



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:38 AM UTC

PDB ID : 4IXQ / pdb_00004ixq
Title : RT fs X-ray diffraction of Photosystem II, dark state
Authors : Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on : 2013-01-27
Resolution : 5.70 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)

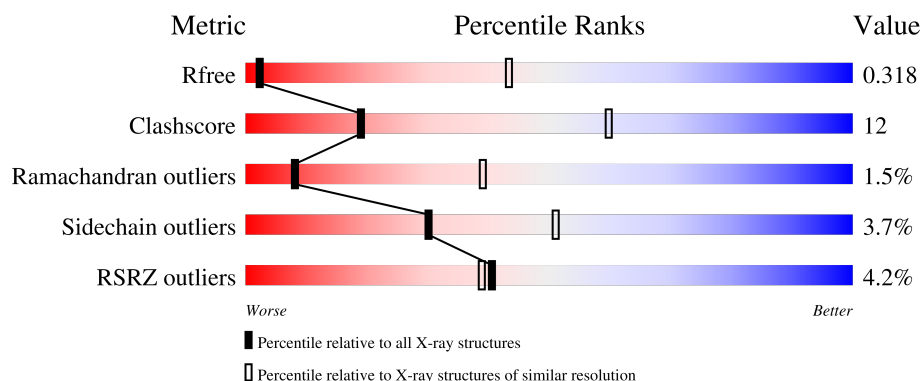
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.70 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	1109 (7.40-4.00)
Clashscore	190562	1170 (7.40-4.00)
Ramachandran outliers	187476	1005 (7.40-4.00)
Sidechain outliers	187428	1035 (7.40-3.96)
RSRZ outliers	180081	1102 (7.40-4.00)

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	A	360	 4% 65% 27% • 7%
1	a	360	 3% 66% 26% • 7%

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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

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Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	J	101	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	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	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	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	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	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	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	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	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	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	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	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	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	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	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	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	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	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	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	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	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

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

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

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

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

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

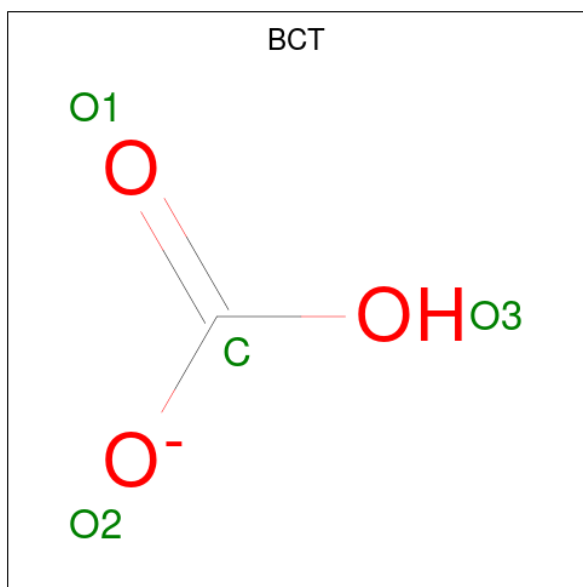
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

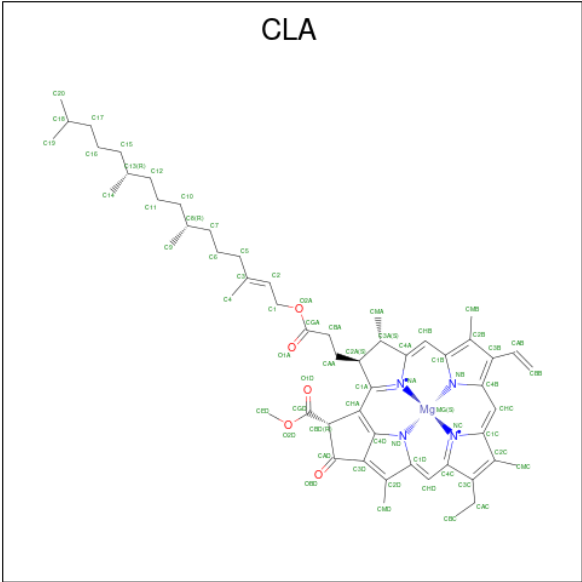
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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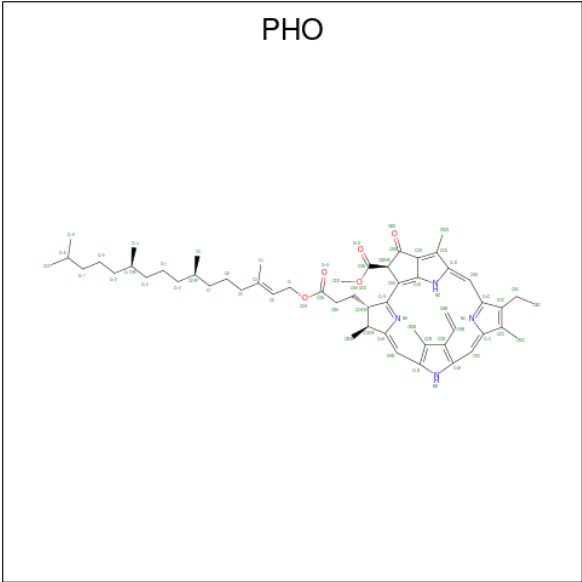
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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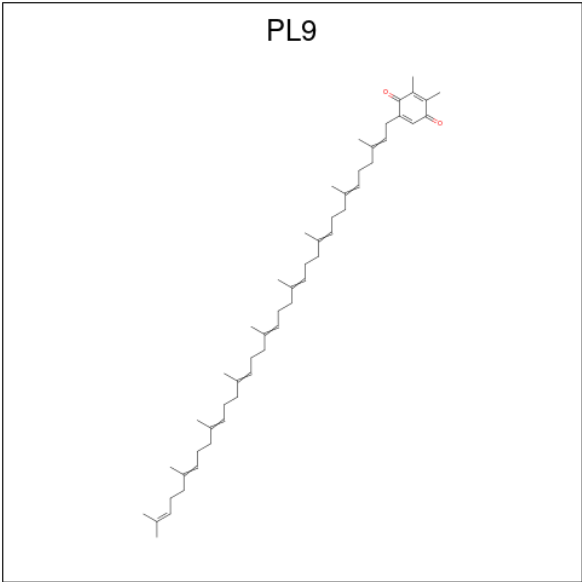
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



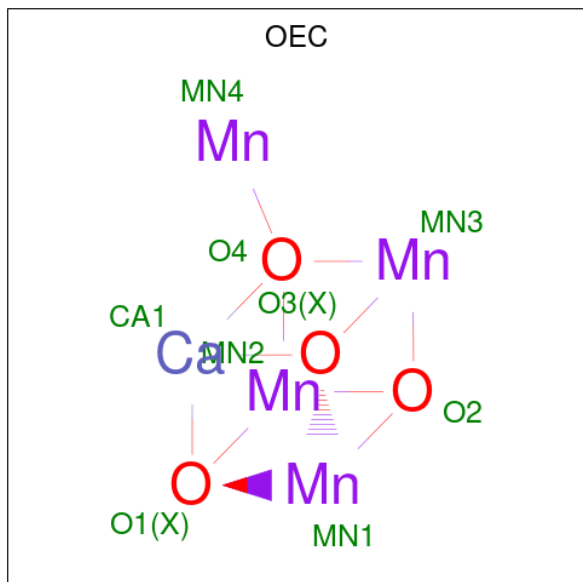
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



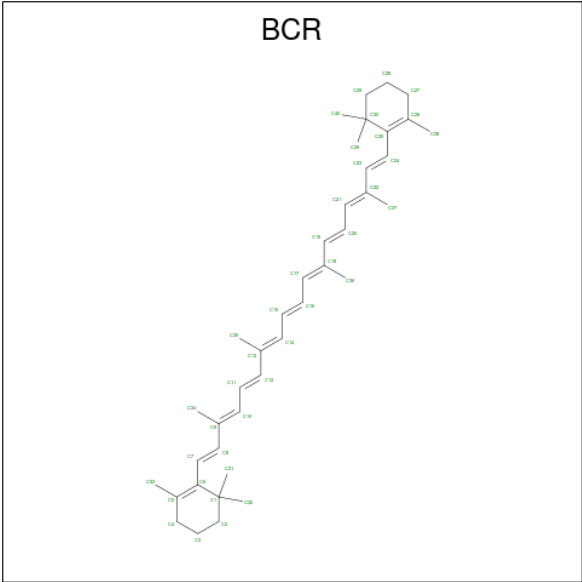
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	J	1	Total	C	O	0	0
			35	33	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			55	53	2		
25	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



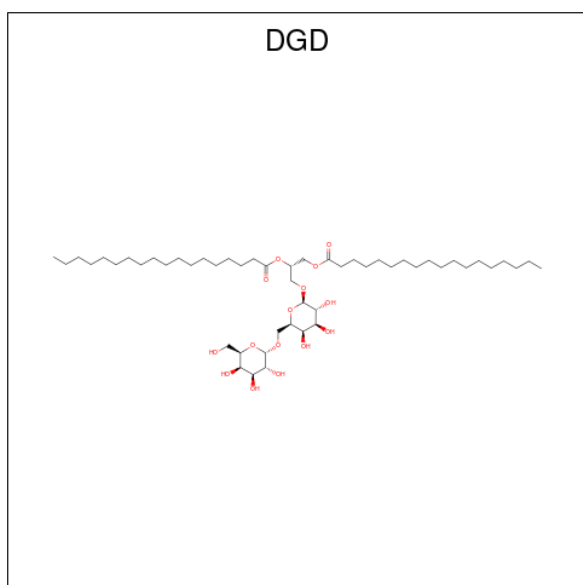
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Z	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	f	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

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



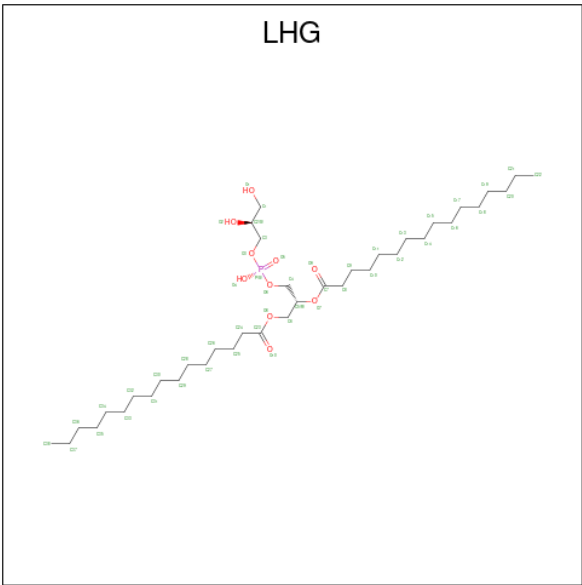
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0

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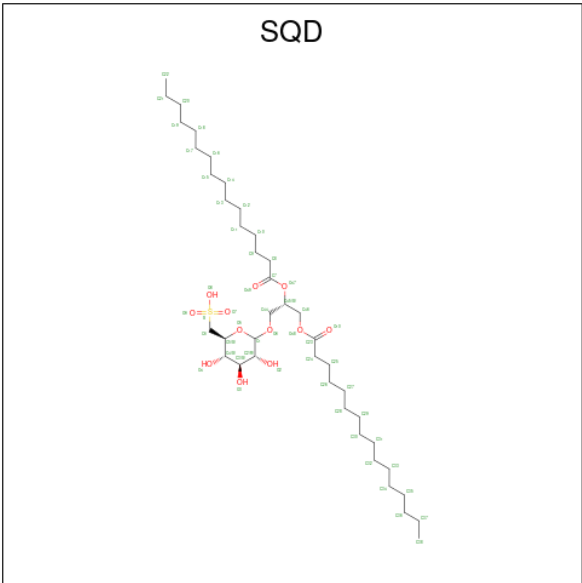
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			58	43	15		
28	B	1	Total	C	O	0	0
			52	37	15		
28	C	1	Total	C	O	0	0
			53	38	15		
28	C	1	Total	C	O	0	0
			62	47	15		
28	C	1	Total	C	O	0	0
			66	51	15		
28	D	1	Total	C	O	0	0
			63	48	15		
28	a	1	Total	C	O	0	0
			56	41	15		
28	b	1	Total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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



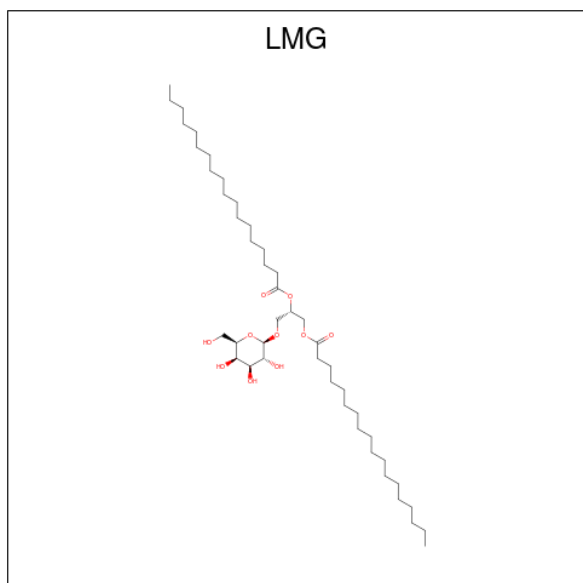
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			51	41	10		

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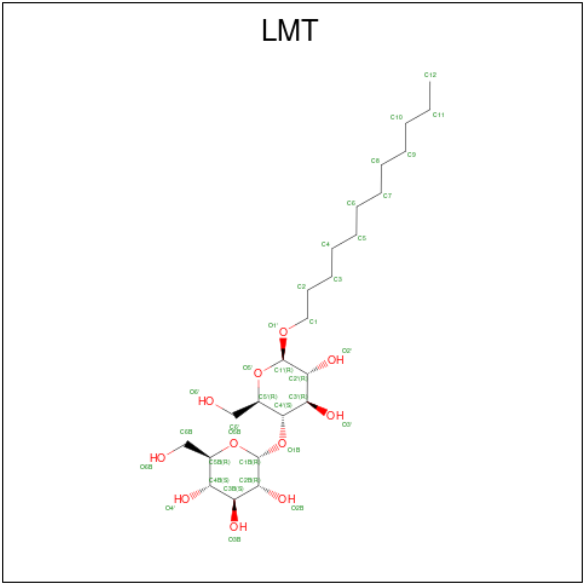
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			42	32	10		
31	B	1	Total	C	O	0	0
			49	39	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	C	1	Total	C	O	0	0
			45	35	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	D	1	Total	C	O	0	0
			49	39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

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



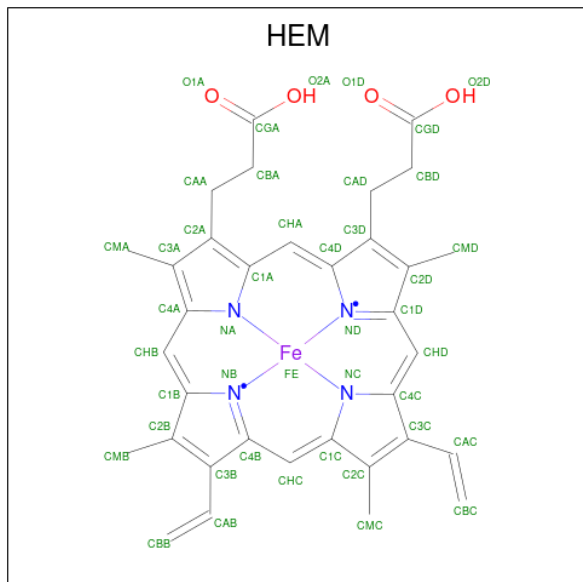
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	D	1	Total	C	O	0	0
			31	20	11		
33	I	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	T	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	b	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	i	1	Total	C	O	0	0
			35	24	11		
33	m	1	Total	C	O	0	0
			35	24	11		
33	x	1	Total	C	O	0	0
			31	20	11		

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



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

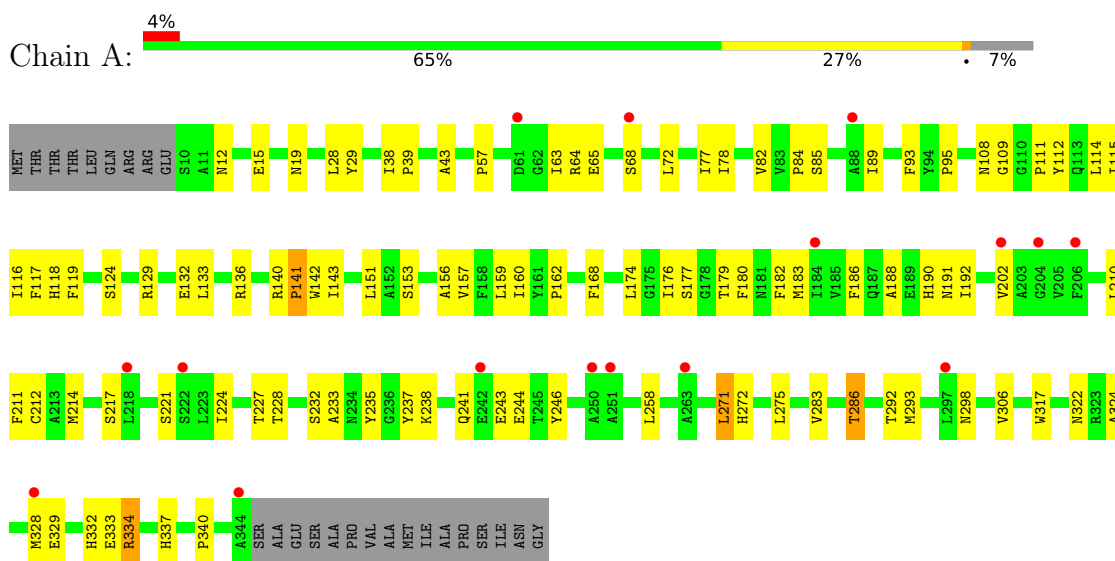
- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

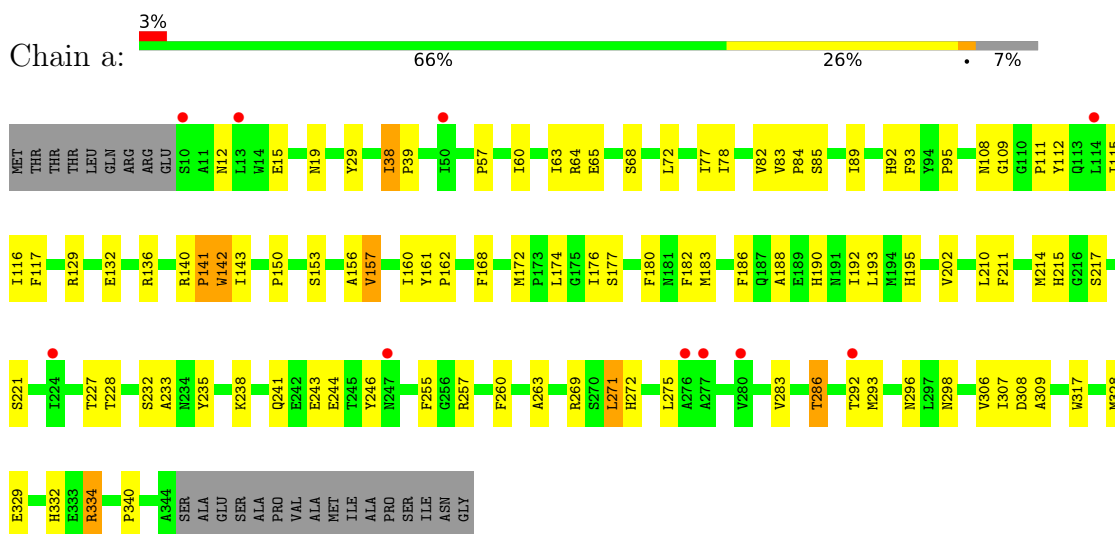
3 Residue-property plots [i](#)

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

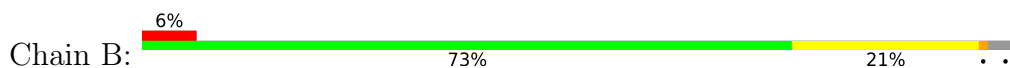
- Molecule 1: Photosystem Q(B) protein 1

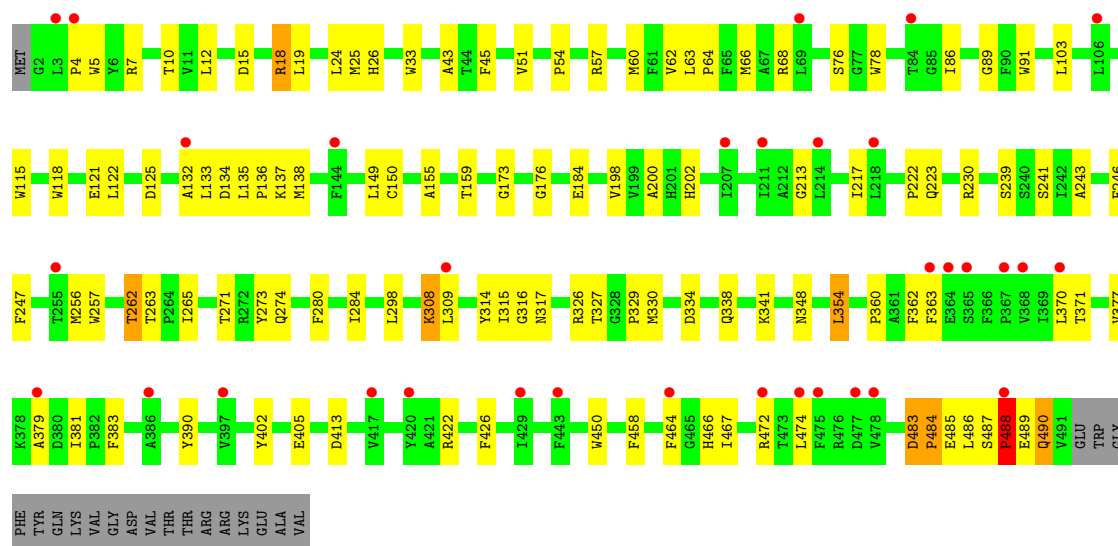


- Molecule 1: Photosystem Q(B) protein 1

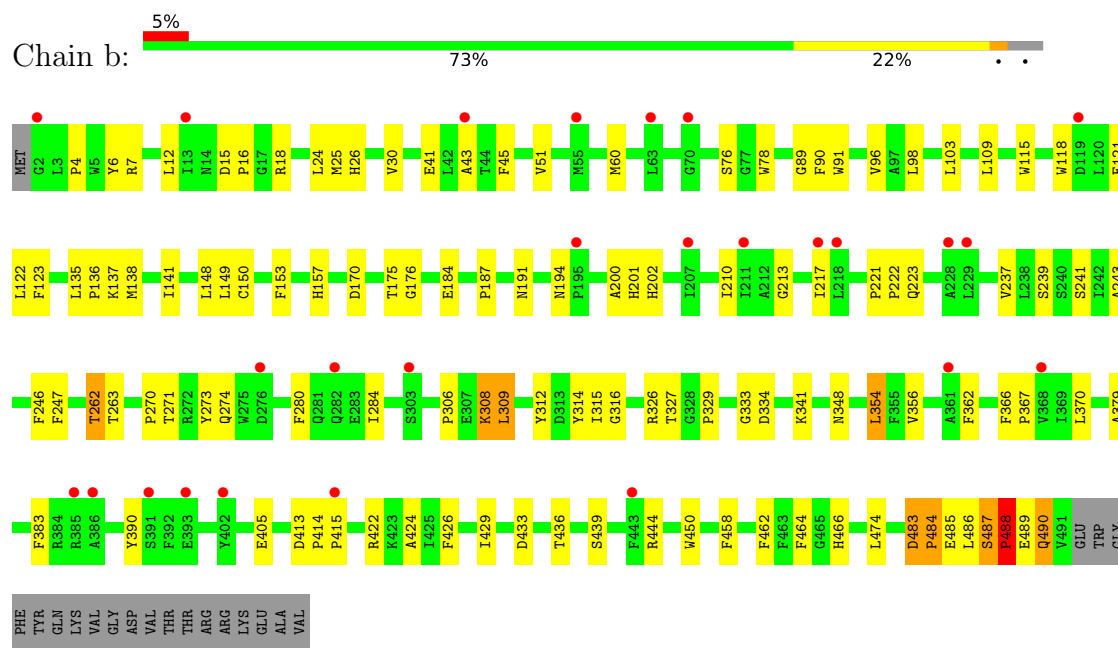


- Molecule 2: Photosystem II core light harvesting protein

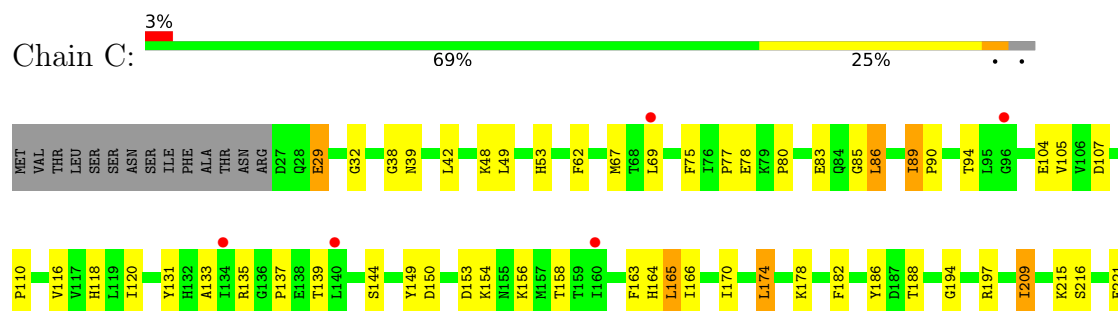


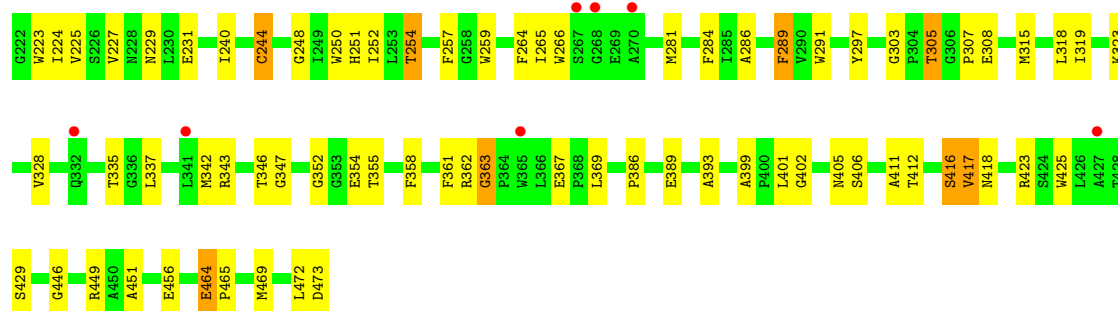


• Molecule 2: Photosystem II core light harvesting protein

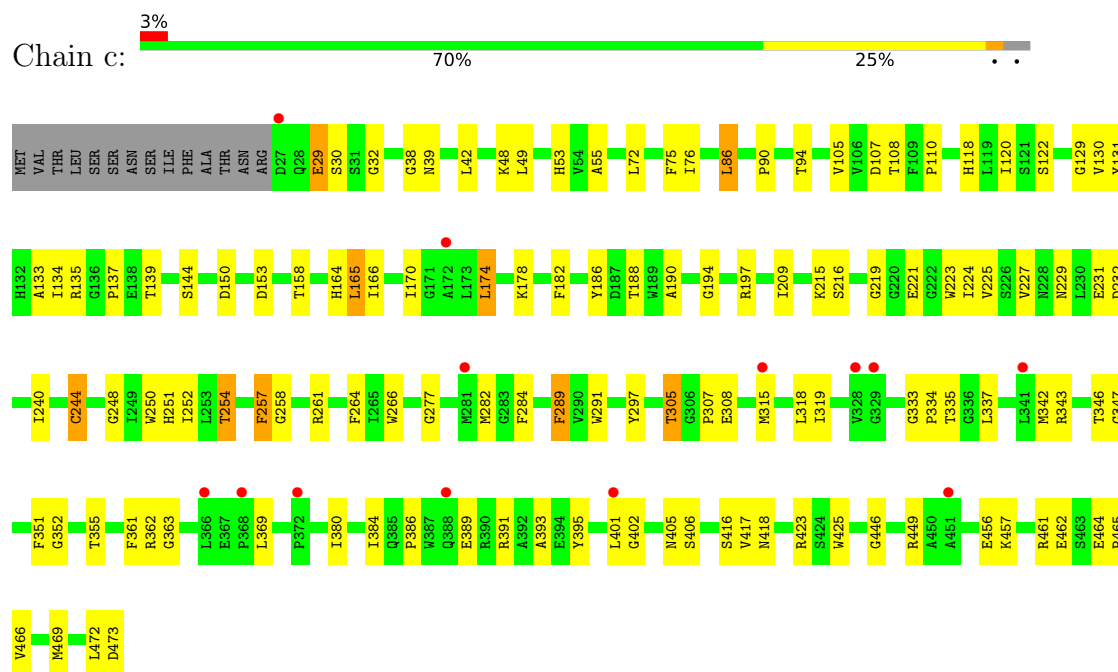


• Molecule 3: Photosystem II CP43 protein

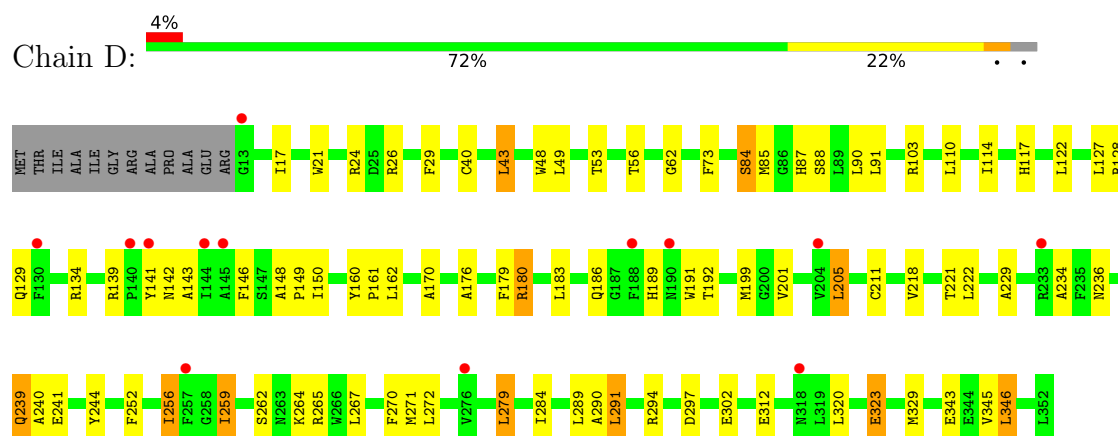




• Molecule 3: Photosystem II CP43 protein

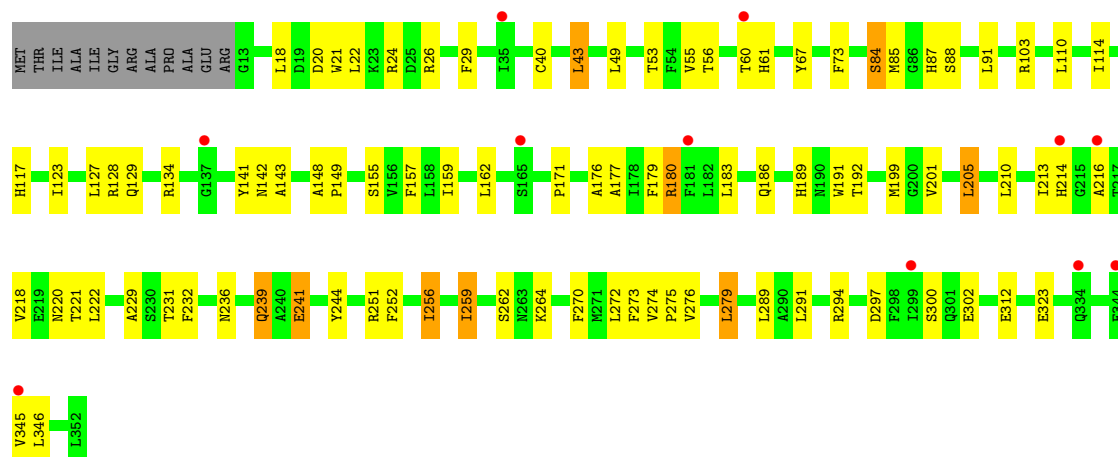


• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein





• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha



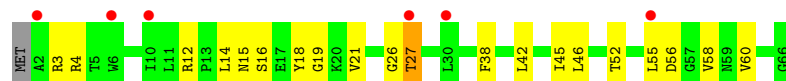
• Molecule 6: Cytochrome b559 subunit beta



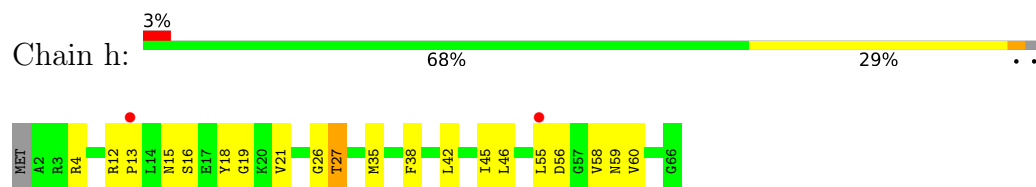
• Molecule 6: Cytochrome b559 subunit beta



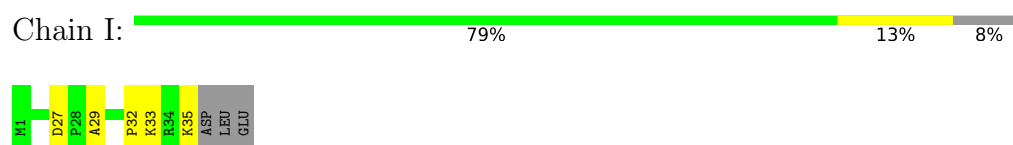
• Molecule 7: Photosystem II reaction center protein H



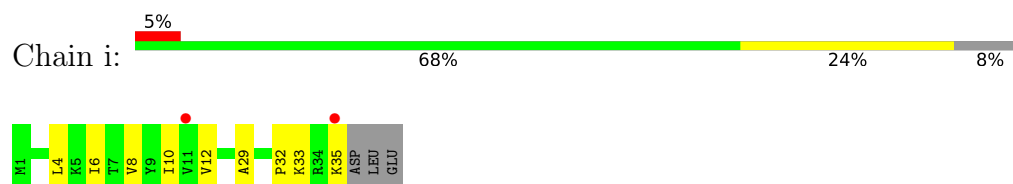
- Molecule 7: Photosystem II reaction center protein H



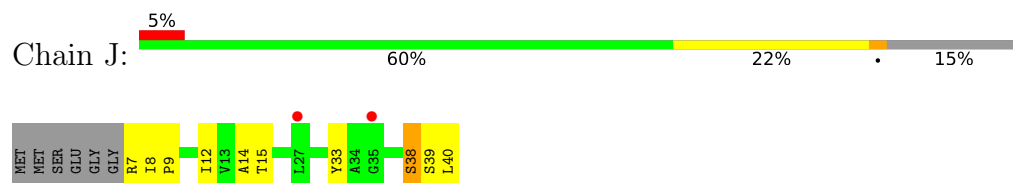
- Molecule 8: Photosystem II reaction center protein I



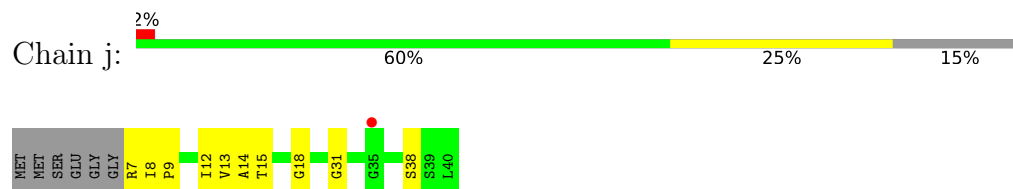
- Molecule 8: Photosystem II reaction center protein I



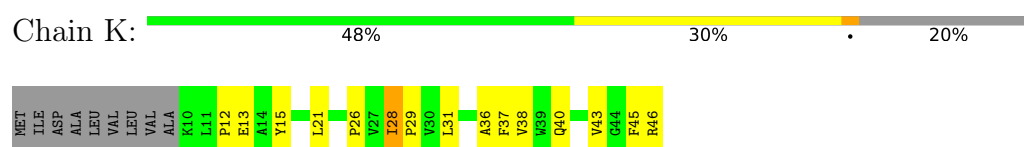
- Molecule 9: Photosystem II reaction center protein J



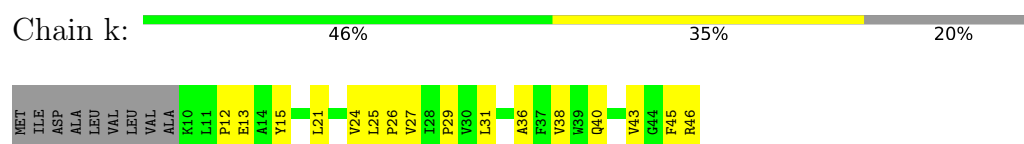
- Molecule 9: Photosystem II reaction center protein J



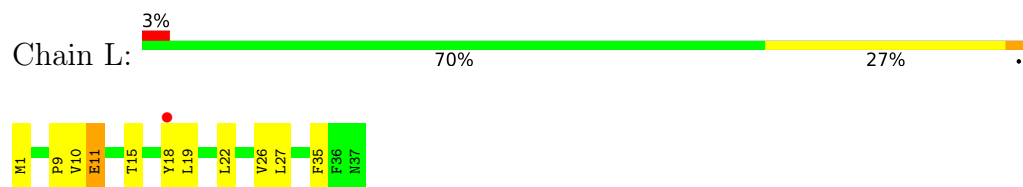
- Molecule 10: Photosystem II reaction center protein K



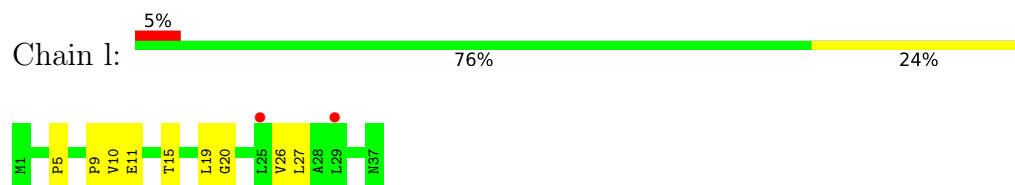
- Molecule 10: Photosystem II reaction center protein K



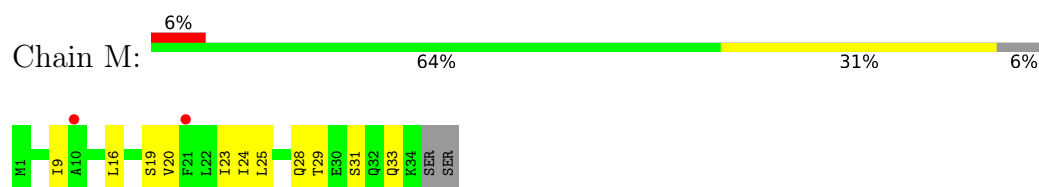
- Molecule 11: Photosystem II reaction center protein L



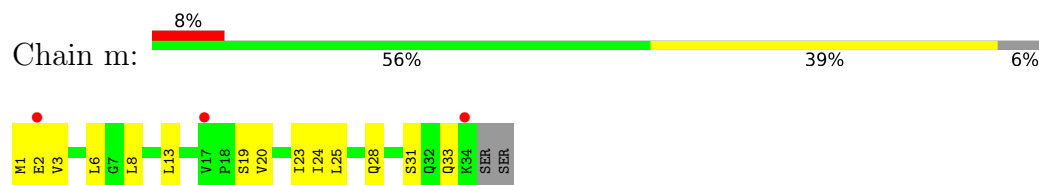
- Molecule 11: Photosystem II reaction center protein L



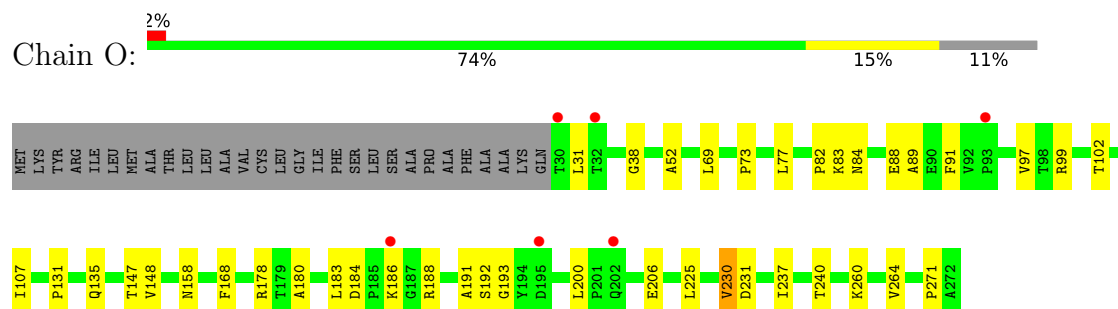
- Molecule 12: Photosystem II reaction center protein M



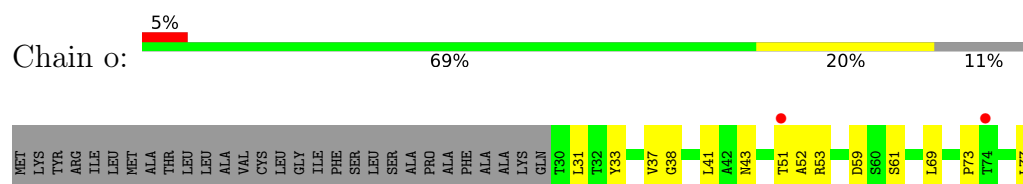
- Molecule 12: Photosystem II reaction center protein M

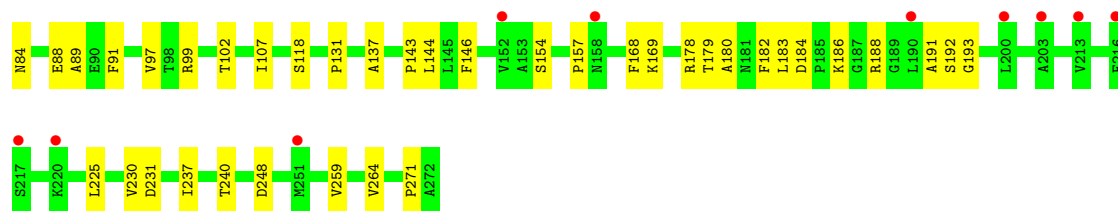


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

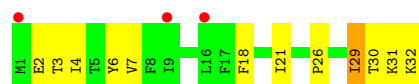




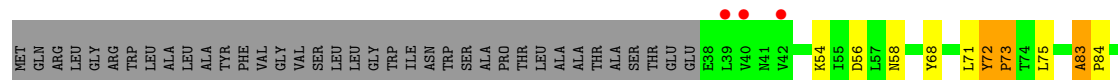
• Molecule 14: Photosystem II reaction center protein T



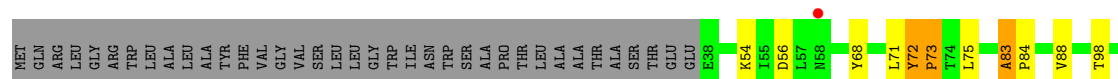
• Molecule 14: Photosystem II reaction center protein T



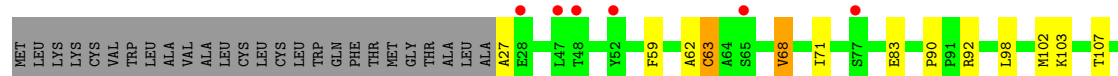
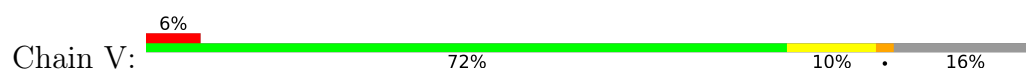
• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

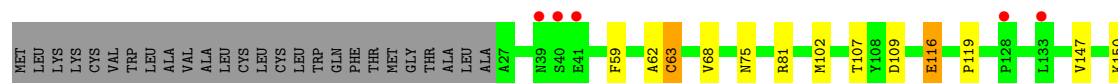
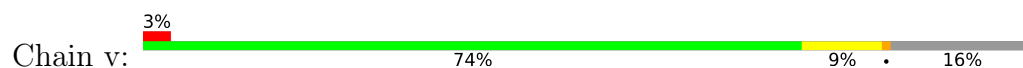


• Molecule 16: Cytochrome c-550

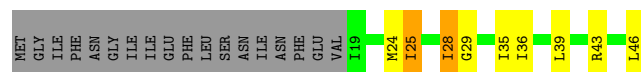




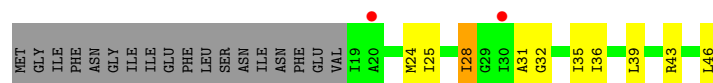
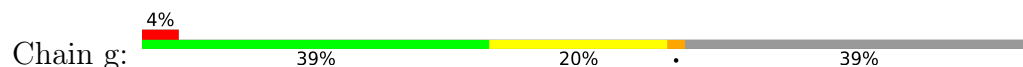
• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein ycf12



• Molecule 17: Photosystem II reaction center protein ycf12



• Molecule 18: Photosystem II reaction center X protein



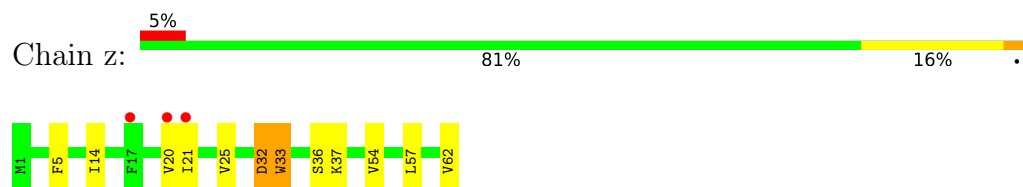
• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.86Å 227.51Å 307.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.94 – 5.70 82.94 – 5.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.94-5.70) 98.3 (82.94-5.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.277 , 0.314 0.281 , 0.318	Depositor DCC
R_{free} test set	1325 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	3.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, CL, PL9, CLA, BCT, FE2, LMT, DGD, HEM, BCR, CA, LMG, LHG, PHO, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/2712	0.85	0/3700
1	a	0.38	0/2712	0.86	5/3700 (0.1%)
2	B	0.39	0/3986	0.86	8/5433 (0.1%)
2	b	0.38	0/3986	0.87	10/5433 (0.2%)
3	C	0.38	0/3556	0.84	5/4842 (0.1%)
3	c	0.39	0/3556	0.85	8/4842 (0.2%)
4	D	0.36	0/2801	0.82	0/3818
4	d	0.37	0/2801	0.83	1/3818 (0.0%)
5	E	0.36	0/685	0.88	0/933
5	e	0.36	0/685	0.87	0/933
6	F	0.39	0/291	0.83	0/397
6	f	0.41	0/291	0.82	0/397
7	H	0.37	0/520	0.77	1/709 (0.1%)
7	h	0.37	0/520	0.78	0/709
8	I	0.36	0/293	0.82	0/395
8	i	0.37	0/293	0.87	0/395
9	J	0.35	0/255	0.89	0/346
9	j	0.42	0/255	0.94	0/346
10	K	0.43	0/303	0.92	1/416 (0.2%)
10	k	0.46	0/303	0.93	0/416
11	L	0.38	0/311	0.75	0/422
11	l	0.33	0/311	0.78	0/422
12	M	0.53	0/270	1.07	0/367
12	m	0.53	0/270	1.08	0/367
13	O	0.33	0/1876	0.74	2/2548 (0.1%)
13	o	0.36	0/1876	0.77	0/2548
14	T	0.38	0/284	0.84	0/381
14	t	0.40	0/284	0.81	0/381
15	U	0.37	0/785	0.84	0/1064
15	u	0.43	0/785	0.91	0/1064
16	V	0.39	0/1081	0.86	2/1468 (0.1%)
16	v	0.38	0/1081	0.82	2/1468 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.39	0/202	0.88	0/272
17	y	0.40	0/202	0.82	0/272
18	X	0.47	0/273	0.85	0/370
18	x	0.47	0/273	0.89	0/370
19	Z	0.36	0/490	0.86	0/669
19	z	0.35	0/490	0.86	0/669
All	All	0.38	0/41948	0.84	45/57100 (0.1%)

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.80	133.34	119.84
2	b	483	ASP	C-N-CA	10.80	133.34	119.84
2	B	483	ASP	CA-C-N	10.41	132.85	119.84
2	B	483	ASP	C-N-CA	10.41	132.85	119.84
2	b	194	ASN	CA-C-N	6.55	126.32	119.05

There are no chirality outliers.

There are no planarity outliers.

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	A	2627	0	2524	87	0
1	a	2627	0	2524	84	0
2	B	3850	0	3718	82	0
2	b	3850	0	3718	89	0
3	C	3444	0	3365	95	0
3	c	3444	0	3365	90	0
4	D	2706	0	2608	71	0
4	d	2706	0	2608	78	0
5	E	666	0	651	15	0
5	e	666	0	651	19	0
6	F	282	0	291	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	10	0
7	H	507	0	521	16	0
7	h	507	0	521	16	0
8	I	286	0	308	3	0
8	i	286	0	308	4	0
9	J	249	0	262	7	0
9	j	249	0	262	7	0
10	K	293	0	305	11	0
10	k	293	0	305	14	0
11	L	304	0	316	11	0
11	l	304	0	316	8	0
12	M	267	0	289	13	0
12	m	267	0	289	16	0
13	O	1845	0	1801	24	0
13	o	1845	0	1801	35	0
14	T	275	0	288	10	0
14	t	275	0	288	10	0
15	U	774	0	773	11	0
15	u	774	0	773	10	0
16	V	1060	0	1068	13	0
16	v	1060	0	1068	10	0
17	g	201	0	226	8	0
17	y	201	0	226	5	0
18	X	270	0	299	10	0
18	x	270	0	299	9	0
19	Z	479	0	516	15	0
19	z	479	0	516	9	0
20	G	140	0	32	1	0
20	Y	140	0	32	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	1	0	0
22	d	4	0	1	0	0
23	A	260	0	288	29	0
23	B	1040	0	1152	73	0
23	C	845	0	936	36	0
23	D	130	0	144	11	0
23	a	260	0	288	32	0
23	b	1040	0	1152	73	0
23	c	845	0	936	38	0
23	d	130	0	144	12	0
24	A	64	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	64	0	74	7	0
24	a	128	0	148	14	0
25	A	45	0	61	2	0
25	D	55	0	80	5	0
25	J	35	0	45	2	0
25	a	45	0	61	5	0
25	d	55	0	80	7	0
25	j	35	0	45	0	0
26	A	5	0	0	0	0
26	a	5	0	0	0	0
27	A	40	0	56	5	0
27	B	160	0	224	24	0
27	C	80	0	112	16	0
27	D	40	0	56	3	0
27	H	40	0	56	2	0
27	J	40	0	56	5	0
27	K	40	0	56	9	0
27	T	80	0	112	14	0
27	Z	40	0	56	4	0
27	a	40	0	56	2	0
27	b	80	0	112	12	0
27	c	120	0	168	14	0
27	f	40	0	56	3	0
27	j	40	0	56	4	0
27	k	40	0	56	7	0
27	x	40	0	56	4	0
28	A	56	0	70	1	0
28	B	110	0	136	5	0
28	C	181	0	245	14	0
28	D	63	0	87	3	0
28	a	56	0	70	0	0
28	b	110	0	136	8	0
28	c	181	0	245	11	0
28	d	63	0	87	0	0
29	A	76	0	95	6	0
29	a	76	0	95	7	0
30	A	105	0	147	12	0
30	B	47	0	61	1	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	6	0
30	b	47	0	61	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	43	0	50	4	0
30	f	45	0	54	2	0
31	A	93	0	124	6	0
31	B	49	0	67	4	0
31	C	93	0	124	4	0
31	D	143	0	194	10	0
31	E	44	0	57	1	0
31	I	43	0	55	3	0
31	M	84	0	107	6	0
31	a	93	0	124	7	0
31	b	98	0	134	7	0
31	c	45	0	59	2	0
31	d	94	0	126	9	0
31	e	44	0	58	0	0
31	i	43	0	55	2	0
31	k	48	0	66	2	0
32	A	1	0	0	0	0
32	d	1	0	0	0	0
33	B	140	0	184	4	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	0	0
33	T	35	0	46	2	0
33	b	105	0	138	6	0
33	i	35	0	46	1	0
33	m	35	0	46	0	0
33	x	31	0	35	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50232	0	51358	1198	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 12.

The worst 5 of 1198 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)
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.50	0.91
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.51	0.89
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.54	0.89
3:C:362:ARG:H	28:C:516:DGD:HE4	1.40	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.57	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	311 (93%)	18 (5%)	4 (1%)	10	43
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	10	43
2	B	488/510 (96%)	448 (92%)	35 (7%)	5 (1%)	12	48
2	b	488/510 (96%)	448 (92%)	36 (7%)	4 (1%)	16	53
3	C	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	9	41
3	c	445/461 (96%)	405 (91%)	33 (7%)	7 (2%)	7	37
4	D	338/352 (96%)	315 (93%)	20 (6%)	3 (1%)	14	50
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	21	59
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	41
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	41
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
8	I	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	3	22
8	i	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	21
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	21
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1	13
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1	13
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	207 (86%)	30 (12%)	4 (2%)	7	35
13	o	241/272 (89%)	209 (87%)	29 (12%)	3 (1%)	10	43
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	20
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	20
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	3	21
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	3	21
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	19
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1	13
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1	13
19	Z	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	3	20
19	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
All	All	5138/5650 (91%)	4681 (91%)	382 (7%)	75 (2%)	8	39

5 of 75 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/291 (93%)	262 (97%)	9 (3%)	33	54
1	a	271/291 (93%)	262 (97%)	9 (3%)	33	54
2	B	390/407 (96%)	377 (97%)	13 (3%)	33	54
2	b	390/407 (96%)	379 (97%)	11 (3%)	38	59
3	C	347/362 (96%)	334 (96%)	13 (4%)	30	51
3	c	347/362 (96%)	335 (96%)	12 (4%)	32	53
4	D	275/283 (97%)	261 (95%)	14 (5%)	21	42
4	d	275/283 (97%)	260 (94%)	15 (6%)	19	41
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	36
5	e	72/73 (99%)	67 (93%)	5 (7%)	14	36
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	50 (94%)	3 (6%)	18	40
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	40
8	I	32/35 (91%)	31 (97%)	1 (3%)	35	56
8	i	32/35 (91%)	31 (97%)	1 (3%)	35	56
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	48
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	48
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	57
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	57
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	199 (98%)	3 (2%)	57	71
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	29/29 (100%)	28 (97%)	1 (3%)	32	54
14	t	29/29 (100%)	28 (97%)	1 (3%)	32	54
15	U	84/112 (75%)	81 (96%)	3 (4%)	31	52
15	u	84/112 (75%)	80 (95%)	4 (5%)	23	44
16	V	116/138 (84%)	113 (97%)	3 (3%)	40	61
16	v	116/138 (84%)	113 (97%)	3 (3%)	40	61
17	g	20/37 (54%)	16 (80%)	4 (20%)	1	7
17	y	20/37 (54%)	16 (80%)	4 (20%)	1	7
18	X	30/34 (88%)	27 (90%)	3 (10%)	7	24
18	x	30/34 (88%)	27 (90%)	3 (10%)	7	24
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	39
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	39
All	All	4244/4616 (92%)	4086 (96%)	158 (4%)	30	51

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	91	LEU
15	u	114	VAL
4	d	241	GLU
5	e	82	GLN
17	g	36	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
4	d	98	GLN
2	b	343	HIS
3	c	56	HIS
4	d	142	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	CLA	B	615	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
33	LMT	b	626	-	36,36,36	0.44	0	47,47,47	0.68	1 (2%)
23	CLA	b	615	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	5 (6%)
27	BCR	c	516	-	41,41,41	0.69	0	56,56,56	1.95	15 (26%)
24	PHO	D	402	-	58,69,69	2.21	11 (18%)	55,99,99	1.49	5 (9%)
28	DGD	c	519	-	67,67,67	1.16	7 (10%)	81,81,81	1.43	10 (12%)
34	HEM	F	101	6,5	50,50,50	1.85	9 (18%)	67,82,82	1.33	7 (10%)
25	PL9	A	408	-	45,45,55	1.30	7 (15%)	56,57,69	1.57	13 (23%)
28	DGD	d	408	-	64,64,67	1.14	7 (10%)	78,78,81	1.40	9 (11%)
27	BCR	J	102	-	41,41,41	0.72	0	56,56,56	3.43	24 (42%)
33	LMT	D	411	-	32,32,36	0.49	1 (3%)	43,43,47	0.72	1 (2%)
31	LMG	c	520	-	45,45,55	1.22	7 (15%)	53,53,63	1.40	8 (15%)
31	LMG	C	520	-	45,45,55	1.21	7 (15%)	53,53,63	1.44	8 (15%)
23	CLA	B	606	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
33	LMT	b	625	-	36,36,36	0.41	0	47,47,47	0.76	1 (2%)
30	SQD	A	413	-	49,51,54	0.99	4 (8%)	59,62,65	1.48	10 (16%)
27	BCR	a	412	-	41,41,41	0.71	0	56,56,56	1.91	15 (26%)
27	BCR	b	621	-	41,41,41	0.72	0	56,56,56	2.19	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	403	-	69,73,73	1.20	6 (8%)	82,113,113	1.26	5 (6%)
31	LMG	d	406	-	48,48,55	1.17	7 (14%)	56,56,63	1.38	7 (12%)
33	LMT	m	101	-	36,36,36	0.39	0	47,47,47	0.72	1 (2%)
27	BCR	f	102	-	41,41,41	0.69	0	56,56,56	2.19	17 (30%)
34	HEM	V	201	16	50,50,50	1.83	8 (16%)	67,82,82	1.14	2 (2%)
23	CLA	C	509	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
28	DGD	D	410	-	64,64,67	1.15	7 (10%)	78,78,81	1.38	8 (10%)
23	CLA	C	501	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	5 (6%)
33	LMT	i	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.65	0
31	LMG	M	101	-	42,42,55	1.33	7 (16%)	50,50,63	1.50	8 (16%)
25	PL9	a	410	-	45,45,55	1.25	7 (15%)	56,57,69	1.66	13 (23%)
27	BCR	k	102	-	41,41,41	0.71	0	56,56,56	1.90	13 (23%)
23	CLA	B	601	-	69,73,73	1.23	8 (11%)	82,113,113	1.26	6 (7%)
23	CLA	B	603	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
23	CLA	B	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	5 (6%)
25	PL9	d	404	-	55,55,55	1.28	8 (14%)	68,69,69	1.68	15 (22%)
29	LHG	A	415	-	36,36,48	1.09	2 (5%)	39,42,54	1.08	2 (5%)
27	BCR	B	620	-	41,41,41	0.72	1 (2%)	56,56,56	2.14	17 (30%)
23	CLA	c	501	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	6 (7%)
23	CLA	B	616	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	4 (4%)
23	CLA	c	510	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	4 (4%)
23	CLA	b	606	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
31	LMG	e	101	-	44,44,55	1.23	7 (15%)	52,52,63	1.30	8 (15%)
23	CLA	c	512	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	5 (6%)
23	CLA	b	607	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
28	DGD	B	621	-	59,59,67	1.29	9 (15%)	73,73,81	1.14	6 (8%)
23	CLA	D	403	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
30	SQD	a	401	-	52,54,54	0.98	4 (7%)	62,65,65	1.56	10 (16%)
23	CLA	a	406	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	7 (8%)
23	CLA	b	618	-	69,73,73	1.18	5 (7%)	82,113,113	1.31	6 (7%)
23	CLA	C	507	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	6 (7%)
27	BCR	K	102	-	41,41,41	0.74	0	56,56,56	1.86	11 (19%)
27	BCR	H	101	-	41,41,41	0.72	0	56,56,56	1.73	15 (26%)
27	BCR	A	410	-	41,41,41	0.75	1 (2%)	56,56,56	1.99	14 (25%)
23	CLA	C	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	D	409	-	41,43,54	1.12	4 (9%)	51,54,65	1.96	10 (19%)
22	BCT	A	402	21	3,3,3	0.66	0	2,3,3	0.04	0
25	PL9	D	404	-	55,55,55	1.25	8 (14%)	68,69,69	1.70	19 (27%)
23	CLA	B	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	7 (8%)
25	PL9	j	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.61	8 (18%)
28	DGD	c	518	-	63,63,67	1.23	9 (14%)	77,77,81	1.25	7 (9%)
23	CLA	B	612	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
28	DGD	C	518	-	67,67,67	1.16	7 (10%)	81,81,81	1.45	9 (11%)
23	CLA	b	619	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	6 (7%)
24	PHO	a	408	-	58,69,69	2.17	9 (15%)	55,99,99	1.34	5 (9%)
27	BCR	C	514	-	41,41,41	0.77	0	56,56,56	2.42	20 (35%)
23	CLA	a	409	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
28	DGD	b	602	-	53,53,67	1.26	6 (11%)	67,67,81	1.38	9 (13%)
23	CLA	b	605	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	4 (4%)
31	LMG	k	103	-	48,48,55	1.16	6 (12%)	56,56,63	1.29	6 (10%)
24	PHO	a	407	-	58,69,69	2.11	11 (18%)	55,99,99	1.43	7 (12%)
23	CLA	B	608	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
33	LMT	M	103	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
23	CLA	B	610	-	69,73,73	1.20	7 (10%)	82,113,113	1.33	6 (7%)
23	CLA	b	616	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
22	BCT	d	401	21	3,3,3	0.67	0	2,3,3	0.17	0
23	CLA	b	610	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
31	LMG	M	102	-	42,42,55	1.30	7 (16%)	50,50,63	1.48	8 (16%)
23	CLA	B	602	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
29	LHG	a	417	-	36,36,48	1.08	2 (5%)	39,42,54	1.08	2 (5%)
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.69	1 (2%)
31	LMG	C	519	-	48,48,55	1.15	6 (12%)	56,56,63	1.35	7 (12%)
23	CLA	c	508	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
27	BCR	j	102	-	41,41,41	0.74	0	56,56,56	3.44	23 (41%)
23	CLA	c	509	-	69,73,73	1.19	5 (7%)	82,113,113	1.31	5 (6%)
27	BCR	c	514	-	41,41,41	0.71	0	56,56,56	2.46	19 (33%)
28	DGD	A	411	-	57,57,67	1.25	8 (14%)	71,71,81	1.60	12 (16%)
27	BCR	Z	101	-	41,41,41	0.64	0	56,56,56	1.89	16 (28%)
23	CLA	c	513	-	69,73,73	1.18	6 (8%)	82,113,113	1.34	6 (7%)
27	BCR	T	102	-	41,41,41	0.76	0	56,56,56	1.93	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	604	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	7 (8%)
28	DGD	b	622	-	59,59,67	1.26	9 (15%)	73,73,81	1.16	6 (8%)
31	LMG	d	405	-	46,46,55	1.20	7 (15%)	54,54,63	1.36	6 (11%)
33	LMT	B	624	-	36,36,36	0.44	0	47,47,47	0.71	1 (2%)
23	CLA	C	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.27	4 (4%)
27	BCR	B	617	-	41,41,41	0.74	0	56,56,56	1.95	12 (21%)
23	CLA	C	506	-	69,73,73	1.20	5 (7%)	82,113,113	1.36	6 (7%)
23	CLA	b	613	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	5 (6%)
23	CLA	c	503	-	69,73,73	1.21	6 (8%)	82,113,113	1.25	5 (6%)
23	CLA	A	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	5 (6%)
31	LMG	i	101	-	43,43,55	1.29	7 (16%)	51,51,63	1.31	7 (13%)
23	CLA	c	502	-	69,73,73	1.19	7 (10%)	82,113,113	1.33	5 (6%)
23	CLA	a	404	-	69,73,73	1.20	7 (10%)	82,113,113	1.32	6 (7%)
28	DGD	a	413	-	57,57,67	1.23	7 (12%)	71,71,81	1.57	12 (16%)
23	CLA	B	605	-	69,73,73	1.15	7 (10%)	82,113,113	1.28	5 (6%)
29	LHG	A	412	-	38,38,48	1.07	2 (5%)	41,44,54	0.99	2 (4%)
23	CLA	C	511	3	69,73,73	1.18	7 (10%)	82,113,113	1.36	6 (7%)
33	LMT	b	603	-	36,36,36	0.40	0	47,47,47	0.62	0
30	SQD	a	415	-	49,51,54	1.01	3 (6%)	59,62,65	1.51	10 (16%)
23	CLA	B	609	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
23	CLA	b	604	-	69,73,73	1.22	7 (10%)	82,113,113	1.29	6 (7%)
31	LMG	b	624	-	49,49,55	1.18	7 (14%)	57,57,63	1.39	8 (14%)
27	BCR	C	515	-	41,41,41	0.69	0	56,56,56	1.99	15 (26%)
23	CLA	A	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	6 (7%)
30	SQD	B	625	-	45,47,54	1.04	4 (8%)	55,58,65	1.50	8 (14%)
25	PL9	J	101	-	35,35,55	1.21	5 (14%)	44,45,69	1.59	7 (15%)
23	CLA	A	403	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	5 (6%)
23	CLA	b	617	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	4 (4%)
23	CLA	C	512	-	69,73,73	1.19	7 (10%)	82,113,113	1.32	5 (6%)
30	SQD	A	417	-	52,54,54	1.02	4 (7%)	62,65,65	1.55	10 (16%)
28	DGD	C	517	-	63,63,67	1.23	10 (15%)	77,77,81	1.22	7 (9%)
27	BCR	c	515	-	41,41,41	0.64	0	56,56,56	1.81	15 (26%)
27	BCR	b	620	-	41,41,41	0.66	0	56,56,56	1.95	14 (25%)
24	PHO	A	406	-	58,69,69	2.21	9 (15%)	55,99,99	1.66	8 (14%)
23	CLA	c	506	-	69,73,73	1.21	7 (10%)	82,113,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	402	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
33	LMT	T	101	-	36,36,36	0.41	0	47,47,47	0.86	1 (2%)
33	LMT	B	623	-	36,36,36	0.41	0	47,47,47	0.74	1 (2%)
27	BCR	B	619	-	41,41,41	0.65	0	56,56,56	1.89	15 (26%)
31	LMG	a	402	-	42,42,55	1.25	6 (14%)	50,50,63	1.48	8 (16%)
23	CLA	B	614	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	4 (4%)
30	SQD	d	407	-	41,43,54	1.14	3 (7%)	51,54,65	1.97	9 (17%)
23	CLA	a	405	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	7 (8%)
27	BCR	D	405	-	41,41,41	0.67	0	56,56,56	2.24	18 (32%)
23	CLA	C	513	-	69,73,73	1.19	6 (8%)	82,113,113	1.31	6 (7%)
23	CLA	C	502	-	69,73,73	1.18	8 (11%)	82,113,113	1.32	5 (6%)
23	CLA	C	503	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	6 (7%)
30	SQD	b	601	-	45,47,54	1.04	3 (6%)	55,58,65	1.53	9 (16%)
31	LMG	E	101	-	44,44,55	1.23	7 (15%)	52,52,63	1.36	8 (15%)
31	LMG	a	416	-	51,51,55	1.15	6 (11%)	59,59,63	1.41	5 (8%)
23	CLA	b	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	4 (4%)
31	LMG	b	623	-	49,49,55	1.22	7 (14%)	57,57,63	1.35	7 (12%)
33	LMT	B	628	-	36,36,36	0.47	0	47,47,47	0.64	0
27	BCR	B	618	-	41,41,41	0.73	0	56,56,56	2.29	14 (25%)
23	CLA	b	614	-	69,73,73	1.21	8 (11%)	82,113,113	1.29	6 (7%)
28	DGD	C	516	-	54,54,67	1.26	7 (12%)	68,68,81	1.28	9 (13%)
27	BCR	T	103	-	41,41,41	0.71	0	56,56,56	2.29	17 (30%)
23	CLA	c	504	-	69,73,73	1.21	7 (10%)	82,113,113	1.38	6 (7%)
23	CLA	c	505	-	69,73,73	1.18	6 (8%)	82,113,113	1.40	7 (8%)
23	CLA	D	401	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
31	LMG	D	407	-	49,49,55	1.20	7 (14%)	57,57,63	1.26	8 (14%)
34	HEM	v	201	16	50,50,50	2.02	11 (22%)	67,82,82	1.37	6 (8%)
30	SQD	F	102	-	43,45,54	1.05	2 (4%)	53,56,65	1.62	9 (16%)
27	BCR	x	101	-	41,41,41	0.71	0	56,56,56	1.73	17 (30%)
23	CLA	b	612	-	69,73,73	1.20	6 (8%)	82,113,113	1.21	5 (6%)
23	CLA	b	609	-	69,73,73	1.20	6 (8%)	82,113,113	1.29	5 (6%)
23	CLA	c	511	-	69,73,73	1.22	6 (8%)	82,113,113	1.32	4 (4%)
31	LMG	B	622	-	49,49,55	1.20	7 (14%)	57,57,63	1.38	8 (14%)
31	LMG	D	406	-	46,46,55	1.18	6 (13%)	54,54,63	1.36	6 (11%)
23	CLA	B	607	-	69,73,73	1.16	6 (8%)	82,113,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	507	-	69,73,73	1.18	6 (8%)	82,113,113	1.30	6 (7%)
34	HEM	f	101	6,5	50,50,50	1.85	10 (20%)	67,82,82	1.35	4 (5%)
31	LMG	A	418	-	42,42,55	1.25	6 (14%)	50,50,63	1.53	11 (22%)
31	LMG	I	101	-	43,43,55	1.28	8 (18%)	51,51,63	1.34	8 (15%)
29	LHG	a	414	-	38,38,48	1.09	2 (5%)	41,44,54	0.97	3 (7%)
28	DGD	c	517	-	54,54,67	1.28	7 (12%)	68,68,81	1.28	8 (11%)
28	DGD	B	626	-	53,53,67	1.26	7 (13%)	67,67,81	1.39	9 (13%)
31	LMG	D	408	-	48,48,55	1.22	7 (14%)	56,56,63	1.38	7 (12%)
23	CLA	A	407	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
30	SQD	f	103	-	43,45,54	1.04	2 (4%)	53,56,65	1.59	11 (20%)
33	LMT	x	102	-	32,32,36	0.49	1 (3%)	43,43,47	0.67	1 (2%)
23	CLA	b	611	-	69,73,73	1.20	7 (10%)	82,113,113	1.35	9 (10%)
31	LMG	A	414	-	51,51,55	1.18	6 (11%)	59,59,63	1.35	5 (8%)
33	LMT	B	627	-	36,36,36	0.45	0	47,47,47	0.80	1 (2%)
23	CLA	C	504	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
23	CLA	C	508	-	69,73,73	1.20	8 (11%)	82,113,113	1.28	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	615	-	1/1/15/20	10/39/115/115	-
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
23	CLA	b	615	-	1/1/15/20	9/39/115/115	-
27	BCR	c	516	-	-	8/29/63/63	0/2/2/2
24	PHO	D	402	-	-	8/37/103/103	0/5/6/6
28	DGD	c	519	-	-	21/55/95/95	0/2/2/2
34	HEM	F	101	6,5	-	2/14/54/54	-
25	PL9	A	408	-	-	22/41/61/73	0/1/1/1
28	DGD	d	408	-	-	29/52/92/95	0/2/2/2
27	BCR	J	102	-	-	2/29/63/63	0/2/2/2
33	LMT	D	411	-	-	0/17/57/61	0/2/2/2
31	LMG	c	520	-	-	21/40/60/70	0/1/1/1
31	LMG	C	520	-	-	19/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	606	-	1/1/15/20	13/39/115/115	-
33	LMT	b	625	-	-	2/21/61/61	0/2/2/2
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
27	BCR	a	412	-	-	3/29/63/63	0/2/2/2
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	10/39/115/115	-
31	LMG	d	406	-	-	20/43/63/70	0/1/1/1
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
27	BCR	f	102	-	-	6/29/63/63	0/2/2/2
34	HEM	V	201	16	-	4/14/54/54	-
23	CLA	C	509	-	1/1/15/20	18/39/115/115	-
28	DGD	D	410	-	-	31/52/92/95	0/2/2/2
23	CLA	C	501	-	1/1/15/20	14/39/115/115	-
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
25	PL9	a	410	-	-	23/41/61/73	0/1/1/1
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
23	CLA	B	601	-	1/1/15/20	14/39/115/115	-
23	CLA	B	603	-	1/1/15/20	15/39/115/115	-
23	CLA	B	611	-	1/1/15/20	12/39/115/115	-
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
29	LHG	A	415	-	-	12/41/41/53	-
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
23	CLA	c	501	-	1/1/15/20	15/39/115/115	-
23	CLA	B	616	-	1/1/15/20	19/39/115/115	-
23	CLA	c	510	-	1/1/15/20	17/39/115/115	-
23	CLA	b	606	-	1/1/15/20	15/39/115/115	-
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	c	512	-	1/1/15/20	19/39/115/115	-
23	CLA	b	607	-	1/1/15/20	9/39/115/115	-
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
23	CLA	D	403	-	1/1/15/20	9/39/115/115	-
30	SQD	a	401	-	-	15/49/69/69	0/1/1/1
23	CLA	a	406	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	618	-	1/1/15/20	8/39/115/115	-
23	CLA	C	507	-	1/1/15/20	13/39/115/115	-
27	BCR	K	102	-	-	8/29/63/63	0/2/2/2
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/15/20	20/39/115/115	-
30	SQD	D	409	-	-	11/38/58/69	0/1/1/1
25	PL9	D	404	-	-	12/53/73/73	0/1/1/1
23	CLA	B	613	-	1/1/15/20	15/39/115/115	-
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
23	CLA	B	612	-	1/1/15/20	10/39/115/115	-
28	DGD	C	518	-	-	24/55/95/95	0/2/2/2
23	CLA	b	619	-	1/1/15/20	19/39/115/115	-
24	PHO	a	408	-	-	10/37/103/103	0/5/6/6
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
23	CLA	a	409	-	1/1/15/20	8/39/115/115	-
28	DGD	b	602	-	-	18/41/81/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	18/39/115/115	-
31	LMG	k	103	-	-	17/43/63/70	0/1/1/1
24	PHO	a	407	-	-	11/37/103/103	0/5/6/6
23	CLA	B	608	-	1/1/15/20	15/39/115/115	-
33	LMT	M	103	-	-	0/21/61/61	0/2/2/2
23	CLA	B	610	-	1/1/15/20	18/39/115/115	-
23	CLA	b	616	-	1/1/15/20	15/39/115/115	-
23	CLA	b	610	-	1/1/15/20	9/39/115/115	-
31	LMG	M	102	-	-	17/37/57/70	0/1/1/1
23	CLA	B	602	-	1/1/15/20	13/39/115/115	-
29	LHG	a	417	-	-	13/41/41/53	-
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
31	LMG	C	519	-	-	16/43/63/70	0/1/1/1
23	CLA	c	508	-	1/1/15/20	13/39/115/115	-
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
28	DGD	A	411	-	-	11/45/85/95	0/2/2/2
27	BCR	Z	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/15/20	21/39/115/115	-
27	BCR	T	102	-	-	2/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	10/39/115/115	-
28	DGD	b	622	-	-	19/47/87/95	0/2/2/2
31	LMG	d	405	-	-	10/41/61/70	0/1/1/1
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
23	CLA	C	510	-	1/1/15/20	16/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	C	506	-	1/1/15/20	18/39/115/115	-
23	CLA	b	613	-	1/1/15/20	17/39/115/115	-
23	CLA	c	503	-	1/1/15/20	13/39/115/115	-
23	CLA	A	405	-	1/1/15/20	10/39/115/115	-
31	LMG	i	101	-	-	19/38/58/70	0/1/1/1
23	CLA	c	502	-	1/1/15/20	12/39/115/115	-
23	CLA	a	404	-	1/1/15/20	8/39/115/115	-
28	DGD	a	413	-	-	11/45/85/95	0/2/2/2
23	CLA	B	605	-	1/1/15/20	15/39/115/115	-
29	LHG	A	412	-	-	17/43/43/53	-
23	CLA	C	511	3	1/1/15/20	13/39/115/115	-
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
30	SQD	a	415	-	-	17/46/66/69	0/1/1/1
23	CLA	B	609	-	1/1/15/20	9/39/115/115	-
23	CLA	b	604	-	1/1/15/20	13/39/115/115	-
31	LMG	b	624	-	-	15/44/64/70	0/1/1/1
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	CLA	A	404	-	1/1/15/20	15/39/115/115	-
30	SQD	B	625	-	-	14/42/62/69	0/1/1/1
25	PL9	J	101	-	-	11/29/49/73	0/1/1/1
23	CLA	A	403	-	1/1/15/20	9/39/115/115	-
23	CLA	b	617	-	1/1/15/20	14/39/115/115	-
23	CLA	C	512	-	1/1/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	A	417	-	-	15/49/69/69	0/1/1/1
28	DGD	C	517	-	-	21/51/91/95	0/2/2/2
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	PHO	A	406	-	-	11/37/103/103	0/5/6/6
23	CLA	c	506	-	1/1/15/20	15/39/115/115	-
23	CLA	d	402	-	1/1/15/20	13/39/115/115	-
33	LMT	T	101	-	-	3/21/61/61	0/2/2/2
33	LMT	B	623	-	-	2/21/61/61	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	14/39/115/115	-
30	SQD	d	407	-	-	11/38/58/69	0/1/1/1
23	CLA	a	405	-	1/1/15/20	15/39/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
23	CLA	C	513	-	1/1/15/20	18/39/115/115	-
23	CLA	C	502	-	1/1/15/20	10/39/115/115	-
23	CLA	C	503	-	1/1/15/20	14/39/115/115	-
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
31	LMG	a	416	-	-	22/46/66/70	0/1/1/1
23	CLA	b	608	-	1/1/15/20	17/39/115/115	-
31	LMG	b	623	-	-	22/44/64/70	0/1/1/1
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
28	DGD	C	516	-	-	18/42/82/95	0/2/2/2
27	BCR	T	103	-	-	9/29/63/63	0/2/2/2
23	CLA	c	504	-	1/1/15/20	13/39/115/115	-
23	CLA	c	505	-	1/1/15/20	19/39/115/115	-
23	CLA	D	401	-	1/1/15/20	14/39/115/115	-
31	LMG	D	407	-	-	24/44/64/70	0/1/1/1
34	HEM	v	201	16	-	4/14/54/54	-
30	SQD	F	102	-	-	17/40/60/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	x	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	612	-	-	9/39/115/115	-
23	CLA	b	609	-	1/1/15/20	14/39/115/115	-
23	CLA	c	511	-	1/1/15/20	13/39/115/115	-
31	LMG	B	622	-	-	15/44/64/70	0/1/1/1
31	LMG	D	406	-	-	10/41/61/70	0/1/1/1
23	CLA	B	607	-	1/1/15/20	9/39/115/115	-
23	CLA	c	507	-	1/1/15/20	14/39/115/115	-
34	HEM	f	101	6,5	-	2/14/54/54	-
31	LMG	A	418	-	-	15/37/57/70	0/1/1/1
31	LMG	I	101	-	-	21/38/58/70	0/1/1/1
29	LHG	a	414	-	-	17/43/43/53	-
28	DGD	c	517	-	-	20/42/82/95	0/2/2/2
28	DGD	B	626	-	-	18/41/81/95	0/2/2/2
31	LMG	D	408	-	-	21/43/63/70	0/1/1/1
23	CLA	A	407	-	1/1/15/20	8/39/115/115	-
30	SQD	f	103	-	-	15/40/60/69	0/1/1/1
33	LMT	x	102	-	-	0/17/57/61	0/2/2/2
23	CLA	b	611	-	1/1/15/20	18/39/115/115	-
31	LMG	A	414	-	-	20/46/66/70	0/1/1/1
33	LMT	B	627	-	-	3/21/61/61	0/2/2/2
23	CLA	C	504	-	1/1/15/20	11/39/115/115	-
23	CLA	C	508	-	1/1/15/20	13/39/115/115	-

The worst 5 of 908 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C1B-C2B	10.10	1.50	1.39
24	a	407	PHO	C1B-C2B	9.66	1.50	1.39
24	A	406	PHO	C1B-C2B	9.61	1.50	1.39
24	a	408	PHO	C1B-C2B	9.51	1.49	1.39
24	A	406	PHO	C3B-C4B	8.88	1.50	1.41

The worst 5 of 1292 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	102	BCR	C32-C1-C6	-14.03	88.24	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	j	102	BCR	C32-C1-C6	-13.95	88.37	110.24
27	j	102	BCR	C32-C1-C31	-9.26	82.13	108.63
27	J	102	BCR	C32-C1-C31	-9.17	82.39	108.63
27	B	618	BCR	C7-C8-C9	-8.76	113.28	126.23

5 of 69 chirality outliers are listed below:

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

5 of 2107 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	C3A-C2A-CAA-CBA
23	A	405	CLA	C2B-C3B-CAB-CBB
23	A	405	CLA	C4B-C3B-CAB-CBB
23	B	601	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

