC	511	CLA	C4A-NA-C1A	12.77	112.50	106.68
22	AC	503	CLA	C4A-NA-C1A	12.70	112.47	106.68

5 of 156 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AA	402	CLA	ND
22	AA	403	CLA	ND
22	AA	404	CLA	ND
22	AA	406	CLA	ND
22	AB	601	CLA	ND

5 of 2261 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AA	403	CLA	C1A-C2A-CAA-CBA
22	AA	403	CLA	C3A-C2A-CAA-CBA
22	AA	403	CLA	C1-C2-C3-C4
22	AA	403	CLA	C1-C2-C3-C5
22	AA	403	CLA	C4-C3-C5-C6

There are no ring outliers.

165 monomers are involved in 591 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	AB	622	LMG	1	0
22	BA	407	CLA	3	0
26	AD	406	BCR	3	0
22	AB	614	CLA	1	0
22	AC	511	CLA	7	0
32	AT	101	LMT	3	0
22	BB	619	CLA	5	0
22	BC	510	CLA	1	0
27	AB	626	DGD	3	0
24	BD	405	PL9	8	0
26	AH	101	BCR	2	0
22	BA	404	CLA	7	0
22	BD	404	CLA	3	0
26	AB	617	BCR	3	0
29	BB	601	SQD	2	0
26	AC	515	BCR	5	0
30	BB	624	LMG	1	0
22	BC	511	CLA	9	0
22	AB	616	CLA	4	0
22	BC	502	CLA	2	0
22	AC	506	CLA	2	0
24	AA	407	PL9	5	0
22	BC	501	CLA	2	0
34	BV	201	HEM	3	0
27	AC	516	DGD	3	0
26	BX	101	BCR	4	0
29	BL	101	SQD	2	0
30	AB	621	LMG	1	0
22	BC	508	CLA	7	0
22	AC	507	CLA	3	0
22	BB	608	CLA	3	0
22	BB	615	CLA	4	0
29	AD	409	SQD	2	0
23	AA	405	PHO	5	0
22	BB	612	CLA	5	0
33	BD	401	BCT	1	0
26	BB	620	BCR	3	0
30	AI	101	LMG	3	0
22	BD	402	CLA	8	0
22	AC	512	CLA	8	0
32	AD	411	LMT	1	0
28	BC	521	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	AC	518	DGD	8	0
27	AC	517	DGD	8	0
28	AA	411	LHG	3	0
32	BB	626	LMT	2	0
34	AE	101	HEM	5	0
22	AC	508	CLA	8	0
22	AA	402	CLA	8	0
22	AC	501	CLA	2	0
22	BB	614	CLA	8	0
22	BC	503	CLA	2	0
23	BA	406	PHO	5	0
34	AV	201	HEM	3	0
22	BB	605	CLA	6	0
30	AB	623	LMG	2	0
30	BC	520	LMG	5	0
22	BC	512	CLA	6	0
30	AA	413	LMG	1	0
22	AB	607	CLA	13	0
26	AK	102	BCR	13	0
30	BC	519	LMG	3	0
22	AD	404	CLA	3	0
32	AM	102	LMT	1	0
22	AB	601	CLA	3	0
30	AM	101	LMG	4	0
32	AB	625	LMT	2	0
26	BZ	101	BCR	4	0
26	BK	102	BCR	13	0
29	AF	101	SQD	2	0
30	BM	102	LMG	4	0
23	AD	403	PHO	3	0
22	AB	603	CLA	7	0
22	BA	403	CLA	8	0
22	AB	608	CLA	10	0
22	AA	404	CLA	2	0
34	BE	101	HEM	6	0
26	BJ	102	BCR	5	0
29	AA	412	SQD	5	0
22	AB	610	CLA	4	0
26	AB	620	BCR	2	0
30	AE	102	LMG	4	0
23	BD	403	PHO	6	0
22	AC	513	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BB	617	CLA	1	0
33	AD	401	BCT	1	0
28	BA	412	LHG	4	0
30	AC	520	LMG	4	0
22	AC	505	CLA	9	0
27	BC	517	DGD	10	0
24	BA	408	PL9	6	0
26	AJ	102	BCR	5	0
22	AC	504	CLA	5	0
32	BT	101	LMT	3	0
26	AA	409	BCR	6	0
22	AB	615	CLA	5	0
22	BC	506	CLA	2	0
26	BB	622	BCR	2	0
32	BB	625	LMT	1	0
24	AD	405	PL9	9	0
29	BA	401	SQD	2	0
22	AB	613	CLA	1	0
22	BC	513	CLA	3	0
22	AA	406	CLA	3	0
26	AC	514	BCR	8	0
22	AB	602	CLA	5	0
22	AB	609	CLA	4	0
22	AB	612	CLA	4	0
30	BA	414	LMG	2	0
22	BB	616	CLA	1	0
22	BB	618	CLA	4	0
28	AC	521	LHG	5	0
30	AD	408	LMG	7	0
32	AI	102	LMT	4	0
26	AB	618	BCR	4	0
30	AA	416	LMG	4	0
22	BC	507	CLA	4	0
22	AD	402	CLA	7	0
27	BH	101	DGD	1	0
22	BB	613	CLA	4	0
30	BB	623	LMG	1	0
22	AB	606	CLA	4	0
26	AZ	101	BCR	4	0
22	BB	609	CLA	5	0
26	BD	406	BCR	3	0
22	BC	505	CLA	10	0

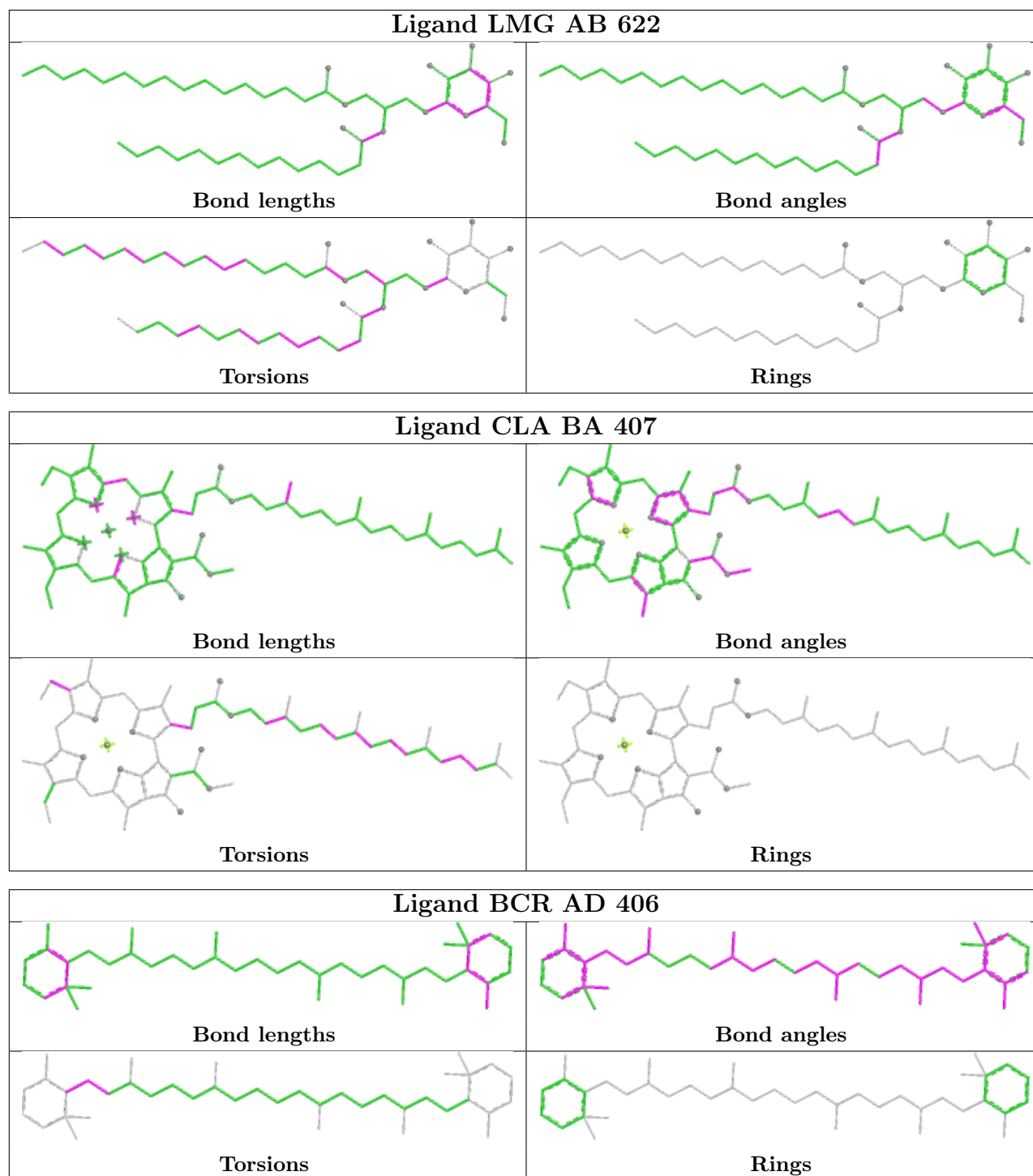
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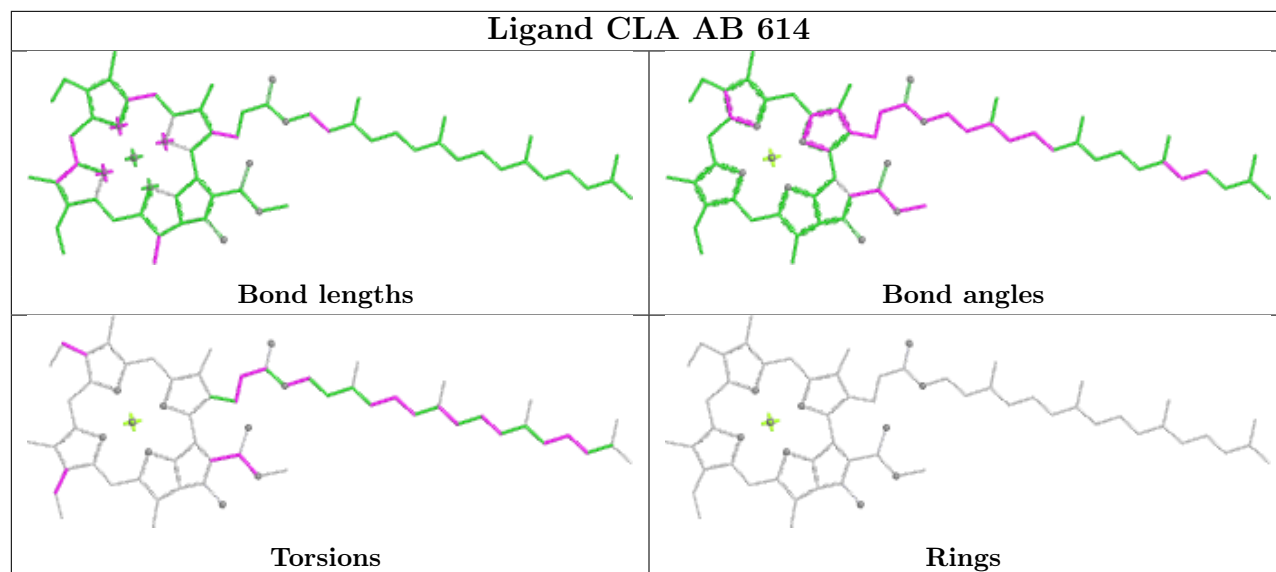
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	BM	101	LMT	1	0
22	AC	509	CLA	2	0
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32	AB	627	LMT	3	0
29	BD	409	SQD	2	0
22	BB	611	CLA	10	0
32	AB	624	LMT	2	0
32	BI	102	LMT	3	0
27	BC	516	DGD	4	0
29	BF	101	SQD	1	0
22	AC	510	CLA	1	0
22	BC	504	CLA	5	0
22	AC	502	CLA	3	0
29	AA	415	SQD	5	0
30	BD	408	LMG	8	0
22	AA	403	CLA	7	0
22	AC	503	CLA	2	0
27	AH	102	DGD	1	0
27	BB	602	DGD	3	0
30	BI	101	LMG	3	0
22	AB	604	CLA	5	0
26	BA	410	BCR	3	0
26	BC	514	BCR	10	0
22	BA	405	CLA	3	0
29	BA	413	SQD	4	0
30	AC	519	LMG	2	0
22	AB	611	CLA	5	0
30	BD	407	LMG	2	0
30	AD	407	LMG	2	0
27	BC	518	DGD	8	0
30	BE	102	LMG	4	0
22	AB	605	CLA	3	0
22	BB	610	CLA	12	0
22	BB	604	CLA	3	0
26	BC	515	BCR	6	0
22	BC	509	CLA	2	0
22	BB	607	CLA	5	0
22	BB	606	CLA	7	0
32	BB	603	LMT	3	0

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

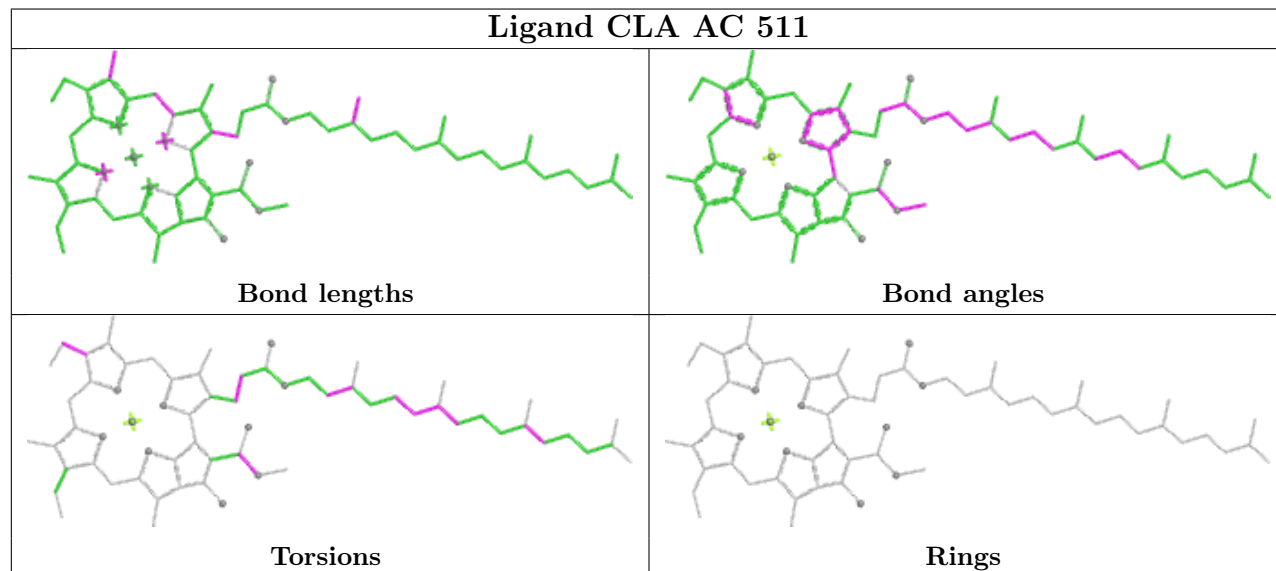
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



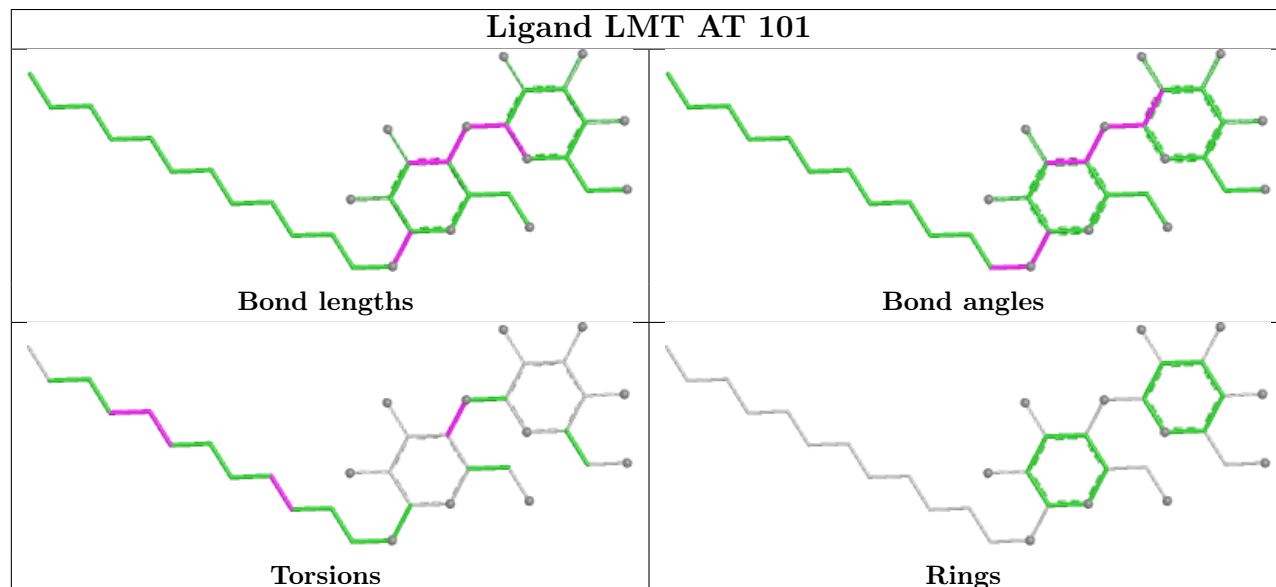
Ligand CLA AB 614

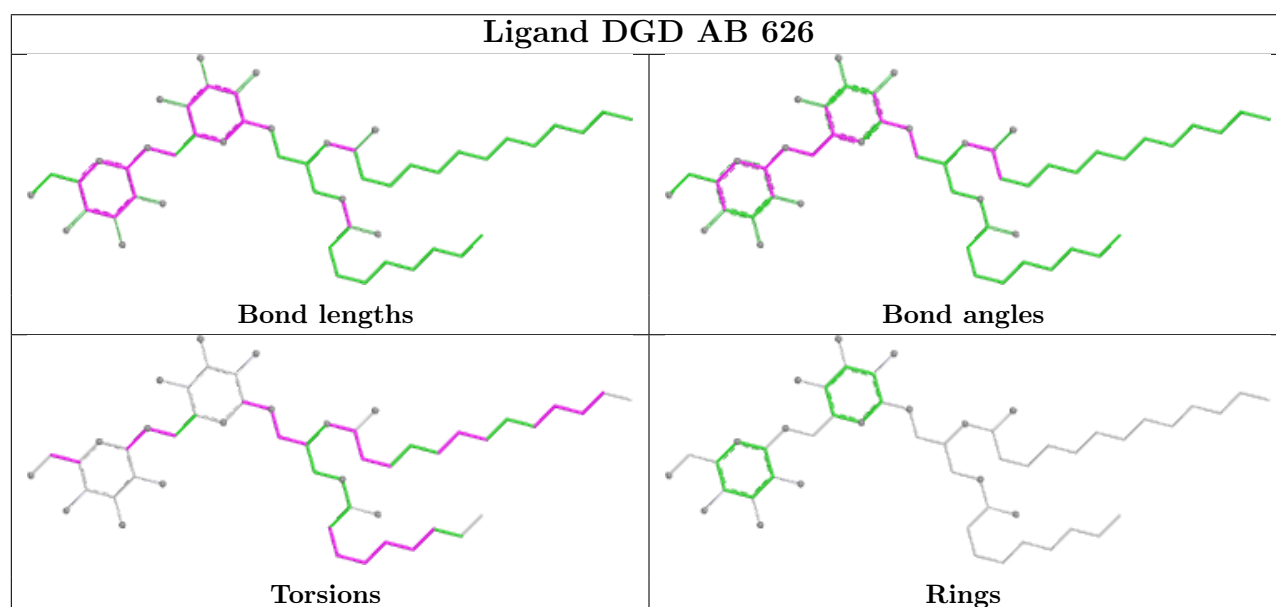
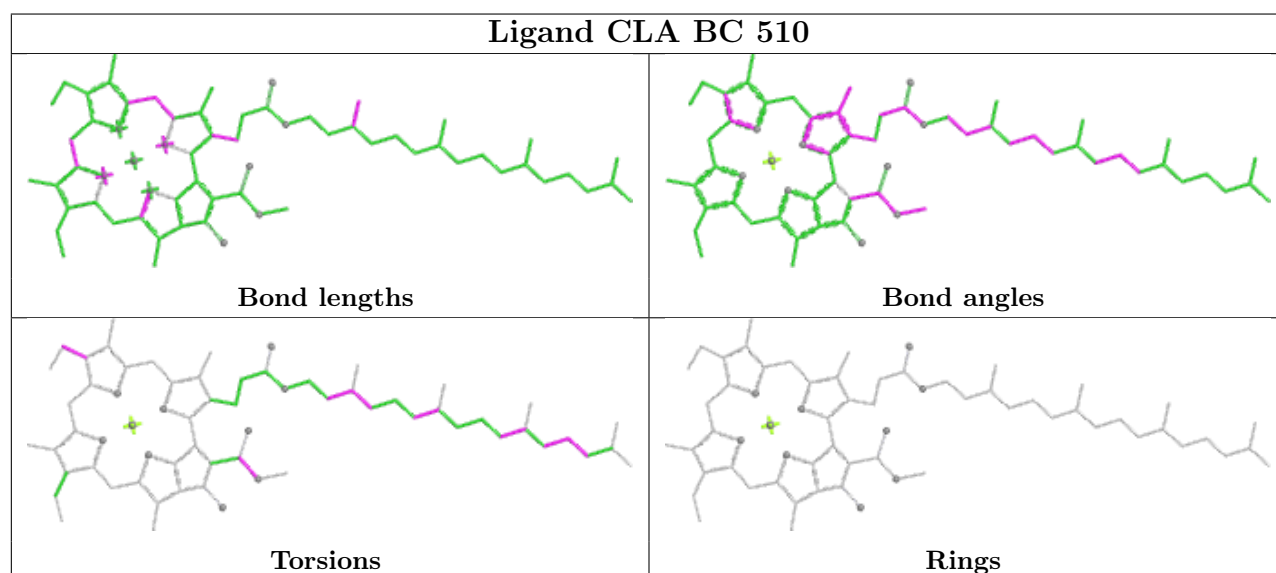
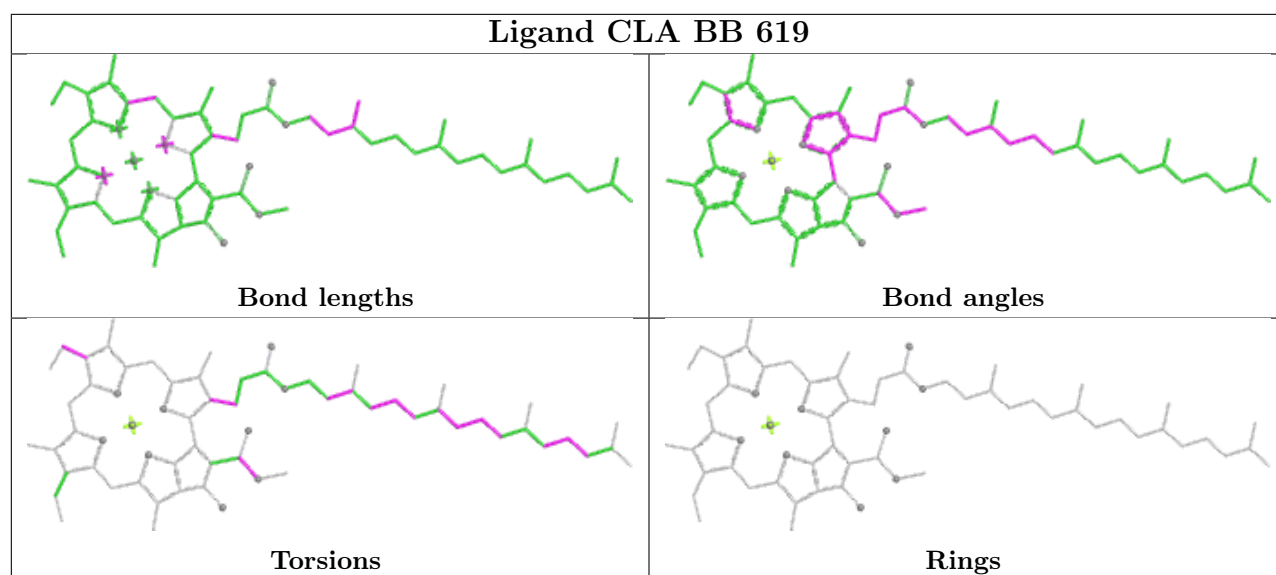


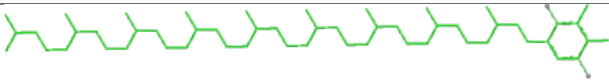
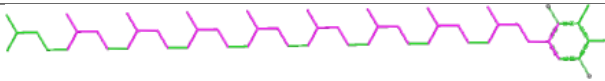
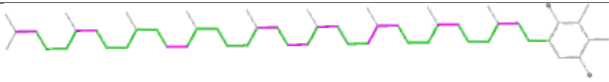
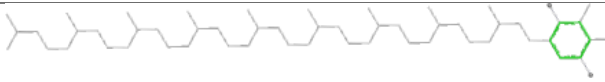
Ligand CLA AC 511

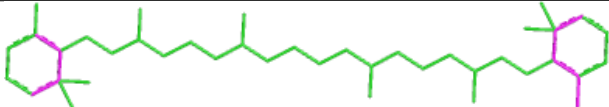
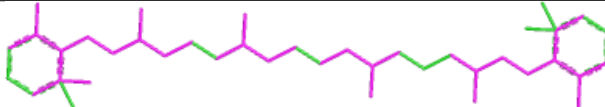
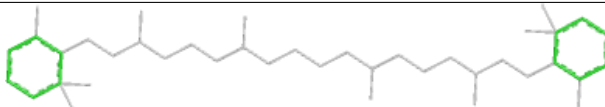


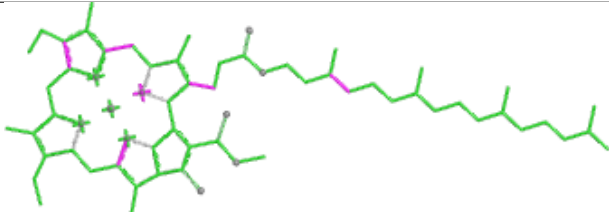
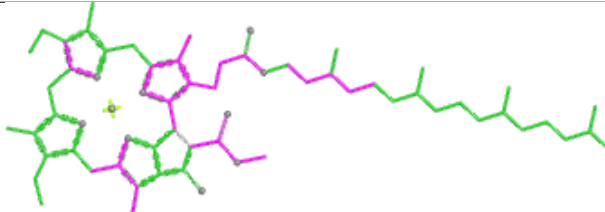
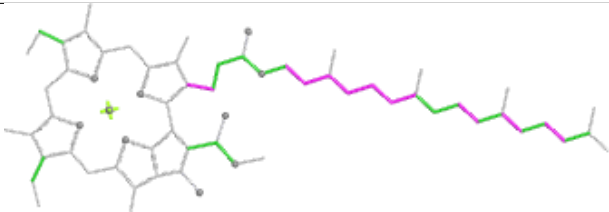
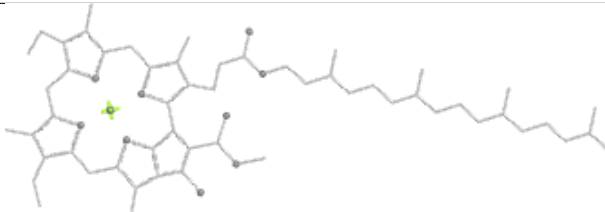
Ligand LMT AT 101

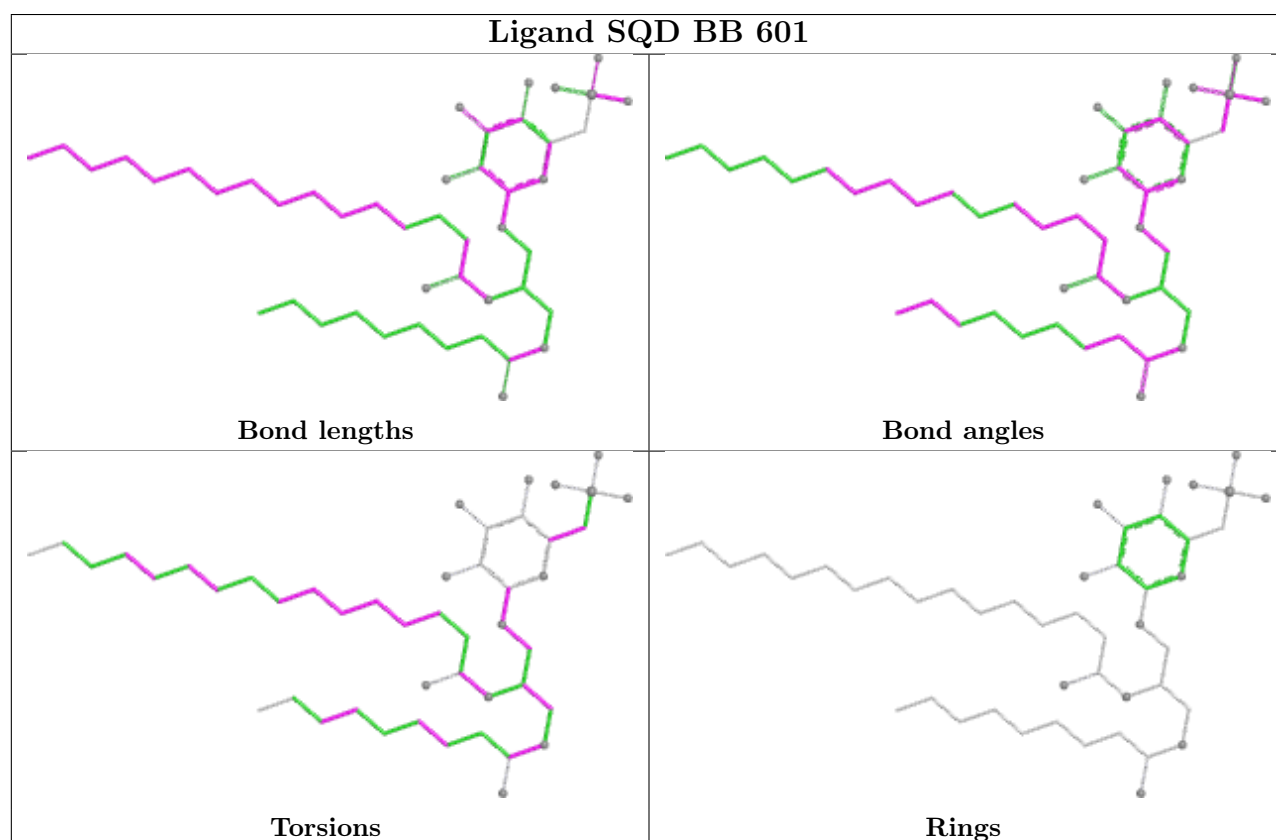
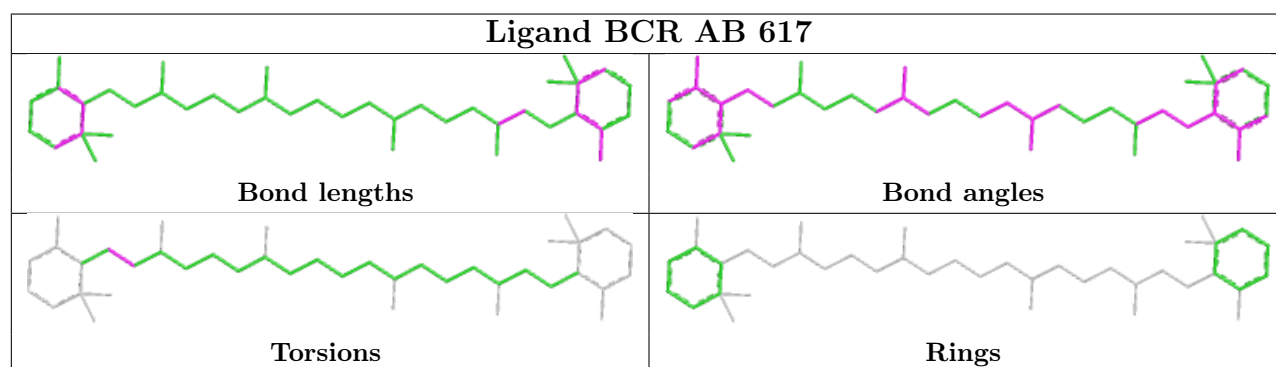
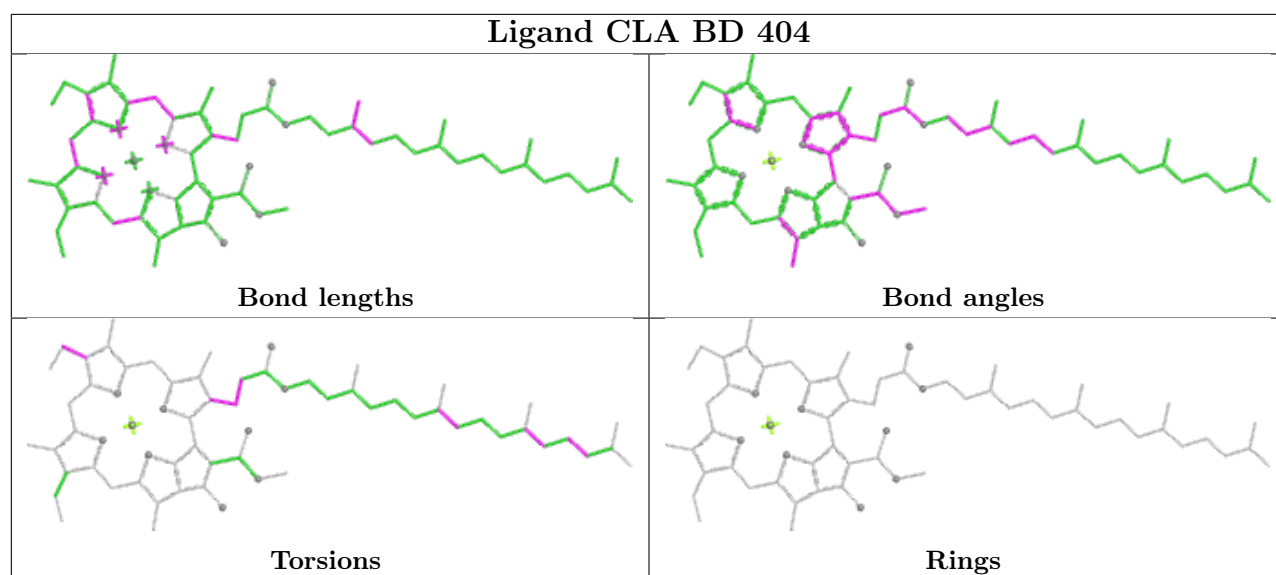


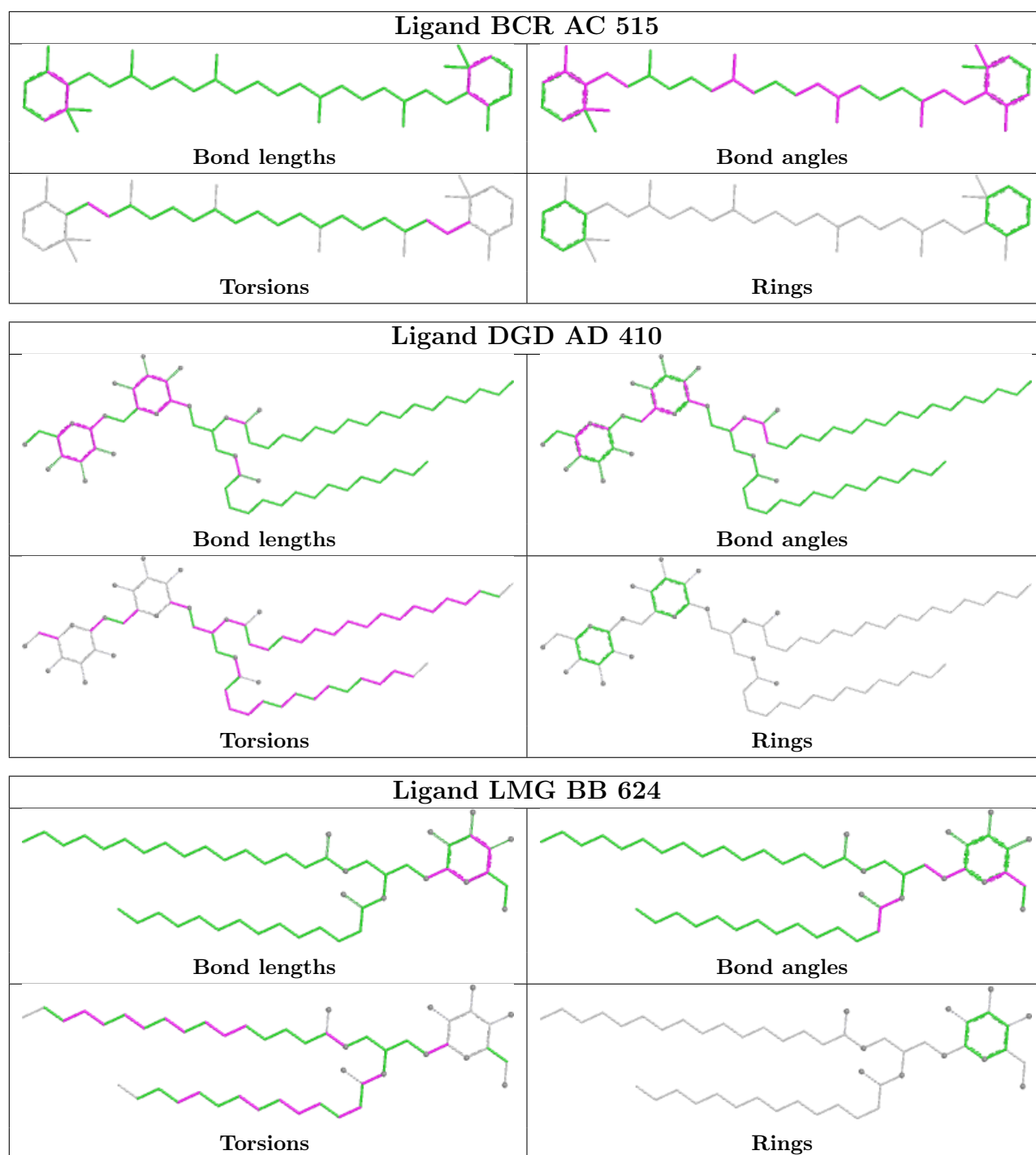


Ligand PL9 BD 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

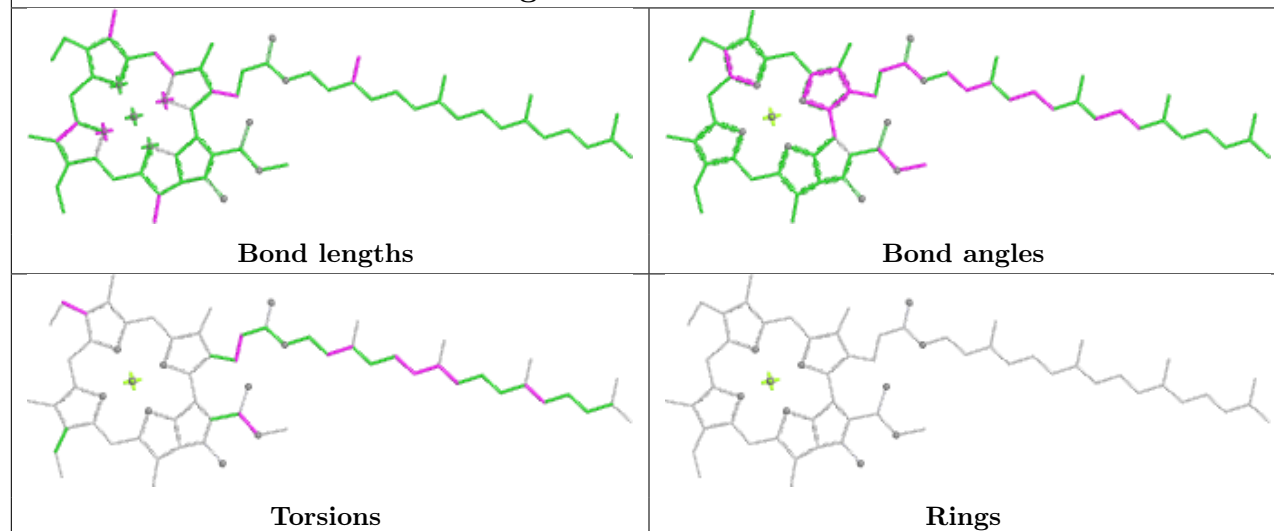
Ligand BCR AH 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BA 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

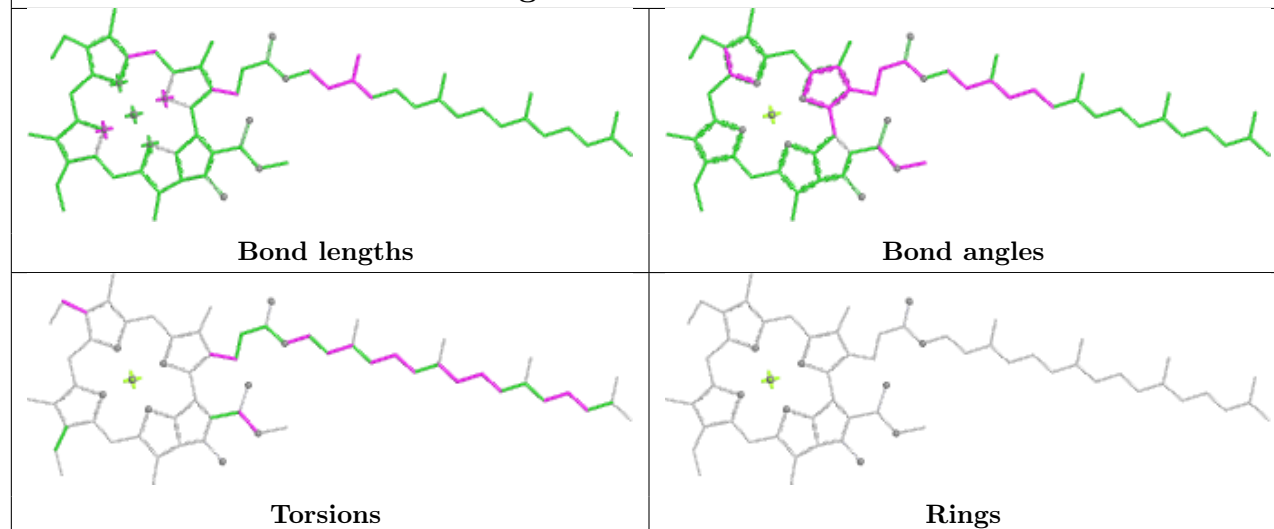




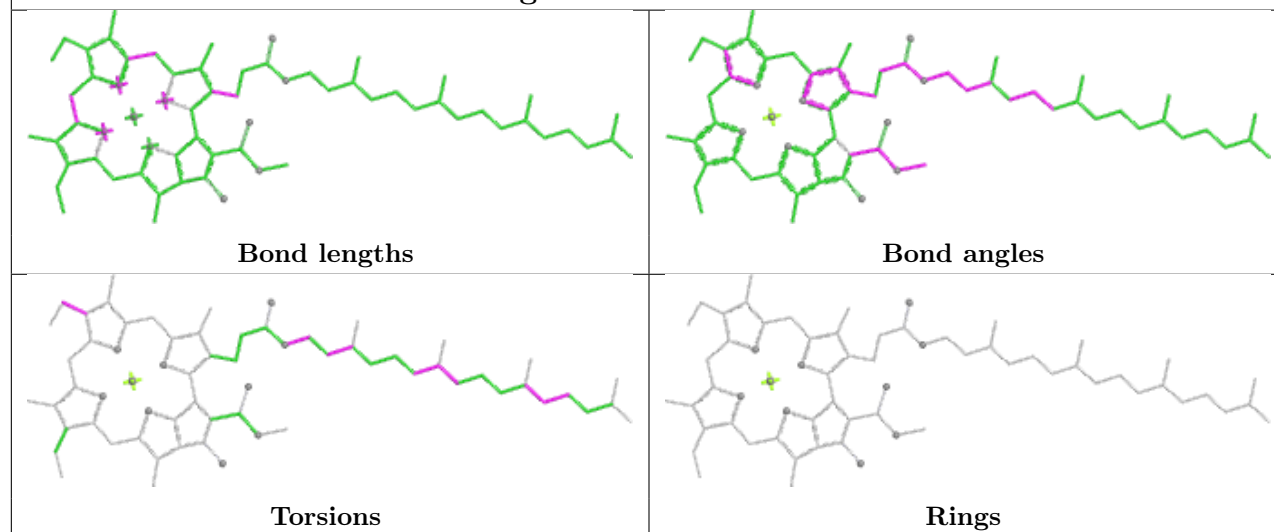
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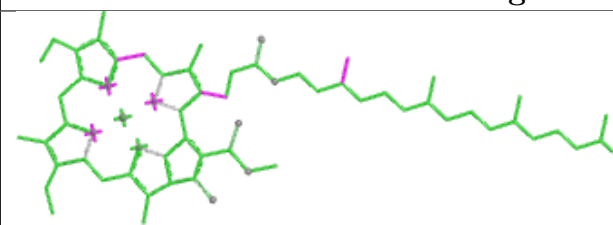
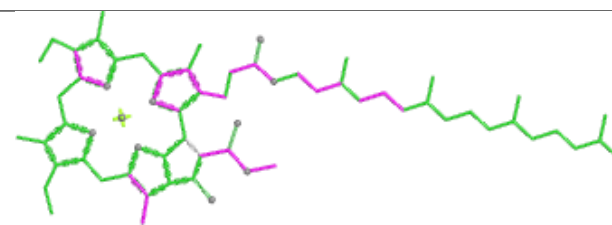
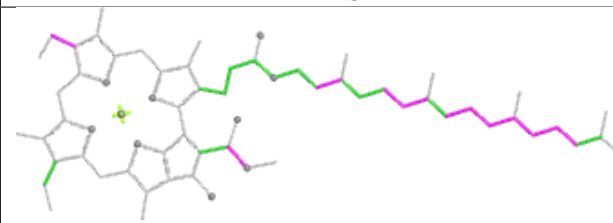
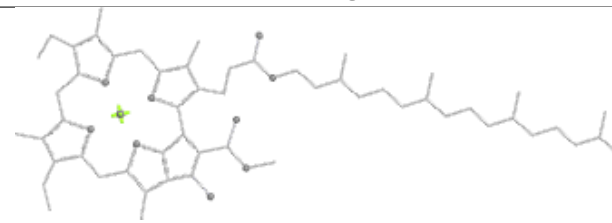


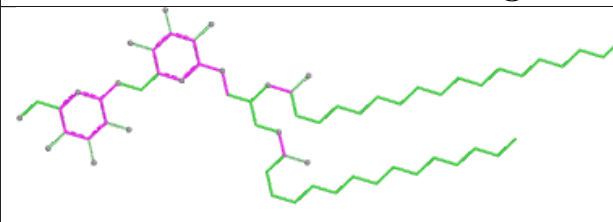
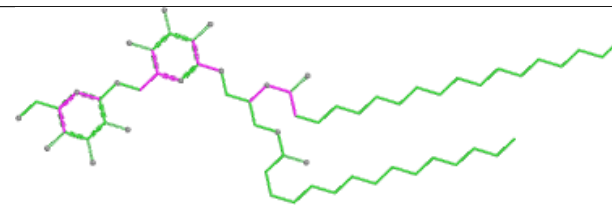
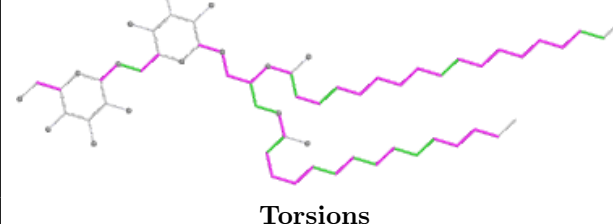
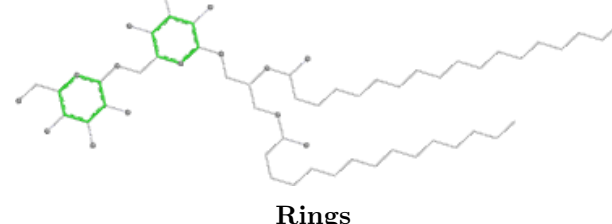
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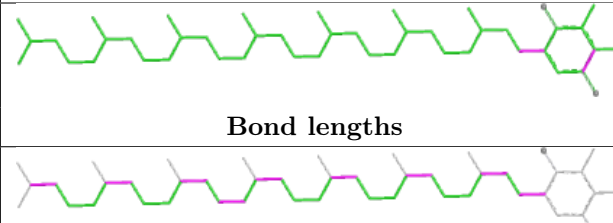
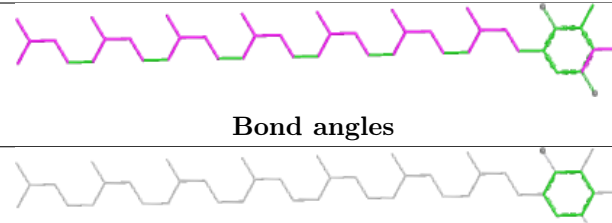
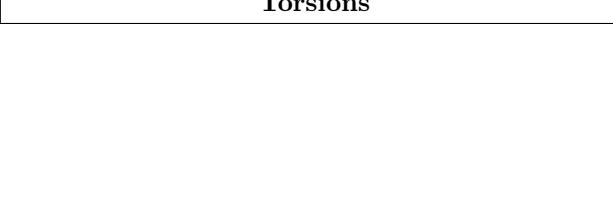
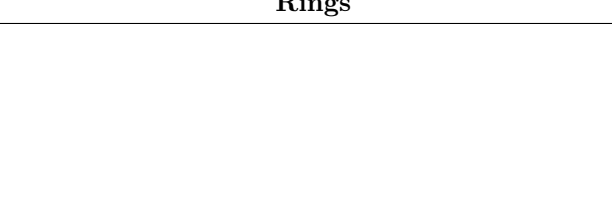


Ligand CLA BC 502

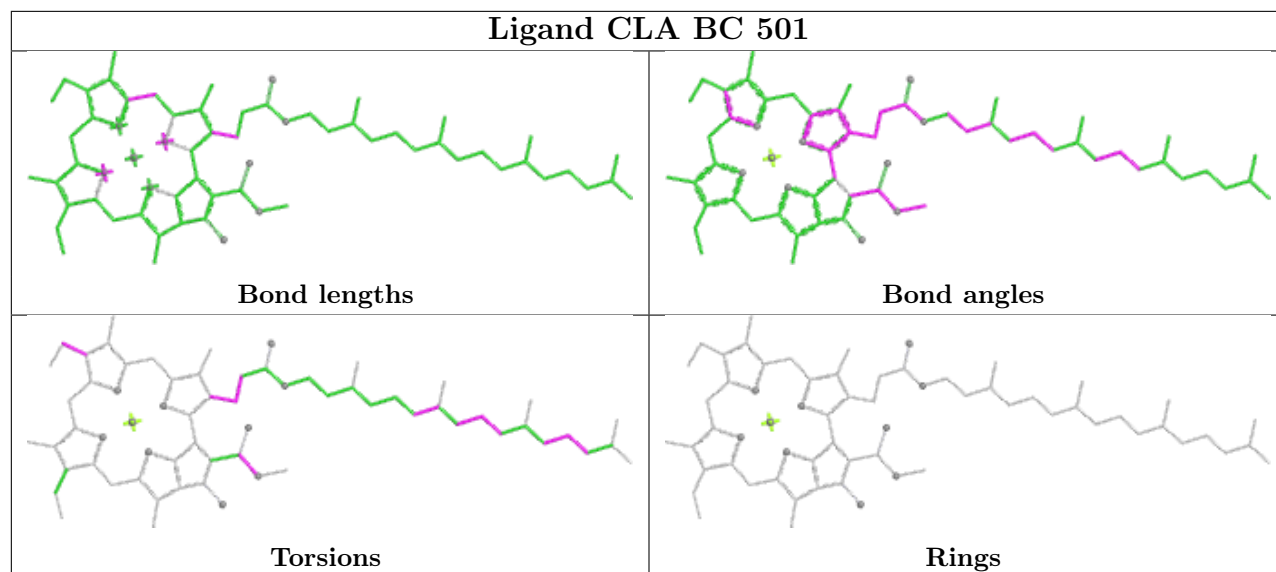


Ligand CLA AC 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

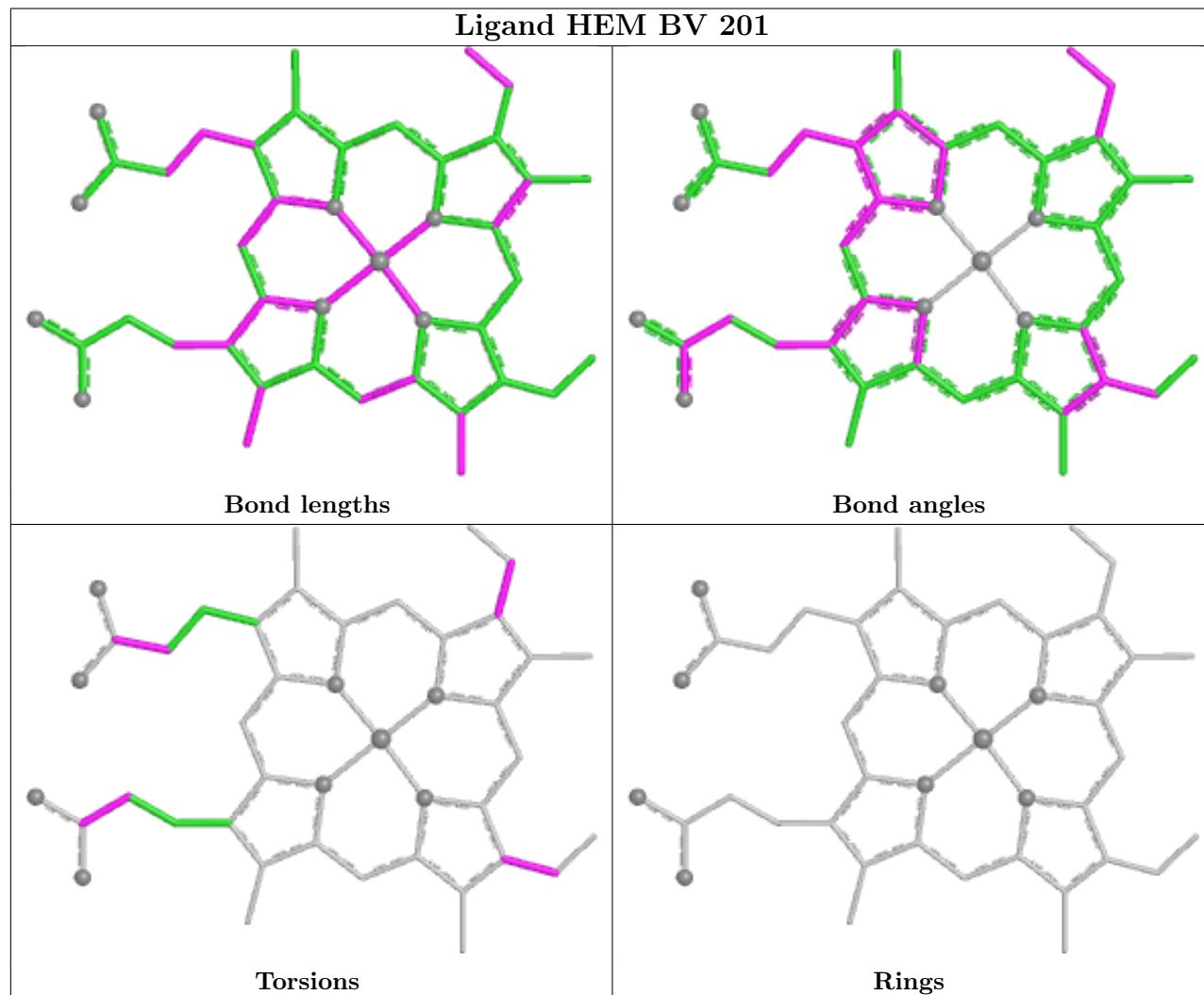
Ligand DGD BD 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

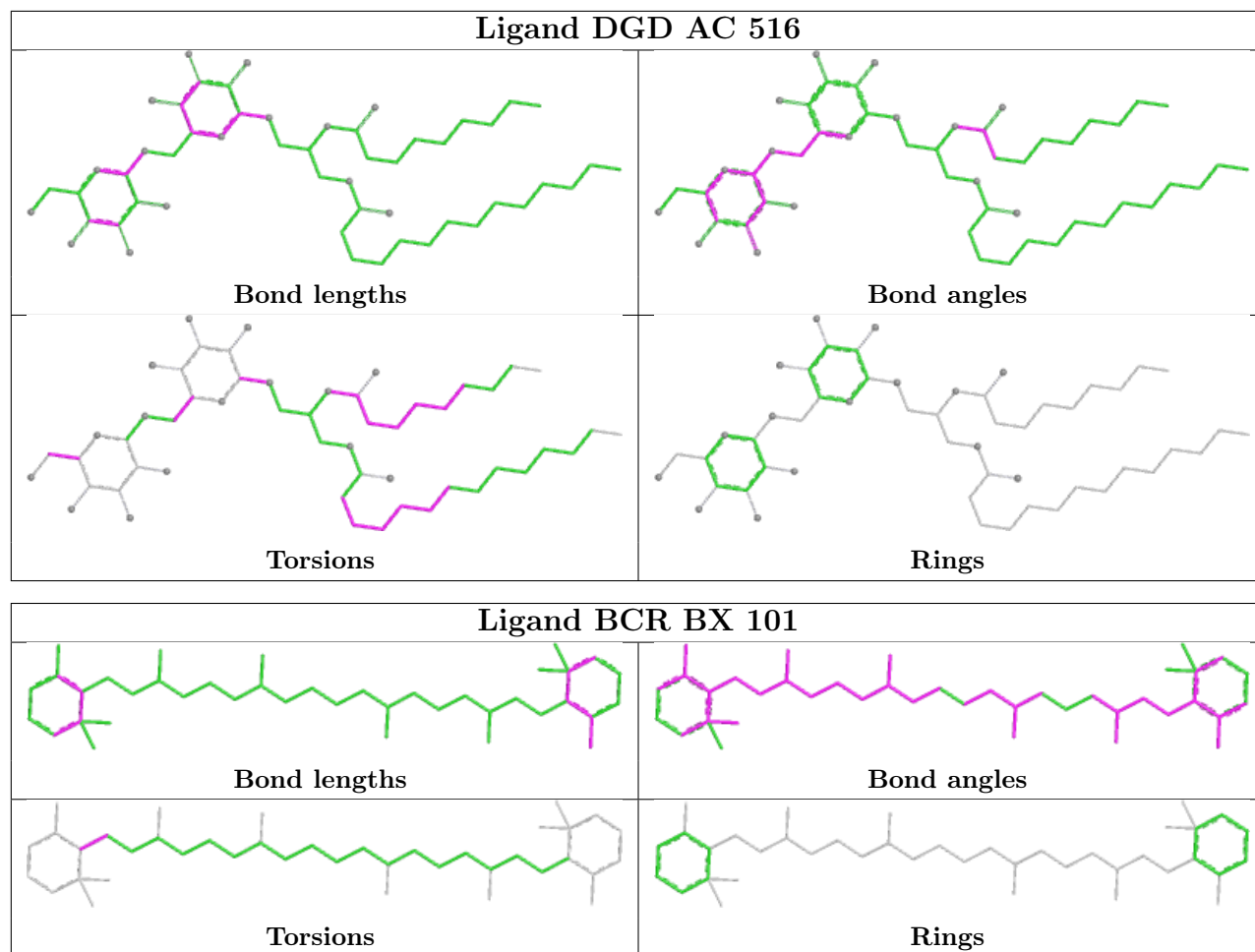
Ligand PL9 AA 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

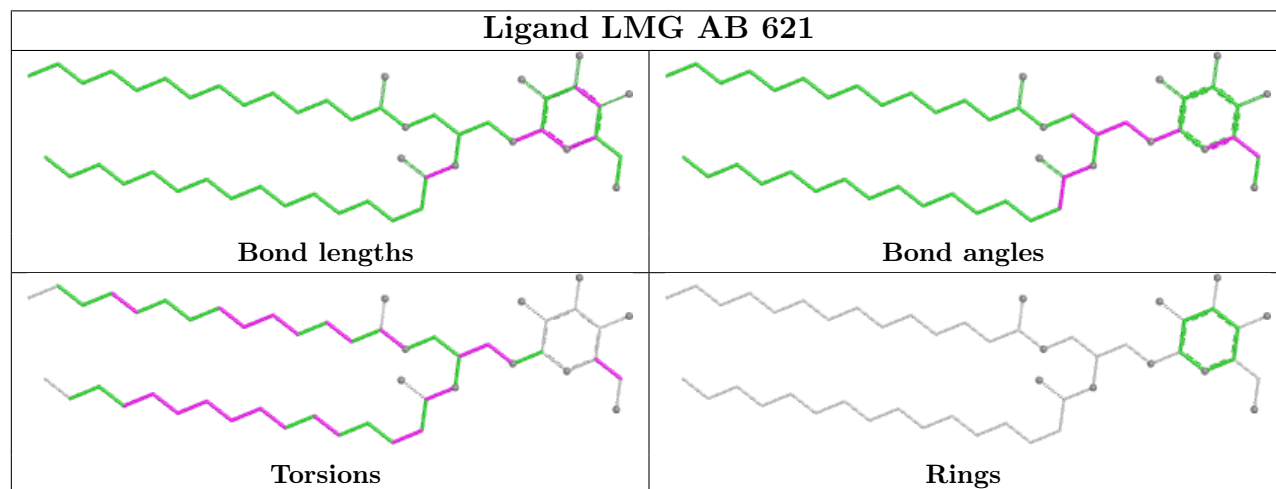
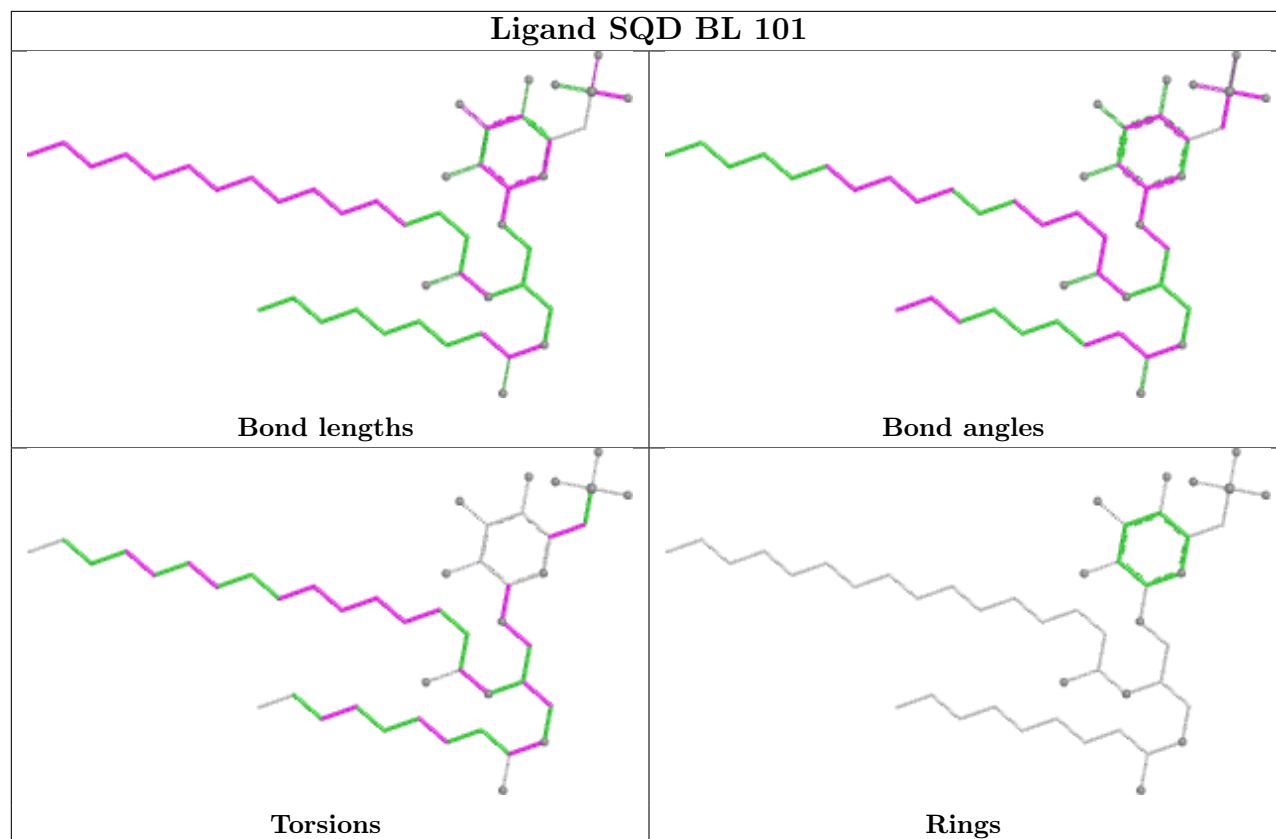
Ligand CLA BC 501



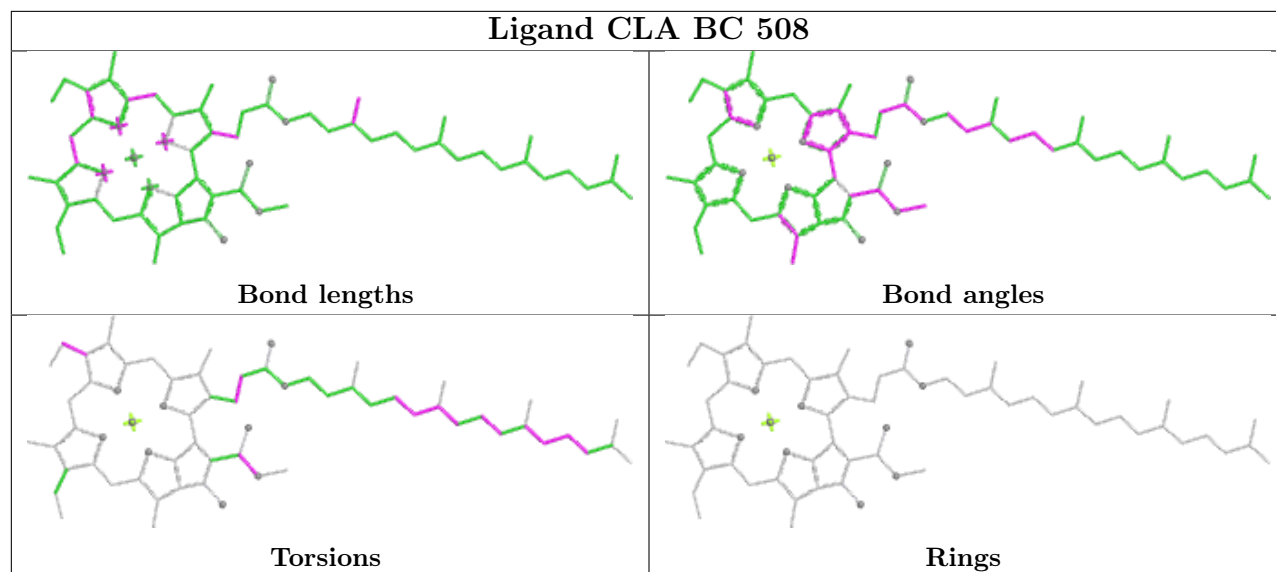
Ligand HEM BV 201



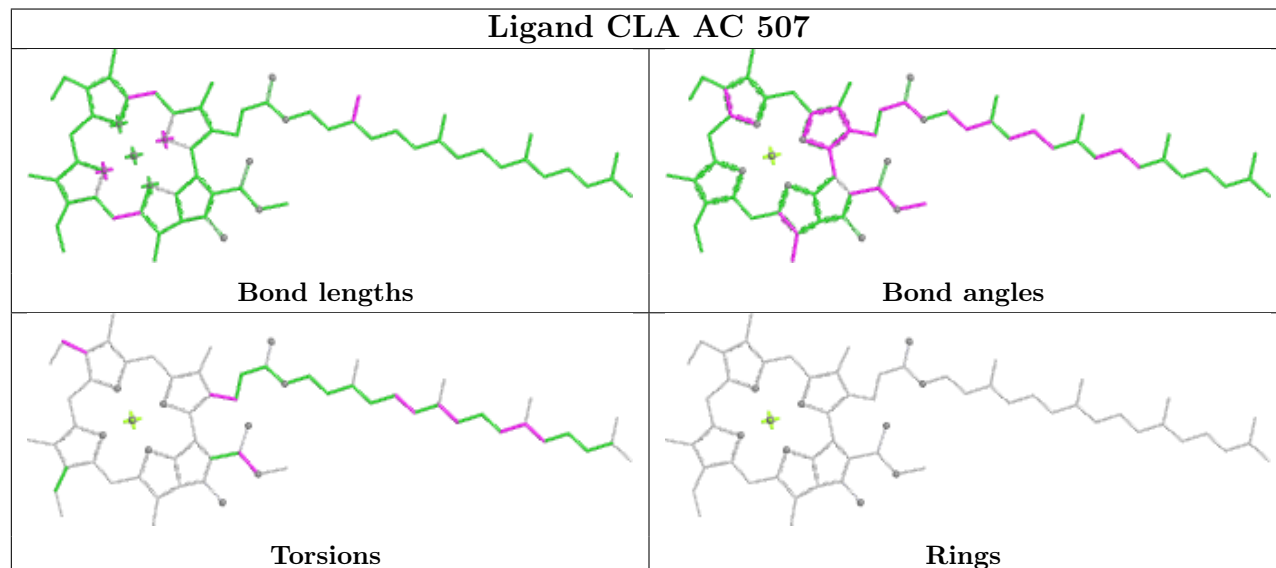




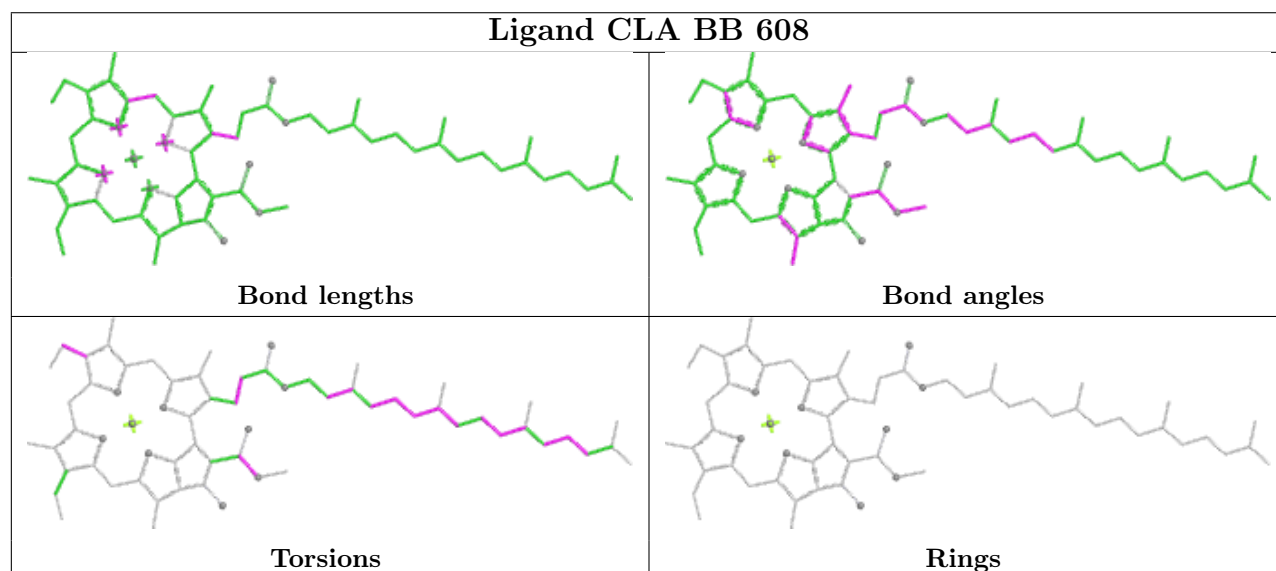
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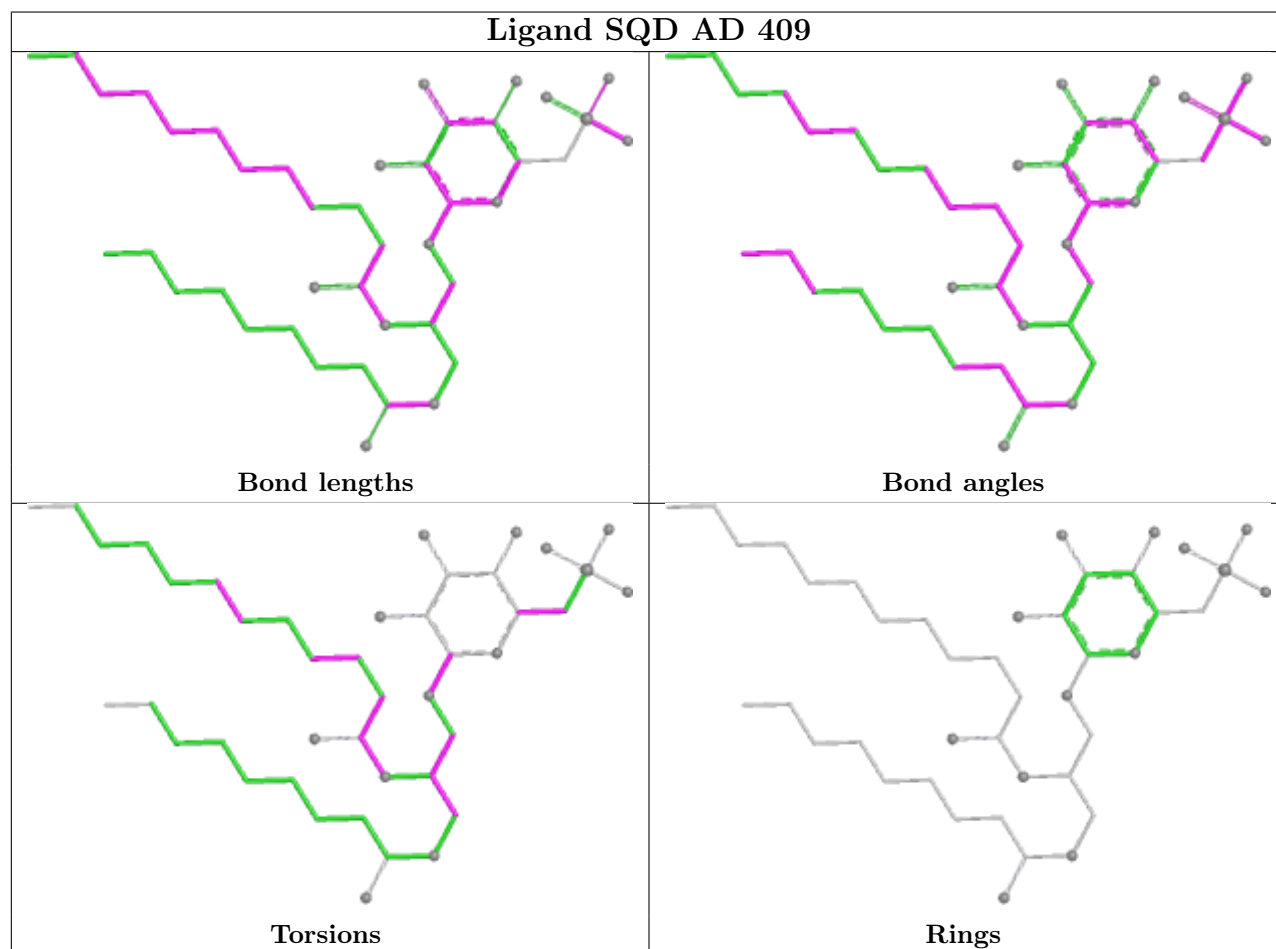
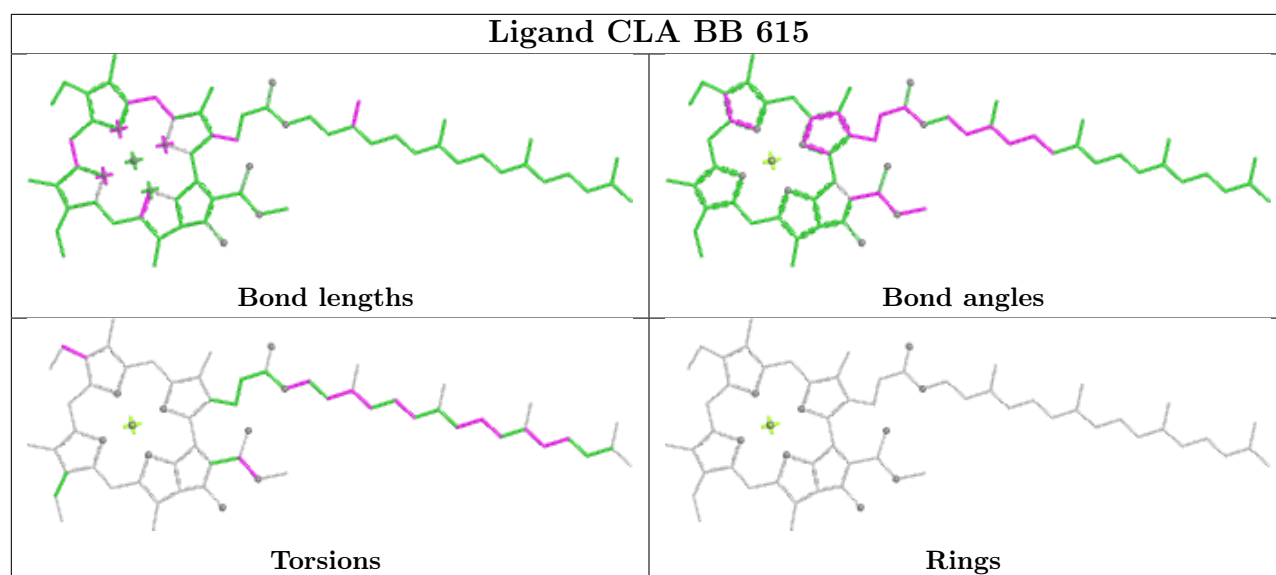


