



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:08 PM EDT

PDB ID : 4IXR / pdb_00004ixr
Title : RT fs X-ray diffraction of Photosystem II, first illuminated state
Authors : Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on : 2013-01-27
Resolution : 5.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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)

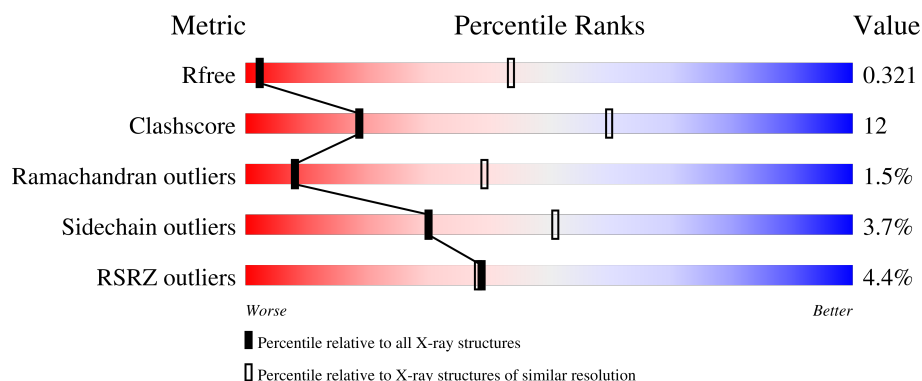
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1135 (7.80-4.00)
Clashscore	190562	1201 (7.80-4.00)
Ramachandran outliers	187476	1026 (7.80-4.00)
Sidechain outliers	187428	1017 (7.82-3.98)
RSRZ outliers	180081	1128 (7.80-4.00)

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	
1	a	360	

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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	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	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	J	101	-	-	-	X
27	BCR	j	102	-	-	-	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			

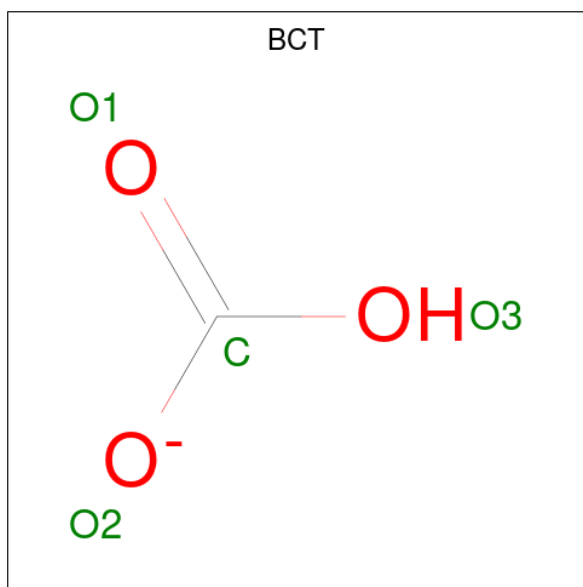
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

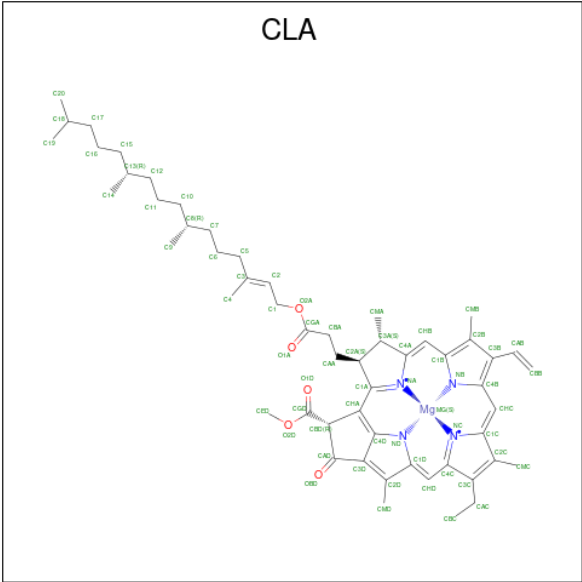
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- 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 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
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	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

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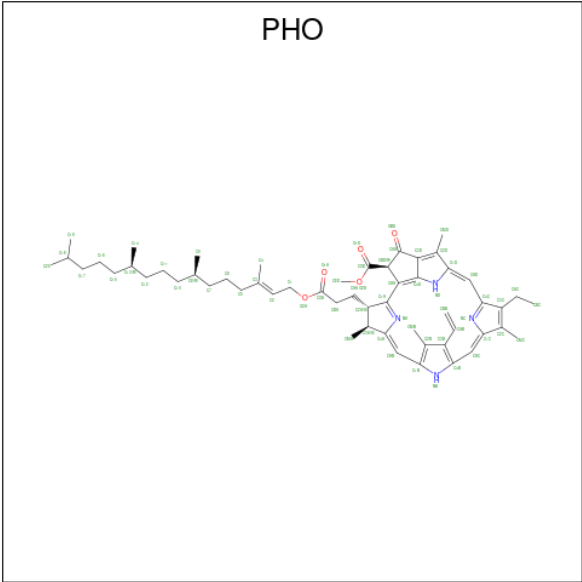
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 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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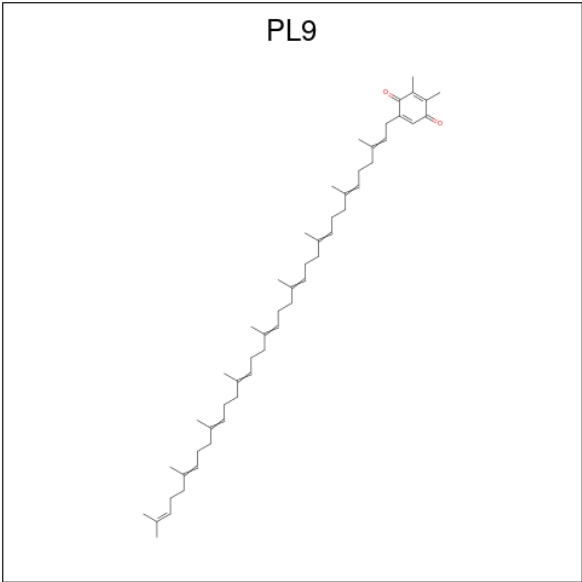
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 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: $C_{55}H_{74}N_4O_5$).



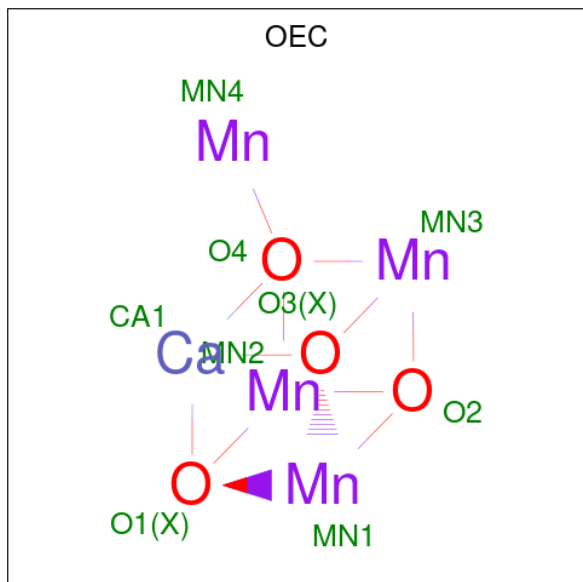
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- 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).



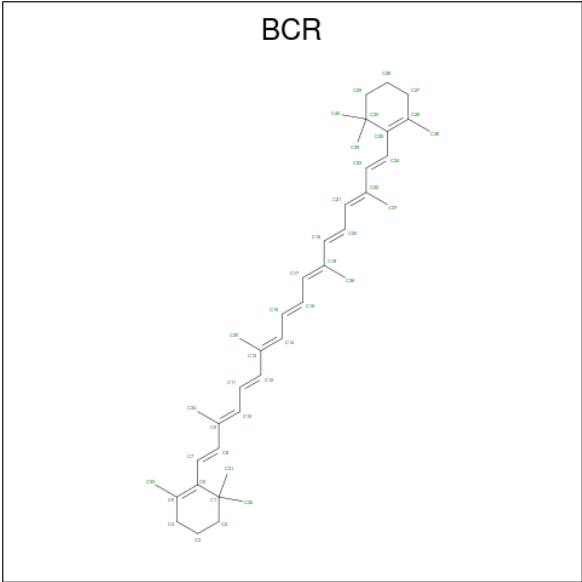
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	J	1	Total	C	O	0	0
			35	33	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			55	53	2		
25	j	1	Total	C	O	0	0
			35	33	2		

- 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: $\text{C}_{40}\text{H}_{56}$).



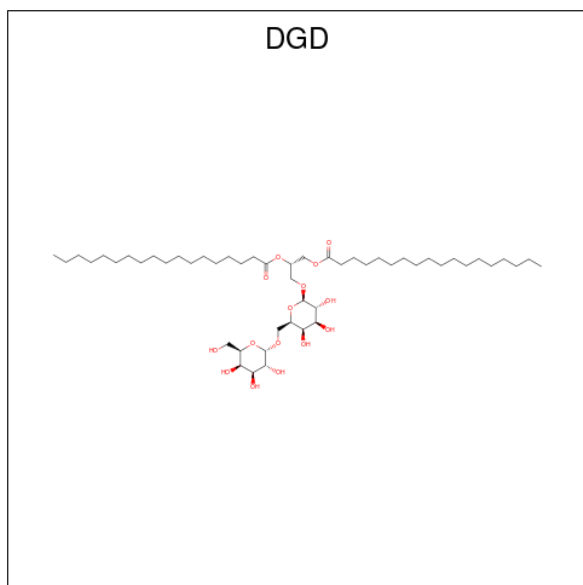
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total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

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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	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	z	1	Total C 40 40	0	0

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



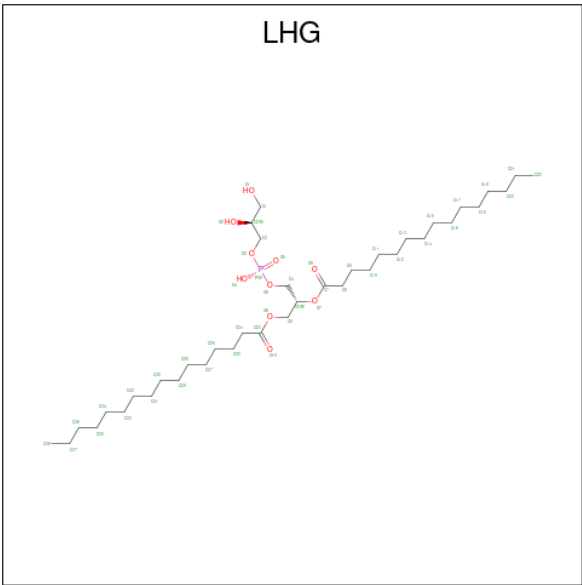
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0

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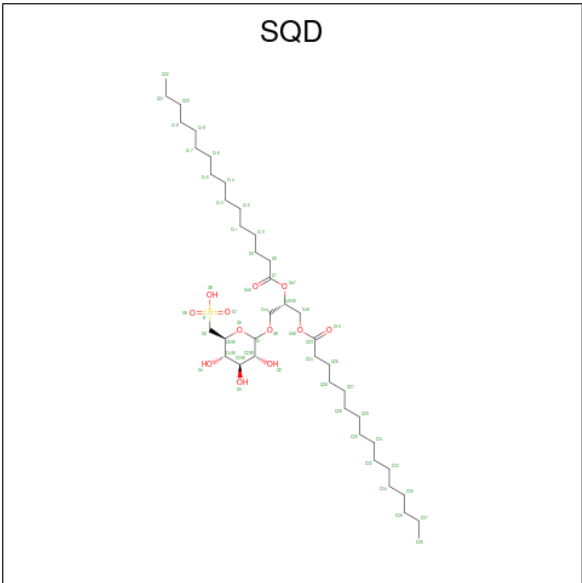
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			58	43	15		
28	B	1	Total	C	O	0	0
			52	37	15		
28	C	1	Total	C	O	0	0
			53	38	15		
28	C	1	Total	C	O	0	0
			62	47	15		
28	C	1	Total	C	O	0	0
			66	51	15		
28	D	1	Total	C	O	0	0
			63	48	15		
28	a	1	Total	C	O	0	0
			56	41	15		
28	b	1	Total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



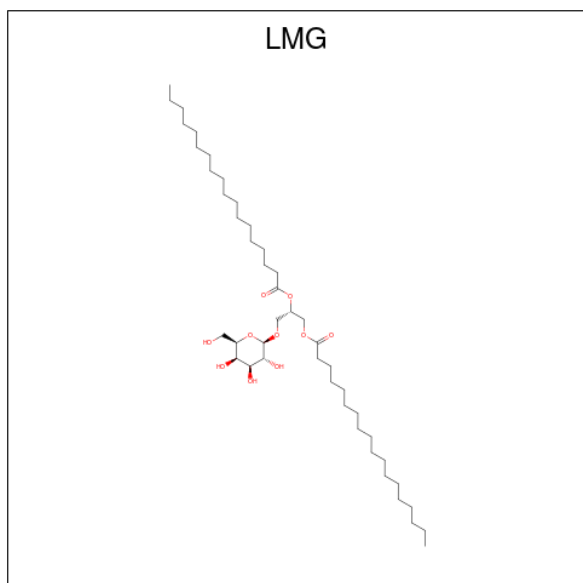
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- 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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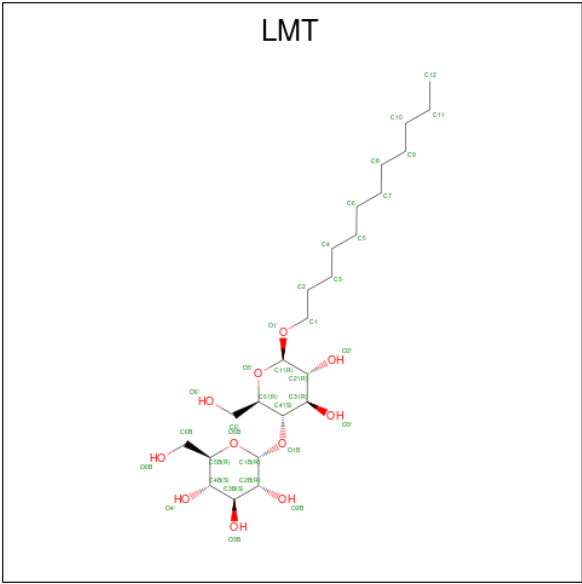
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			42	32	10		
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	C	1	Total	C	O	0	0
			45	35	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	D	1	Total	C	O	0	0
			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	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		
31	m	1	Total	C	O	0	0
			42	32	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	a	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	b	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 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	d	1	Total C O 31 20 11	0	0
33	i	1	Total C O 35 24 11	0	0
33	m	1	Total C O 35 24 11	0	0

- # HEM

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

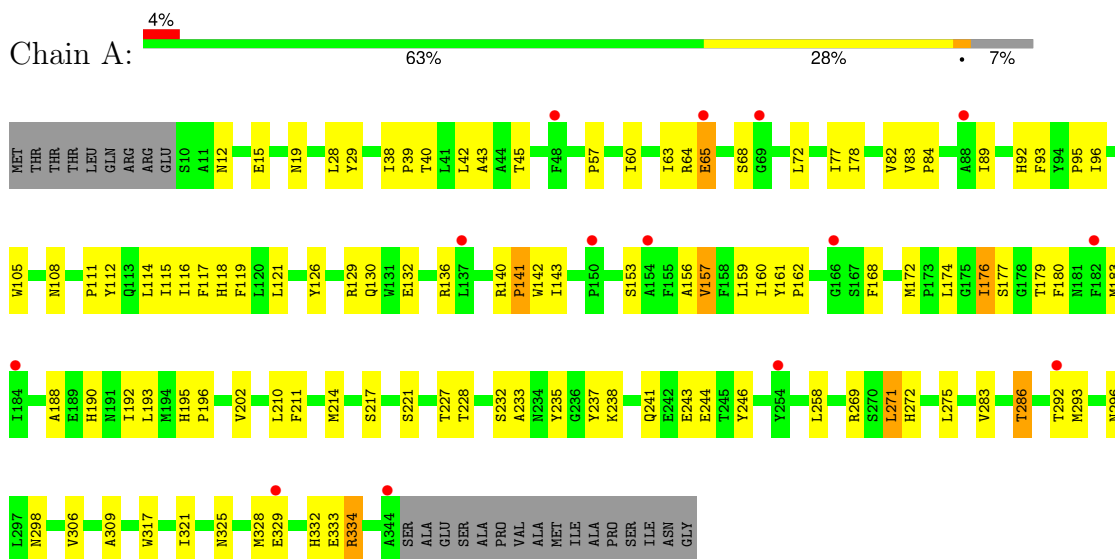
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

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

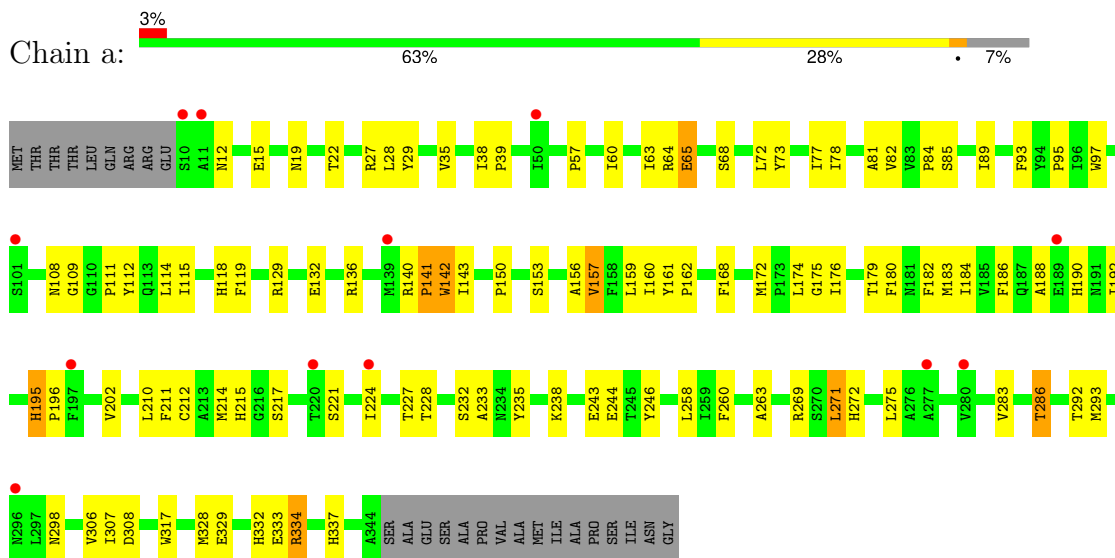
3 Residue-property plots [i](#)

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.

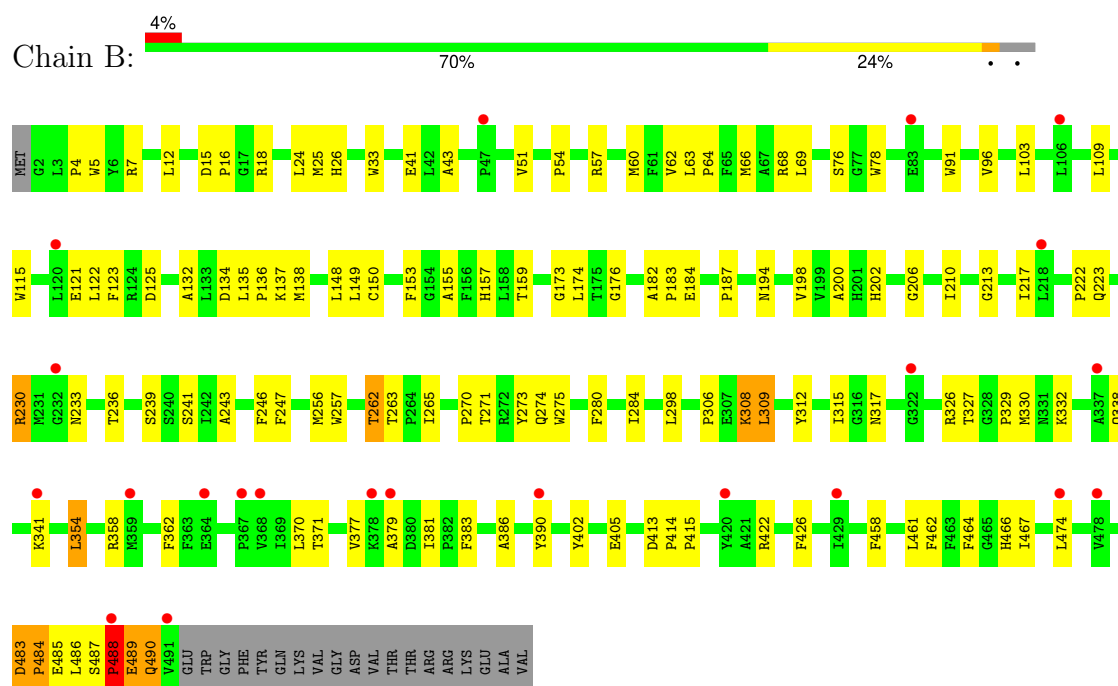
- Molecule 1: Photosystem Q(B) protein 1



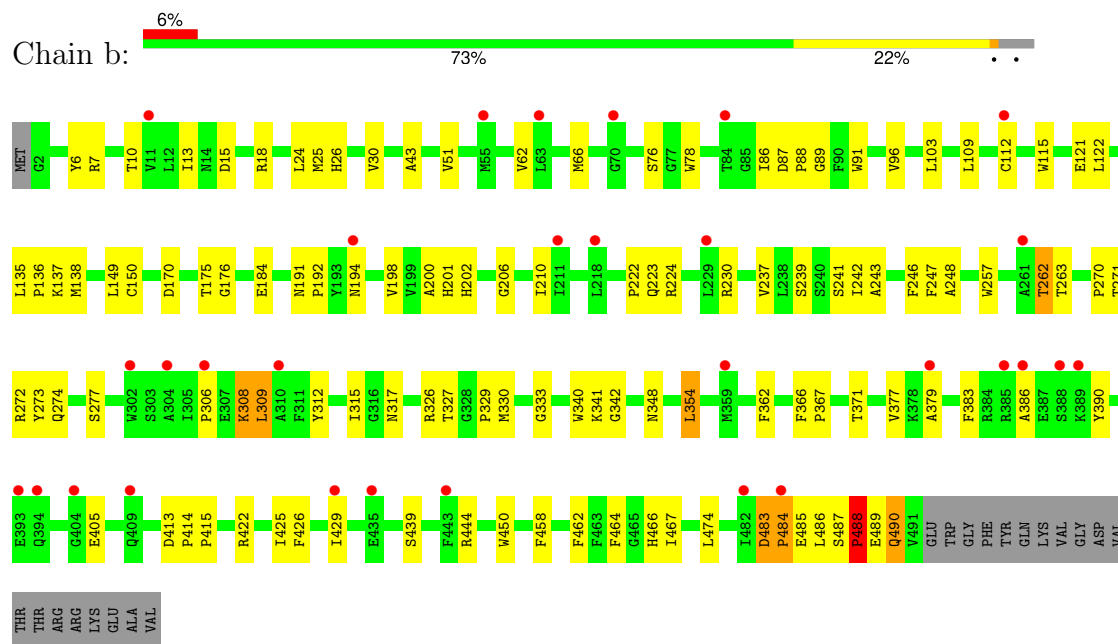
- Molecule 1: Photosystem Q(B) protein 1



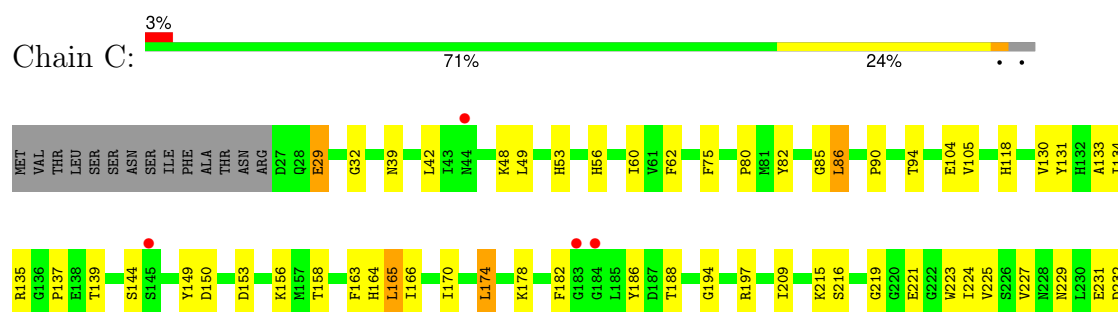
- Molecule 2: Photosystem II core light harvesting protein

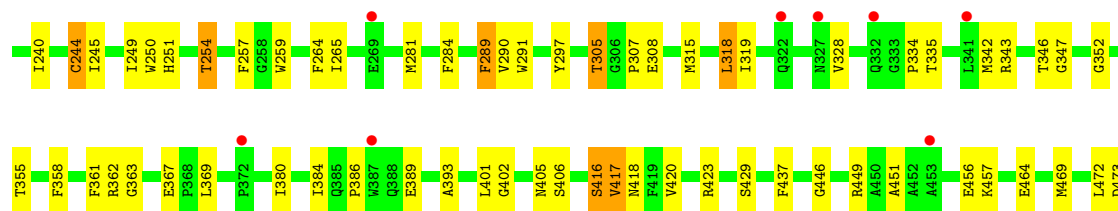


• Molecule 2: Photosystem II core light harvesting protein

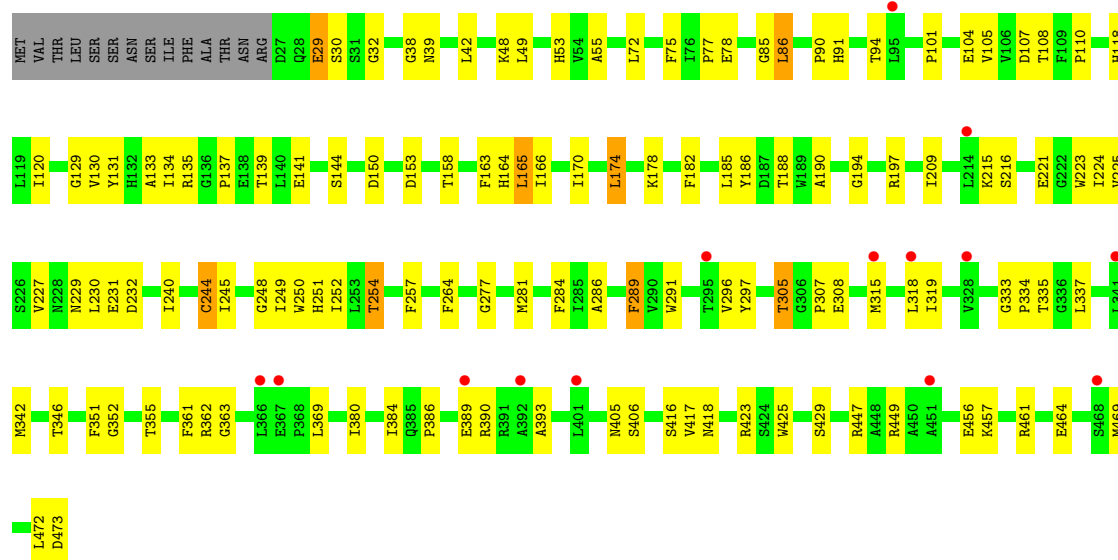


• Molecule 3: Photosystem II CP43 protein

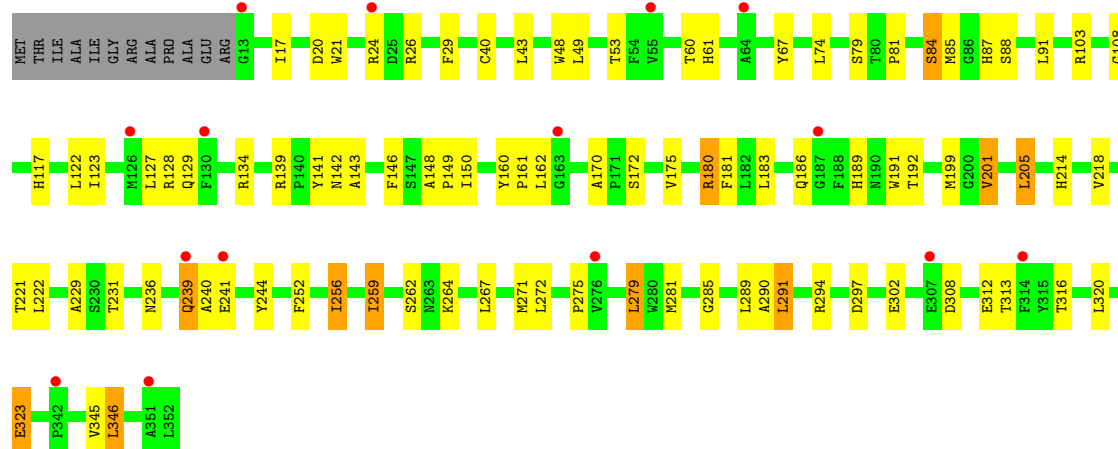




• Molecule 3: Photosystem II CP43 protein

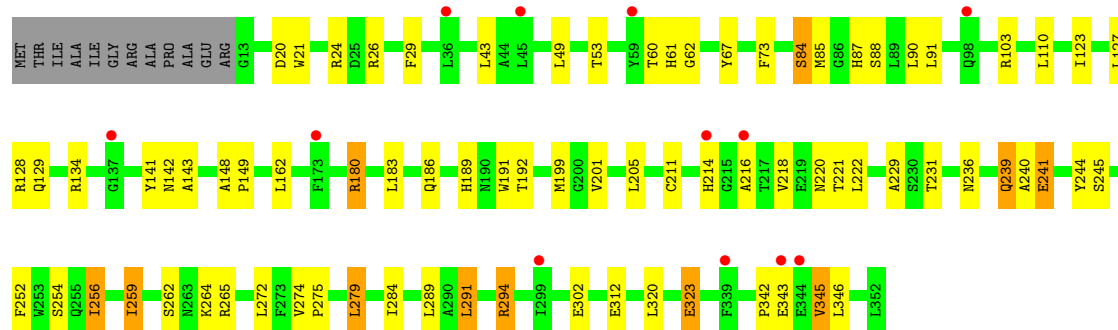


• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein





• Molecule 5: Cytochrome b559 subunit alpha



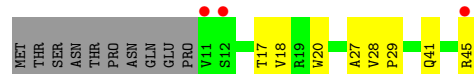
• Molecule 5: Cytochrome b559 subunit alpha



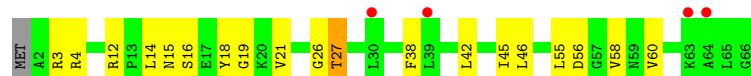
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta



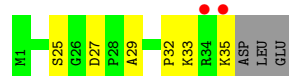
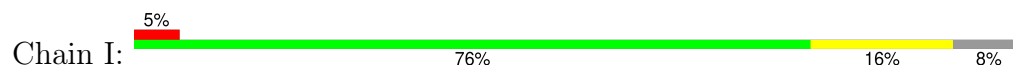
• Molecule 7: Photosystem II reaction center protein H



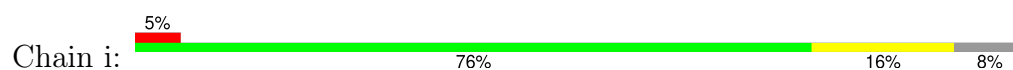
• Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



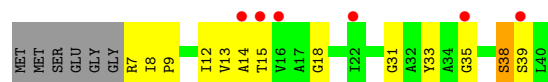
- Molecule 8: Photosystem II reaction center protein I



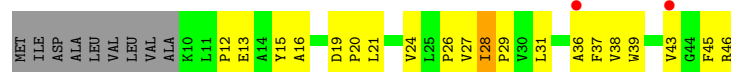
- Molecule 9: Photosystem II reaction center protein J



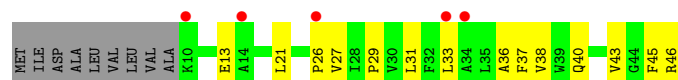
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



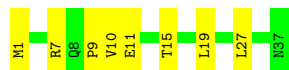
- Molecule 11: Photosystem II reaction center protein L

Chain L:  76% 24%



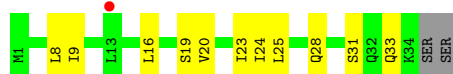
- Molecule 11: Photosystem II reaction center protein L

Chain l:  78% 22%



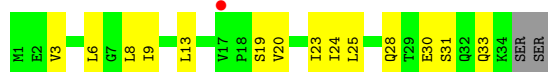
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 64% 31% 6%



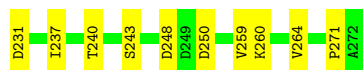
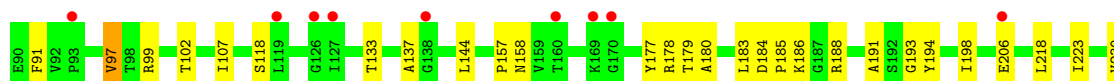
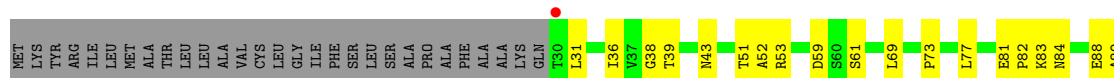
- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 56% 39% 6%



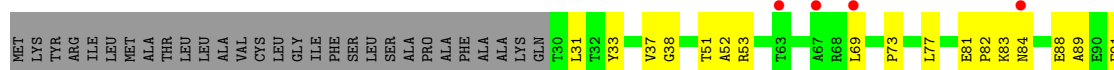
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

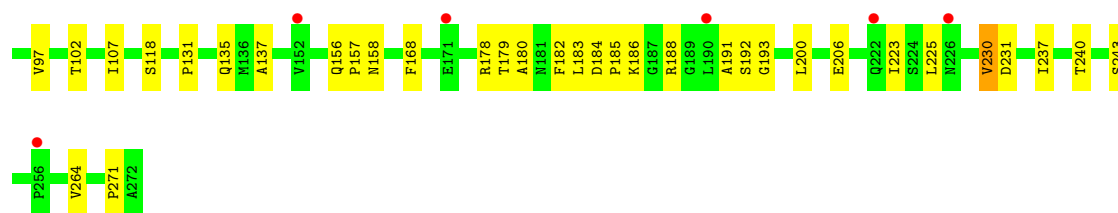
Chain O:  4% 68% 21% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  4% 71% 18% 11%





• Molecule 14: Photosystem II reaction center protein T

Chain T: 59% 38%



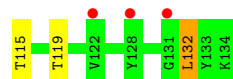
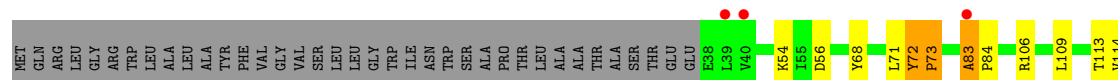
• Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 59% 41%



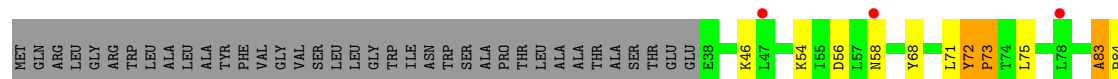
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 4% 61% 8% 28%



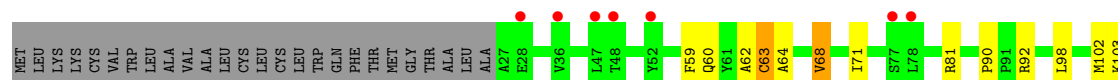
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 2% 56% 13% 28%



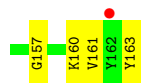
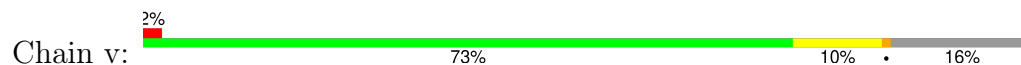
• Molecule 16: Cytochrome c-550

Chain V: 6% 71% 11% 16%

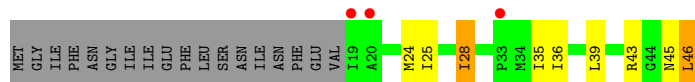
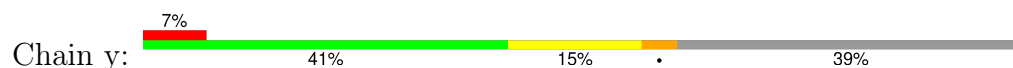




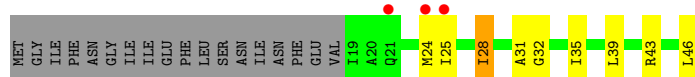
• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein ycf12



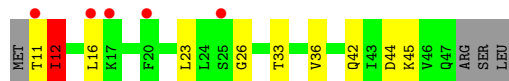
• Molecule 17: Photosystem II reaction center protein ycf12



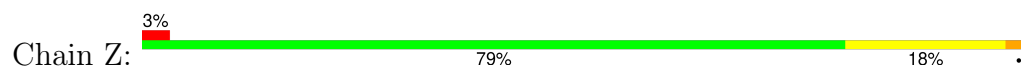
• Molecule 18: Photosystem II reaction center X protein

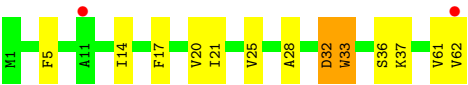


• Molecule 18: Photosystem II reaction center X protein

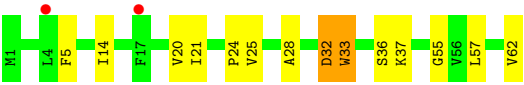
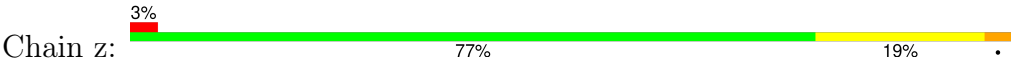


• Molecule 19: Photosystem II reaction center protein Z

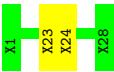




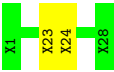
● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II reaction center protein Y



● 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	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.4 (82.97-5.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.285 , 0.313 0.288 , 0.321	Depositor DCC
R_{free} test set	1200 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	3/3700 (0.1%)
1	a	0.38	0/2712	0.86	5/3700 (0.1%)
2	B	0.37	0/3986	0.85	12/5433 (0.2%)
2	b	0.37	0/3986	0.86	8/5433 (0.1%)
3	C	0.37	0/3556	0.82	3/4842 (0.1%)
3	c	0.37	0/3556	0.85	6/4842 (0.1%)
4	D	0.35	0/2801	0.81	2/3818 (0.1%)
4	d	0.36	0/2801	0.84	0/3818
5	E	0.37	0/685	0.88	3/933 (0.3%)
5	e	0.37	0/685	0.89	0/933
6	F	0.46	0/291	0.83	0/397
6	f	0.46	0/291	0.85	0/397
7	H	0.38	0/520	0.74	0/709
7	h	0.38	0/520	0.78	0/709
8	I	0.37	0/293	0.83	0/395
8	i	0.37	0/293	0.88	0/395
9	J	0.39	0/255	0.91	0/346
9	j	0.38	0/255	0.90	0/346
10	K	0.51	0/303	0.91	1/416 (0.2%)
10	k	0.44	0/303	0.92	0/416
11	L	0.33	0/311	0.76	0/422
11	l	0.33	0/311	0.78	0/422
12	M	0.55	0/270	1.08	0/367
12	m	0.53	0/270	1.10	0/367
13	O	0.35	0/1876	0.74	0/2548
13	o	0.36	0/1876	0.77	4/2548 (0.2%)
14	T	0.40	0/284	0.83	0/381
14	t	0.37	0/284	0.81	0/381
15	U	0.35	0/785	0.83	0/1064
15	u	0.43	0/785	0.89	0/1064
16	V	0.39	0/1081	0.85	2/1468 (0.1%)
16	v	0.37	0/1081	0.82	4/1468 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.40	0/202	0.86	0/272
17	y	0.38	0/202	0.84	0/272
18	X	0.47	0/273	0.87	0/370
18	x	0.50	0/273	0.88	0/370
19	Z	0.37	0/490	0.86	0/669
19	z	0.35	0/490	0.88	0/669
All	All	0.38	0/41948	0.84	53/57100 (0.1%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.73	133.25	119.84
2	b	483	ASP	C-N-CA	10.73	133.25	119.84
2	B	483	ASP	CA-C-N	10.40	132.84	119.84
2	B	483	ASP	C-N-CA	10.40	132.84	119.84
2	B	413	ASP	CA-C-N	6.75	127.33	120.38

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	85	0
1	a	2627	0	2524	91	0
2	B	3850	0	3718	95	0
2	b	3850	0	3718	90	0
3	C	3444	0	3365	86	0
3	c	3444	0	3365	90	0
4	D	2706	0	2608	72	0
4	d	2706	0	2608	71	0
5	E	666	0	651	16	0
5	e	666	0	651	20	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	8	0
7	H	507	0	521	15	0
7	h	507	0	521	15	0
8	I	286	0	308	2	0
8	i	286	0	308	3	0
9	J	249	0	262	6	0
9	j	249	0	262	8	0
10	K	293	0	305	18	0
10	k	293	0	305	11	0
11	L	304	0	316	10	0
11	l	304	0	316	7	0
12	M	267	0	289	13	0
12	m	267	0	289	16	0
13	O	1845	0	1801	36	0
13	o	1845	0	1801	32	0
14	T	275	0	288	11	0
14	t	275	0	288	11	0
15	U	774	0	773	9	0
15	u	774	0	773	13	0
16	V	1060	0	1068	12	0
16	v	1060	0	1068	12	0
17	g	201	0	226	8	0
17	y	201	0	226	6	0
18	X	270	0	299	10	0
18	x	270	0	299	8	0
19	Z	479	0	516	12	0
19	z	479	0	516	11	0
20	G	140	0	32	1	0
20	Y	140	0	32	1	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	25	0
23	B	1040	0	1152	75	0
23	C	845	0	936	46	0
23	D	130	0	144	9	0
23	a	260	0	288	34	0
23	b	1040	0	1152	70	0
23	c	845	0	936	41	0
23	d	130	0	144	9	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	6	0
24	a	128	0	148	13	0
25	A	45	0	61	2	0
25	D	55	0	80	6	0
25	J	35	0	45	0	0
25	a	45	0	61	5	0
25	d	55	0	80	9	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	6	0
27	B	160	0	224	22	0
27	C	120	0	168	14	0
27	D	40	0	56	3	0
27	H	40	0	56	3	0
27	J	40	0	56	3	0
27	T	80	0	112	15	0
27	a	40	0	56	7	0
27	b	80	0	112	8	0
27	c	80	0	112	14	0
27	d	40	0	56	2	0
27	h	40	0	56	4	0
27	j	40	0	56	4	0
27	k	40	0	56	8	0
27	y	40	0	56	6	0
27	z	40	0	56	3	0
28	A	56	0	70	1	0
28	B	110	0	136	2	0
28	C	181	0	245	15	0
28	D	63	0	87	1	0
28	a	56	0	70	2	0
28	b	110	0	136	5	0
28	c	181	0	244	14	0
28	d	63	0	87	1	0
29	A	76	0	95	7	0
29	a	76	0	95	5	0
30	A	105	0	147	11	0
30	B	47	0	61	2	0
30	D	43	0	50	4	0
30	F	45	0	54	2	0
30	a	105	0	147	10	0
30	b	47	0	61	4	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	125	5	0
31	B	98	0	135	8	0
31	C	93	0	126	5	0
31	D	94	0	126	4	0
31	E	44	0	58	1	0
31	I	43	0	55	2	0
31	M	42	0	53	4	0
31	a	93	0	124	6	0
31	b	98	0	135	8	0
31	c	45	0	59	2	0
31	d	94	0	126	8	0
31	e	44	0	58	1	0
31	i	43	0	55	3	0
31	k	48	0	66	3	0
31	m	42	0	53	4	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	B	140	0	184	5	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	1	0
33	b	140	0	184	5	0
33	d	31	0	35	1	0
33	i	35	0	46	2	0
33	m	35	0	46	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	5	0
34	v	43	0	30	4	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	51361	1211	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 1211 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)
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.54	0.88
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.57	0.86
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.57	0.86
27:T:101:BCR:H383	30:b:601:SQD:H92	1.57	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.58	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%)	17 (5%)	5 (2%)	8	39
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	10	43
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	12	48
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	12	48
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	9	42
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	9	42
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	21	59
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	21	59
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	42
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	42
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%)	4 (12%)	2 (6%)	1	12
8	i	33/38 (87%)	28 (85%)	4 (12%)	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	22
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	1	12
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%)	34 (97%)	1 (3%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	206 (86%)	31 (13%)	4 (2%)	7	36
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	7	36
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
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%)	125 (93%)	10 (7%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
17	y	26/46 (56%)	19 (73%)	6 (23%)	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%)	5 (8%)	1 (2%)	7	36
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	1	15
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	8	39

5 of 79 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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	55
1	a	271/291 (93%)	262 (97%)	9 (3%)	33	55
2	B	390/407 (96%)	378 (97%)	12 (3%)	35	56
2	b	390/407 (96%)	377 (97%)	13 (3%)	33	55
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%)	260 (94%)	15 (6%)	19	41
4	d	275/283 (97%)	259 (94%)	16 (6%)	18	39
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%)	51 (96%)	2 (4%)	29	50
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	58
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	58
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	68	77
13	o	202/228 (89%)	199 (98%)	3 (2%)	57	71

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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%)	82 (98%)	2 (2%)	43	63
15	u	84/112 (75%)	81 (96%)	3 (4%)	31	52
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%)	17 (85%)	3 (15%)	3	12
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%)	4087 (96%)	157 (4%)	30	51

5 of 157 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	80	LEU
17	g	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	409	GLN
4	d	250	ASN
3	c	44	ASN
3	c	229	ASN
4	d	301	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	PL9	j	101	-	35,35,55	1.21	5 (14%)	44,45,69	1.55	8 (18%)
24	PHO	a	408	-	58,69,69	2.16	9 (15%)	55,99,99	1.41	6 (10%)
27	BCR	J	102	-	41,41,41	0.75	0	56,56,56	3.44	25 (44%)
33	LMT	m	101	-	36,36,36	0.42	0	47,47,47	0.66	0
23	CLA	A	404	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
23	CLA	c	504	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	4 (4%)
23	CLA	D	403	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
23	CLA	C	511	3	69,73,73	1.19	6 (8%)	82,113,113	1.37	6 (7%)
23	CLA	B	605	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)
23	CLA	c	506	-	69,73,73	1.19	5 (7%)	82,113,113	1.33	6 (7%)
31	LMG	B	622	-	49,49,55	1.14	7 (14%)	57,57,63	1.30	6 (10%)
28	DGD	d	409	-	64,64,67	1.14	6 (9%)	78,78,81	1.41	10 (12%)
28	DGD	c	518	-	67,67,67	1.11	6 (8%)	81,81,81	1.45	13 (16%)
23	CLA	C	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	5 (6%)
28	DGD	C	517	-	54,54,67	1.22	6 (11%)	68,68,81	1.24	5 (7%)
30	SQD	B	626	-	45,47,54	1.03	3 (6%)	55,58,65	1.49	9 (16%)
31	LMG	A	414	-	51,51,55	1.15	6 (11%)	59,59,63	1.34	5 (8%)
28	DGD	D	409	-	64,64,67	1.15	6 (9%)	78,78,81	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMT	b	627	-	36,36,36	0.44	0	47,47,47	0.66	1 (2%)
27	BCR	C	516	-	41,41,41	0.70	0	56,56,56	1.96	15 (26%)
27	BCR	T	102	-	41,41,41	0.71	0	56,56,56	2.27	17 (30%)
23	CLA	B	616	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
23	CLA	b	611	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
23	CLA	B	614	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
30	SQD	F	102	-	43,45,54	1.04	2 (4%)	53,56,65	1.60	10 (18%)
23	CLA	a	404	-	69,73,73	1.21	7 (10%)	82,113,113	1.34	6 (7%)
29	LHG	a	417	-	36,36,48	1.09	2 (5%)	39,42,54	1.02	2 (5%)
27	BCR	y	101	-	41,41,41	0.74	0	56,56,56	1.95	13 (23%)
31	LMG	d	406	-	46,46,55	1.19	7 (15%)	54,54,63	1.32	6 (11%)
28	DGD	B	627	-	53,53,67	1.22	6 (11%)	67,67,81	1.42	9 (13%)
23	CLA	b	608	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	6 (7%)
23	CLA	A	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	7 (8%)
23	CLA	b	616	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	4 (4%)
33	LMT	D	410	-	32,32,36	0.51	1 (3%)	43,43,47	0.71	1 (2%)
33	LMT	B	629	-	36,36,36	0.46	0	47,47,47	0.66	0
27	BCR	B	619	-	41,41,41	0.67	0	56,56,56	1.87	15 (26%)
27	BCR	c	514	-	41,41,41	0.71	0	56,56,56	2.39	20 (35%)
23	CLA	B	607	-	69,73,73	1.16	6 (8%)	82,113,113	1.38	7 (8%)
33	LMT	B	628	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
23	CLA	c	502	-	69,73,73	1.19	10 (14%)	82,113,113	1.31	7 (8%)
23	CLA	c	510	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
27	BCR	A	410	-	41,41,41	0.73	0	56,56,56	1.89	11 (19%)
31	LMG	a	416	-	51,51,55	1.12	6 (11%)	59,59,63	1.38	6 (10%)
30	SQD	A	417	-	52,54,54	1.01	5 (9%)	62,65,65	1.60	11 (17%)
22	BCT	d	401	21	3,3,3	0.62	0	2,3,3	0.26	0
27	BCR	C	514	-	41,41,41	0.75	0	56,56,56	2.37	22 (39%)
23	CLA	B	603	-	69,73,73	1.19	8 (11%)	82,113,113	1.27	4 (4%)
33	LMT	b	604	-	36,36,36	0.40	0	47,47,47	0.64	0
30	SQD	b	601	-	45,47,54	1.02	3 (6%)	55,58,65	1.53	9 (16%)
23	CLA	C	506	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	5 (6%)
28	DGD	C	519	-	67,67,67	1.12	7 (10%)	81,81,81	1.41	9 (11%)
30	SQD	a	401	-	52,54,54	1.00	5 (9%)	62,65,65	1.63	10 (16%)
23	CLA	B	611	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	D	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	6 (7%)
27	BCR	k	102	-	41,41,41	0.74	0	56,56,56	1.97	16 (28%)
25	PL9	d	404	-	55,55,55	1.27	8 (14%)	68,69,69	1.72	19 (27%)
27	BCR	z	101	-	41,41,41	0.63	0	56,56,56	1.85	13 (23%)
23	CLA	c	501	-	69,73,73	1.17	6 (8%)	82,113,113	1.30	6 (7%)
27	BCR	d	405	-	41,41,41	0.67	0	56,56,56	2.17	17 (30%)
25	PL9	J	101	-	35,35,55	1.22	5 (14%)	44,45,69	1.56	7 (15%)
31	LMG	d	407	-	48,48,55	1.17	8 (16%)	56,56,63	1.48	7 (12%)
23	CLA	a	409	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
31	LMG	C	520	-	48,48,55	1.13	6 (12%)	56,56,63	1.30	5 (8%)
25	PL9	D	404	-	55,55,55	1.28	8 (14%)	68,69,69	1.64	16 (23%)
24	PHO	D	402	-	58,69,69	2.18	10 (17%)	55,99,99	1.48	6 (10%)
30	SQD	D	408	-	41,43,54	1.12	4 (9%)	51,54,65	1.93	10 (19%)
31	LMG	m	102	-	42,42,55	1.34	7 (16%)	50,50,63	1.56	7 (14%)
28	DGD	c	516	-	54,54,67	1.24	5 (9%)	68,68,81	1.26	8 (11%)
23	CLA	b	619	-	69,73,73	1.17	6 (8%)	82,113,113	1.29	6 (7%)
23	CLA	B	610	-	69,73,73	1.19	7 (10%)	82,113,113	1.28	7 (8%)
30	SQD	A	413	-	49,51,54	0.98	4 (8%)	59,62,65	1.47	10 (16%)
23	CLA	C	513	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	a	406	-	69,73,73	1.18	6 (8%)	82,113,113	1.36	7 (8%)
28	DGD	a	413	-	57,57,67	1.20	7 (12%)	71,71,81	1.49	12 (16%)
23	CLA	C	503	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
23	CLA	C	502	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
31	LMG	i	101	-	43,43,55	1.27	7 (16%)	51,51,63	1.30	7 (13%)
27	BCR	H	101	-	41,41,41	0.70	0	56,56,56	1.76	16 (28%)
31	LMG	a	402	-	42,42,55	1.23	6 (14%)	50,50,63	1.51	9 (18%)
33	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
28	DGD	C	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.26	7 (9%)
28	DGD	B	621	-	59,59,67	1.23	9 (15%)	73,73,81	1.09	5 (6%)
23	CLA	C	508	-	69,73,73	1.19	8 (11%)	82,113,113	1.27	5 (6%)
31	LMG	E	101	-	44,44,55	1.19	6 (13%)	52,52,63	1.33	8 (15%)
23	CLA	b	620	-	69,73,73	1.19	9 (13%)	82,113,113	1.21	5 (6%)
23	CLA	B	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.19	4 (4%)
27	BCR	b	621	-	41,41,41	0.64	0	56,56,56	1.97	16 (28%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	B	623	-	49,49,55	1.19	7 (14%)	57,57,63	1.38	8 (14%)
33	LMT	i	102	-	36,36,36	0.48	1 (2%)	47,47,47	0.68	1 (2%)
31	LMG	D	407	-	48,48,55	1.18	8 (16%)	56,56,63	1.41	7 (12%)
24	PHO	a	407	-	58,69,69	2.14	11 (18%)	55,99,99	1.49	5 (9%)
28	DGD	b	623	-	59,59,67	1.21	9 (15%)	73,73,81	1.13	6 (8%)
23	CLA	B	615	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
33	LMT	B	624	-	36,36,36	0.42	0	47,47,47	0.70	0
23	CLA	b	609	-	69,73,73	1.17	6 (8%)	82,113,113	1.24	5 (6%)
23	CLA	d	403	-	69,73,73	1.20	6 (8%)	82,113,113	1.27	5 (6%)
23	CLA	A	403	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
23	CLA	c	507	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	6 (7%)
34	HEM	v	201	16	50,50,50	2.01	11 (22%)	67,82,82	1.39	5 (7%)
23	CLA	b	607	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
24	PHO	A	406	-	58,69,69	2.20	9 (15%)	55,99,99	1.55	8 (14%)
29	LHG	A	412	-	38,38,48	1.05	2 (5%)	41,44,54	1.00	2 (4%)
23	CLA	B	606	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
34	HEM	V	201	16	50,50,50	1.92	11 (22%)	67,82,82	1.27	1 (1%)
23	CLA	C	501	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	6 (7%)
23	CLA	c	513	-	69,73,73	1.19	7 (10%)	82,113,113	1.29	6 (7%)
27	BCR	B	617	-	41,41,41	0.71	0	56,56,56	1.86	13 (23%)
23	CLA	c	509	-	69,73,73	1.21	5 (7%)	82,113,113	1.29	5 (6%)
27	BCR	D	405	-	41,41,41	0.65	0	56,56,56	2.20	16 (28%)
23	CLA	A	407	-	69,73,73	1.18	9 (13%)	82,113,113	1.23	5 (6%)
23	CLA	c	512	-	69,73,73	1.19	6 (8%)	82,113,113	1.32	5 (6%)
30	SQD	f	102	-	43,45,54	1.02	2 (4%)	53,56,65	1.61	11 (20%)
29	LHG	A	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.10	2 (5%)
23	CLA	C	510	-	69,73,73	1.21	8 (11%)	82,113,113	1.26	5 (6%)
31	LMG	b	625	-	49,49,55	1.18	7 (14%)	57,57,63	1.41	9 (15%)
33	LMT	M	102	-	36,36,36	0.44	0	47,47,47	0.68	0
31	LMG	I	101	-	43,43,55	1.26	8 (18%)	51,51,63	1.31	8 (15%)
33	LMT	d	410	-	32,32,36	0.49	1 (3%)	43,43,47	0.70	1 (2%)
23	CLA	b	617	-	69,73,73	1.18	7 (10%)	82,113,113	1.36	6 (7%)
31	LMG	e	101	-	44,44,55	1.21	7 (15%)	52,52,63	1.35	9 (17%)
23	CLA	b	605	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	6 (7%)
23	CLA	C	509	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
33	LMT	I	102	-	36,36,36	0.43	0	47,47,47	0.68	1 (2%)
23	CLA	c	503	-	69,73,73	1.20	6 (8%)	82,113,113	1.22	5 (6%)
23	CLA	b	606	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
28	DGD	b	602	-	53,53,67	1.23	6 (11%)	67,67,81	1.36	8 (11%)
23	CLA	c	508	-	69,73,73	1.19	7 (10%)	82,113,113	1.31	6 (7%)
23	CLA	B	608	-	69,73,73	1.20	8 (11%)	82,113,113	1.28	6 (7%)
23	CLA	a	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.35	8 (9%)
27	BCR	T	101	-	41,41,41	0.71	0	56,56,56	1.79	12 (21%)
23	CLA	c	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
27	BCR	C	515	-	41,41,41	0.63	0	56,56,56	1.92	16 (28%)
23	CLA	c	511	-	69,73,73	1.22	5 (7%)	82,113,113	1.28	6 (7%)
31	LMG	c	519	-	45,45,55	1.21	7 (15%)	53,53,63	1.32	6 (11%)
23	CLA	C	504	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
23	CLA	B	612	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
23	CLA	b	613	-	69,73,73	1.18	6 (8%)	82,113,113	1.22	7 (8%)
31	LMG	A	418	-	42,42,55	1.23	6 (14%)	50,50,63	1.50	9 (18%)
34	HEM	f	101	6,5	50,50,50	1.96	10 (20%)	67,82,82	1.45	9 (13%)
23	CLA	B	609	-	69,73,73	1.18	5 (7%)	82,113,113	1.28	5 (6%)
33	LMT	b	603	-	36,36,36	0.44	0	47,47,47	0.76	1 (2%)
27	BCR	a	412	-	41,41,41	0.75	0	56,56,56	1.90	12 (21%)
23	CLA	B	601	-	69,73,73	1.21	9 (13%)	82,113,113	1.31	5 (6%)
31	LMG	D	406	-	46,46,55	1.17	7 (15%)	54,54,63	1.38	6 (11%)
23	CLA	b	610	-	69,73,73	1.20	7 (10%)	82,113,113	1.27	5 (6%)
25	PL9	a	410	-	45,45,55	1.27	7 (15%)	56,57,69	1.65	14 (25%)
29	LHG	a	414	-	38,38,48	1.07	2 (5%)	41,44,54	1.01	3 (7%)
23	CLA	b	618	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	4 (4%)
23	CLA	C	507	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	B	604	-	69,73,73	1.19	8 (11%)	82,113,113	1.30	6 (7%)
31	LMG	C	521	-	45,45,55	1.19	7 (15%)	53,53,63	1.36	8 (15%)
30	SQD	d	408	-	41,43,54	1.12	2 (4%)	51,54,65	1.91	10 (19%)
23	CLA	b	615	-	69,73,73	1.20	9 (13%)	82,113,113	1.30	5 (6%)
31	LMG	k	103	-	48,48,55	1.13	6 (12%)	56,56,63	1.27	6 (10%)
27	BCR	c	515	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	c	517	-	63,63,67	1.21	11 (17%)	77,77,81	1.29	7 (9%)
23	CLA	B	602	-	69,73,73	1.18	5 (7%)	82,113,113	1.24	5 (6%)
27	BCR	B	620	-	41,41,41	0.71	0	56,56,56	2.15	17 (30%)
34	HEM	F	101	6,5	50,50,50	1.87	8 (16%)	67,82,82	1.38	6 (8%)
28	DGD	A	411	-	57,57,67	1.23	7 (12%)	71,71,81	1.56	12 (16%)
23	CLA	d	402	-	69,73,73	1.18	5 (7%)	82,113,113	1.35	5 (6%)
22	BCT	A	402	21	3,3,3	0.61	0	2,3,3	0.26	0
27	BCR	b	622	-	41,41,41	0.70	0	56,56,56	2.22	17 (30%)
25	PL9	A	408	-	45,45,55	1.30	7 (15%)	56,57,69	1.58	13 (23%)
30	SQD	a	415	-	49,51,54	0.97	2 (4%)	59,62,65	1.50	10 (16%)
23	CLA	b	614	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
31	LMG	M	101	-	42,42,55	1.28	7 (16%)	50,50,63	1.50	6 (12%)
23	CLA	C	512	-	69,73,73	1.17	5 (7%)	82,113,113	1.33	5 (6%)
27	BCR	B	618	-	41,41,41	0.68	0	56,56,56	2.29	18 (32%)
27	BCR	h	101	-	41,41,41	0.72	0	56,56,56	1.77	14 (25%)
27	BCR	j	102	-	41,41,41	0.72	0	56,56,56	3.44	22 (39%)