163 monomers are involved in 556 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	615	CLA	4	0
33	b	626	LMT	1	0
23	b	615	CLA	5	0
27	c	516	BCR	2	0
24	D	402	PHO	7	0
28	c	519	DGD	4	0
34	F	101	HEM	4	0
25	A	408	PL9	2	0
27	J	102	BCR	5	0
33	D	411	LMT	1	0
31	c	520	LMG	2	0
31	C	520	LMG	2	0
23	B	606	CLA	8	0
33	b	625	LMT	4	0
30	A	413	SQD	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	412	BCR	2	0
27	b	621	BCR	5	0
23	d	403	CLA	3	0
31	d	406	LMG	6	0
27	f	102	BCR	3	0
34	V	201	HEM	3	0
23	C	509	CLA	1	0
28	D	410	DGD	3	0
23	C	501	CLA	3	0
33	i	102	LMT	1	0
31	M	101	LMG	2	0
25	a	410	PL9	5	0
27	k	102	BCR	7	0
23	B	603	CLA	11	0
23	B	611	CLA	6	0
25	d	404	PL9	7	0
29	A	415	LHG	3	0
27	B	620	BCR	5	0
23	c	501	CLA	5	0
23	B	616	CLA	4	0
23	c	510	CLA	3	0
23	b	606	CLA	10	0
23	c	512	CLA	3	0
23	b	607	CLA	4	0
28	B	621	DGD	1	0
23	D	403	CLA	4	0
30	a	401	SQD	2	0
23	a	406	CLA	3	0
23	b	618	CLA	2	0
23	C	507	CLA	4	0
27	K	102	BCR	9	0
27	H	101	BCR	2	0
27	A	410	BCR	5	0
23	C	505	CLA	4	0
30	D	409	SQD	3	0
25	D	404	PL9	5	0
23	B	613	CLA	1	0
28	c	518	DGD	2	0
23	B	612	CLA	4	0
28	C	518	DGD	4	0
23	b	619	CLA	4	0
24	a	408	PHO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	514	BCR	10	0
23	a	409	CLA	2	0
28	b	602	DGD	6	0
23	b	605	CLA	9	0
31	k	103	LMG	2	0
24	a	407	PHO	9	0
23	B	608	CLA	8	0
23	B	610	CLA	3	0
23	b	616	CLA	3	0
23	b	610	CLA	9	0
31	M	102	LMG	4	0
23	B	602	CLA	8	0
29	a	417	LHG	3	0
33	I	102	LMT	2	0
31	C	519	LMG	2	0
23	c	508	CLA	3	0
27	j	102	BCR	4	0
23	c	509	CLA	4	0
27	c	514	BCR	9	0
28	A	411	DGD	1	0
27	Z	101	BCR	4	0
23	c	513	CLA	2	0
27	T	102	BCR	7	0
23	B	604	CLA	6	0
28	b	622	DGD	2	0
31	d	405	LMG	3	0
23	C	510	CLA	3	0
27	B	617	BCR	8	0
23	C	506	CLA	1	0
23	b	613	CLA	1	0
23	c	503	CLA	4	0
23	A	405	CLA	4	0
31	i	101	LMG	2	0
23	c	502	CLA	2	0
23	a	404	CLA	14	0
23	B	605	CLA	9	0
29	A	412	LHG	3	0
23	C	511	CLA	6	0
33	b	603	LMT	1	0
30	a	415	SQD	4	0
23	B	609	CLA	5	0
23	b	604	CLA	2	0

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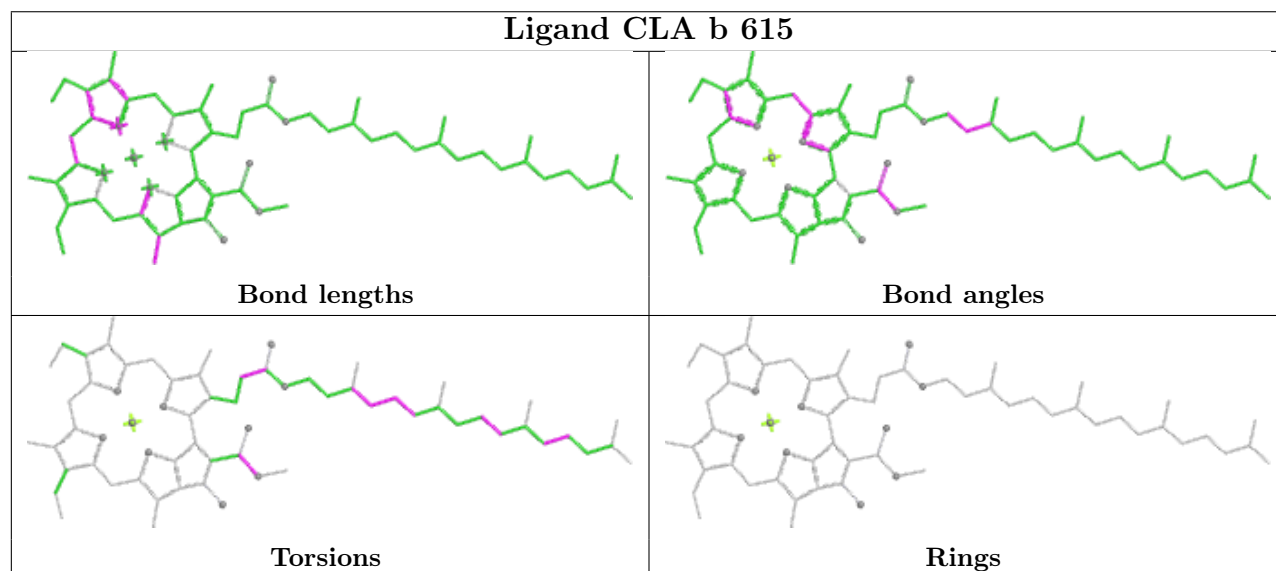
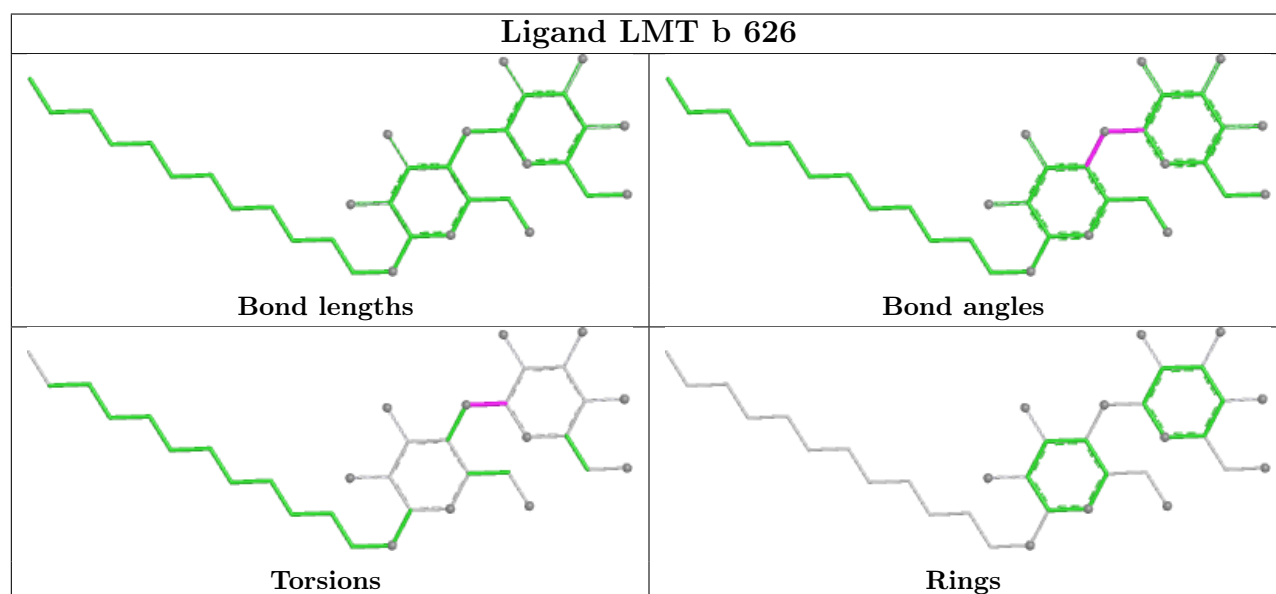
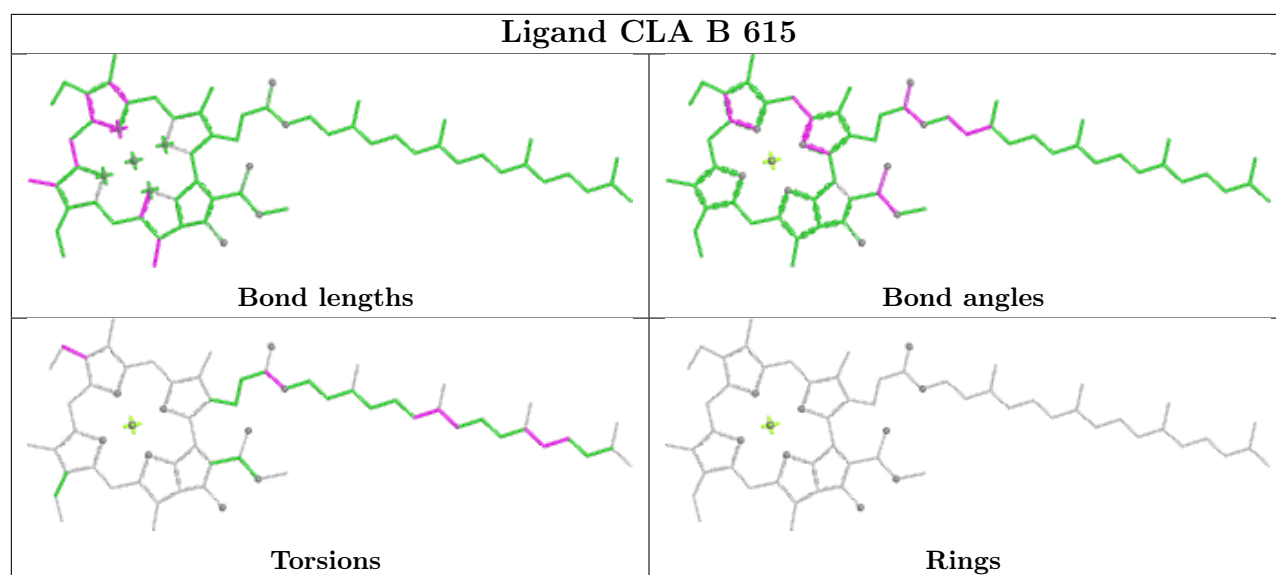
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	624	LMG	4	0
27	C	515	BCR	6	0
23	A	404	CLA	14	0
30	B	625	SQD	1	0
25	J	101	PL9	2	0
23	A	403	CLA	13	0
23	b	617	CLA	2	0
23	C	512	CLA	3	0
30	A	417	SQD	6	0
28	C	517	DGD	6	0
27	c	515	BCR	3	0
27	b	620	BCR	7	0
24	A	406	PHO	5	0
23	c	506	CLA	2	0
23	d	402	CLA	9	0
33	T	101	LMT	2	0
33	B	623	LMT	1	0
27	B	619	BCR	5	0
31	a	402	LMG	2	0
23	B	614	CLA	6	0
30	d	407	SQD	4	0
23	a	405	CLA	15	0
27	D	405	BCR	3	0
23	C	513	CLA	3	0
23	C	502	CLA	2	0
23	C	503	CLA	3	0
30	b	601	SQD	2	0
31	E	101	LMG	1	0
31	a	416	LMG	5	0
23	b	608	CLA	11	0
31	b	623	LMG	3	0
33	B	628	LMT	2	0
27	B	618	BCR	9	0
23	b	614	CLA	5	0
28	C	516	DGD	4	0
27	T	103	BCR	7	0
23	c	504	CLA	5	0
23	c	505	CLA	4	0
23	D	401	CLA	7	0
31	D	407	LMG	2	0
34	v	201	HEM	5	0
30	F	102	SQD	2	0

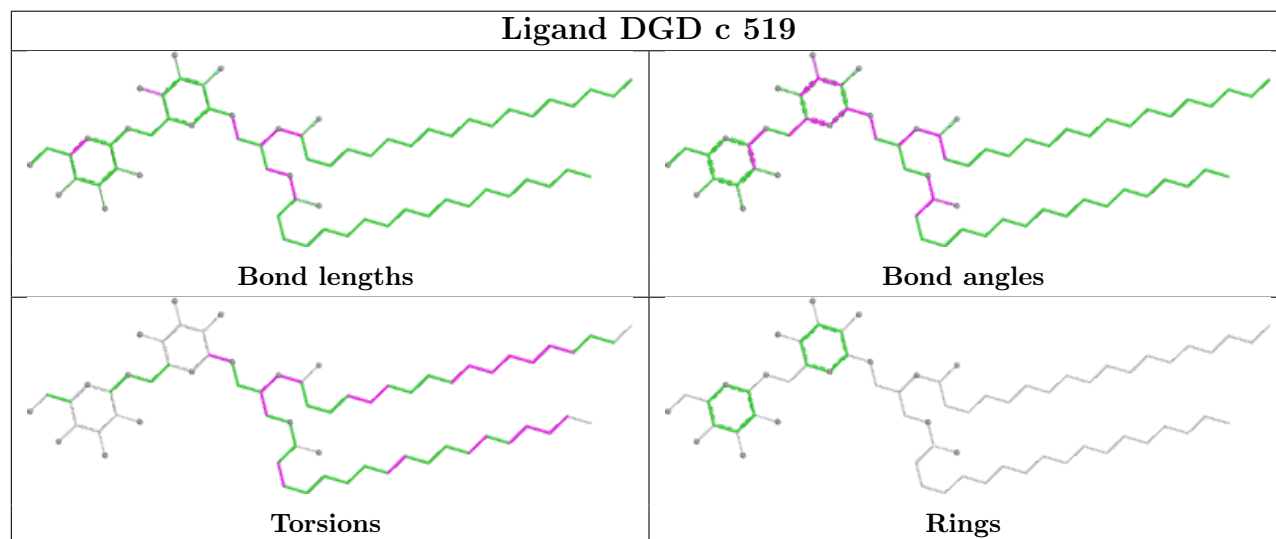
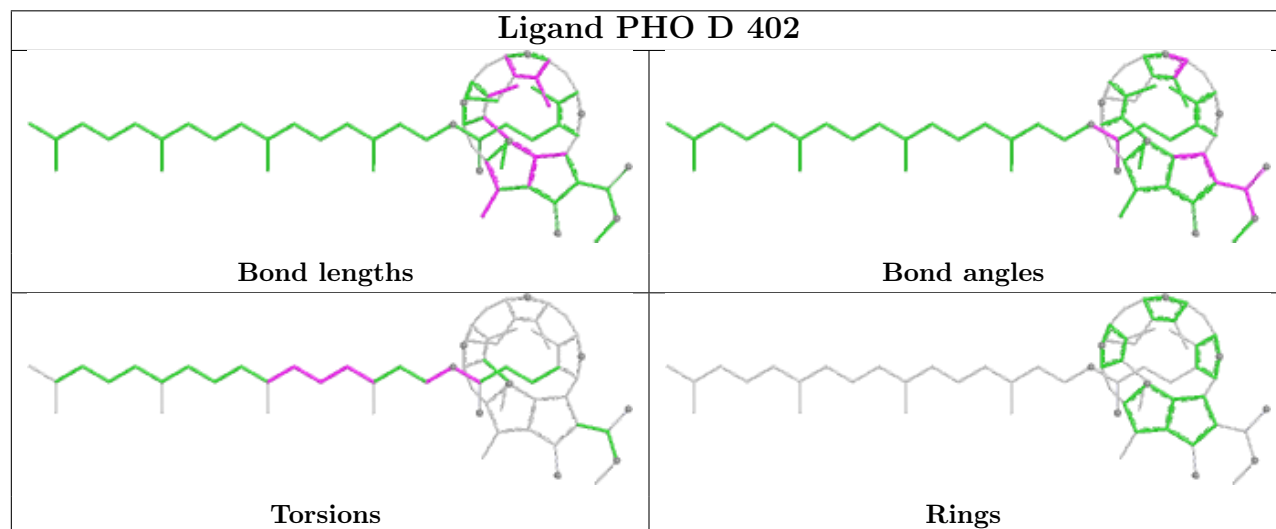
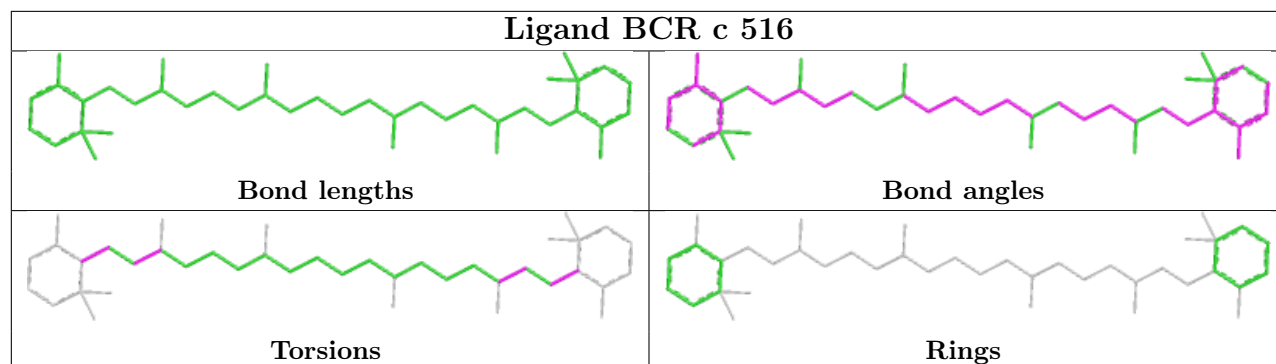
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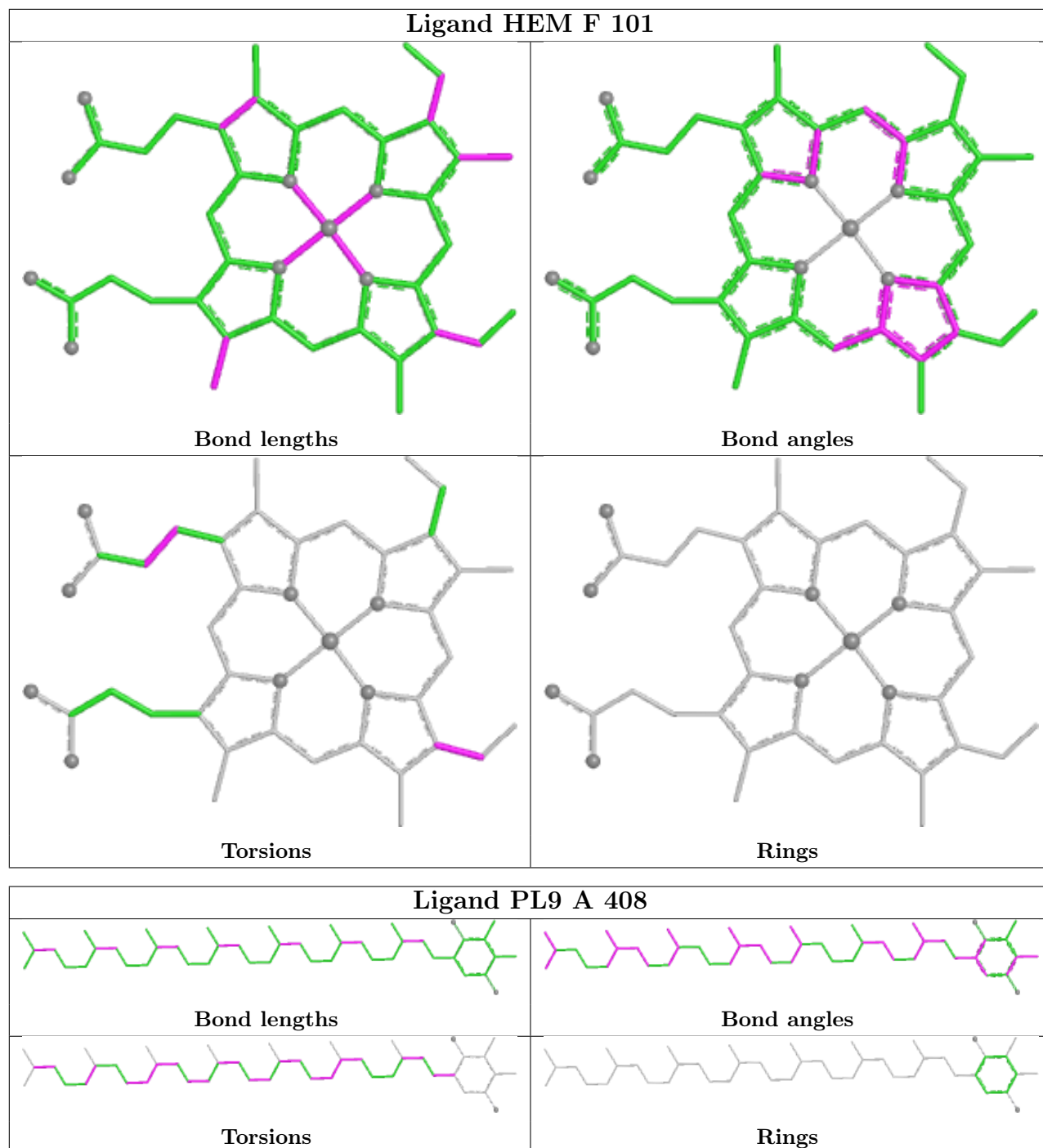
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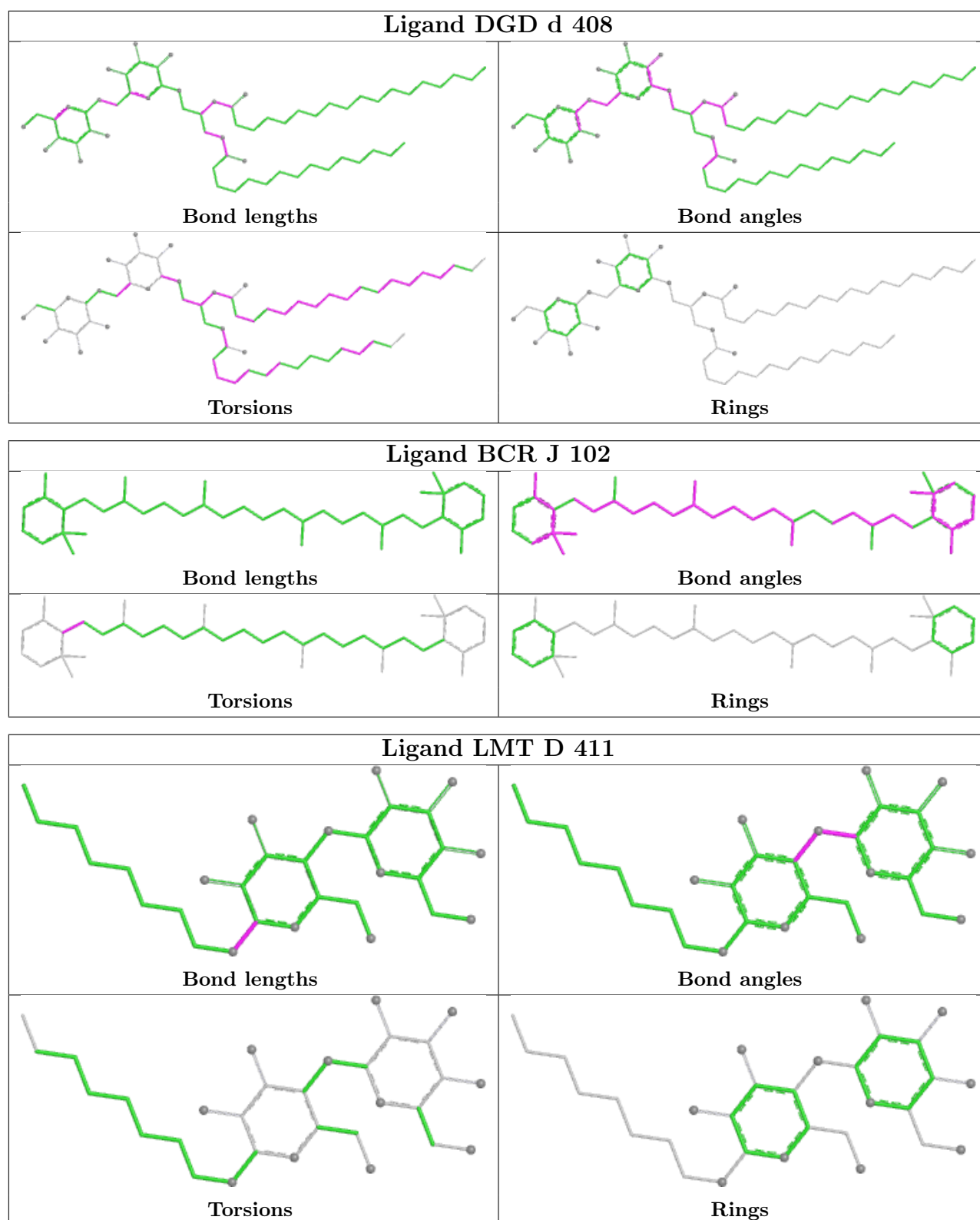
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	x	101	BCR	4	0
23	b	612	CLA	4	0
23	b	609	CLA	8	0
23	c	511	CLA	4	0
31	B	622	LMG	4	0
31	D	406	LMG	1	0
23	B	607	CLA	8	0
23	c	507	CLA	5	0
34	f	101	HEM	4	0
31	A	418	LMG	2	0
31	I	101	LMG	3	0
29	a	414	LHG	4	0
28	c	517	DGD	5	0
28	B	626	DGD	4	0
31	D	408	LMG	7	0
23	A	407	CLA	1	0
30	f	103	SQD	2	0
23	b	611	CLA	7	0
31	A	414	LMG	4	0
33	B	627	LMT	1	0
23	C	504	CLA	6	0
23	C	508	CLA	3	0

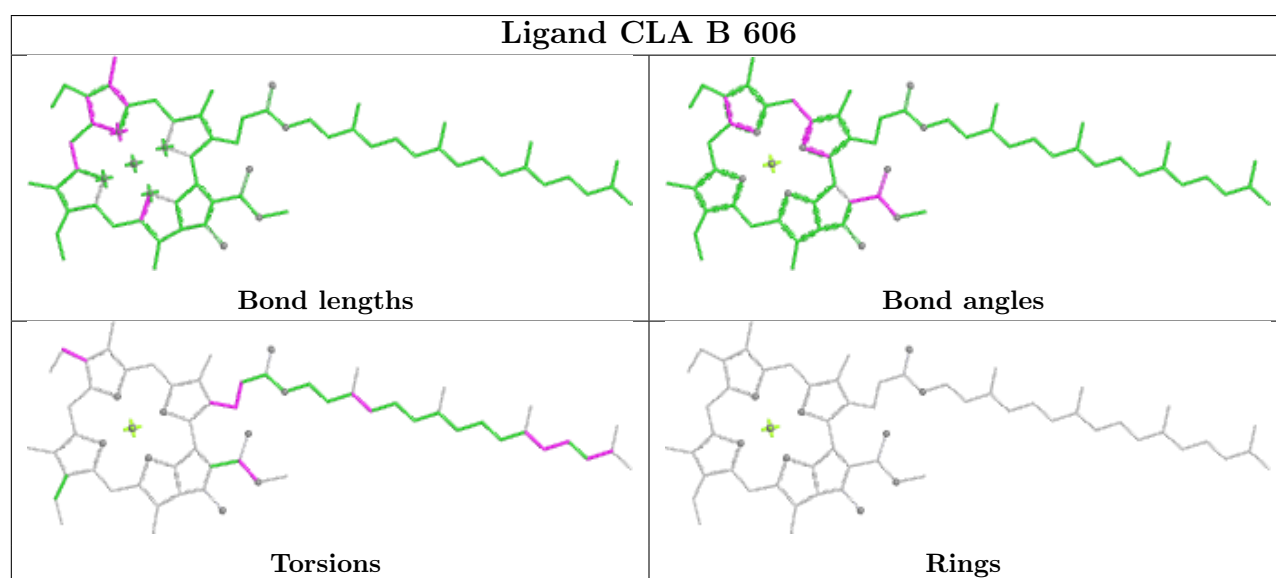
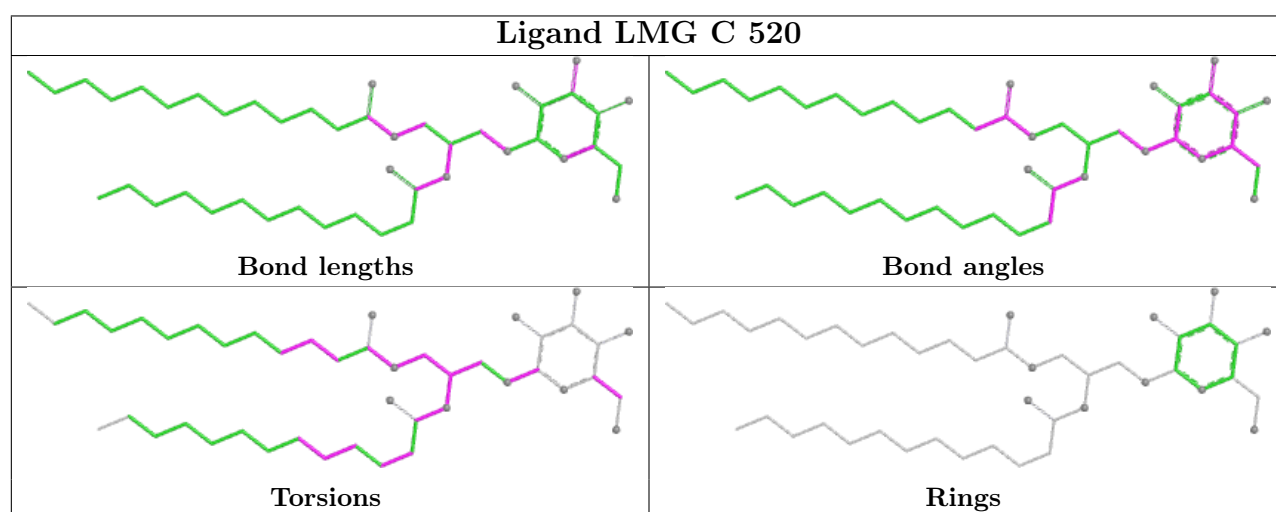
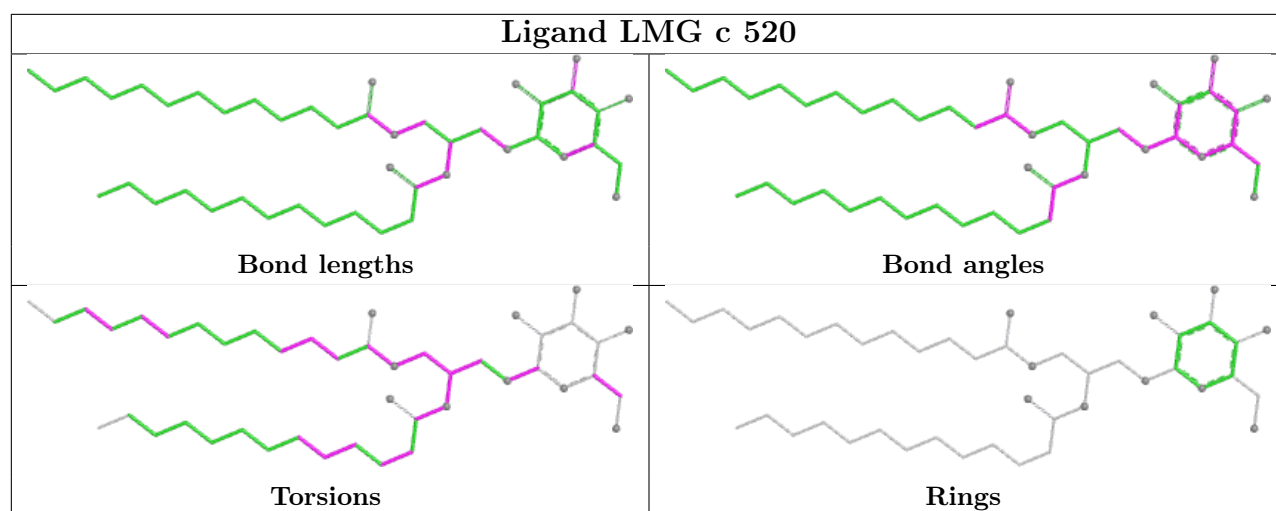
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

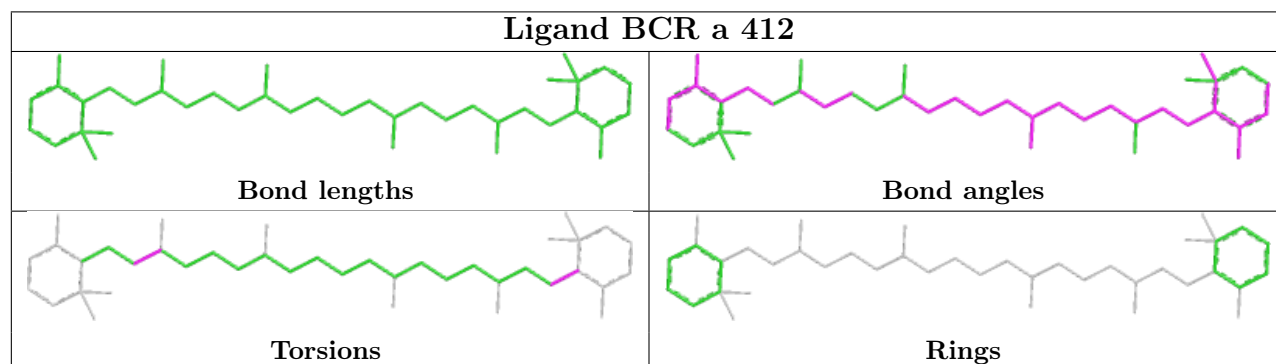
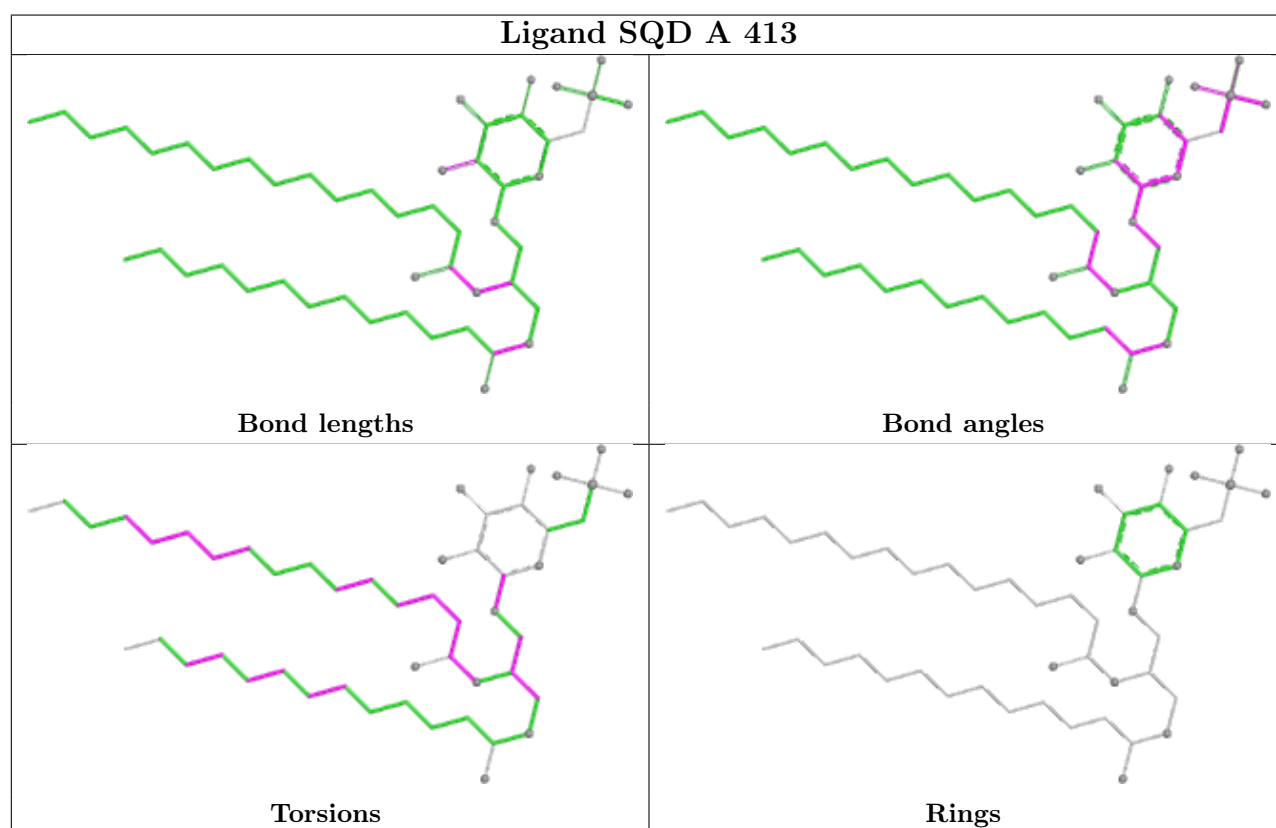
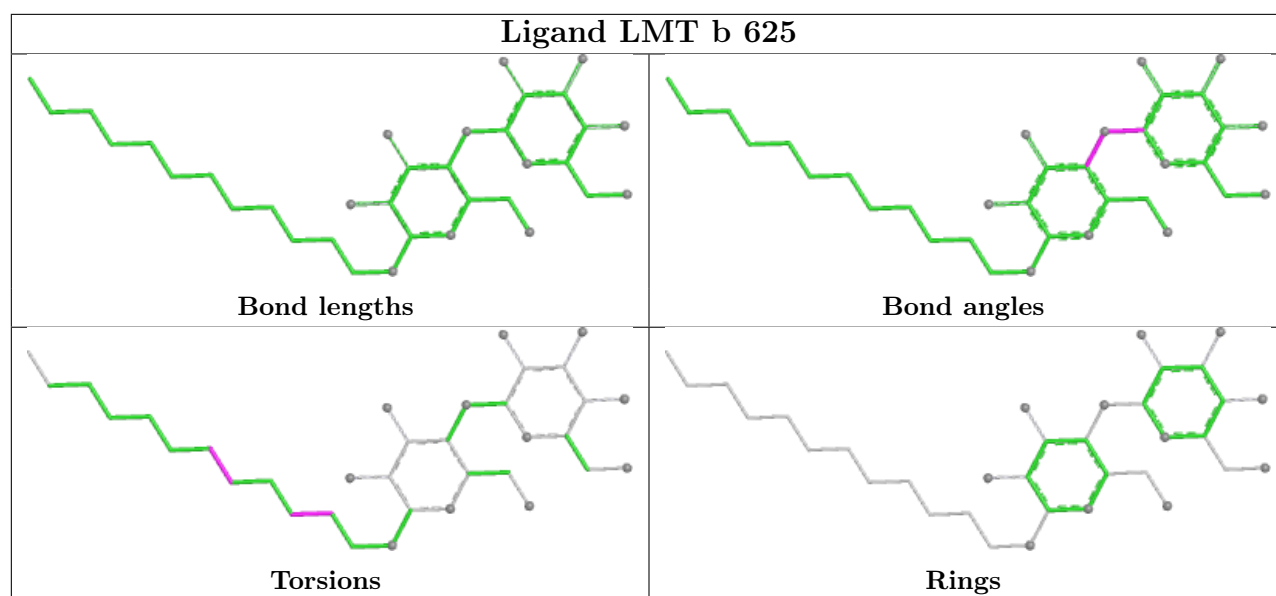


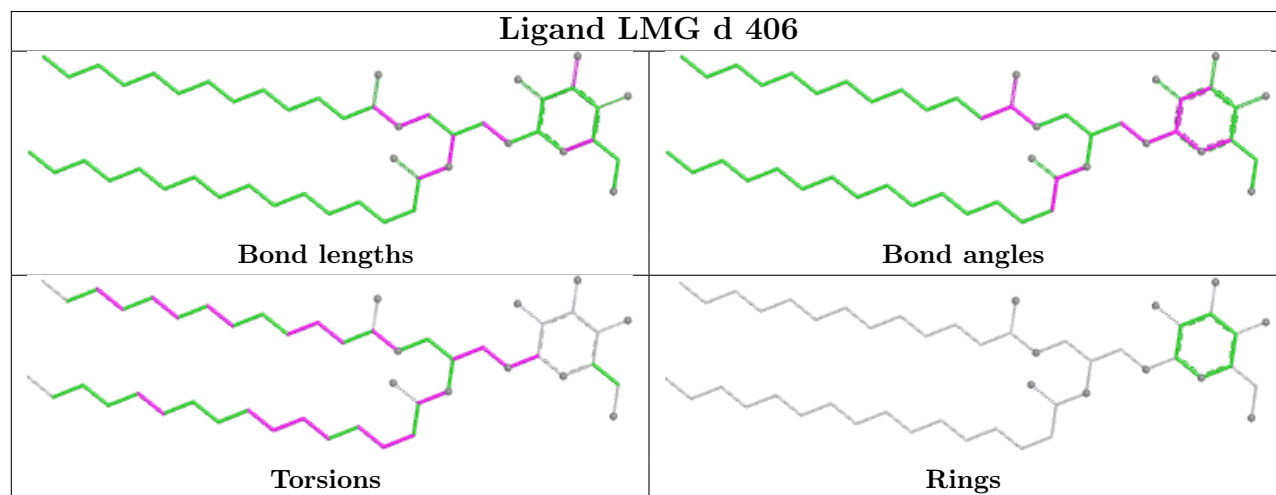
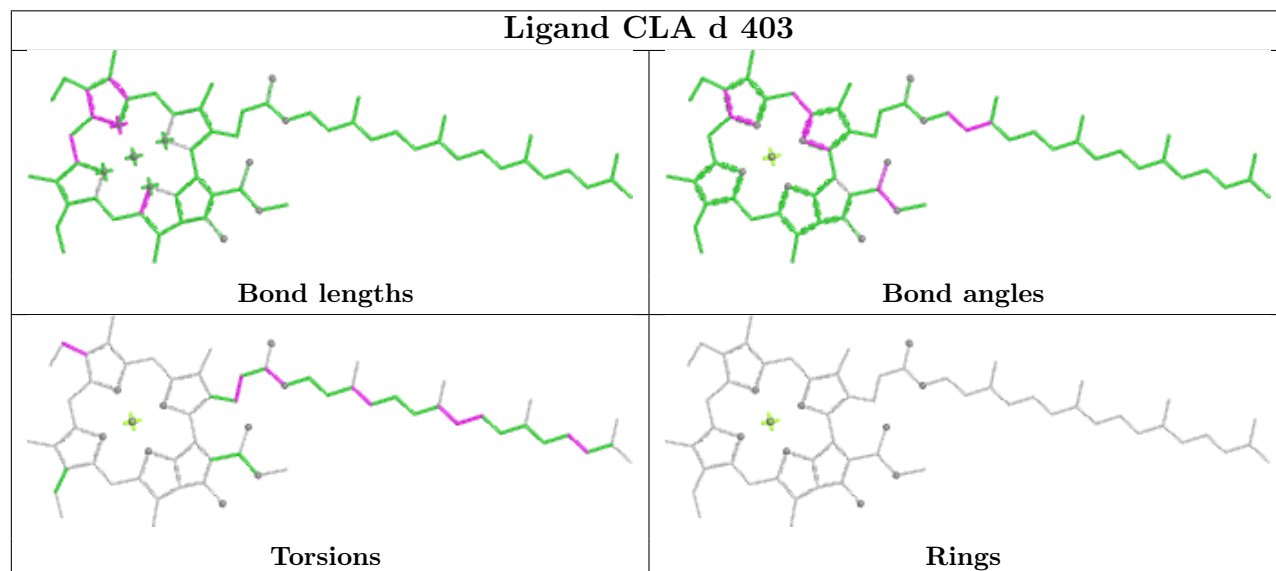
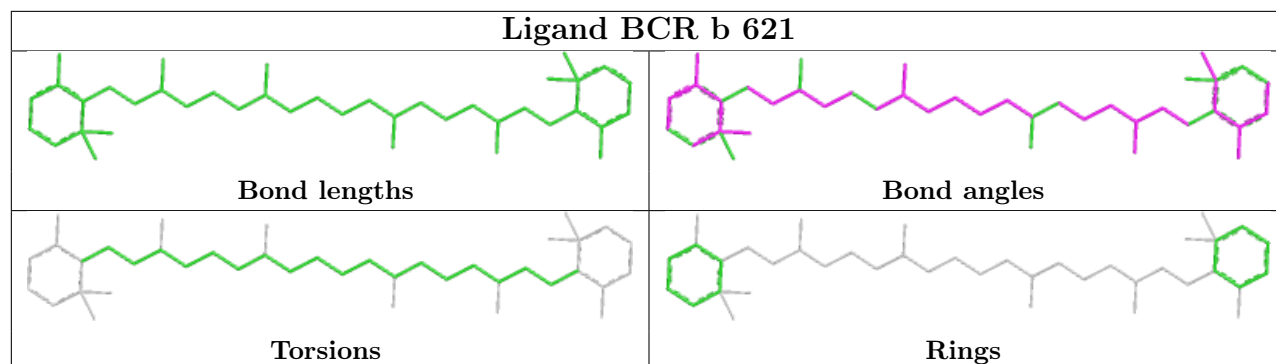


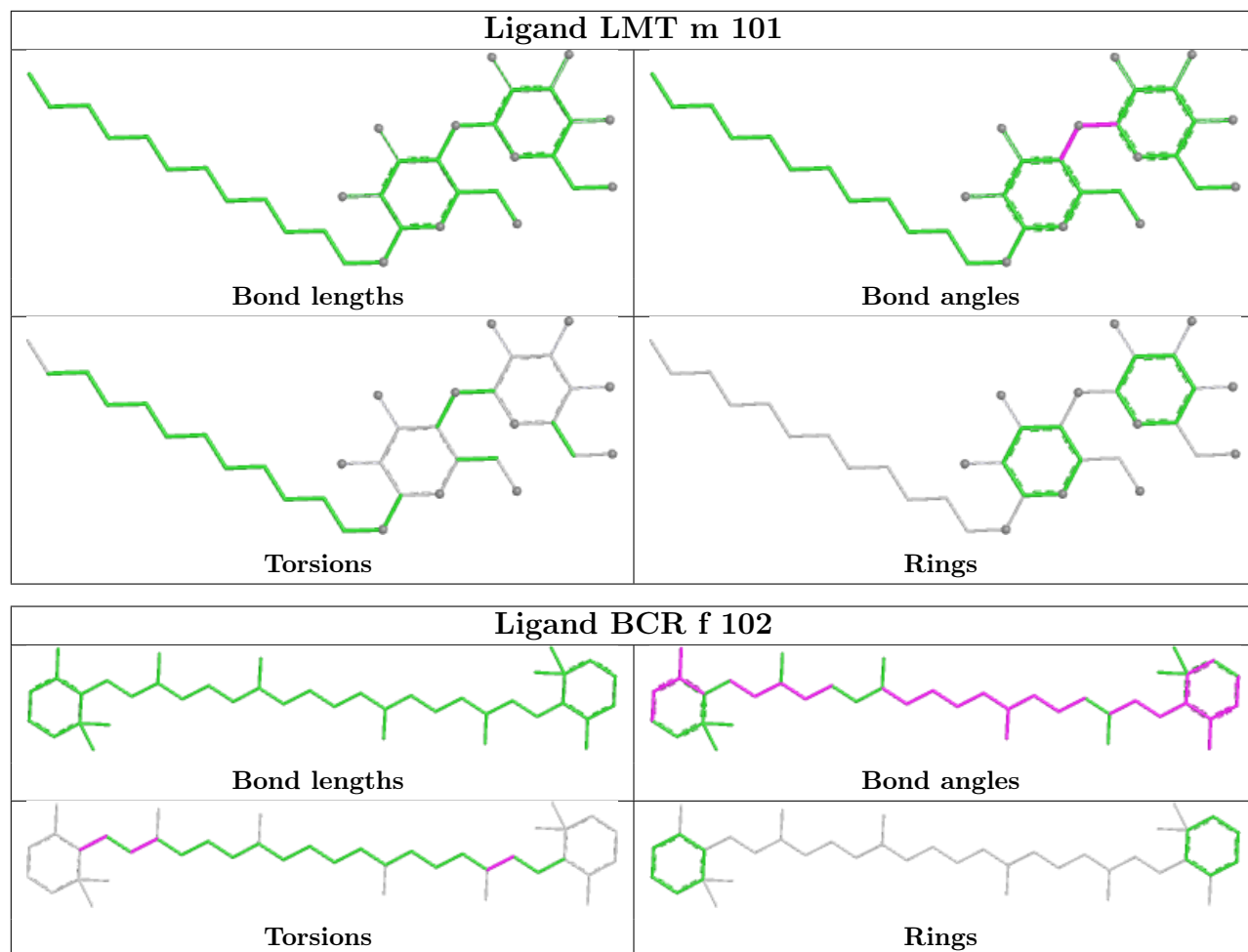




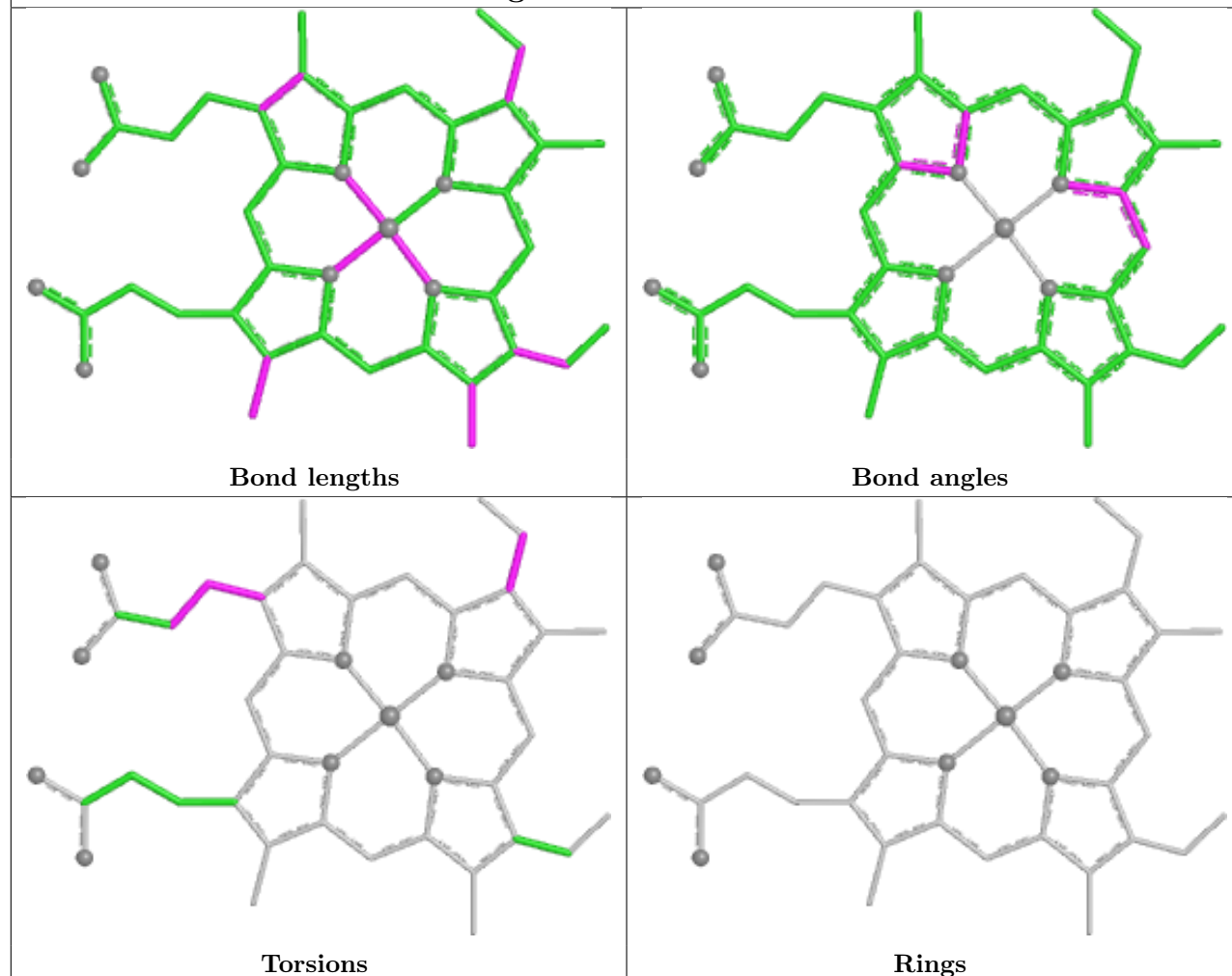




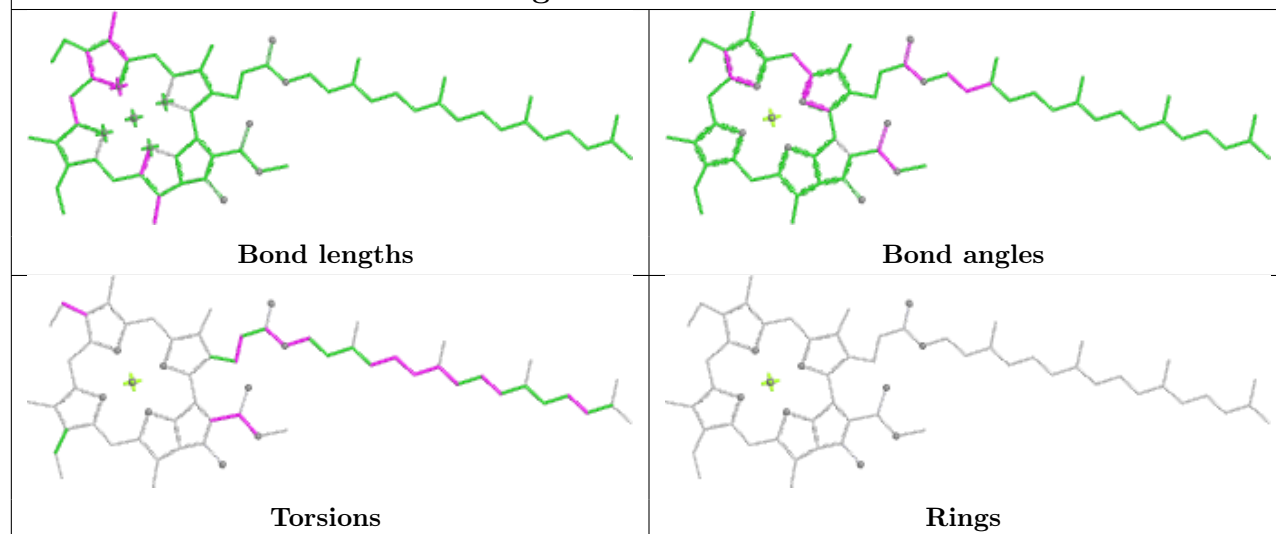


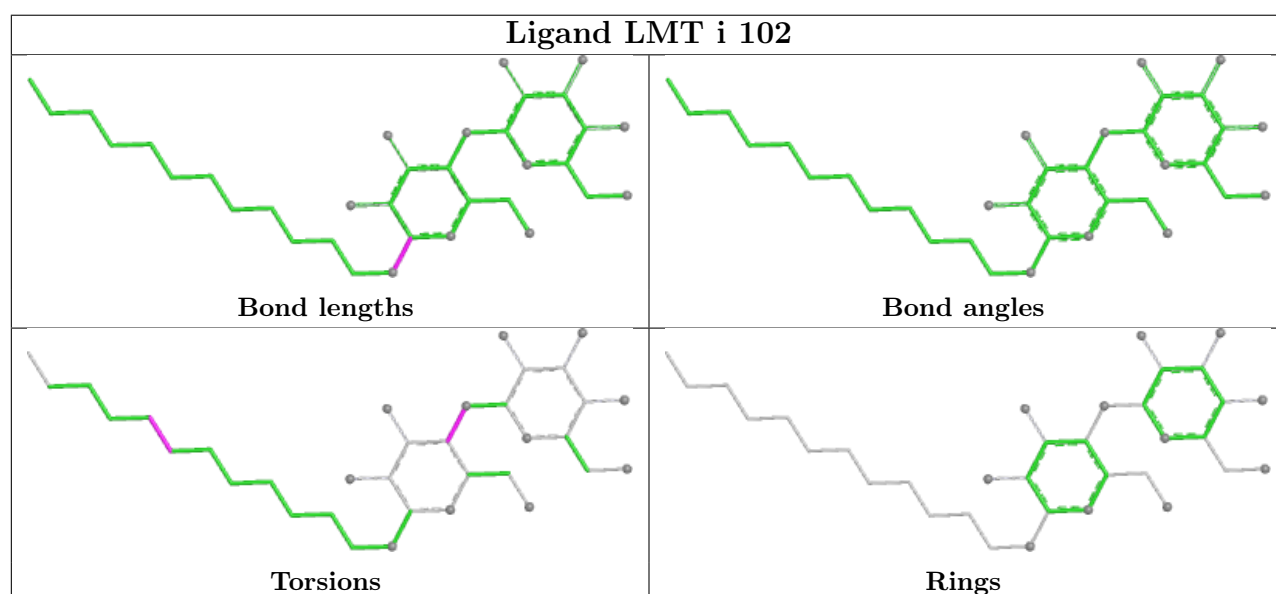
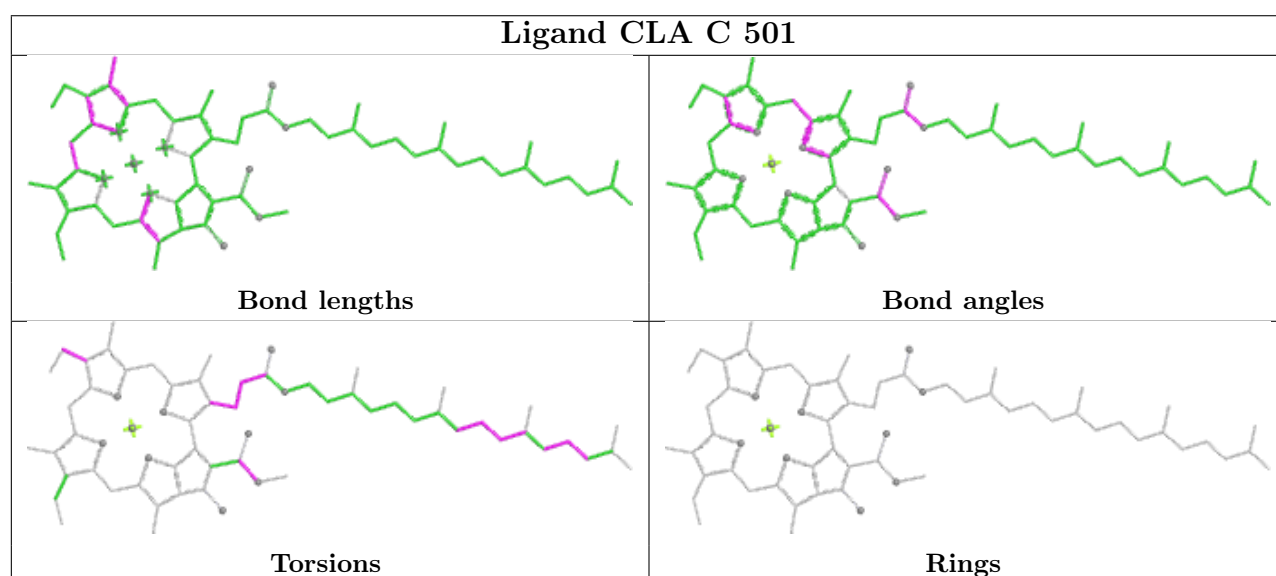
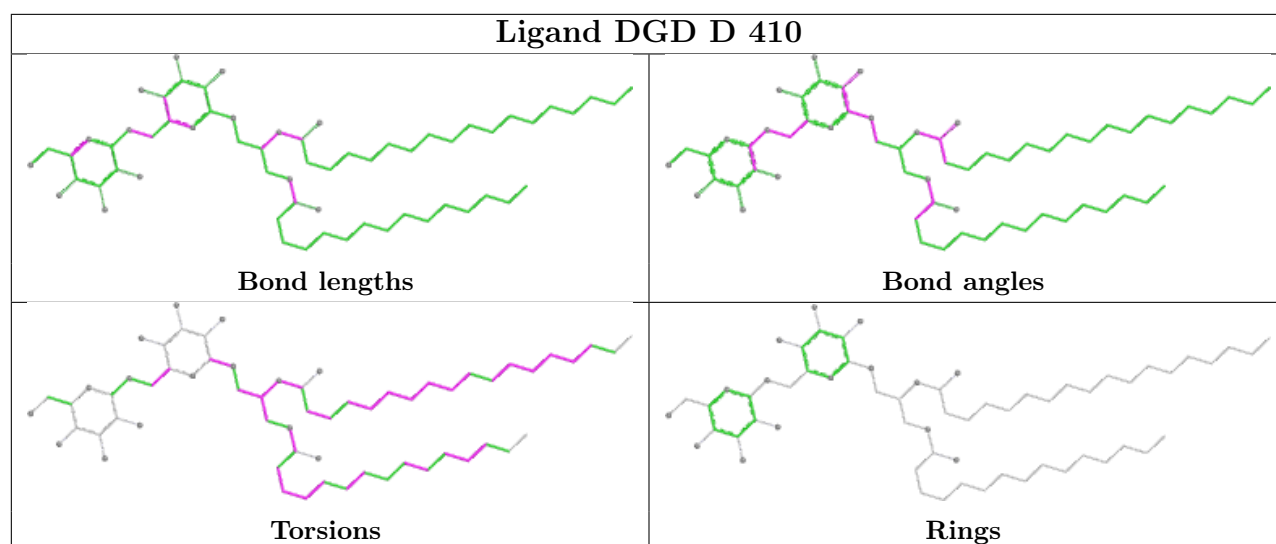


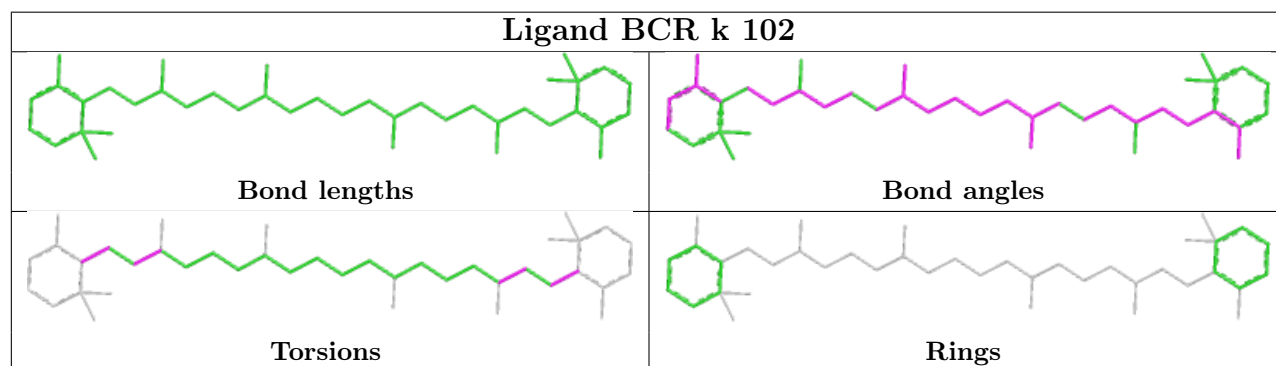
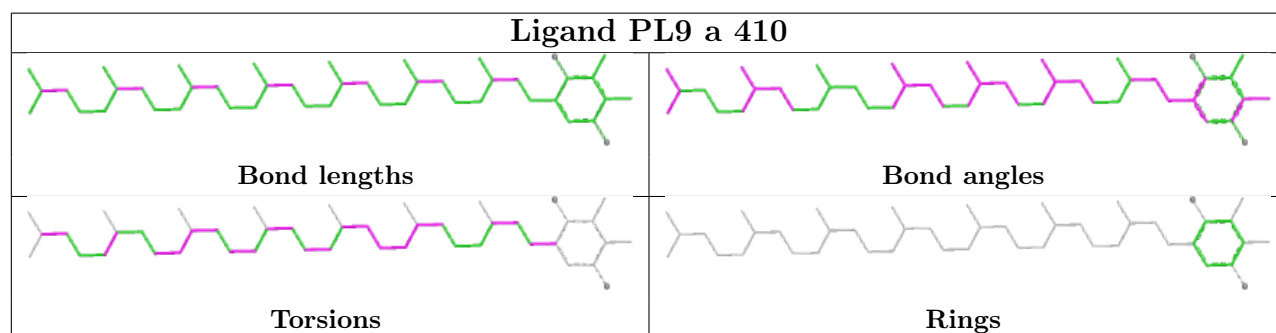
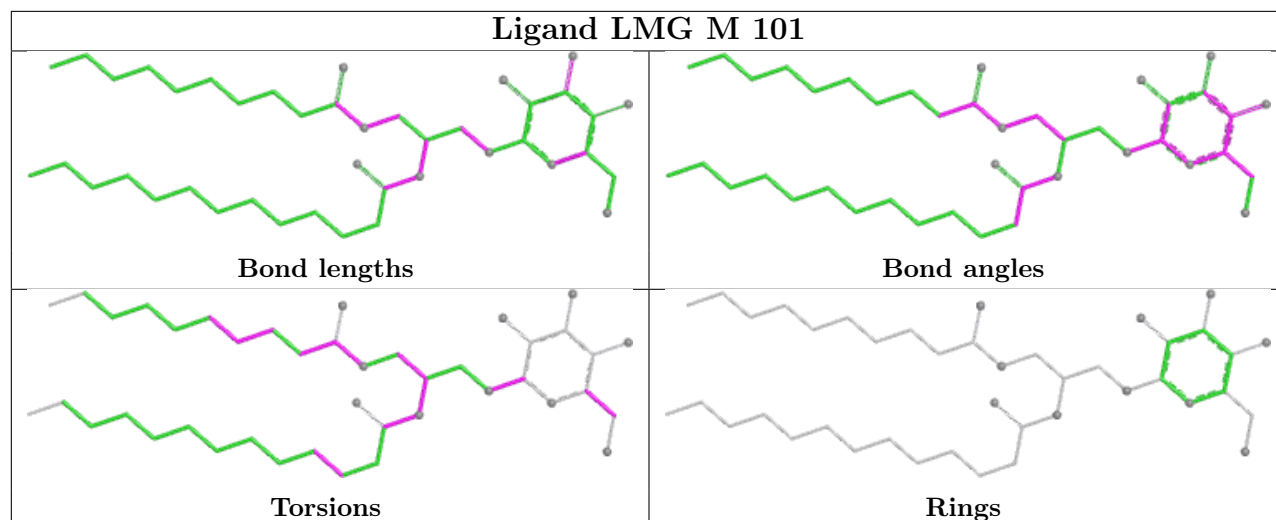
Ligand HEM V 201



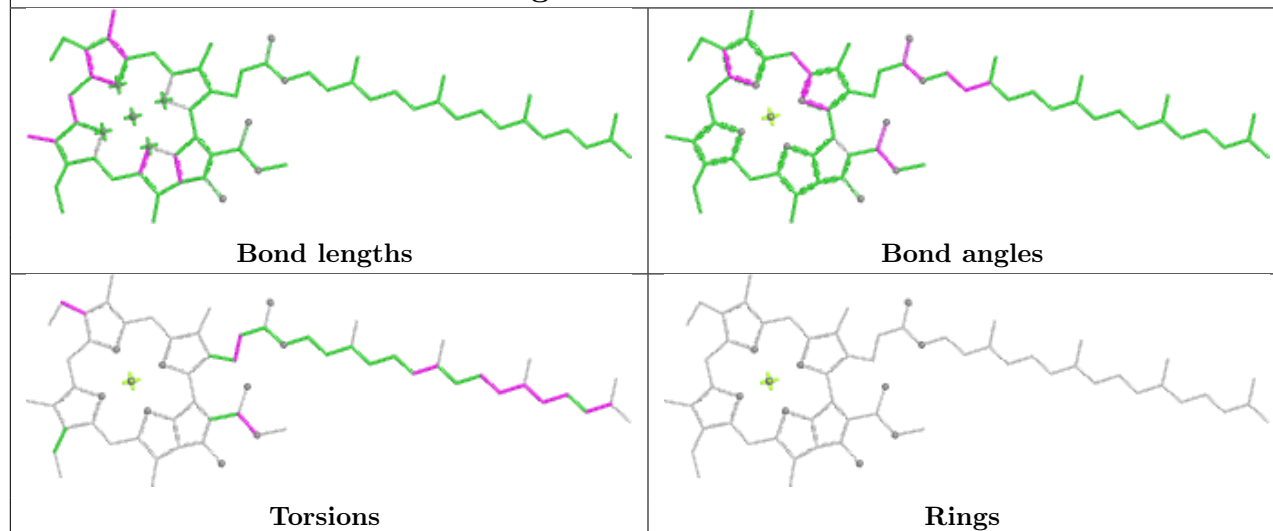
Ligand CLA C 509



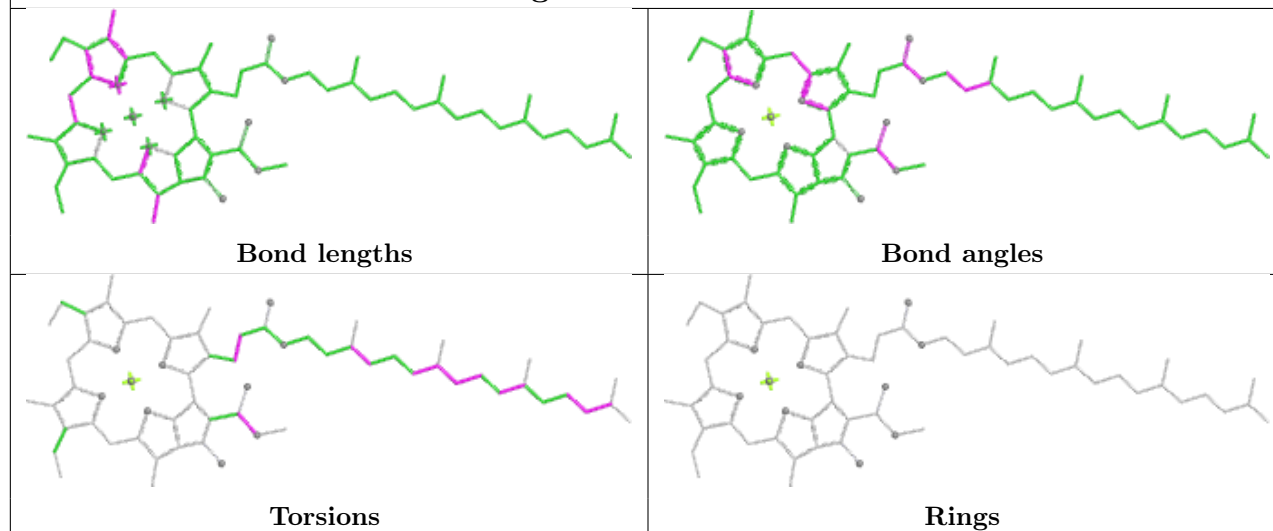




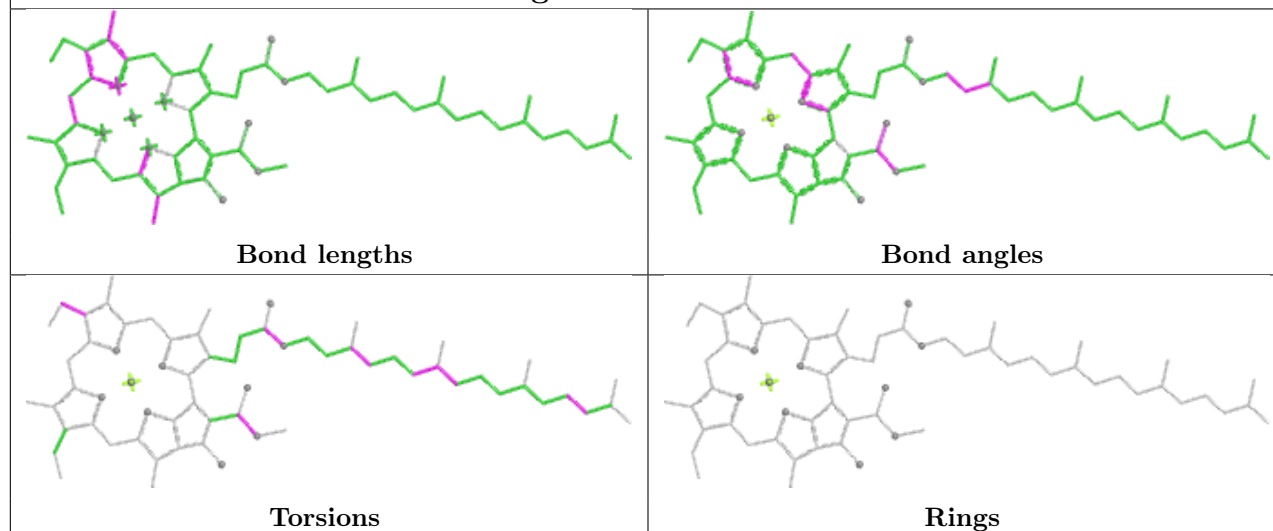
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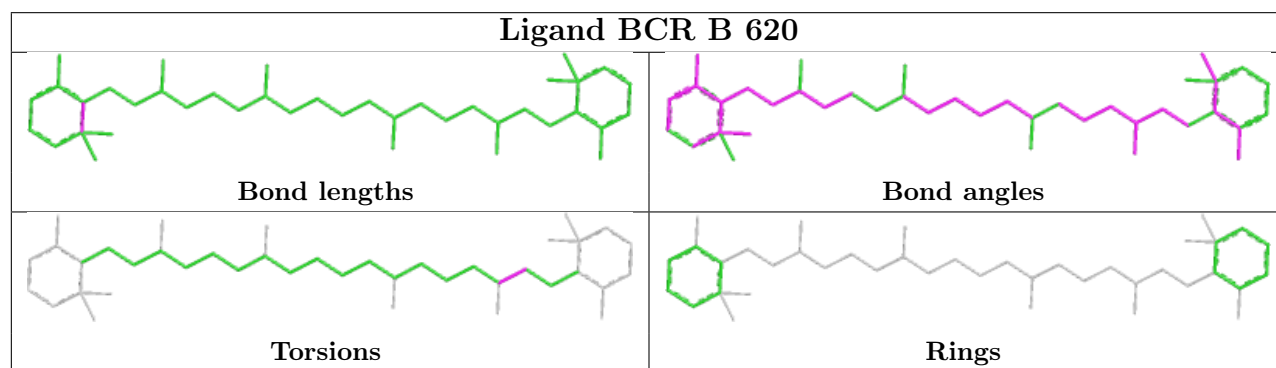
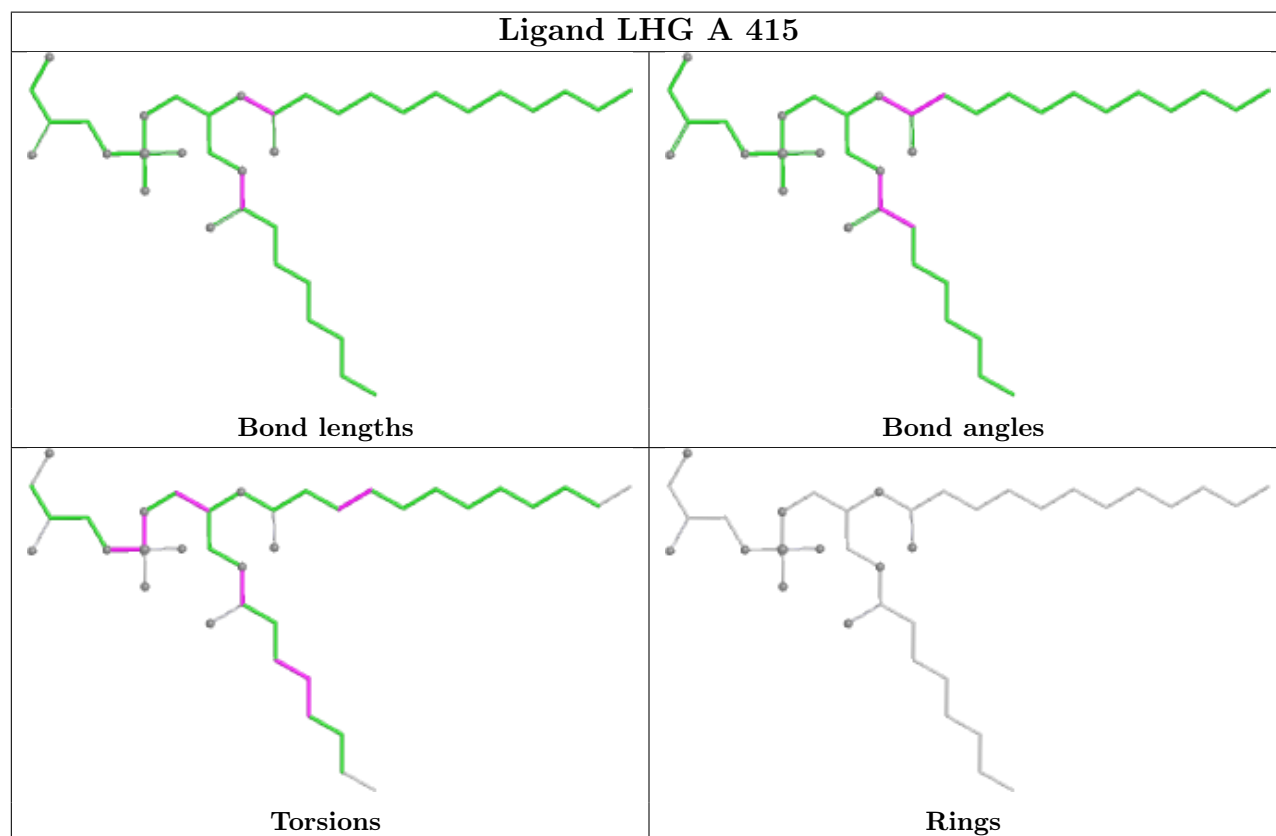
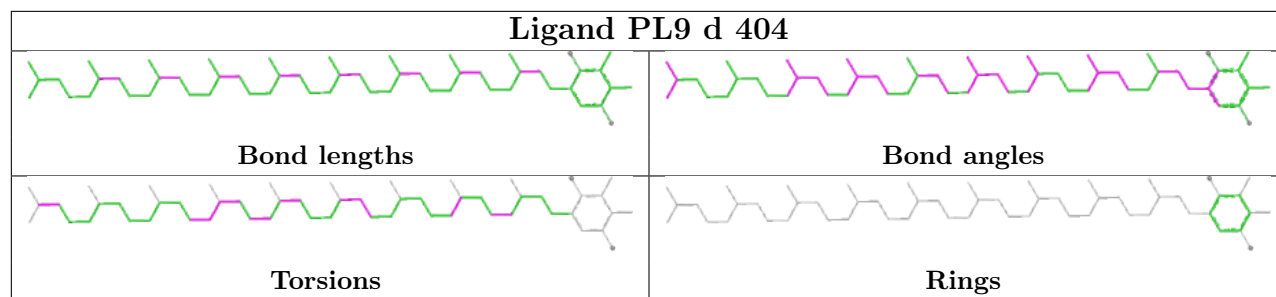


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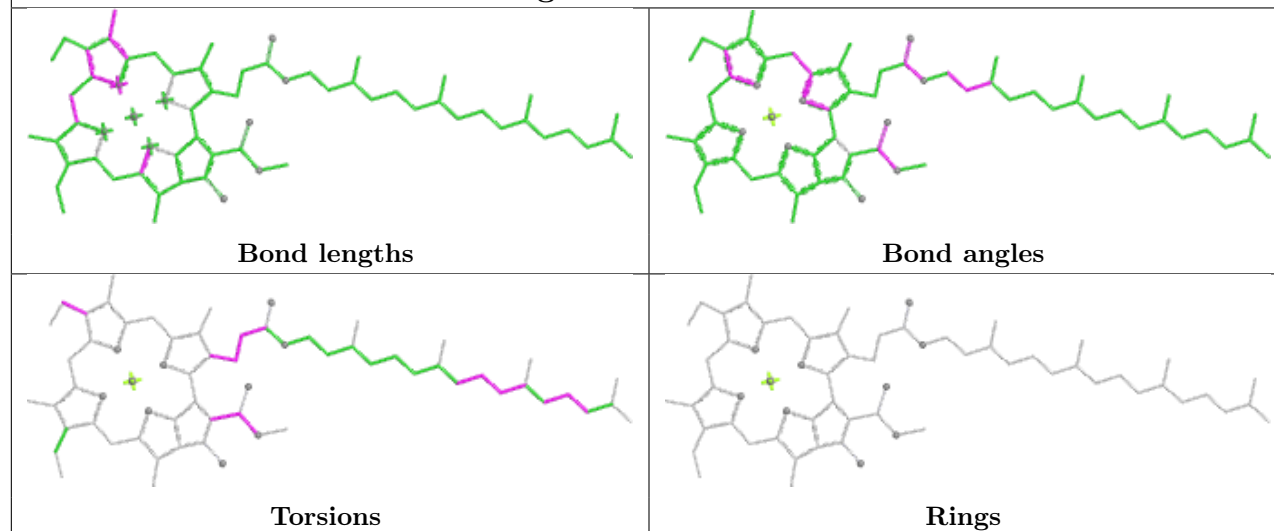


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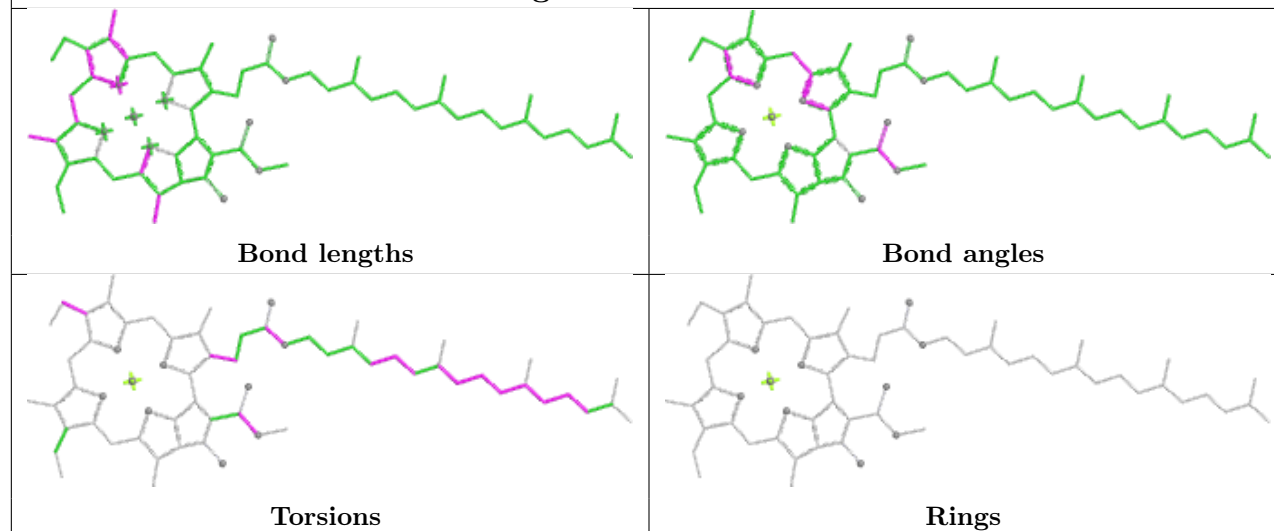