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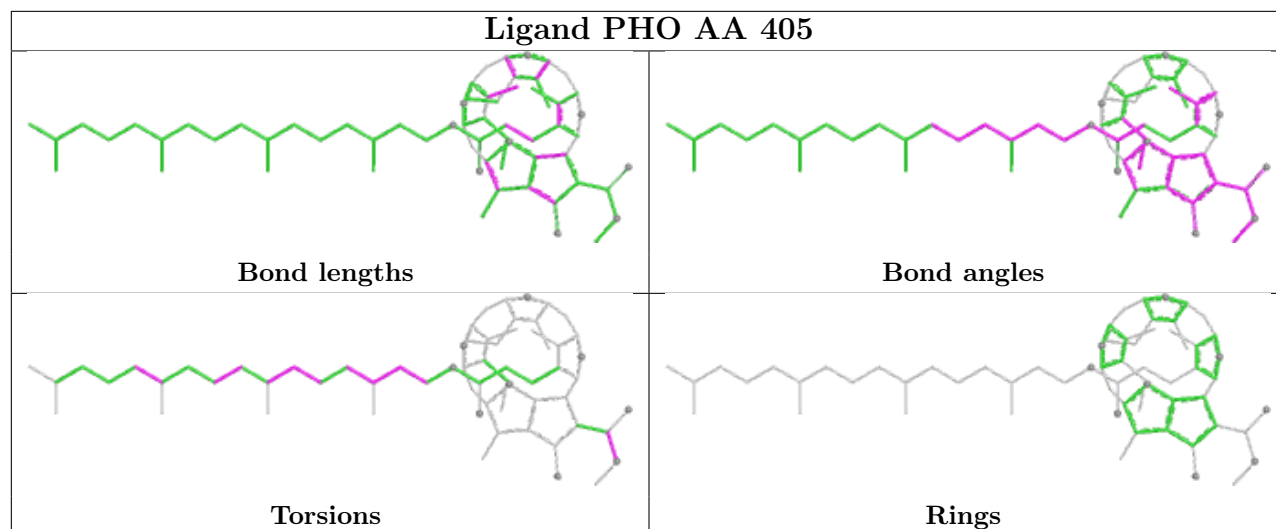


Ligand CLA BB 608

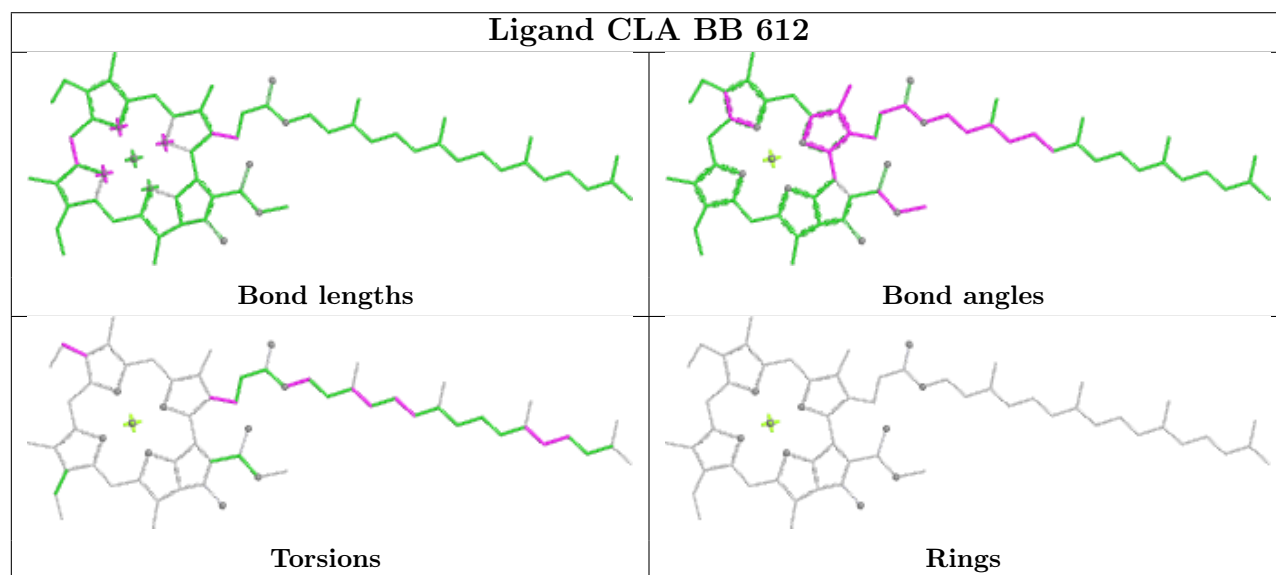




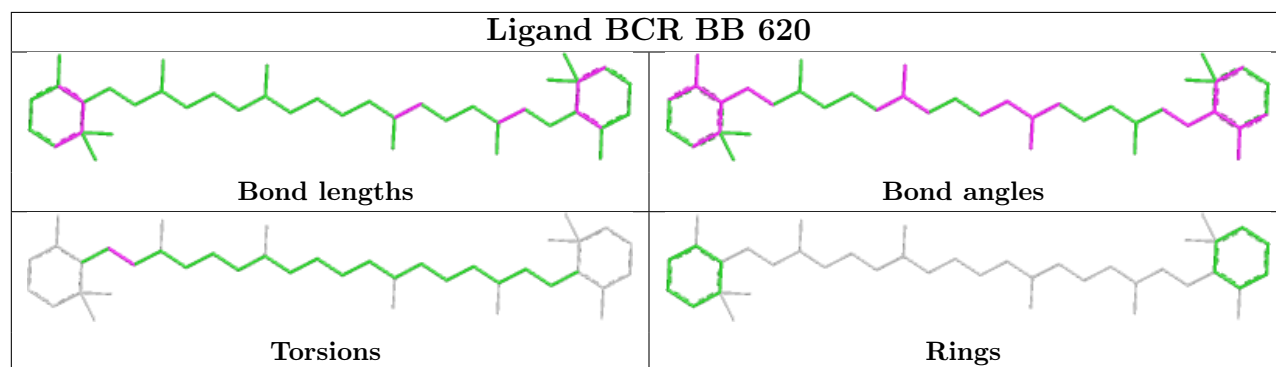
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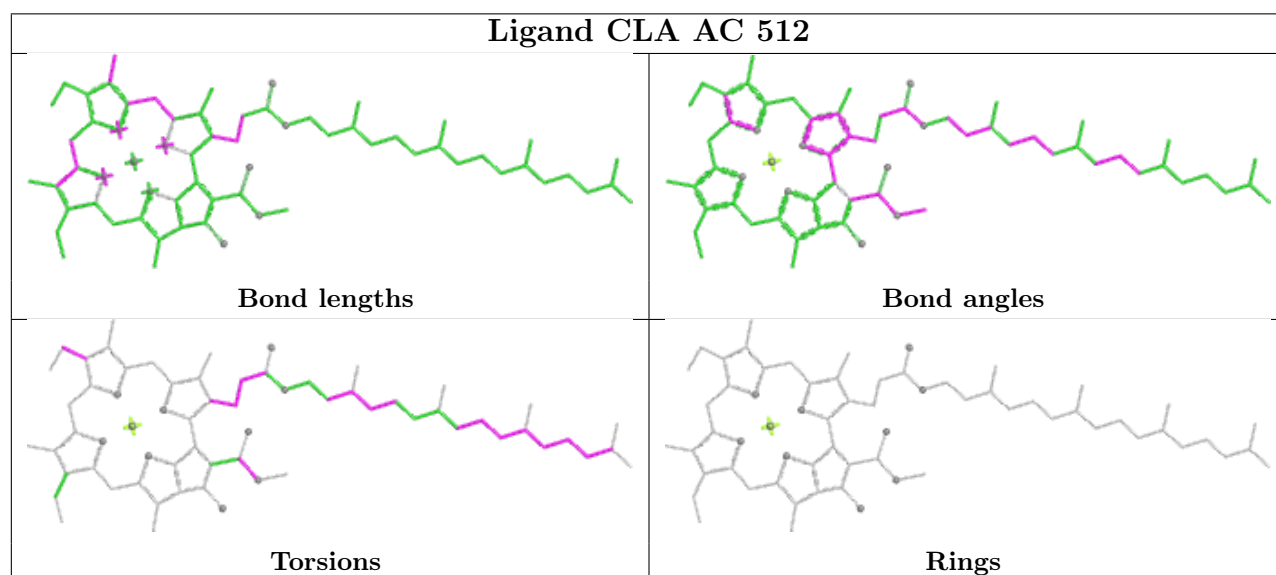
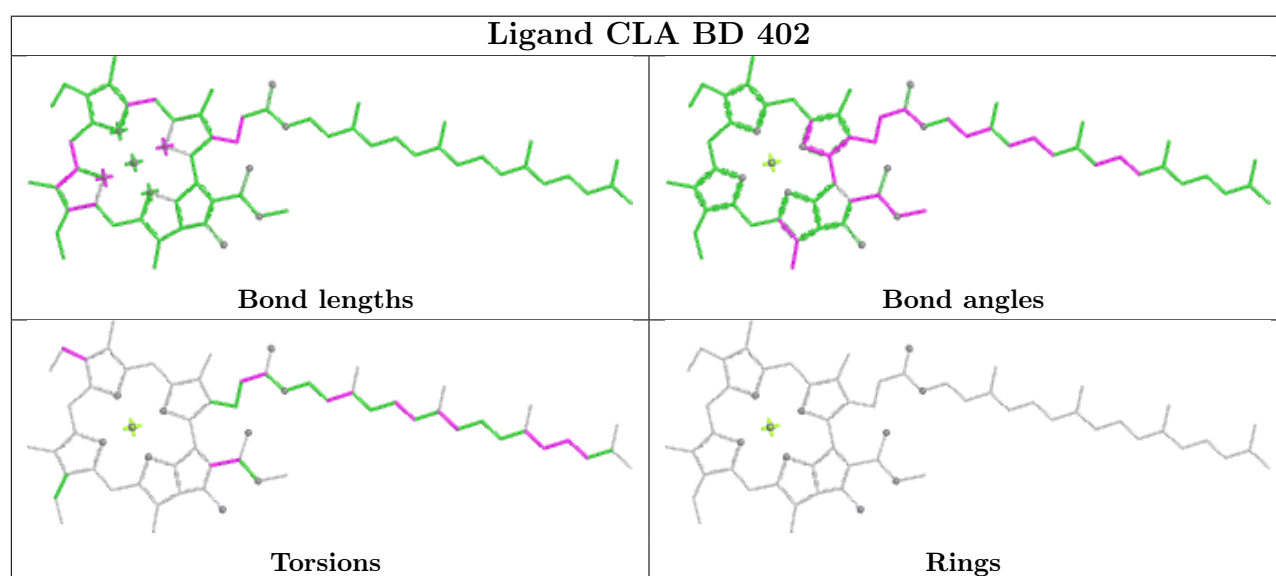
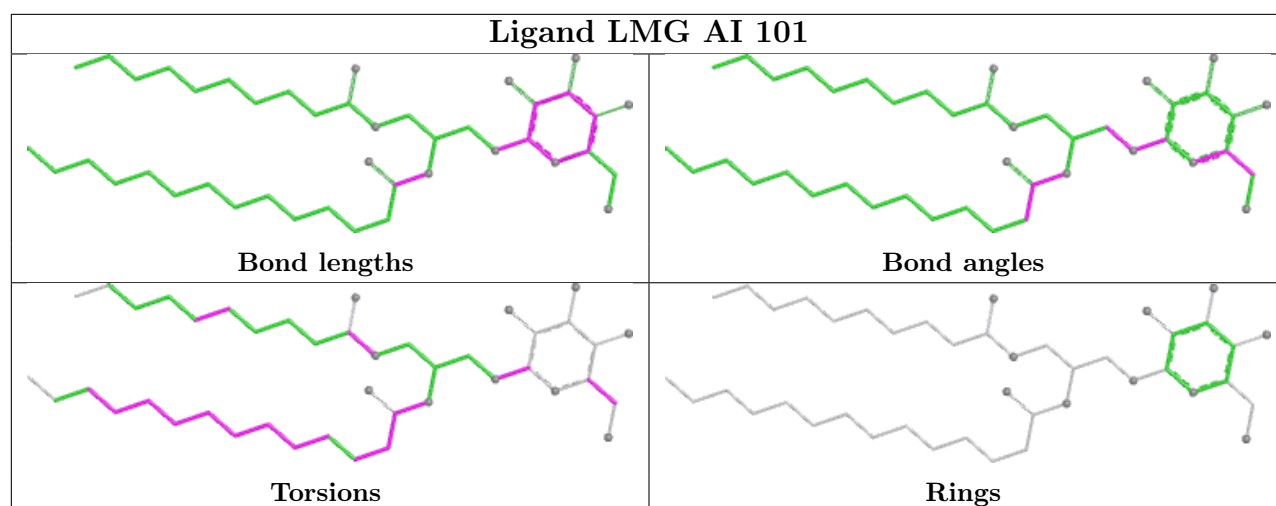


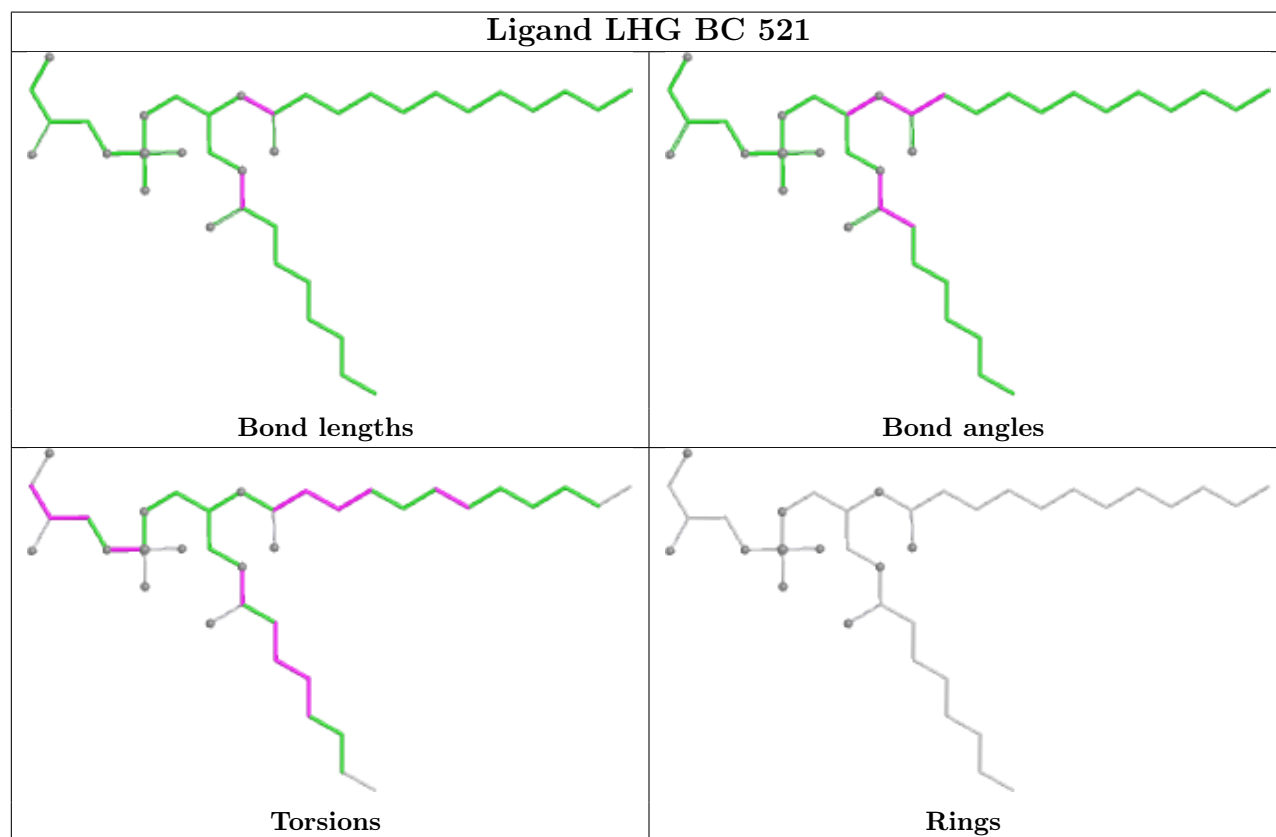
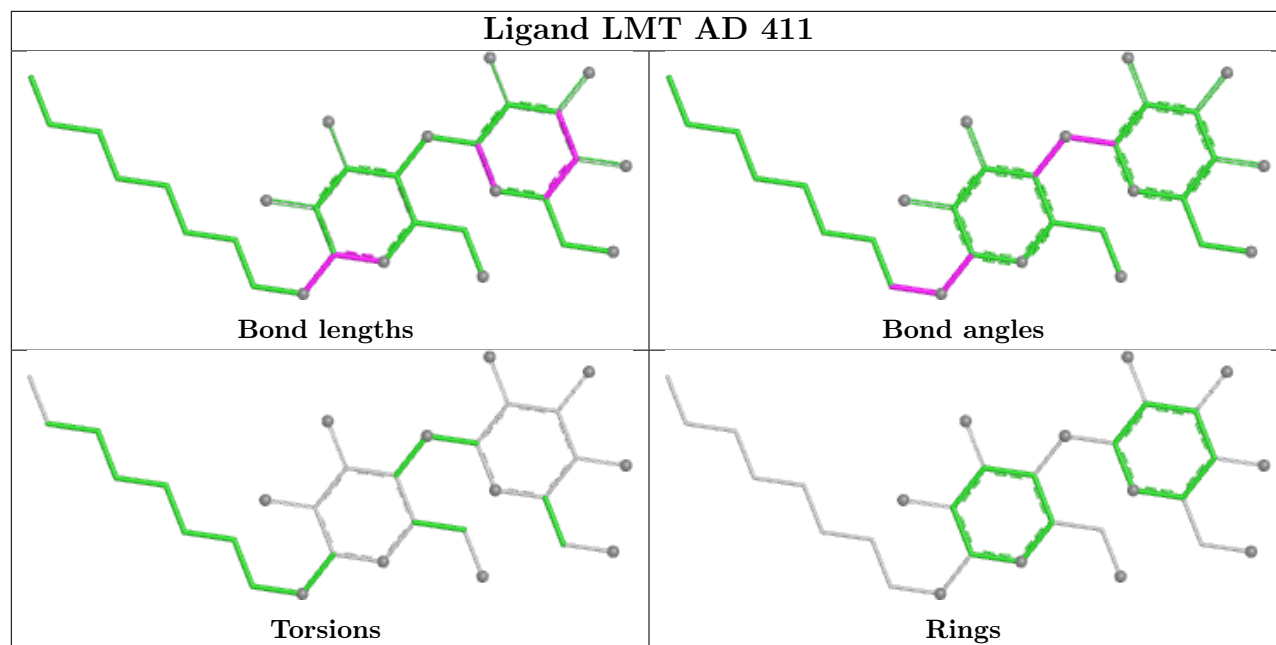
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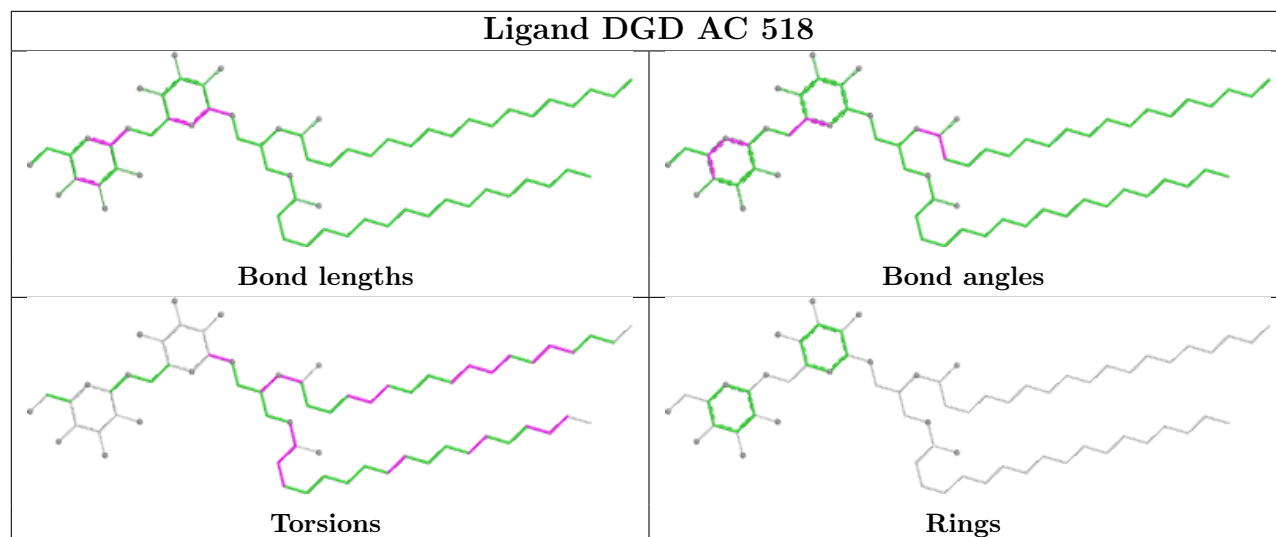
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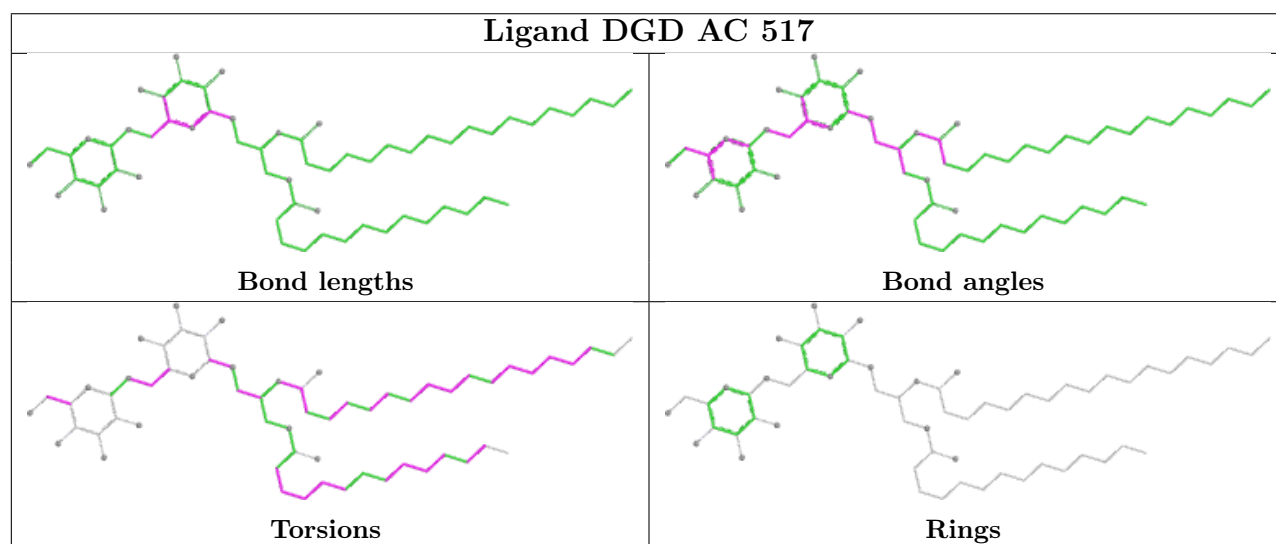


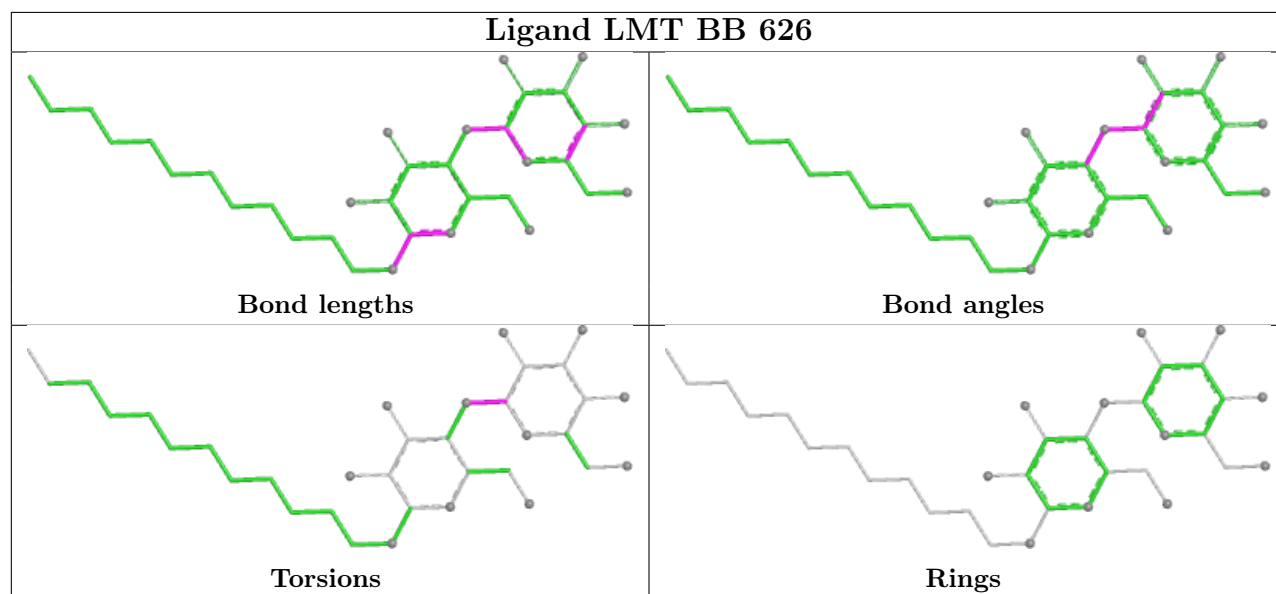
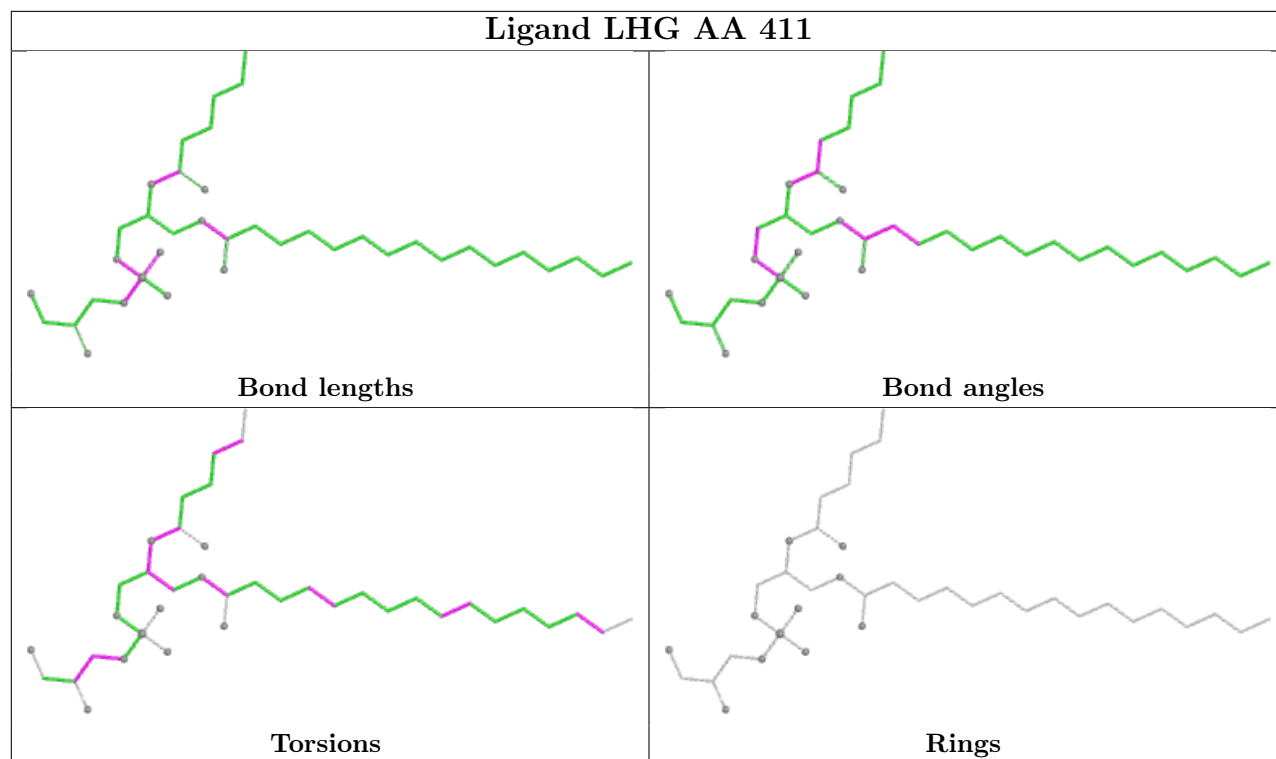


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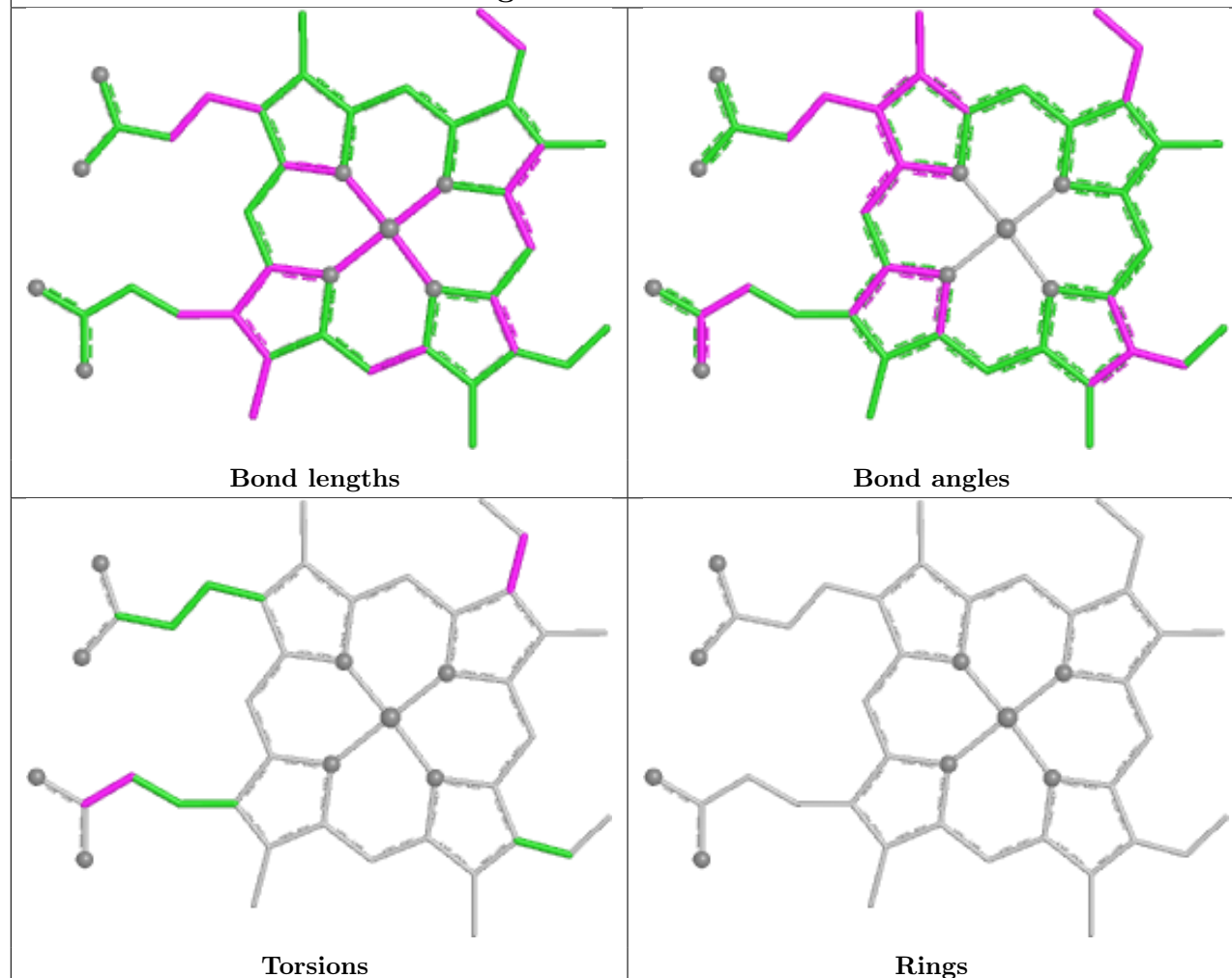


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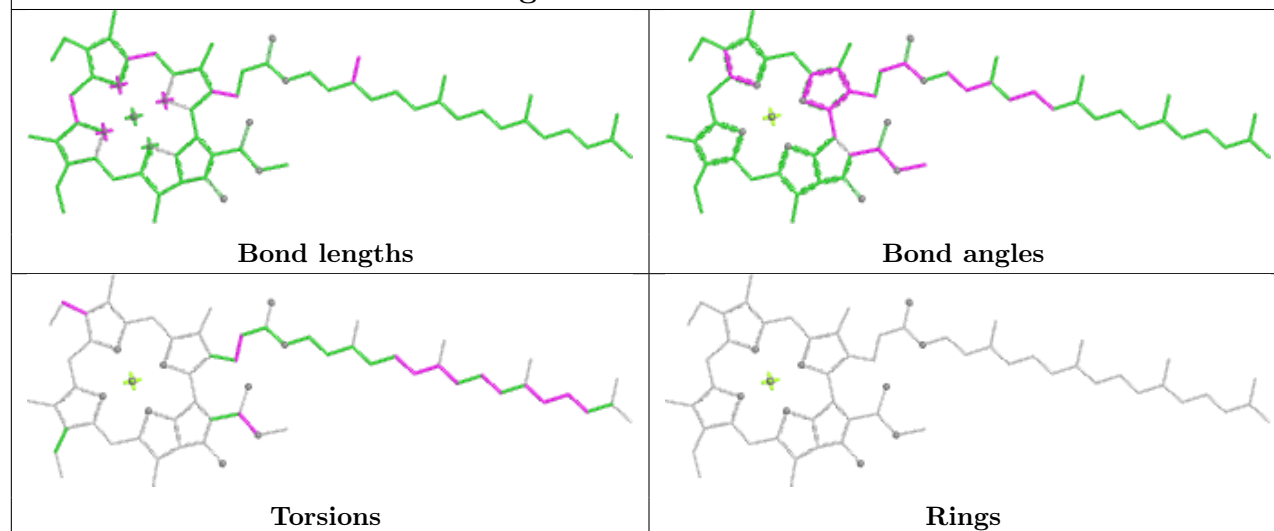


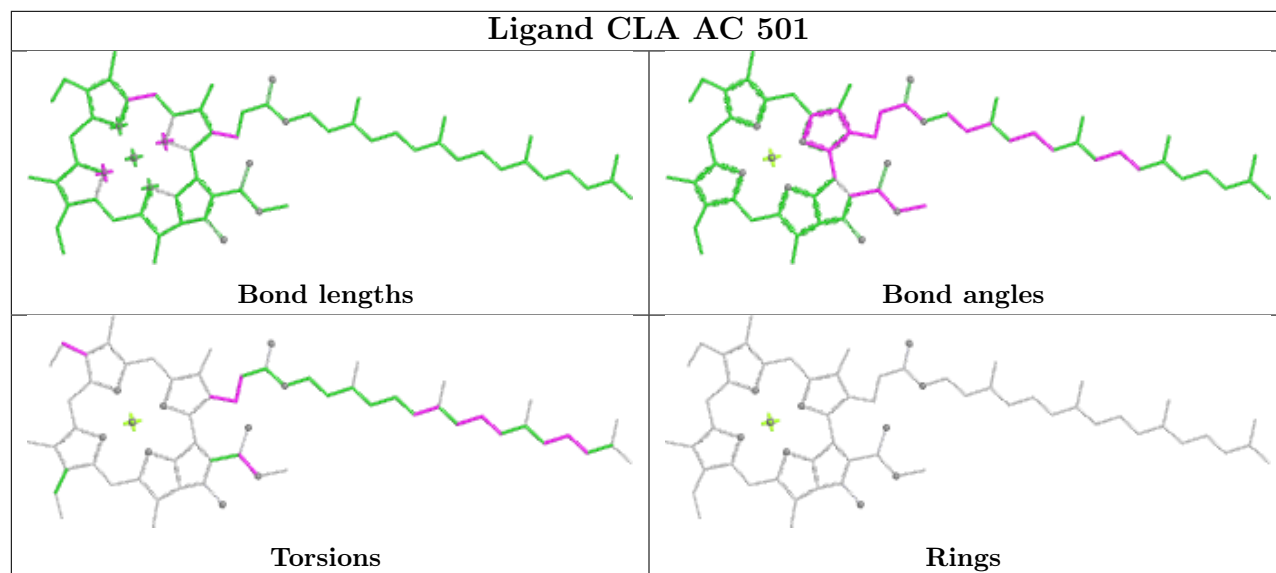
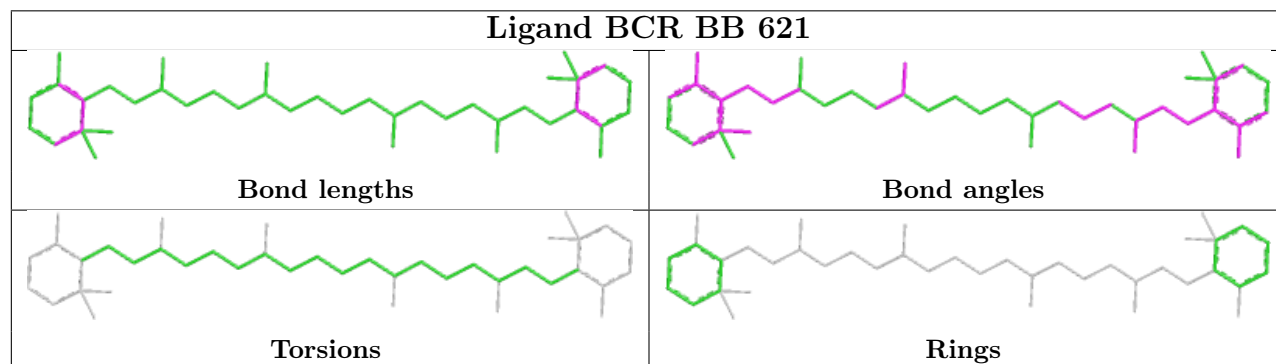
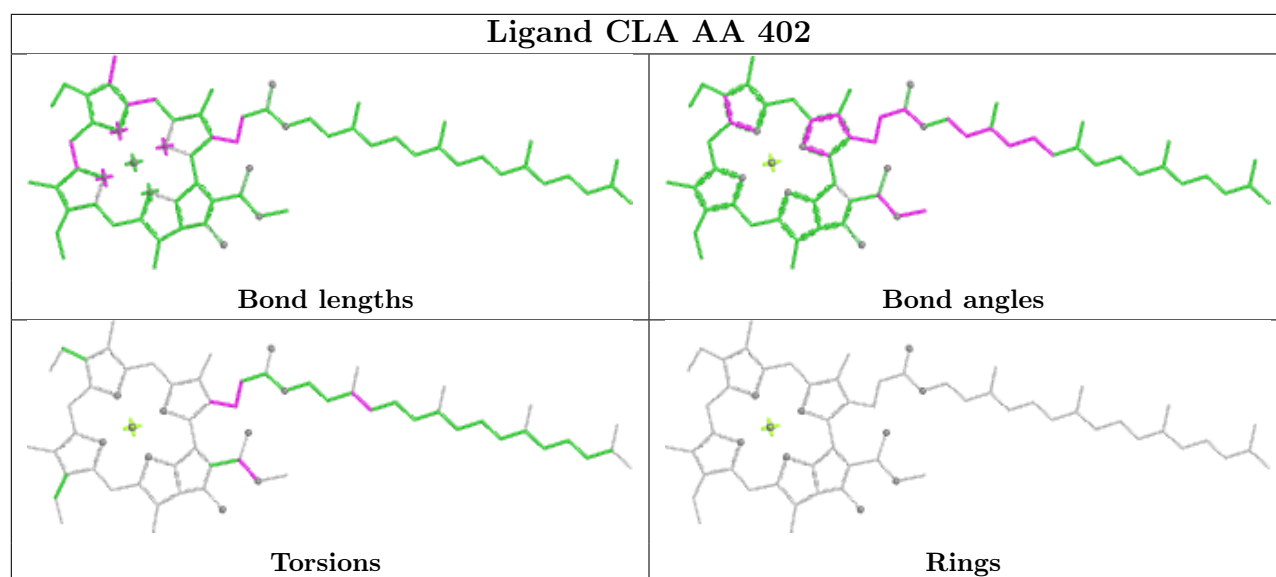


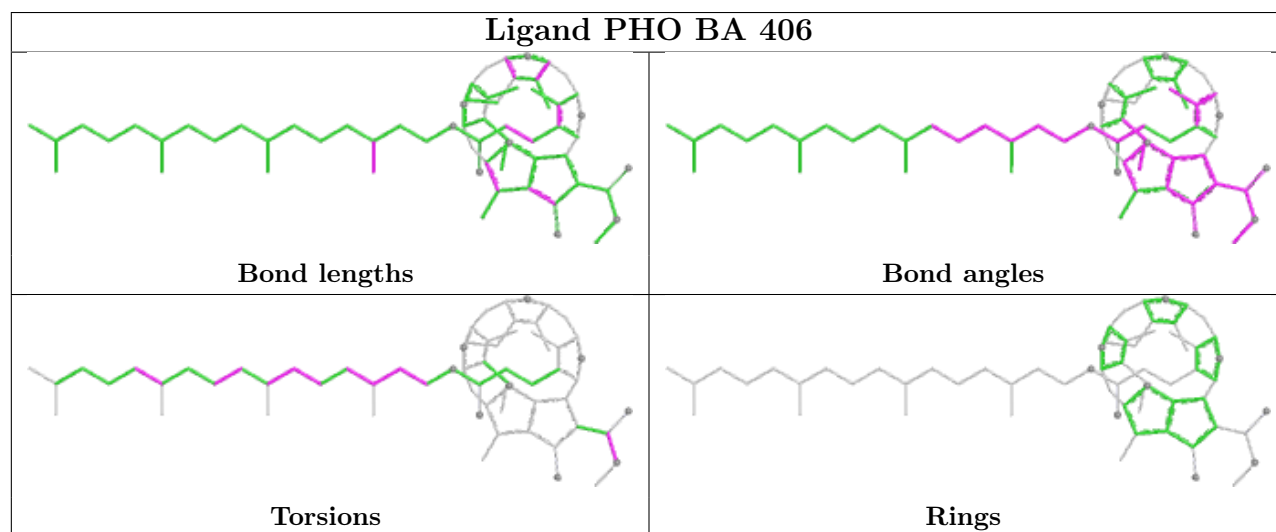
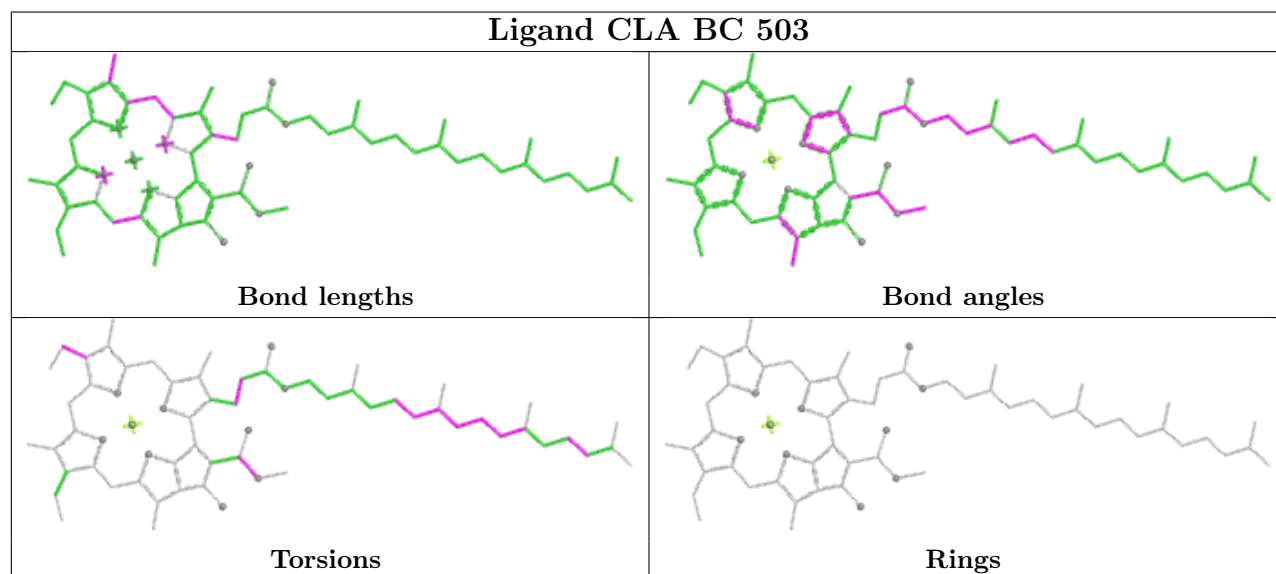
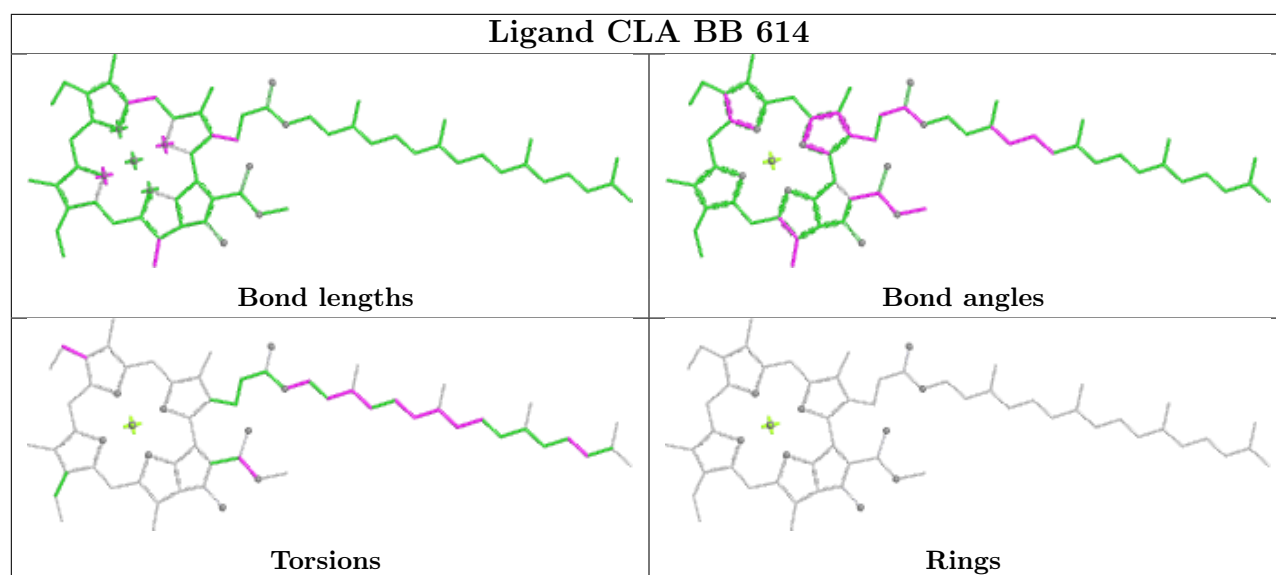
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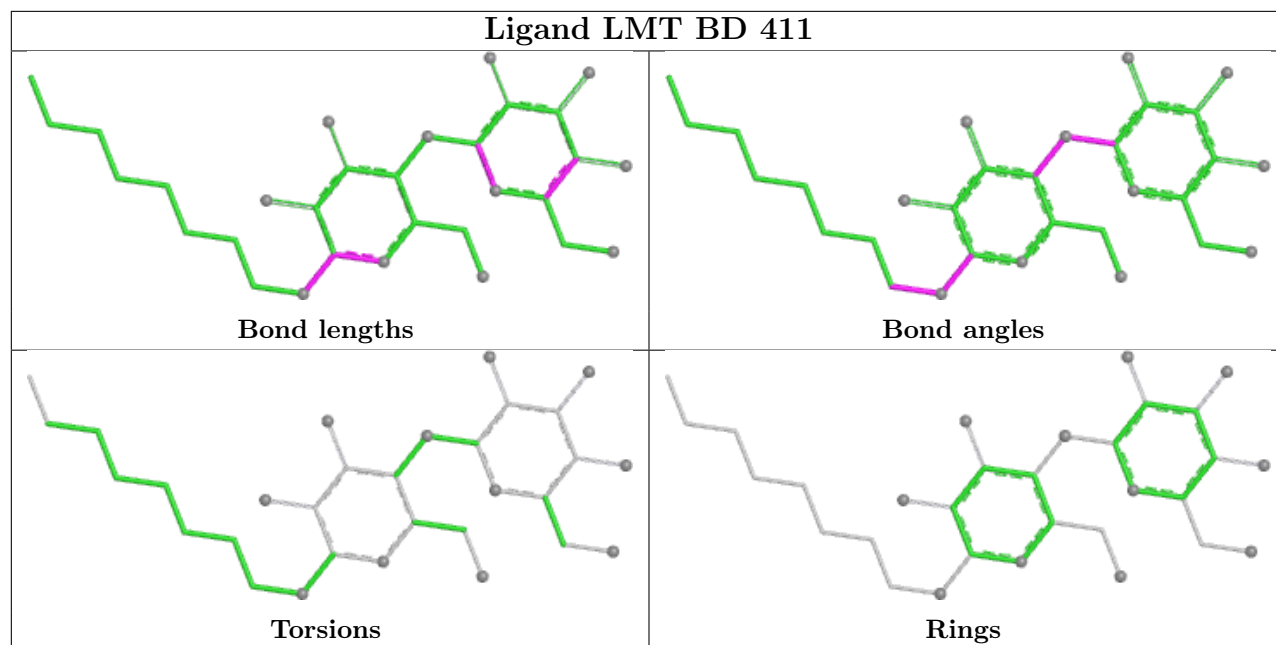
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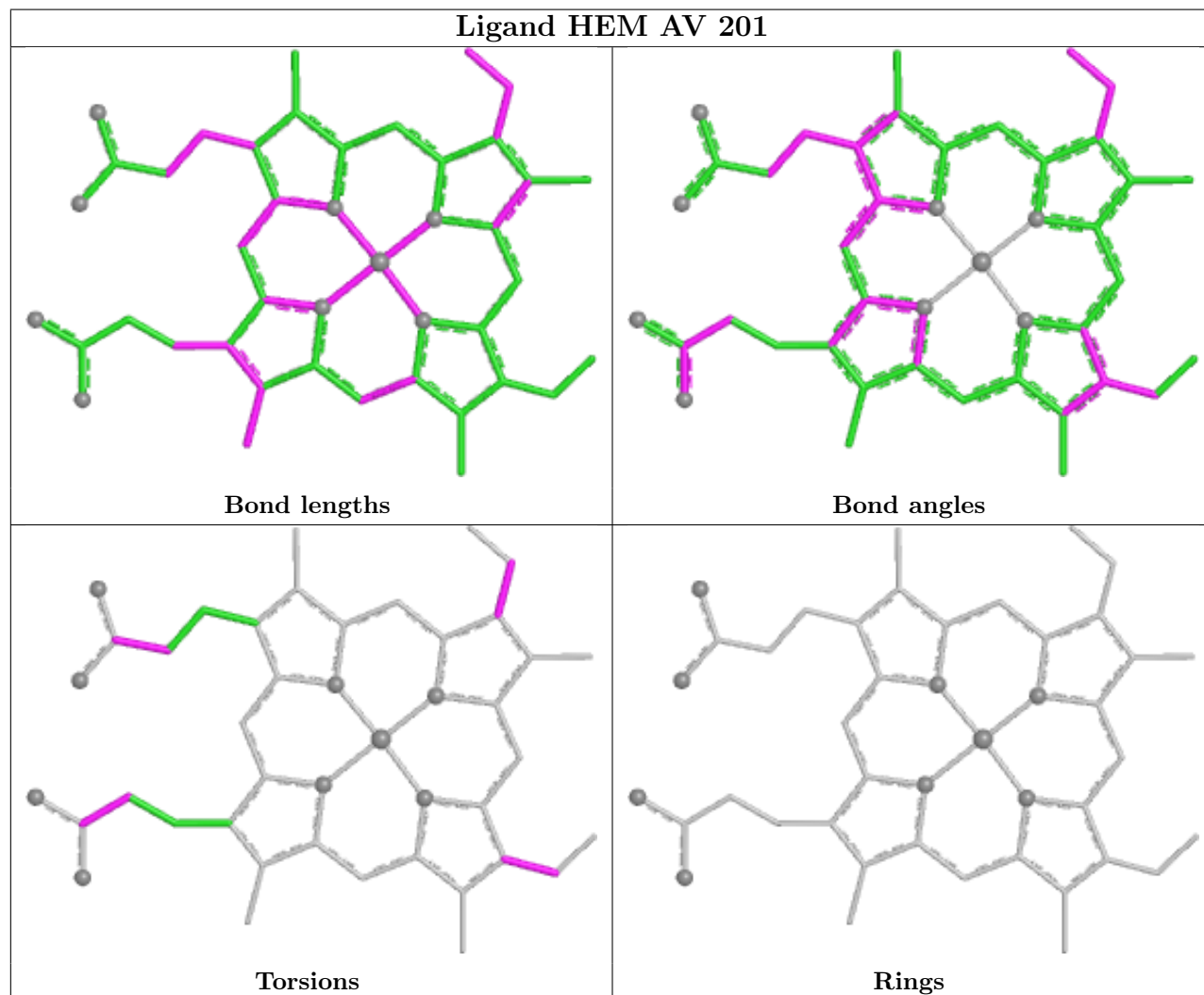


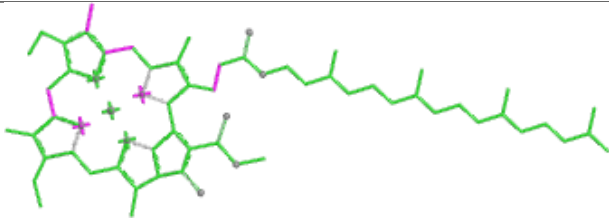
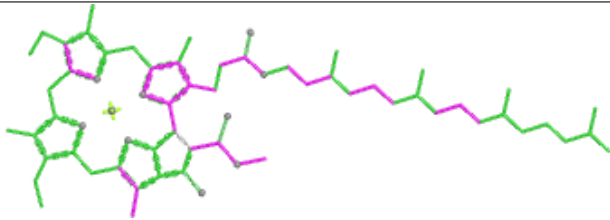
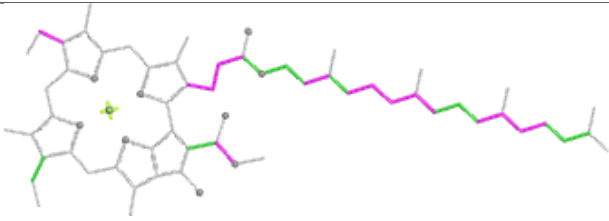
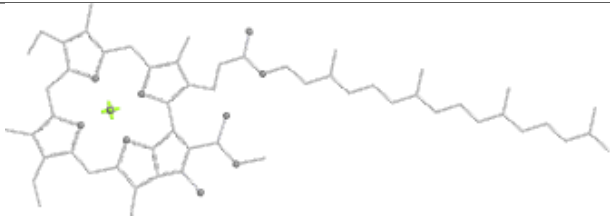


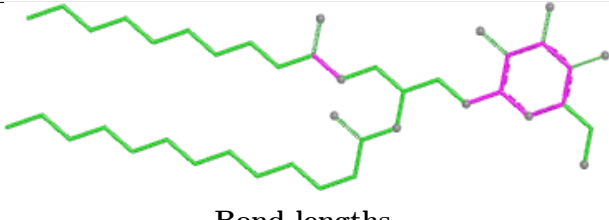
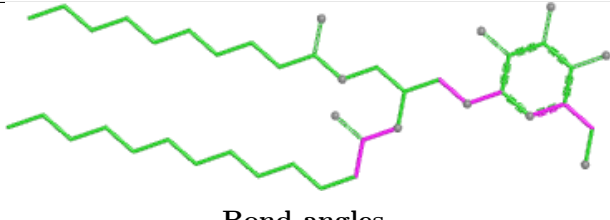
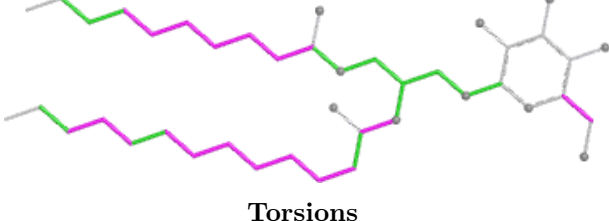
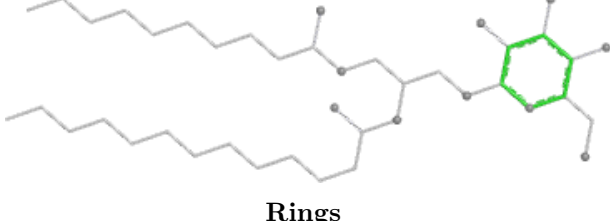
Ligand LMT BD 411

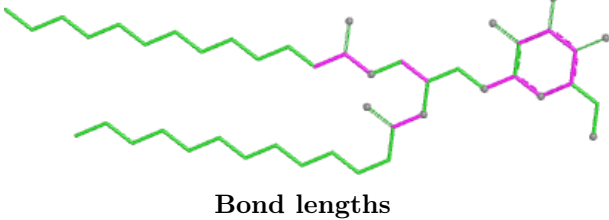
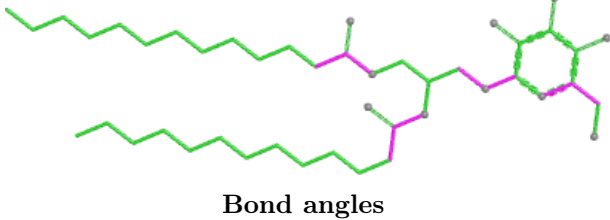
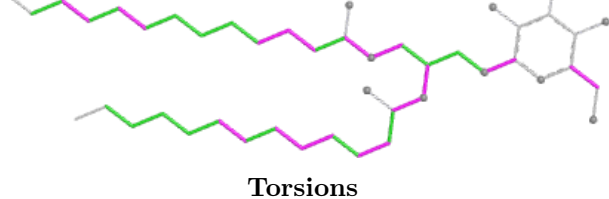
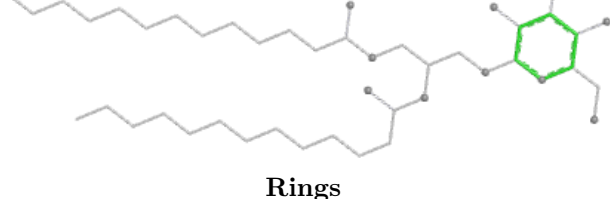


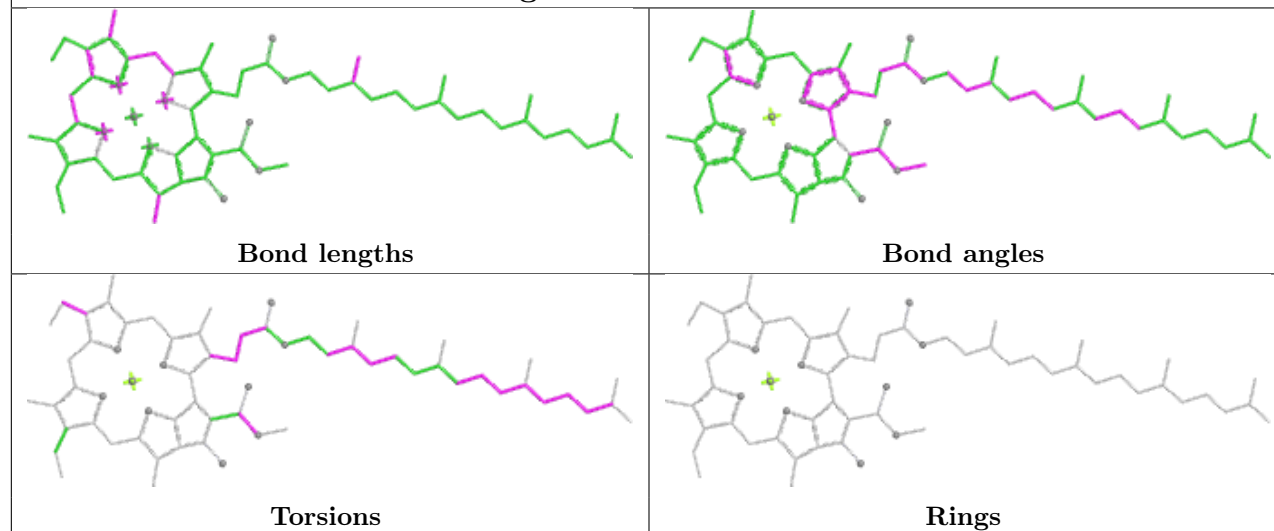
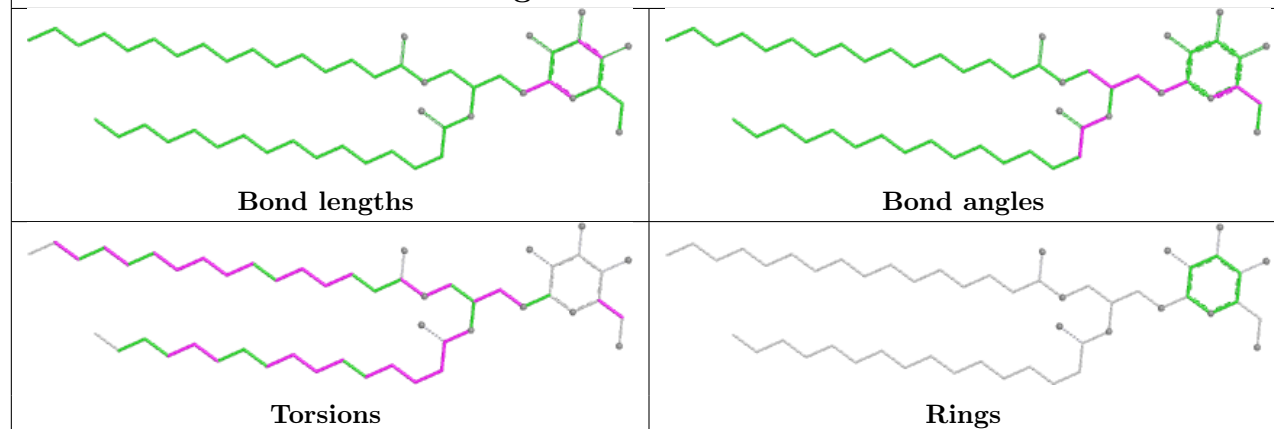
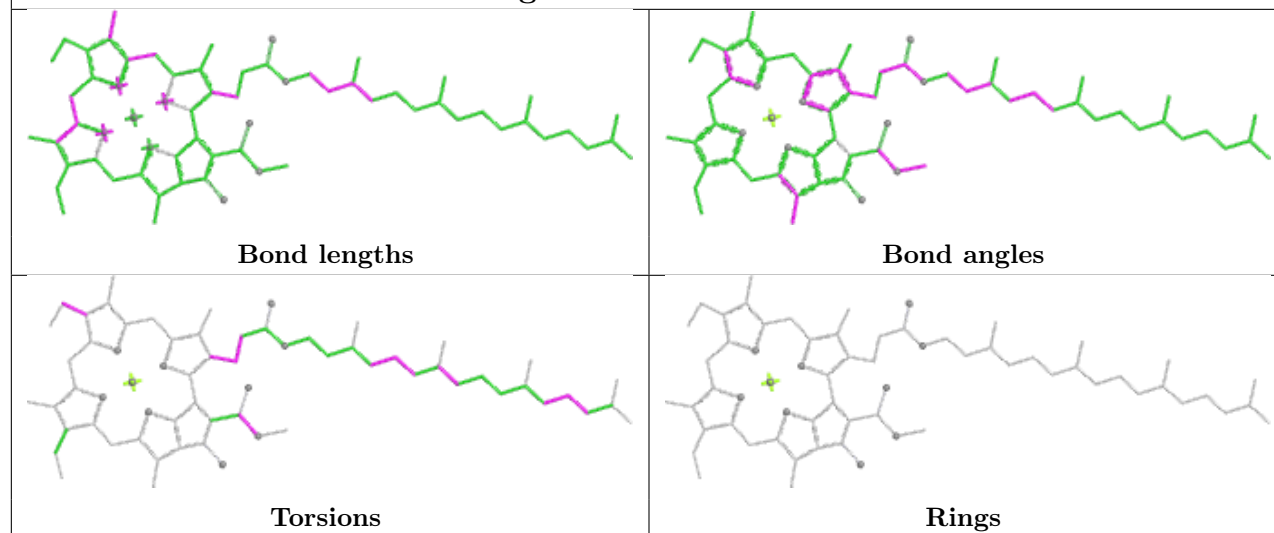
Ligand HEM AV 201



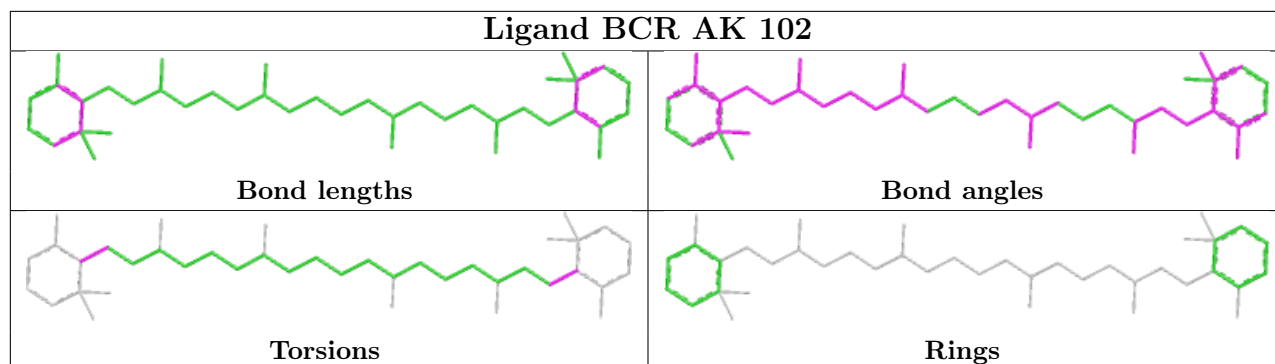
Ligand CLA BB 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG AB 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

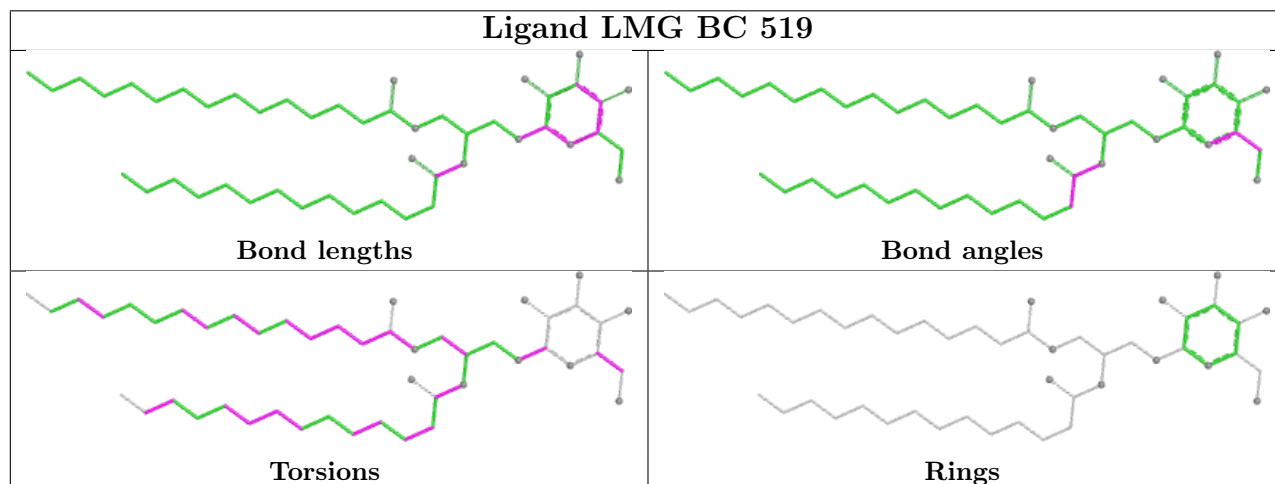
Ligand LMG BC 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BC 512**Ligand LMG AA 413****Ligand CLA AB 607**