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
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
24	PHO	a	408	-	-	13/37/103/103	0/5/6/6
27	BCR	J	102	-	-	6/29/63/63	0/2/2/2
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
23	CLA	A	404	-	1/1/15/20	17/39/115/115	-
23	CLA	c	504	-	1/1/15/20	12/39/115/115	-
23	CLA	D	403	-	1/1/15/20	9/39/115/115	-
23	CLA	C	511	3	1/1/15/20	14/39/115/115	-
23	CLA	B	605	-	1/1/15/20	16/39/115/115	-
23	CLA	c	506	-	1/1/15/20	16/39/115/115	-
31	LMG	B	622	-	-	21/44/64/70	0/1/1/1
28	DGD	d	409	-	-	31/52/92/95	0/2/2/2
28	DGD	c	518	-	-	21/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	-	1/1/15/20	18/39/115/115	-
28	DGD	C	517	-	-	19/42/82/95	0/2/2/2
30	SQD	B	626	-	-	14/42/62/69	0/1/1/1
31	LMG	A	414	-	-	20/46/66/70	0/1/1/1
28	DGD	D	409	-	-	30/52/92/95	0/2/2/2
33	LMT	b	627	-	-	2/21/61/61	0/2/2/2
27	BCR	C	516	-	-	8/29/63/63	0/2/2/2
27	BCR	T	102	-	-	7/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/15/20	19/39/115/115	-
23	CLA	b	611	-	1/1/15/20	9/39/115/115	-
23	CLA	B	614	-	1/1/15/20	14/39/115/115	-
30	SQD	F	102	-	-	17/40/60/69	0/1/1/1
23	CLA	a	404	-	1/1/15/20	8/39/115/115	-
29	LHG	a	417	-	-	13/41/41/53	-
27	BCR	y	101	-	-	8/29/63/63	0/2/2/2
31	LMG	d	406	-	-	10/41/61/70	0/1/1/1
28	DGD	B	627	-	-	17/41/81/95	0/2/2/2
23	CLA	b	608	-	1/1/15/20	9/39/115/115	-
23	CLA	A	405	-	1/1/15/20	12/39/115/115	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
33	LMT	B	629	-	-	3/21/61/61	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
23	CLA	B	607	-	1/1/15/20	9/39/115/115	-
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
23	CLA	c	502	-	1/1/15/20	10/39/115/115	-
23	CLA	c	510	-	1/1/15/20	17/39/115/115	-
27	BCR	A	410	-	-	1/29/63/63	0/2/2/2
31	LMG	a	416	-	-	19/46/66/70	0/1/1/1
30	SQD	A	417	-	-	14/49/69/69	0/1/1/1
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/15/20	16/39/115/115	-
33	LMT	b	604	-	-	3/21/61/61	0/2/2/2
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	506	-	1/1/15/20	18/39/115/115	-
28	DGD	C	519	-	-	22/55/95/95	0/2/2/2
30	SQD	a	401	-	-	17/49/69/69	0/1/1/1
23	CLA	B	611	-	1/1/15/20	11/39/115/115	-
23	CLA	D	401	-	1/1/15/20	13/39/115/115	-
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
27	BCR	z	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	501	-	1/1/15/20	14/39/115/115	-
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2
25	PL9	J	101	-	-	12/29/49/73	0/1/1/1
31	LMG	d	407	-	-	19/43/63/70	0/1/1/1
23	CLA	a	409	-	1/1/15/20	7/39/115/115	-
31	LMG	C	520	-	-	18/43/63/70	0/1/1/1
25	PL9	D	404	-	-	13/53/73/73	0/1/1/1
24	PHO	D	402	-	-	8/37/103/103	0/5/6/6
30	SQD	D	408	-	-	11/38/58/69	0/1/1/1
31	LMG	m	102	-	-	15/37/57/70	0/1/1/1
28	DGD	c	516	-	-	19/42/82/95	0/2/2/2
23	CLA	b	619	-	1/1/15/20	8/39/115/115	-
23	CLA	B	610	-	1/1/15/20	18/39/115/115	-
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
23	CLA	C	513	-	1/1/15/20	17/39/115/115	-
23	CLA	a	406	-	1/1/15/20	11/39/115/115	-
28	DGD	a	413	-	-	12/45/85/95	0/2/2/2
23	CLA	C	503	-	1/1/15/20	14/39/115/115	-
23	CLA	C	502	-	1/1/15/20	11/39/115/115	-
31	LMG	i	101	-	-	20/38/58/70	0/1/1/1
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
31	LMG	a	402	-	-	18/37/57/70	0/1/1/1
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
28	DGD	C	518	-	-	22/51/91/95	0/2/2/2
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
23	CLA	C	508	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
23	CLA	b	620	-	1/1/15/20	19/39/115/115	-
23	CLA	B	613	-	1/1/15/20	15/39/115/115	-
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
31	LMG	b	624	-	-	22/44/64/70	0/1/1/1
31	LMG	B	623	-	-	15/44/64/70	0/1/1/1
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMG	D	407	-	-	20/43/63/70	0/1/1/1
24	PHO	a	407	-	-	11/37/103/103	0/5/6/6
28	DGD	b	623	-	-	19/47/87/95	0/2/2/2
23	CLA	B	615	-	1/1/15/20	10/39/115/115	-
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
23	CLA	b	609	-	1/1/15/20	16/39/115/115	-
23	CLA	d	403	-	1/1/15/20	10/39/115/115	-
23	CLA	A	403	-	1/1/15/20	8/39/115/115	-
23	CLA	c	507	-	1/1/15/20	13/39/115/115	-
34	HEM	v	201	16	-	4/14/54/54	-
23	CLA	b	607	-	1/1/15/20	14/39/115/115	-
24	PHO	A	406	-	-	11/37/103/103	0/5/6/6
29	LHG	A	412	-	-	16/43/43/53	-
23	CLA	B	606	-	1/1/15/20	12/39/115/115	-
34	HEM	V	201	16	-	4/14/54/54	-
23	CLA	C	501	-	1/1/15/20	14/39/115/115	-
23	CLA	c	513	-	1/1/15/20	19/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	18/39/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/15/20	7/39/115/115	-
23	CLA	c	512	-	1/1/15/20	19/39/115/115	-
30	SQD	f	102	-	-	16/40/60/69	0/1/1/1
29	LHG	A	415	-	-	13/41/41/53	-
23	CLA	C	510	-	1/1/15/20	15/39/115/115	-
31	LMG	b	625	-	-	16/44/64/70	0/1/1/1
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	I	101	-	-	20/38/58/70	0/1/1/1
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
23	CLA	b	617	-	1/1/15/20	15/39/115/115	-
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	b	605	-	1/1/15/20	14/39/115/115	-
23	CLA	C	509	-	1/1/15/20	18/39/115/115	-
23	CLA	b	612	-	1/1/15/20	17/39/115/115	-
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
23	CLA	c	503	-	1/1/15/20	14/39/115/115	-
23	CLA	b	606	-	1/1/15/20	15/39/115/115	-
28	DGD	b	602	-	-	18/41/81/95	0/2/2/2
23	CLA	c	508	-	1/1/15/20	13/39/115/115	-
23	CLA	B	608	-	1/1/15/20	17/39/115/115	-
23	CLA	a	405	-	1/1/15/20	16/39/115/115	-
27	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	505	-	1/1/15/20	18/39/115/115	-
27	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	c	511	-	1/1/15/20	13/39/115/115	-
31	LMG	c	519	-	-	21/40/60/70	0/1/1/1
23	CLA	C	504	-	1/1/15/20	12/39/115/115	-
33	LMT	B	625	-	-	2/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	9/39/115/115	-
23	CLA	b	613	-	1/1/15/20	9/39/115/115	-
31	LMG	A	418	-	-	16/37/57/70	0/1/1/1
34	HEM	f	101	6,5	-	3/14/54/54	-
23	CLA	B	609	-	1/1/15/20	8/39/115/115	-
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
27	BCR	a	412	-	-	1/29/63/63	0/2/2/2
23	CLA	B	601	-	1/1/15/20	16/39/115/115	-
31	LMG	D	406	-	-	12/41/61/70	0/1/1/1
23	CLA	b	610	-	1/1/15/20	15/39/115/115	-
25	PL9	a	410	-	-	22/41/61/73	0/1/1/1
29	LHG	a	414	-	-	17/43/43/53	-
23	CLA	b	618	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	507	-	1/1/15/20	9/39/115/115	-
23	CLA	B	604	-	1/1/15/20	11/39/115/115	-
31	LMG	C	521	-	-	20/40/60/70	0/1/1/1
30	SQD	d	408	-	-	12/38/58/69	0/1/1/1
23	CLA	b	615	-	1/1/15/20	12/39/115/115	-
31	LMG	k	103	-	-	18/43/63/70	0/1/1/1
27	BCR	c	515	-	-	8/29/63/63	0/2/2/2
28	DGD	c	517	-	-	23/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	13/39/115/115	-
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
34	HEM	F	101	6,5	-	3/14/54/54	-
28	DGD	A	411	-	-	10/45/85/95	0/2/2/2
23	CLA	d	402	-	1/1/15/20	12/39/115/115	-
27	BCR	b	622	-	-	2/29/63/63	0/2/2/2
25	PL9	A	408	-	-	22/41/61/73	0/1/1/1
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
23	CLA	b	614	-	1/1/15/20	18/39/115/115	-
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
23	CLA	C	512	-	1/1/15/20	19/39/115/115	-
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2

The worst 5 of 903 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C1B-C2B	9.99	1.50	1.39
24	D	402	PHO	C1B-C2B	9.98	1.50	1.39
24	a	408	PHO	C1B-C2B	9.46	1.49	1.39
24	A	406	PHO	C1B-C2B	9.28	1.49	1.39
24	A	406	PHO	C3B-C4B	9.01	1.50	1.41

The worst 5 of 1294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	j	102	BCR	C32-C1-C6	-14.09	88.14	110.24
27	J	102	BCR	C32-C1-C6	-13.79	88.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	102	BCR	C32-C1-C31	-9.11	82.55	108.63
27	j	102	BCR	C32-C1-C31	-9.08	82.62	108.63
27	T	102	BCR	C7-C8-C9	-8.97	112.96	126.23

5 of 70 chirality outliers are listed below:

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

5 of 2110 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-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
23	B	602	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

166 monomers are involved in 561 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	408	PHO	5	0
27	J	102	BCR	3	0
23	A	404	CLA	10	0
23	c	504	CLA	5	0
23	D	403	CLA	2	0
23	C	511	CLA	8	0
23	B	605	CLA	11	0
23	c	506	CLA	3	0
31	B	622	LMG	3	0
28	d	409	DGD	1	0
28	c	518	DGD	4	0
23	C	505	CLA	5	0
28	C	517	DGD	4	0
30	B	626	SQD	2	0
31	A	414	LMG	3	0
28	D	409	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	b	627	LMT	1	0
27	C	516	BCR	4	0
27	T	102	BCR	8	0
23	B	616	CLA	3	0
23	b	611	CLA	9	0
23	B	614	CLA	3	0
30	F	102	SQD	2	0
23	a	404	CLA	16	0
29	a	417	LHG	3	0
27	y	101	BCR	6	0
31	d	406	LMG	2	0
28	B	627	DGD	2	0
23	b	608	CLA	4	0
23	A	405	CLA	3	0
23	b	616	CLA	4	0
33	D	410	LMT	1	0
33	B	629	LMT	2	0
27	B	619	BCR	6	0
27	c	514	BCR	10	0
23	B	607	CLA	9	0
33	B	628	LMT	2	0
23	c	502	CLA	2	0
23	c	510	CLA	3	0
27	A	410	BCR	6	0
31	a	416	LMG	3	0
30	A	417	SQD	7	0
27	C	514	BCR	6	0
23	B	603	CLA	14	0
33	b	604	LMT	1	0
30	b	601	SQD	4	0
23	C	506	CLA	2	0
28	C	519	DGD	5	0
30	a	401	SQD	6	0
23	B	611	CLA	5	0
23	D	401	CLA	7	0
27	k	102	BCR	8	0
25	d	404	PL9	9	0
27	z	101	BCR	3	0
23	c	501	CLA	3	0
27	d	405	BCR	2	0
31	d	407	LMG	6	0
23	a	409	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	520	LMG	3	0
25	D	404	PL9	6	0
24	D	402	PHO	6	0
30	D	408	SQD	4	0
31	m	102	LMG	4	0
28	c	516	DGD	4	0
23	b	619	CLA	4	0
23	B	610	CLA	1	0
30	A	413	SQD	4	0
23	C	513	CLA	4	0
23	a	406	CLA	4	0
28	a	413	DGD	2	0
23	C	503	CLA	4	0
23	C	502	CLA	1	0
31	i	101	LMG	3	0
27	H	101	BCR	3	0
31	a	402	LMG	3	0
33	b	626	LMT	1	0
28	C	518	DGD	6	0
23	C	508	CLA	5	0
31	E	101	LMG	1	0
23	b	620	CLA	5	0
23	B	613	CLA	3	0
27	b	621	BCR	4	0
31	b	624	LMG	3	0
31	B	623	LMG	5	0
33	i	102	LMT	2	0
31	D	407	LMG	4	0
24	a	407	PHO	8	0
28	b	623	DGD	2	0
23	B	615	CLA	1	0
33	B	624	LMT	1	0
23	b	609	CLA	9	0
23	d	403	CLA	3	0
23	A	403	CLA	13	0
23	c	507	CLA	6	0
34	v	201	HEM	4	0
23	b	607	CLA	9	0
24	A	406	PHO	5	0
29	A	412	LHG	4	0
23	B	606	CLA	8	0
34	V	201	HEM	3	0

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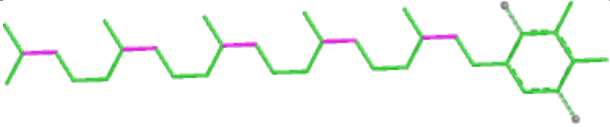
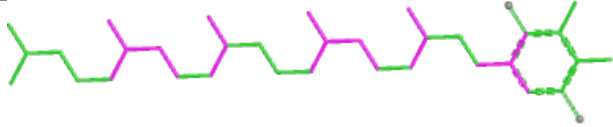
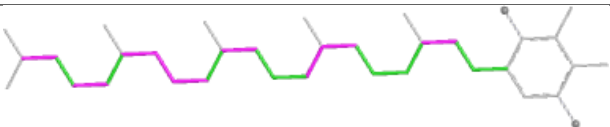
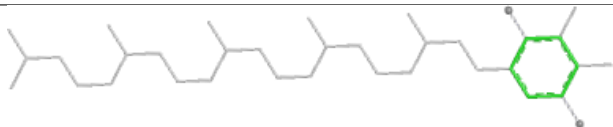
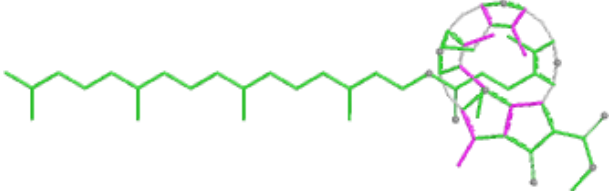
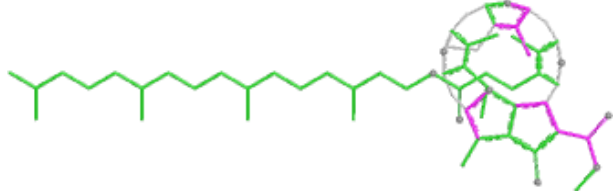
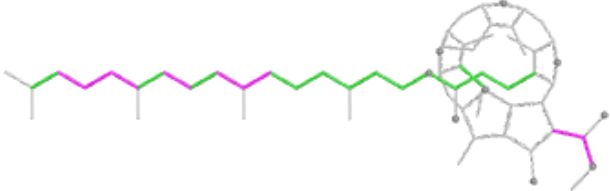
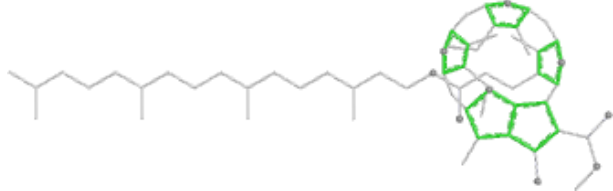
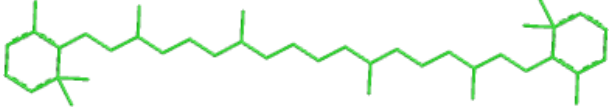
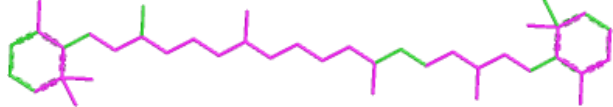
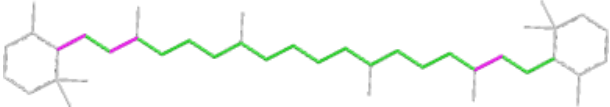
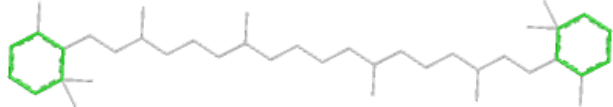
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	501	CLA	3	0
23	c	513	CLA	2	0
27	B	617	BCR	5	0
23	c	509	CLA	2	0
27	D	405	BCR	3	0
23	A	407	CLA	1	0
23	c	512	CLA	3	0
30	f	102	SQD	2	0
29	A	415	LHG	3	0
23	C	510	CLA	5	0
31	b	625	LMG	5	0
33	M	102	LMT	1	0
31	I	101	LMG	2	0
33	d	410	LMT	1	0
23	b	617	CLA	2	0
31	e	101	LMG	1	0
23	b	605	CLA	1	0
23	C	509	CLA	4	0
23	b	612	CLA	8	0
33	I	102	LMT	2	0
23	c	503	CLA	4	0
23	b	606	CLA	7	0
28	b	602	DGD	3	0
23	c	508	CLA	5	0
23	B	608	CLA	8	0
23	a	405	CLA	14	0
27	T	101	BCR	8	0
23	c	505	CLA	4	0
27	C	515	BCR	4	0
23	c	511	CLA	6	0
31	c	519	LMG	2	0
23	C	504	CLA	3	0
23	B	612	CLA	5	0
23	b	613	CLA	4	0
31	A	418	LMG	2	0
34	f	101	HEM	5	0
23	B	609	CLA	4	0
33	b	603	LMT	2	0
27	a	412	BCR	7	0
23	B	601	CLA	2	0
23	b	610	CLA	6	0
25	a	410	PL9	5	0

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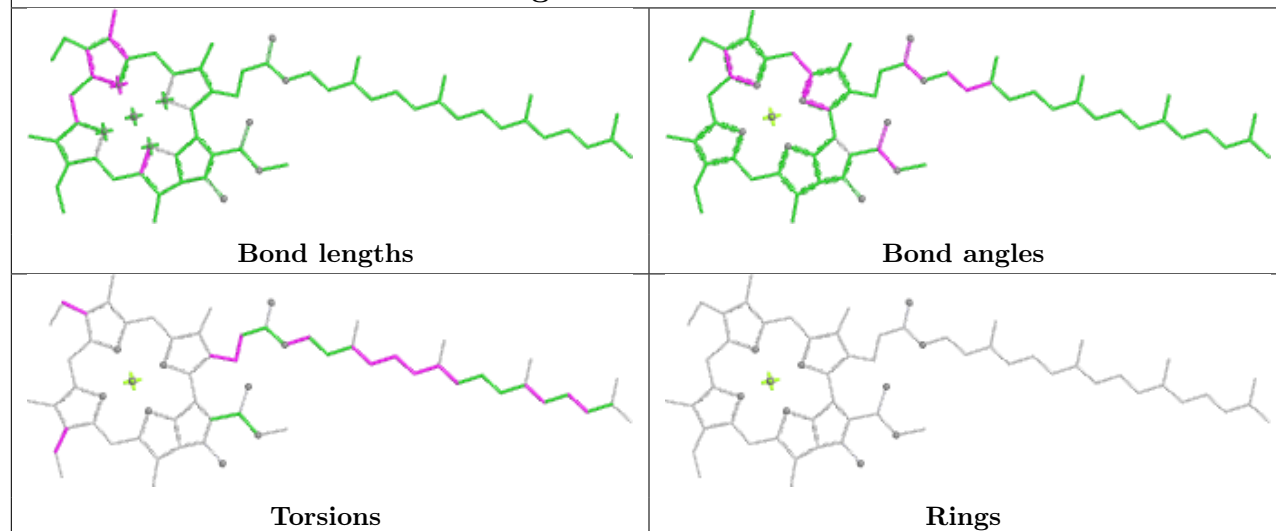
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	414	LHG	2	0
23	b	618	CLA	6	0
23	C	507	CLA	5	0
23	B	604	CLA	8	0
31	C	521	LMG	2	0
30	d	408	SQD	4	0
23	b	615	CLA	4	0
31	k	103	LMG	3	0
27	c	515	BCR	4	0
28	c	517	DGD	6	0
23	B	602	CLA	6	0
27	B	620	BCR	4	0
34	F	101	HEM	4	0
28	A	411	DGD	1	0
23	d	402	CLA	6	0
27	b	622	BCR	4	0
25	A	408	PL9	2	0
30	a	415	SQD	4	0
23	b	614	CLA	2	0
31	M	101	LMG	4	0
23	C	512	CLA	5	0
27	B	618	BCR	10	0
27	h	101	BCR	4	0
27	j	102	BCR	4	0

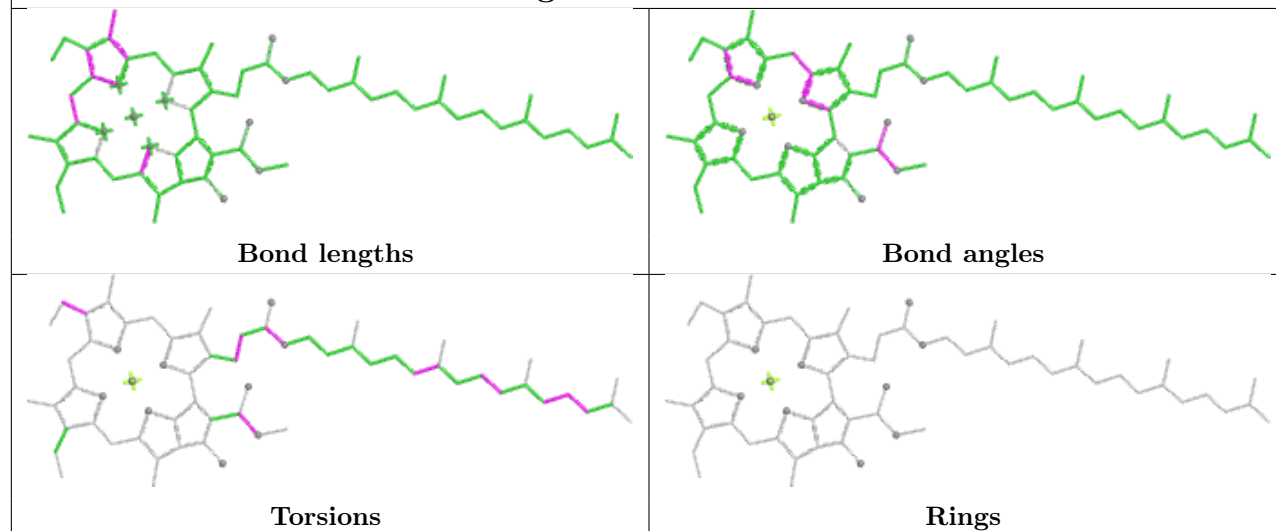
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PL9 j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

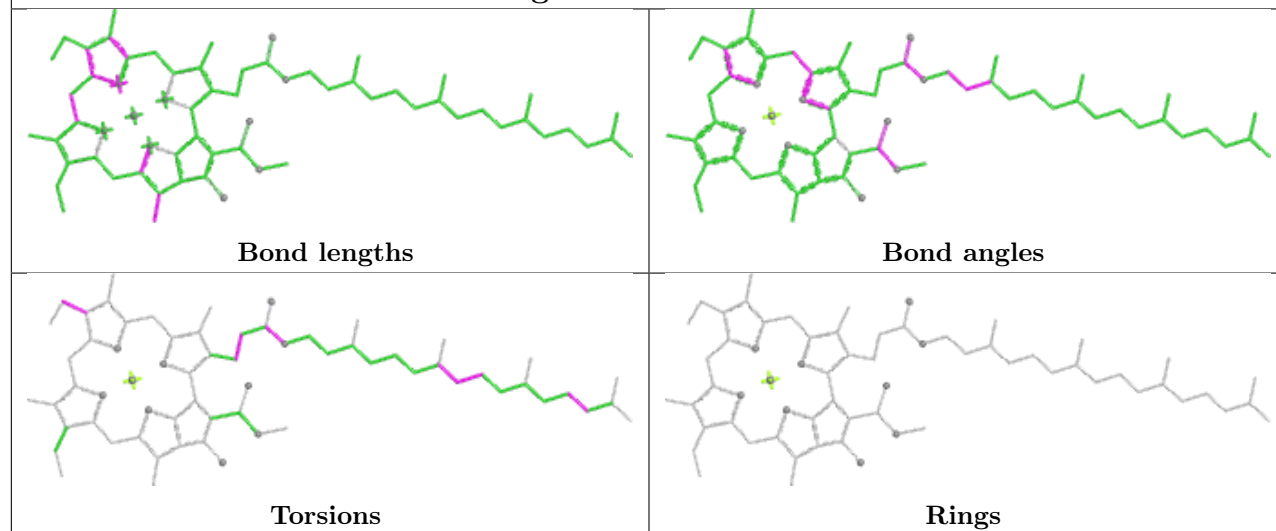
Ligand CLA A 404

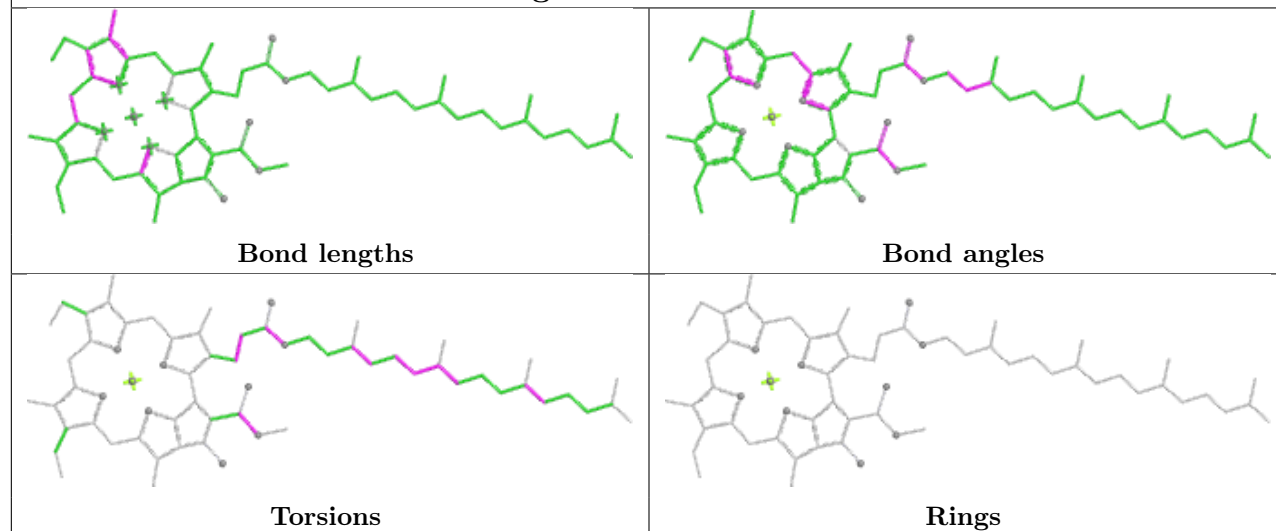
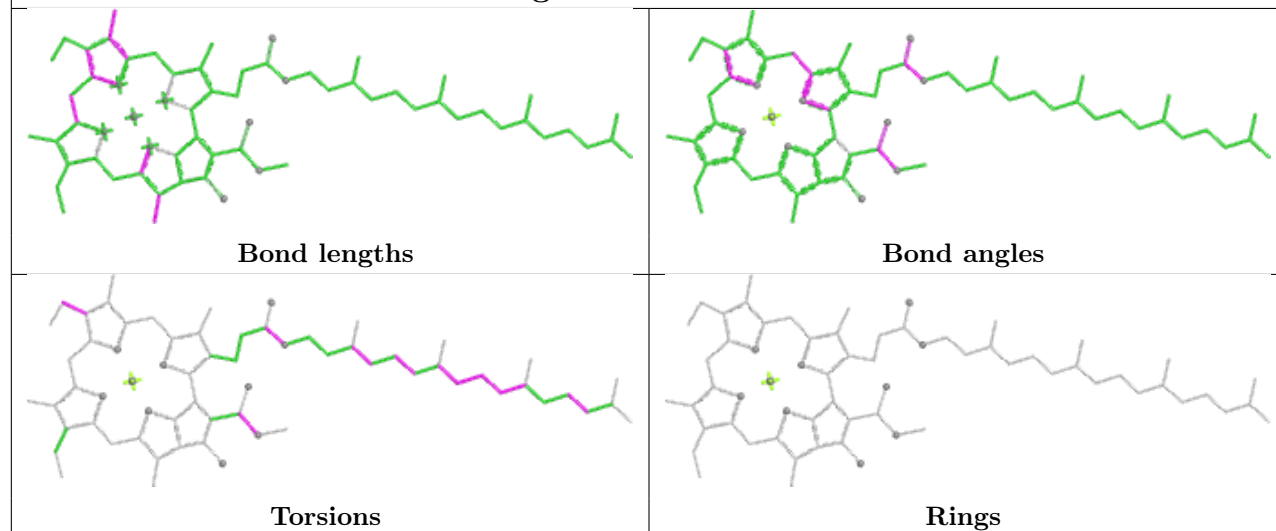
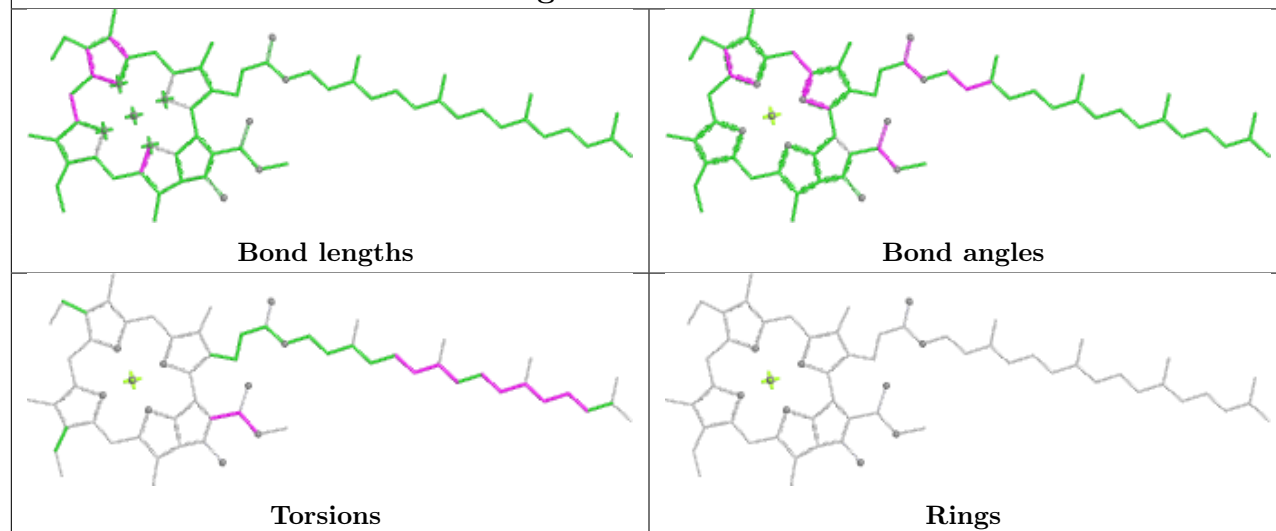


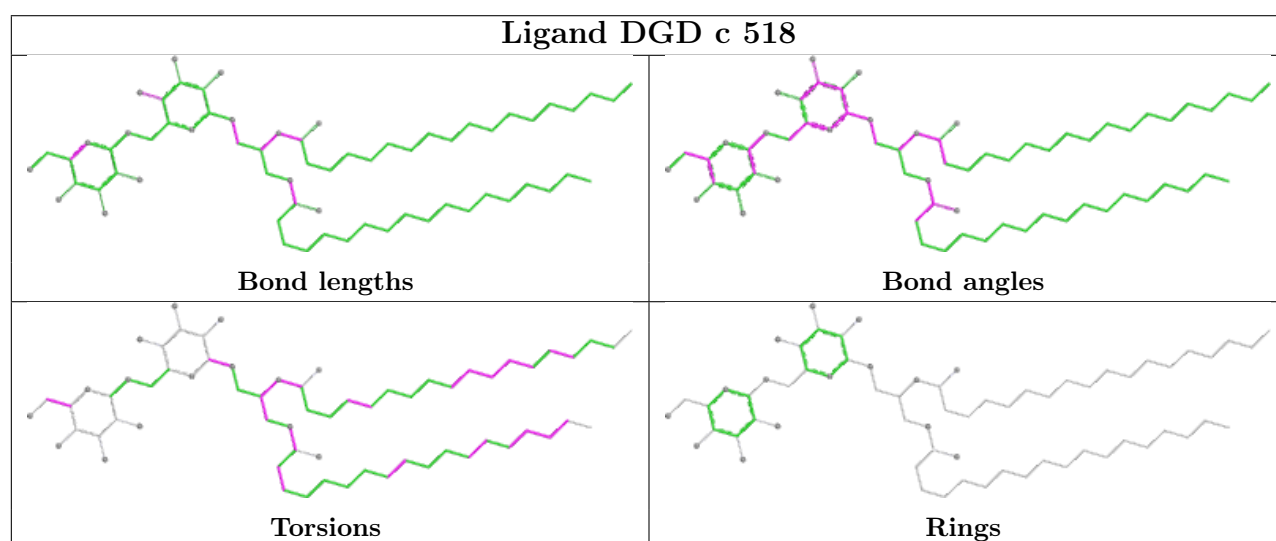
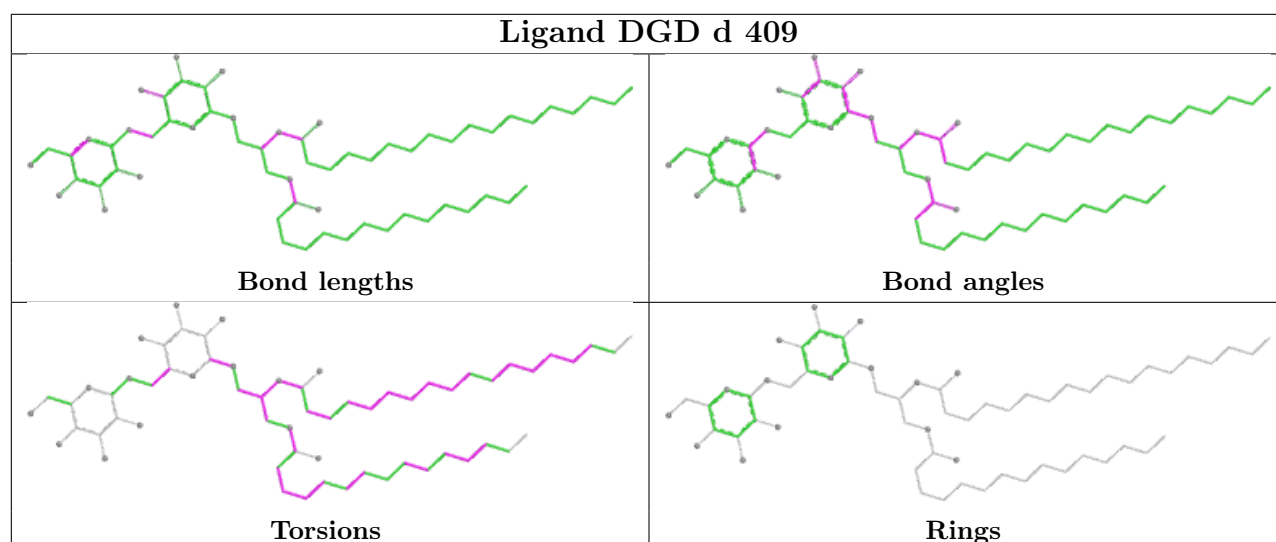
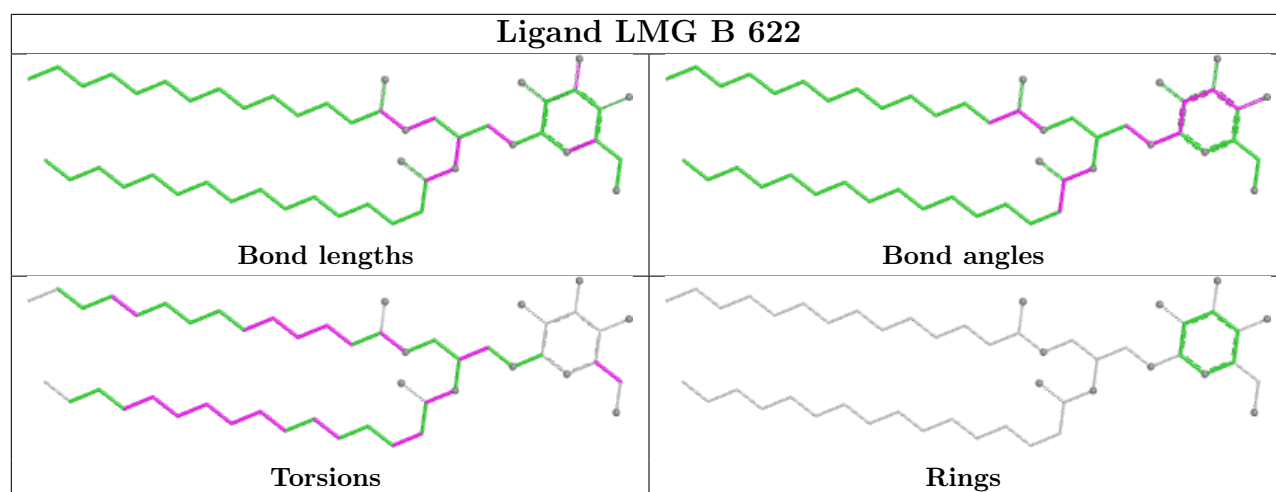
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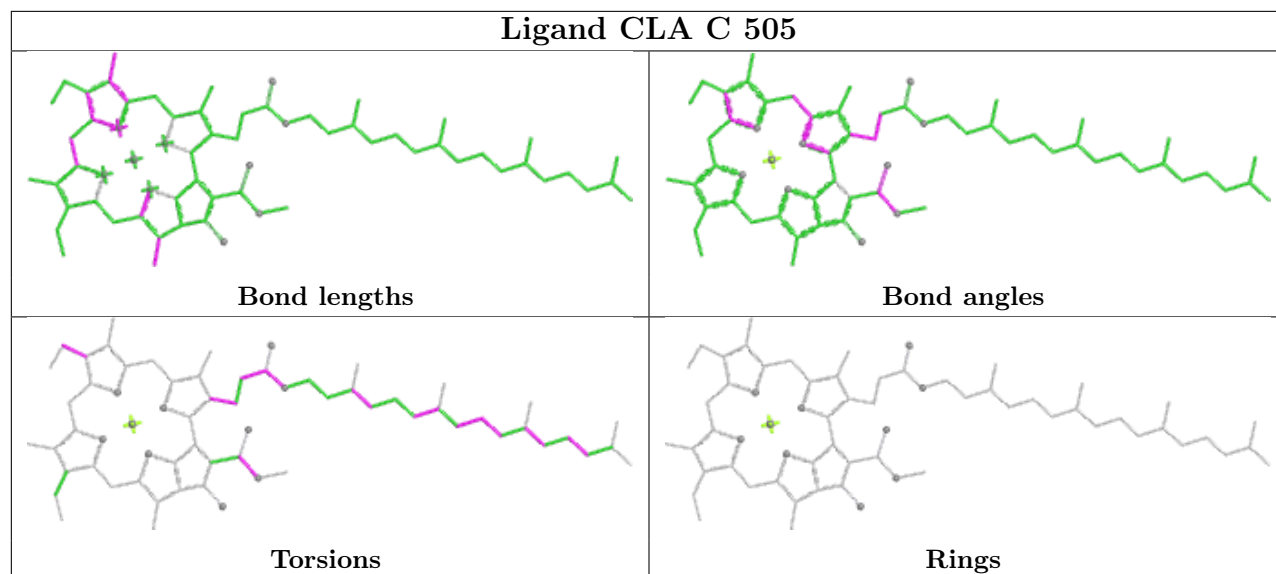
Ligand CLA D 403



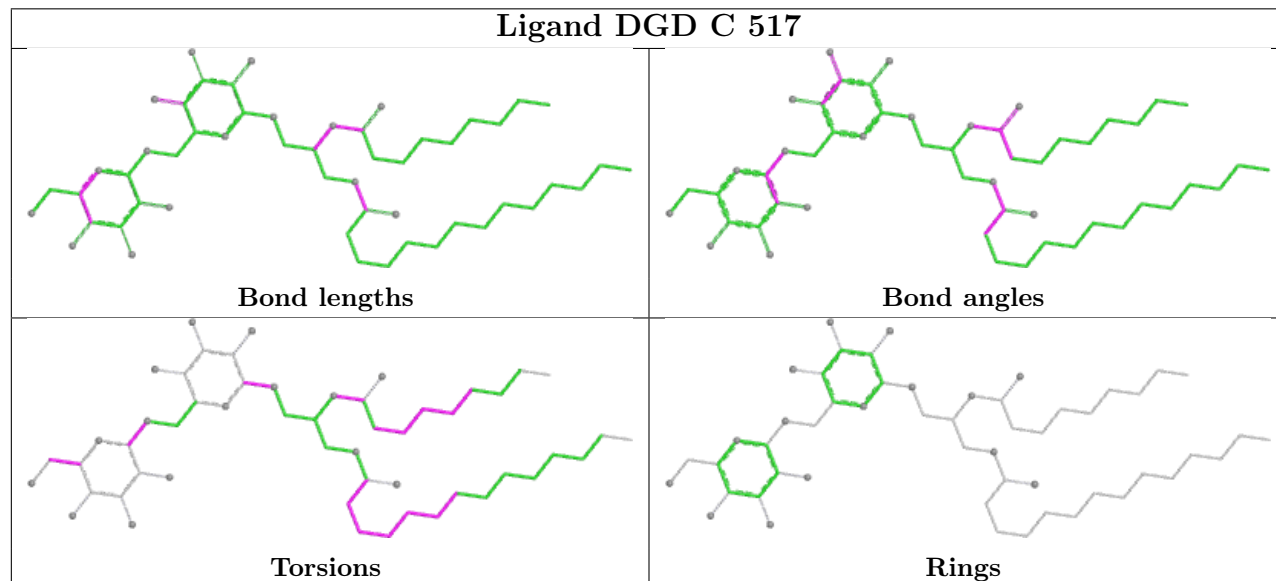
Ligand CLA C 511**Ligand CLA B 605****Ligand CLA c 506**

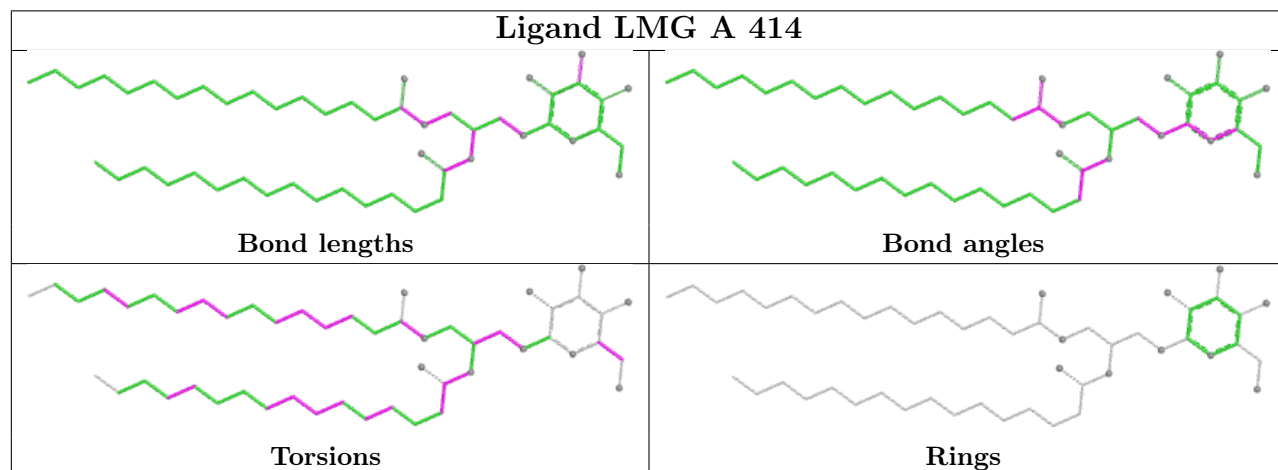
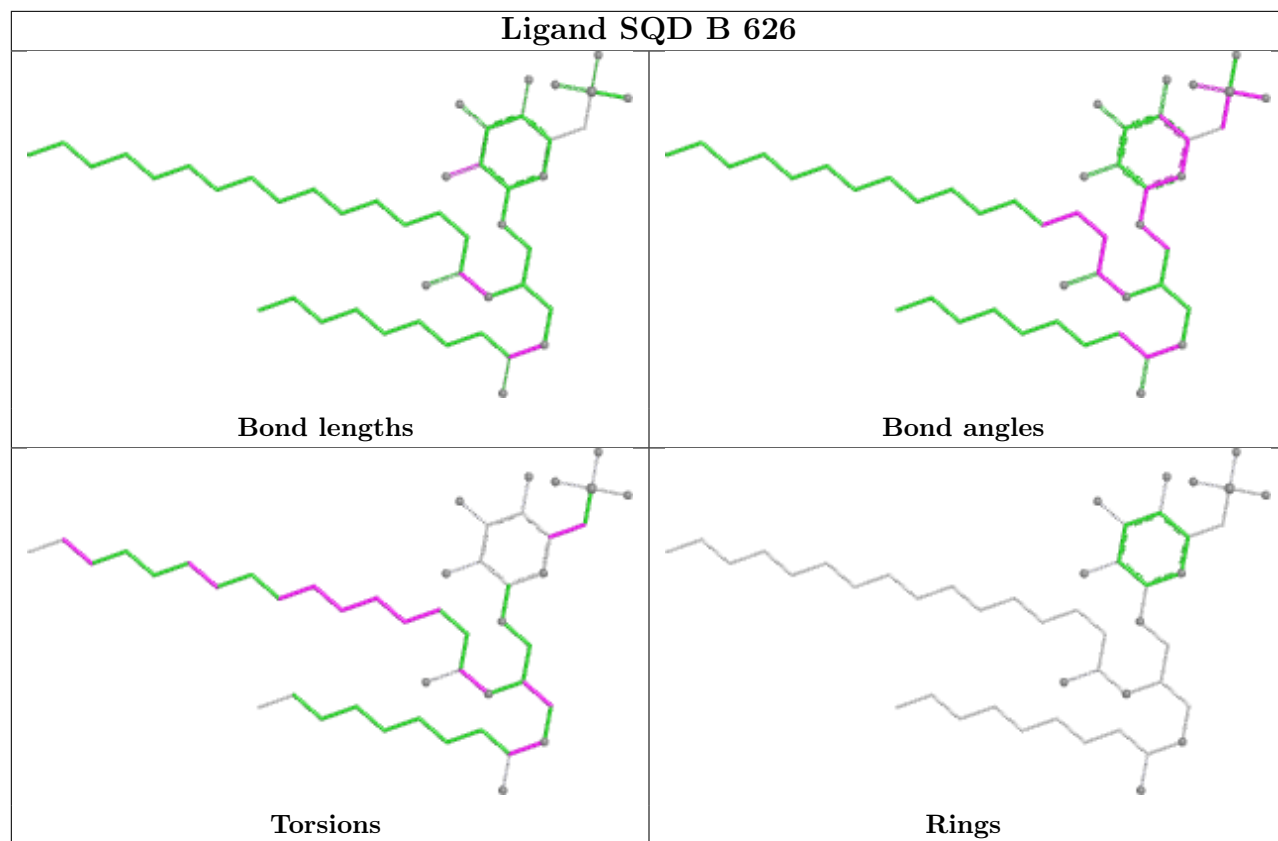


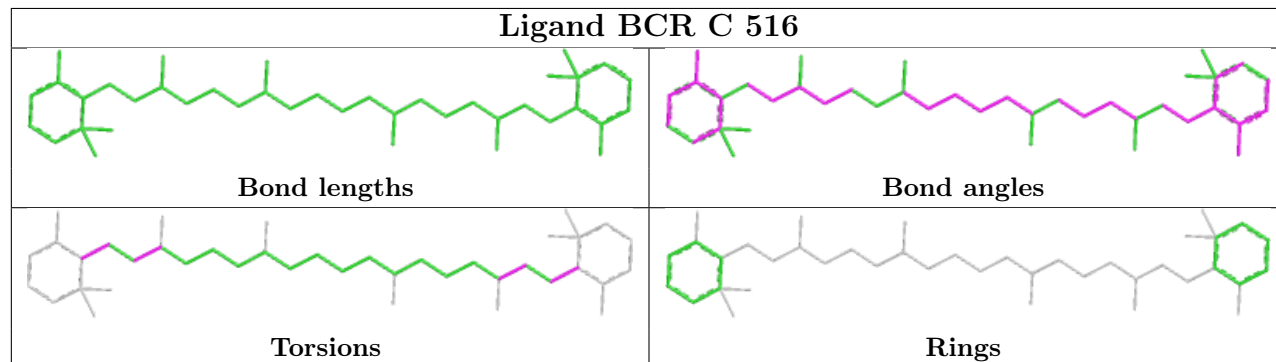
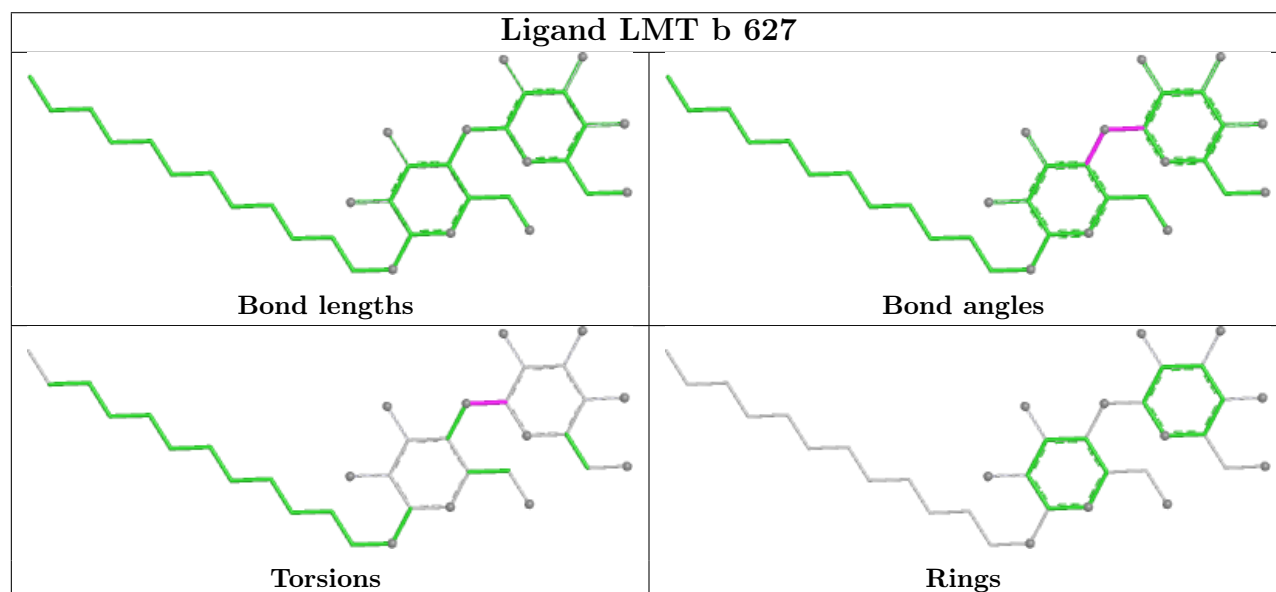
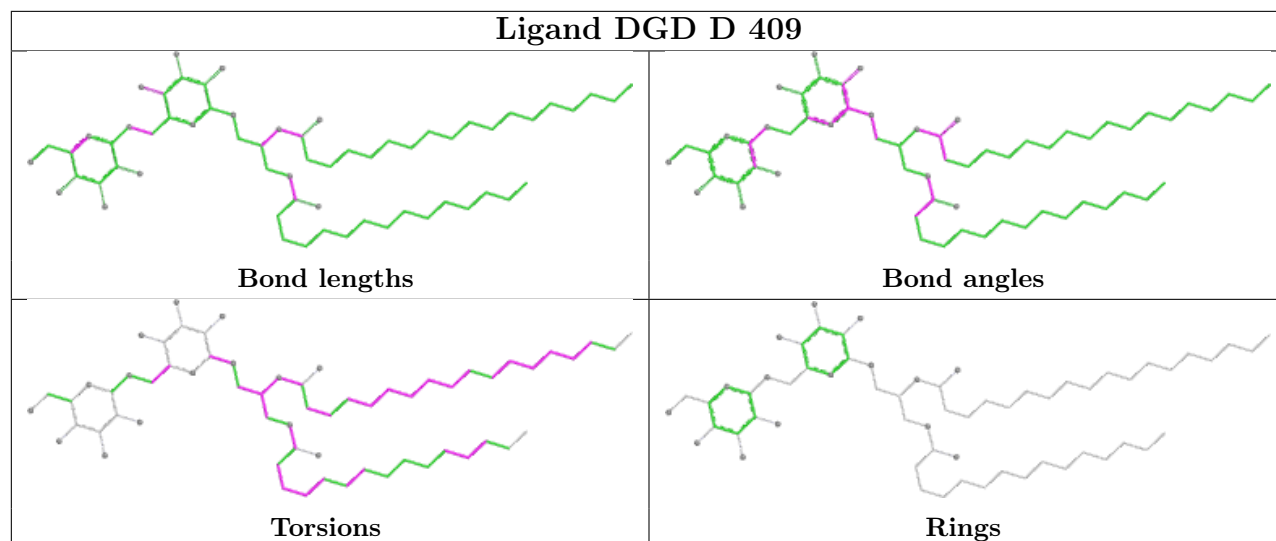
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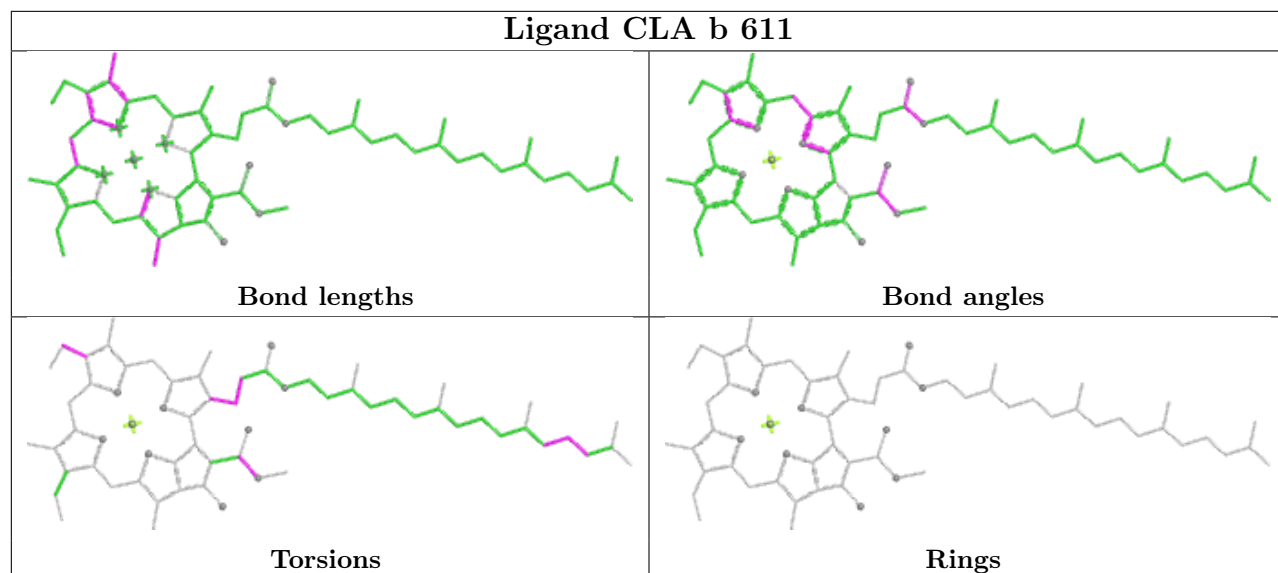
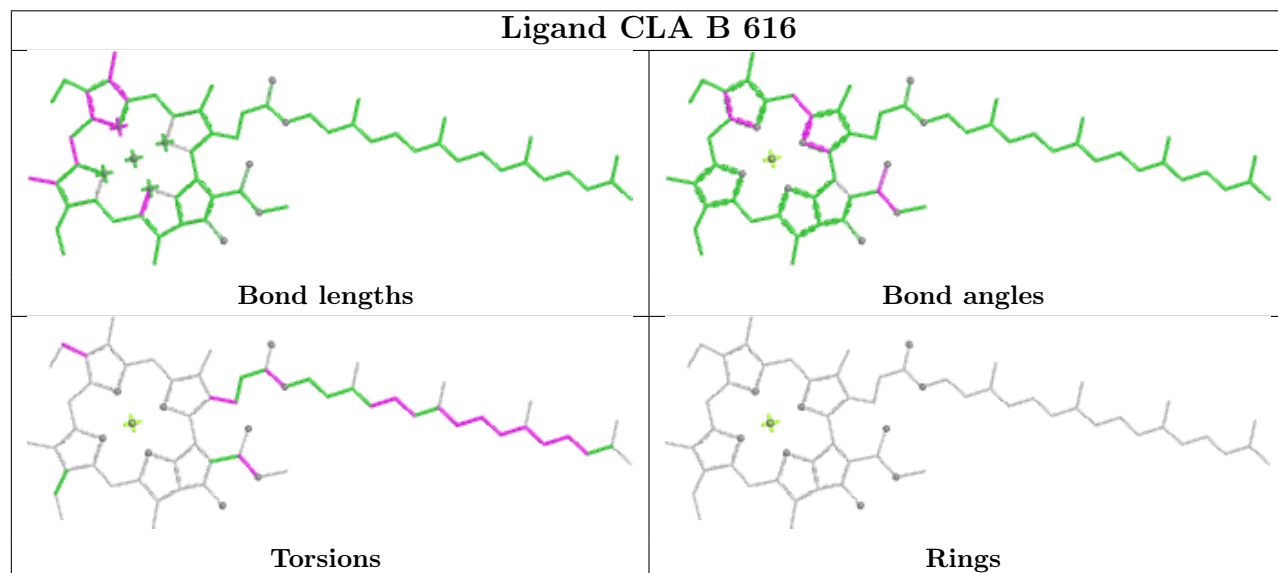
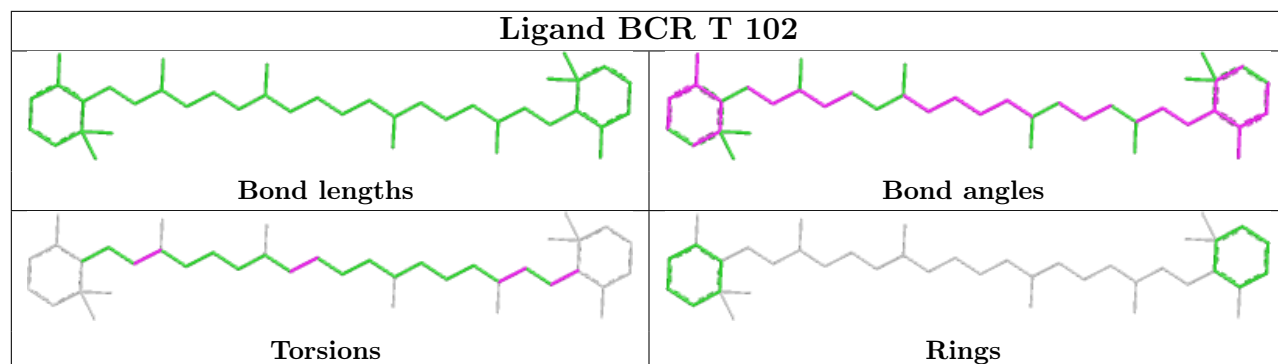


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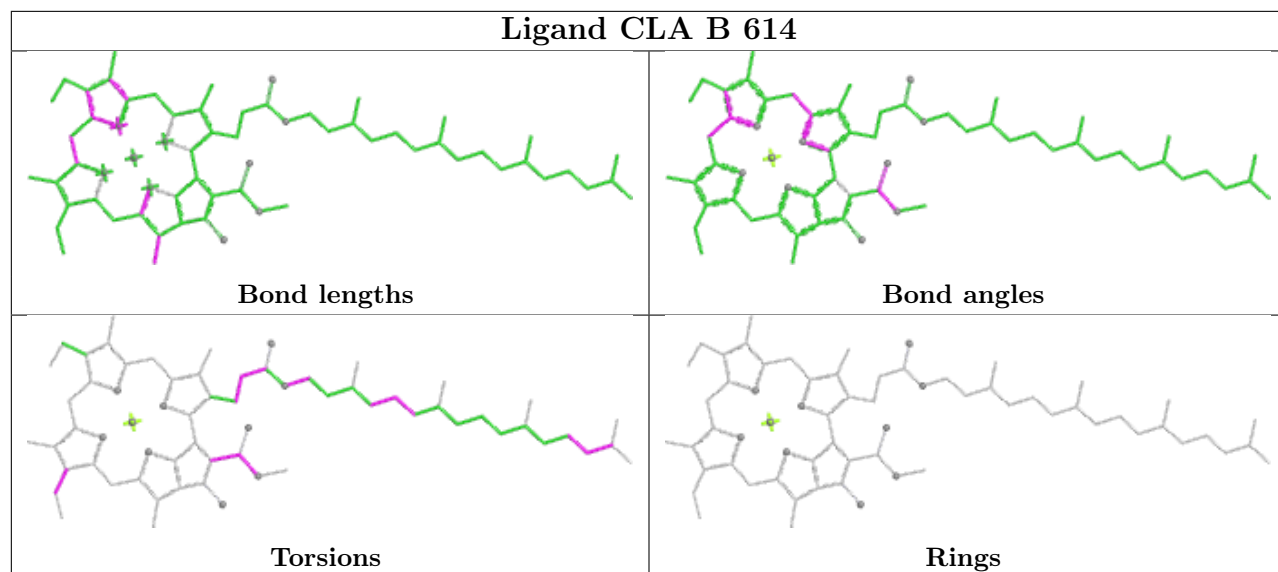




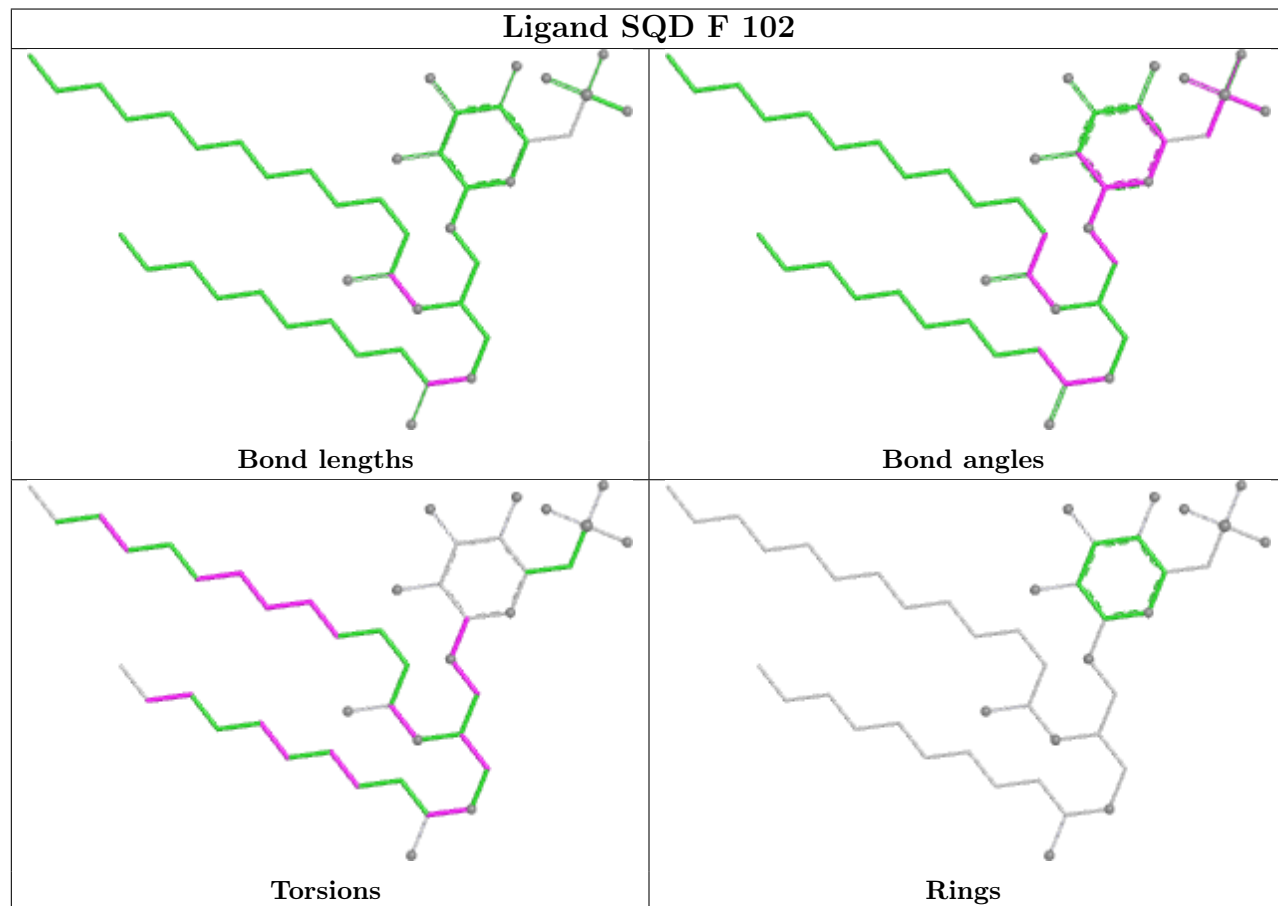




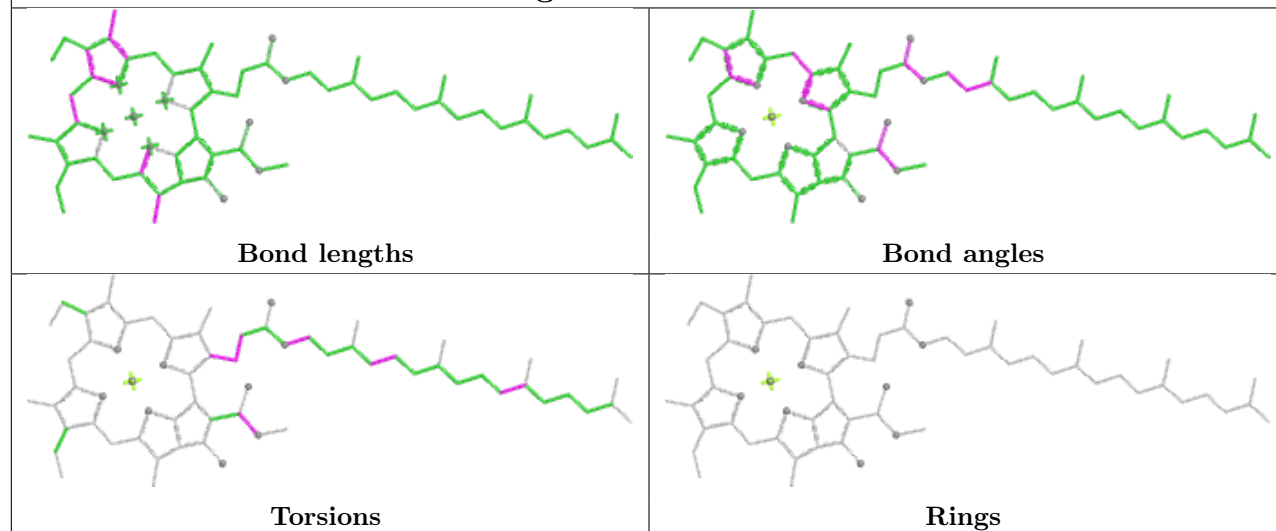
Ligand CLA B 614



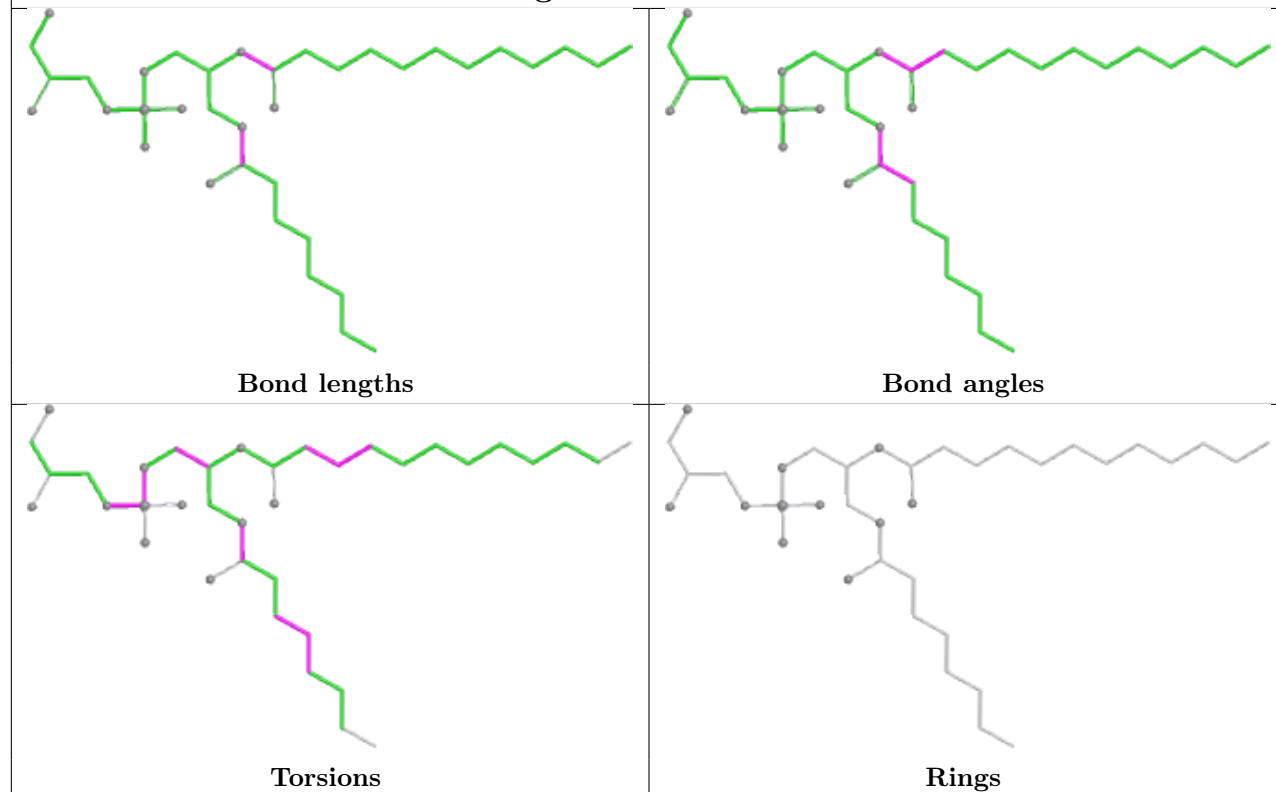
Ligand SQD F 102



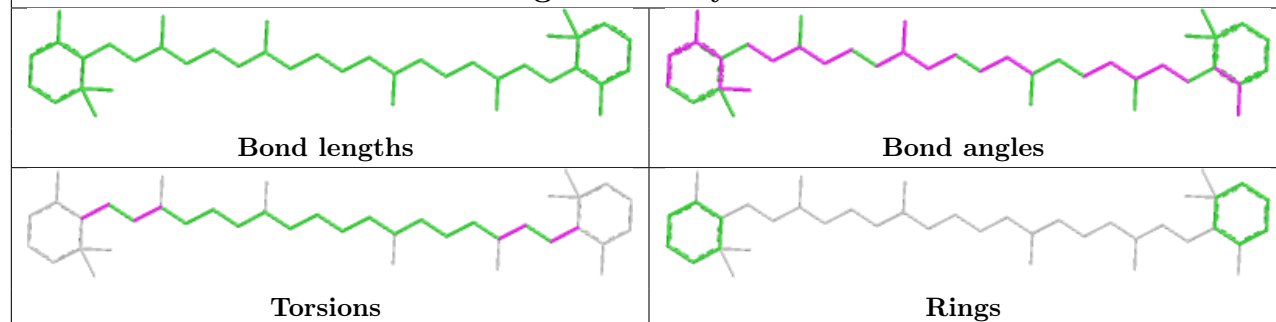
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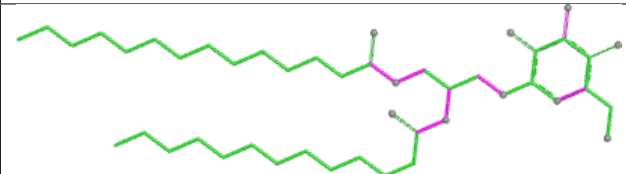
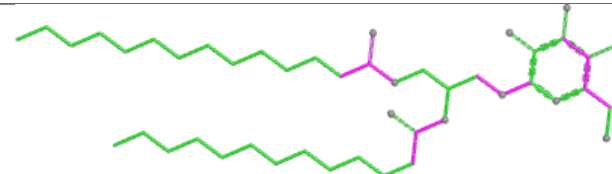
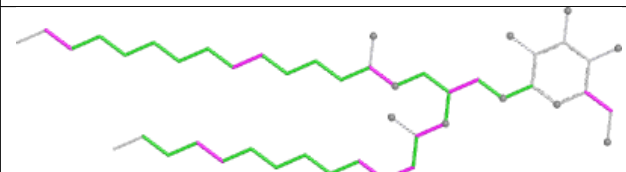
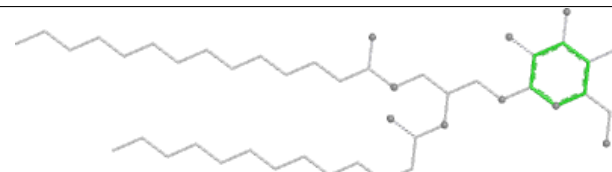