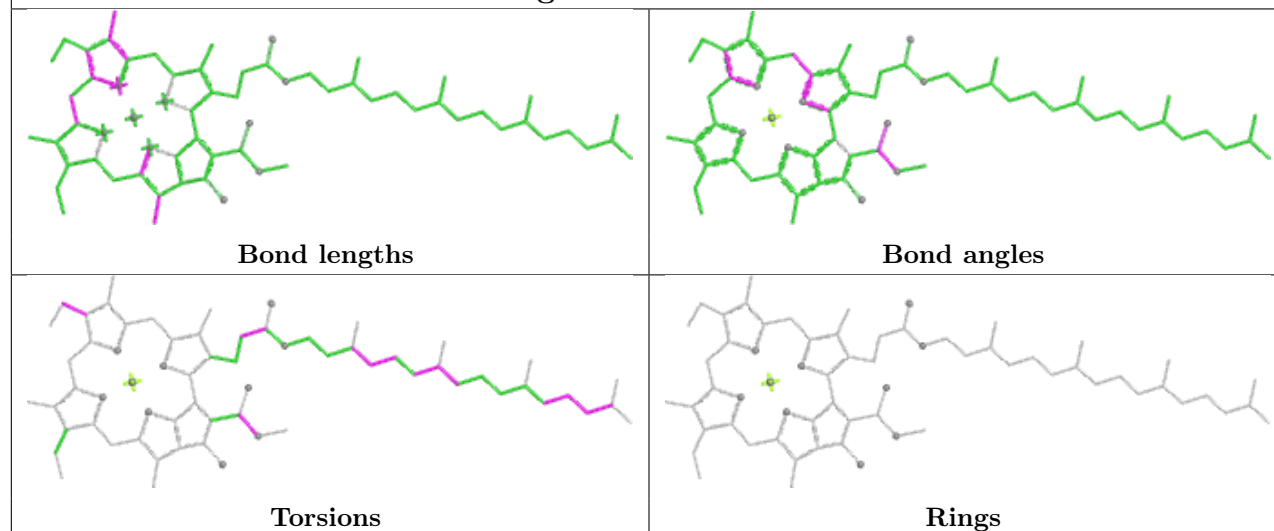
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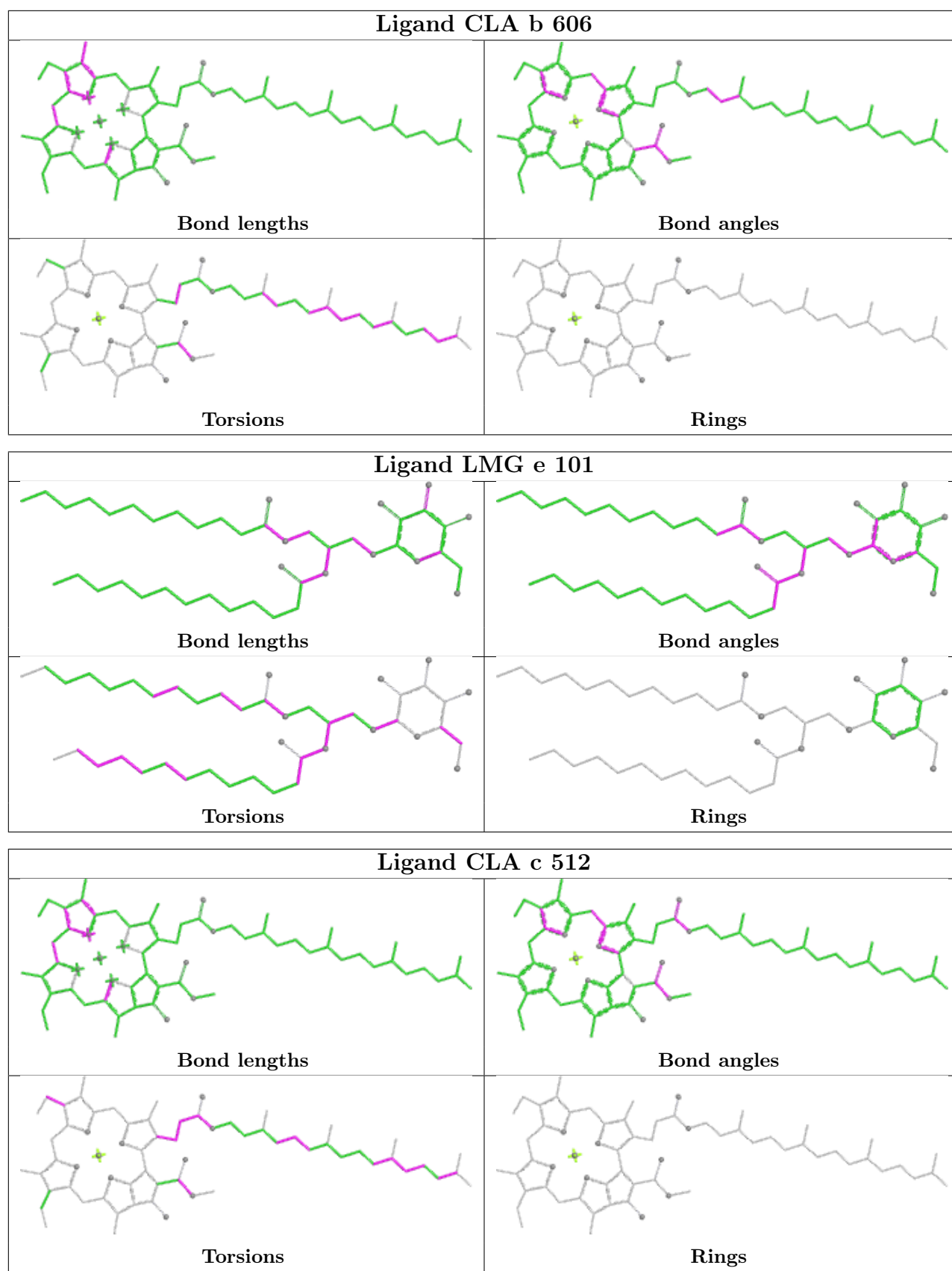


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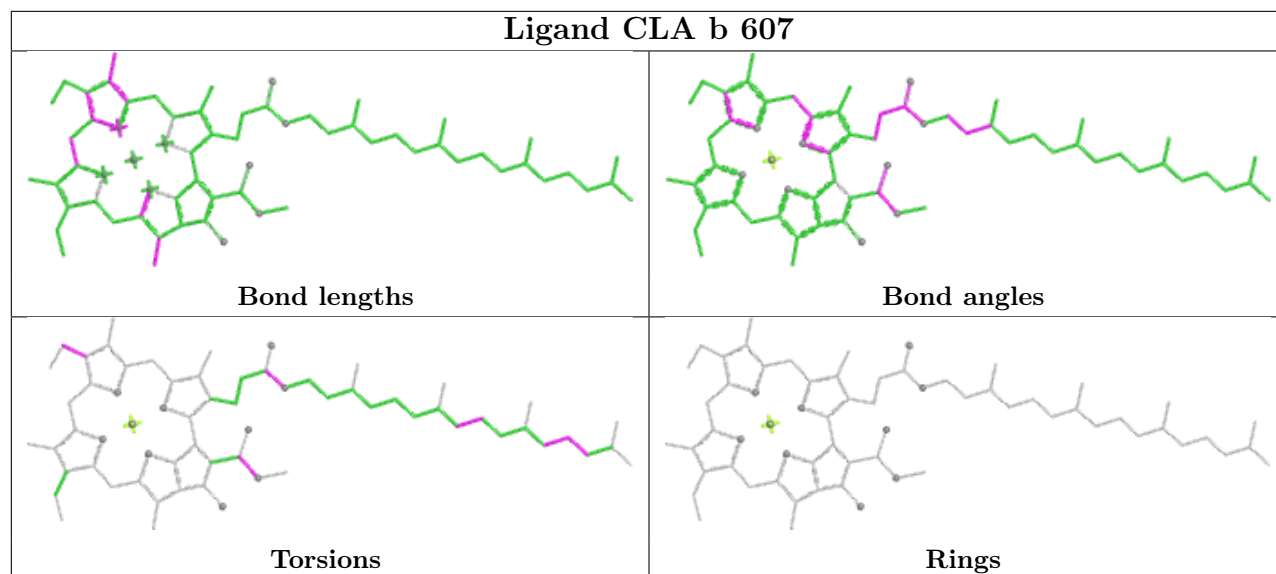


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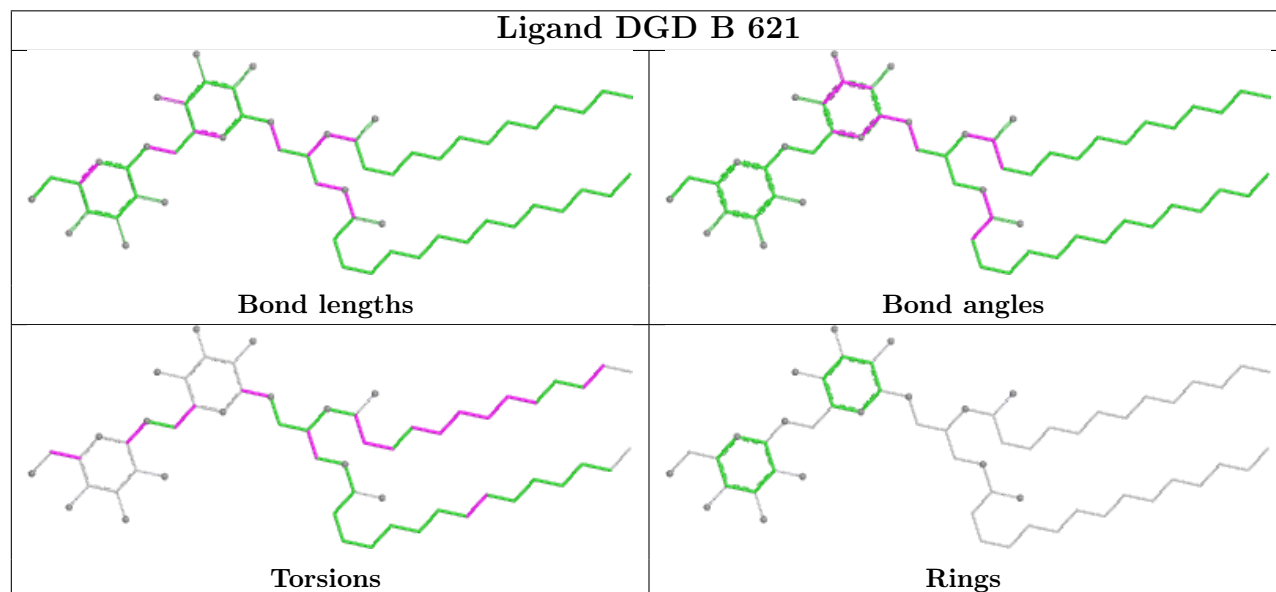




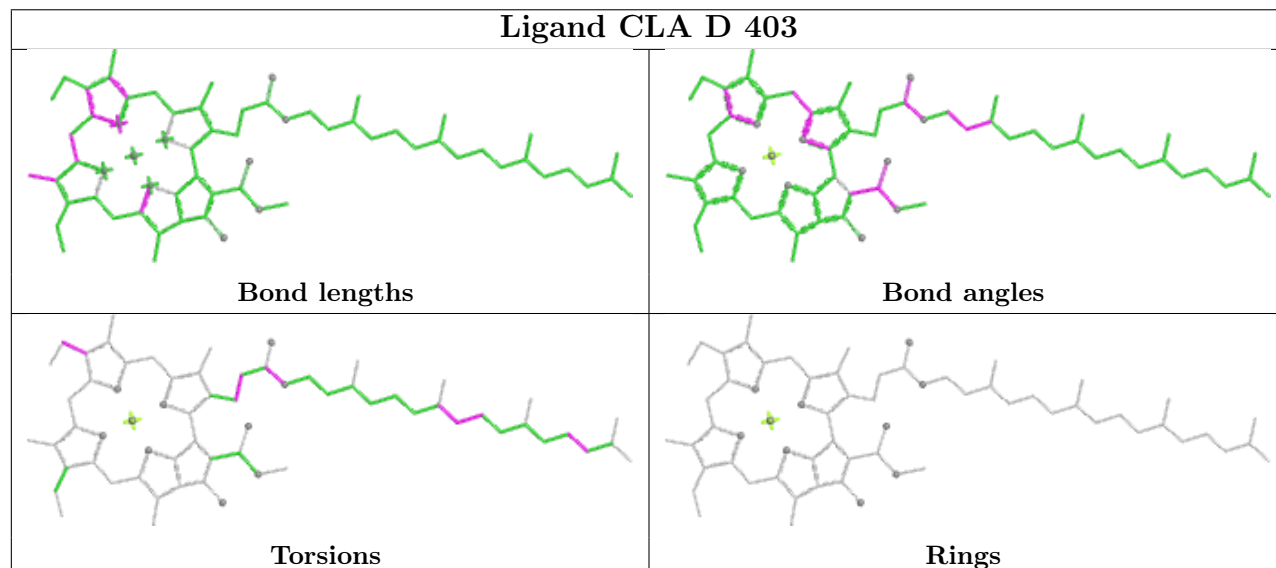
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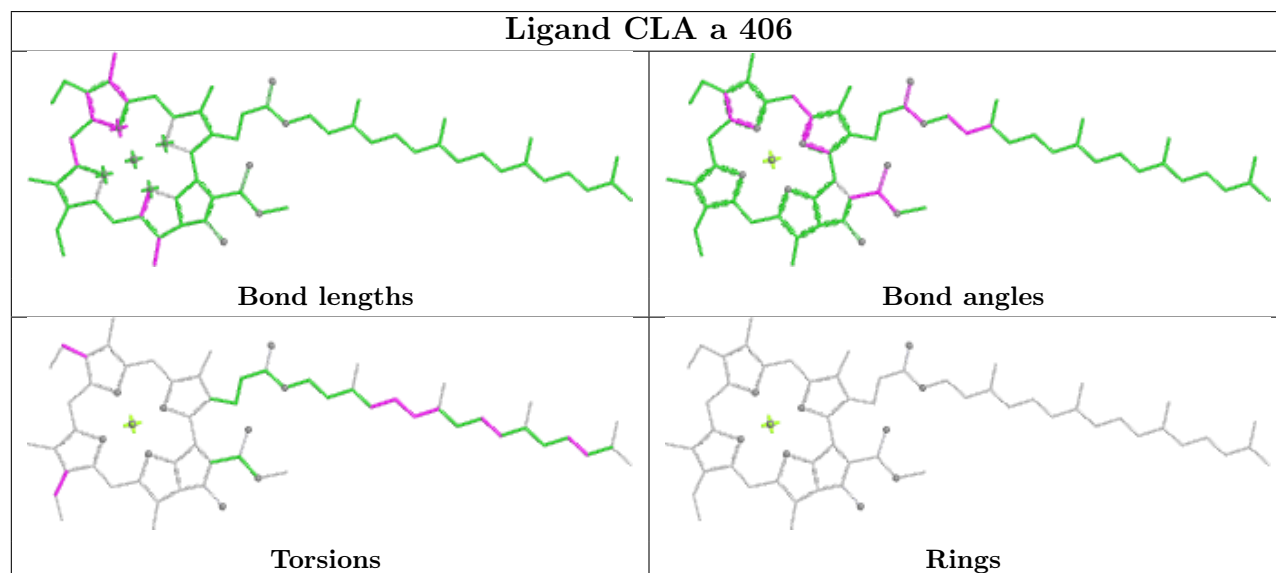
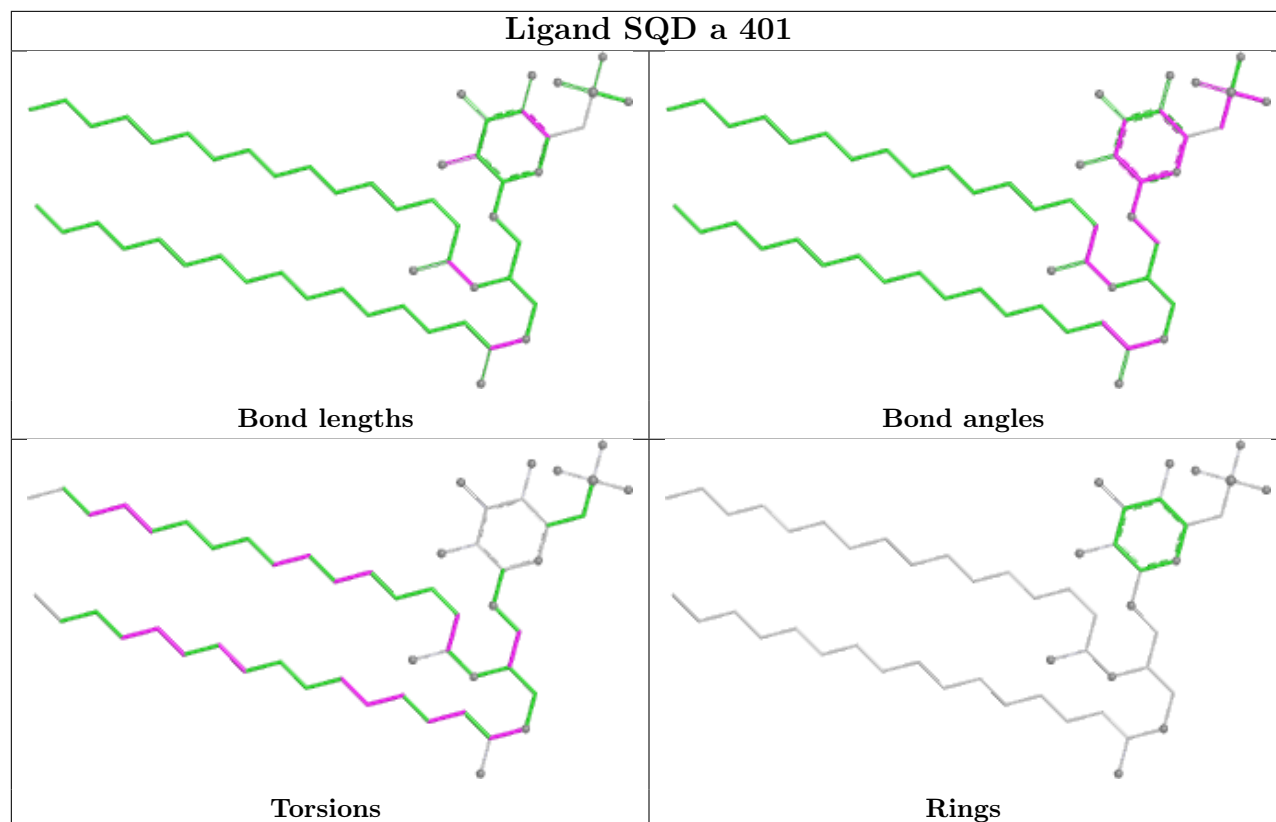


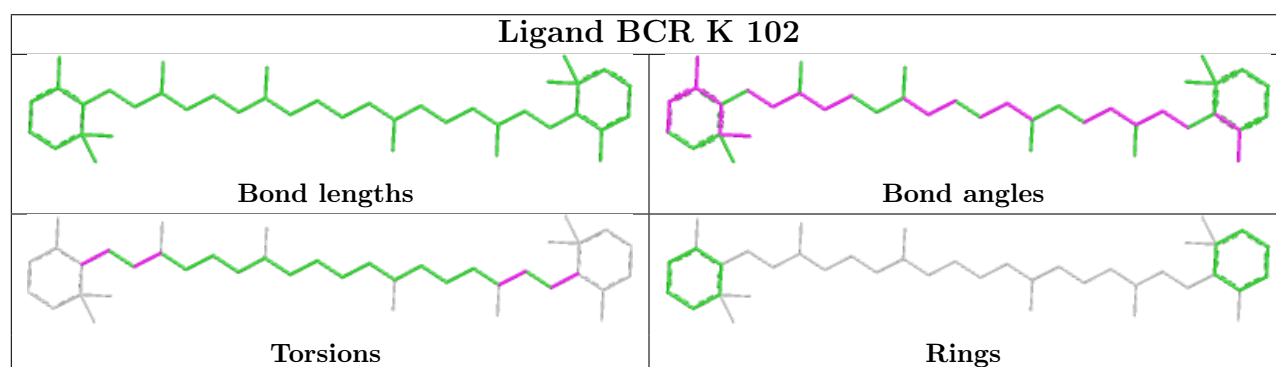
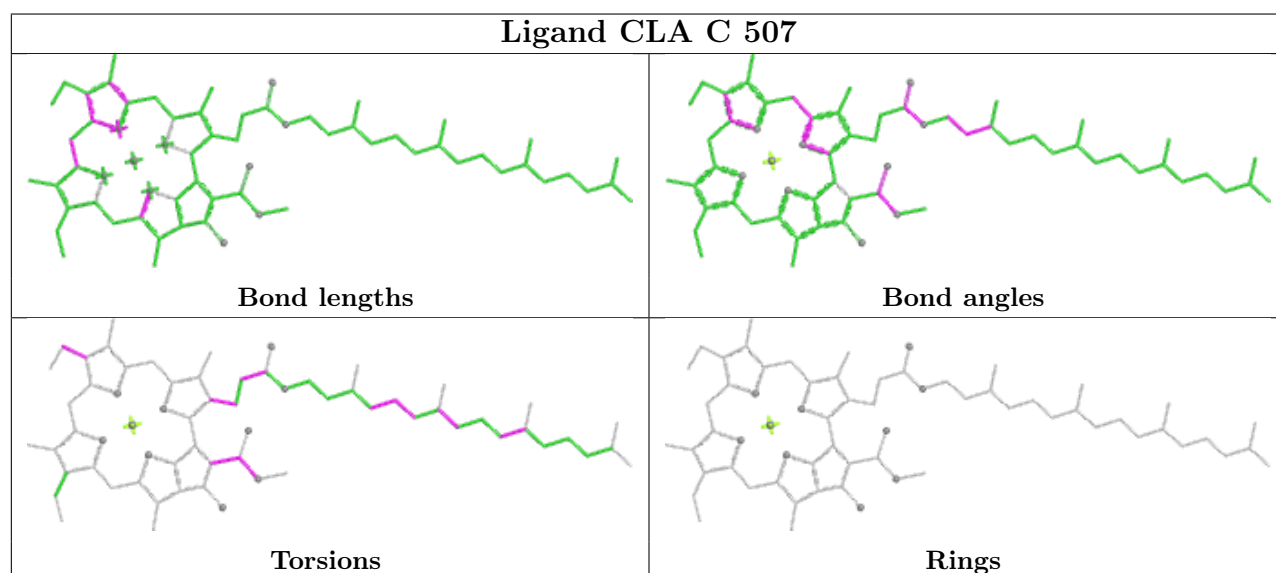
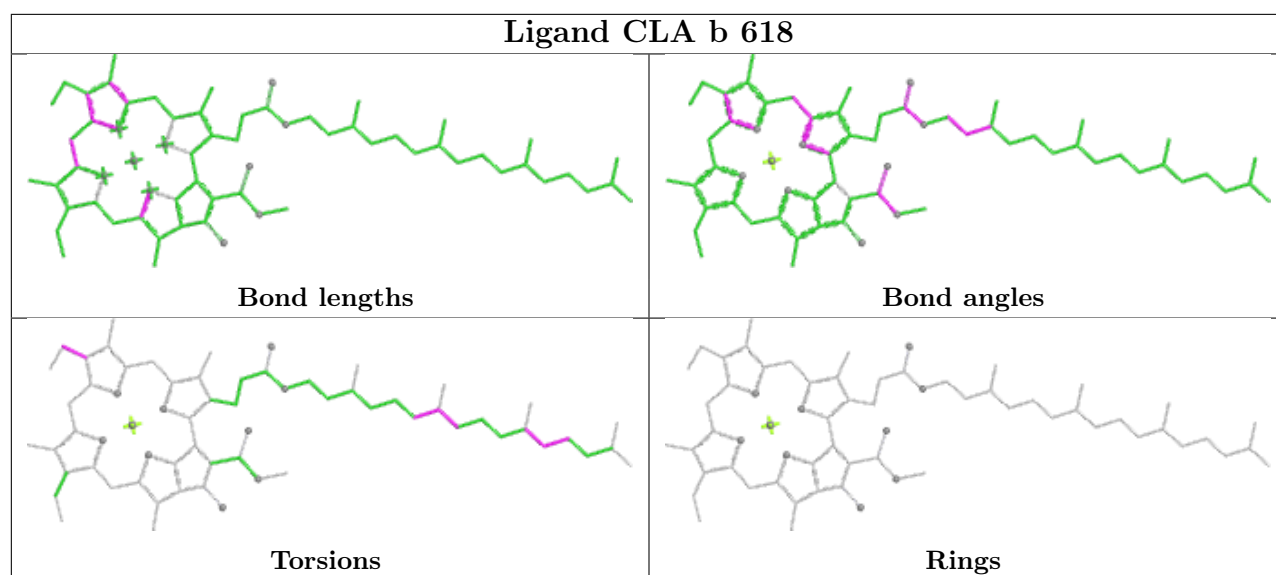
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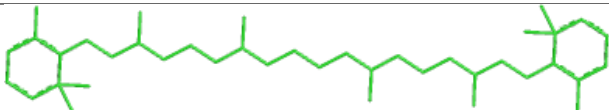
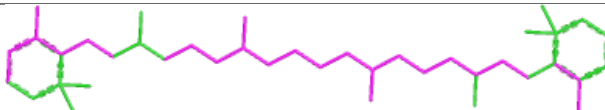
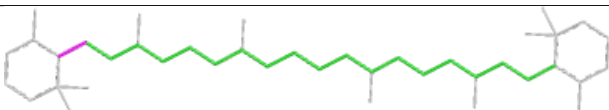
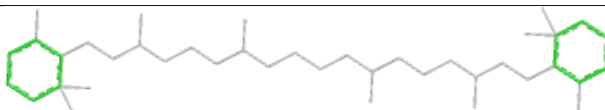


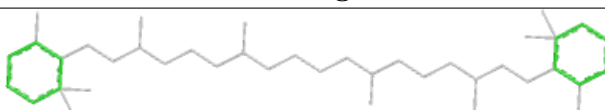
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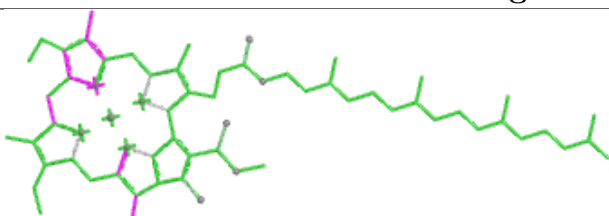
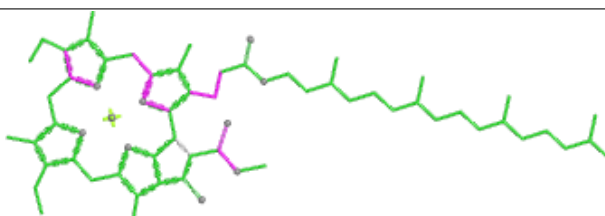
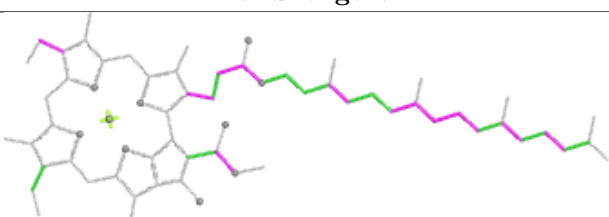
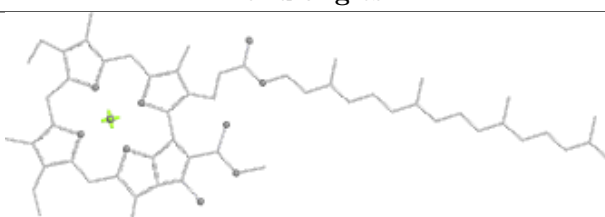


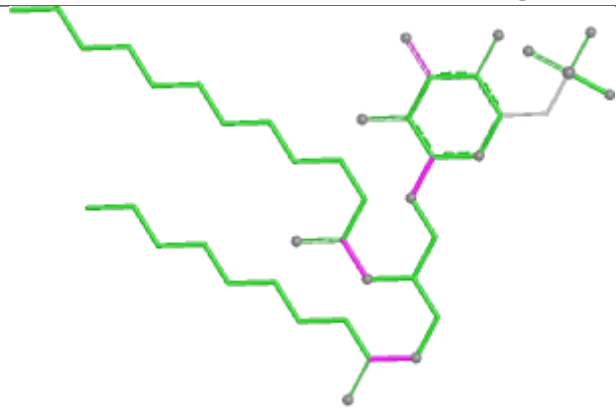
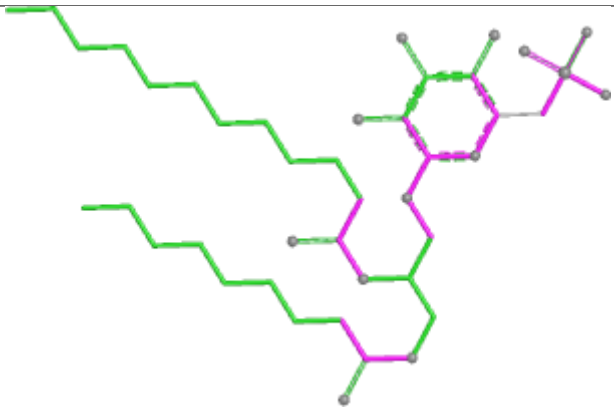
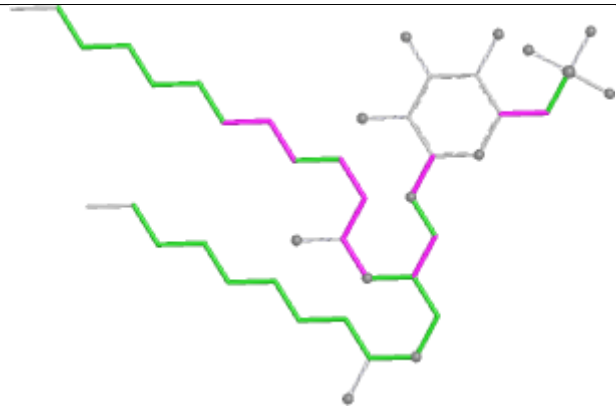
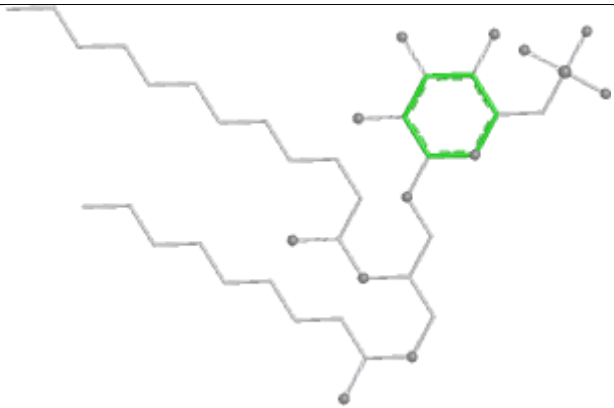


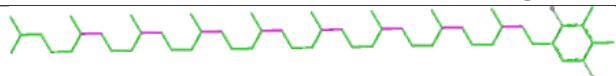
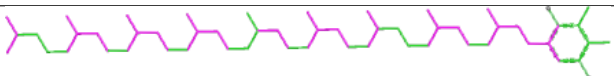
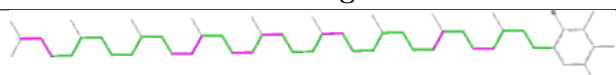
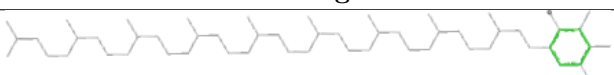


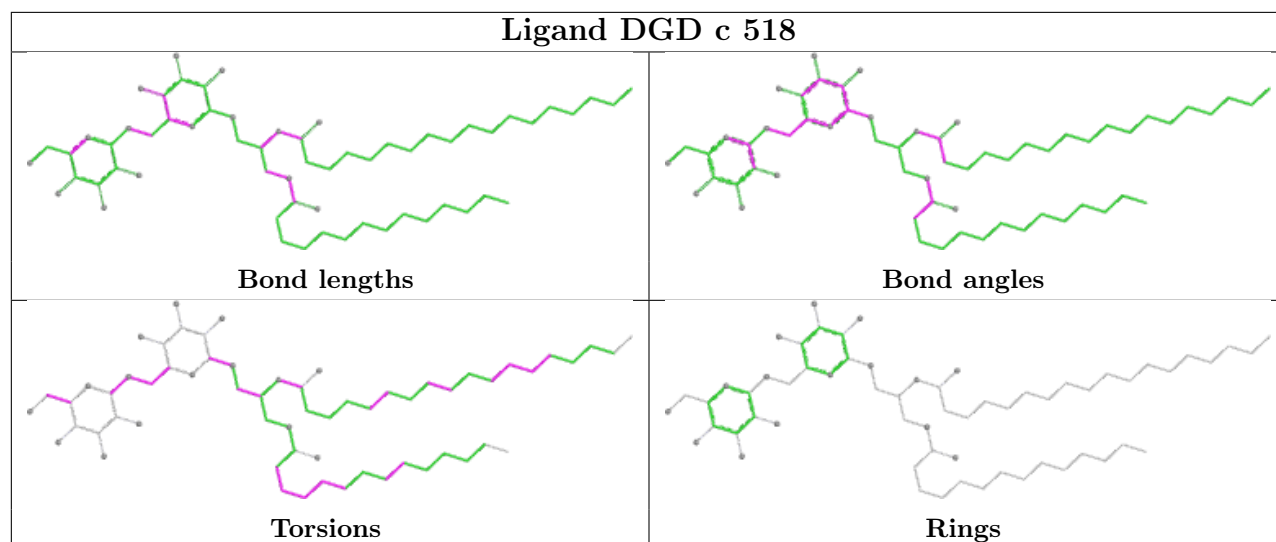
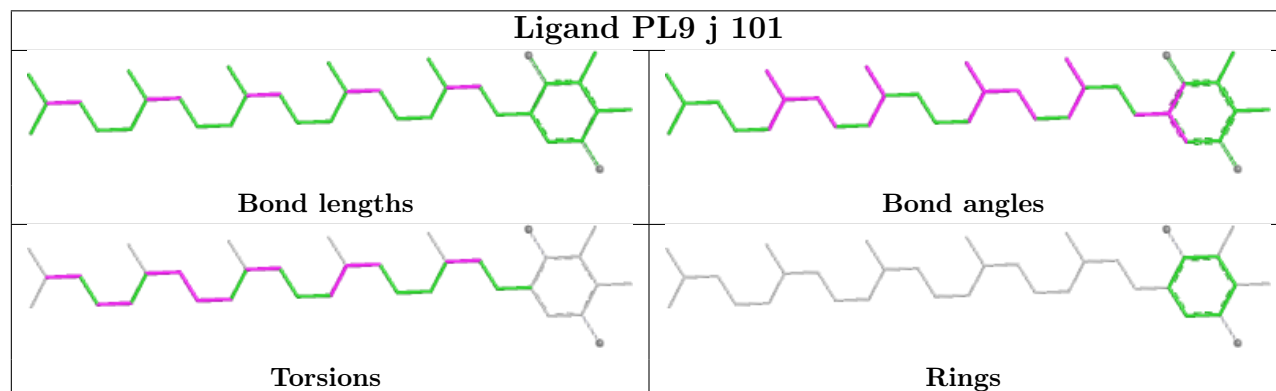
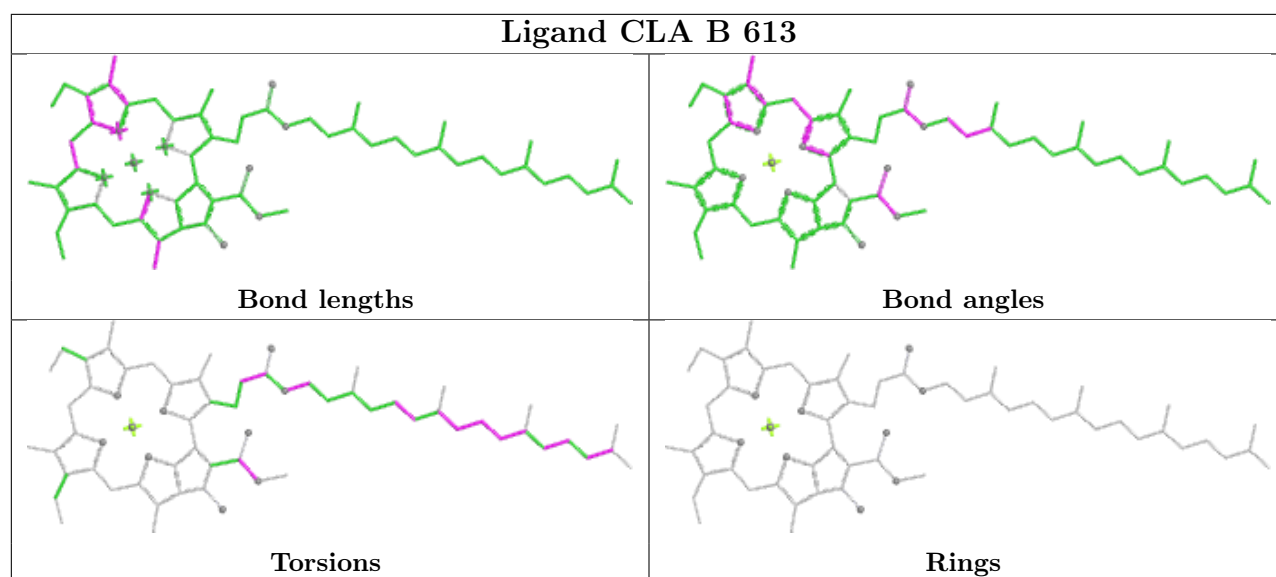
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

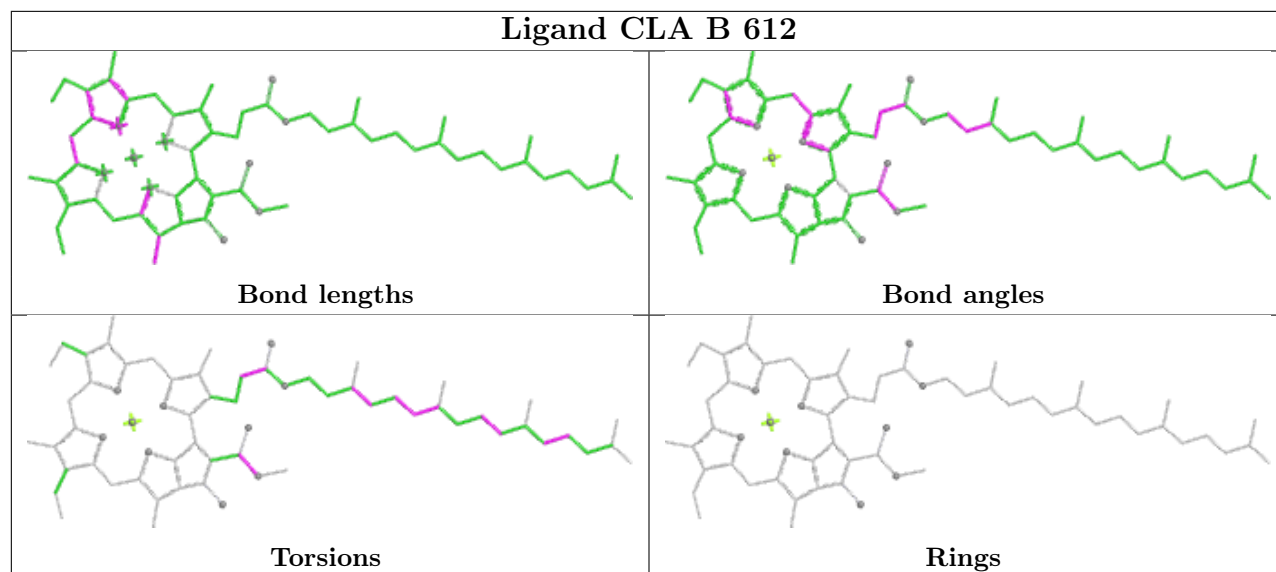
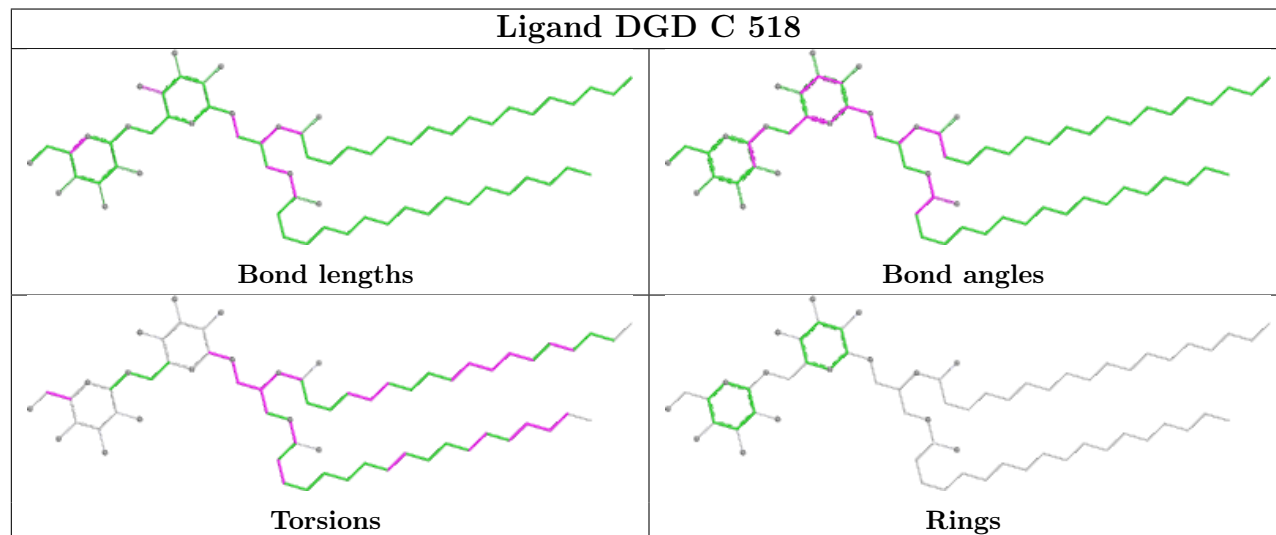
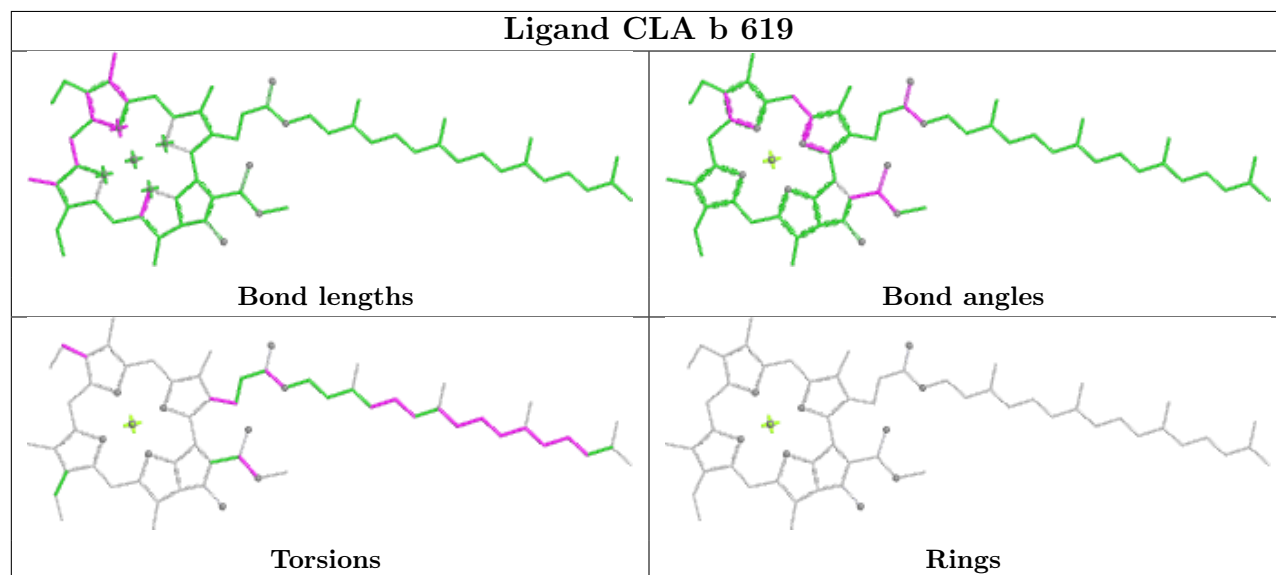
Ligand BCR A 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

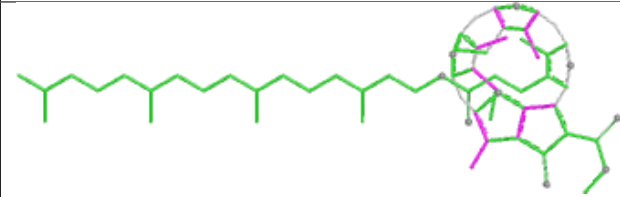
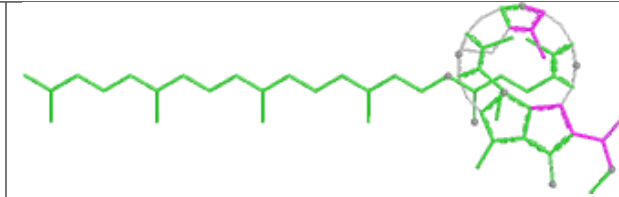
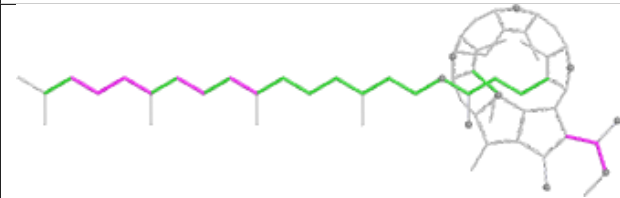
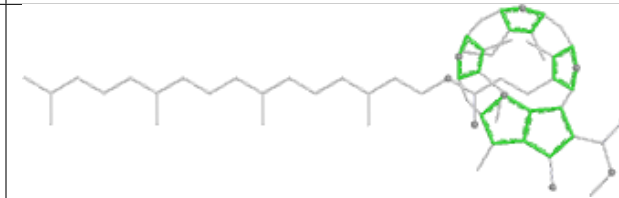
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Bond lengths	Bond angles
	
Torsions	Rings

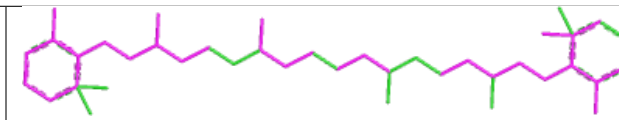
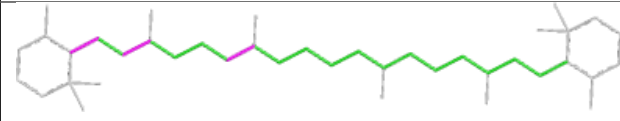
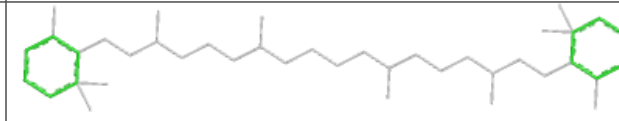
Ligand SQD D 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

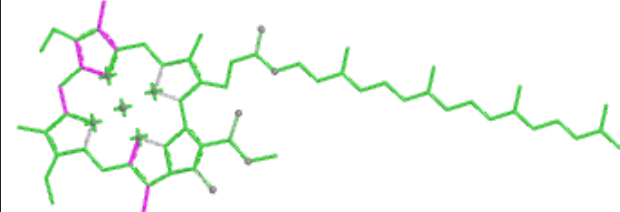
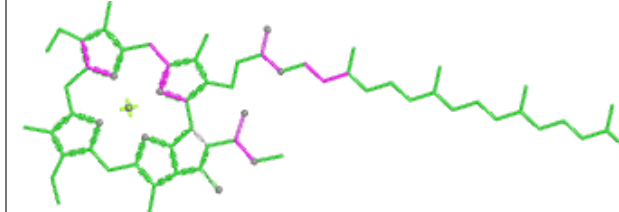
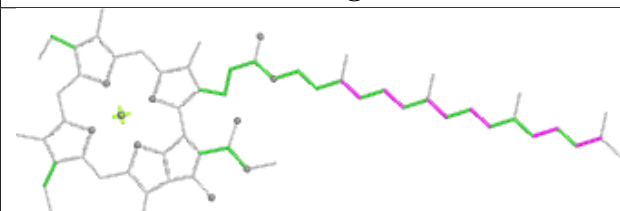
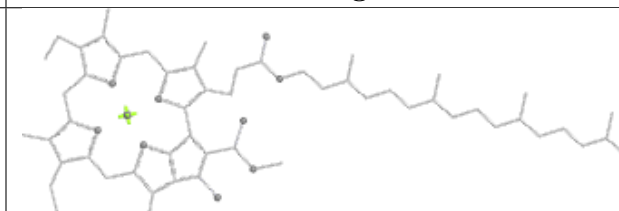
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Bond lengths	Bond angles
	
Torsions	Rings

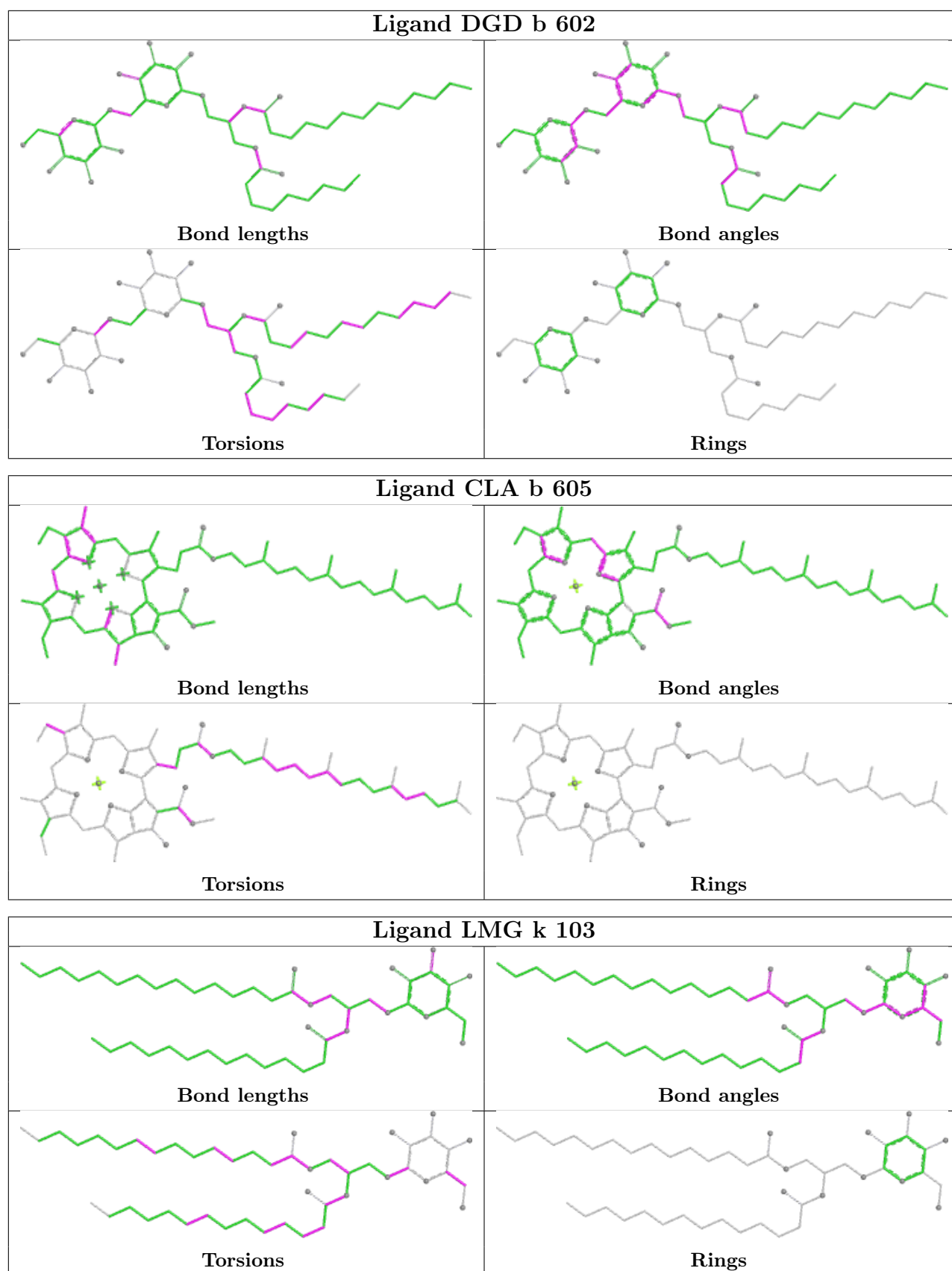


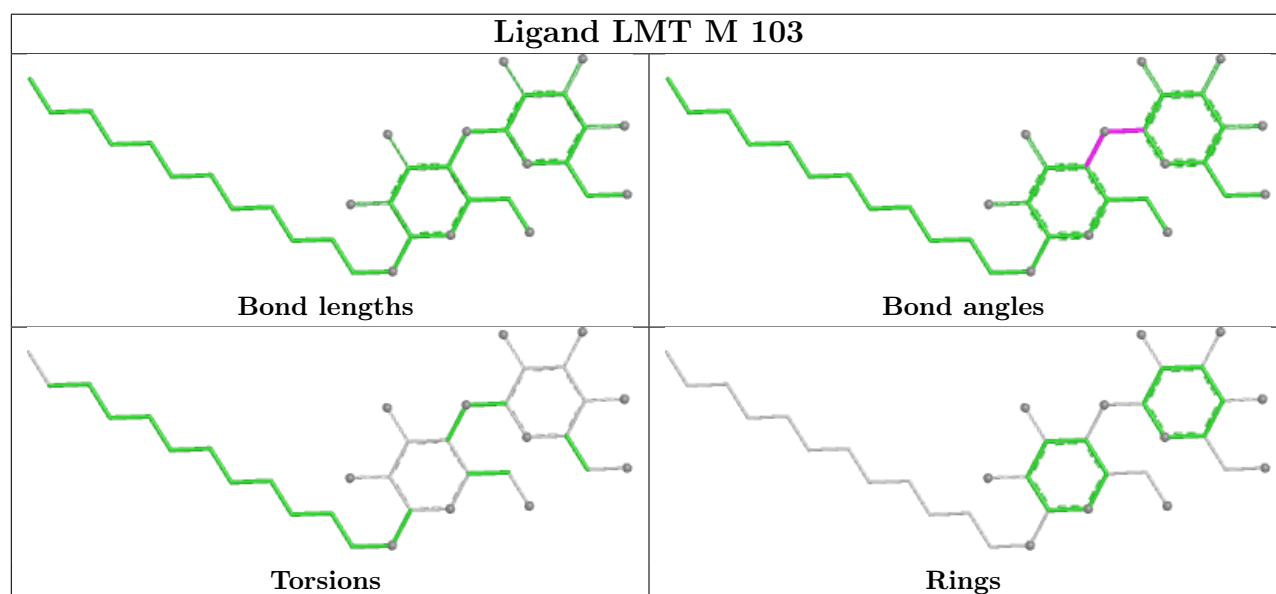
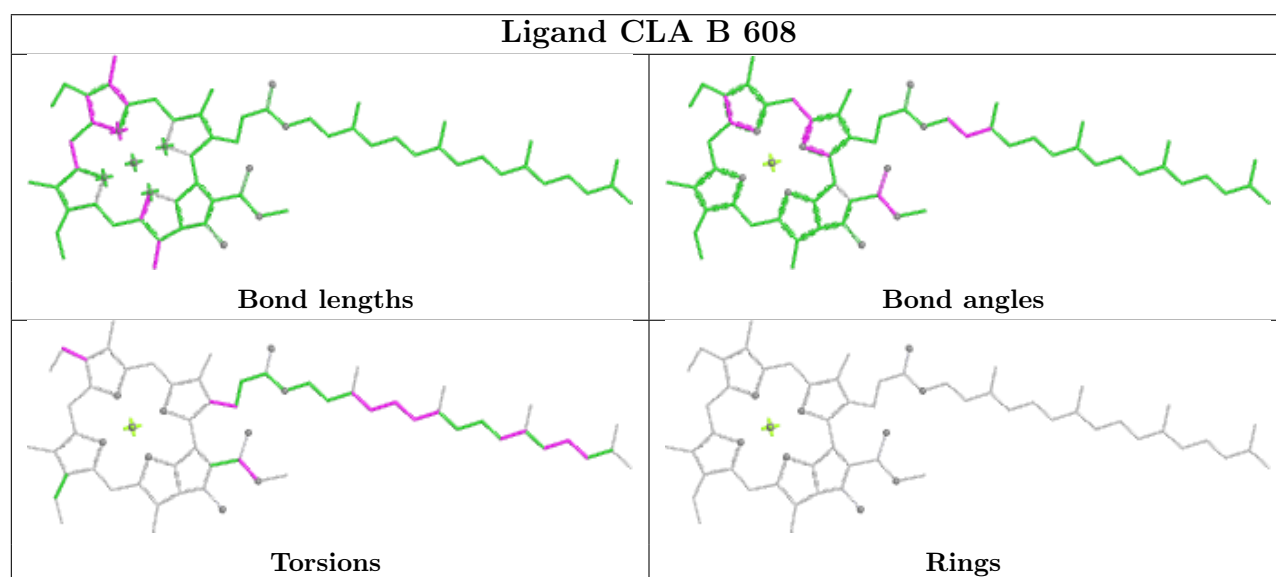
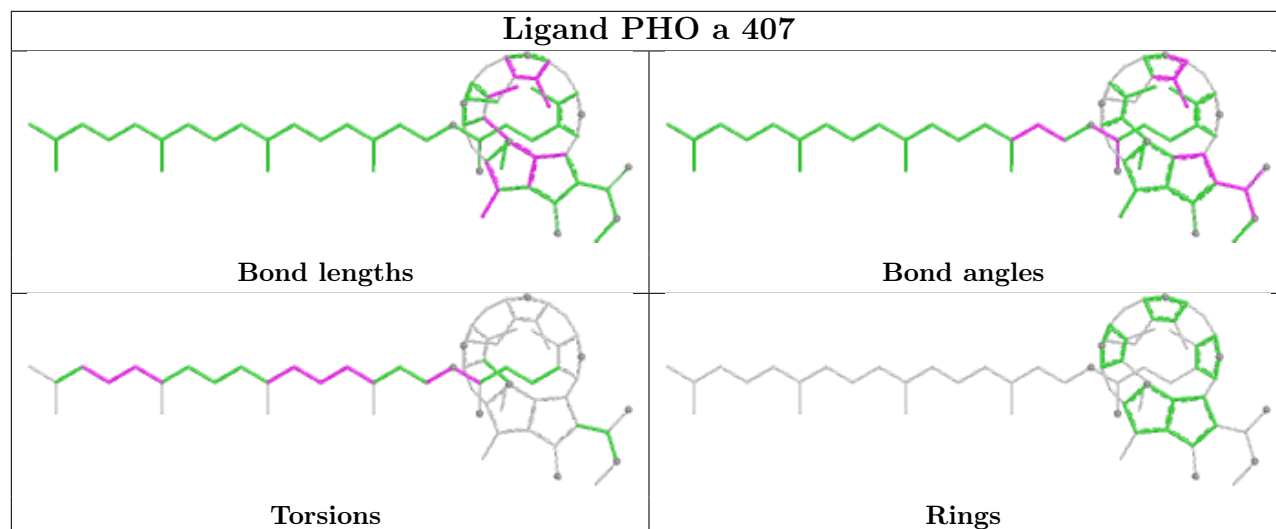
Ligand CLA B 612**Ligand DGD C 518****Ligand CLA b 619**

Ligand PHO a 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

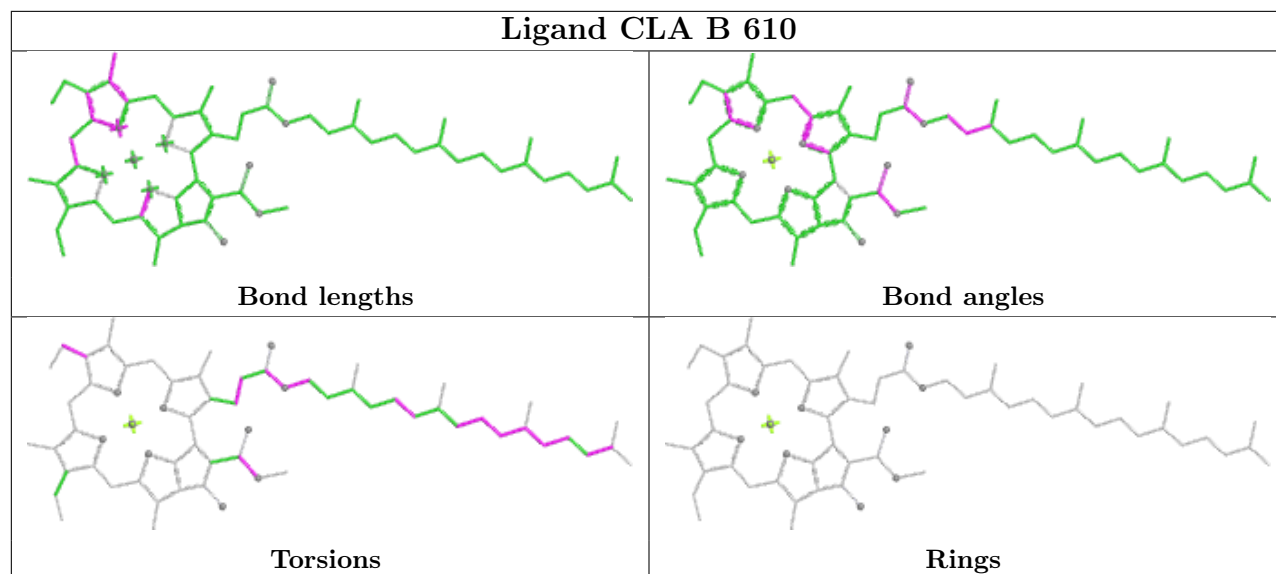
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

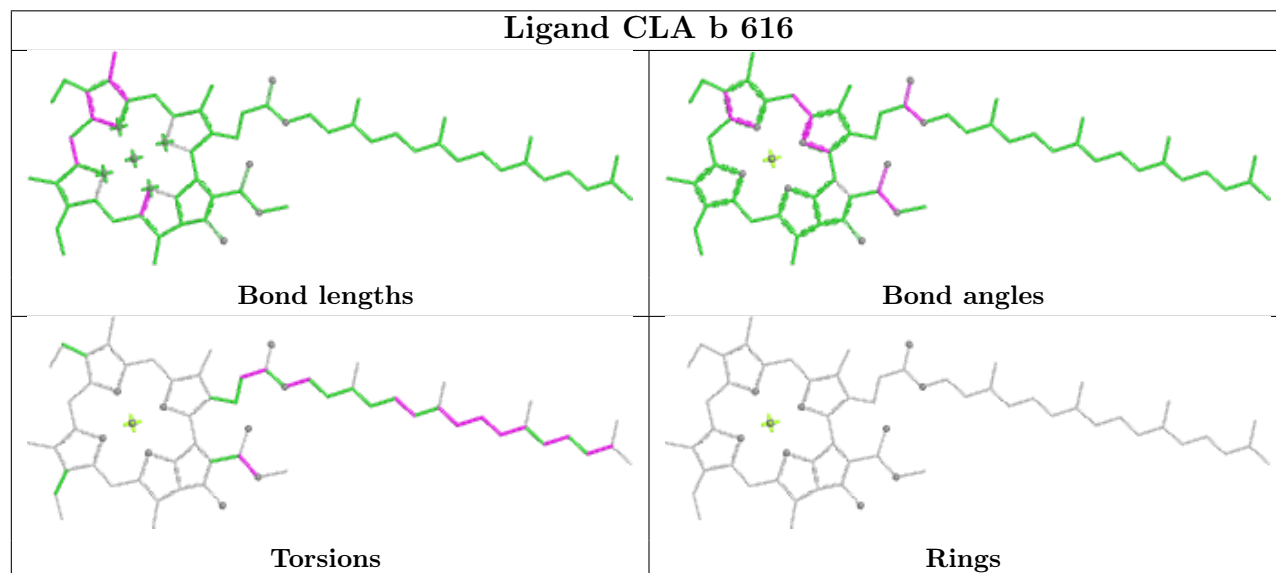




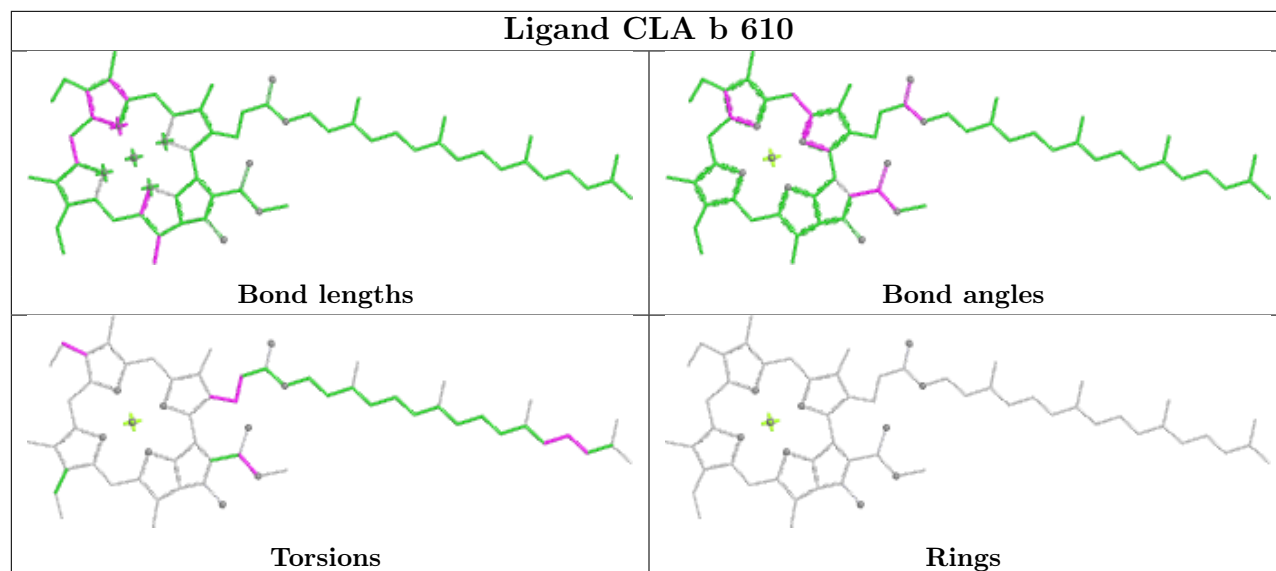
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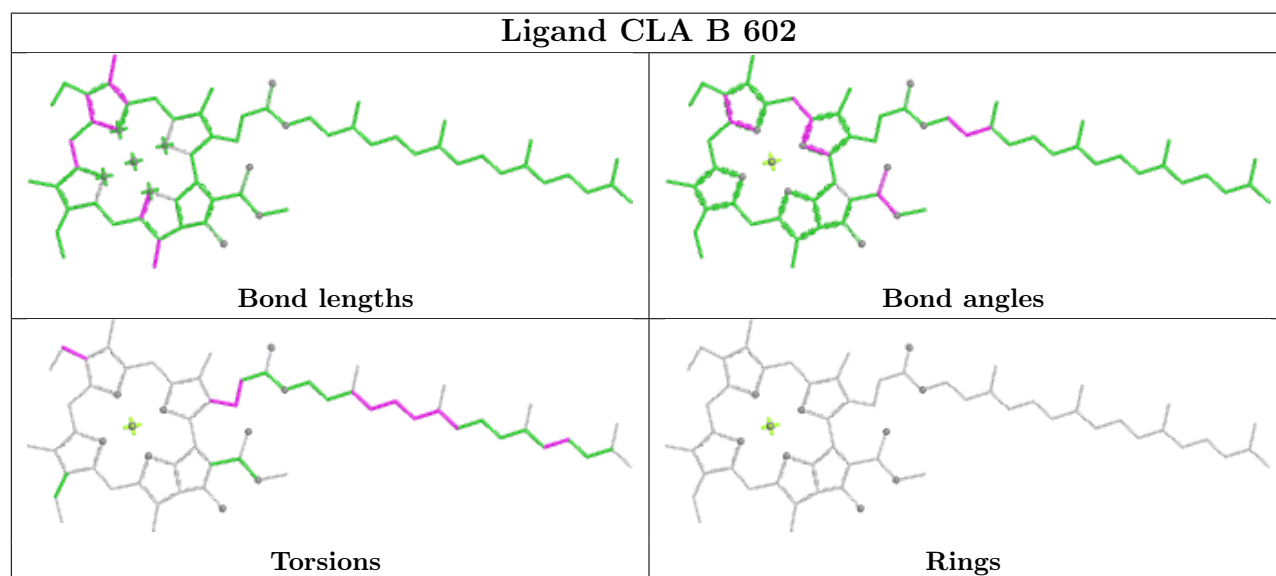
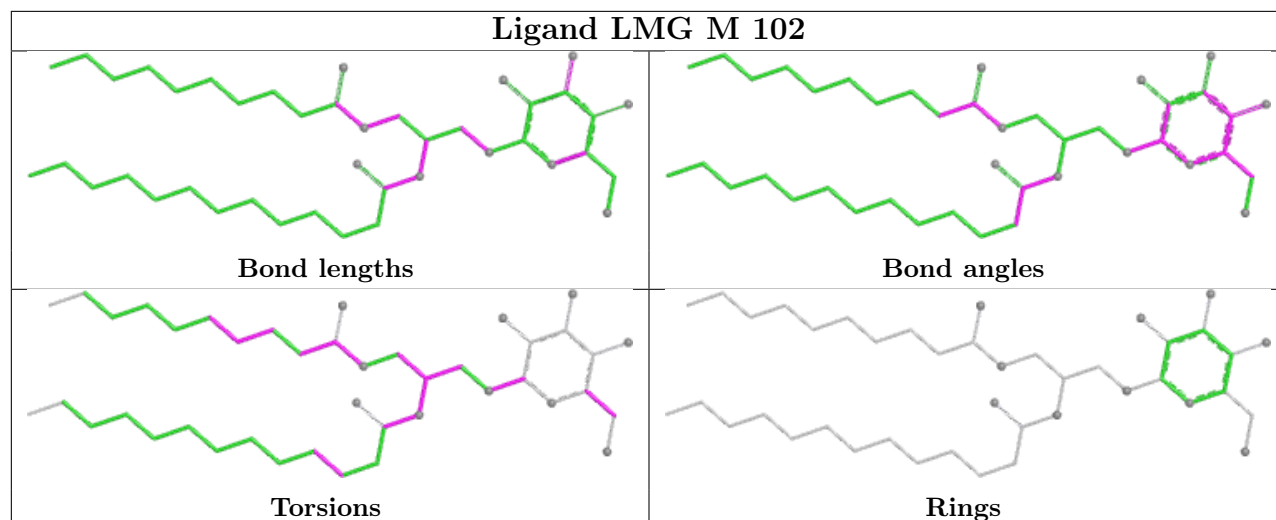


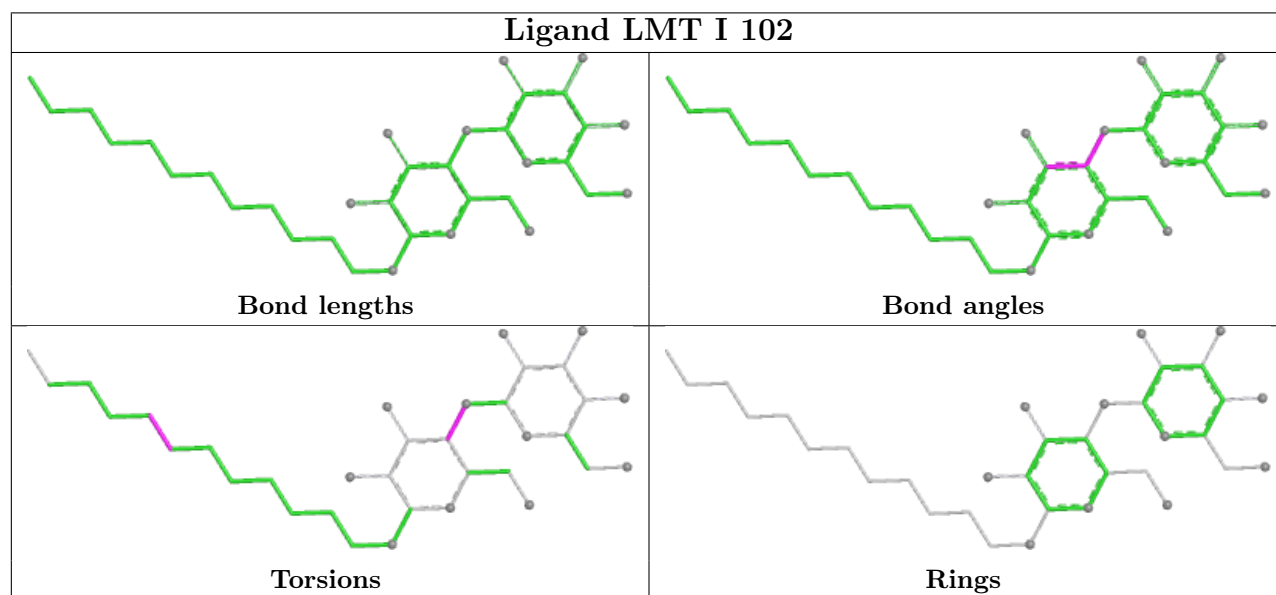
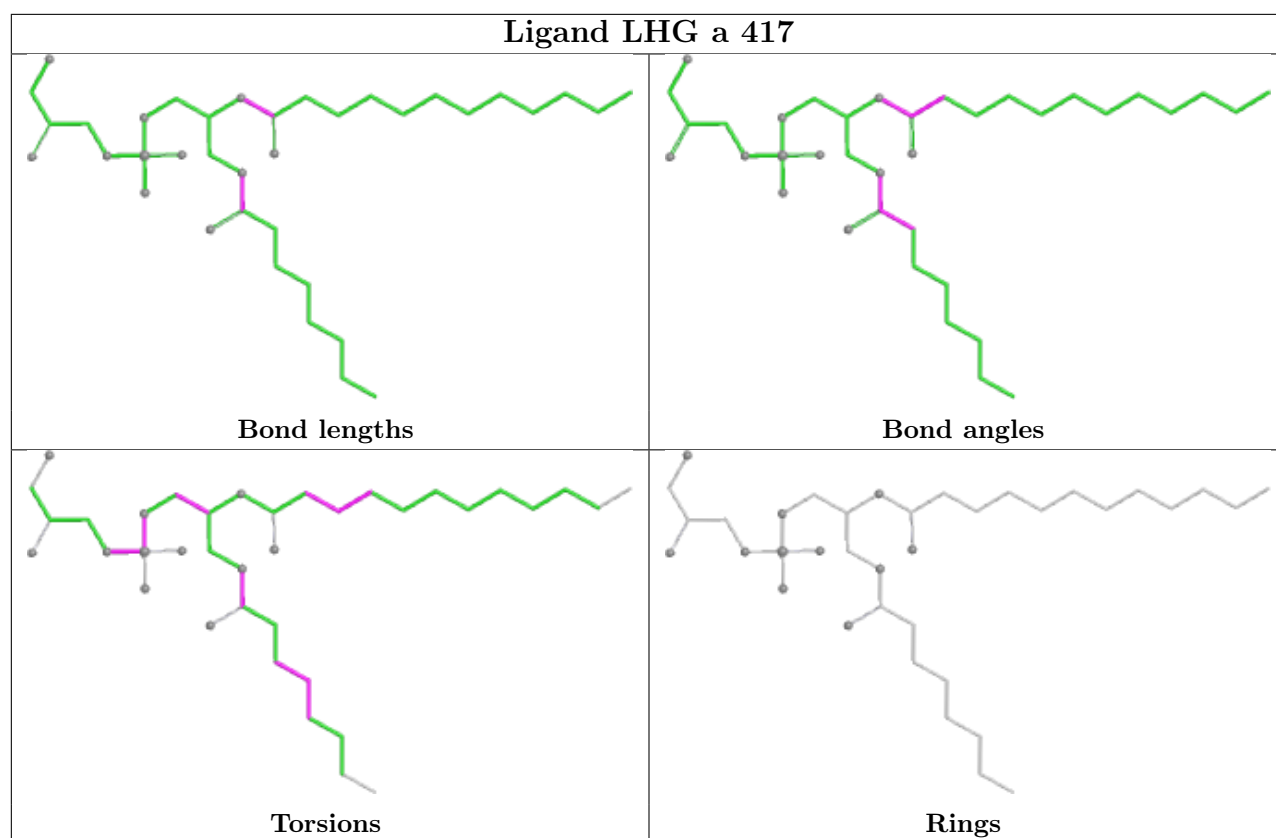
Ligand CLA b 616

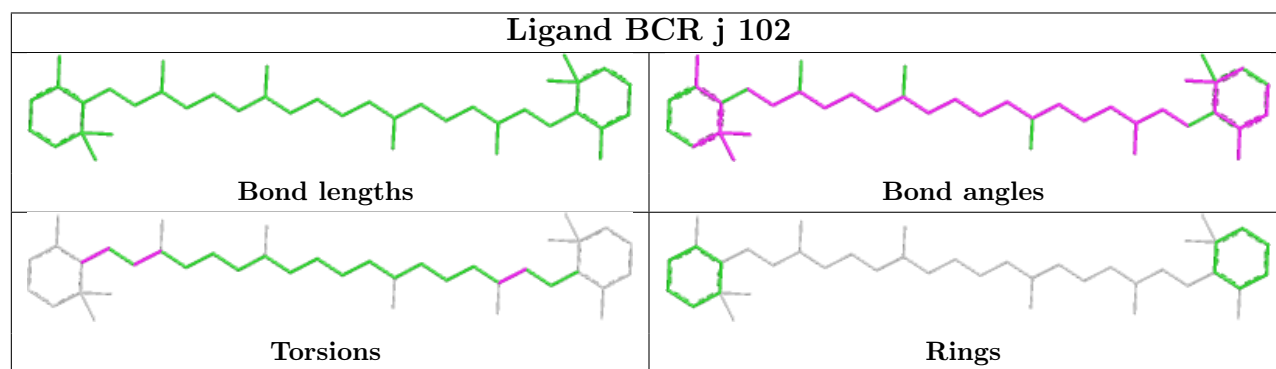
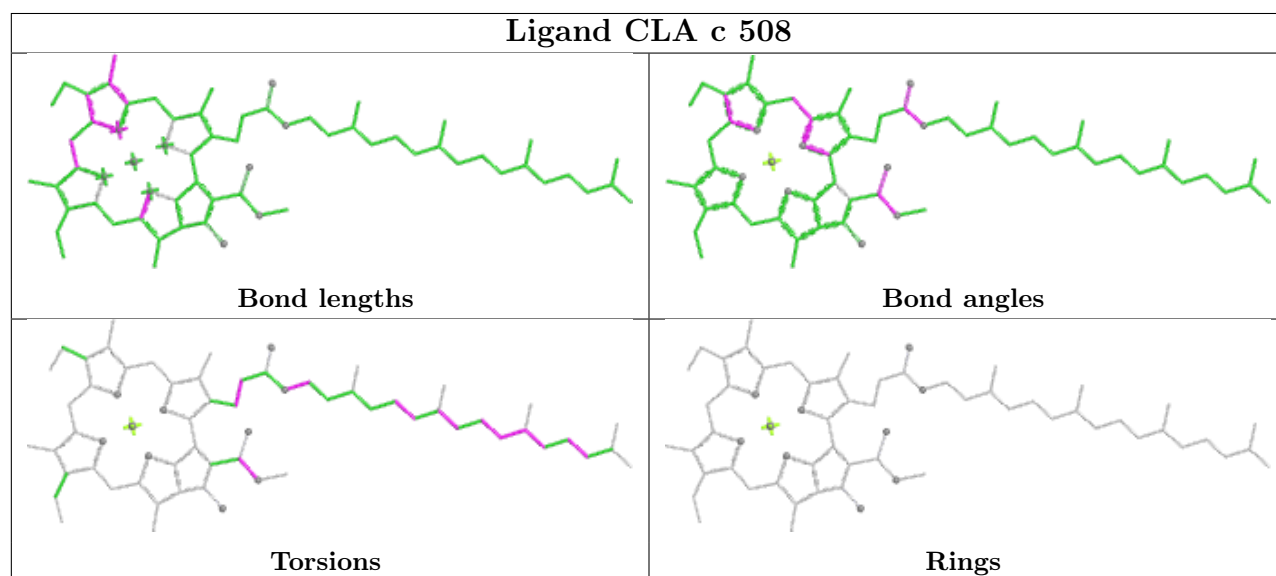
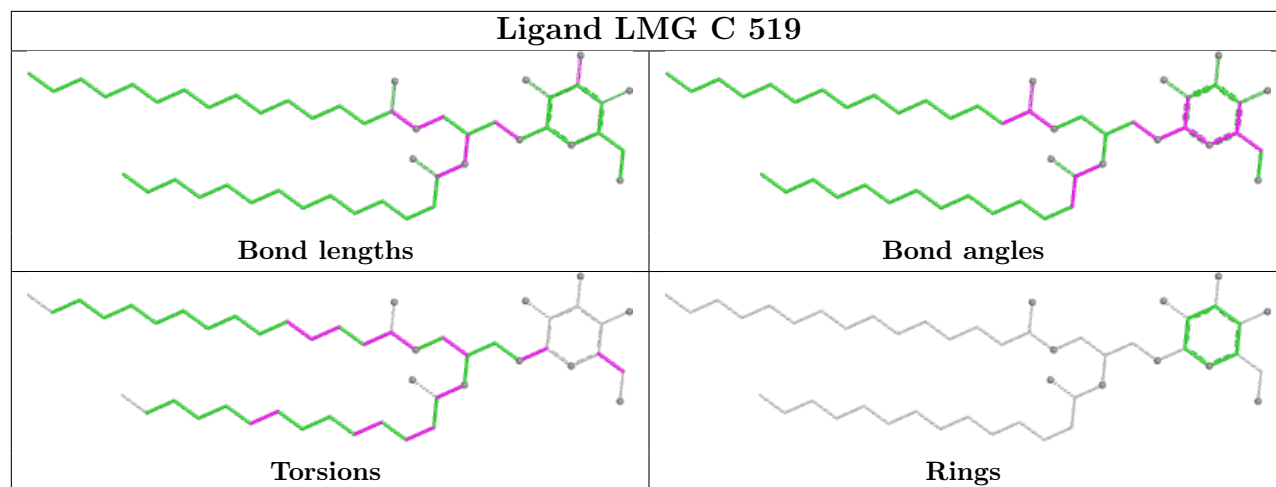