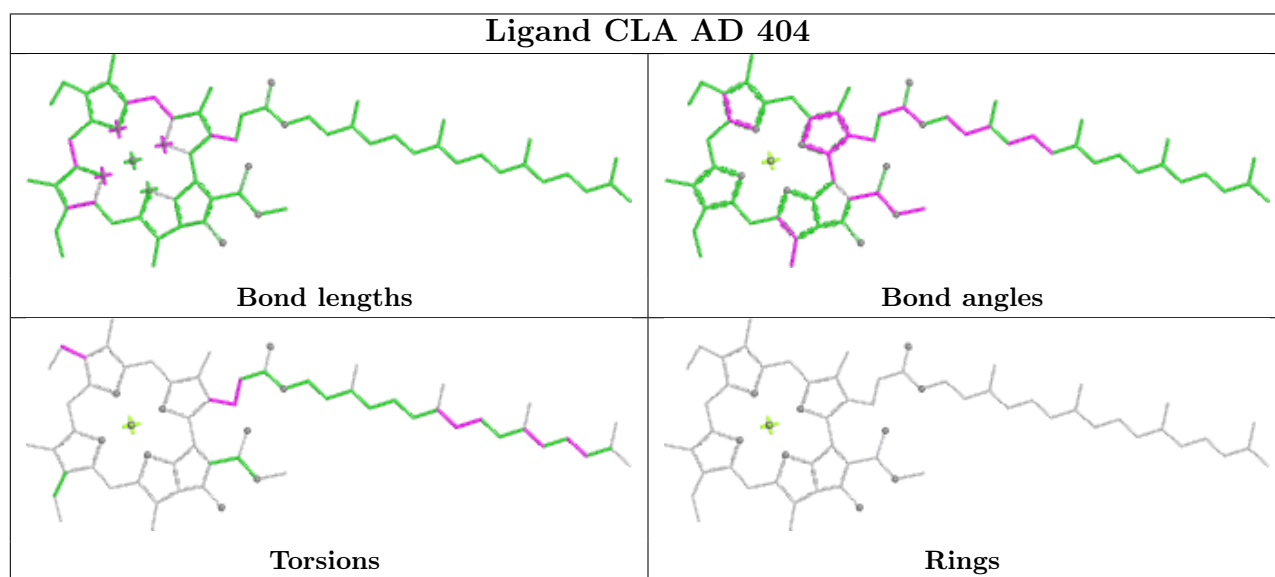
Ligand BCR AK 102

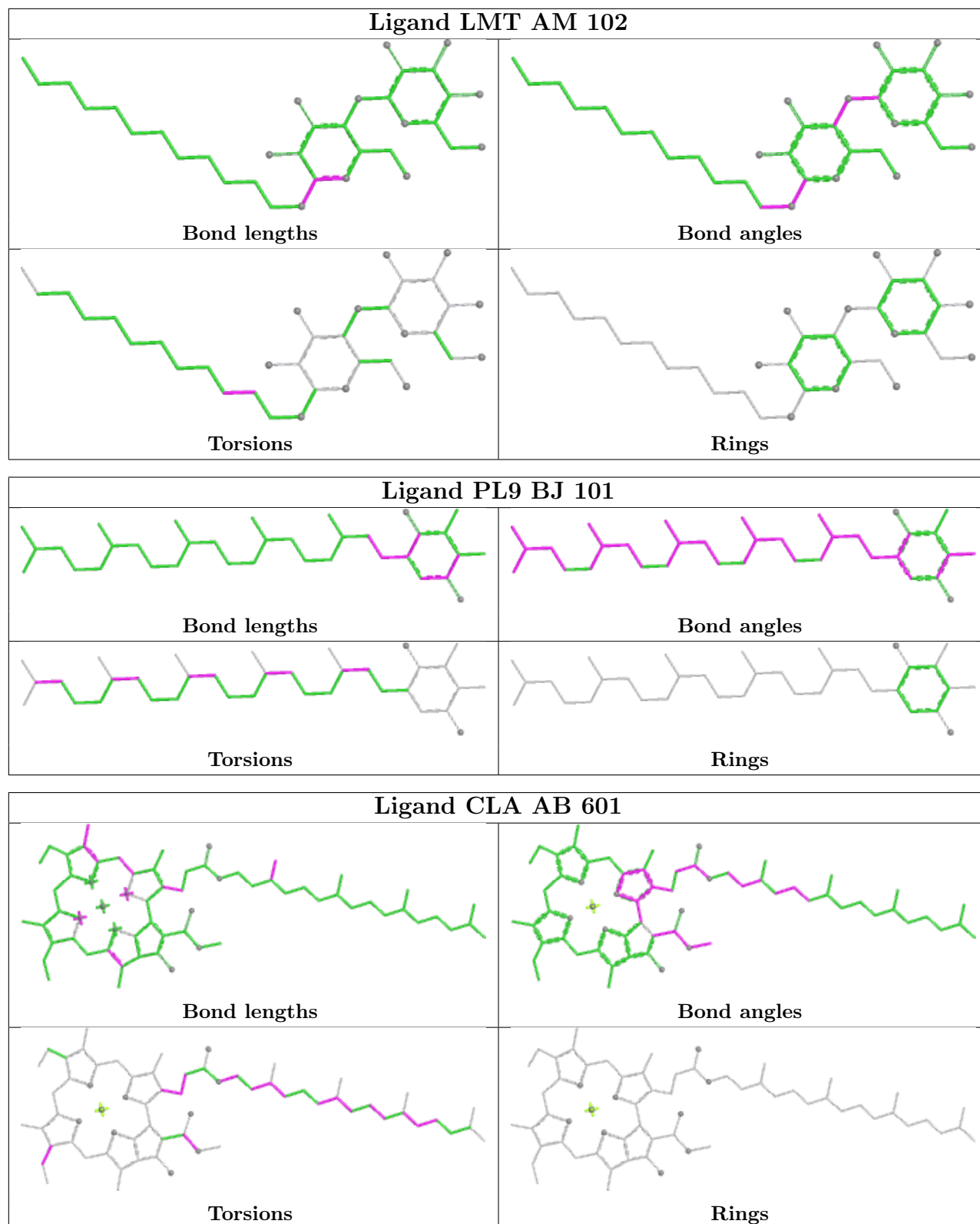


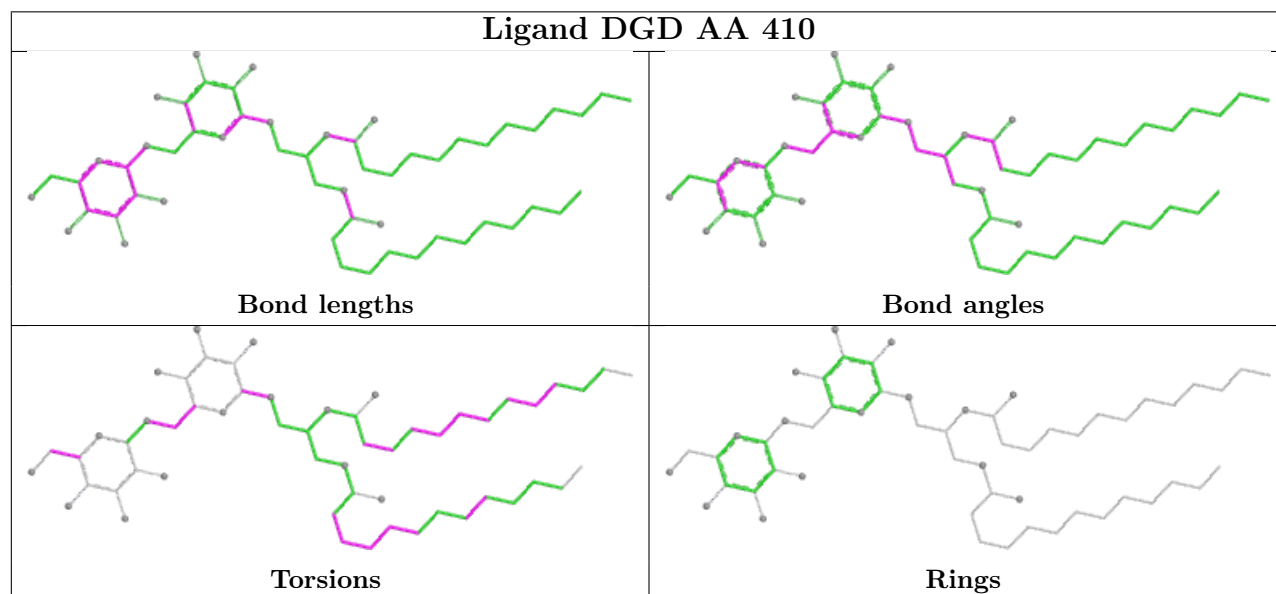
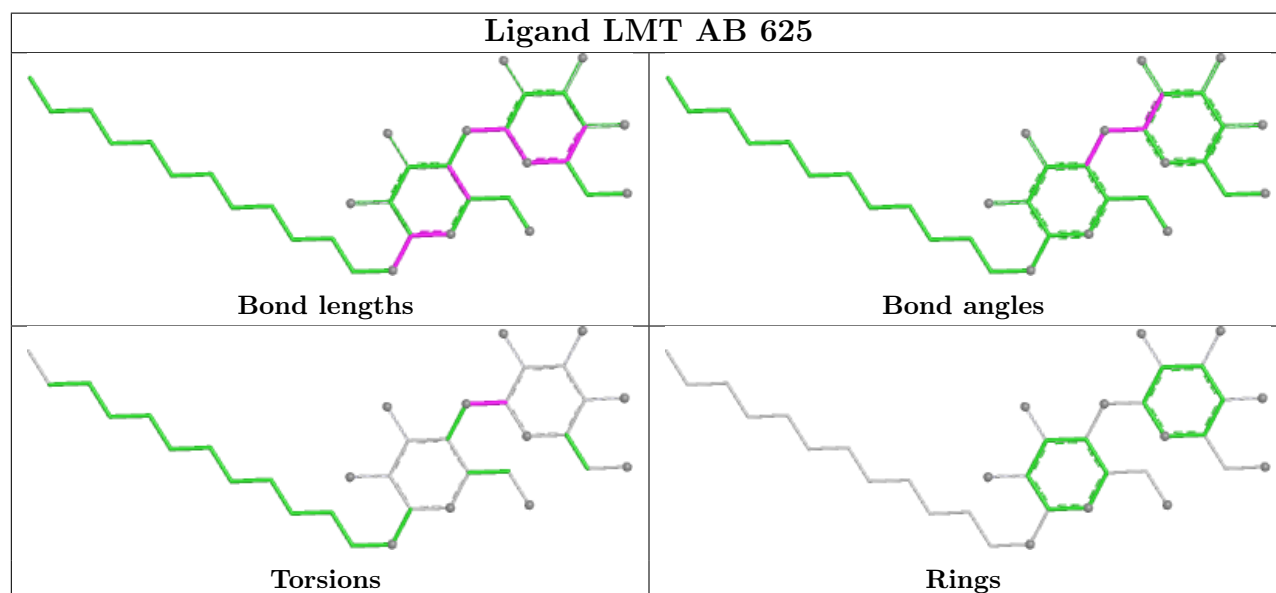
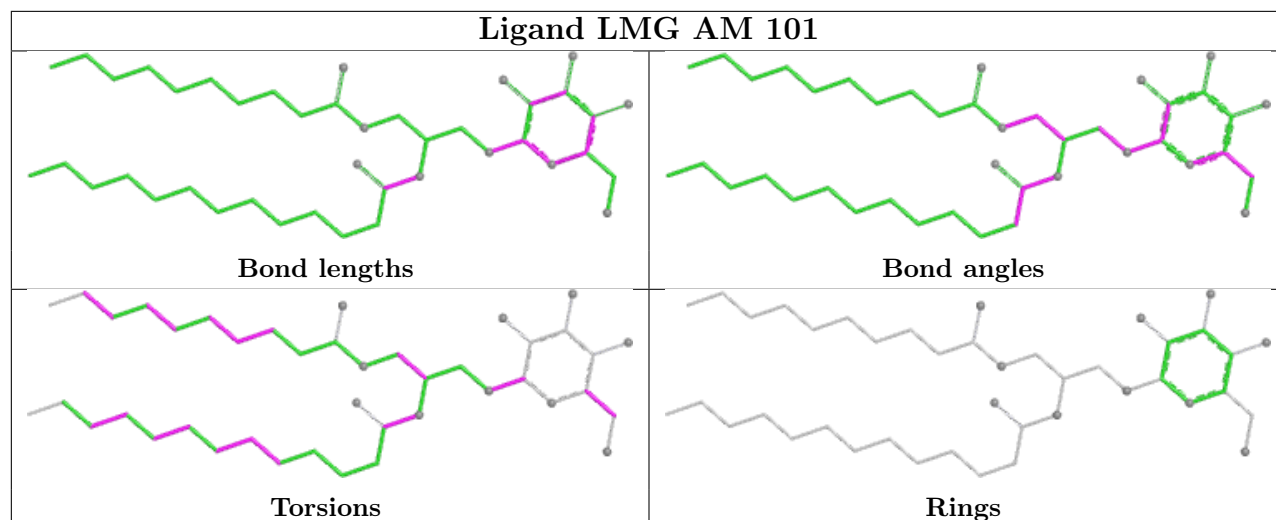
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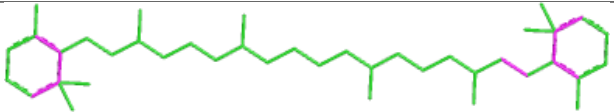
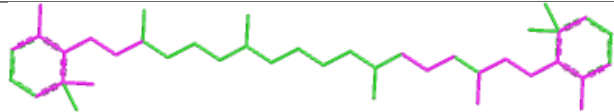
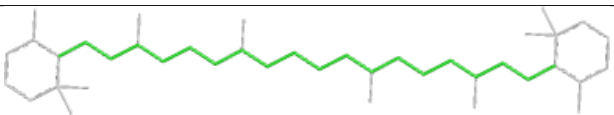
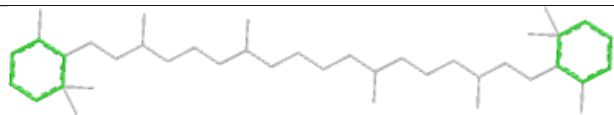


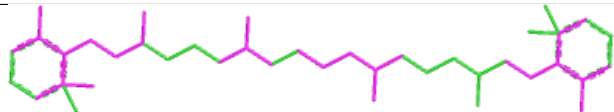
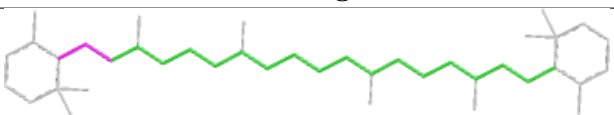
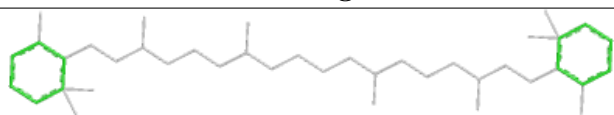
Ligand CLA AD 404

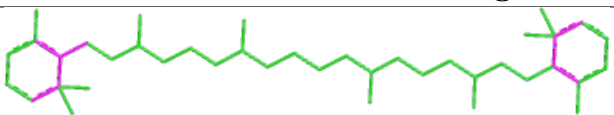
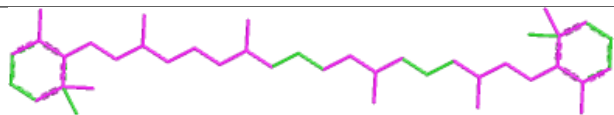
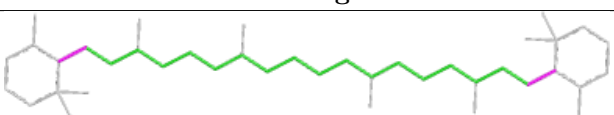
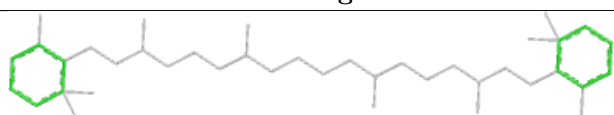


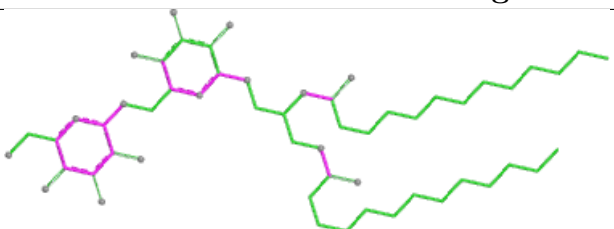
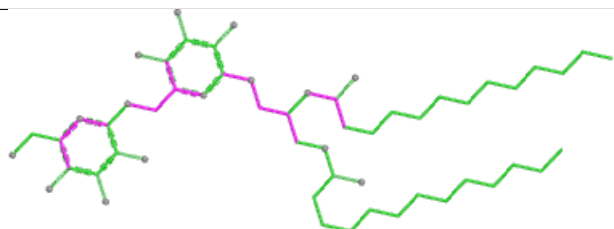
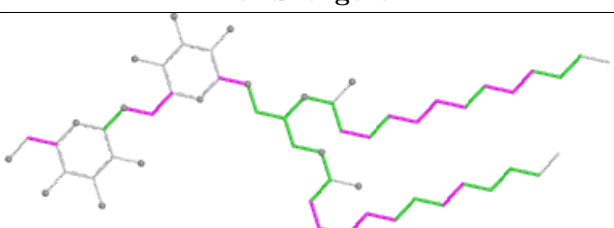
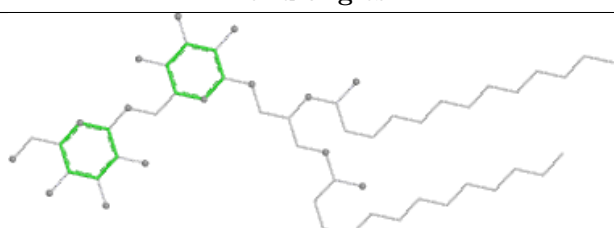


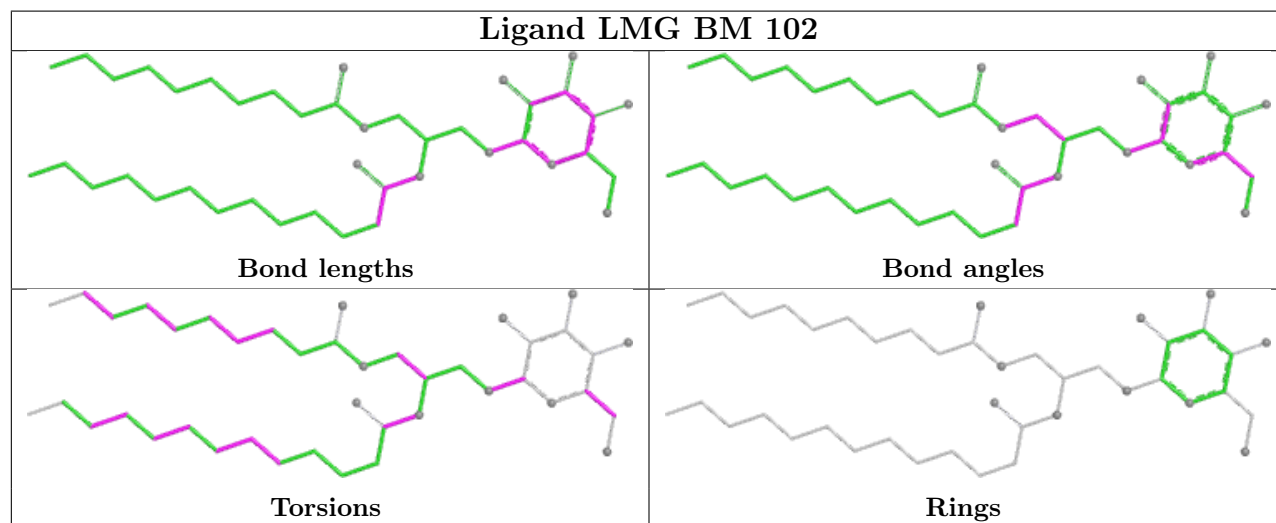
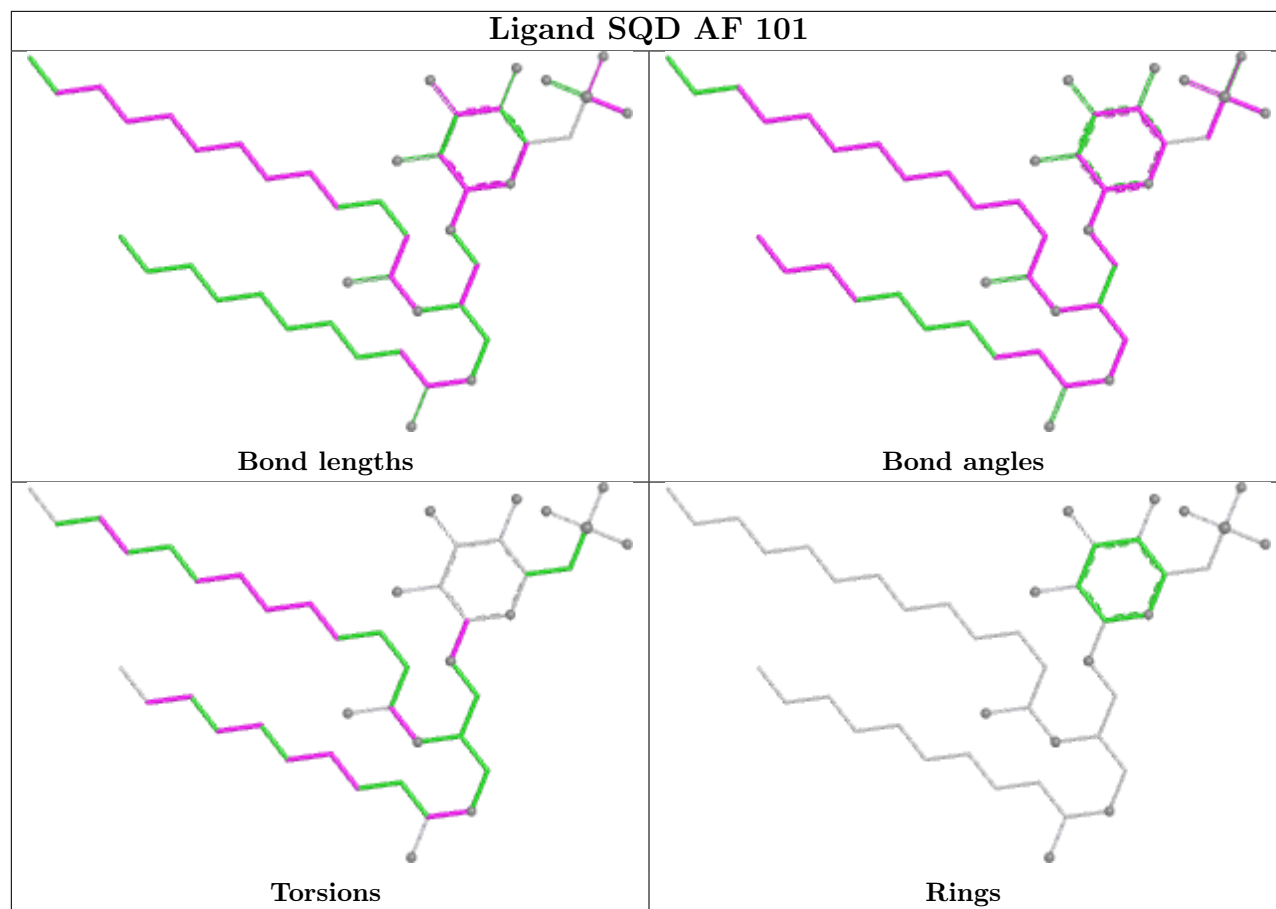


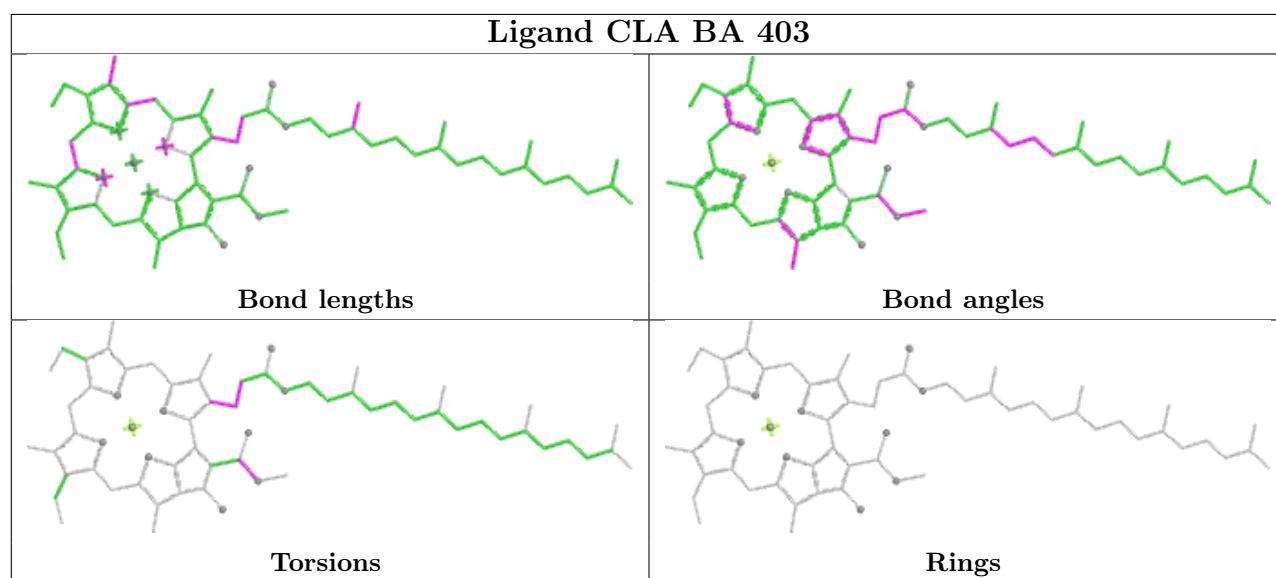
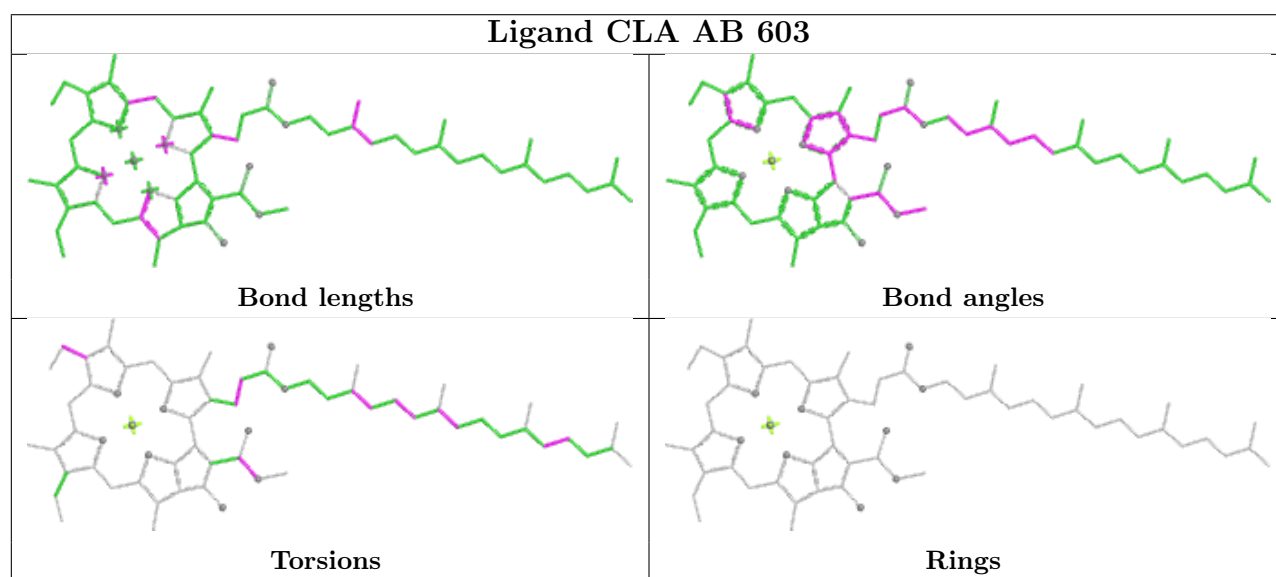
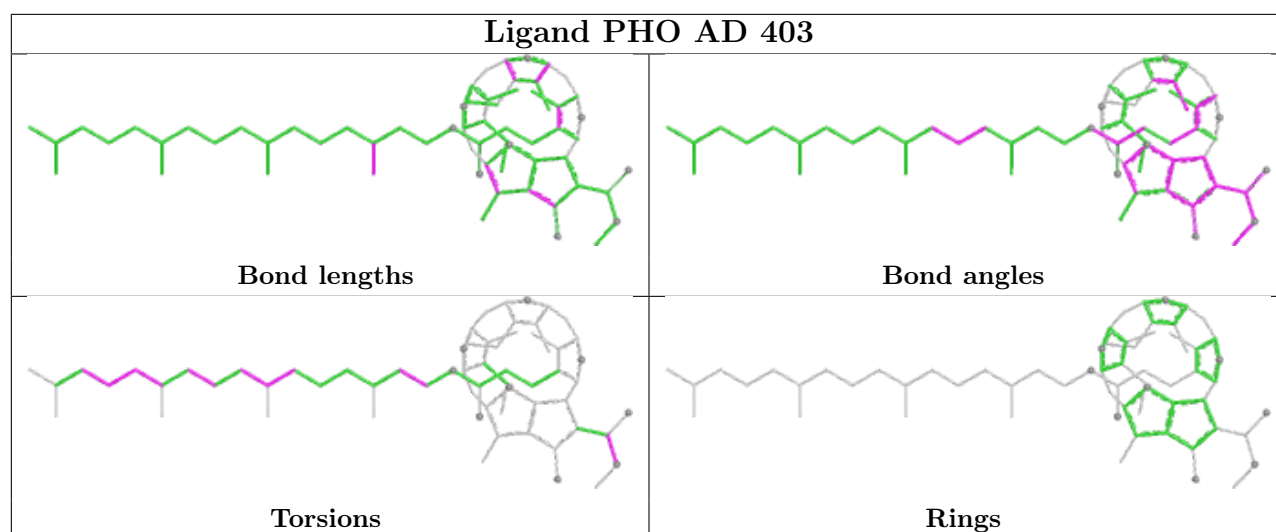
Ligand BCR AB 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

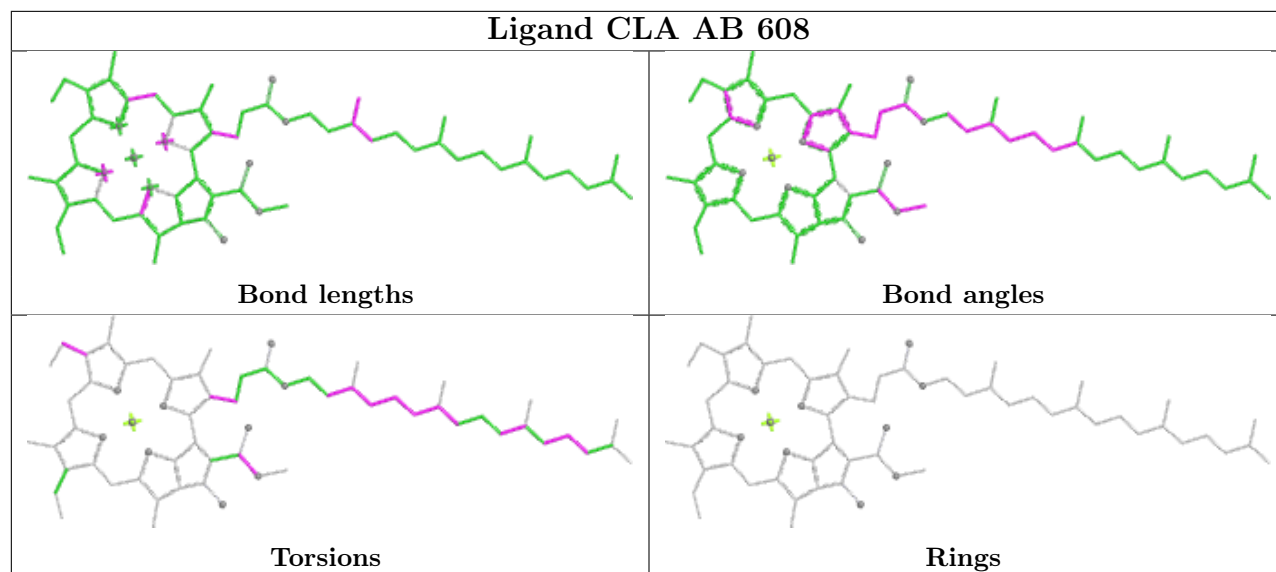
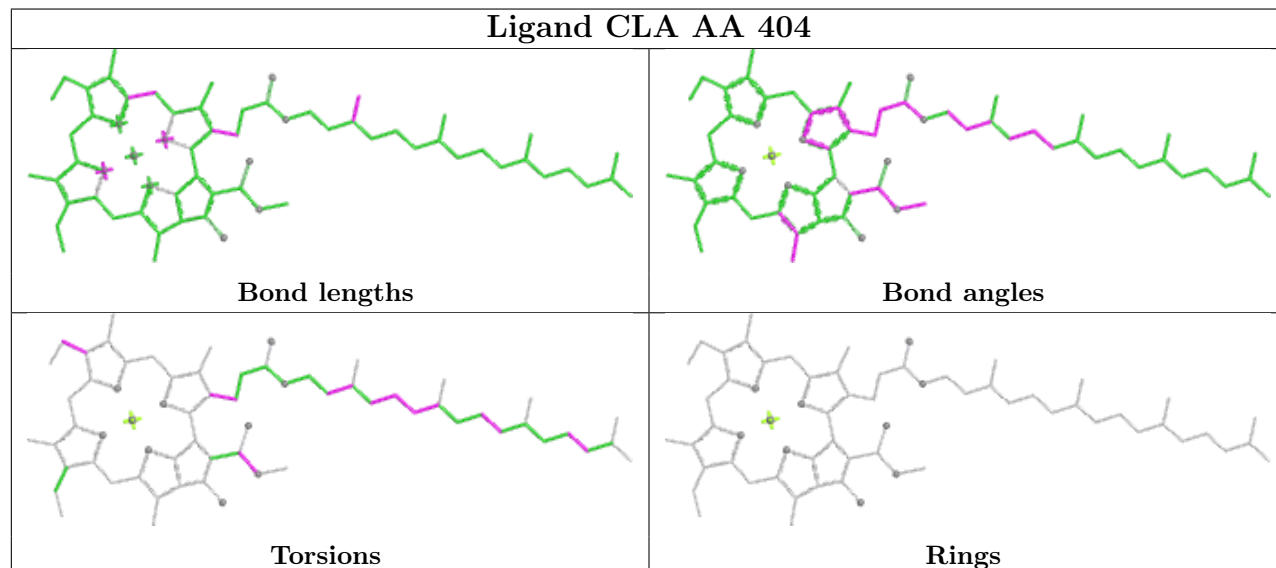
Ligand BCR BZ 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BK 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

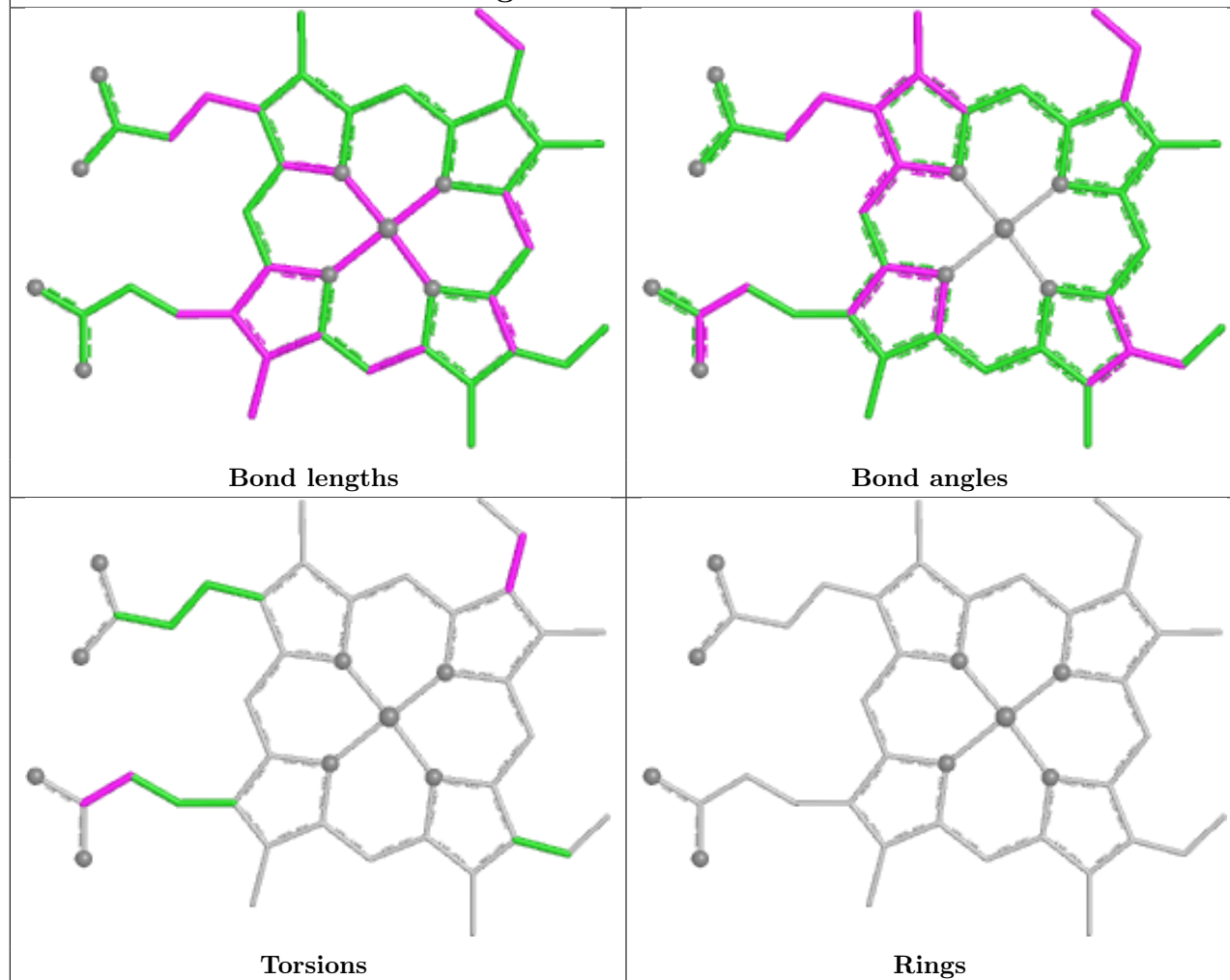
Ligand DGD BA 411	
	
Bond lengths	Bond angles
	
Torsions	Rings



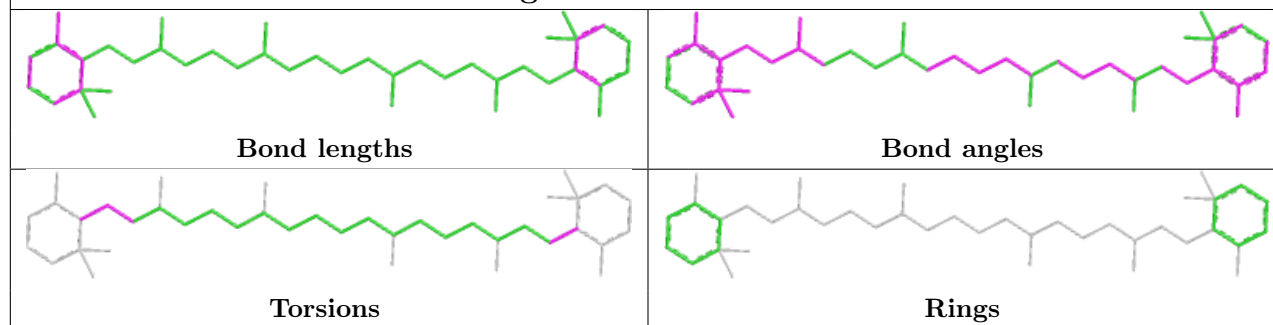


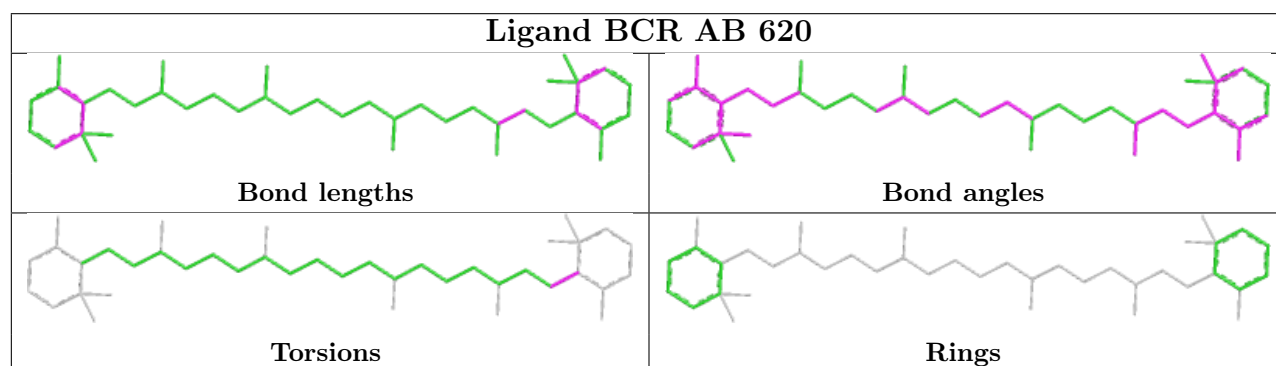
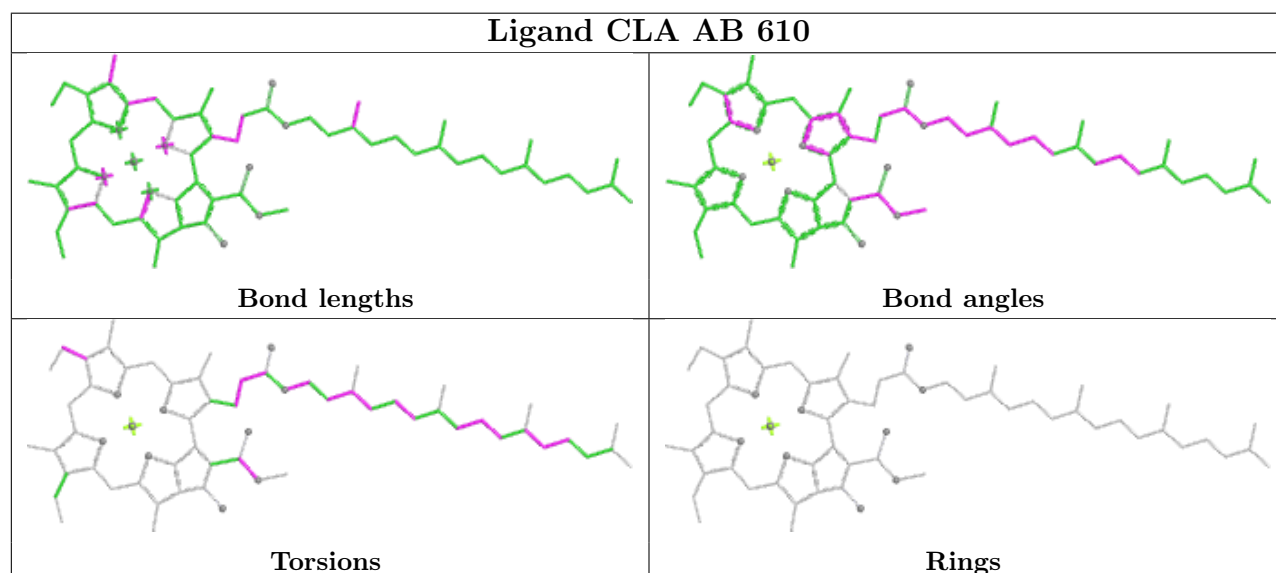
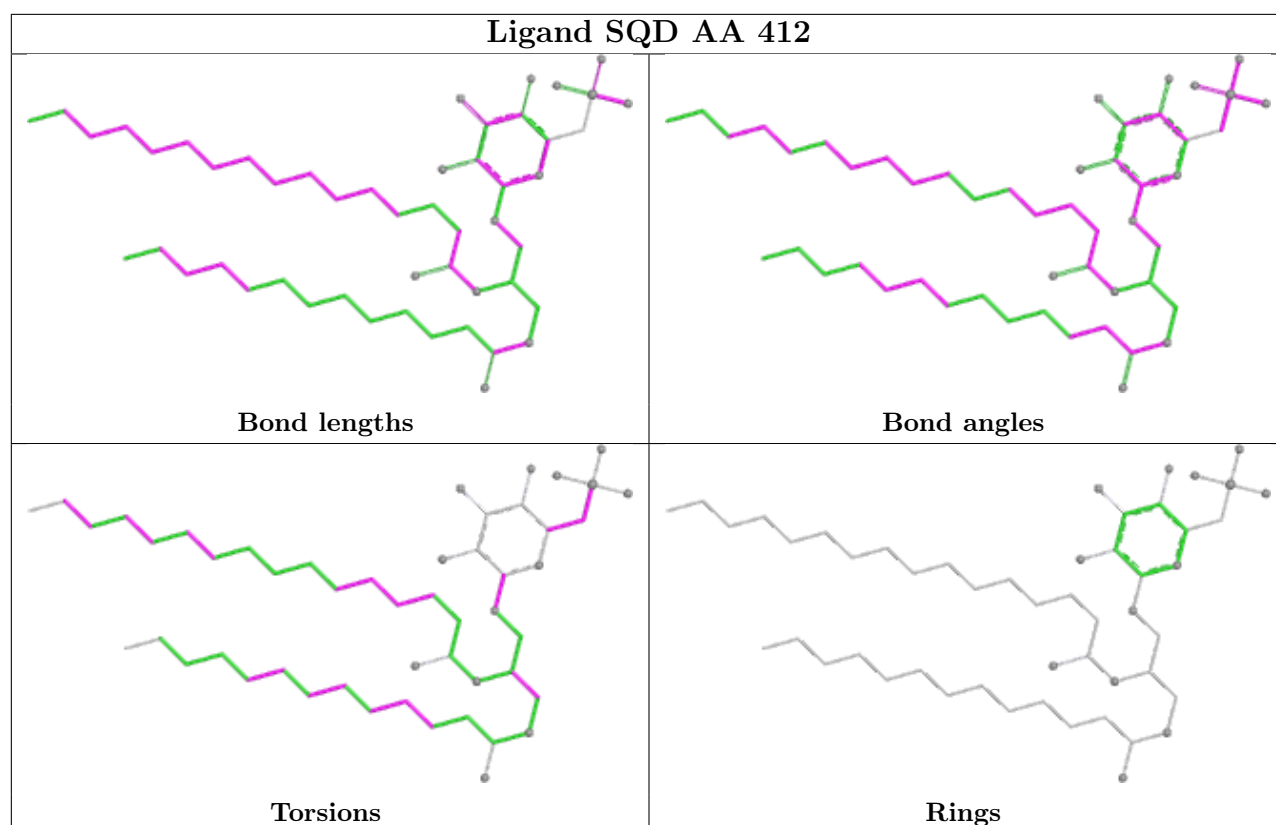
Ligand CLA AB 608**Ligand CLA AA 404**

Ligand HEM BE 101

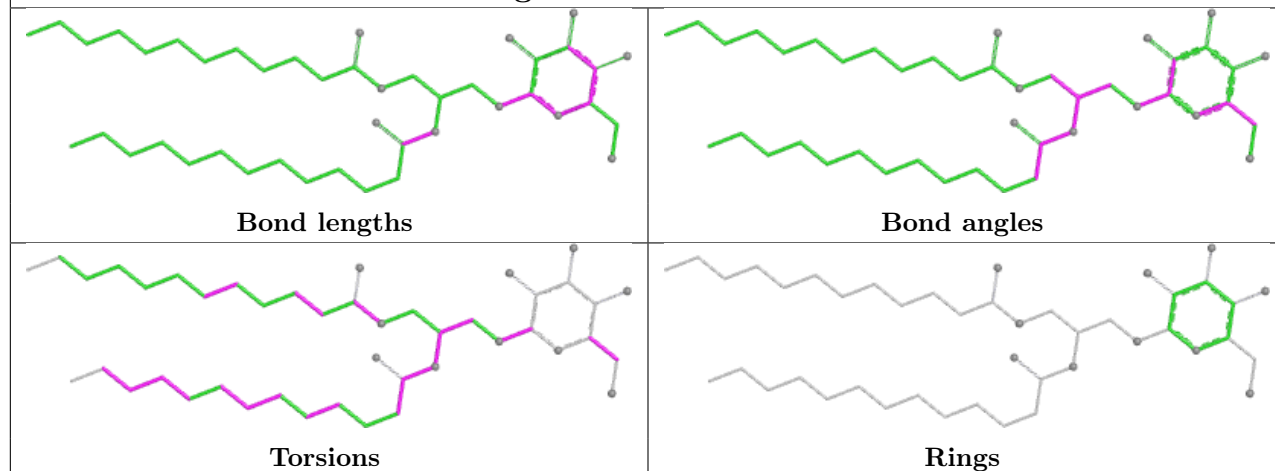


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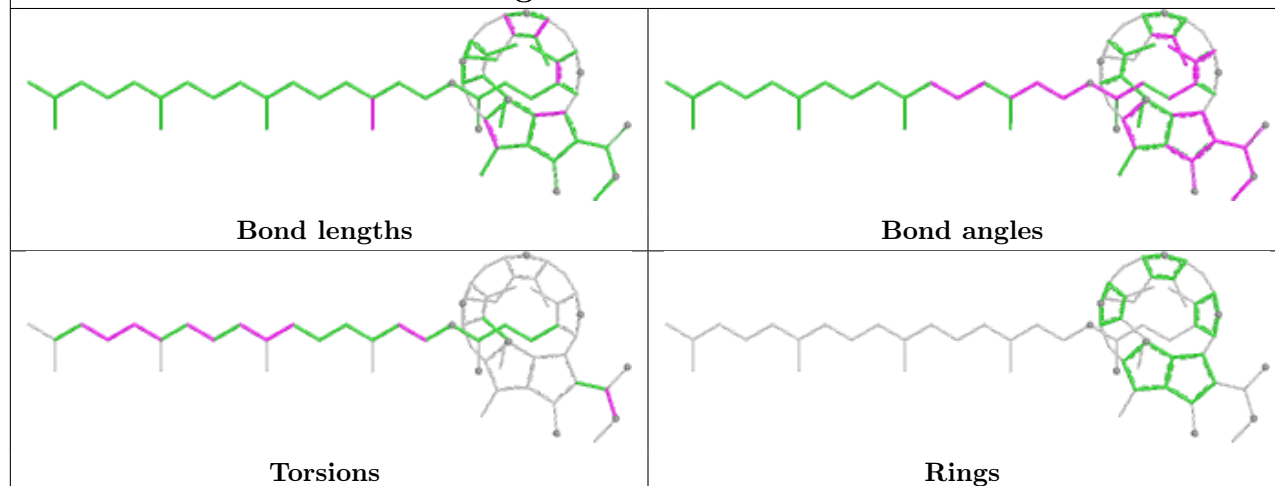




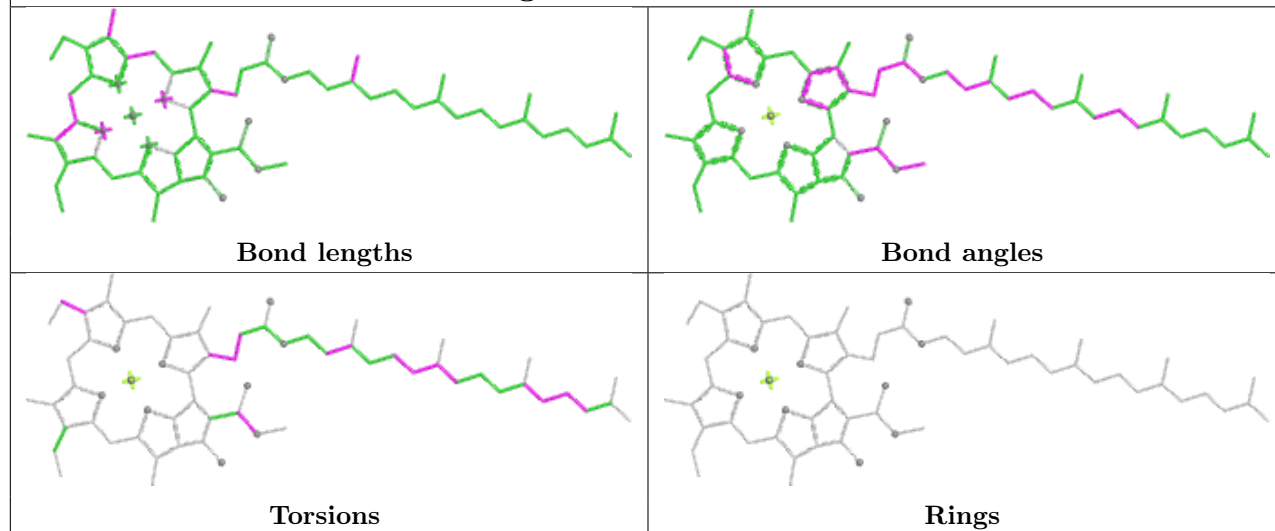
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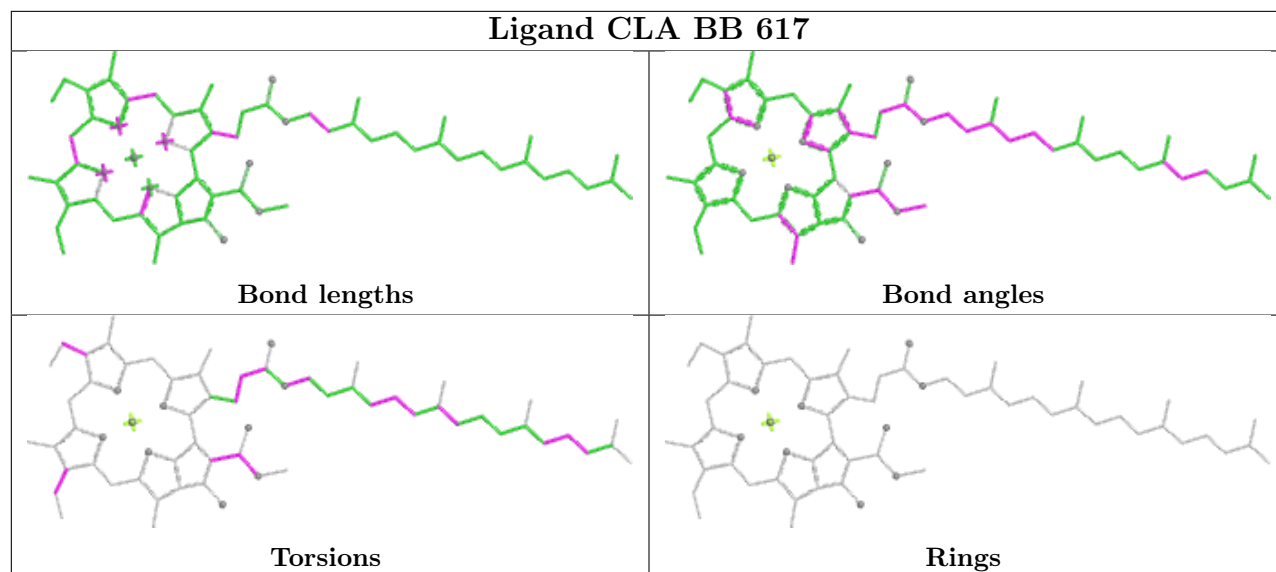
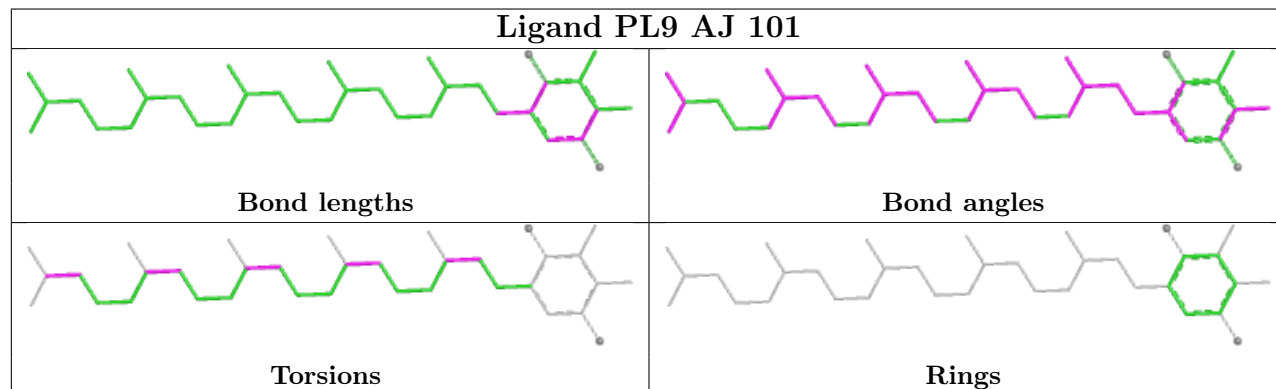
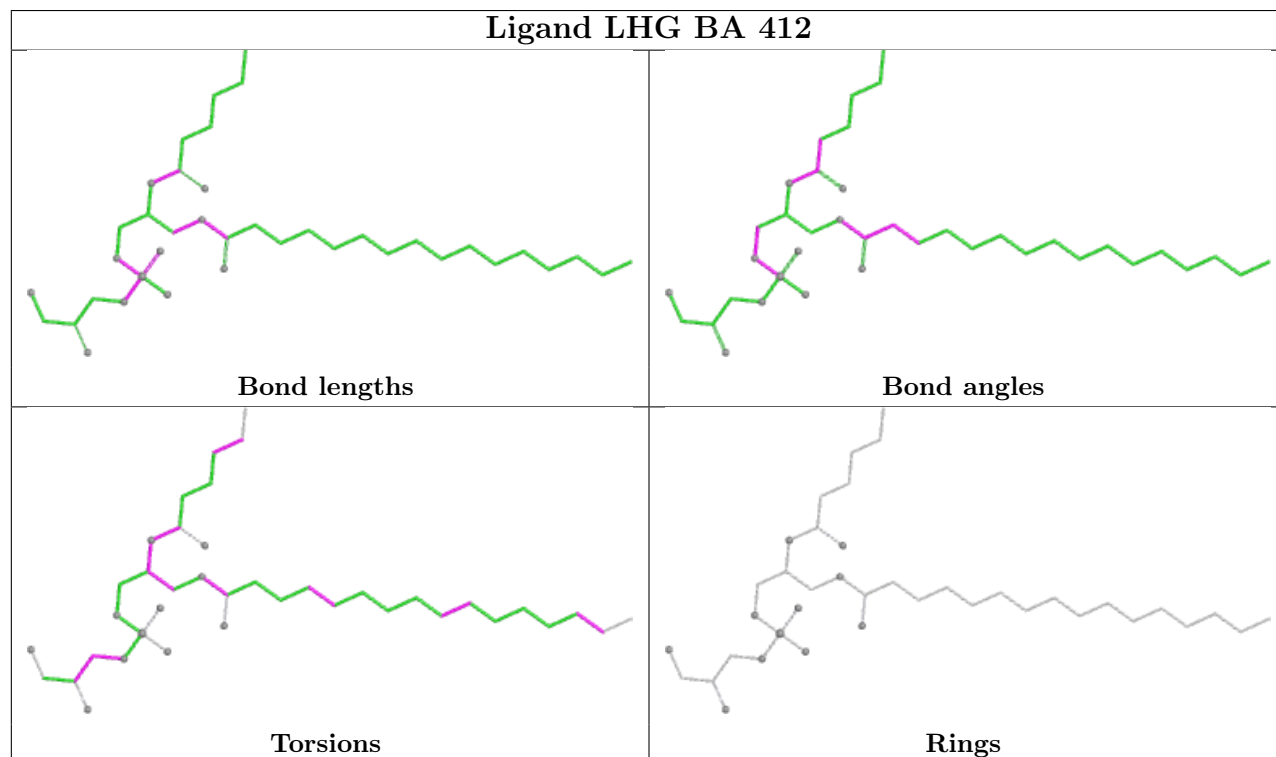


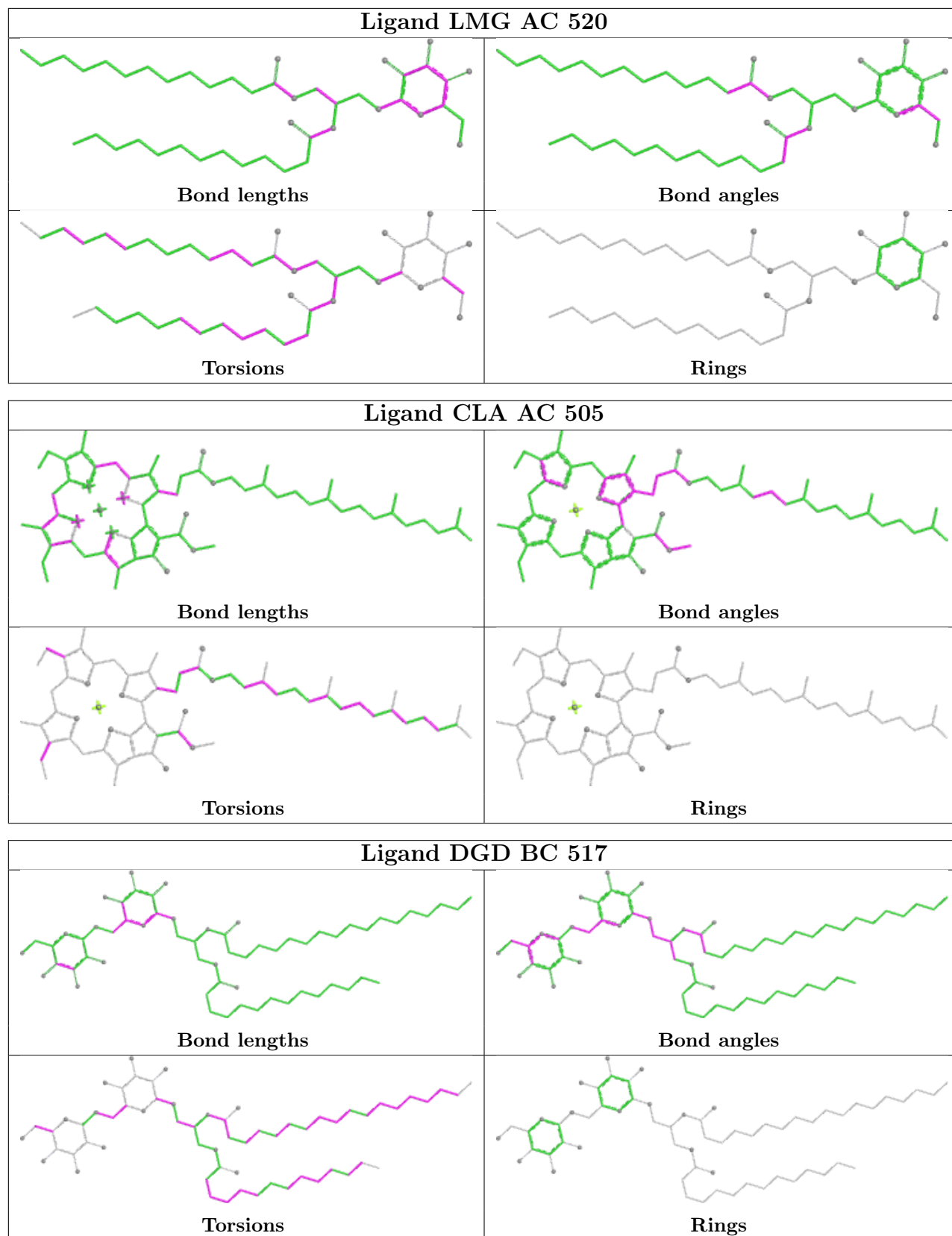
Ligand PHO BD 403

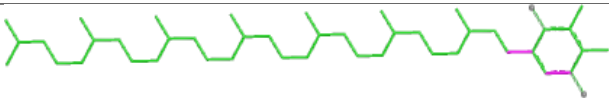
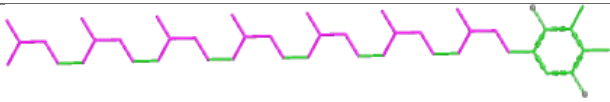
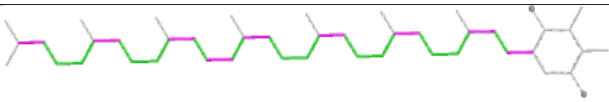
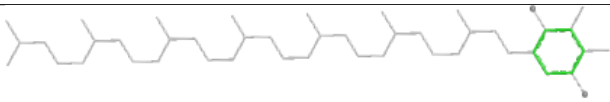


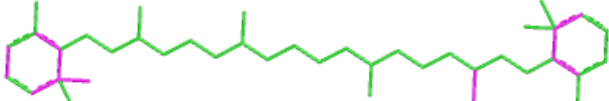
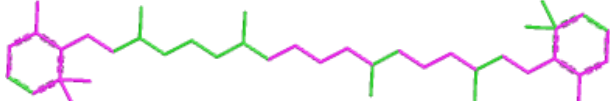
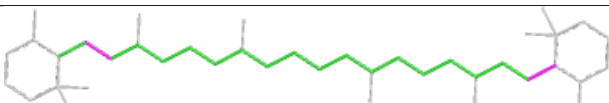
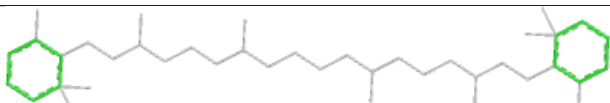
Ligand CLA AC 513

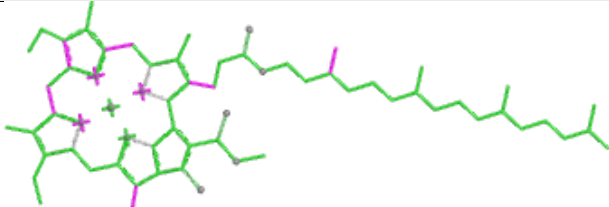
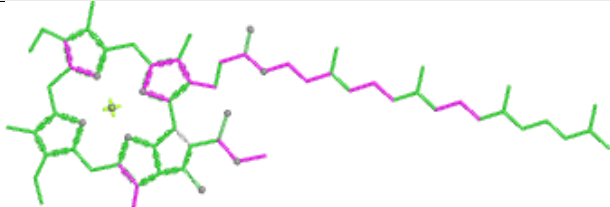
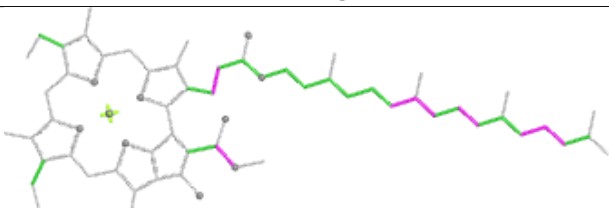
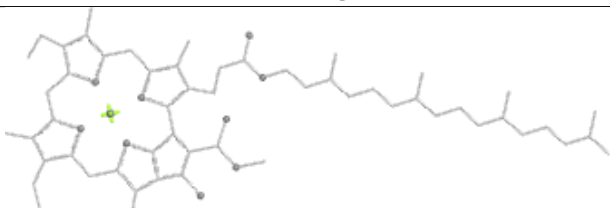


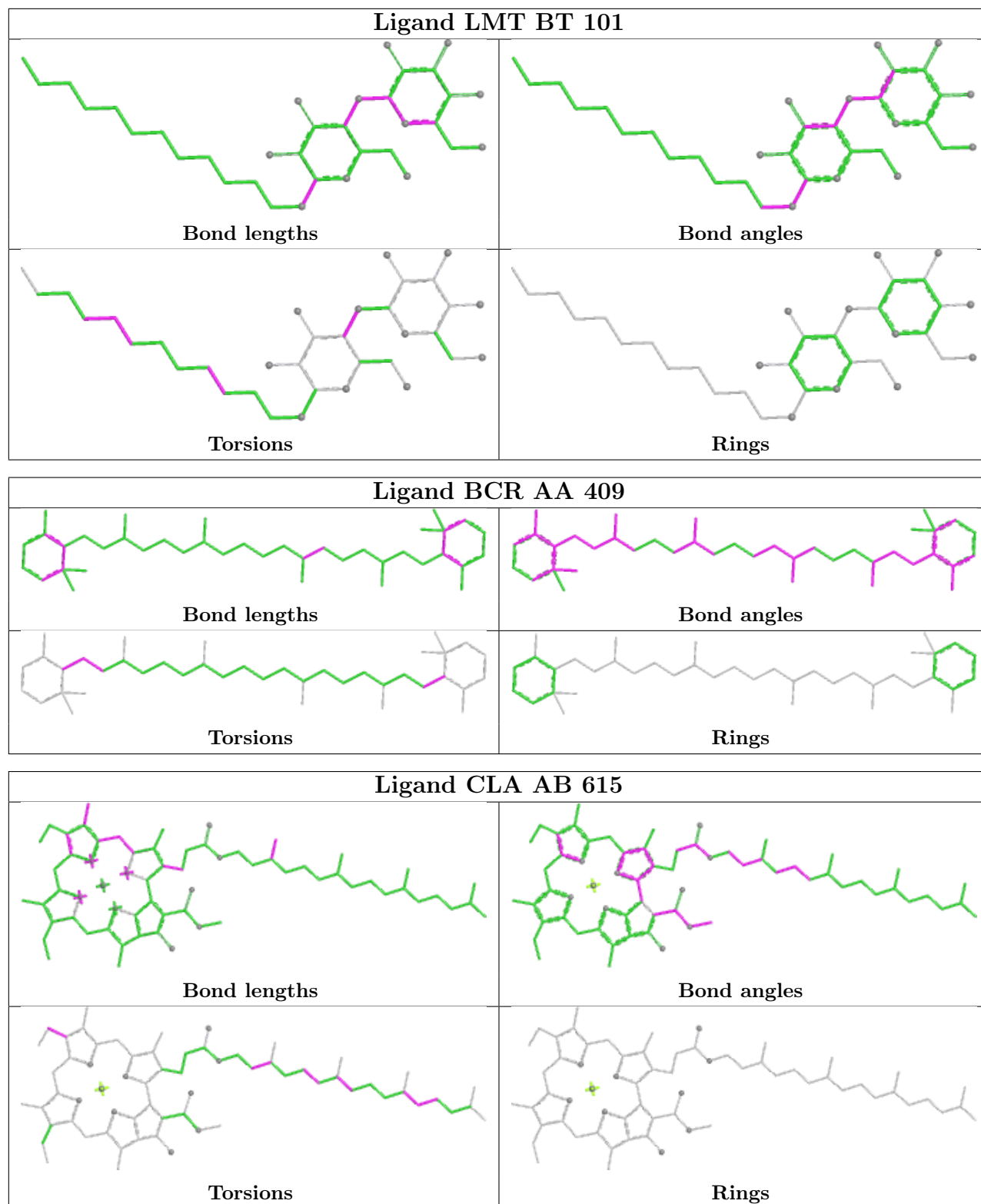
Ligand CLA BB 617**Ligand PL9 AJ 101****Ligand LHG BA 412**

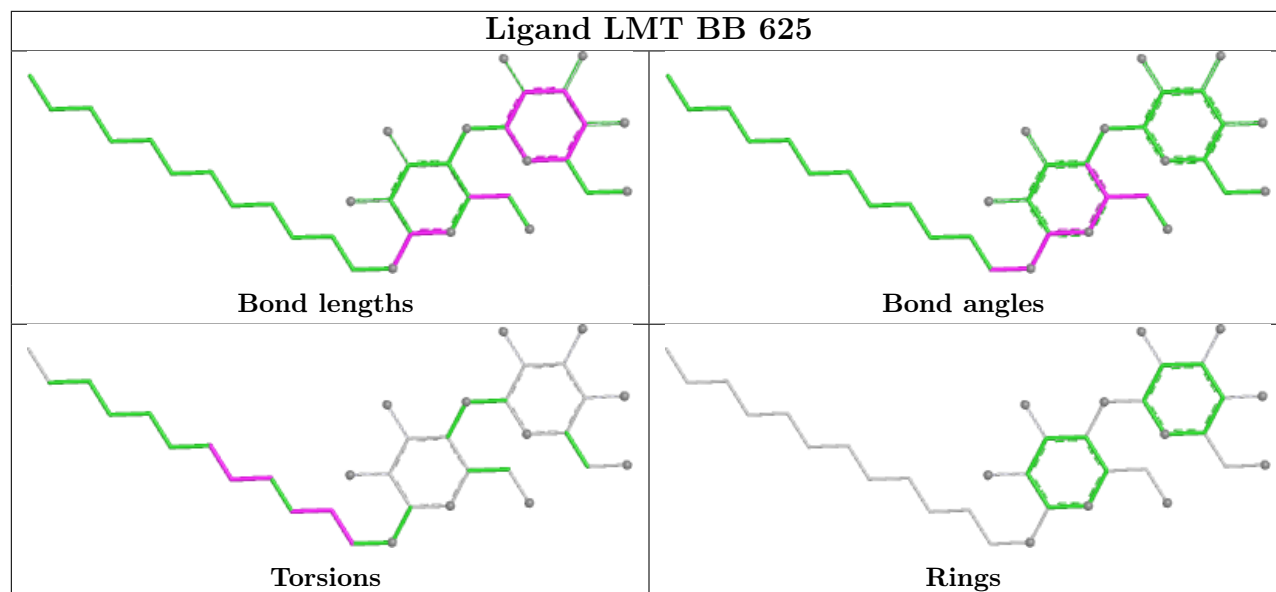
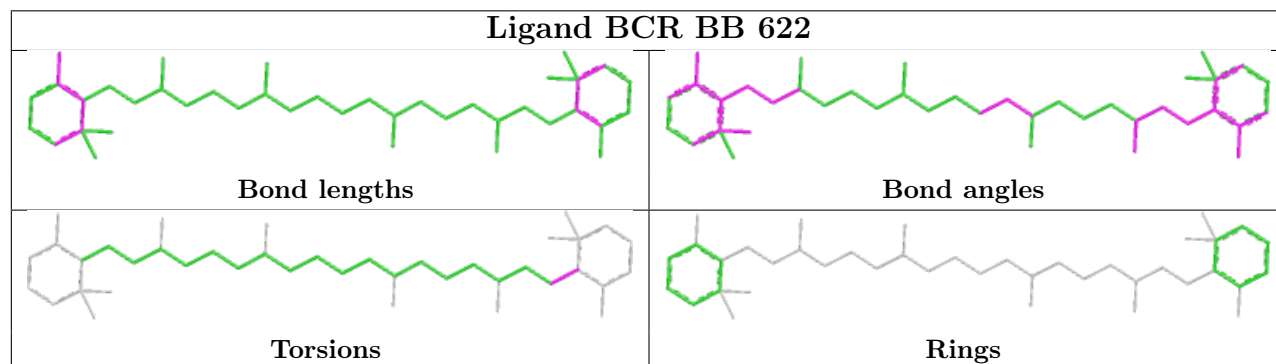
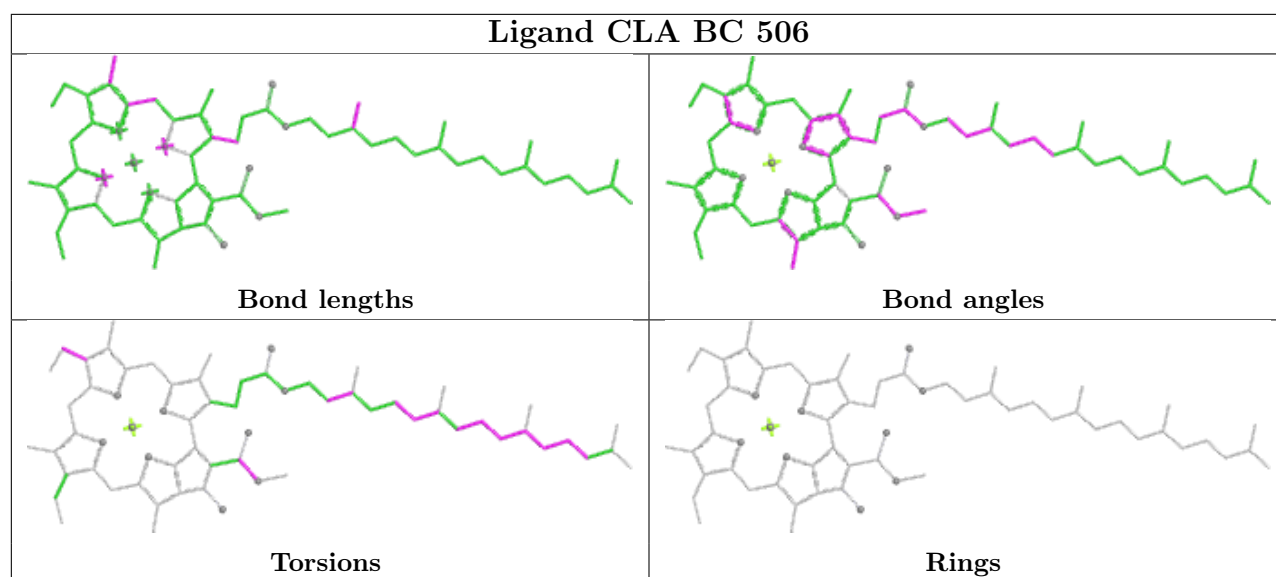


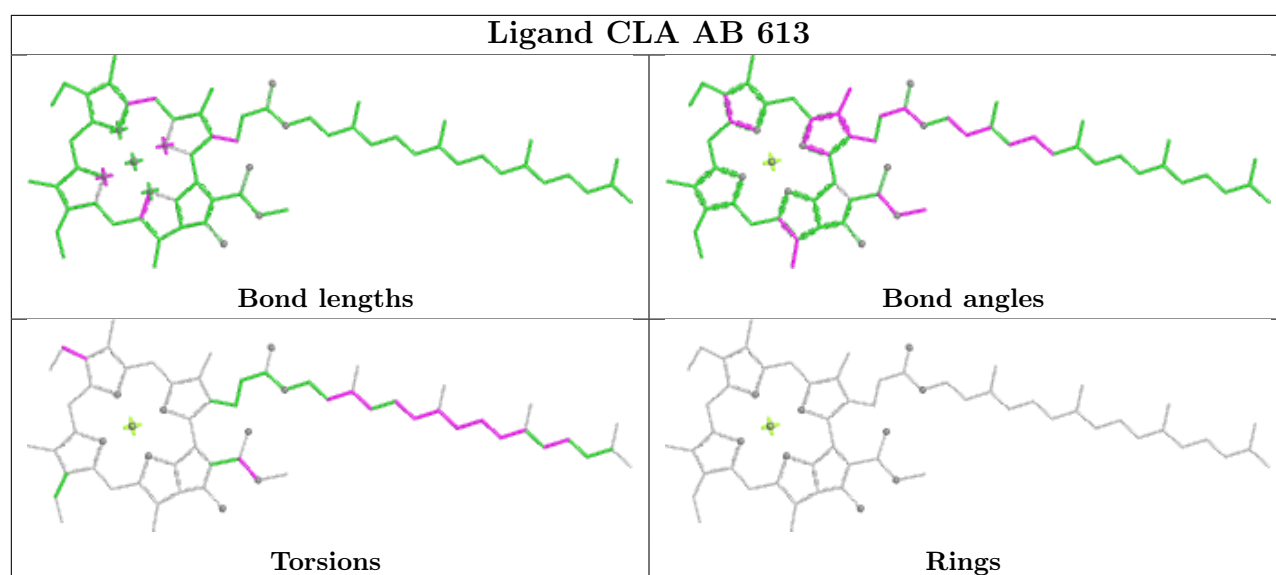
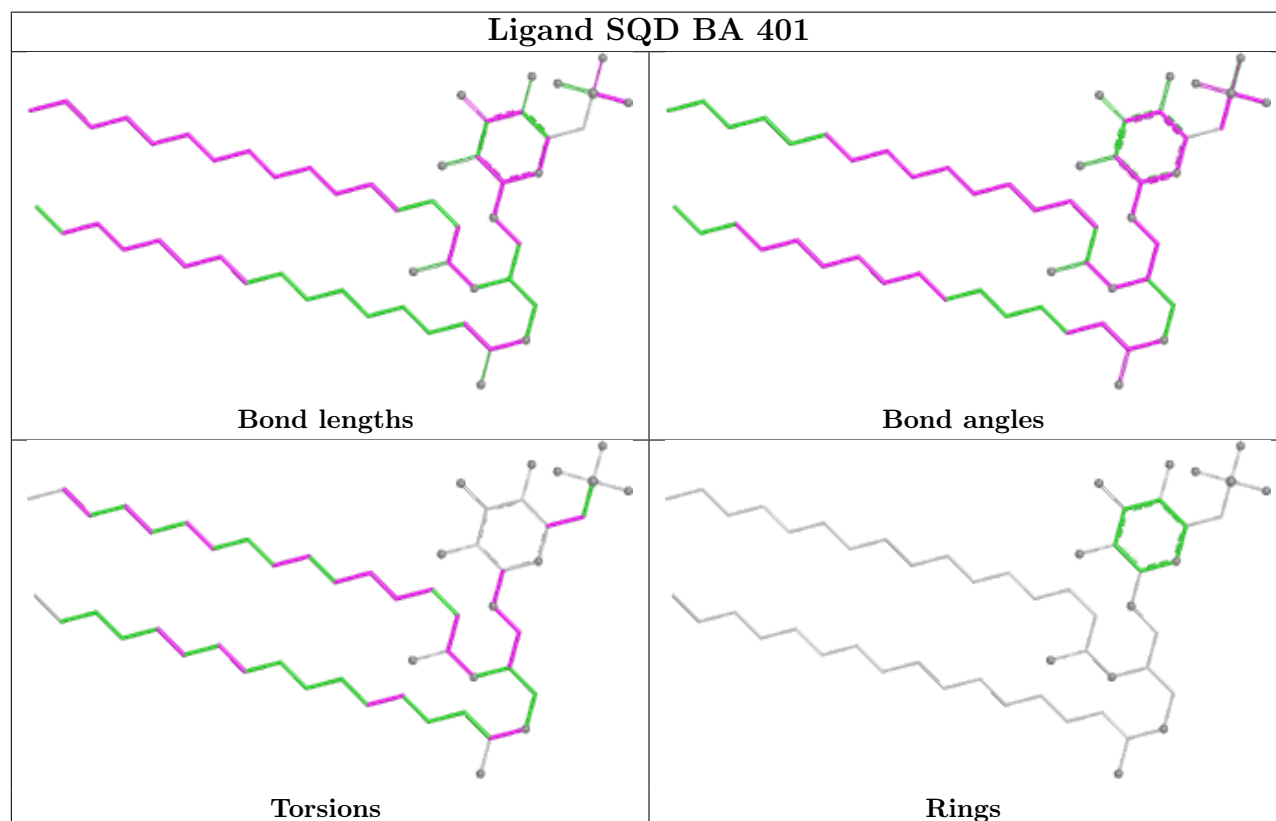
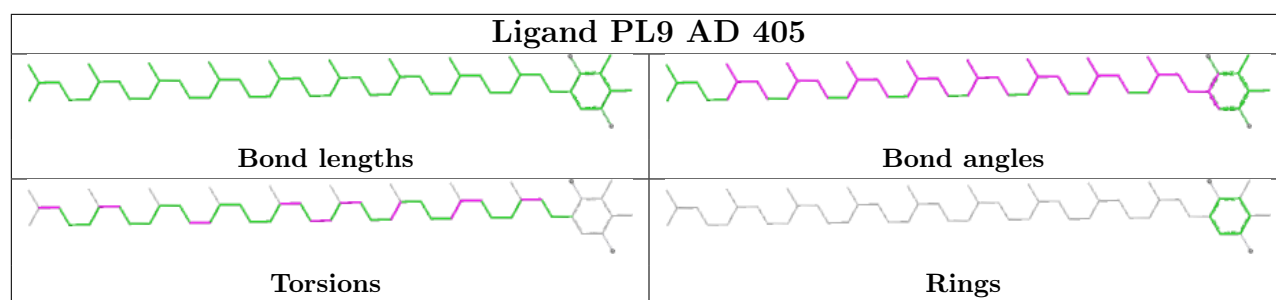
Ligand PL9 BA 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