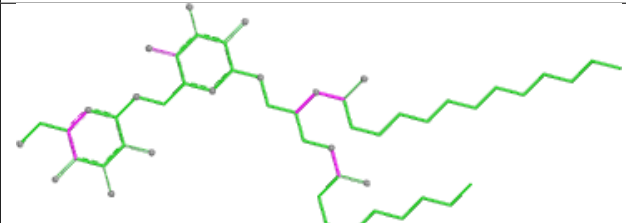
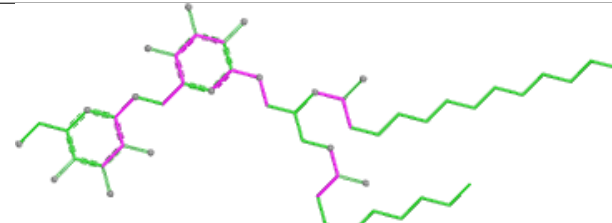
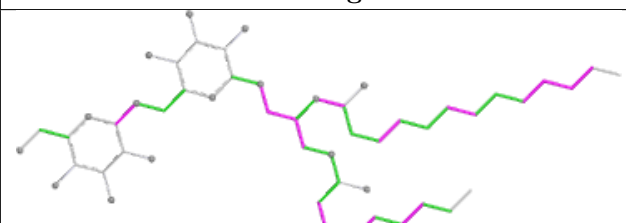
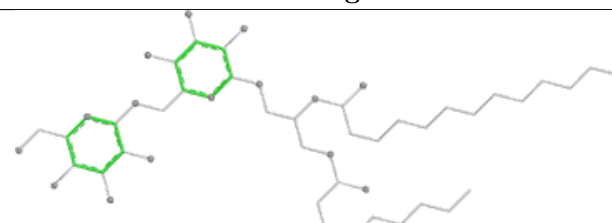
Ligand LHG a 417

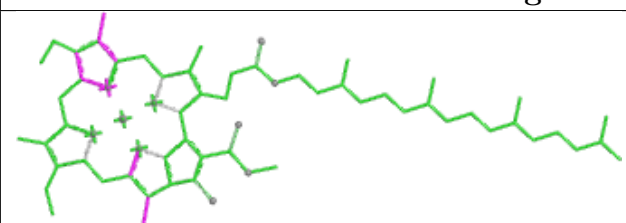
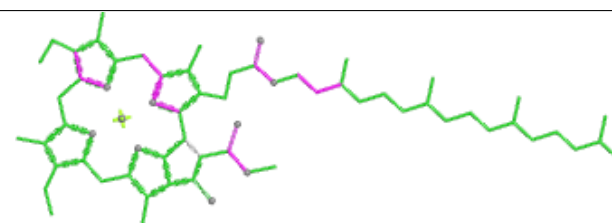
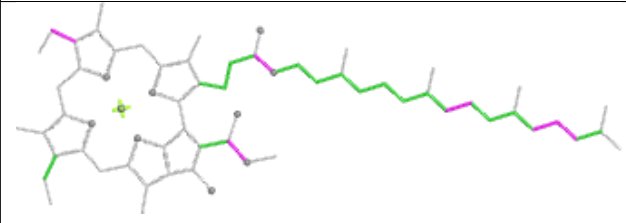
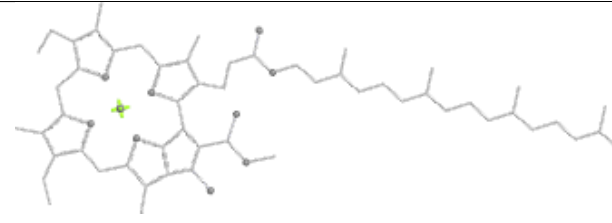


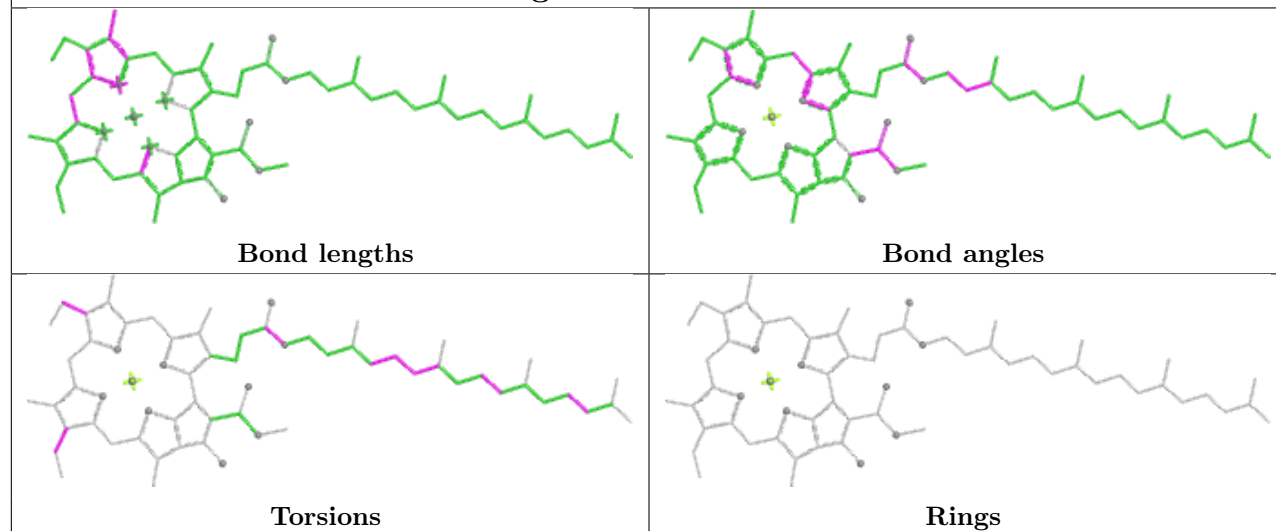
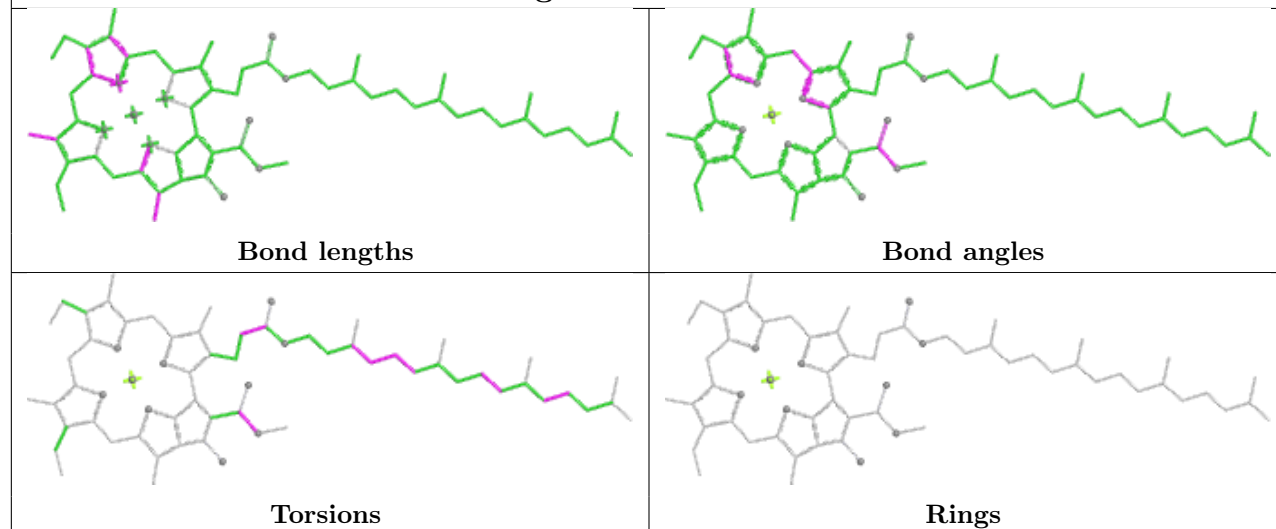
Ligand BCR y 101

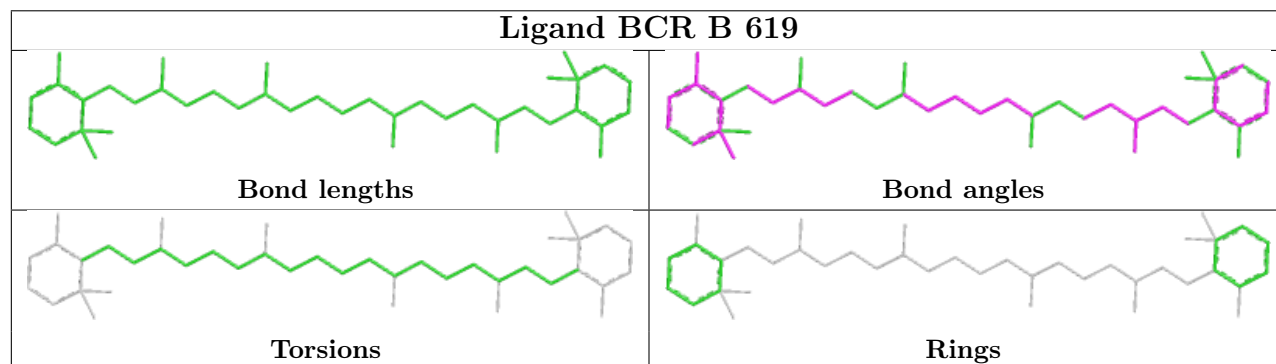
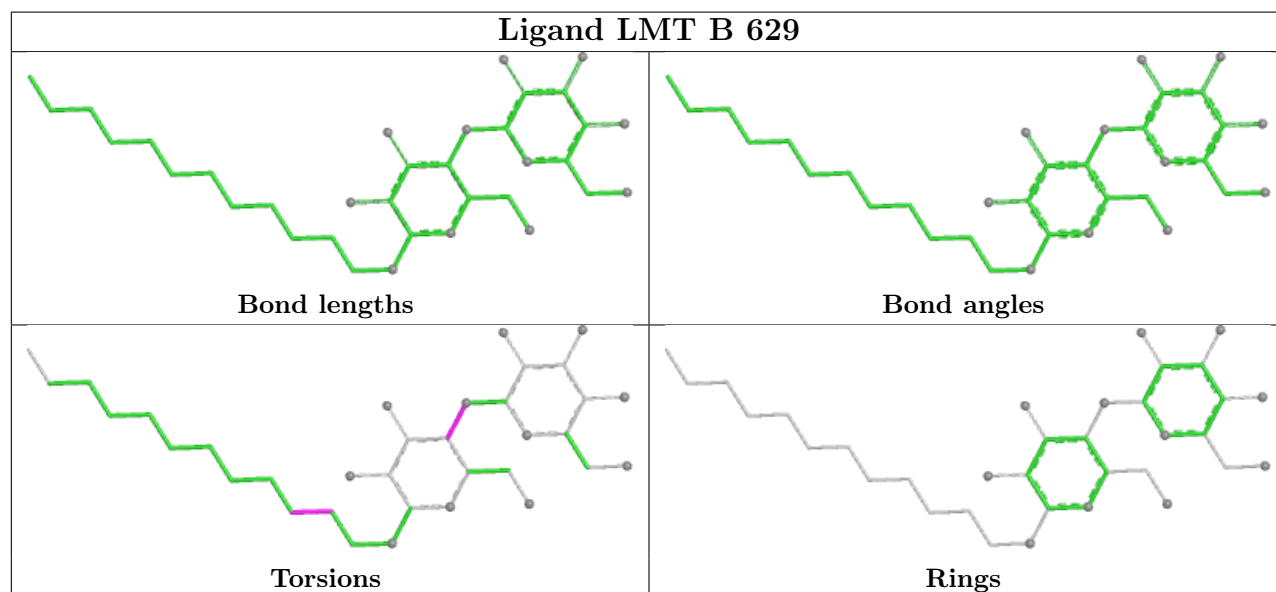
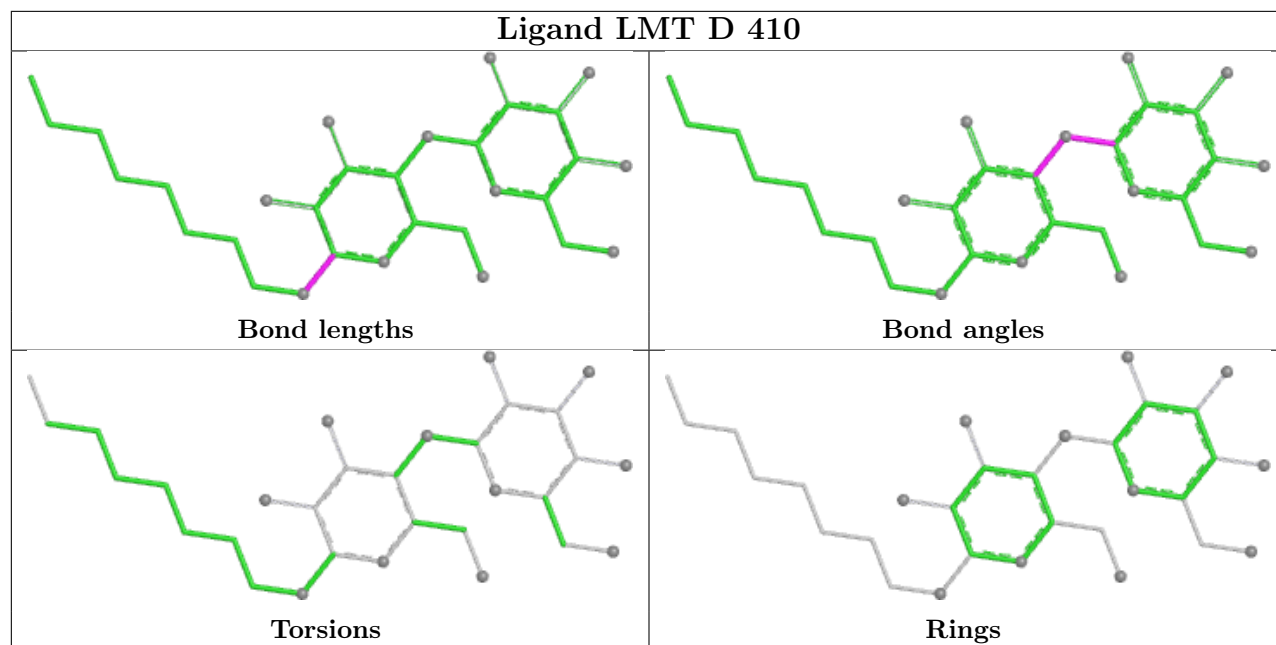


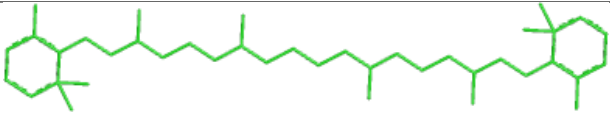
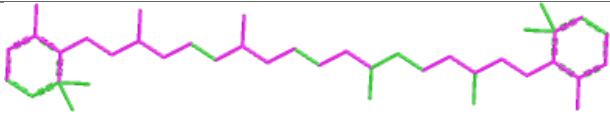
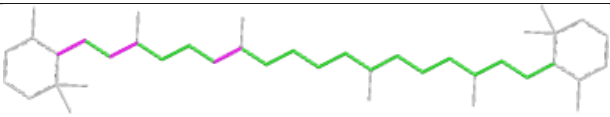
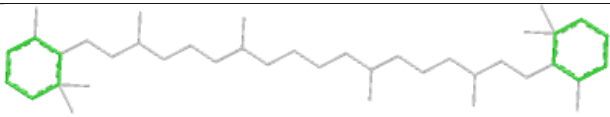
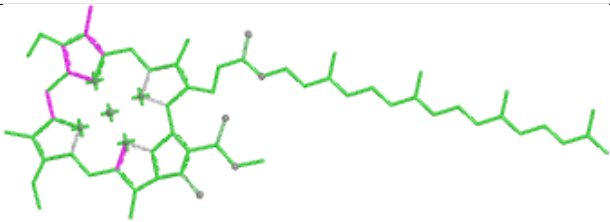
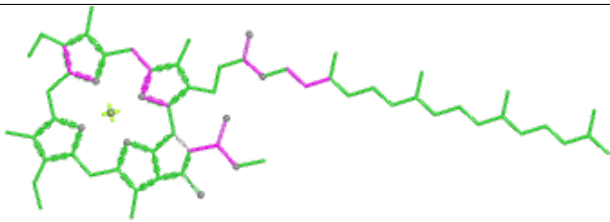
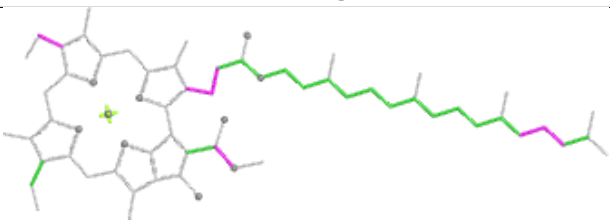
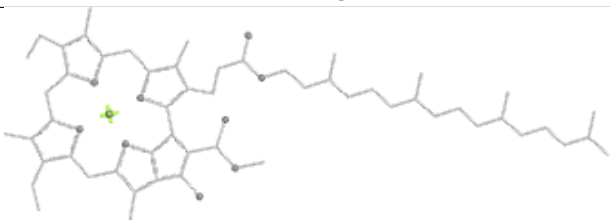
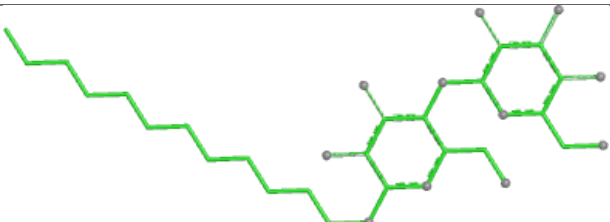
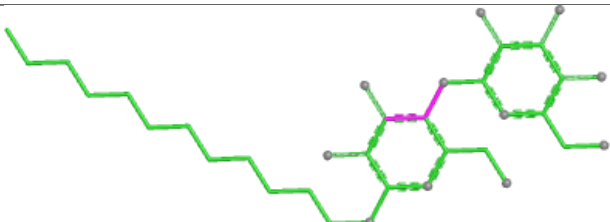
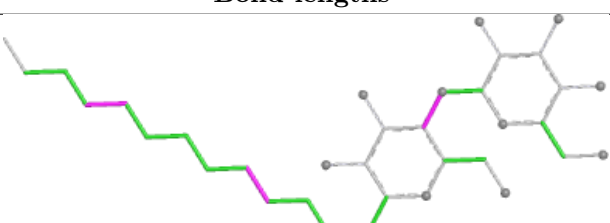
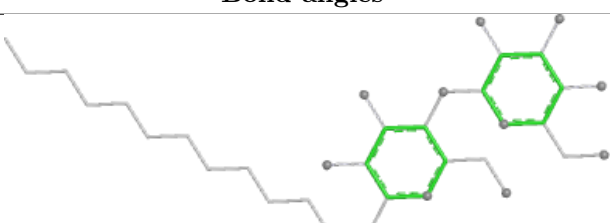
Ligand LMG d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

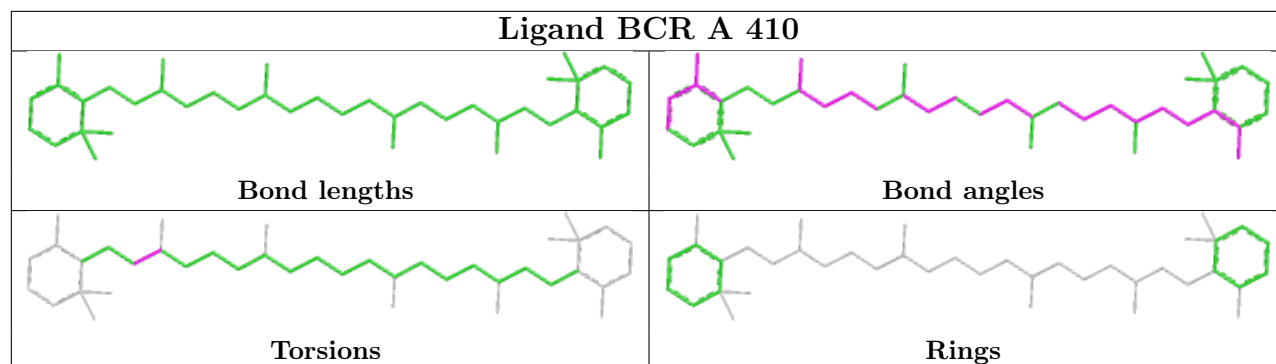
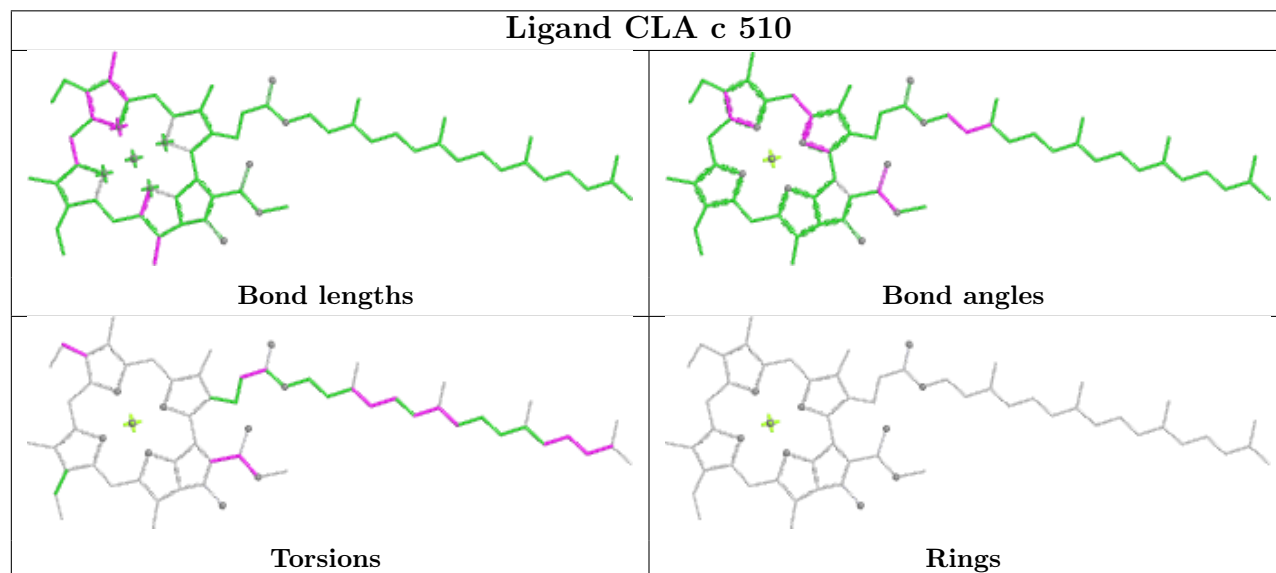
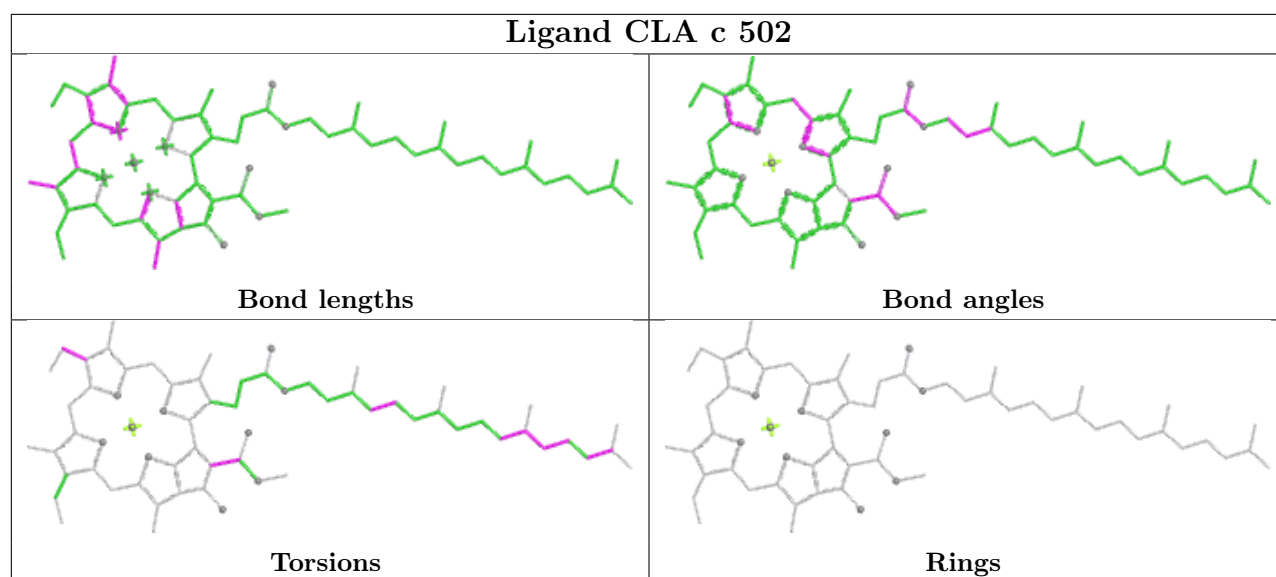
Ligand DGD B 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

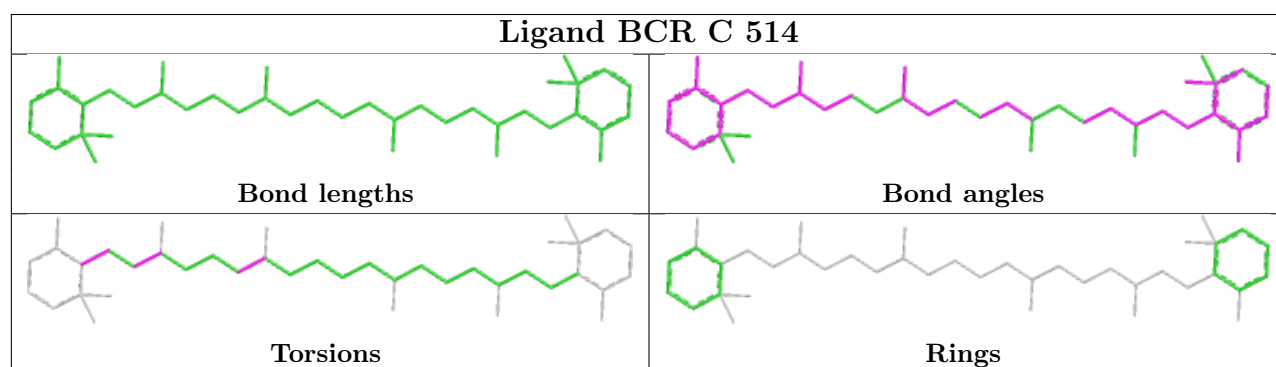
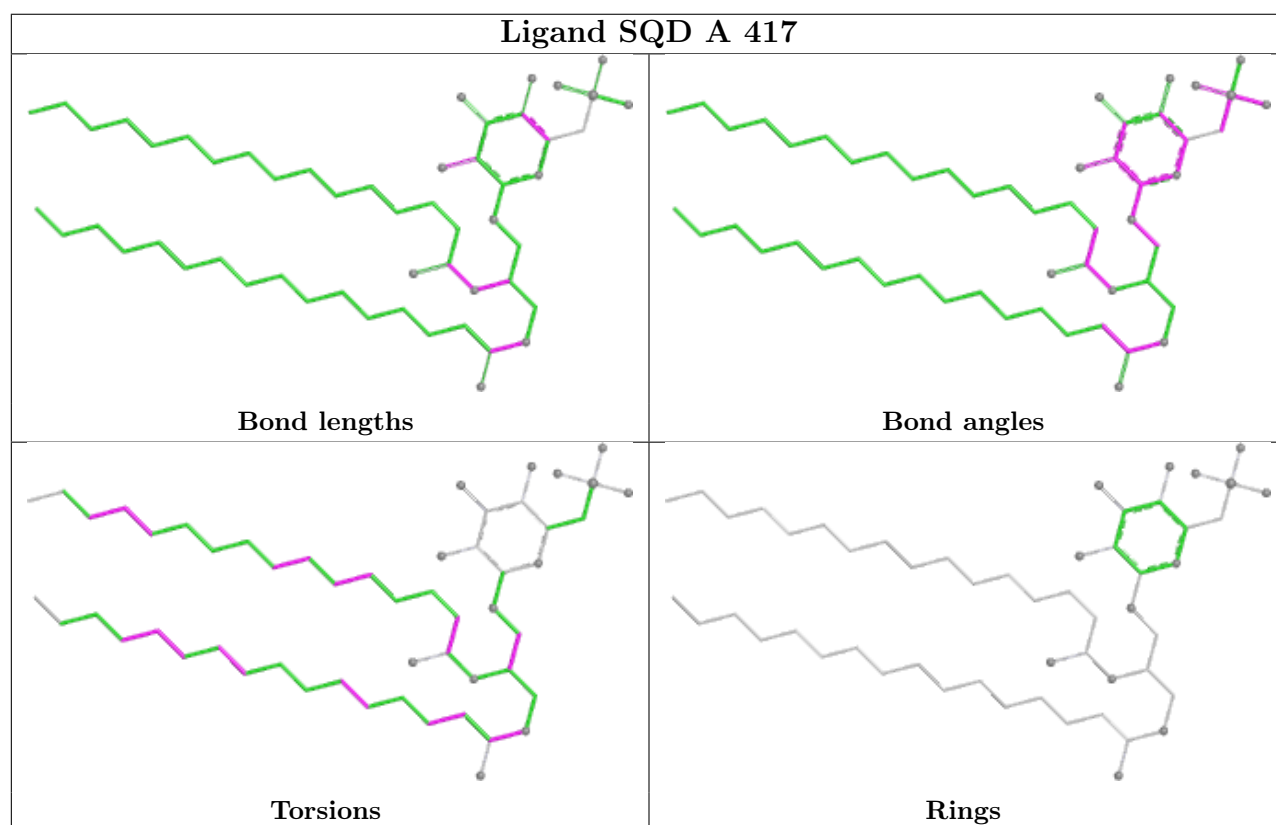
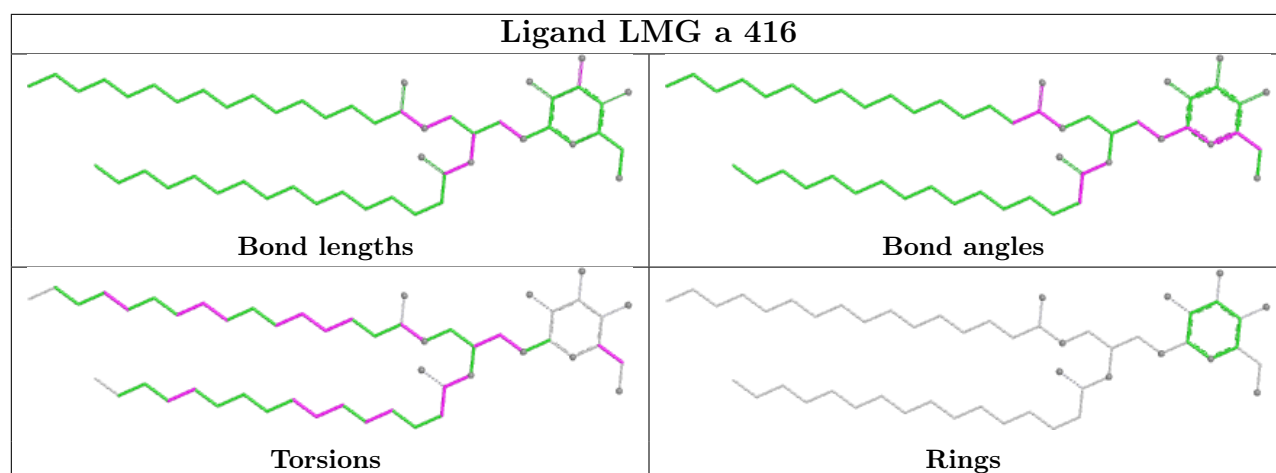
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Bond lengths	Bond angles
	
Torsions	Rings

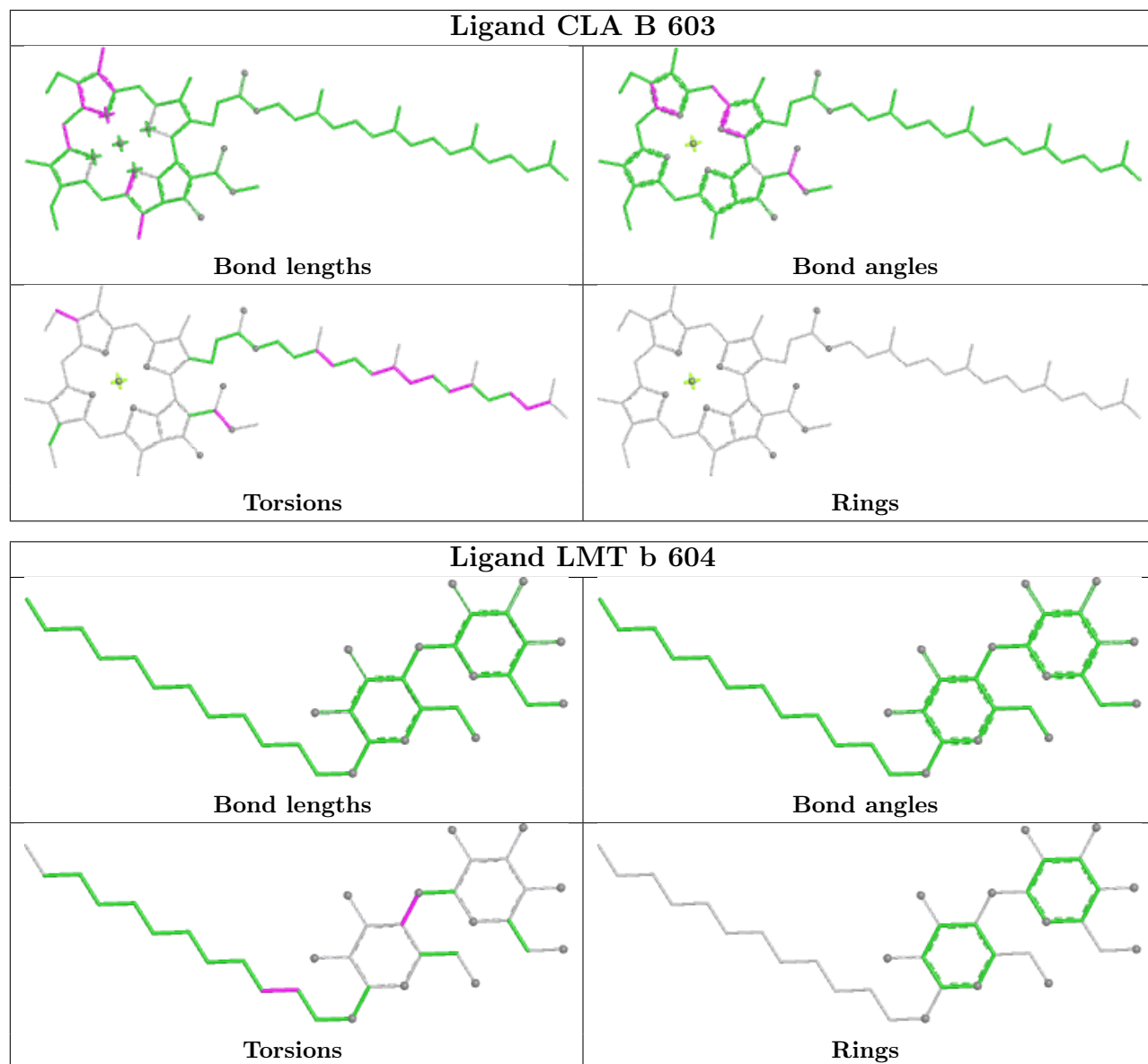
Ligand CLA A 405**Ligand CLA b 616**

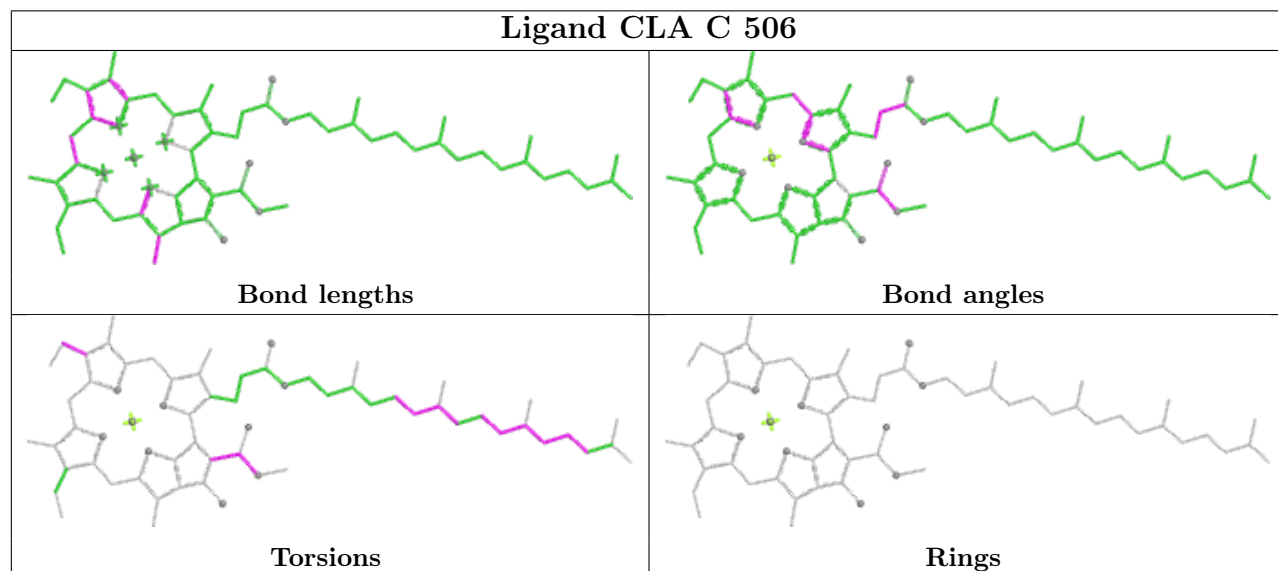
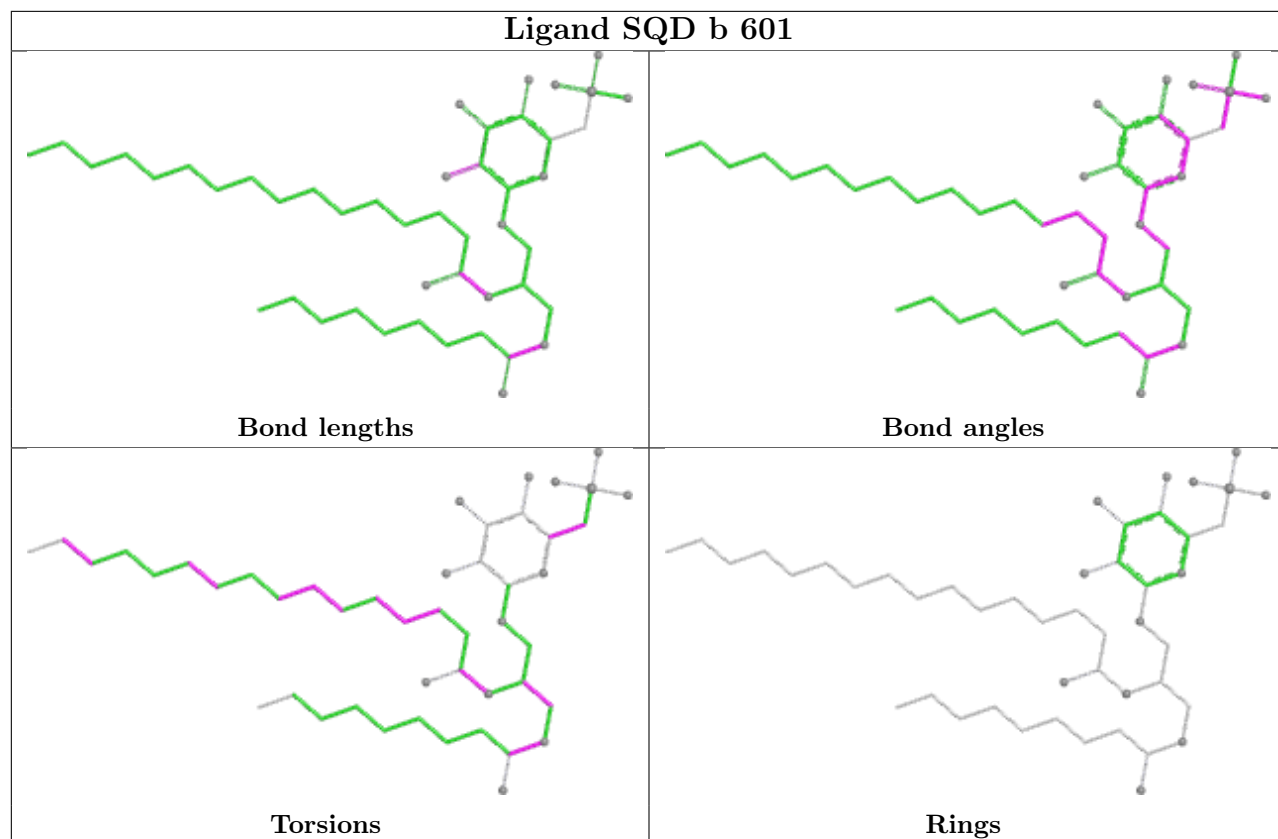


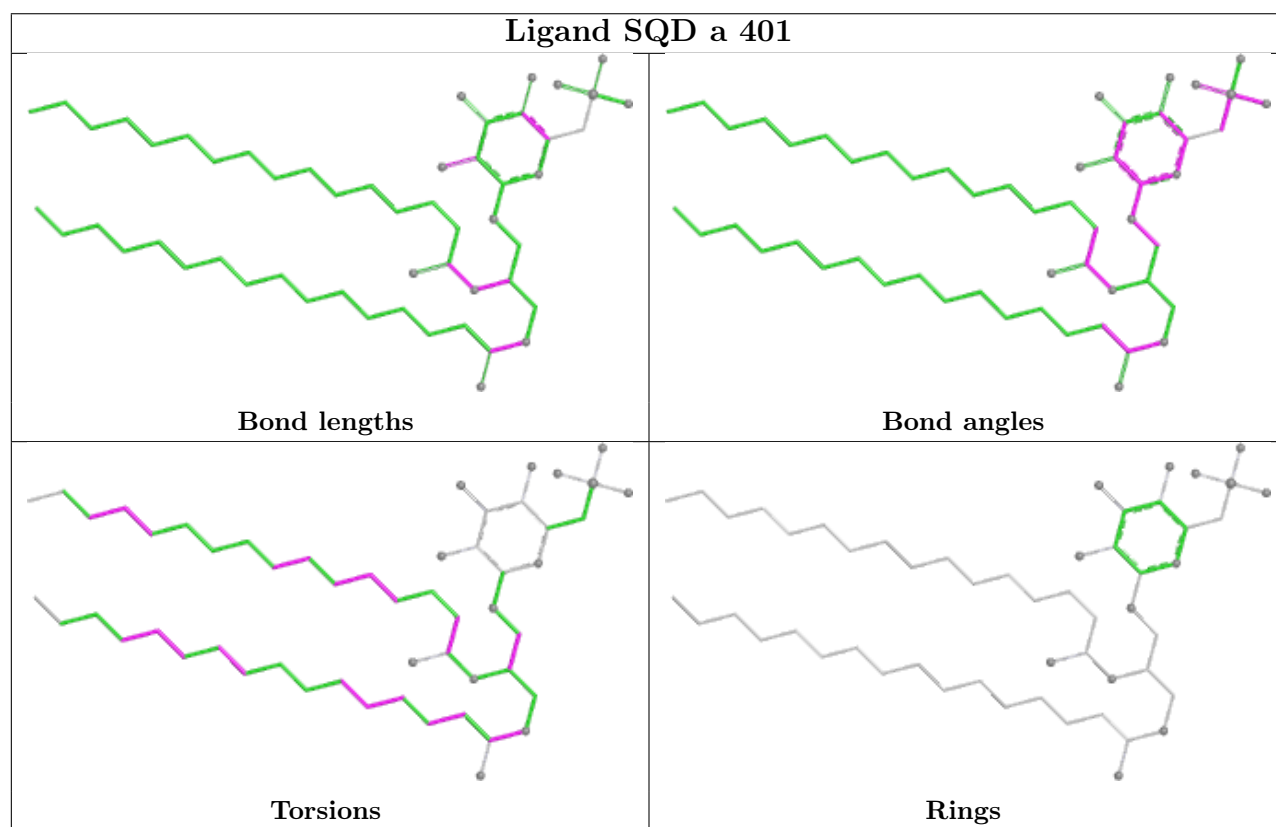
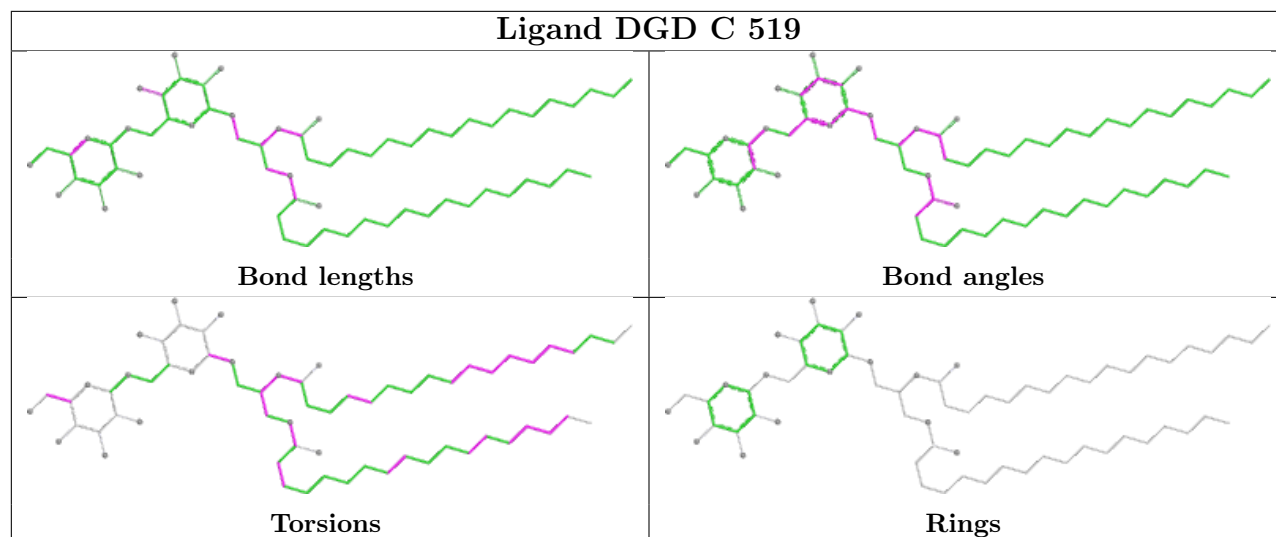
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT B 628	
 Bond lengths	 Bond angles
 Torsions	 Rings

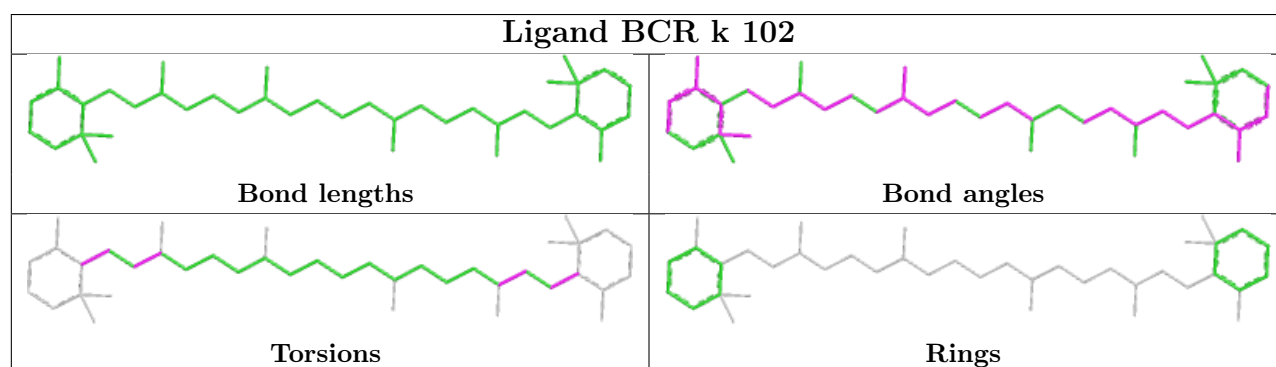
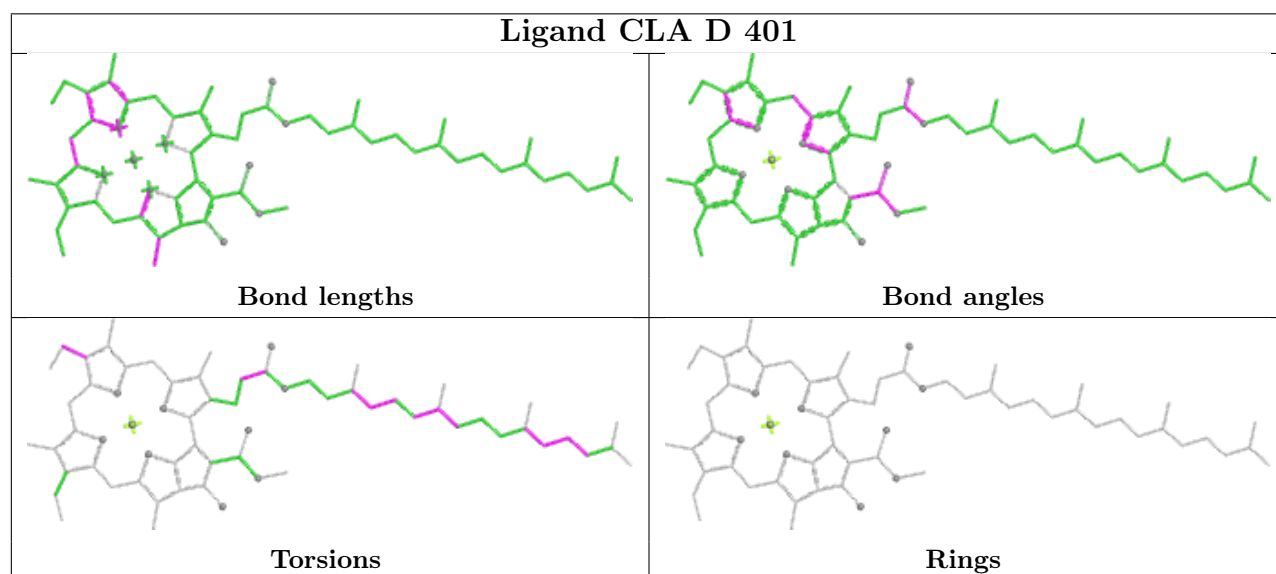
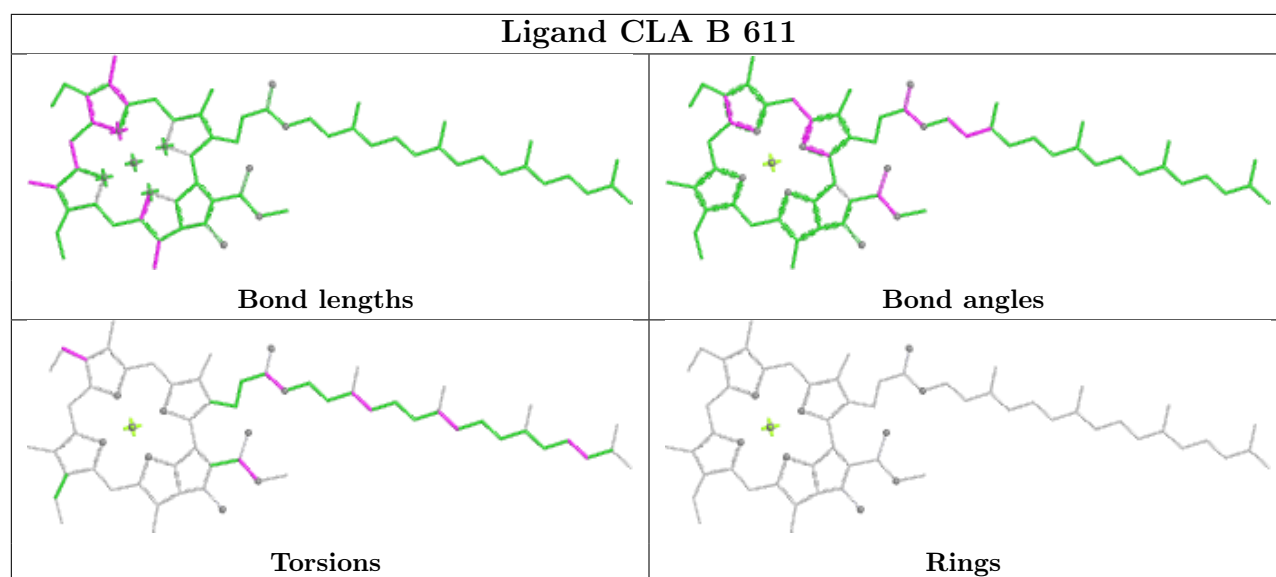


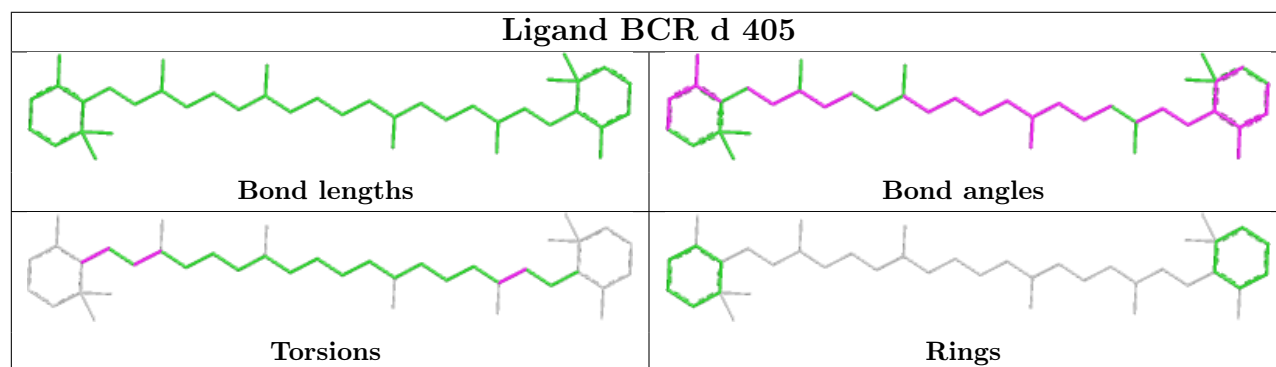
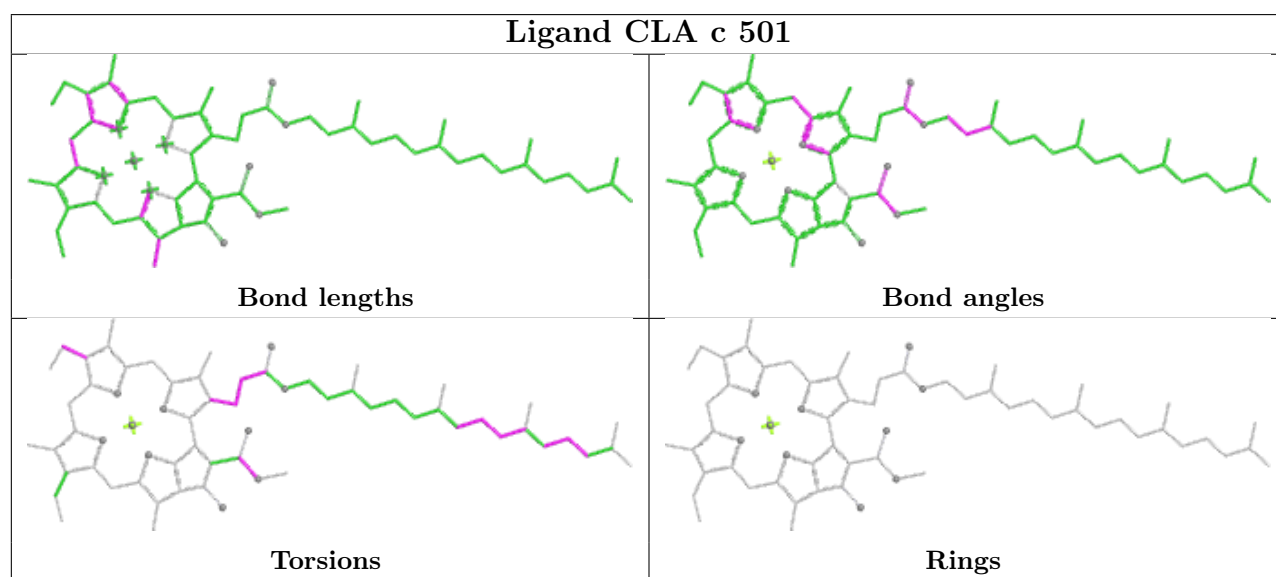
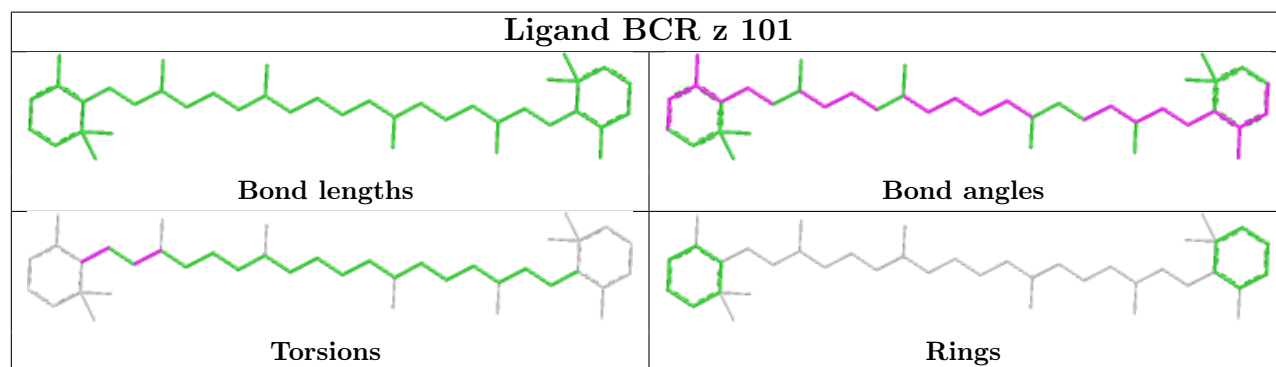
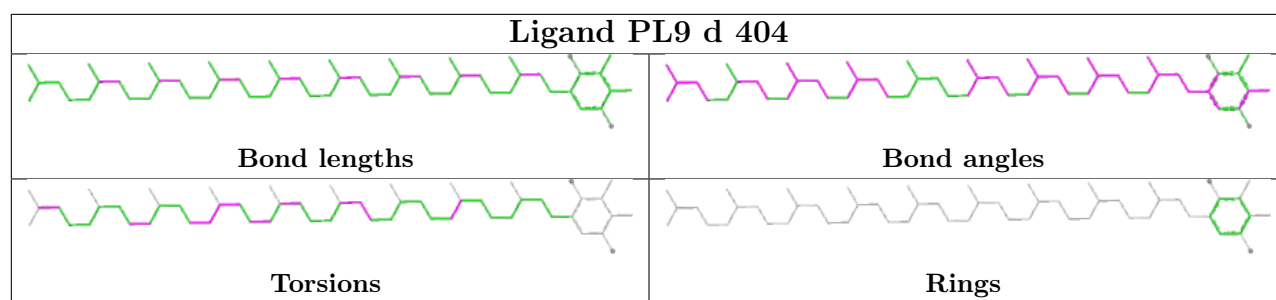