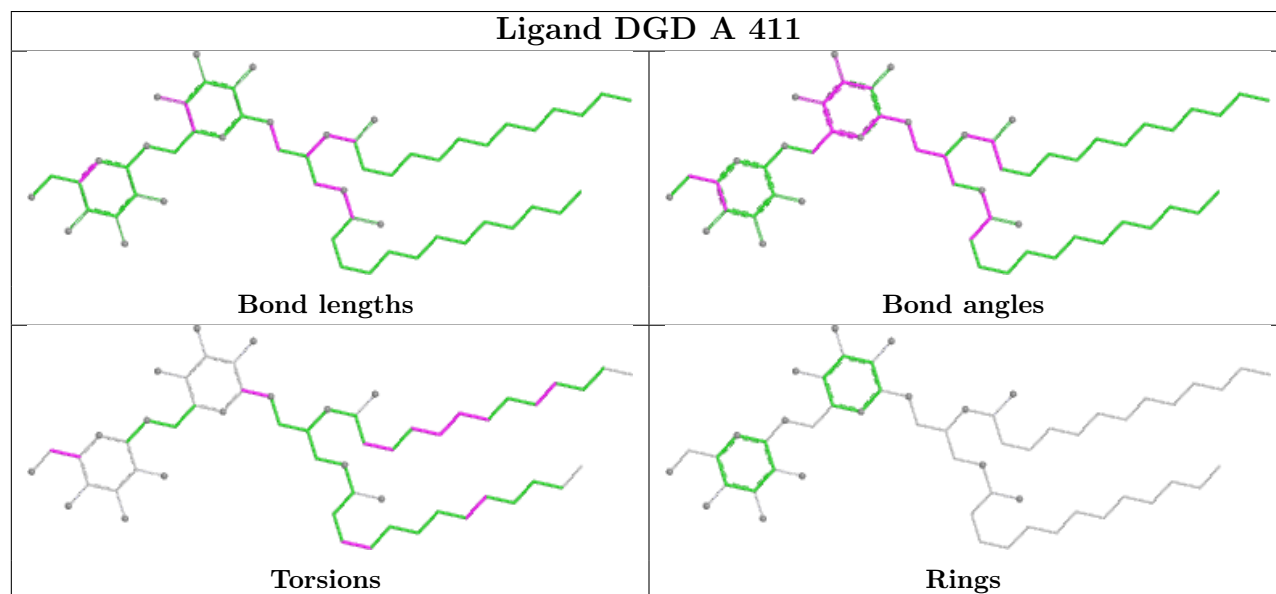
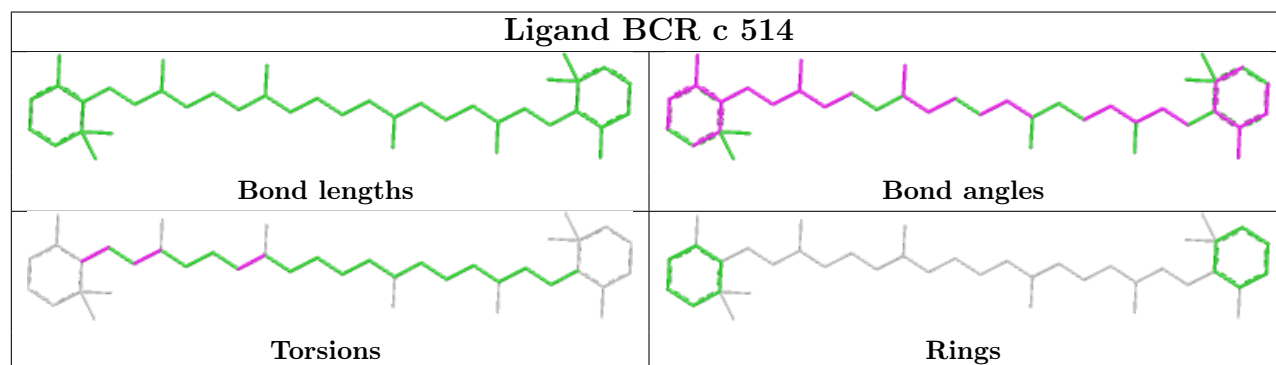
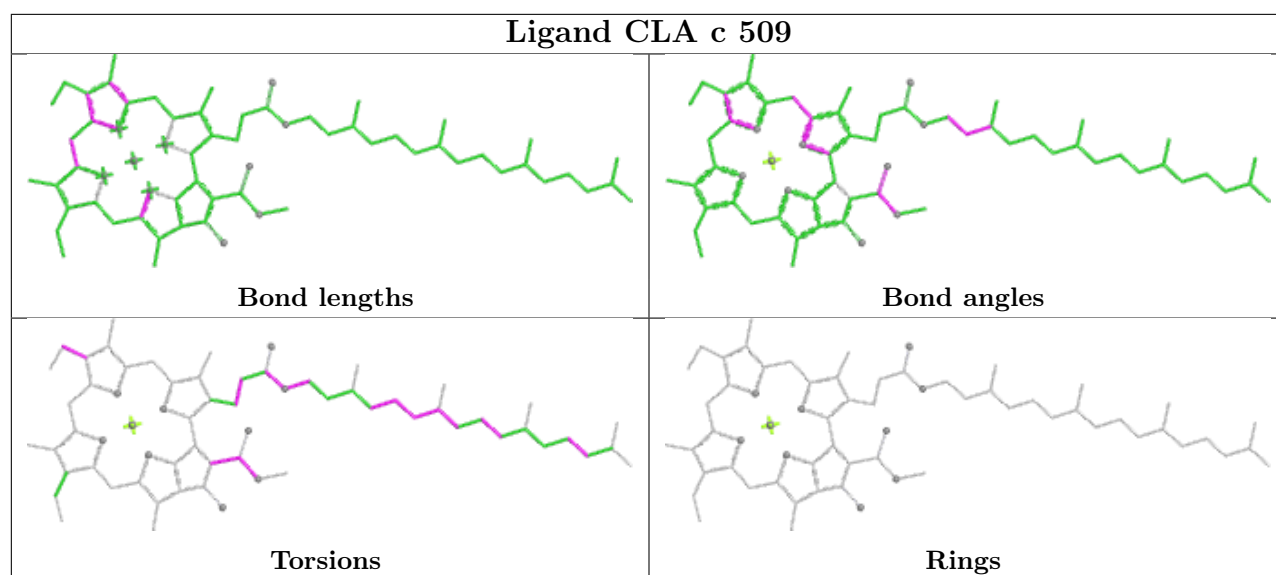
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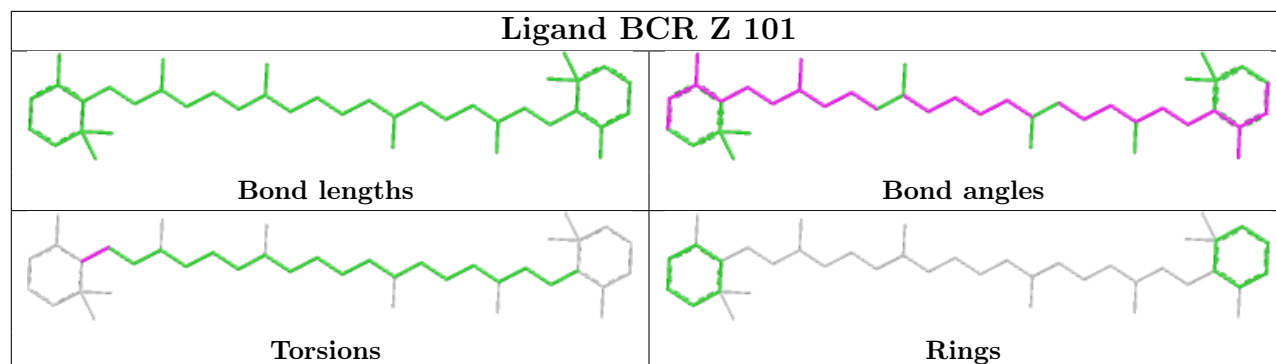
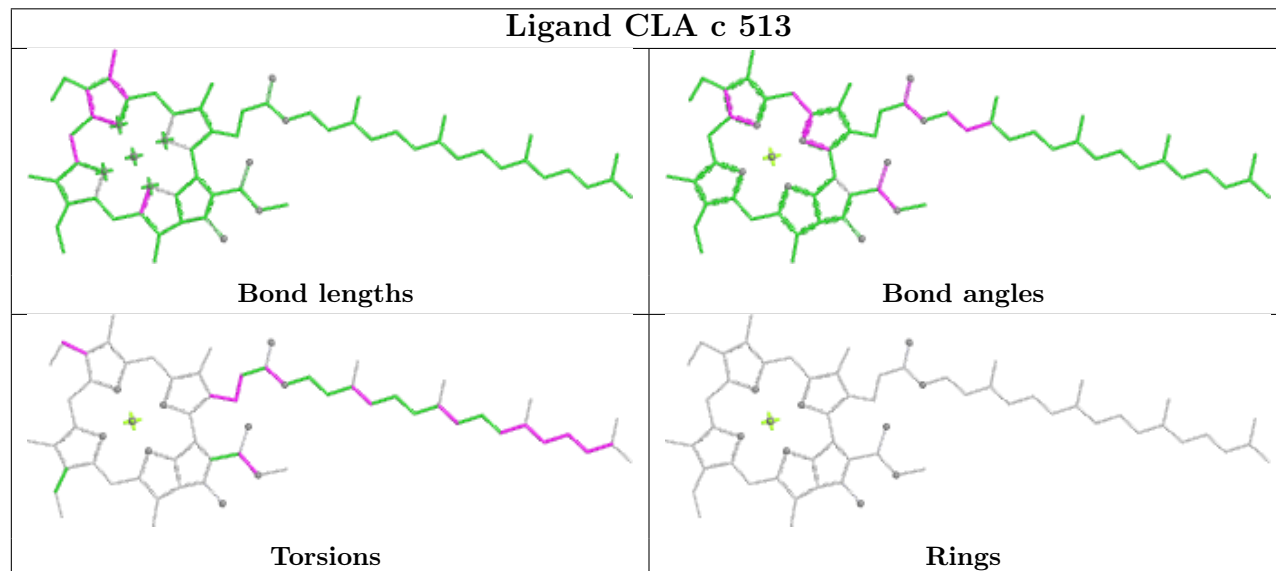
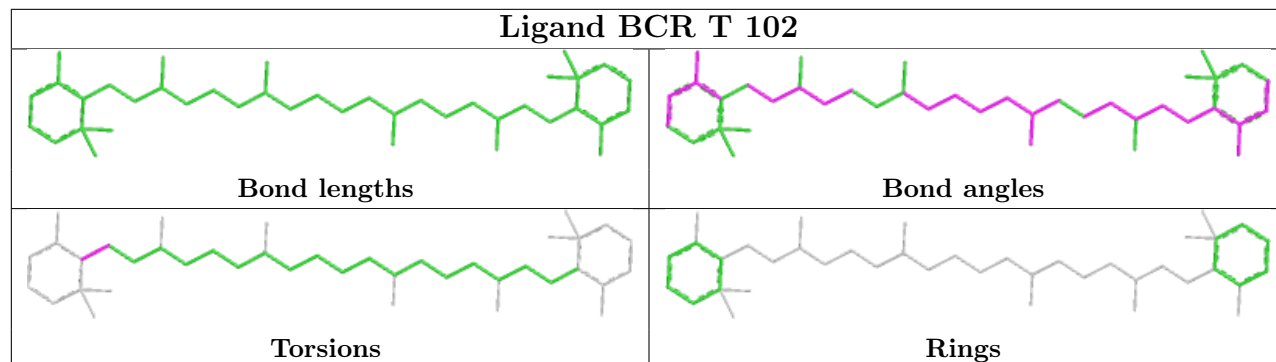


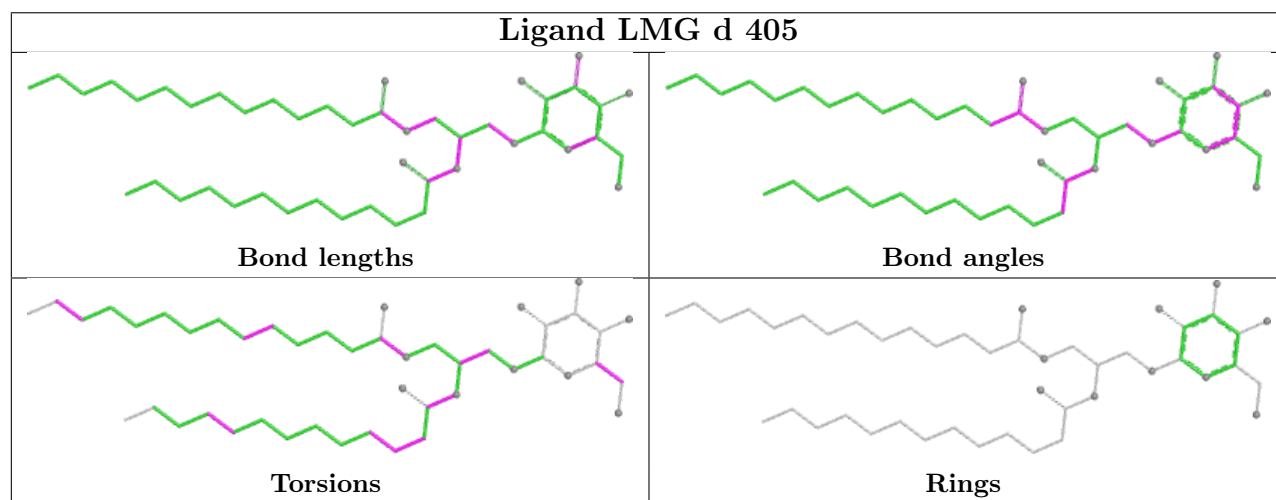
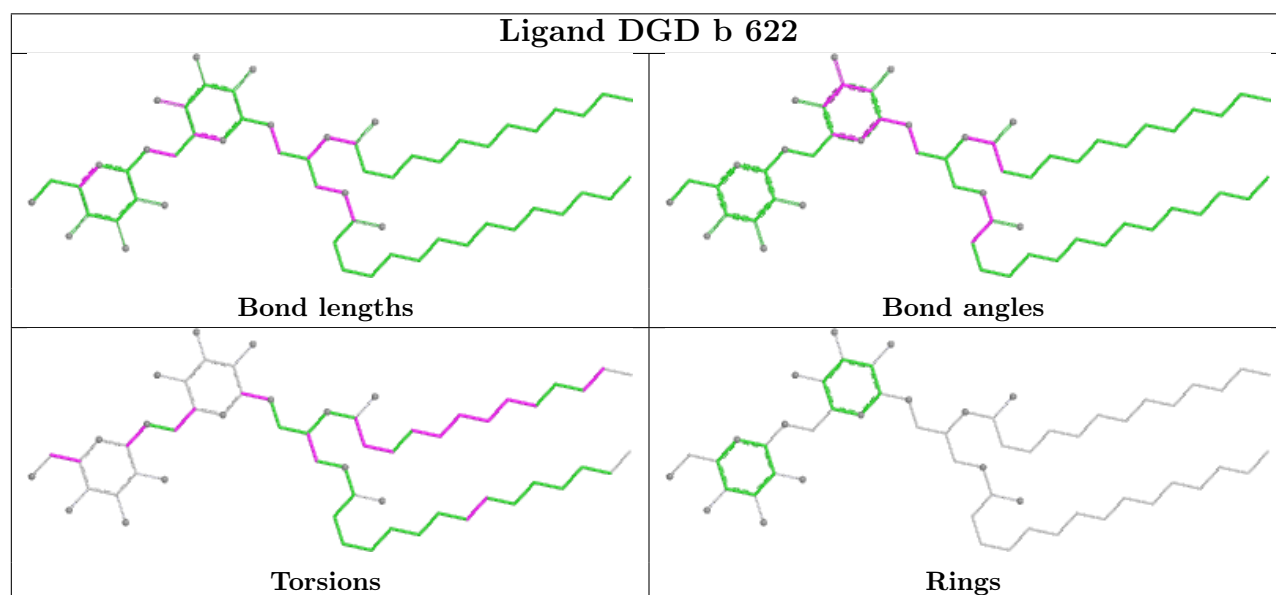
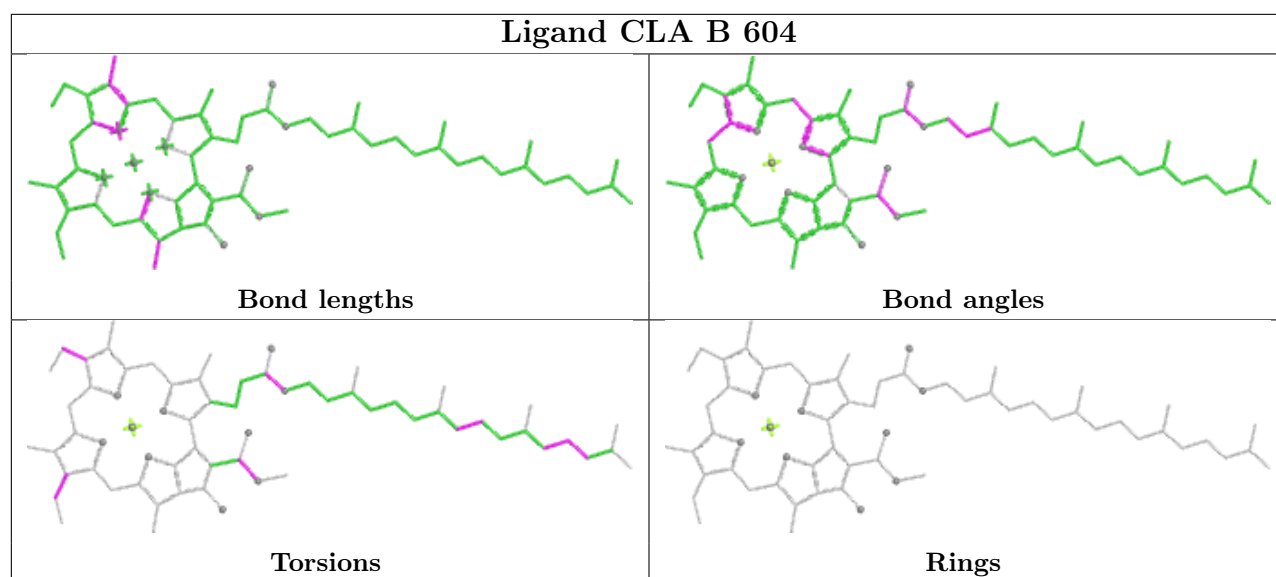


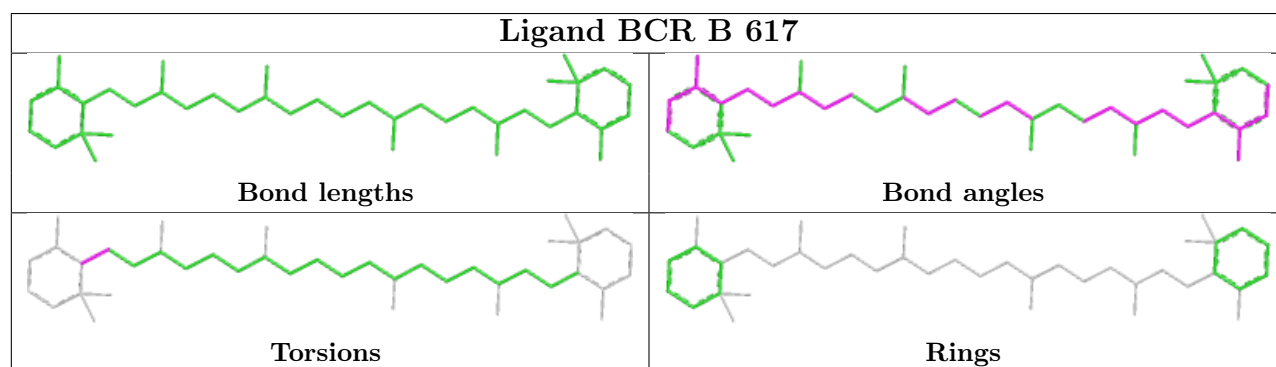
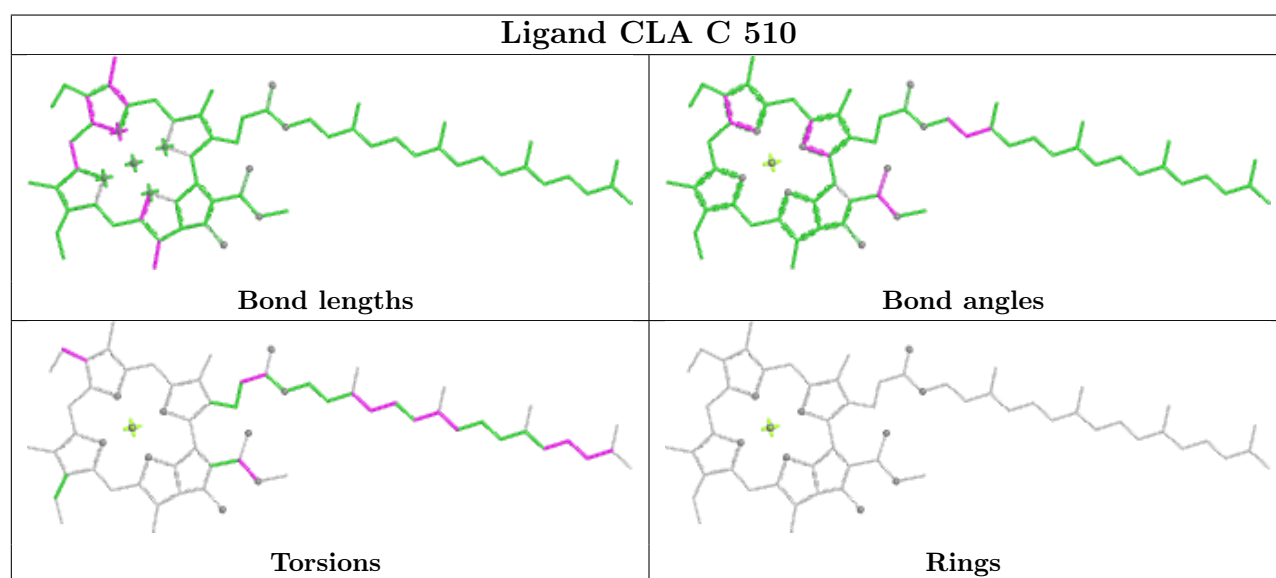
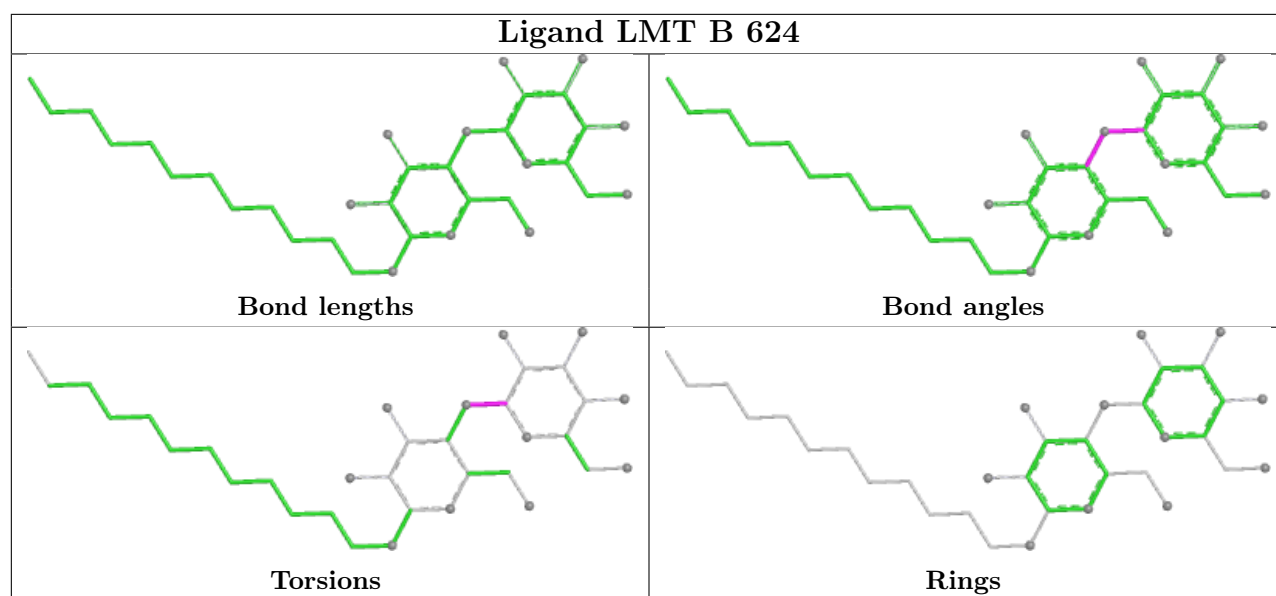


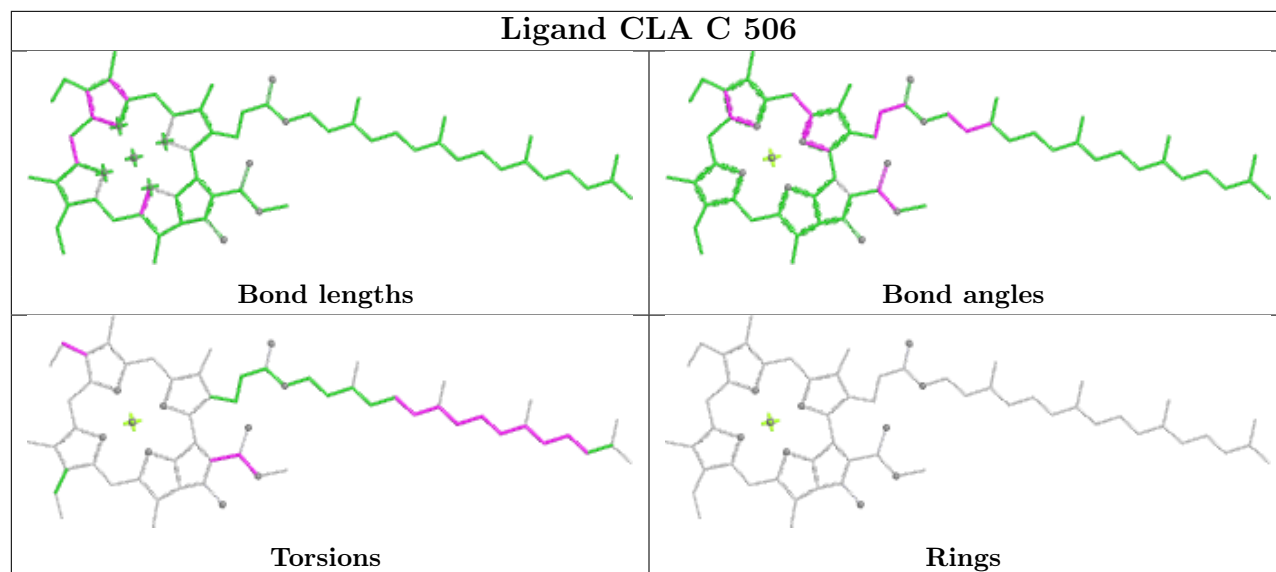
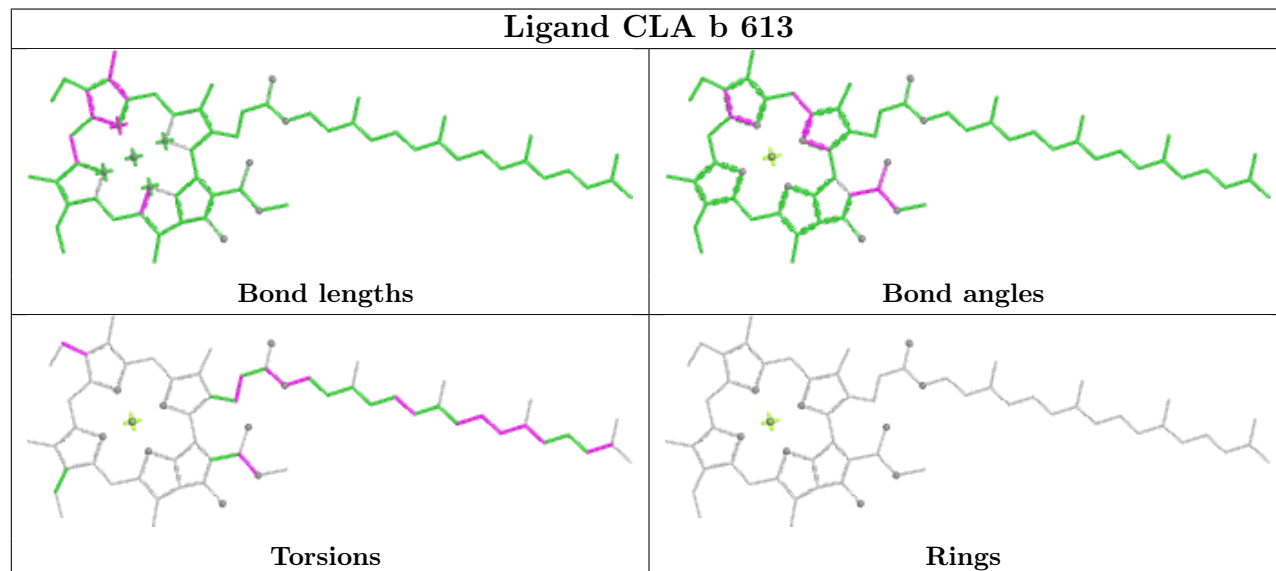
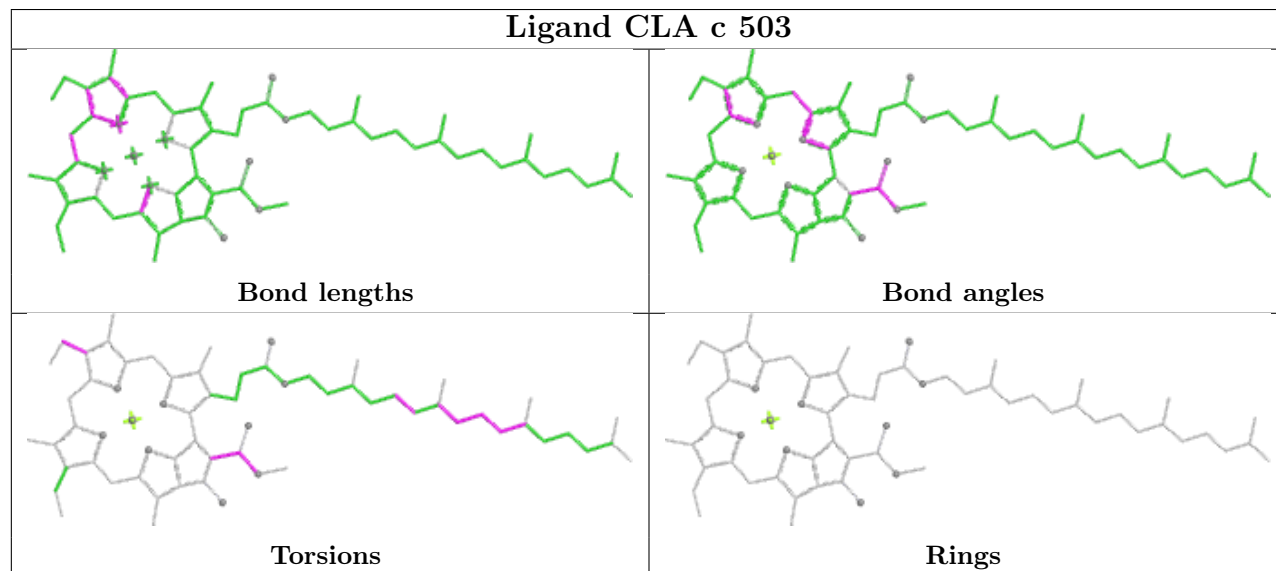


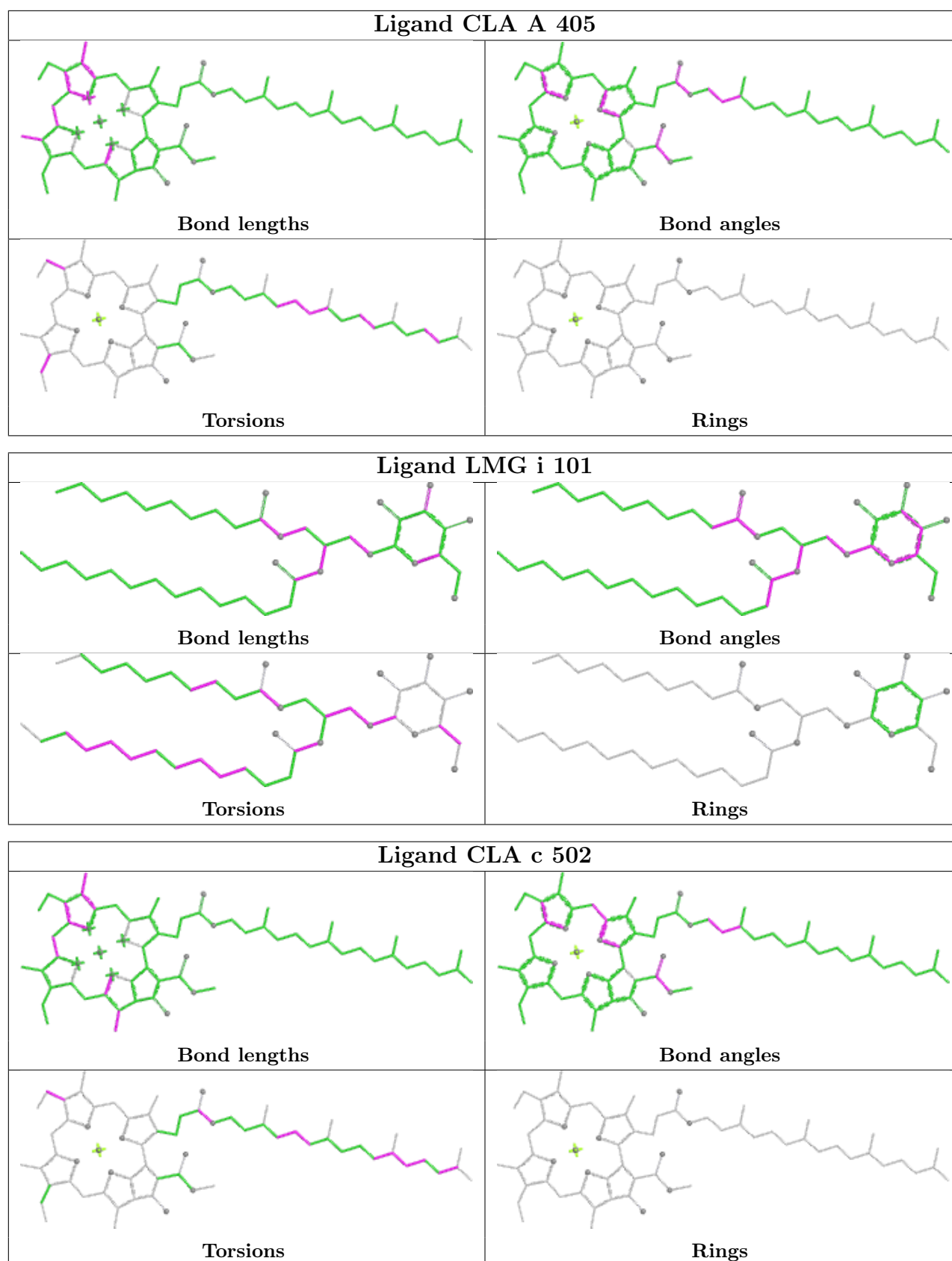


Ligand BCR Z 101**Ligand CLA c 513****Ligand BCR T 102**

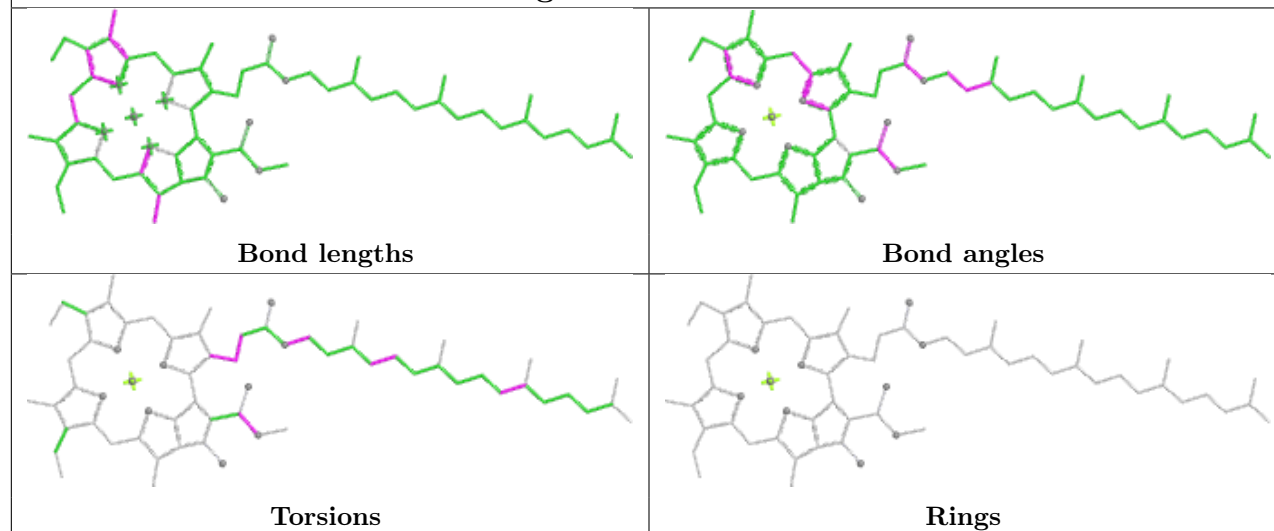




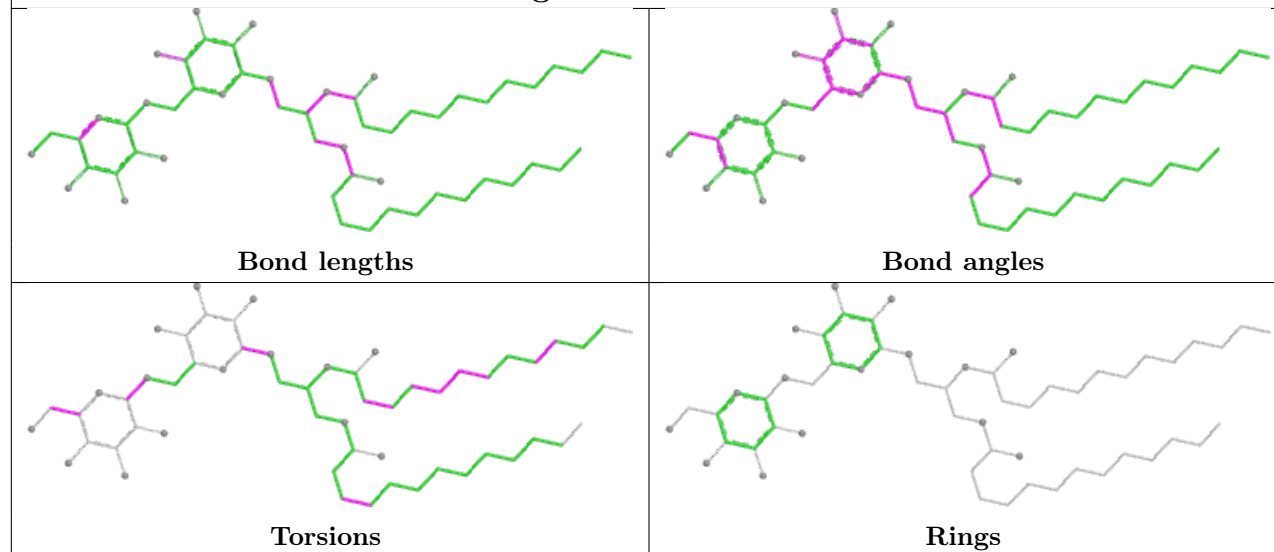
Ligand CLA C 506**Ligand CLA b 613****Ligand CLA c 503**



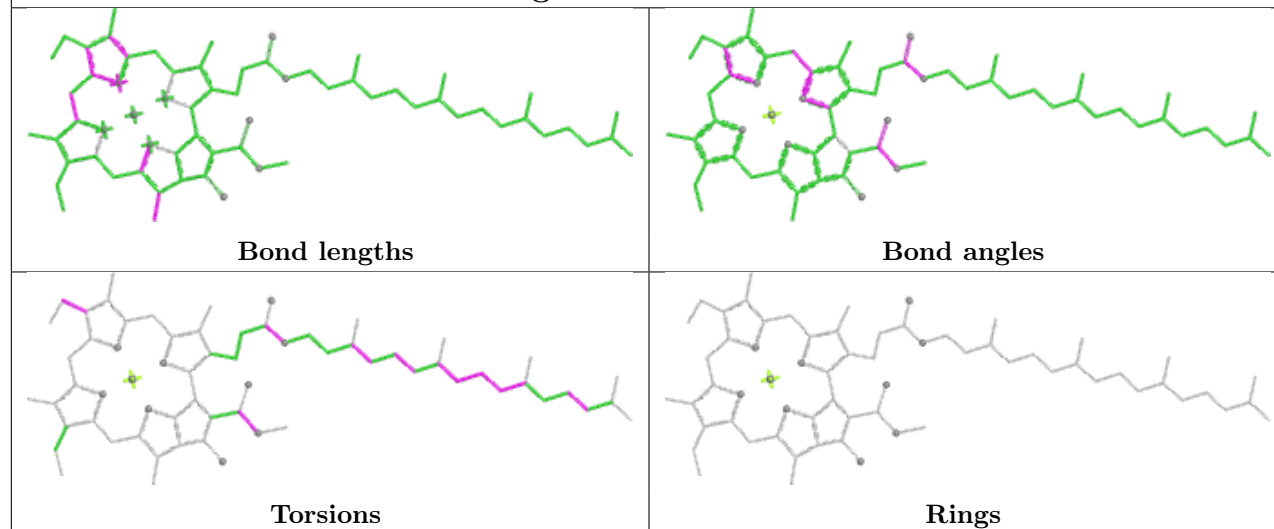
Ligand CLA a 404

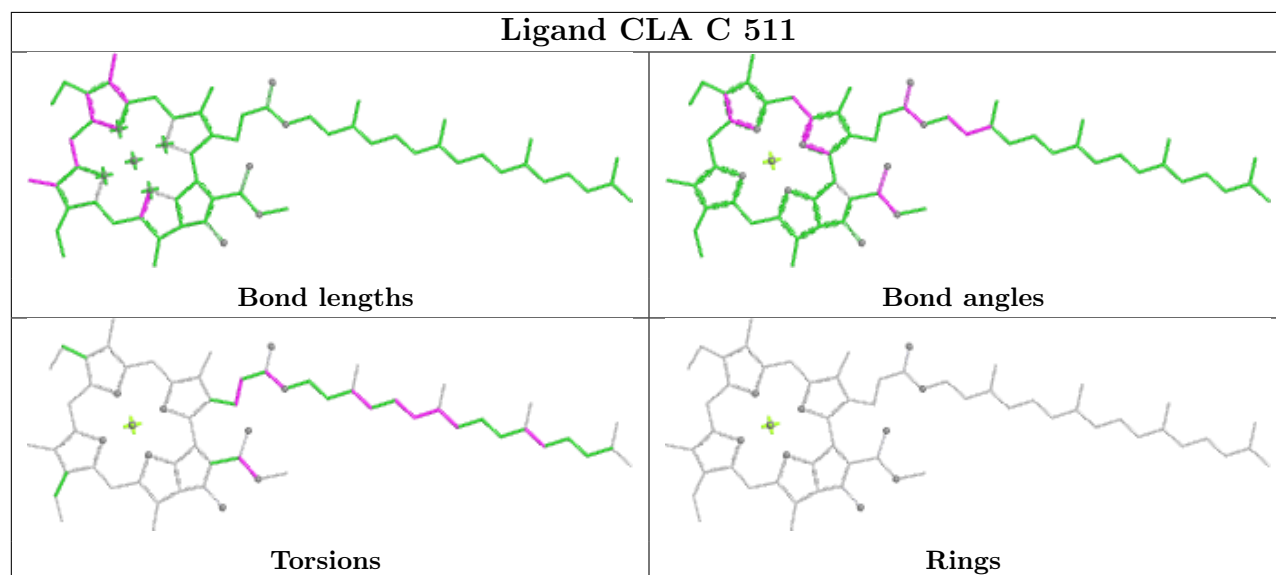
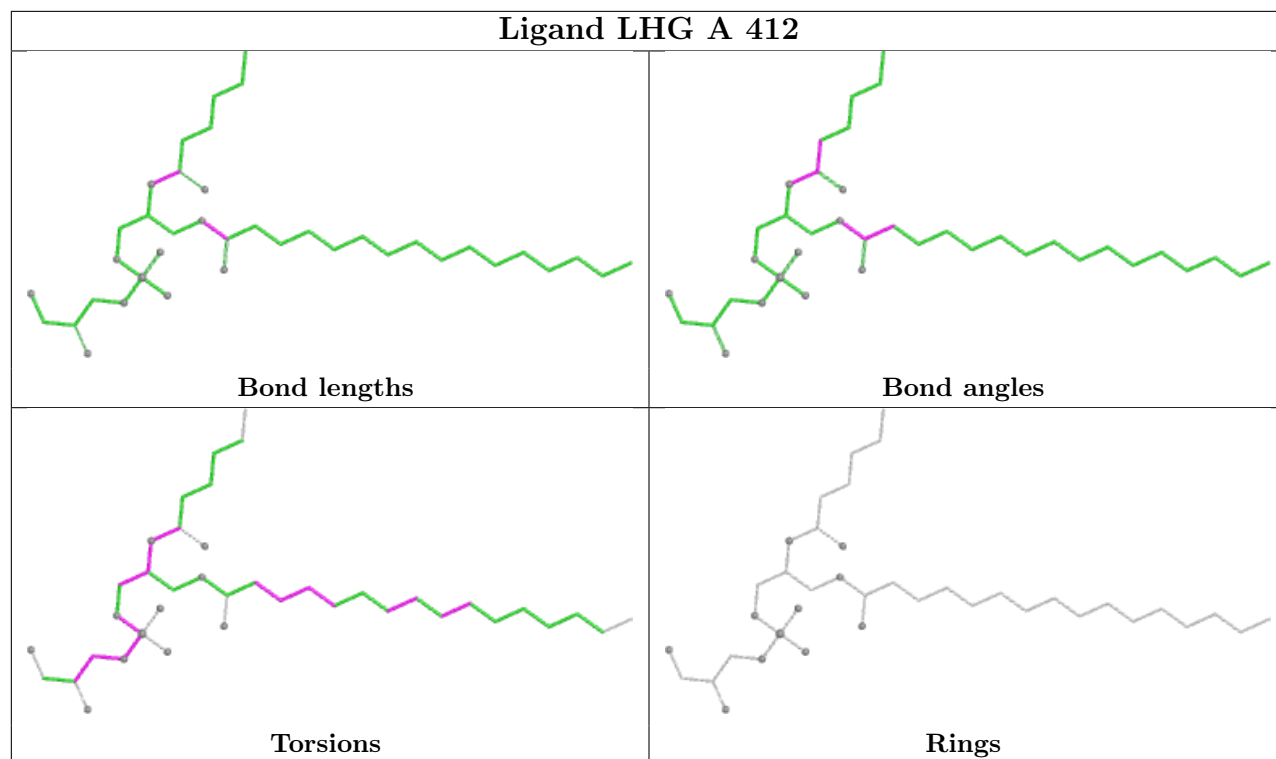


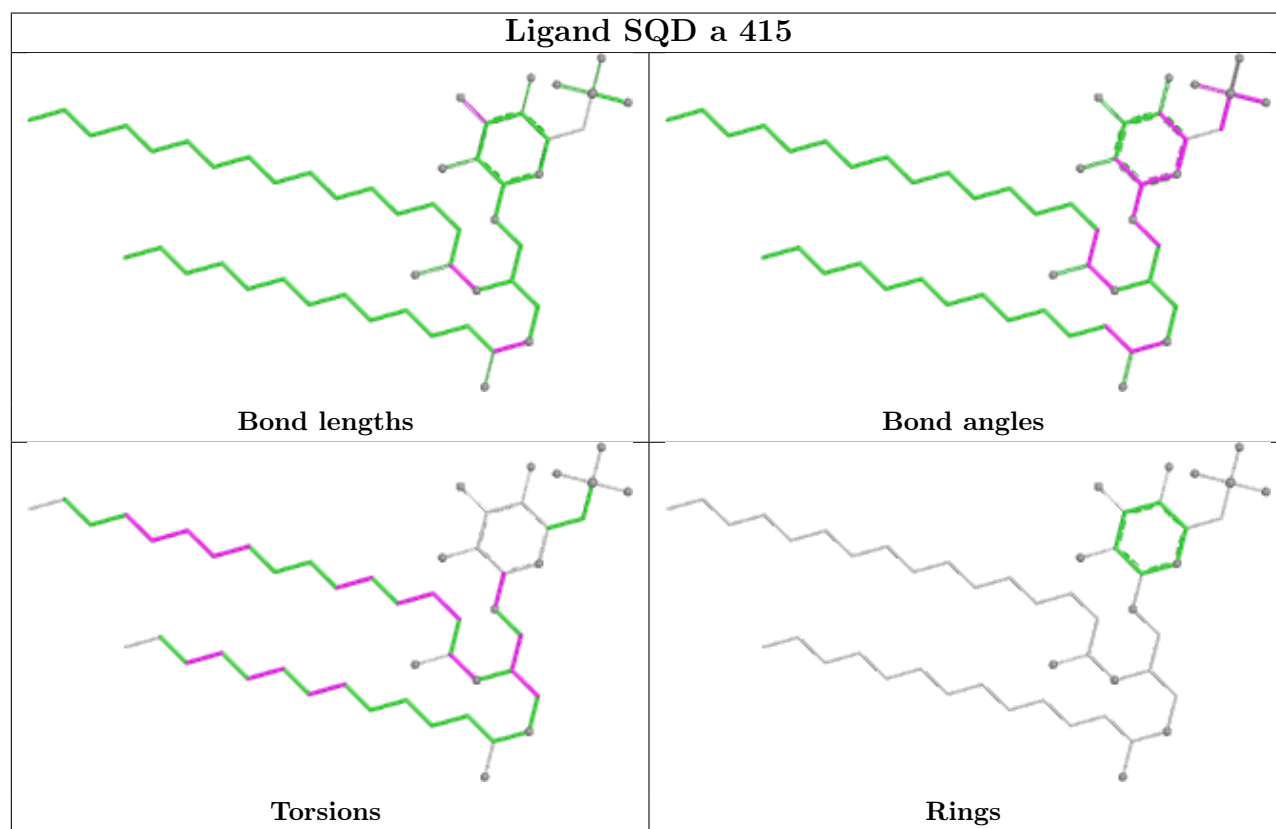
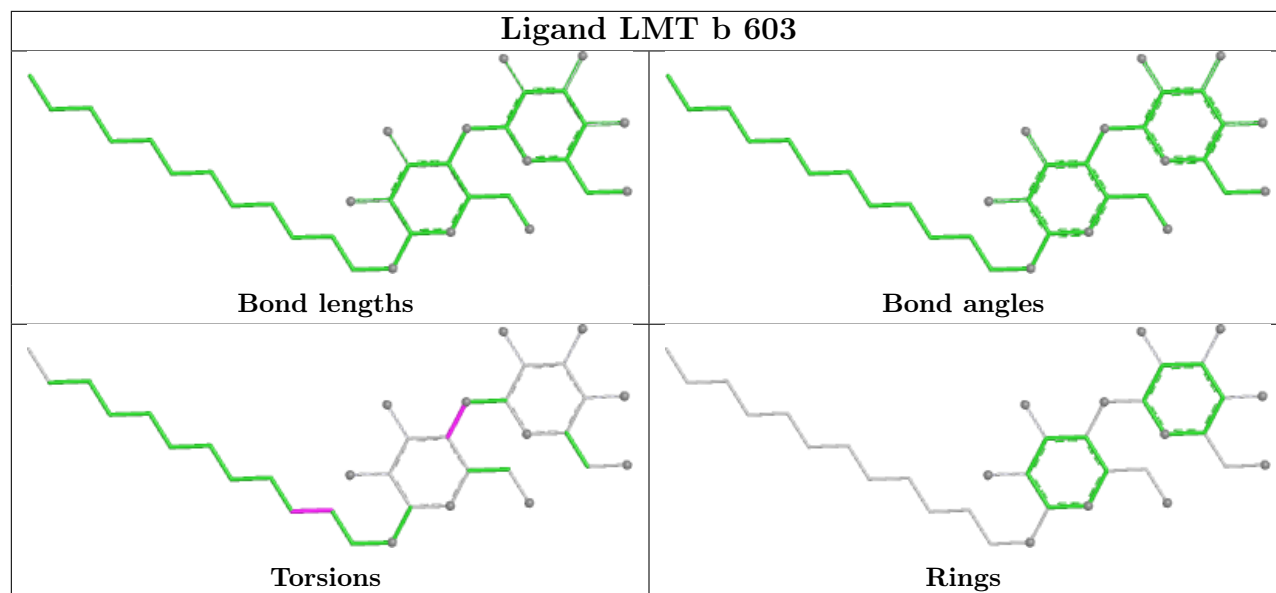
Ligand DGD a 413

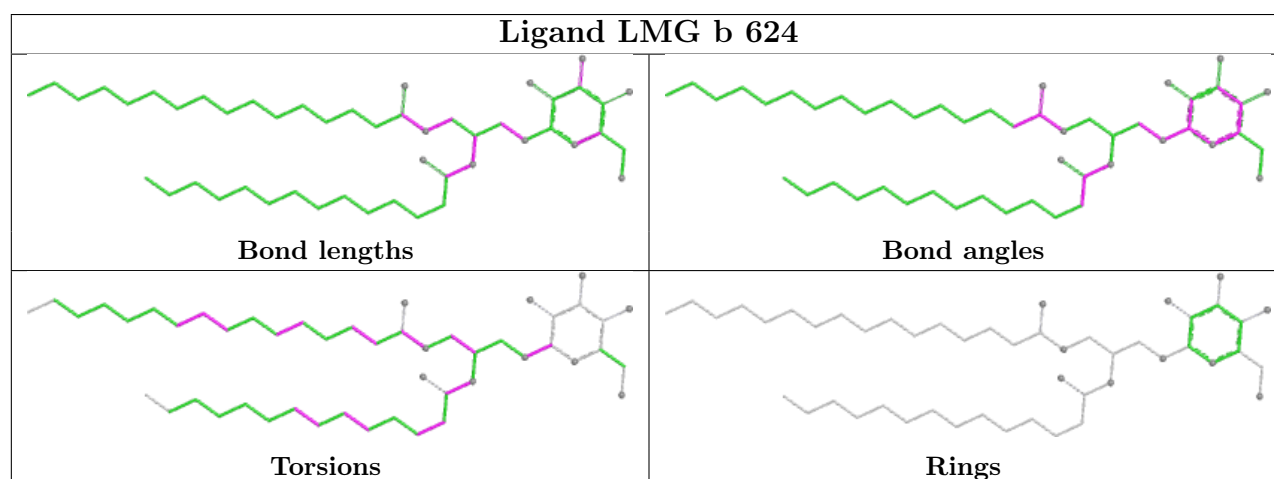
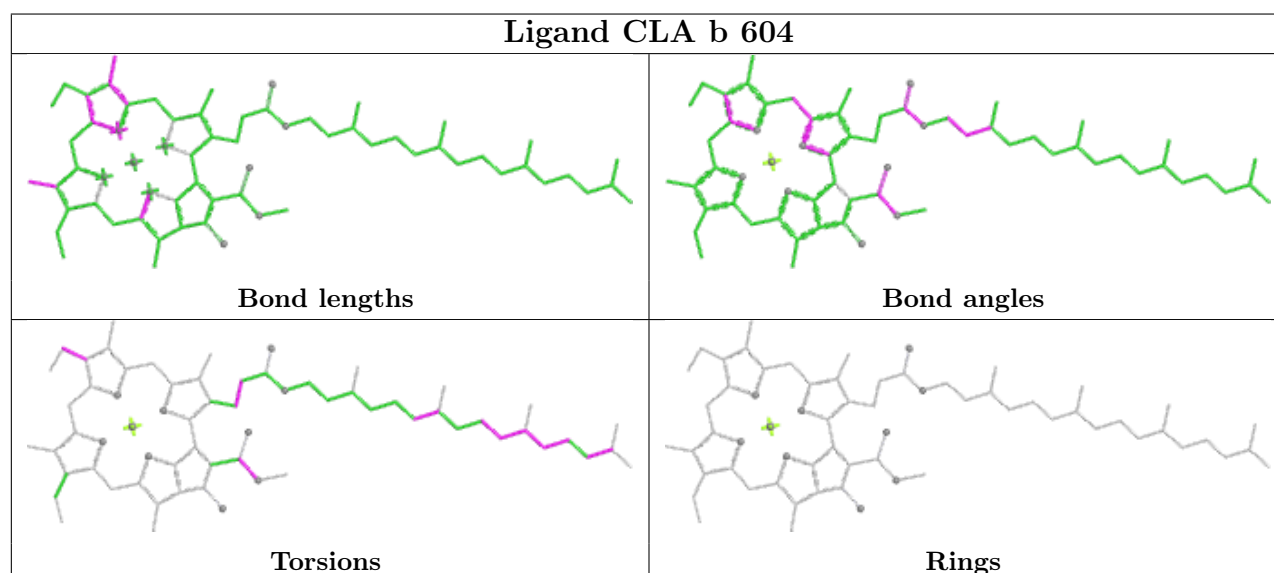
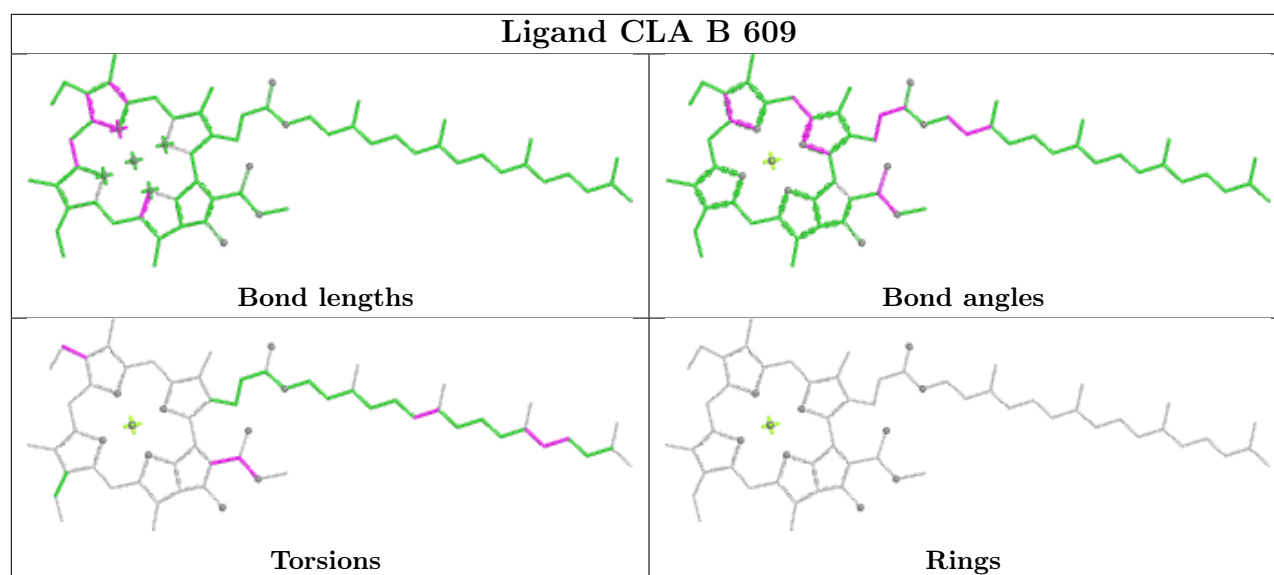


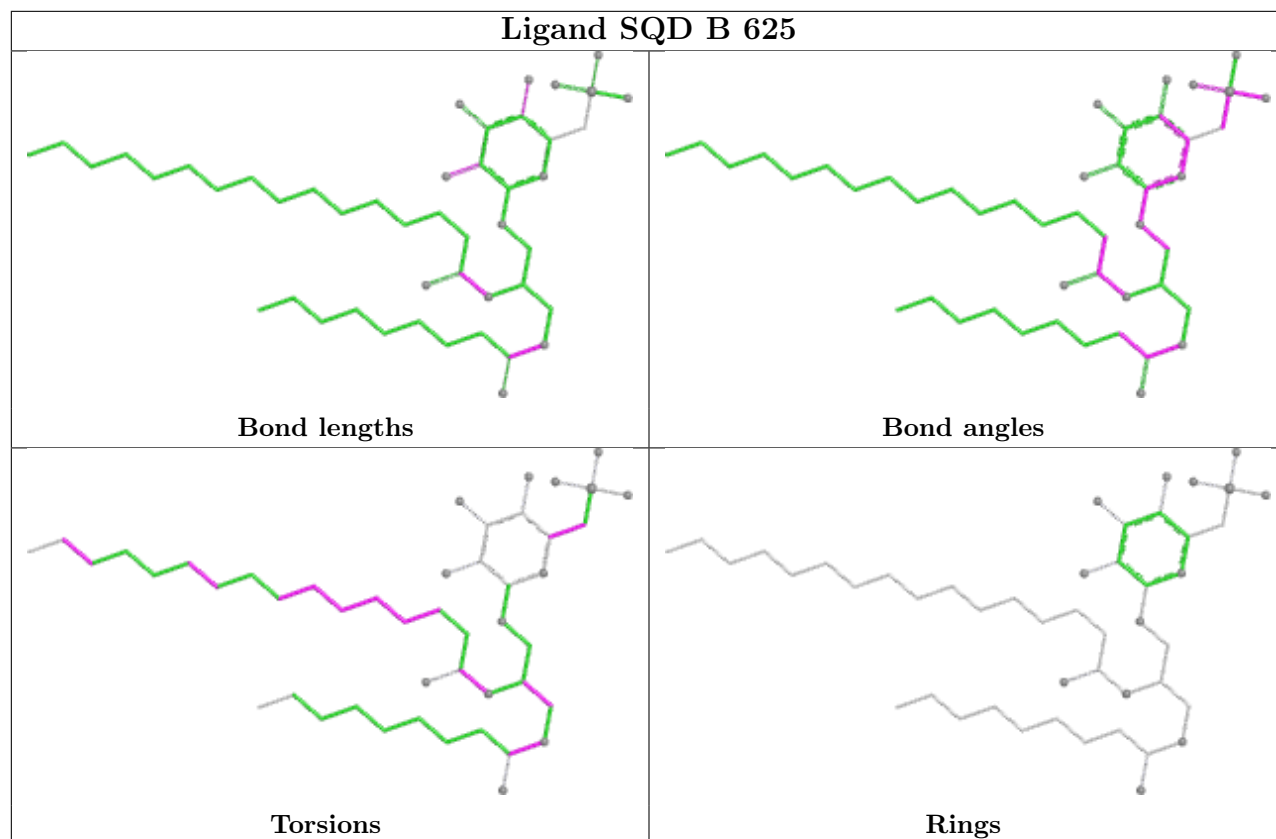
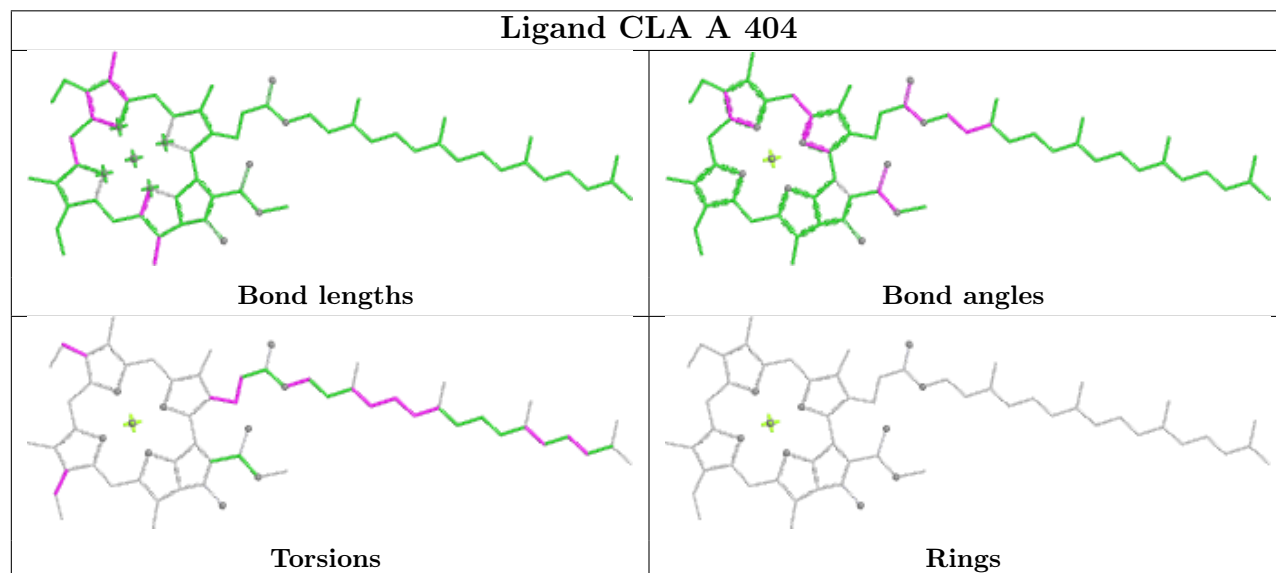
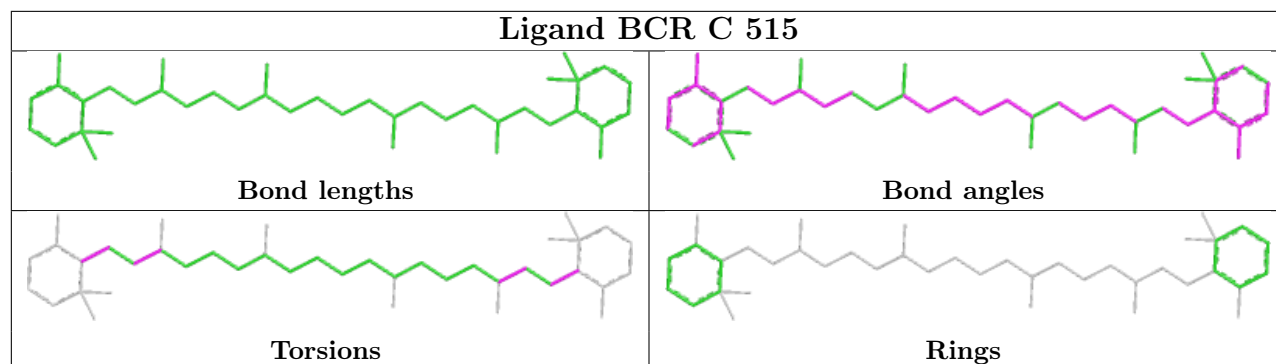
Ligand CLA B 605

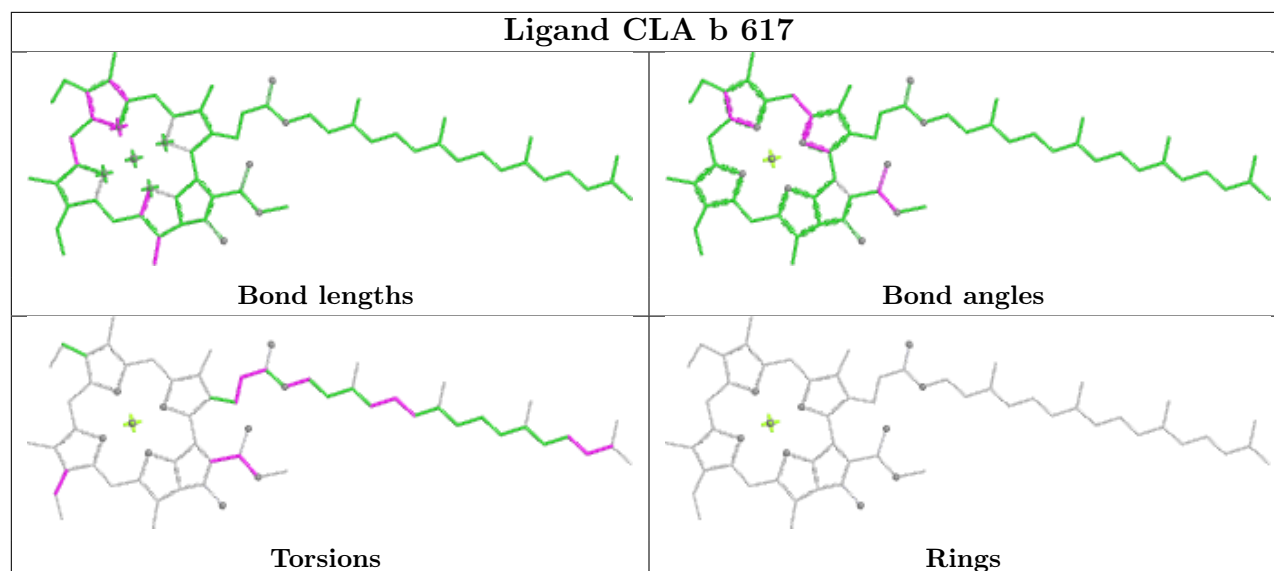
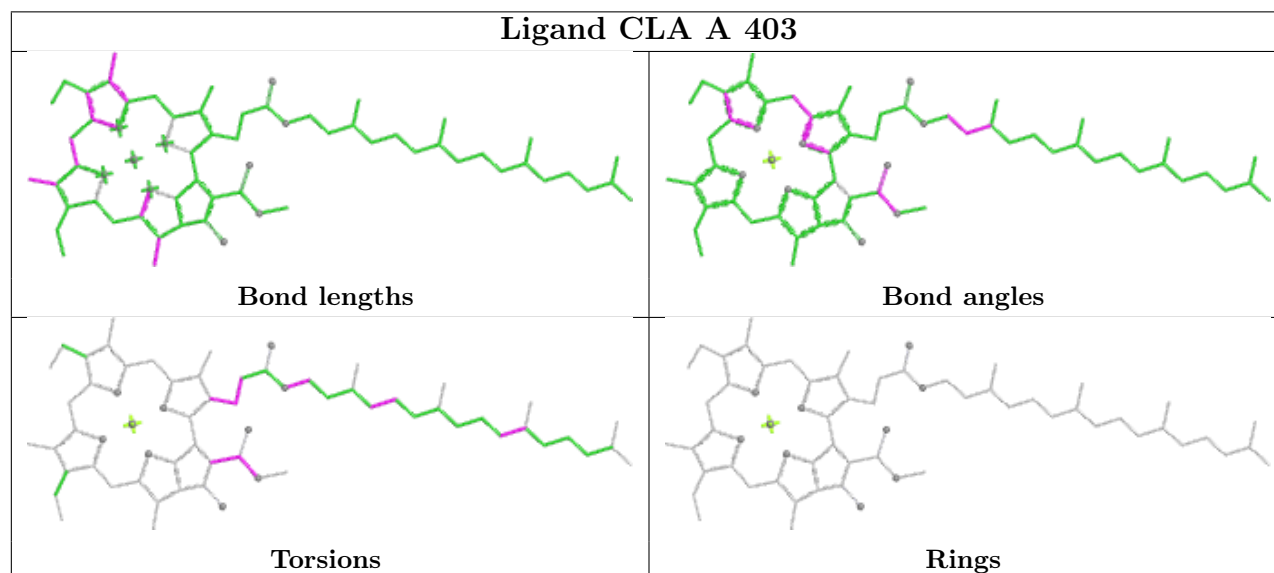
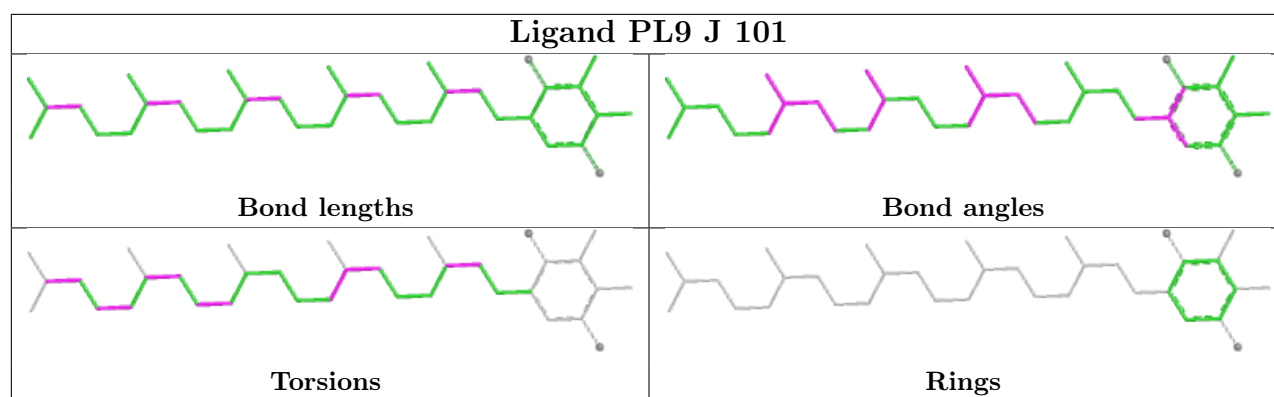




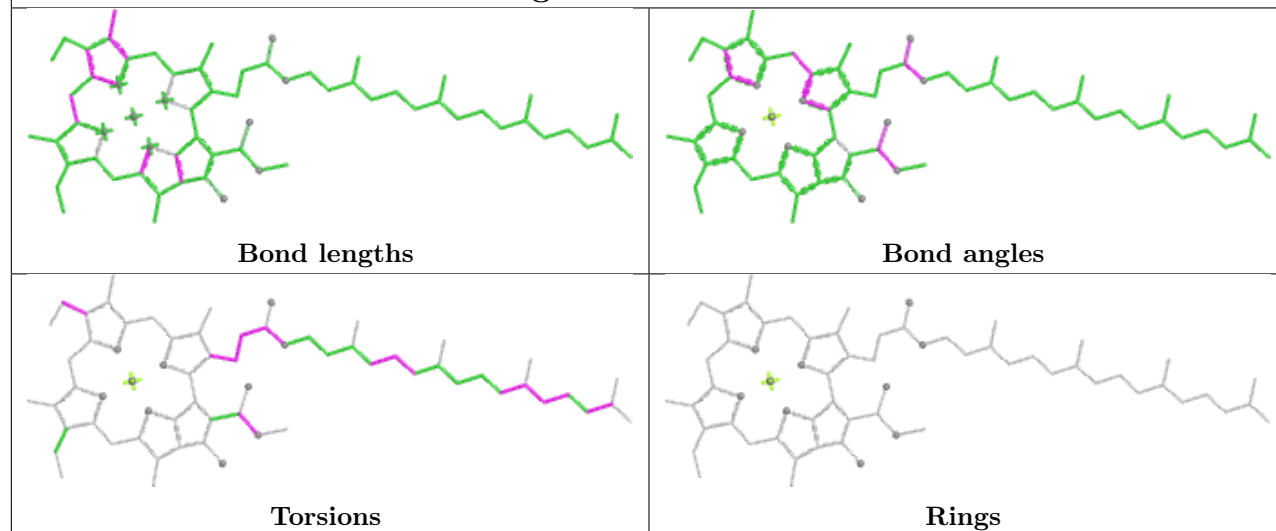




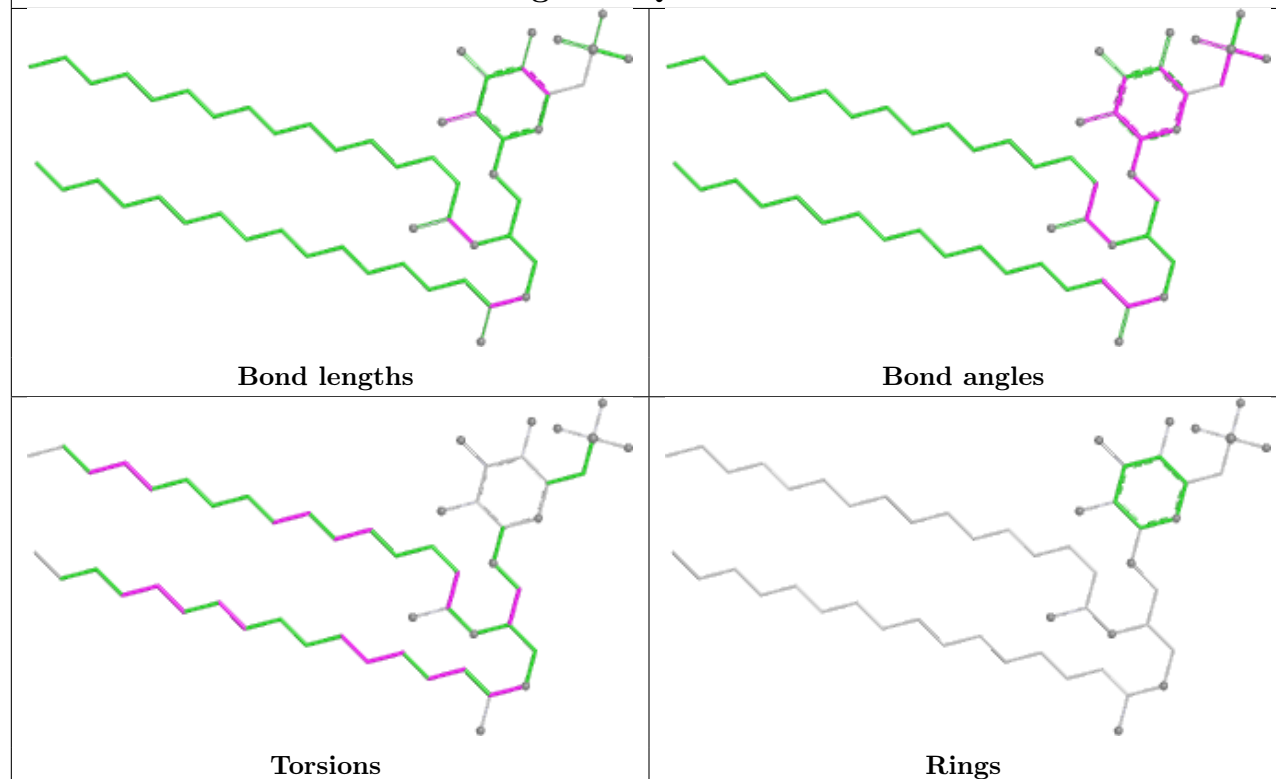


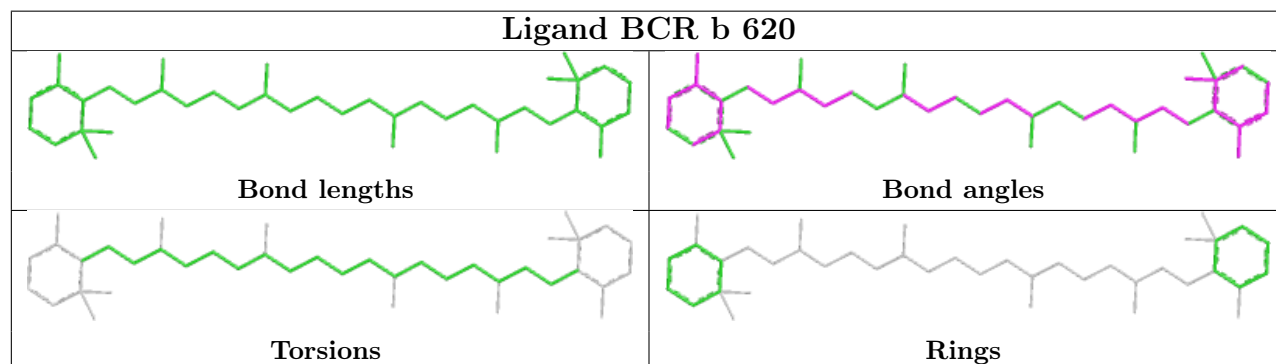
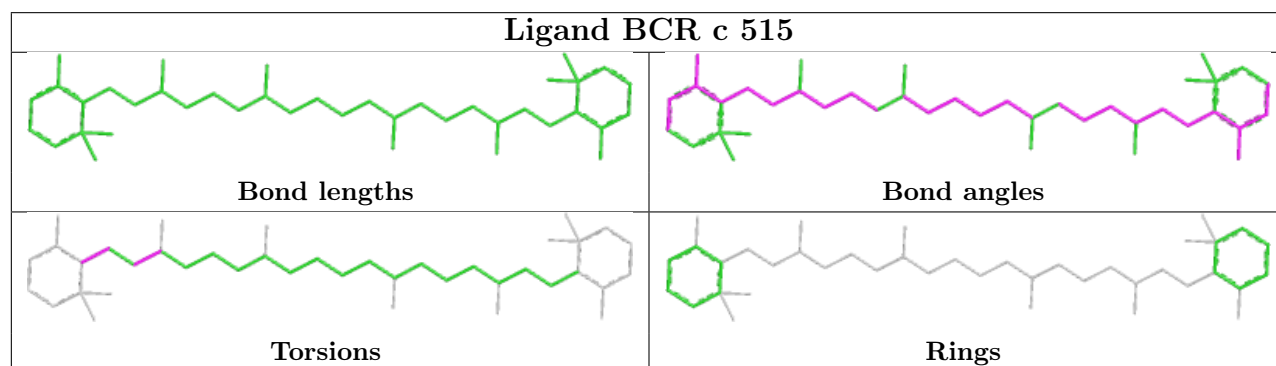
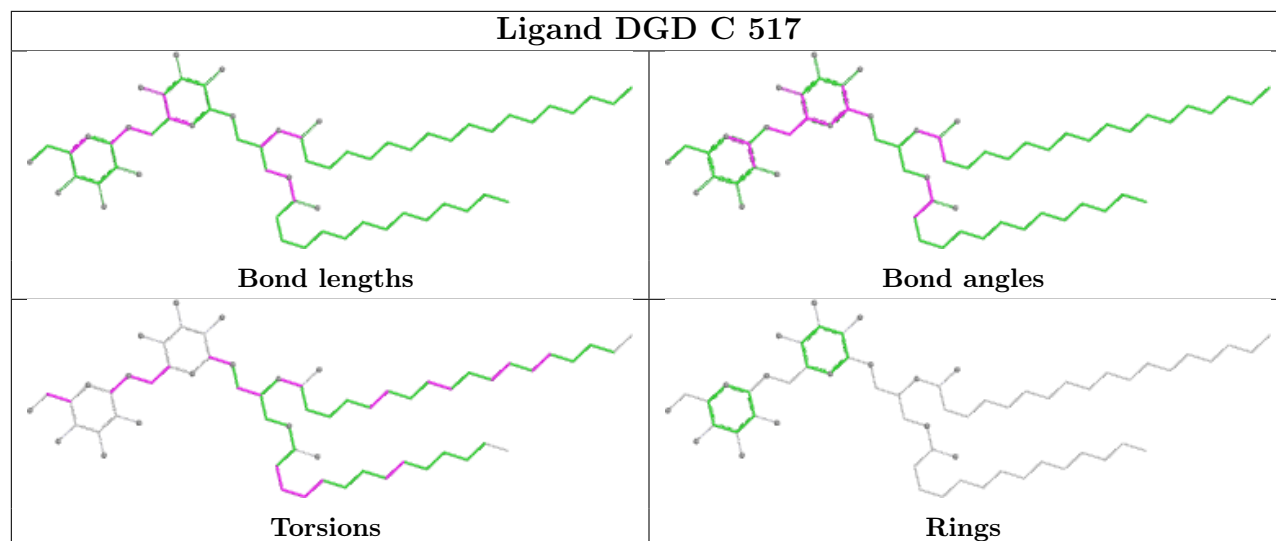