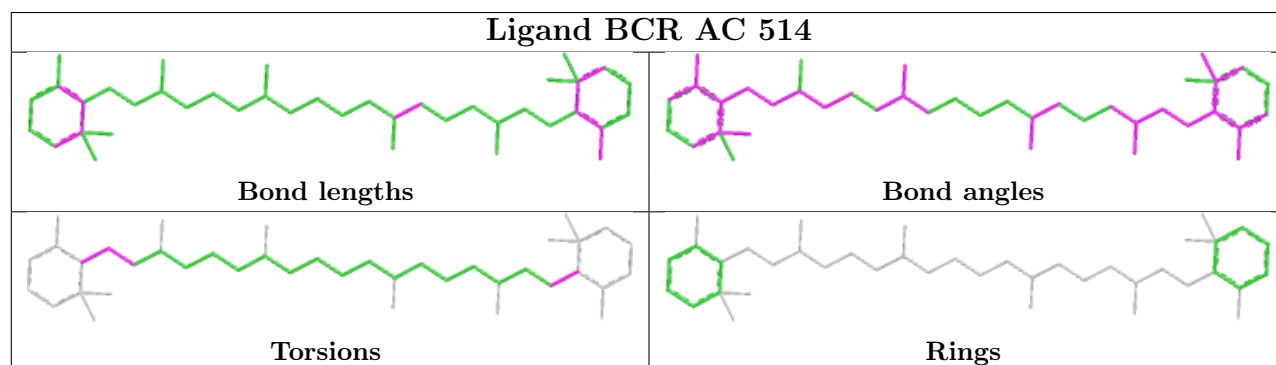
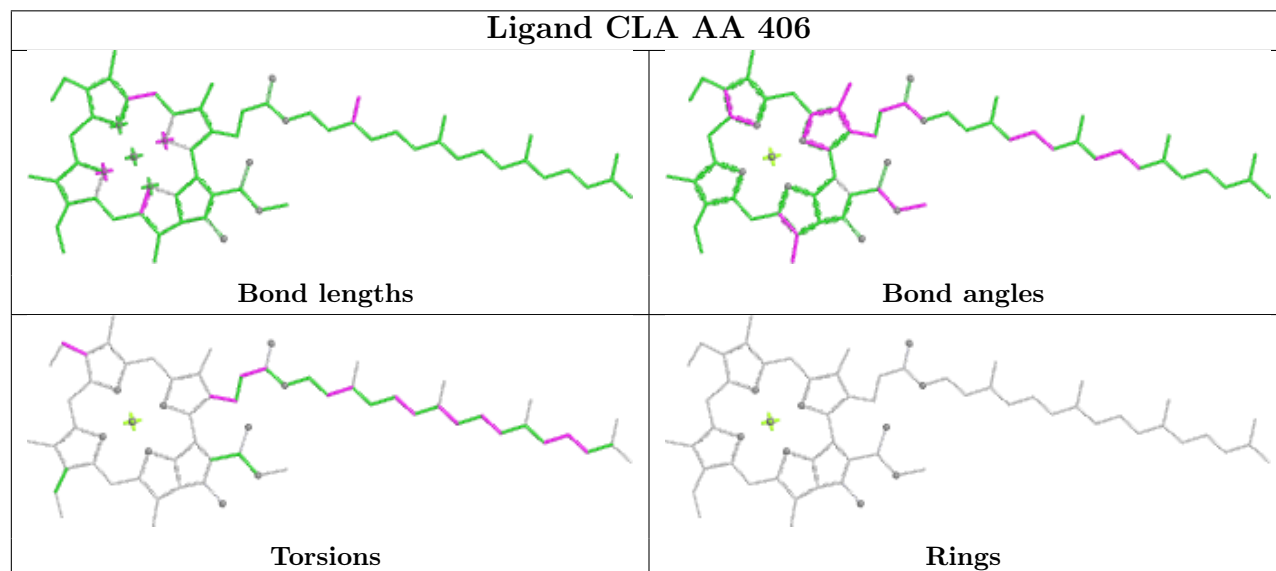
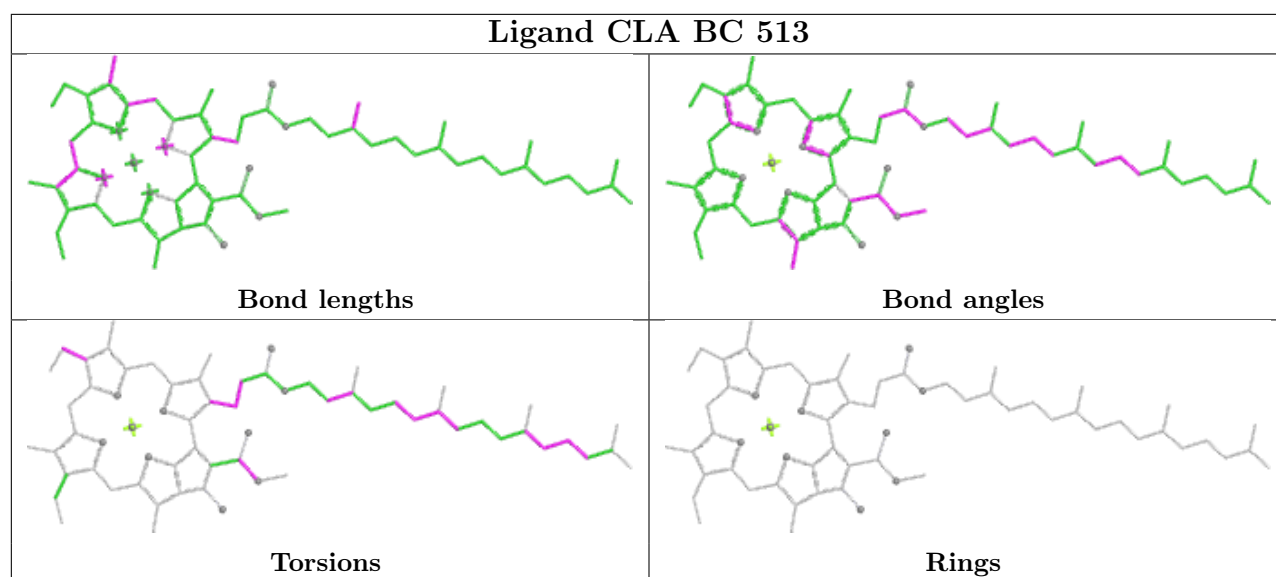
Ligand BCR AJ 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AC 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

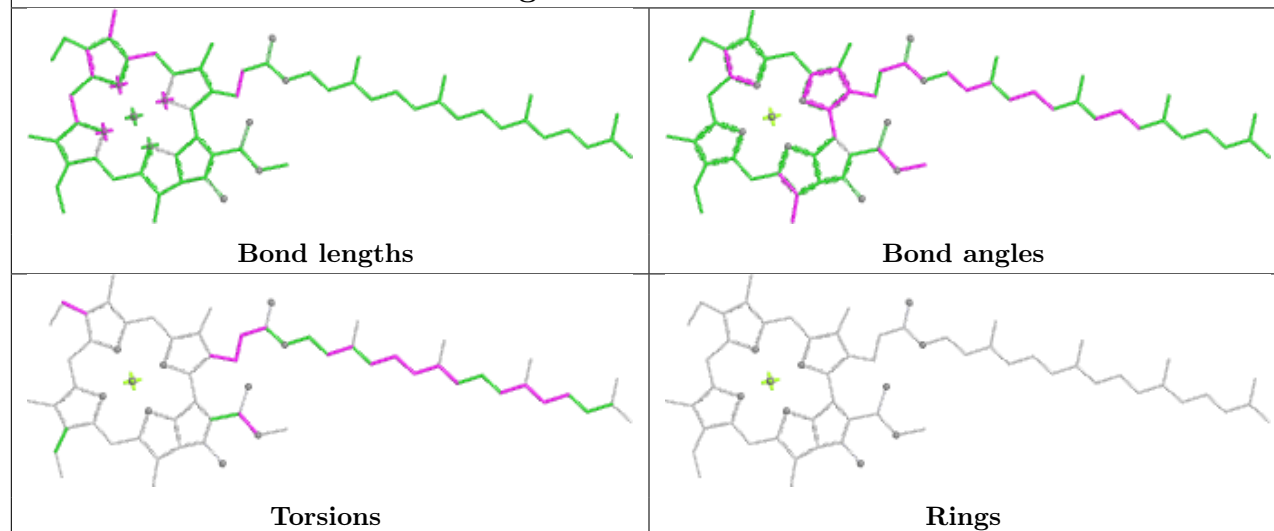




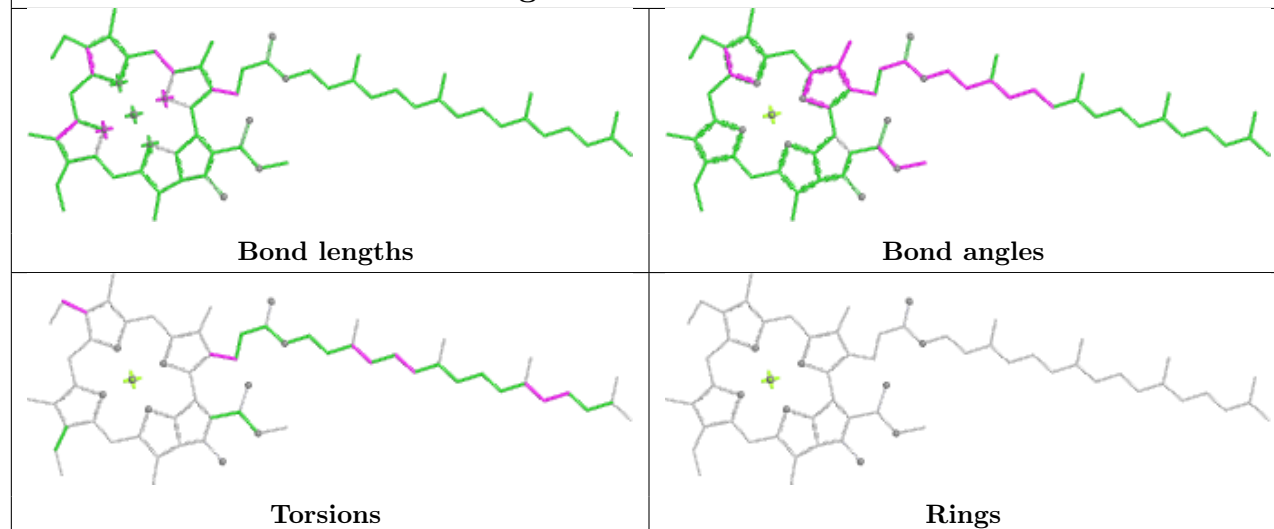




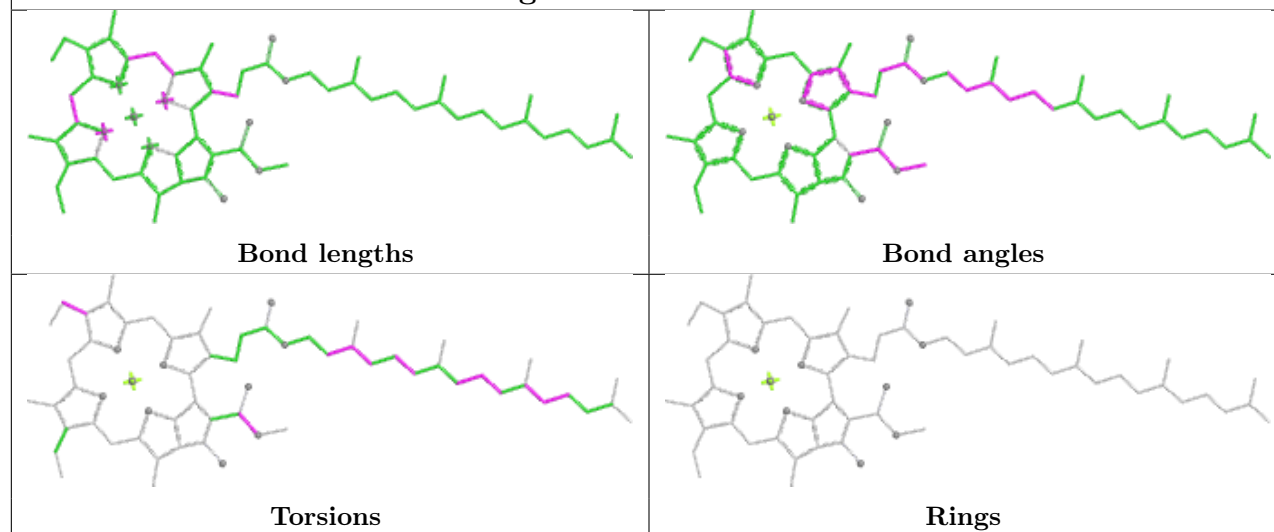
Ligand CLA AB 602

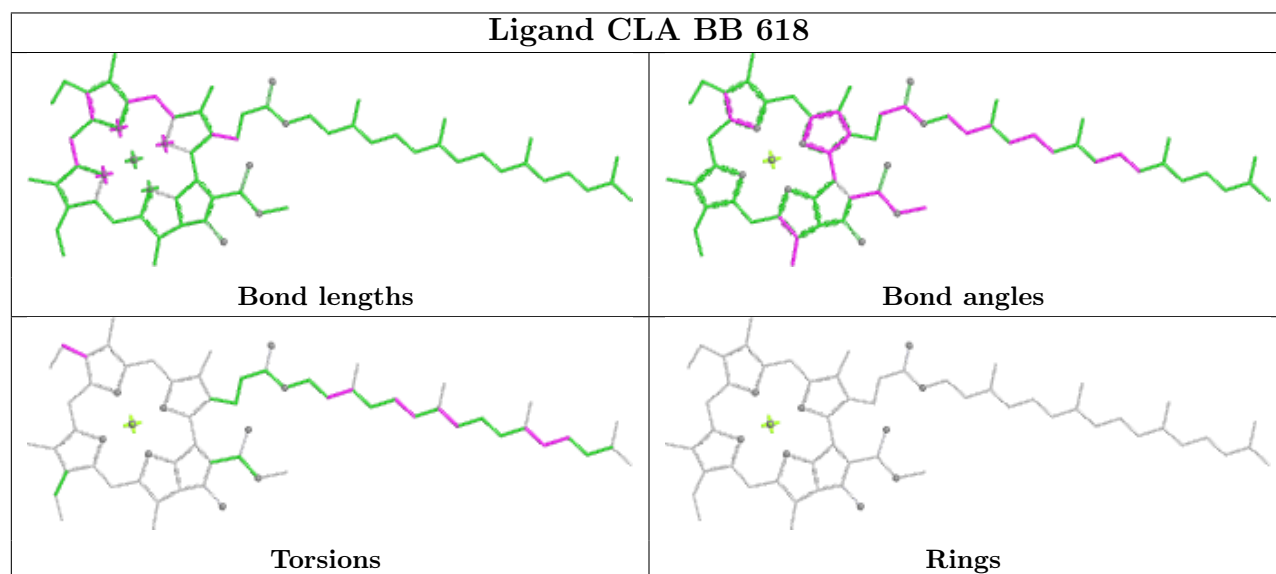
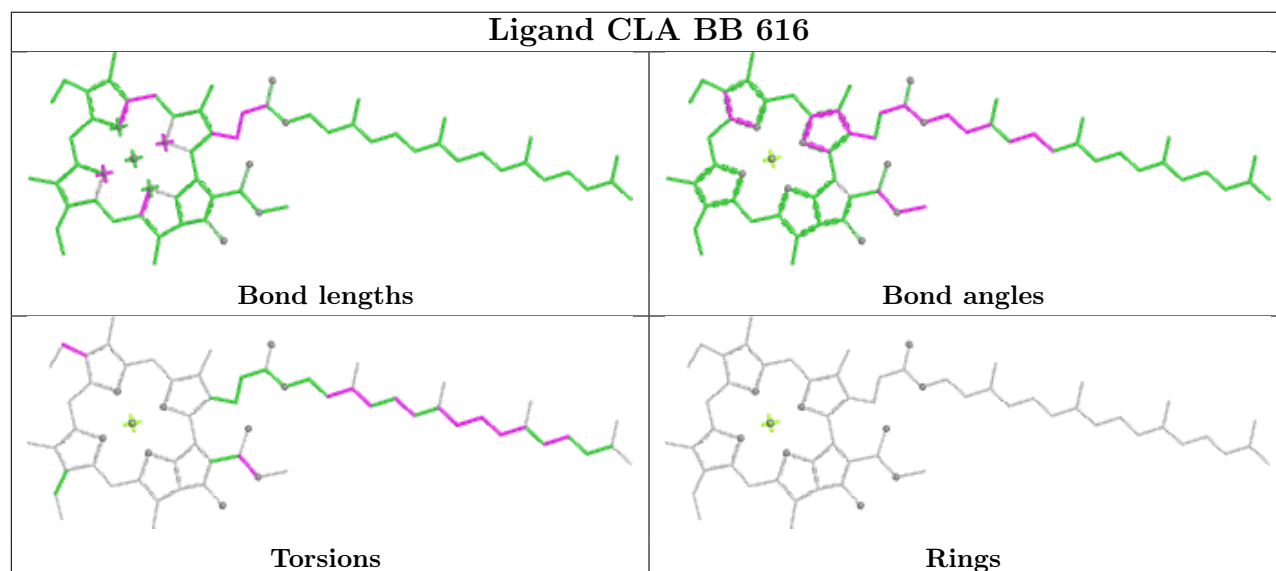
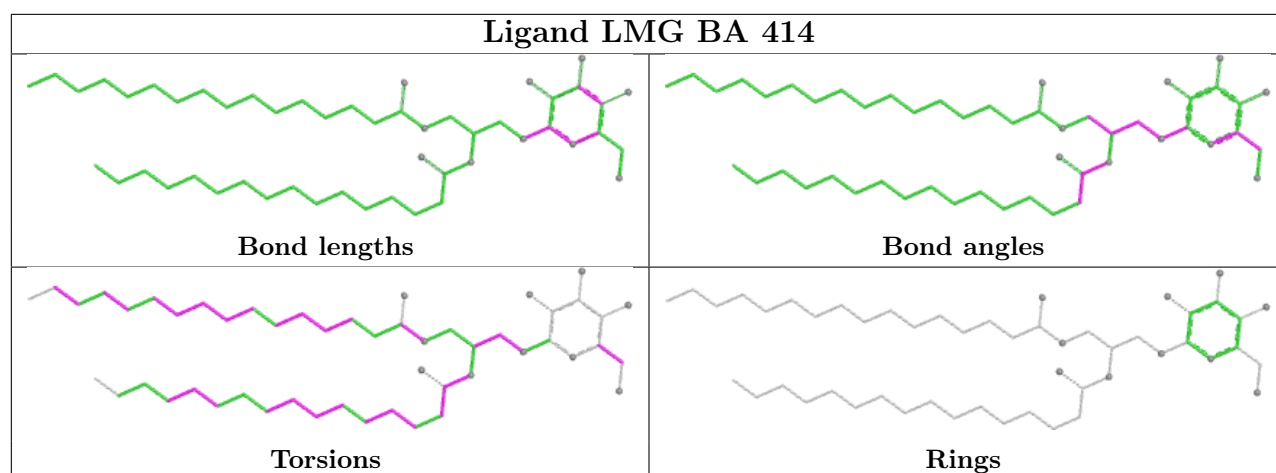


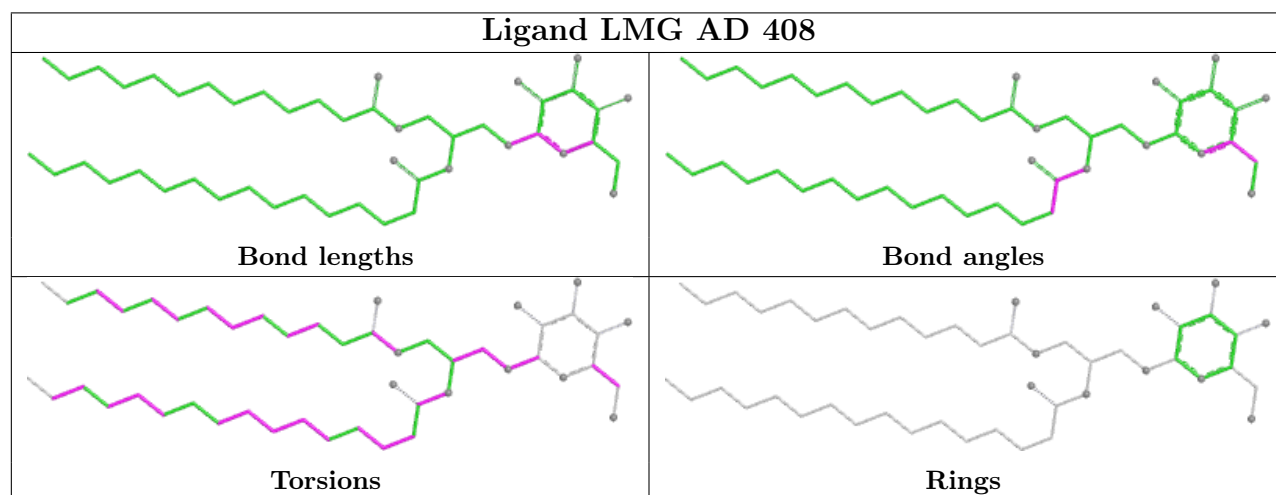
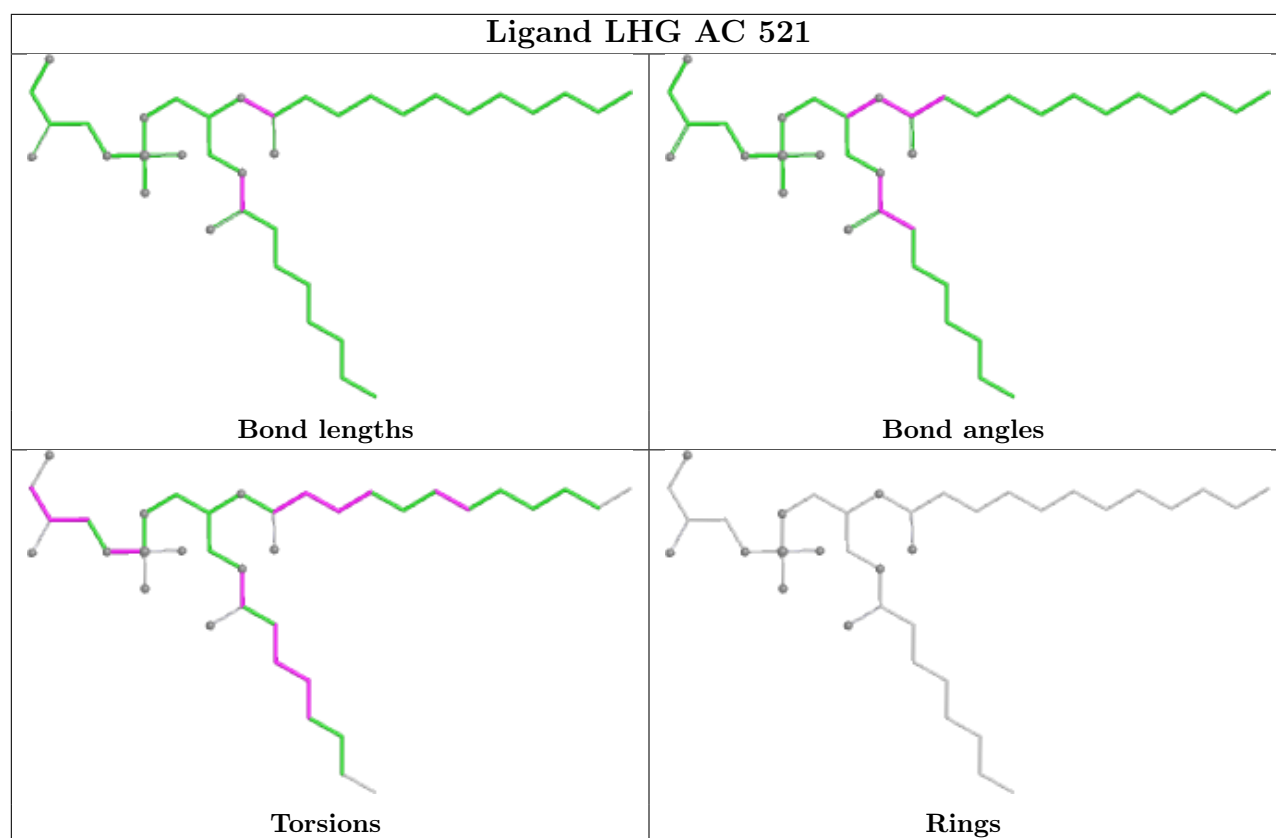
Ligand CLA AB 609

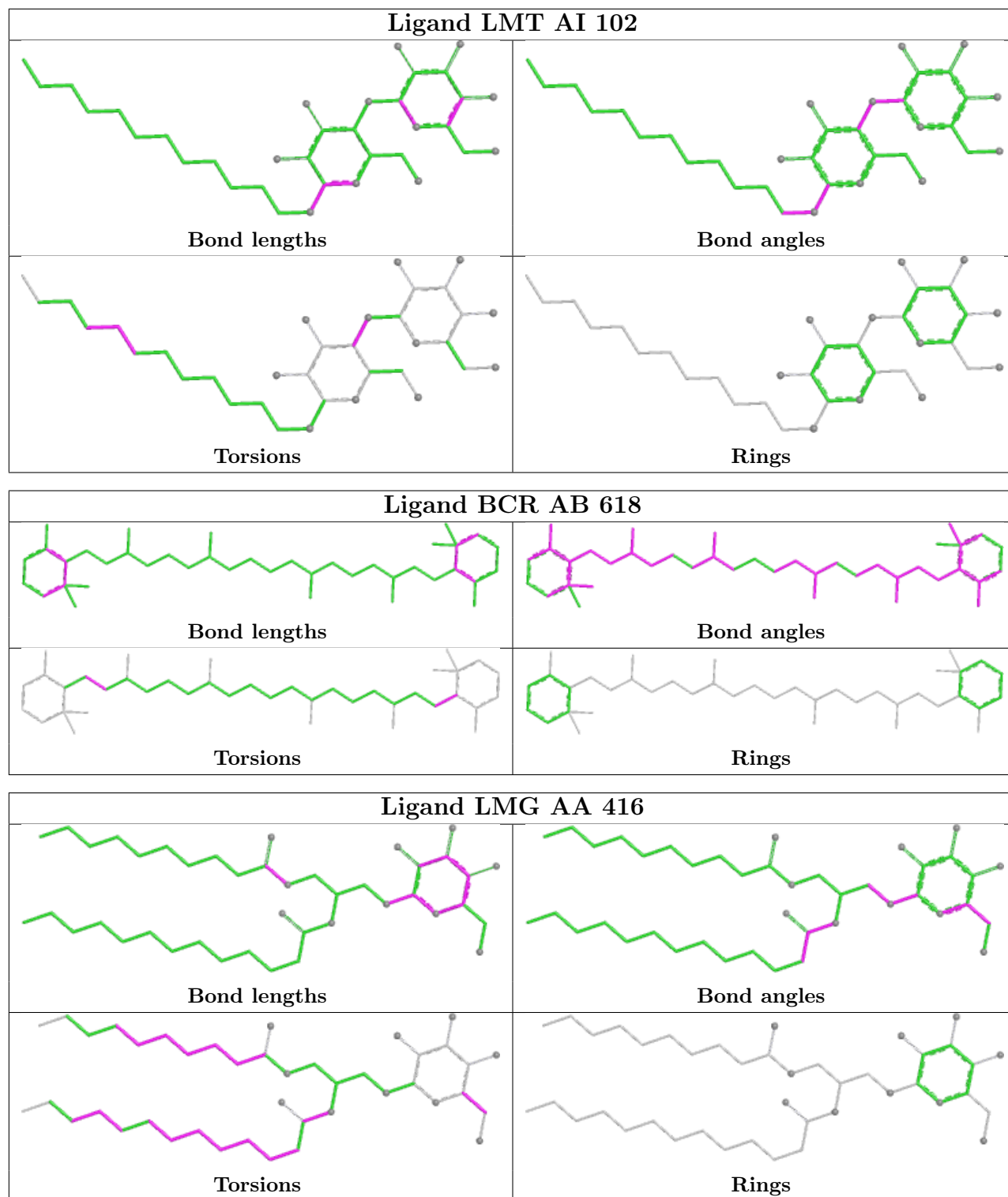


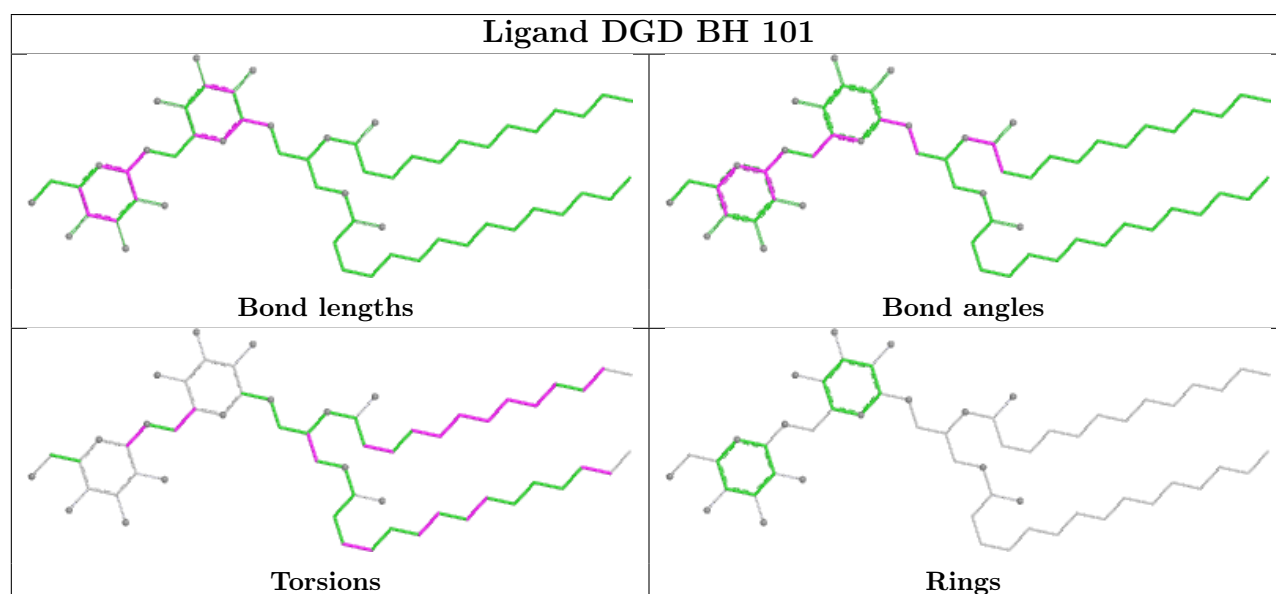
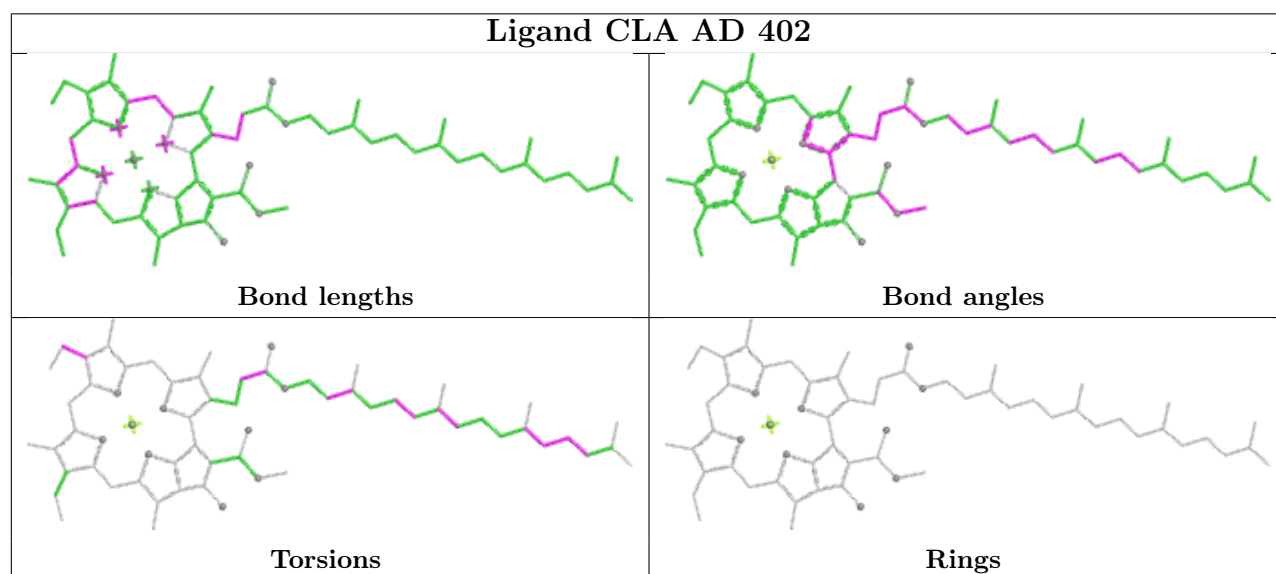
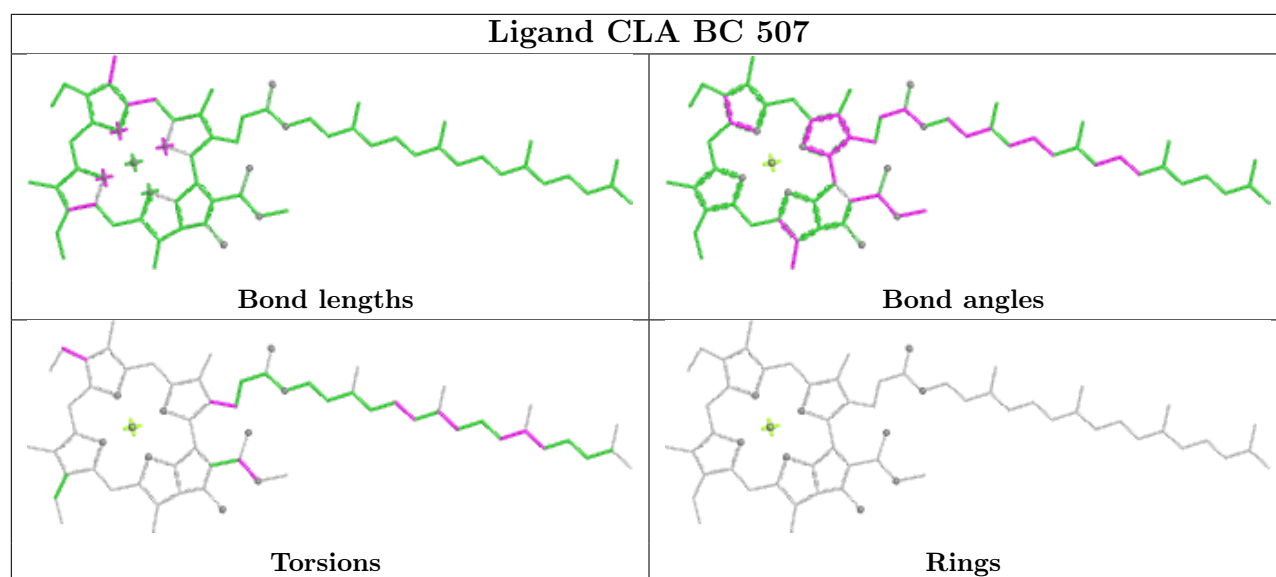
Ligand CLA AB 612

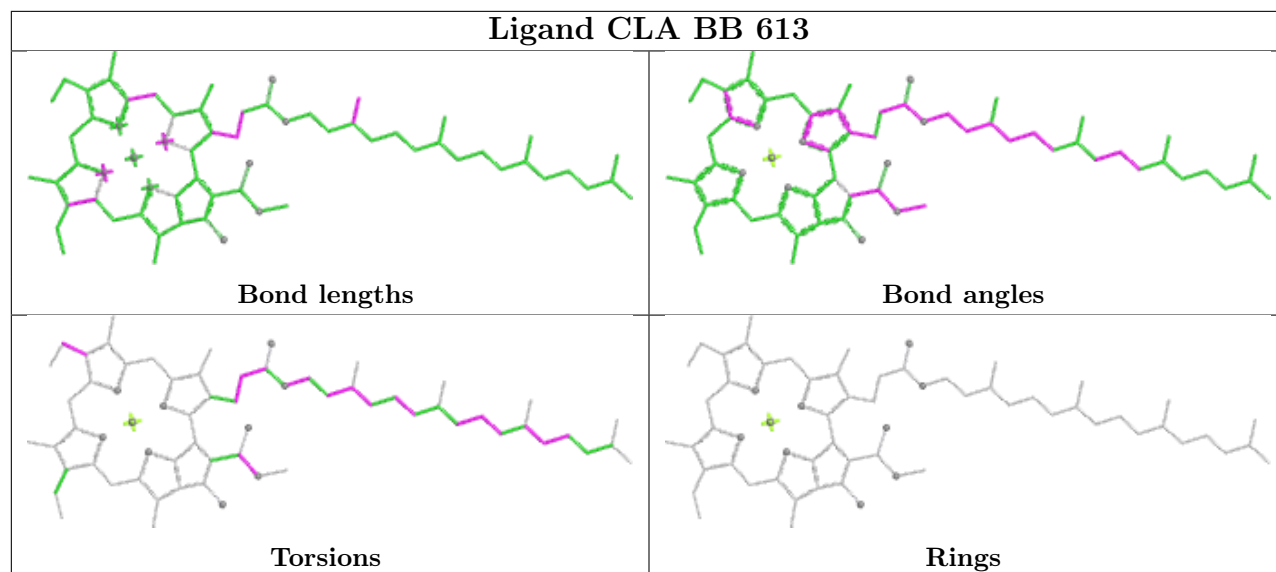
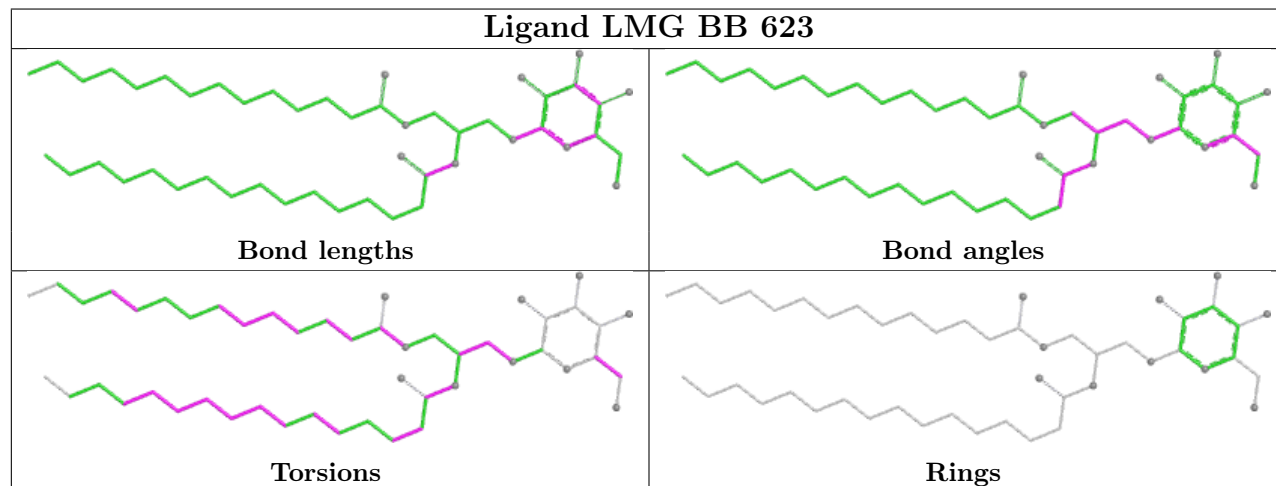
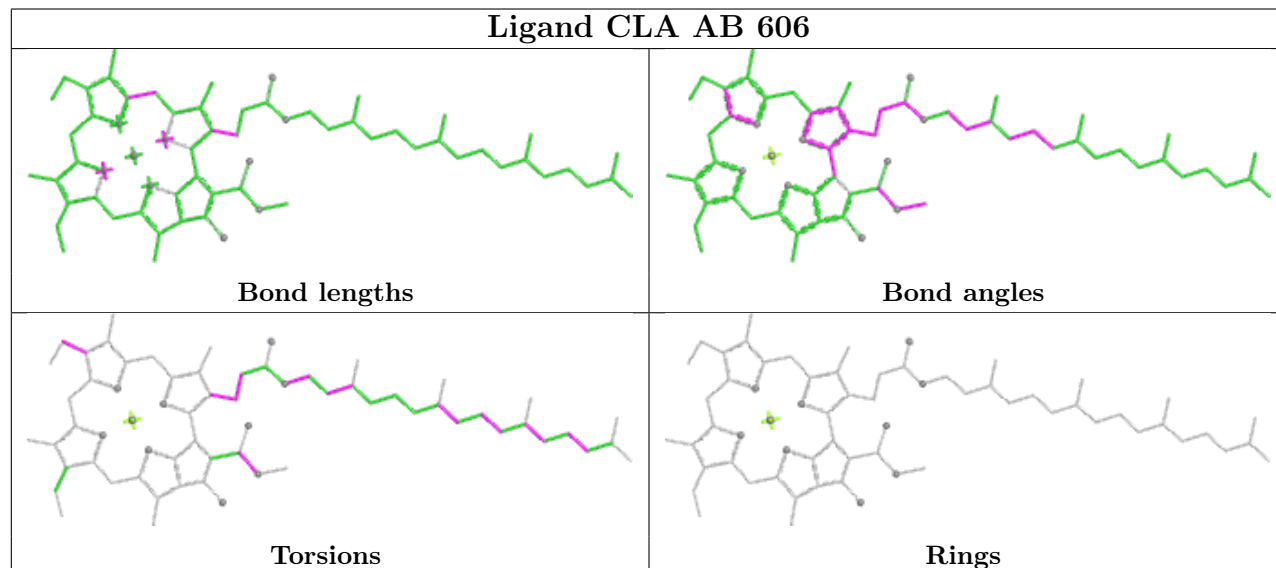


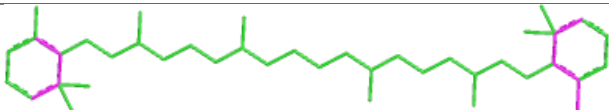
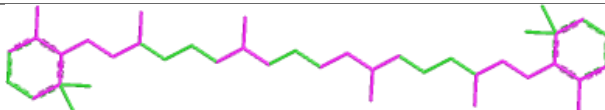
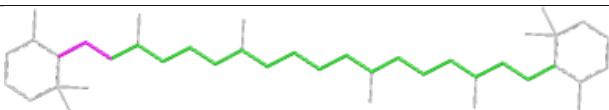
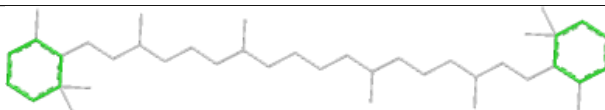


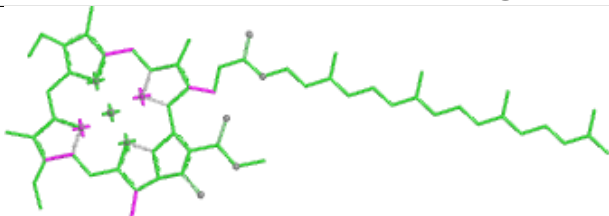
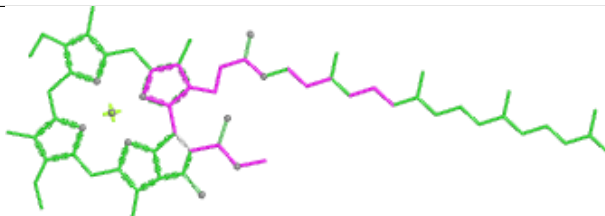
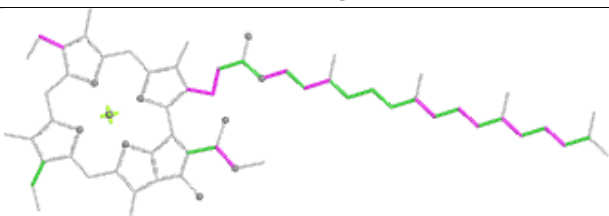
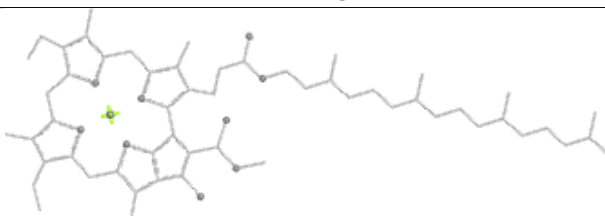


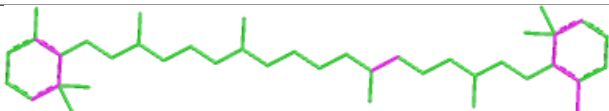
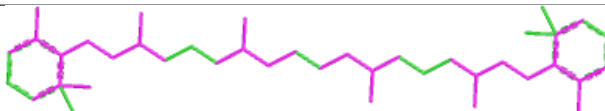
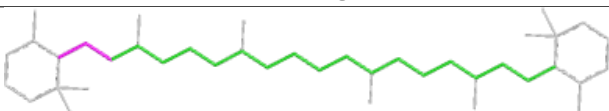
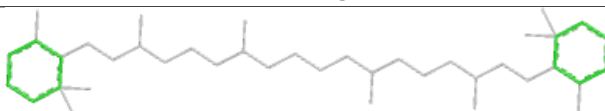


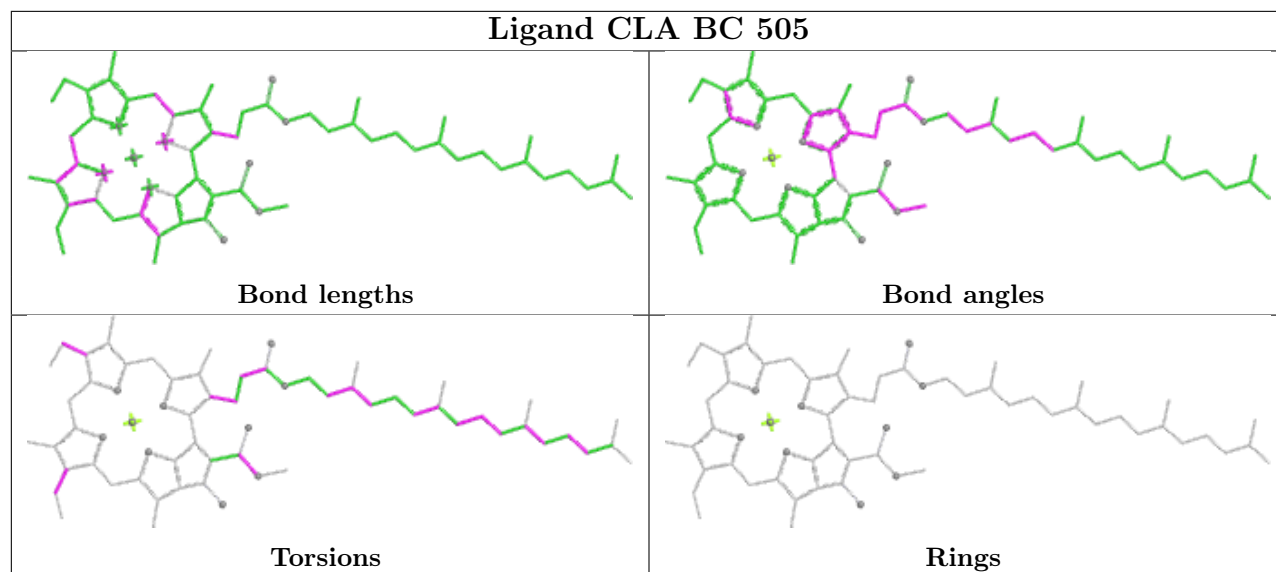
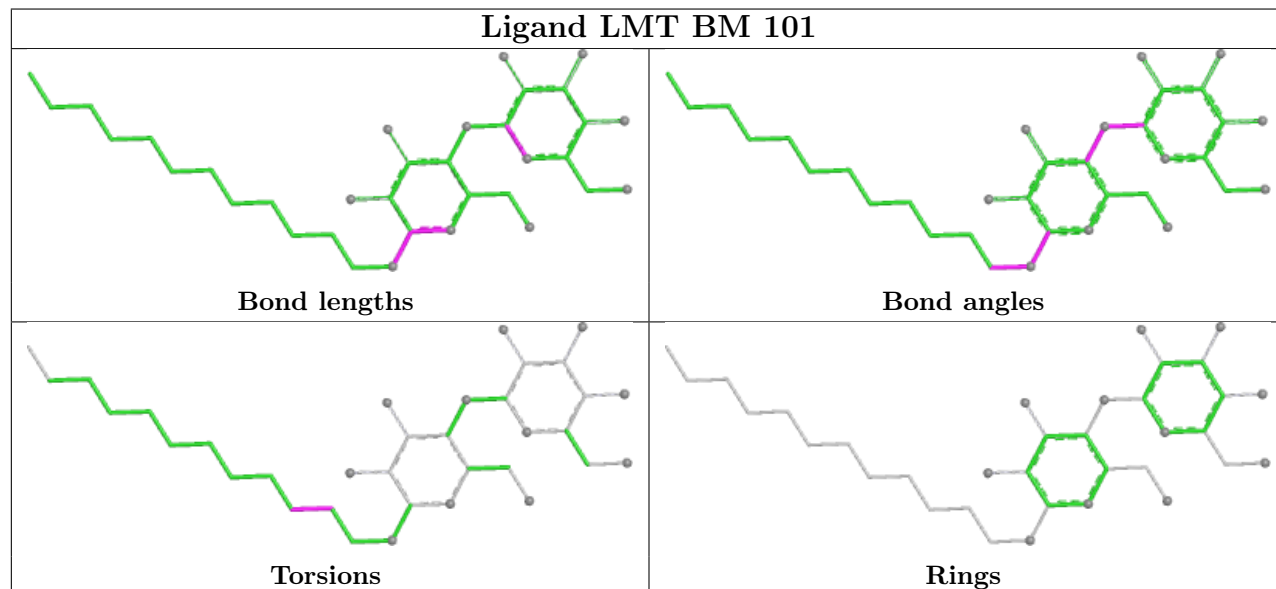
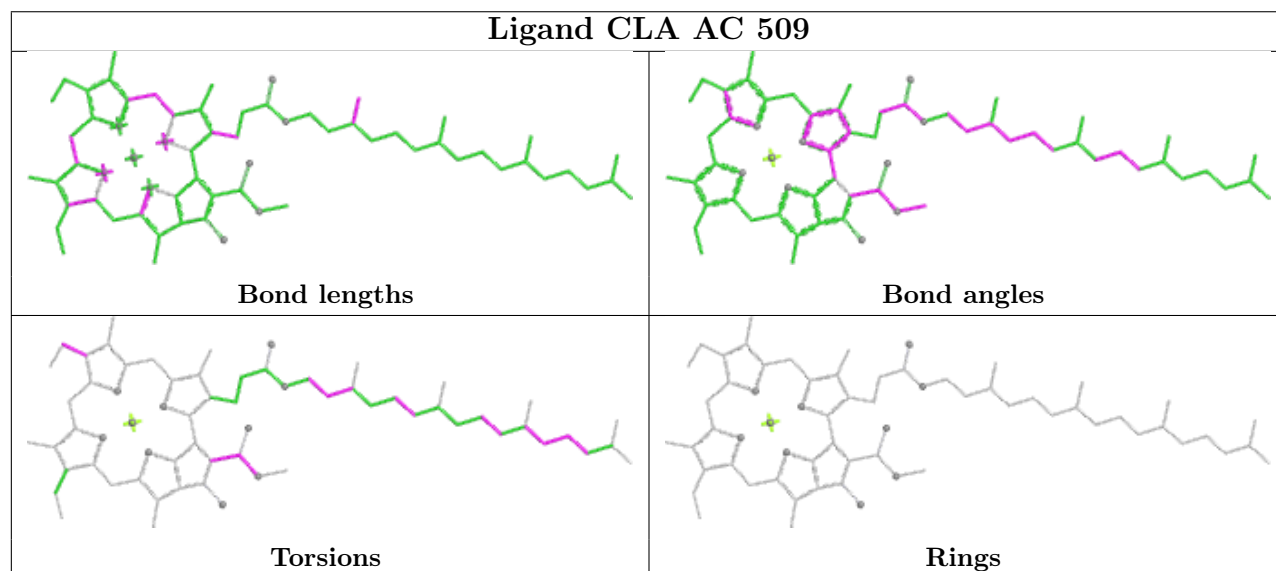


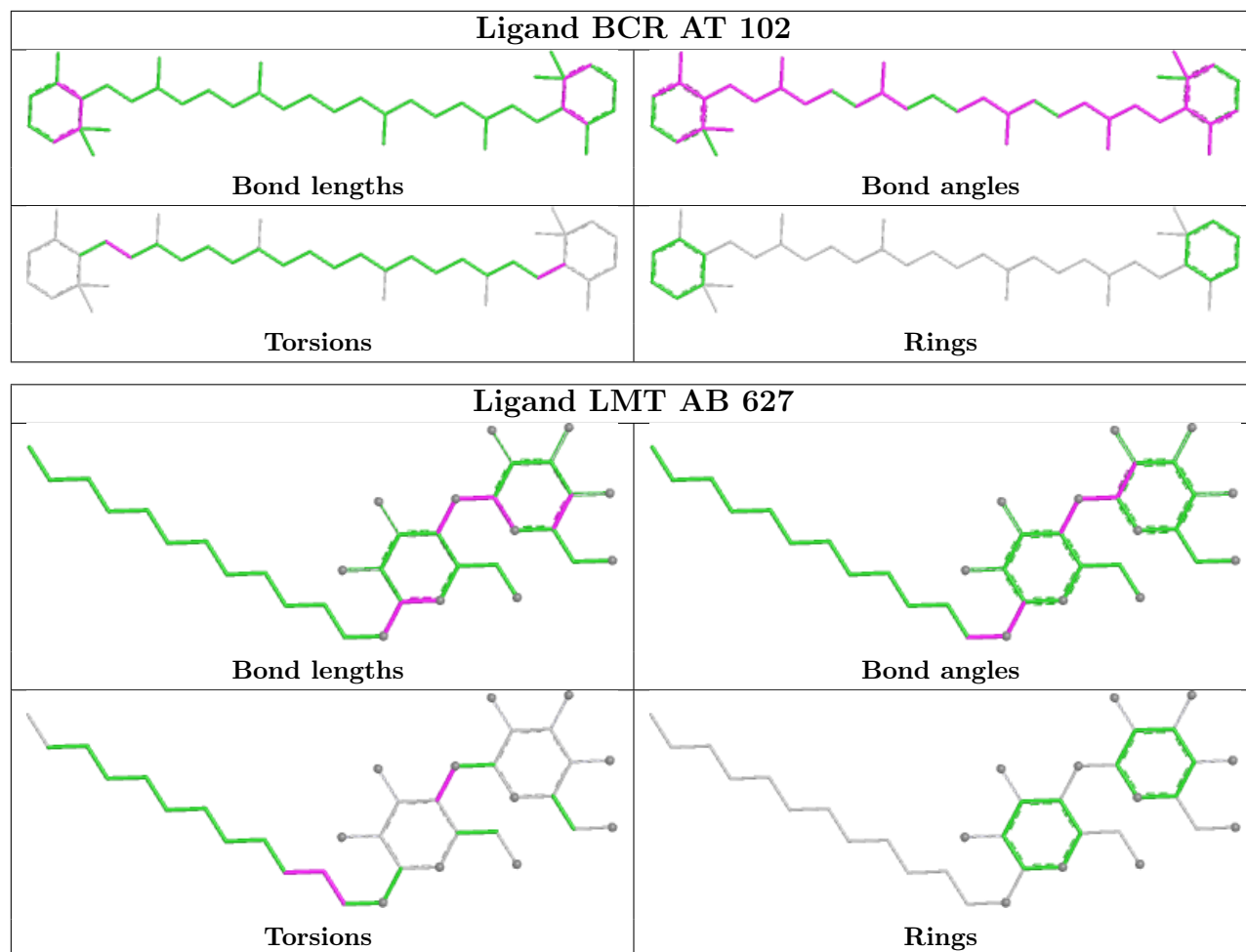
Ligand CLA BB 613**Ligand LMG BB 623****Ligand CLA AB 606**

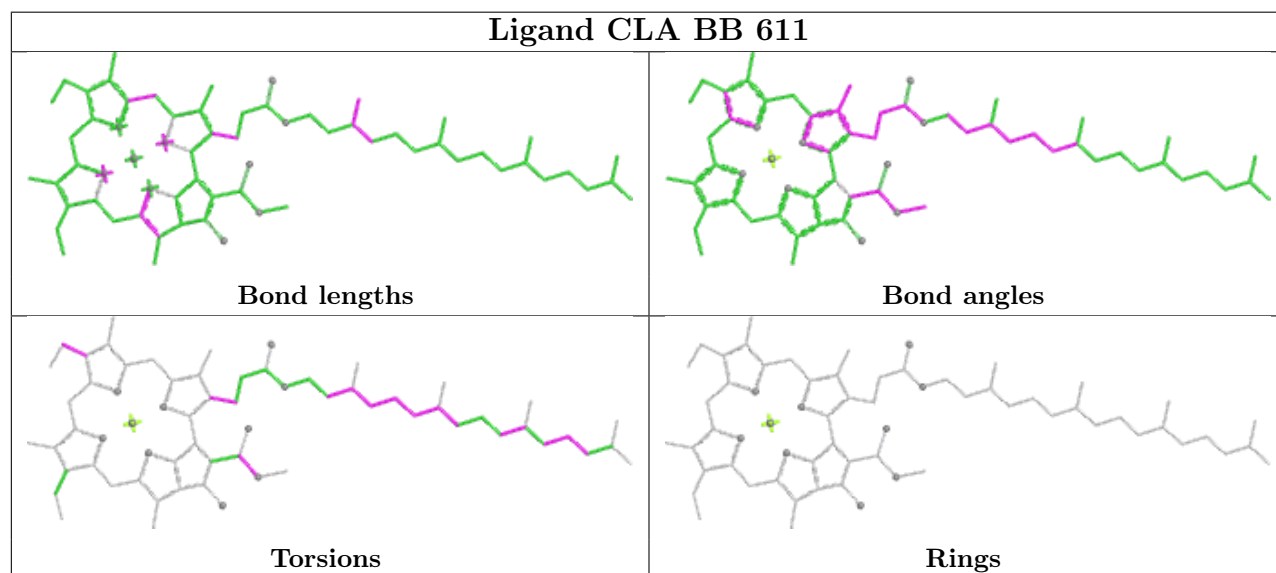
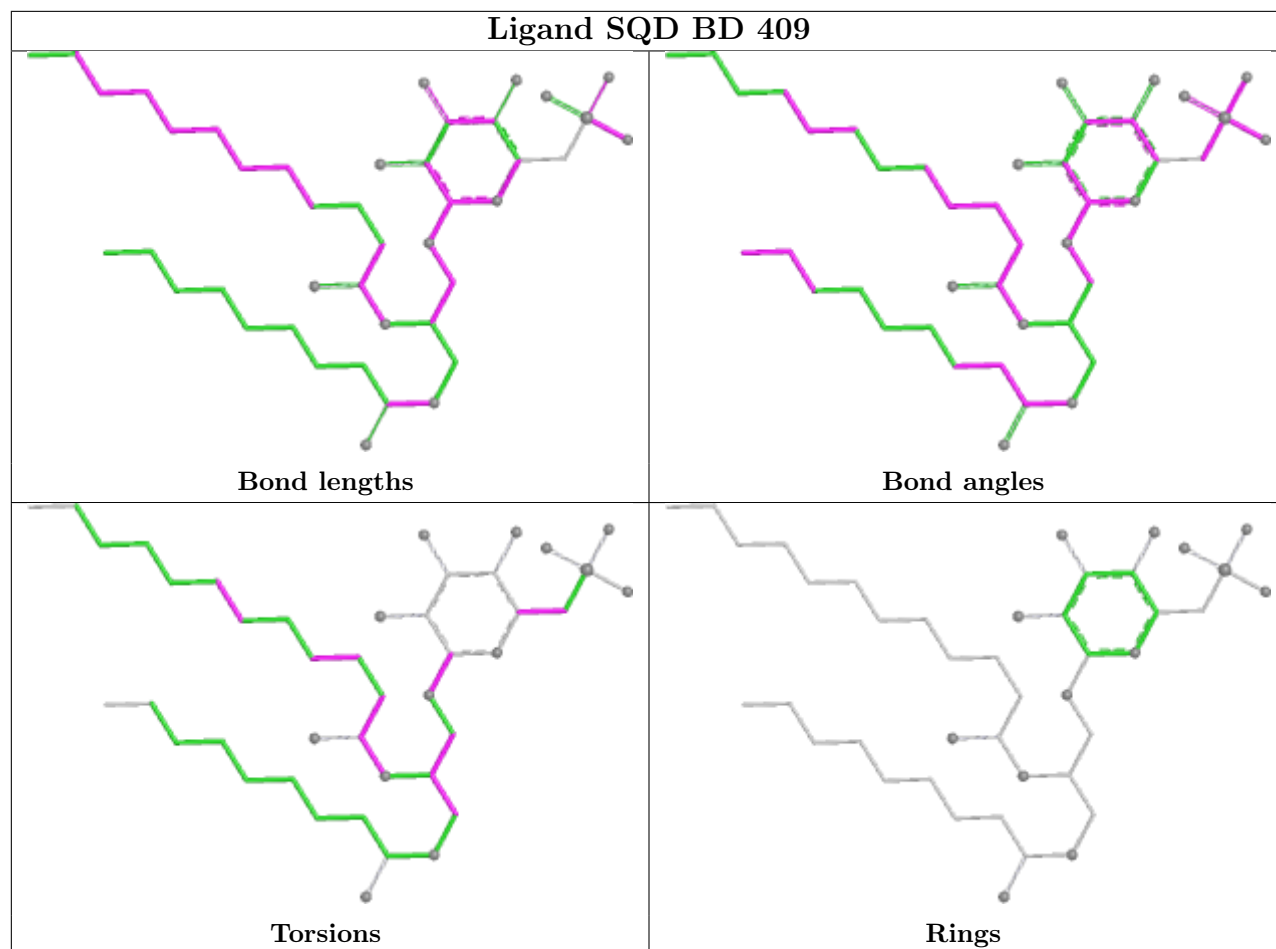
Ligand BCR AZ 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

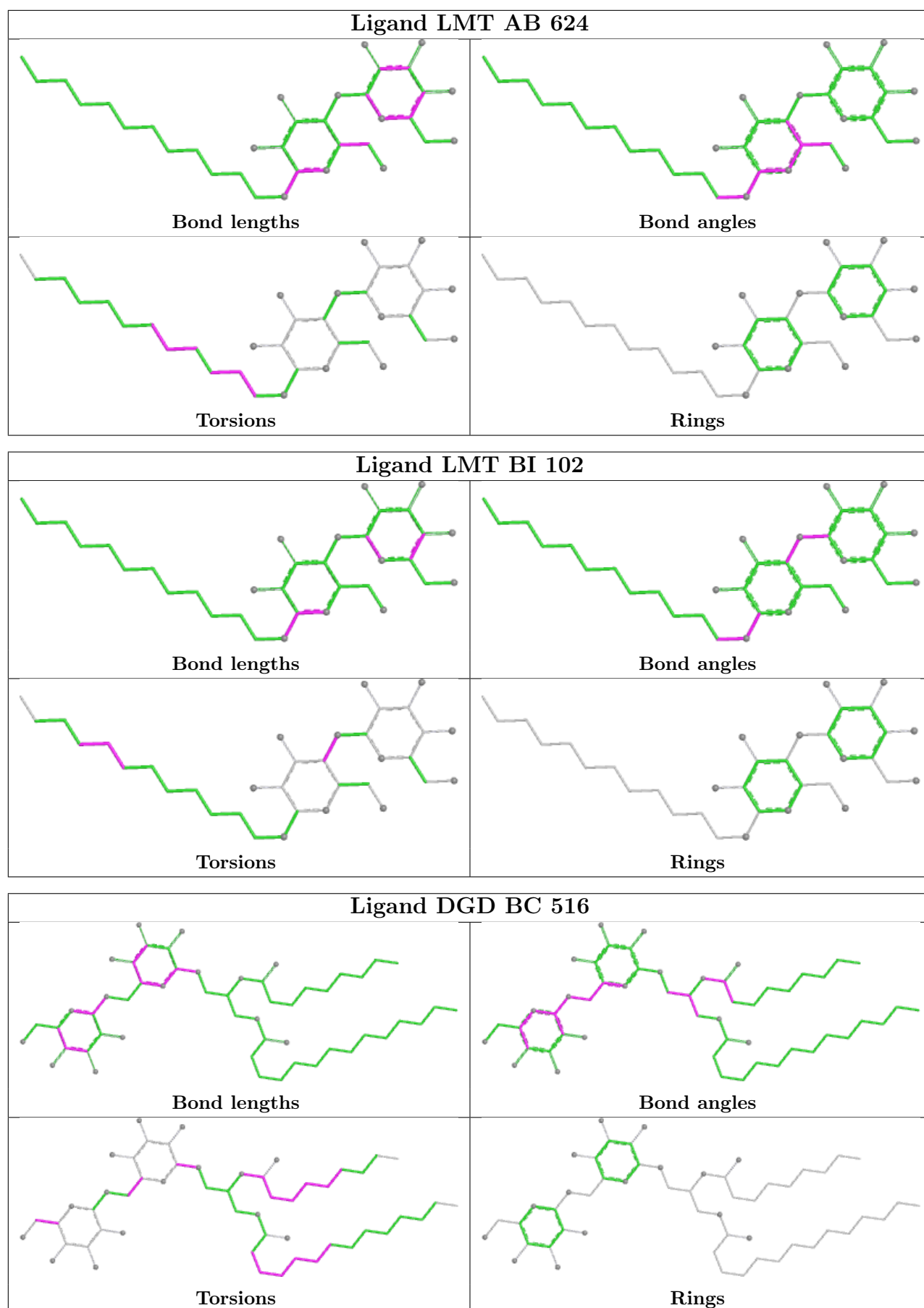
Ligand CLA BB 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

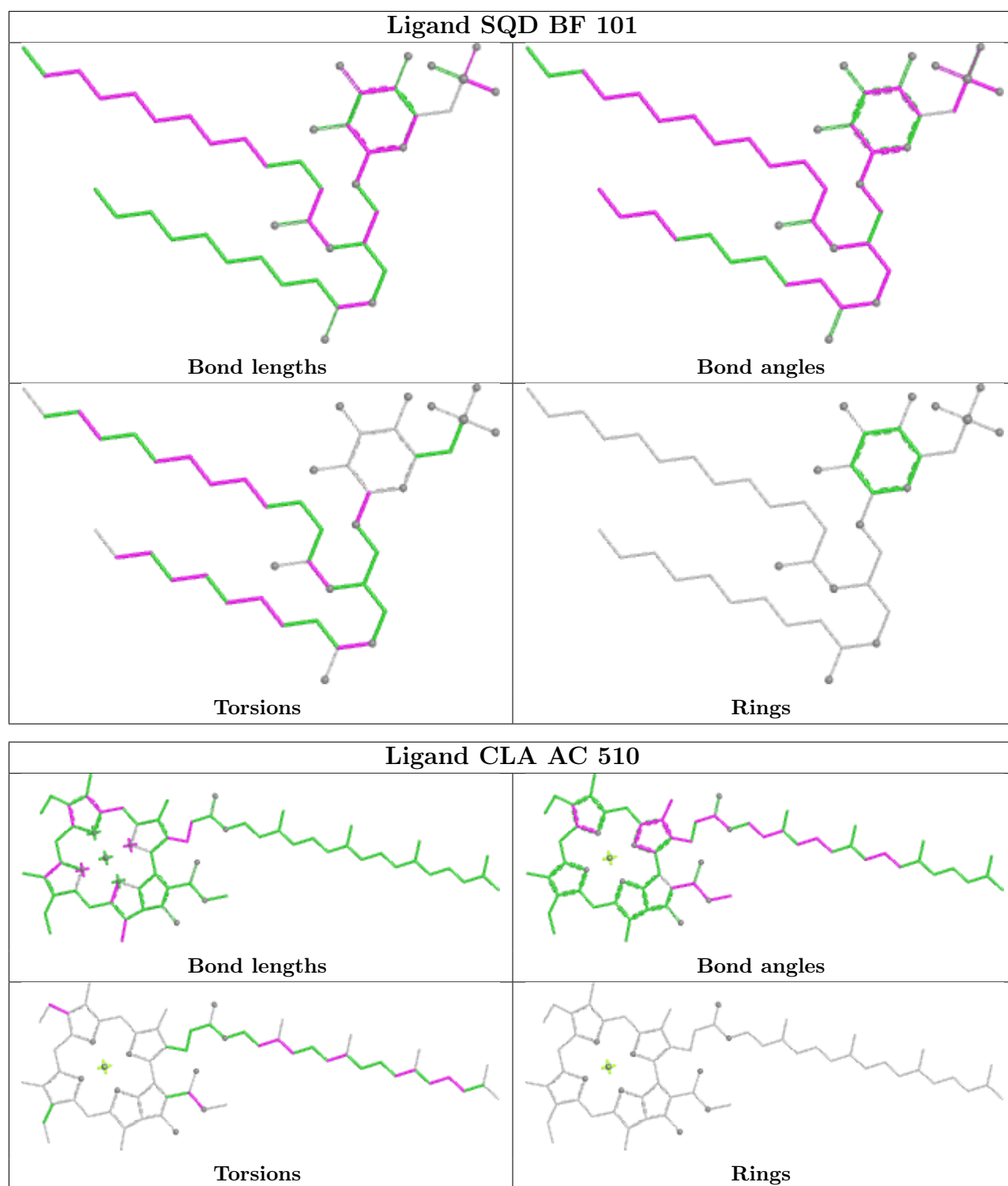
Ligand BCR BD 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

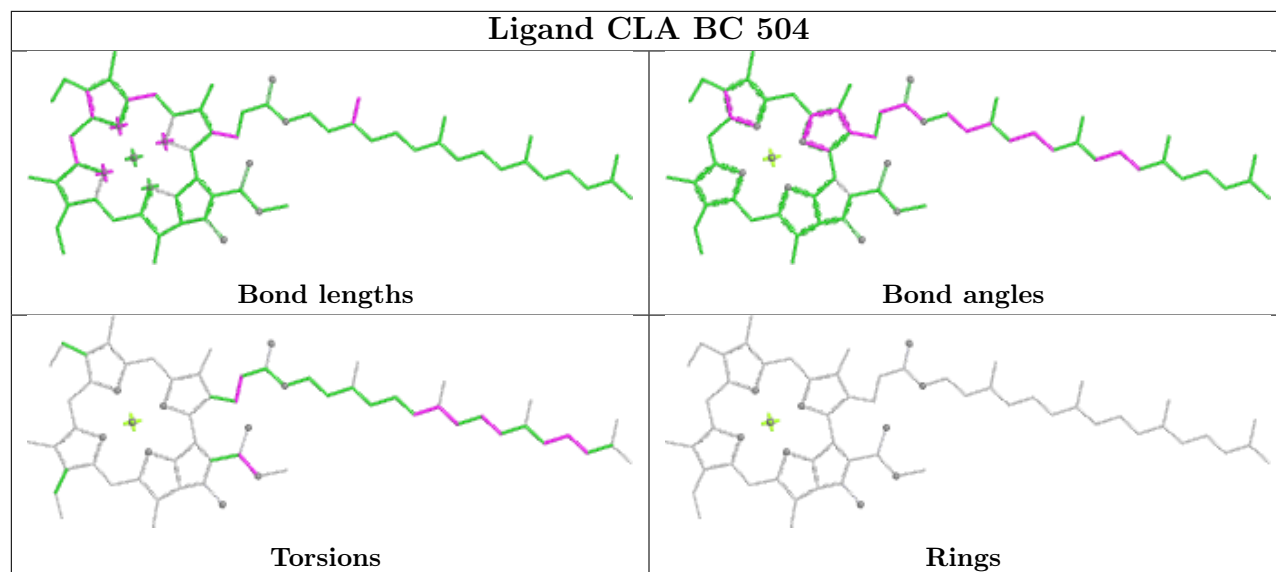
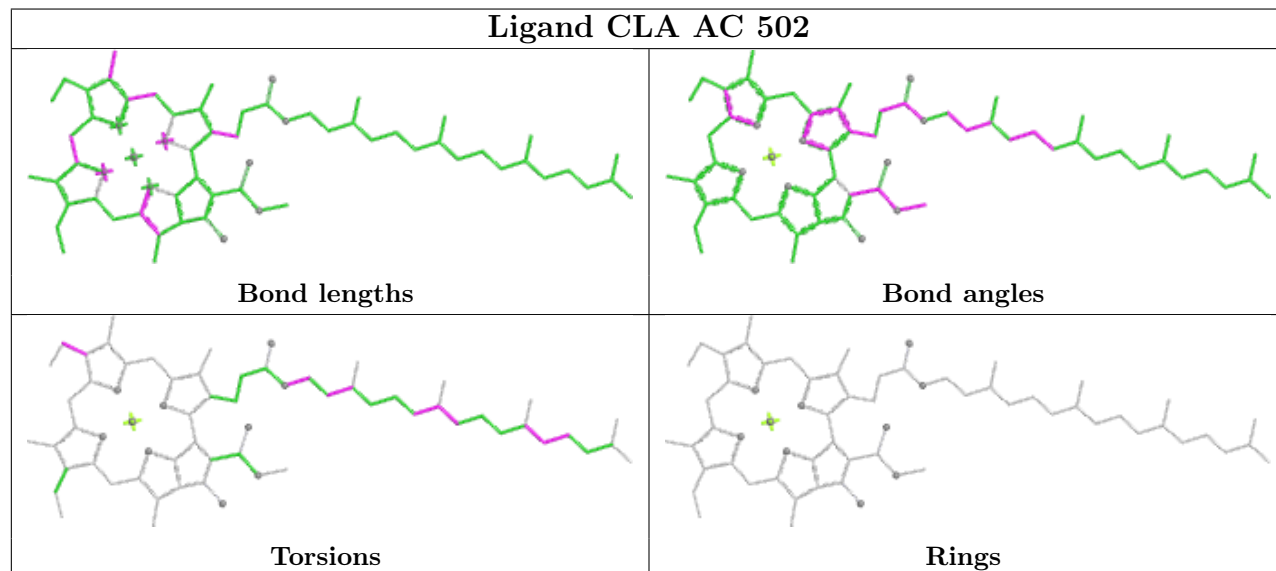
Ligand CLA BC 505**Ligand LMT BM 101****Ligand CLA AC 509**