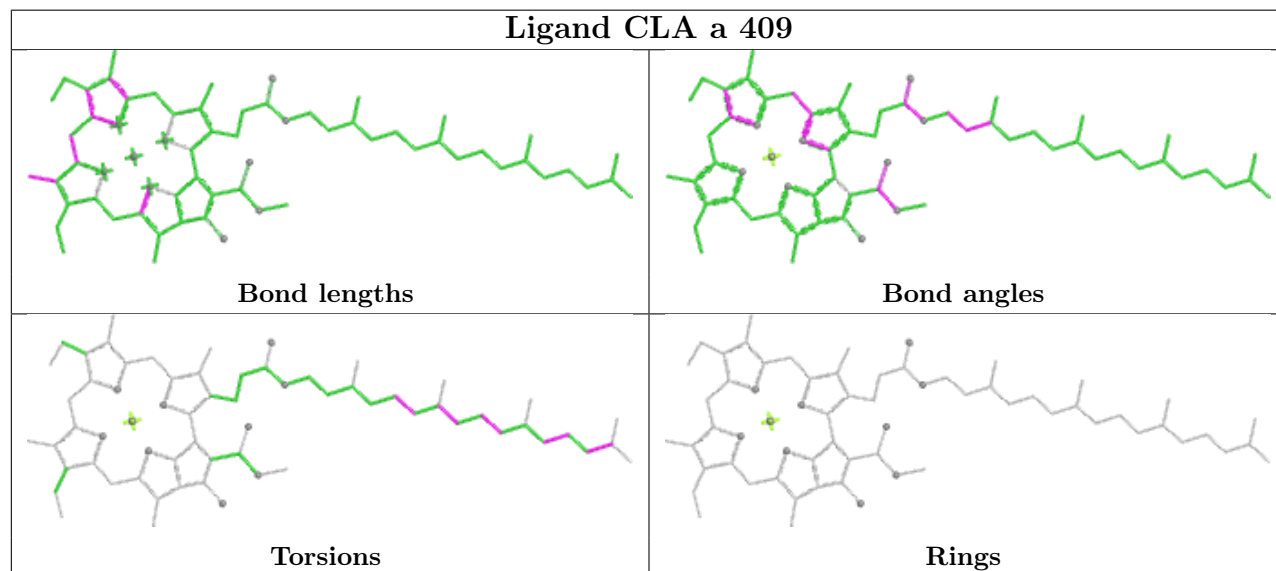
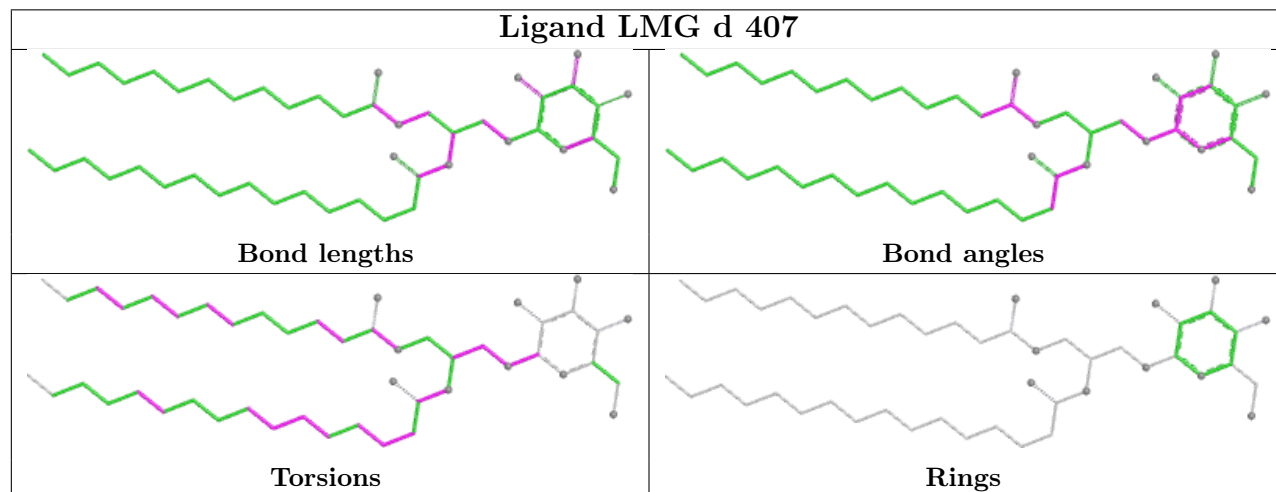
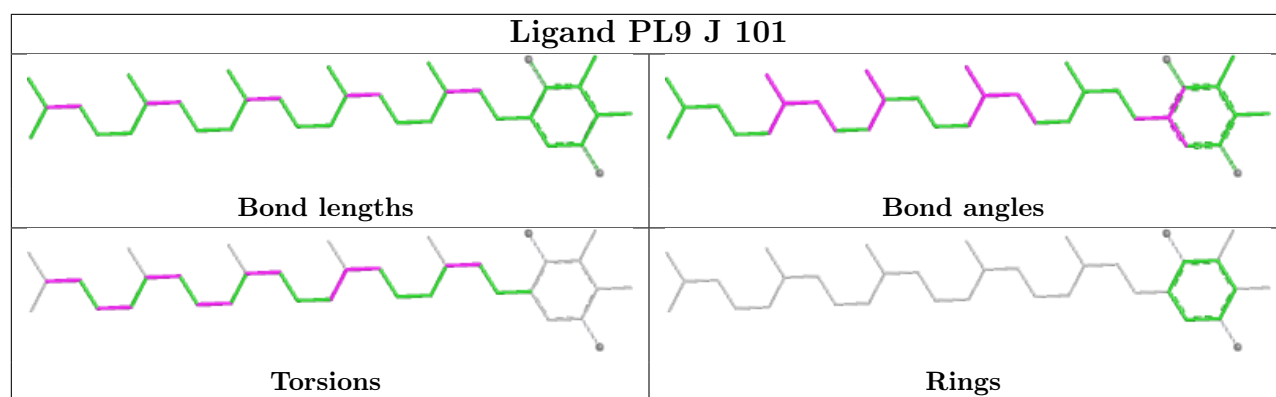


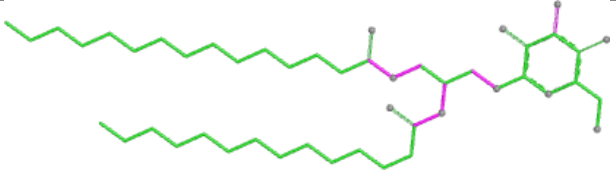
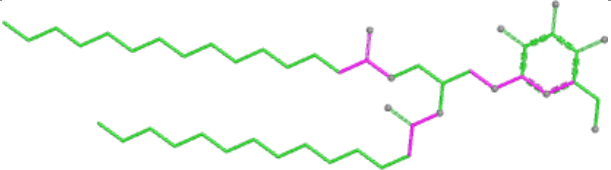
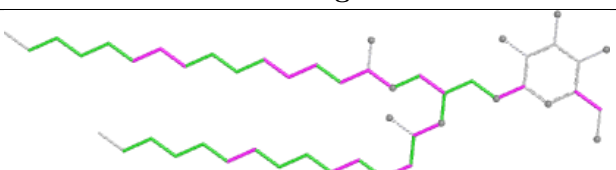
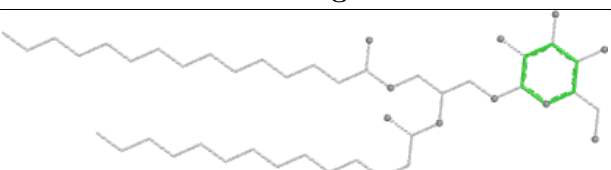


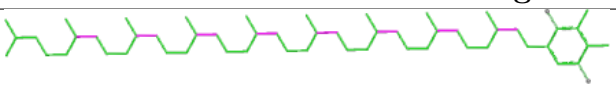
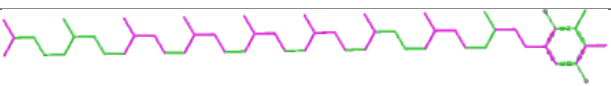
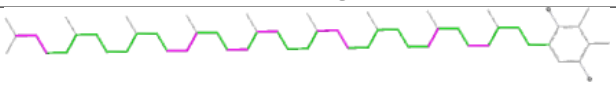
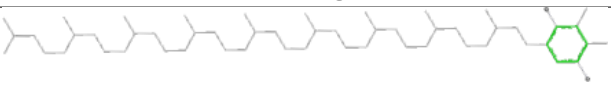


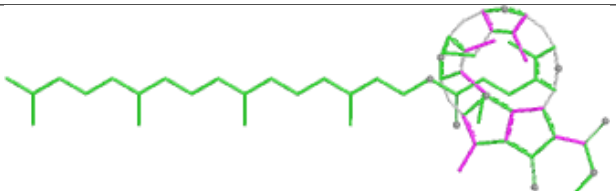
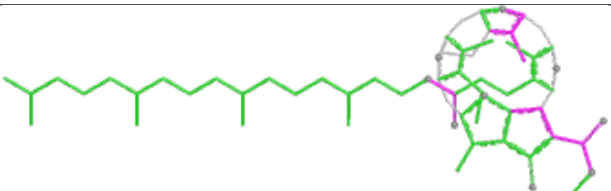
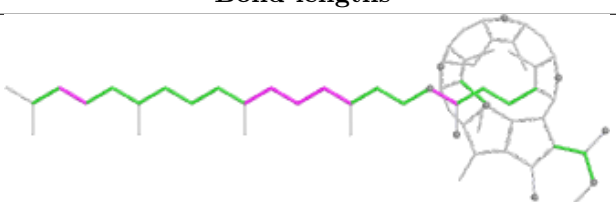
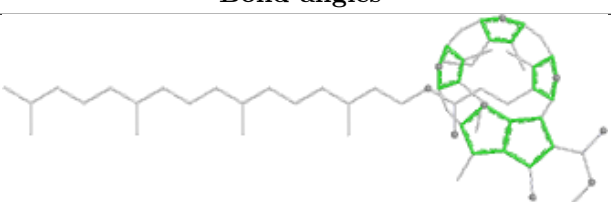




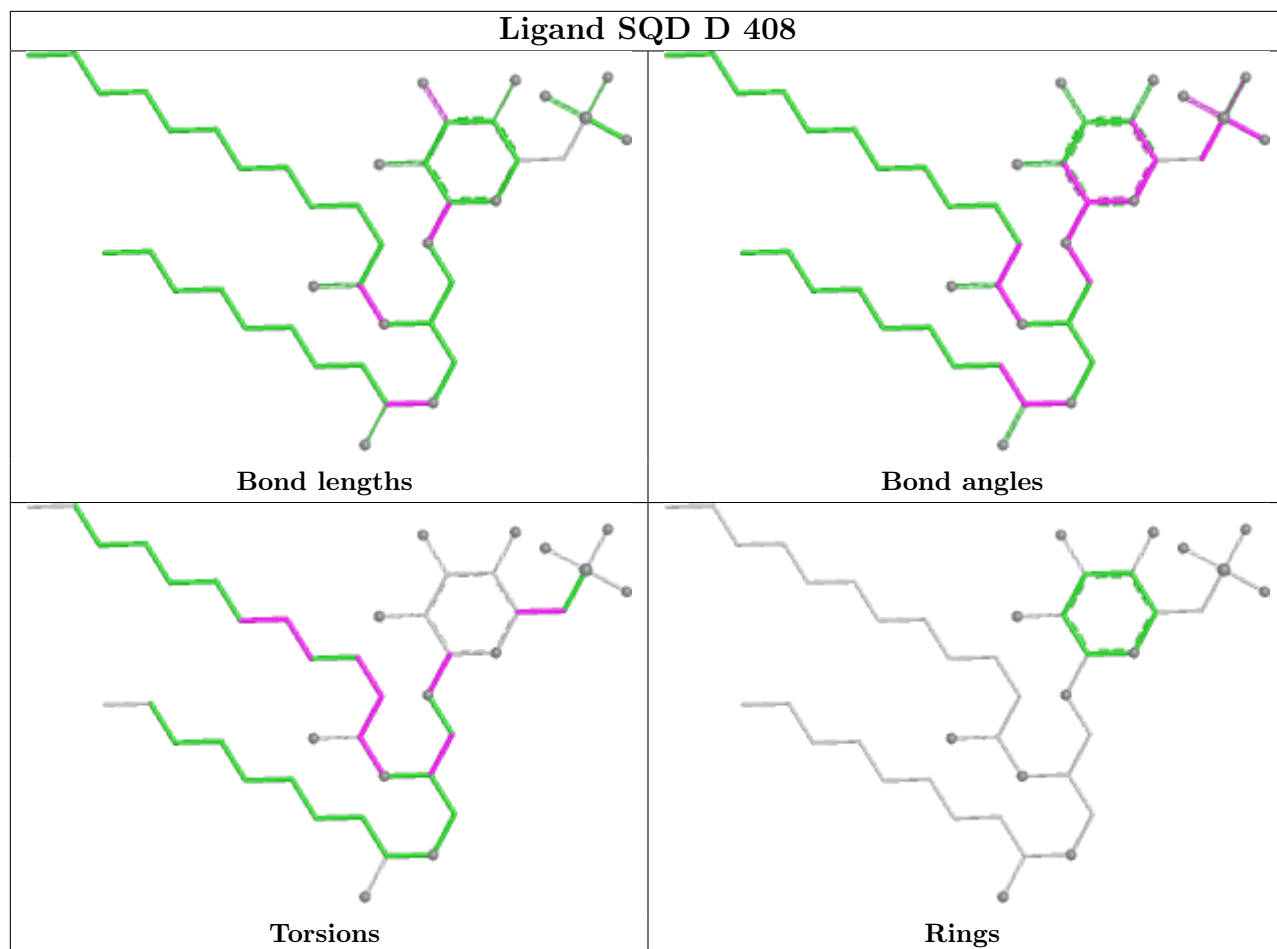


Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

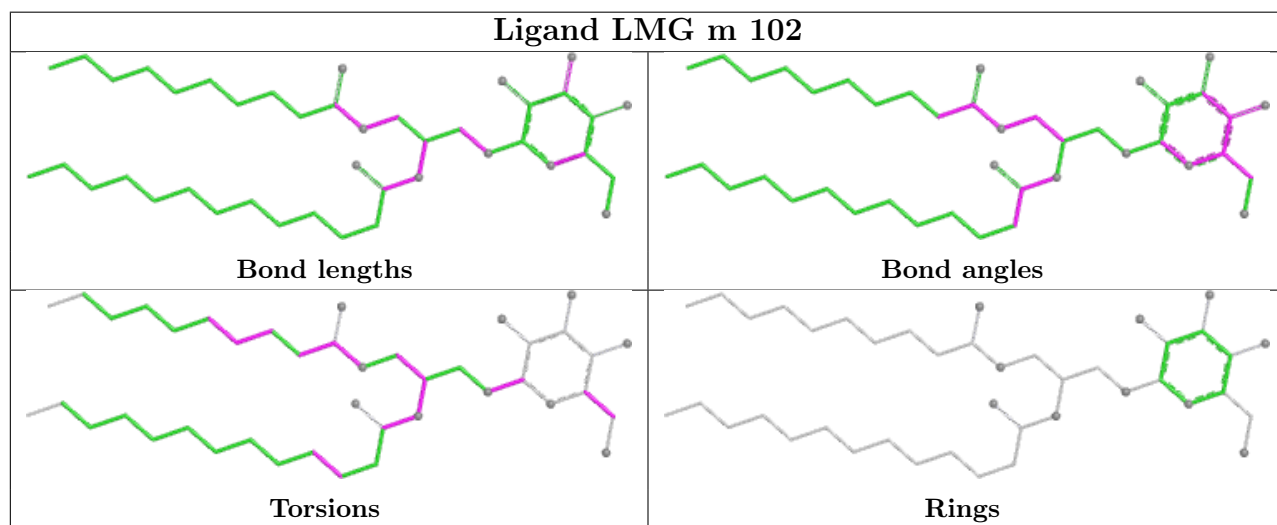
Ligand PL9 D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

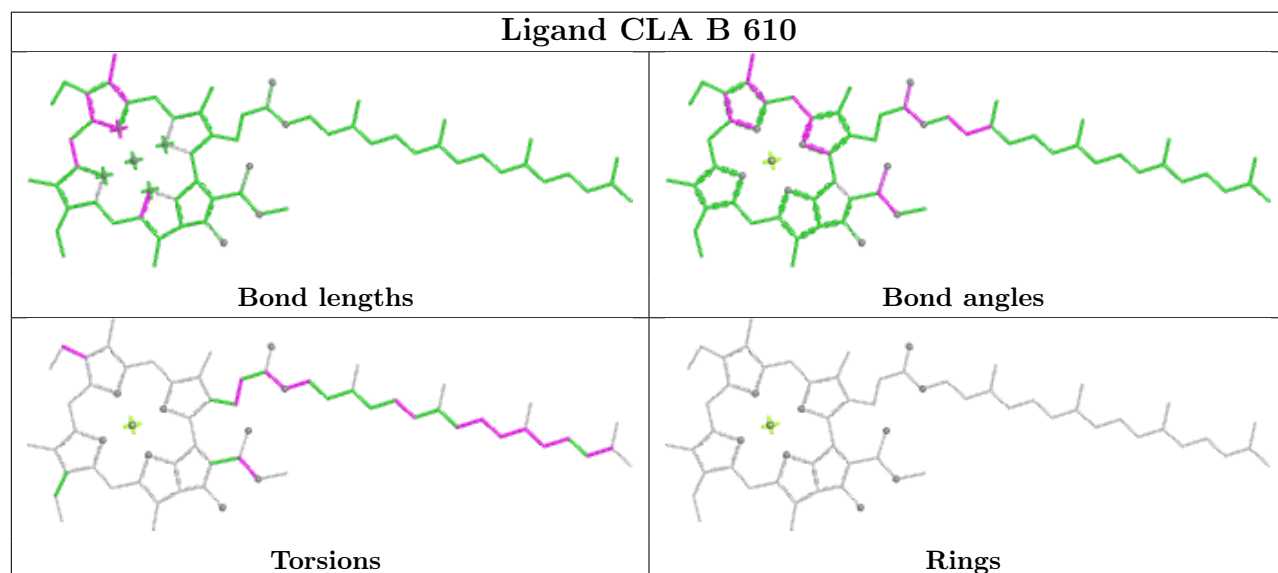
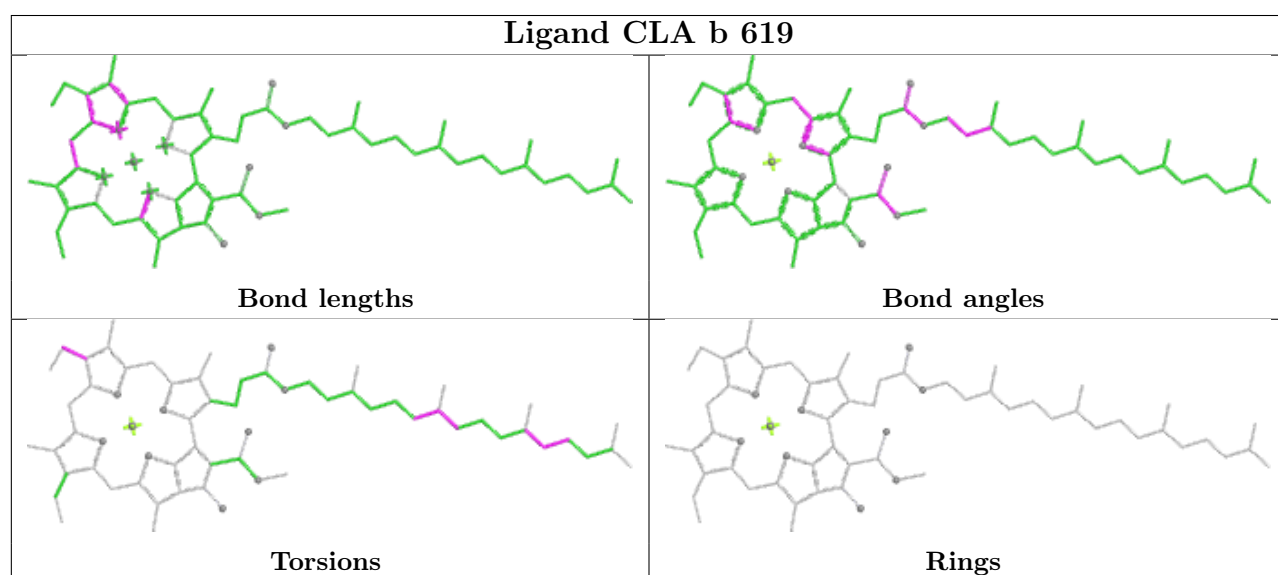
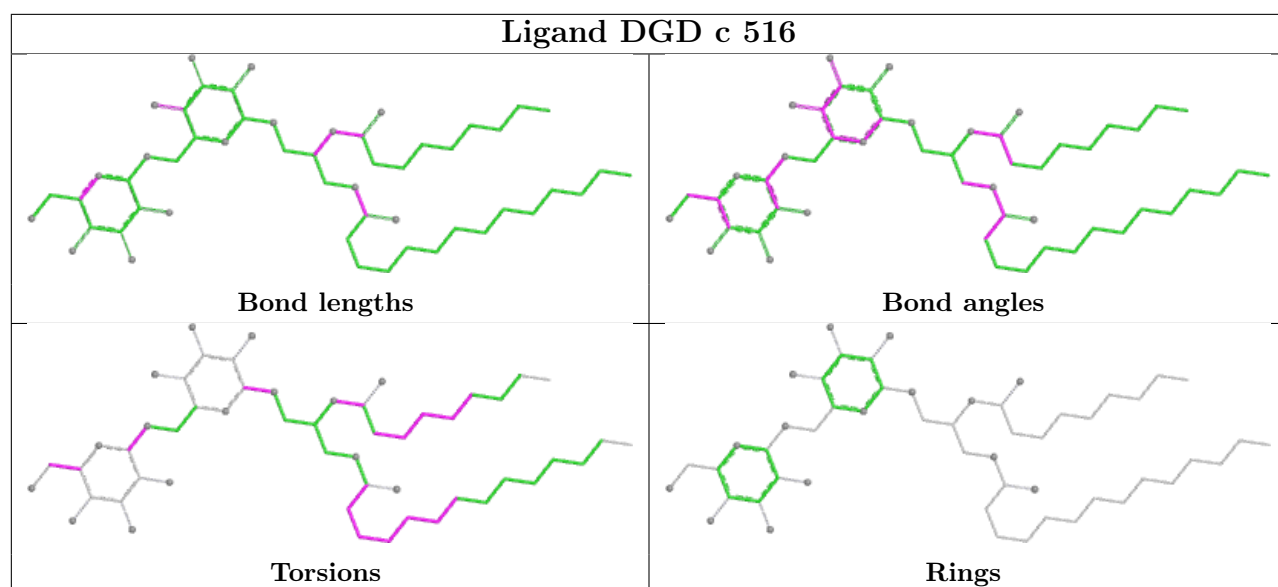
Ligand PHO D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

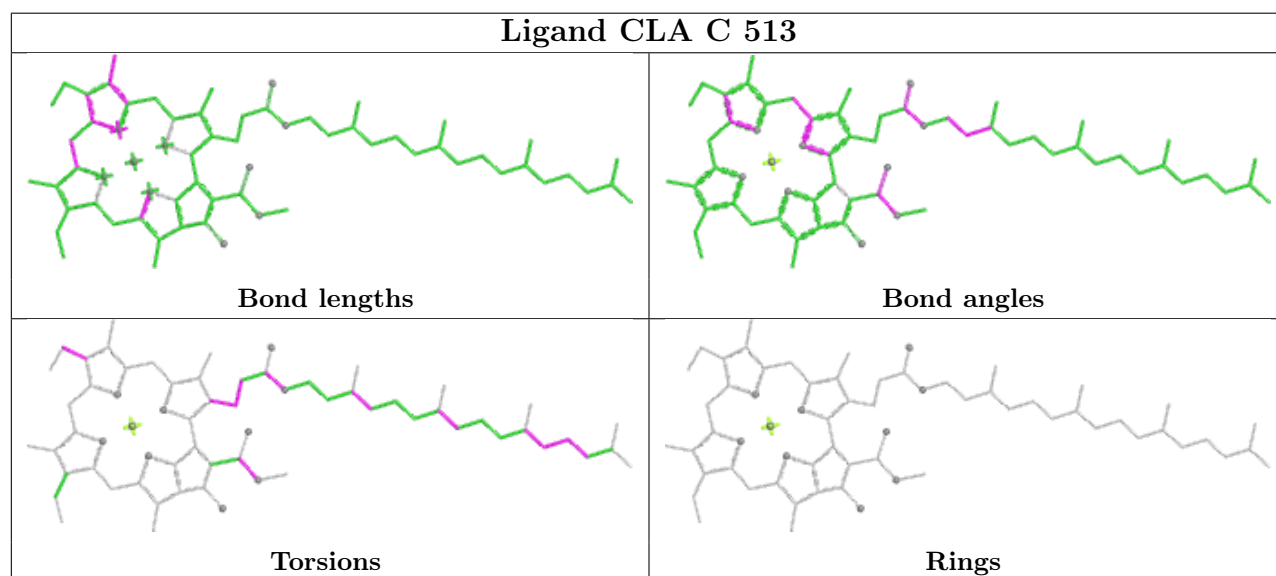
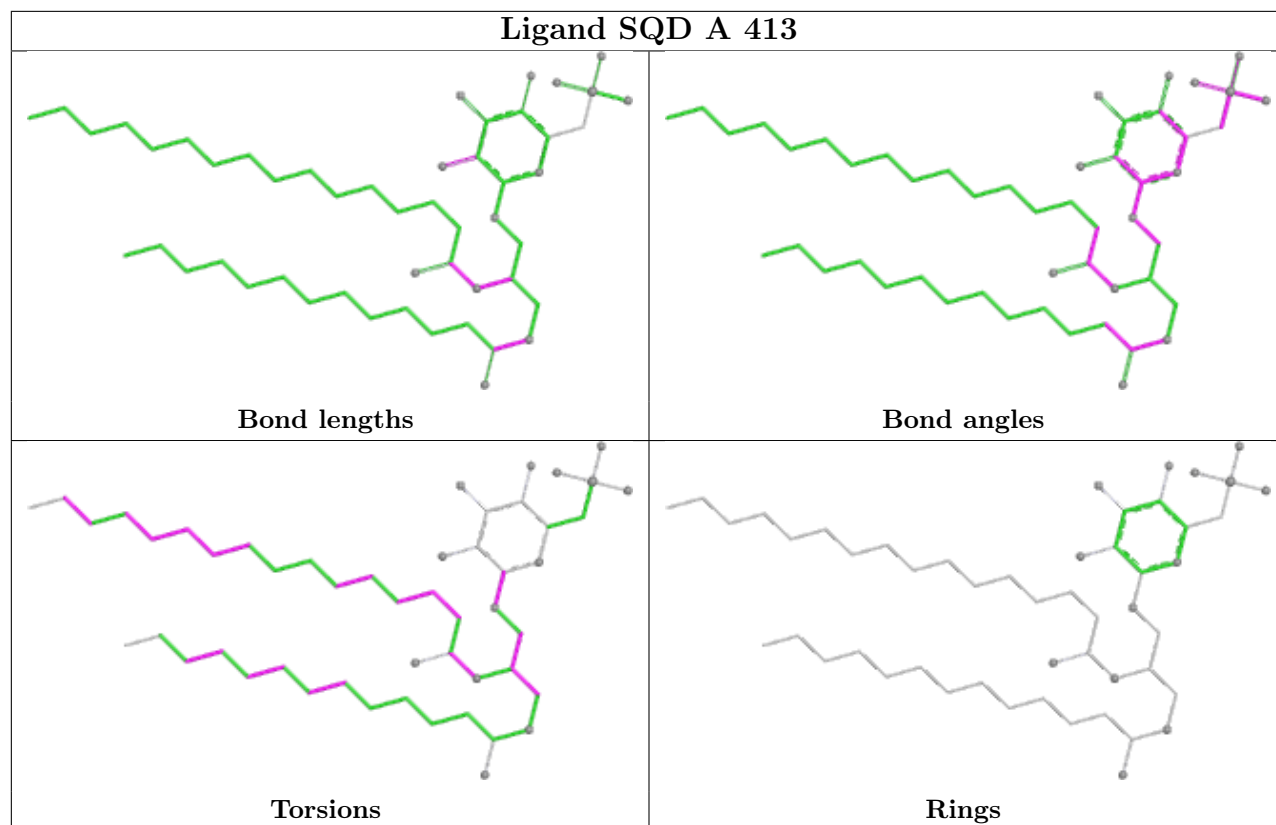
Ligand SQD D 408



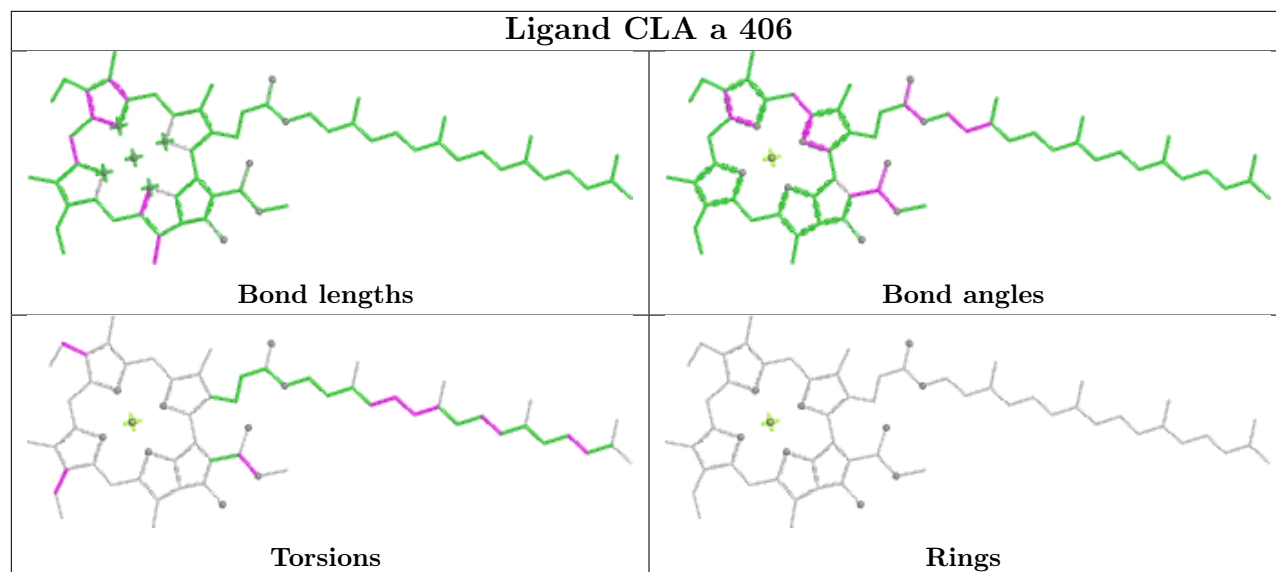
Ligand LMG m 102



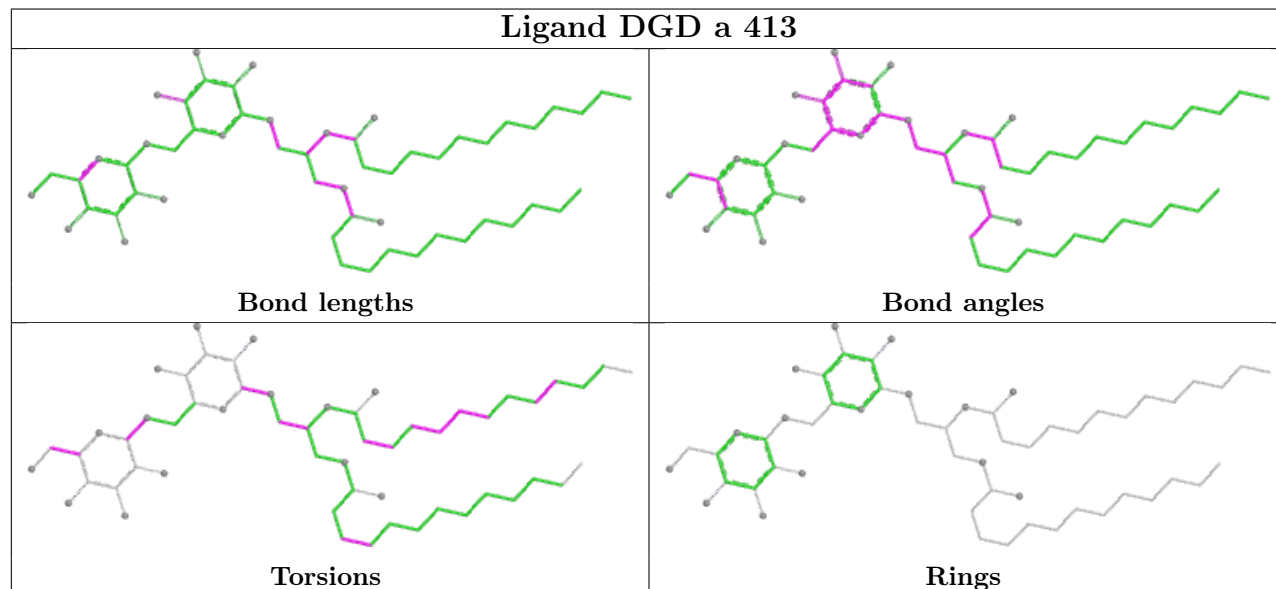




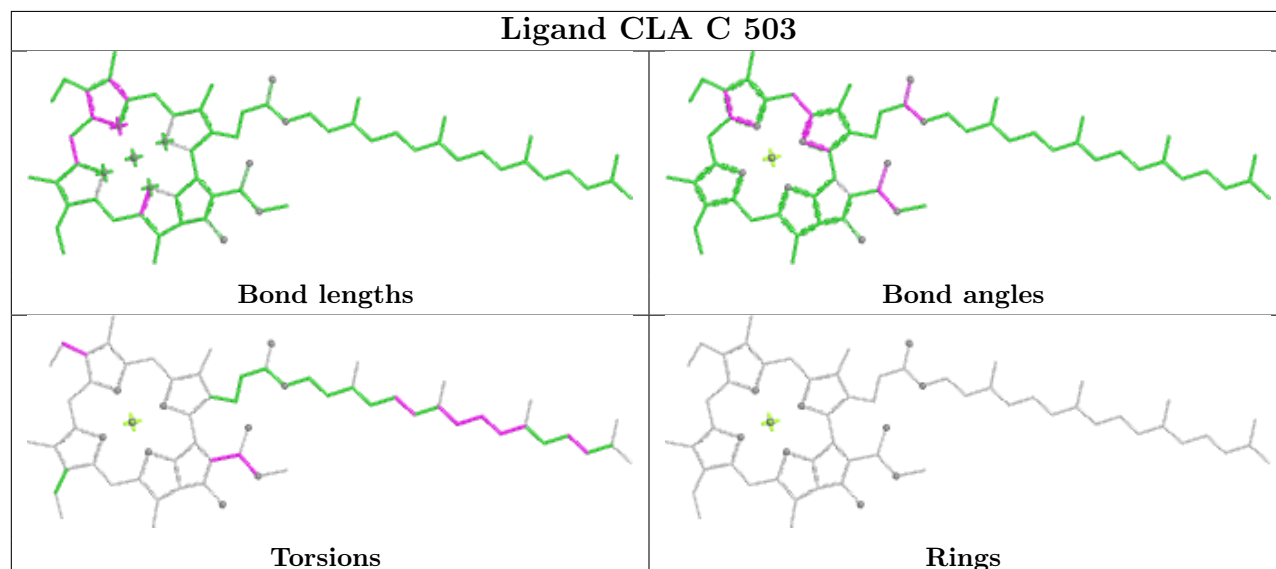
Ligand CLA a 406

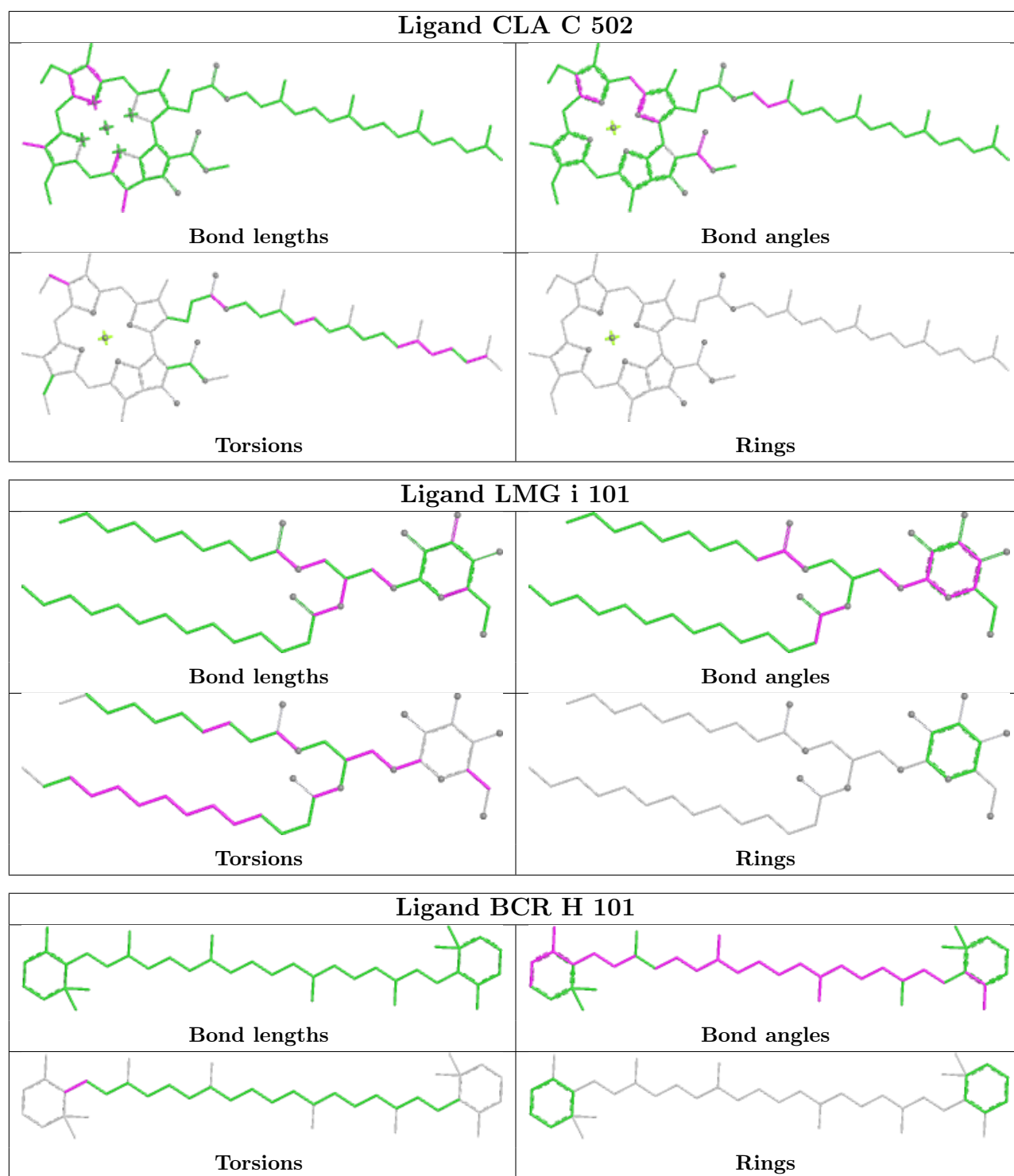


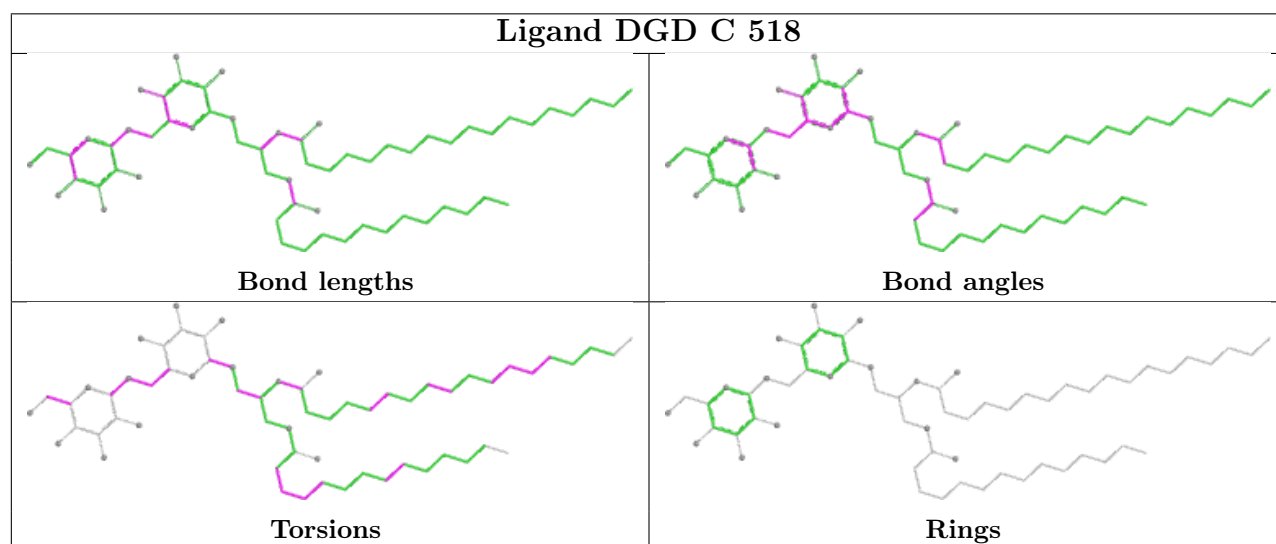
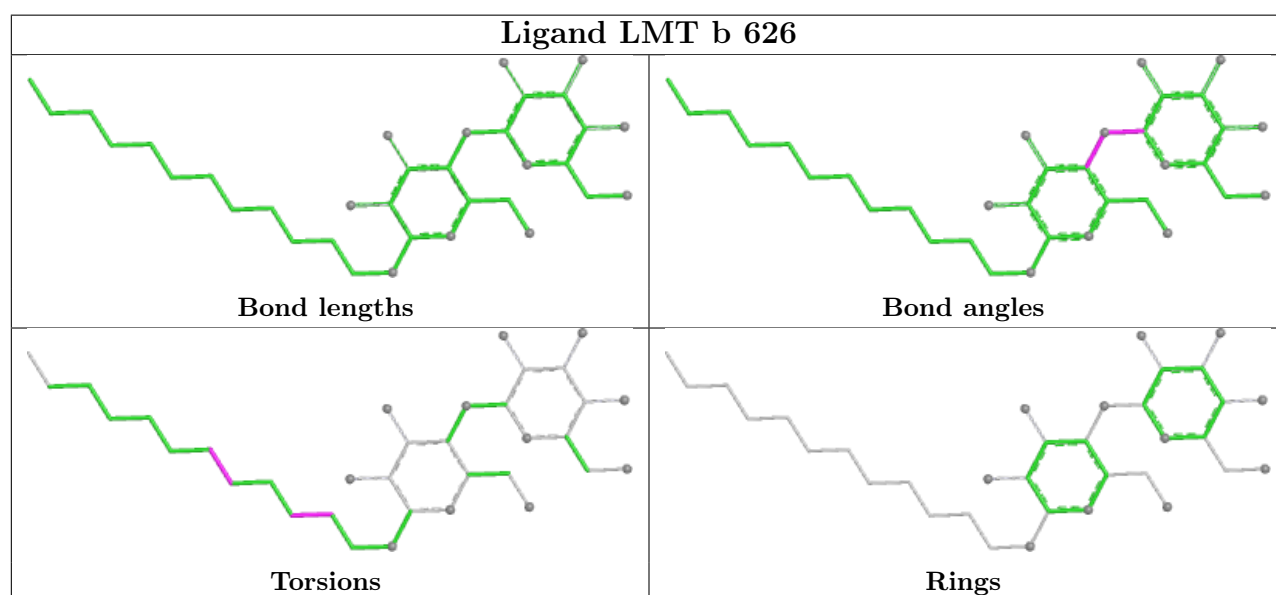
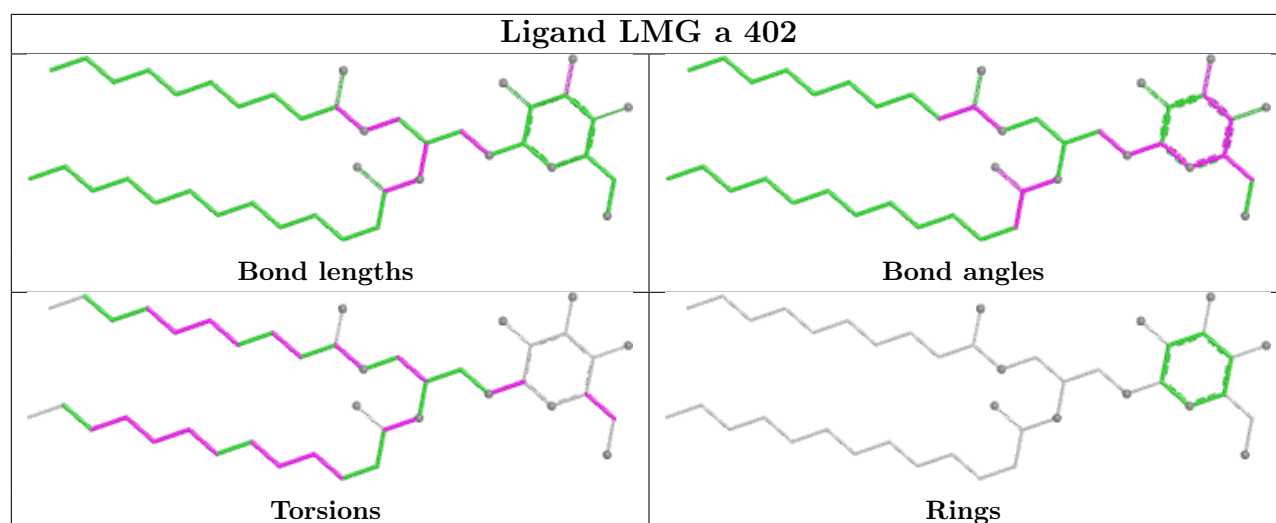
Ligand DGD a 413

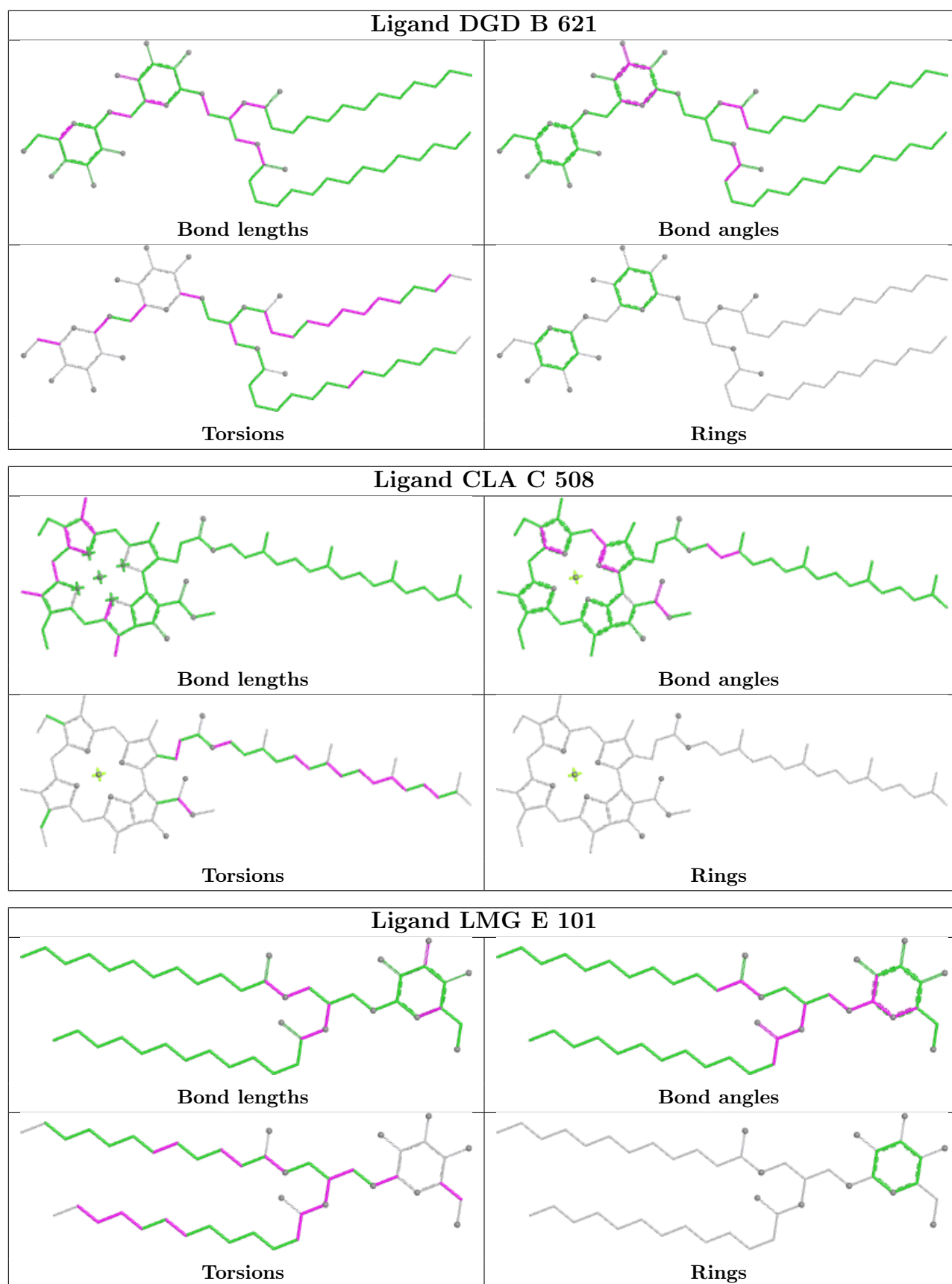


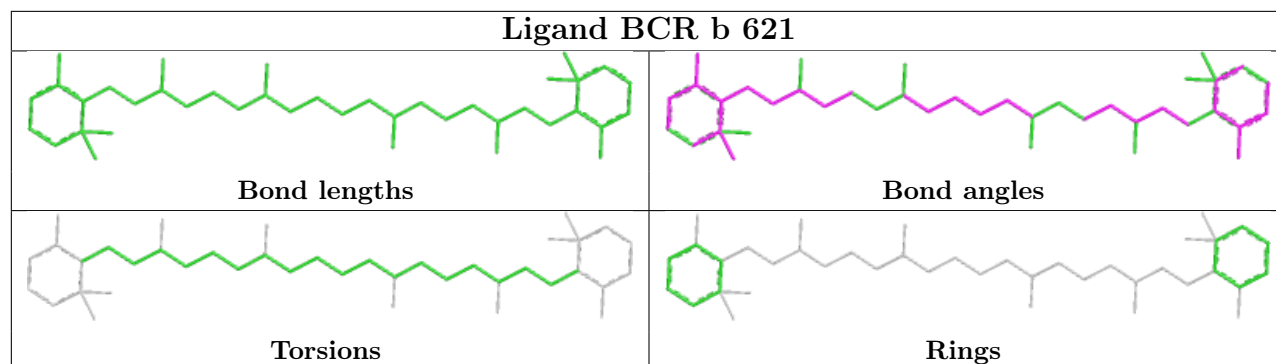
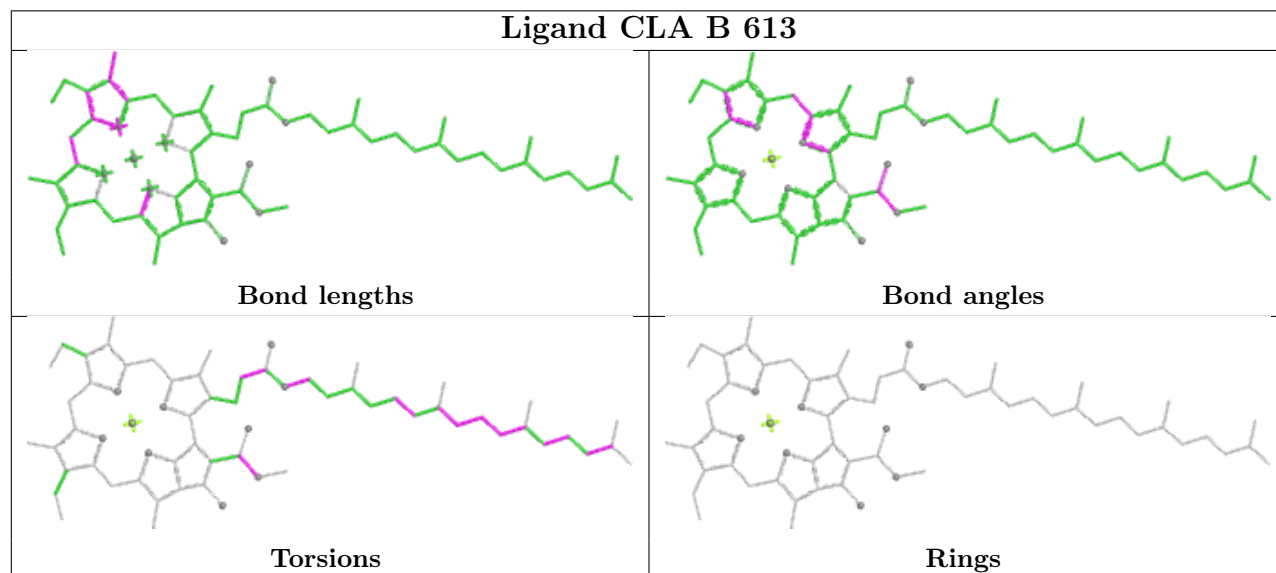
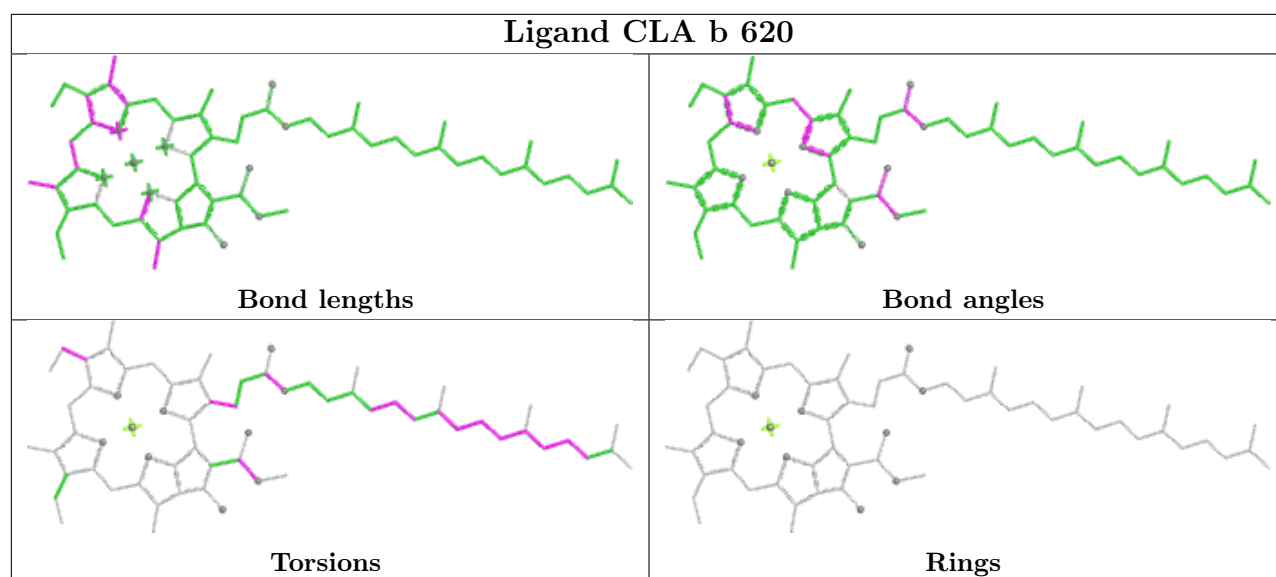
Ligand CLA C 503

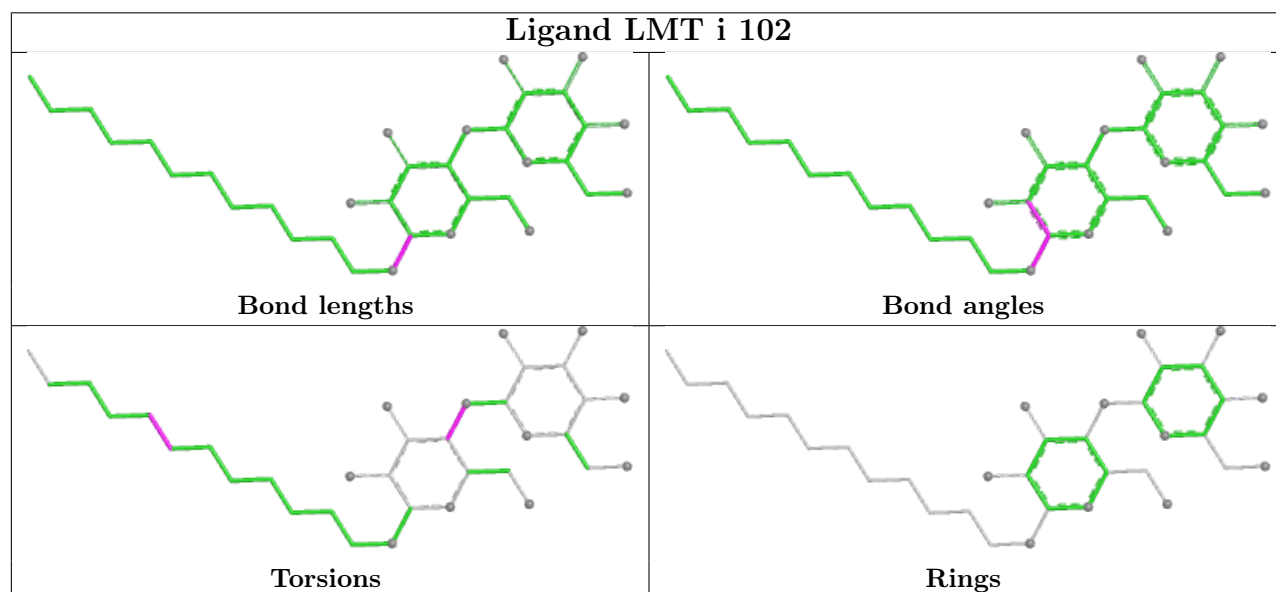
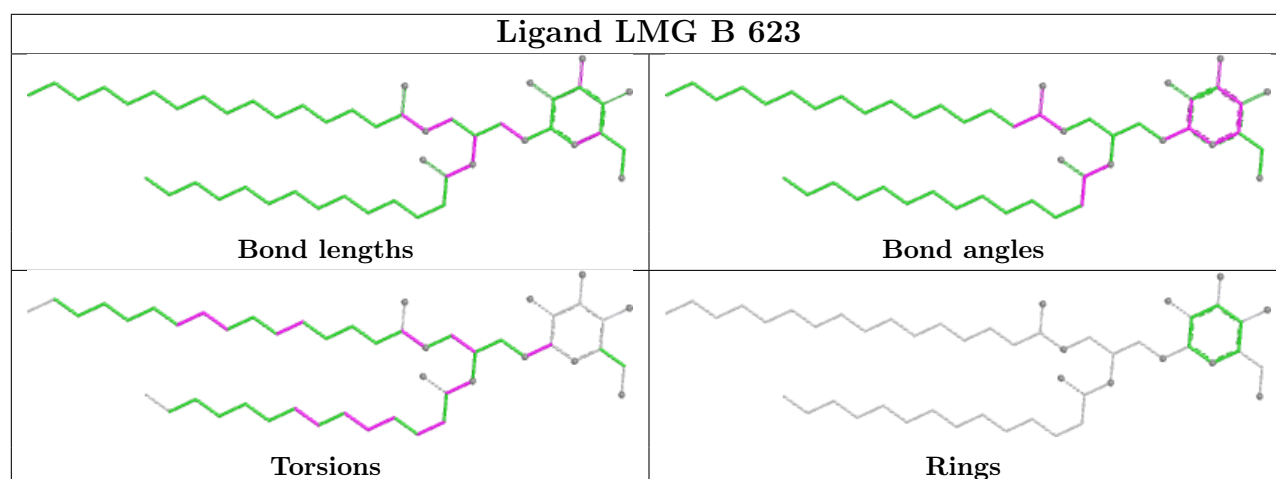
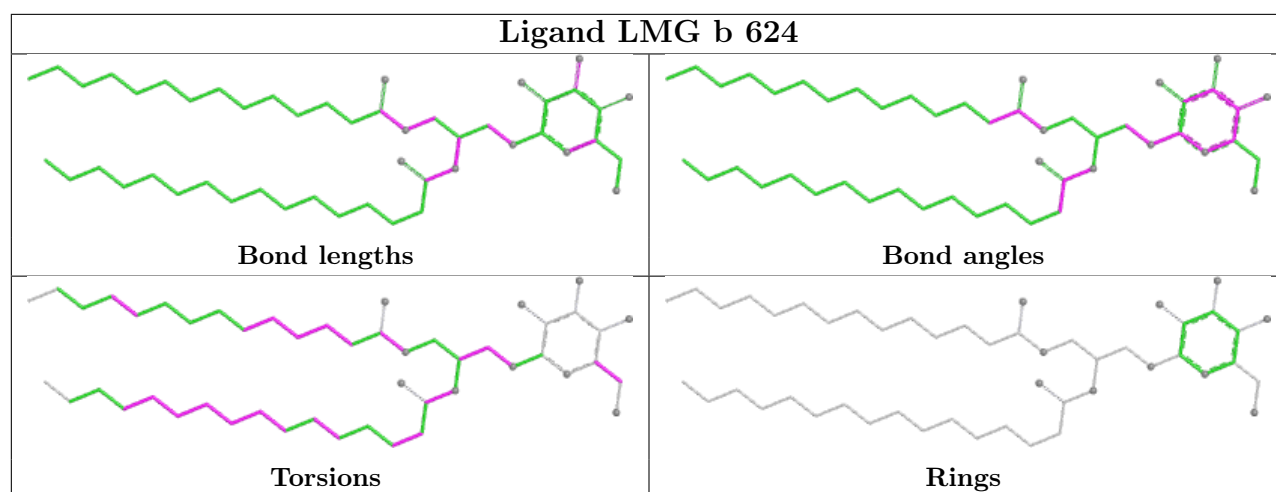