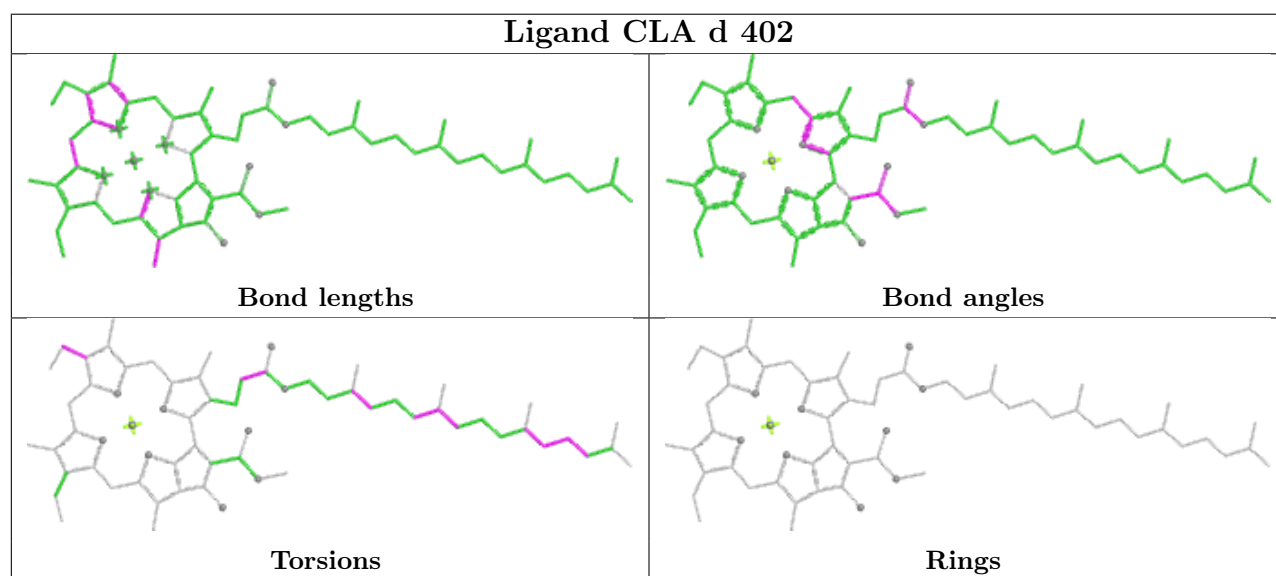
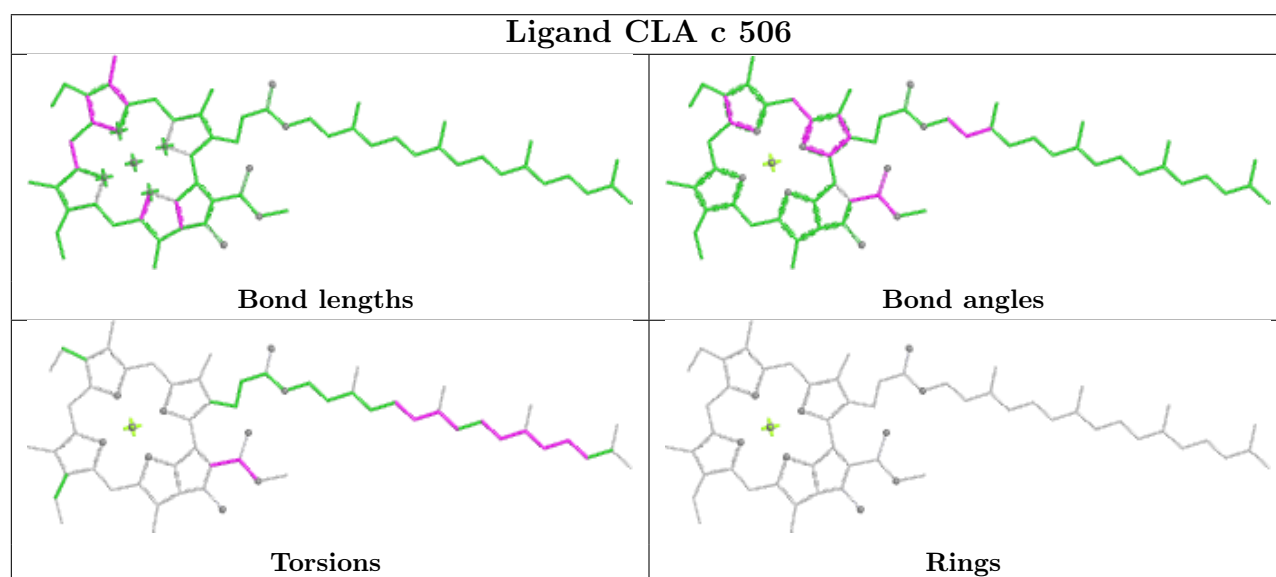
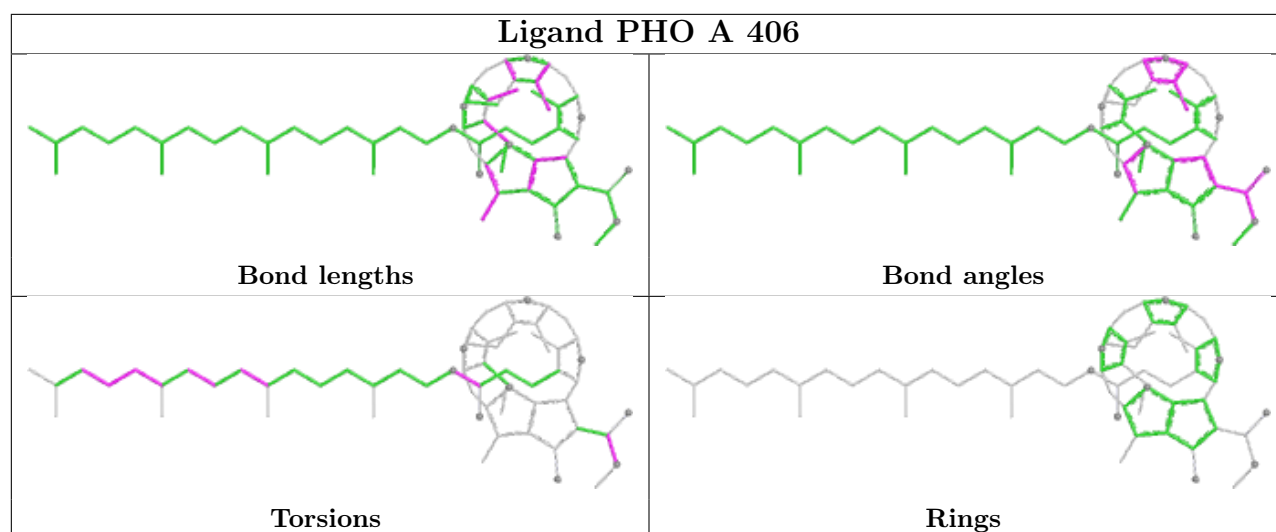
Ligand CLA C 512

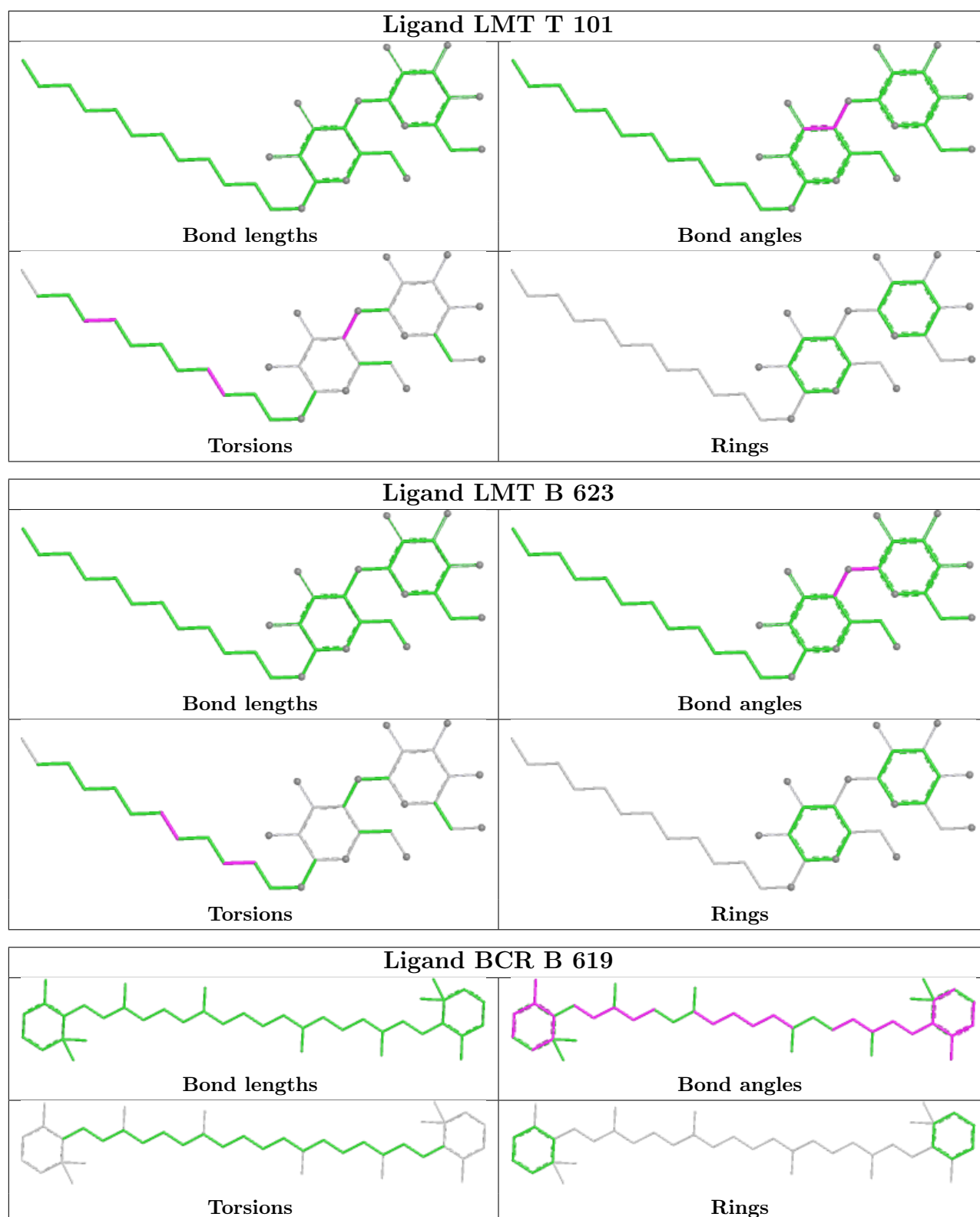


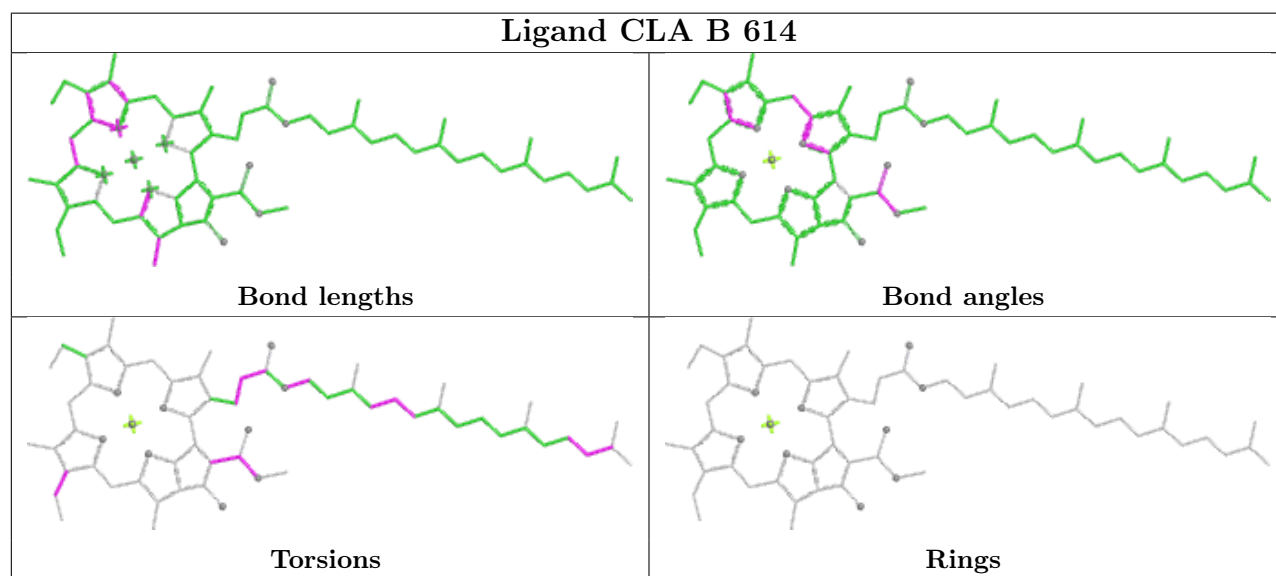
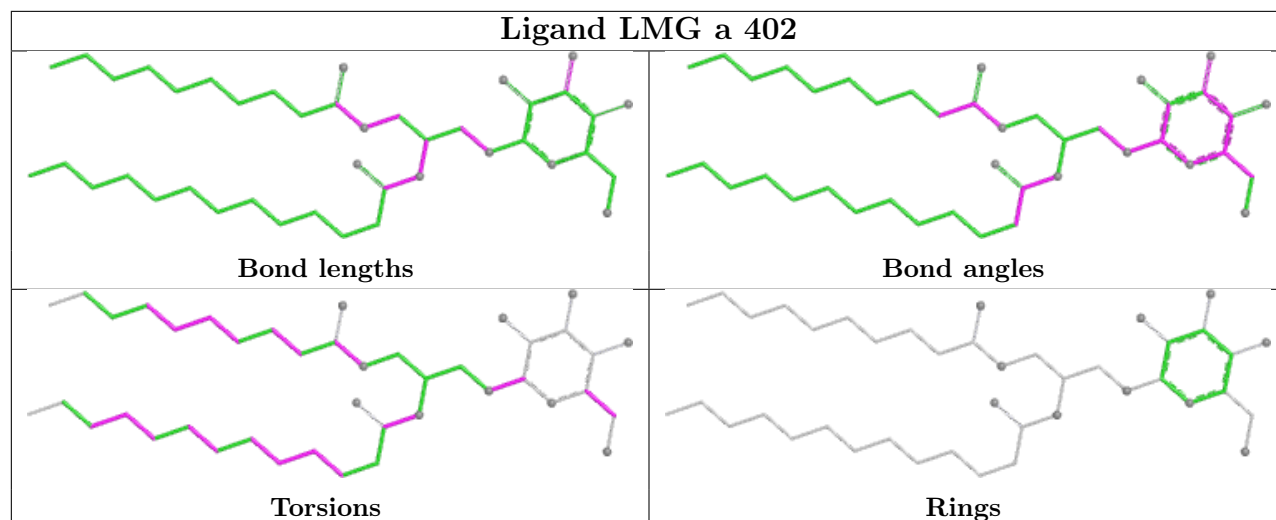
Ligand SQD A 417



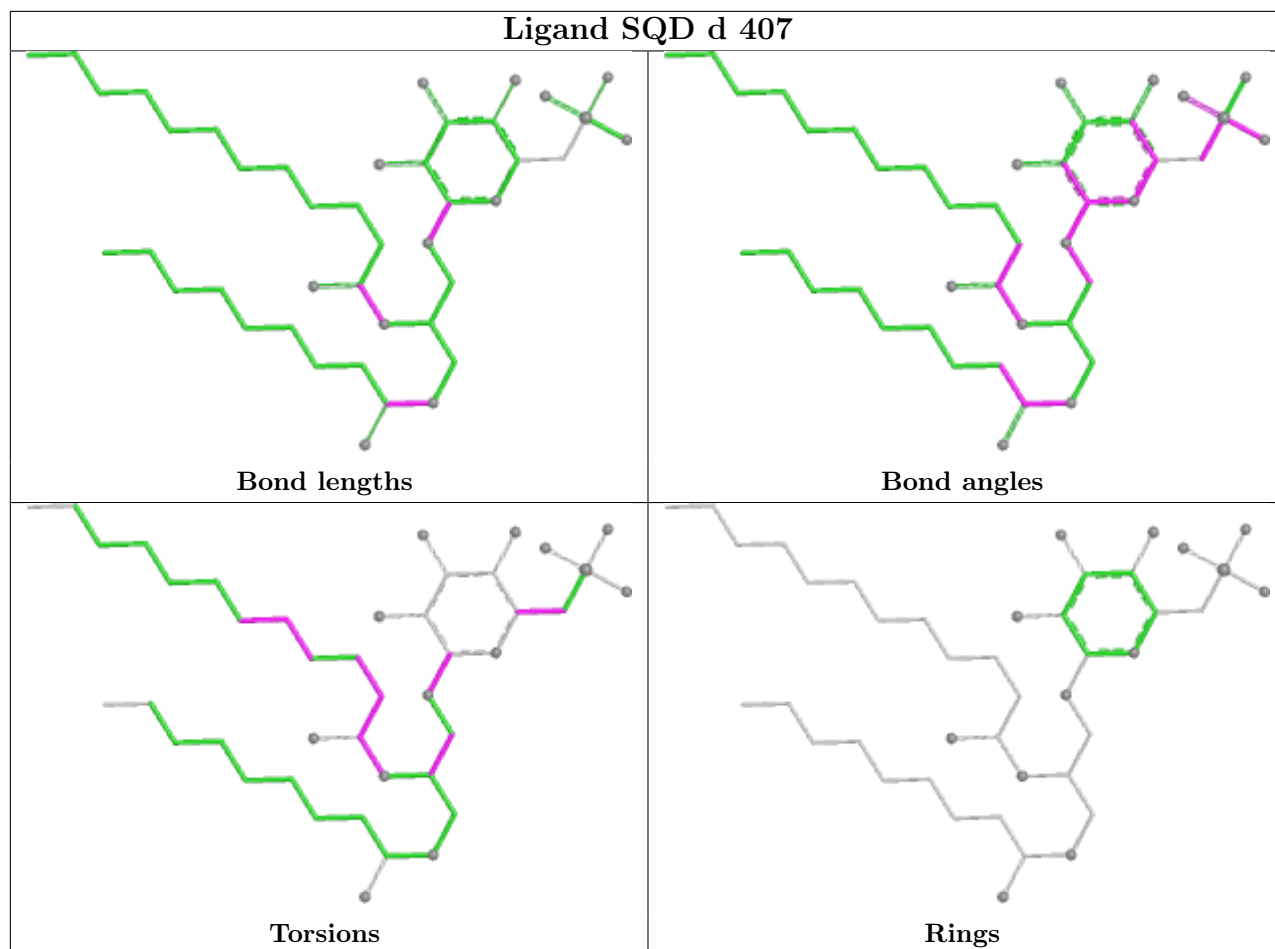




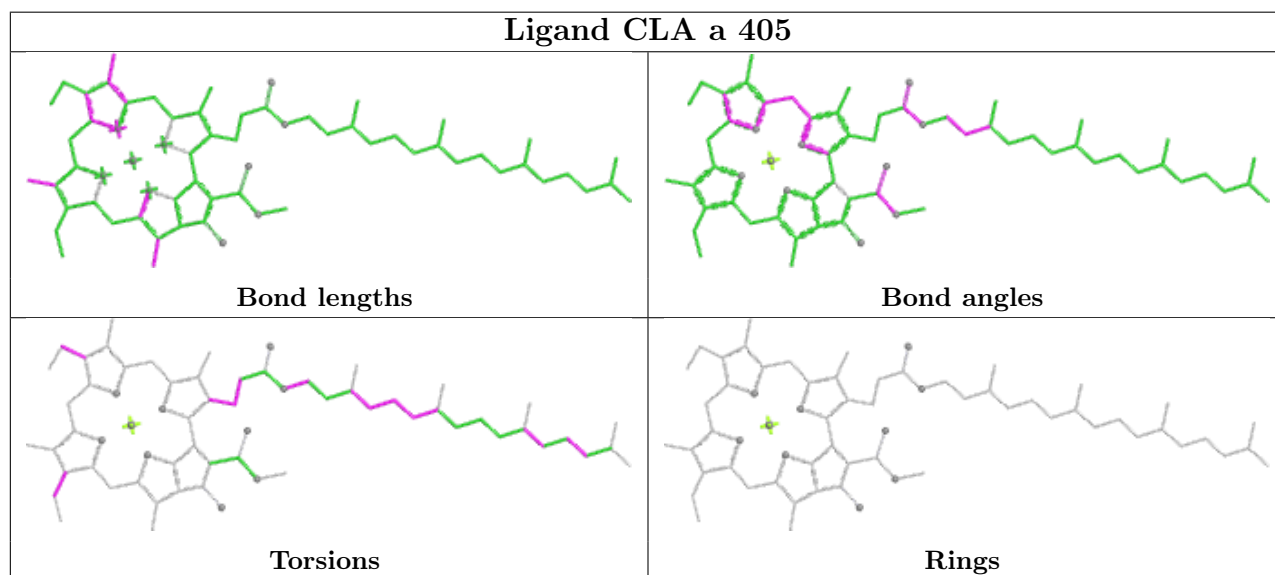


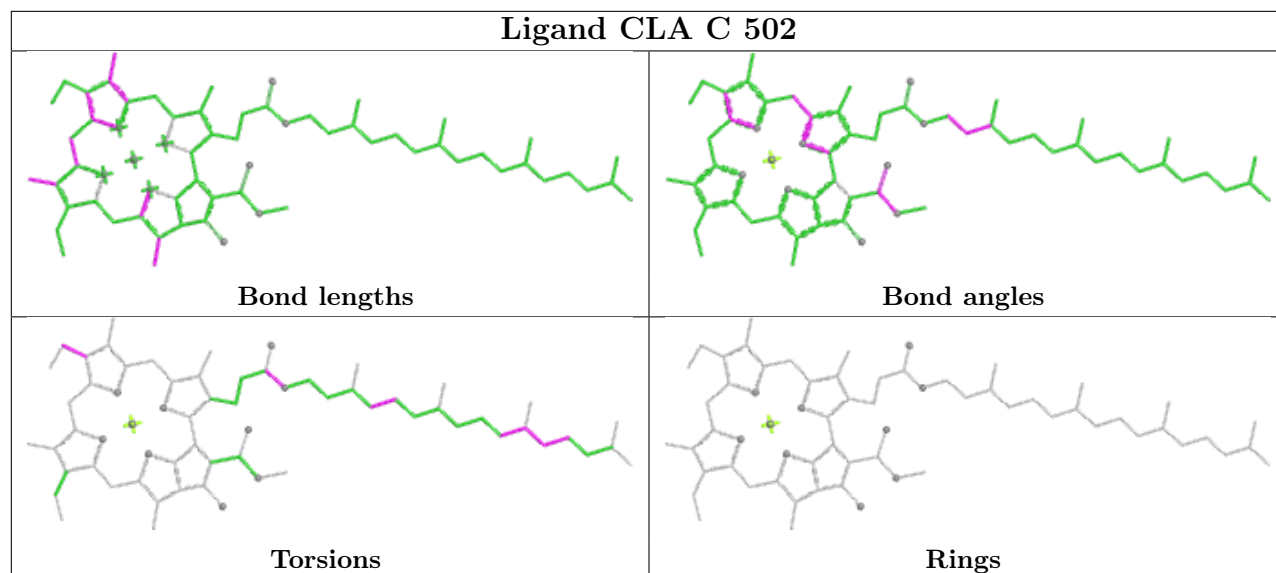
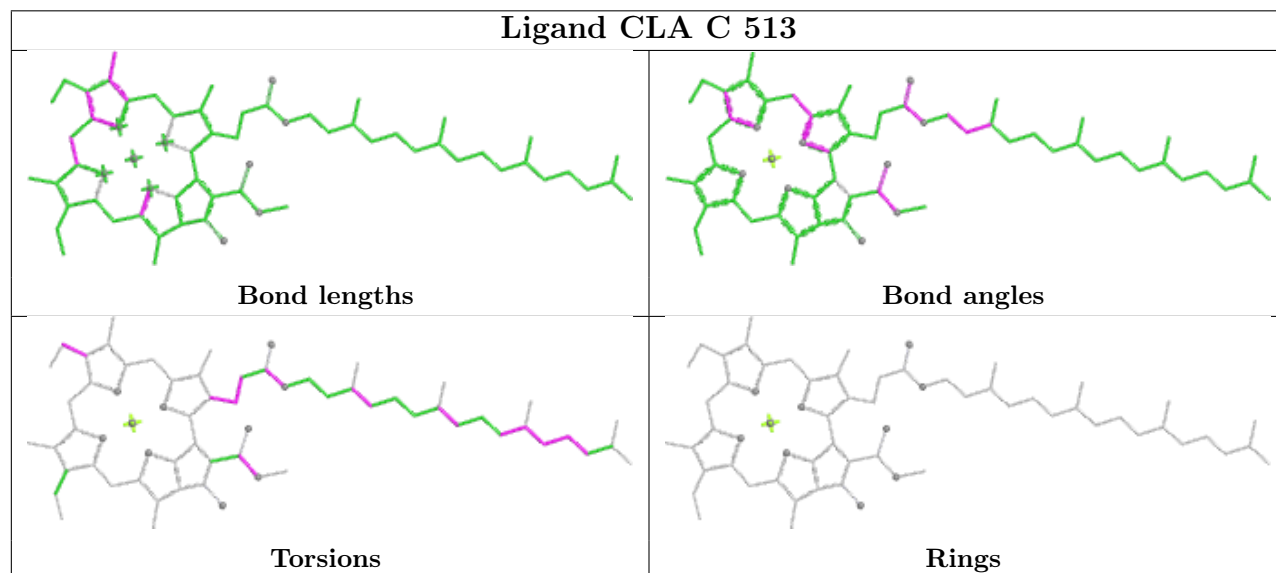
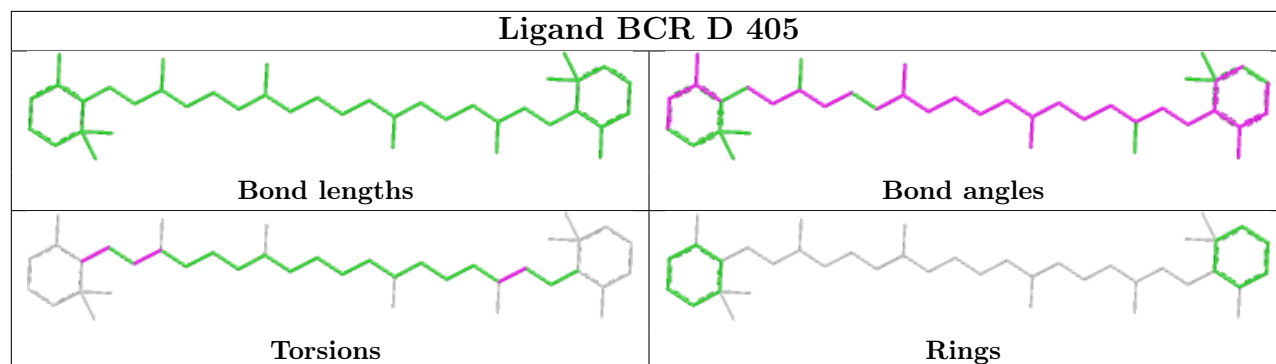


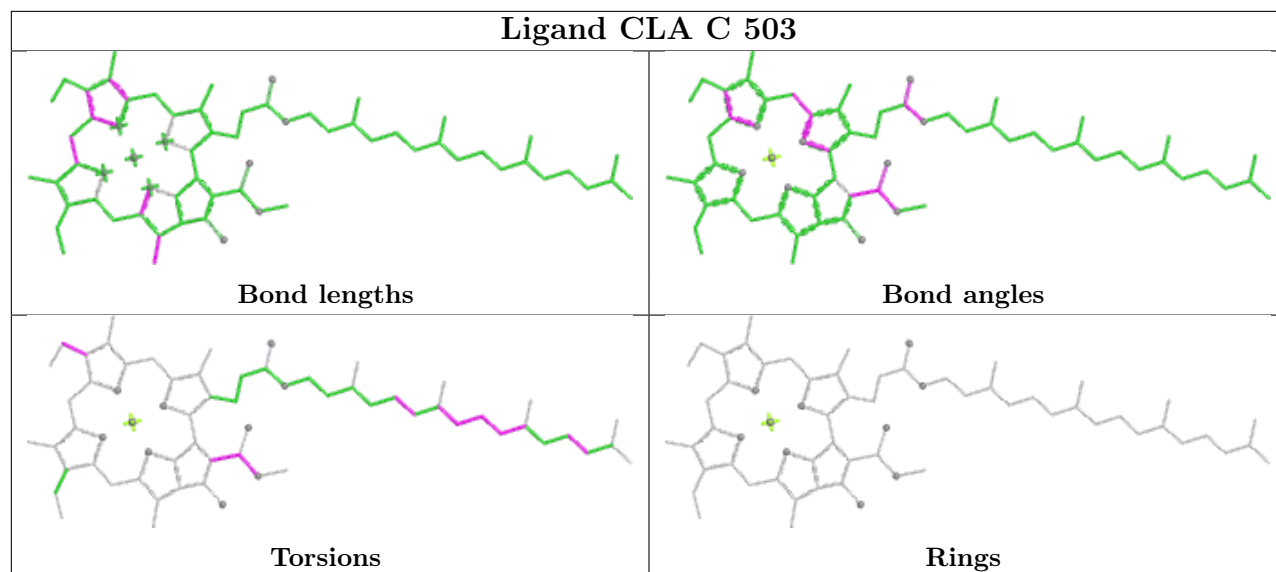
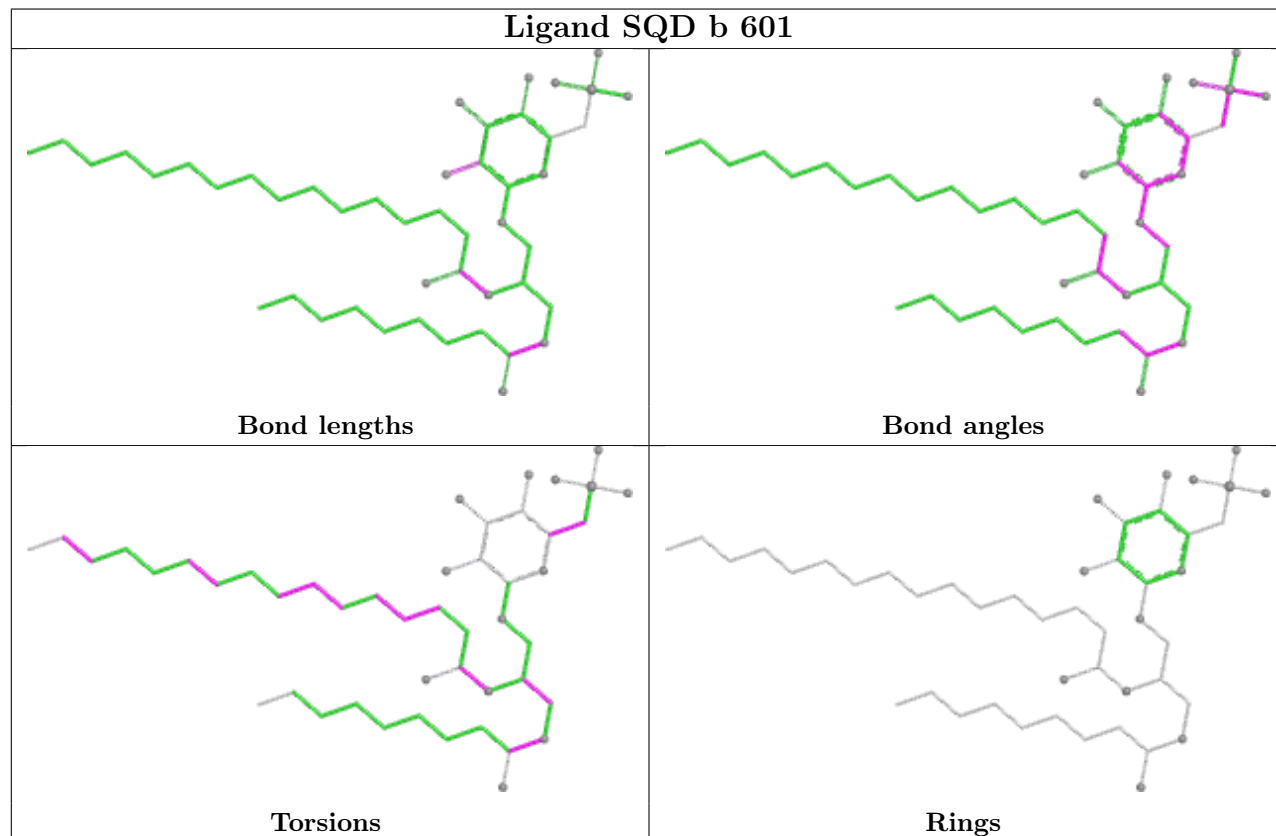
Ligand SQD d 407

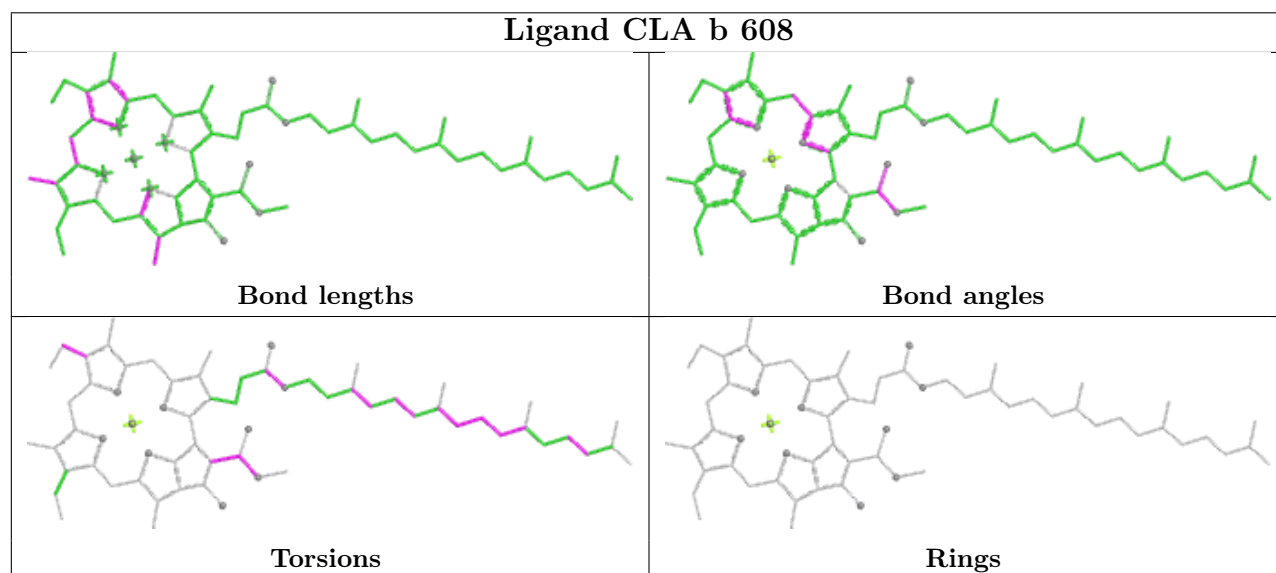
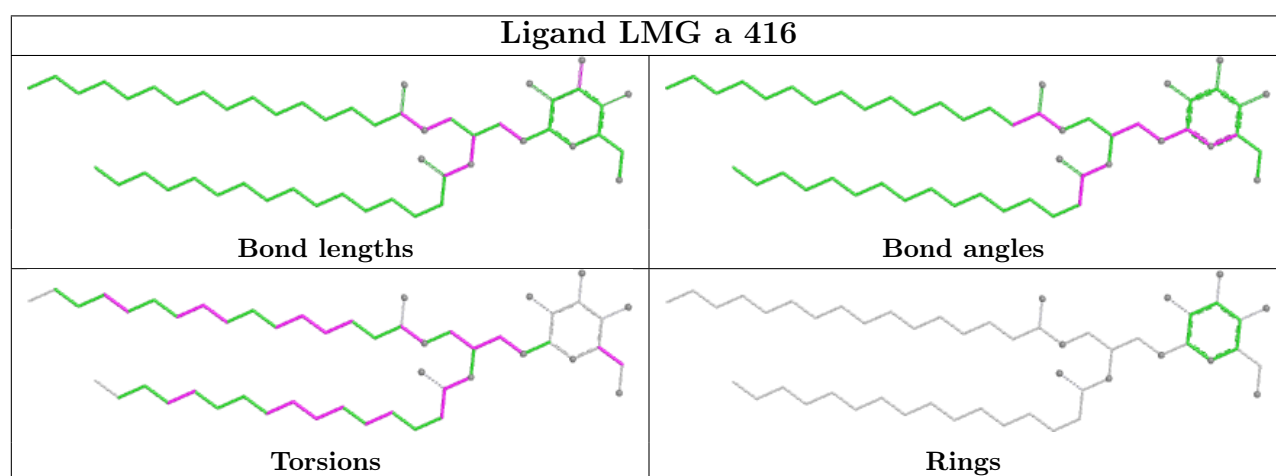
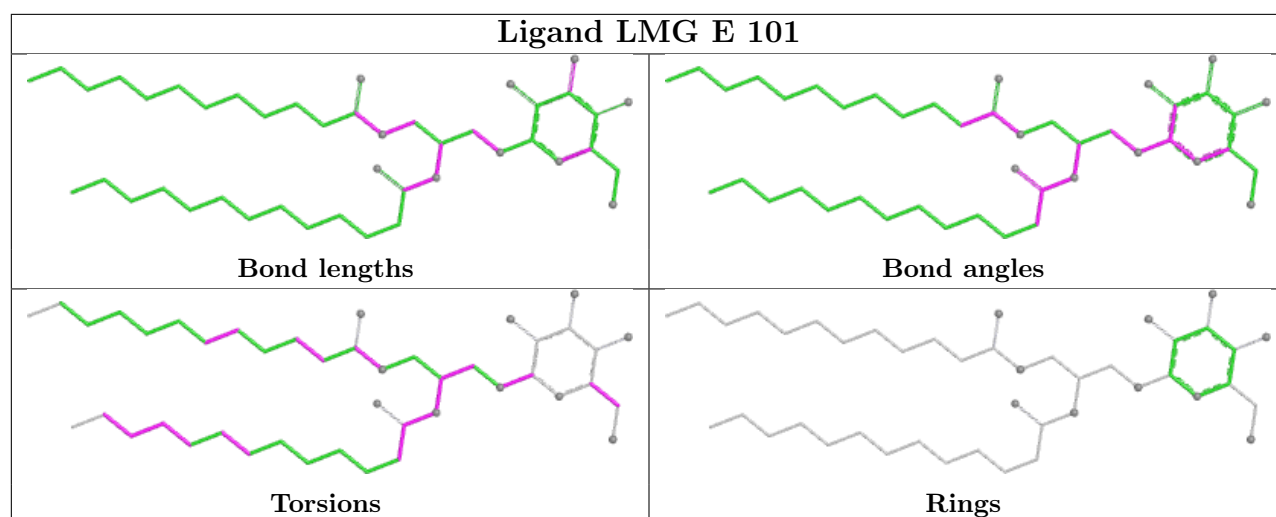


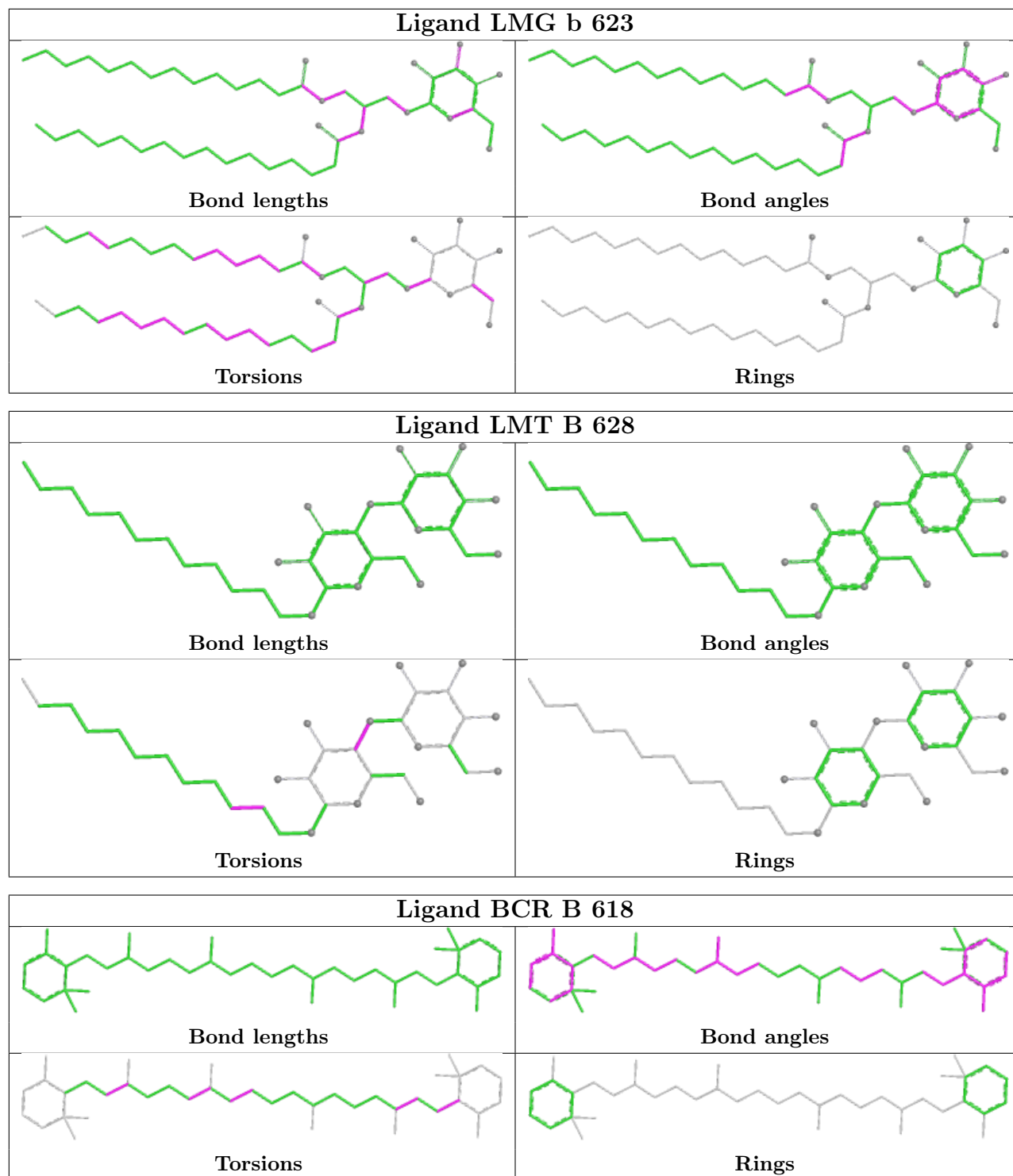
Ligand CLA a 405

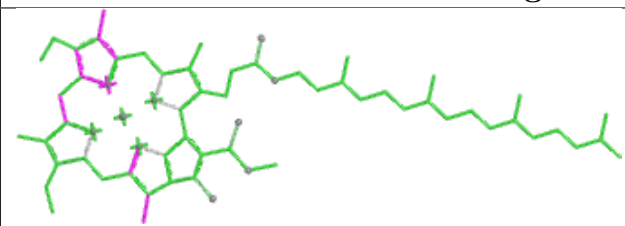
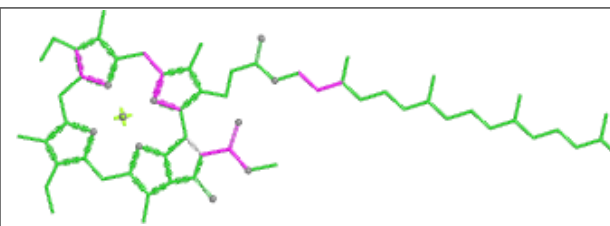
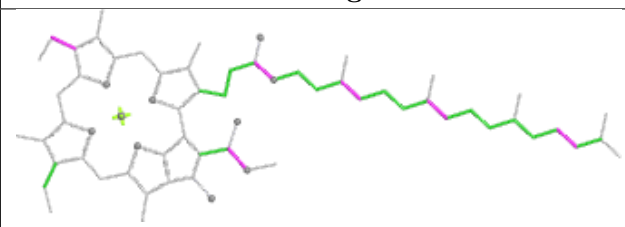
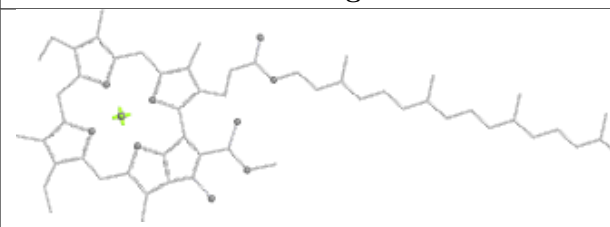


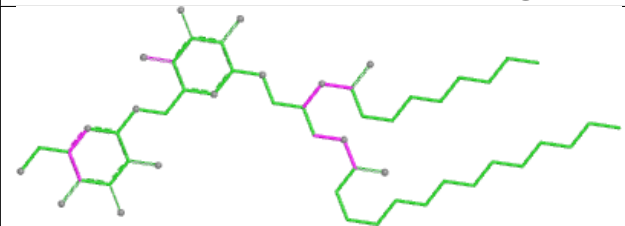
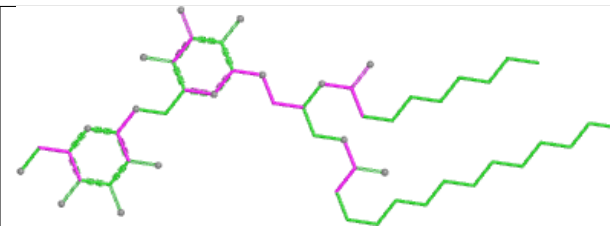
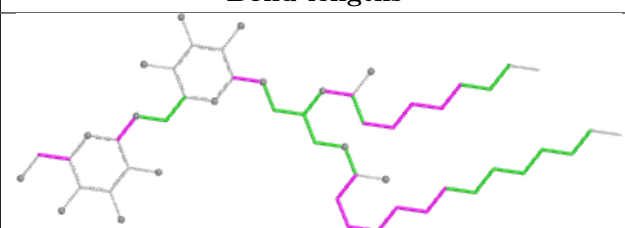
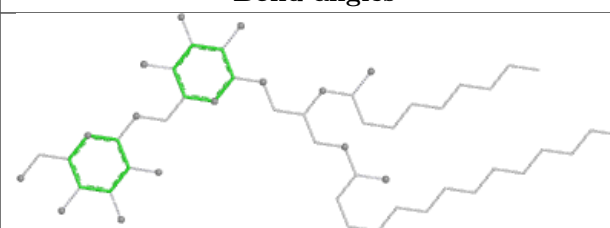


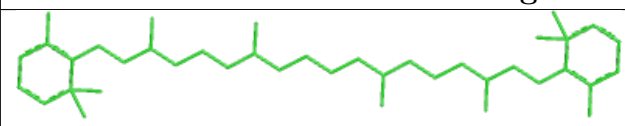
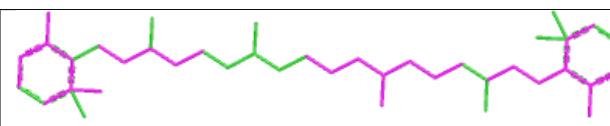
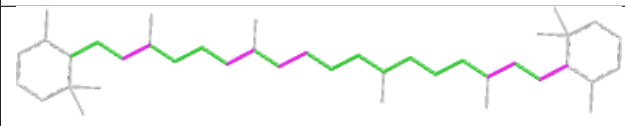
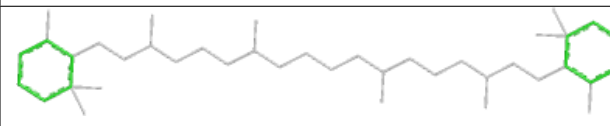
Ligand CLA C 503**Ligand SQD b 601**



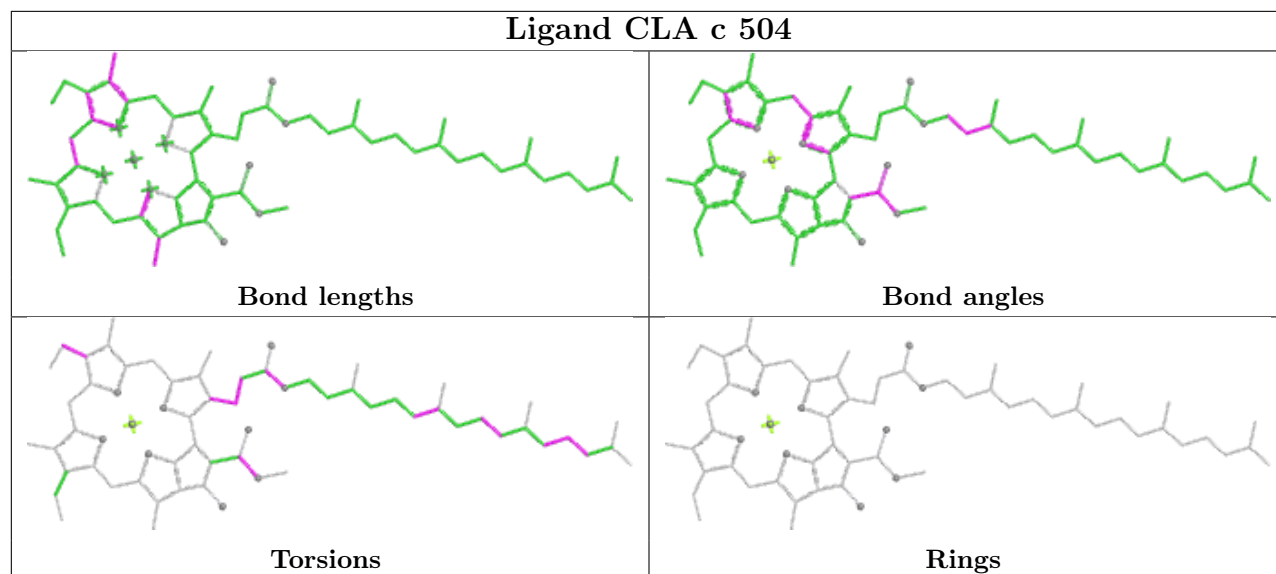


Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

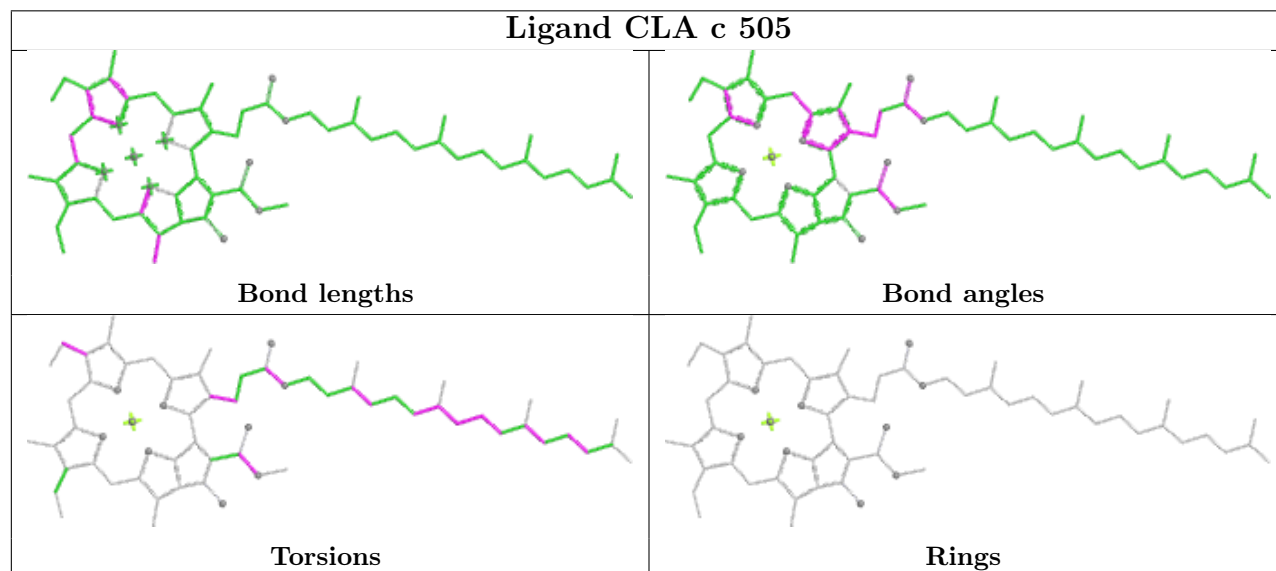
Ligand DGD C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

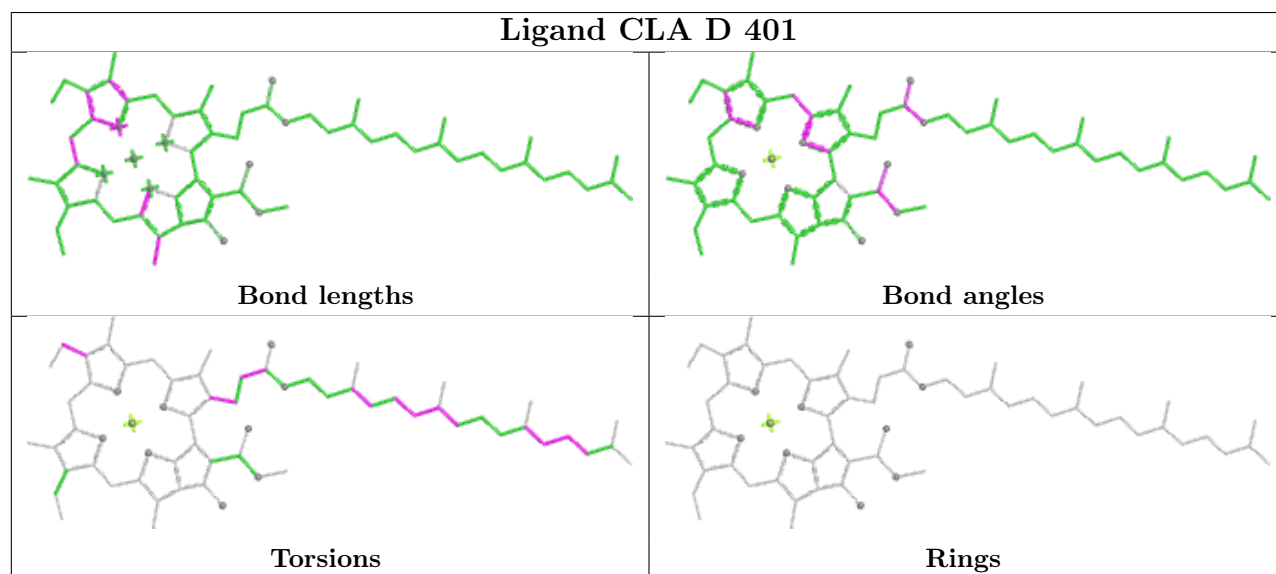
Ligand CLA c 504

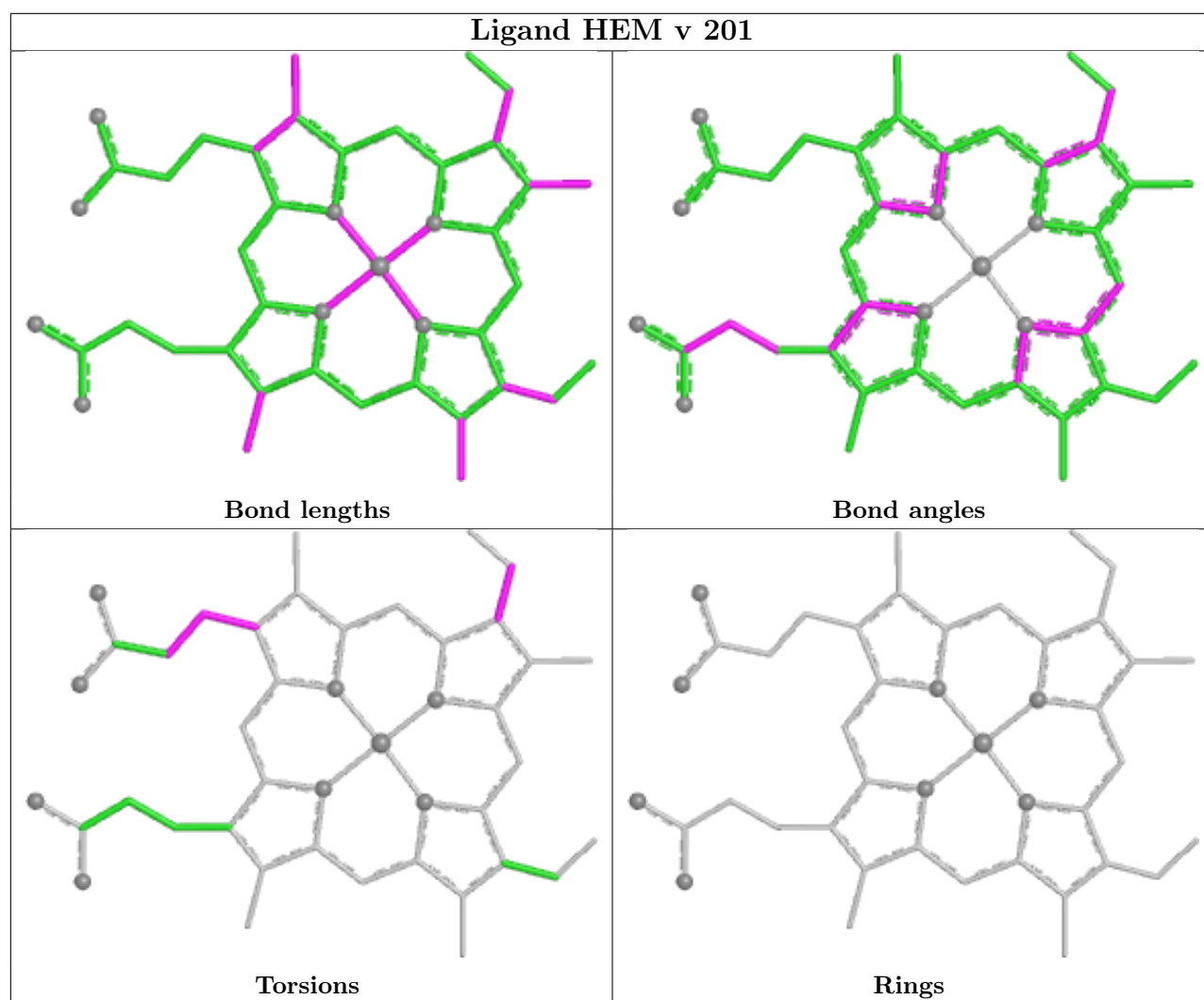
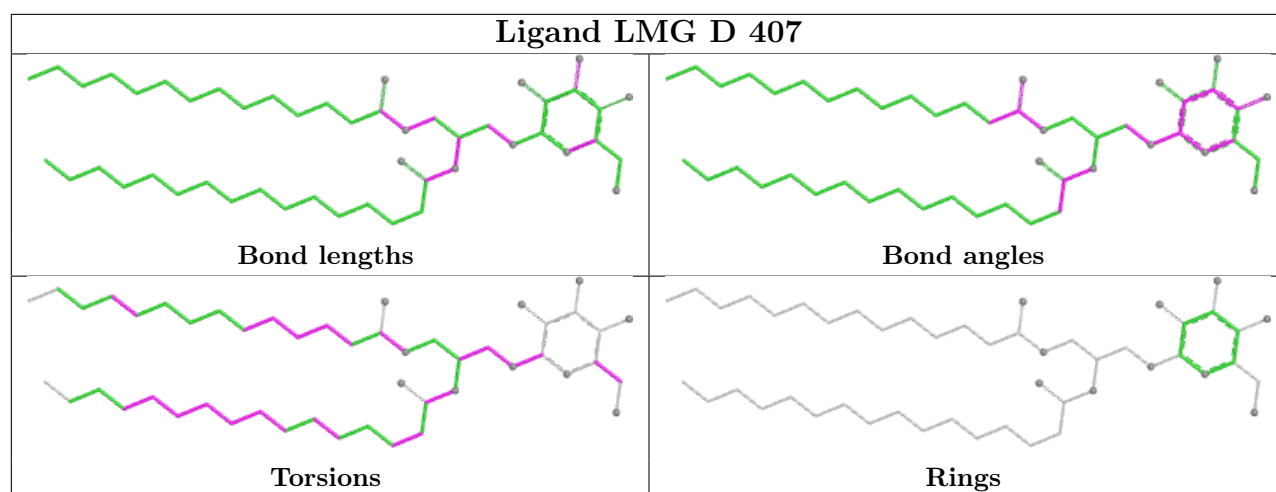


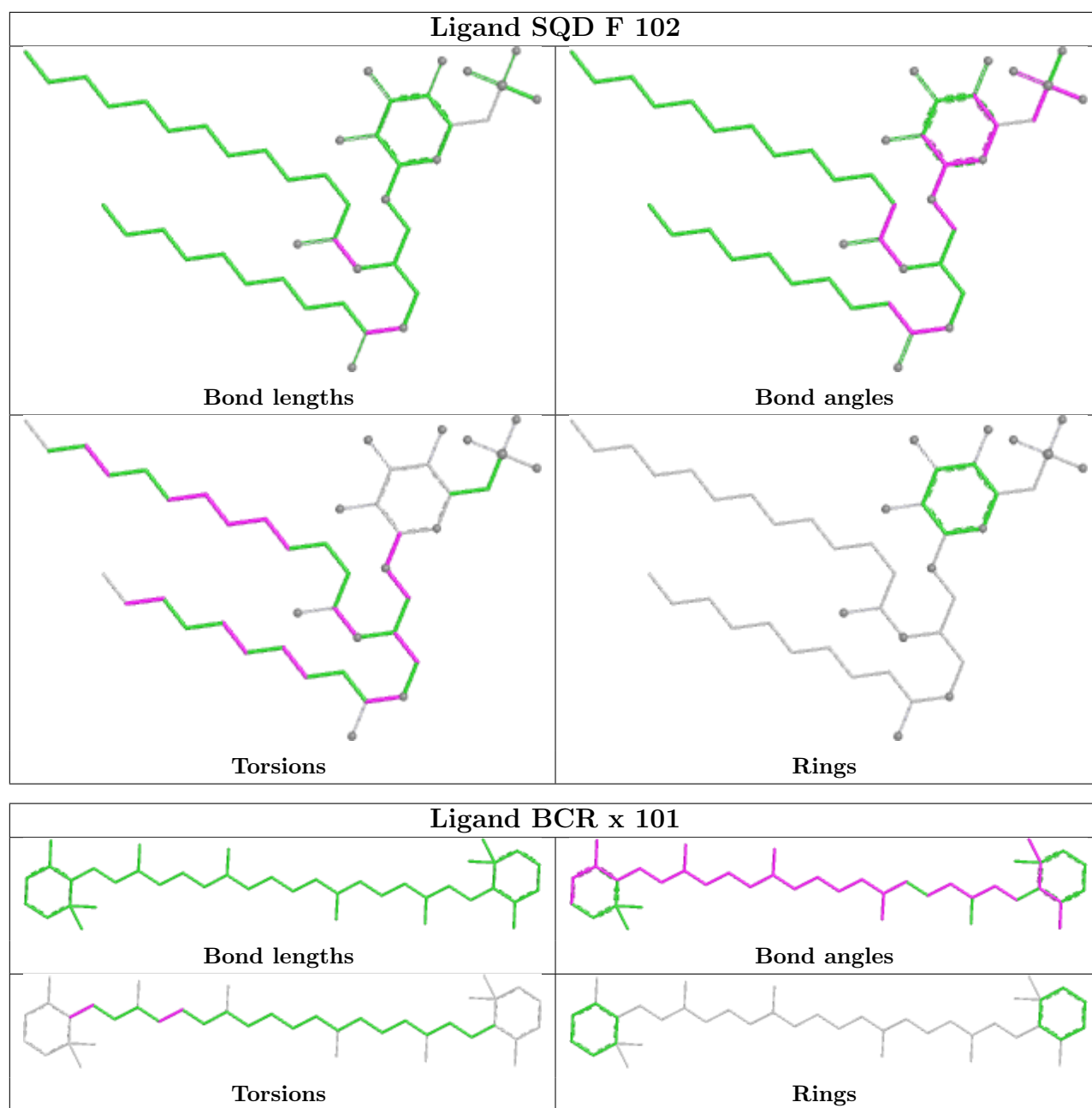
Ligand CLA c 505

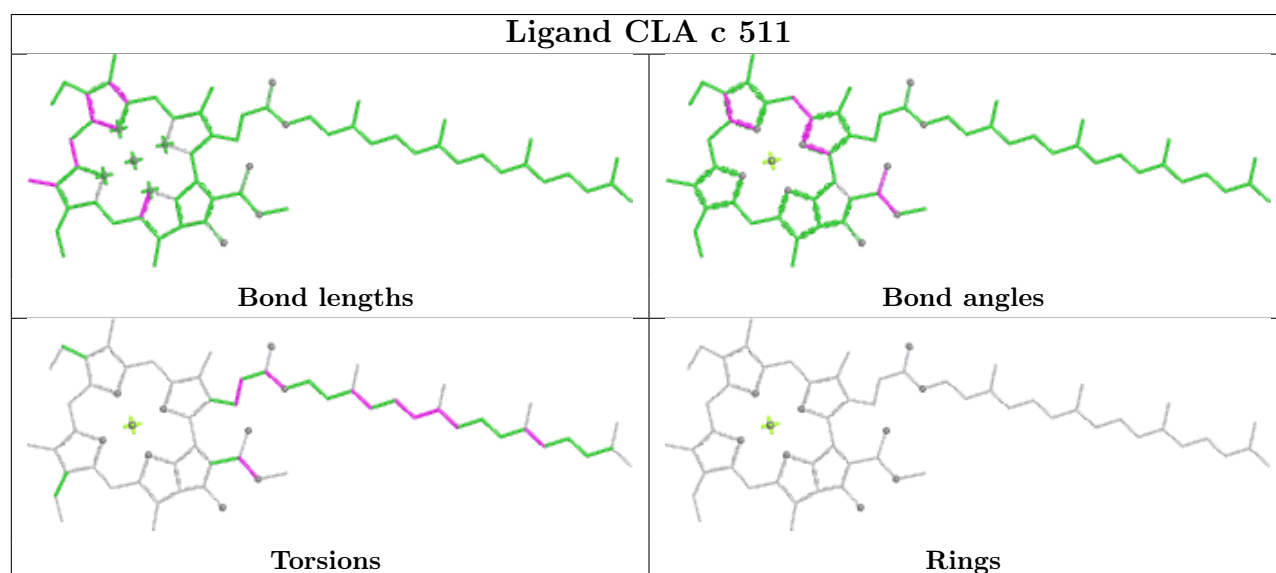
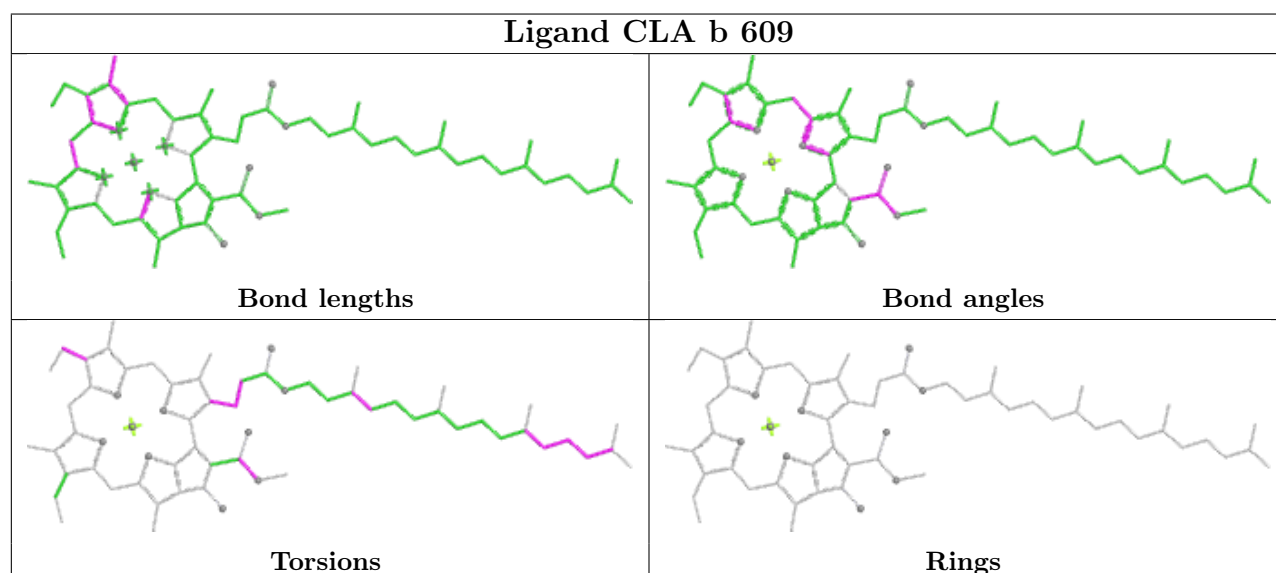
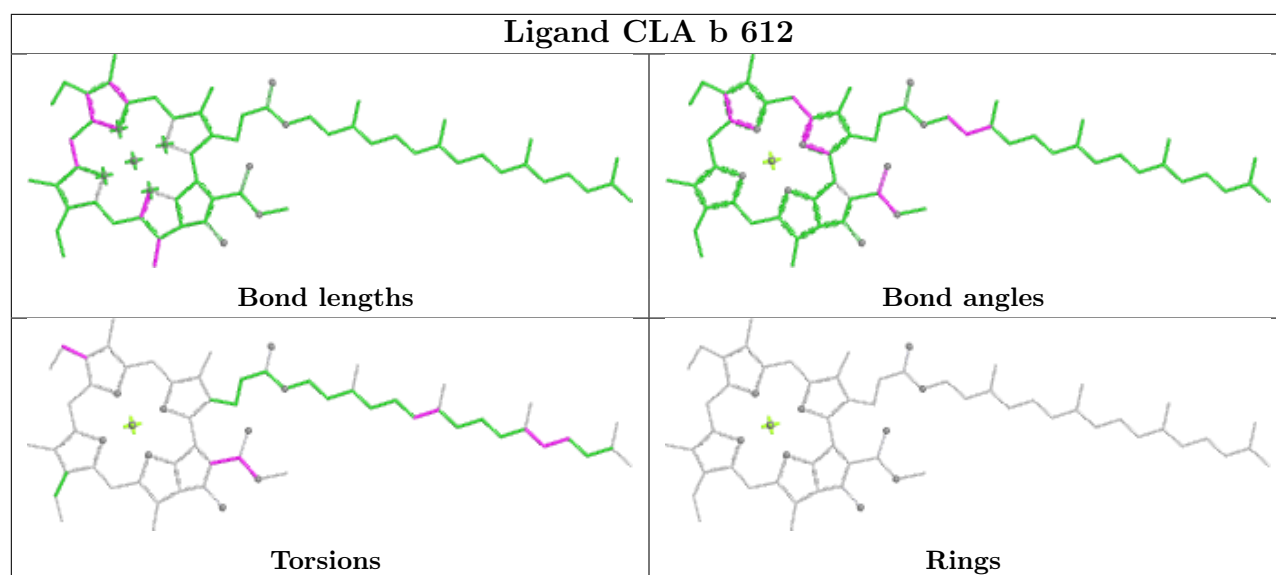