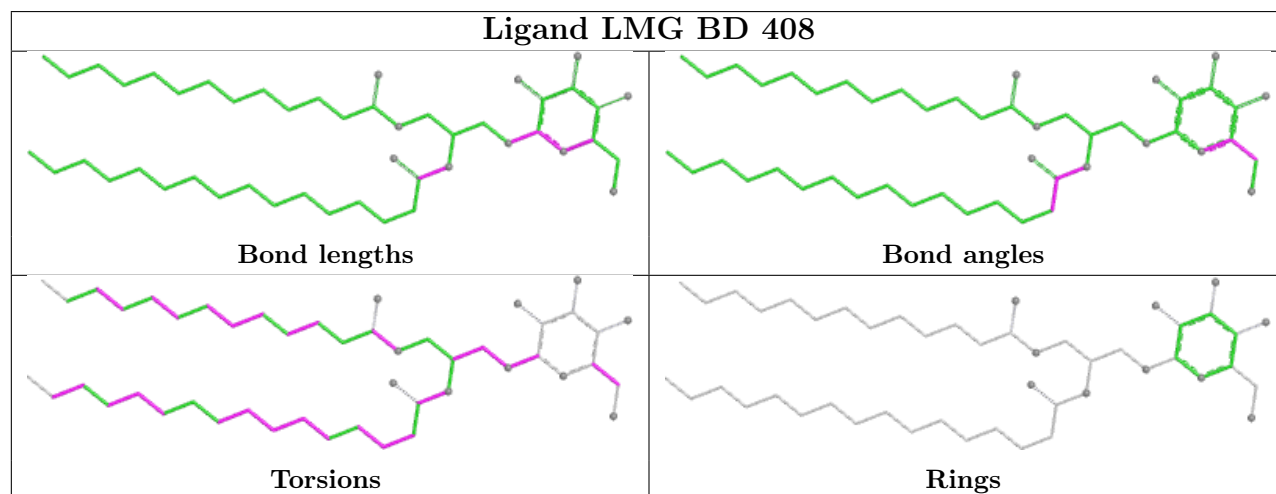
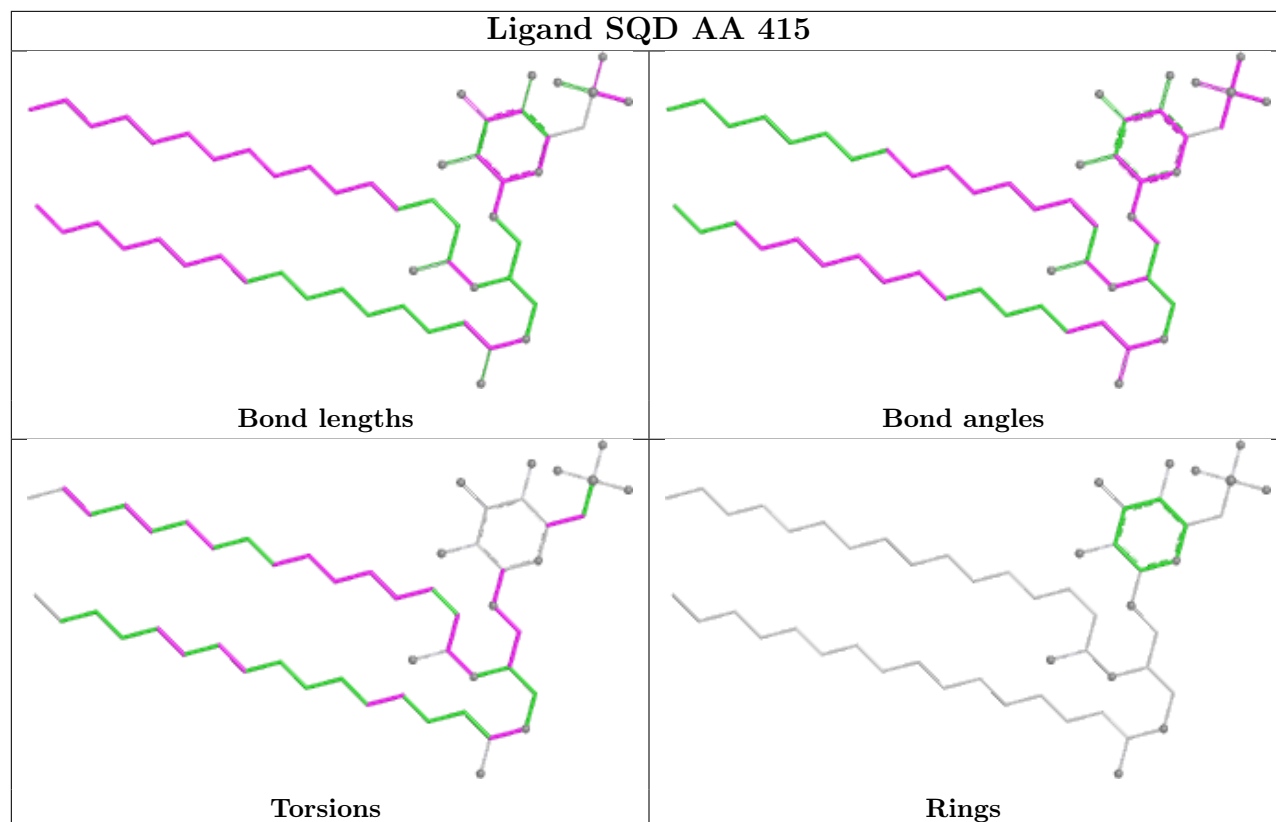




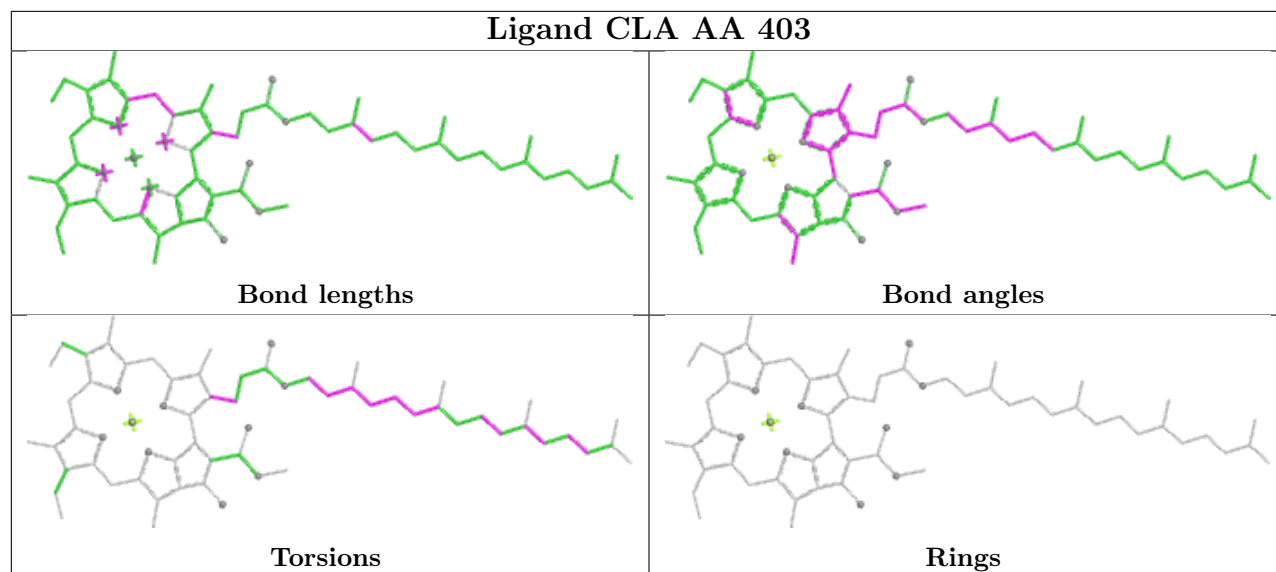




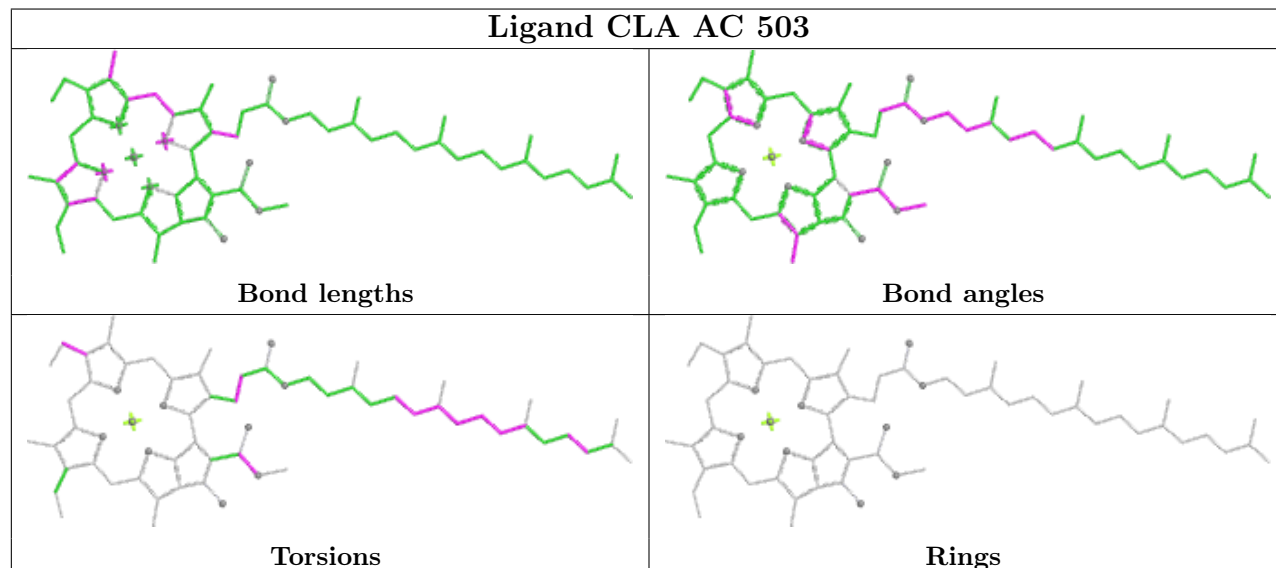
Ligand CLA BC 504**Ligand CLA AC 502**



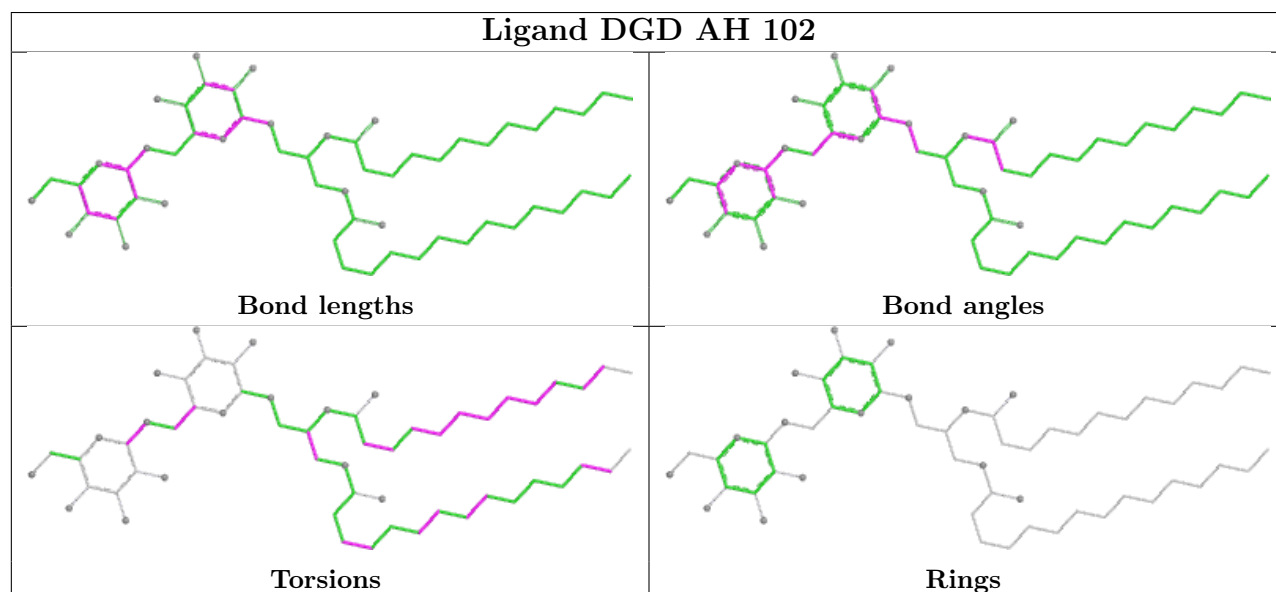
Ligand CLA AA 403

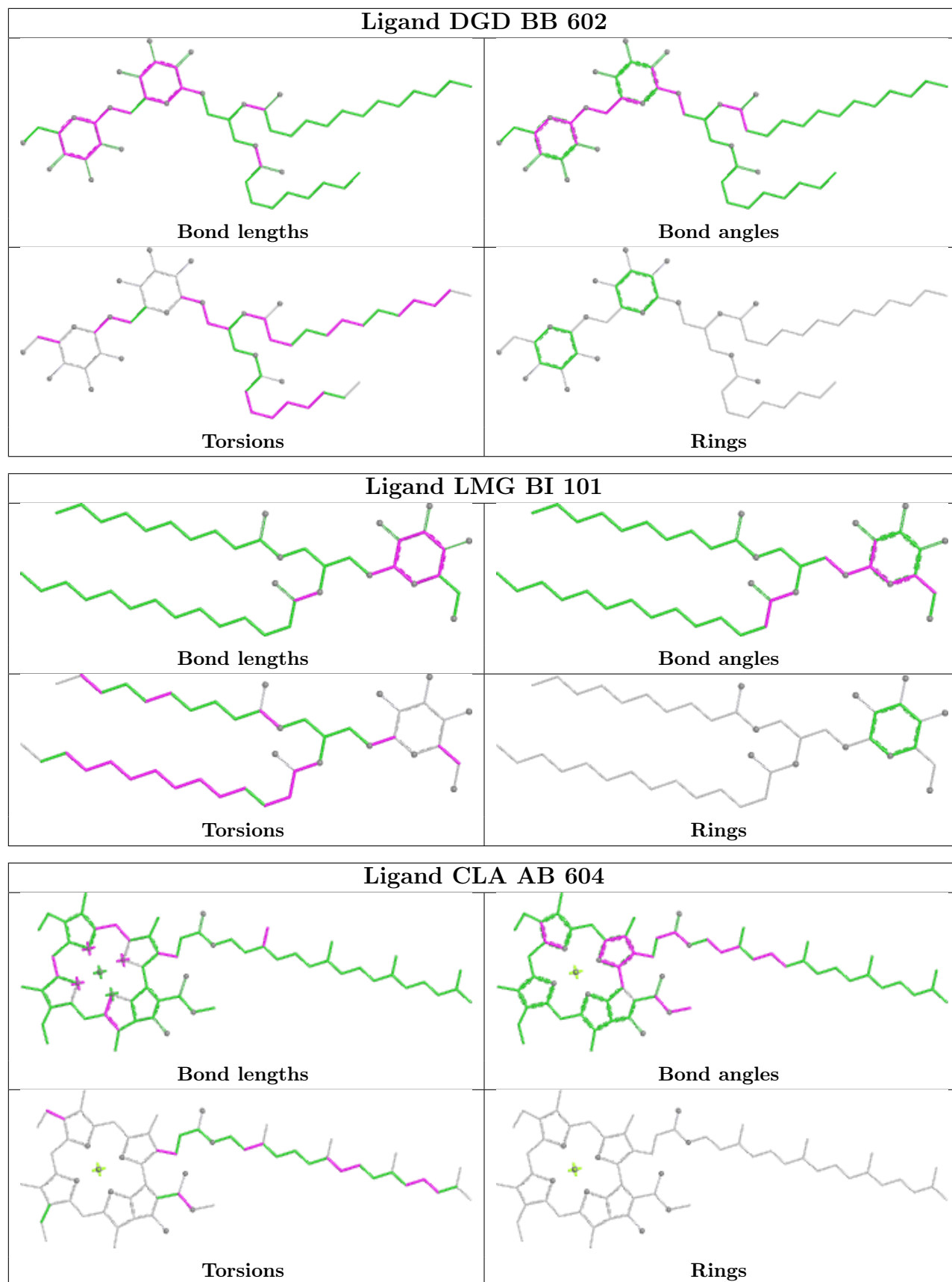


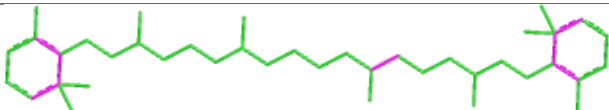
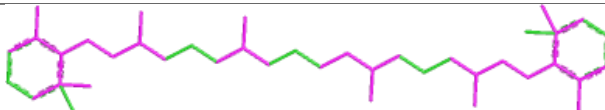
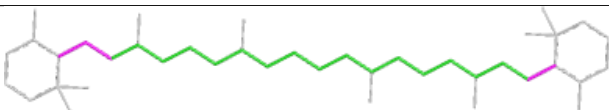
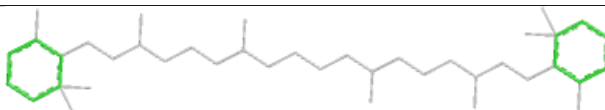
Ligand CLA AC 503

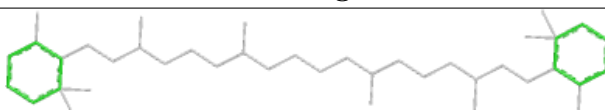


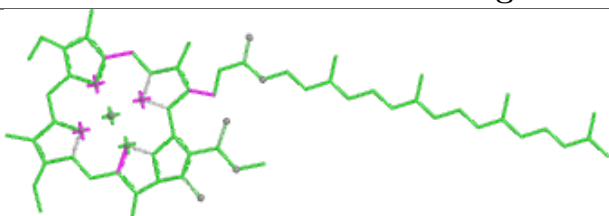
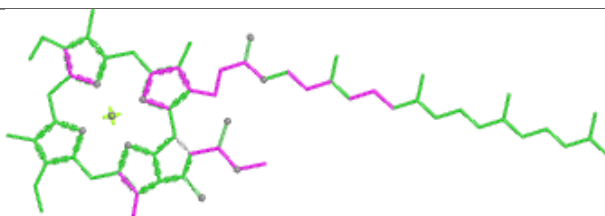
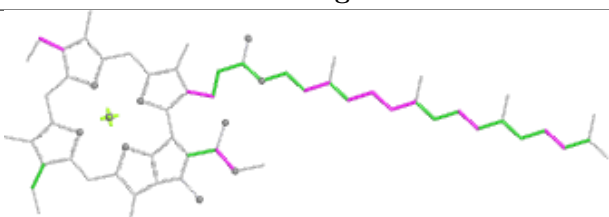
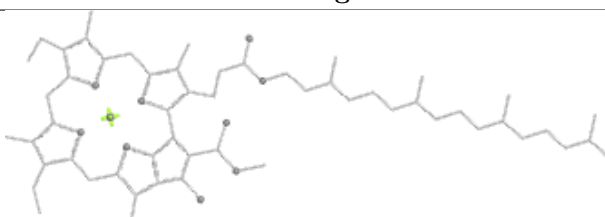
Ligand DGD AH 102

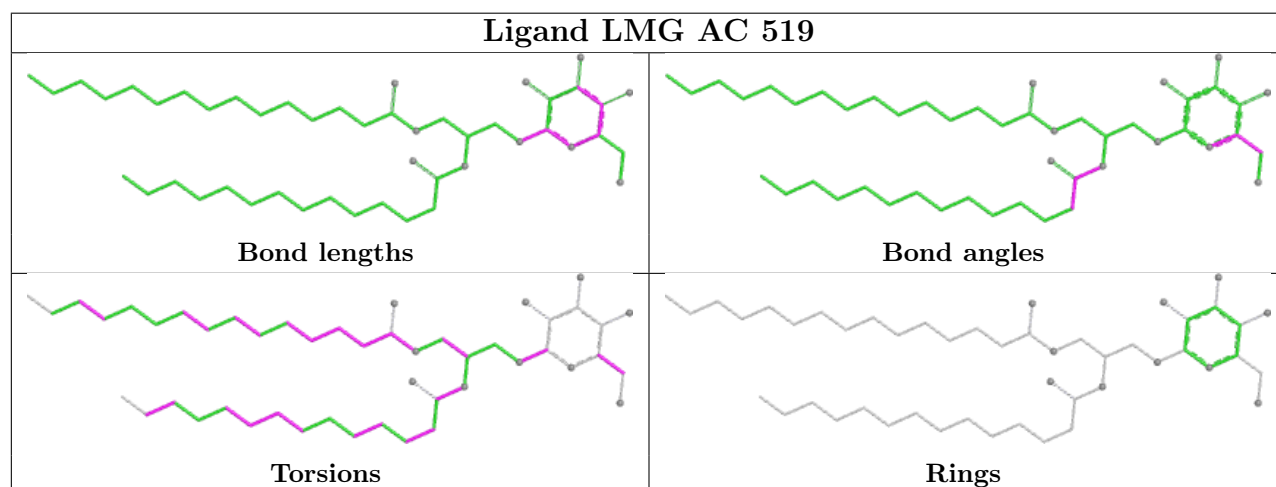
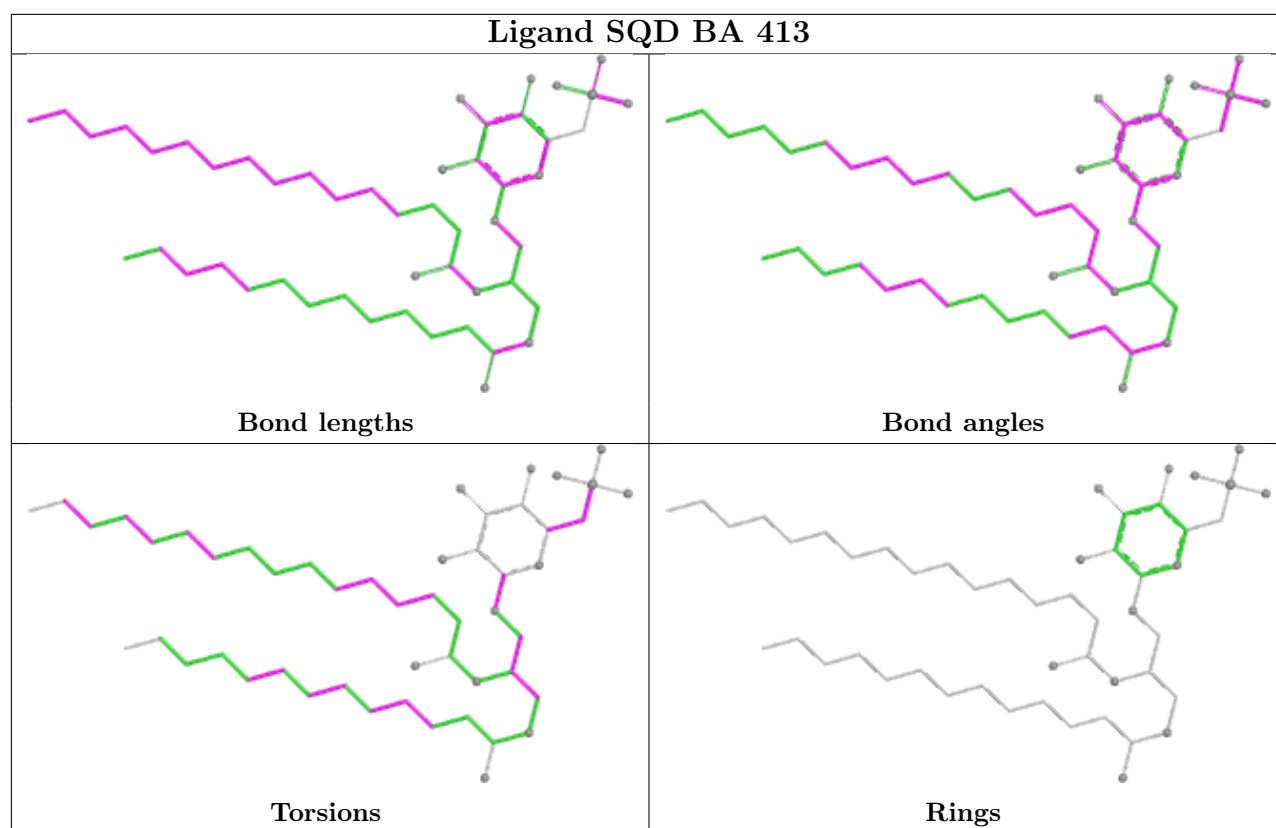


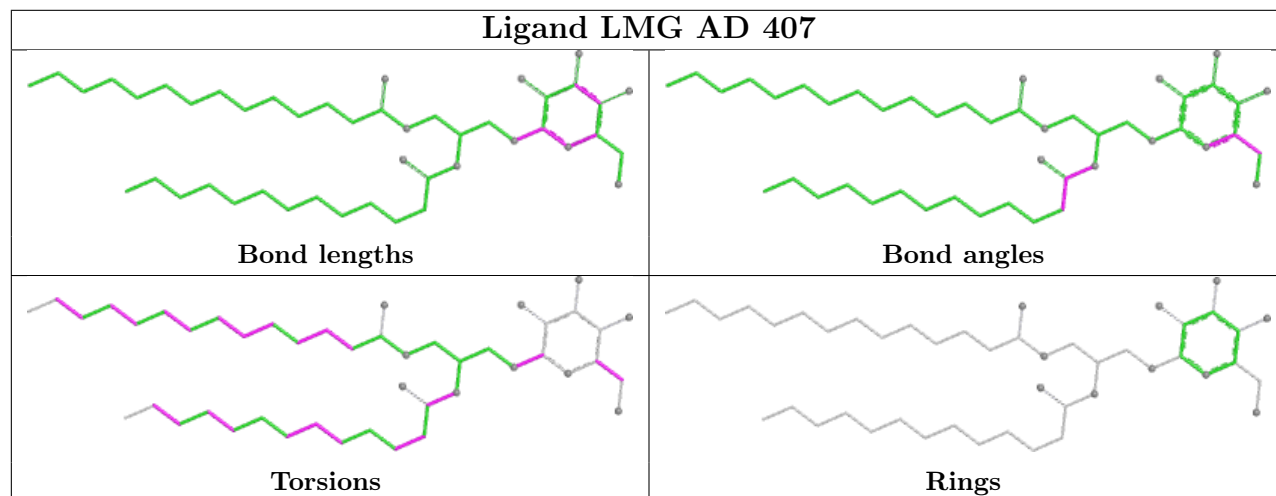
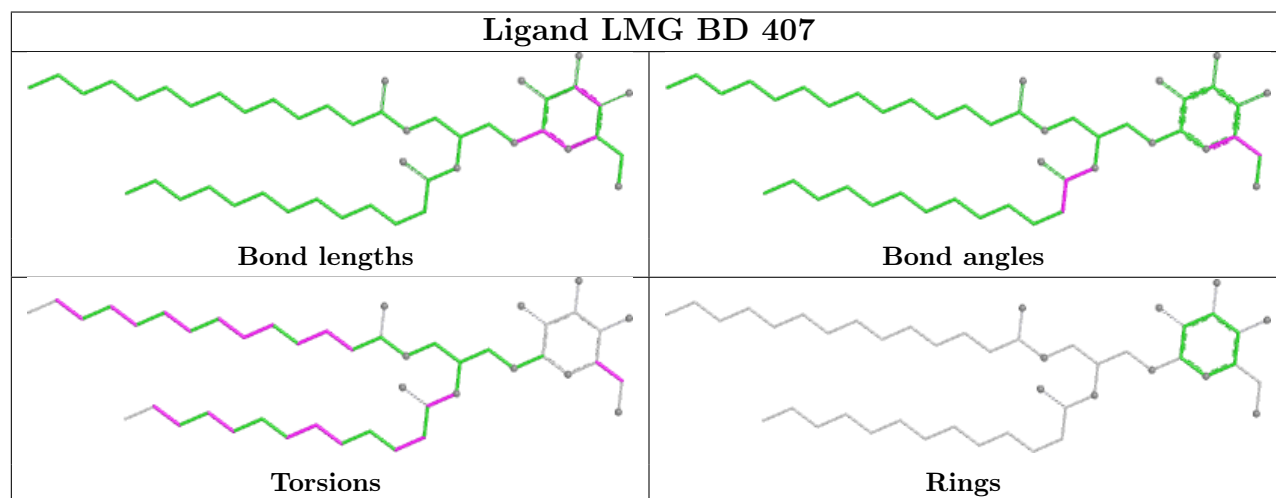
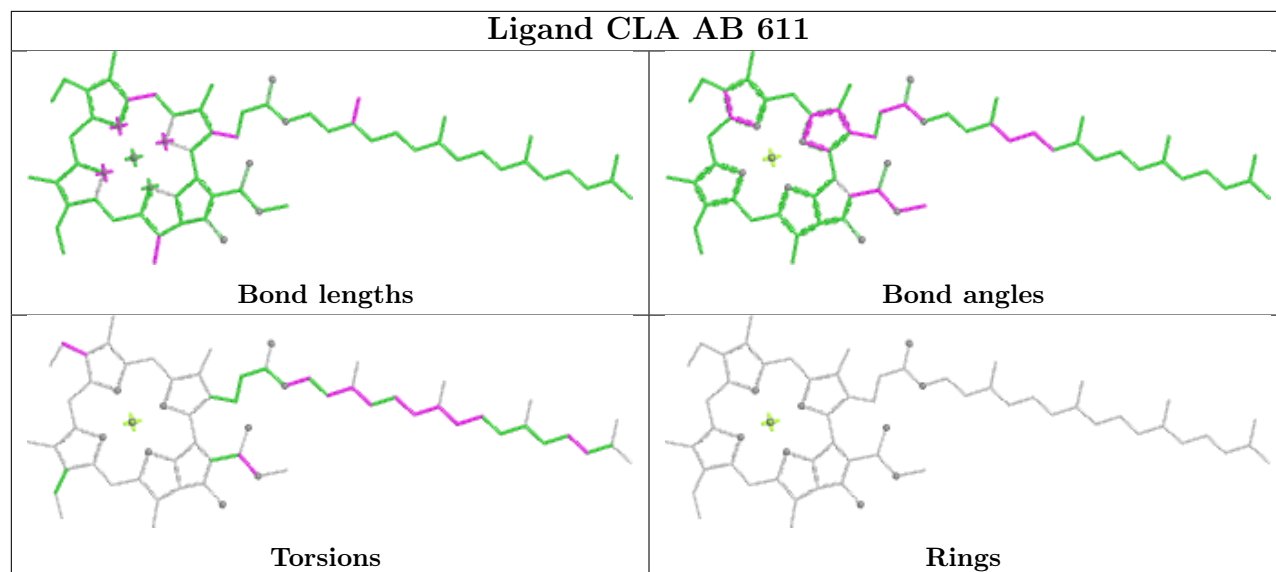


Ligand BCR BA 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

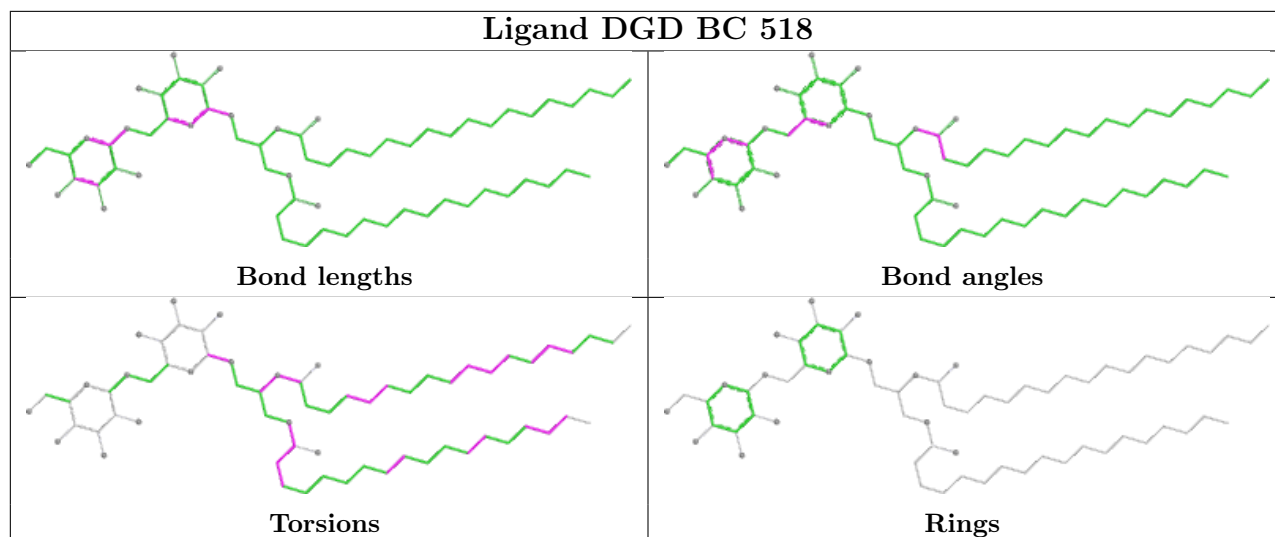
Ligand BCR BC 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BA 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

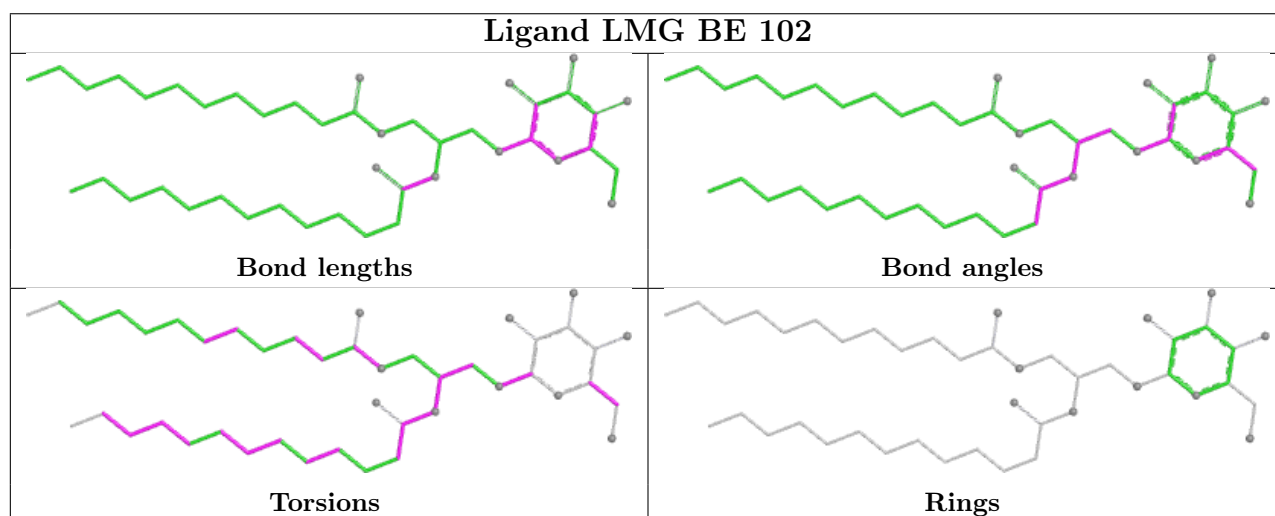




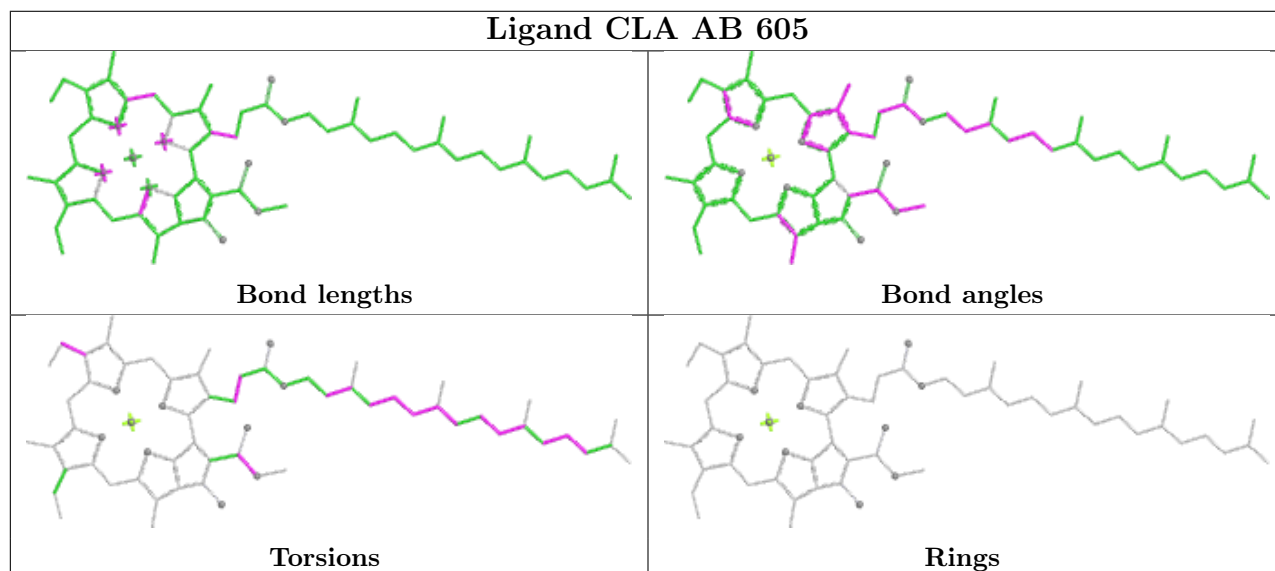
Ligand DGD BC 518

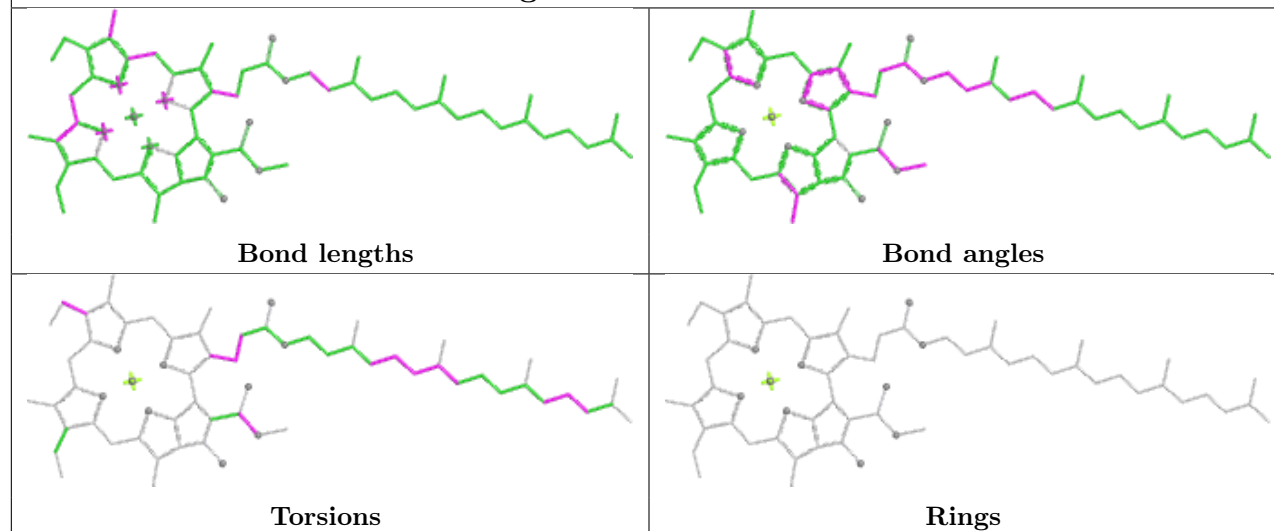
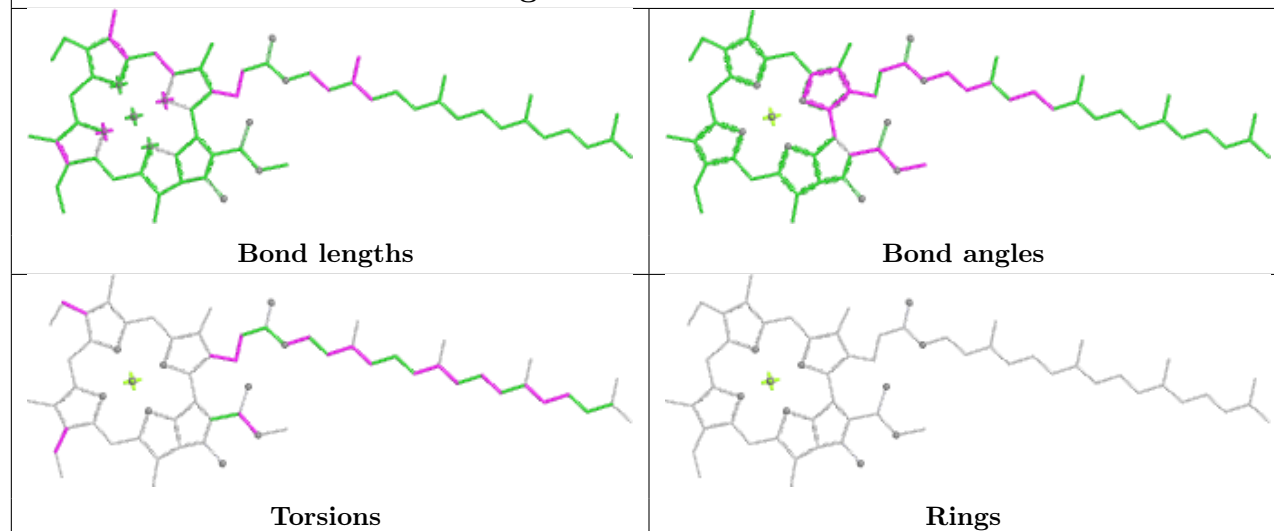
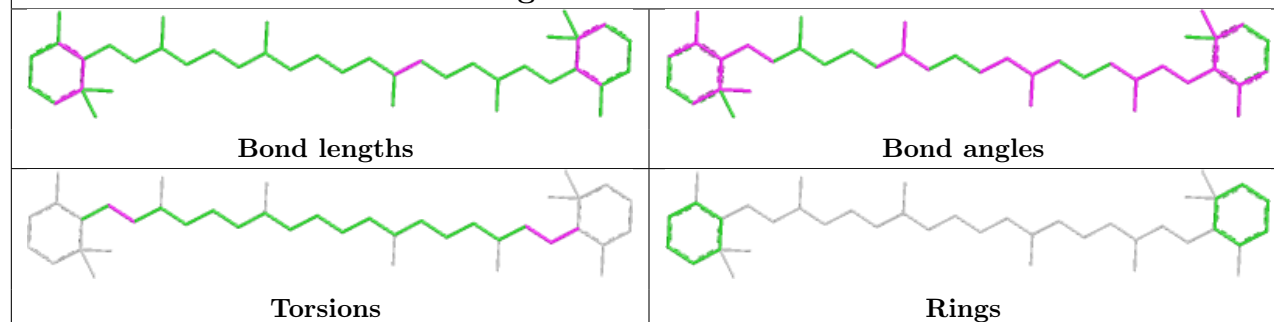


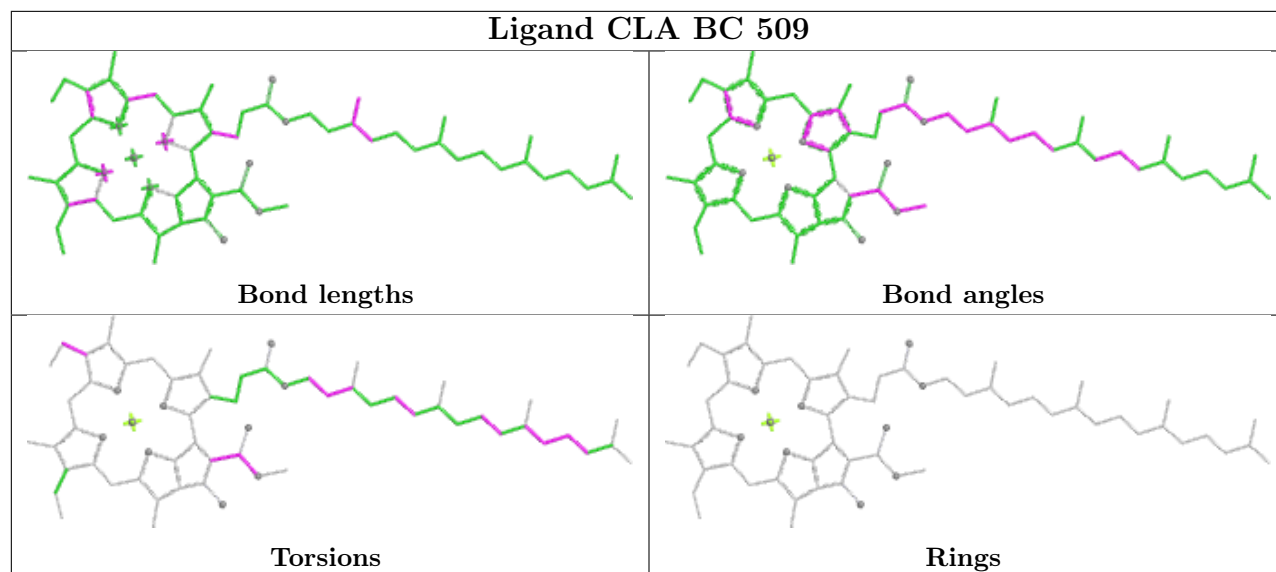
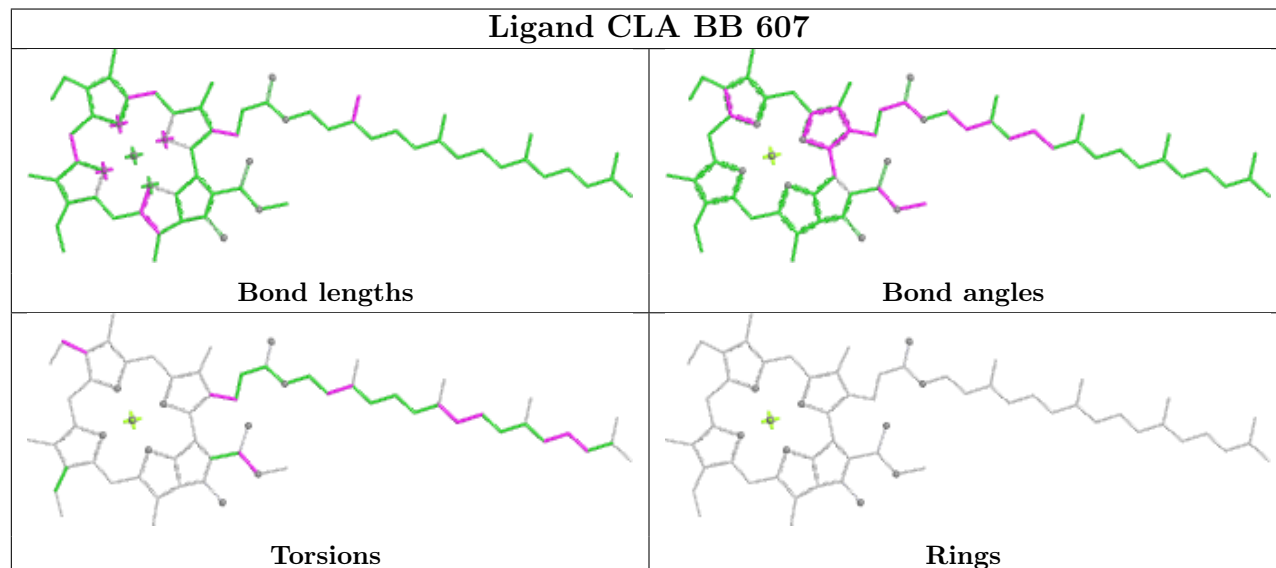
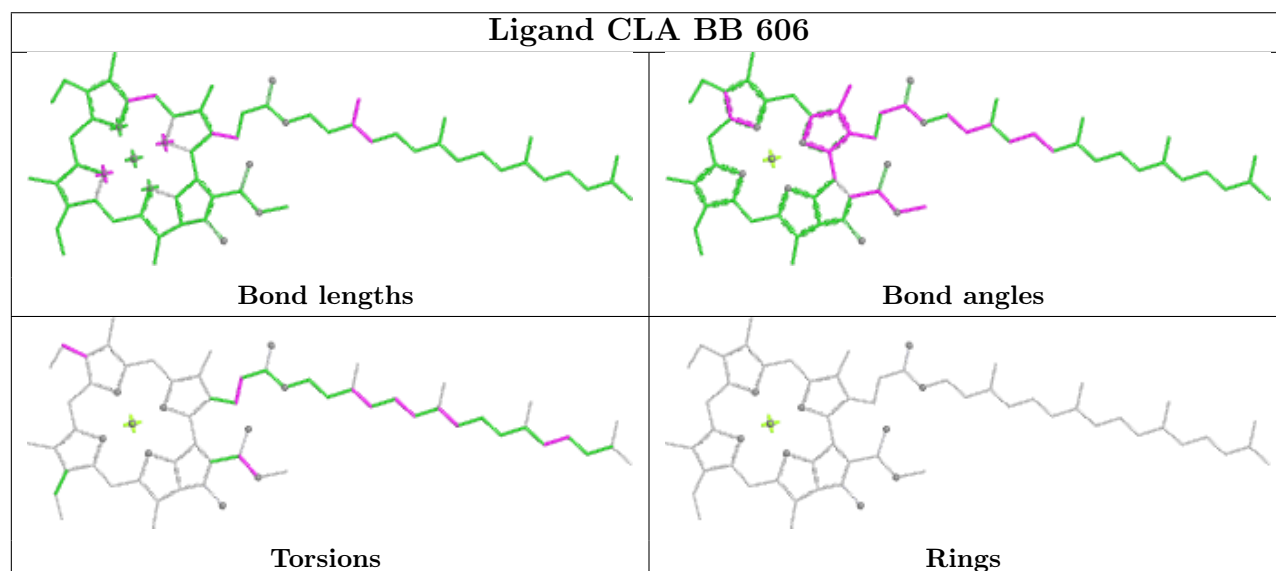
Ligand LMG BE 102

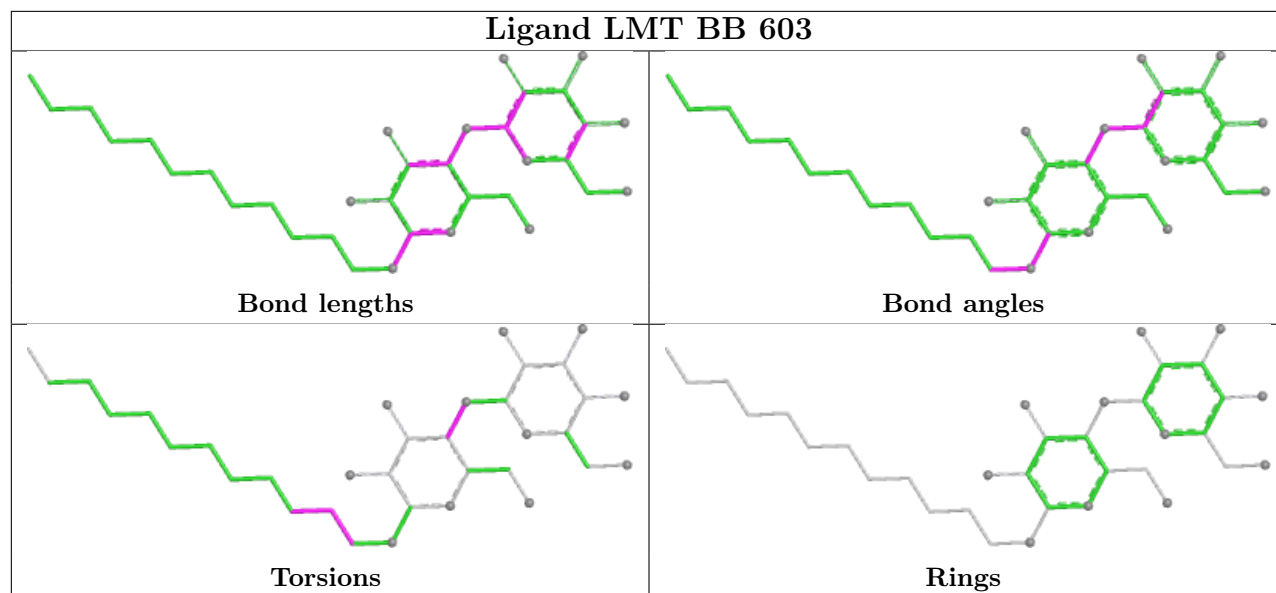


Ligand CLA AB 605



Ligand CLA BB 610**Ligand CLA BB 604****Ligand BCR BC 515**

Ligand CLA BC 509**Ligand CLA BB 607****Ligand CLA BB 606**



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%)	-0.56	0 100 100	23, 59, 88, 103	0
1	BA	335/344 (97%)	-0.42	1 (0%) 90 87	47, 70, 89, 103	0
2	AB	490/510 (96%)	-0.48	1 (0%) 91 89	37, 63, 86, 99	0
2	BB	490/510 (96%)	-0.51	0 100 100	41, 64, 87, 103	0
3	AC	447/473 (94%)	-0.42	2 (0%) 88 85	43, 72, 87, 102	0
3	BC	447/473 (94%)	-0.24	4 (0%) 81 75	54, 83, 95, 101	0
4	AD	340/352 (96%)	-0.61	1 (0%) 90 87	29, 59, 84, 95	0
4	BD	340/352 (96%)	-0.49	0 100 100	40, 69, 91, 101	0
5	AE	82/84 (97%)	-0.10	1 (1%) 76 69	54, 75, 93, 99	0
5	BE	82/84 (97%)	-0.15	1 (1%) 76 69	71, 85, 98, 104	0
6	AF	35/45 (77%)	-0.48	0 100 100	56, 73, 94, 97	0
6	BF	35/45 (77%)	-0.13	1 (2%) 53 45	75, 82, 97, 99	0
7	AH	65/66 (98%)	-0.21	0 100 100	57, 76, 92, 97	0
7	BH	65/66 (98%)	-0.23	1 (1%) 72 64	62, 80, 91, 103	0
8	AI	35/38 (92%)	-0.31	0 100 100	57, 70, 87, 94	0
8	BI	35/38 (92%)	-0.22	0 100 100	69, 80, 92, 95	0
9	AJ	34/40 (85%)	-0.09	1 (2%) 53 45	65, 74, 83, 89	0
9	BJ	34/40 (85%)	-0.23	0 100 100	73, 81, 93, 98	0
10	AK	37/37 (100%)	-0.51	0 100 100	67, 75, 86, 93	0
10	BK	37/37 (100%)	-0.24	0 100 100	84, 90, 96, 101	0
11	AL	37/37 (100%)	-0.43	0 100 100	45, 60, 98, 107	0
11	BL	37/37 (100%)	-0.41	0 100 100	46, 62, 94, 102	0
12	AM	34/36 (94%)	-0.42	0 100 100	51, 65, 94, 100	0
12	BM	34/36 (94%)	-0.55	0 100 100	55, 61, 76, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	-0.35	1 (0%) 88 85	39, 70, 93, 107	0
13	BO	243/247 (98%)	-0.23	3 (1%) 76 69	48, 76, 97, 107	0
14	AT	32/32 (100%)	-0.23	1 (3%) 51 42	53, 63, 102, 104	0
14	BT	32/32 (100%)	-0.25	0 100 100	57, 67, 93, 103	0
15	AU	97/104 (93%)	-0.47	0 100 100	43, 63, 78, 86	0
15	BU	97/104 (93%)	-0.48	0 100 100	55, 67, 77, 87	0
16	AV	137/137 (100%)	-0.53	1 (0%) 84 79	49, 66, 76, 79	0
16	BV	137/137 (100%)	-0.32	1 (0%) 84 79	64, 79, 95, 102	0
17	Ay	28/46 (60%)	0.08	1 (3%) 46 38	79, 91, 97, 99	0
17	By	28/46 (60%)	0.14	0 100 100	89, 98, 102, 106	0
18	AX	37/50 (74%)	-0.10	0 100 100	70, 79, 93, 95	0
18	BX	37/50 (74%)	-0.25	0 100 100	75, 82, 91, 94	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	-0.17	0 100 100	76, 85, 103, 110	0
20	BZ	62/62 (100%)	0.25	0 100 100	86, 96, 105, 110	0
All	All	5214/5536 (94%)	-0.39	22 (0%) 88 85	23, 71, 94, 110	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	AT	30	THR	3.2
6	BF	17	THR	3.0
3	AC	32	GLY	2.7
1	BA	11	ALA	2.7
3	AC	31	SER	2.5

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 oligosaccharides 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
24	PL9	AJ	101	35/55	0.39	0.15	93,101,107,109	0
24	PL9	BJ	101	35/55	0.44	0.14	78,99,111,112	0
26	BCR	BJ	102	40/40	0.46	0.14	93,98,101,102	0
28	LHG	AC	521	37/49	0.50	0.13	78,99,109,109	0
28	LHG	BC	521	37/49	0.50	0.14	90,100,113,114	0
27	DGD	BD	410	63/66	0.53	0.11	84,100,105,105	0
25	OEC	BA	409	5/9	0.54	0.10	30,74,79,92	0
27	DGD	AD	410	63/66	0.55	0.12	91,97,107,108	0
22	CLA	BB	604	65/65	0.55	0.15	86,98,107,109	0
30	LMG	AI	101	43/55	0.56	0.13	83,92,97,98	0
32	LMT	BI	102	35/35	0.56	0.11	90,104,106,106	0
30	LMG	BI	101	43/55	0.59	0.11	84,90,99,100	0
30	LMG	AC	520	45/55	0.62	0.10	75,92,97,98	0
32	LMT	AB	627	35/35	0.64	0.12	73,103,106,107	0
32	LMT	AI	102	35/35	0.64	0.10	74,92,95,95	0
26	BCR	AJ	102	40/40	0.64	0.12	85,91,101,102	0
27	DGD	BB	602	52/66	0.65	0.12	71,85,104,105	0
32	LMT	AB	624	35/35	0.66	0.12	71,100,106,107	0
27	DGD	AB	626	52/66	0.68	0.11	79,94,105,107	0
29	SQD	AD	409	43/54	0.69	0.11	68,92,108,111	0
32	LMT	BB	625	35/35	0.69	0.12	66,103,111,111	0
22	CLA	AB	601	65/65	0.69	0.12	88,97,102,105	0
32	LMT	BB	603	35/35	0.70	0.10	68,86,95,96	0
30	LMG	BC	520	45/55	0.71	0.09	86,93,101,102	0
32	LMT	BD	411	31/35	0.71	0.12	67,91,99,100	0
32	LMT	AD	411	31/35	0.71	0.13	52,96,104,104	0
29	SQD	BD	409	43/54	0.72	0.10	73,88,110,111	0
29	SQD	BF	101	45/54	0.73	0.10	95,98,103,104	0
32	LMT	AT	101	35/35	0.73	0.12	72,91,97,98	0
29	SQD	AF	101	45/54	0.73	0.10	82,97,102,103	0
30	LMG	AM	101	42/55	0.74	0.10	68,86,93,95	0
27	DGD	AA	410	56/66	0.74	0.12	78,86,91,92	0
30	LMG	AA	416	42/55	0.74	0.11	67,92,96,99	0
27	DGD	BA	411	56/66	0.75	0.10	76,85,103,104	0
30	LMG	BE	102	44/55	0.77	0.11	75,92,98,99	0
29	SQD	BA	401	54/54	0.77	0.09	82,91,107,108	0
30	LMG	BM	102	42/55	0.77	0.09	72,90,95,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	LMG	AC	519	48/55	0.77	0.09	75,84,89,90	0
30	LMG	BC	519	48/55	0.78	0.08	83,90,94,95	0
26	BCR	BZ	101	40/40	0.78	0.10	81,90,93,94	0
32	LMT	AB	625	35/35	0.79	0.09	82,98,100,101	0
30	LMG	AB	623	42/55	0.79	0.10	70,89,92,93	0
30	LMG	AE	102	44/55	0.79	0.10	81,91,96,96	0
32	LMT	BT	101	35/35	0.79	0.11	77,91,94,95	0
27	DGD	BC	517	62/66	0.80	0.12	78,82,100,101	0
30	LMG	BB	623	49/55	0.80	0.10	70,78,88,91	0
29	SQD	BA	413	51/54	0.80	0.09	73,90,103,104	0
29	SQD	BL	101	47/54	0.81	0.09	75,91,115,116	0
29	SQD	AA	415	54/54	0.81	0.09	71,87,105,105	0
32	LMT	BM	101	35/35	0.81	0.09	70,88,97,101	0
32	LMT	BB	626	35/35	0.81	0.09	76,93,101,102	0
29	SQD	AA	412	51/54	0.82	0.10	73,83,98,99	0
31	CL	AA	414	1/1	0.82	0.07	73,73,73,73	0
30	LMG	BD	407	46/55	0.82	0.10	70,80,92,94	0
26	BCR	BC	515	40/40	0.82	0.08	74,80,91,92	0
24	PL9	AA	407	45/55	0.82	0.09	83,87,94,95	0
26	BCR	AK	102	40/40	0.83	0.10	73,77,81,81	0
22	CLA	AC	513	65/65	0.83	0.10	92,98,104,106	0
22	CLA	BB	617	65/65	0.83	0.12	75,79,99,100	0
30	LMG	BD	408	48/55	0.83	0.09	68,75,85,87	0
22	CLA	BC	505	65/65	0.83	0.09	88,93,94,95	0
22	CLA	BC	508	65/65	0.83	0.09	92,97,101,106	0
22	CLA	BC	513	65/65	0.83	0.10	96,99,106,107	0
26	BCR	BX	101	40/40	0.84	0.10	76,79,89,90	0
22	CLA	BC	512	65/65	0.84	0.10	95,99,109,110	0
22	CLA	AC	512	65/65	0.84	0.10	91,95,106,106	0
30	LMG	AA	413	51/55	0.84	0.09	70,74,77,79	0
22	CLA	BD	404	65/65	0.84	0.10	89,92,101,102	0
27	DGD	AC	516	53/66	0.84	0.10	57,72,91,92	0
22	CLA	AB	614	65/65	0.84	0.11	78,85,98,99	0
22	CLA	AC	506	65/65	0.84	0.09	83,87,101,102	0
24	PL9	BA	408	45/55	0.84	0.07	82,88,90,92	0
26	BCR	BK	102	40/40	0.84	0.08	76,81,85,85	0
29	SQD	BB	601	47/54	0.84	0.08	74,87,109,111	0
26	BCR	AZ	101	40/40	0.85	0.08	75,82,90,91	0
27	DGD	BC	518	66/66	0.85	0.09	71,78,89,90	0
30	LMG	AD	408	48/55	0.85	0.09	63,68,74,80	0
26	BCR	AH	101	40/40	0.85	0.10	76,88,95,95	0
22	CLA	BB	619	65/65	0.85	0.09	75,81,93,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	BC	511	65/65	0.85	0.09	91,99,104,105	0
27	DGD	BC	516	53/66	0.85	0.10	69,77,96,97	0
28	LHG	AA	411	39/49	0.86	0.09	63,68,76,78	0
30	LMG	BA	414	51/55	0.86	0.08	62,71,78,80	0
22	CLA	BC	506	65/65	0.86	0.09	81,85,97,99	0
27	DGD	AC	517	62/66	0.86	0.11	70,78,91,92	0
30	LMG	AB	621	49/55	0.86	0.08	62,75,80,83	0
26	BCR	BD	406	40/40	0.86	0.08	66,78,92,92	0
25	OEC	AA	408	5/9	0.87	0.07	56,62,67,75	0
22	CLA	AB	616	65/65	0.87	0.09	73,85,105,106	0
30	LMG	AD	407	46/55	0.87	0.08	63,71,90,92	0
27	DGD	BH	101	58/66	0.87	0.09	66,73,80,81	0
22	CLA	AC	511	65/65	0.87	0.09	77,85,89,90	0
22	CLA	BB	618	65/65	0.88	0.10	69,84,87,88	0
22	CLA	AC	507	65/65	0.88	0.09	83,90,95,97	0
22	CLA	AB	609	65/65	0.88	0.08	76,87,91,92	0
22	CLA	AB	615	65/65	0.88	0.09	83,93,97,99	0
22	CLA	BC	507	65/65	0.88	0.09	84,92,96,97	0
32	LMT	AM	102	35/35	0.88	0.07	67,89,93,96	0
27	DGD	AC	518	66/66	0.88	0.09	62,68,84,86	0
35	CA	BO	301	1/1	0.88	0.07	100,100,100,100	0
28	LHG	BA	412	39/49	0.89	0.07	72,77,80,81	0
26	BCR	AB	620	40/40	0.89	0.08	75,77,83,84	0
26	BCR	AD	406	40/40	0.89	0.07	64,72,85,85	0
22	CLA	AB	604	65/65	0.89	0.09	67,73,91,91	0
22	CLA	AC	504	65/65	0.89	0.10	78,86,107,107	0
22	CLA	BC	503	65/65	0.89	0.10	82,97,100,101	0
27	DGD	AH	102	58/66	0.89	0.09	57,72,85,86	0
22	CLA	AB	606	65/65	0.89	0.09	73,87,96,96	0
26	BCR	BB	620	40/40	0.89	0.08	66,69,72,73	0
22	CLA	AB	608	65/65	0.89	0.08	72,79,87,91	0
22	CLA	BB	609	65/65	0.89	0.10	72,80,96,96	0
22	CLA	BB	612	65/65	0.89	0.08	82,89,92,95	0
22	CLA	BC	510	65/65	0.89	0.11	79,83,92,92	0
22	CLA	AC	508	65/65	0.89	0.09	80,86,99,101	0
26	BCR	AB	618	40/40	0.89	0.07	75,78,82,83	0
35	CA	BK	101	1/1	0.89	0.06	90,90,90,90	0
26	BCR	AB	619	40/40	0.89	0.08	62,70,82,83	0
30	LMG	AB	622	49/55	0.90	0.08	64,73,80,83	0
22	CLA	BC	501	65/65	0.90	0.07	76,80,87,88	0
22	CLA	AB	612	65/65	0.90	0.09	63,75,81,83	0
26	BCR	AC	515	40/40	0.90	0.07	69,75,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	BC	504	65/65	0.90	0.09	87,92,102,102	0
23	PHO	BD	403	64/64	0.90	0.10	77,88,92,93	0
22	CLA	BB	610	65/65	0.90	0.08	60,70,77,81	0
22	CLA	BB	611	65/65	0.90	0.08	67,74,81,85	0
26	BCR	AT	102	40/40	0.90	0.09	72,79,91,91	0
22	CLA	AD	404	65/65	0.90	0.08	80,83,102,103	0
22	CLA	BA	407	65/65	0.90	0.09	72,76,103,104	0
30	LMG	BB	624	49/55	0.90	0.08	68,72,78,79	0
26	BCR	BB	622	40/40	0.90	0.07	67,71,79,80	0
22	CLA	BC	509	65/65	0.90	0.09	73,83,93,94	0
22	CLA	AA	404	65/65	0.90	0.09	63,72,97,99	0
26	BCR	AA	409	40/40	0.90	0.09	59,67,70,71	0
26	BCR	AB	617	40/40	0.90	0.07	56,67,75,76	0
22	CLA	BB	606	65/65	0.90	0.08	58,61,74,76	0
22	CLA	BB	613	65/65	0.91	0.09	69,77,82,84	0
22	CLA	AB	613	65/65	0.91	0.08	65,69,84,87	0
22	CLA	AB	610	65/65	0.91	0.08	60,67,79,80	0
31	CL	BA	415	1/1	0.91	0.06	81,81,81,81	0
22	CLA	BA	405	65/65	0.91	0.08	72,76,104,105	0
23	PHO	AD	403	64/64	0.91	0.08	39,56,70,72	0
23	PHO	BA	406	64/64	0.91	0.07	54,61,70,74	0
22	CLA	AC	505	65/65	0.91	0.07	69,73,77,79	0
34	HEM	BE	101	43/43	0.91	0.12	93,95,104,107	0
22	CLA	BC	502	65/65	0.91	0.08	81,85,101,103	0
22	CLA	AB	603	65/65	0.91	0.08	54,60,72,74	0
22	CLA	AC	501	65/65	0.92	0.08	78,83,85,86	0
22	CLA	BB	605	65/65	0.92	0.09	77,82,86,89	0
22	CLA	AB	611	65/65	0.92	0.07	62,68,71,73	0
22	CLA	BB	616	65/65	0.92	0.07	49,54,79,82	0
22	CLA	AB	607	65/65	0.92	0.07	50,55,74,74	0
22	CLA	AA	406	65/65	0.92	0.08	54,60,89,90	0
26	BCR	BA	410	40/40	0.92	0.07	61,74,82,83	0
22	CLA	BA	403	65/65	0.93	0.08	57,64,71,75	0
22	CLA	BB	614	65/65	0.93	0.08	59,68,75,77	0
22	CLA	BB	615	65/65	0.93	0.08	60,72,77,81	0
22	CLA	AB	602	65/65	0.93	0.07	81,85,88,90	0
22	CLA	AB	605	65/65	0.93	0.08	68,76,84,85	0
22	CLA	AD	402	65/65	0.93	0.08	47,58,69,71	0
26	BCR	BB	621	40/40	0.93	0.07	57,69,82,83	0
26	BCR	AC	514	40/40	0.93	0.07	56,66,73,74	0
26	BCR	BC	514	40/40	0.93	0.08	81,83,87,87	0
34	HEM	AE	101	43/43	0.93	0.11	85,92,103,106	0

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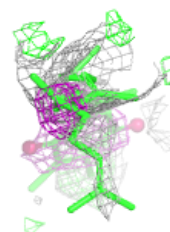
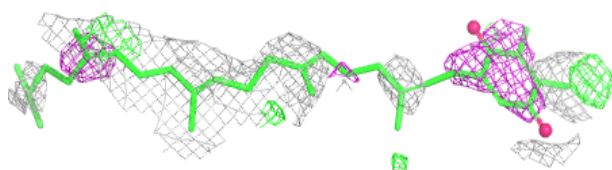
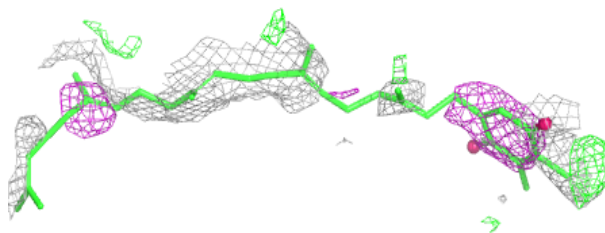
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PL9	BD	405	55/55	0.93	0.07	63,70,76,78	0
22	CLA	AC	503	65/65	0.93	0.10	78,86,92,95	0
23	PHO	AA	405	64/64	0.93	0.07	40,64,67,69	0
22	CLA	BB	607	65/65	0.94	0.06	53,64,86,87	0
22	CLA	BB	608	65/65	0.94	0.07	45,53,76,78	0
22	CLA	BD	402	65/65	0.94	0.07	50,57,79,83	0
22	CLA	BA	404	65/65	0.94	0.07	55,60,68,70	0
22	CLA	AA	402	65/65	0.94	0.07	51,58,66,69	0
22	CLA	AC	502	65/65	0.94	0.07	50,58,81,84	0
22	CLA	AC	509	65/65	0.94	0.08	59,74,86,89	0
22	CLA	AC	510	65/65	0.94	0.07	48,56,70,72	0
35	CA	AO	301	1/1	0.94	0.04	87,87,87,87	0
22	CLA	AA	403	65/65	0.94	0.07	41,48,56,60	0
24	PL9	AD	405	55/55	0.94	0.07	52,67,71,73	0
33	BCT	BD	401	4/4	0.96	0.05	84,86,87,88	0
34	HEM	AV	201	43/43	0.96	0.07	60,63,66,67	0
33	BCT	AD	401	4/4	0.97	0.04	90,91,91,92	0
34	HEM	BV	201	43/43	0.97	0.07	58,67,76,79	0
35	CA	AK	101	1/1	0.97	0.07	95,95,95,95	0
21	FE2	AA	401	1/1	0.98	0.05	69,69,69,69	0
21	FE2	BA	402	1/1	0.99	0.06	81,81,81,81	0

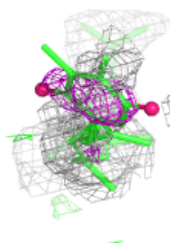
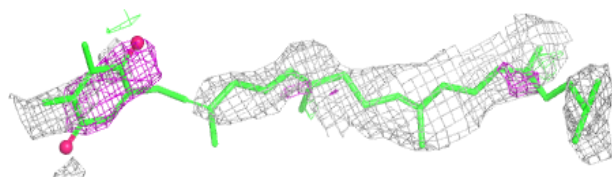
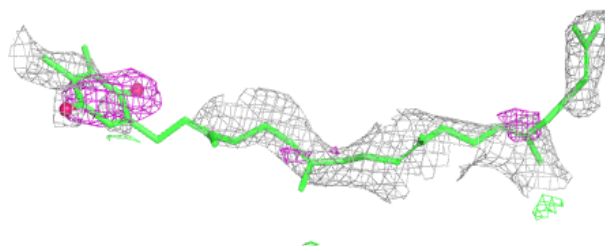
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PL9 AJ 101:

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

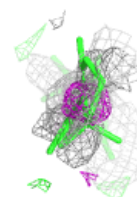
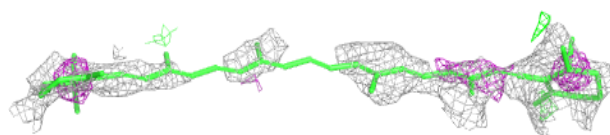
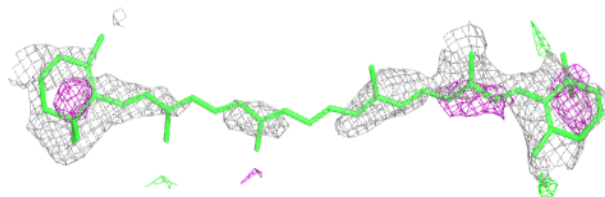
**Electron density around PL9 BJ 101:**

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

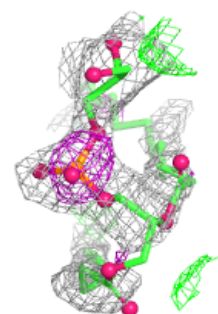
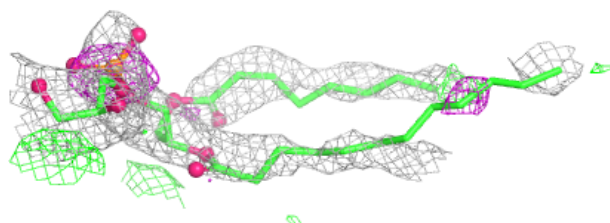
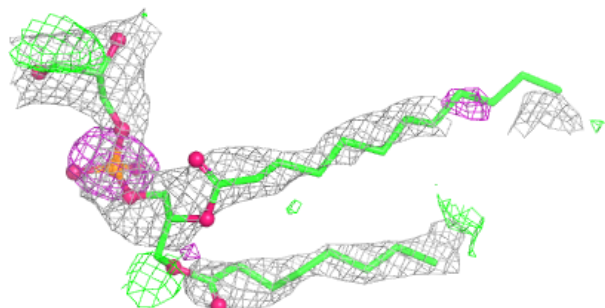


Electron density around BCR BJ 102:

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

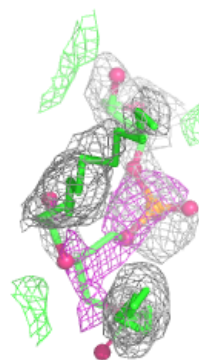
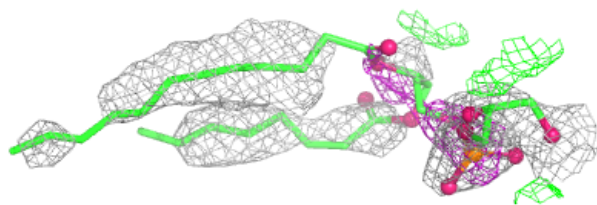
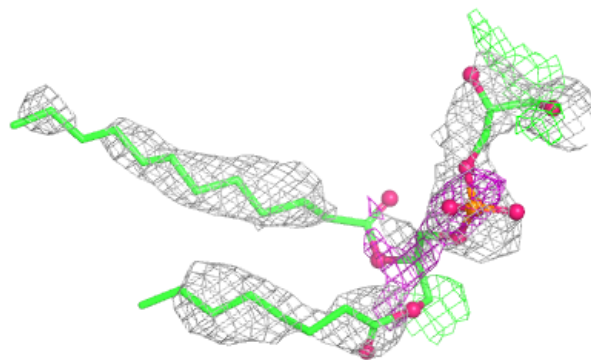
**Electron density around LHG AC 521:**