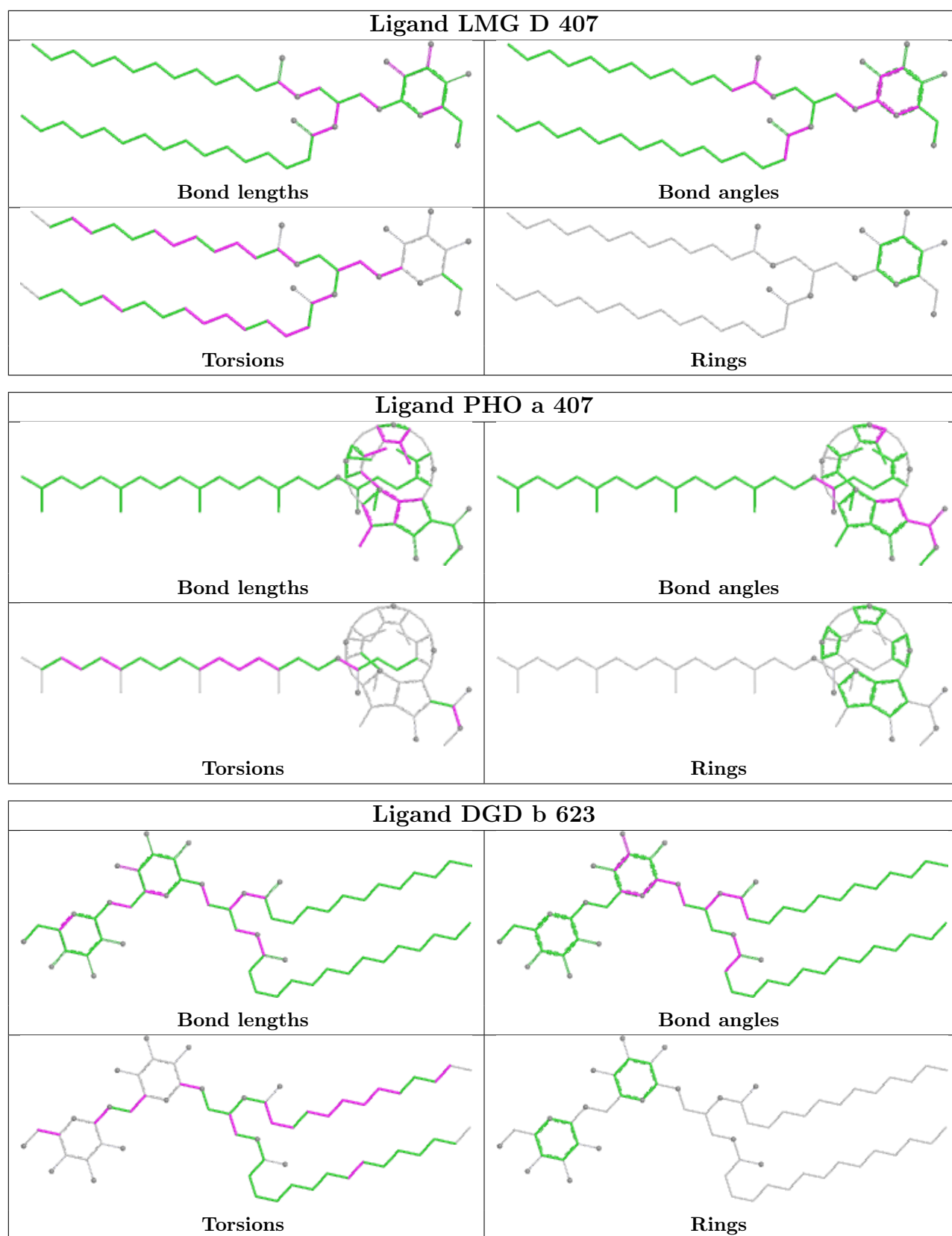




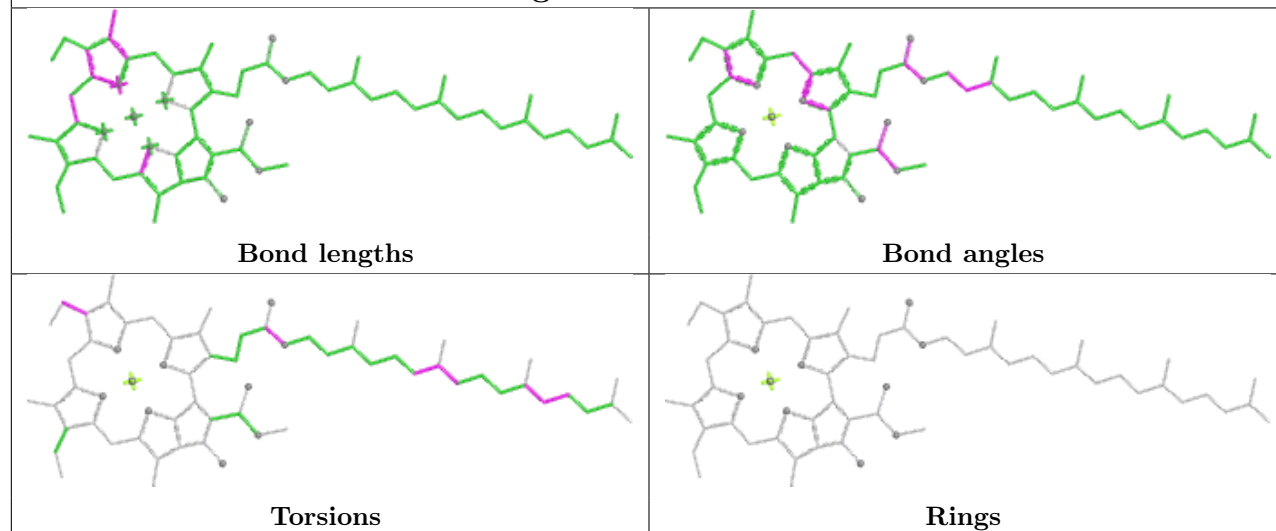




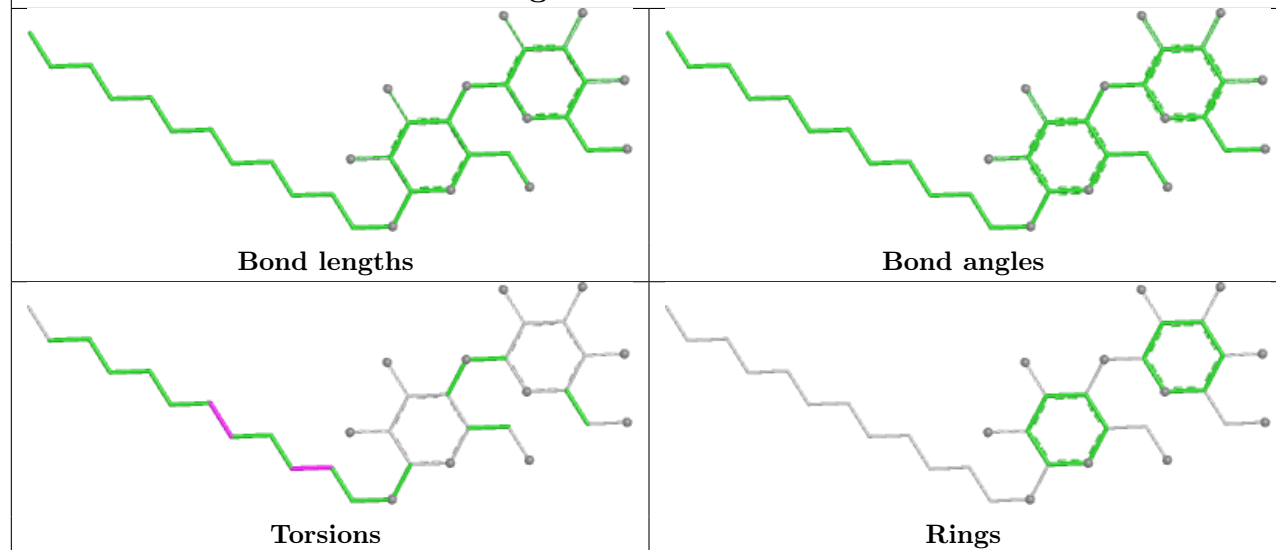




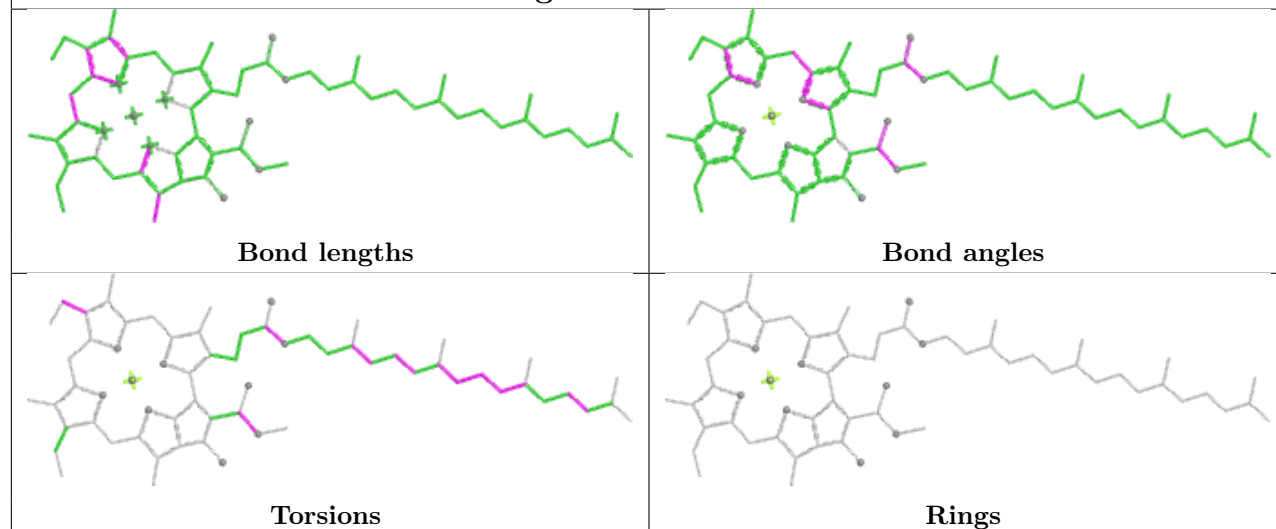
Ligand CLA B 615



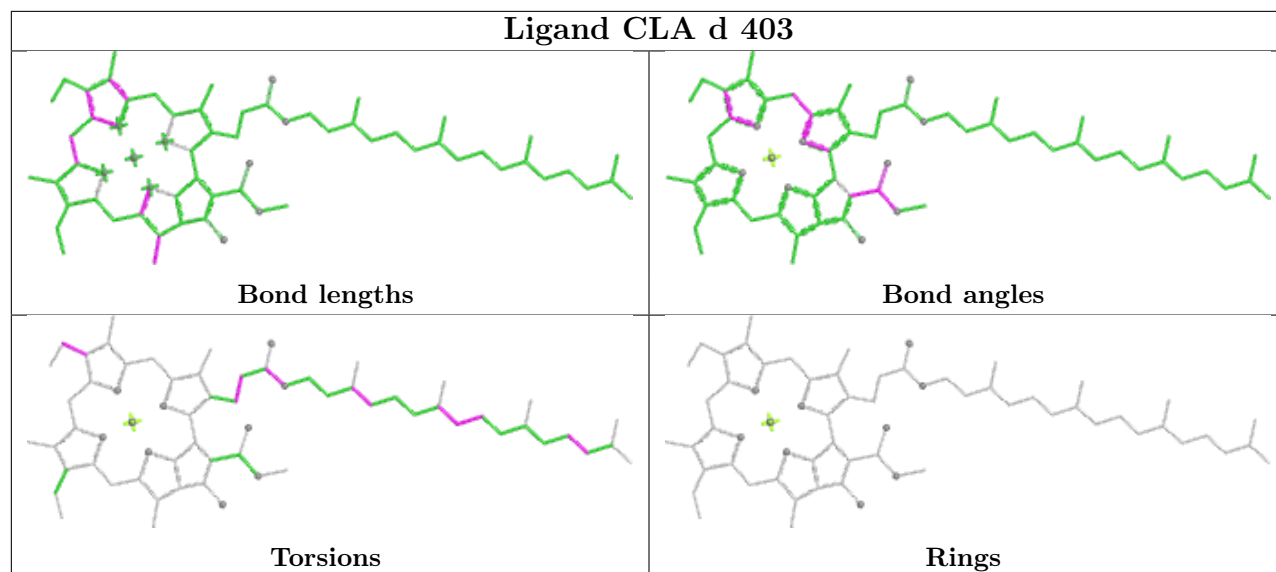
Ligand LMT B 624



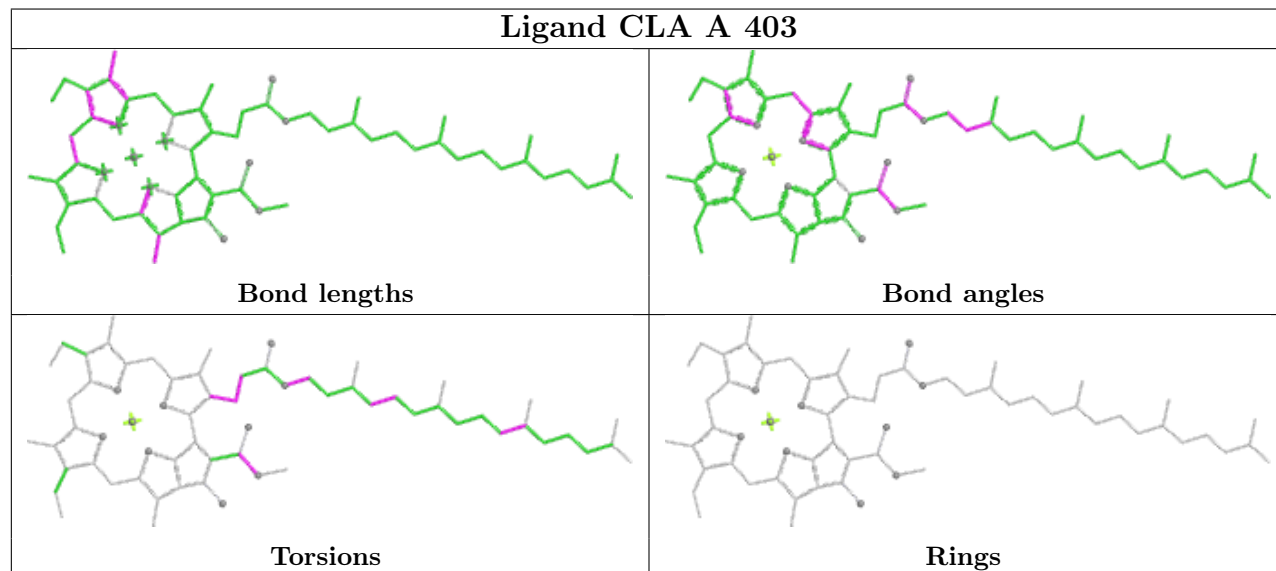
Ligand CLA b 609



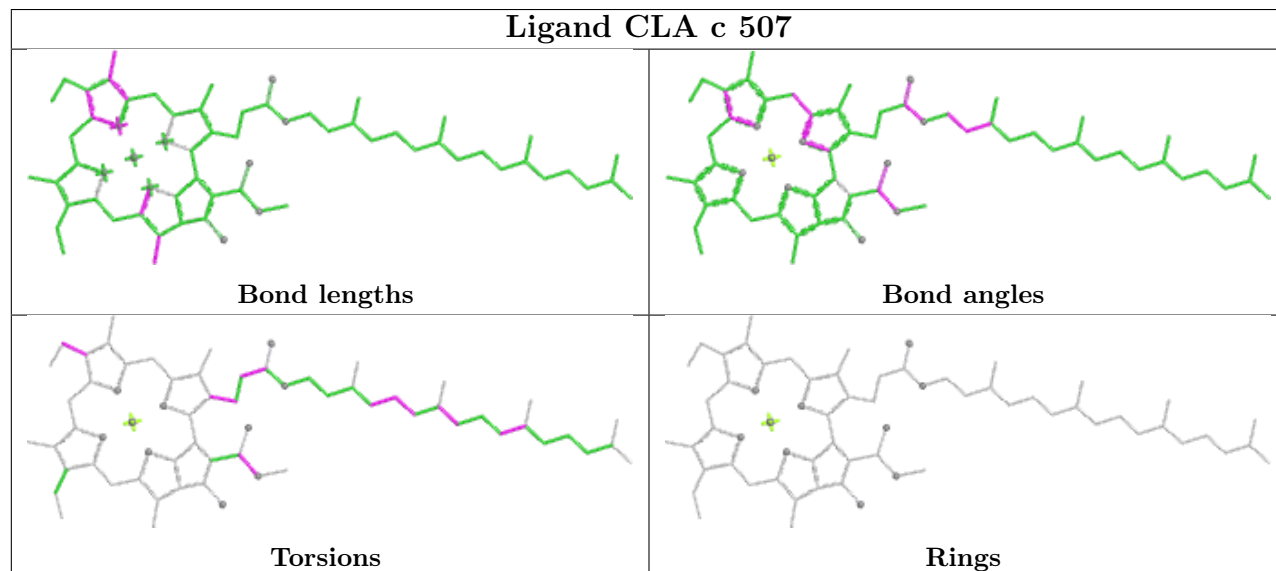
Ligand CLA d 403



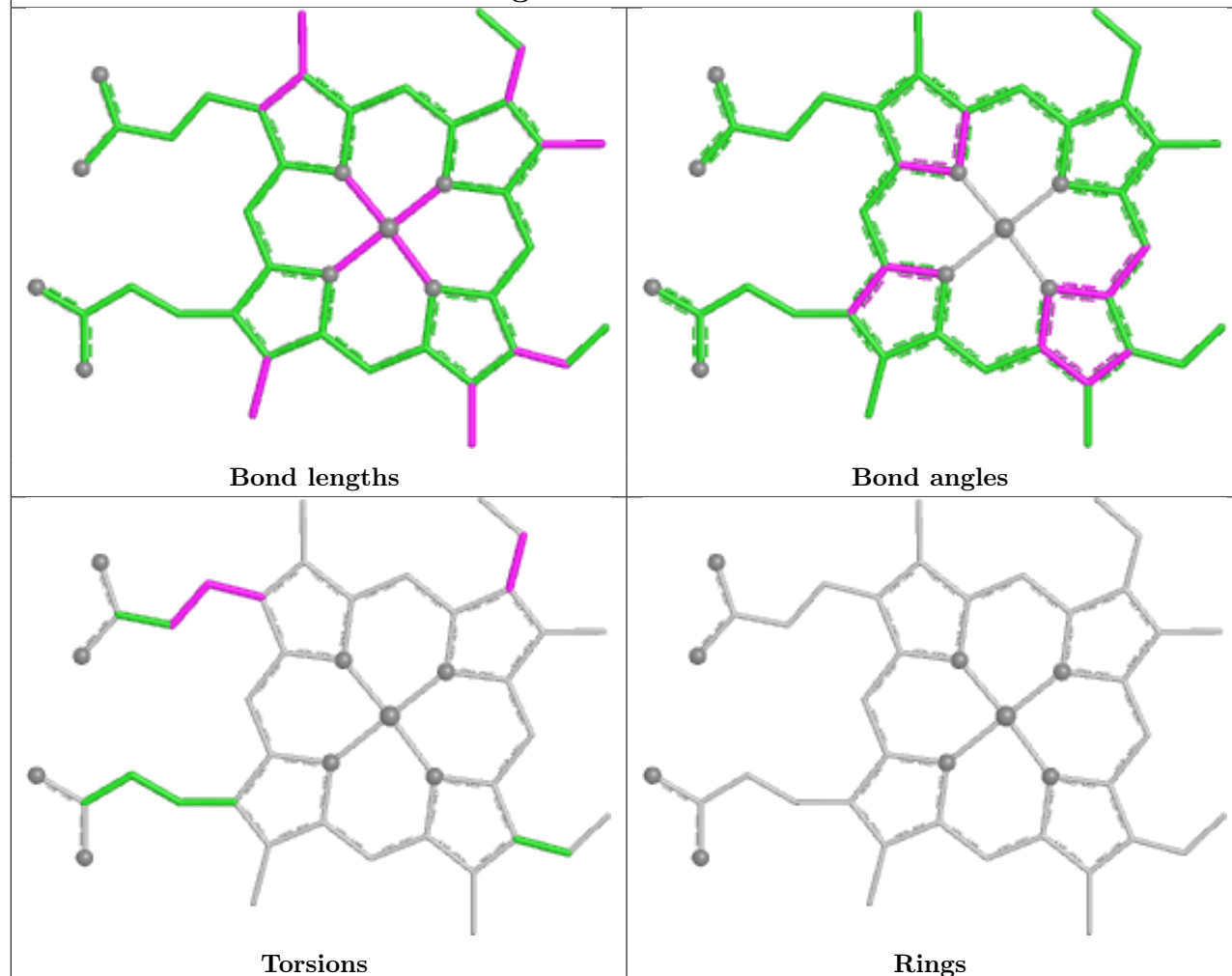
Ligand CLA A 403



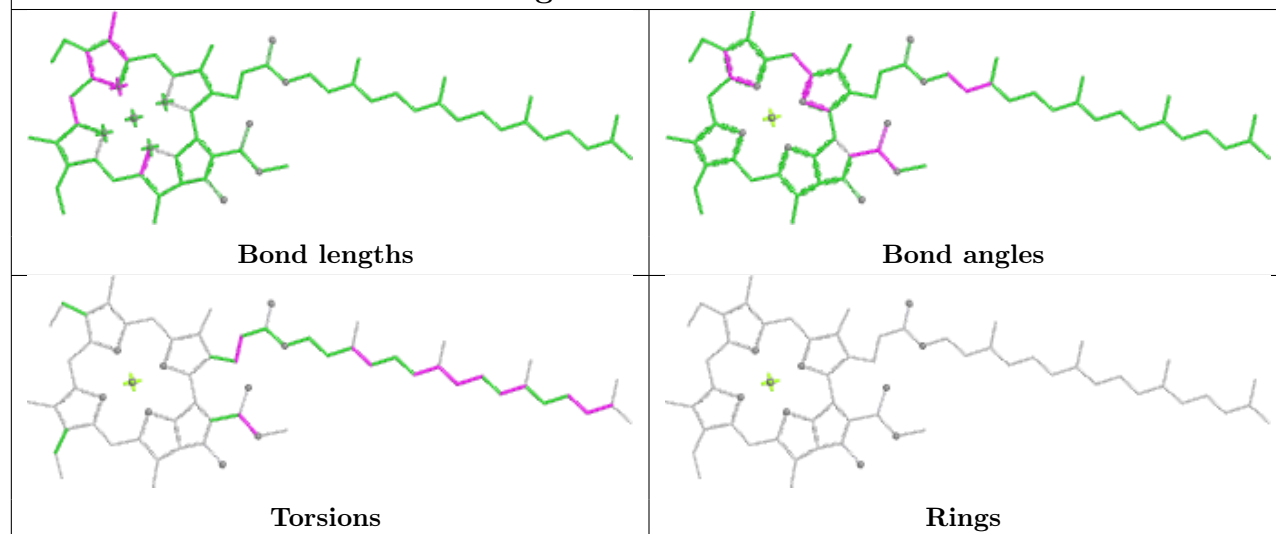
Ligand CLA c 507

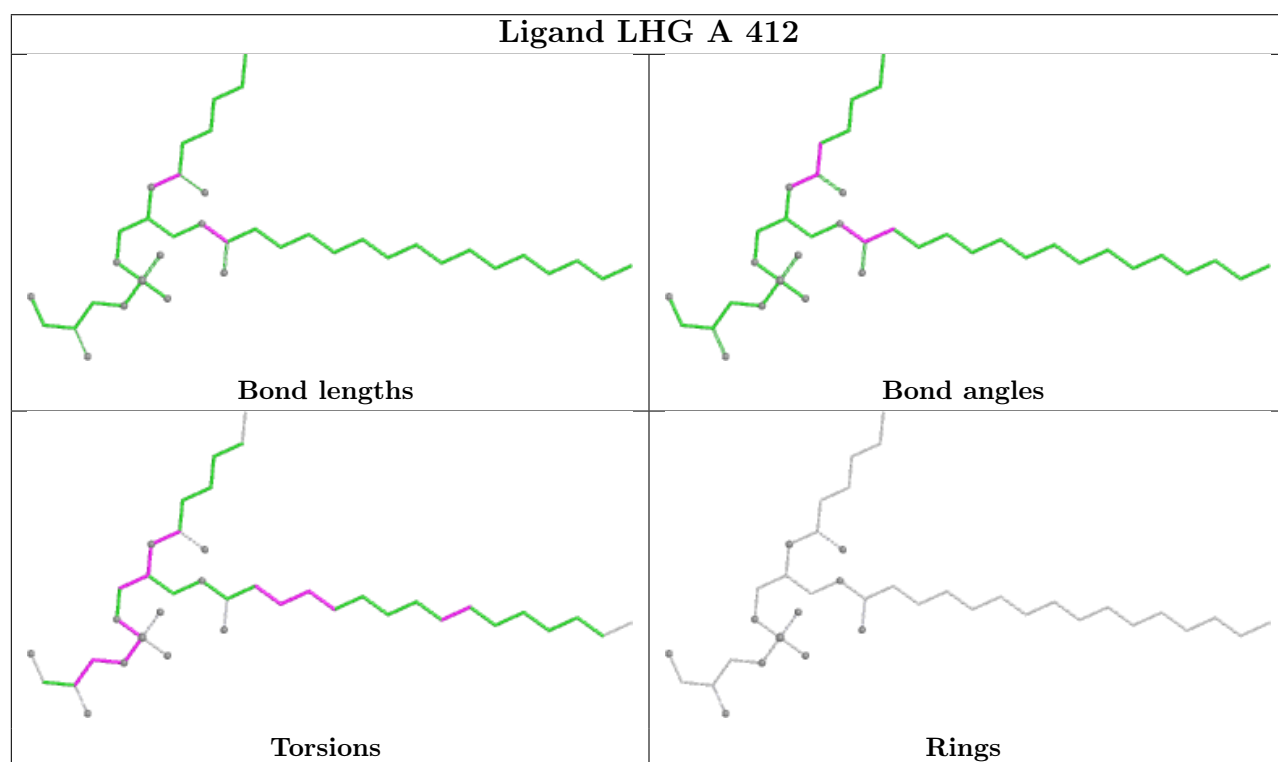
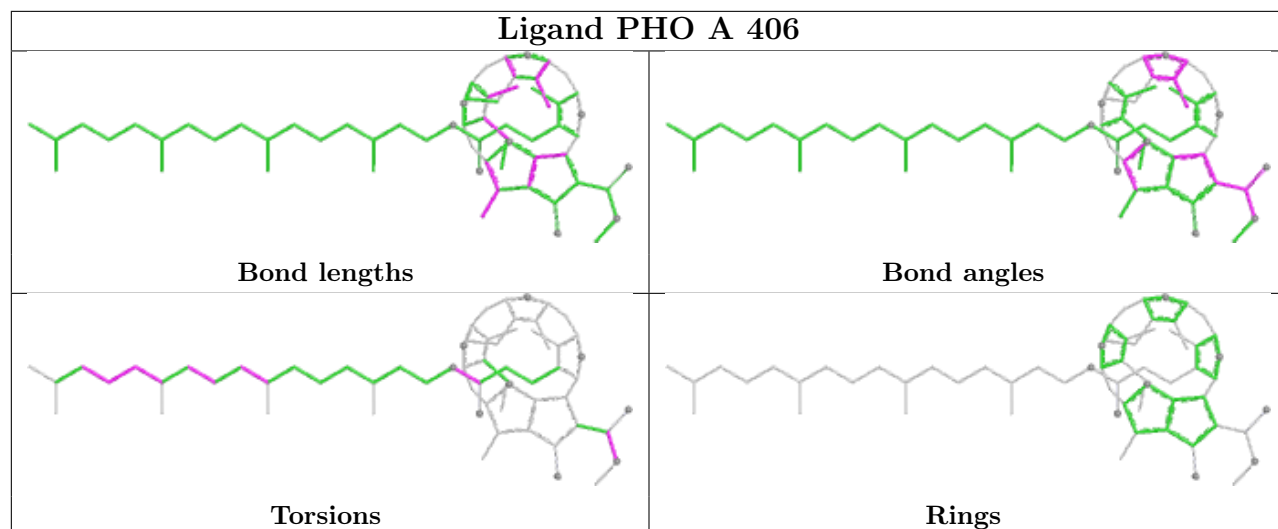


Ligand HEM v 201

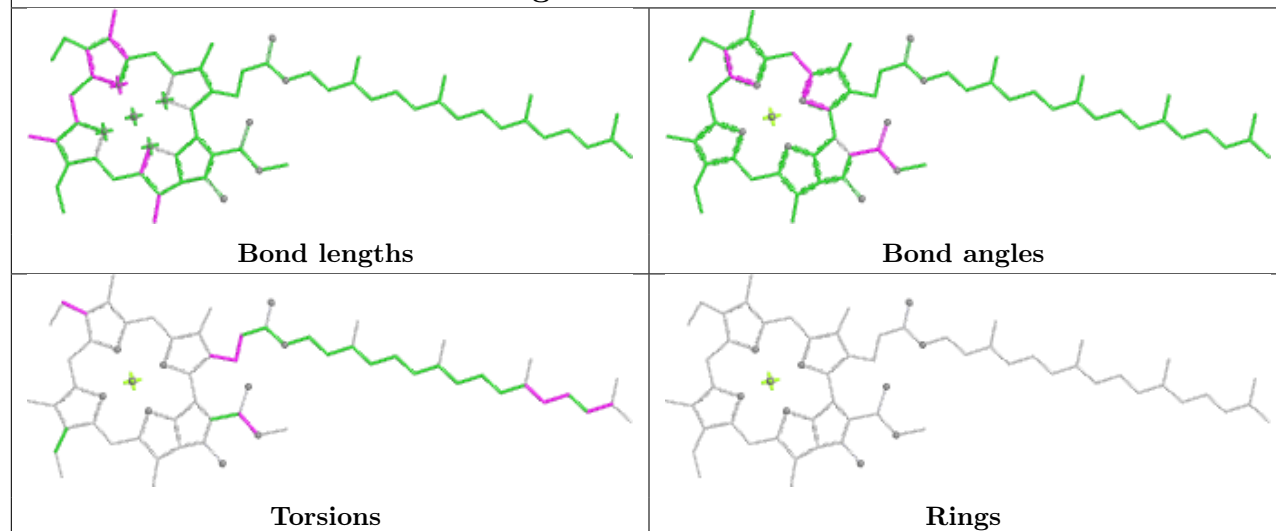


Ligand CLA b 607

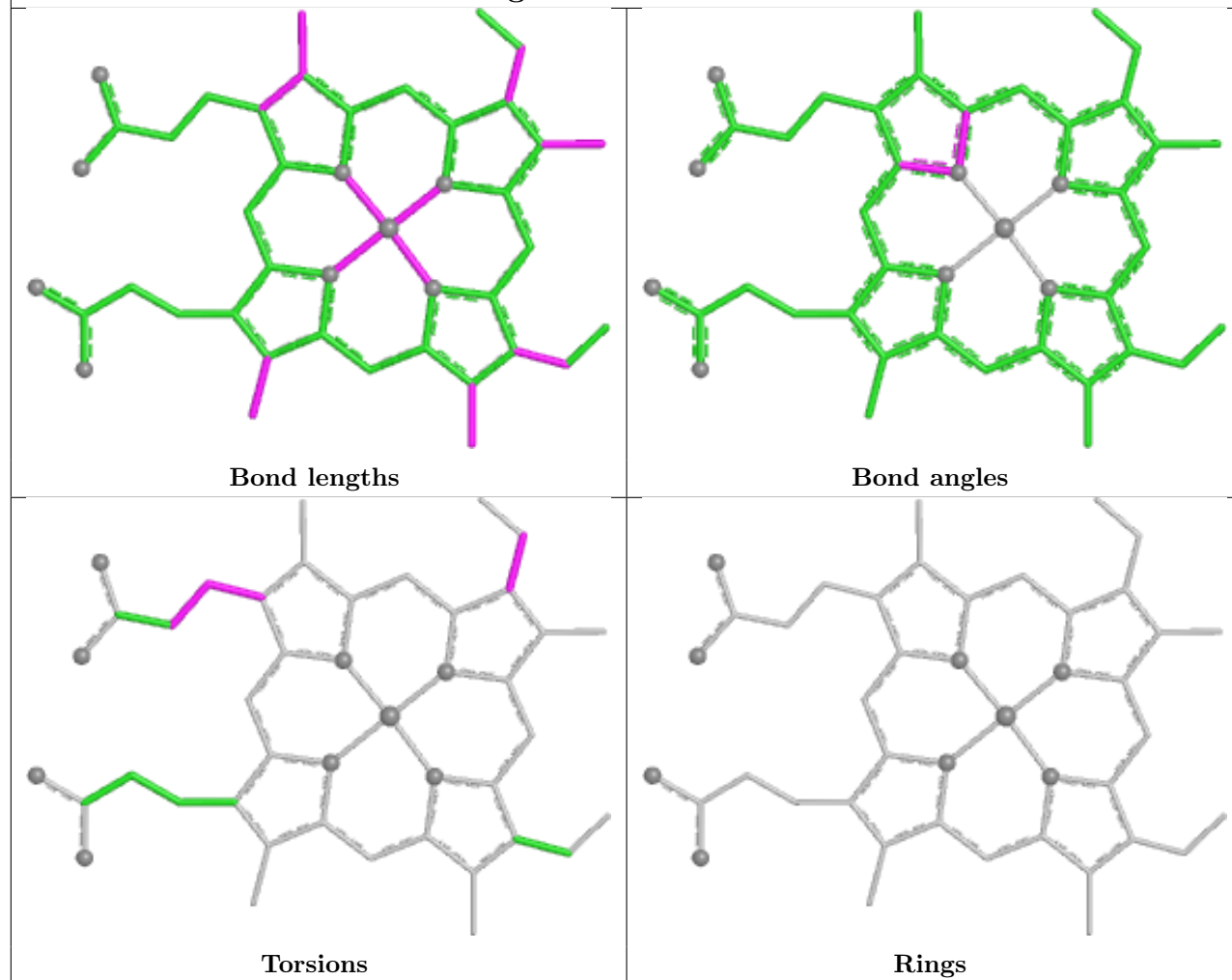


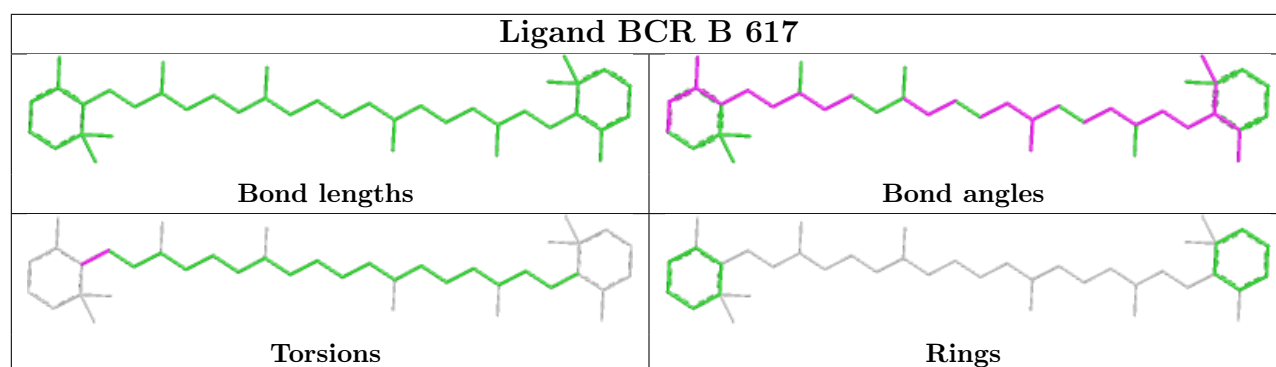
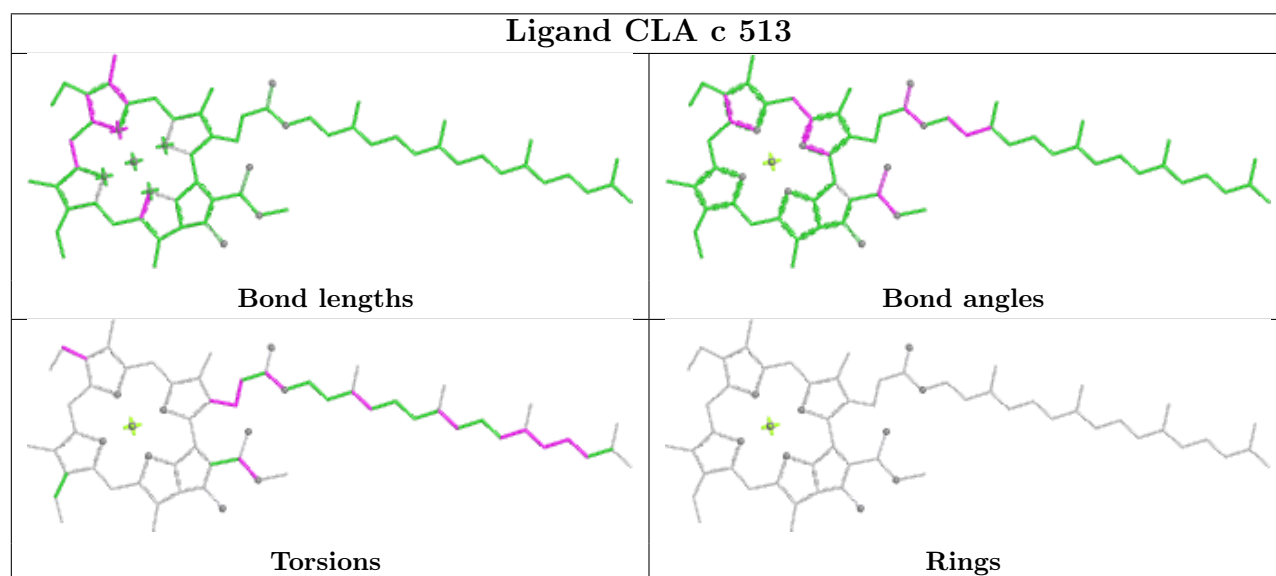
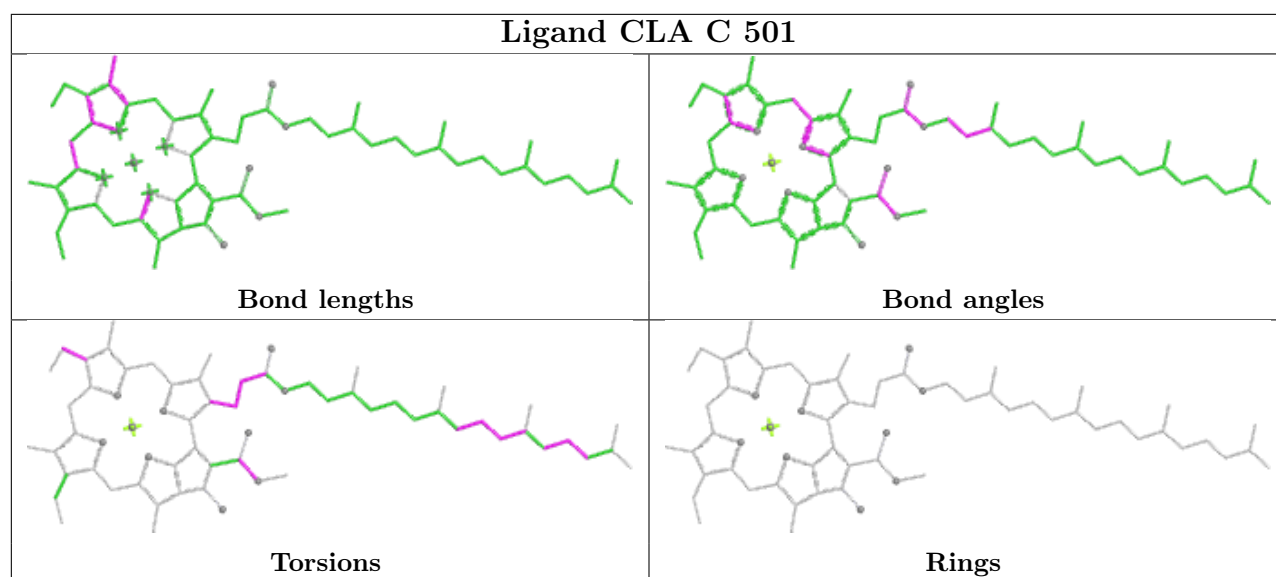


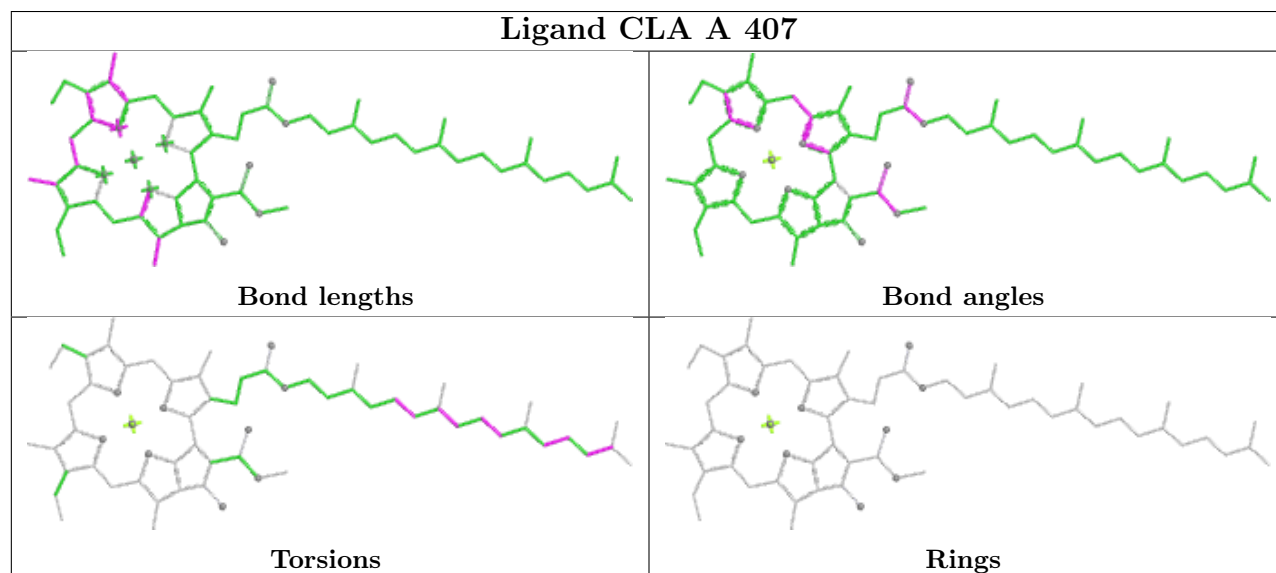
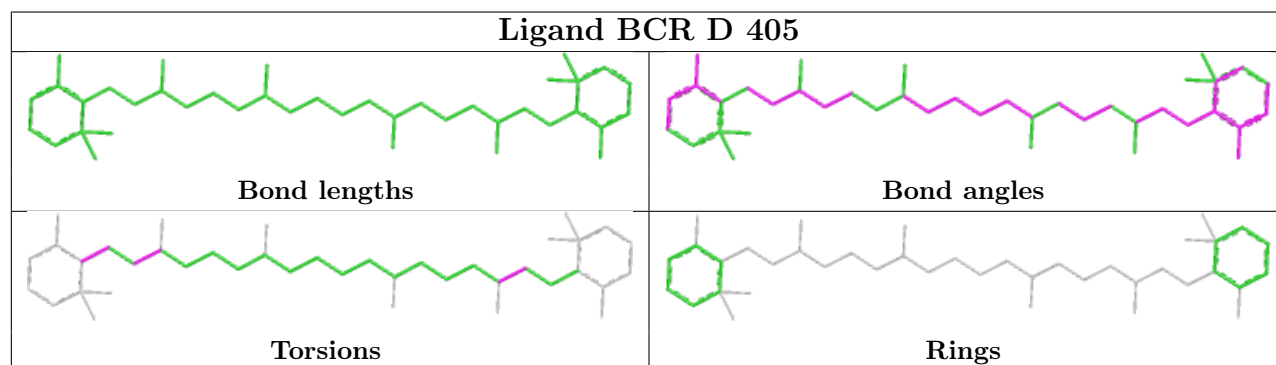
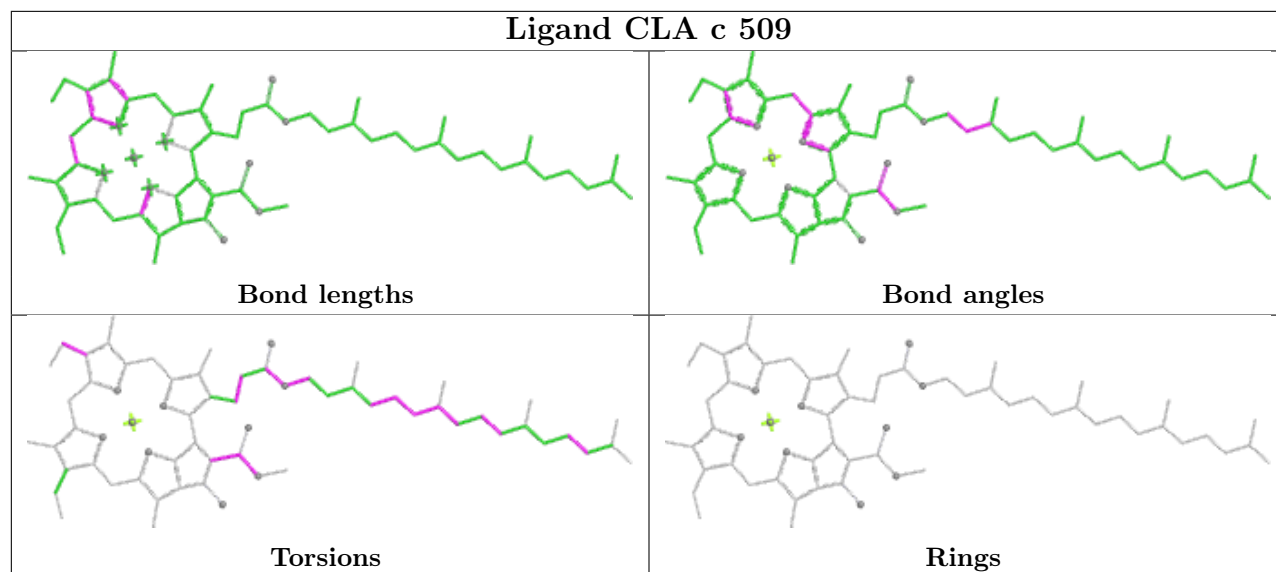
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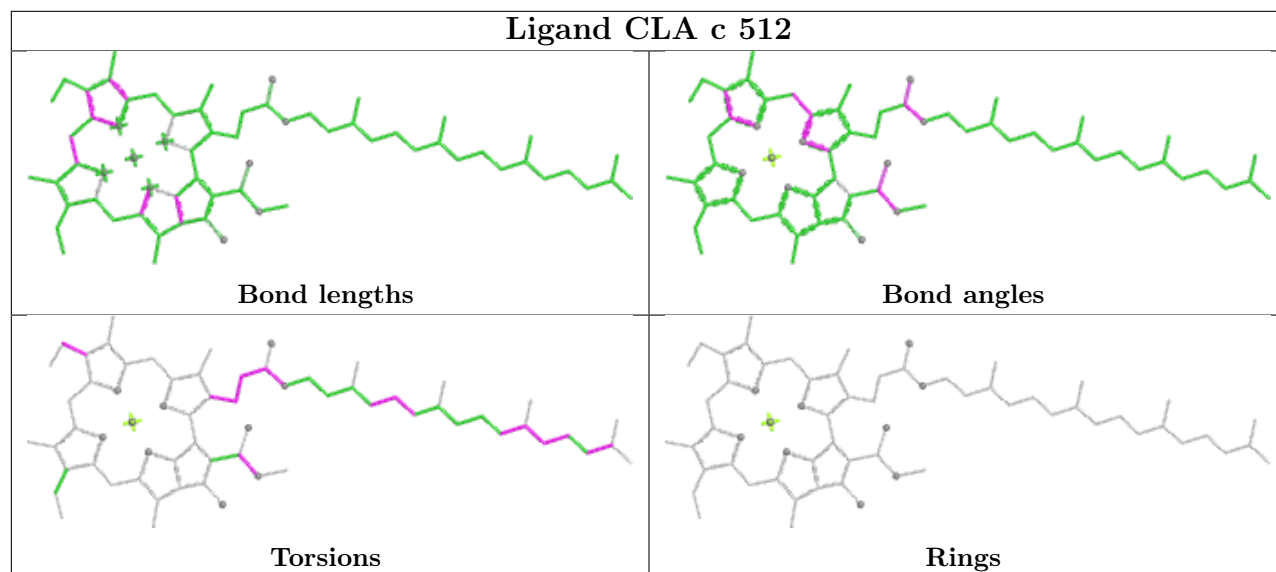
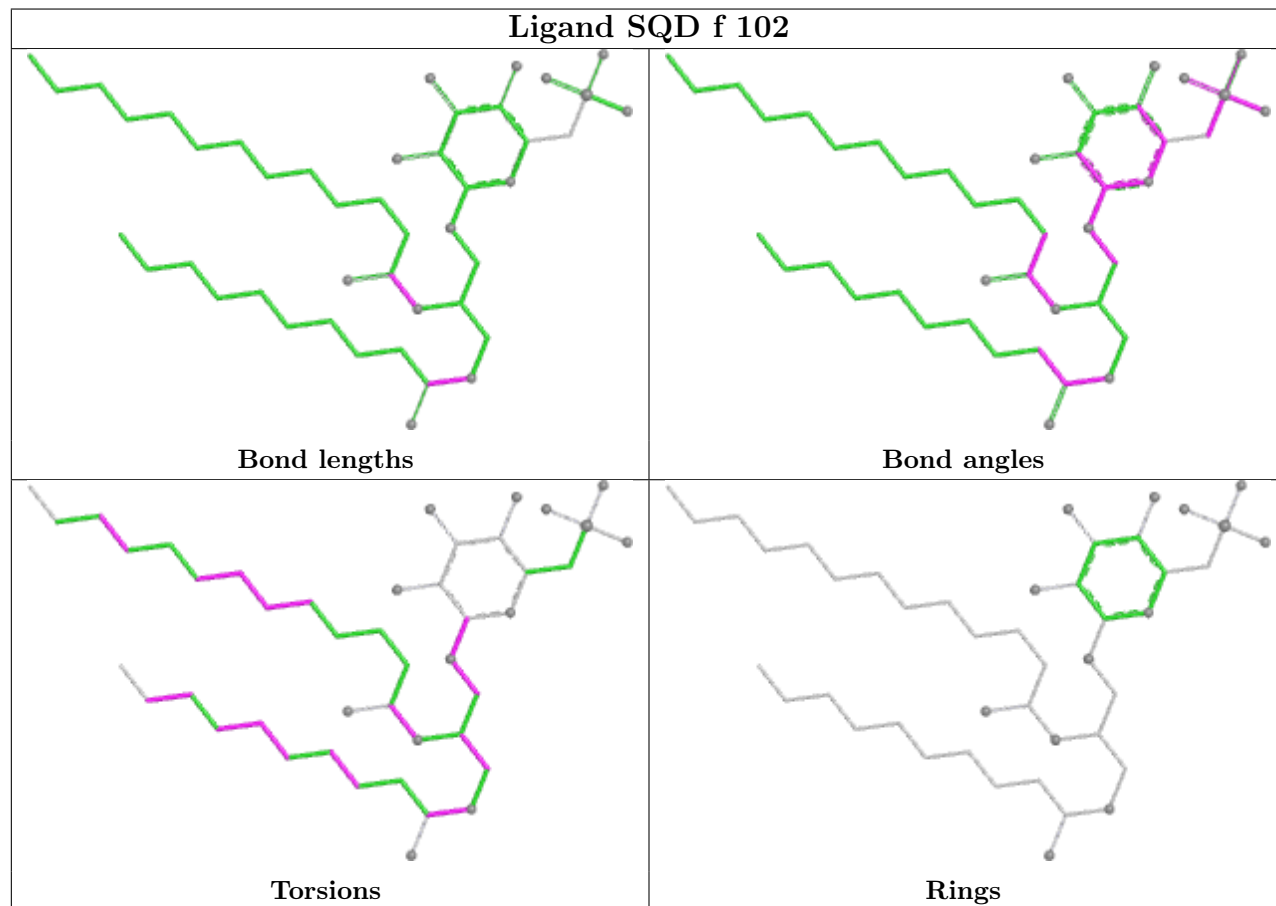


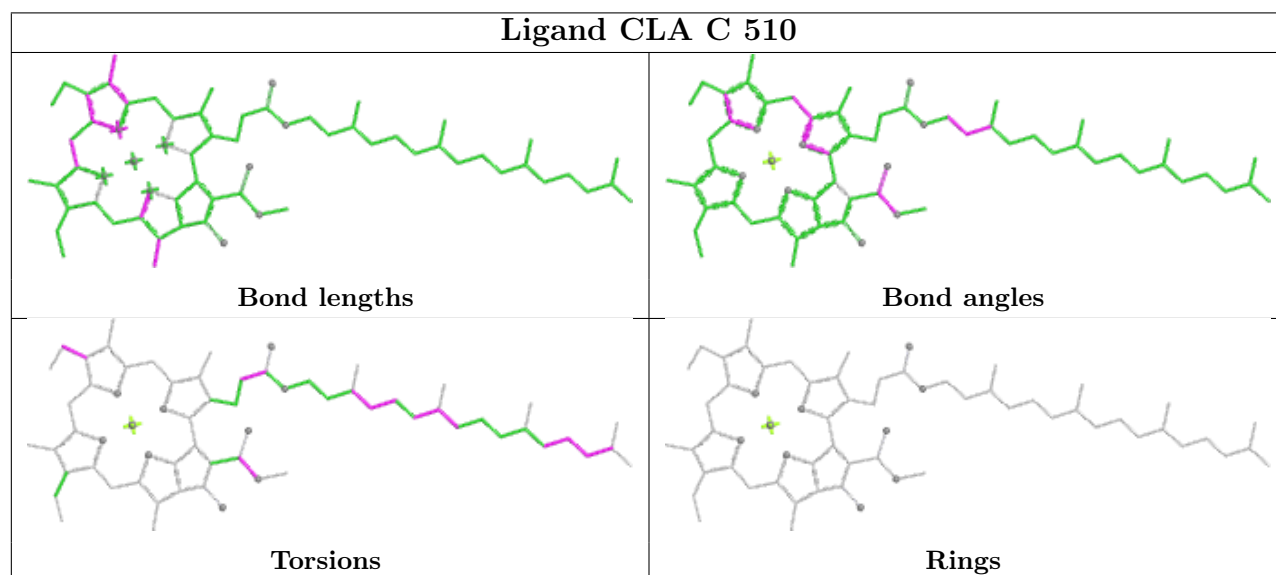
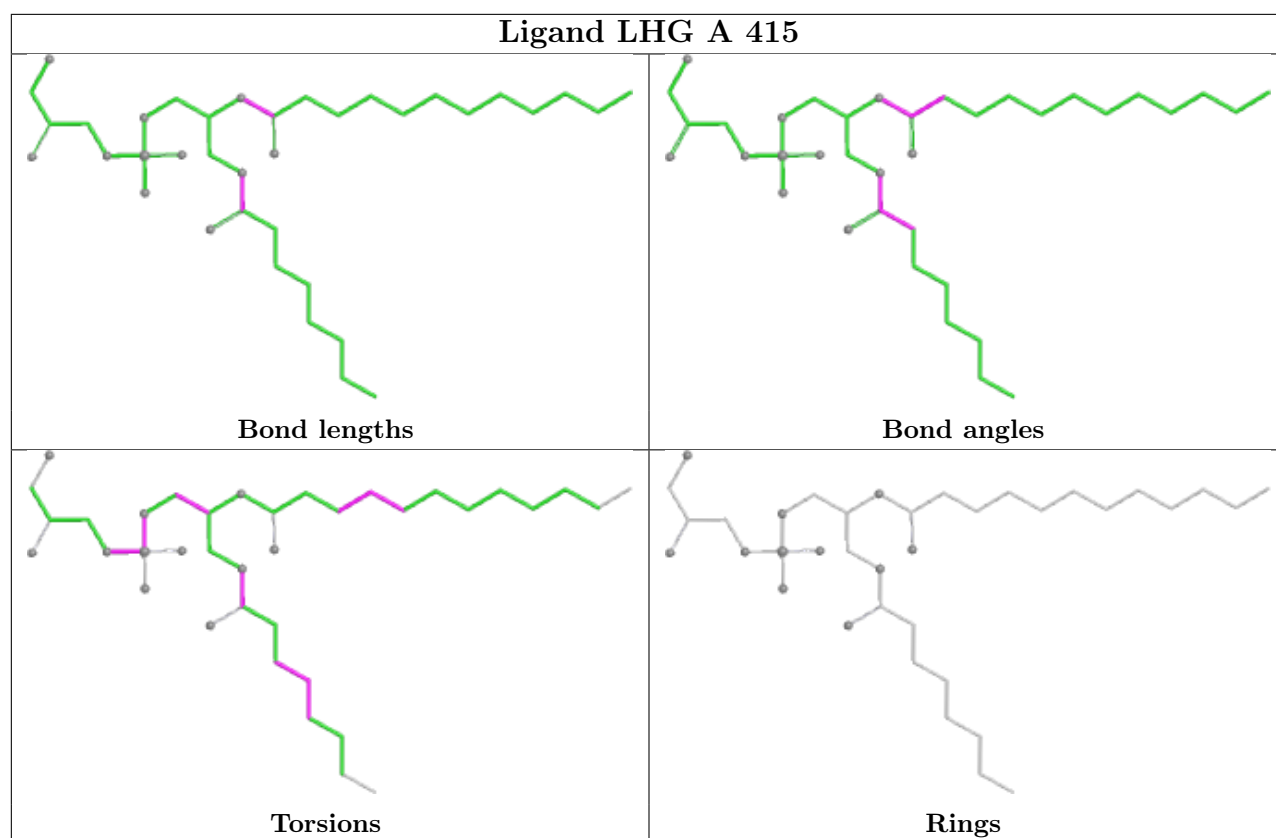
Ligand HEM V 201

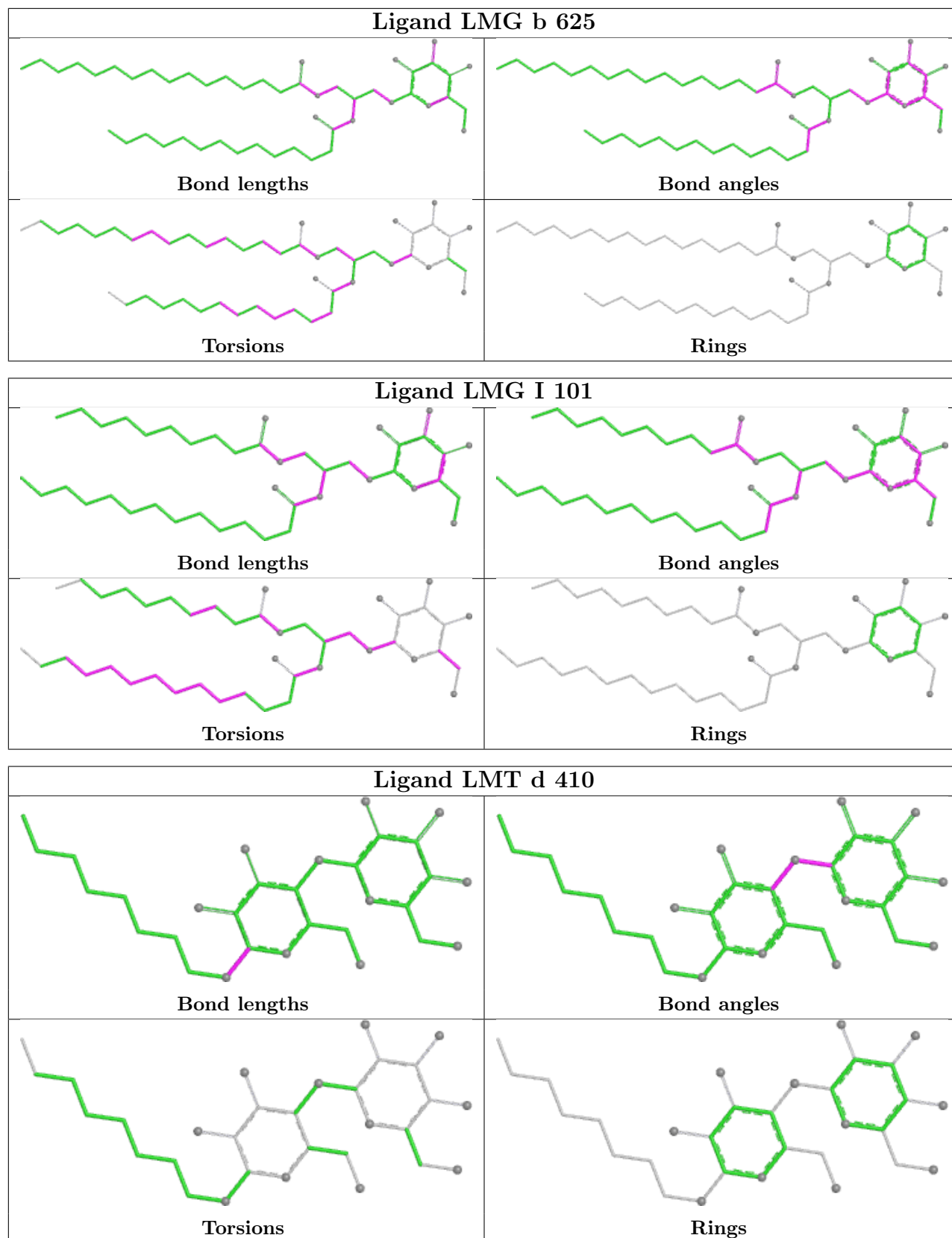




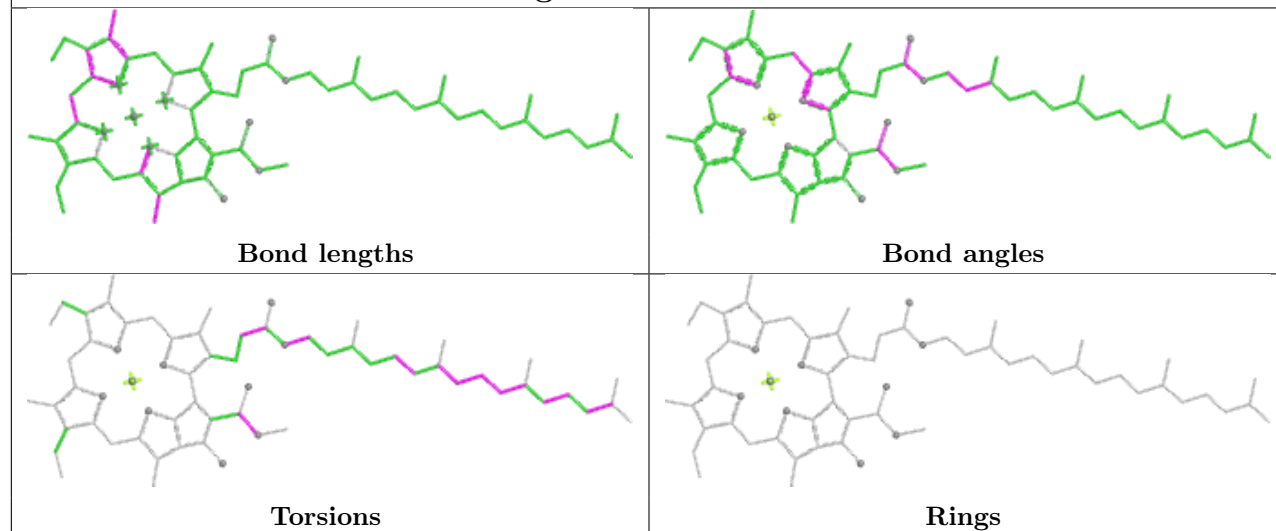


Ligand CLA c 512**Ligand SQD f 102**

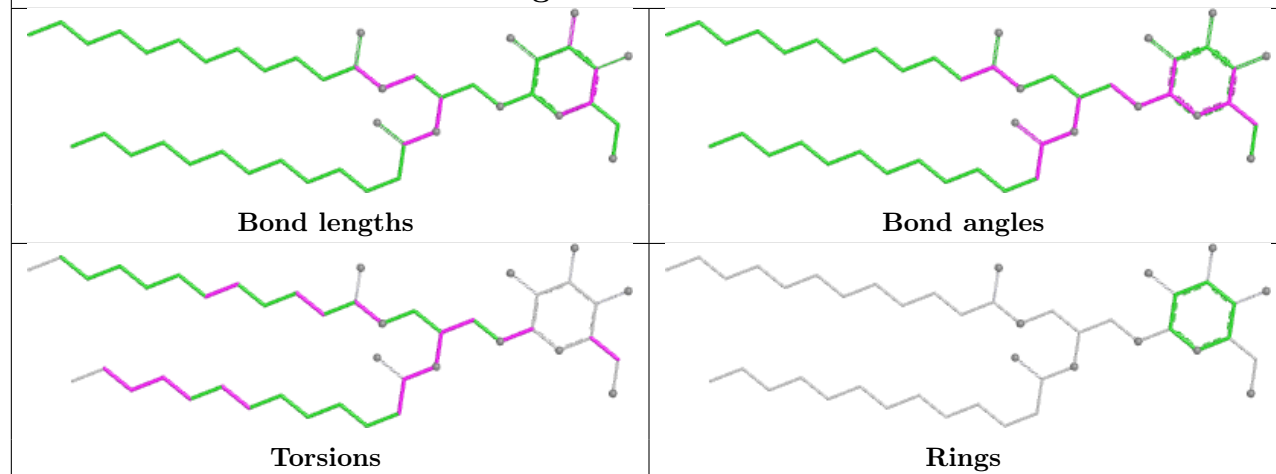




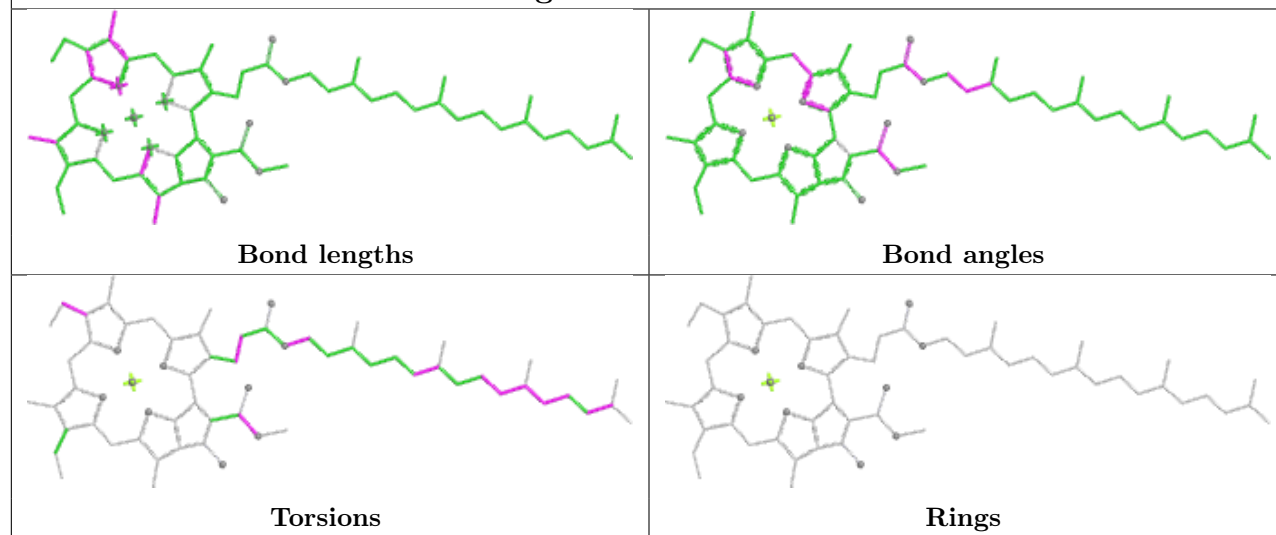
Ligand CLA b 617

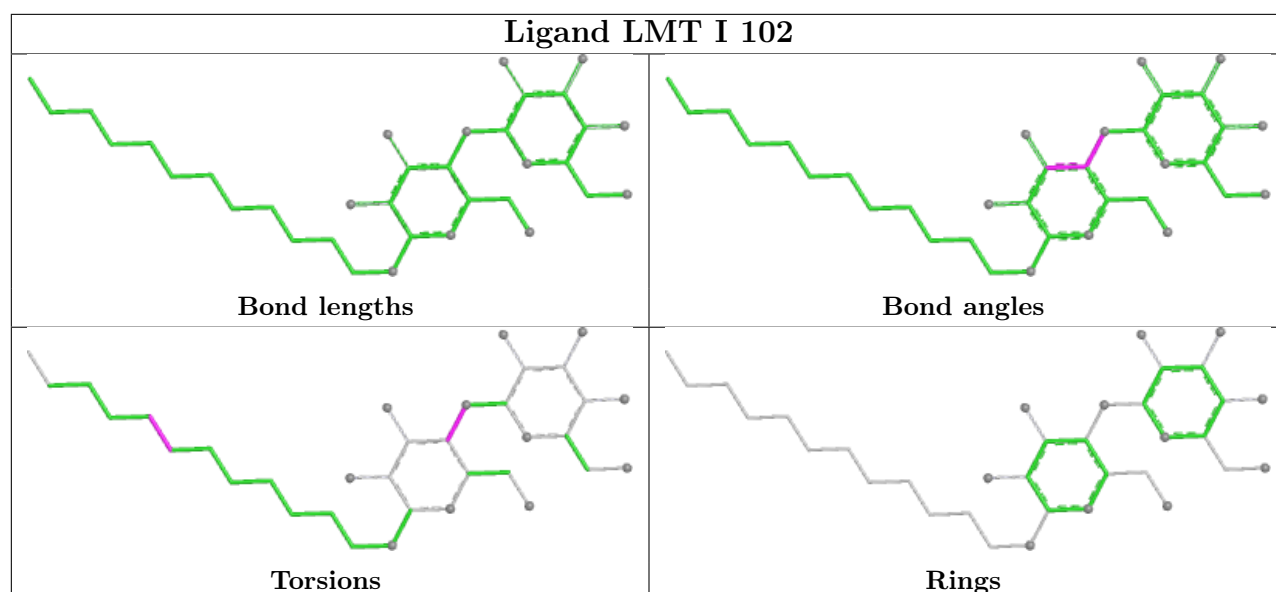
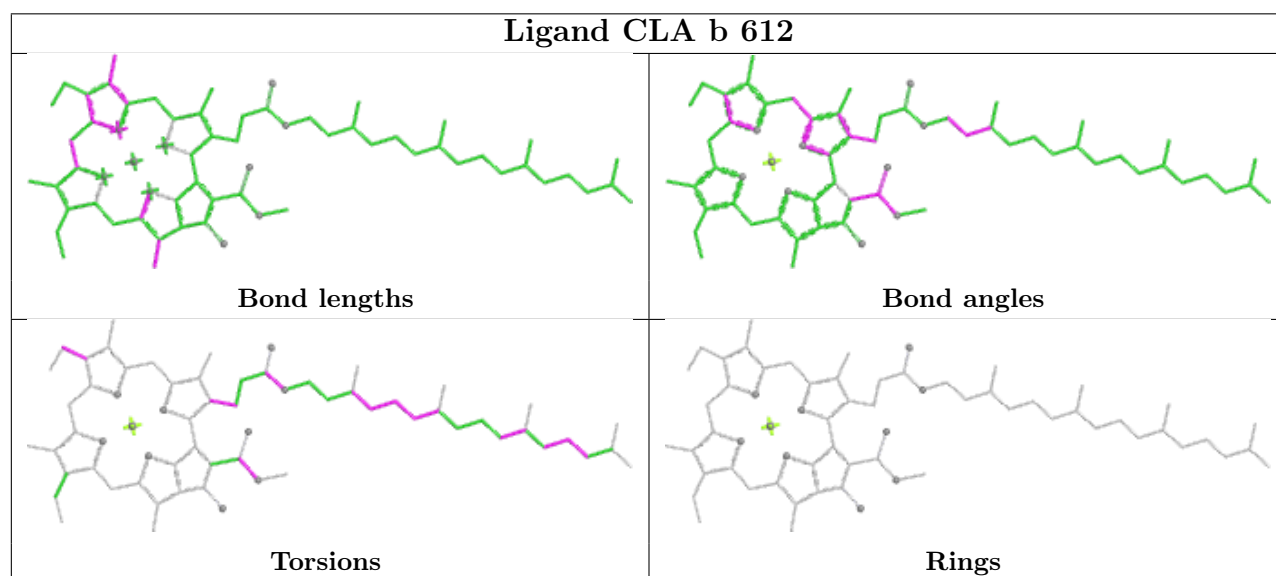
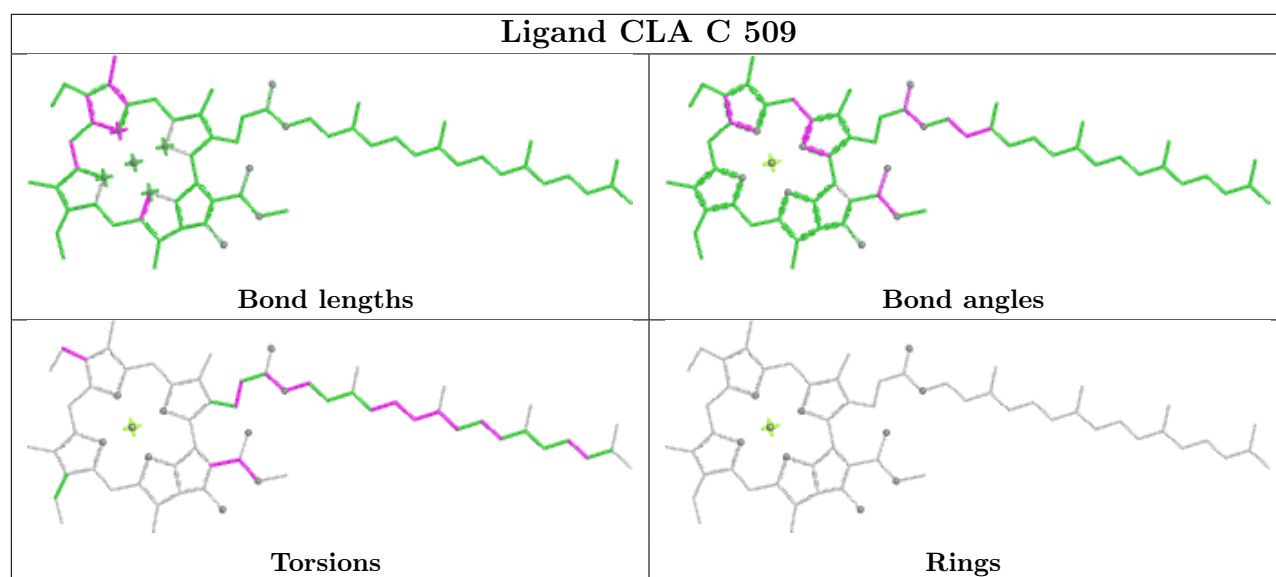