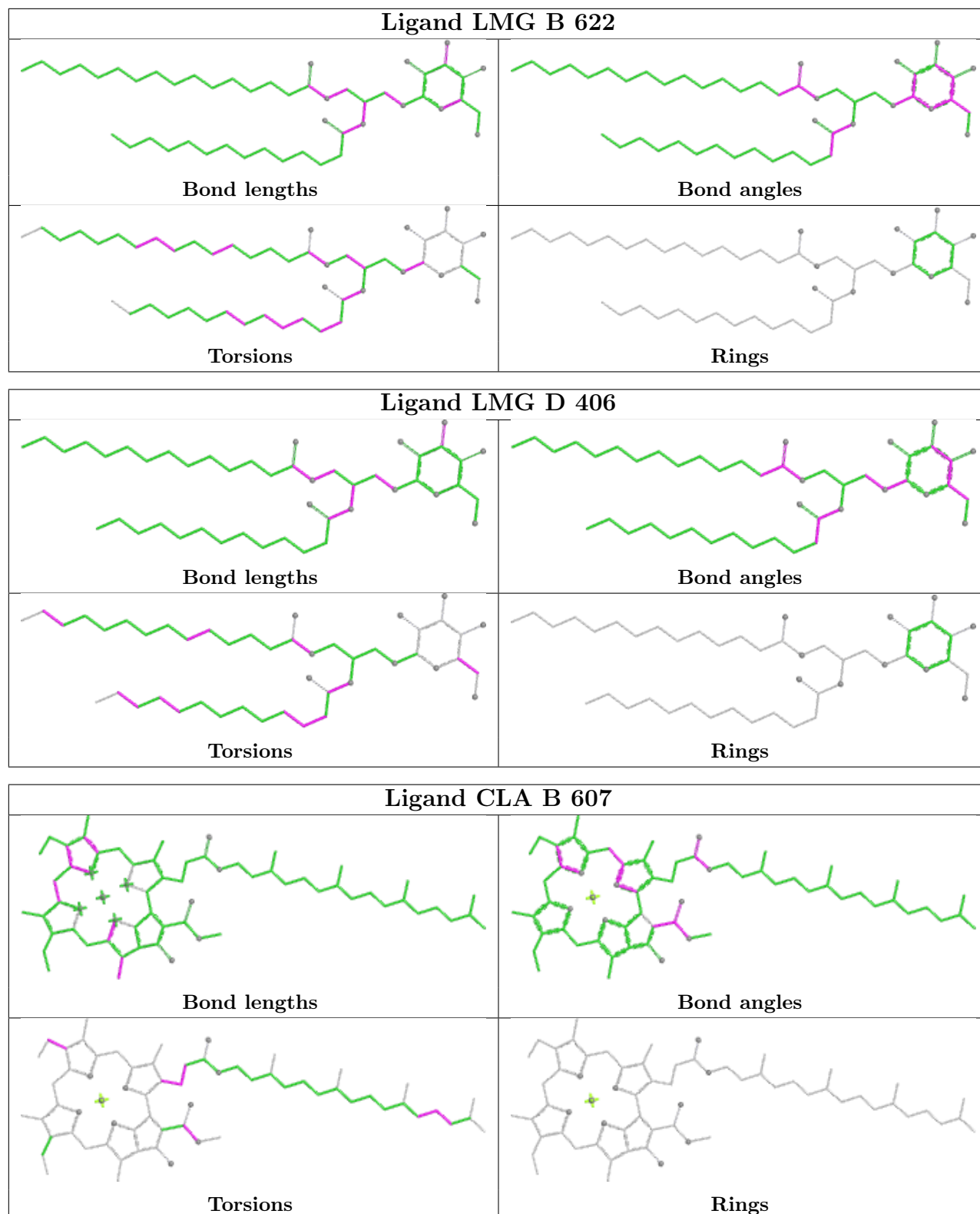
Ligand CLA D 401



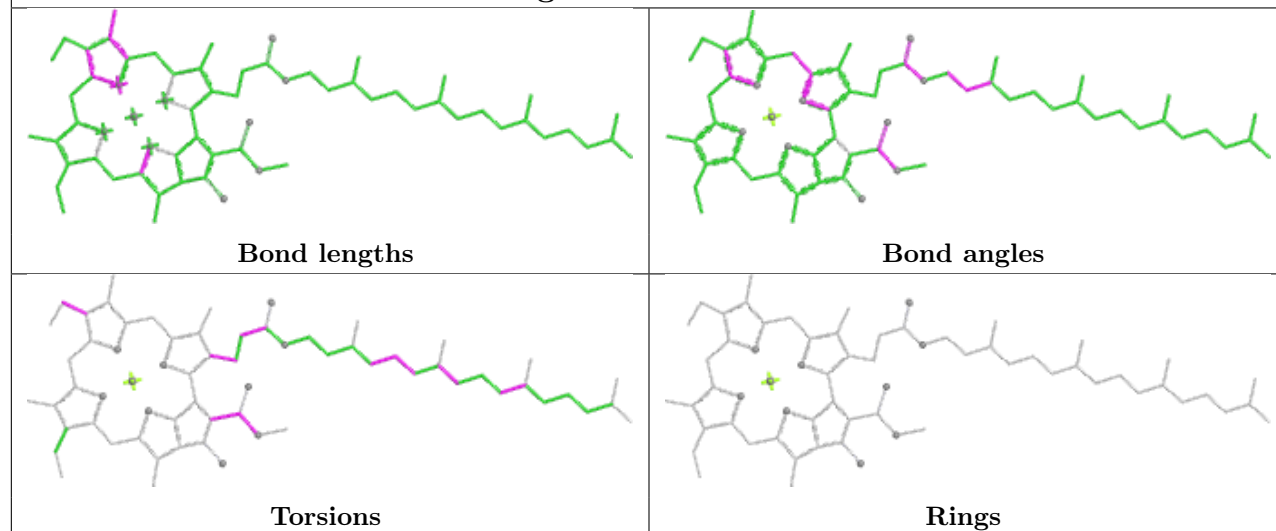




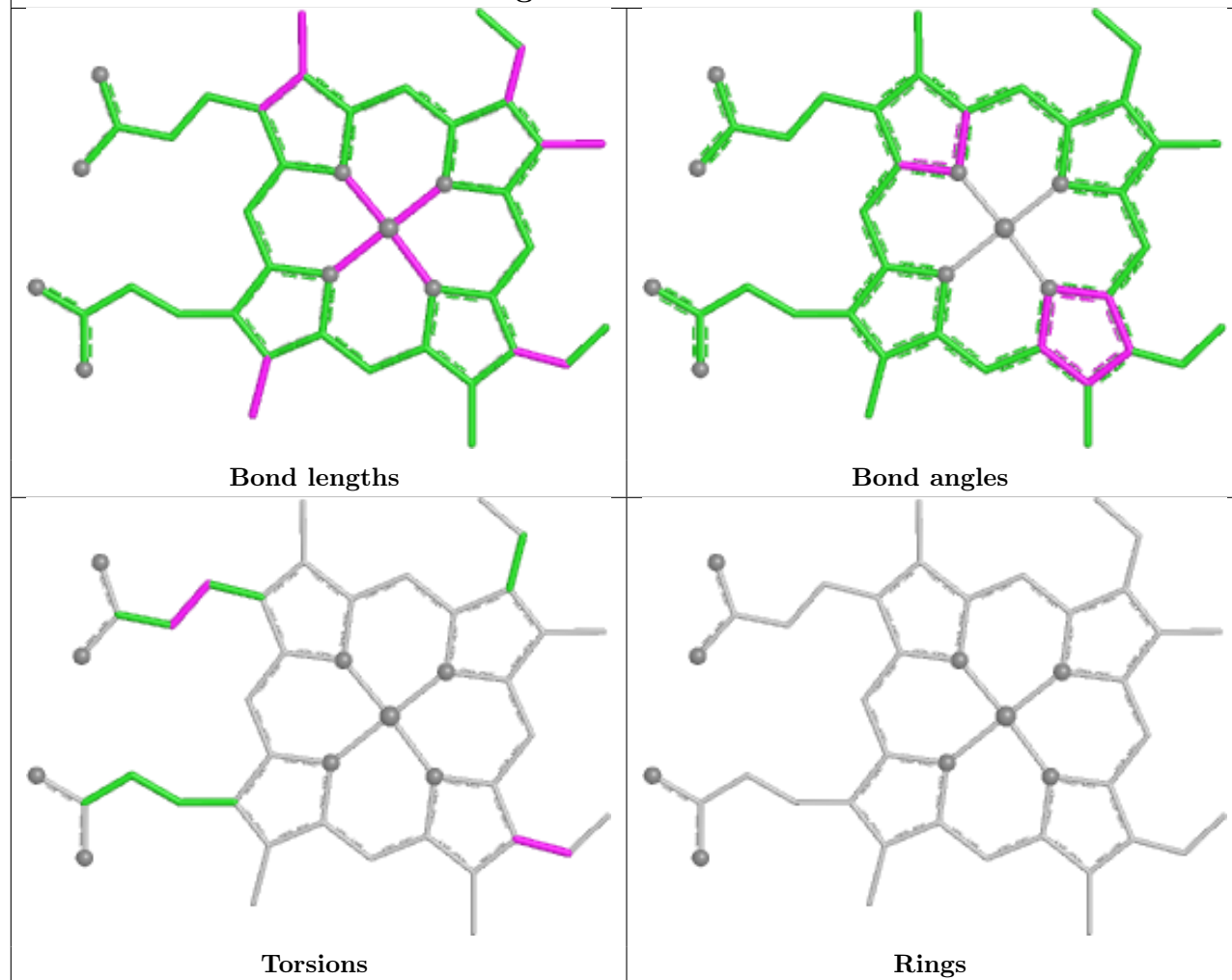


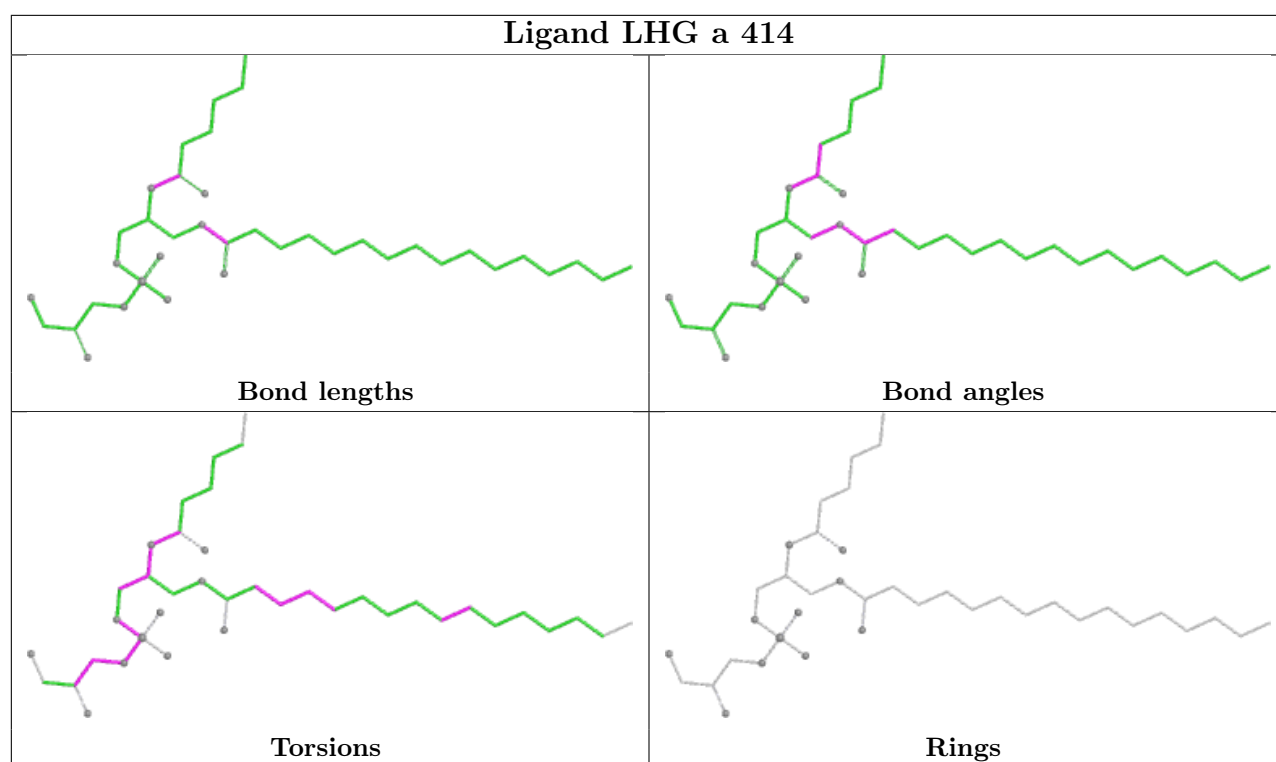
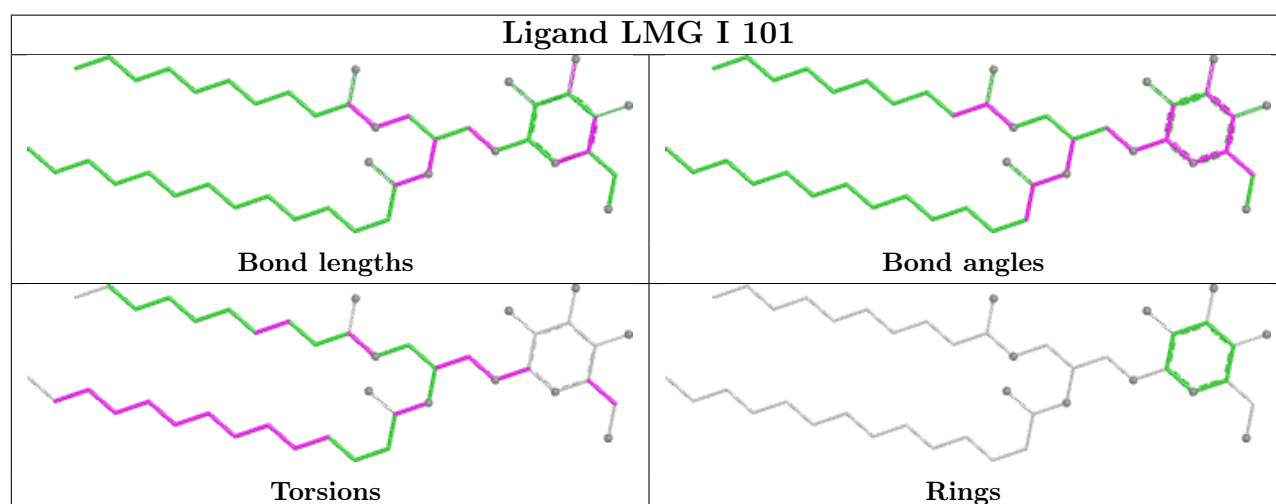
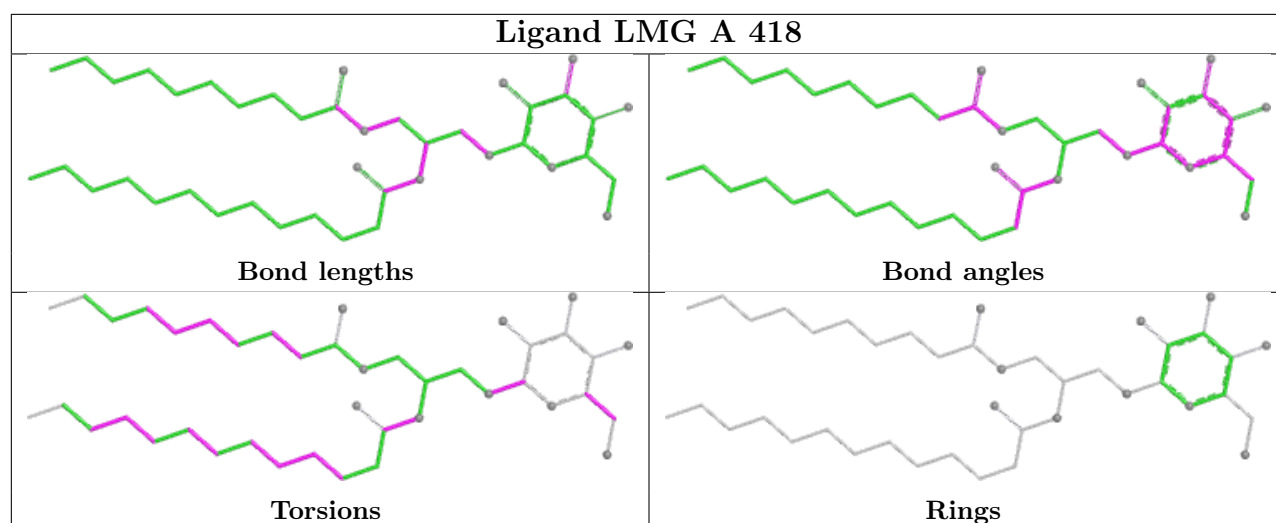


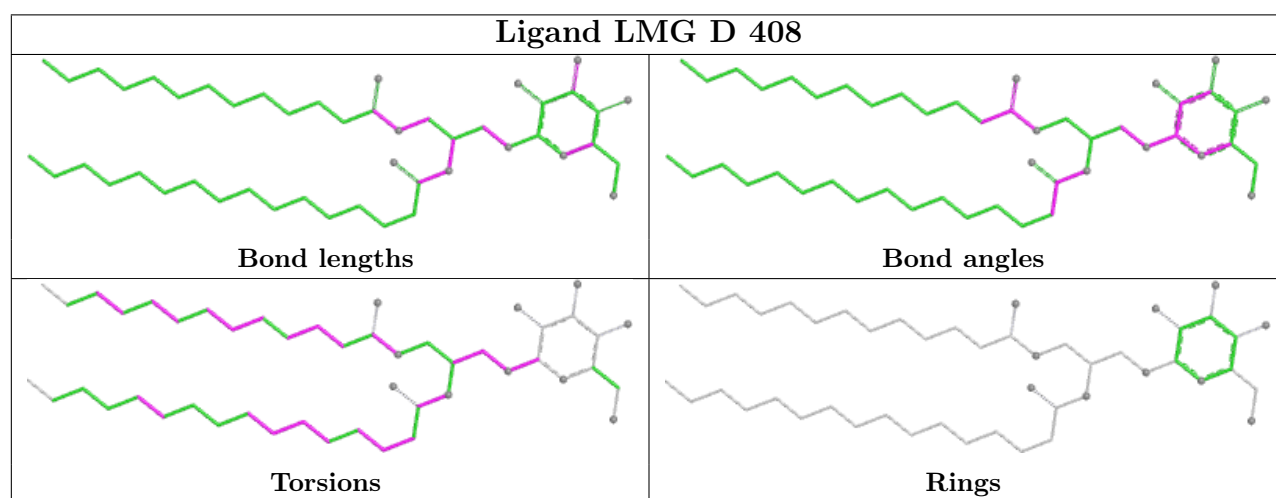
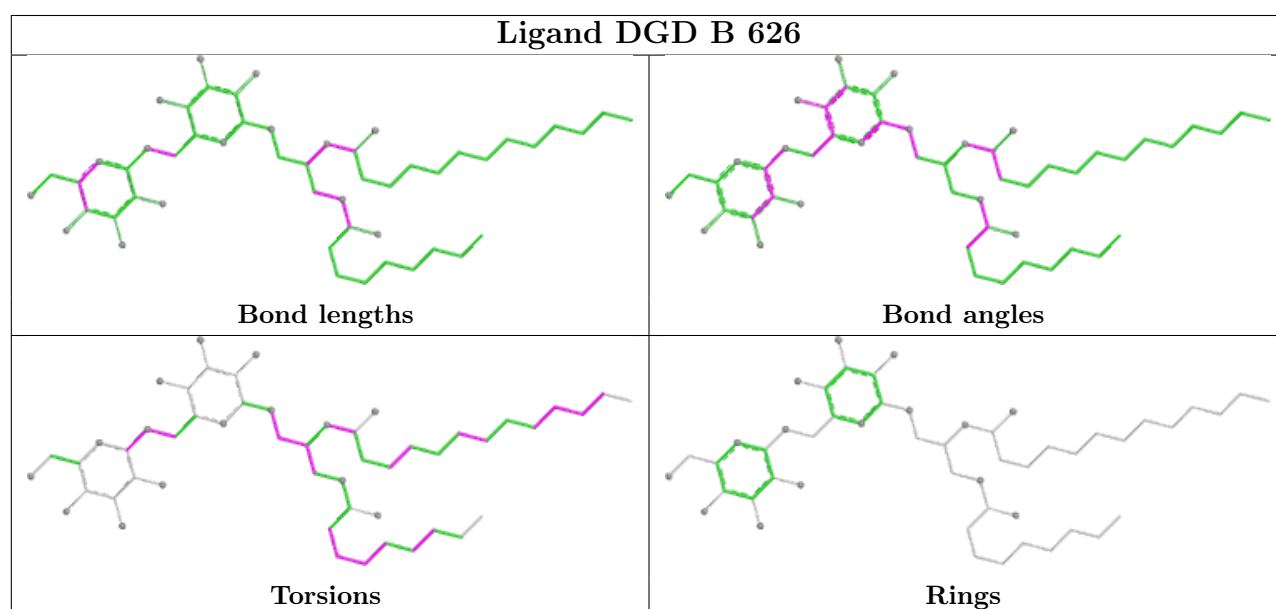
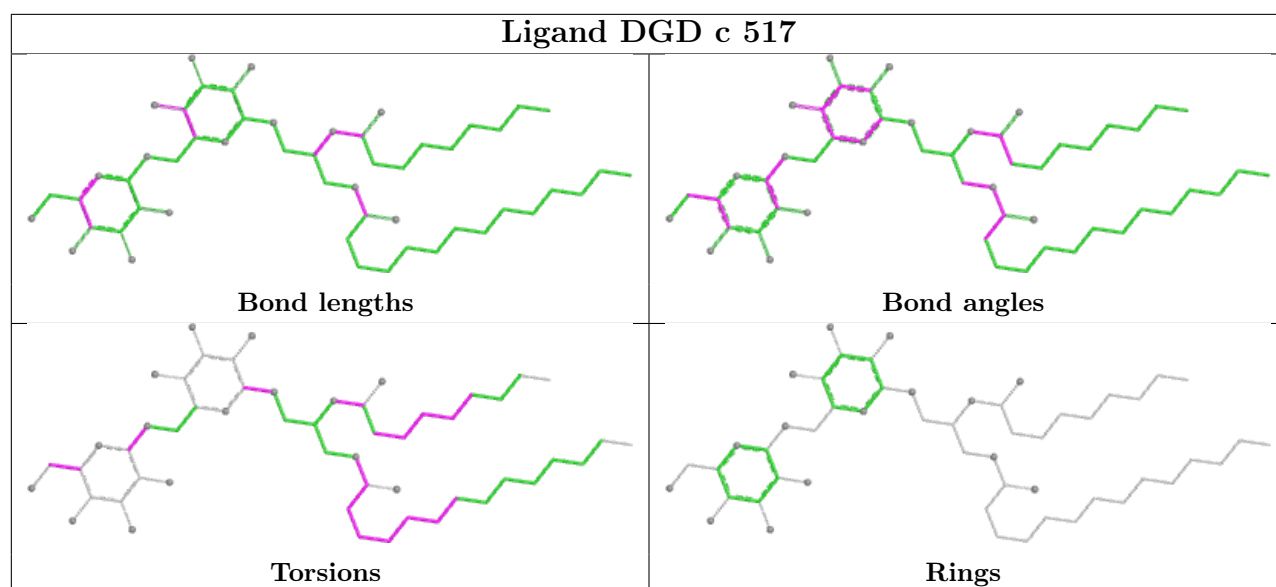
Ligand CLA c 507



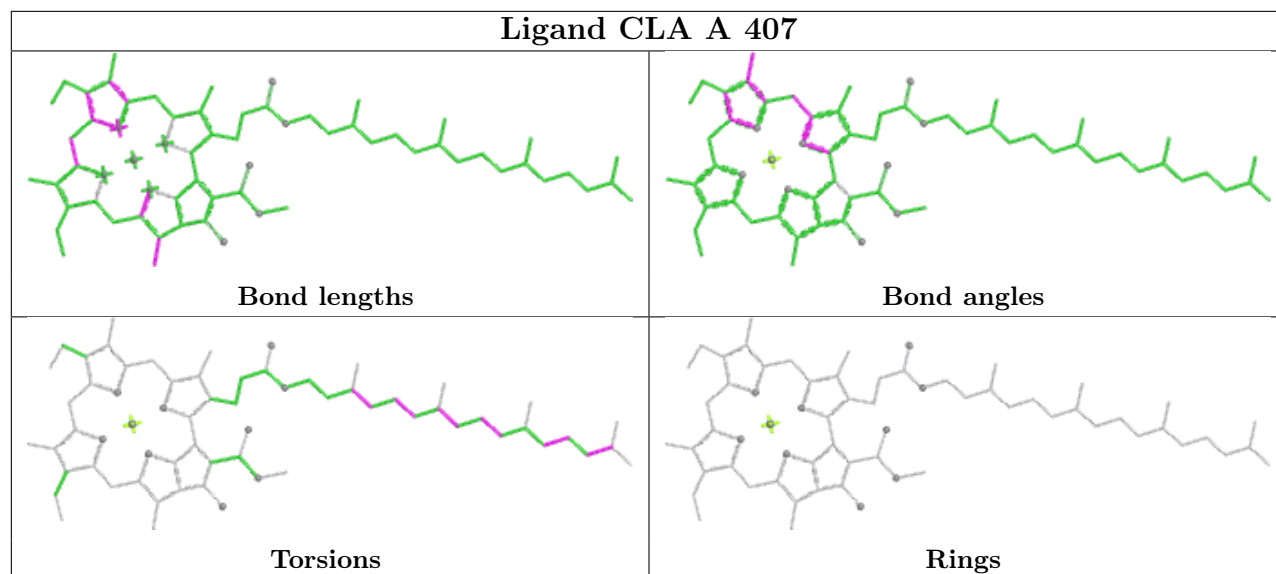
Ligand HEM f 101



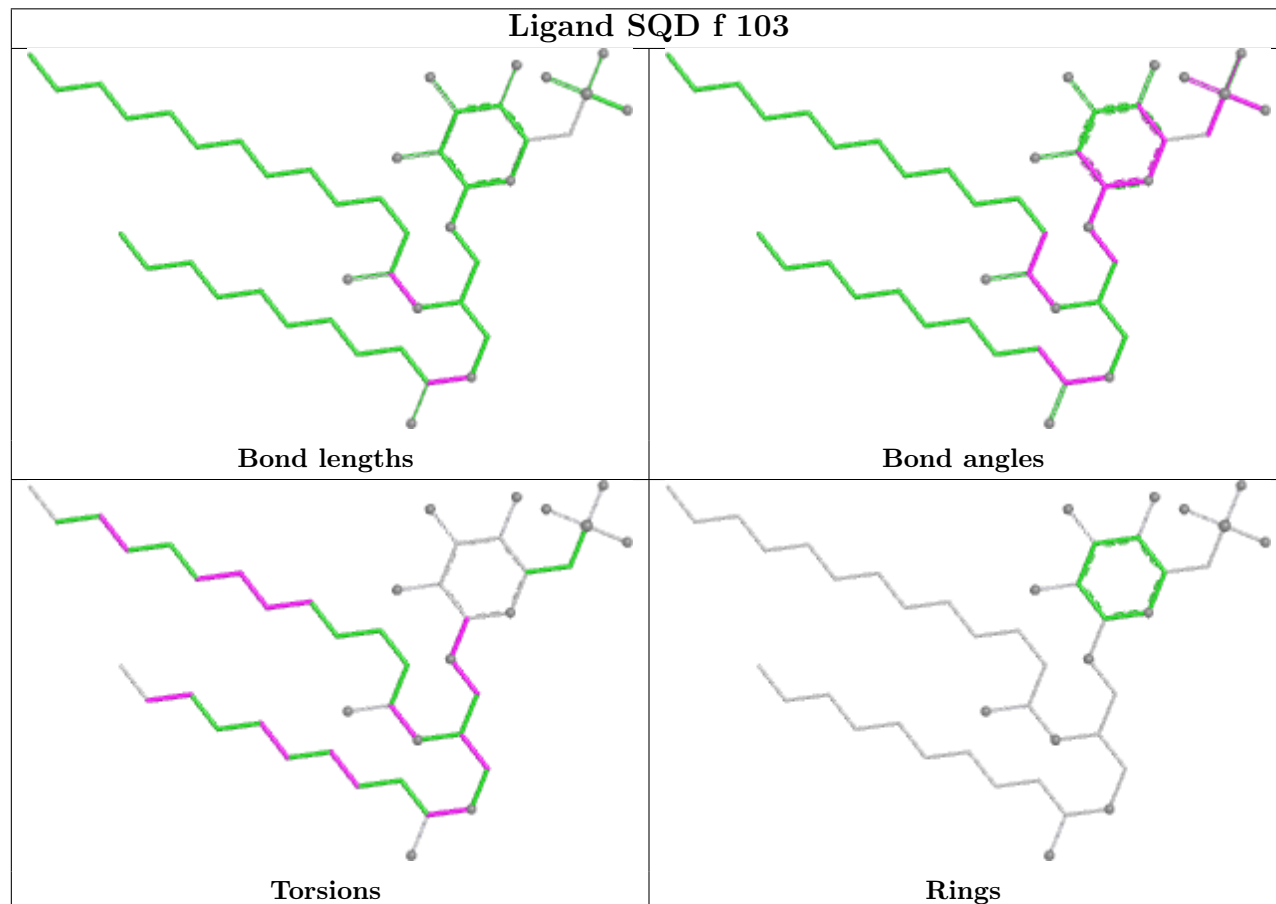


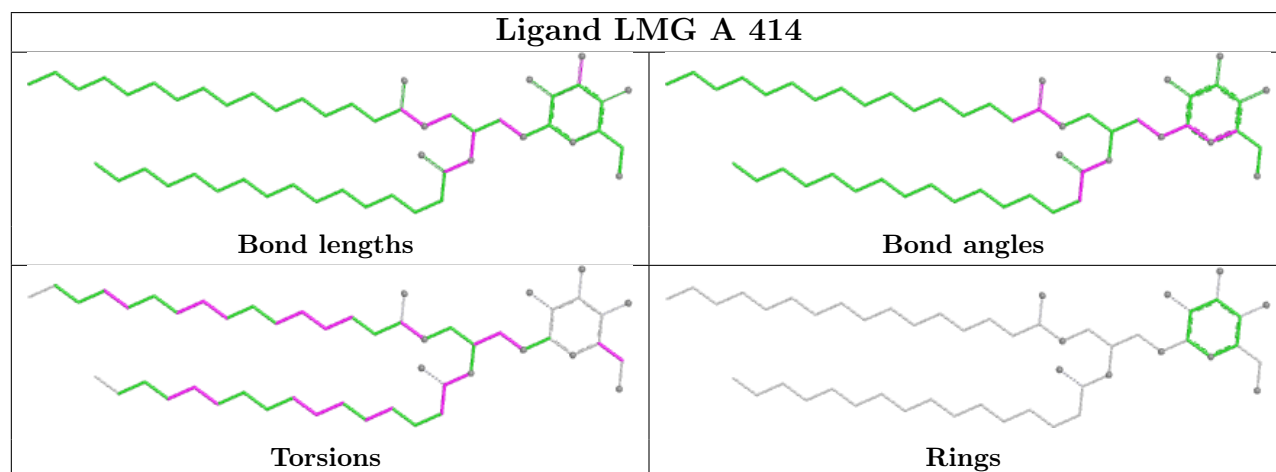
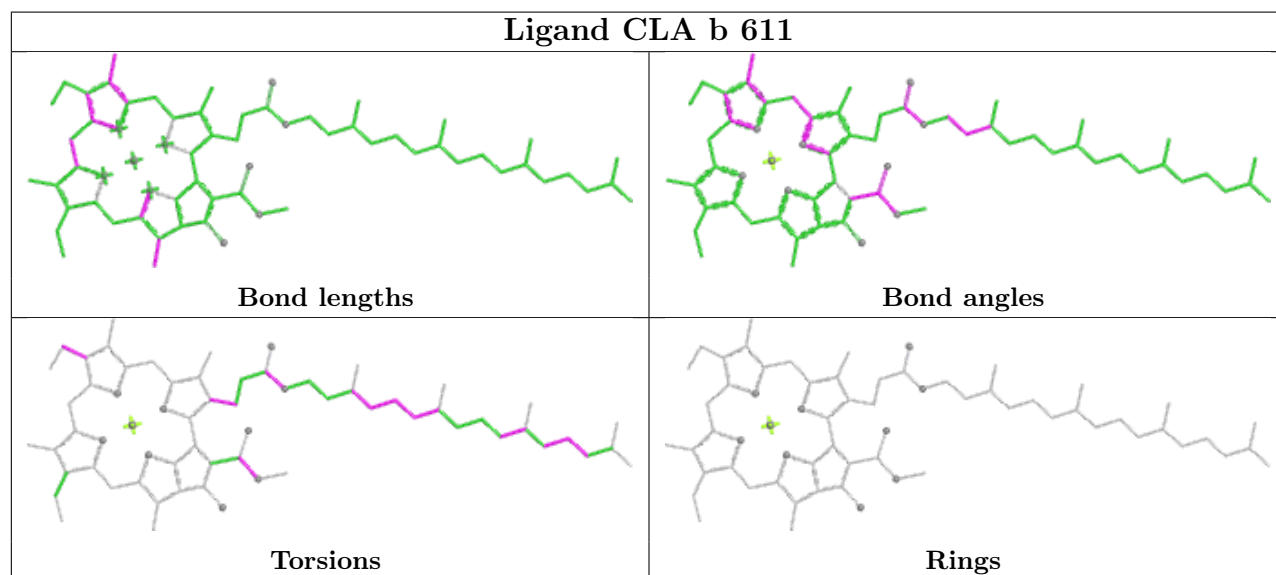
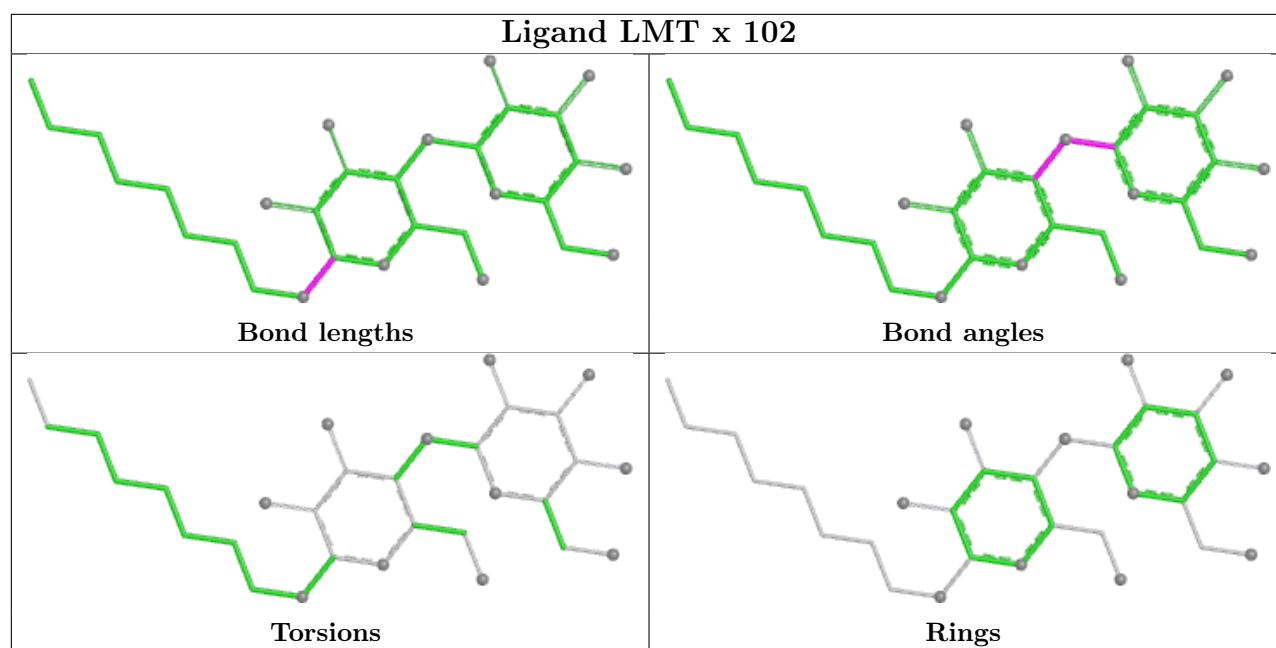


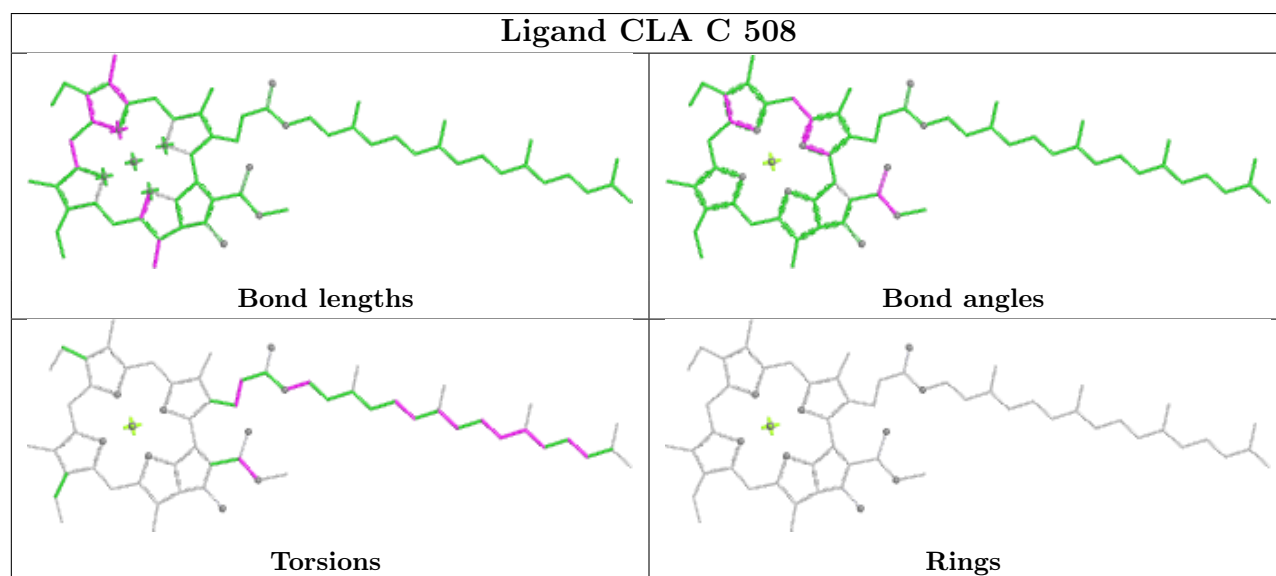
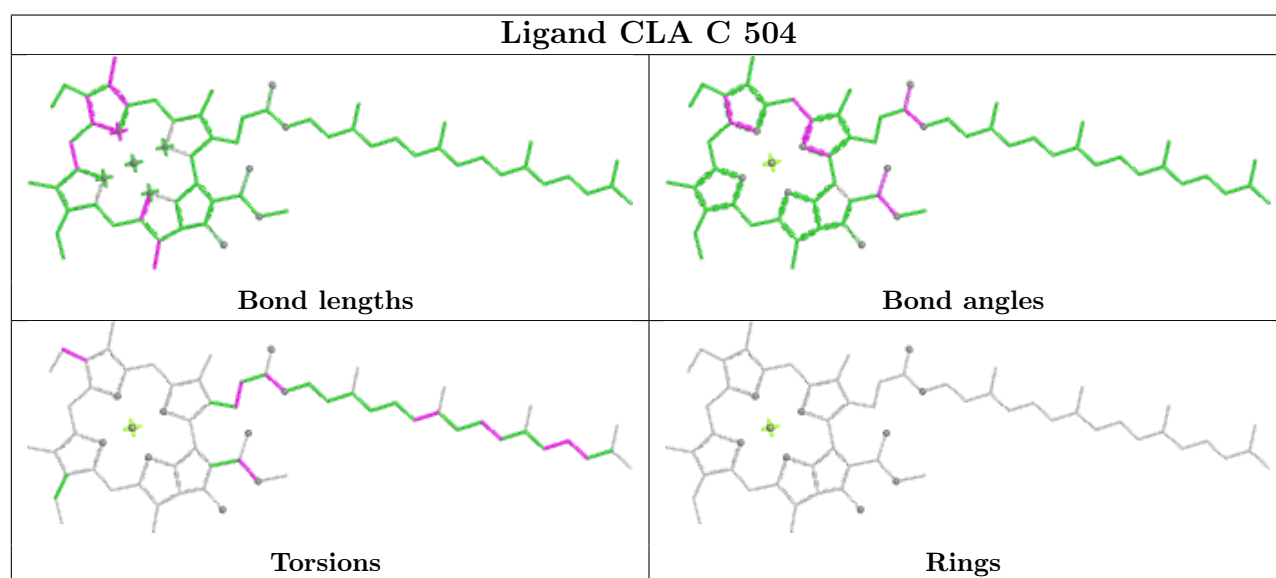
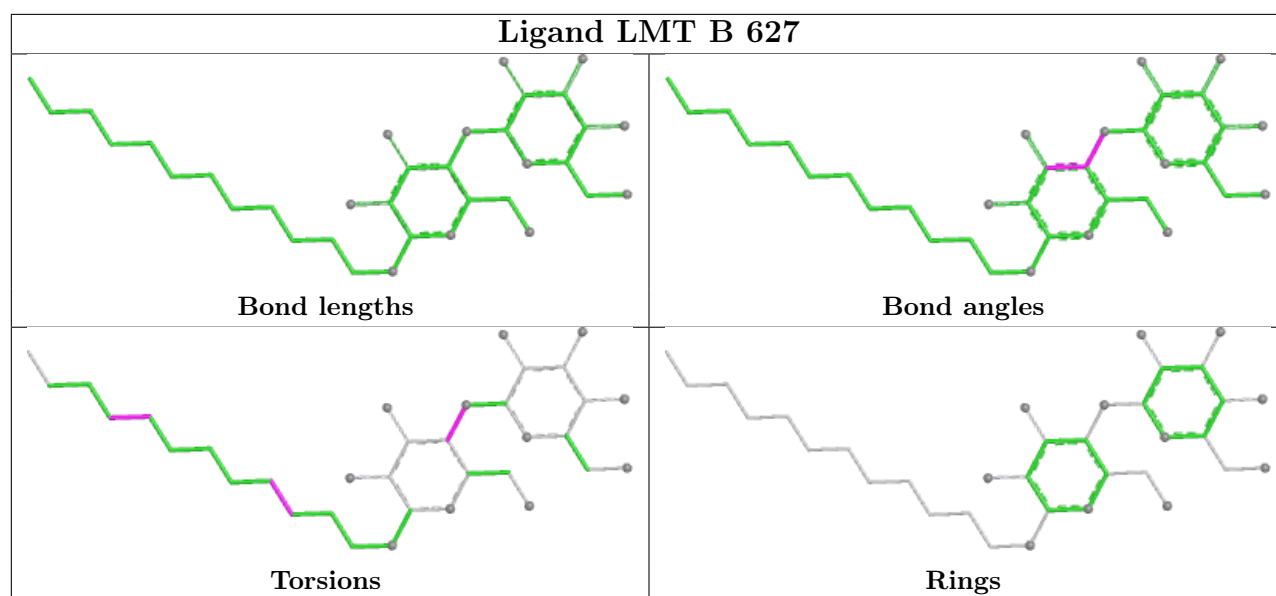
Ligand CLA A 407



Ligand SQD f 103







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	A	335/360 (93%)	0.35	16 (4%) 35 36	44, 65, 104, 152	0
1	a	335/360 (93%)	0.26	10 (2%) 52 45	46, 65, 104, 153	0
2	B	490/510 (96%)	0.38	33 (6%) 24 28	46, 70, 103, 156	0
2	b	490/510 (96%)	0.40	26 (5%) 32 33	43, 70, 103, 160	0
3	C	447/461 (96%)	0.31	12 (2%) 56 47	52, 79, 105, 133	0
3	c	447/461 (96%)	0.25	13 (2%) 53 46	56, 81, 106, 135	0
4	D	340/352 (96%)	0.35	13 (3%) 44 41	44, 66, 102, 139	0
4	d	340/352 (96%)	0.22	11 (3%) 50 44	43, 66, 102, 135	0
5	E	82/84 (97%)	0.36	1 (1%) 76 64	68, 92, 123, 132	0
5	e	82/84 (97%)	0.16	1 (1%) 76 64	70, 92, 123, 127	0
6	F	35/45 (77%)	0.61	4 (11%) 10 17	67, 84, 119, 143	0
6	f	35/45 (77%)	0.21	0 100 100	72, 83, 121, 141	0
7	H	65/66 (98%)	0.72	6 (9%) 14 21	74, 93, 119, 145	0
7	h	65/66 (98%)	0.46	2 (3%) 51 44	73, 94, 119, 148	0
8	I	35/38 (92%)	0.25	0 100 100	65, 80, 106, 120	0
8	i	35/38 (92%)	0.33	2 (5%) 29 32	68, 80, 105, 120	0
9	J	34/40 (85%)	0.40	2 (5%) 28 31	72, 85, 95, 112	0
9	j	34/40 (85%)	0.51	1 (2%) 53 46	77, 87, 96, 115	0
10	K	37/46 (80%)	0.18	0 100 100	76, 88, 99, 125	0
10	k	37/46 (80%)	0.20	0 100 100	73, 89, 104, 126	0
11	L	37/37 (100%)	0.40	1 (2%) 56 47	50, 63, 126, 156	0
11	l	37/37 (100%)	0.46	2 (5%) 31 33	51, 63, 127, 155	0
12	M	34/36 (94%)	0.52	2 (5%) 28 31	53, 69, 107, 165	0
12	m	34/36 (94%)	0.56	3 (8%) 15 21	55, 69, 109, 163	0

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Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.26	6 (2%) 58 49	49, 79, 122, 167	0
13	o	243/272 (89%)	0.42	13 (5%) 32 33	49, 79, 121, 167	0
14	T	32/32 (100%)	0.30	0 100 100	57, 69, 159, 169	0
14	t	32/32 (100%)	0.78	3 (9%) 14 20	56, 67, 158, 170	0
15	U	97/134 (72%)	0.43	4 (4%) 41 39	56, 70, 90, 112	0
15	u	97/134 (72%)	0.32	2 (2%) 63 54	56, 70, 89, 111	0
16	V	137/163 (84%)	0.34	9 (6%) 24 28	55, 71, 85, 100	0
16	v	137/163 (84%)	0.25	5 (3%) 46 42	58, 71, 86, 96	0
17	g	28/46 (60%)	0.85	2 (7%) 22 27	96, 108, 125, 129	0
17	y	28/46 (60%)	0.24	0 100 100	92, 108, 128, 129	0
18	X	37/41 (90%)	0.25	1 (2%) 56 47	77, 92, 120, 140	0
18	x	37/41 (90%)	0.43	1 (2%) 56 47	75, 90, 124, 145	0
19	Z	62/62 (100%)	0.51	7 (11%) 10 17	87, 103, 170, 186	0
19	z	62/62 (100%)	0.38	3 (4%) 35 36	88, 104, 169, 184	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.34	217 (4%) 40 39	43, 75, 115, 186	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	393	GLU	7.5
13	O	195	ASP	5.5
1	a	280	VAL	5.4
2	B	214	LEU	5.1
4	D	188	PHE	5.0

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
33	LMT	x	102	31/35	0.53	0.21	79,130,156,157	0
33	LMT	i	102	35/35	0.55	0.21	99,136,146,150	0
23	CLA	b	604	65/65	0.59	0.22	93,108,130,134	0
33	LMT	D	411	31/35	0.60	0.18	82,132,156,156	0
33	LMT	I	102	35/35	0.60	0.24	94,136,147,149	0
31	LMG	C	520	45/55	0.61	0.26	80,119,142,171	0
27	BCR	J	102	40/40	0.63	0.35	109,129,176,177	0
33	LMT	B	623	35/35	0.63	0.17	76,136,170,172	0
32	CL	A	416	1/1	0.64	0.15	49,49,49,49	0
33	LMT	B	628	35/35	0.66	0.23	72,137,162,163	0
23	CLA	B	601	65/65	0.68	0.20	94,108,129,134	0
33	LMT	b	626	35/35	0.69	0.20	99,143,152,153	0
23	CLA	C	507	65/65	0.69	0.23	77,92,101,105	0
27	BCR	j	102	40/40	0.69	0.37	107,125,176,178	0
28	DGD	B	626	52/66	0.72	0.23	77,104,179,183	0
25	PL9	J	101	35/55	0.74	0.45	119,157,183,185	0
31	LMG	c	520	45/55	0.75	0.17	82,119,140,168	0
30	SQD	B	625	47/54	0.76	0.23	73,102,139,146	0
25	PL9	A	408	45/55	0.76	0.30	84,103,119,127	0
33	LMT	b	625	35/35	0.76	0.16	78,139,172,176	0
28	DGD	C	518	66/66	0.78	0.23	58,72,106,121	0
33	LMT	b	603	35/35	0.78	0.20	76,131,155,156	0
27	BCR	k	102	40/40	0.79	0.22	69,85,106,109	0
29	LHG	a	417	37/49	0.79	0.19	111,134,197,206	0
27	BCR	H	101	40/40	0.79	0.24	82,95,131,132	0
31	LMG	b	624	49/55	0.80	0.29	56,76,88,91	0
28	DGD	b	602	52/66	0.80	0.21	81,104,177,178	0
23	CLA	c	513	65/65	0.80	0.17	94,107,138,149	0
29	LHG	A	415	37/49	0.81	0.17	108,137,192,202	0
30	SQD	d	407	43/54	0.81	0.20	73,107,144,149	0
28	DGD	d	408	63/66	0.81	0.26	104,127,184,187	0
33	LMT	B	624	35/35	0.82	0.20	91,142,154,155	0
33	LMT	B	627	35/35	0.82	0.23	71,122,138,140	0
31	LMG	k	103	48/55	0.82	0.29	80,100,118,120	0
28	DGD	D	410	63/66	0.82	0.26	104,127,181,188	0
28	DGD	c	518	62/66	0.82	0.22	65,86,138,143	0
23	CLA	a	409	65/65	0.83	0.23	55,69,129,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SQD	a	415	51/54	0.83	0.22	81,102,128,134	0
30	SQD	b	601	47/54	0.83	0.22	86,99,139,146	0
27	BCR	c	514	40/40	0.83	0.21	66,80,89,91	0
27	BCR	D	405	40/40	0.83	0.24	65,80,101,108	0
31	LMG	M	101	42/55	0.83	0.23	78,110,135,144	0
23	CLA	b	619	65/65	0.83	0.20	78,99,142,147	0
30	SQD	F	102	45/54	0.84	0.25	86,129,153,154	0
29	LHG	A	412	39/49	0.84	0.23	61,80,92,94	0
24	PHO	A	406	64/64	0.84	0.20	57,69,74,76	0
33	LMT	T	101	35/35	0.84	0.25	63,115,136,143	0
25	PL9	j	101	35/55	0.84	0.33	120,159,178,180	0
31	LMG	A	418	42/55	0.84	0.24	76,107,120,142	0
31	LMG	B	622	49/55	0.84	0.24	50,74,85,91	0
28	DGD	A	411	56/66	0.84	0.20	79,100,145,149	0
31	LMG	E	101	44/55	0.84	0.22	85,123,134,138	0
31	LMG	a	402	42/55	0.85	0.23	76,105,121,142	0
31	LMG	a	416	51/55	0.85	0.27	61,80,92,99	0
28	DGD	C	517	62/66	0.85	0.17	61,84,132,147	0
23	CLA	b	618	65/65	0.85	0.16	78,97,109,116	0
23	CLA	C	503	65/65	0.85	0.19	76,88,99,101	0
27	BCR	x	101	40/40	0.85	0.21	81,97,129,130	0
23	CLA	c	509	65/65	0.85	0.17	73,82,91,98	0
30	SQD	a	401	54/54	0.85	0.23	75,116,152,156	0
23	CLA	b	609	65/65	0.85	0.17	71,86,111,121	0
22	BCT	d	401	4/4	0.86	0.13	77,80,82,85	0
23	CLA	b	613	65/65	0.86	0.16	71,81,88,91	0
23	CLA	C	512	65/65	0.86	0.19	83,101,147,151	0
23	CLA	A	407	65/65	0.86	0.21	57,69,128,131	0
27	BCR	c	515	40/40	0.86	0.21	83,95,112,115	0
23	CLA	C	506	65/65	0.86	0.21	75,91,123,134	0
27	BCR	B	618	40/40	0.86	0.25	68,80,90,92	0
33	LMT	m	101	35/35	0.86	0.25	71,95,109,109	0
27	BCR	B	620	40/40	0.86	0.22	77,87,92,92	0
35	CA	o	301	1/1	0.86	0.11	106,106,106,106	0
27	BCR	Z	101	40/40	0.87	0.23	81,93,117,118	0
29	LHG	a	414	39/49	0.87	0.20	62,79,91,94	0
23	CLA	C	511	65/65	0.87	0.18	73,90,100,109	0
23	CLA	c	511	65/65	0.87	0.15	72,91,102,106	0
30	SQD	D	409	43/54	0.87	0.24	72,103,147,151	0
31	LMG	i	101	43/55	0.87	0.21	85,120,158,176	0
31	LMG	C	519	48/55	0.87	0.23	86,99,110,116	0
23	CLA	C	513	65/65	0.87	0.15	93,108,142,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	D	407	49/55	0.87	0.26	59,80,109,117	0
27	BCR	T	103	40/40	0.87	0.23	69,79,87,95	0
35	CA	K	101	1/1	0.87	0.30	72,72,72,72	0
31	LMG	I	101	43/55	0.87	0.20	87,115,159,171	0
27	BCR	a	412	40/40	0.88	0.21	51,71,82,84	0
27	BCR	C	514	40/40	0.88	0.19	70,80,86,90	0
28	DGD	a	413	56/66	0.88	0.18	74,101,145,149	0
31	LMG	M	102	42/55	0.88	0.23	70,109,133,139	0
33	LMT	M	103	35/35	0.88	0.22	68,98,108,115	0
27	BCR	C	515	40/40	0.88	0.20	76,87,95,98	0
23	CLA	c	507	65/65	0.88	0.17	84,94,102,109	0
25	PL9	d	404	55/55	0.88	0.26	48,65,76,86	0
23	CLA	C	504	65/65	0.88	0.20	67,83,133,136	0
27	BCR	K	102	40/40	0.88	0.18	74,85,102,103	0
24	PHO	D	402	64/64	0.88	0.16	48,61,71,77	0
23	CLA	C	501	65/65	0.88	0.18	66,80,90,95	0
30	SQD	A	413	51/54	0.88	0.18	81,95,126,130	0
30	SQD	A	417	54/54	0.88	0.22	81,116,146,153	0
28	DGD	c	519	66/66	0.89	0.18	61,72,104,113	0
27	BCR	T	102	40/40	0.89	0.26	66,73,83,85	0
23	CLA	B	614	65/65	0.89	0.21	64,83,124,132	0
23	CLA	b	611	65/65	0.89	0.17	63,76,96,100	0
23	CLA	c	506	65/65	0.89	0.17	79,94,122,126	0
27	BCR	b	620	40/40	0.89	0.25	59,72,79,80	0
31	LMG	e	101	44/55	0.89	0.18	85,122,133,140	0
27	BCR	b	621	40/40	0.89	0.16	72,83,92,94	0
27	BCR	A	410	40/40	0.89	0.21	53,68,81,91	0
23	CLA	b	612	65/65	0.89	0.17	69,89,104,106	0
31	LMG	D	408	48/55	0.89	0.23	52,73,83,120	0
27	BCR	c	516	40/40	0.89	0.21	76,86,93,103	0
35	CA	k	101	1/1	0.89	0.13	94,94,94,94	0
23	CLA	b	605	65/65	0.89	0.17	73,87,96,98	0
31	LMG	b	623	49/55	0.90	0.23	57,80,96,113	0
27	BCR	f	102	40/40	0.90	0.18	64,83,107,110	0
23	CLA	B	606	65/65	0.90	0.17	68,84,111,123	0
28	DGD	b	622	58/66	0.90	0.19	57,71,97,102	0
23	CLA	a	405	65/65	0.90	0.18	40,54,65,72	0
23	CLA	C	509	65/65	0.90	0.15	65,81,95,98	0
25	PL9	a	410	45/55	0.90	0.21	82,98,119,127	0
23	CLA	B	616	65/65	0.90	0.21	75,93,144,150	0
23	CLA	c	512	65/65	0.90	0.14	90,102,148,154	0
23	CLA	B	610	65/65	0.90	0.16	68,82,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SQD	f	103	45/54	0.90	0.17	88,129,148,155	0
23	CLA	b	607	65/65	0.90	0.17	62,67,112,117	0
23	CLA	b	610	65/65	0.91	0.18	52,64,82,88	0
23	CLA	B	608	65/65	0.91	0.17	62,74,94,97	0
32	CL	d	409	1/1	0.91	0.22	49,49,49,49	0
23	CLA	D	403	65/65	0.91	0.18	73,85,121,124	0
28	DGD	B	621	58/66	0.91	0.17	51,69,99,106	0
23	CLA	B	602	65/65	0.91	0.15	68,87,96,99	0
24	PHO	a	408	64/64	0.91	0.12	58,71,81,87	0
27	BCR	B	619	40/40	0.91	0.24	62,76,82,84	0
23	CLA	c	510	65/65	0.91	0.15	66,74,85,87	0
23	CLA	A	405	65/65	0.91	0.18	48,69,139,145	0
24	PHO	a	407	64/64	0.92	0.17	52,62,71,76	0
31	LMG	D	406	46/55	0.92	0.18	55,74,116,125	0
31	LMG	d	405	46/55	0.92	0.18	65,71,116,128	0
31	LMG	d	406	48/55	0.92	0.18	56,71,86,120	0
23	CLA	c	508	65/65	0.92	0.17	73,84,120,134	0
23	CLA	B	612	65/65	0.92	0.14	56,69,84,87	0
25	PL9	D	404	55/55	0.92	0.21	47,59,70,74	0
23	CLA	B	609	65/65	0.92	0.17	73,89,105,112	0
23	CLA	B	603	65/65	0.92	0.17	65,80,91,105	0
23	CLA	c	503	65/65	0.92	0.11	73,89,97,103	0
34	HEM	f	101	43/43	0.92	0.17	77,103,125,130	0
23	CLA	c	505	65/65	0.92	0.17	66,78,83,86	0
23	CLA	C	510	65/65	0.92	0.14	63,73,85,93	0
23	CLA	b	606	65/65	0.92	0.16	69,79,93,100	0
23	CLA	B	605	65/65	0.93	0.14	58,77,87,92	0
23	CLA	b	614	65/65	0.93	0.16	57,71,79,93	0
23	CLA	b	615	65/65	0.93	0.14	62,72,83,94	0
23	CLA	B	615	65/65	0.93	0.16	82,94,108,116	0
23	CLA	b	608	65/65	0.93	0.15	58,76,85,89	0
27	BCR	B	617	40/40	0.93	0.18	64,73,79,80	0
23	CLA	c	501	65/65	0.93	0.14	68,81,89,95	0
23	CLA	c	502	65/65	0.93	0.11	67,75,101,107	0
23	CLA	a	406	65/65	0.93	0.18	53,70,143,149	0
23	CLA	c	504	65/65	0.93	0.15	69,82,132,136	0
23	CLA	C	508	65/65	0.93	0.16	70,84,123,140	0
28	DGD	c	517	53/66	0.93	0.18	58,75,98,102	0
23	CLA	A	403	65/65	0.93	0.17	47,58,67,68	0
23	CLA	D	401	65/65	0.93	0.14	47,58,85,99	0
23	CLA	d	403	65/65	0.94	0.17	72,88,124,128	0
23	CLA	C	502	65/65	0.94	0.18	62,72,104,112	0

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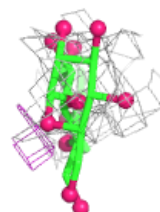
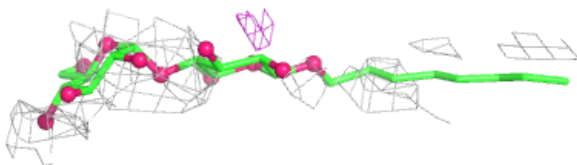
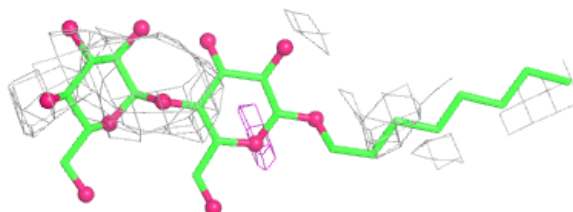
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	A	414	51/55	0.94	0.18	61,74,88,96	0
23	CLA	b	616	65/65	0.94	0.17	54,68,90,92	0
23	CLA	b	617	65/65	0.94	0.18	67,82,130,135	0
23	CLA	B	613	65/65	0.94	0.16	44,63,88,92	0
23	CLA	B	604	65/65	0.94	0.14	55,66,109,121	0
34	HEM	F	101	43/43	0.94	0.17	92,104,127,128	0
23	CLA	C	505	65/65	0.94	0.14	69,77,84,88	0
34	HEM	v	201	43/43	0.94	0.14	61,68,75,78	0
23	CLA	B	607	65/65	0.94	0.14	56,64,84,91	0
35	CA	O	301	1/1	0.94	0.07	123,123,123,123	0
23	CLA	B	611	65/65	0.94	0.13	65,73,80,81	0
22	BCT	A	402	4/4	0.94	0.10	84,88,89,93	0
23	CLA	A	404	65/65	0.95	0.15	39,54,66,70	0
23	CLA	a	404	65/65	0.95	0.12	44,58,65,73	0
28	DGD	C	516	53/66	0.95	0.17	58,75,97,102	0
23	CLA	d	402	65/65	0.95	0.13	49,59,79,91	0
34	HEM	V	201	43/43	0.96	0.18	46,65,74,79	0
26	OEC	a	411	5/9	0.98	0.18	35,44,62,62	0
21	FE2	A	401	1/1	0.99	0.03	60,60,60,60	0
21	FE2	a	403	1/1	0.99	0.06	70,70,70,70	0
26	OEC	A	409	5/9	0.99	0.15	35,44,46,62	0

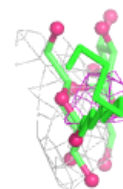
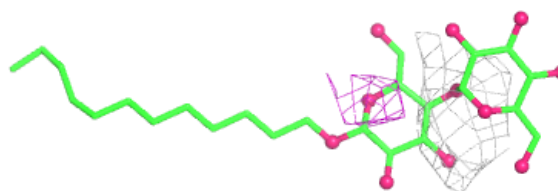
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT x 102:

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

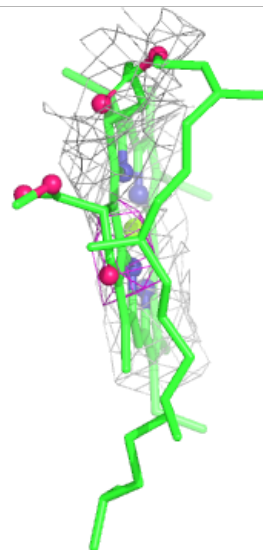
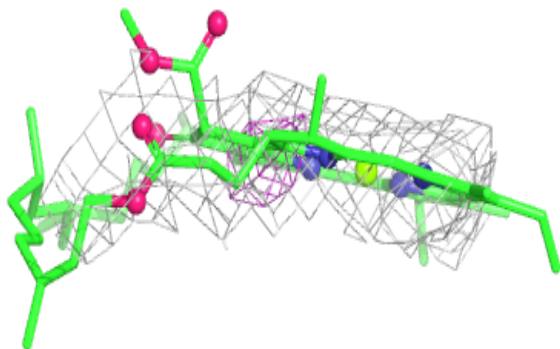
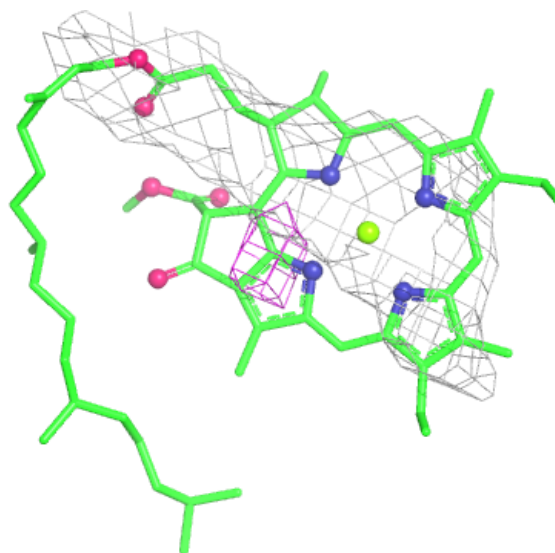
**Electron density around LMT i 102:**

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



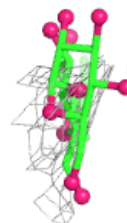
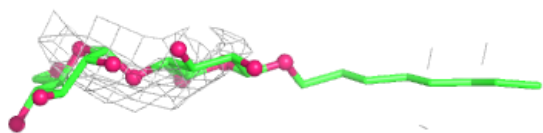
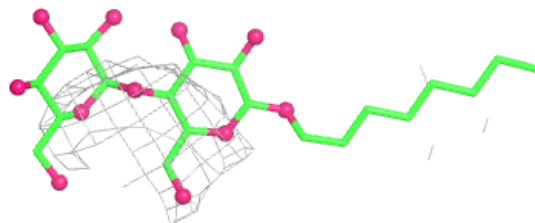
Electron density around CLA b 604:

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

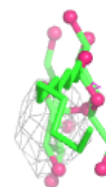
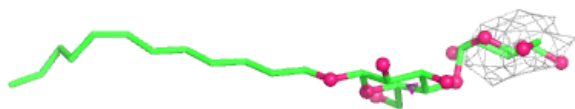
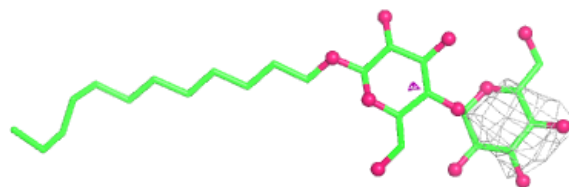


Electron density around LMT D 411:

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

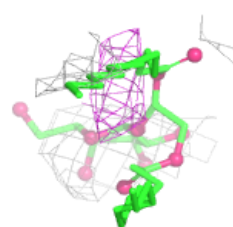
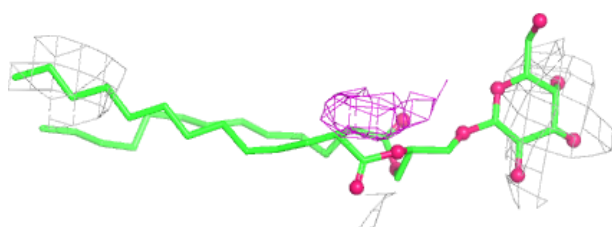
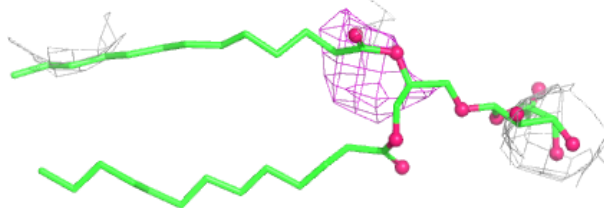
**Electron density around LMT I 102:**

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

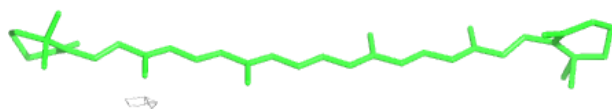
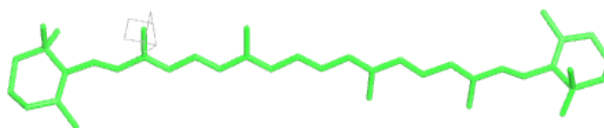


Electron density around LMG C 520:

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

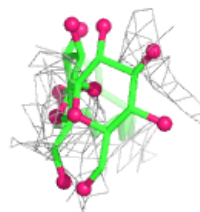
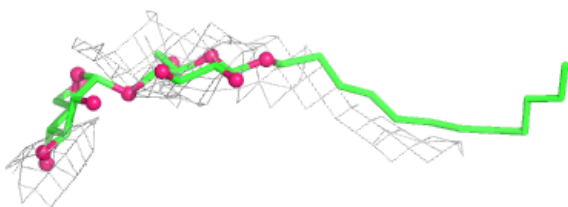
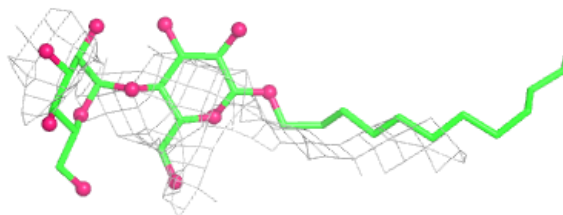
**Electron density around BCR J 102:**

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

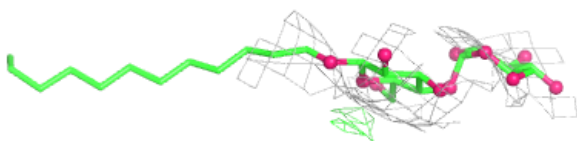
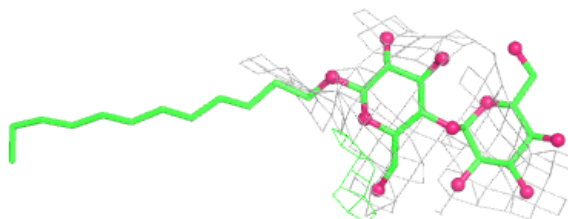


Electron density around LMT B 623:

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

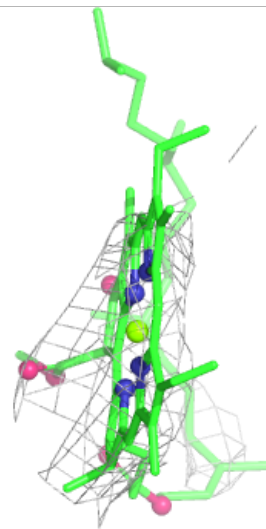
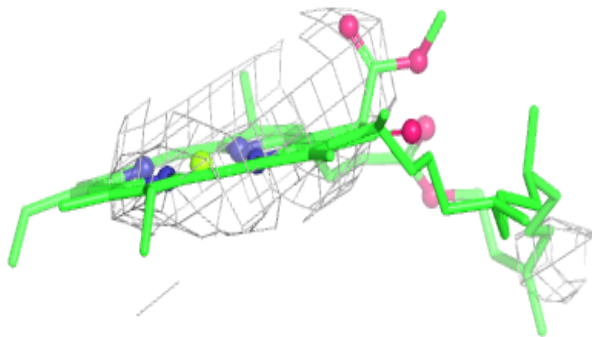
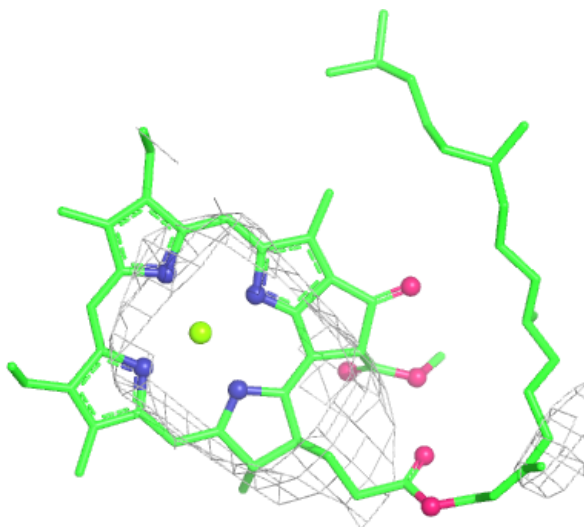
**Electron density around LMT B 628:**

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



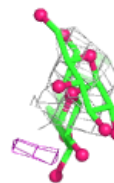
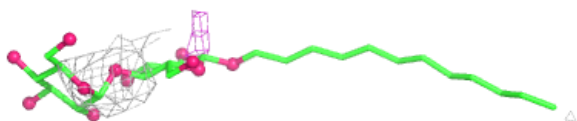
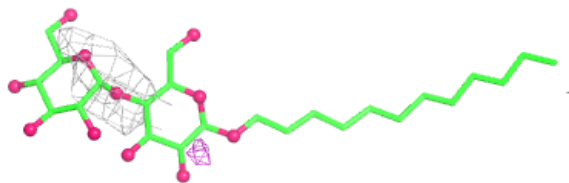
Electron density around CLA B 601:

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



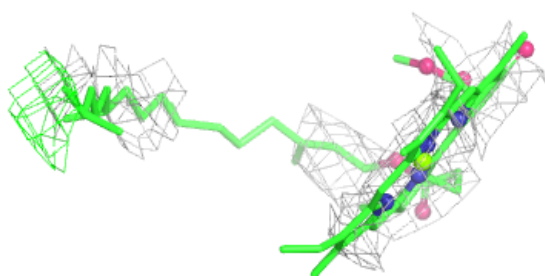
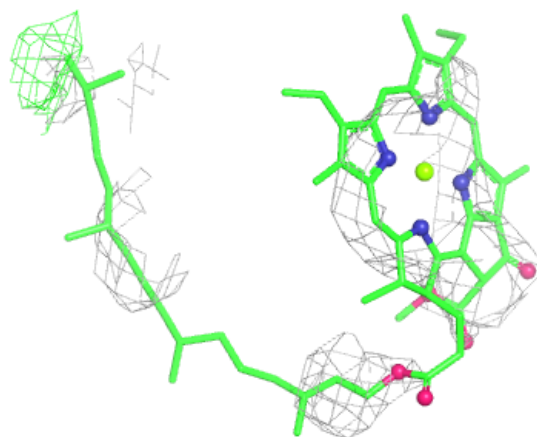
Electron density around LMT b 626:

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

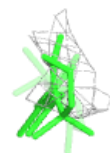
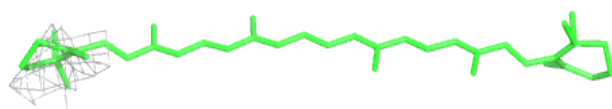
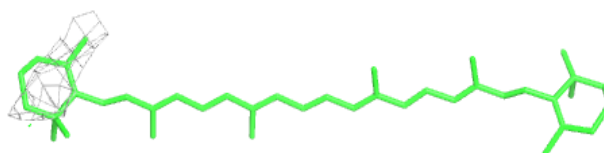


Electron density around CLA C 507:

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

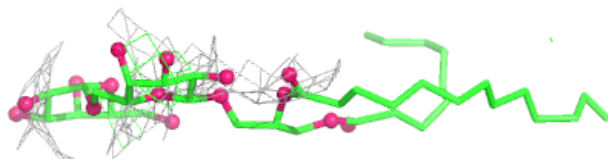
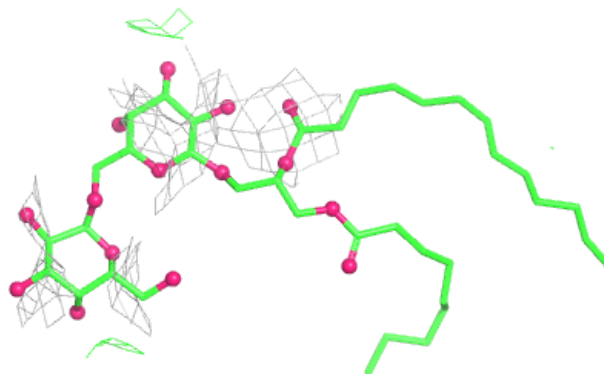
**Electron density around BCR j 102:**

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

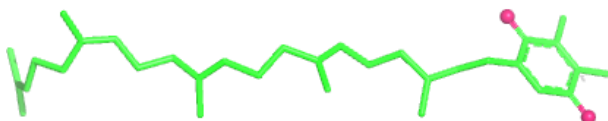
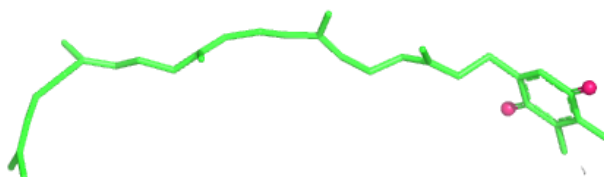


Electron density around DGD B 626:

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

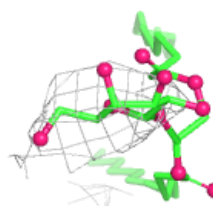
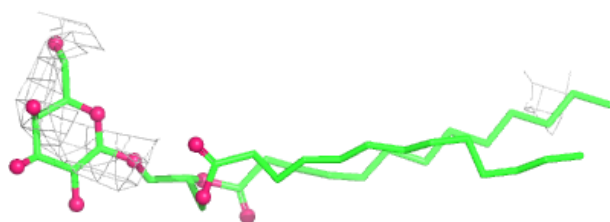
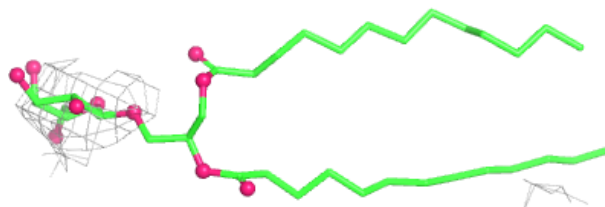
**Electron density around PL9 J 101:**

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

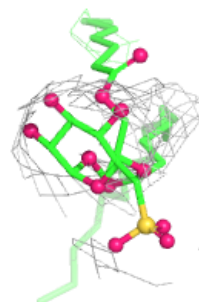
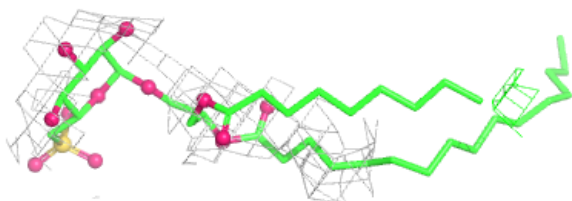
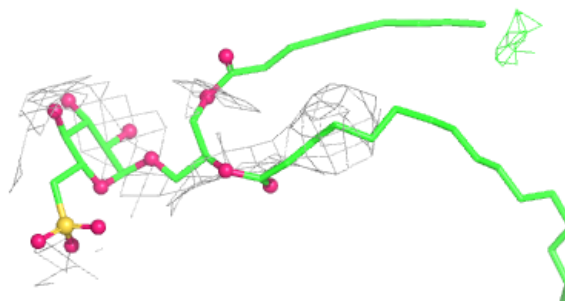


Electron density around LMG c 520:

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

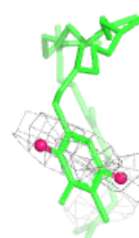
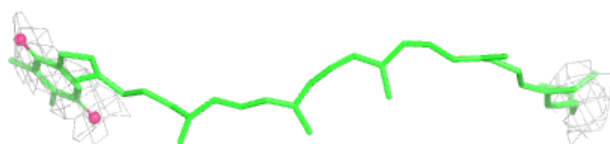
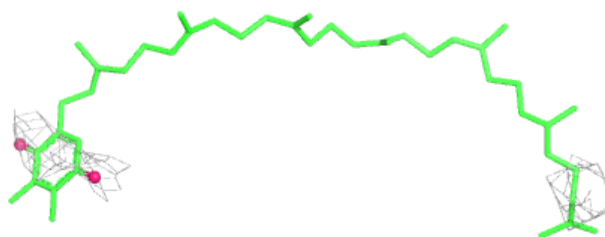
**Electron density around SQD B 625:**

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

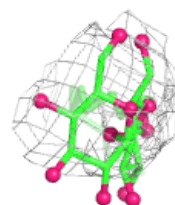
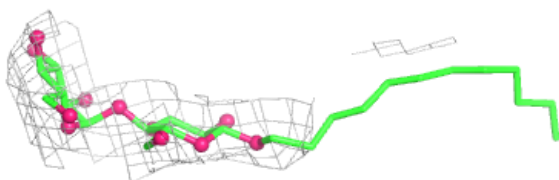
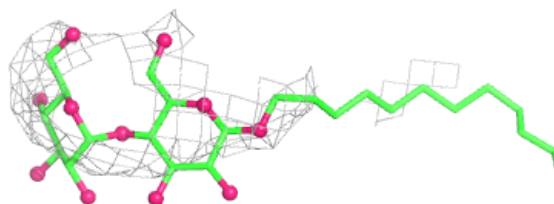


Electron density around PL9 A 408:

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

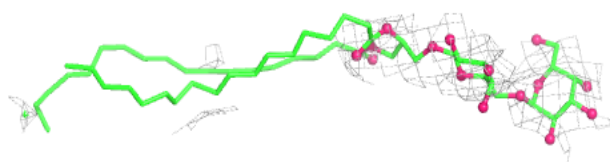
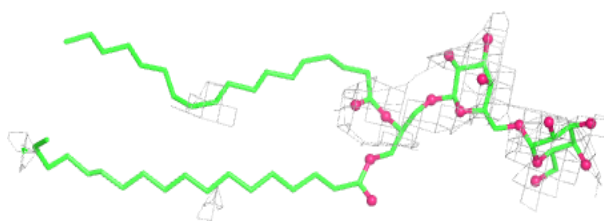
**Electron density around LMT b 625:**

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

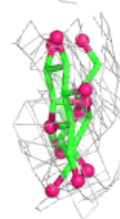
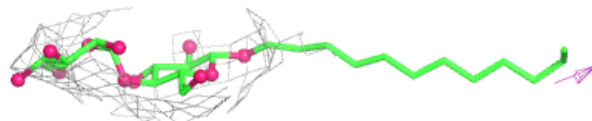
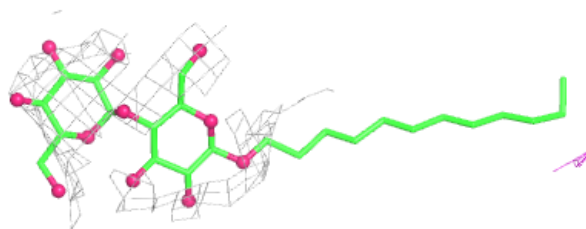


Electron density around DGD C 518:

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

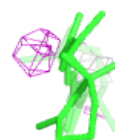
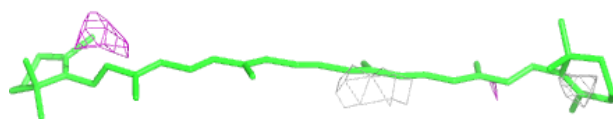
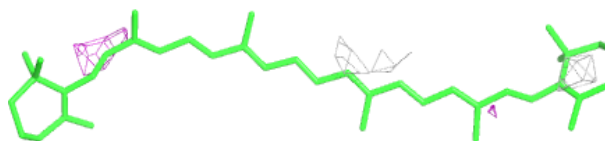
**Electron density around LMT b 603:**

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

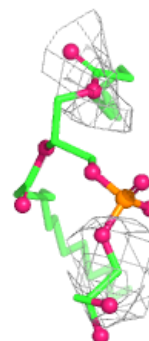
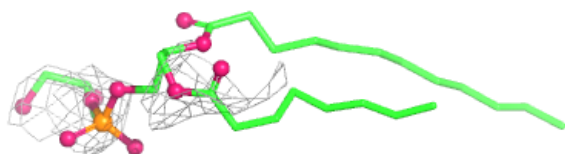
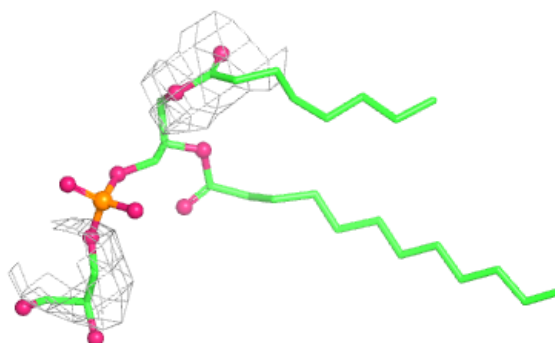


Electron density around BCR k 102:

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

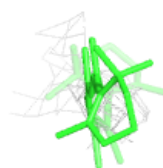
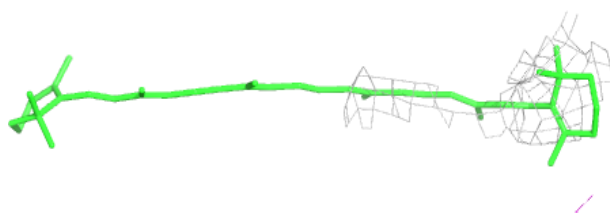
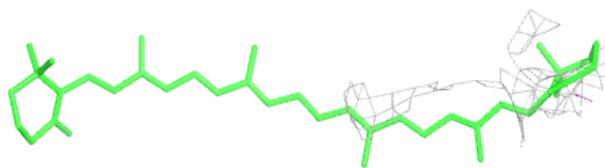
**Electron density around LHG a 417:**

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

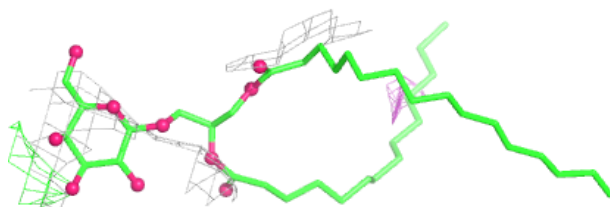
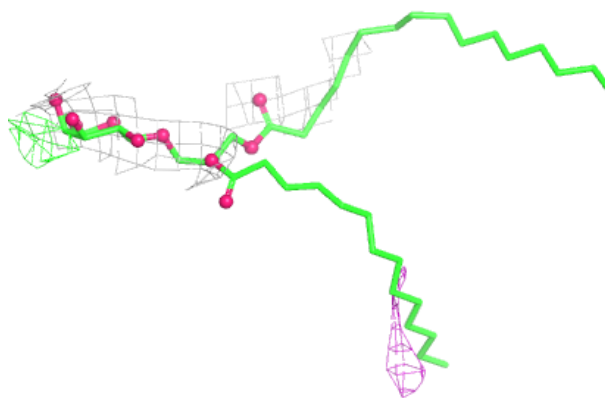


Electron density around BCR H 101:

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

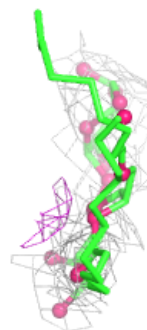
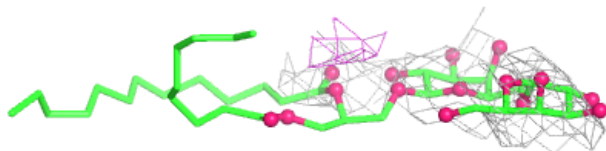
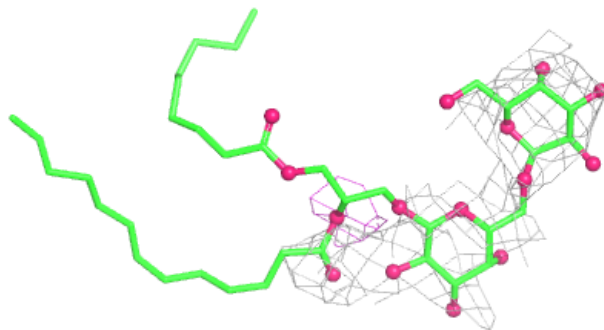
**Electron density around LMG b 624:**

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

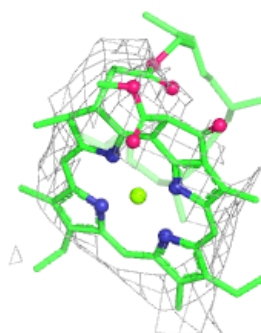


Electron density around DGD b 602:

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

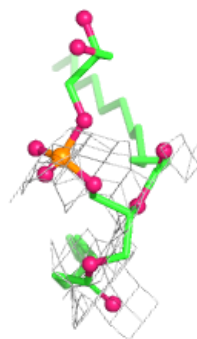
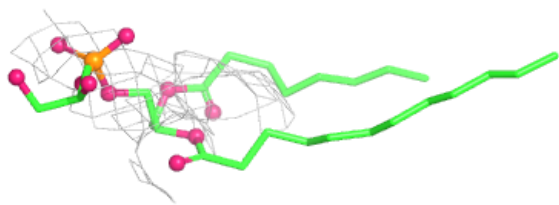
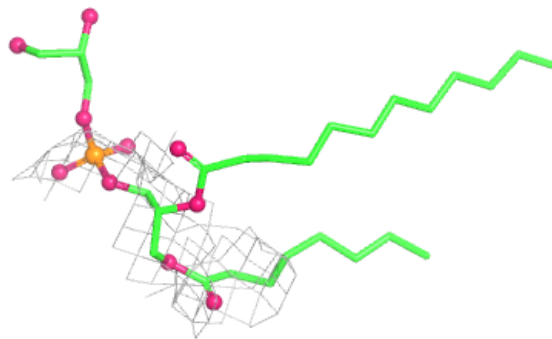
**Electron density around CLA c 513:**