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

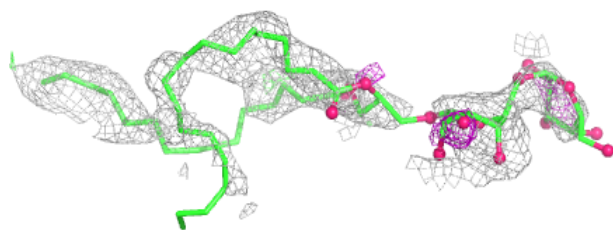
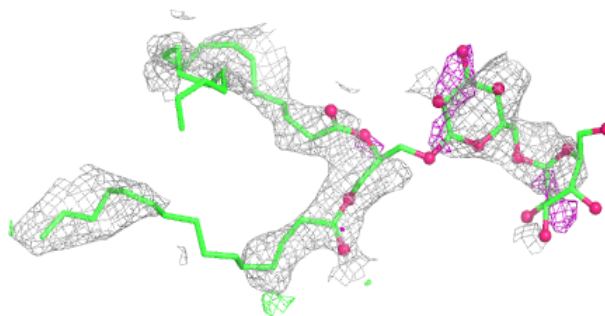


Electron density around LHG BC 521:

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

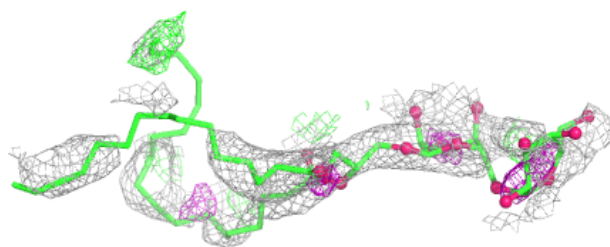
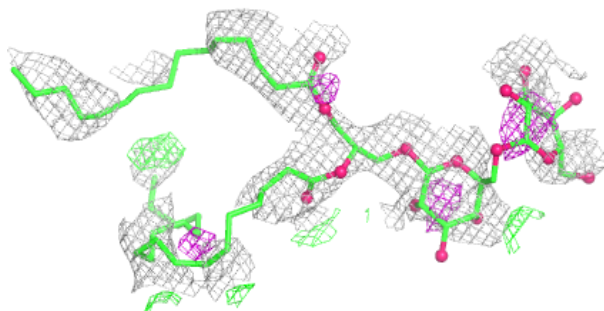
**Electron density around DGD BD 410:**

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



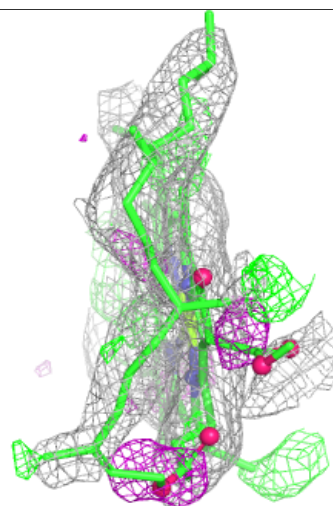
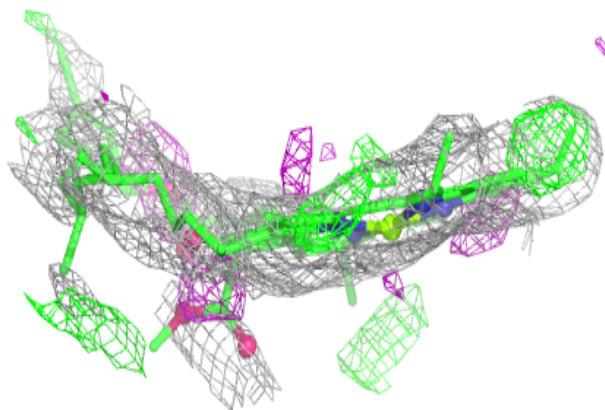
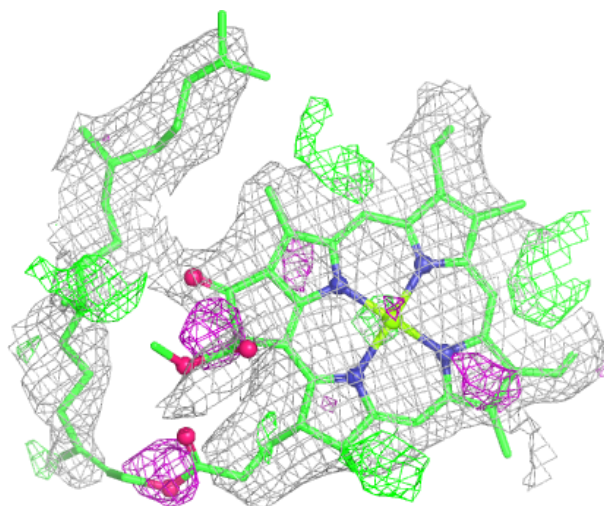
Electron density around DGD AD 410:

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



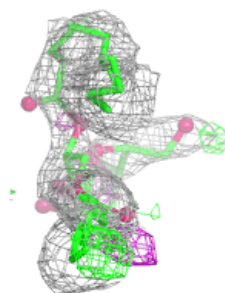
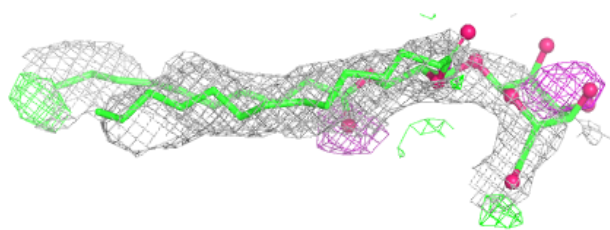
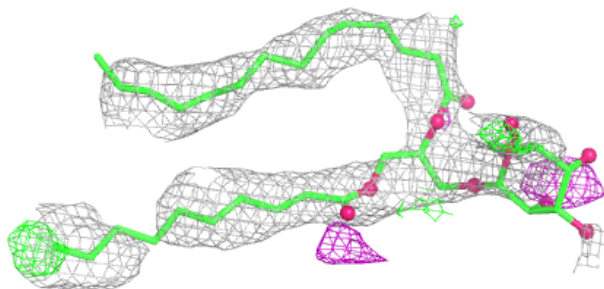
Electron density around CLA BB 604:

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

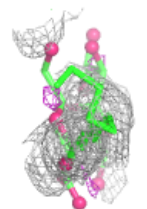
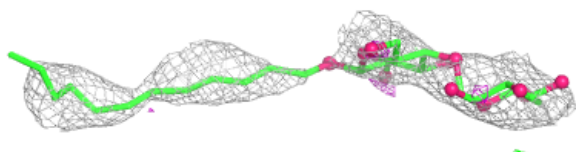
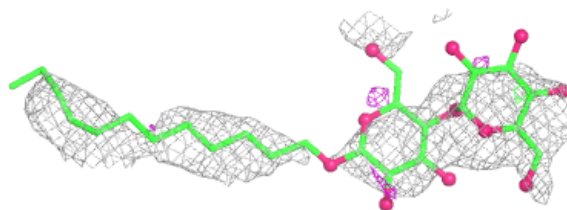


Electron density around LMG AI 101:

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

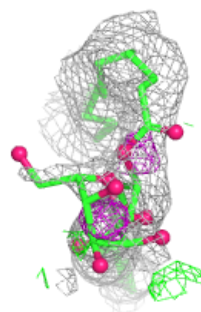
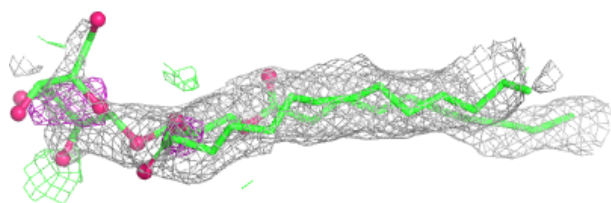
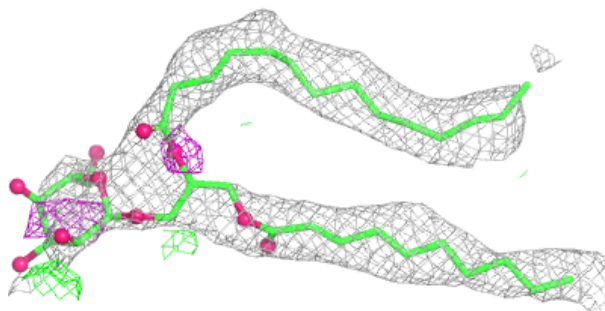
**Electron density around LMT BI 102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

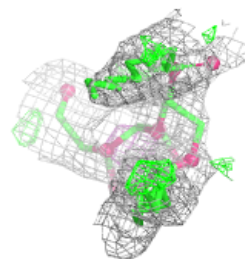
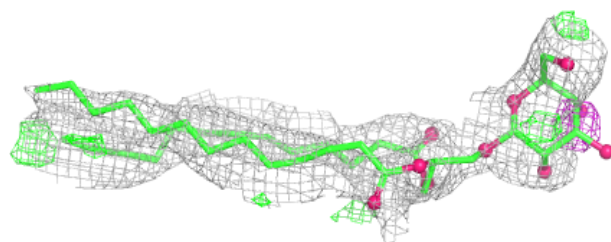
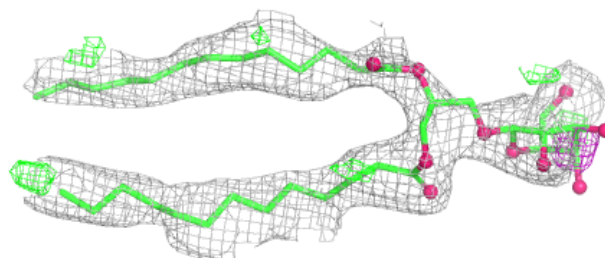


Electron density around LMG BI 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

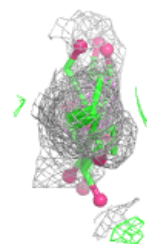
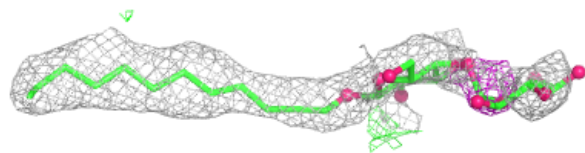
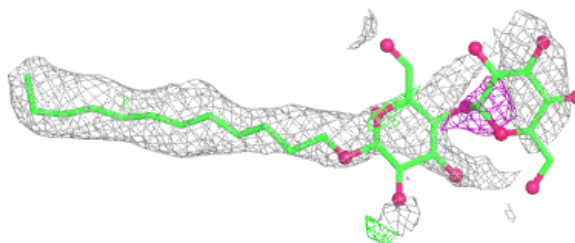
**Electron density around LMG AC 520:**

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

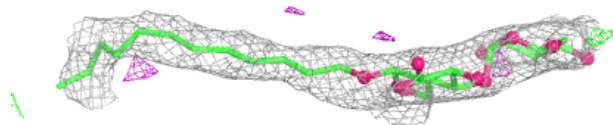
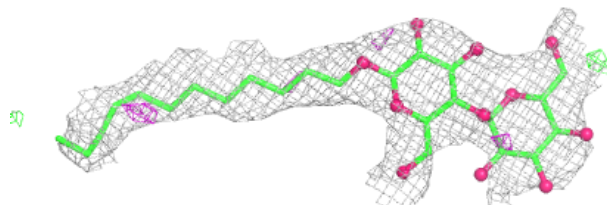


Electron density around LMT AB 627:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

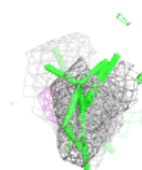
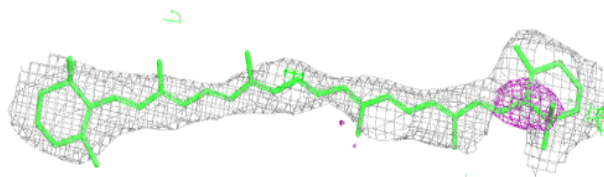
**Electron density around LMT AI 102:**

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

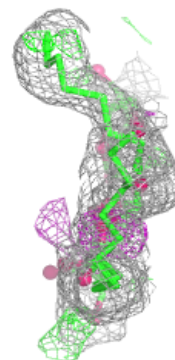
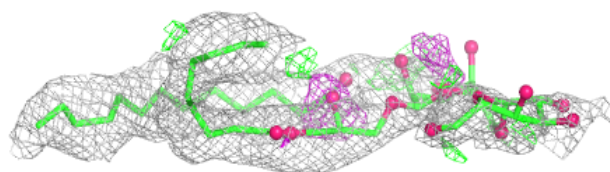
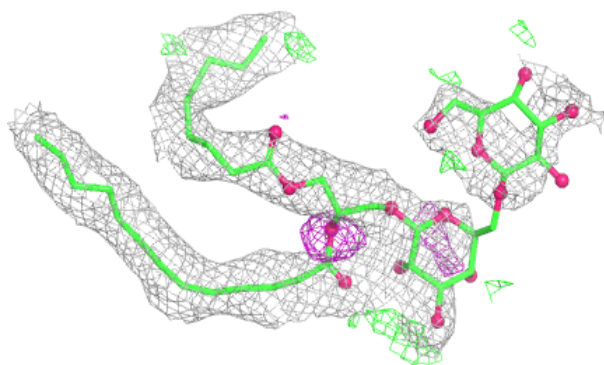


Electron density around BCR AJ 102:

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

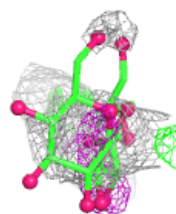
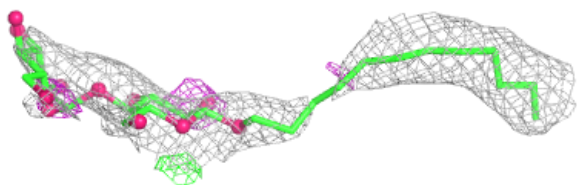
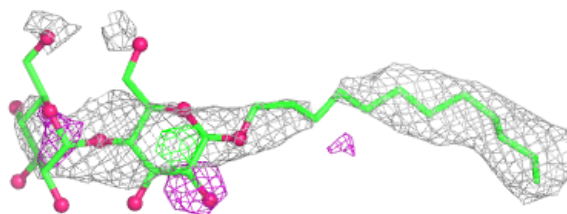
**Electron density around DGD BB 602:**

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

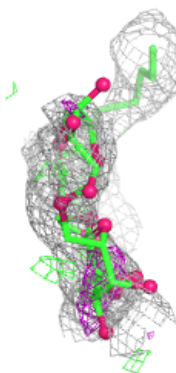
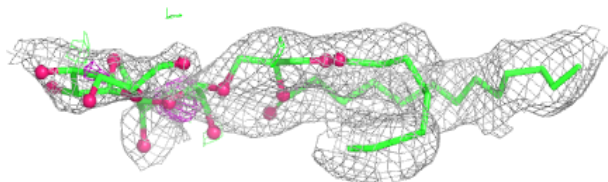
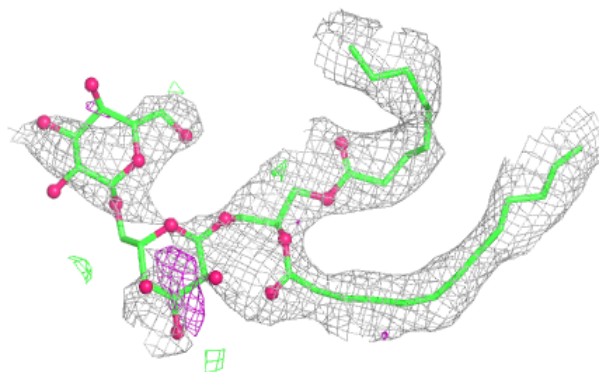


Electron density around LMT AB 624:

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

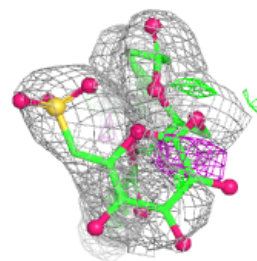
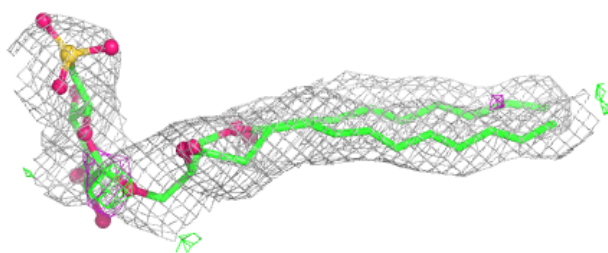
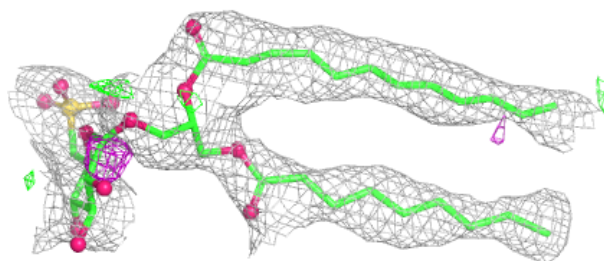
**Electron density around DGD AB 626:**

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

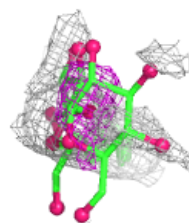
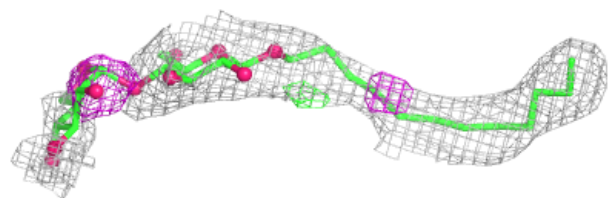
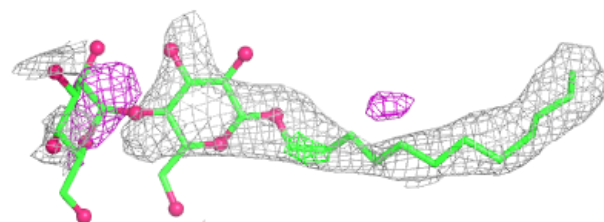


Electron density around SQD AD 409:

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

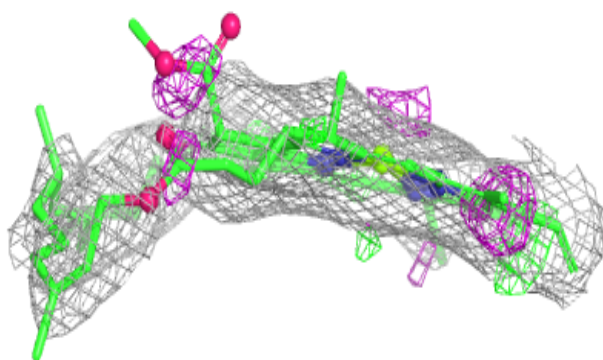
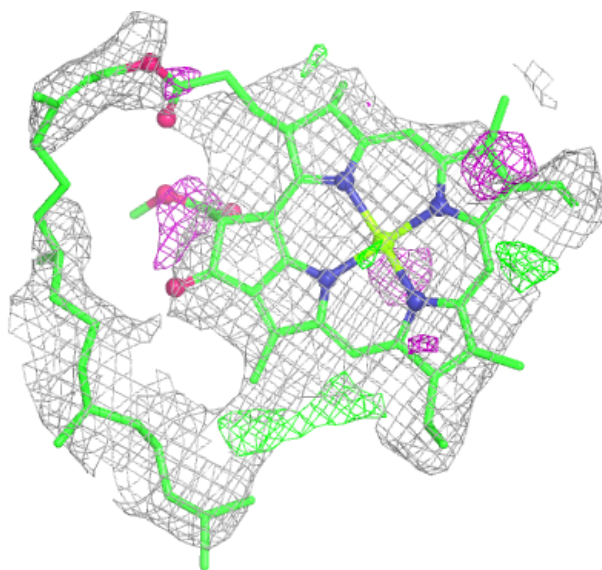
**Electron density around LMT BB 625:**

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



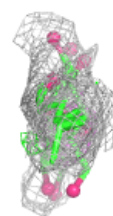
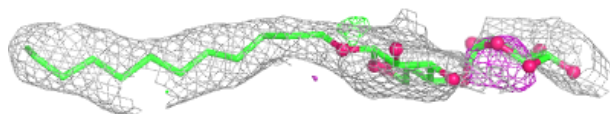
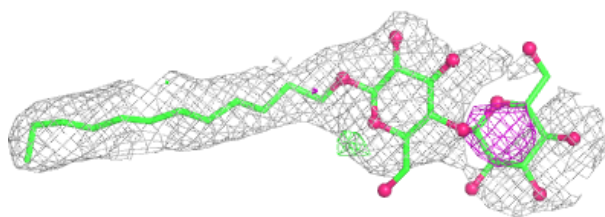
Electron density around CLA AB 601:

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

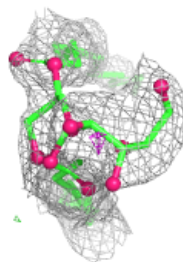
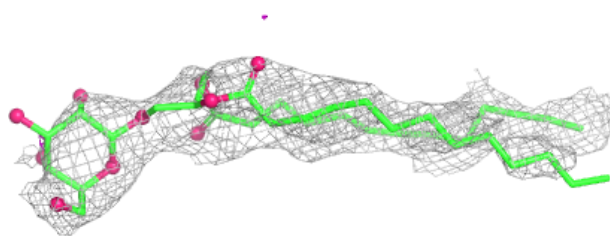
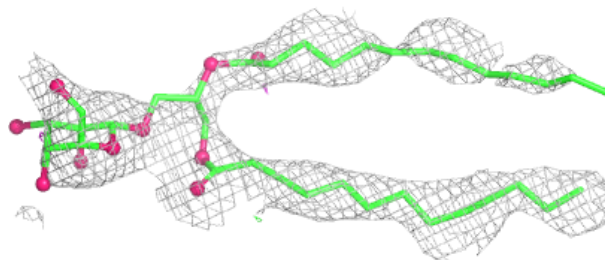


Electron density around LMT BB 603:

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

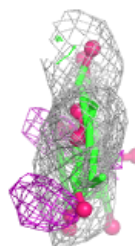
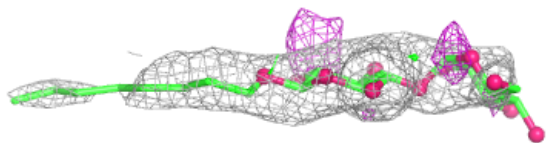
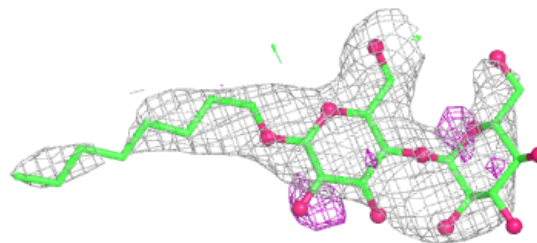
**Electron density around LMG BC 520:**

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

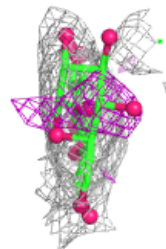
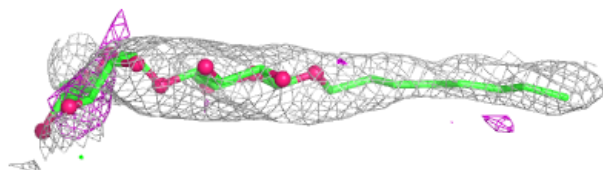
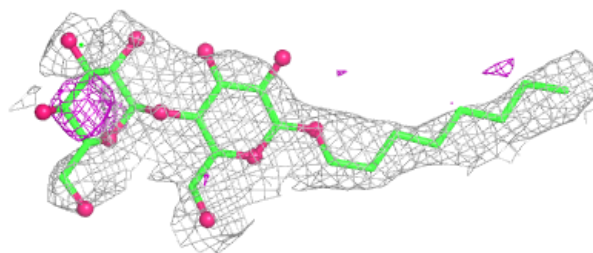


Electron density around LMT BD 411:

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

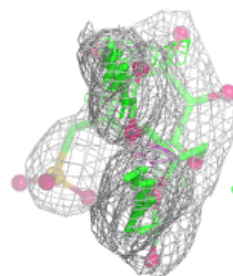
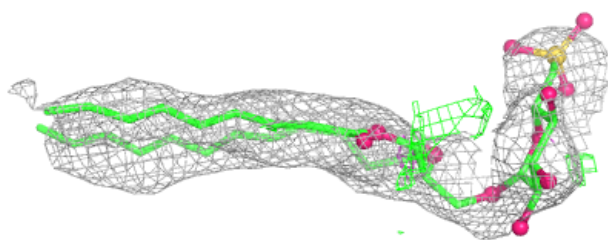
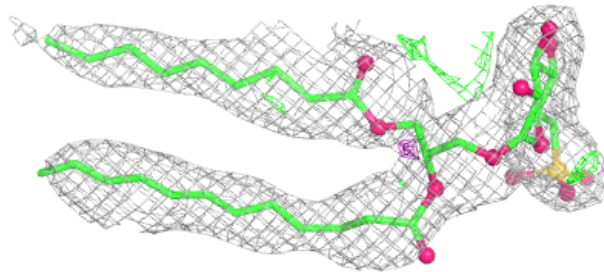
**Electron density around LMT AD 411:**

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

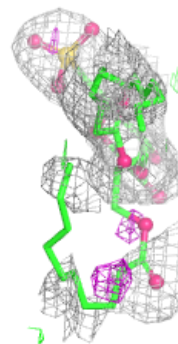
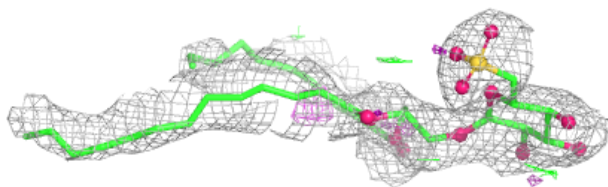
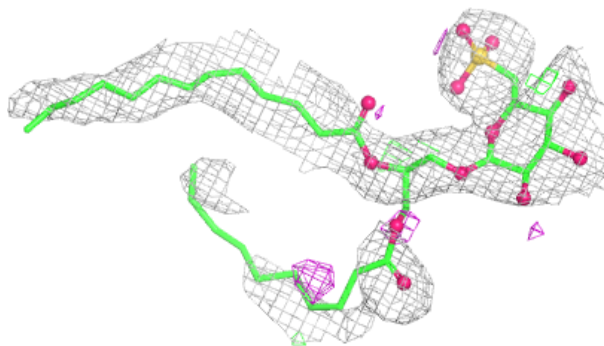


Electron density around SQD BD 409:

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

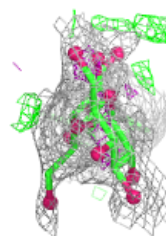
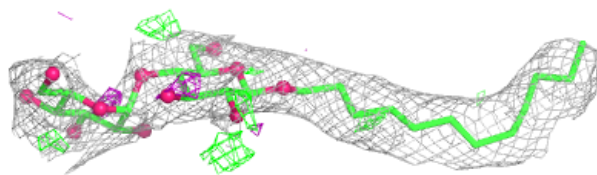
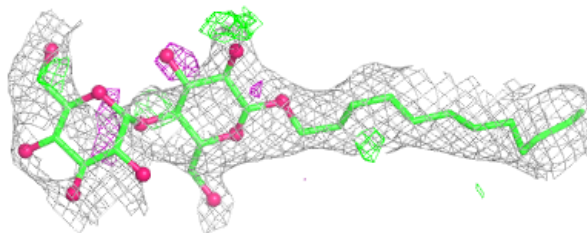
**Electron density around SQD BF 101:**

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

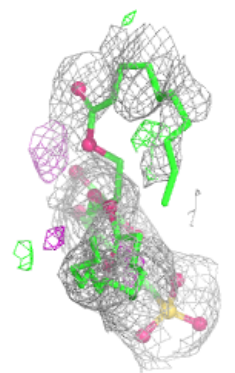
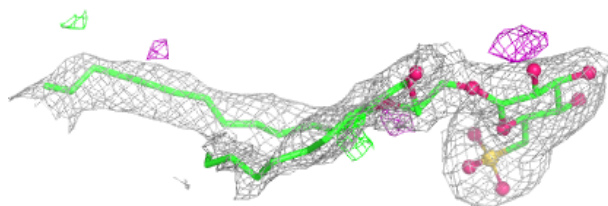
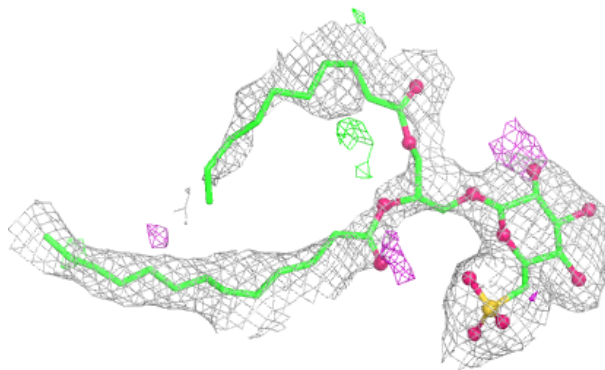


Electron density around LMT AT 101:

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

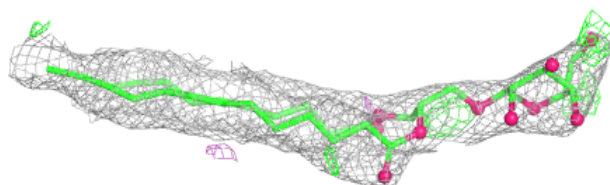
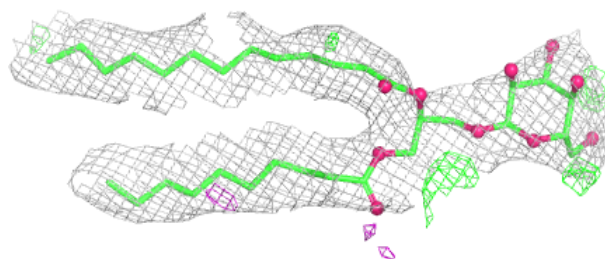
**Electron density around SQD AF 101:**

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

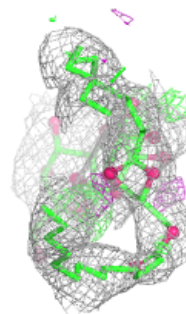
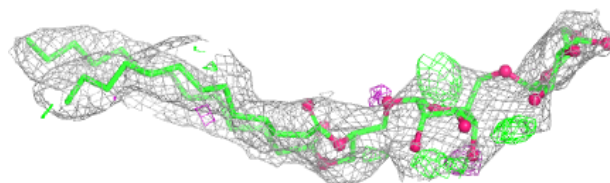
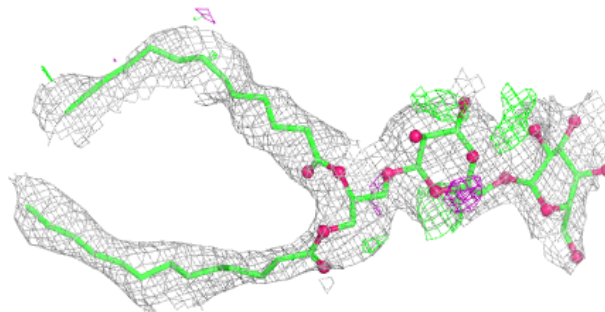


Electron density around LMG AM 101:

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

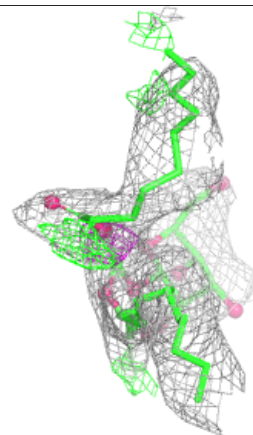
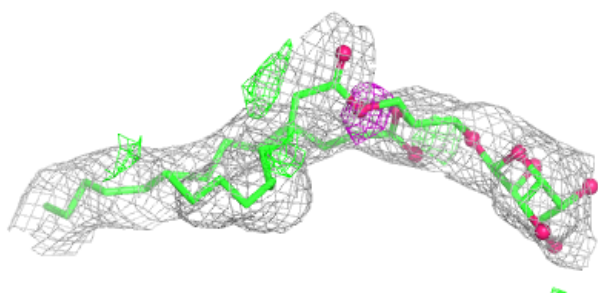
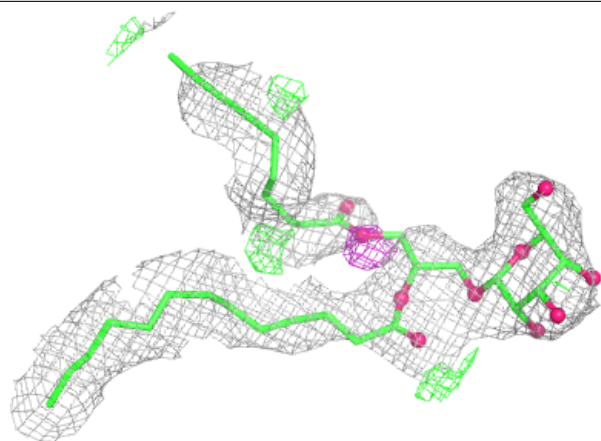
**Electron density around DGD AA 410:**

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

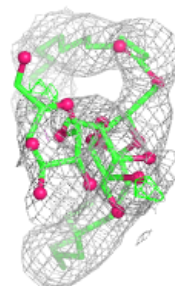
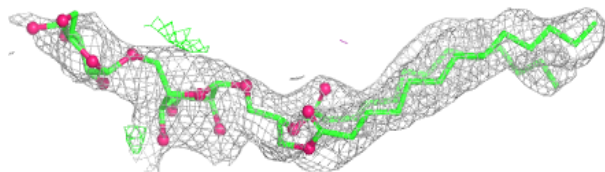
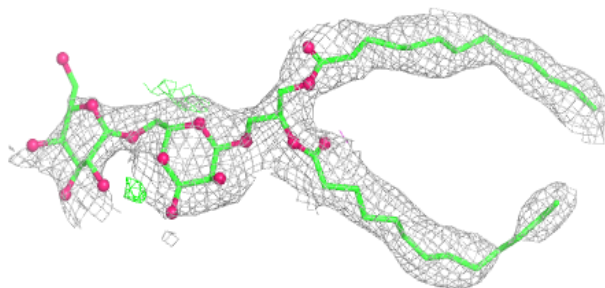


Electron density around LMG AA 416:

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

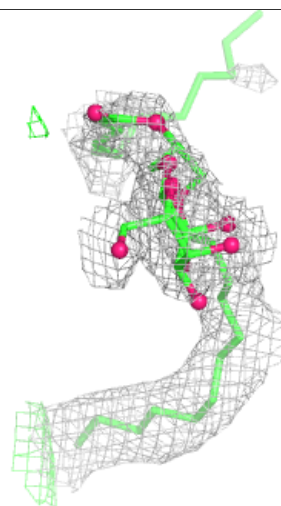
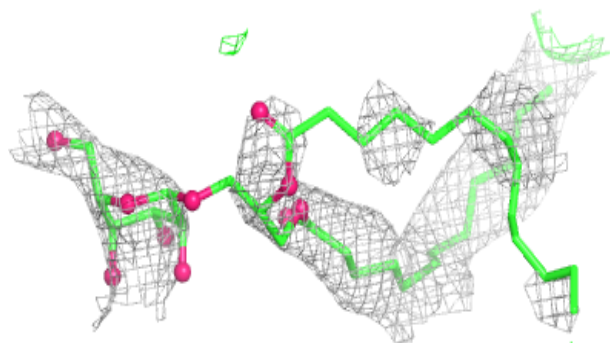
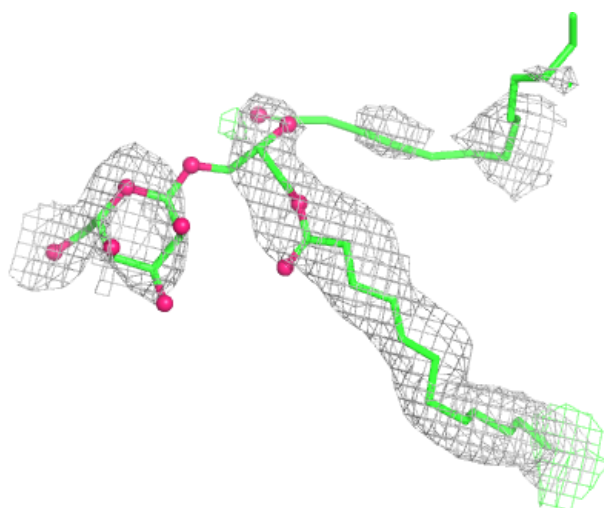
**Electron density around DGD BA 411:**

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



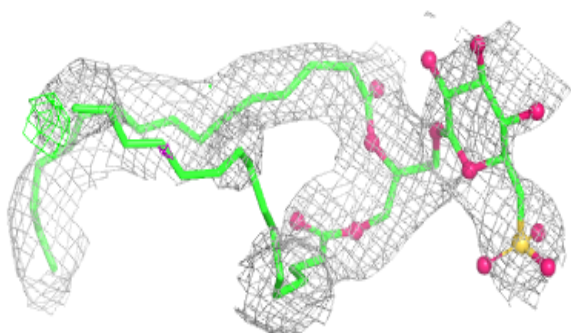
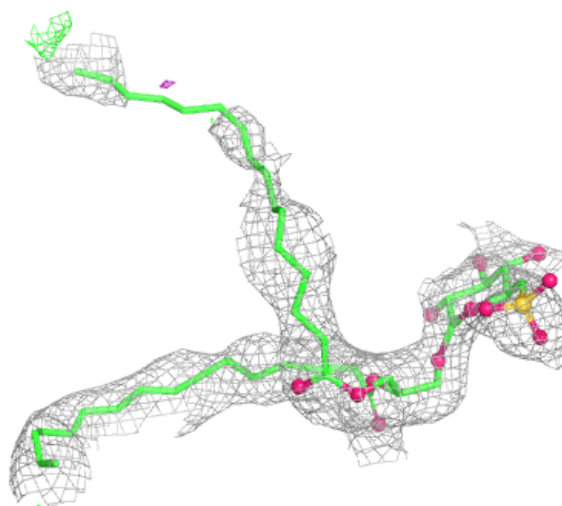
Electron density around LMG BE 102:

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



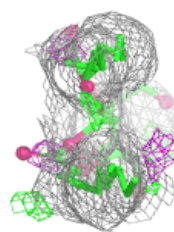
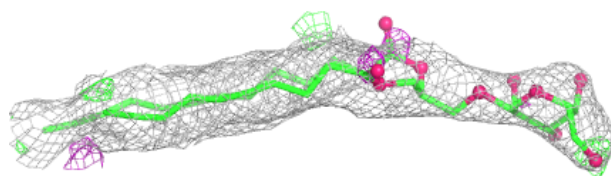
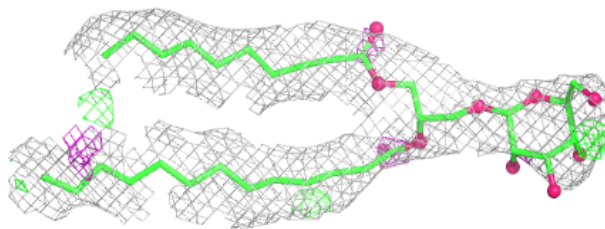
Electron density around SQD BA 401:

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

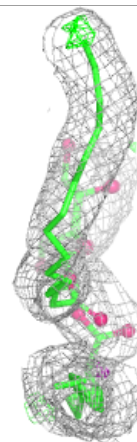
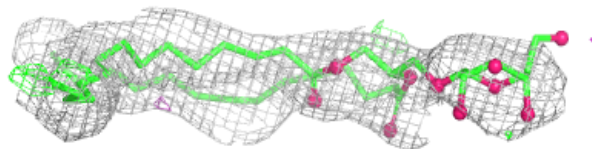
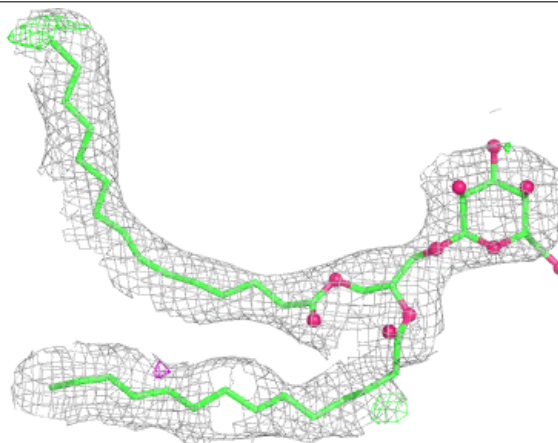


Electron density around LMG BM 102:

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

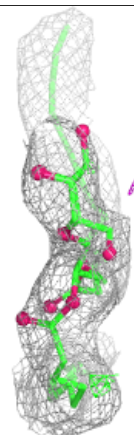
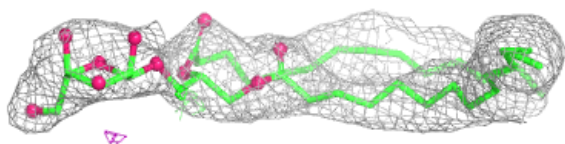
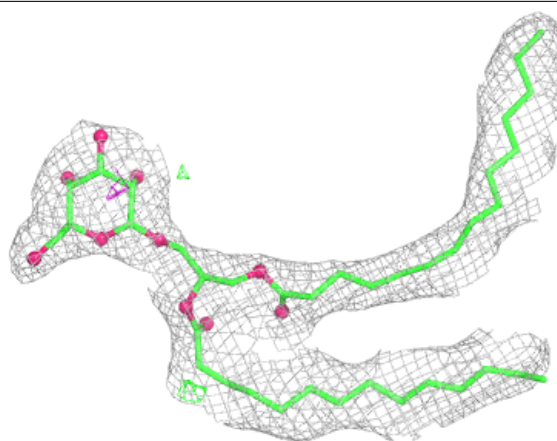
**Electron density around LMG AC 519:**

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

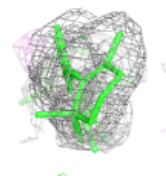
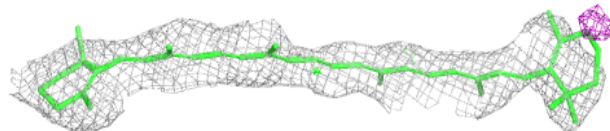
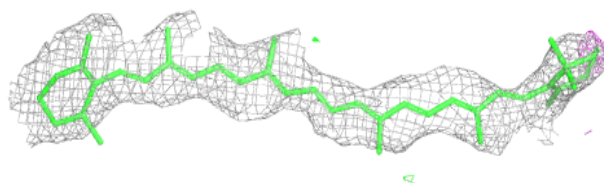


Electron density around LMG BC 519:

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

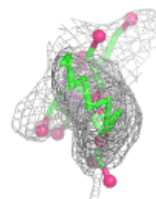
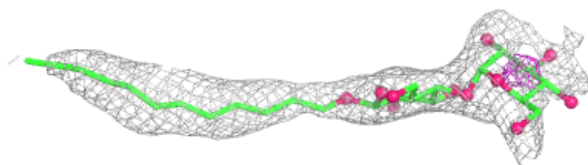
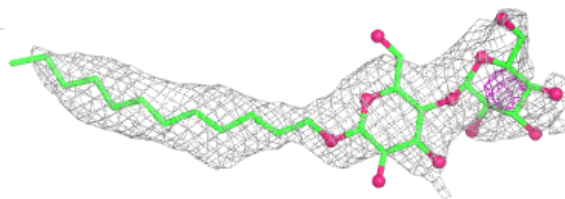
**Electron density around BCR BZ 101:**

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

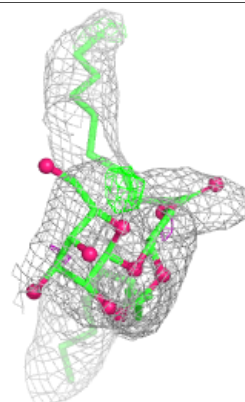
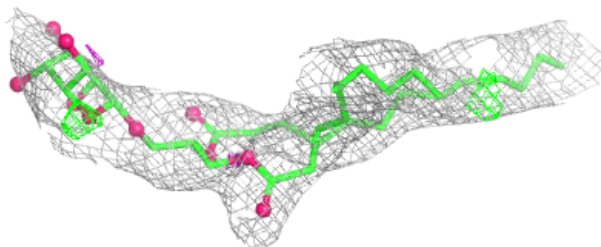
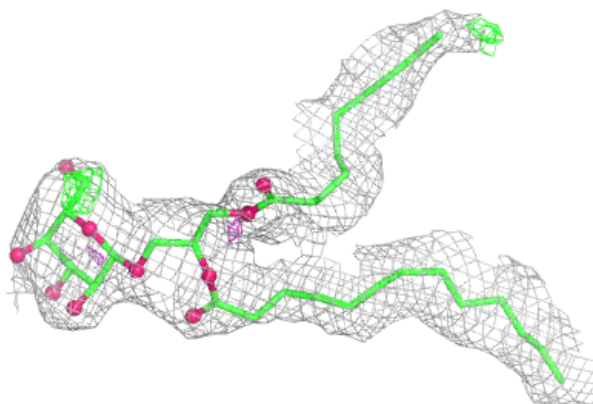


Electron density around LMT AB 625:

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

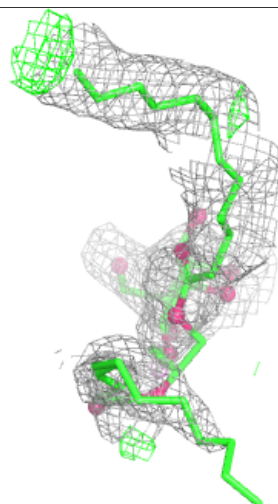
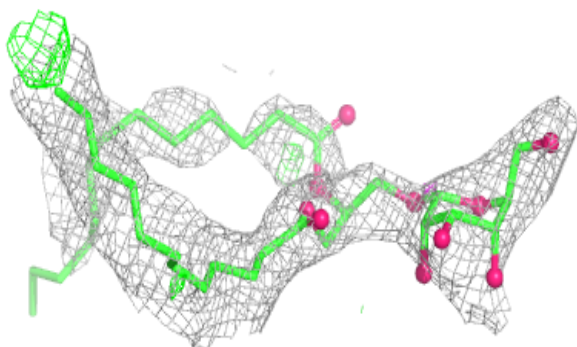
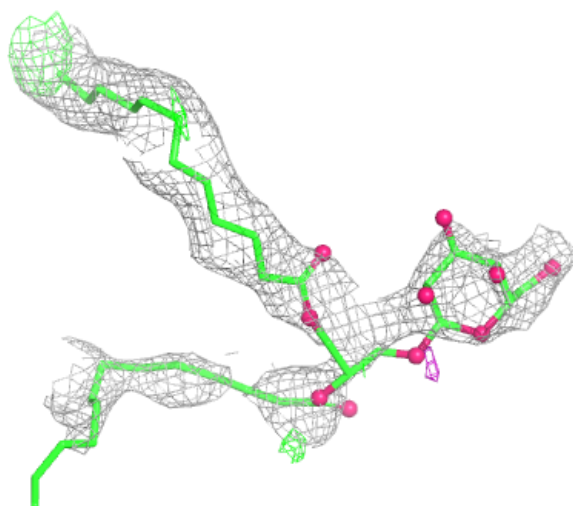
**Electron density around LMG AB 623:**

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



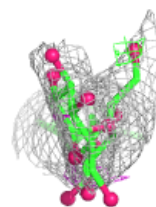
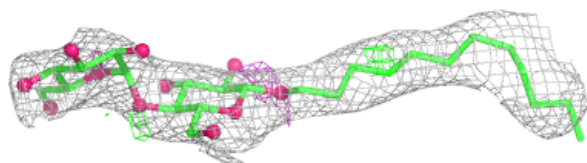
Electron density around LMG AE 102:

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

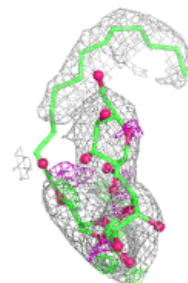
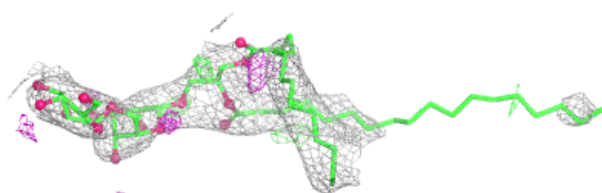
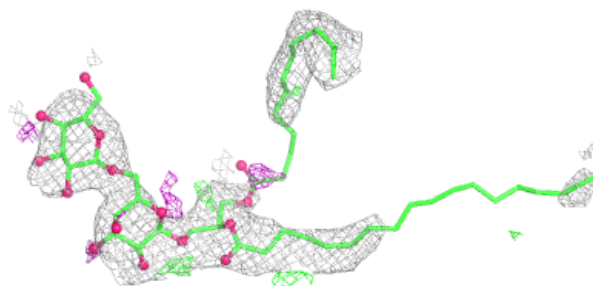


Electron density around LMT BT 101:

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

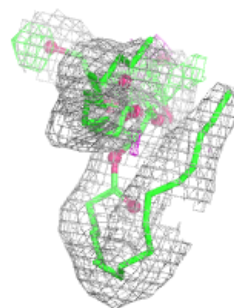
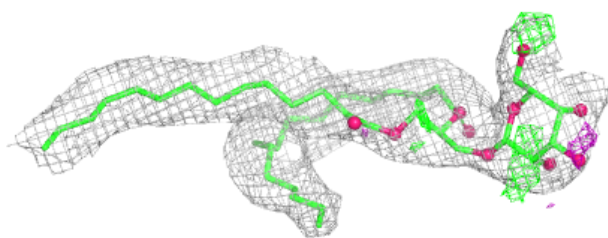
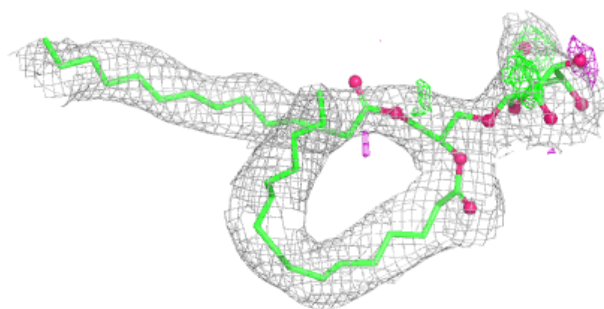
**Electron density around DGD BC 517:**

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

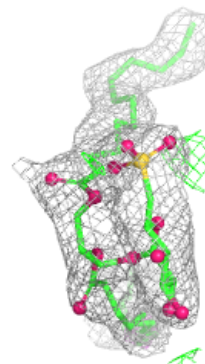
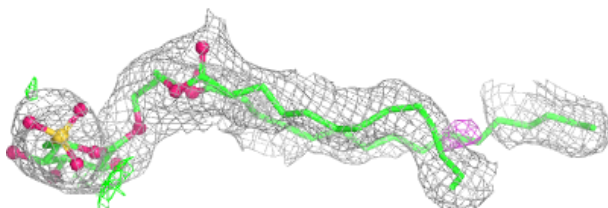
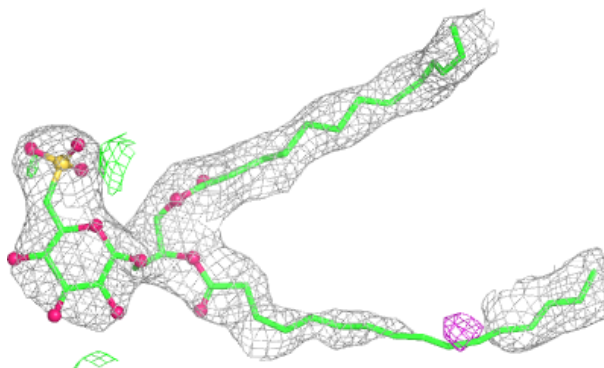


Electron density around LMG BB 623:

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

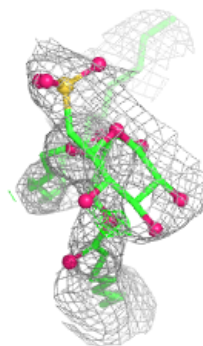
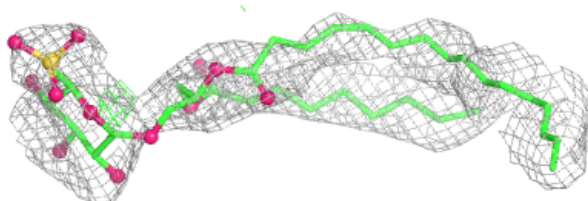
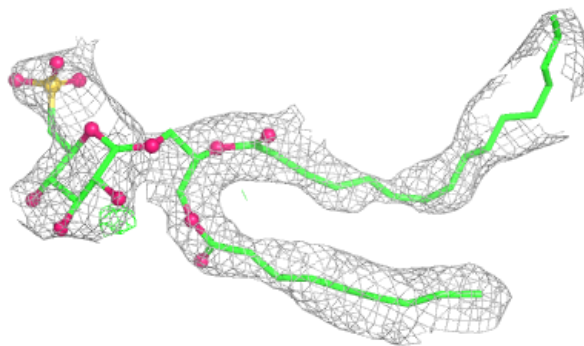
**Electron density around SQD BA 413:**

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



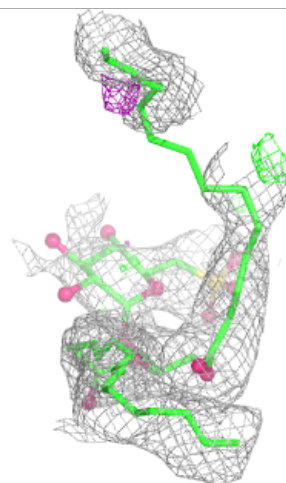
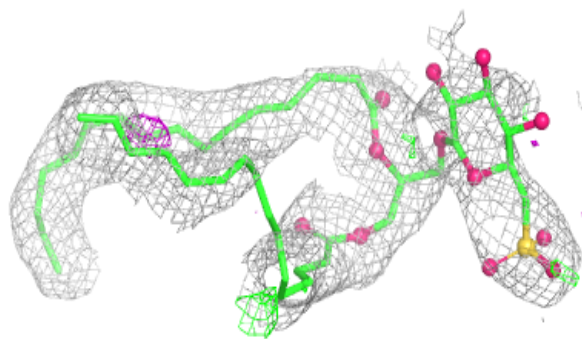
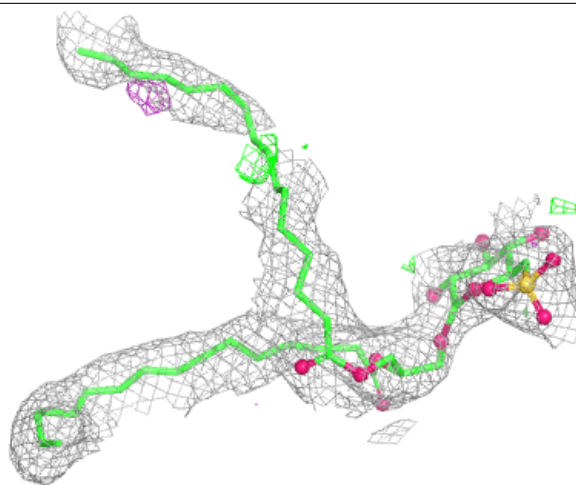
Electron density around SQD BL 101:

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



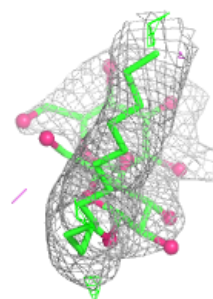
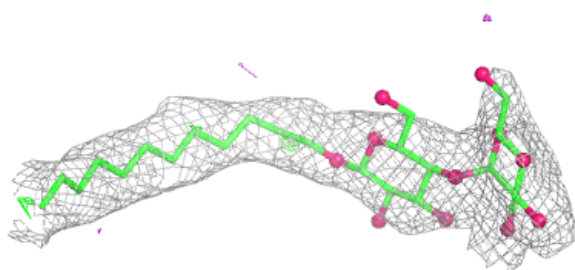
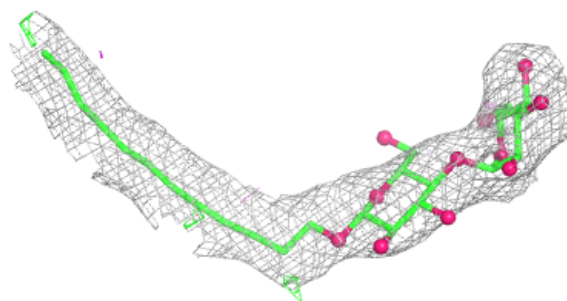
Electron density around SQD AA 415:

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

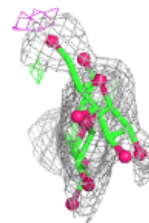
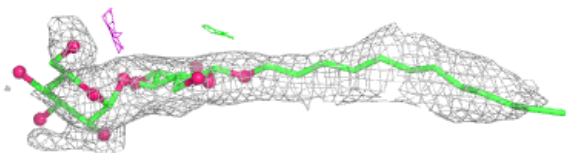
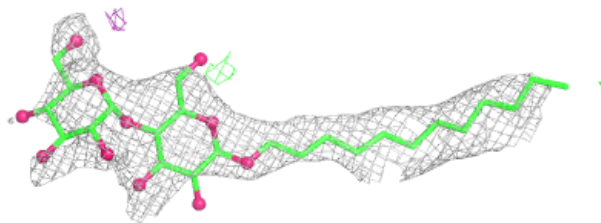


Electron density around LMT BM 101:

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

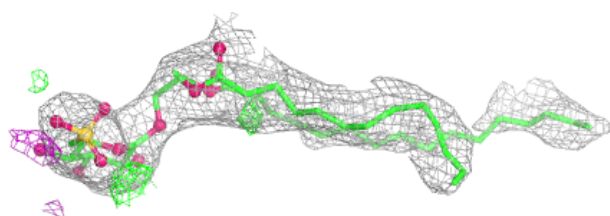
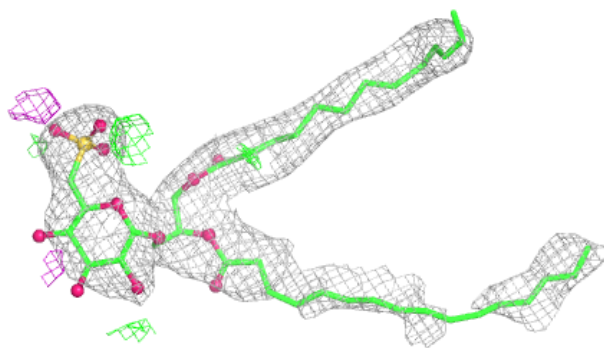
**Electron density around LMT BB 626:**

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

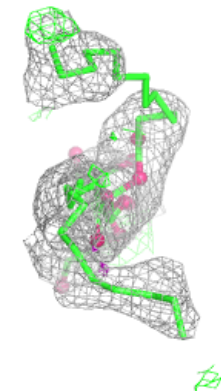
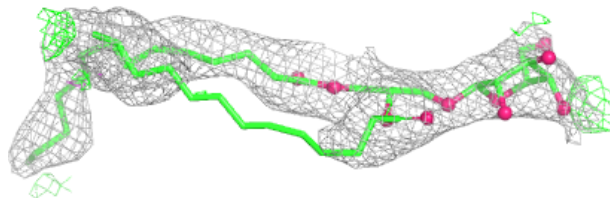
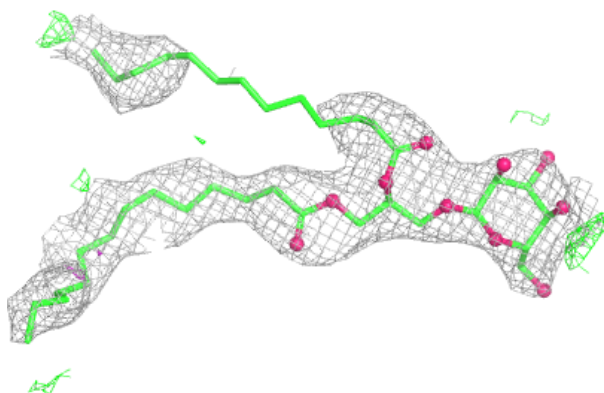


Electron density around SQD AA 412:

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

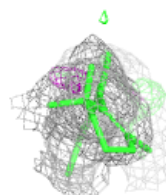
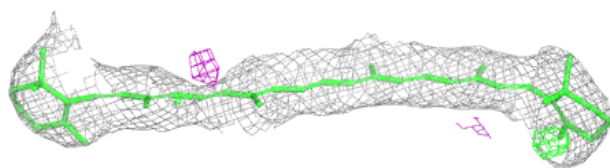
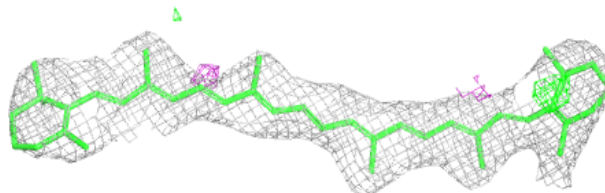
**Electron density around LMG BD 407:**

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

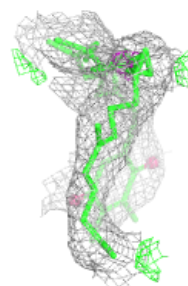
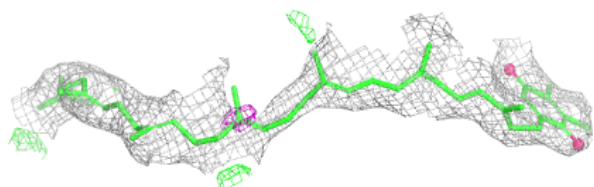
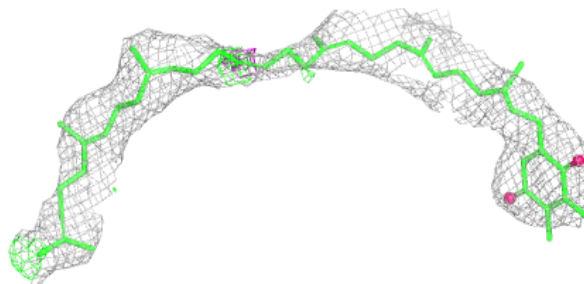


Electron density around BCR BC 515:

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

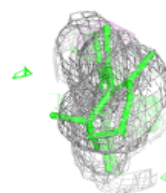
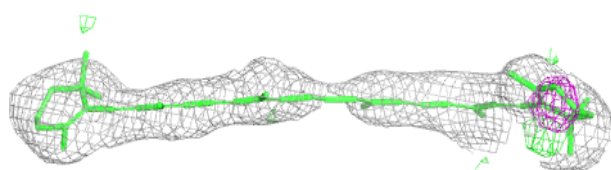
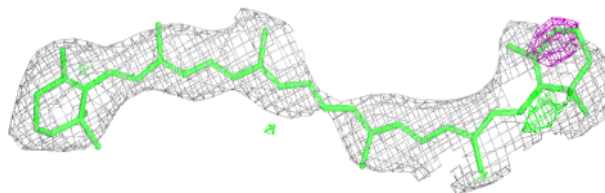
**Electron density around PL9 AA 407:**

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

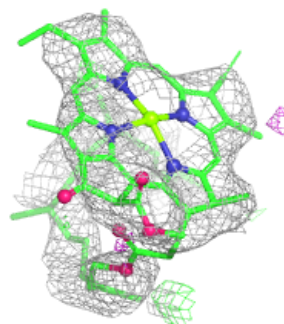
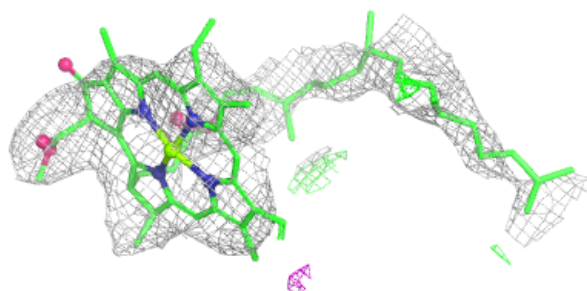
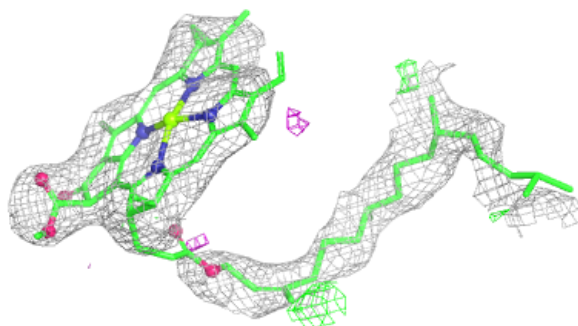


Electron density around BCR AK 102:

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

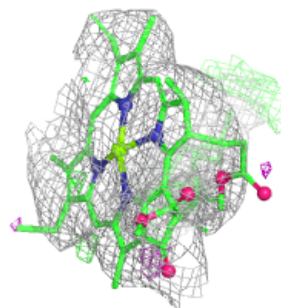
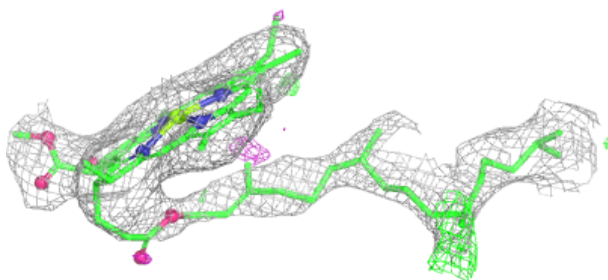
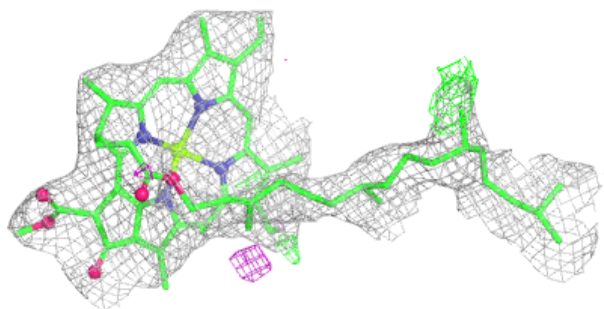
**Electron density around CLA AC 513:**

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

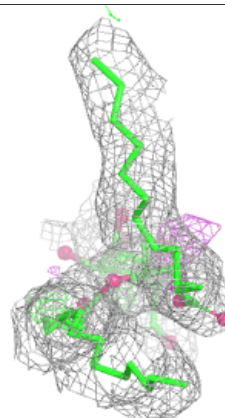
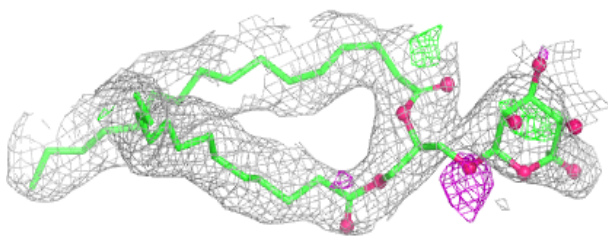
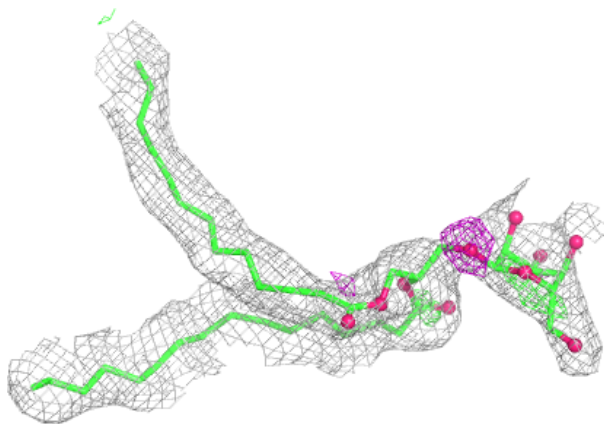


Electron density around CLA BB 617:

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

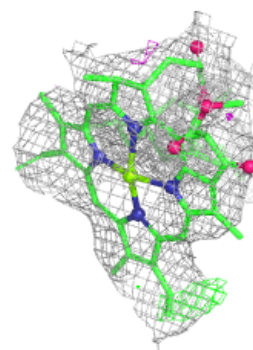
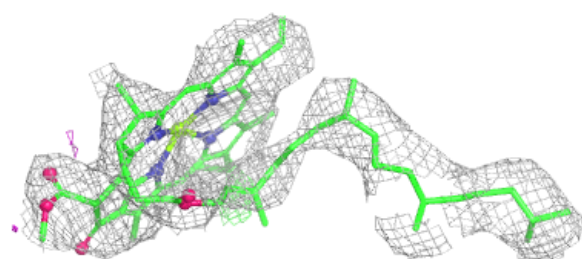
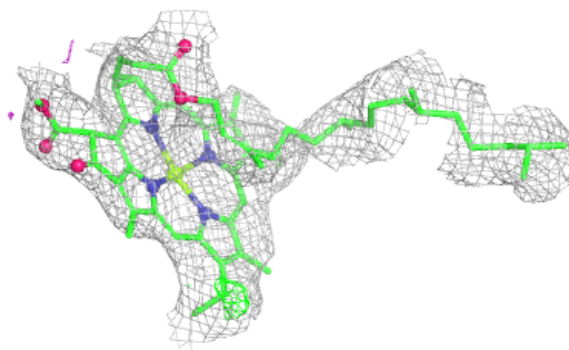
**Electron density around LMG BD 408:**

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

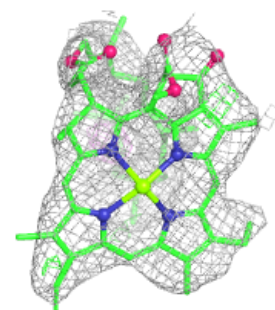
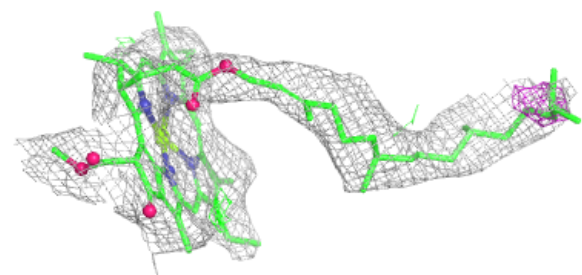
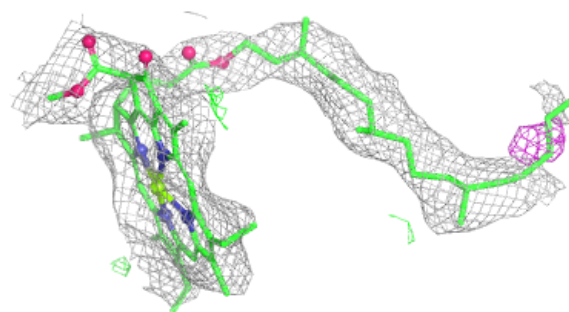


Electron density around CLA BC 505:

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

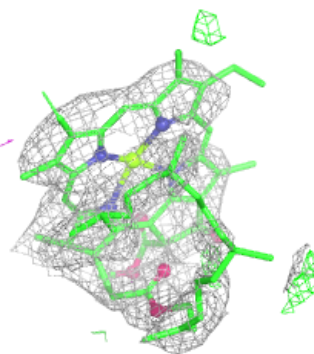
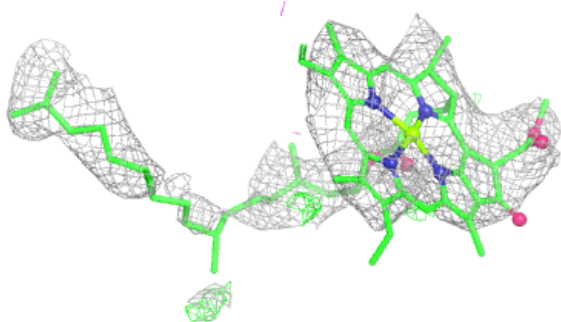
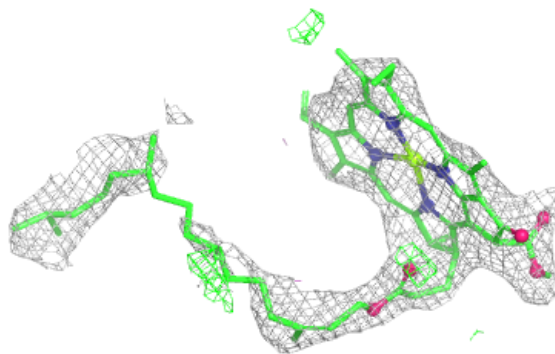
**Electron density around CLA BC 508:**

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

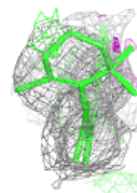
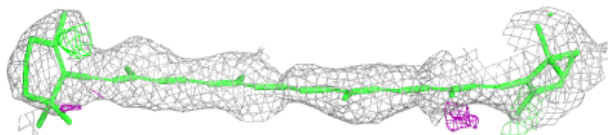


Electron density around CLA BC 513:

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

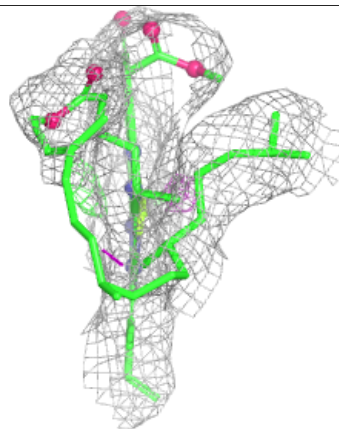
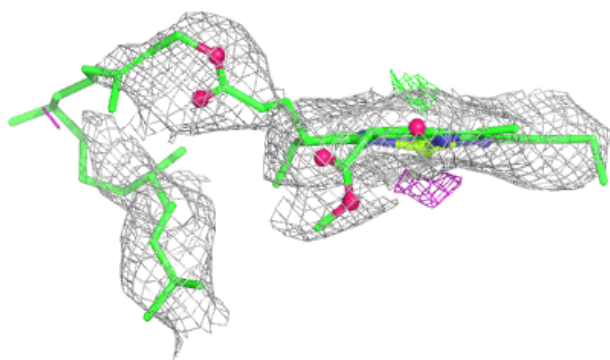
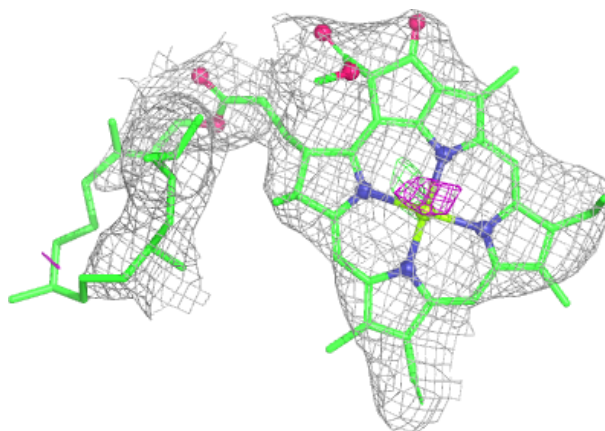
**Electron density around BCR BX 101:**