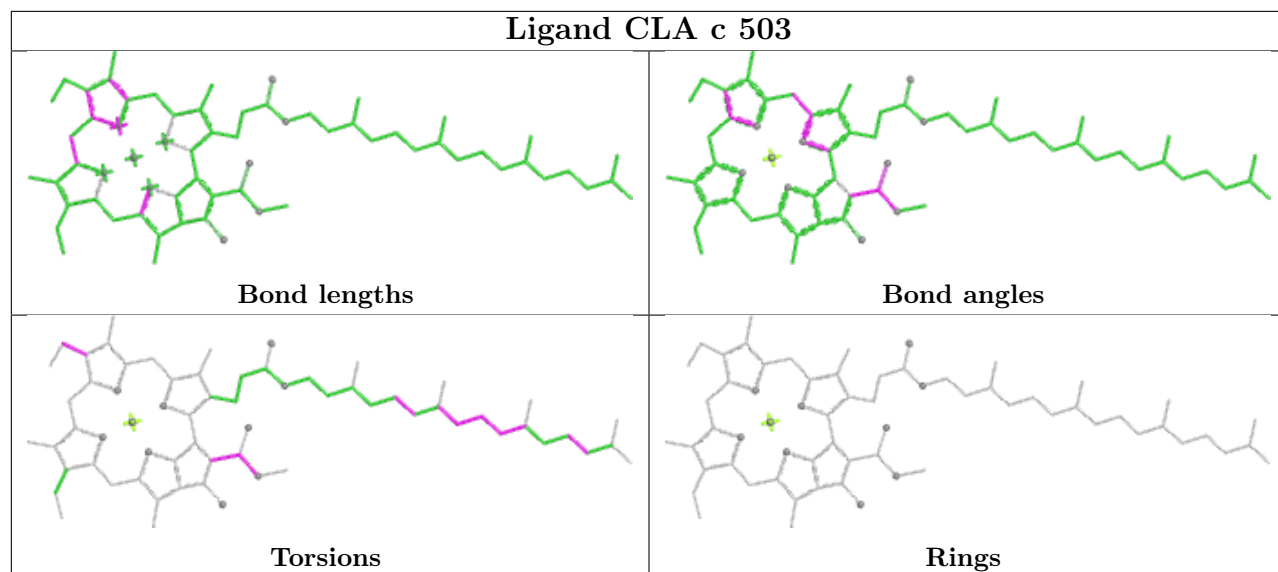
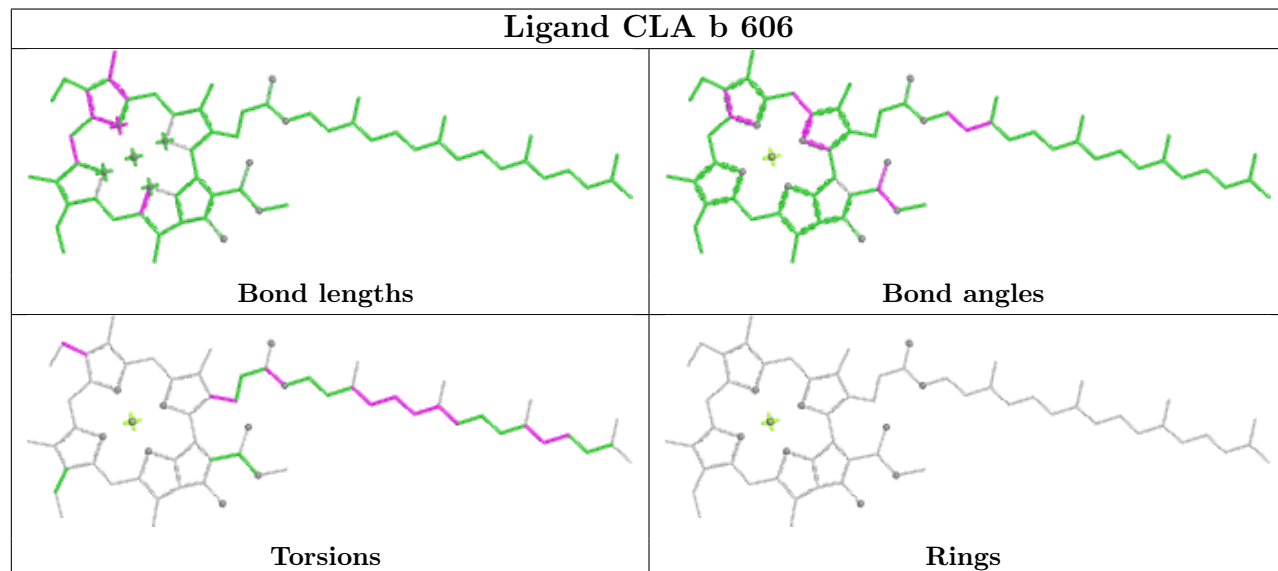
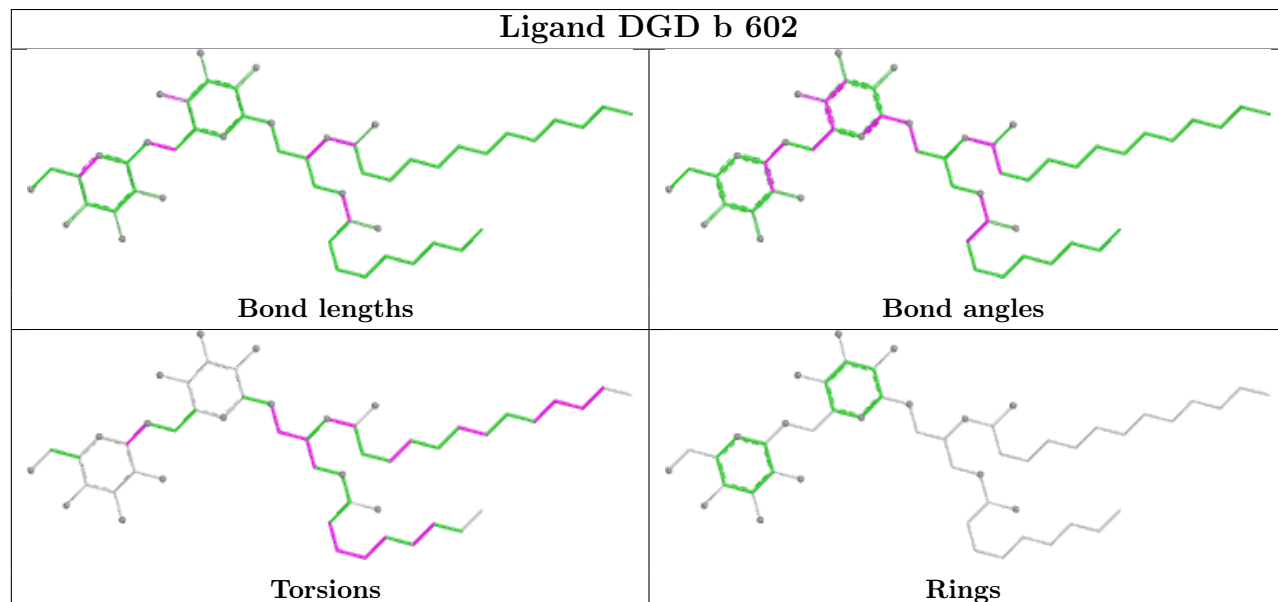
Ligand LMG e 101



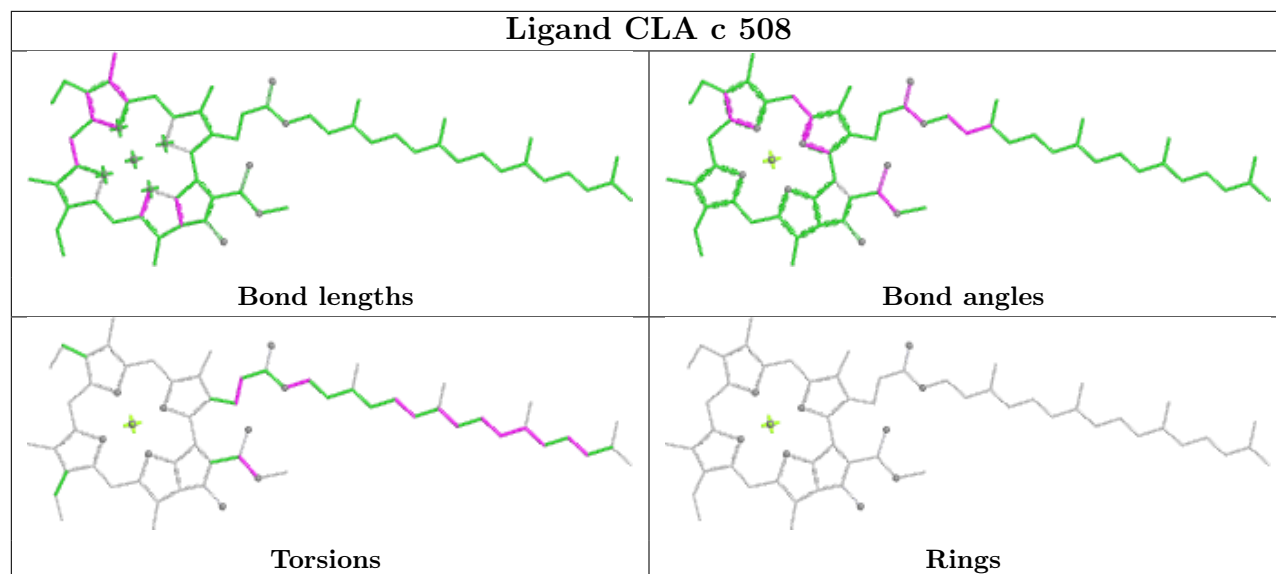
Ligand CLA b 605



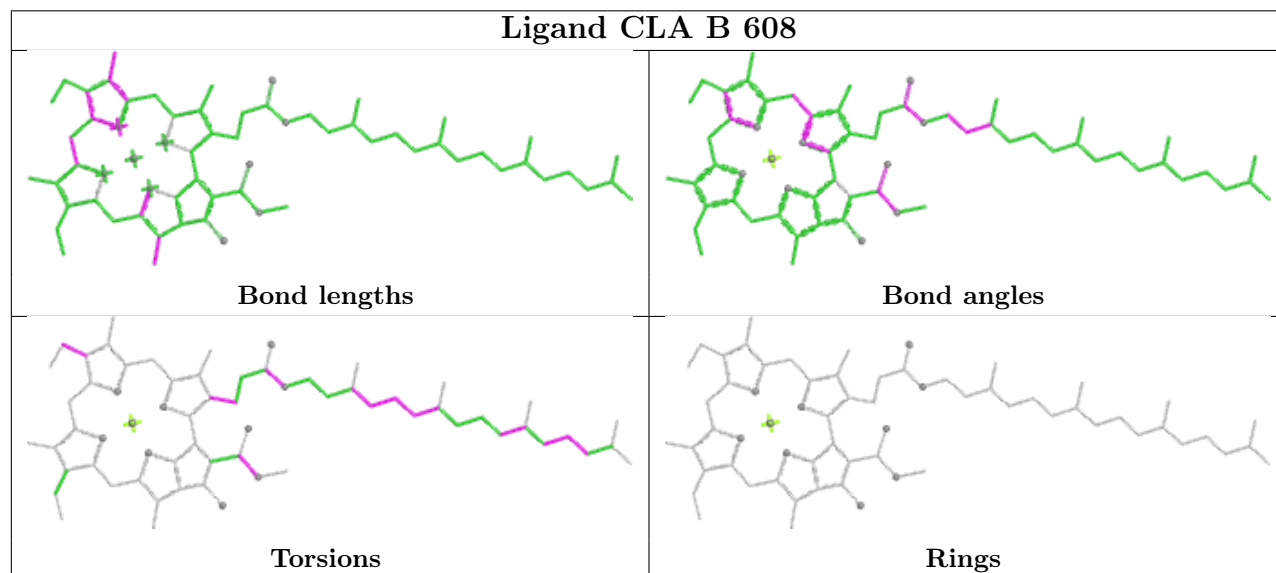


Ligand CLA c 503**Ligand CLA b 606****Ligand DGD b 602**

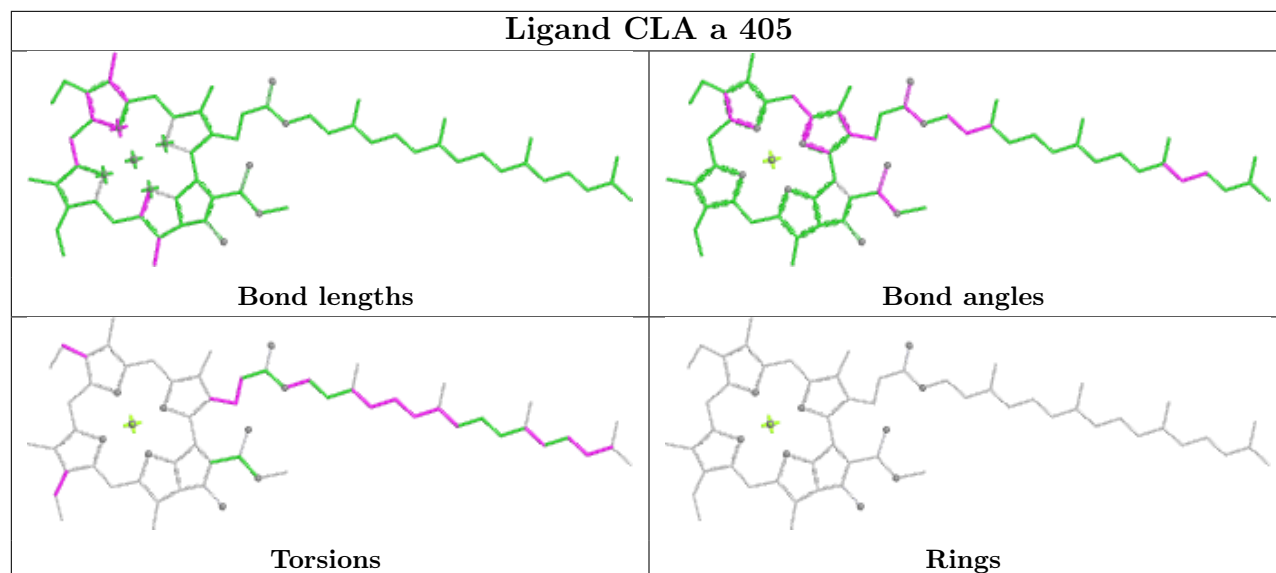
Ligand CLA c 508

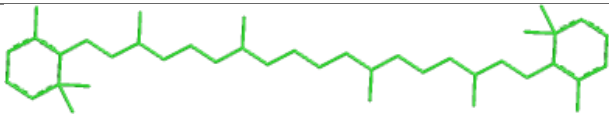
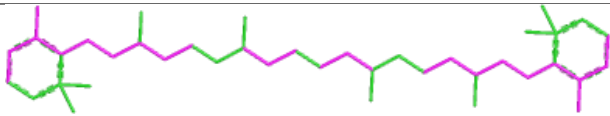
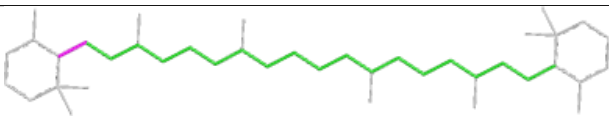
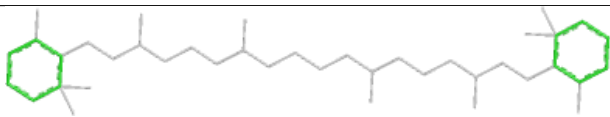


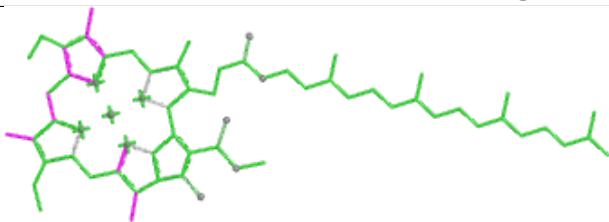
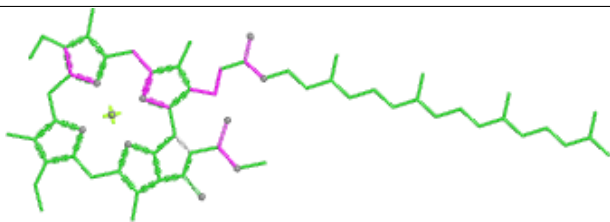
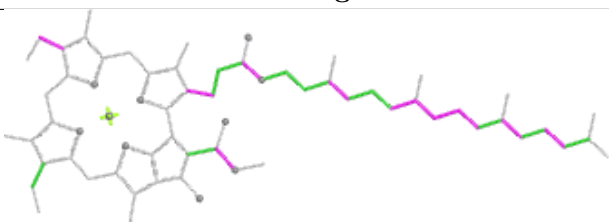
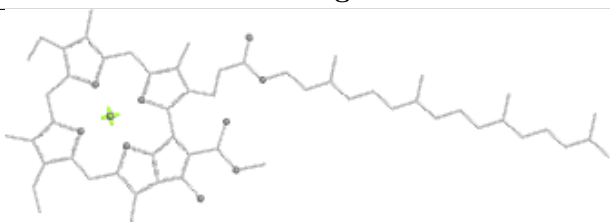
Ligand CLA B 608

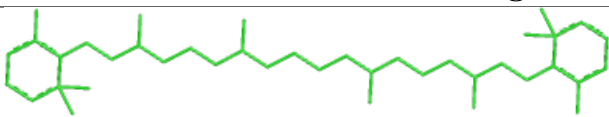
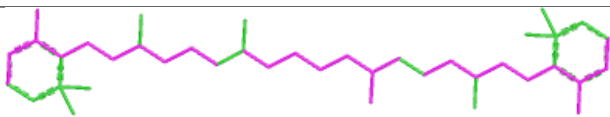
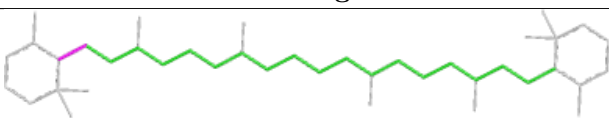
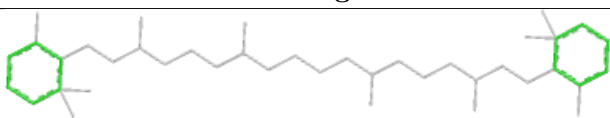


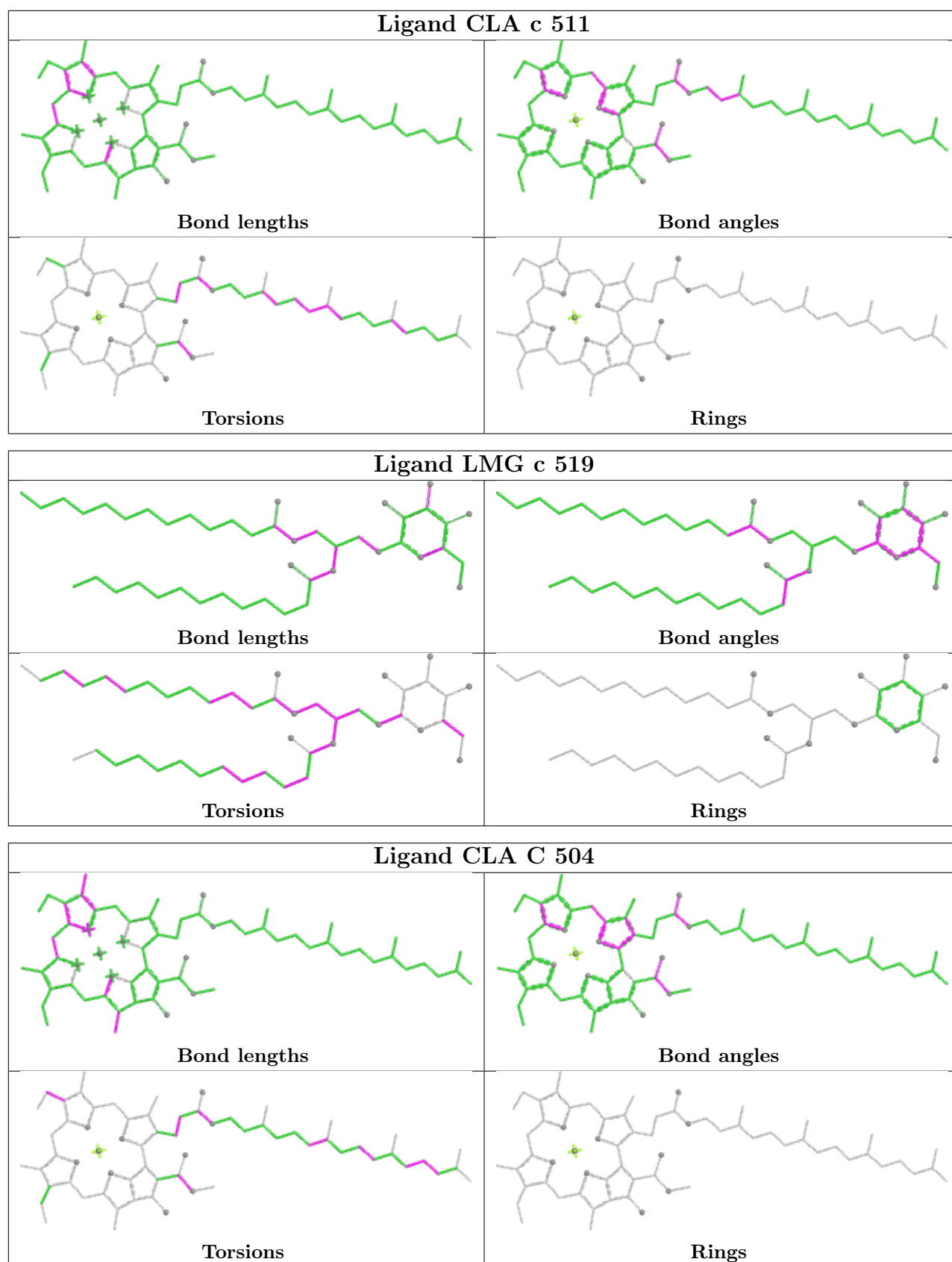
Ligand CLA a 405

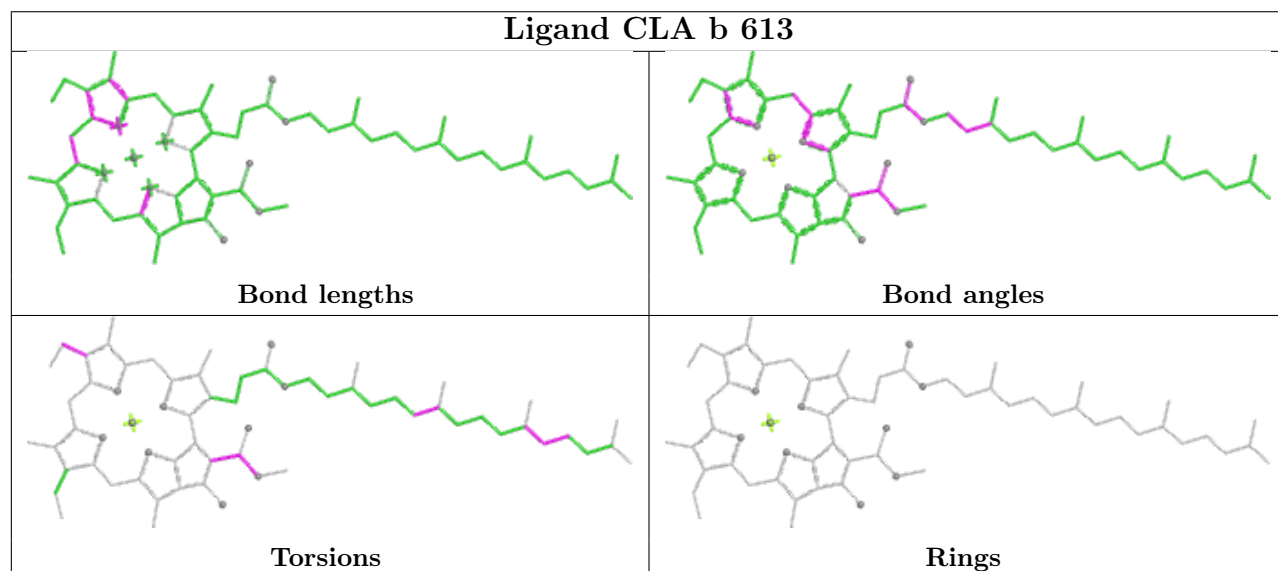
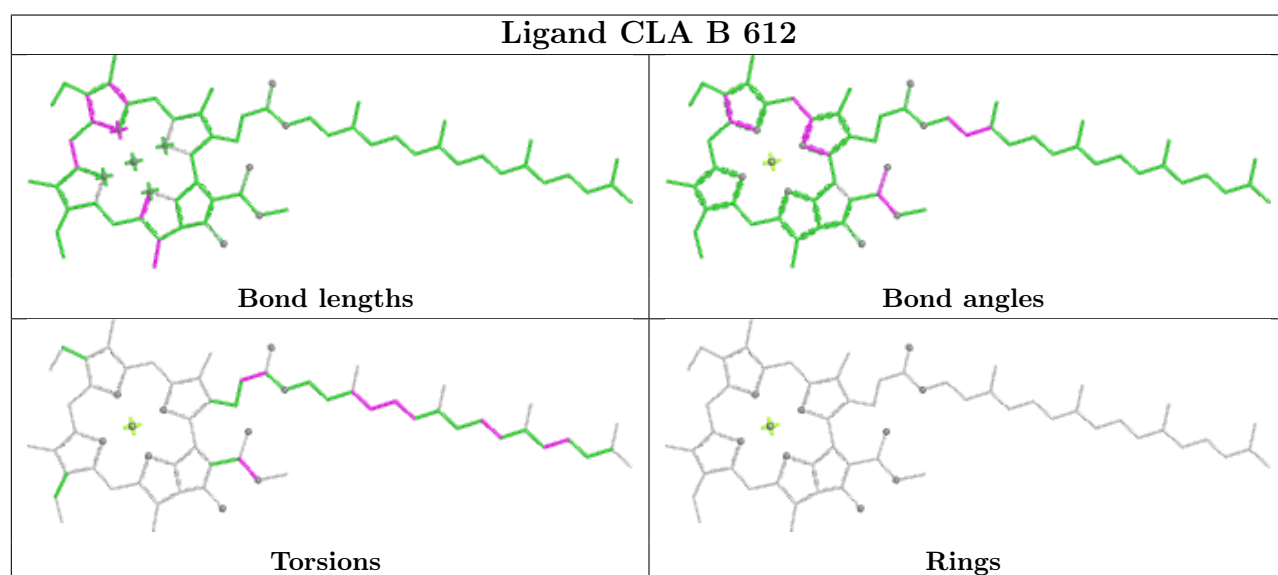
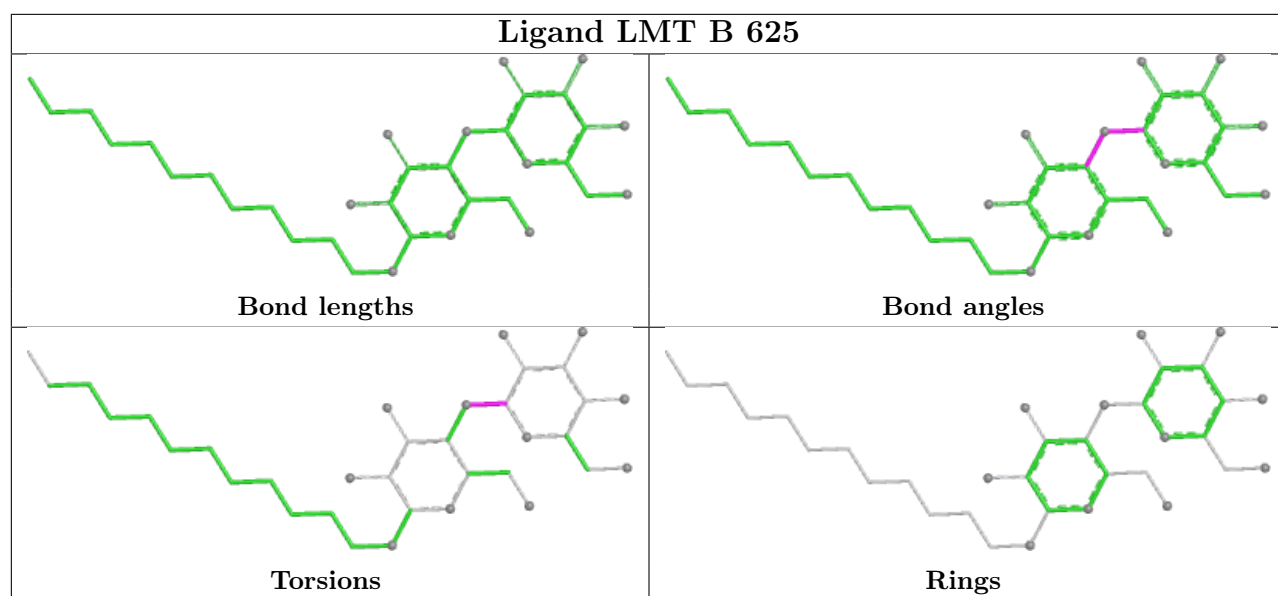


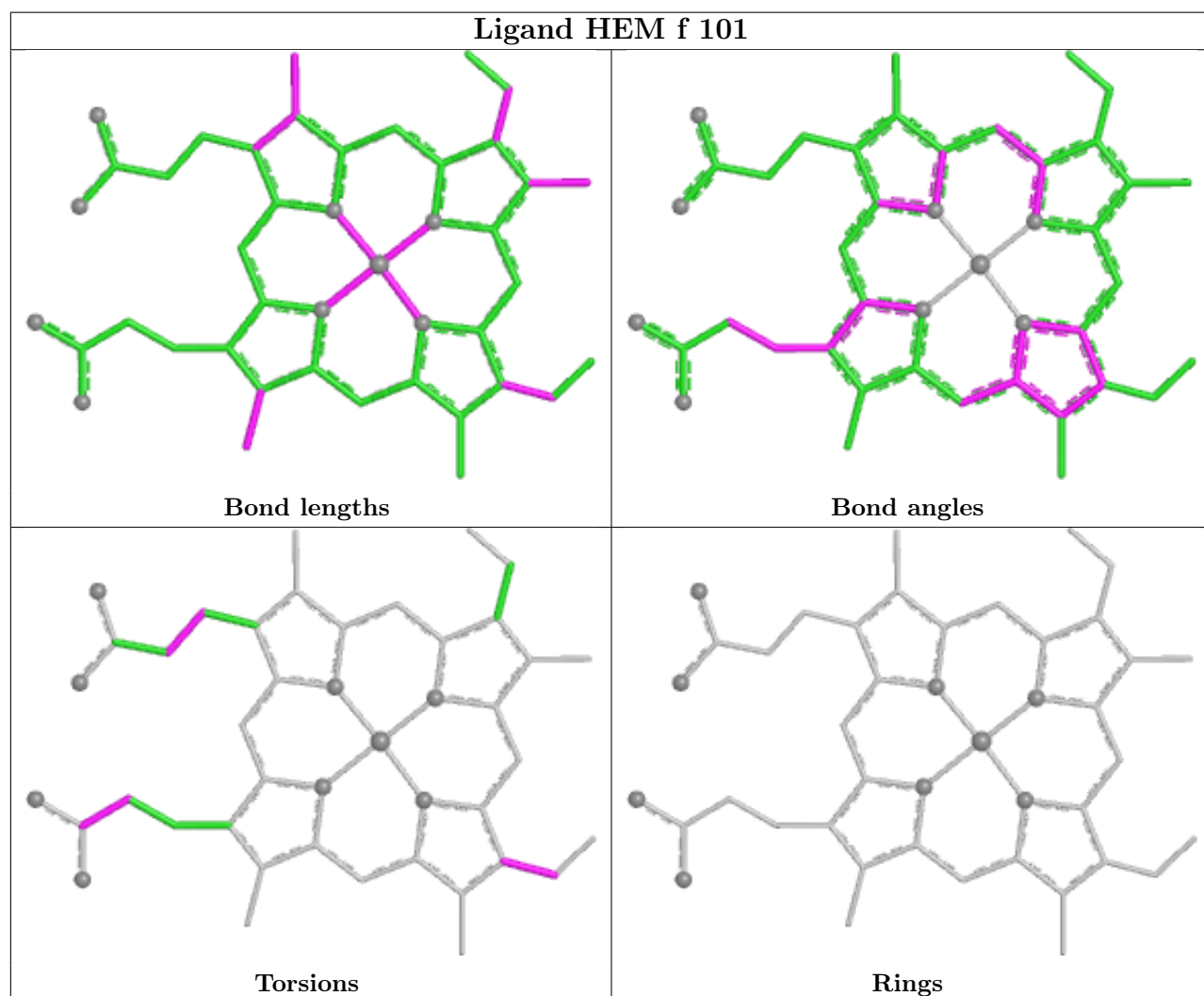
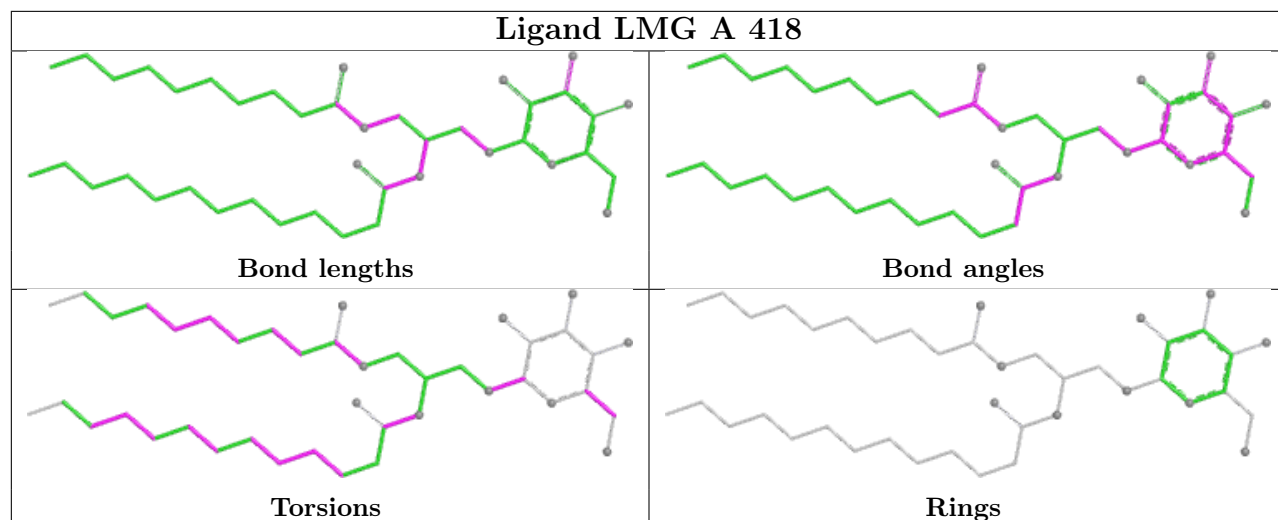
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

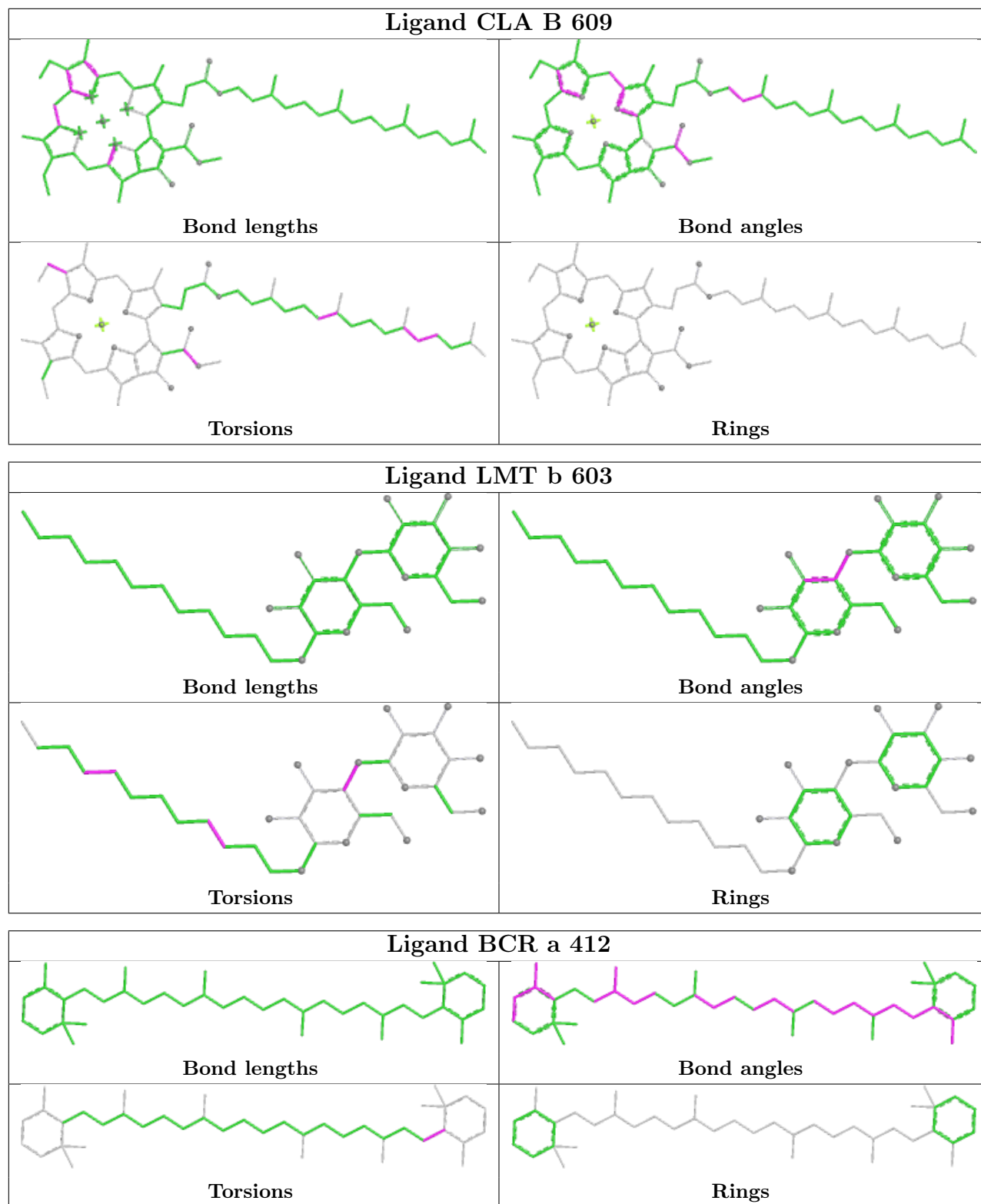
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

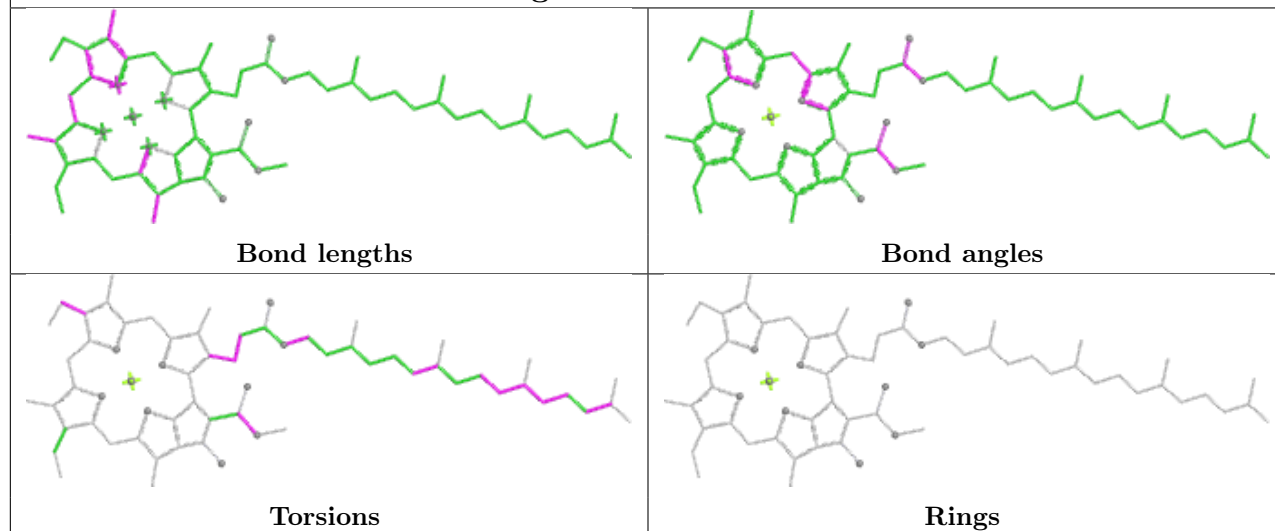




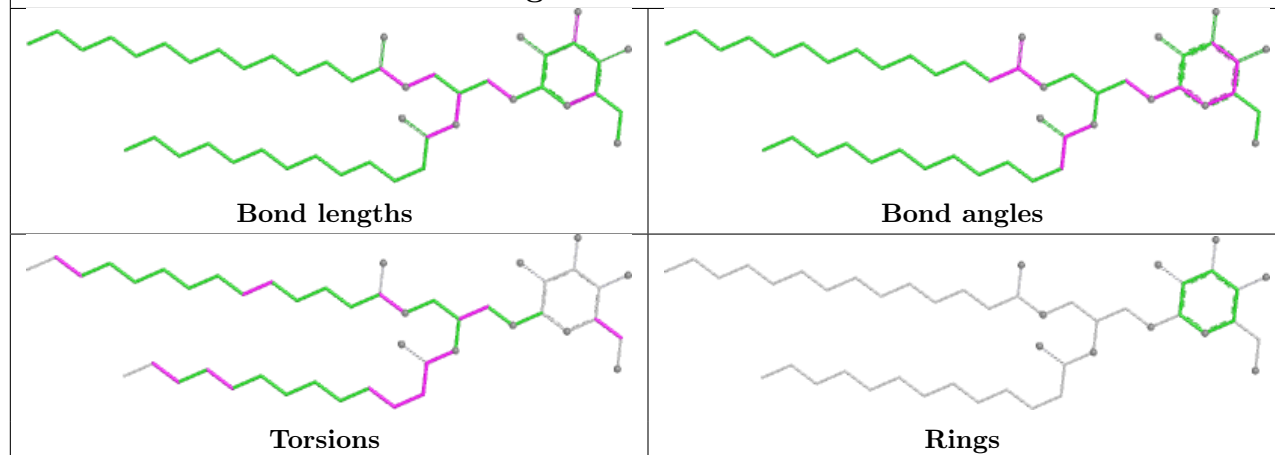




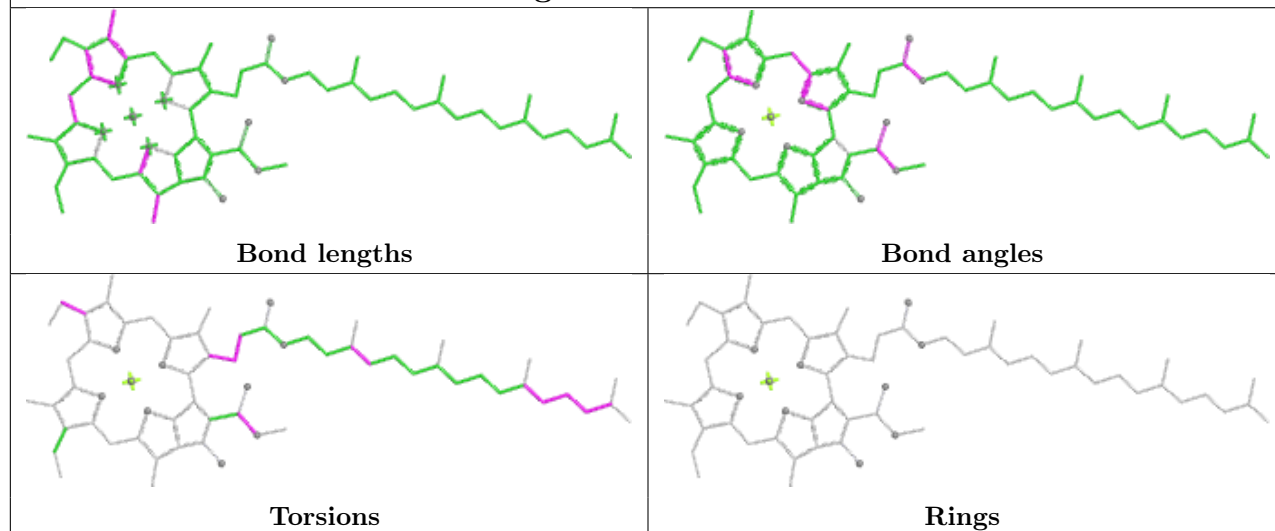
Ligand CLA B 601

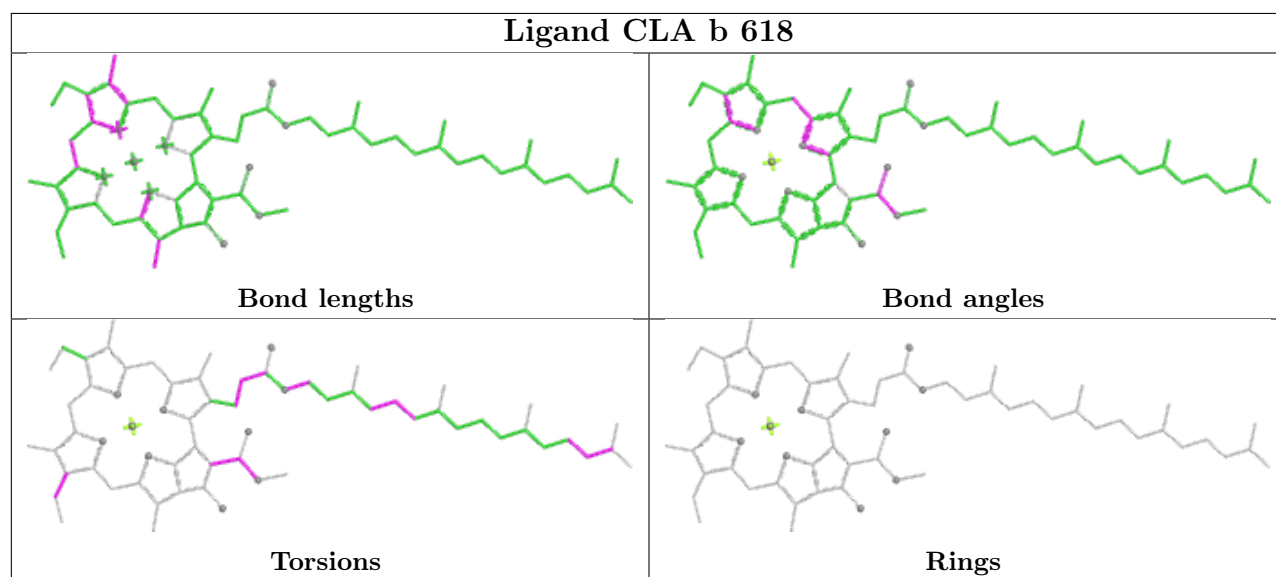
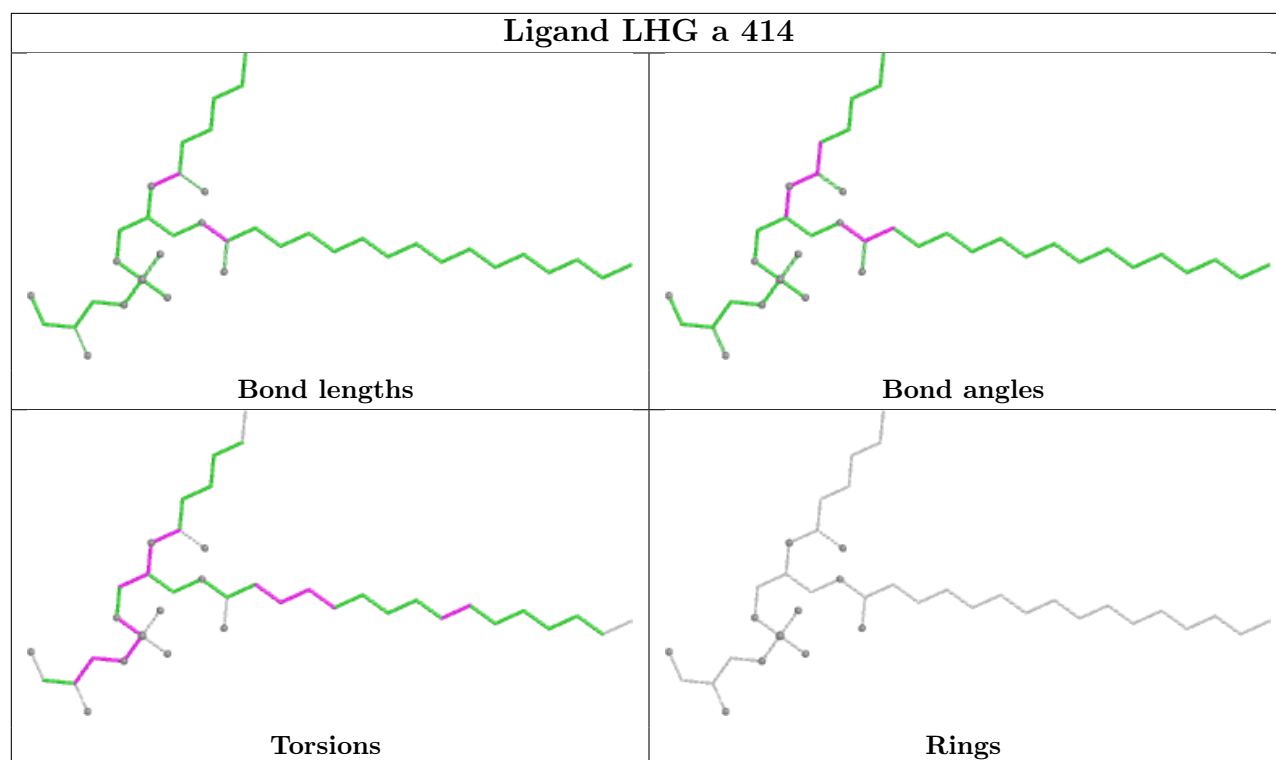
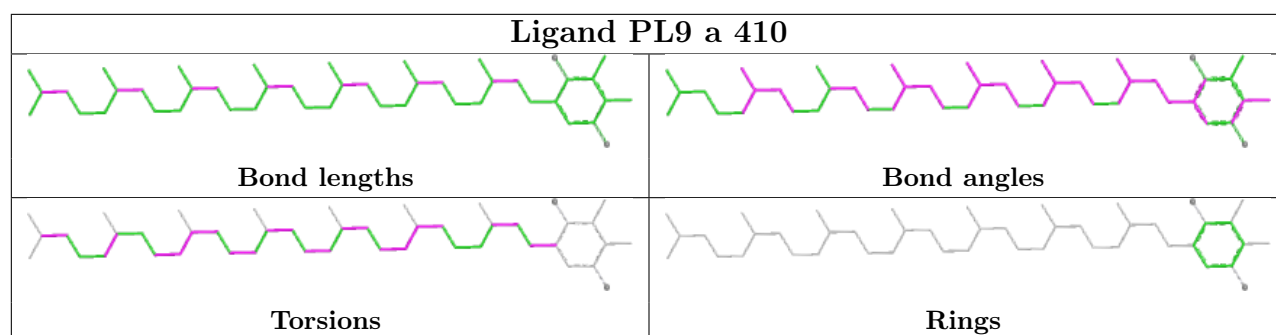