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

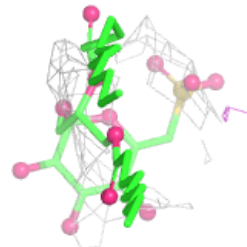
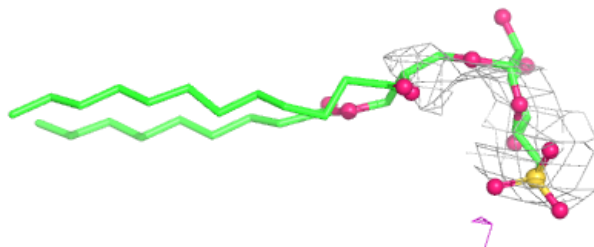
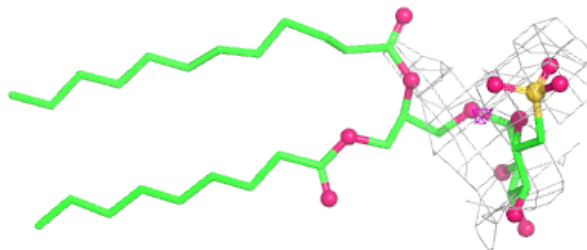


Electron density around LHG A 415:

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

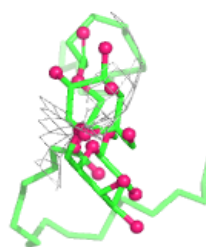
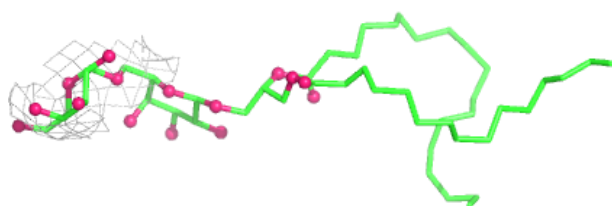
**Electron density around SQD d 407:**

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

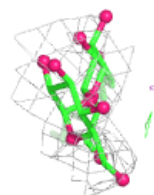
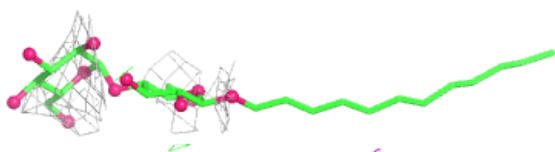
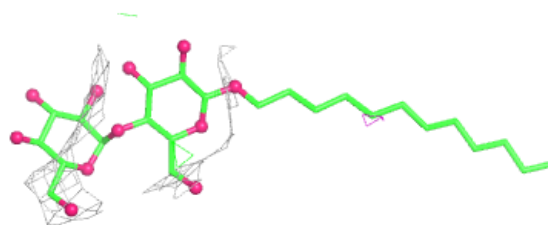


Electron density around DGD d 408:

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

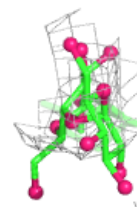
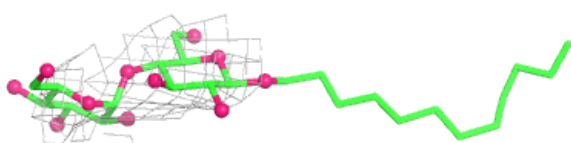
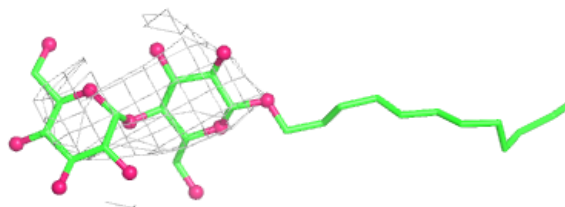
**Electron density around LMT B 624:**

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

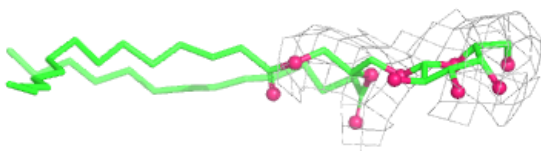
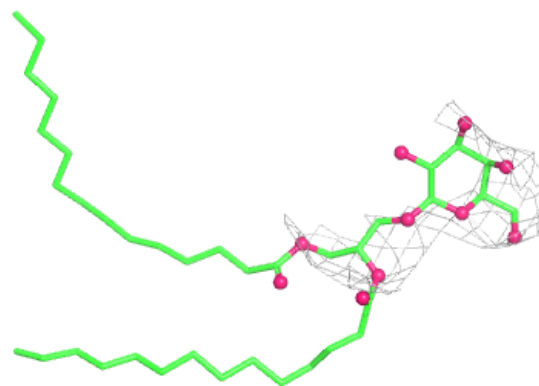


Electron density around LMT B 627:

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

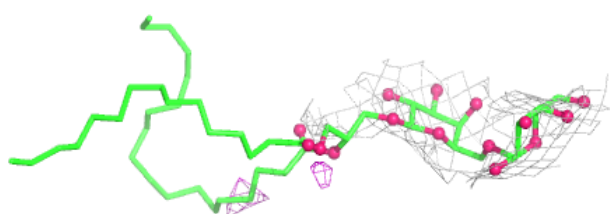
**Electron density around LMG k 103:**

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

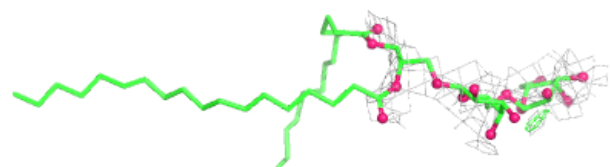


Electron density around DGD D 410:

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

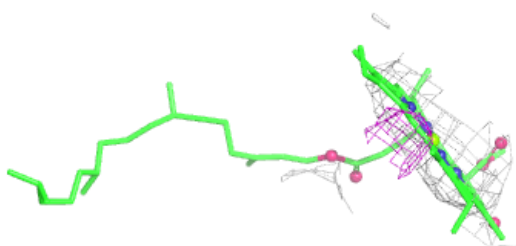
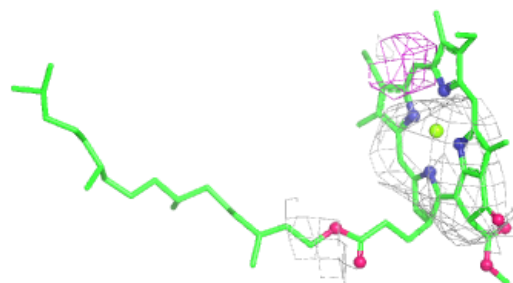
**Electron density around DGD c 518:**

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

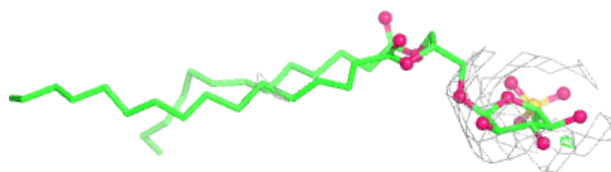
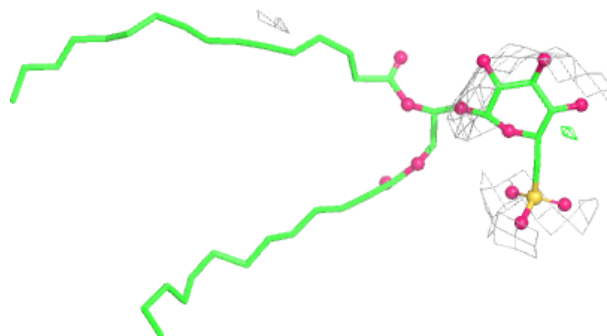


Electron density around CLA a 409:

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

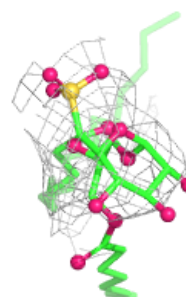
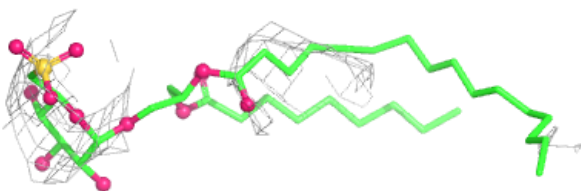
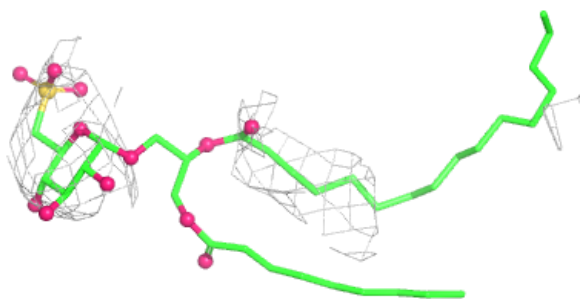
**Electron density around SQD a 415:**

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

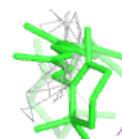
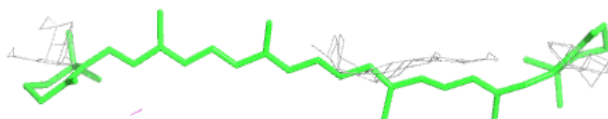
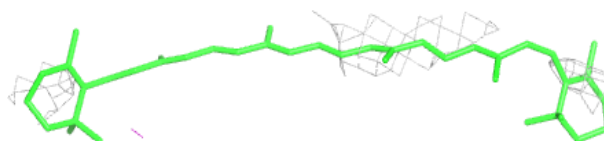


Electron density around SQD b 601:

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

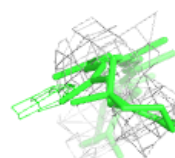
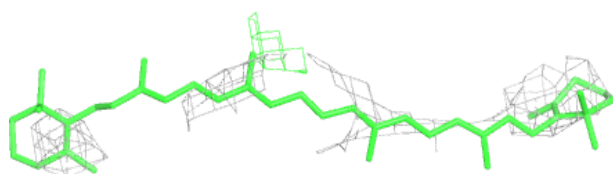
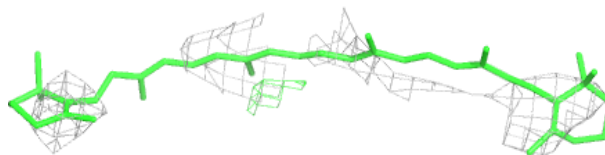
**Electron density around BCR c 514:**

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

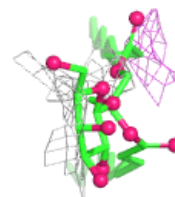
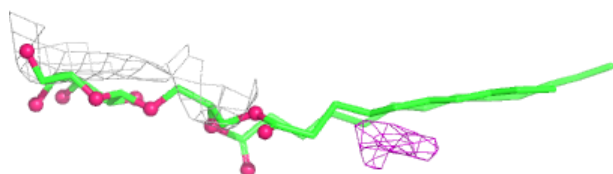
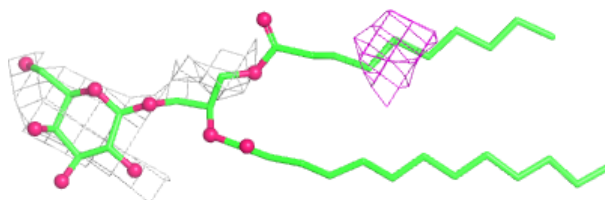


Electron density around BCR D 405:

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

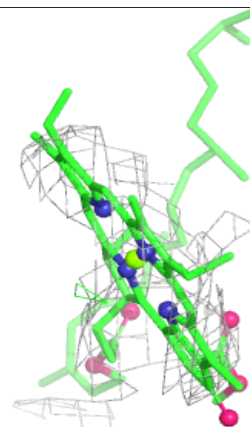
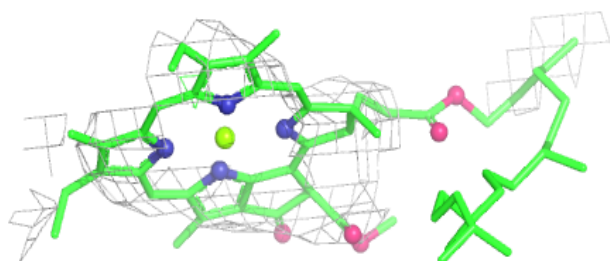
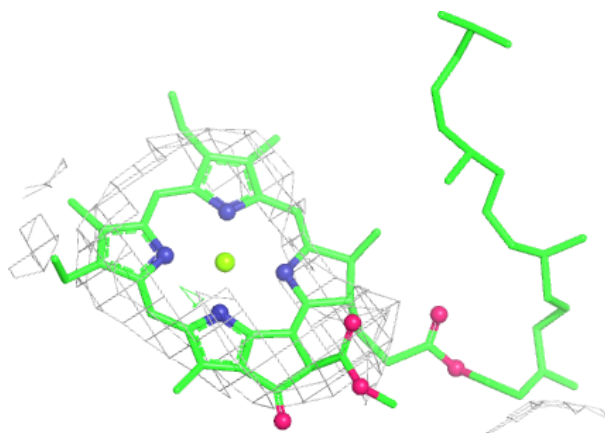
**Electron density around LMG M 101:**

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

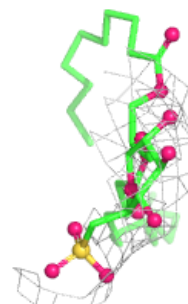
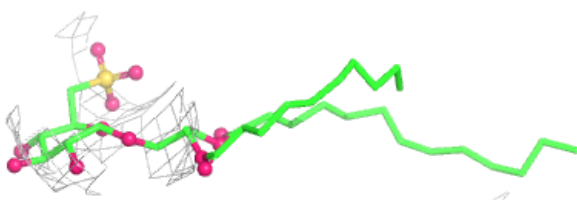


Electron density around CLA b 619:

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

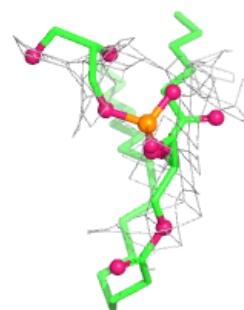
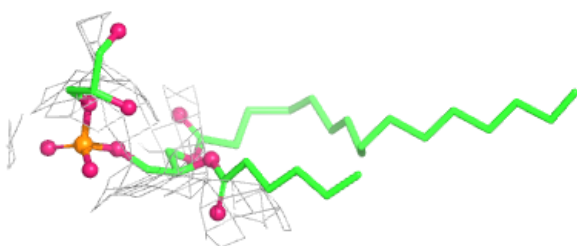
**Electron density around SQD F 102:**

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

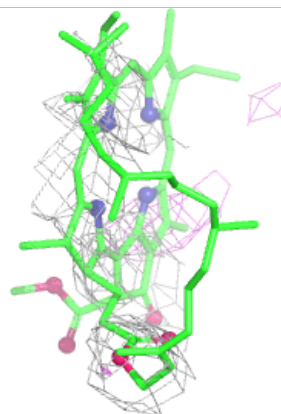
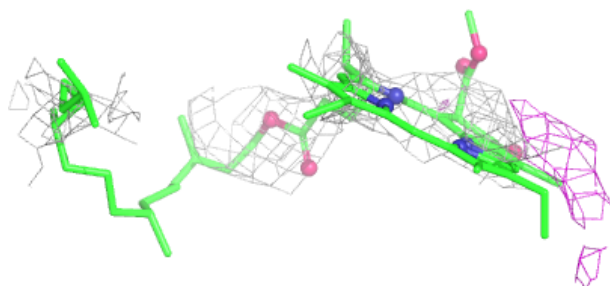
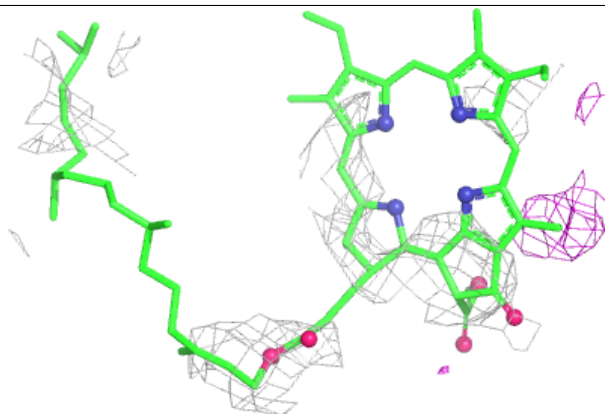


Electron density around LHG A 412:

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

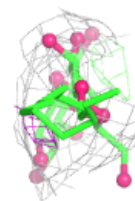
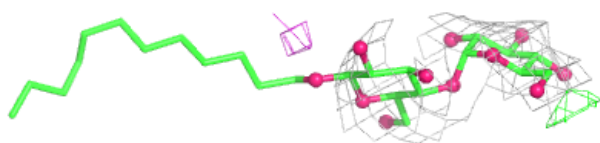
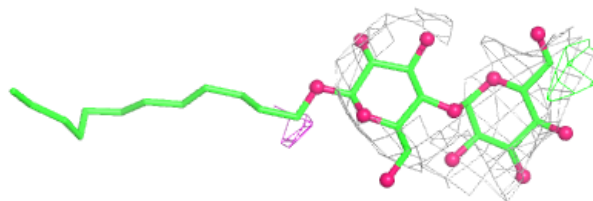
**Electron density around PHO A 406:**

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

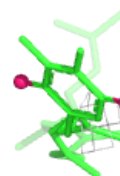
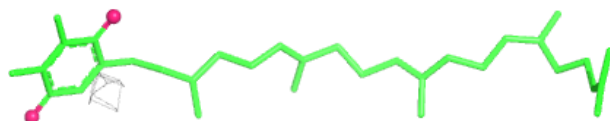
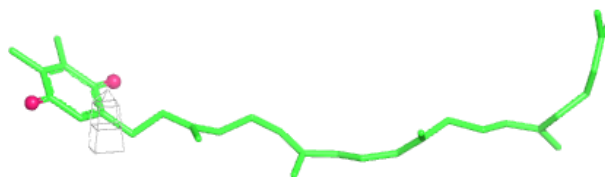


Electron density around LMT T 101:

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

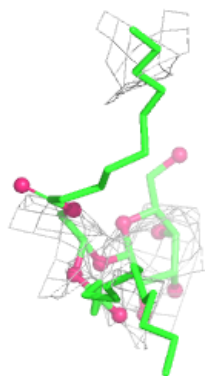
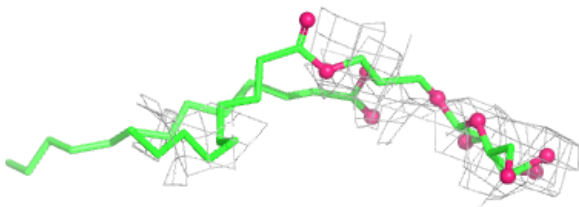
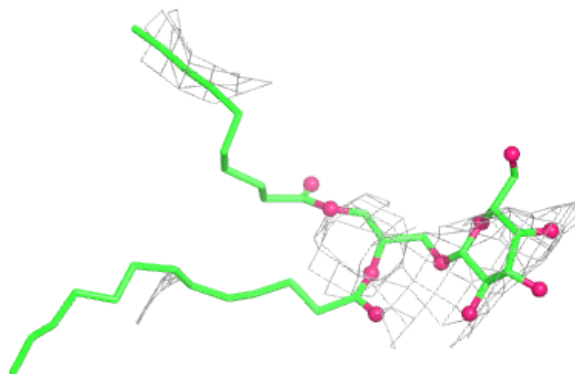
**Electron density around PL9 j 101:**

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

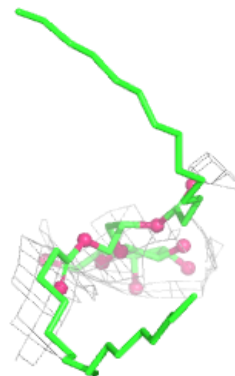
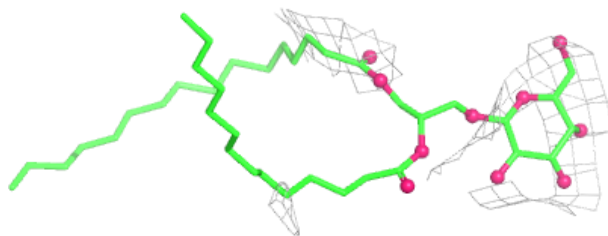
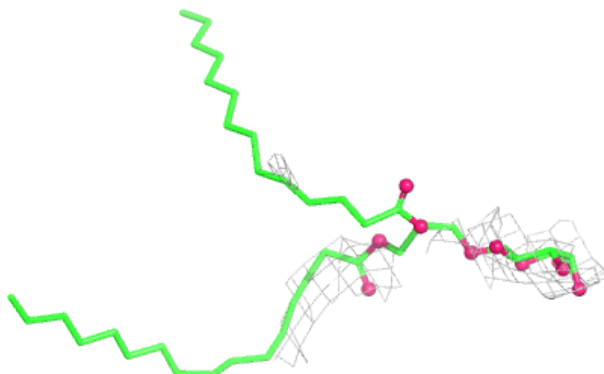


Electron density around LMG A 418:

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

**Electron density around LMG B 622:**

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

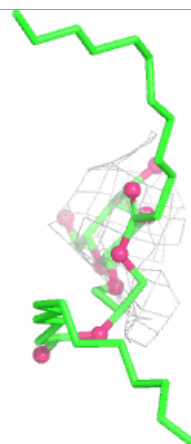
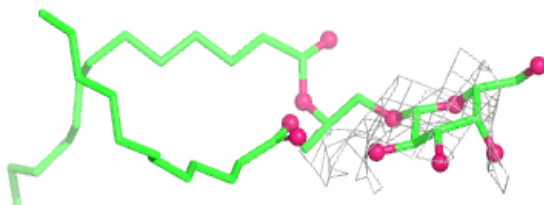
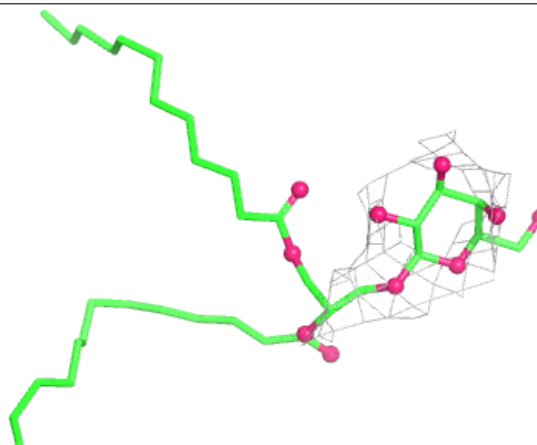


Electron density around DGD A 411:

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

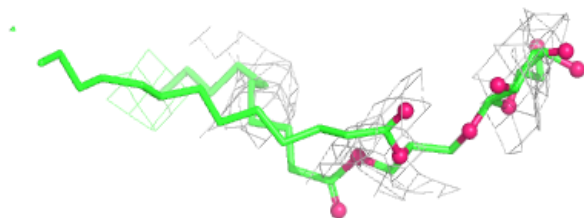
**Electron density around LMG E 101:**

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



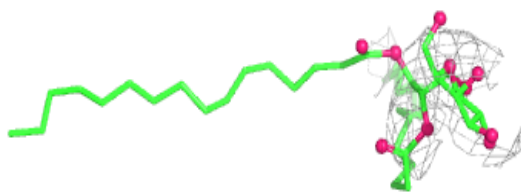
Electron density around LMG a 402:

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



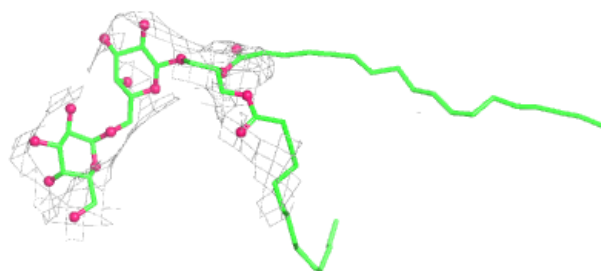
Electron density around LMG a 416:

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



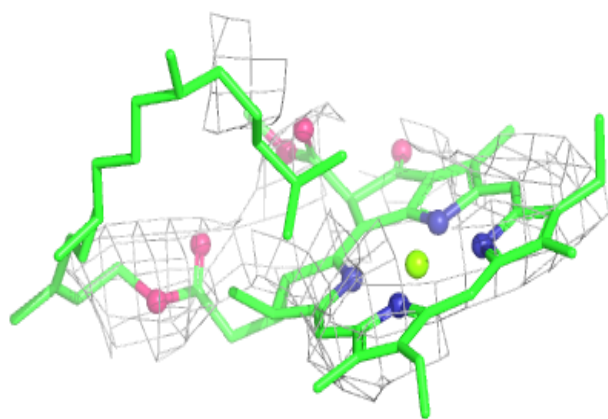
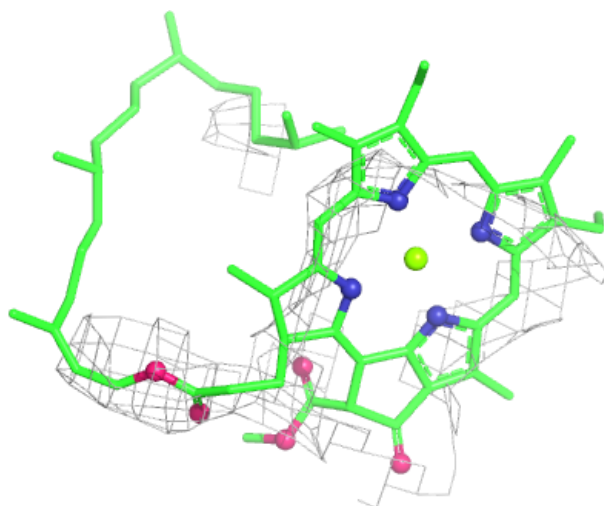
Electron density around DGD C 517:

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



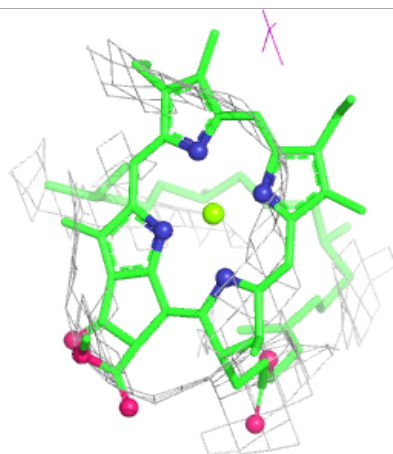
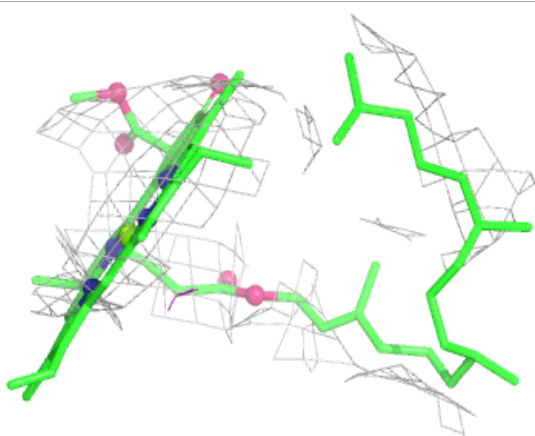
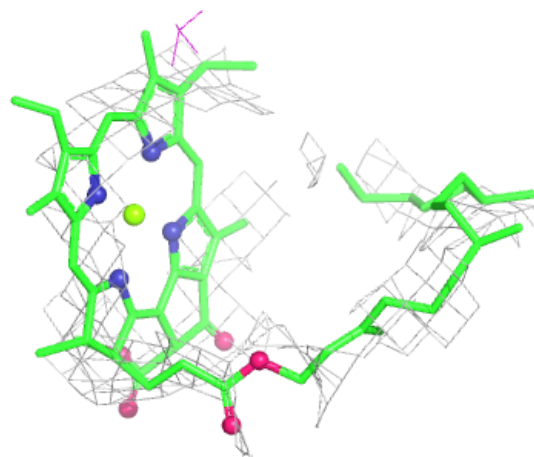
Electron density around CLA b 618:

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



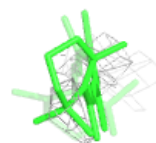
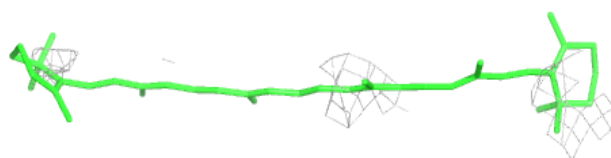
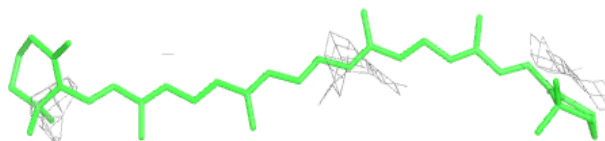
Electron density around CLA C 503:

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

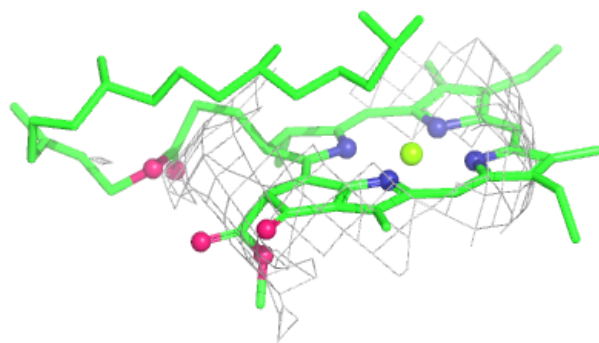
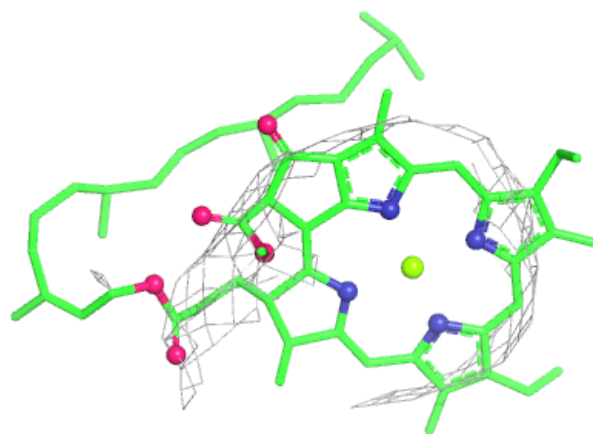


Electron density around BCR x 101:

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

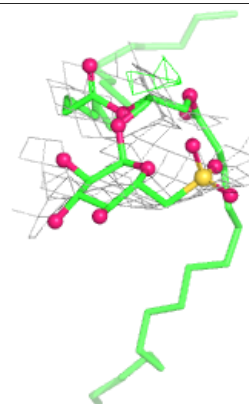
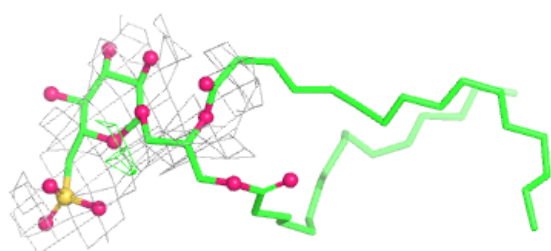
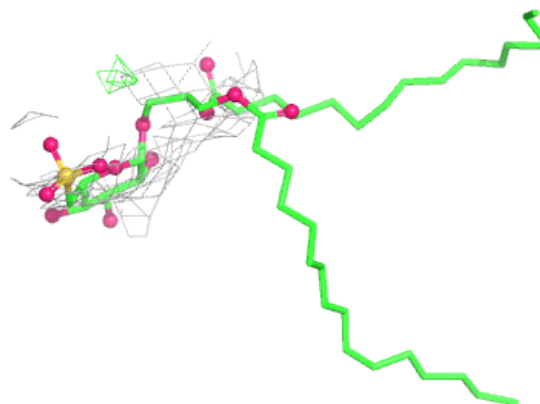
**Electron density around CLA c 509:**

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

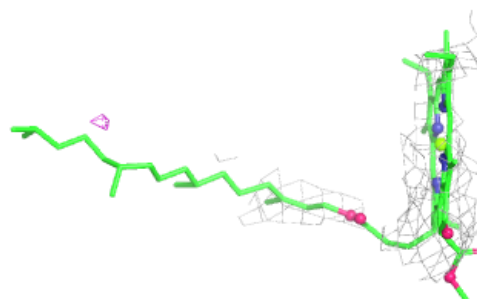


Electron density around SQD a 401:

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

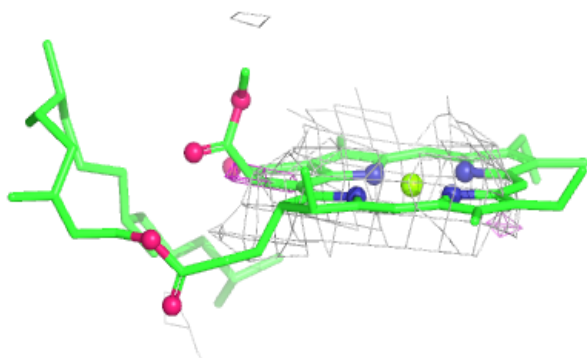
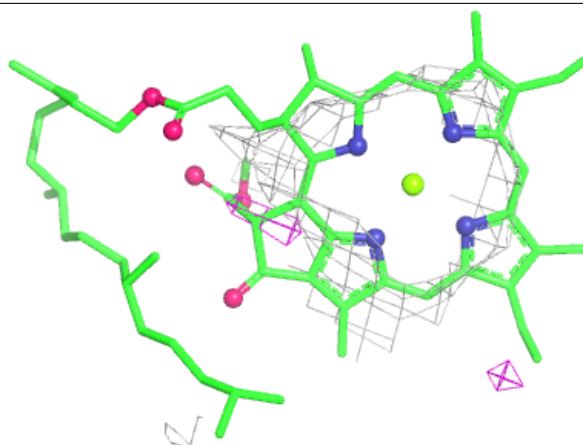
**Electron density around CLA b 609:**

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



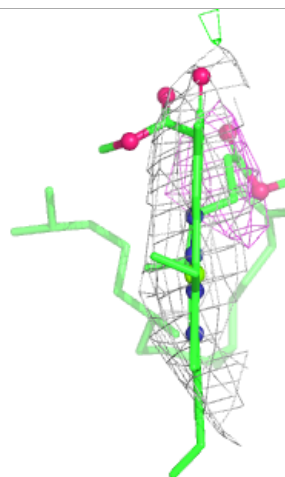
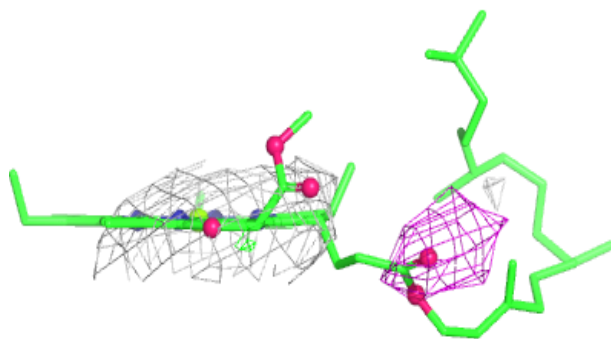
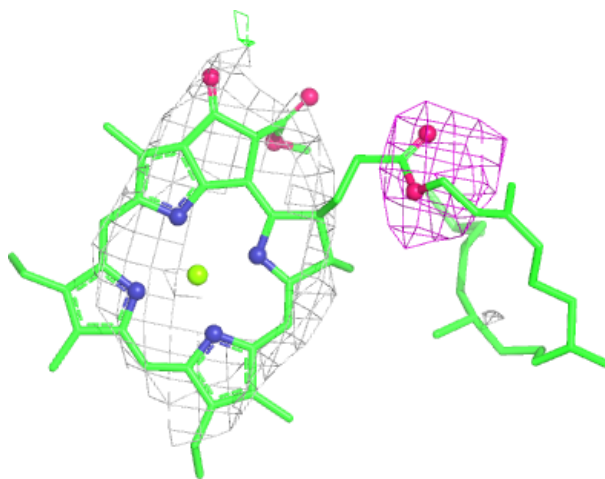
Electron density around CLA b 613:

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



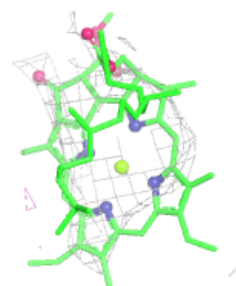
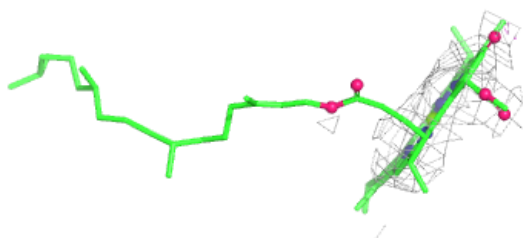
Electron density around CLA C 512:

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

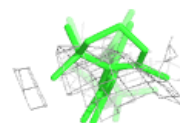
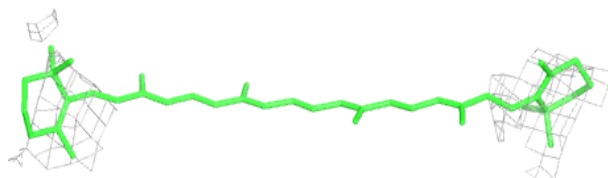
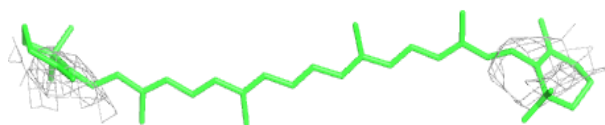


Electron density around CLA A 407:

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

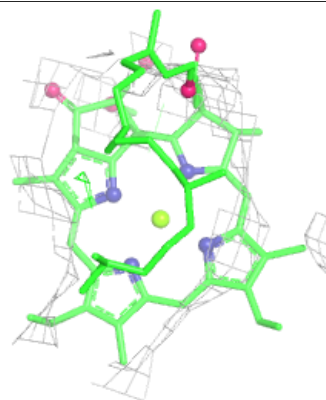
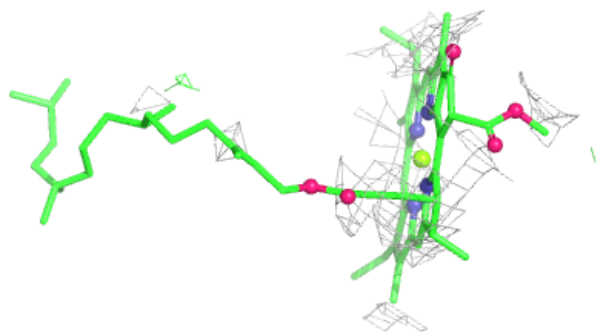
**Electron density around BCR c 515:**

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

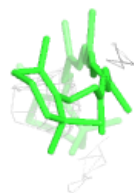
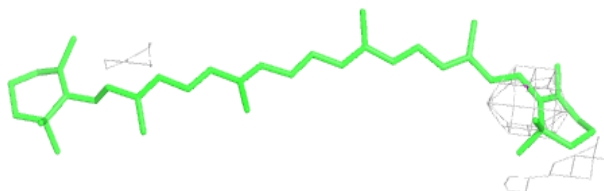


Electron density around CLA C 506:

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

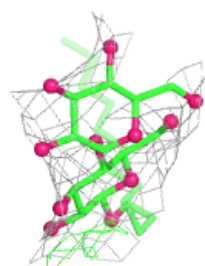
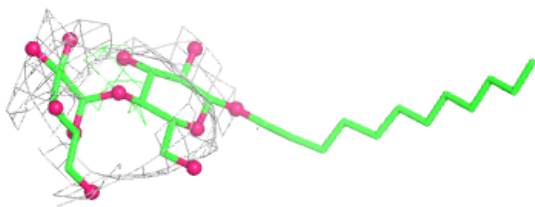
**Electron density around BCR B 618:**

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

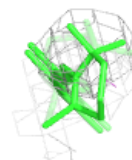
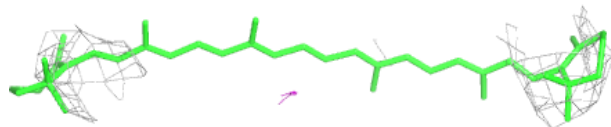
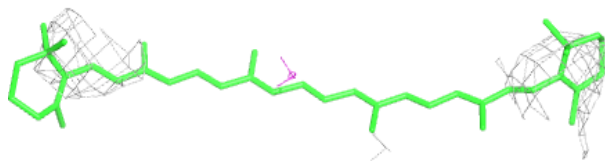


Electron density around LMT m 101:

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

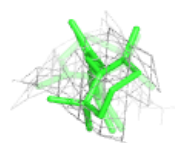
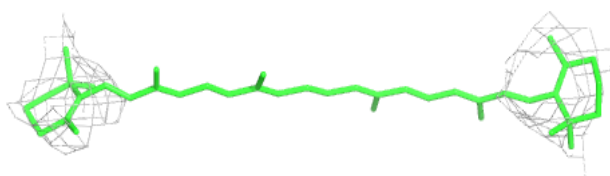
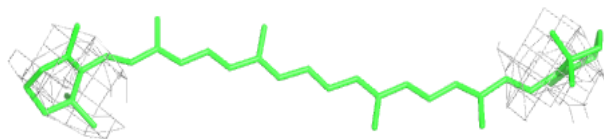
**Electron density around BCR B 620:**

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

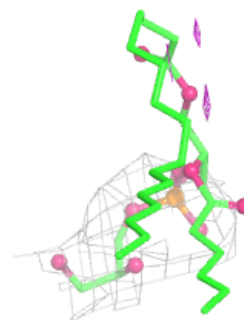
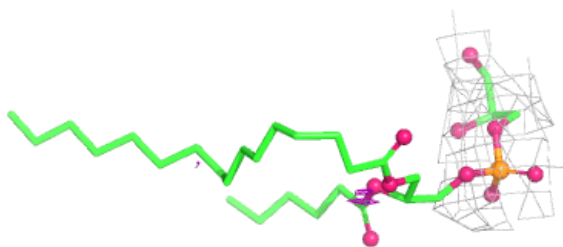
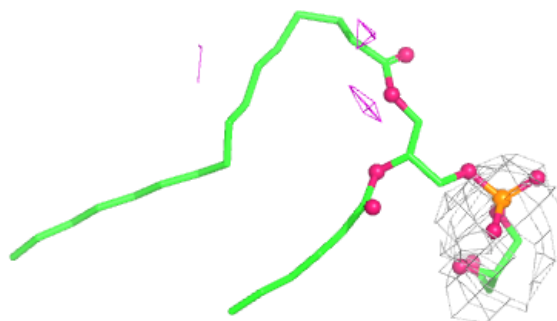


Electron density around BCR Z 101:

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

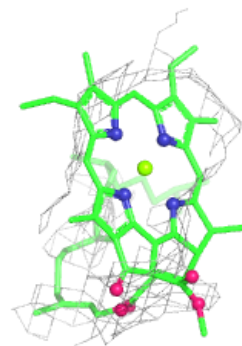
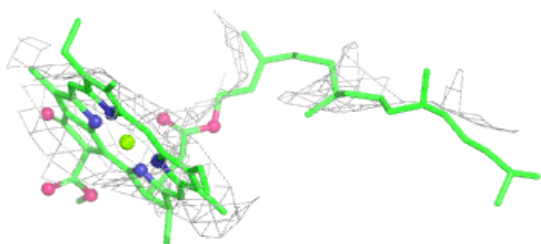
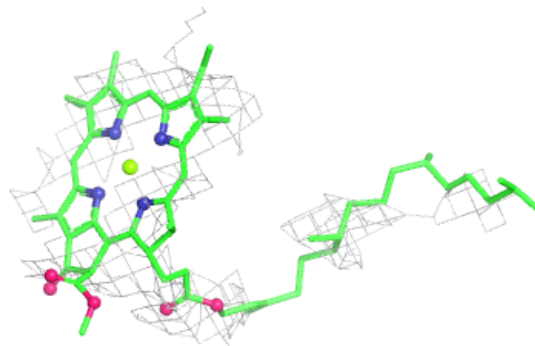
**Electron density around LHG a 414:**

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

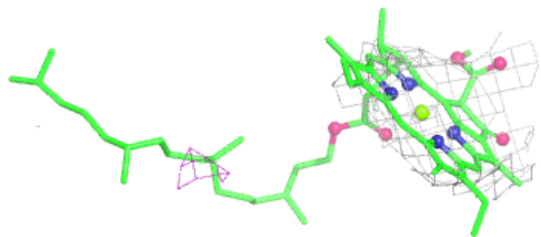
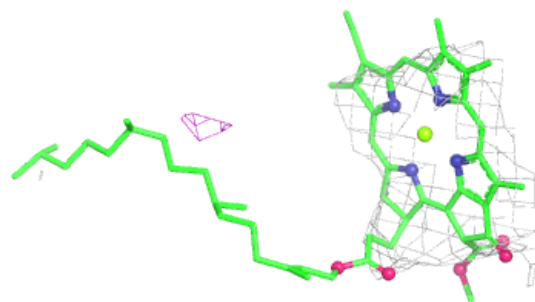


Electron density around CLA C 511:

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

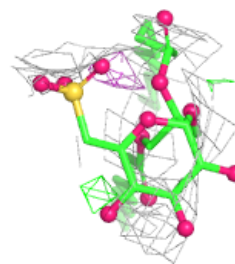
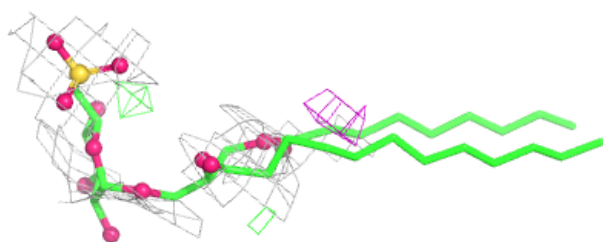
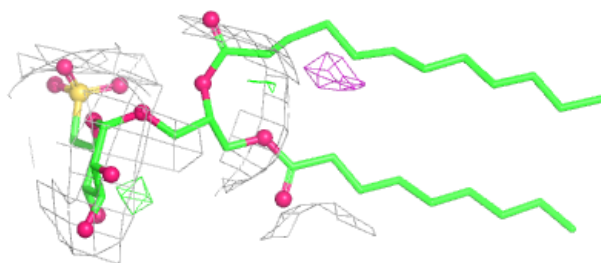
**Electron density around CLA c 511:**

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

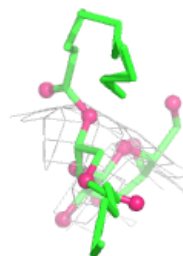
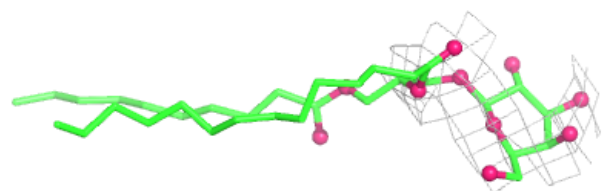
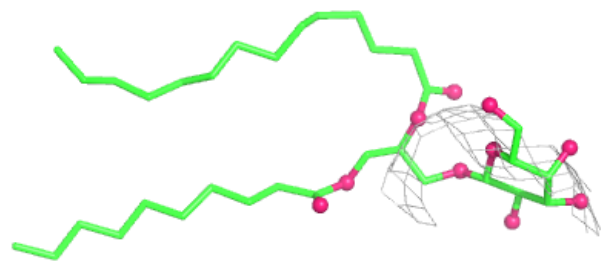


Electron density around SQD D 409:

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

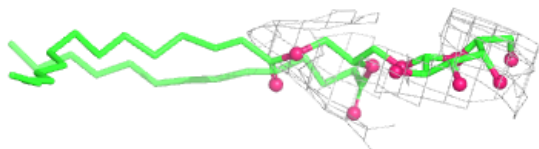
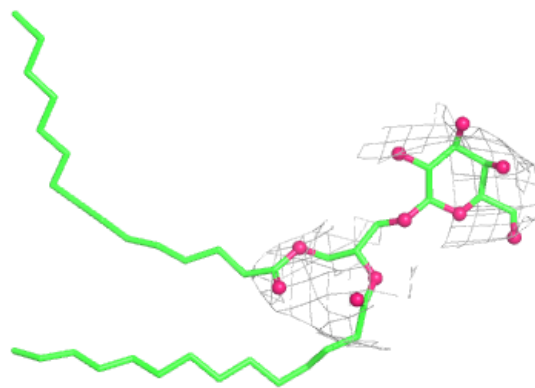
**Electron density around LMG i 101:**

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

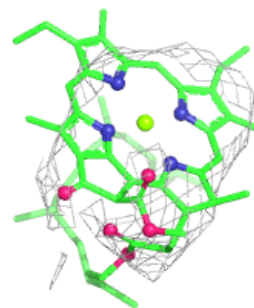
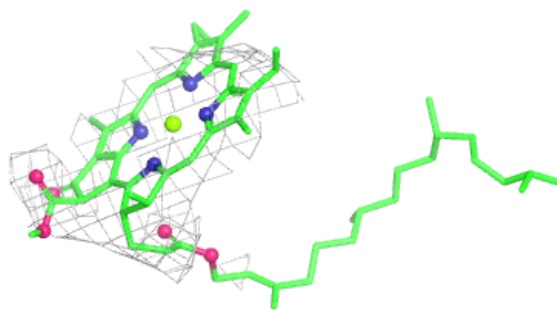


Electron density around LMG C 519:

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

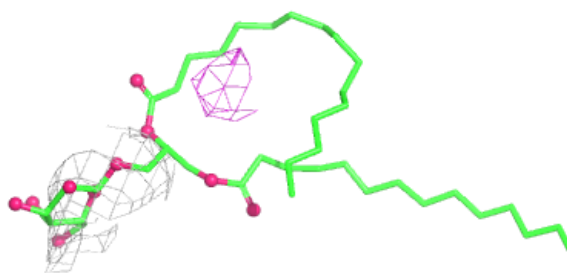
**Electron density around CLA C 513:**

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

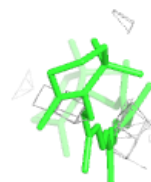
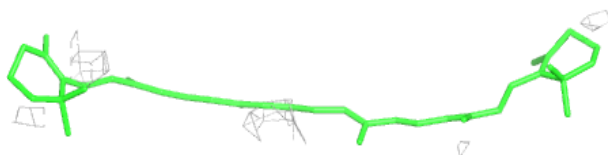
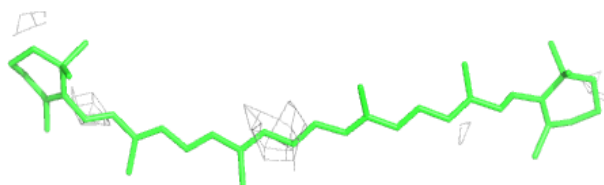


Electron density around LMG D 407:

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

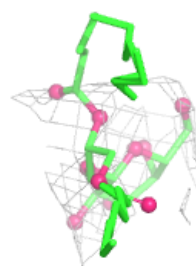
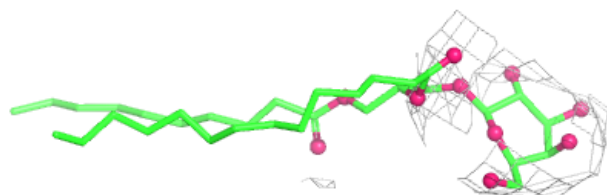
**Electron density around BCR T 103:**

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

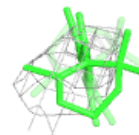
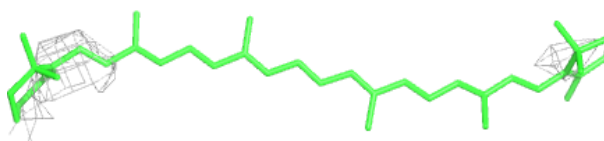


Electron density around LMG I 101:

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

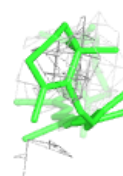
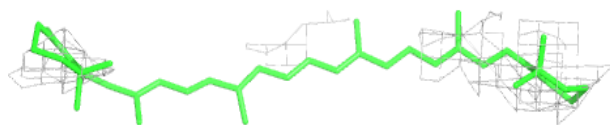
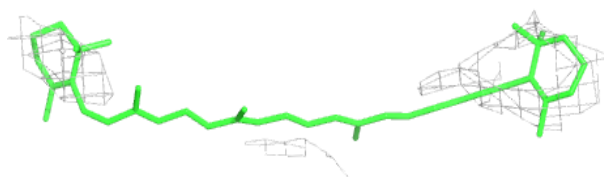
**Electron density around BCR a 412:**

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

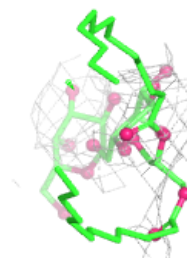
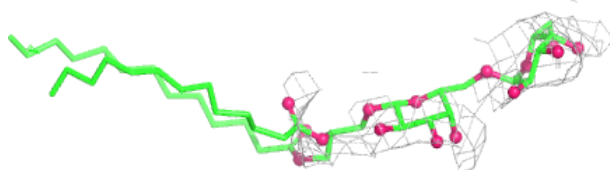
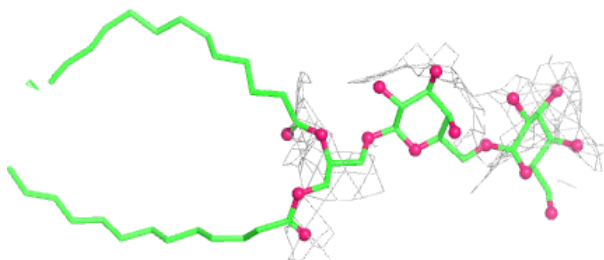


Electron density around BCR C 514:

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

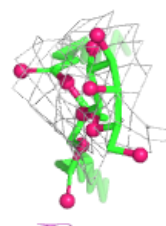
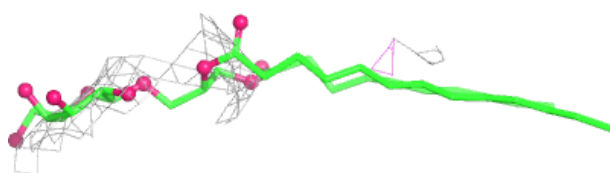
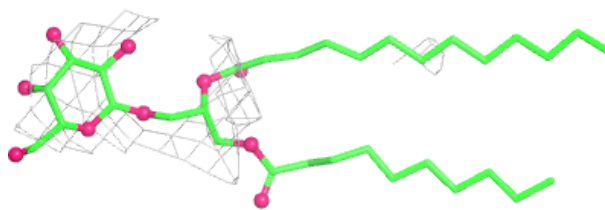
**Electron density around DGD a 413:**

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

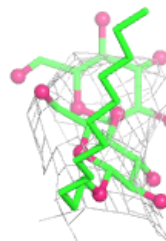
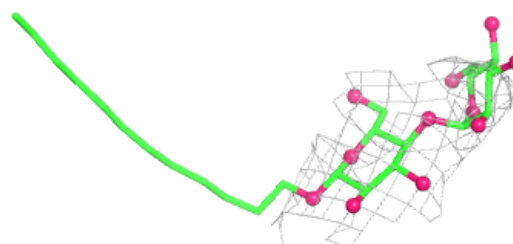


Electron density around LMG M 102:

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

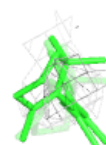
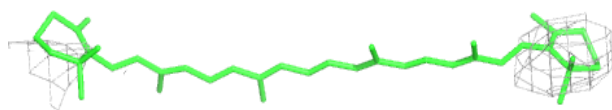
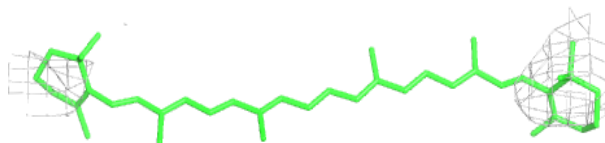
**Electron density around LMT M 103:**

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

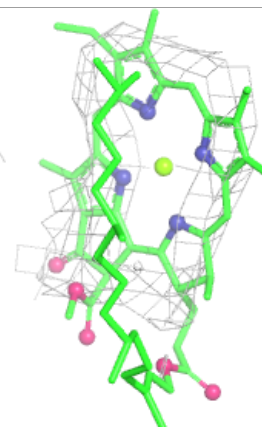
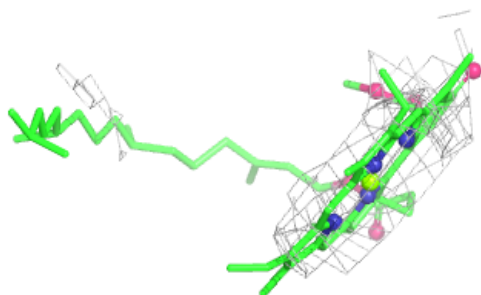
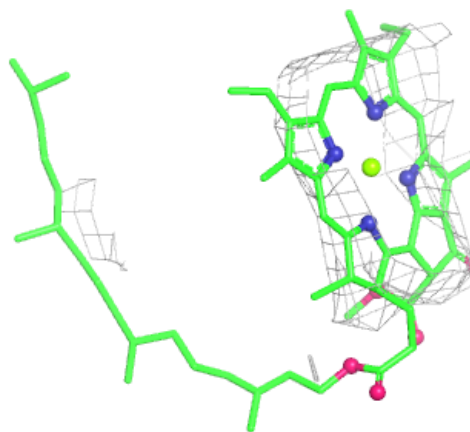


Electron density around BCR C 515:

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

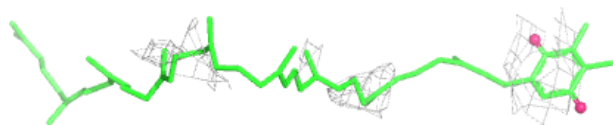
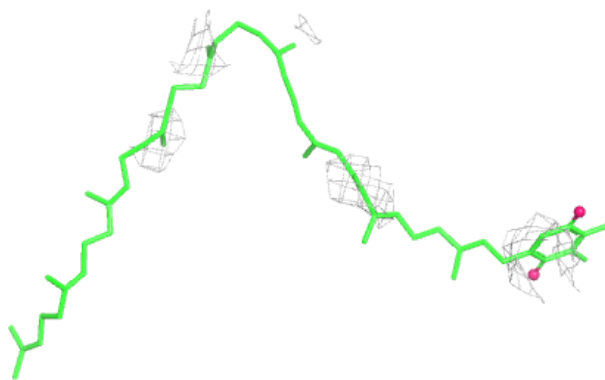
**Electron density around CLA c 507:**

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

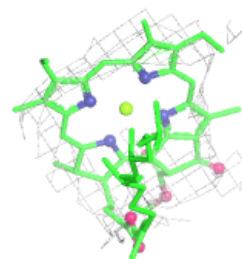
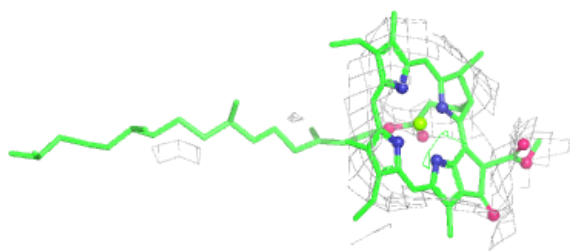
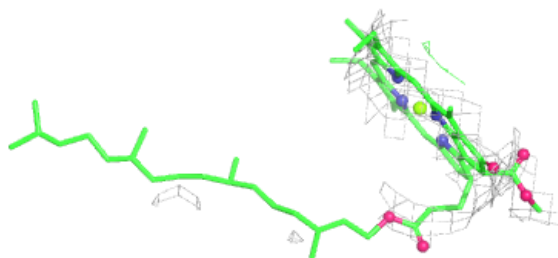


Electron density around PL9 d 404:

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

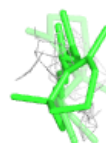
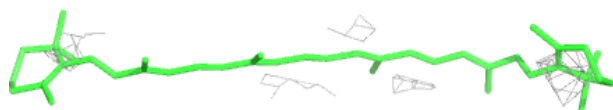
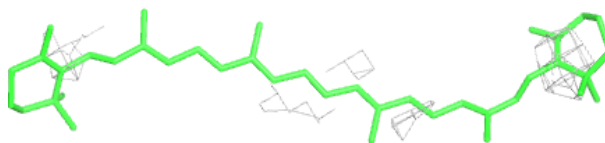
**Electron density around CLA C 504:**

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

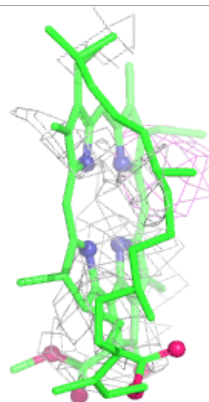
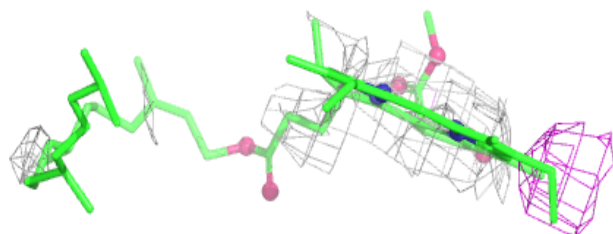
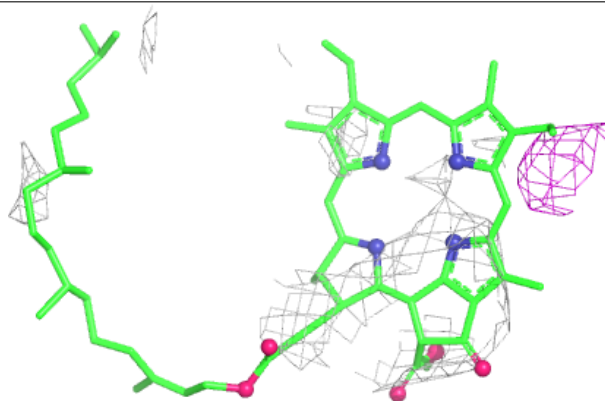


Electron density around BCR K 102:

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

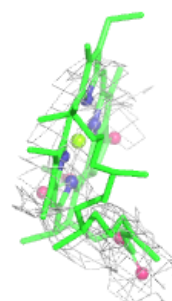
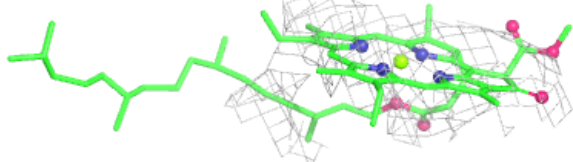
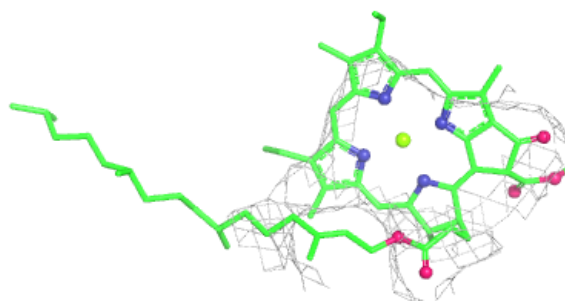
**Electron density around PHO D 402:**

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

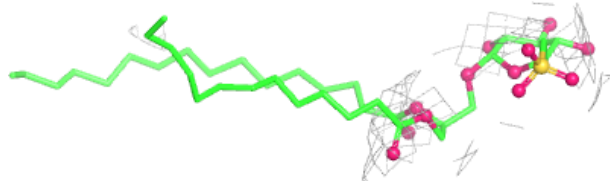
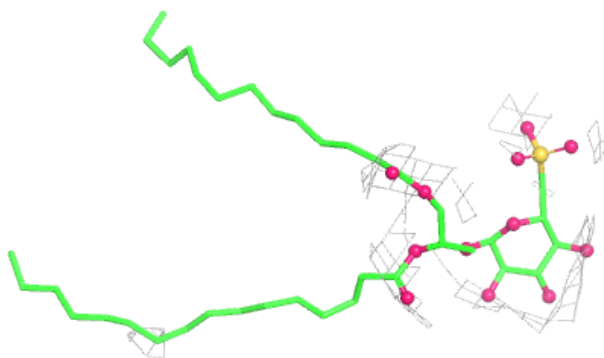


Electron density around CLA C 501:

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

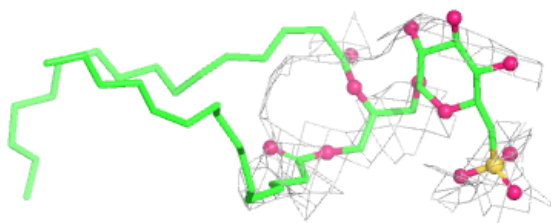
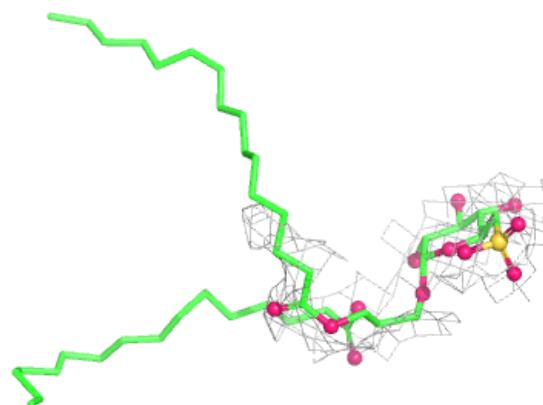
**Electron density around SQD A 413:**

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

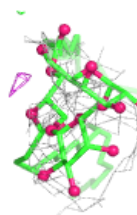
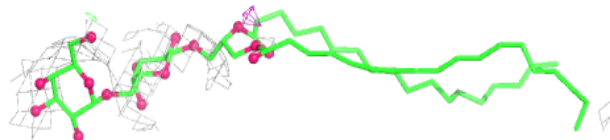
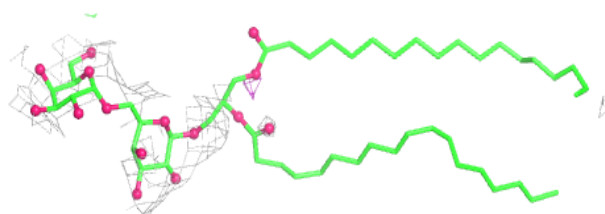


Electron density around SQD A 417:

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

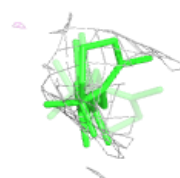
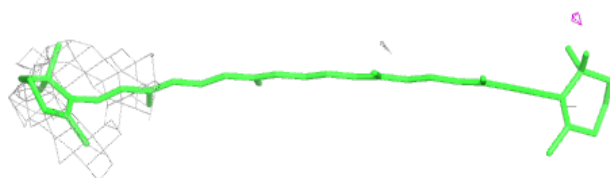
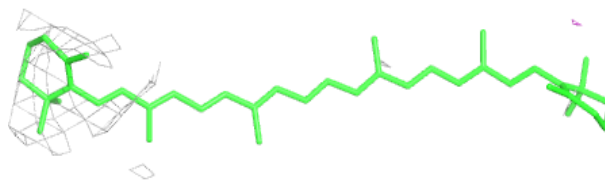
**Electron density around DGD c 519:**

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

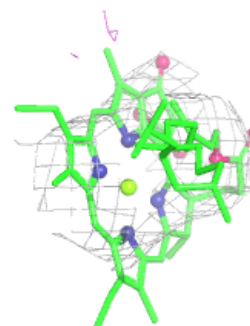
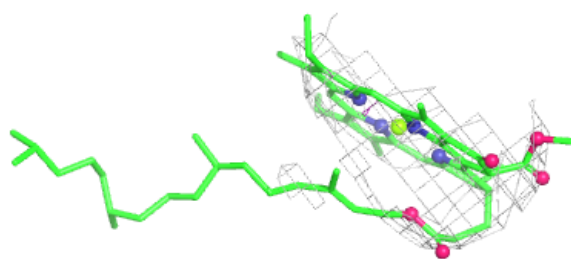
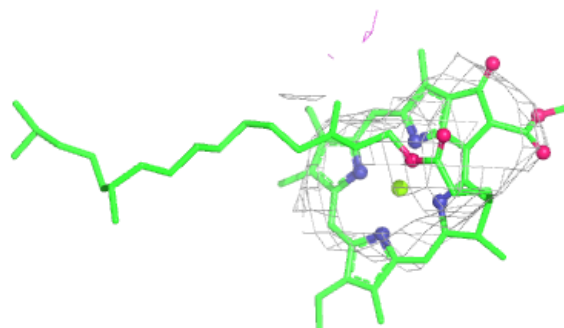


Electron density around BCR T 102:

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

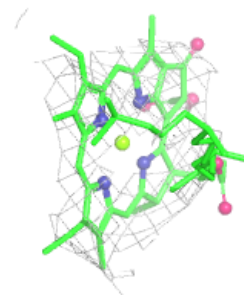
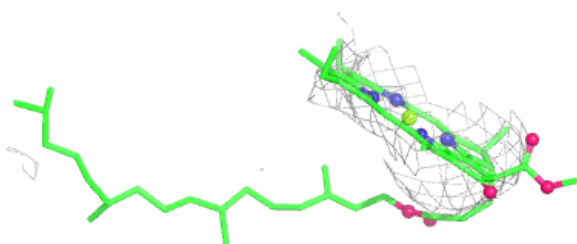
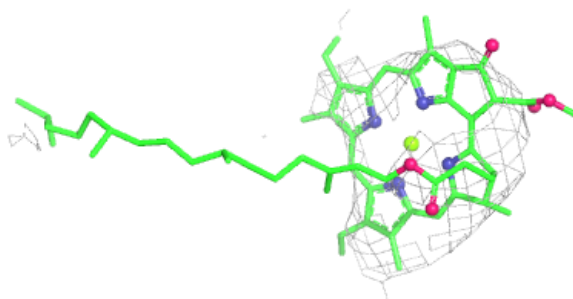
**Electron density around CLA B 614:**

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

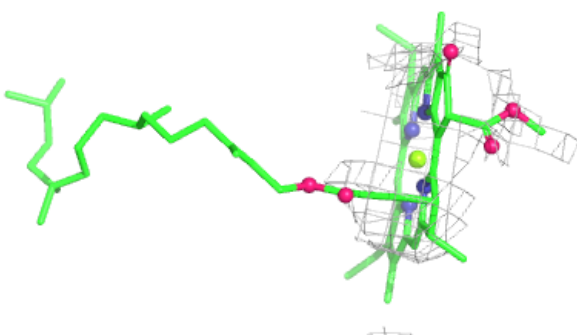


Electron density around CLA b 611:

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

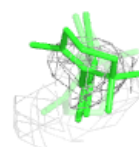
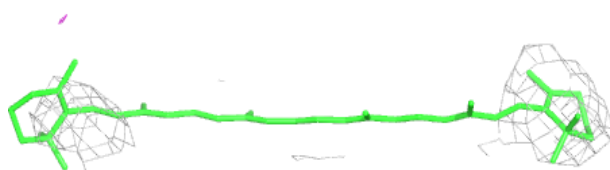
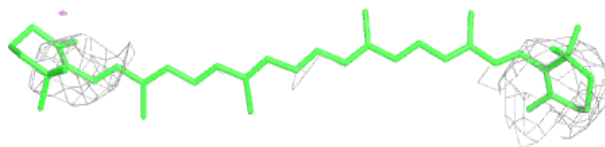
**Electron density around CLA c 506:**

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

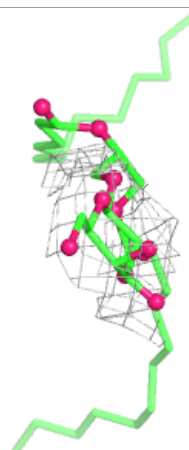
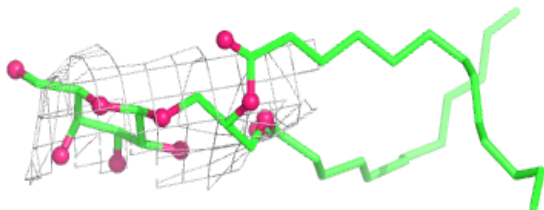
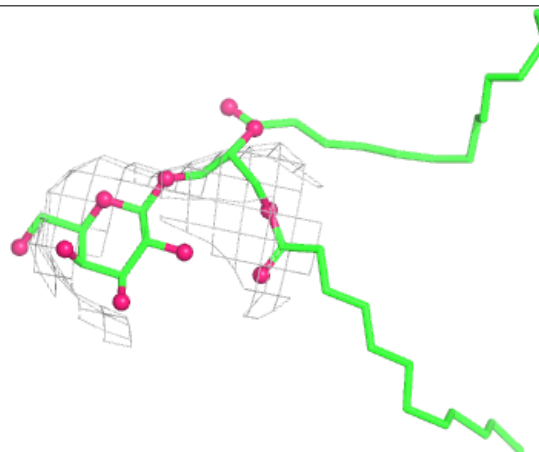


Electron density around BCR b 620:

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

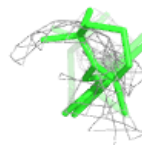
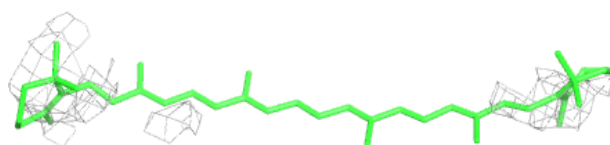
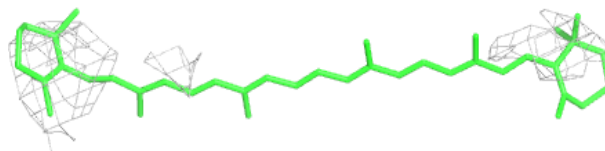
**Electron density around LMG e 101:**

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

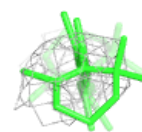
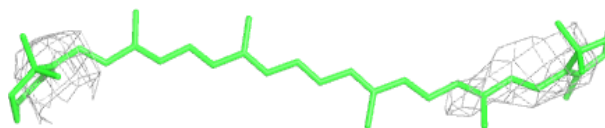


Electron density around BCR b 621:

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

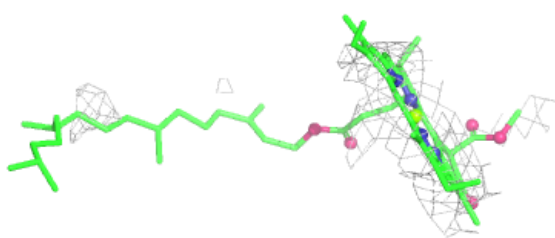
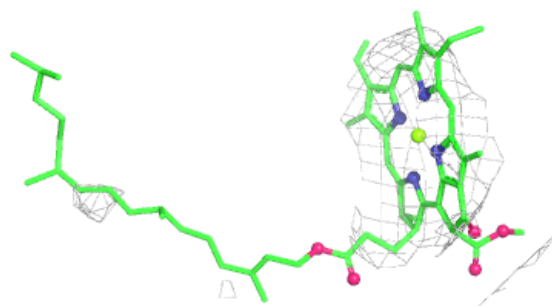
**Electron density around BCR A 410:**

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

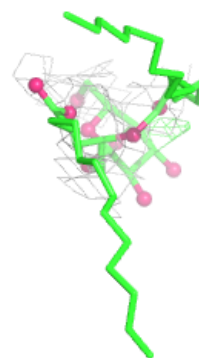
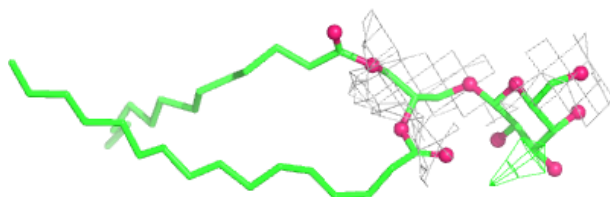


Electron density around CLA b 612:

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

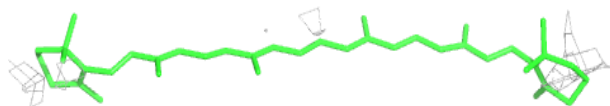
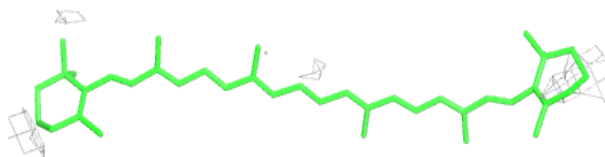
**Electron density around LMG D 408:**

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

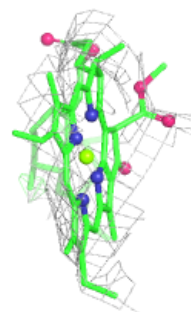
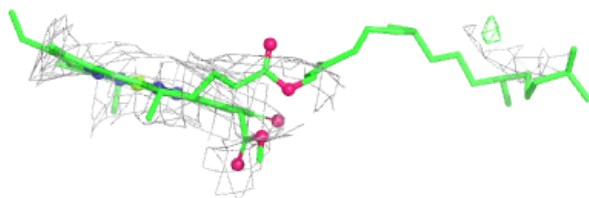
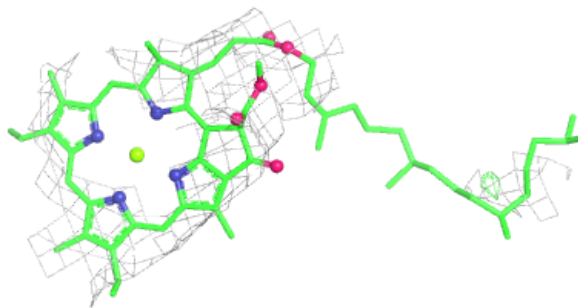


Electron density around BCR c 516:

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

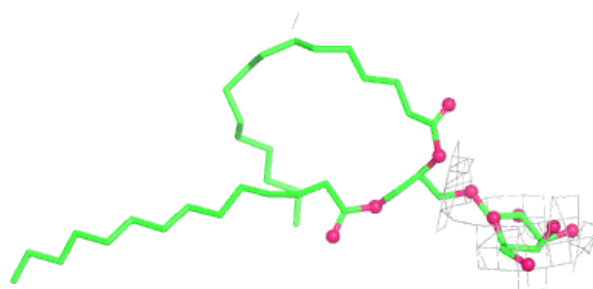
**Electron density around CLA b 605:**

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

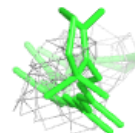
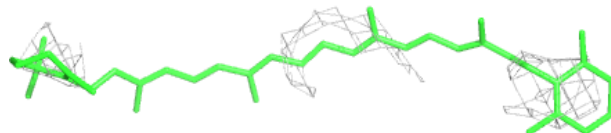
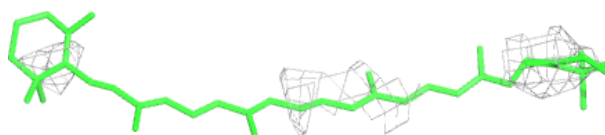


Electron density around LMG b 623:

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

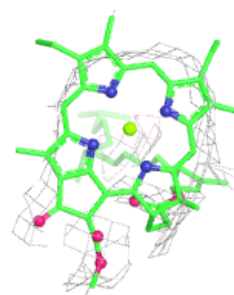
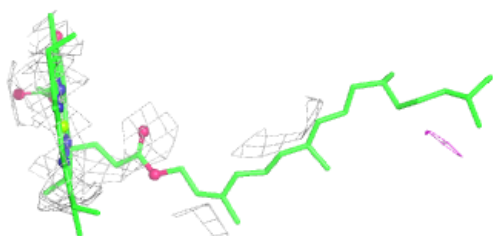
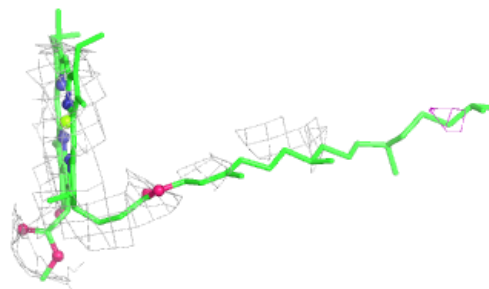
**Electron density around BCR f 102:**

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

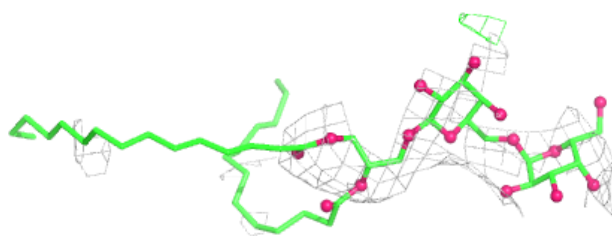


Electron density around CLA B 606:

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

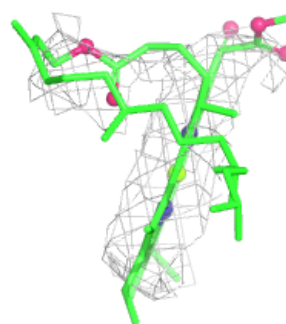
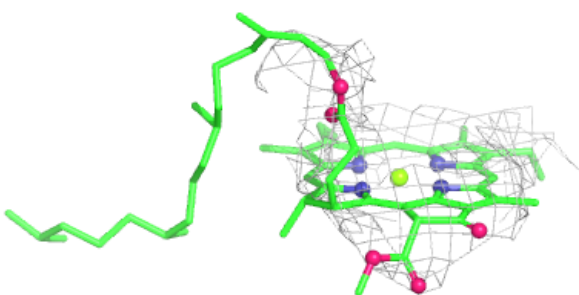
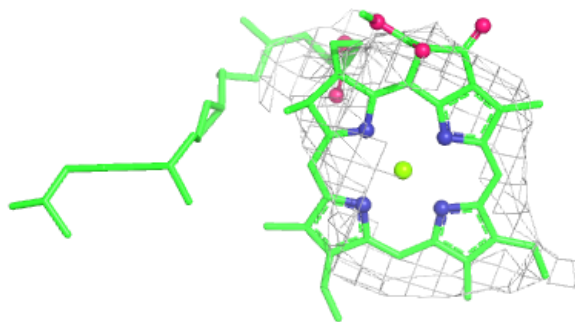
**Electron density around DGD b 622:**