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



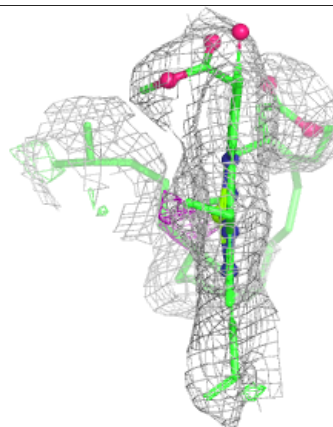
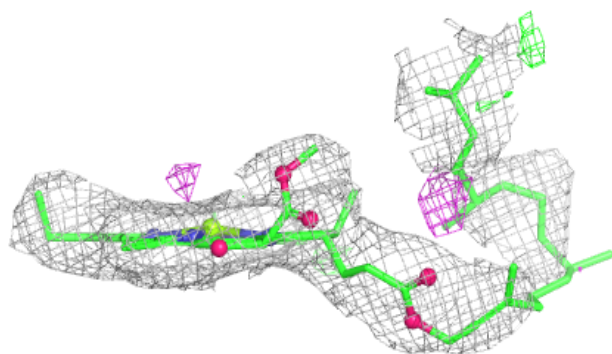
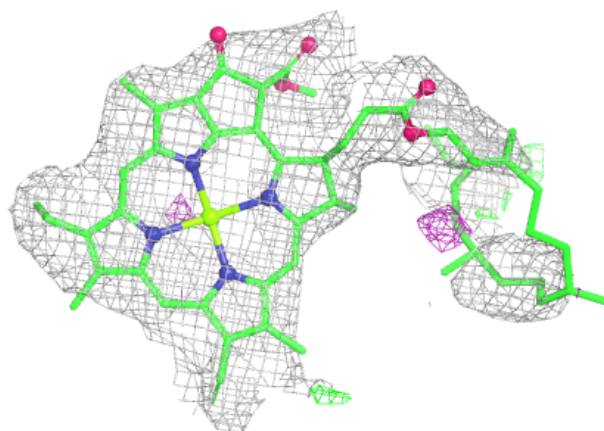
Electron density around CLA BC 512:

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



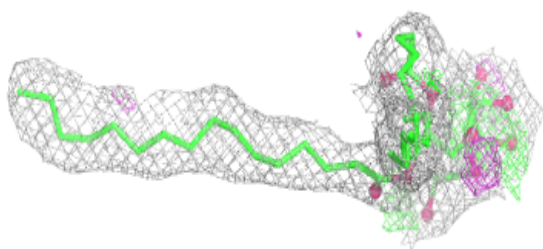
Electron density around CLA AC 512:

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



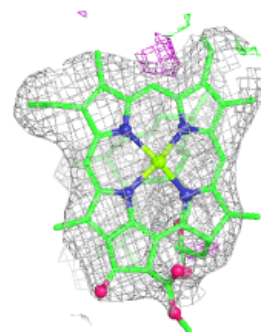
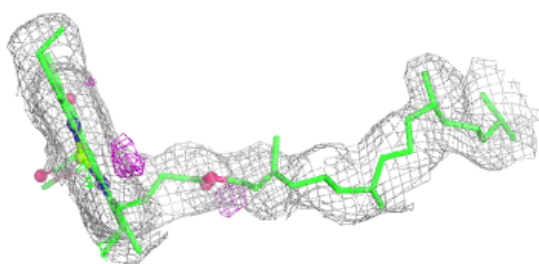
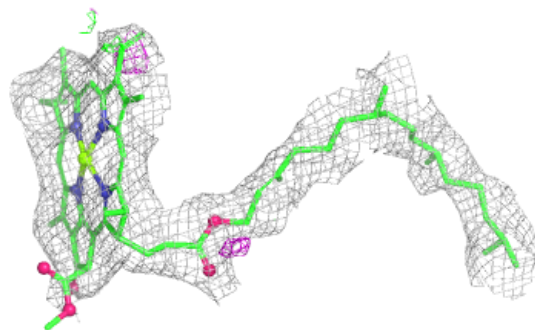
Electron density around LMG AA 413:

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

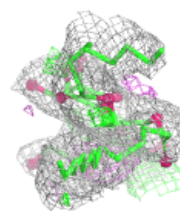
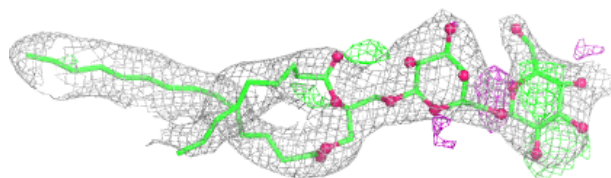
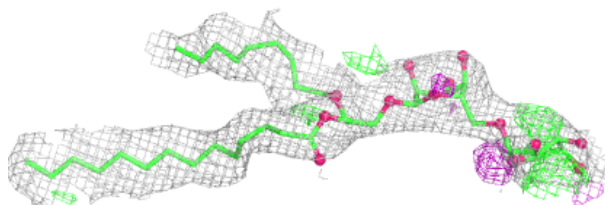


Electron density around CLA BD 404:

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

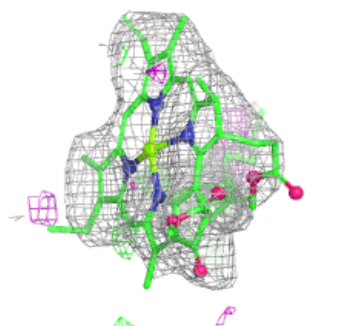
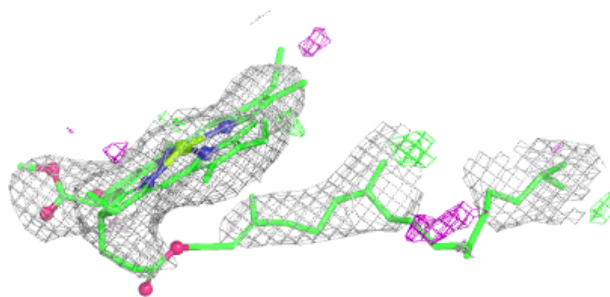
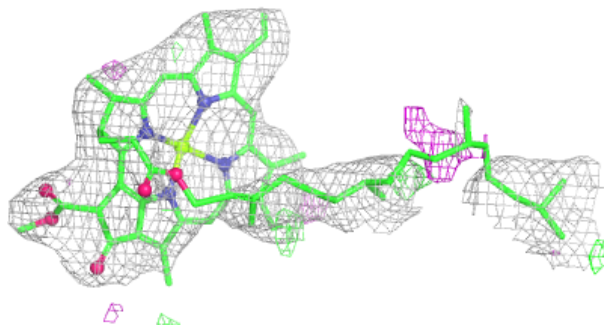
**Electron density around DGD AC 516:**

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

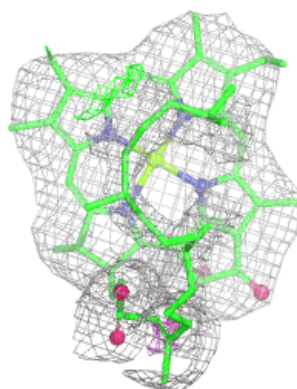
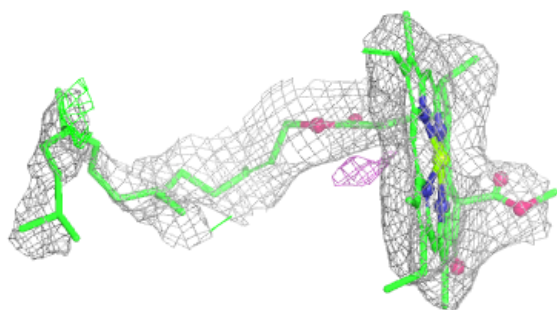
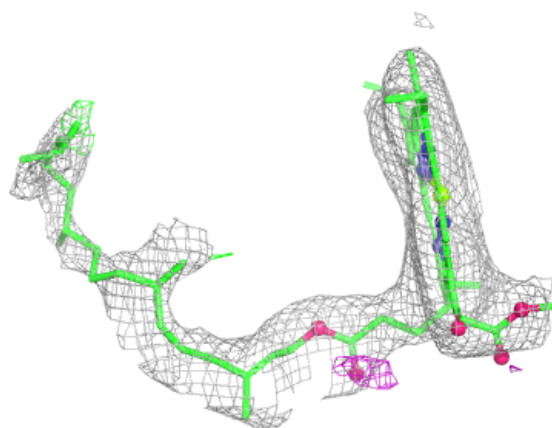


Electron density around CLA AB 614:

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

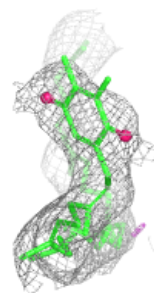
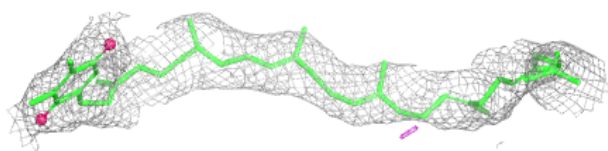
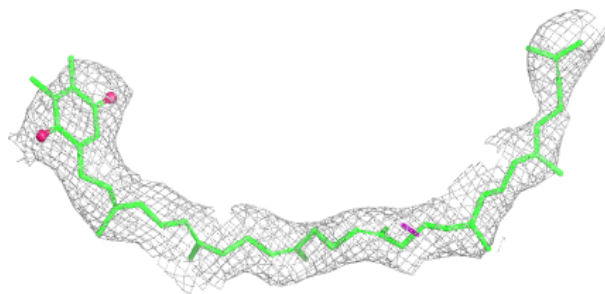
**Electron density around CLA AC 506:**

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

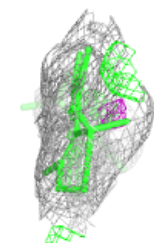
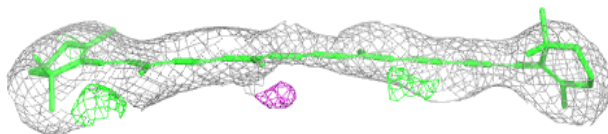
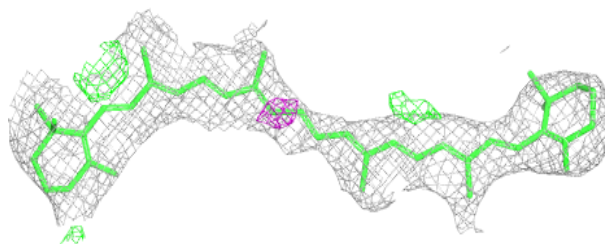


Electron density around PL9 BA 408:

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

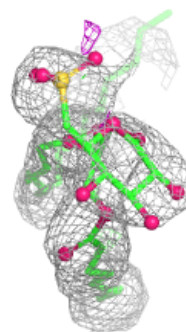
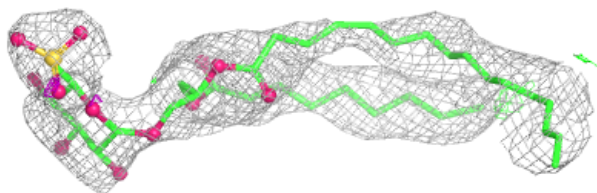
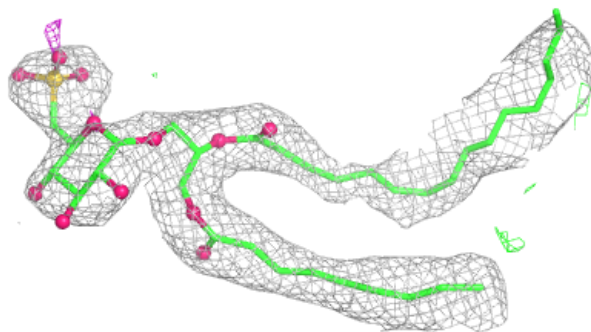
**Electron density around BCR BK 102:**

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

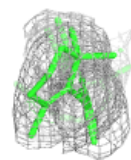
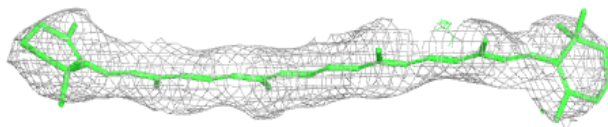
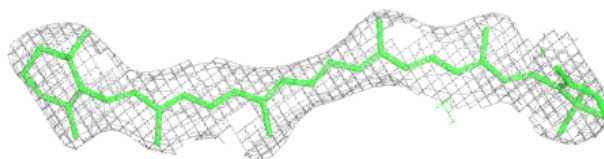


Electron density around SQD BB 601:

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

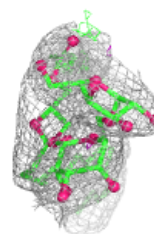
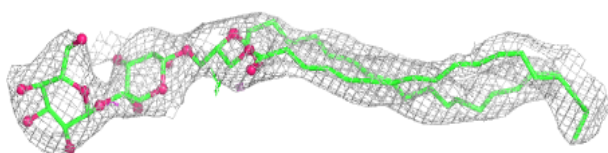
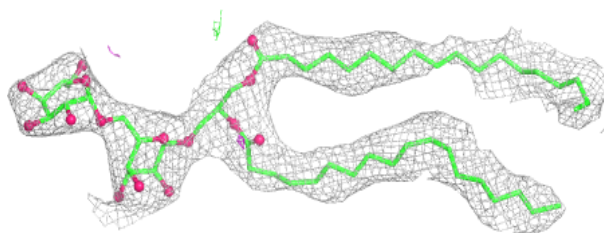
**Electron density around BCR AZ 101:**

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

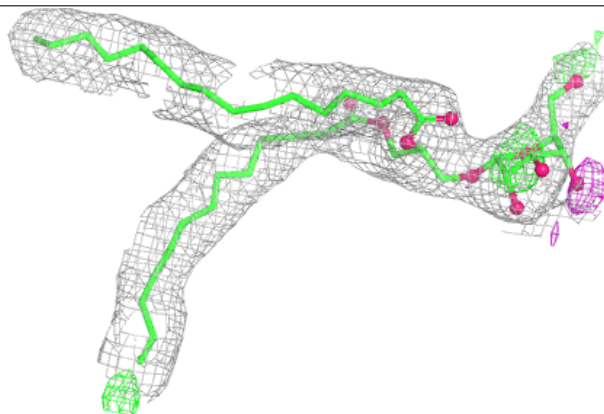


Electron density around DGD BC 518:

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

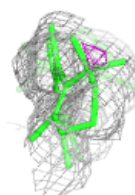
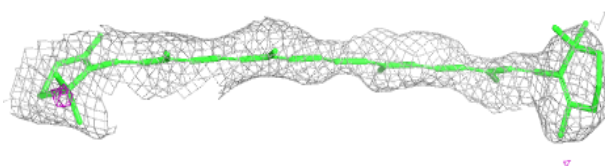
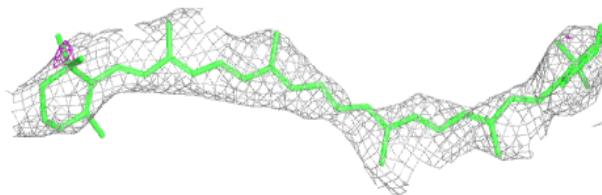
**Electron density around LMG AD 408:**

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

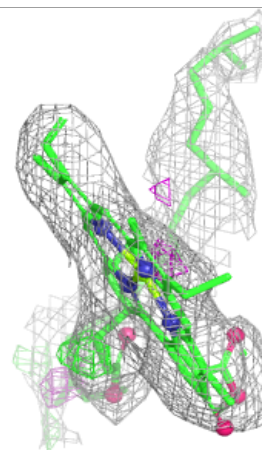
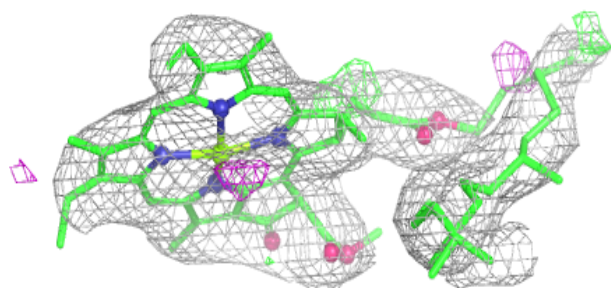
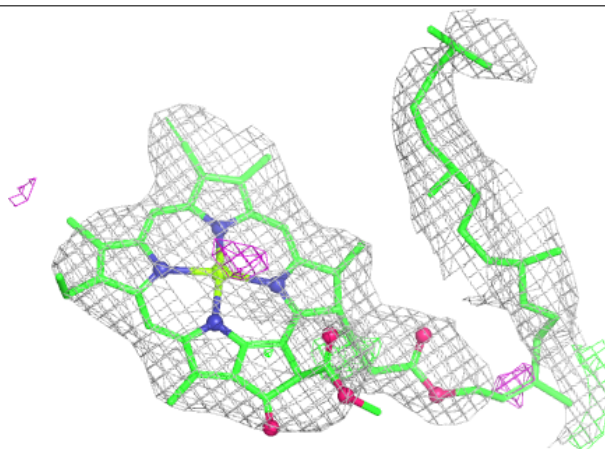


Electron density around BCR AH 101:

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

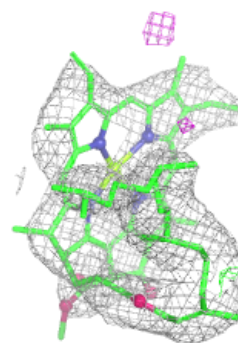
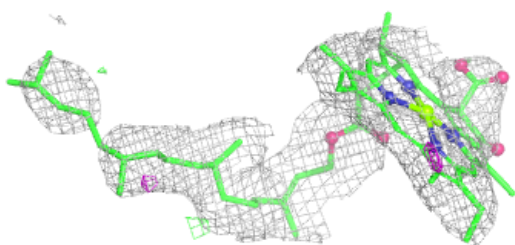
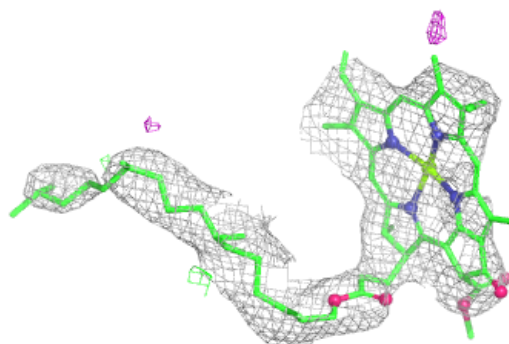
**Electron density around CLA BB 619:**

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

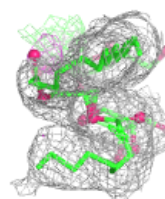
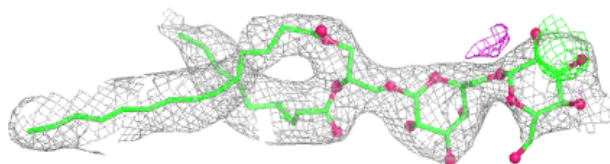
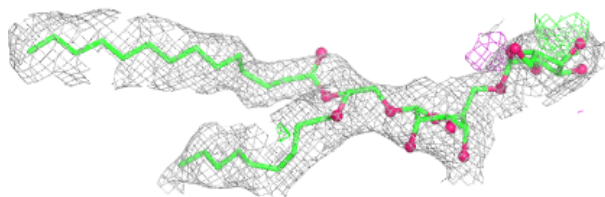


Electron density around CLA BC 511:

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

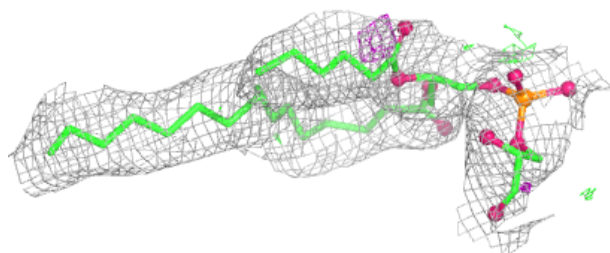
**Electron density around DGD BC 516:**

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



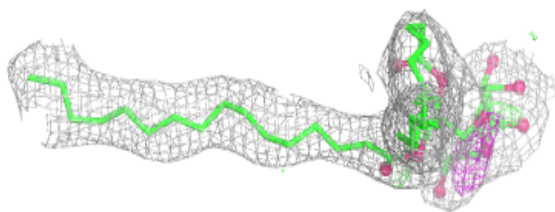
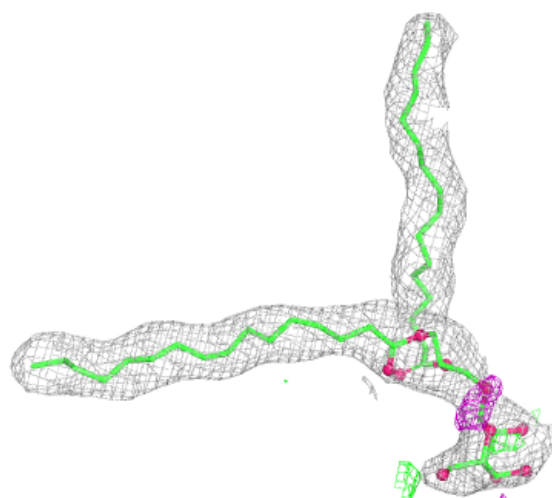
Electron density around LHG AA 411:

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



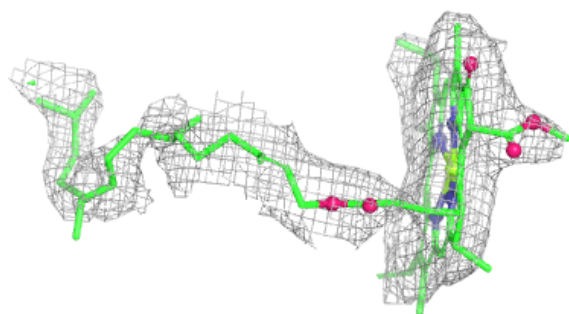
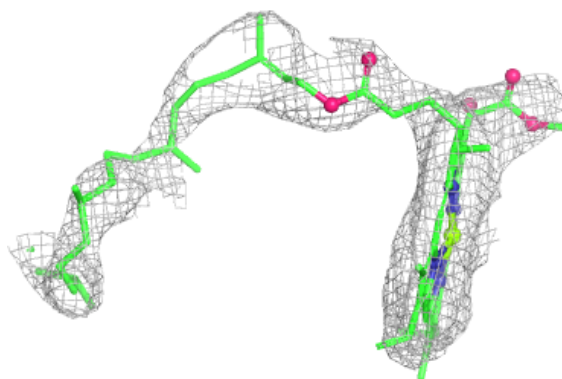
Electron density around LMG BA 414:

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

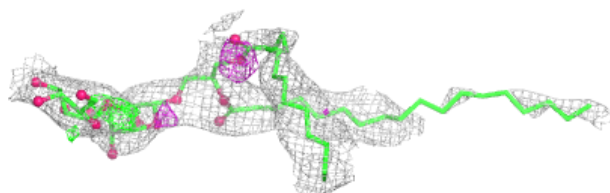
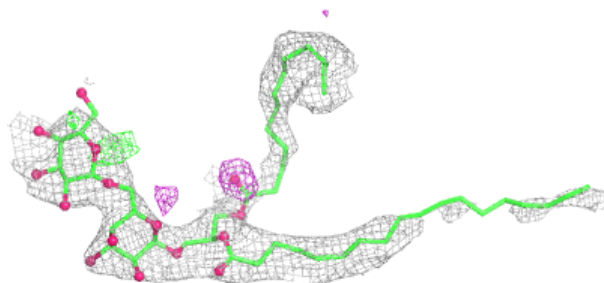


Electron density around CLA BC 506:

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

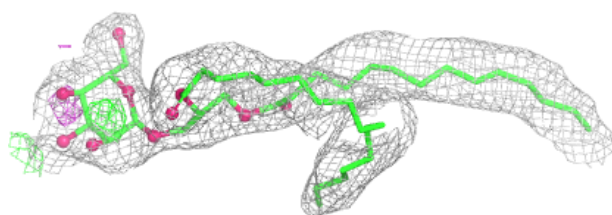
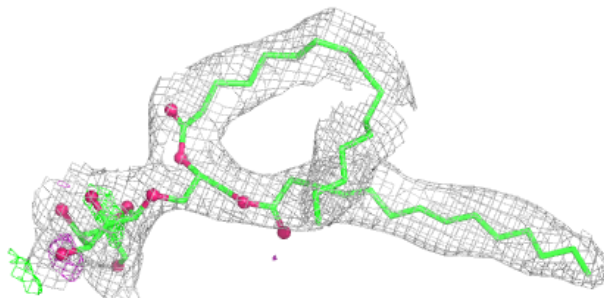
**Electron density around DGD AC 517:**

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

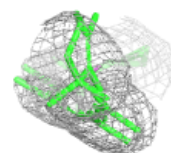
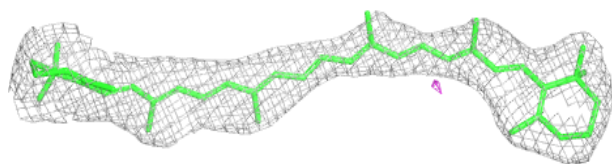
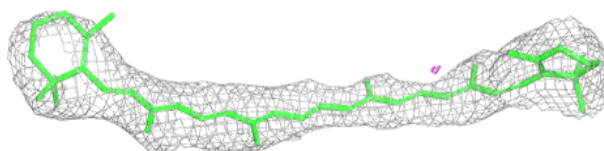


Electron density around LMG AB 621:

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

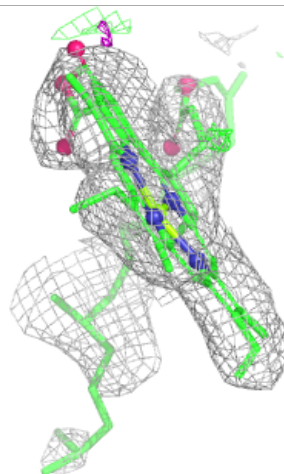
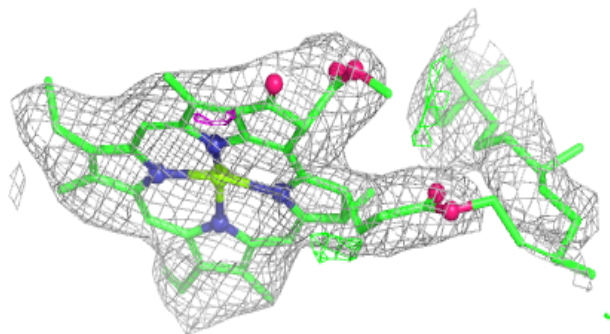
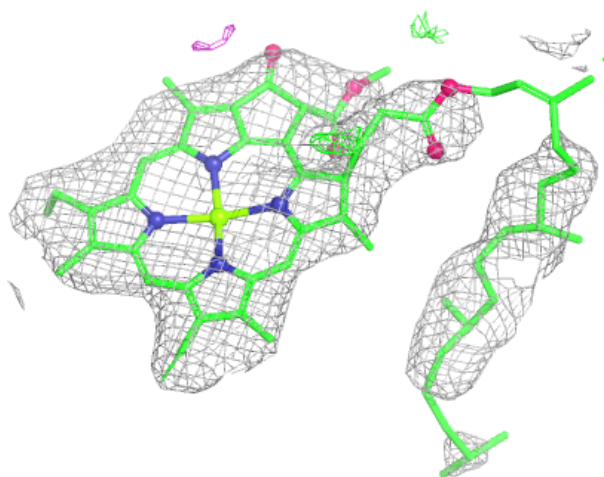
**Electron density around BCR BD 406:**

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



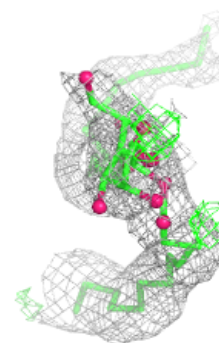
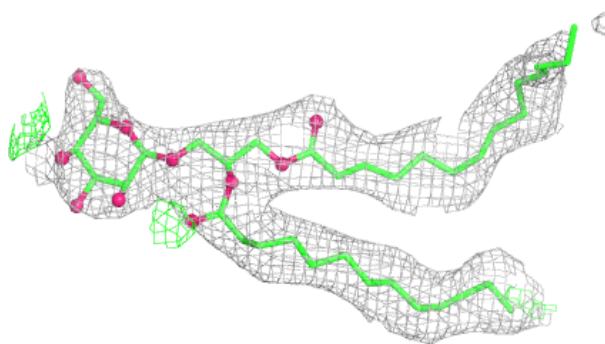
Electron density around CLA AB 616:

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

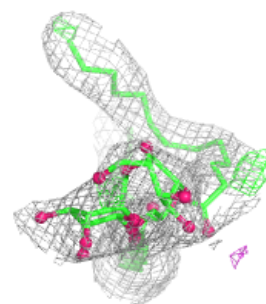
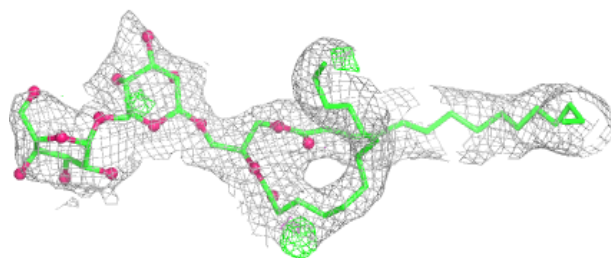
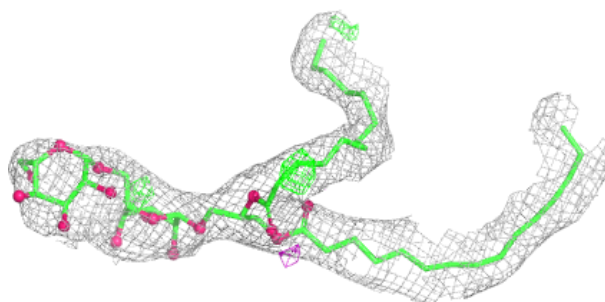


Electron density around LMG AD 407:

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

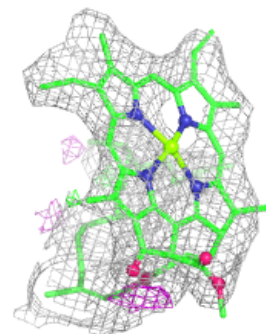
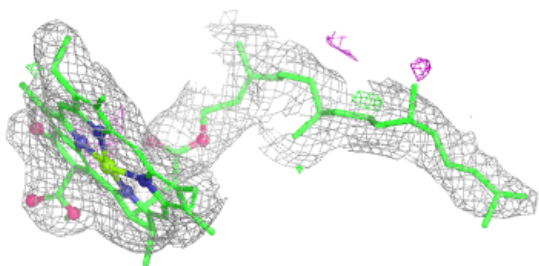
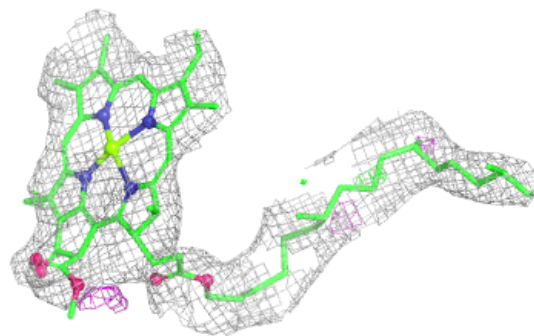
**Electron density around DGD BH 101:**

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



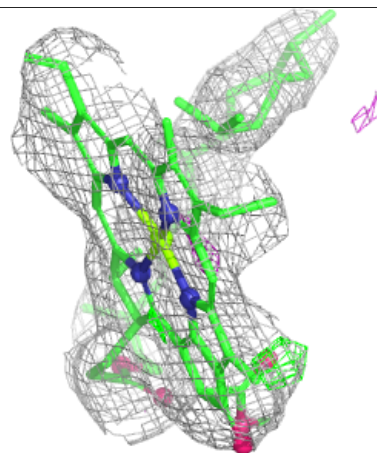
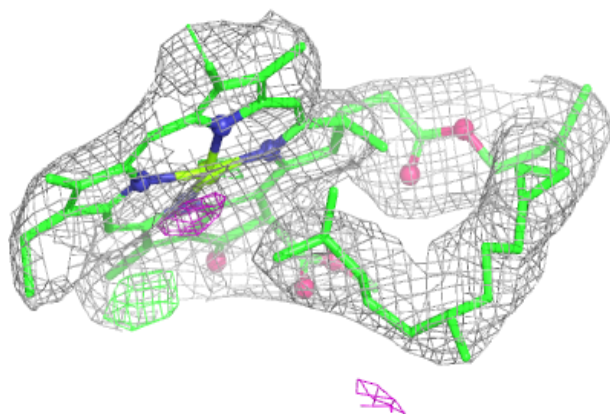
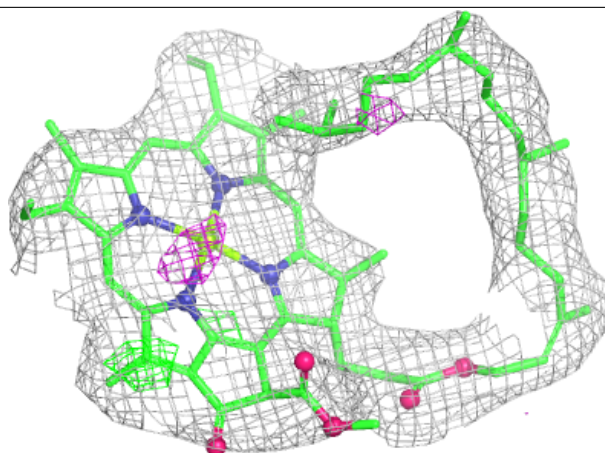
Electron density around CLA AC 511:

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



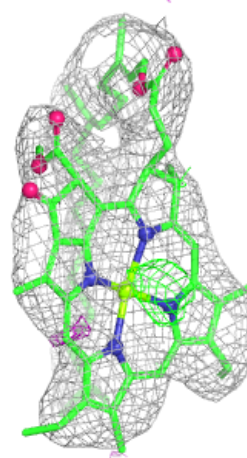
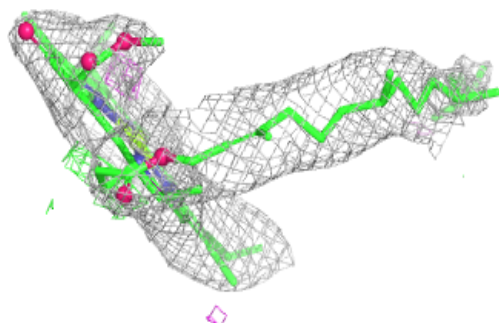
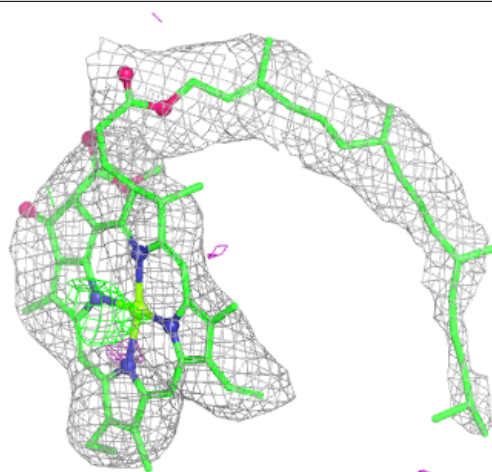
Electron density around CLA BB 618:

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



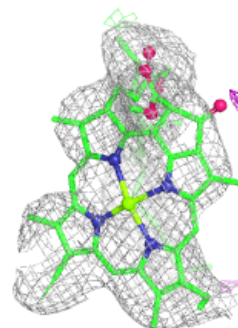
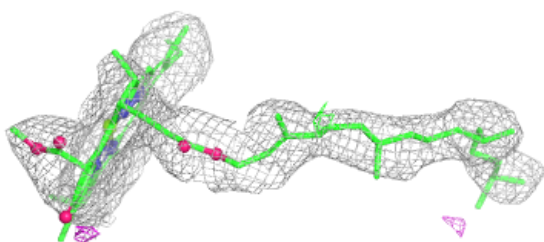
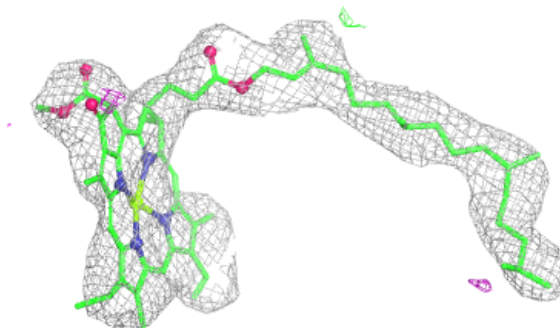
Electron density around CLA AC 507:

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



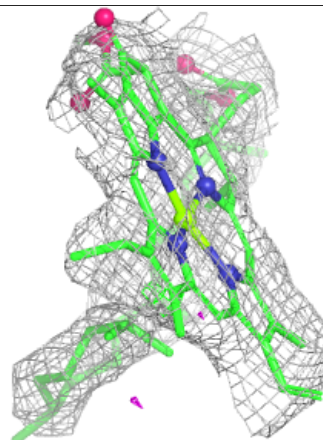
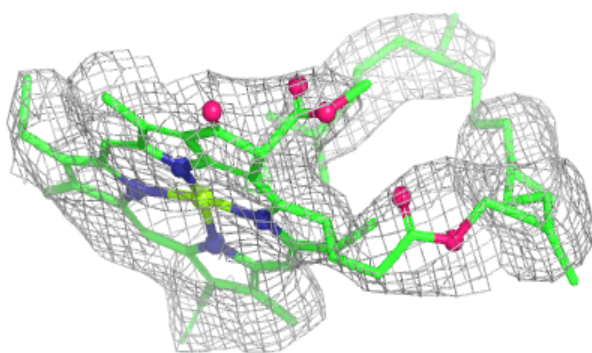
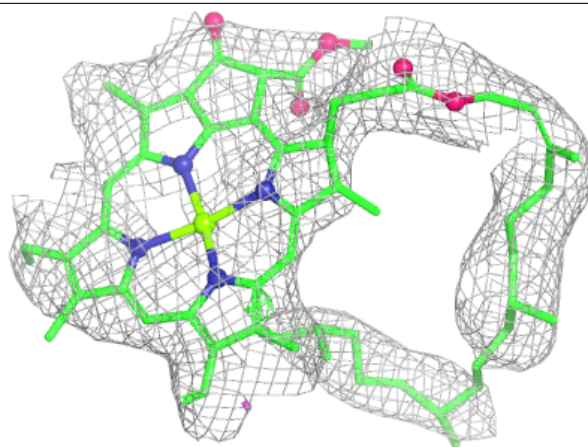
Electron density around CLA AB 609:

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



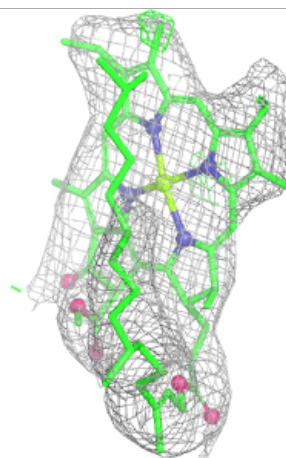
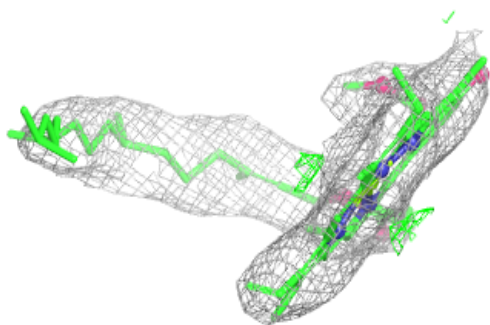
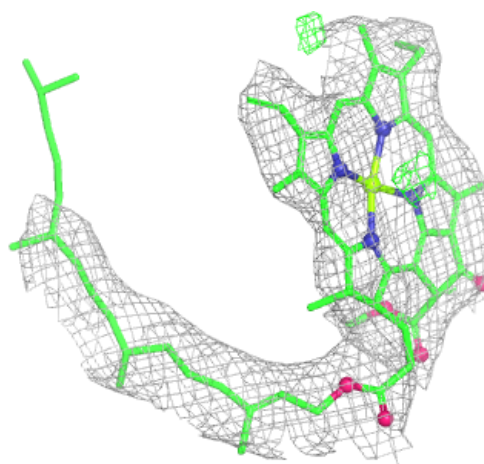
Electron density around CLA AB 615:

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



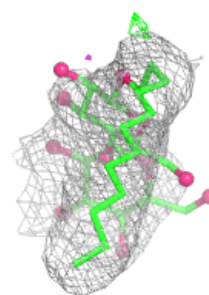
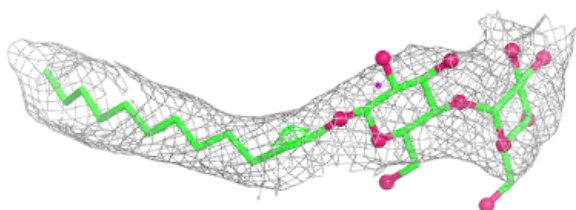
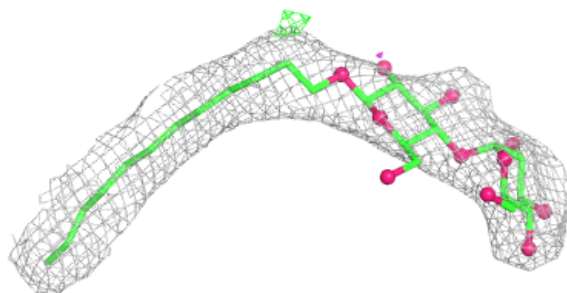
Electron density around CLA BC 507:

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

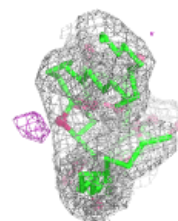
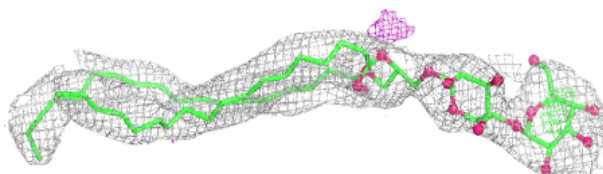
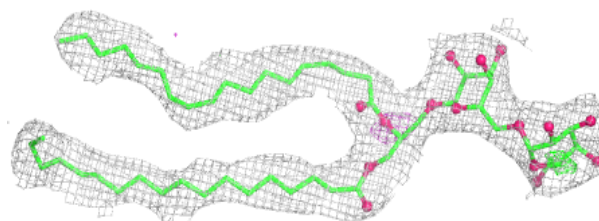


Electron density around LMT AM 102:

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

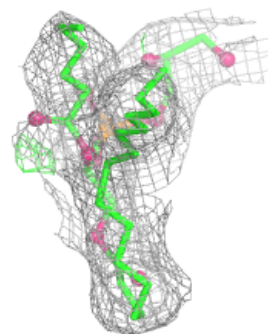
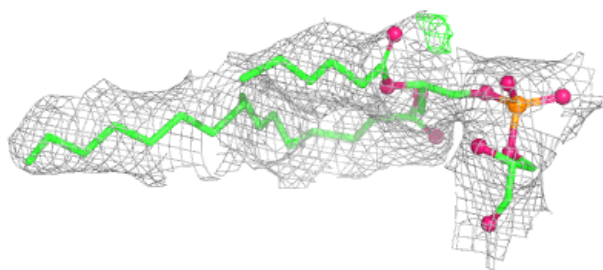
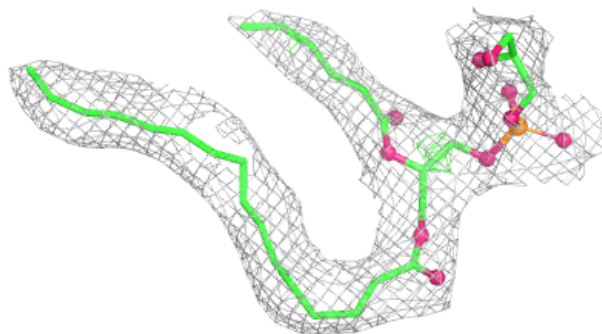
**Electron density around DGD AC 518:**

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

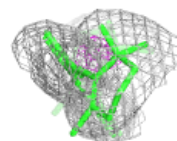
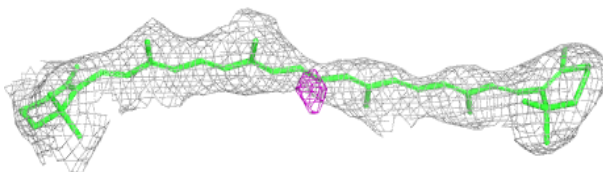
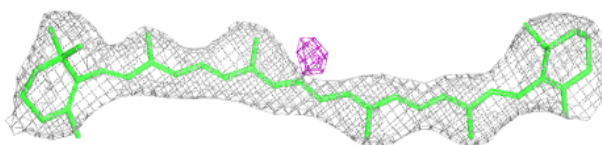


Electron density around LHG BA 412:

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

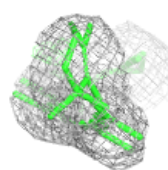
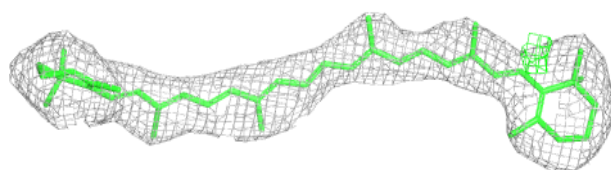
**Electron density around BCR AB 620:**

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

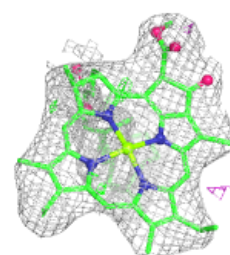
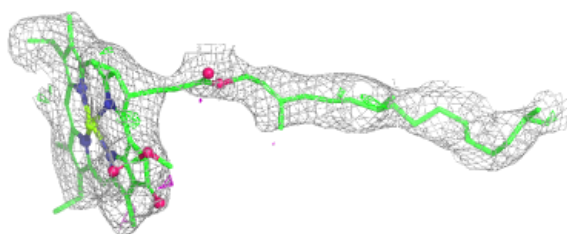
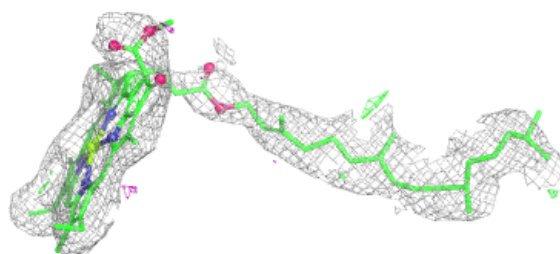


Electron density around BCR AD 406:

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

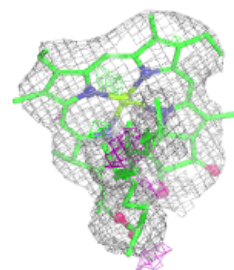
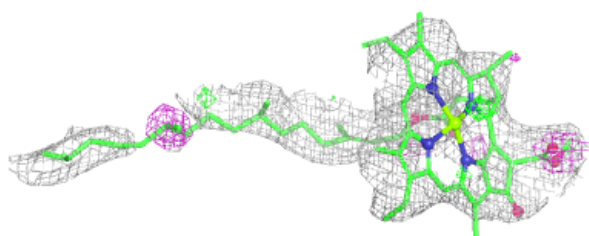
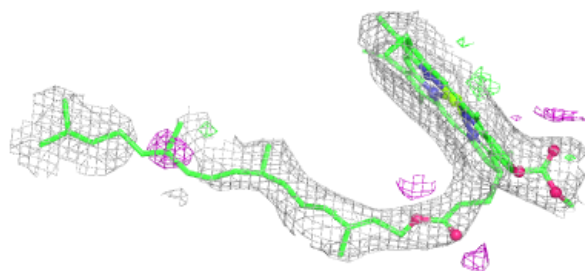
**Electron density around CLA AB 604:**

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



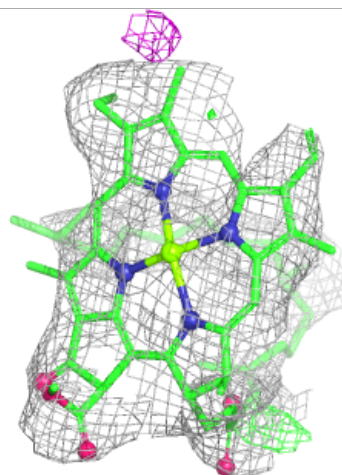
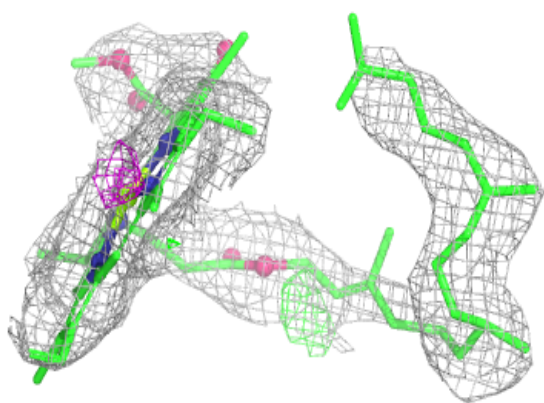
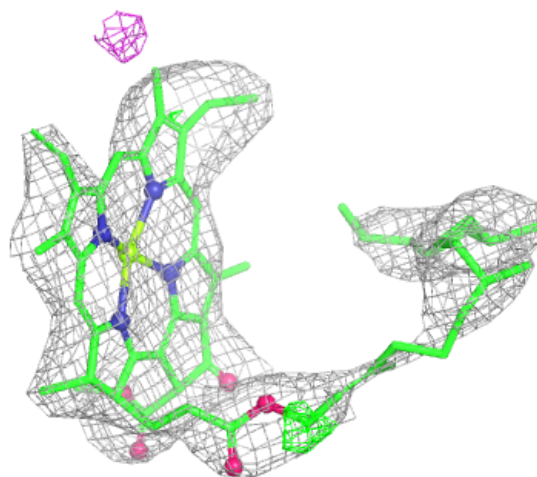
Electron density around CLA AC 504:

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



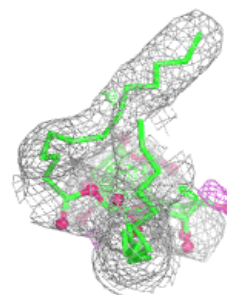
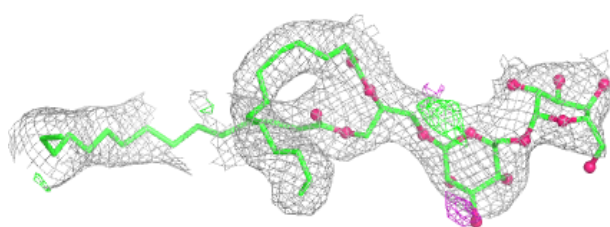
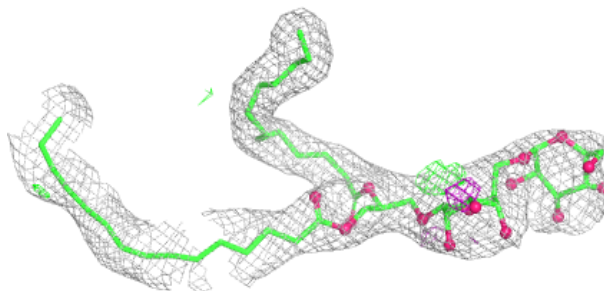
Electron density around CLA BC 503:

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

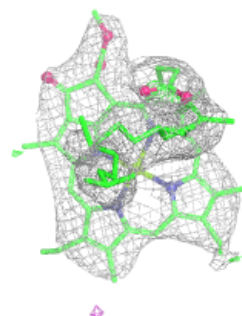
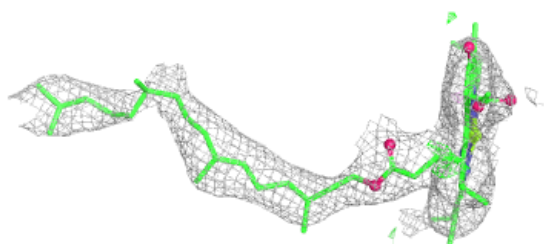
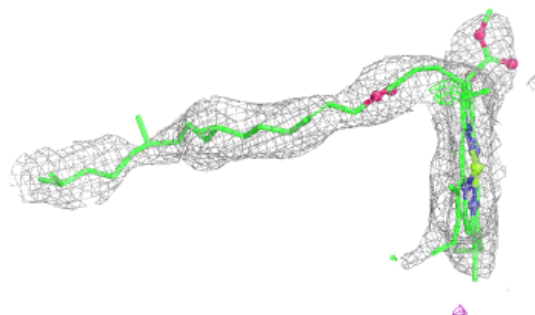


Electron density around DGD AH 102:

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

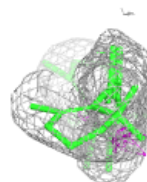
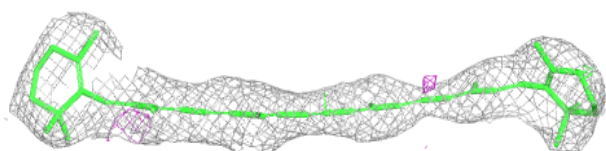
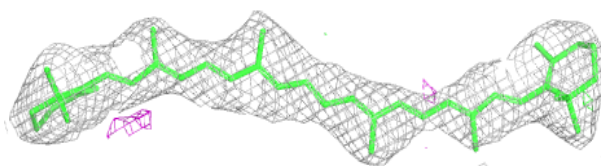
**Electron density around CLA AB 606:**

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

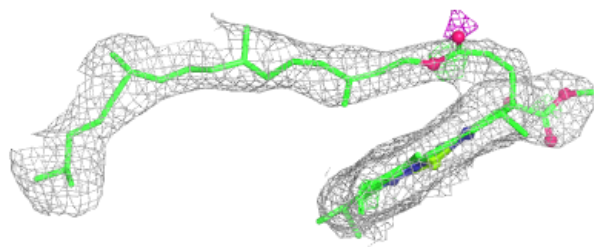
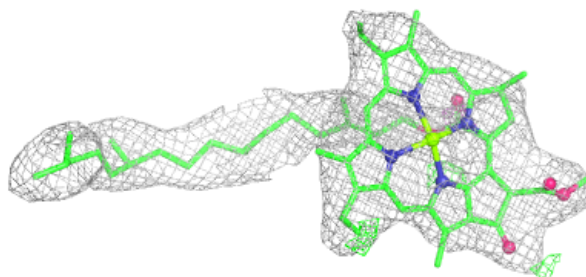


Electron density around BCR BB 620:

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

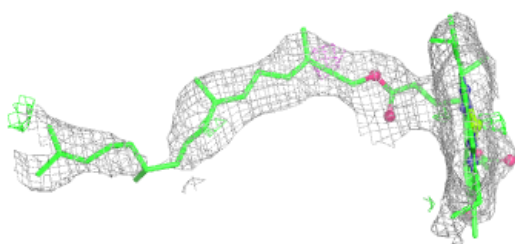
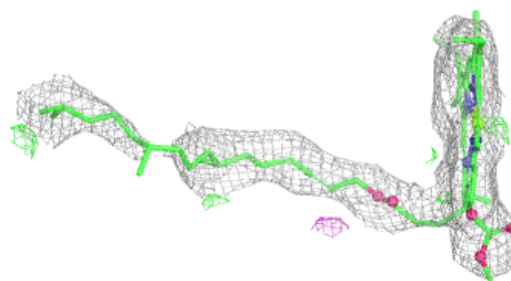
**Electron density around CLA AB 608:**

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

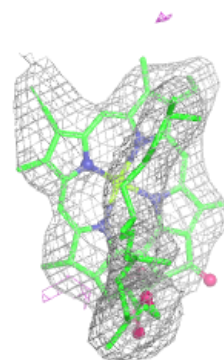
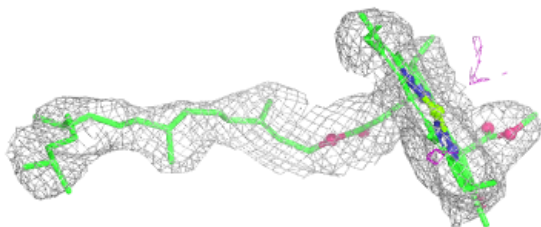
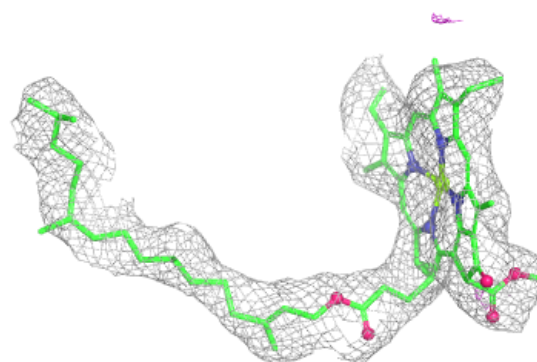


Electron density around CLA BB 609:

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

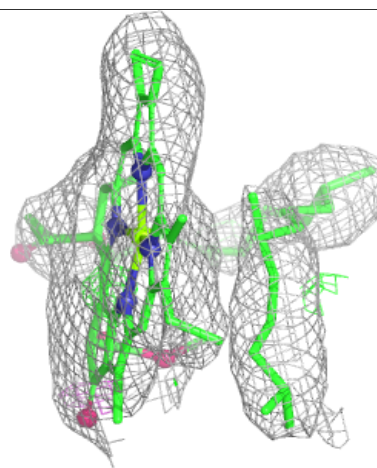
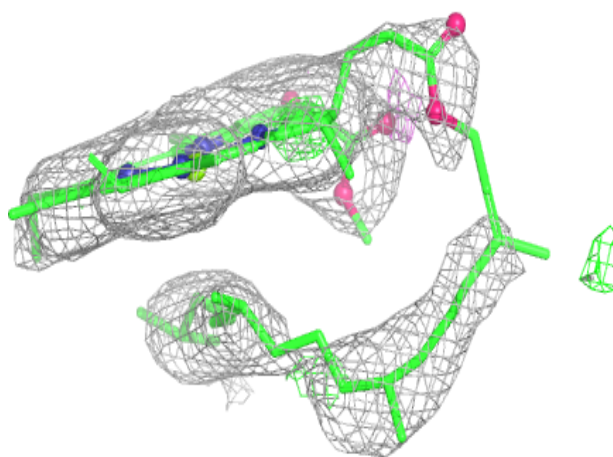
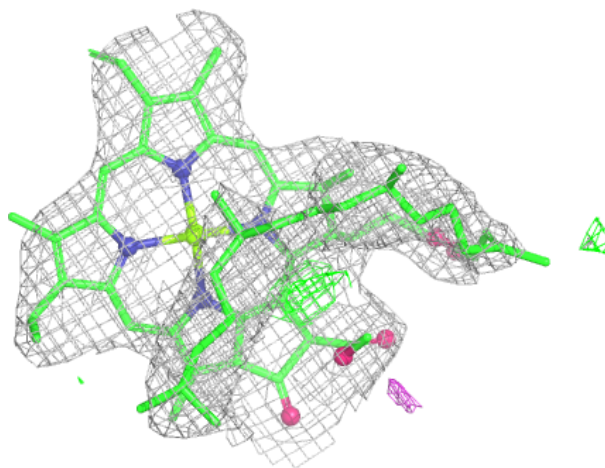
**Electron density around CLA BB 612:**

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



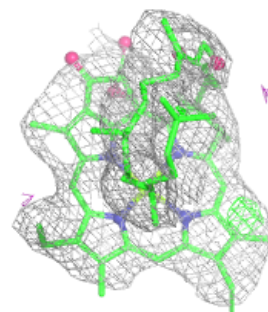
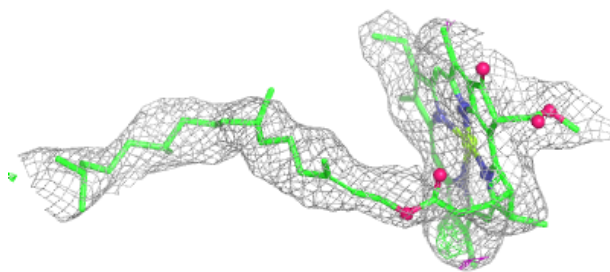
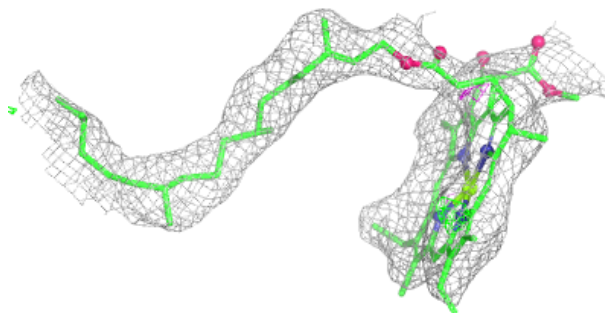
Electron density around CLA BC 510:

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

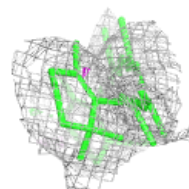
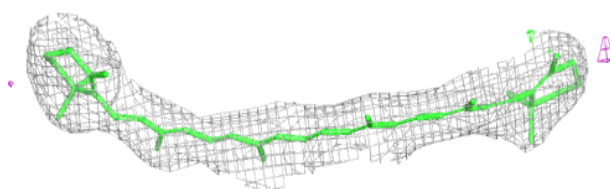
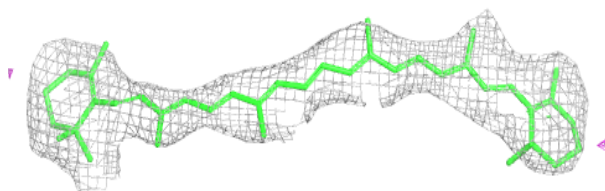


Electron density around CLA AC 508:

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

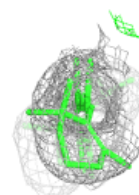
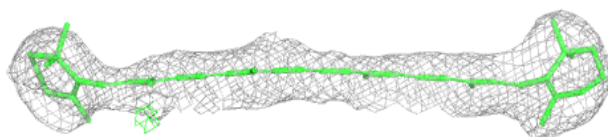
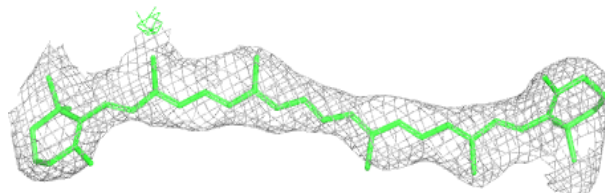
**Electron density around BCR AB 618:**

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

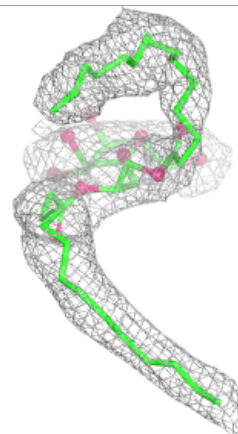
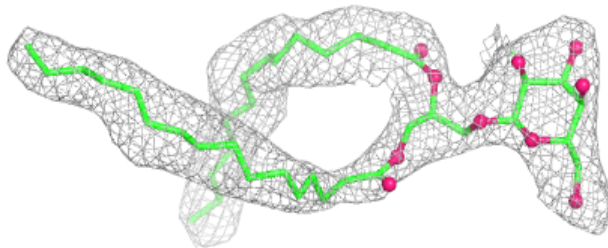
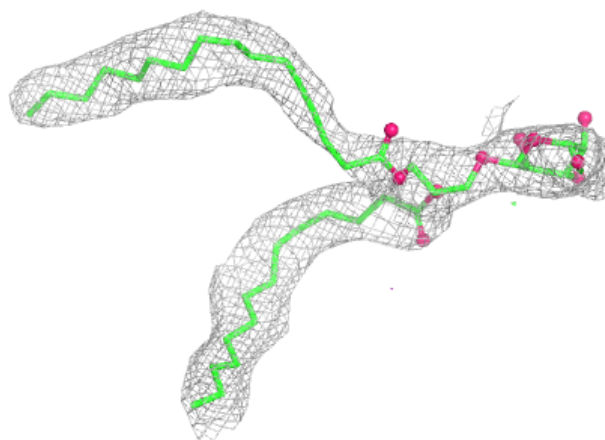


Electron density around BCR AB 619:

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

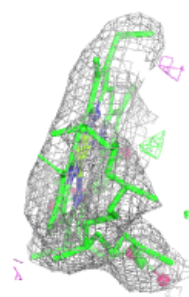
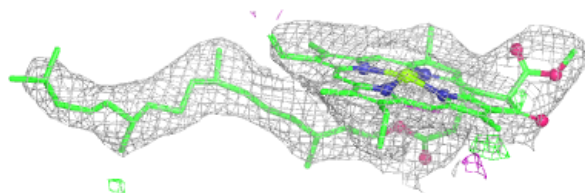
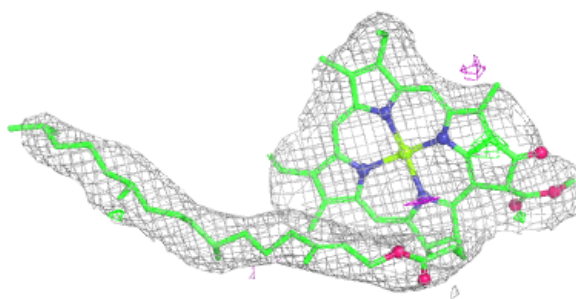
**Electron density around LMG AB 622:**

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

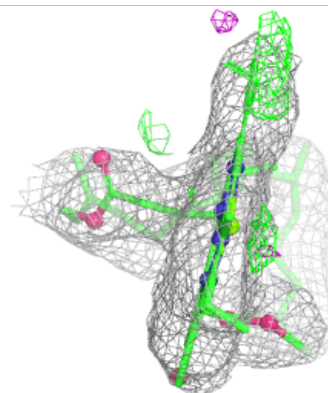
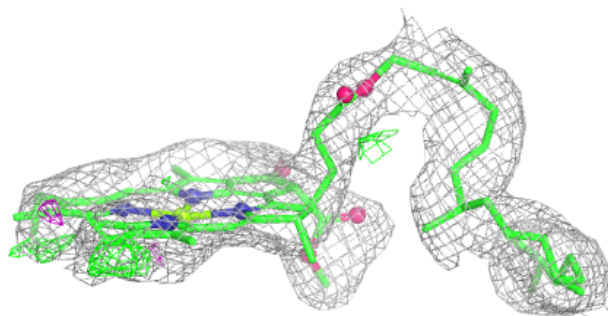
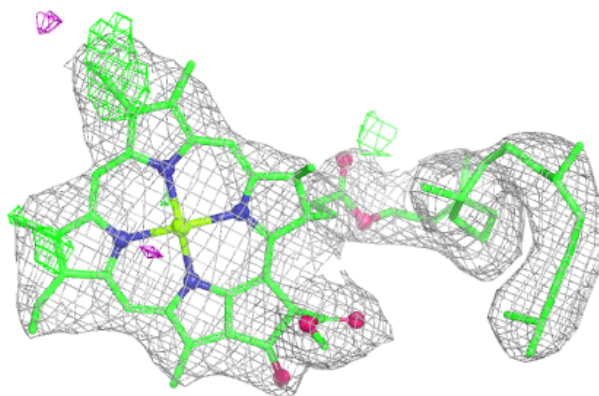


Electron density around CLA BC 501:

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

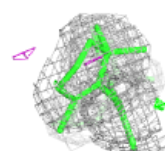
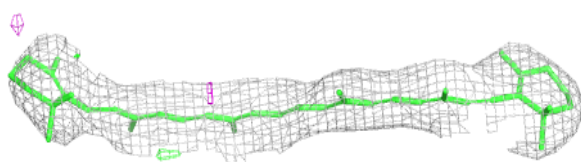
**Electron density around CLA AB 612:**

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

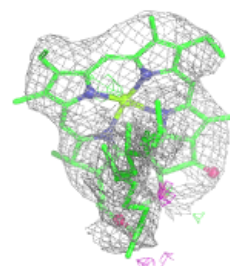
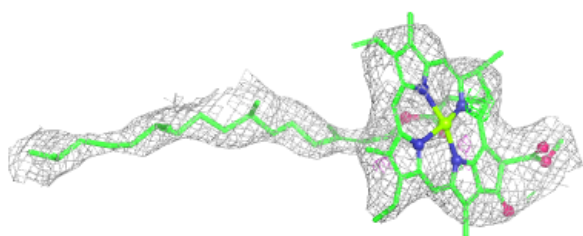
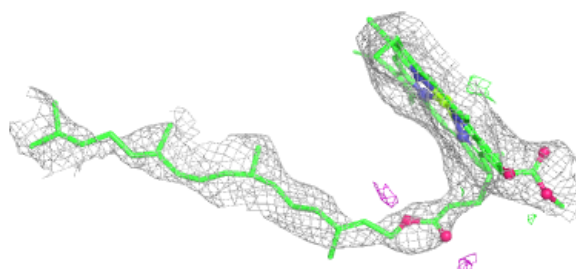


Electron density around BCR AC 515:

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

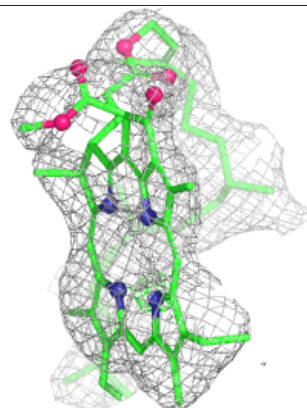
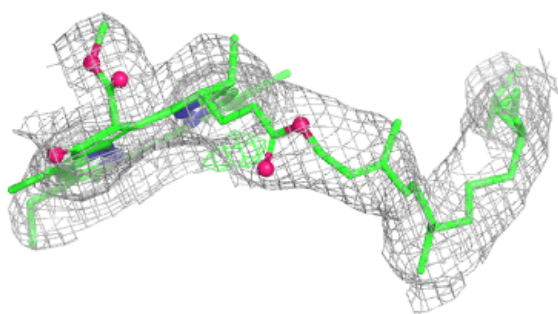
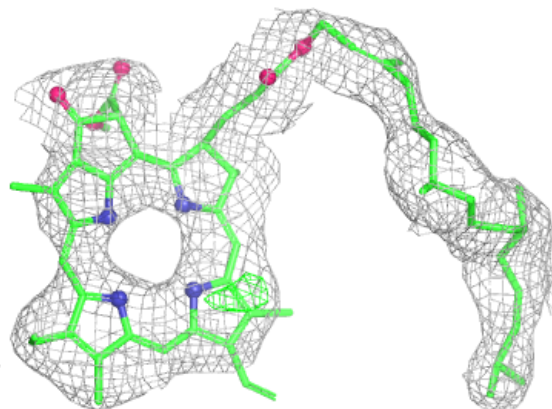
**Electron density around CLA BC 504:**

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

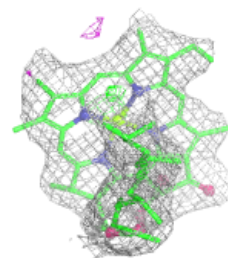
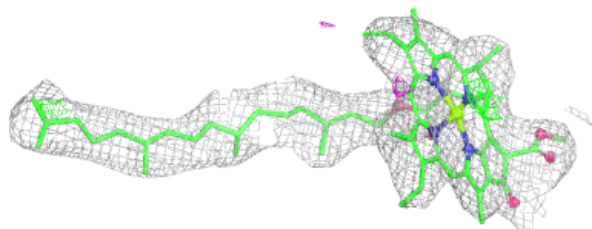
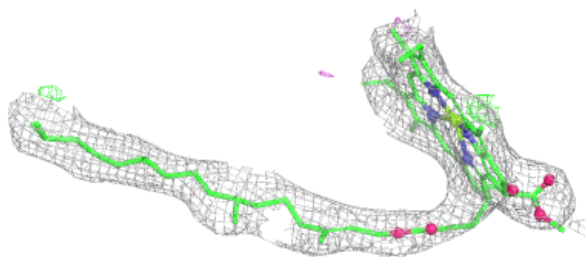


Electron density around PHO BD 403:

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

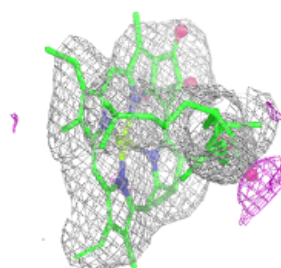
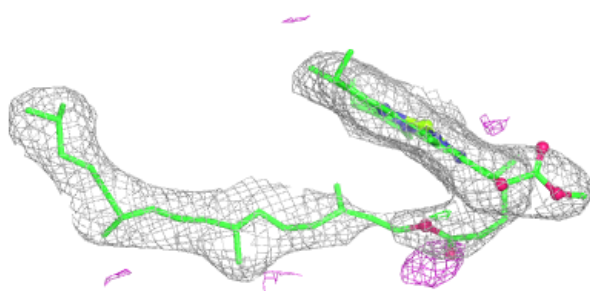
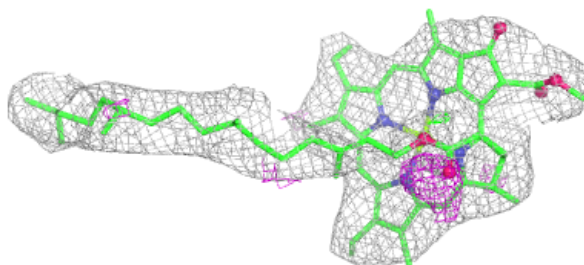
**Electron density around CLA BB 610:**

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

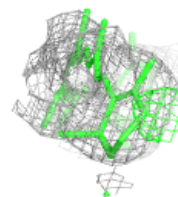
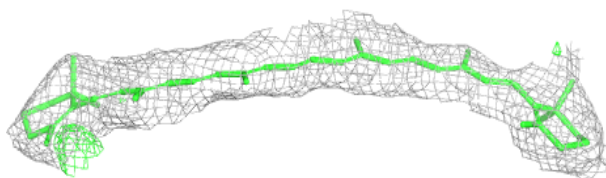
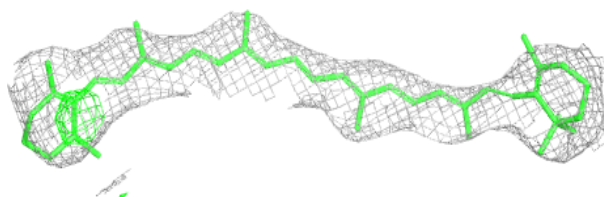


Electron density around CLA BB 611:

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

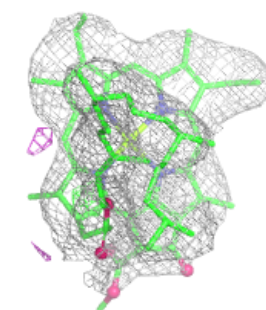
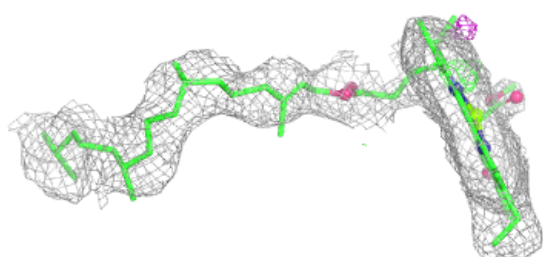
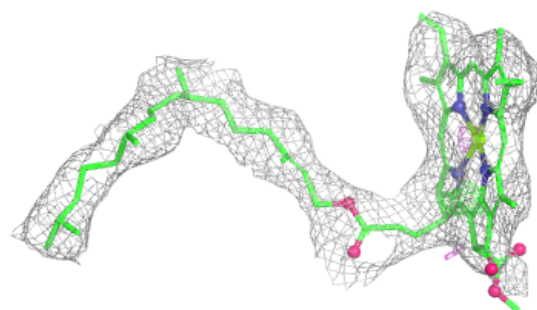
**Electron density around BCR AT 102:**

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

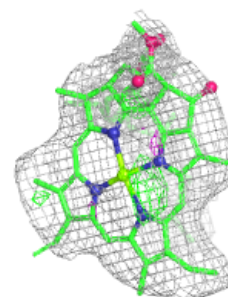
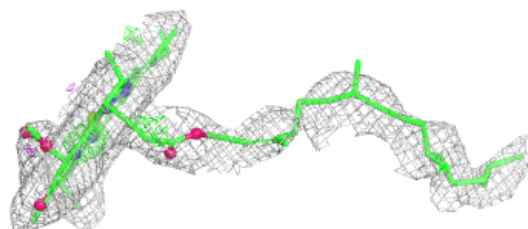
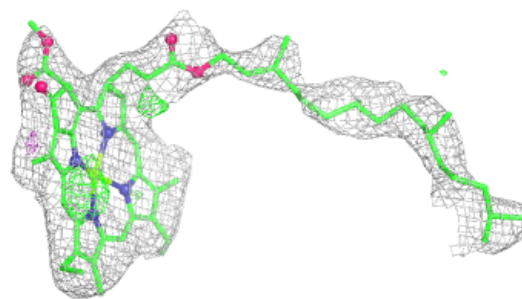


Electron density around CLA AD 404:

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

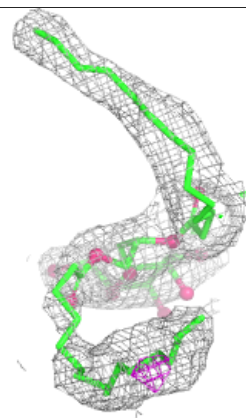
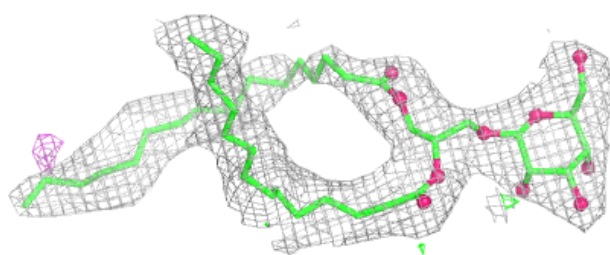
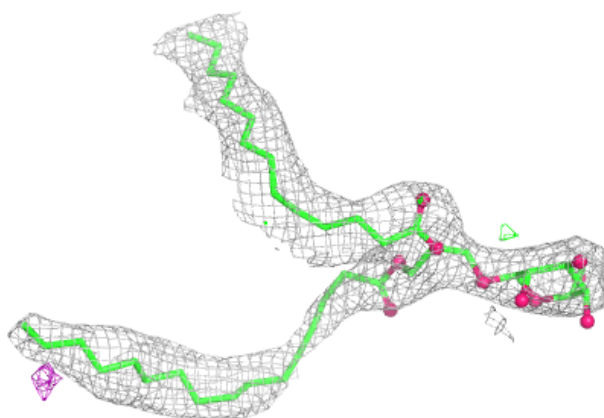
**Electron density around CLA BA 407:**

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

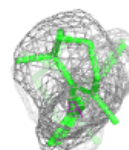
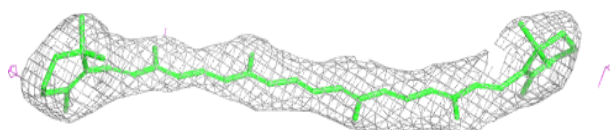
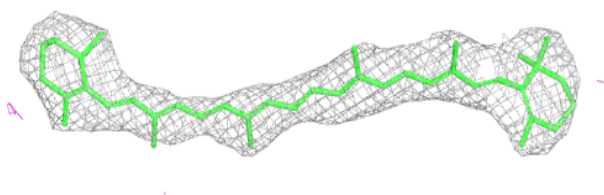


Electron density around LMG BB 624:

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

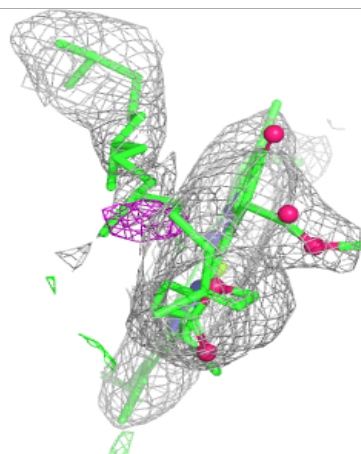
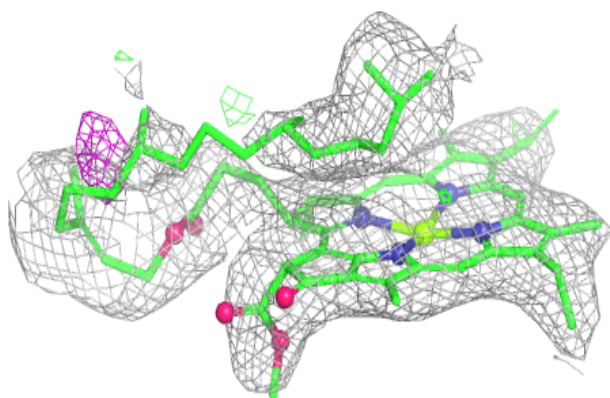
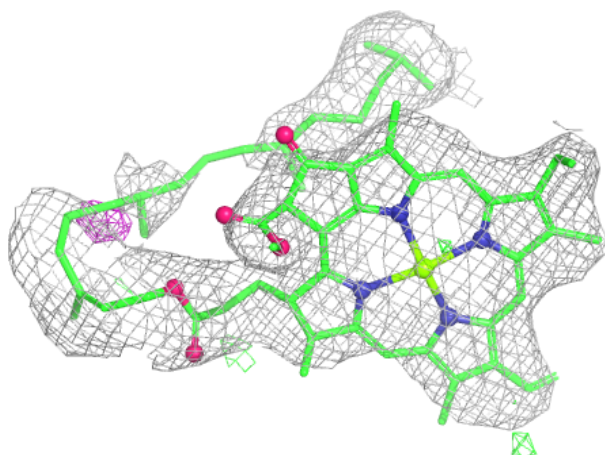
**Electron density around BCR BB 622:**

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



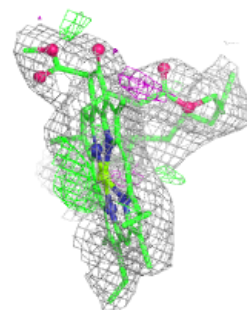
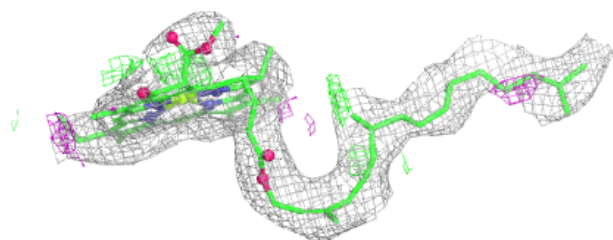
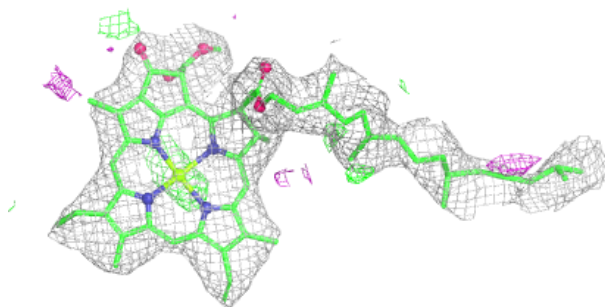
Electron density around CLA BC 509:

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

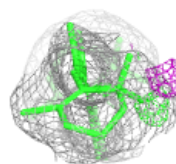
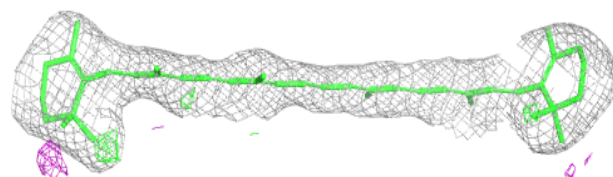
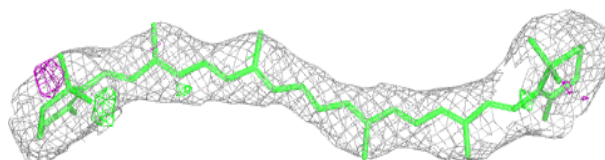


Electron density around CLA AA 404:

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

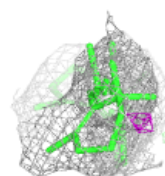
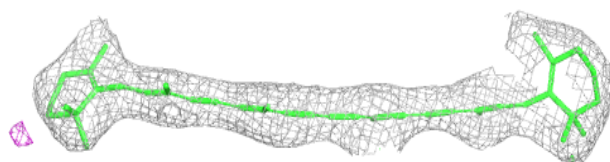
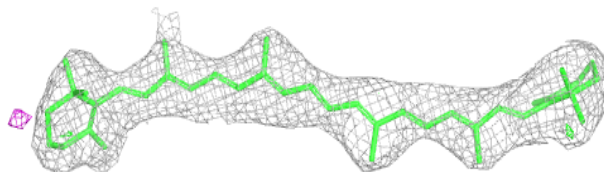
**Electron density around BCR AA 409:**

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

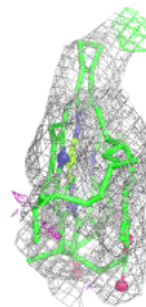
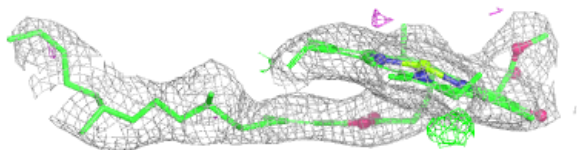
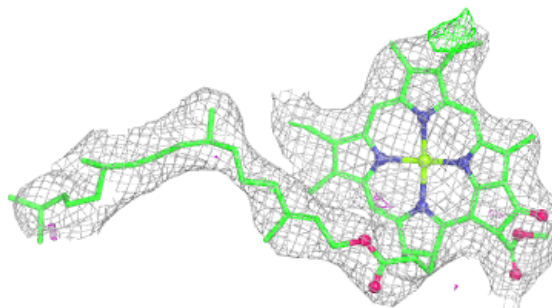


Electron density around BCR AB 617:

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

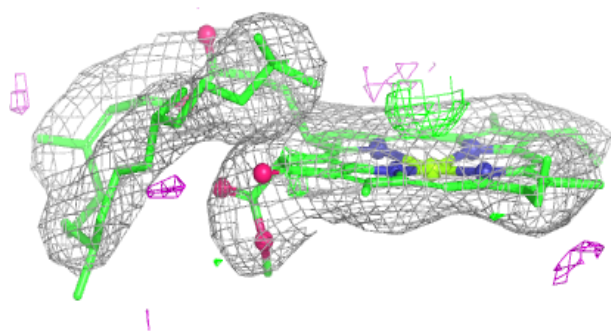
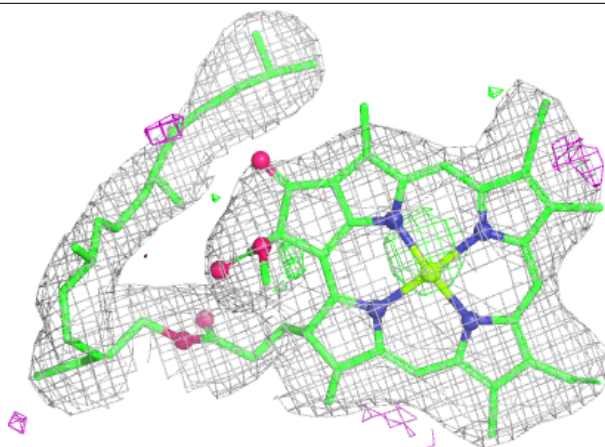
**Electron density around CLA BB 606:**

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



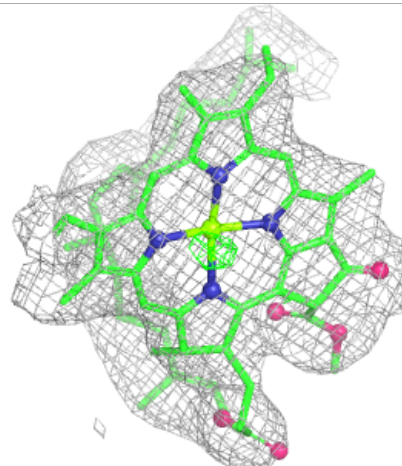
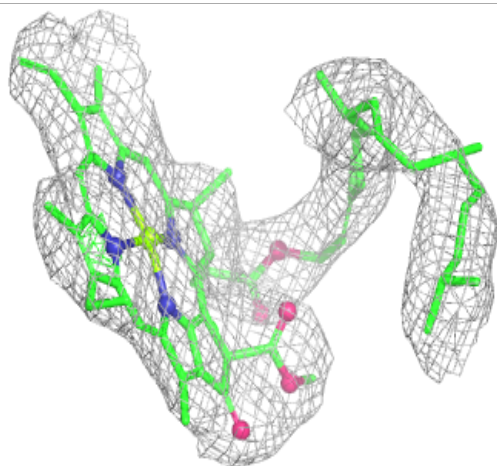
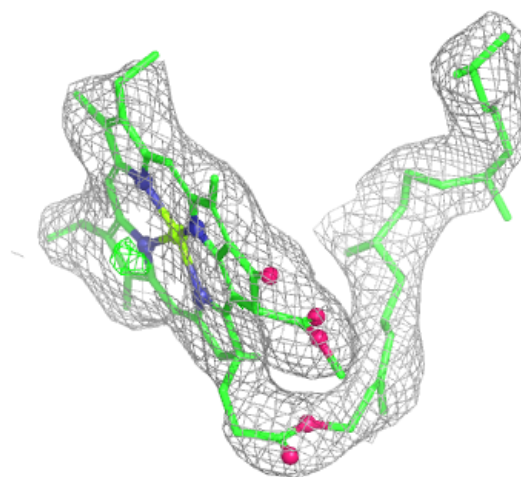
Electron density around CLA BB 613:

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



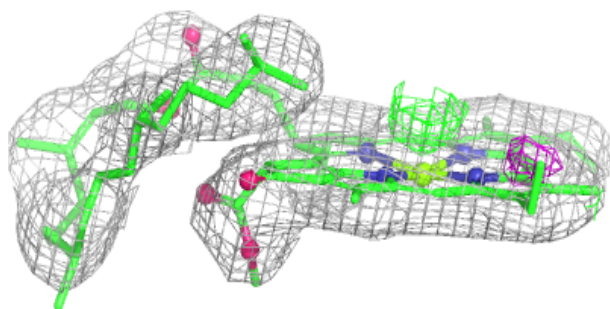
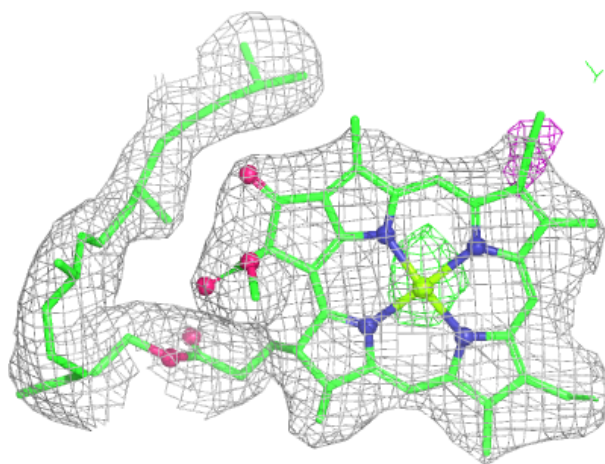
Electron density around CLA AB 613:

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



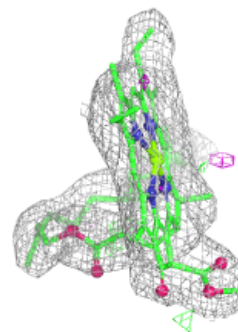
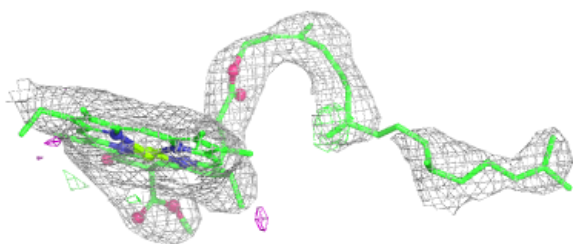
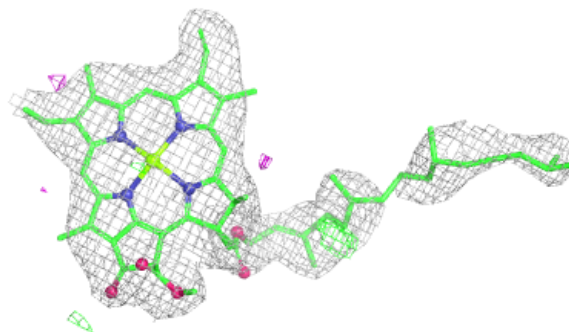
Electron density around CLA AB 610:

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



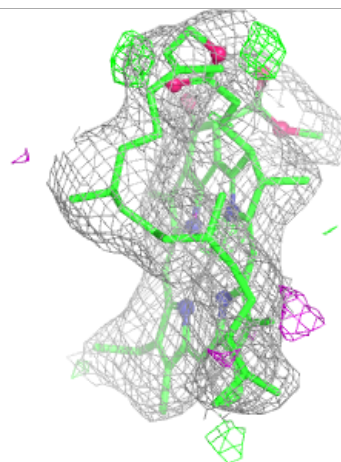
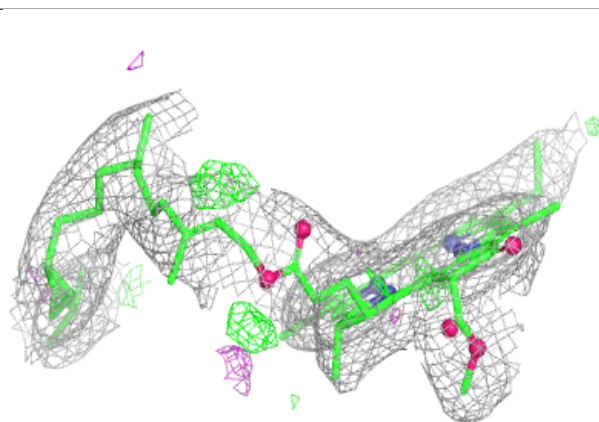
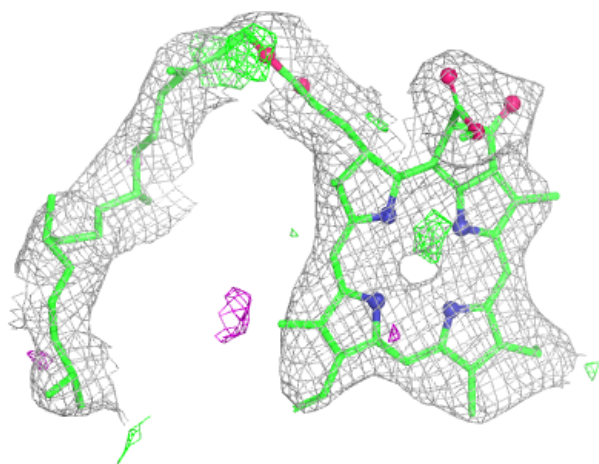
Electron density around CLA BA 405:

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



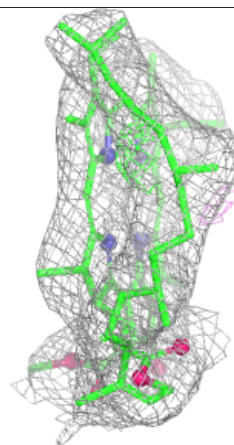
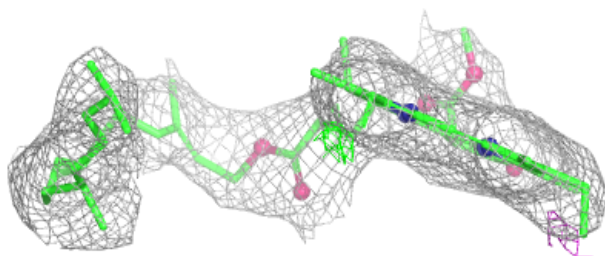
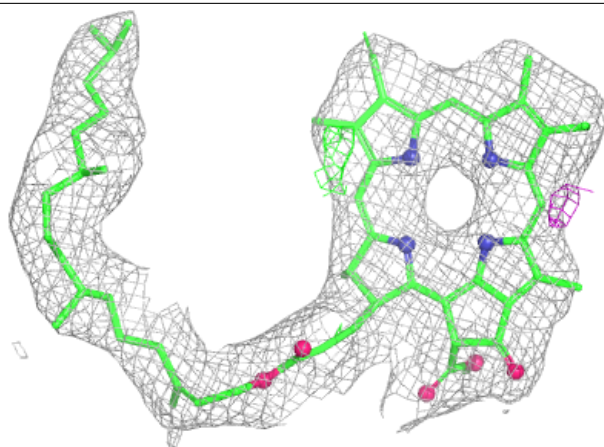
Electron density around PHO AD 403:

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



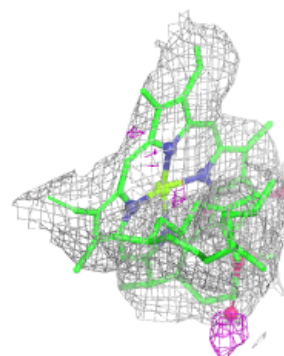
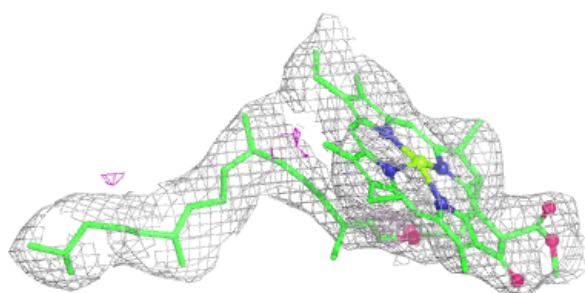
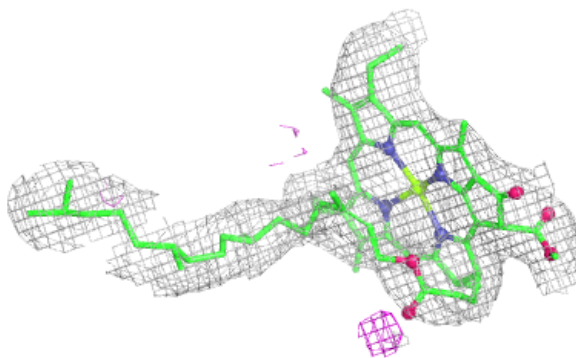
Electron density around PHO BA 406:

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



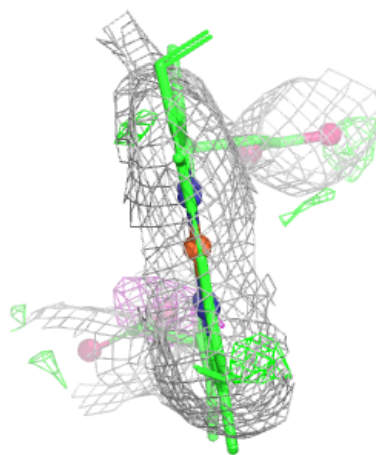
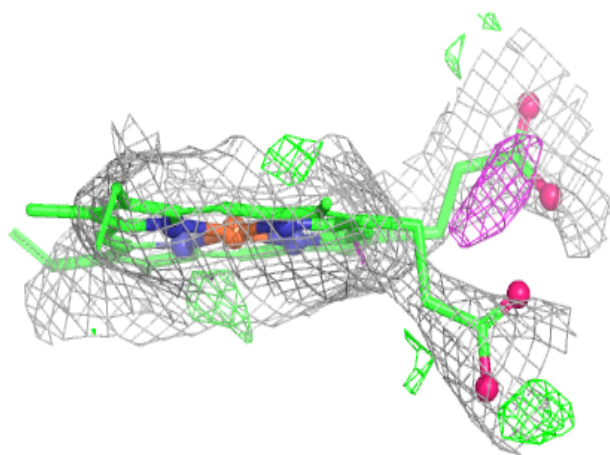
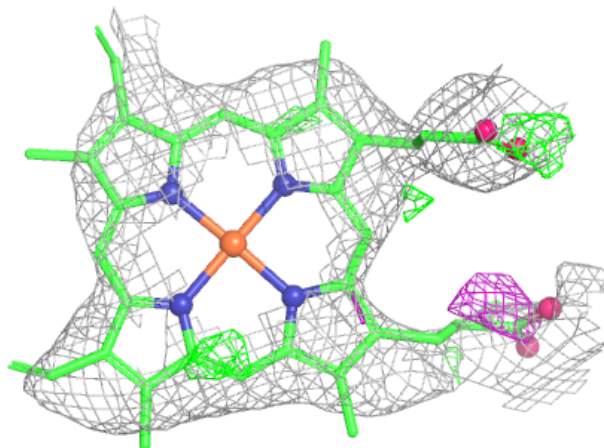
Electron density around CLA AC 505:

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



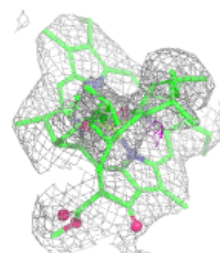
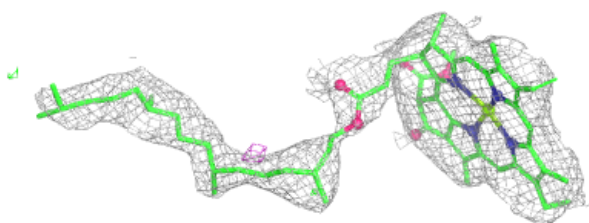
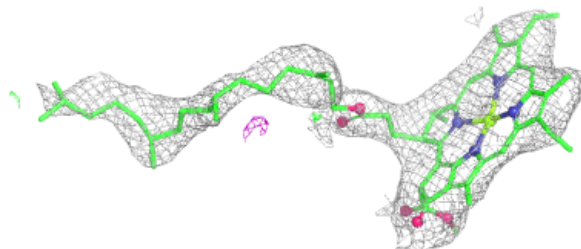
Electron density around HEM BE 101:

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

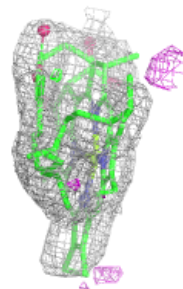
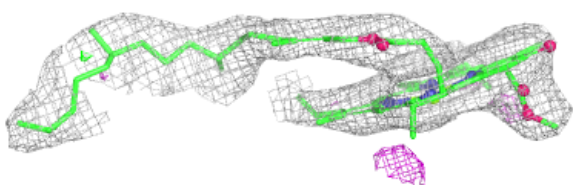
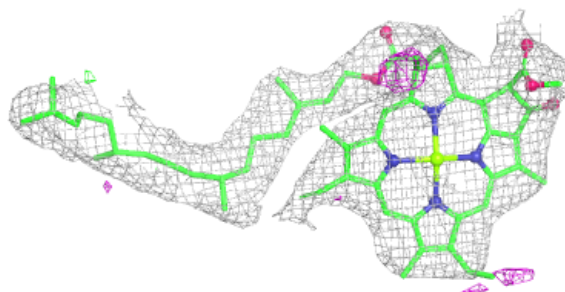


Electron density around CLA BC 502:

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

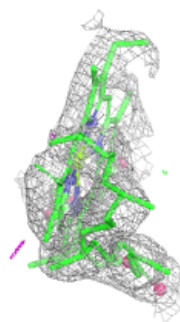
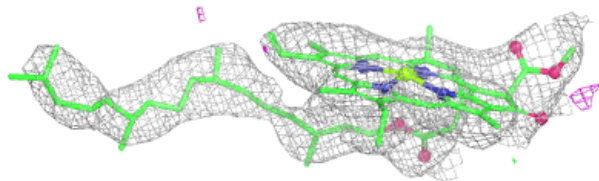
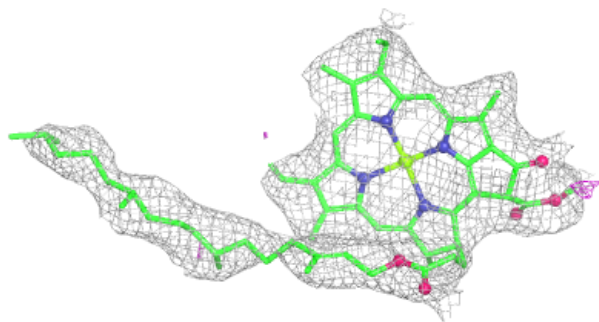
**Electron density around CLA AB 603:**

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

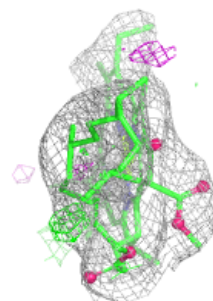
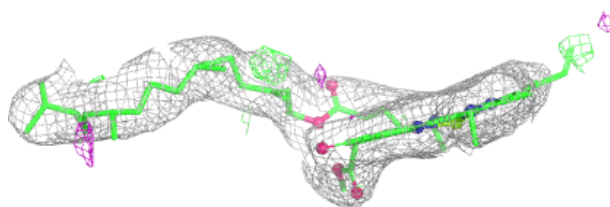
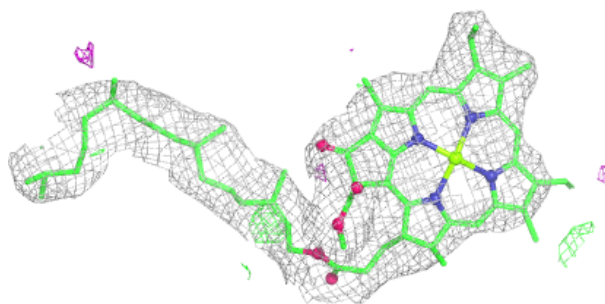


Electron density around CLA AC 501:

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

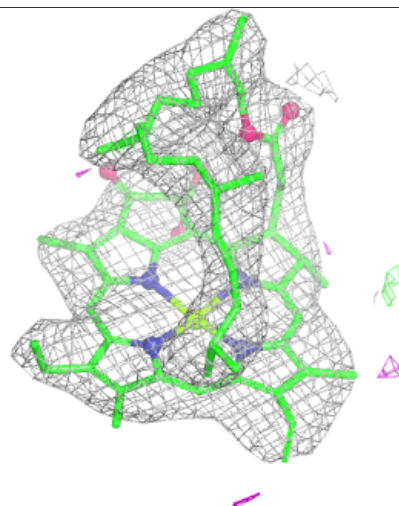
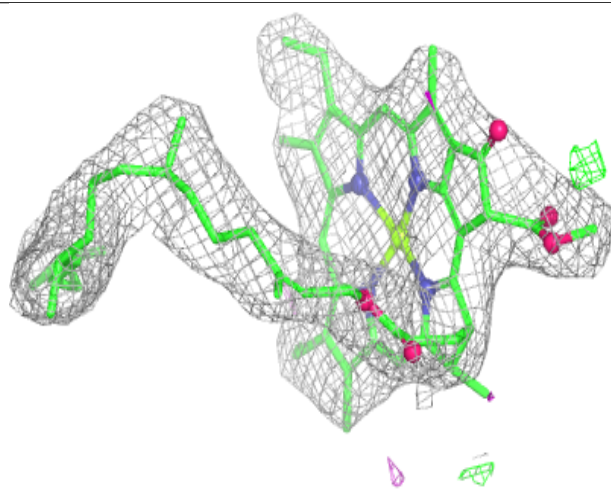
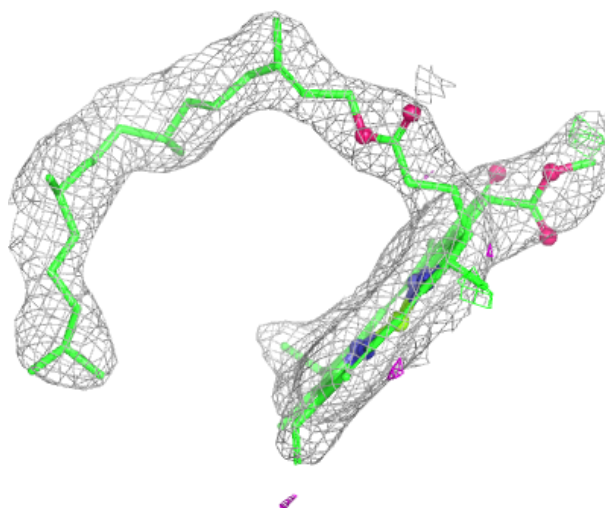
**Electron density around CLA BB 605:**

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



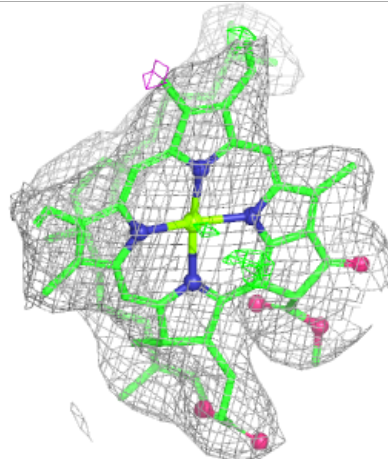
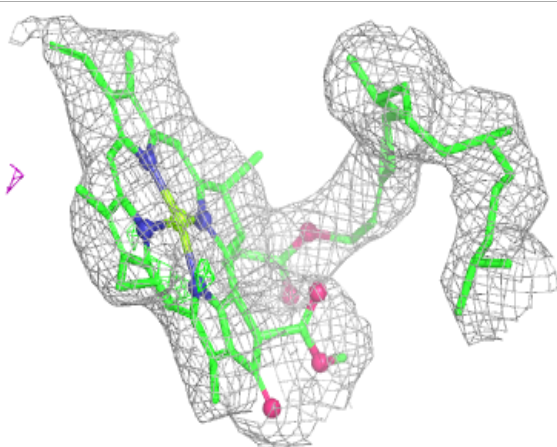
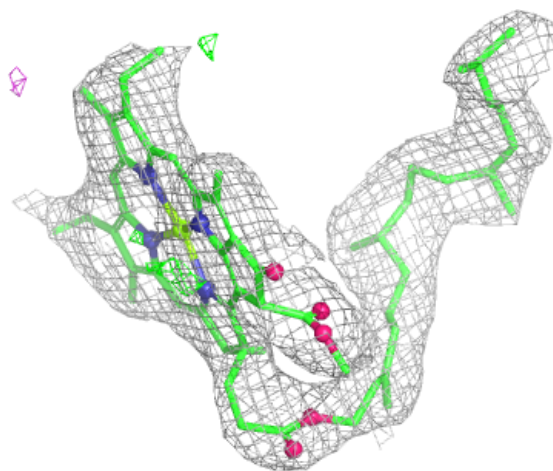
Electron density around CLA AB 611:

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



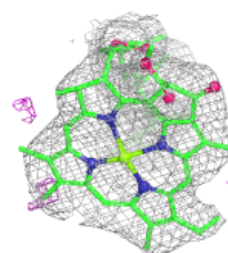
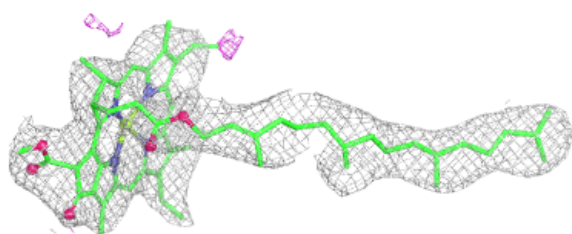
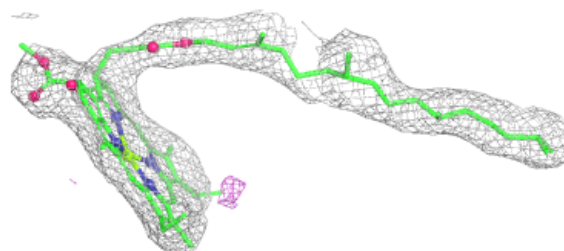
Electron density around CLA BB 616:

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

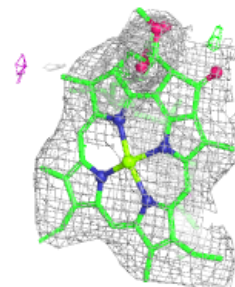
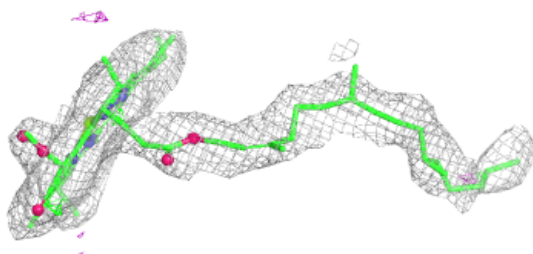
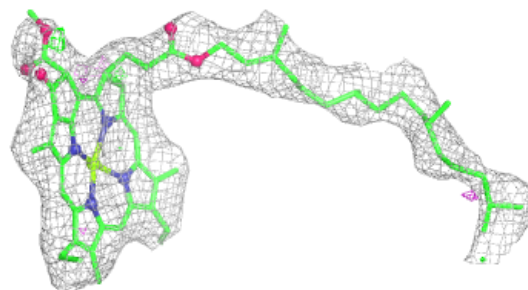


Electron density around CLA AB 607:

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

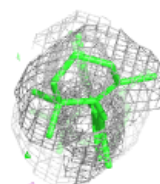
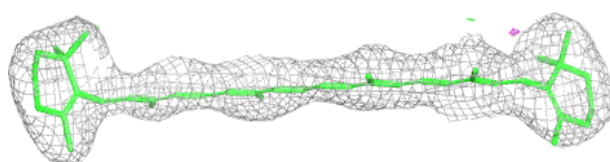
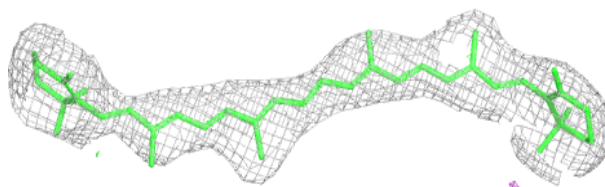
**Electron density around CLA AA 406:**

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

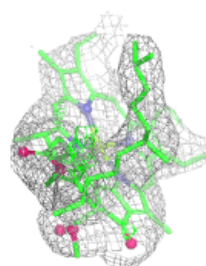
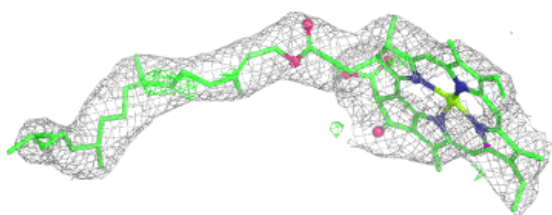
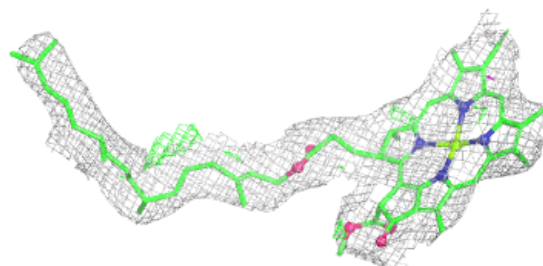


Electron density around BCR BA 410:

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

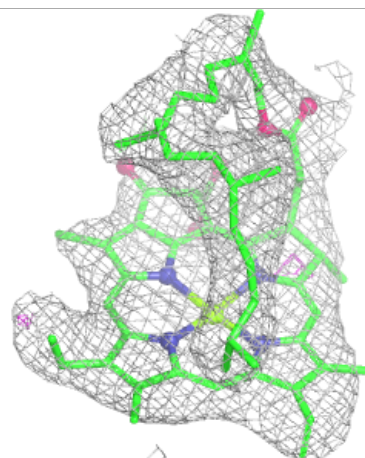
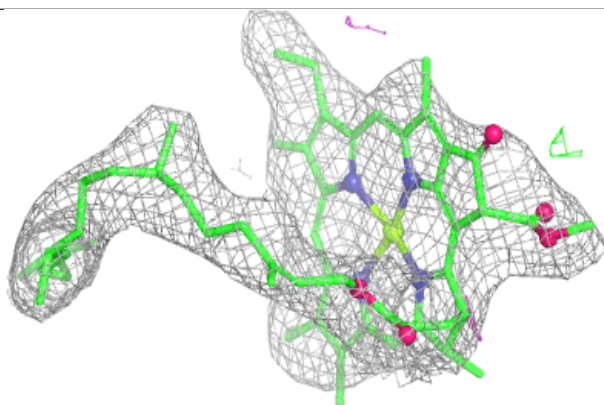
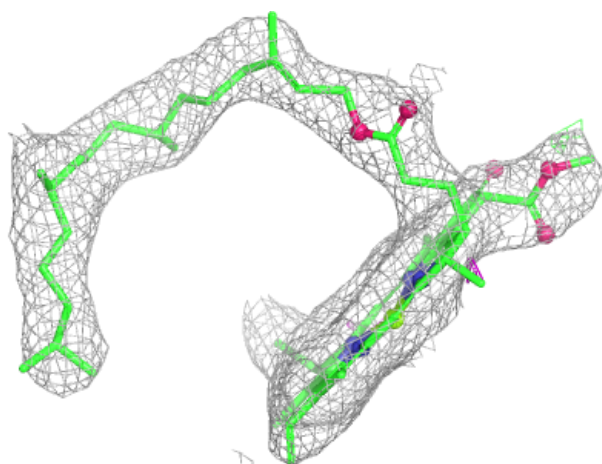
**Electron density around CLA BA 403:**

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



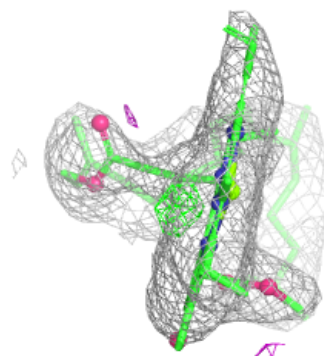
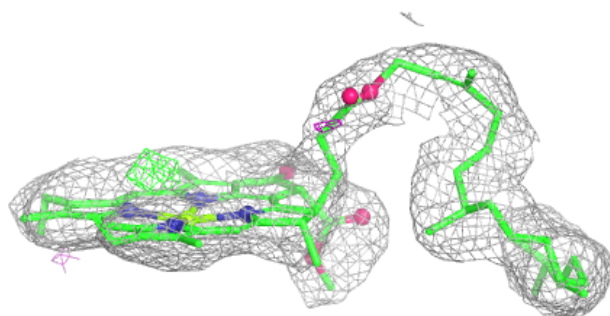
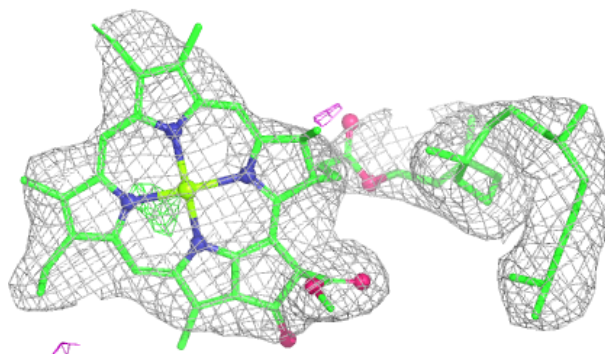
Electron density around CLA BB 614:

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

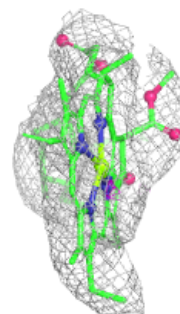
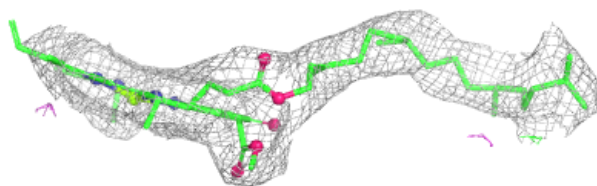
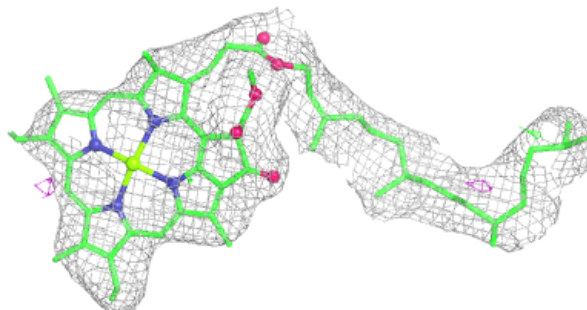


Electron density around CLA BB 615:

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

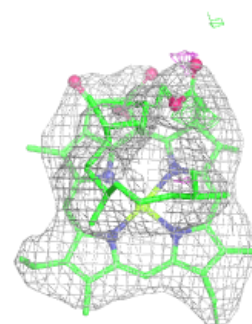
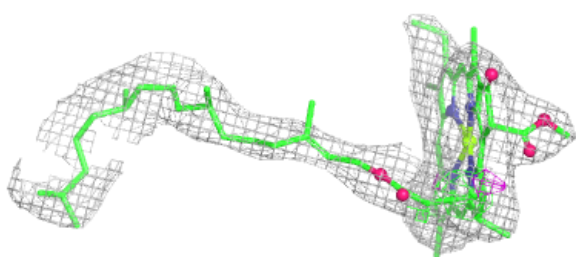
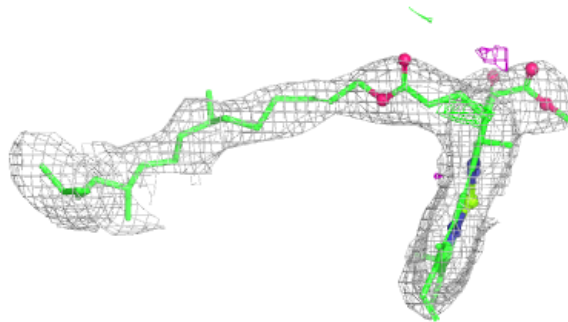
**Electron density around CLA AB 602:**

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

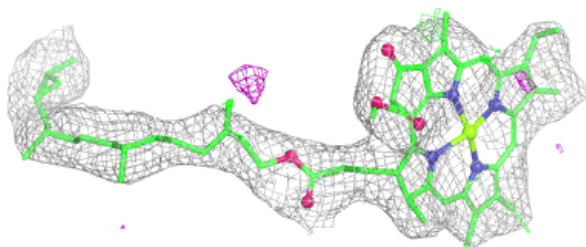
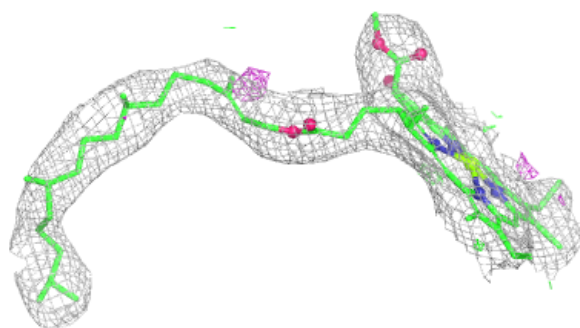


Electron density around CLA AB 605:

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

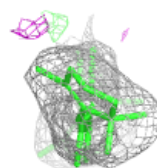
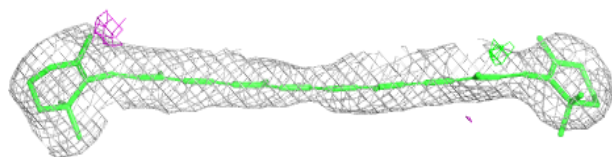
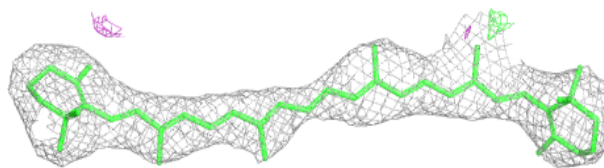
**Electron density around CLA AD 402:**

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

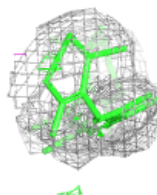
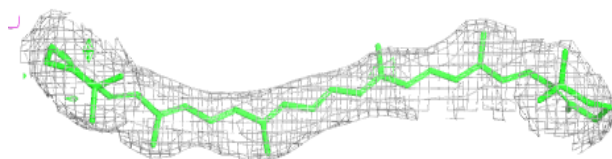
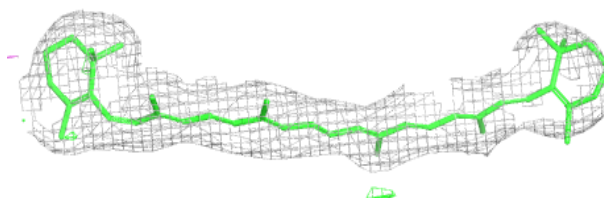


Electron density around BCR BB 621:

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

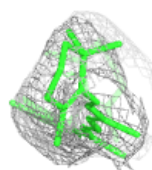
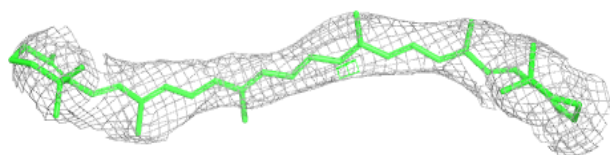
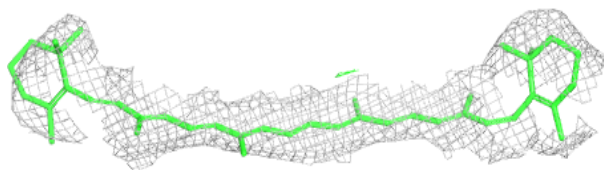
**Electron density around BCR AC 514:**

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



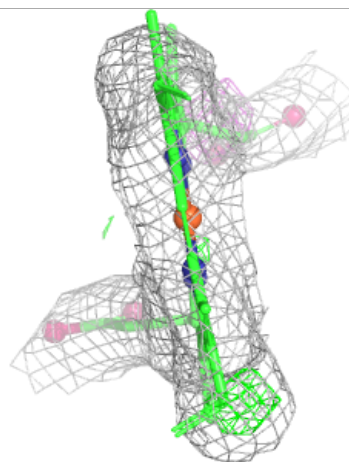
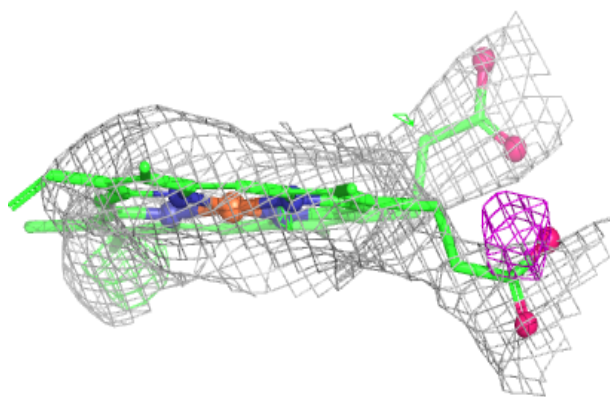
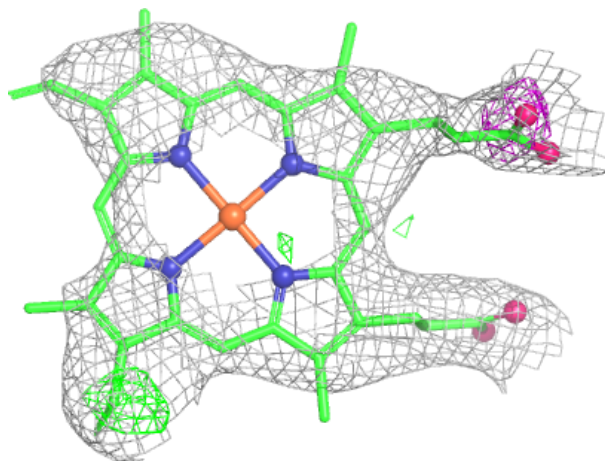
Electron density around BCR BC 514:

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



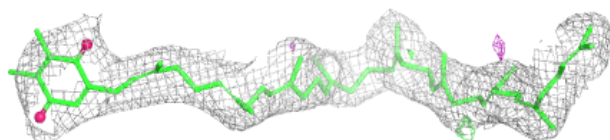
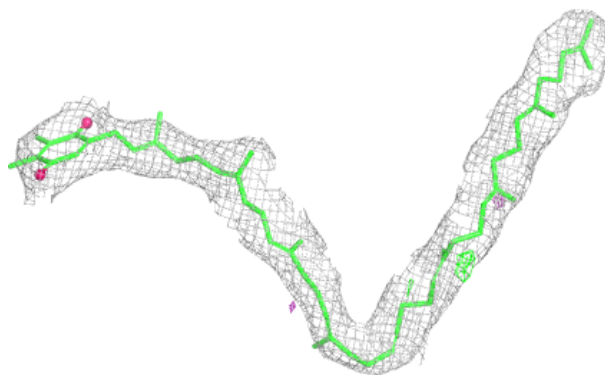
Electron density around HEM AE 101:

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



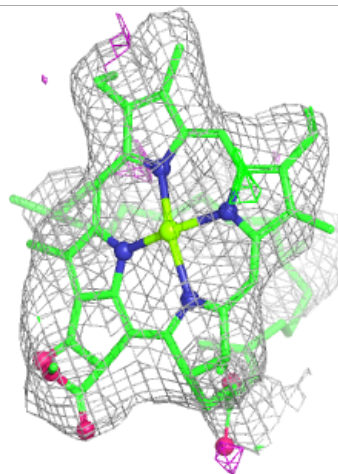
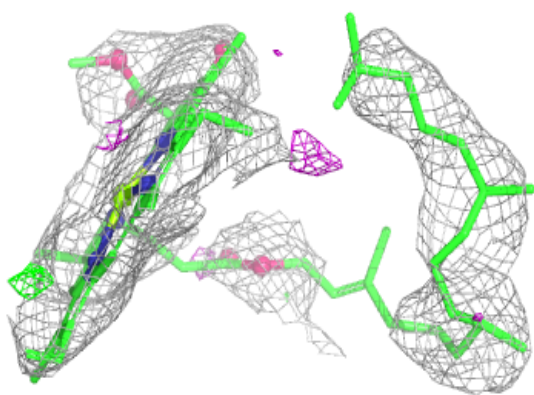
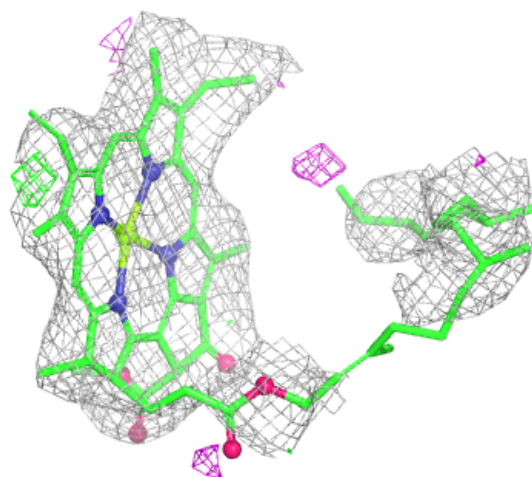
Electron density around PL9 BD 405:

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



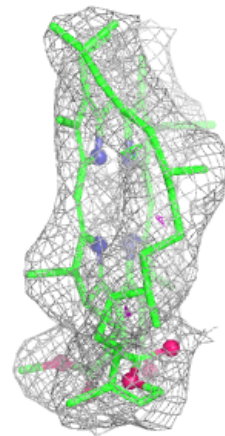
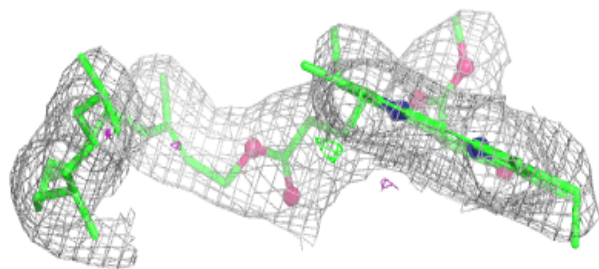
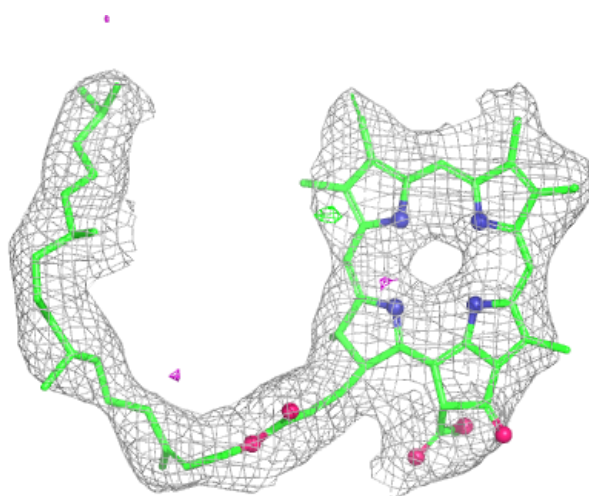
Electron density around CLA AC 503:

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



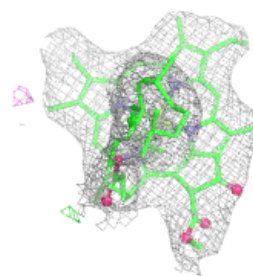
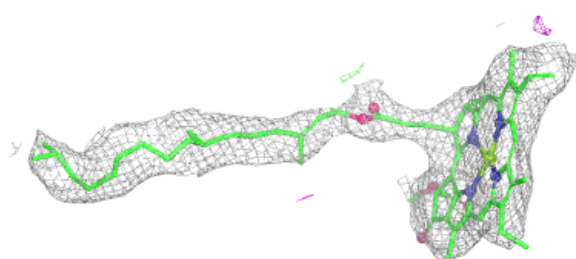
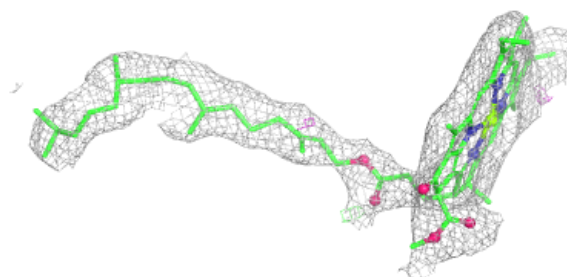
Electron density around PHO AA 405:

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

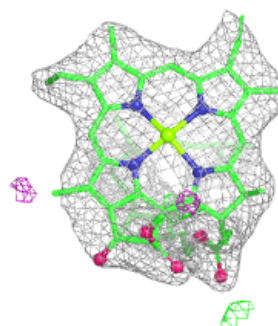
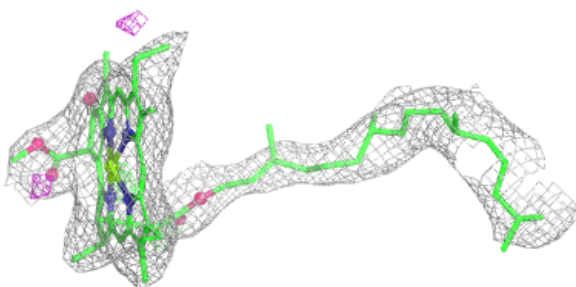
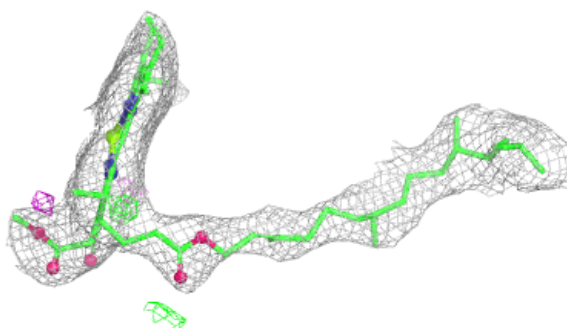


Electron density around CLA BB 607:

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

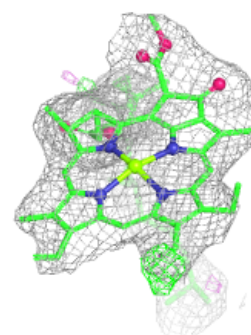
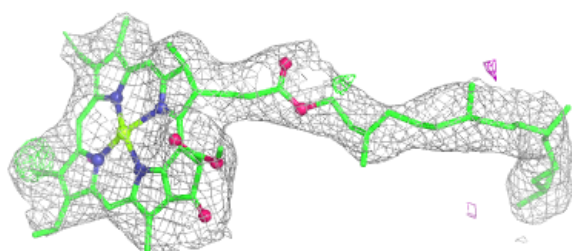
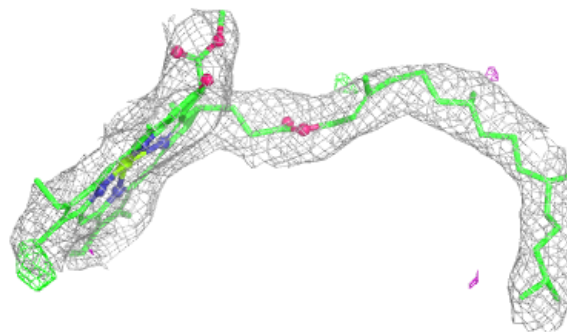
**Electron density around CLA BB 608:**

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

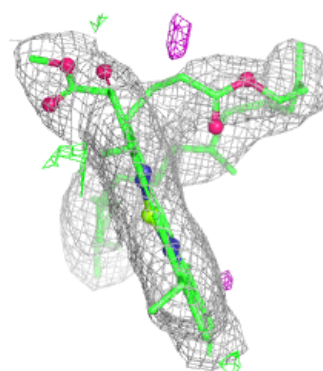
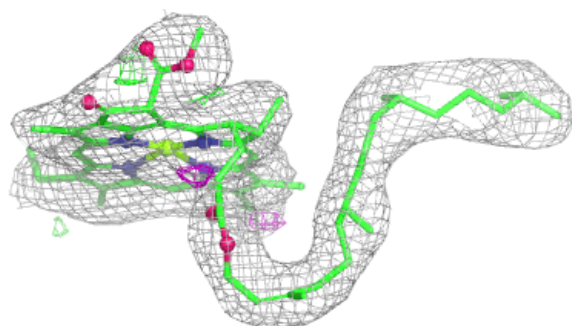
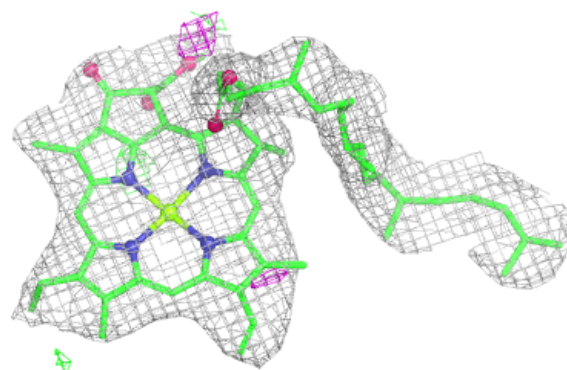


Electron density around CLA BD 402:

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

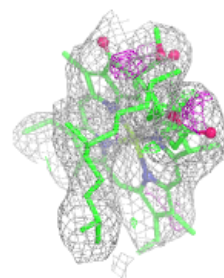
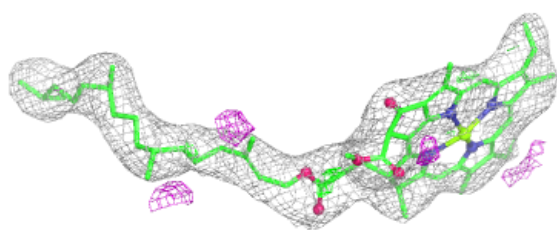
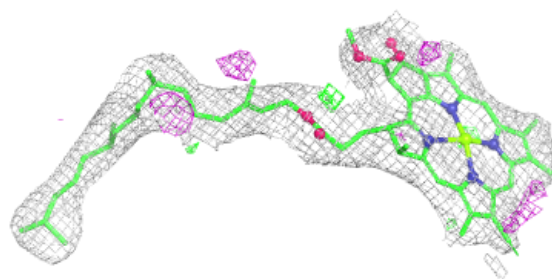
**Electron density around CLA BA 404:**

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

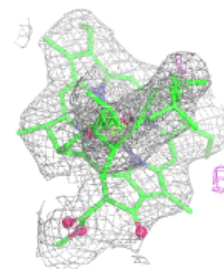
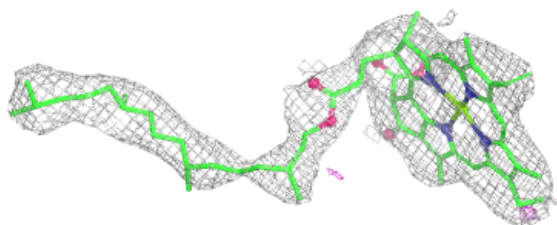
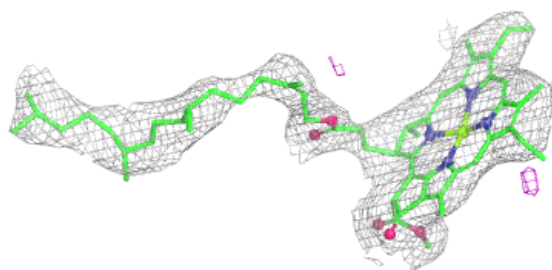


Electron density around CLA AA 402:

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

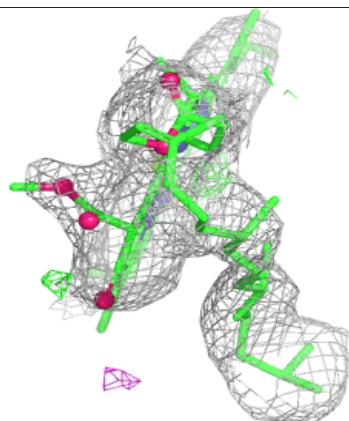
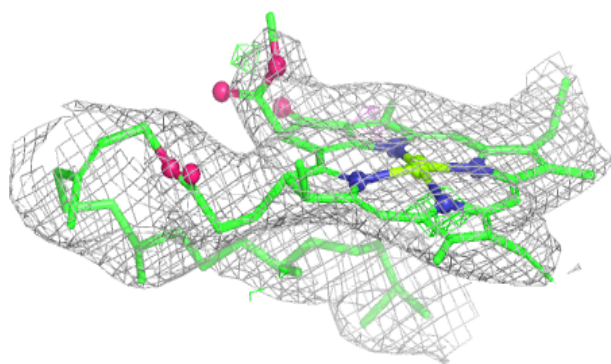
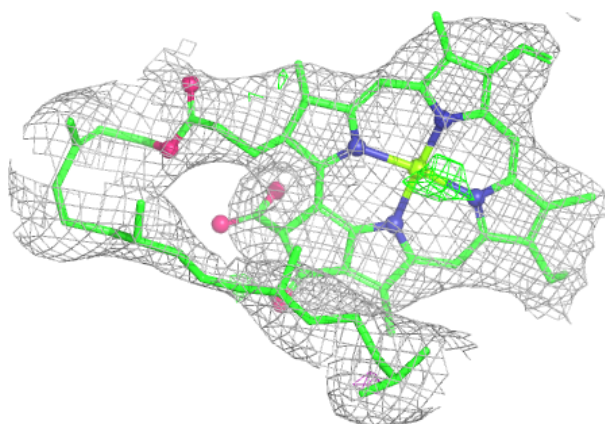
**Electron density around CLA AC 502:**

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



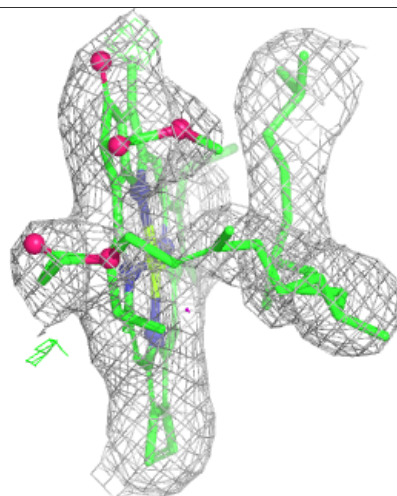
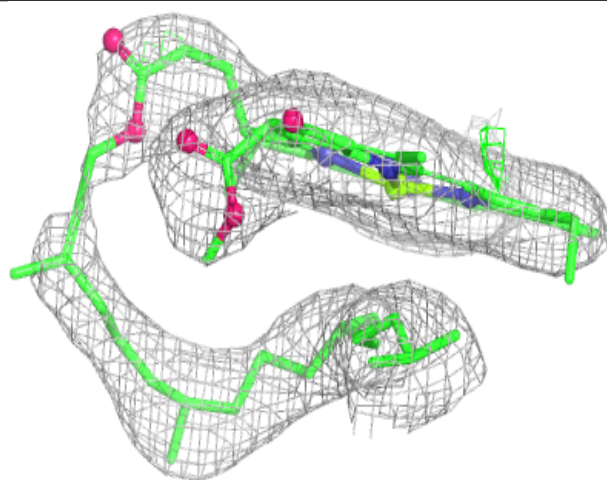
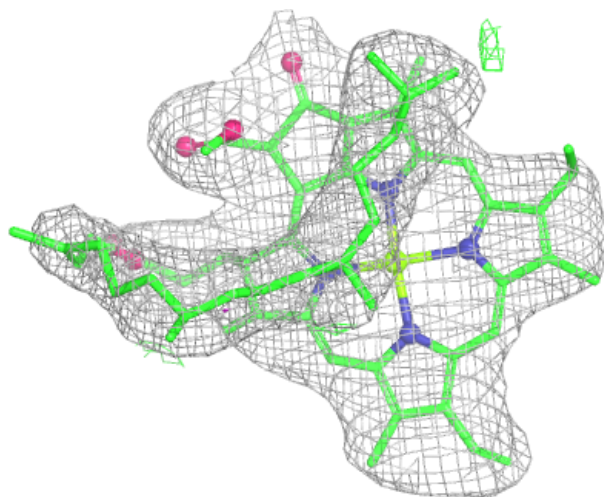
Electron density around CLA AC 509:

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



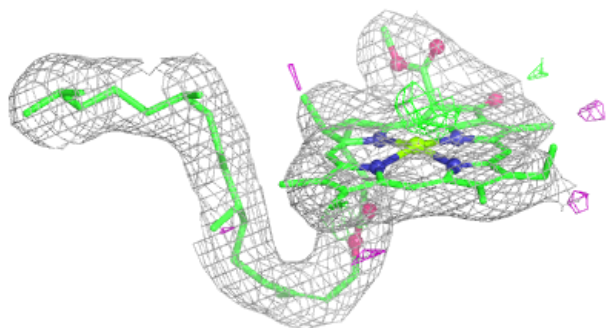
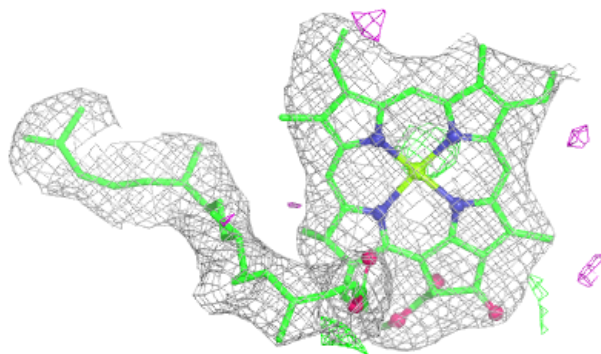
Electron density around CLA AC 510:

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

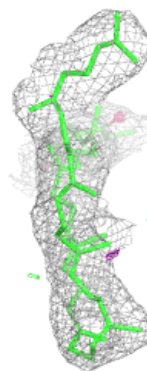
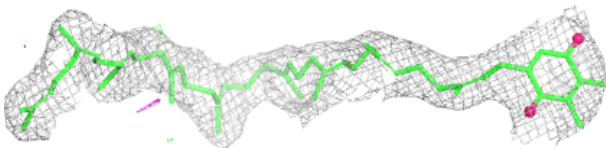
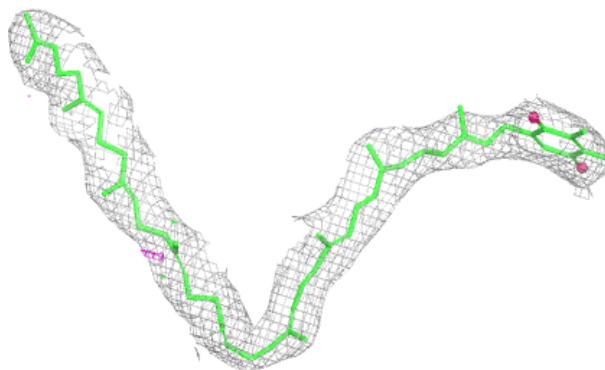


Electron density around CLA AA 403:

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

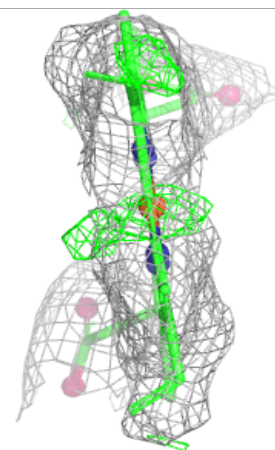
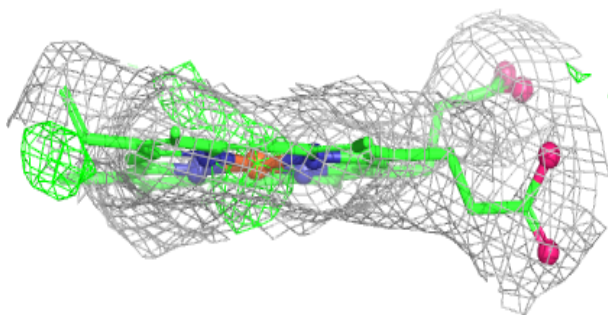
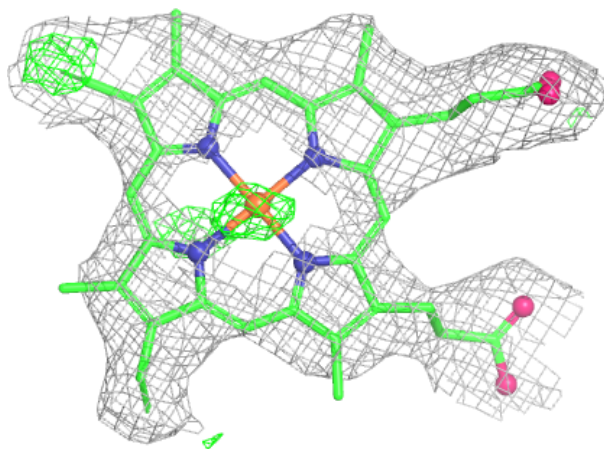
**Electron density around PL9 AD 405:**

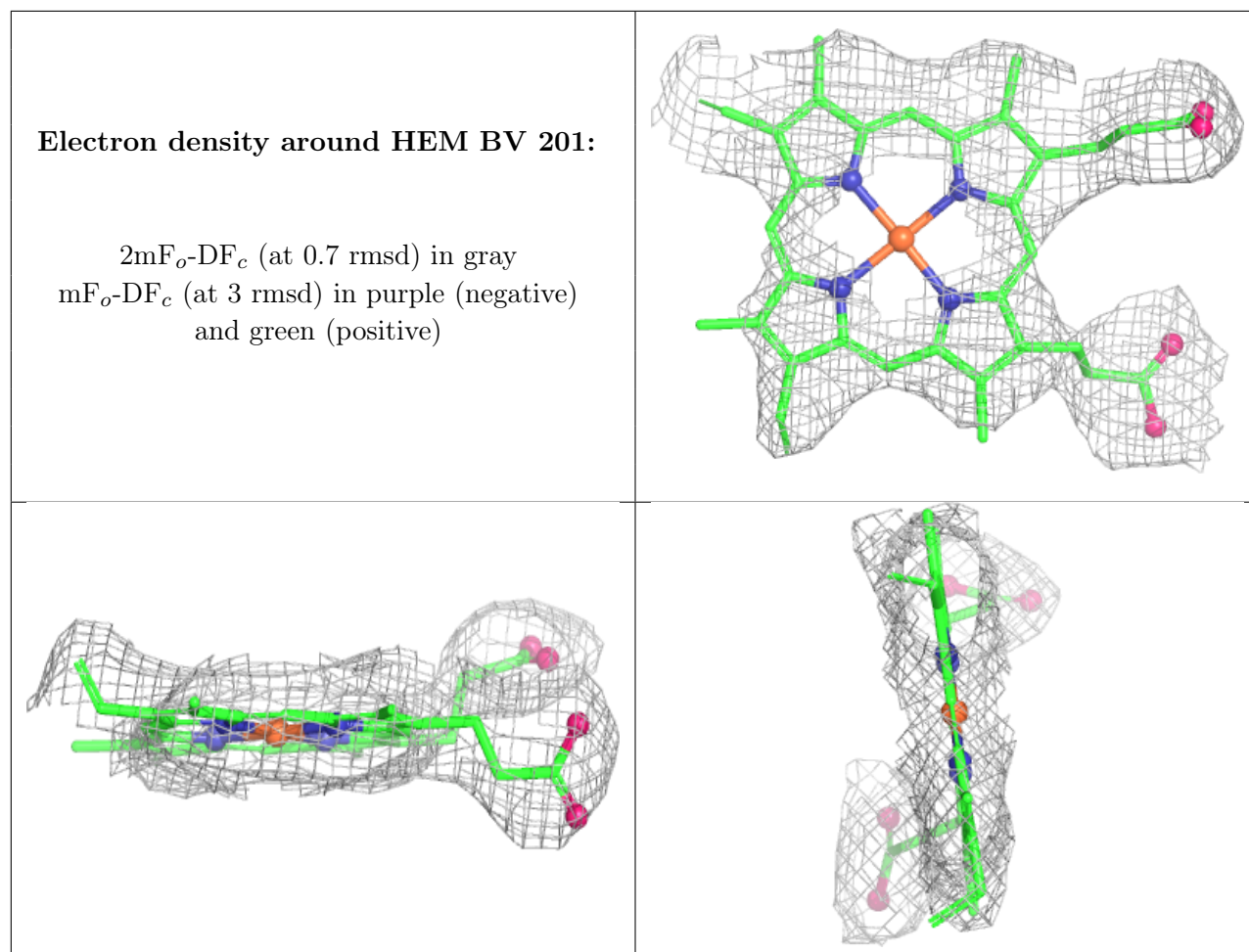
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.