Ligand LMG D 406

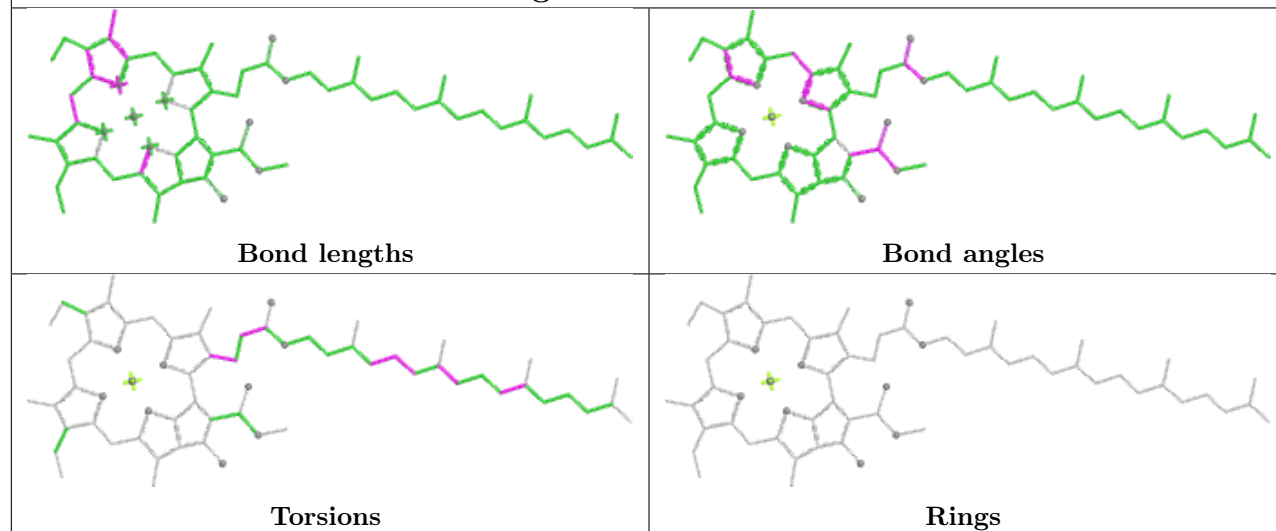


Ligand CLA b 610

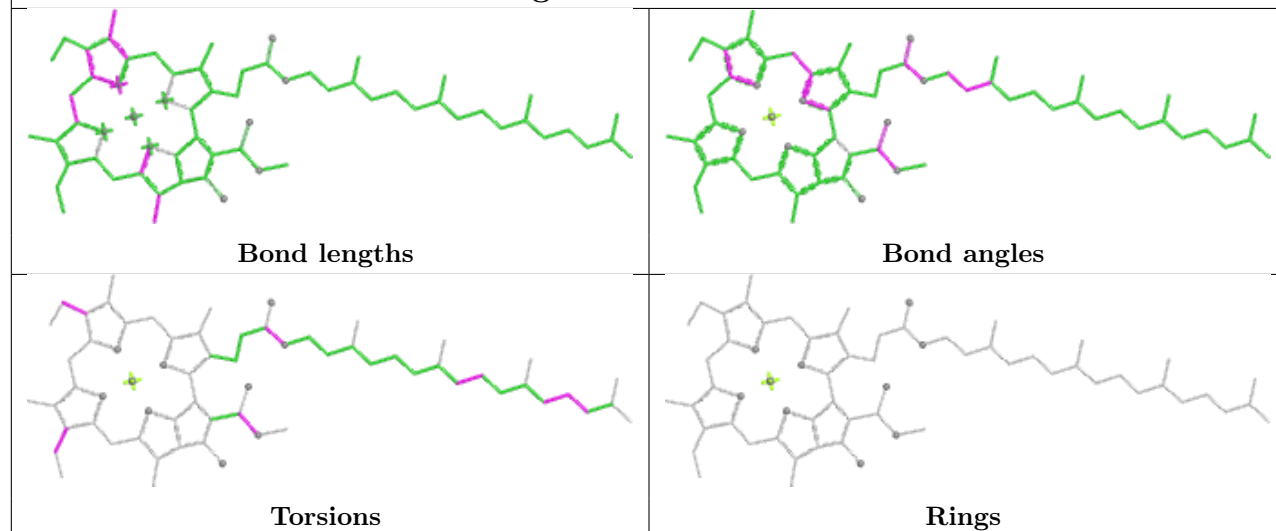




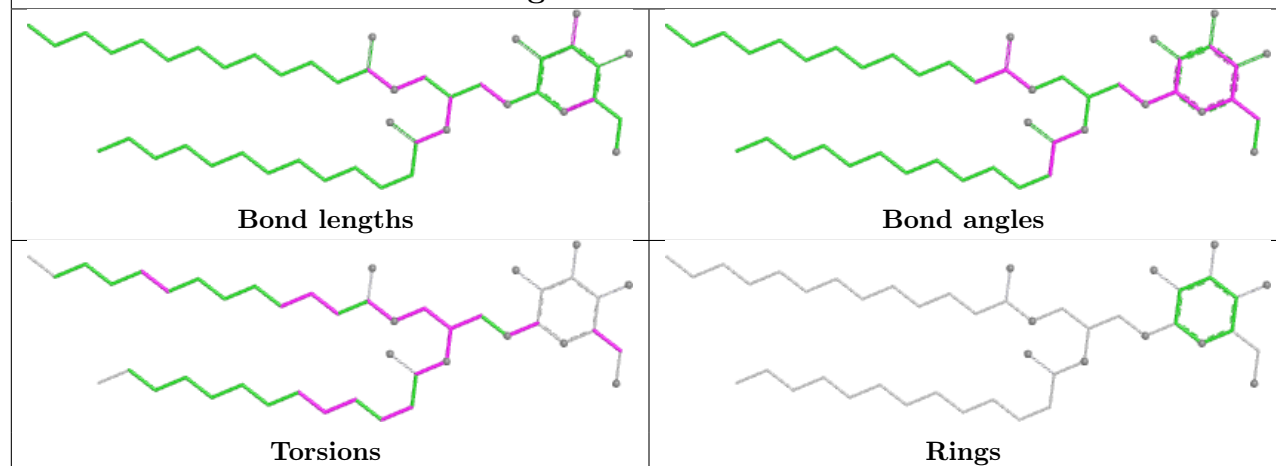
Ligand CLA C 507



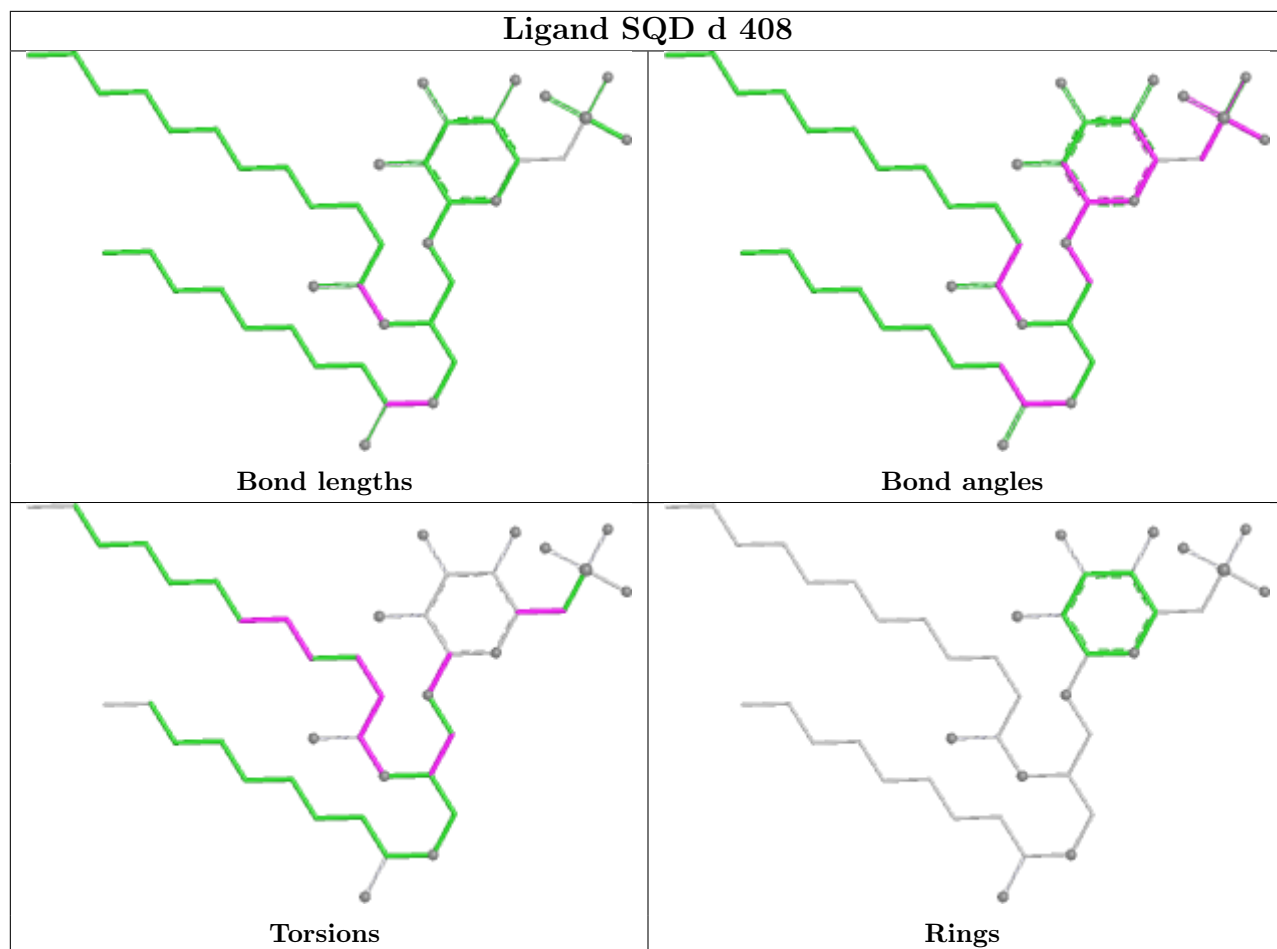
Ligand CLA B 604



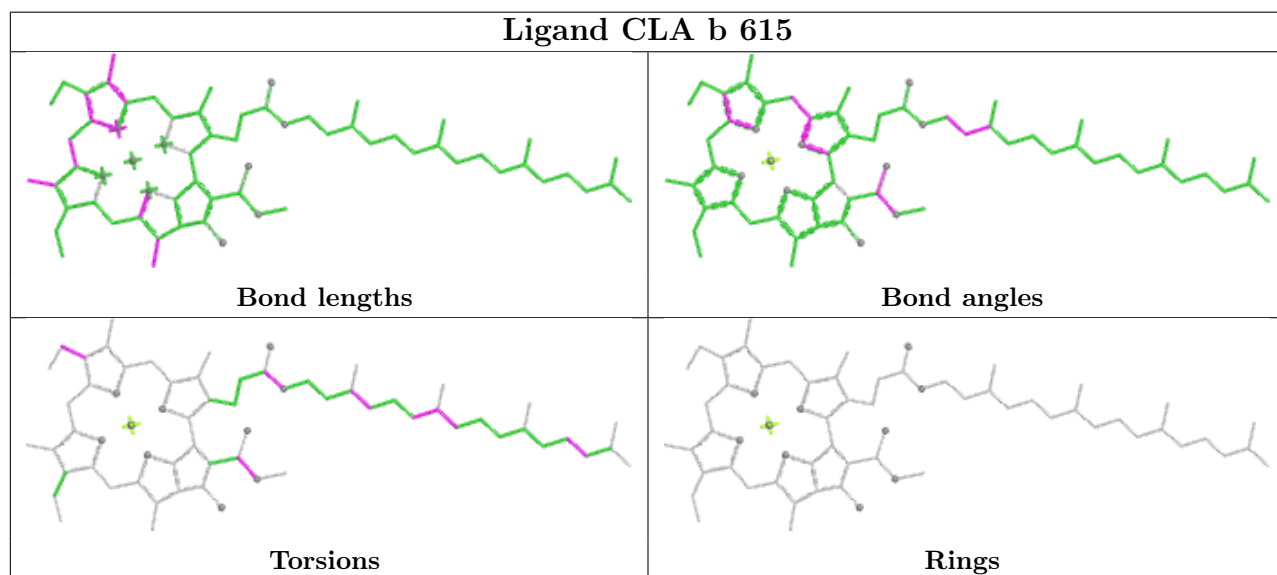
Ligand LMG C 521

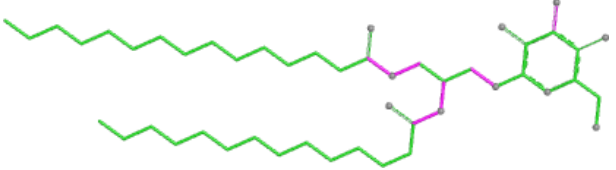
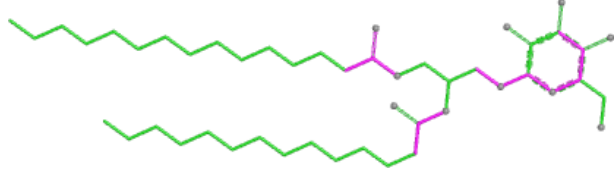
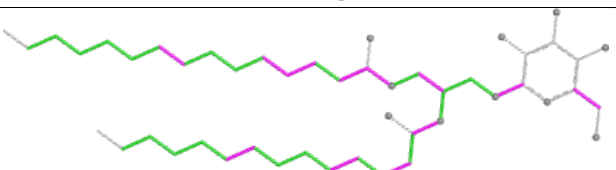
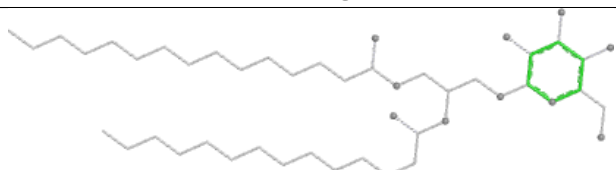
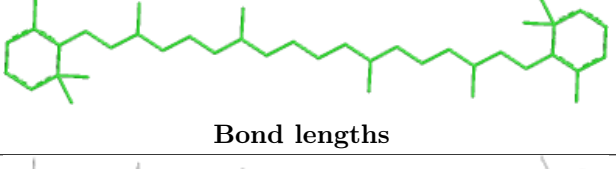
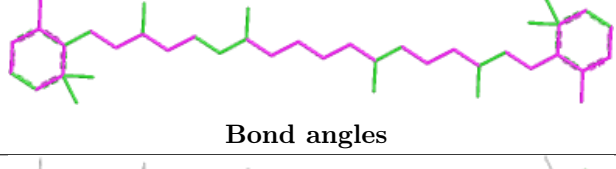
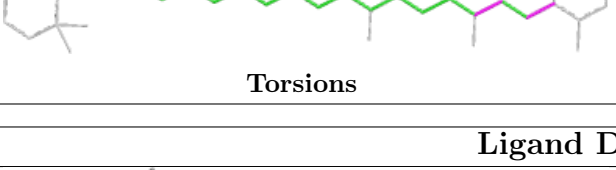
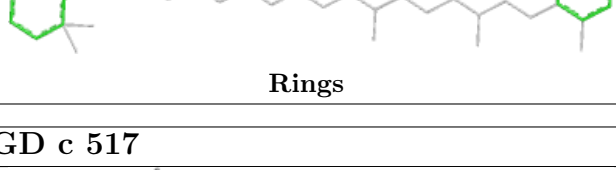
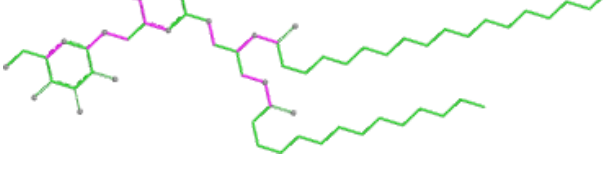
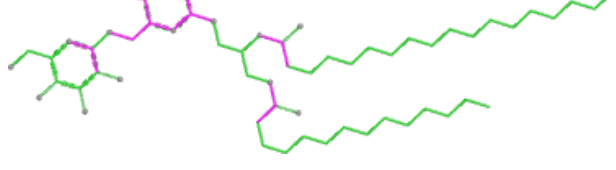
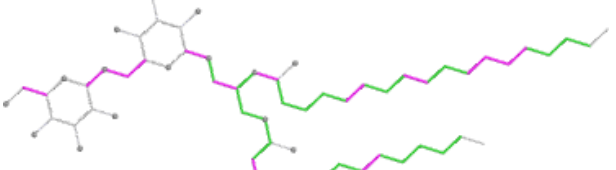
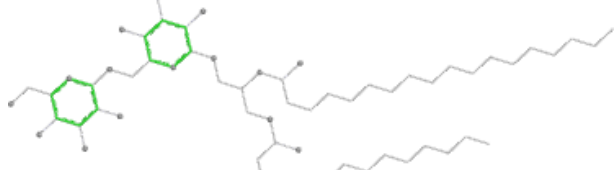


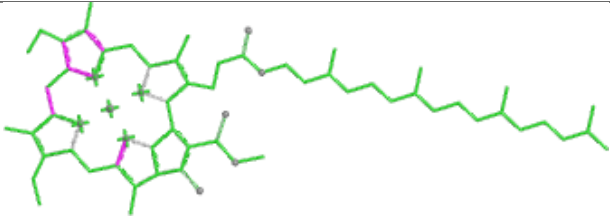
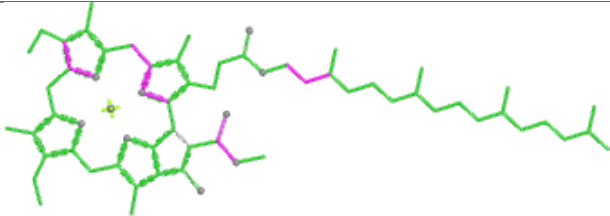
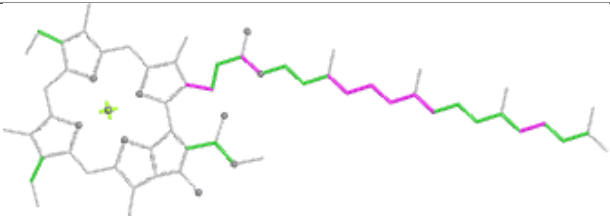
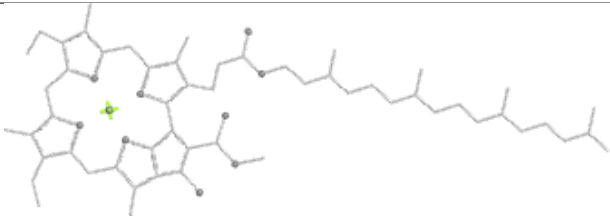
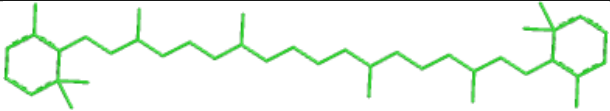
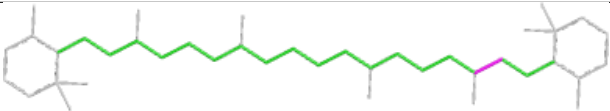
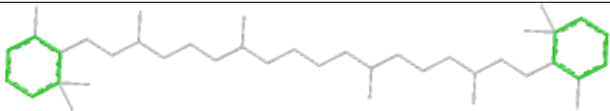
Ligand SQD d 408

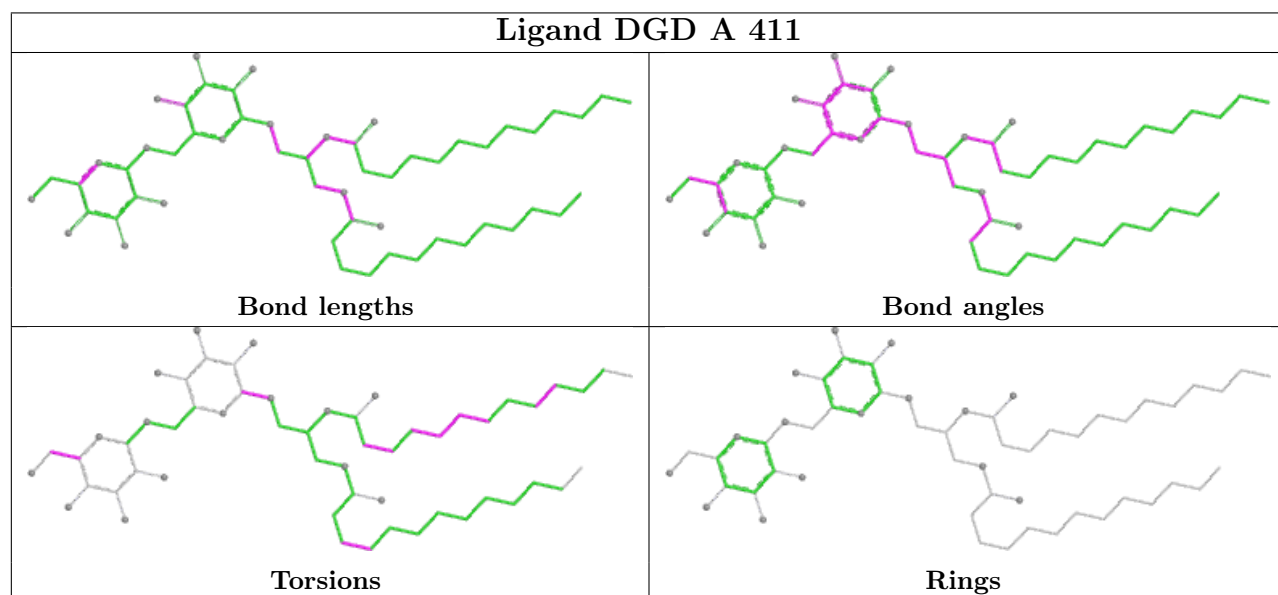
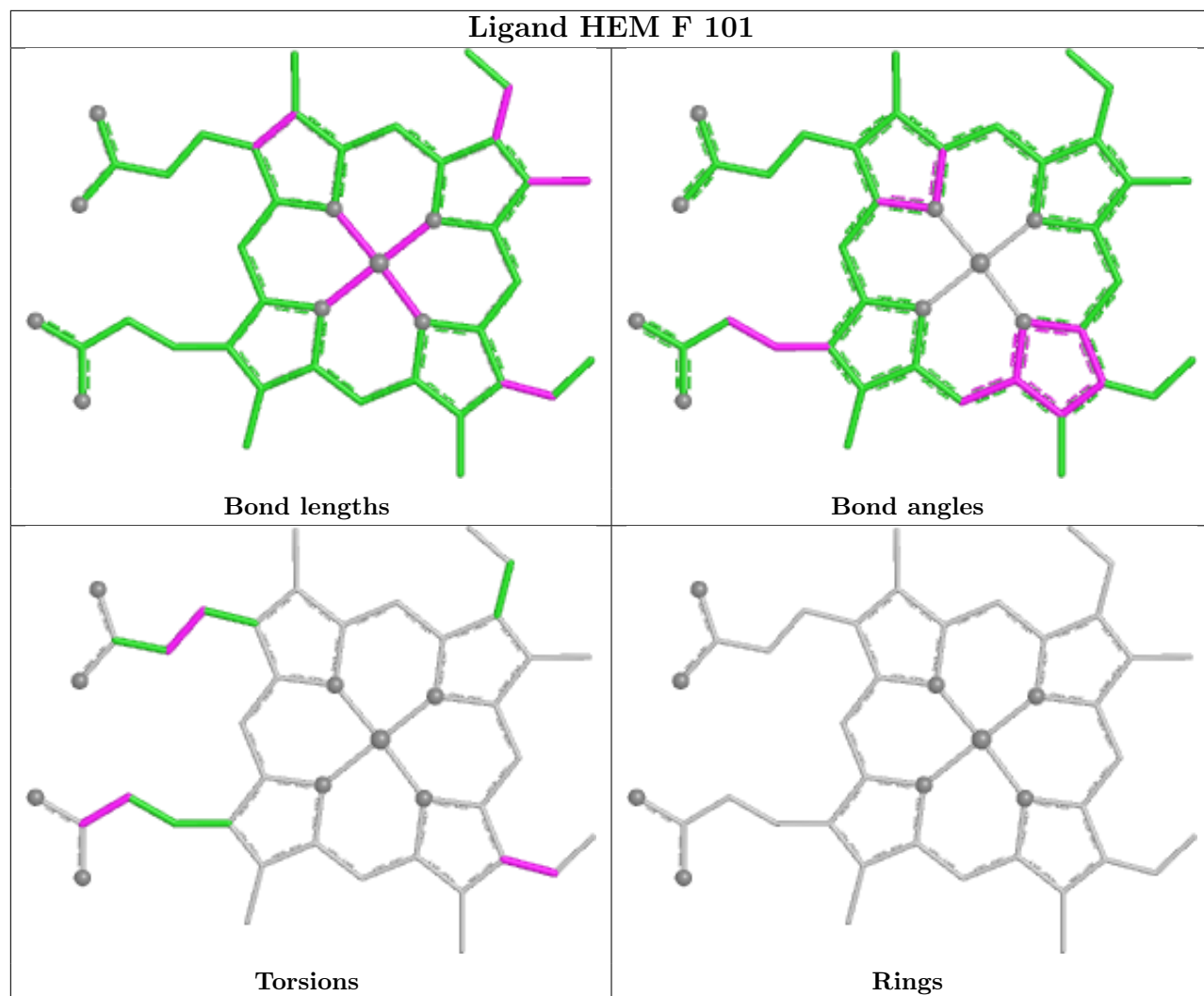


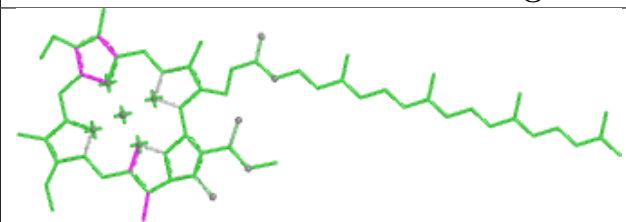
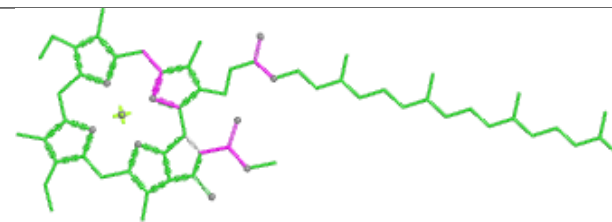
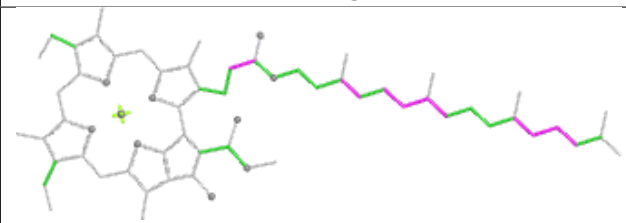
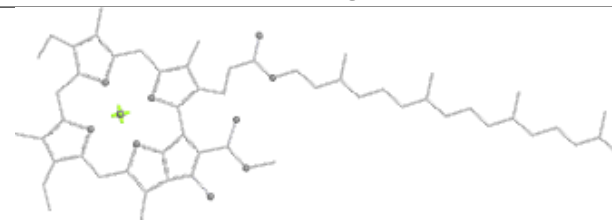
Ligand CLA b 615

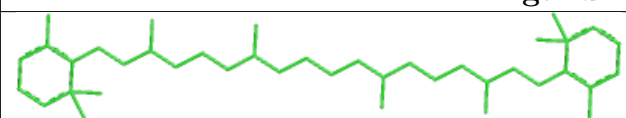
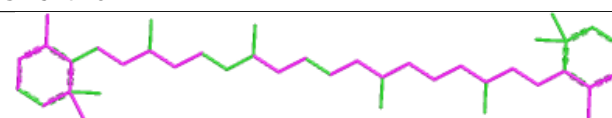
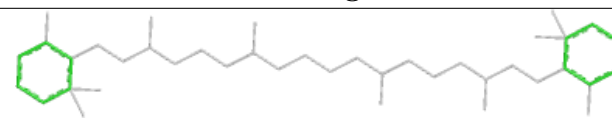


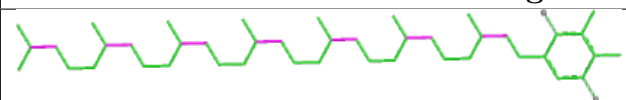
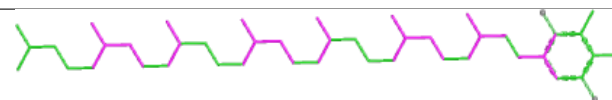
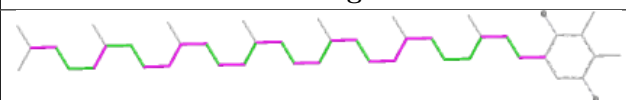
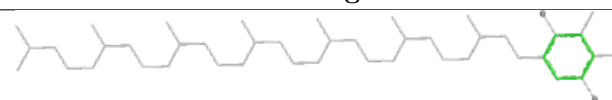
Ligand LMG k 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

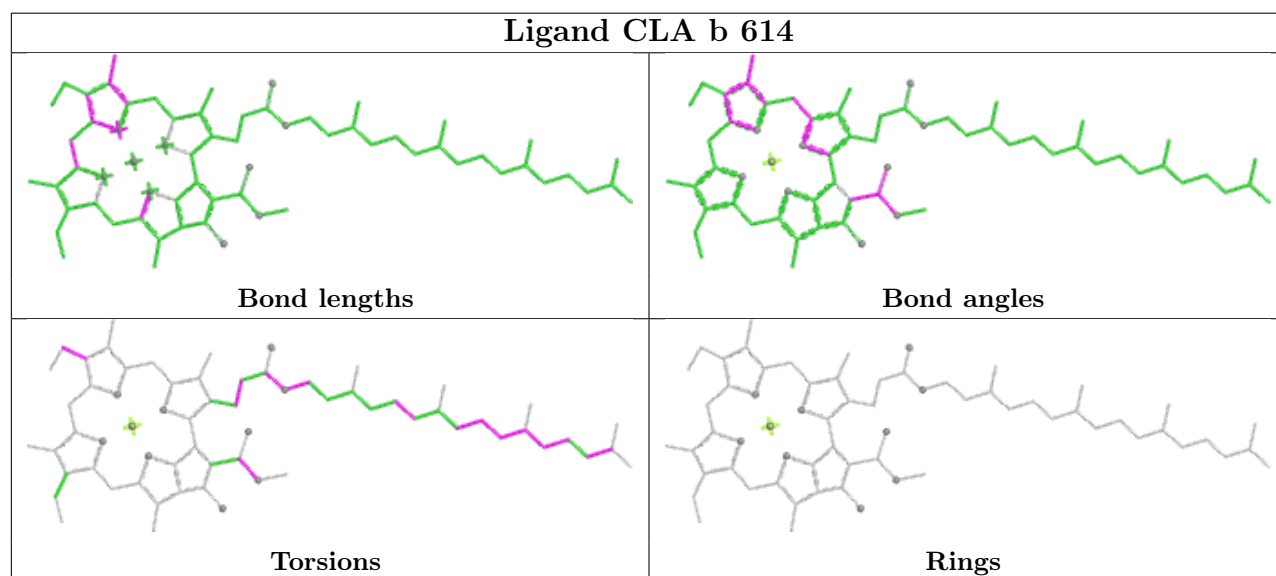
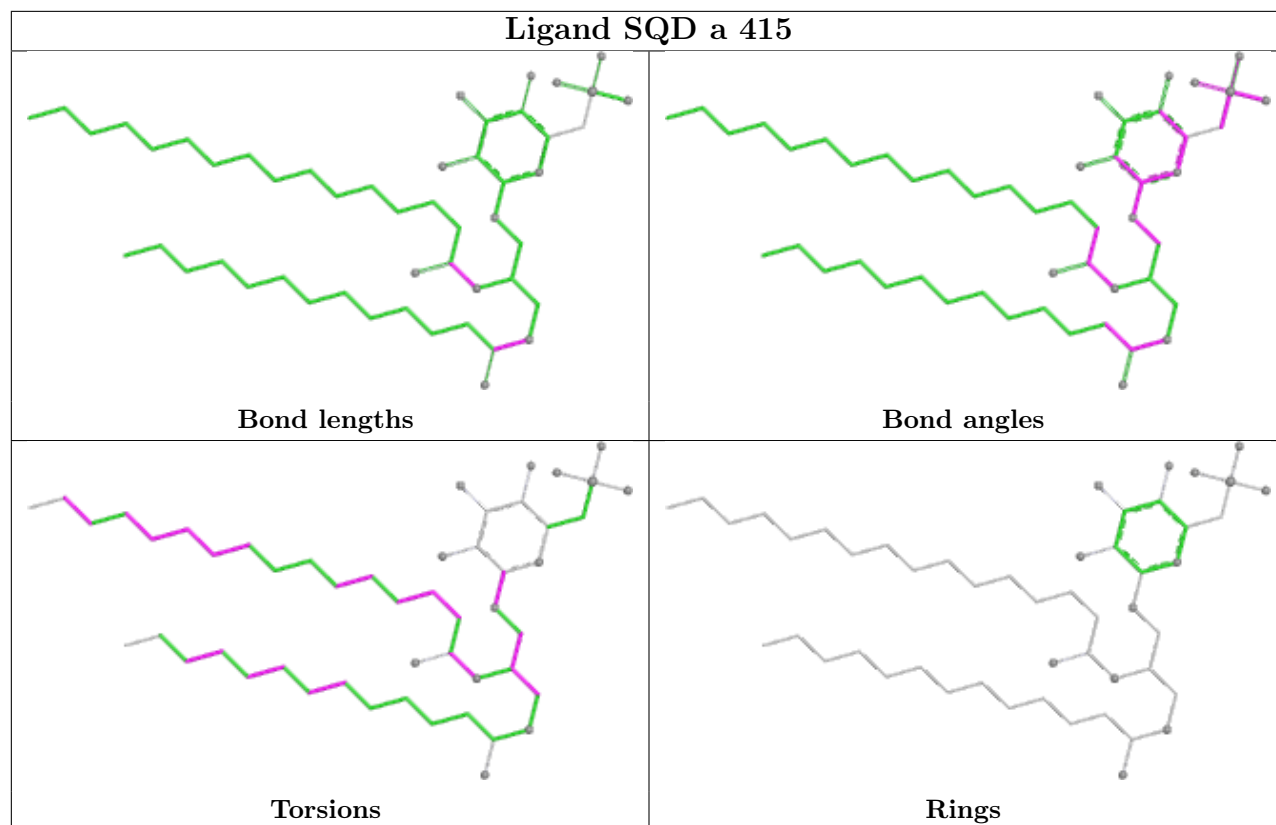
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

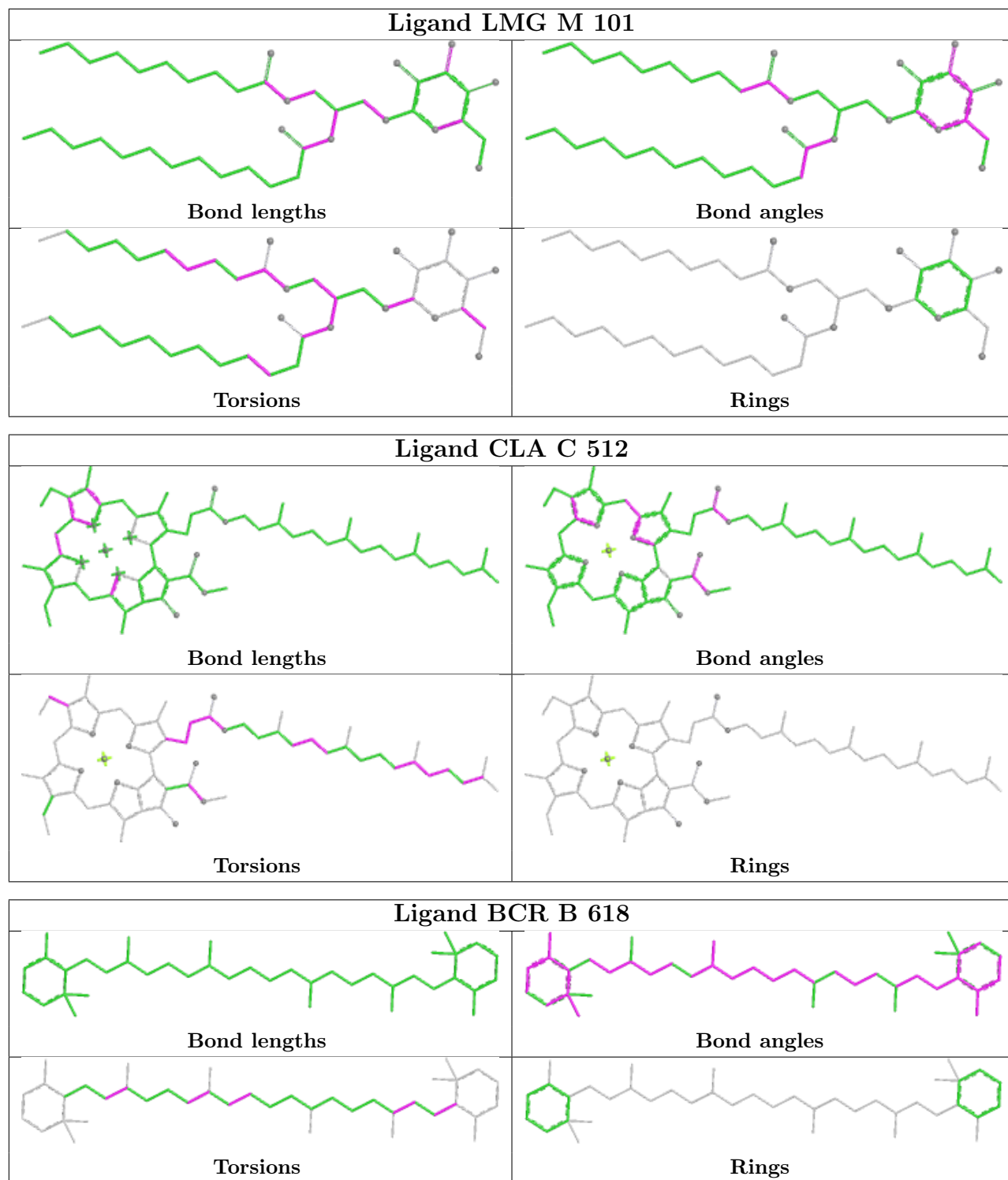


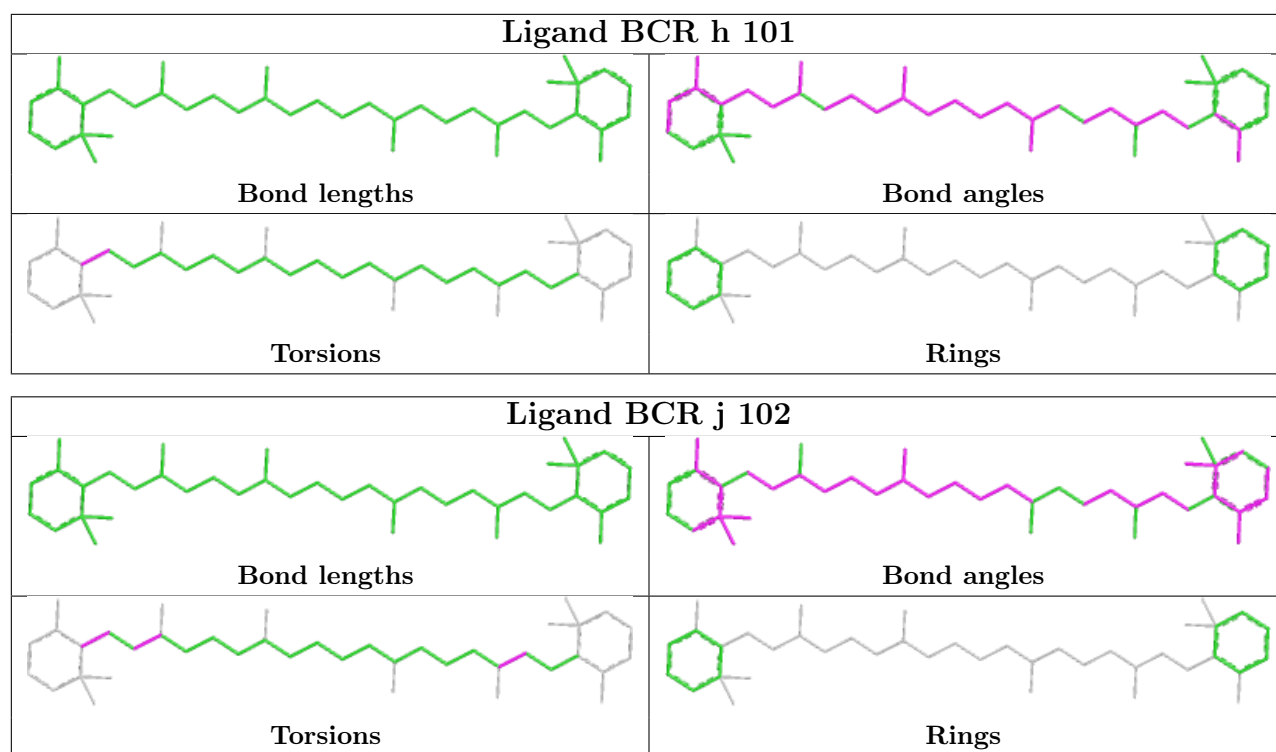
Ligand CLA d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.36	14 (4%) 40 39	43, 64, 104, 149	0
1	a	335/360 (93%)	0.25	12 (3%) 46 42	44, 65, 106, 149	0
2	B	490/510 (96%)	0.31	22 (4%) 38 38	46, 69, 103, 159	0
2	b	490/510 (96%)	0.39	30 (6%) 27 31	47, 71, 104, 159	0
3	C	447/461 (96%)	0.31	12 (2%) 56 48	54, 79, 106, 132	0
3	c	447/461 (96%)	0.28	14 (3%) 51 45	56, 81, 105, 135	0
4	D	340/352 (96%)	0.29	15 (4%) 39 38	44, 66, 103, 137	0
4	d	340/352 (96%)	0.22	12 (3%) 47 43	45, 66, 102, 134	0
5	E	82/84 (97%)	0.44	4 (4%) 35 35	68, 92, 125, 130	0
5	e	82/84 (97%)	0.44	2 (2%) 59 51	70, 92, 125, 129	0
6	F	35/45 (77%)	0.47	3 (8%) 16 22	68, 84, 119, 139	0
6	f	35/45 (77%)	0.37	3 (8%) 16 22	73, 85, 120, 141	0
7	H	65/66 (98%)	0.56	4 (6%) 26 31	77, 94, 122, 138	0
7	h	65/66 (98%)	0.52	2 (3%) 51 45	73, 93, 120, 144	0
8	I	35/38 (92%)	0.48	2 (5%) 29 33	65, 79, 107, 118	0
8	i	35/38 (92%)	0.54	2 (5%) 29 33	66, 81, 106, 120	0
9	J	34/40 (85%)	0.52	2 (5%) 28 32	69, 85, 95, 112	0
9	j	34/40 (85%)	0.70	6 (17%) 4 11	74, 88, 95, 116	0
10	K	37/46 (80%)	0.36	2 (5%) 31 33	77, 87, 101, 122	0
10	k	37/46 (80%)	0.59	5 (13%) 7 14	73, 88, 108, 123	0
11	L	37/37 (100%)	0.16	0 100 100	48, 62, 128, 156	0
11	l	37/37 (100%)	0.31	0 100 100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.35	1 (2%) 53 46	56, 71, 110, 164	0
12	m	34/36 (94%)	0.40	1 (2%) 53 46	55, 69, 108, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.45	10 (4%) 41 40	50, 78, 122, 169	0
13	o	243/272 (89%)	0.38	10 (4%) 41 40	52, 78, 121, 167	0
14	T	32/32 (100%)	0.46	0 100 100	55, 67, 158, 174	0
14	t	32/32 (100%)	0.44	1 (3%) 51 45	54, 69, 159, 168	0
15	U	97/134 (72%)	0.62	6 (6%) 26 31	56, 71, 92, 108	0
15	u	97/134 (72%)	0.42	3 (3%) 51 45	55, 71, 90, 111	0
16	V	137/163 (84%)	0.50	10 (7%) 21 26	53, 71, 86, 101	0
16	v	137/163 (84%)	0.24	4 (2%) 53 46	59, 72, 88, 95	0
17	g	28/46 (60%)	1.02	3 (10%) 11 18	95, 108, 126, 132	0
17	y	28/46 (60%)	0.77	3 (10%) 11 18	89, 107, 126, 131	0
18	X	37/41 (90%)	0.42	2 (5%) 31 33	76, 93, 124, 140	0
18	x	37/41 (90%)	0.56	5 (13%) 7 14	75, 90, 126, 141	0
19	Z	62/62 (100%)	0.44	2 (3%) 50 45	86, 104, 168, 185	0
19	z	62/62 (100%)	0.36	2 (3%) 50 45	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.36	231 (4%) 39 38	43, 75, 115, 187	0

The worst 5 of 231 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	482	ILE	8.2
2	b	393	GLU	5.3
5	E	78	THR	4.9
4	D	64	ALA	4.8
3	c	341	LEU	4.8

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	d	410	31/35	0.32	0.28	83,134,157,157	0
27	BCR	j	102	40/40	0.56	0.44	110,128,180,184	0
33	LMT	D	410	31/35	0.57	0.18	83,133,154,159	0
33	LMT	B	624	35/35	0.58	0.21	80,142,170,171	0
33	LMT	B	629	35/35	0.58	0.21	70,137,165,168	0
33	LMT	i	102	35/35	0.59	0.18	99,137,146,152	0
31	LMG	C	521	45/55	0.60	0.23	84,119,143,175	0
23	CLA	b	605	65/65	0.62	0.24	88,108,124,137	0
27	BCR	J	102	40/40	0.63	0.37	108,125,177,180	0
25	PL9	J	101	35/55	0.67	0.43	119,157,178,182	0
33	LMT	I	102	35/35	0.68	0.18	99,135,144,145	0
33	LMT	b	626	35/35	0.70	0.18	76,139,174,176	0
33	LMT	b	627	35/35	0.70	0.16	100,140,152,154	0
28	DGD	B	627	52/66	0.70	0.25	75,105,178,180	0
22	BCT	d	401	4/4	0.70	0.26	87,91,92,94	0
23	CLA	B	601	65/65	0.72	0.19	92,108,131,137	0
23	CLA	C	507	65/65	0.73	0.23	79,93,100,104	0
23	CLA	c	513	65/65	0.74	0.17	93,109,142,148	0
27	BCR	z	101	40/40	0.74	0.26	86,96,112,115	0
30	SQD	b	601	47/54	0.75	0.21	81,103,147,151	0
33	LMT	B	628	35/35	0.75	0.24	72,126,141,144	0
28	DGD	D	409	63/66	0.75	0.27	104,127,181,188	0
28	DGD	d	409	63/66	0.76	0.27	106,128,181,190	0
27	BCR	B	618	40/40	0.76	0.26	75,82,94,95	0
23	CLA	C	513	65/65	0.76	0.18	95,109,142,149	0
25	PL9	j	101	35/55	0.76	0.37	120,160,178,182	0
32	CL	a	418	1/1	0.77	0.16	49,49,49,49	0
30	SQD	d	408	43/54	0.77	0.20	67,109,152,157	0
30	SQD	B	626	47/54	0.77	0.20	75,100,144,148	0
33	LMT	b	603	35/35	0.77	0.26	73,119,136,138	0
31	LMG	k	103	48/55	0.78	0.27	79,100,112,115	0
28	DGD	C	519	66/66	0.78	0.23	55,72,100,114	0
29	LHG	A	415	37/49	0.78	0.18	104,133,190,202	0
31	LMG	M	101	42/55	0.78	0.21	83,111,135,144	0
31	LMG	E	101	44/55	0.79	0.23	87,123,132,139	0
25	PL9	A	408	45/55	0.79	0.26	89,101,119,127	0
31	LMG	c	519	45/55	0.79	0.19	86,119,142,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	b	625	49/55	0.80	0.30	51,75,86,89	0
25	PL9	a	410	45/55	0.81	0.29	82,103,121,125	0
27	BCR	H	101	40/40	0.81	0.23	83,96,130,131	0
33	LMT	B	625	35/35	0.81	0.20	95,139,149,152	0
27	BCR	k	102	40/40	0.81	0.20	72,80,109,111	0
27	BCR	T	102	40/40	0.82	0.24	71,79,86,86	0
31	LMG	A	418	42/55	0.82	0.25	81,105,123,147	0
27	BCR	a	412	40/40	0.82	0.24	54,71,84,87	0
29	LHG	a	417	37/49	0.82	0.17	110,135,197,206	0
27	BCR	B	620	40/40	0.82	0.20	75,86,98,103	0
31	LMG	a	402	42/55	0.82	0.27	72,100,119,143	0
27	BCR	C	516	40/40	0.82	0.24	74,86,95,100	0
27	BCR	b	621	40/40	0.83	0.28	63,73,84,87	0
28	DGD	b	602	52/66	0.83	0.18	79,107,180,186	0
23	CLA	b	620	65/65	0.84	0.21	75,98,145,147	0
30	SQD	F	102	45/54	0.84	0.23	87,127,149,152	0
30	SQD	a	415	51/54	0.84	0.19	88,101,128,129	0
23	CLA	C	506	65/65	0.84	0.22	79,91,125,133	0
31	LMG	i	101	43/55	0.84	0.19	84,120,162,177	0
33	LMT	b	604	35/35	0.84	0.16	69,133,158,160	0
27	BCR	c	514	40/40	0.84	0.21	76,82,88,89	0
28	DGD	C	518	62/66	0.84	0.19	58,81,134,144	0
23	CLA	b	613	65/65	0.84	0.19	65,93,104,114	0
30	SQD	A	413	51/54	0.84	0.20	81,99,128,131	0
23	CLA	c	511	65/65	0.85	0.16	75,91,102,108	0
23	CLA	c	512	65/65	0.85	0.17	83,104,146,152	0
28	DGD	C	517	53/66	0.85	0.20	61,79,96,101	0
31	LMG	a	416	51/55	0.85	0.24	62,80,93,100	0
23	CLA	B	616	65/65	0.85	0.23	79,93,147,152	0
23	CLA	c	506	65/65	0.85	0.20	78,92,122,128	0
27	BCR	B	619	40/40	0.85	0.26	62,75,83,86	0
33	LMT	m	101	35/35	0.85	0.22	68,93,112,114	0
35	CA	K	101	1/1	0.85	0.16	86,86,86,86	0
32	CL	A	416	1/1	0.86	0.25	49,49,49,49	0
23	CLA	a	406	65/65	0.86	0.25	55,71,140,147	0
28	DGD	A	411	56/66	0.86	0.19	77,102,146,153	0
27	BCR	h	101	40/40	0.86	0.22	85,94,124,127	0
25	PL9	d	404	55/55	0.86	0.23	45,65,78,85	0
30	SQD	a	401	54/54	0.86	0.23	76,114,149,152	0
27	BCR	b	622	40/40	0.86	0.20	72,83,94,96	0
31	LMG	m	102	42/55	0.86	0.26	73,111,128,138	0
28	DGD	c	517	62/66	0.87	0.19	64,84,132,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	B	622	49/55	0.87	0.21	61,79,105,117	0
28	DGD	c	518	66/66	0.87	0.17	54,73,105,118	0
23	CLA	C	504	65/65	0.87	0.19	62,83,138,145	0
31	LMG	I	101	43/55	0.87	0.18	73,118,166,178	0
27	BCR	y	101	40/40	0.87	0.20	79,86,106,109	0
23	CLA	c	502	65/65	0.87	0.17	63,75,100,106	0
27	BCR	C	515	40/40	0.87	0.19	85,92,115,116	0
27	BCR	A	410	40/40	0.87	0.19	52,68,85,90	0
27	BCR	B	617	40/40	0.87	0.19	67,74,81,84	0
31	LMG	e	101	44/55	0.87	0.17	91,122,132,136	0
27	BCR	c	515	40/40	0.87	0.19	75,86,95,101	0
23	CLA	C	511	65/65	0.87	0.18	74,88,102,109	0
28	DGD	a	413	56/66	0.87	0.16	76,100,145,148	0
27	BCR	T	101	40/40	0.87	0.23	68,75,82,83	0
35	CA	k	101	1/1	0.87	0.13	103,103,103,103	0
31	LMG	b	624	49/55	0.88	0.24	59,82,102,113	0
30	SQD	f	102	45/54	0.88	0.18	88,133,148,152	0
23	CLA	b	619	65/65	0.88	0.16	85,97,108,116	0
23	CLA	C	510	65/65	0.88	0.16	67,74,83,93	0
31	LMG	C	520	48/55	0.88	0.21	89,100,109,112	0
23	CLA	a	409	65/65	0.88	0.18	55,67,129,133	0
31	LMG	D	406	46/55	0.88	0.20	58,73,116,129	0
27	BCR	C	514	40/40	0.88	0.18	73,80,87,94	0
23	CLA	B	610	65/65	0.88	0.17	69,81,88,92	0
23	CLA	b	606	65/65	0.88	0.23	70,87,96,97	0
23	CLA	C	509	65/65	0.88	0.17	62,81,95,98	0
23	CLA	b	614	65/65	0.88	0.17	66,82,88,91	0
28	DGD	b	623	58/66	0.89	0.19	57,74,99,107	0
30	SQD	A	417	54/54	0.89	0.20	77,113,147,154	0
28	DGD	c	516	53/66	0.89	0.21	63,77,96,103	0
31	LMG	B	623	49/55	0.89	0.19	58,76,84,87	0
24	PHO	A	406	64/64	0.89	0.15	50,69,77,81	0
23	CLA	B	608	65/65	0.89	0.18	64,75,93,97	0
27	BCR	D	405	40/40	0.89	0.20	68,81,105,110	0
23	CLA	C	505	65/65	0.89	0.19	69,77,86,91	0
23	CLA	c	507	65/65	0.89	0.17	83,93,105,111	0
23	CLA	c	505	65/65	0.90	0.19	70,77,83,85	0
23	CLA	C	501	65/65	0.90	0.14	69,82,90,95	0
23	CLA	b	607	65/65	0.90	0.15	68,82,92,103	0
23	CLA	c	508	65/65	0.90	0.18	70,85,118,134	0
23	CLA	B	603	65/65	0.90	0.19	65,81,94,109	0
23	CLA	B	605	65/65	0.90	0.15	58,78,86,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	614	65/65	0.90	0.17	63,83,125,129	0
23	CLA	d	402	65/65	0.90	0.17	49,57,81,95	0
23	CLA	B	615	65/65	0.90	0.15	83,96,106,116	0
23	CLA	c	501	65/65	0.90	0.15	67,82,92,94	0
25	PL9	D	404	55/55	0.90	0.21	42,61,71,77	0
23	CLA	B	606	65/65	0.90	0.19	67,81,110,121	0
29	LHG	A	412	39/49	0.90	0.18	59,79,89,93	0
23	CLA	c	503	65/65	0.90	0.14	77,89,97,103	0
29	LHG	a	414	39/49	0.90	0.17	60,78,94,102	0
23	CLA	a	405	65/65	0.91	0.17	44,53,69,73	0
23	CLA	A	407	65/65	0.91	0.17	56,66,127,129	0
22	BCT	A	402	4/4	0.91	0.09	85,90,90,94	0
23	CLA	c	509	65/65	0.91	0.13	67,85,91,97	0
23	CLA	A	405	65/65	0.91	0.18	44,69,140,145	0
23	CLA	C	512	65/65	0.91	0.16	89,101,144,149	0
23	CLA	B	604	65/65	0.91	0.15	59,67,104,124	0
23	CLA	b	610	65/65	0.91	0.15	70,83,112,126	0
23	CLA	b	611	65/65	0.91	0.18	54,64,89,92	0
35	CA	O	301	1/1	0.91	0.12	112,112,112,112	0
24	PHO	a	408	64/64	0.91	0.16	58,68,79,86	0
35	CA	o	301	1/1	0.91	0.09	98,98,98,98	0
23	CLA	D	401	65/65	0.92	0.15	49,59,87,97	0
23	CLA	d	403	65/65	0.92	0.16	72,88,121,128	0
33	LMT	M	102	35/35	0.92	0.17	69,96,112,115	0
31	LMG	d	406	46/55	0.92	0.17	63,73,116,130	0
23	CLA	a	404	65/65	0.92	0.15	53,60,67,74	0
23	CLA	C	508	65/65	0.92	0.18	71,86,117,132	0
23	CLA	b	608	65/65	0.92	0.15	61,68,107,117	0
31	LMG	D	407	48/55	0.92	0.19	54,72,81,120	0
23	CLA	B	609	65/65	0.92	0.16	74,89,104,106	0
23	CLA	c	510	65/65	0.92	0.13	67,75,84,89	0
34	HEM	f	101	43/43	0.92	0.12	89,105,124,126	0
23	CLA	B	602	65/65	0.92	0.15	68,87,95,96	0
23	CLA	b	612	65/65	0.92	0.17	63,75,95,98	0
31	LMG	A	414	51/55	0.92	0.16	63,77,92,95	0
23	CLA	c	504	65/65	0.92	0.15	75,83,133,138	0
23	CLA	A	404	65/65	0.93	0.15	44,54,67,74	0
28	DGD	B	621	58/66	0.93	0.17	46,71,101,105	0
31	LMG	d	407	48/55	0.93	0.19	58,70,85,120	0
23	CLA	B	612	65/65	0.93	0.16	61,72,82,86	0
23	CLA	C	503	65/65	0.93	0.13	71,88,99,105	0
24	PHO	D	402	64/64	0.93	0.13	51,62,72,74	0

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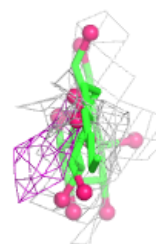
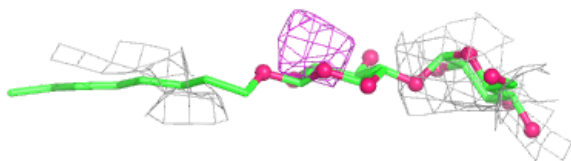
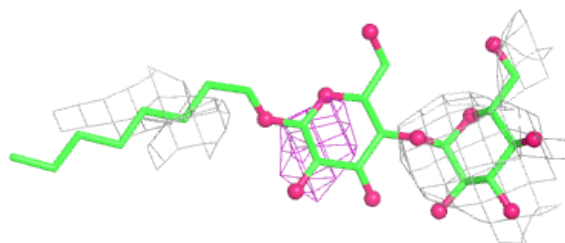
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PHO	a	407	64/64	0.93	0.14	53,63,70,73	0
23	CLA	C	502	65/65	0.94	0.15	59,75,108,111	0
23	CLA	B	607	65/65	0.94	0.13	52,66,82,85	0
23	CLA	b	616	65/65	0.94	0.12	61,73,83,86	0
34	HEM	V	201	43/43	0.94	0.16	58,69,74,76	0
23	CLA	b	617	65/65	0.94	0.15	57,67,91,93	0
23	CLA	b	618	65/65	0.94	0.14	60,82,123,130	0
23	CLA	B	613	65/65	0.94	0.13	46,64,88,93	0
30	SQD	D	408	43/54	0.94	0.17	71,103,148,152	0
23	CLA	B	611	65/65	0.94	0.13	63,72,80,87	0
23	CLA	A	403	65/65	0.95	0.13	52,58,66,70	0
23	CLA	D	403	65/65	0.95	0.15	74,87,123,124	0
34	HEM	v	201	43/43	0.95	0.12	57,68,75,76	0
23	CLA	b	615	65/65	0.95	0.13	54,72,80,87	0
23	CLA	b	609	65/65	0.95	0.12	61,76,84,88	0
27	BCR	d	405	40/40	0.95	0.12	69,82,102,106	0
34	HEM	F	101	43/43	0.95	0.13	89,105,127,130	0
21	FE2	a	403	1/1	0.98	0.12	72,72,72,72	0
26	OEC	a	411	5/9	0.98	0.14	35,44,62,68	0
26	OEC	A	409	5/9	0.99	0.18	35,44,57,62	0
21	FE2	A	401	1/1	0.99	0.06	64,64,64,64	0

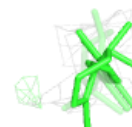
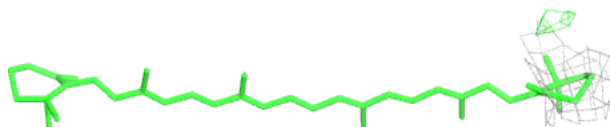
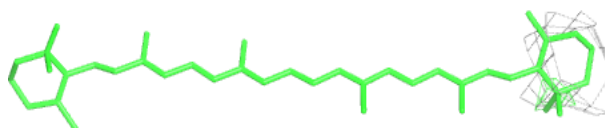
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

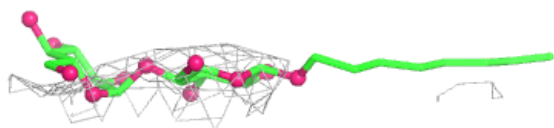
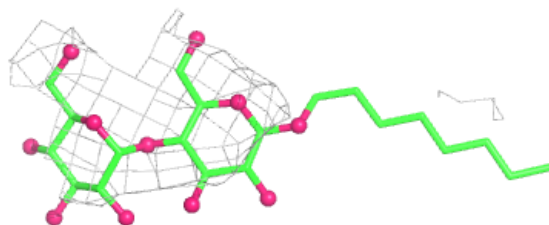
**Electron density around BCR j 102:**

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

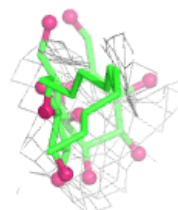
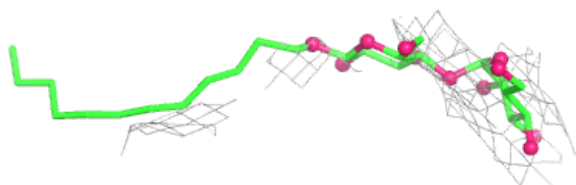
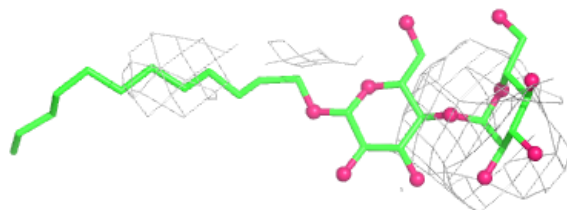


Electron density around LMT D 410:

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

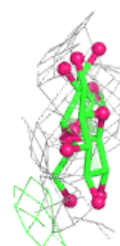
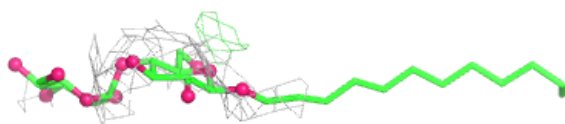
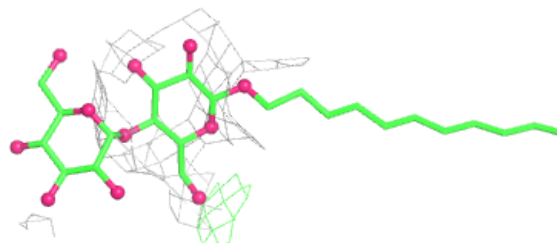
**Electron density around LMT B 624:**

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

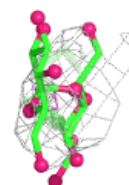
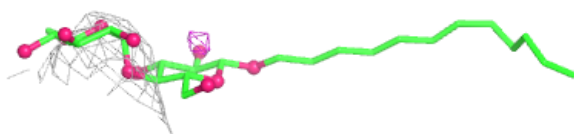
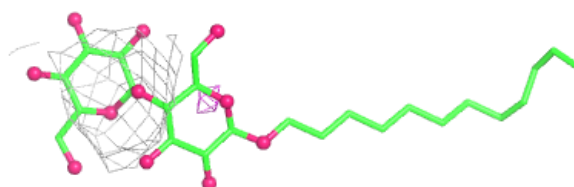


Electron density around LMT B 629:

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

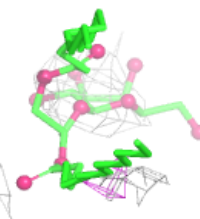
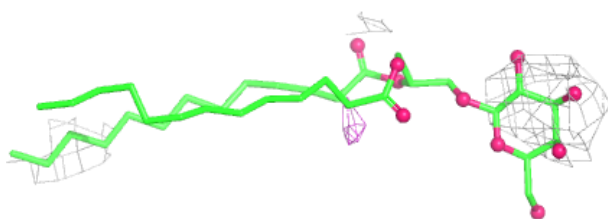
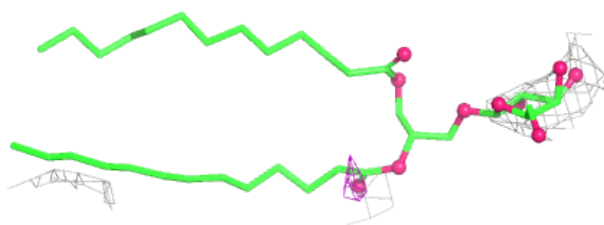
**Electron density around LMT i 102:**

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



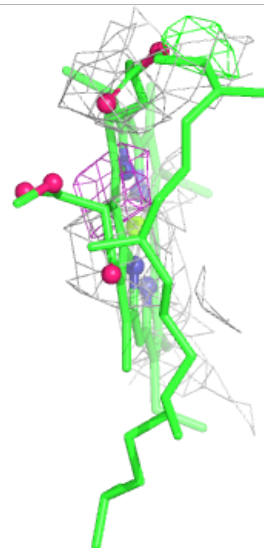
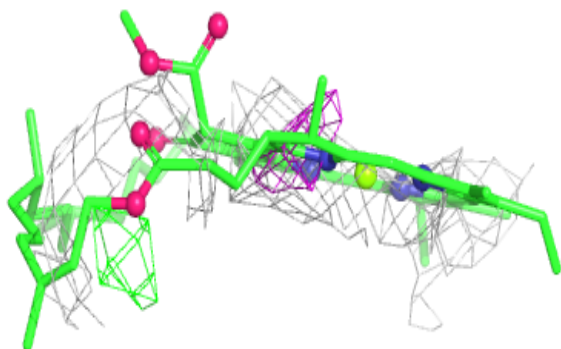
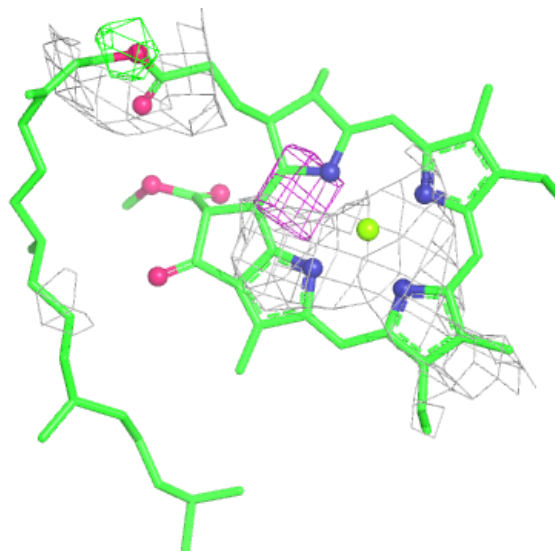
Electron density around LMG C 521:

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



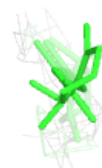
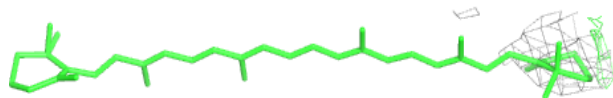
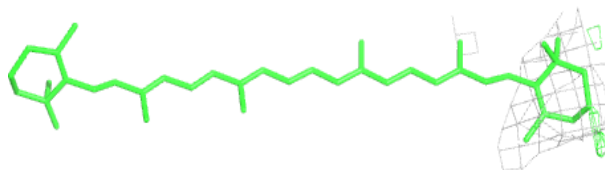
Electron density around CLA b 605:

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

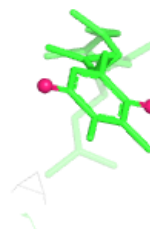
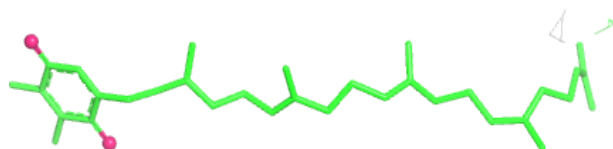
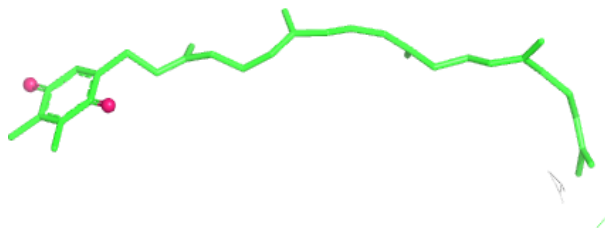


Electron density around BCR J 102:

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

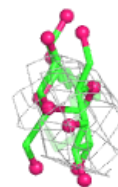
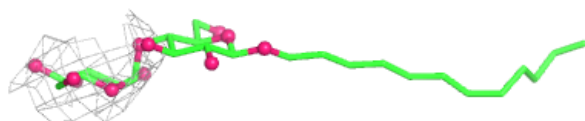
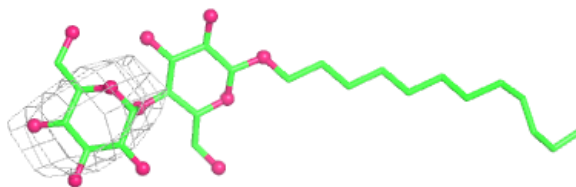
**Electron density around PL9 J 101:**

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

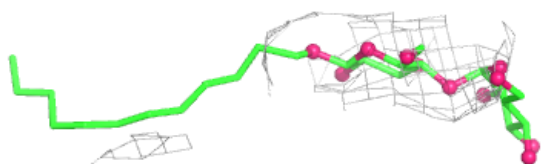
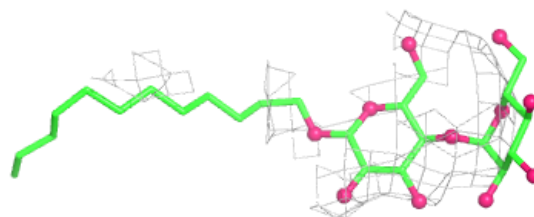