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

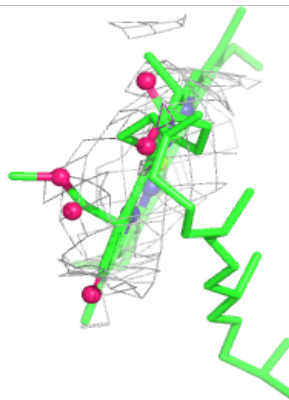
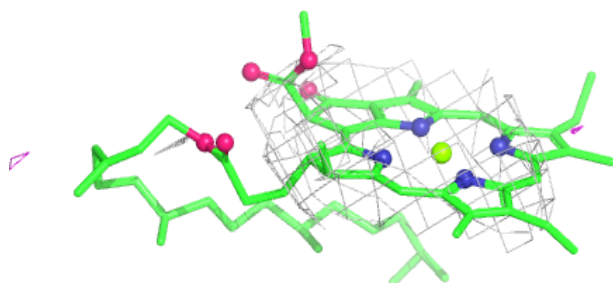
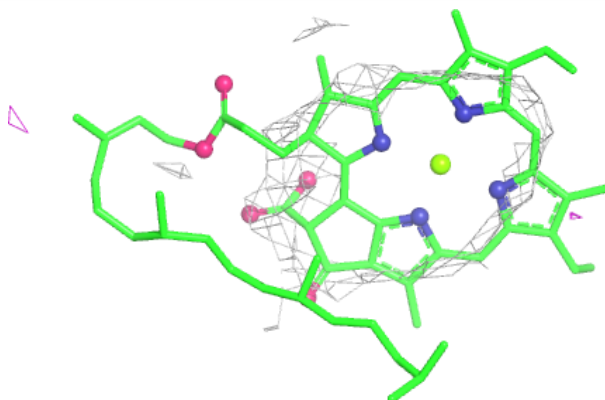


Electron density around CLA a 405:

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

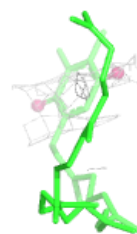
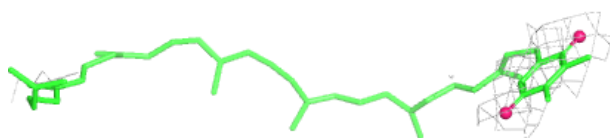
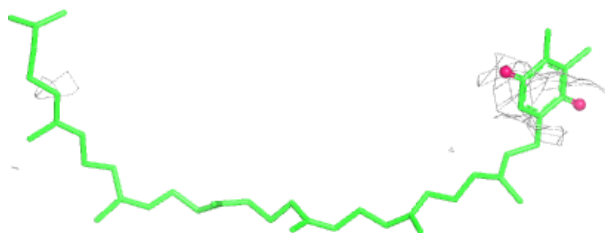
**Electron density around CLA C 509:**

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

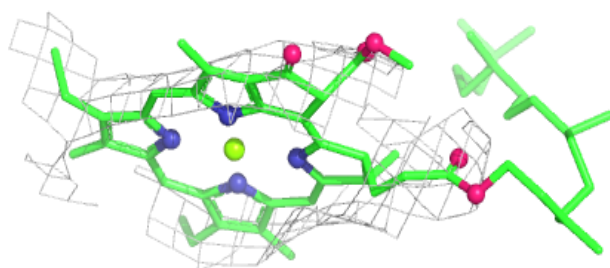
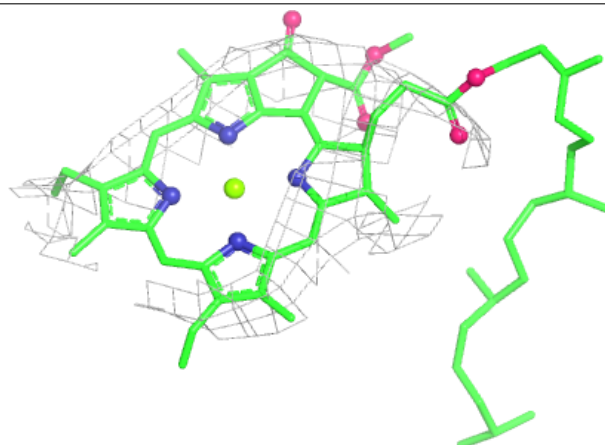


Electron density around PL9 a 410:

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

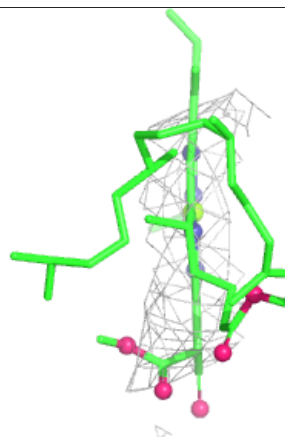
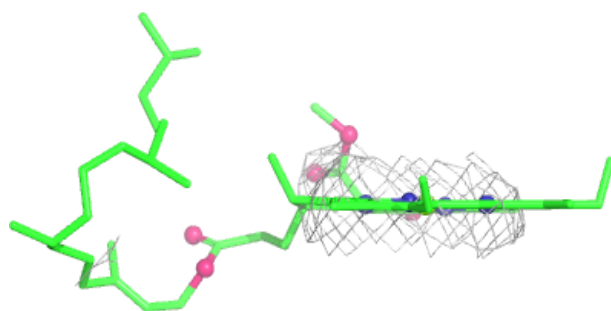
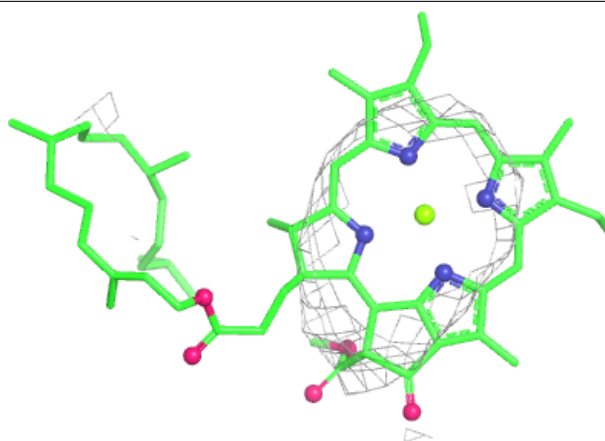
**Electron density around CLA B 616:**

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



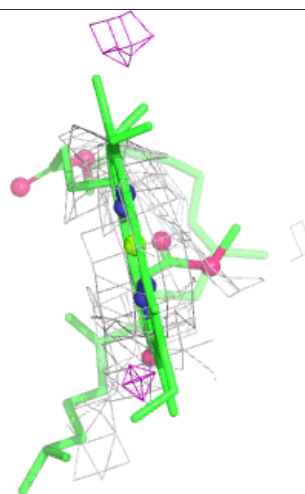
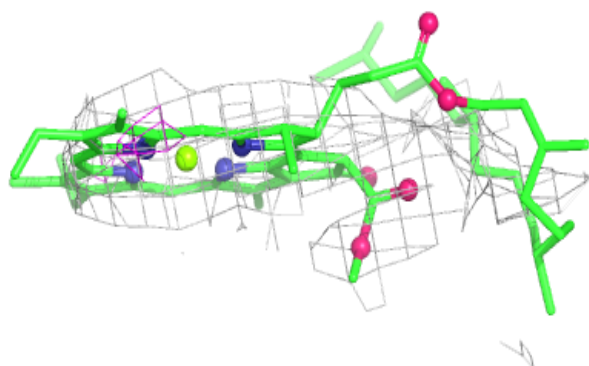
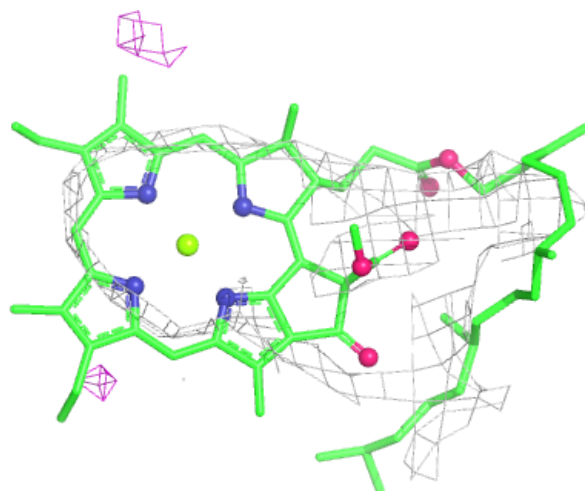
Electron density around CLA c 512:

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



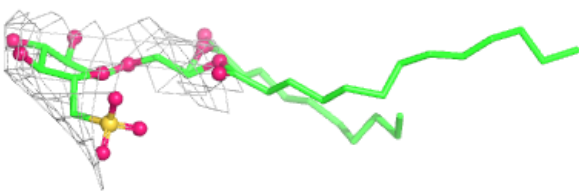
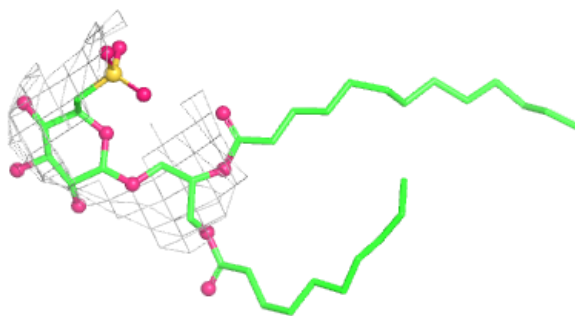
Electron density around CLA B 610:

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

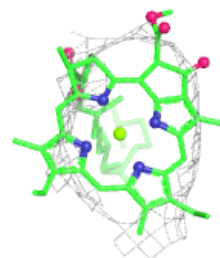
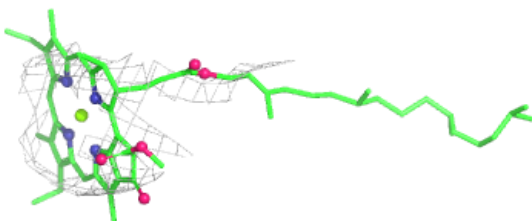
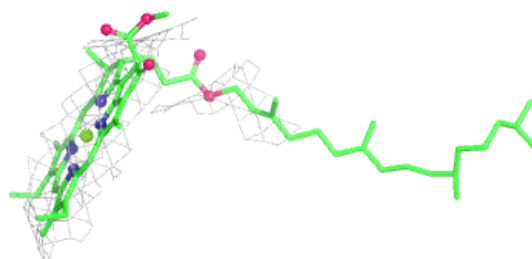


Electron density around SQD f 103:

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

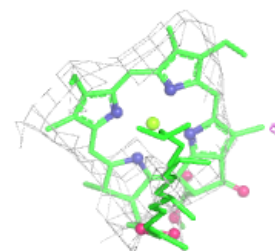
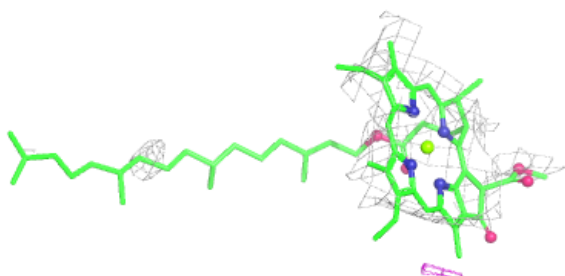
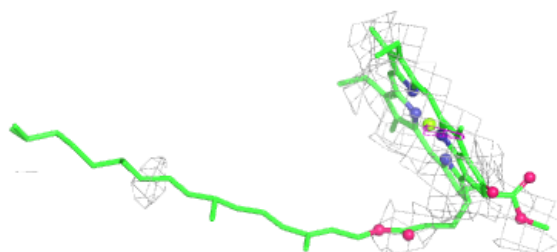
**Electron density around CLA b 607:**

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

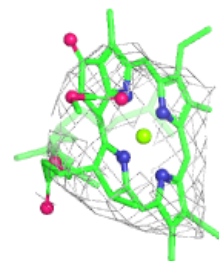
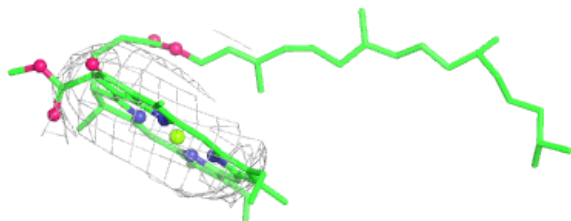
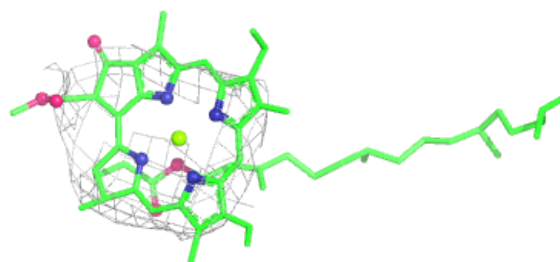


Electron density around CLA b 610:

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

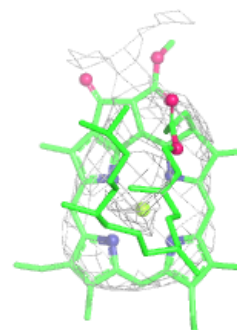
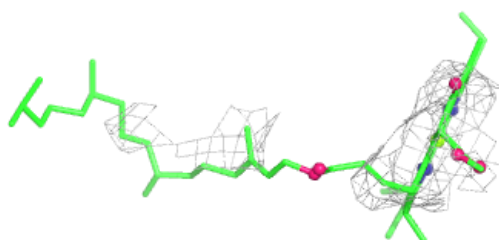
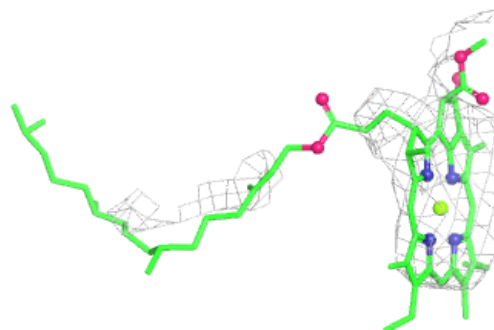
**Electron density around CLA B 608:**

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

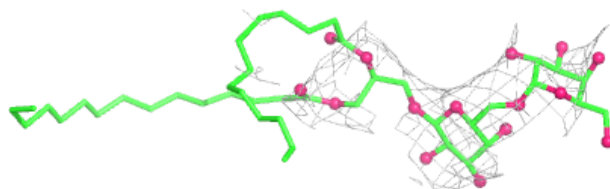
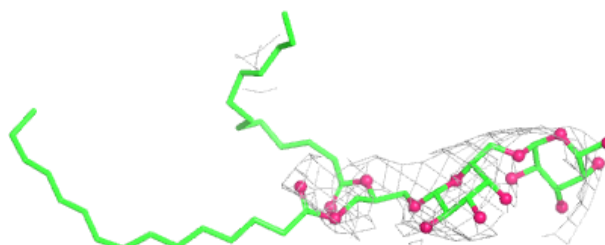


Electron density around CLA D 403:

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

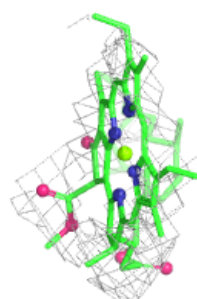
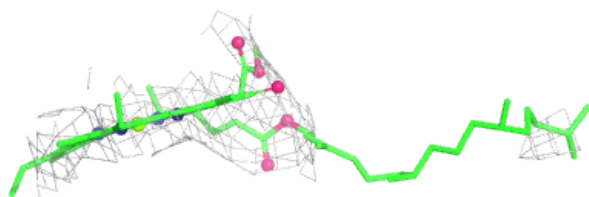
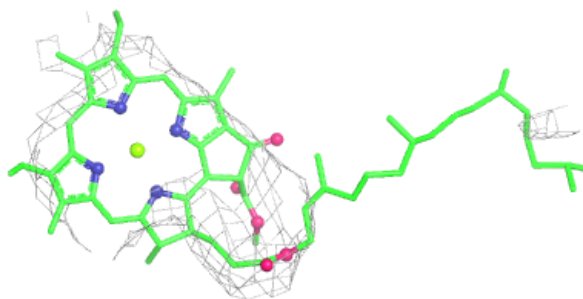
**Electron density around DGD B 621:**

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

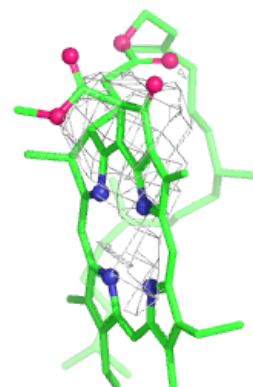
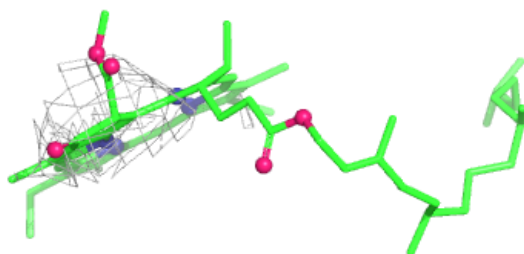
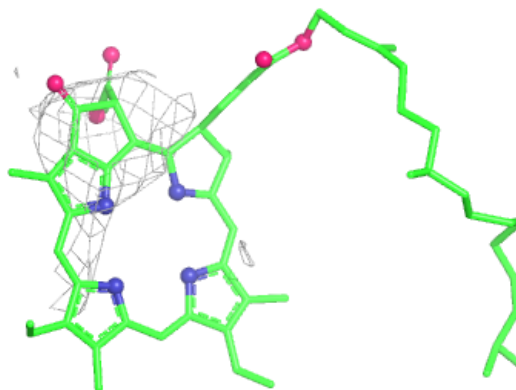


Electron density around CLA B 602:

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

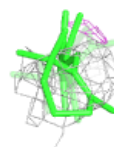
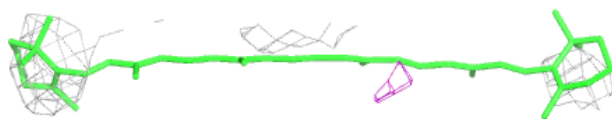
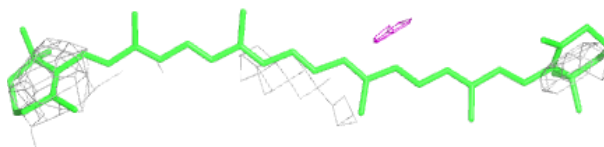
**Electron density around PHO a 408:**

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



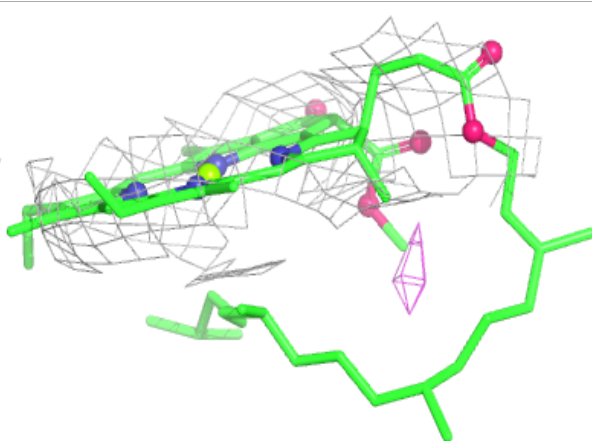
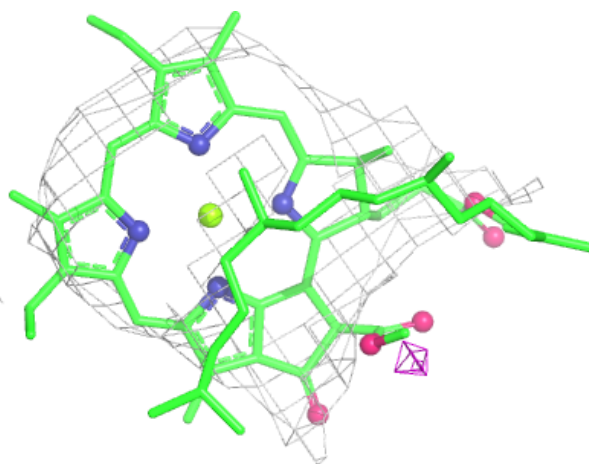
Electron density around BCR B 619:

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



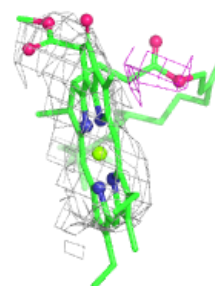
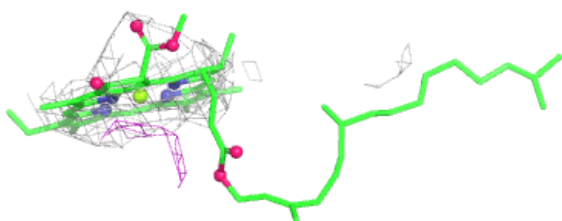
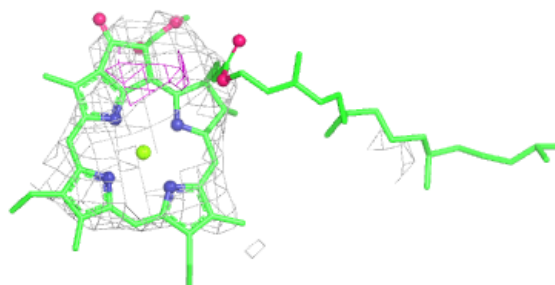
Electron density around CLA c 510:

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

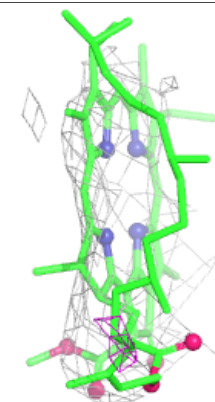
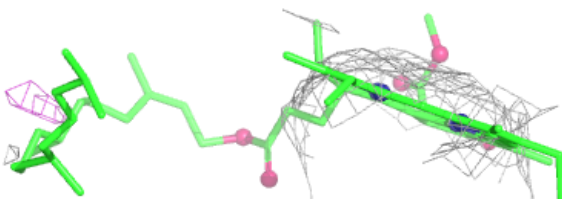
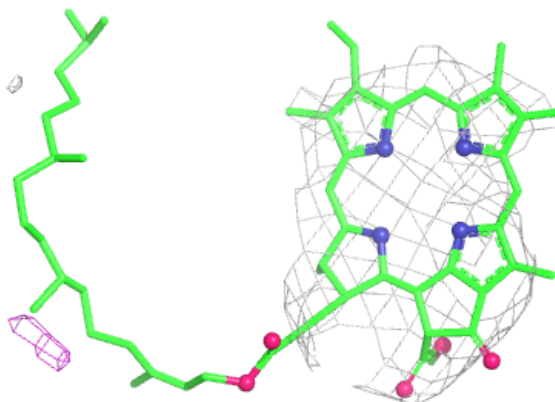


Electron density around CLA A 405:

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

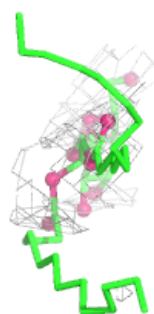
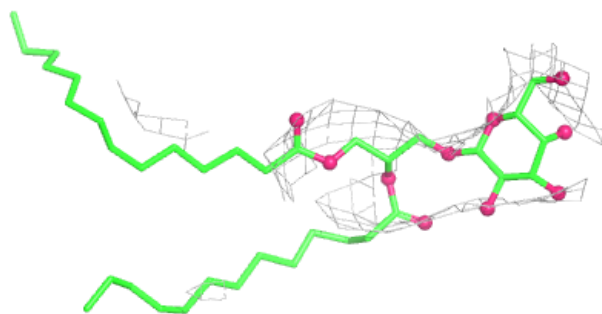
**Electron density around PHO a 407:**

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

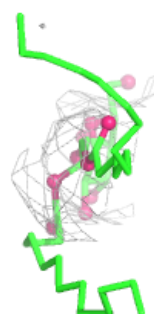
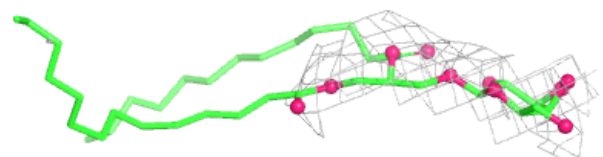
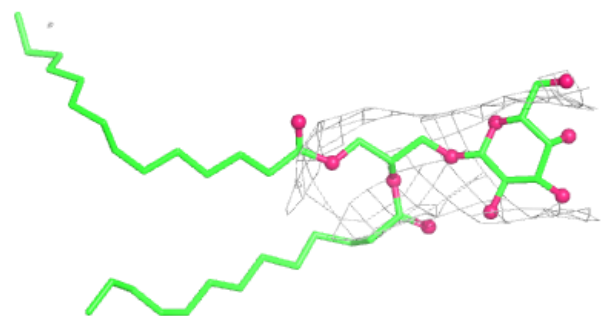


Electron density around LMG D 406:

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

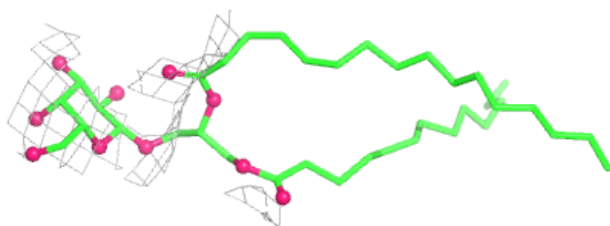
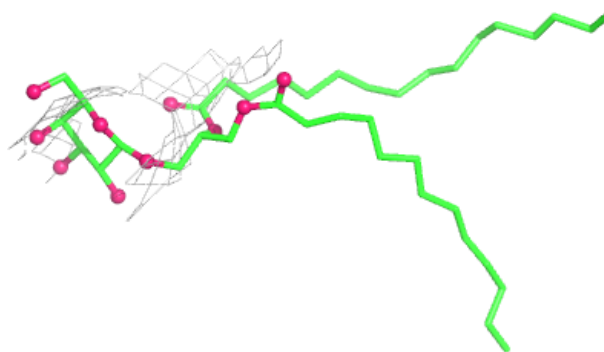
**Electron density around LMG d 405:**

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

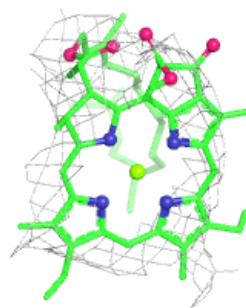
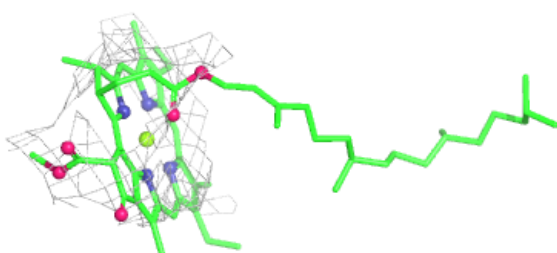
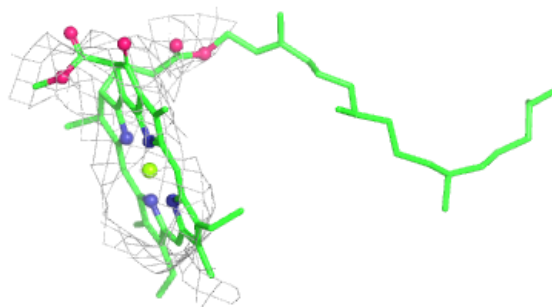


Electron density around LMG d 406:

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

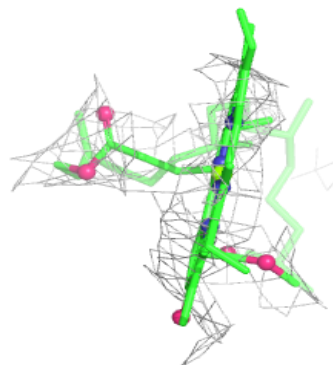
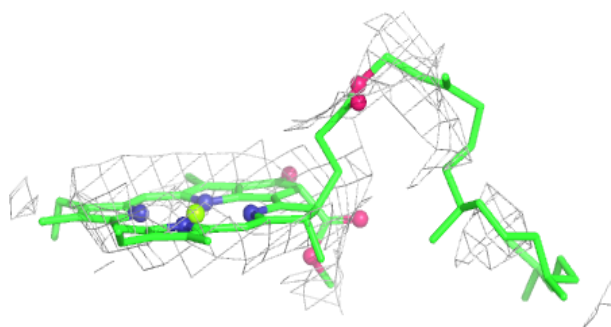
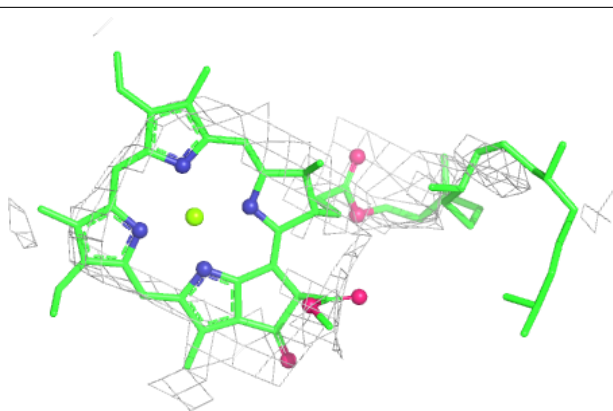
**Electron density around CLA c 508:**

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

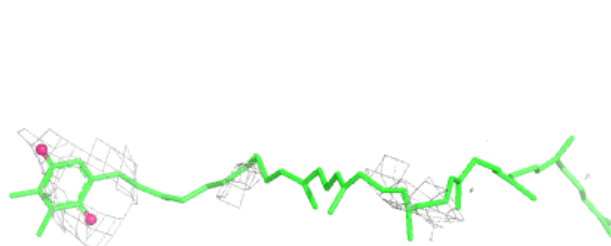
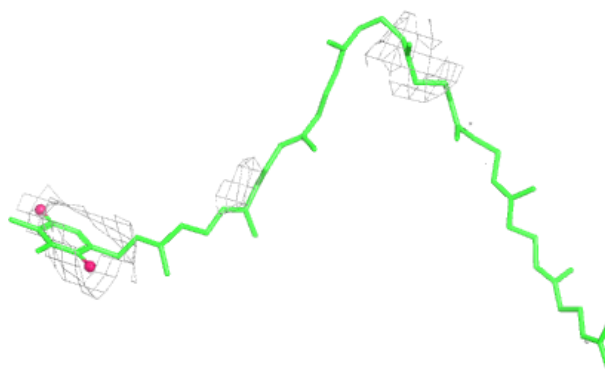


Electron density around CLA B 612:

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

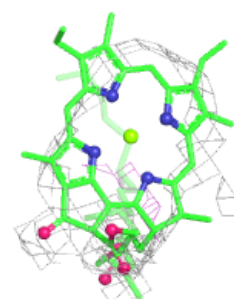
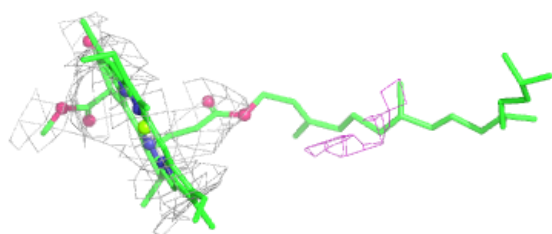
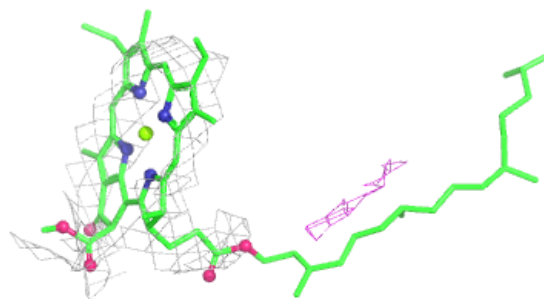
**Electron density around PL9 D 404:**

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

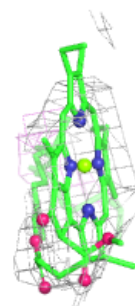
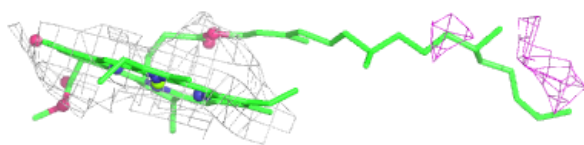
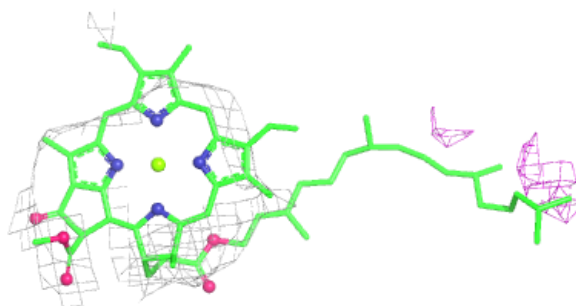


Electron density around CLA B 609:

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

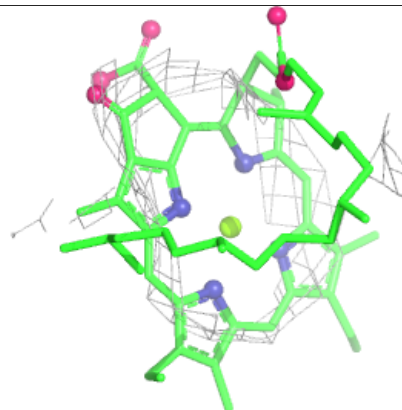
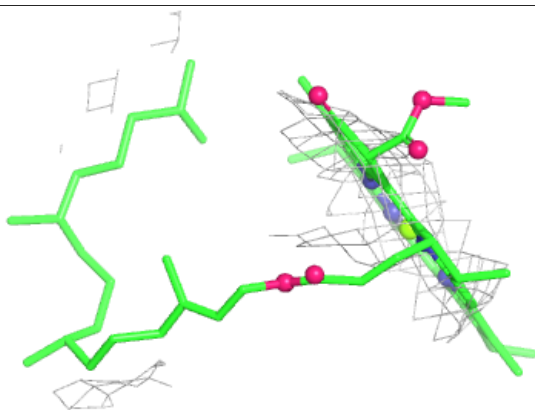
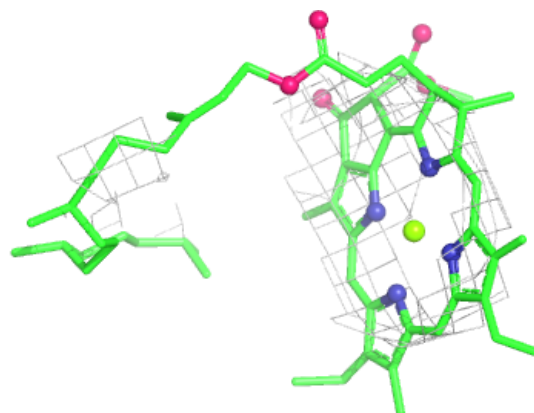
**Electron density around CLA B 603:**

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



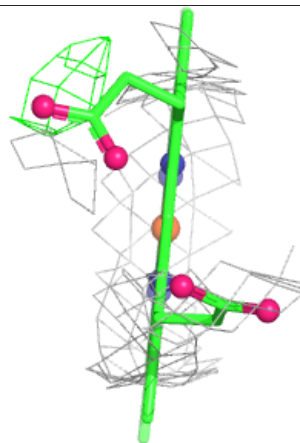
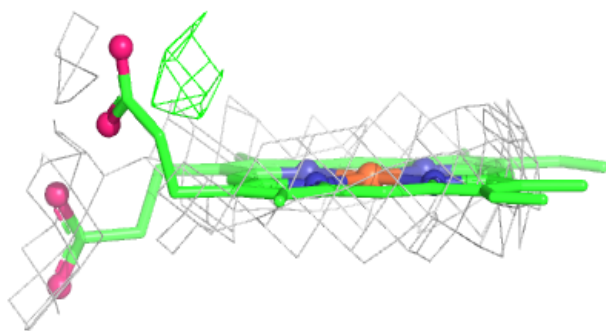
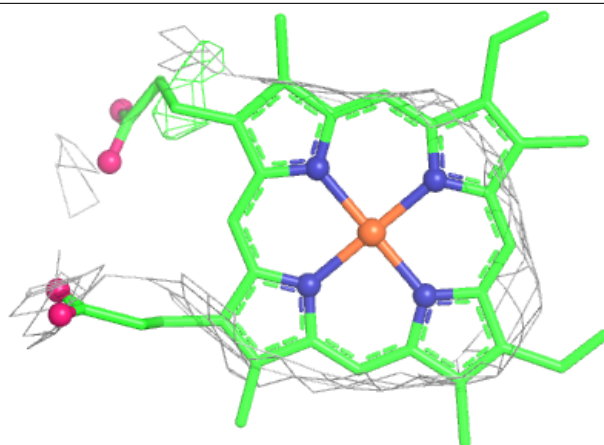
Electron density around CLA c 503:

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



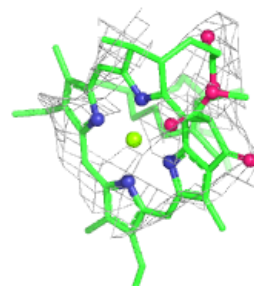
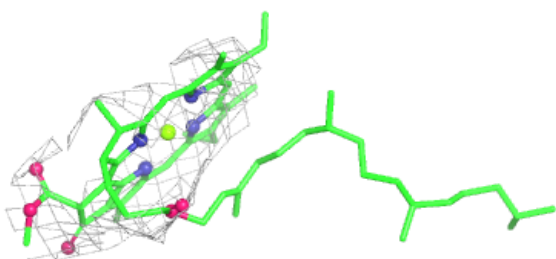
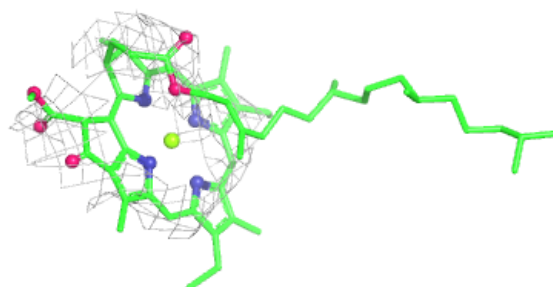
Electron density around HEM f 101:

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



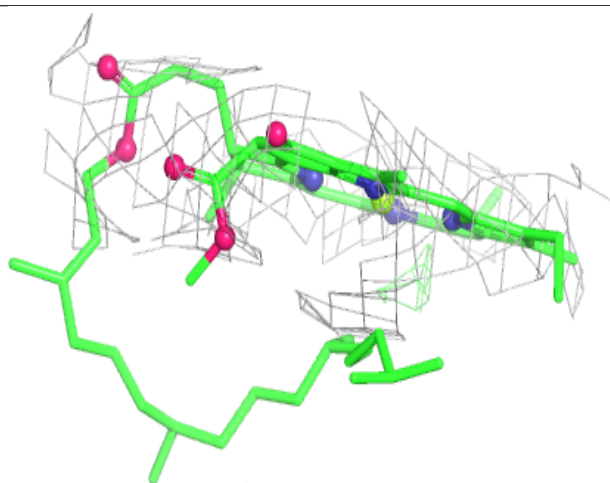
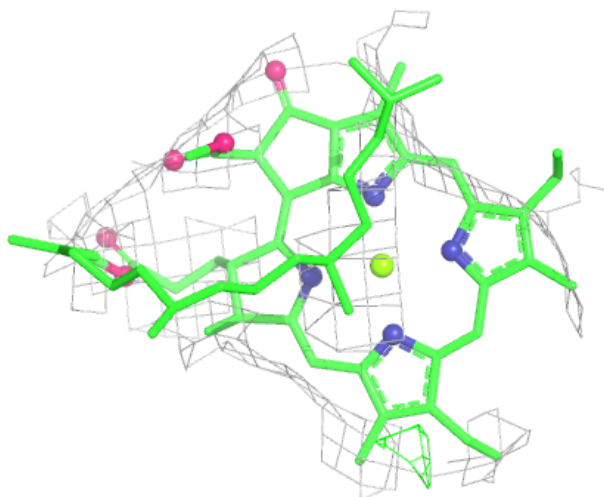
Electron density around CLA c 505:

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



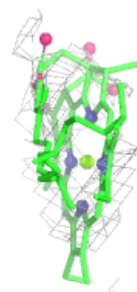
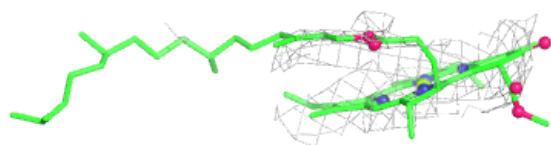
Electron density around CLA C 510:

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

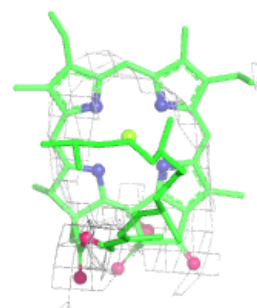
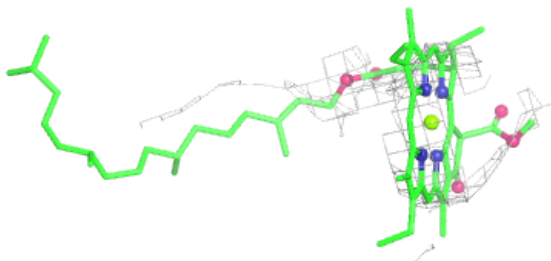


Electron density around CLA b 606:

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

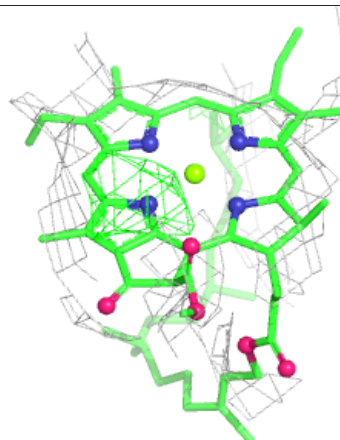
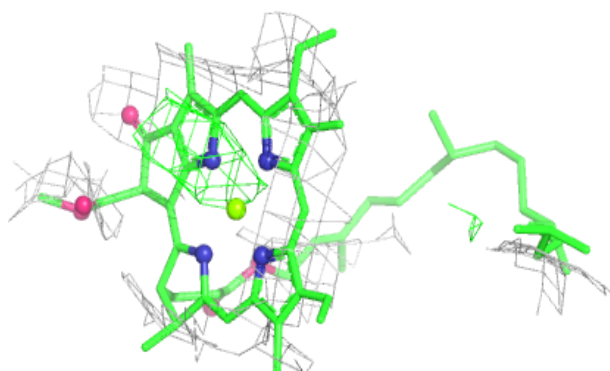
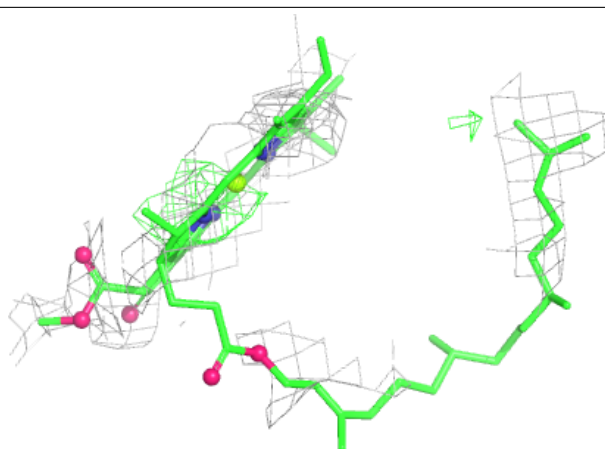
**Electron density around CLA B 605:**

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

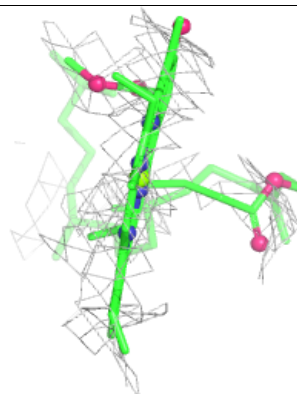
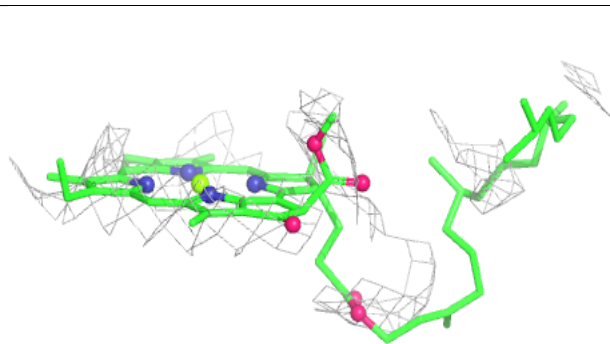
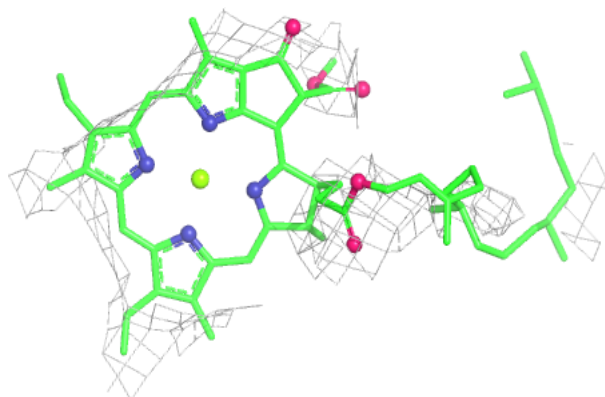


Electron density around CLA b 614:

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

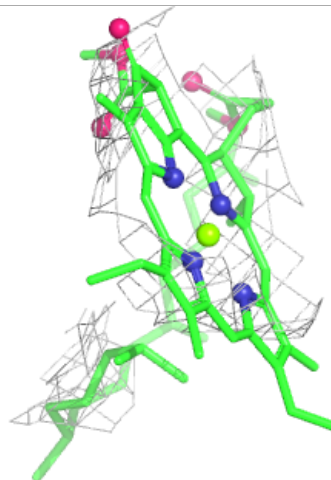
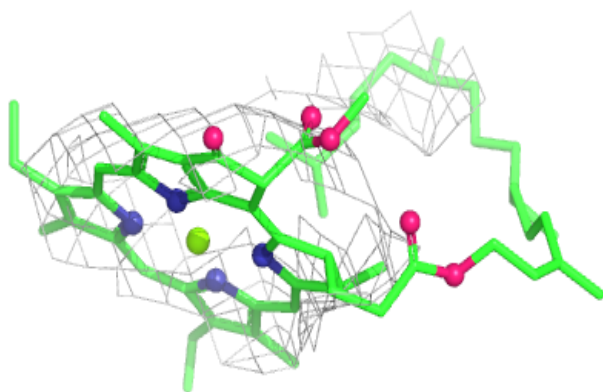
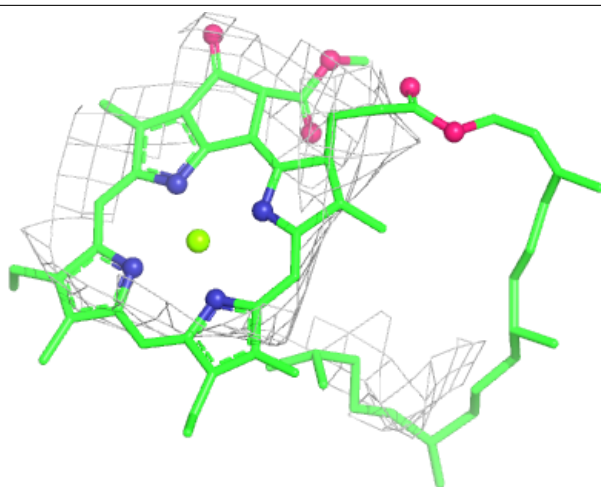
**Electron density around CLA b 615:**

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



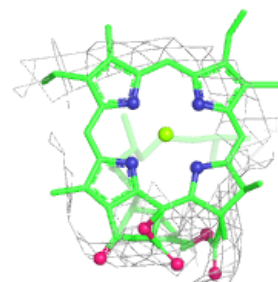
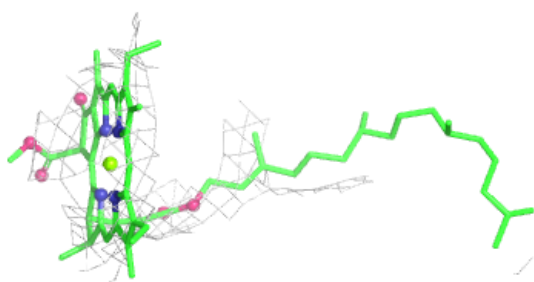
Electron density around CLA B 615:

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

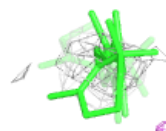
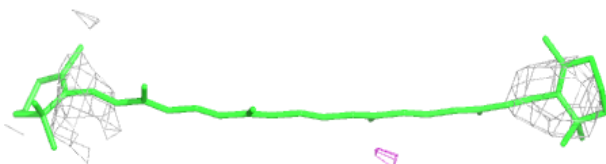
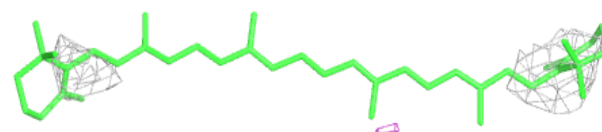


Electron density around CLA b 608:

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

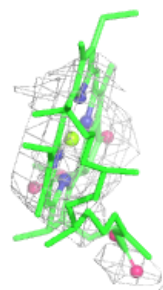
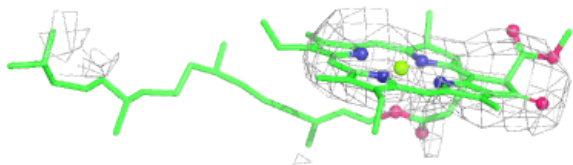
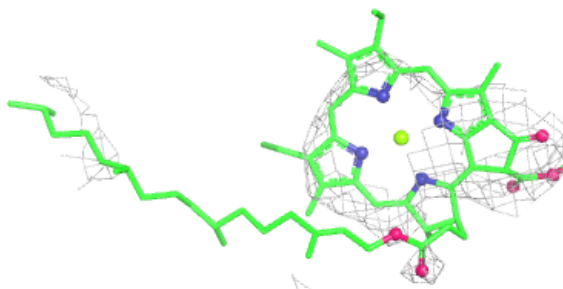
**Electron density around BCR B 617:**

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

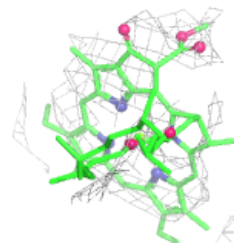
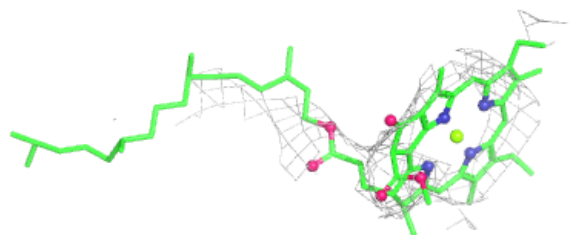
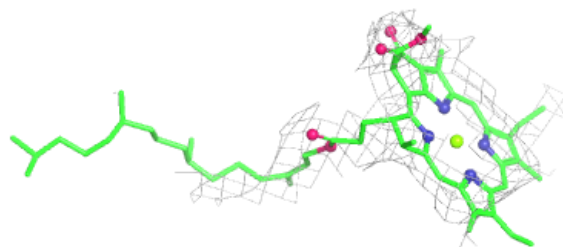


Electron density around CLA c 501:

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

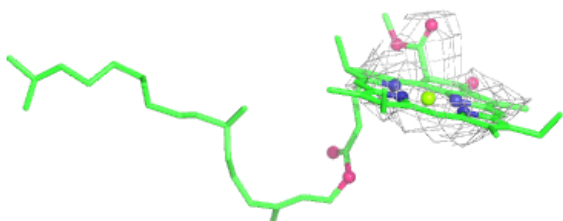
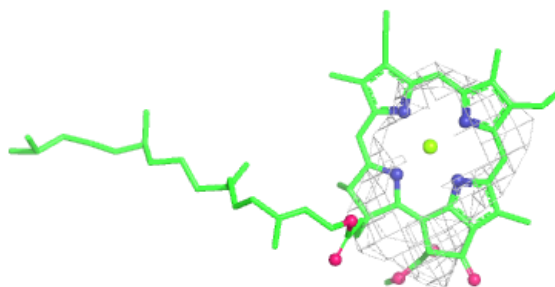
**Electron density around CLA c 502:**

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

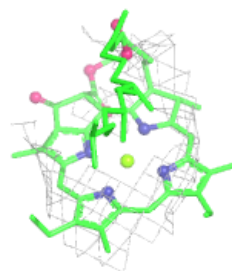
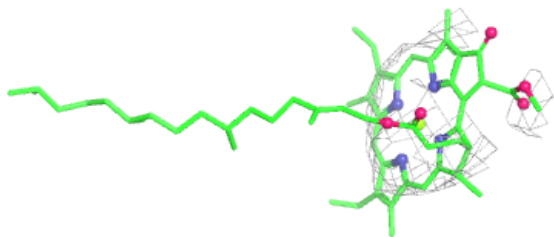
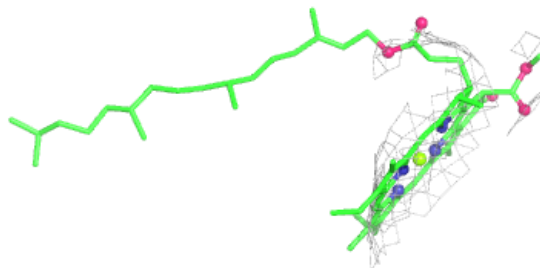


Electron density around CLA a 406:

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

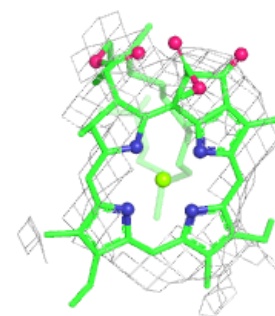
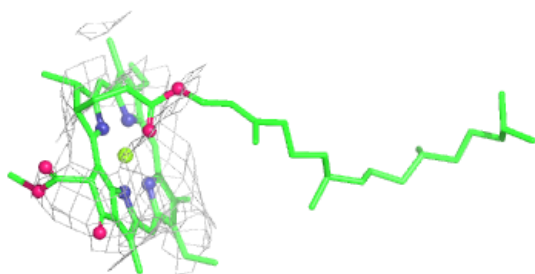
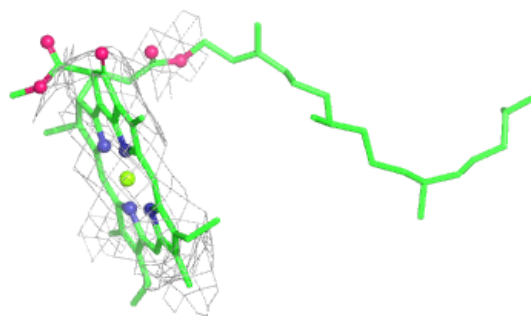
**Electron density around CLA c 504:**

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

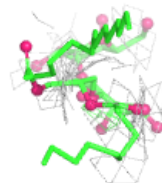
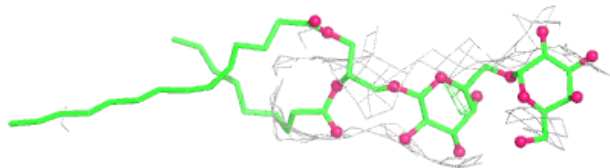
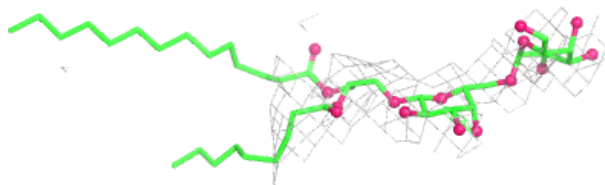


Electron density around CLA C 508:

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

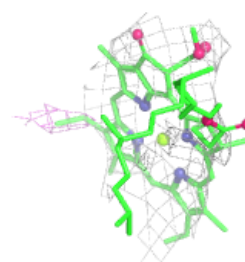
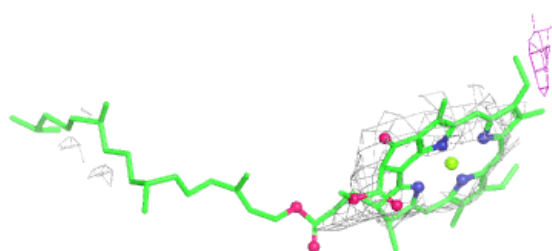
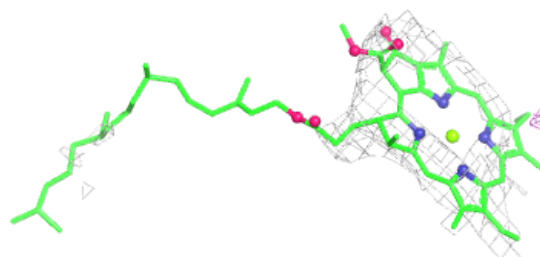
**Electron density around DGD c 517:**

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

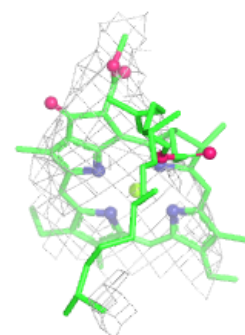
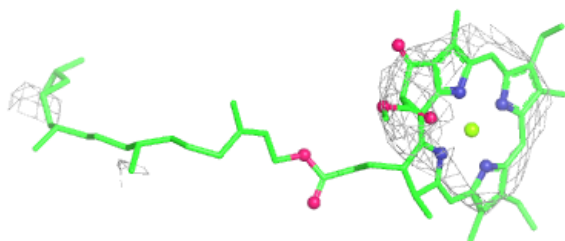
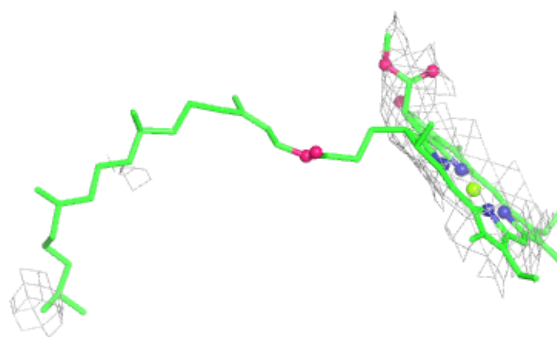


Electron density around CLA A 403:

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

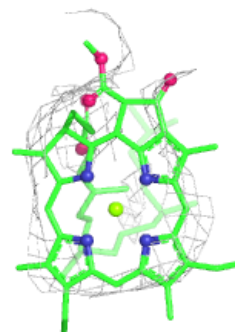
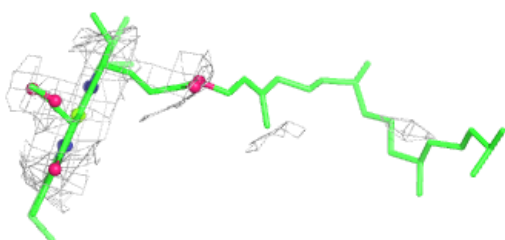
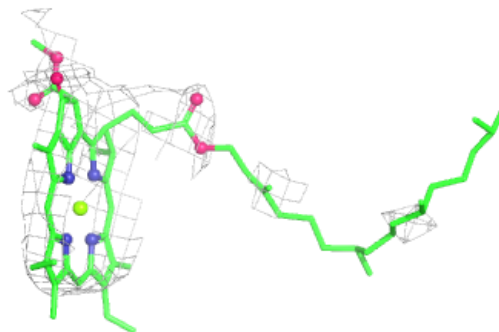
**Electron density around CLA D 401:**

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

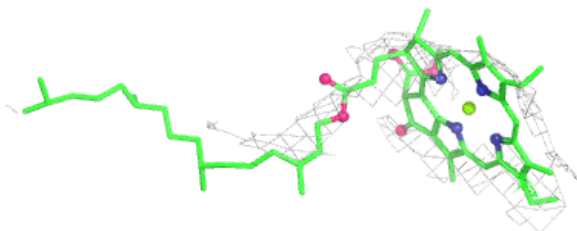


Electron density around CLA d 403:

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

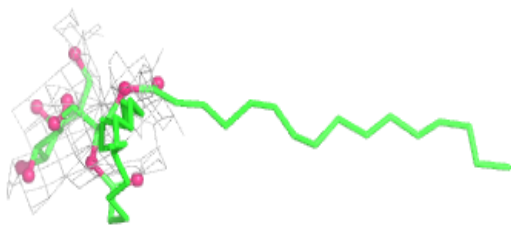
**Electron density around CLA C 502:**

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



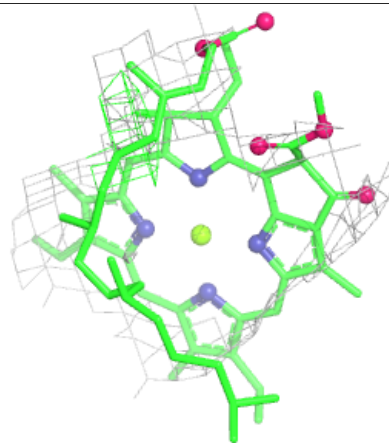
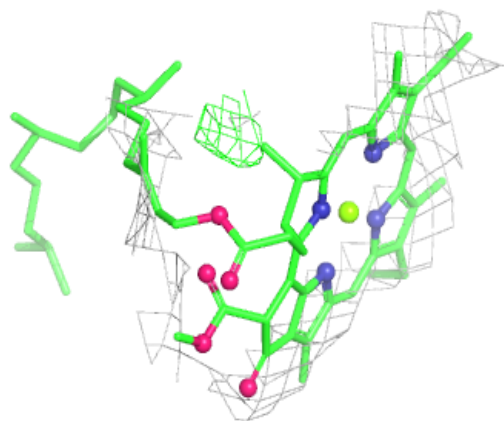
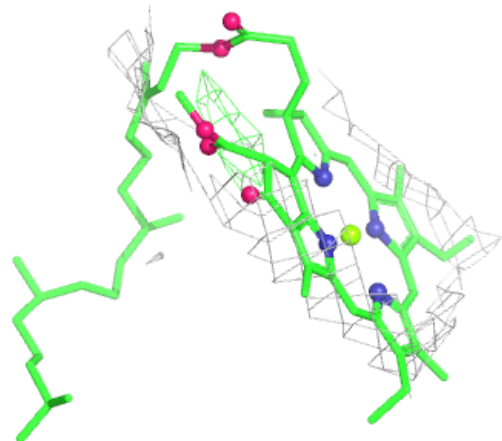
Electron density around LMG A 414:

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



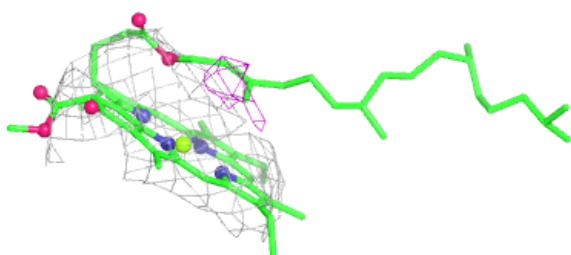
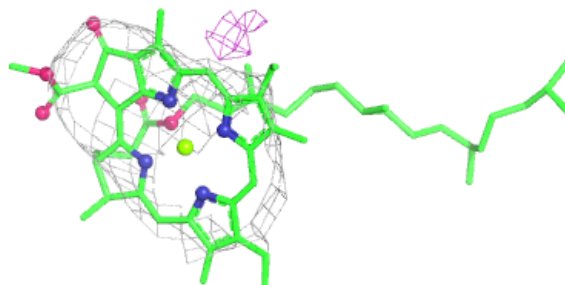
Electron density around CLA b 616:

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



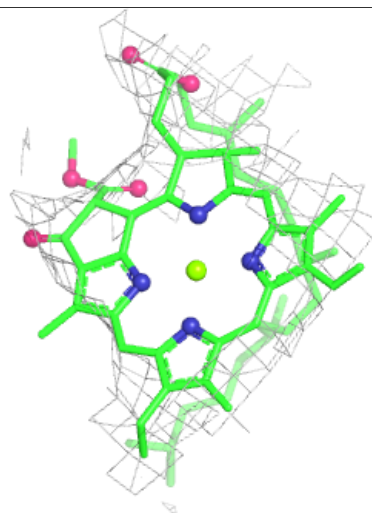
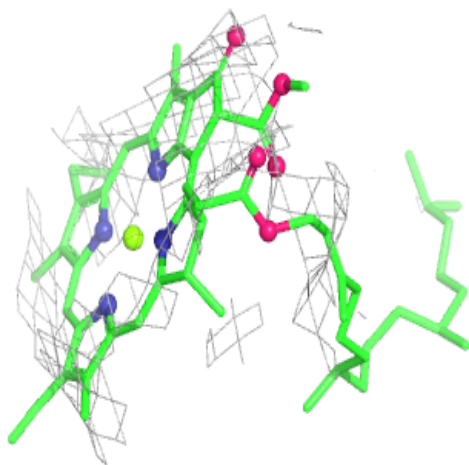
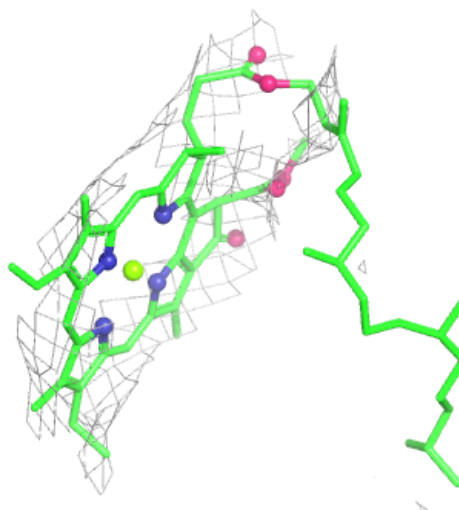
Electron density around CLA b 617:

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



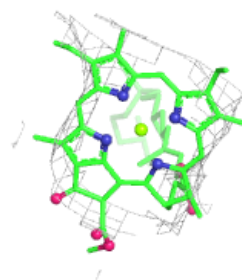
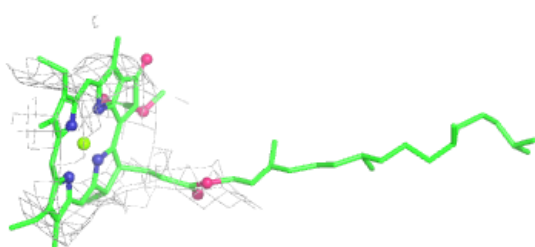
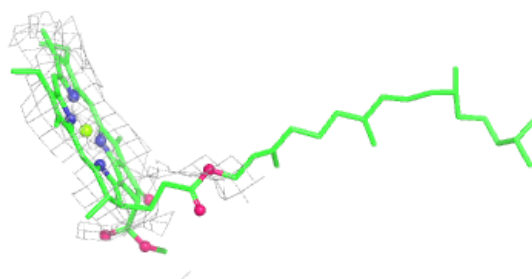
Electron density around CLA B 613:

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

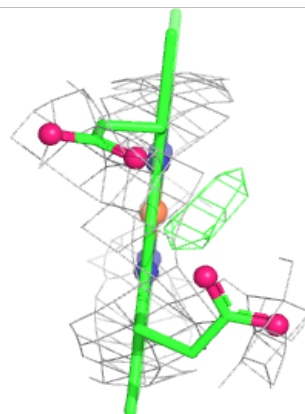
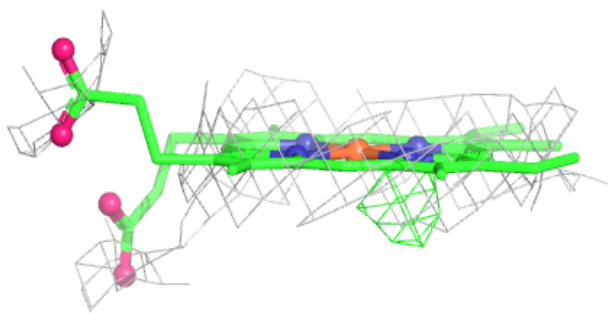
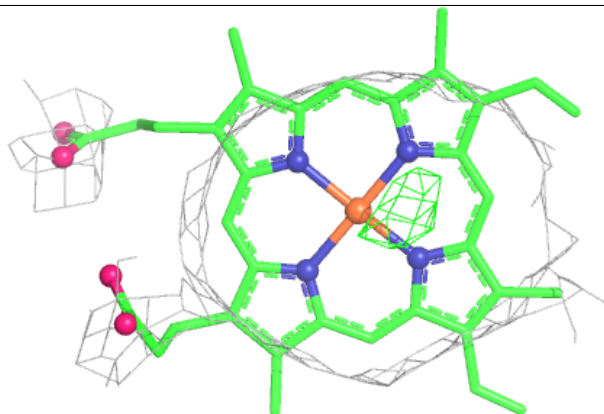


Electron density around CLA B 604:

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

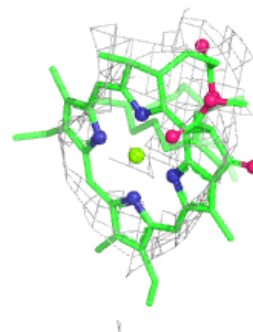
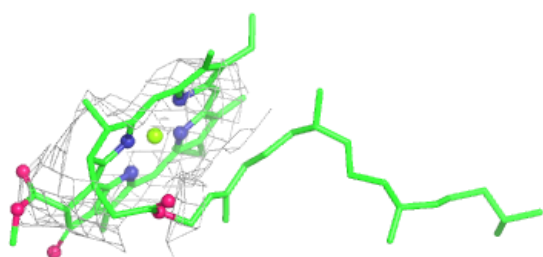
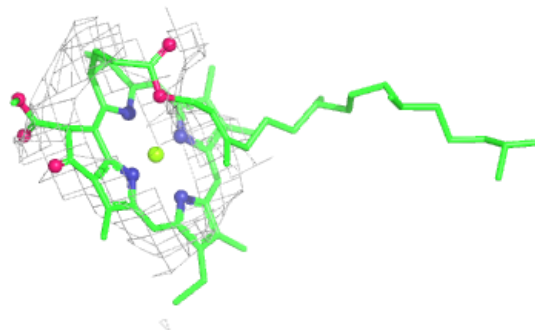
**Electron density around HEM F 101:**

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



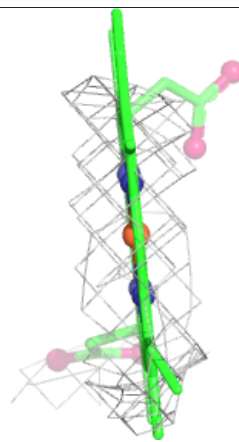
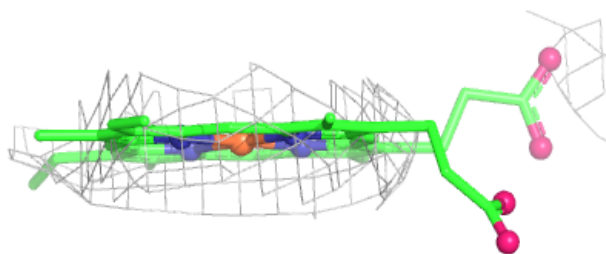
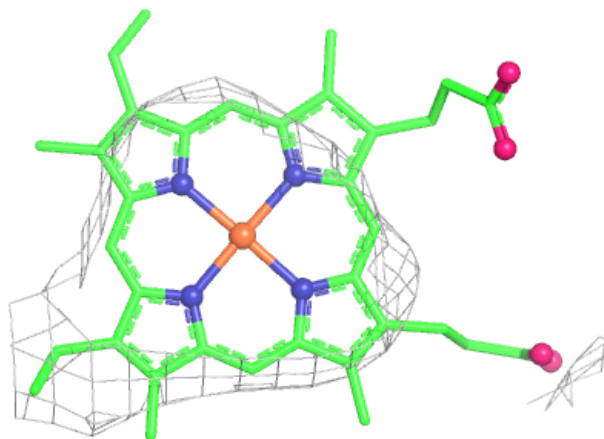
Electron density around CLA C 505:

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



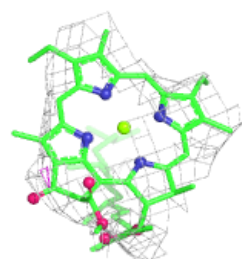
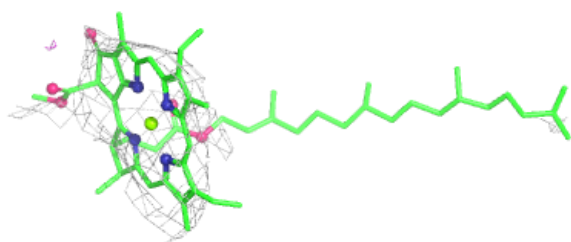
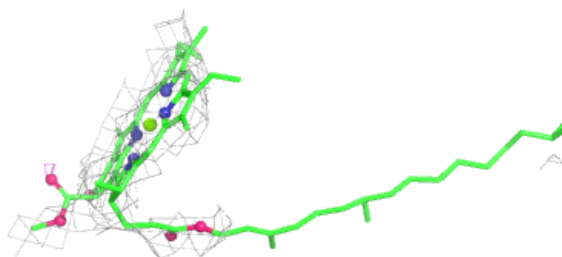
Electron density around HEM v 201:

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



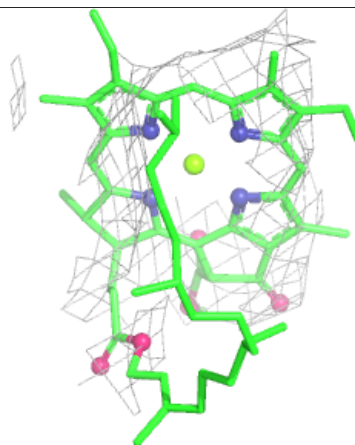
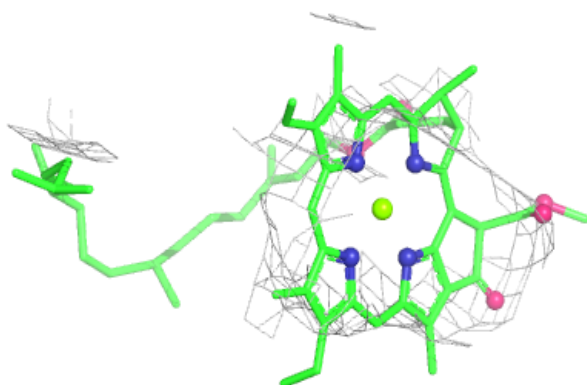
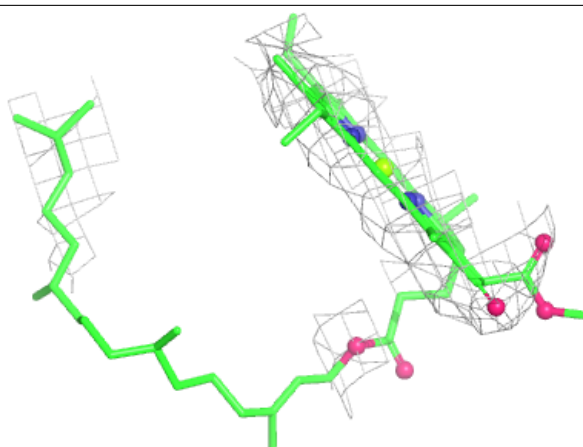
Electron density around CLA B 607:

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



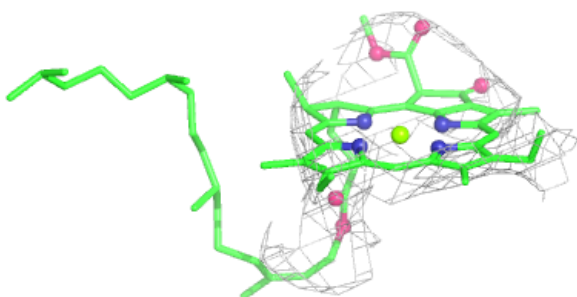
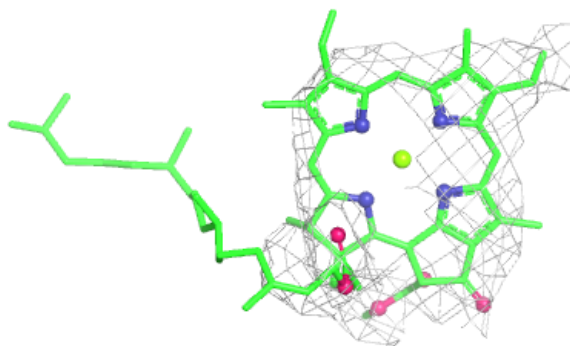
Electron density around CLA B 611:

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

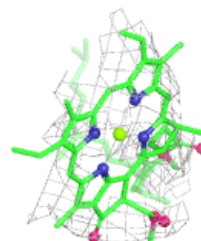


Electron density around CLA A 404:

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

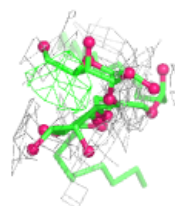
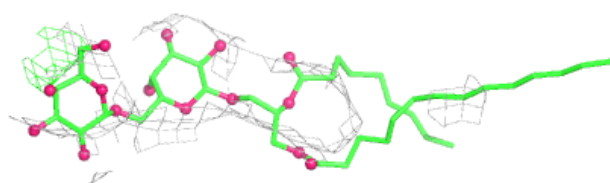
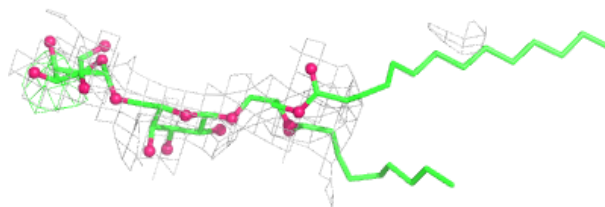
**Electron density around CLA a 404:**

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

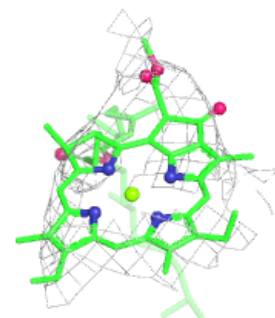
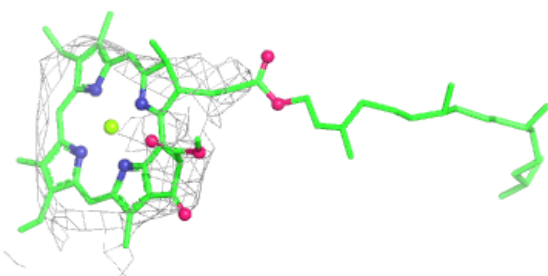
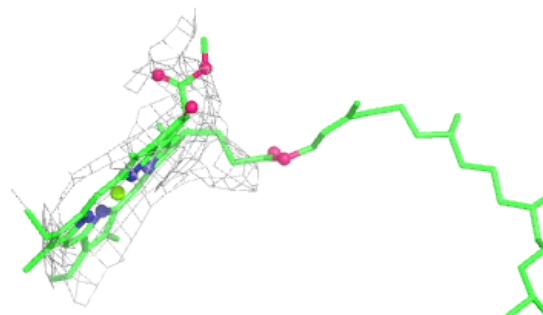


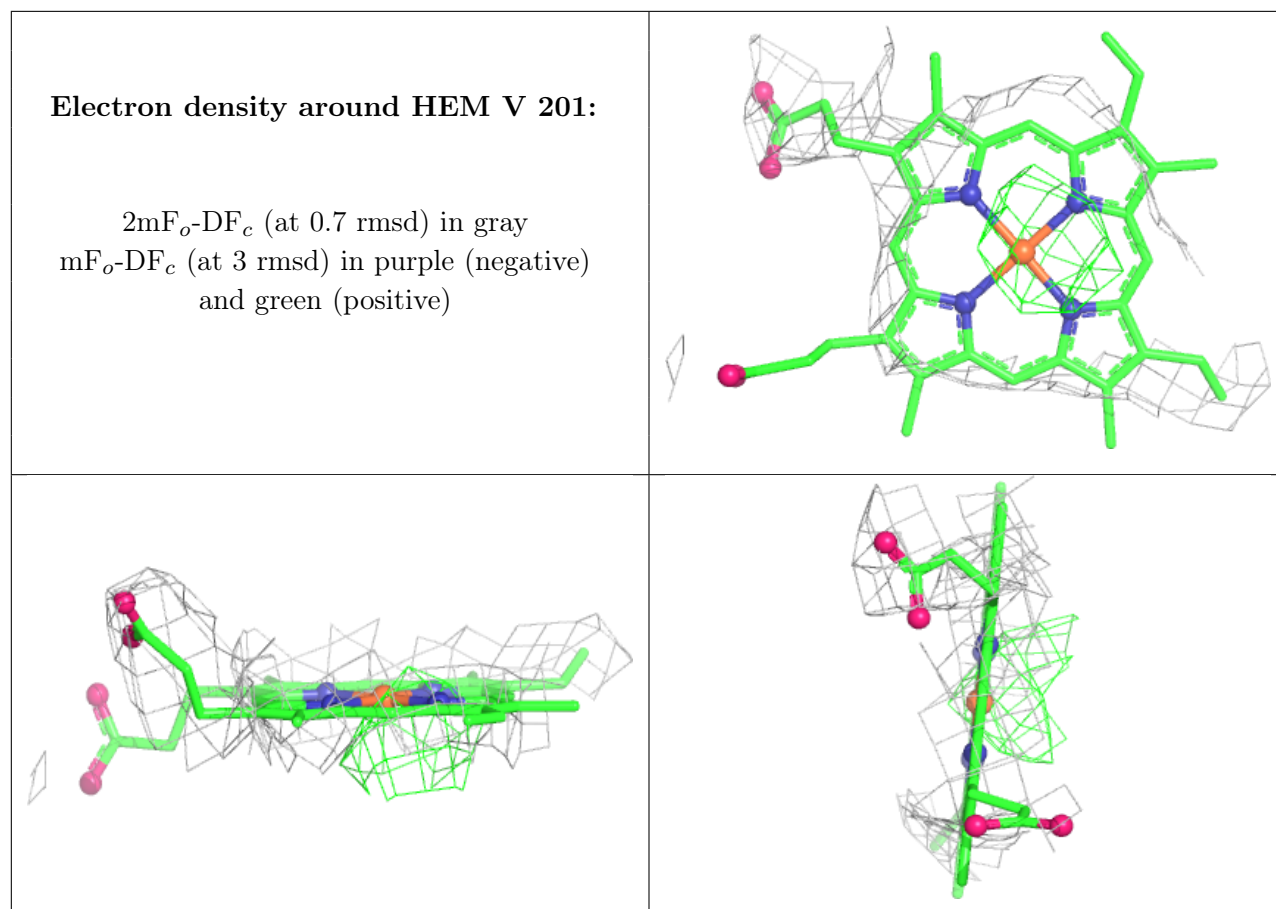
Electron density around DGD C 516:

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

**Electron density around CLA d 402:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.