Electron density around LMT I 102:

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

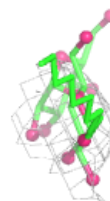
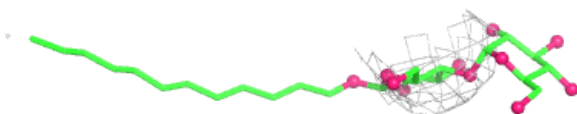
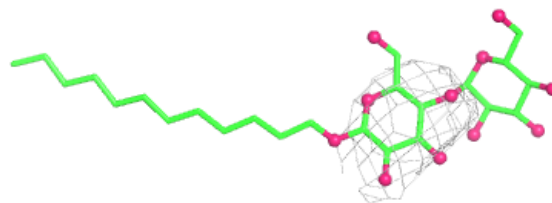
**Electron density around LMT b 626:**

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

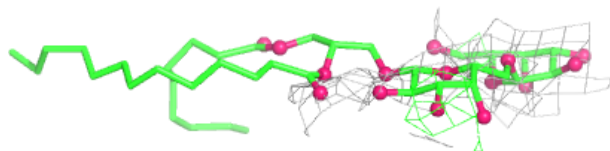
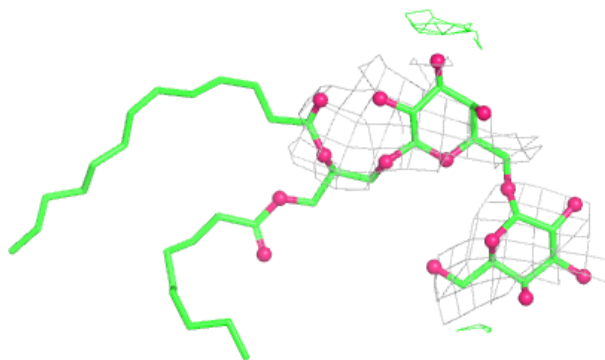


Electron density around LMT b 627:

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

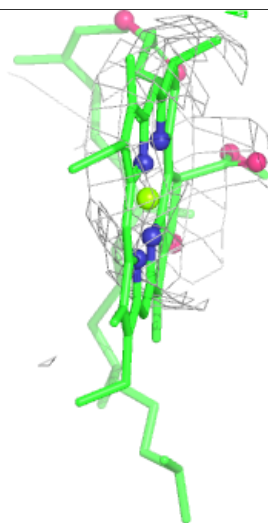
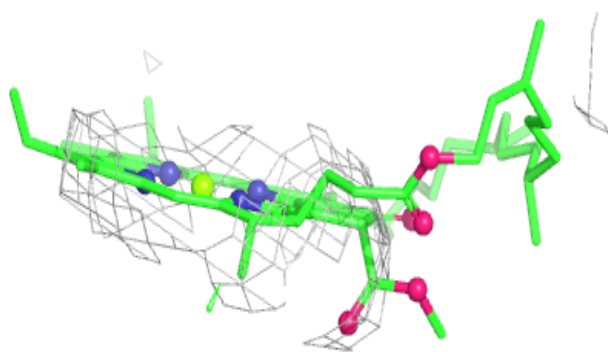
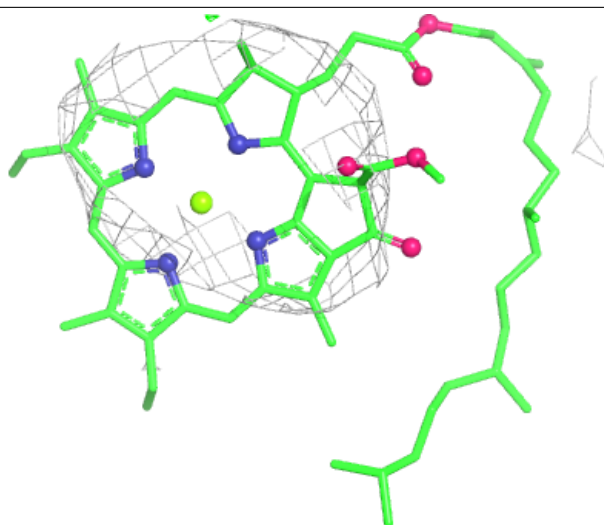
**Electron density around DGD B 627:**

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



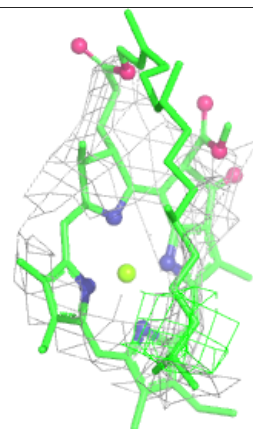
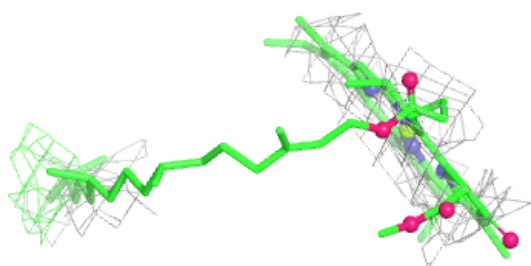
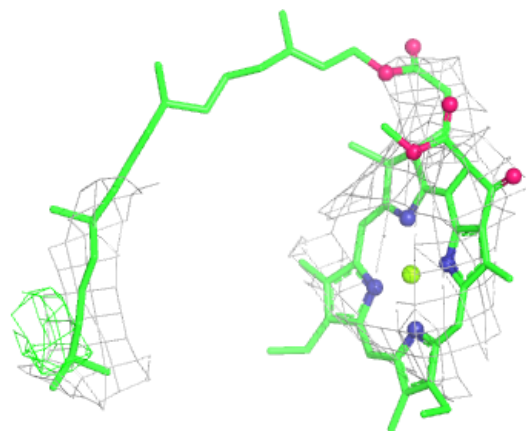
Electron density around CLA B 601:

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

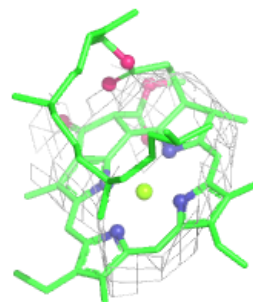
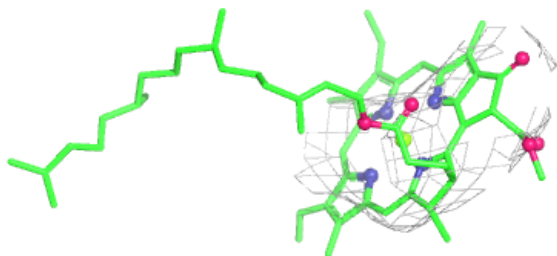
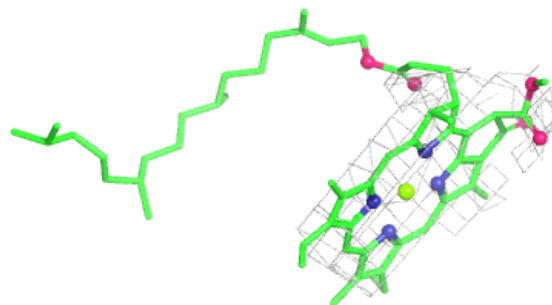


Electron density around CLA C 507:

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

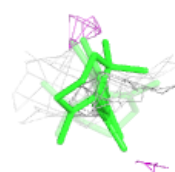
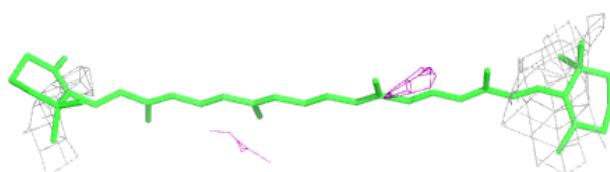
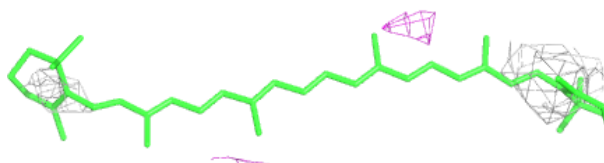
**Electron density around CLA c 513:**

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

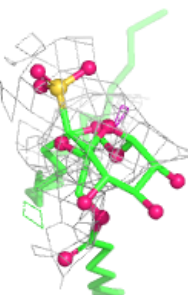
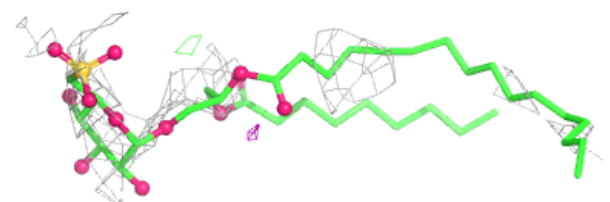
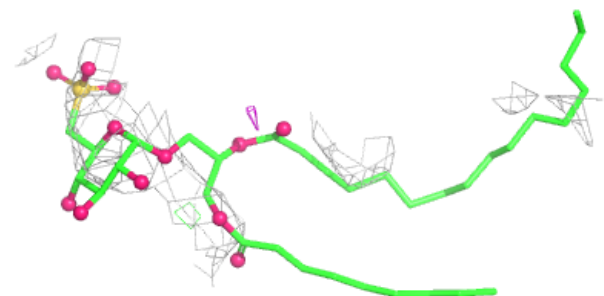


Electron density around BCR z 101:

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

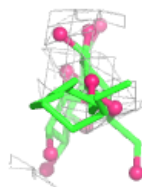
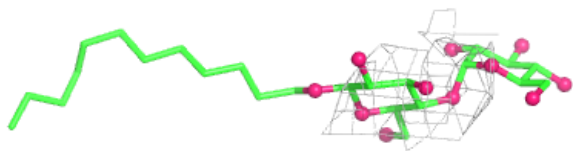
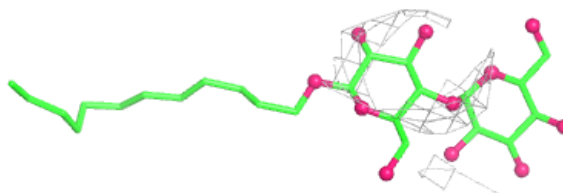
**Electron density around SQD b 601:**

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

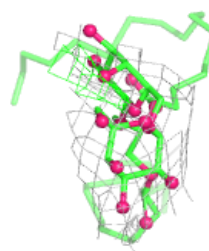
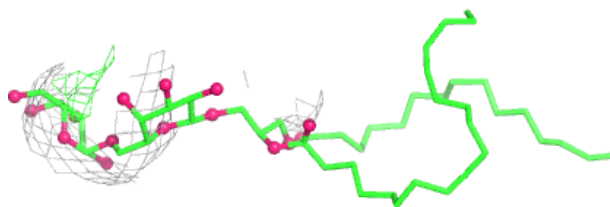
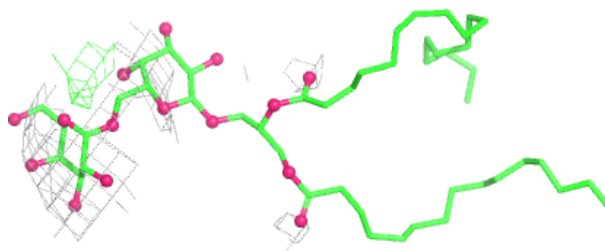


Electron density around LMT B 628:

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

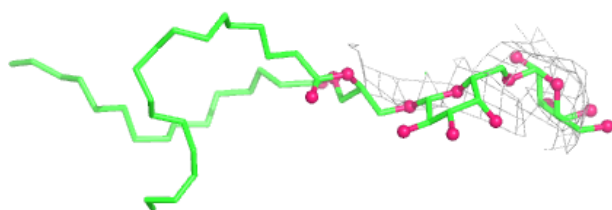
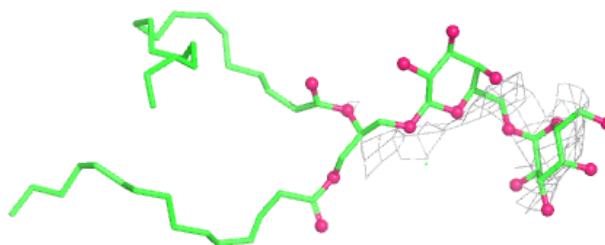
**Electron density around DGD D 409:**

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

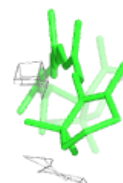
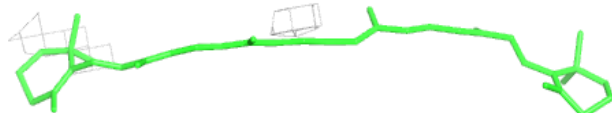
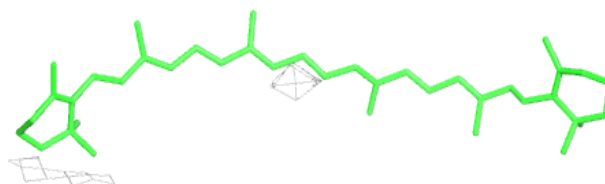


Electron density around DGD d 409:

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

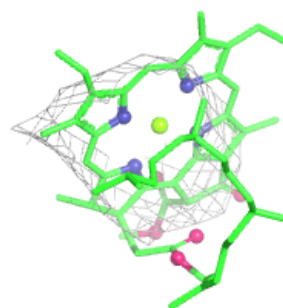
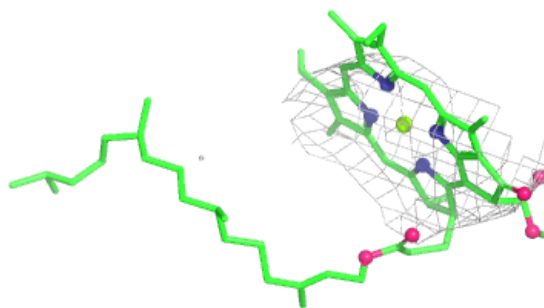
**Electron density around BCR B 618:**

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

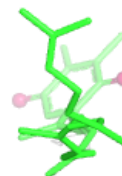
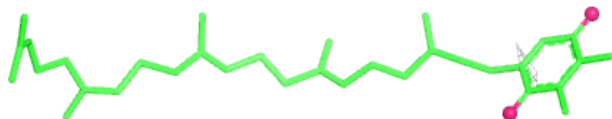
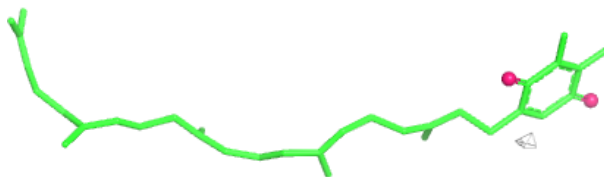


Electron density around CLA C 513:

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

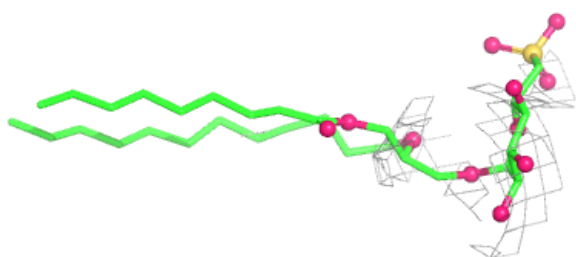
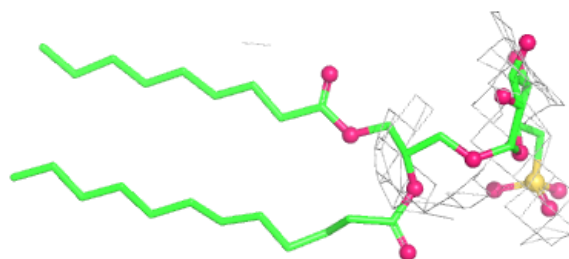
**Electron density around PL9 j 101:**

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

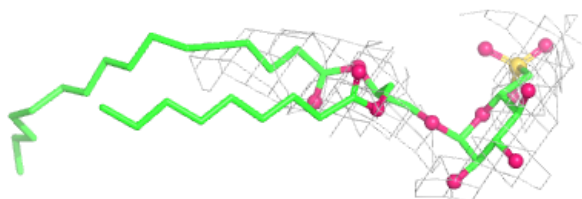
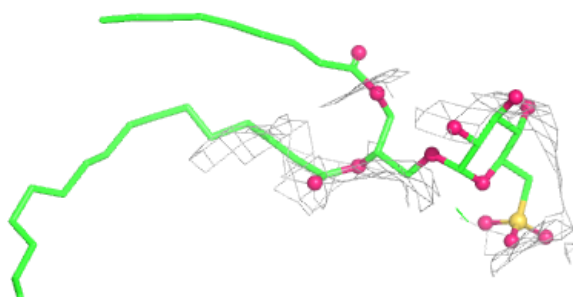


Electron density around SQD d 408:

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

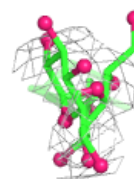
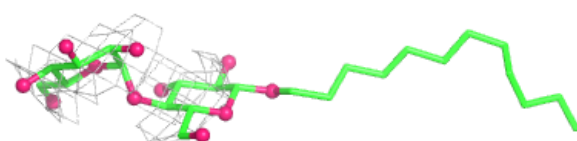
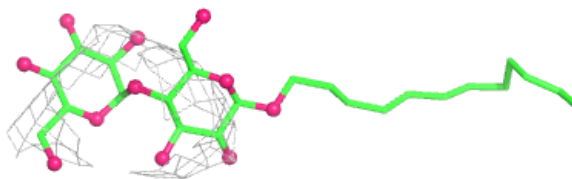
**Electron density around SQD B 626:**

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

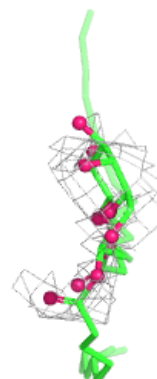
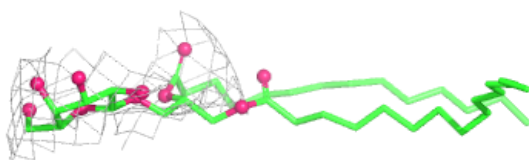
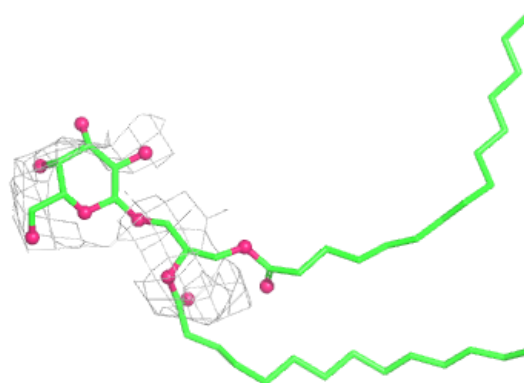


Electron density around LMT b 603:

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

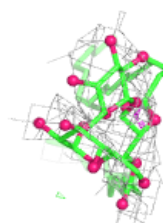
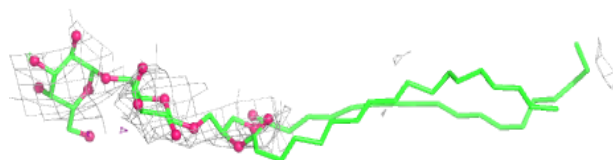
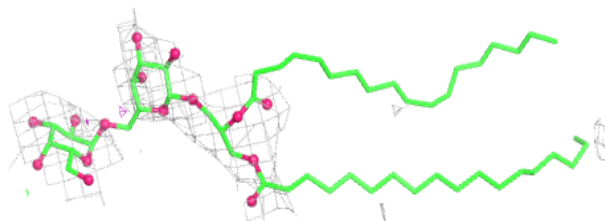
**Electron density around LMG k 103:**

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

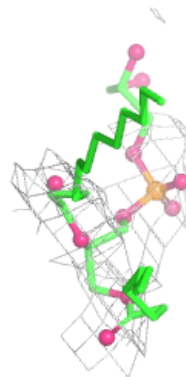
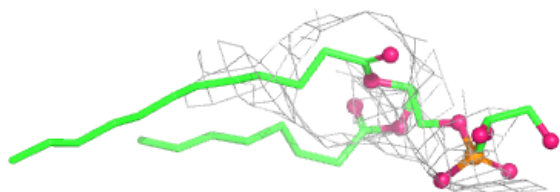


Electron density around DGD C 519:

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

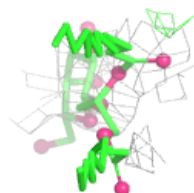
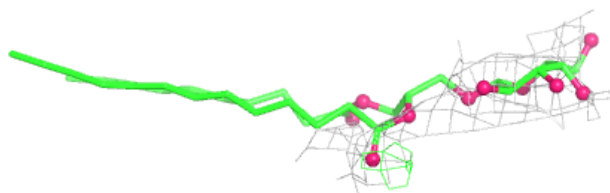
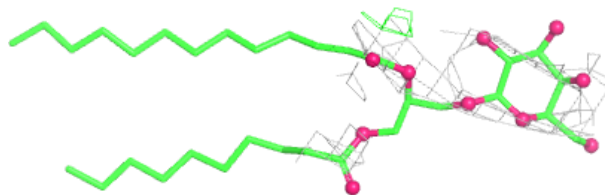
**Electron density around LHG A 415:**

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

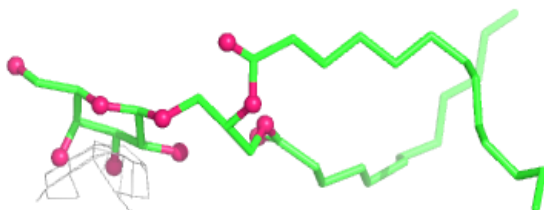
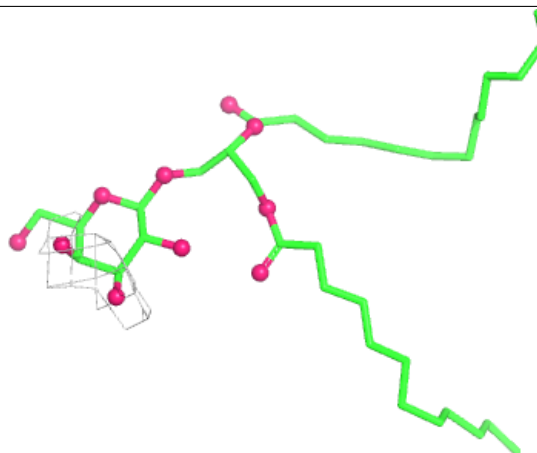


Electron density around LMG M 101:

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

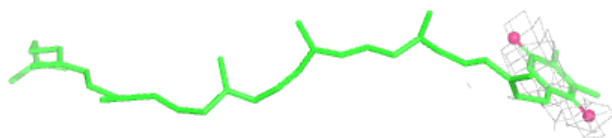
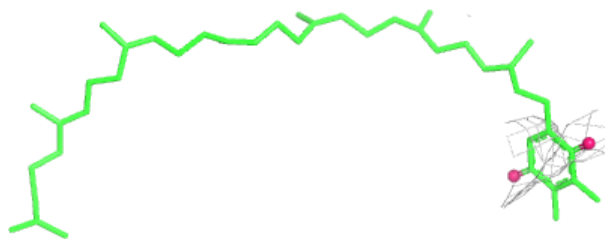
**Electron density around LMG E 101:**

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

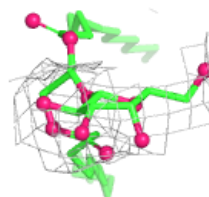
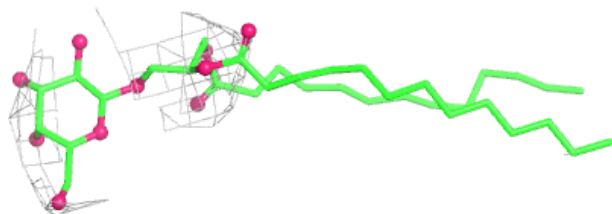
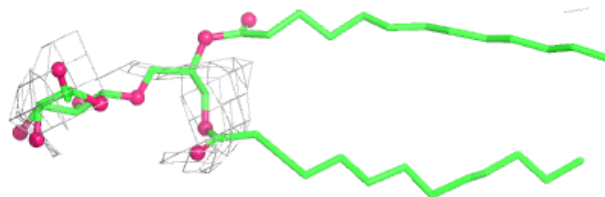


Electron density around PL9 A 408:

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

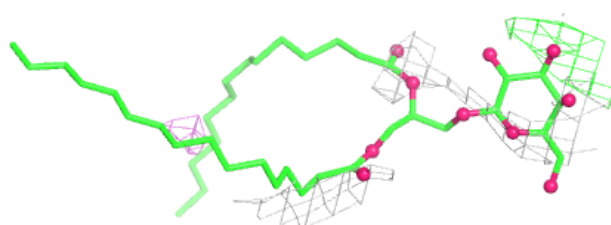
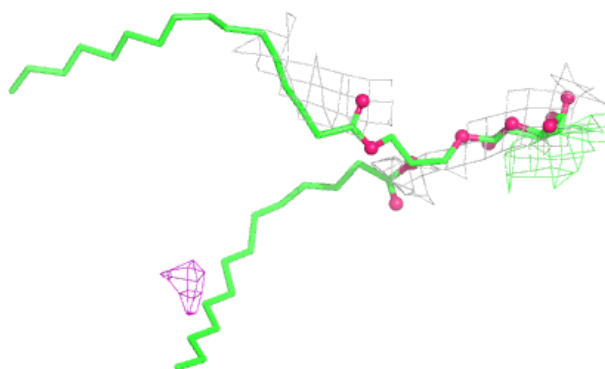
**Electron density around LMG c 519:**

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

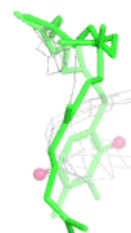
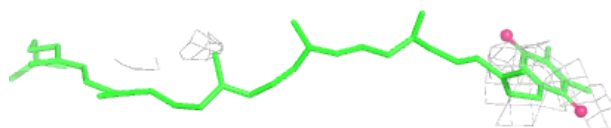
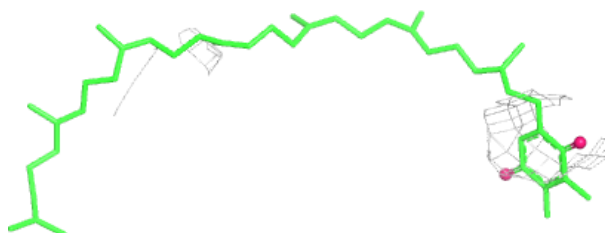


Electron density around LMG b 625:

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

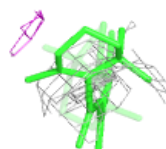
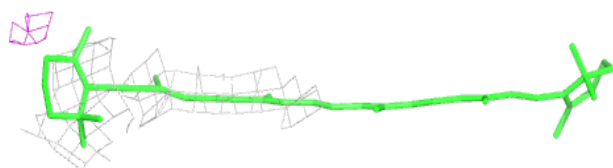
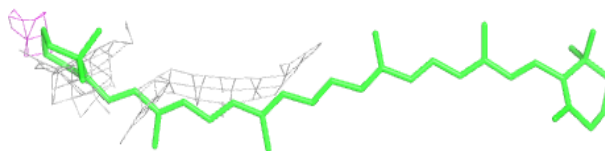
**Electron density around PL9 a 410:**

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

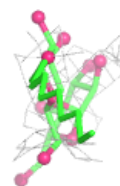
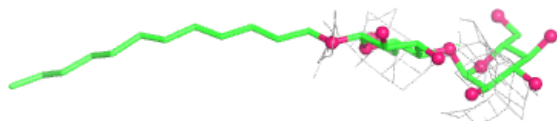
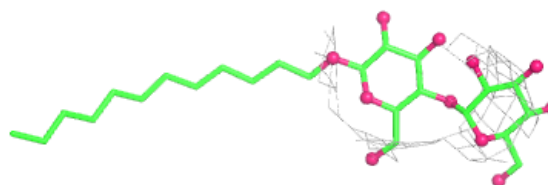


Electron density around BCR H 101:

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

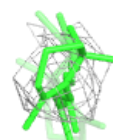
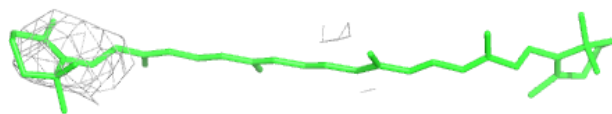
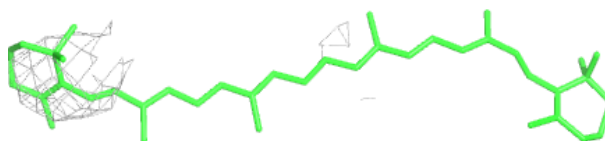
**Electron density around LMT B 625:**

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

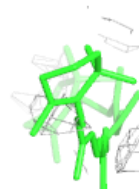
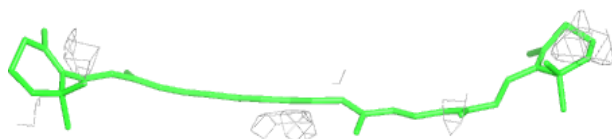
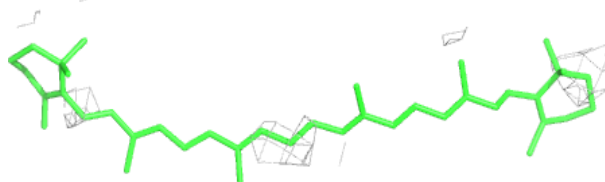


Electron density around BCR k 102:

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

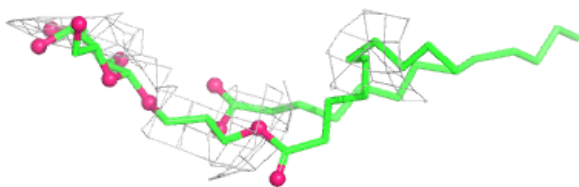
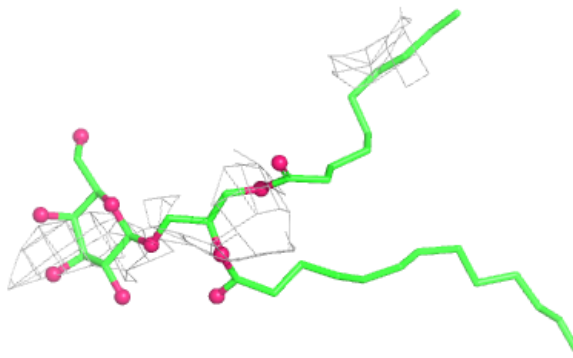
**Electron density around BCR T 102:**

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

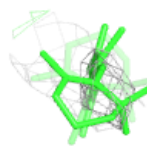
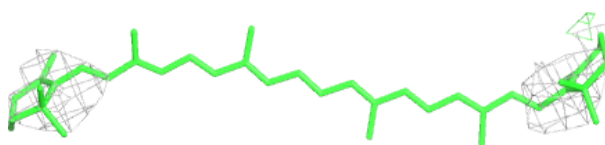


Electron density around LMG A 418:

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

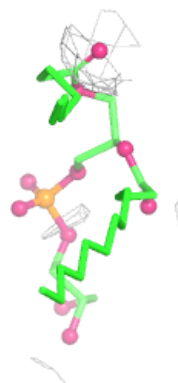
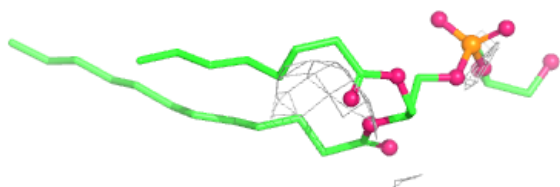
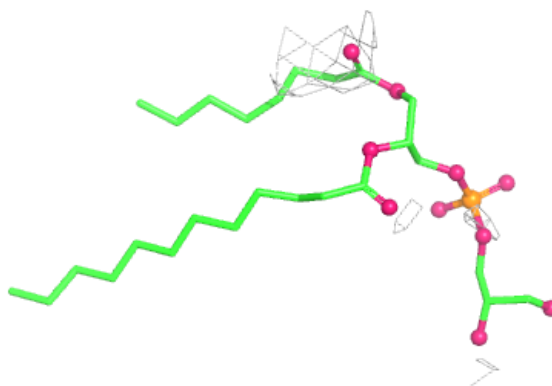
**Electron density around BCR a 412:**

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

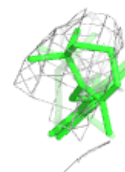
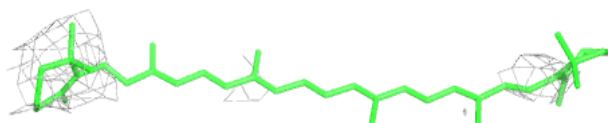
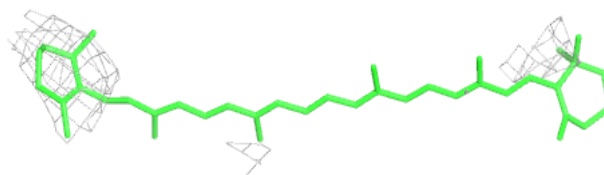


Electron density around LHG a 417:

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

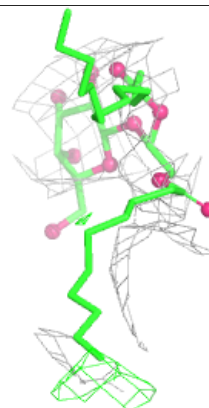
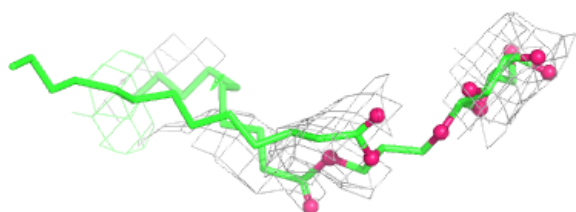
**Electron density around BCR B 620:**

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

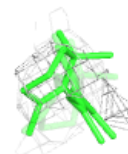
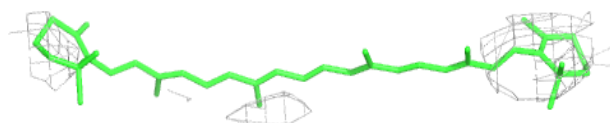
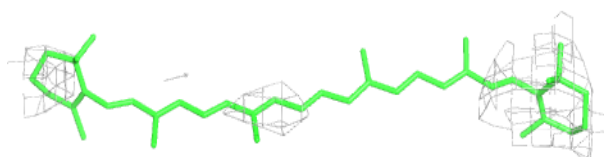


Electron density around LMG a 402:

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

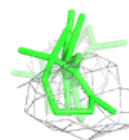
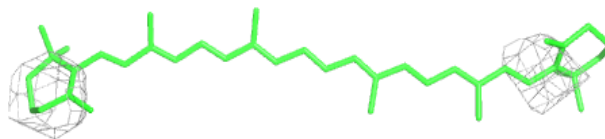
**Electron density around BCR C 516:**

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

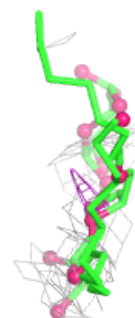
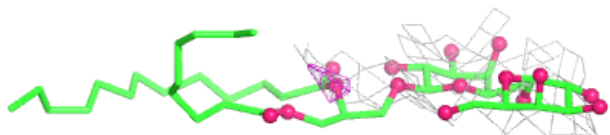
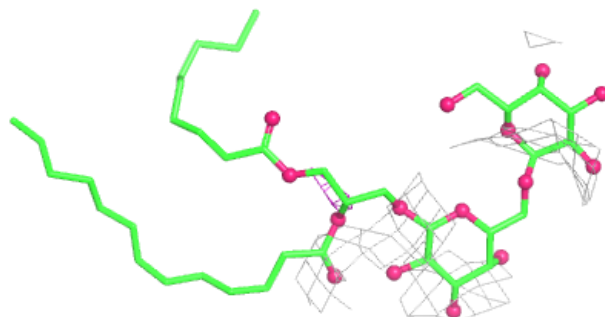


Electron density around BCR b 621:

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

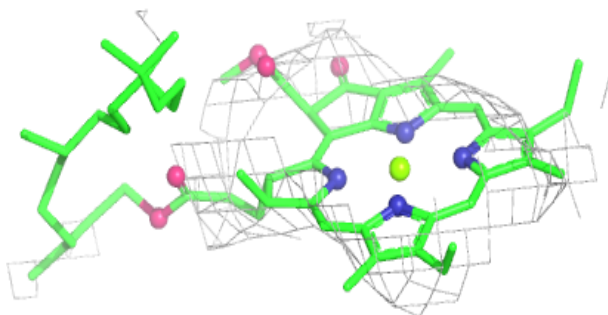
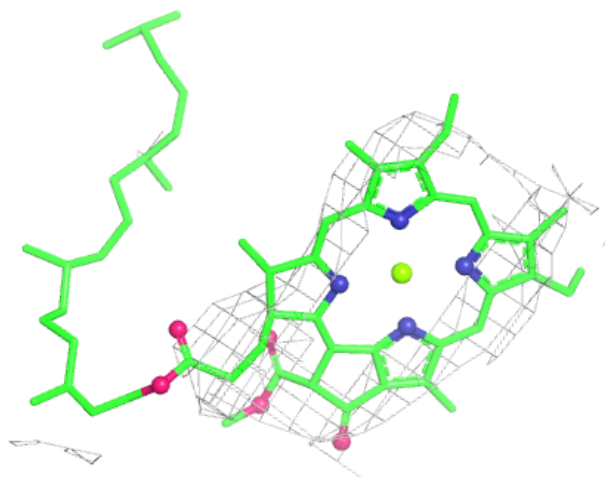
**Electron density around DGD b 602:**

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



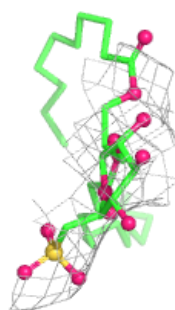
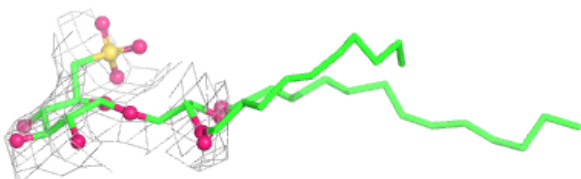
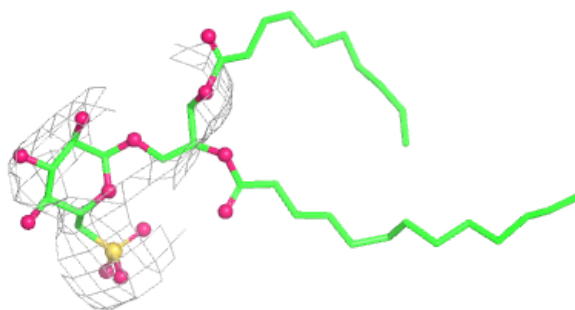
Electron density around CLA b 620:

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

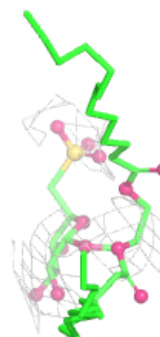
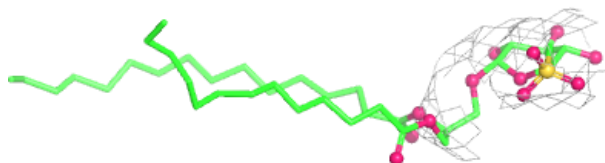


Electron density around SQD F 102:

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

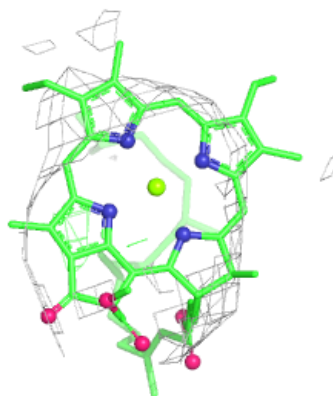
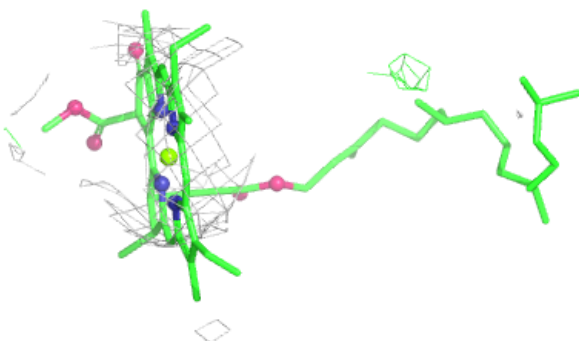
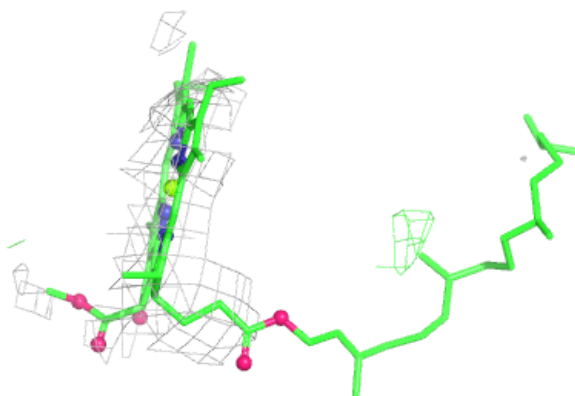
**Electron density around SQD a 415:**

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

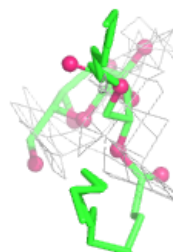
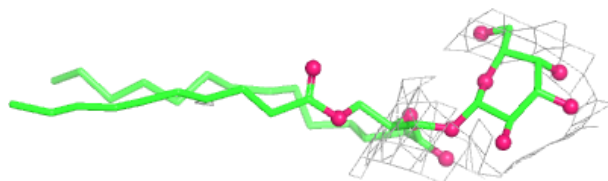
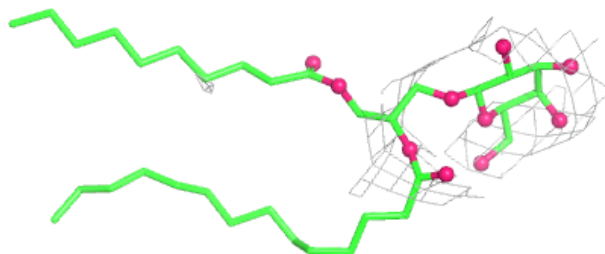


Electron density around CLA C 506:

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

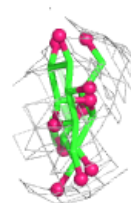
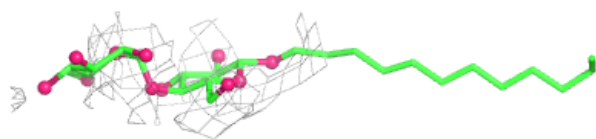
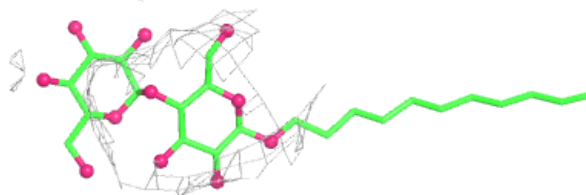
**Electron density around LMG i 101:**

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

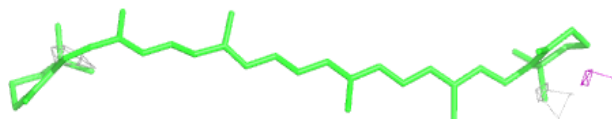
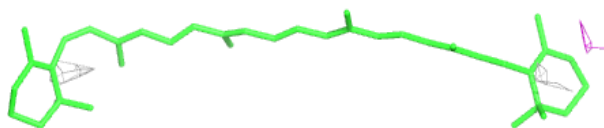


Electron density around LMT b 604:

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

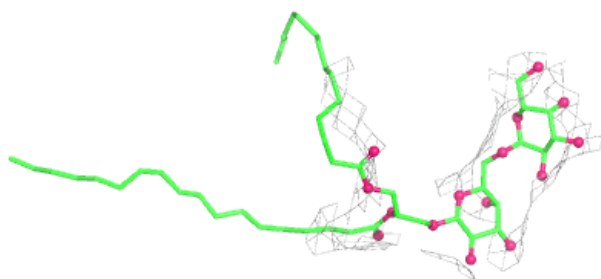
**Electron density around BCR c 514:**

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

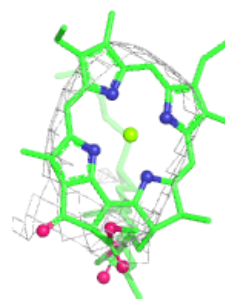
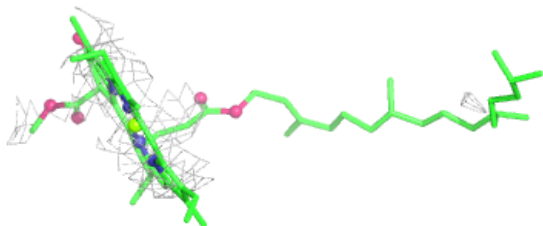
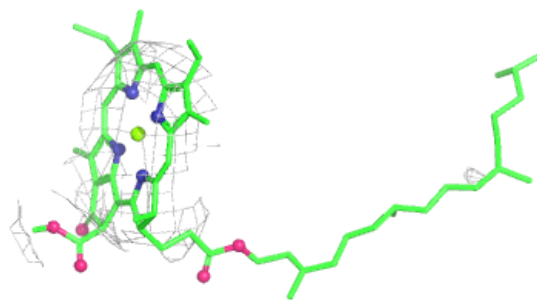


Electron density around DGD C 518:

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

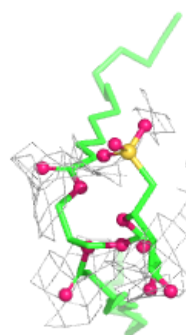
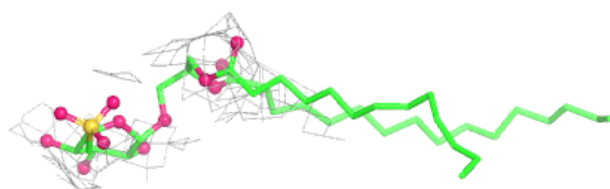
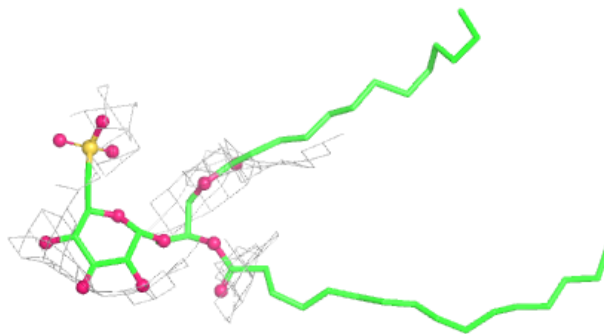
**Electron density around CLA b 613:**

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

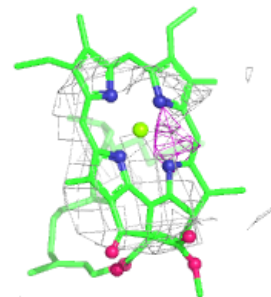
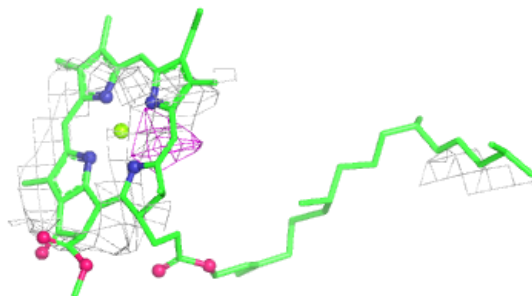


Electron density around SQD A 413:

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

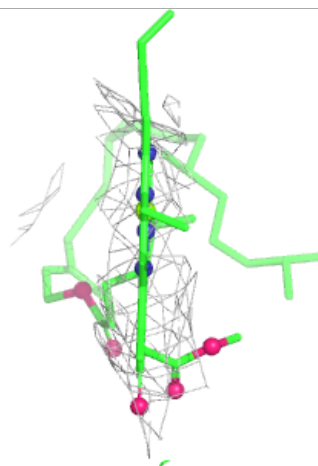
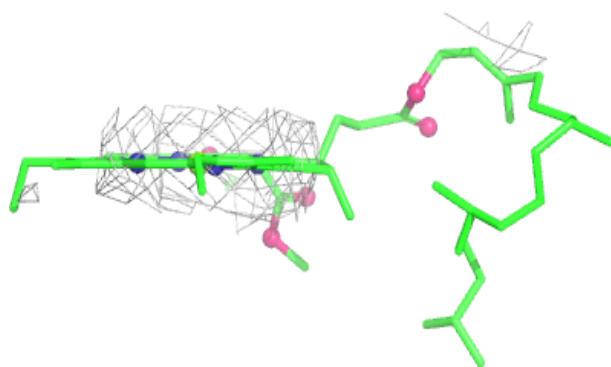
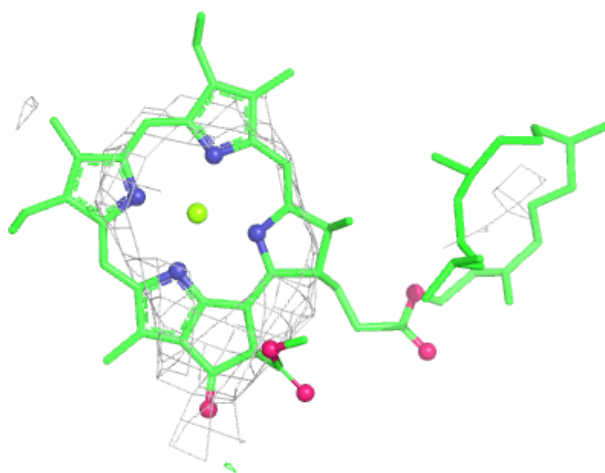
**Electron density around CLA c 511:**

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



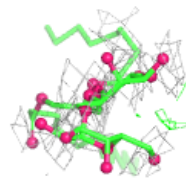
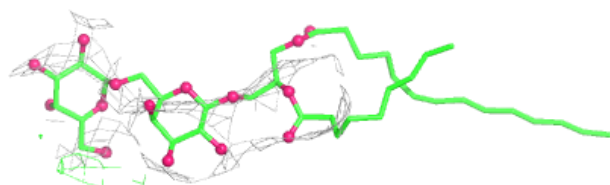
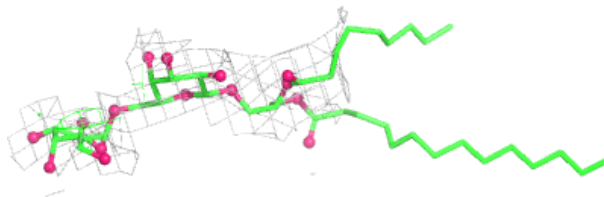
Electron density around CLA c 512:

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



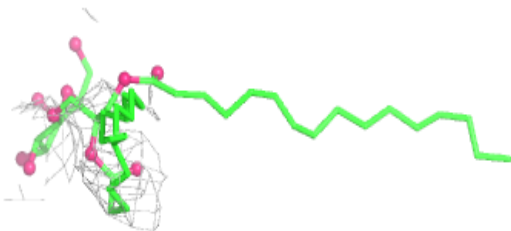
Electron density around DGD C 517:

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



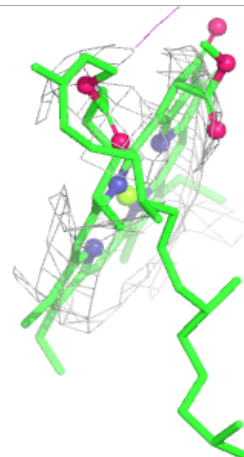
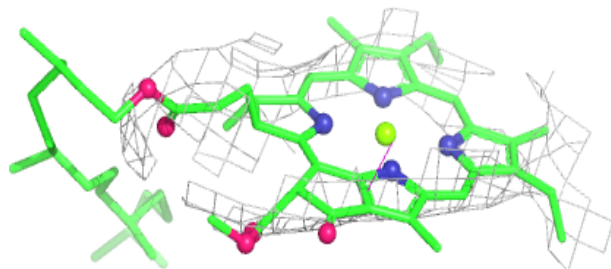
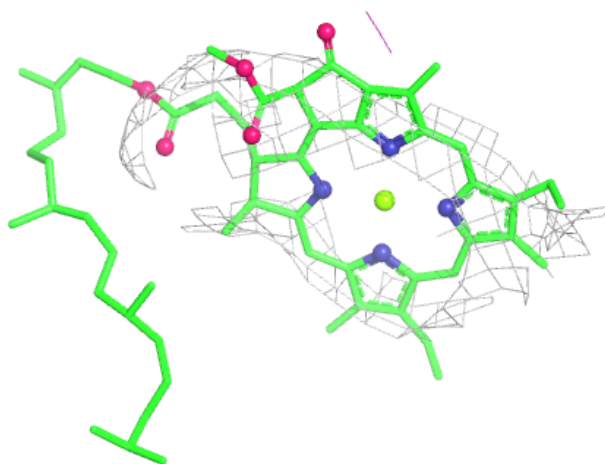
Electron density around LMG a 416:

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



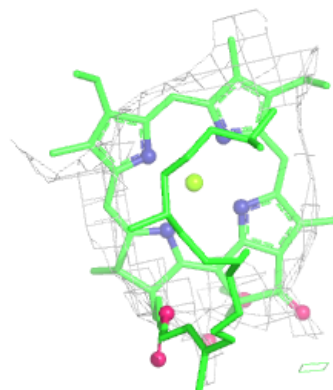
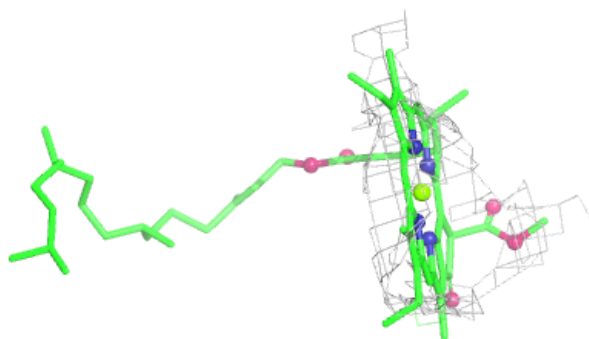
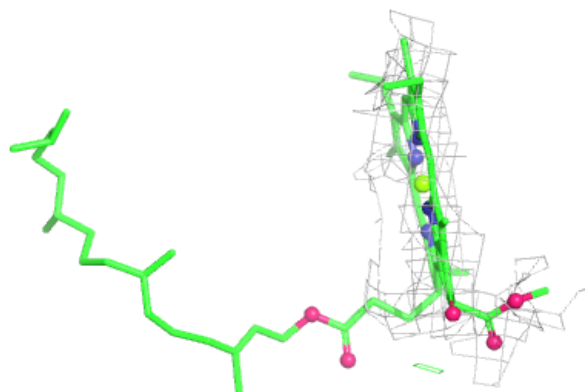
Electron density around CLA B 616:

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

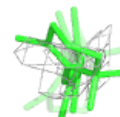
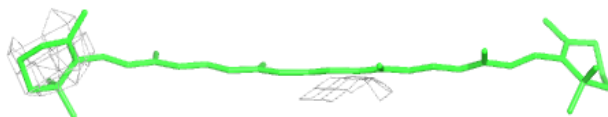
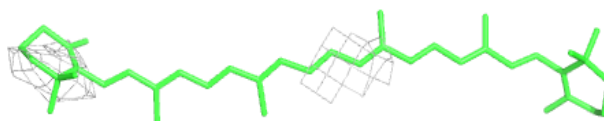


Electron density around CLA c 506:

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

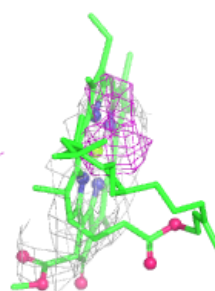
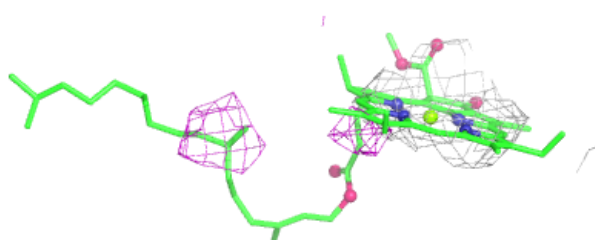
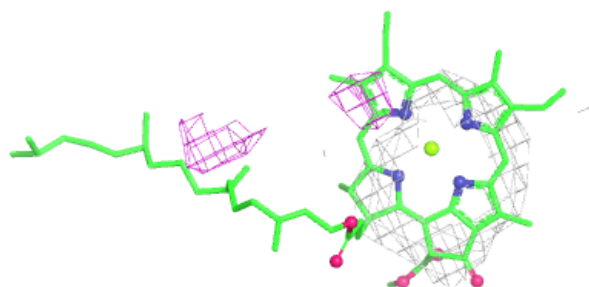
**Electron density around BCR B 619:**

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

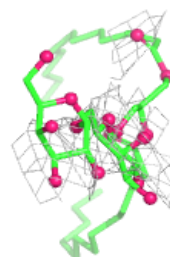
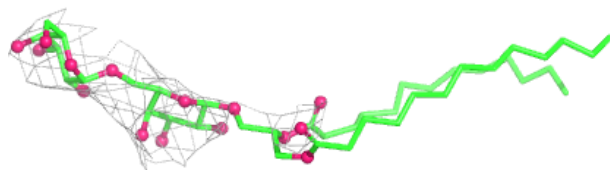
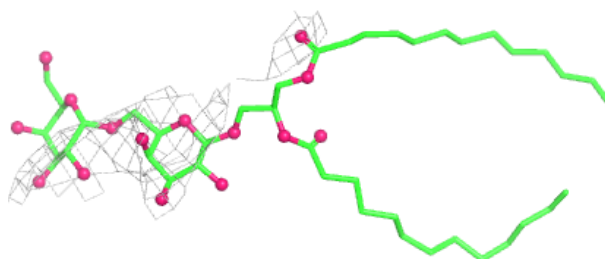


Electron density around CLA a 406:

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

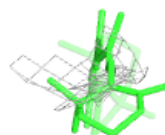
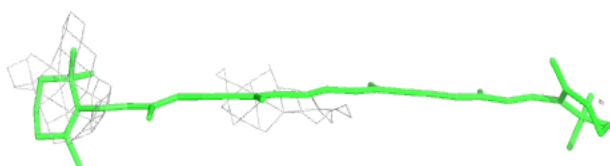
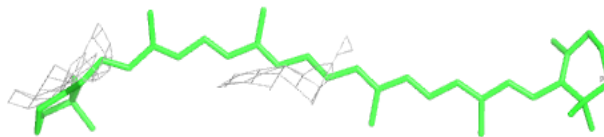
**Electron density around DGD A 411:**

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

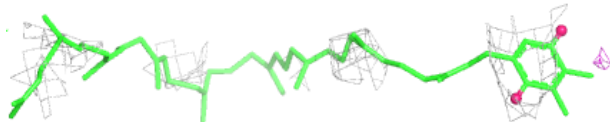
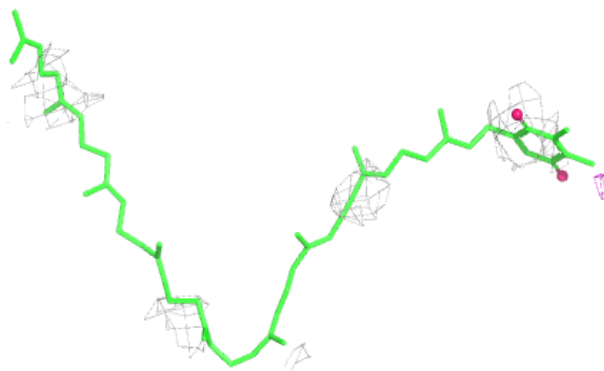


Electron density around BCR h 101:

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

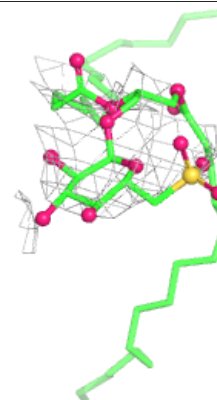
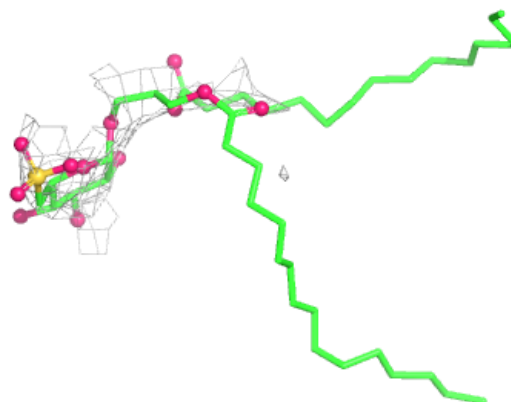
**Electron density around PL9 d 404:**

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

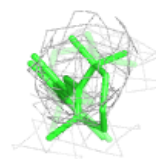
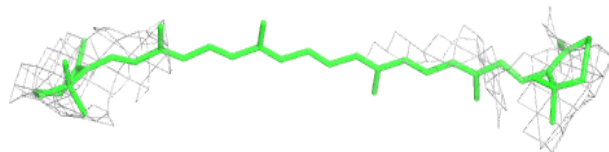
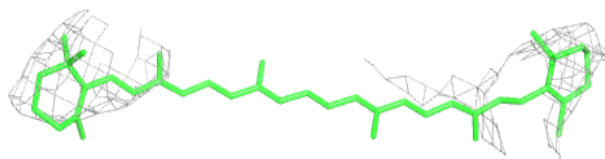


Electron density around SQD a 401:

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

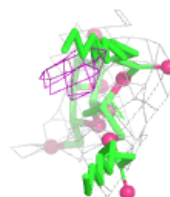
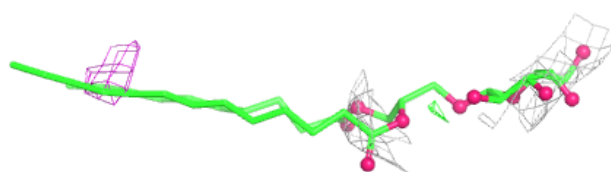
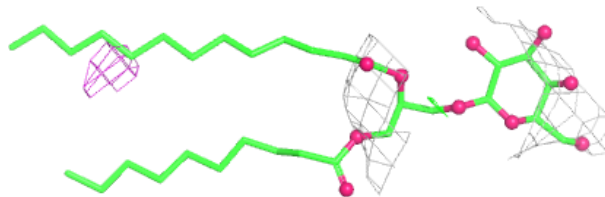
**Electron density around BCR b 622:**

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

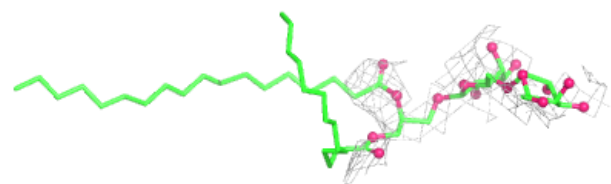


Electron density around LMG m 102:

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

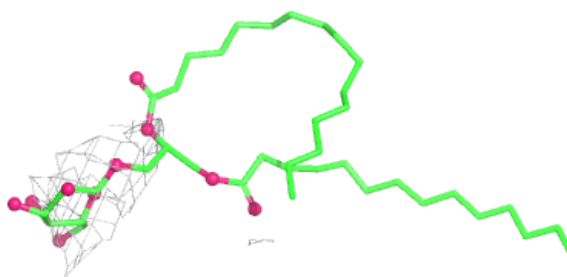
**Electron density around DGD c 517:**

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

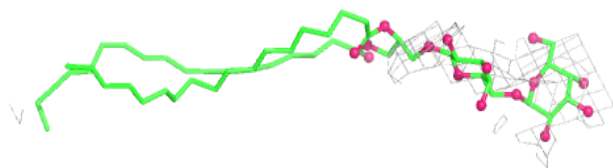
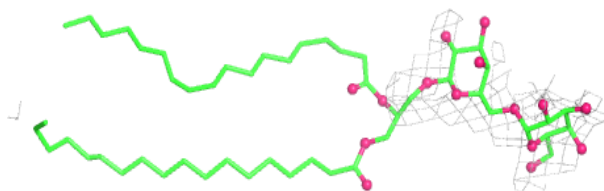


Electron density around LMG B 622:

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

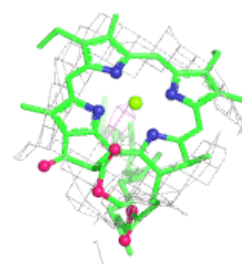
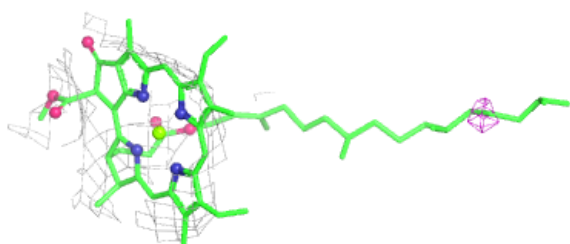
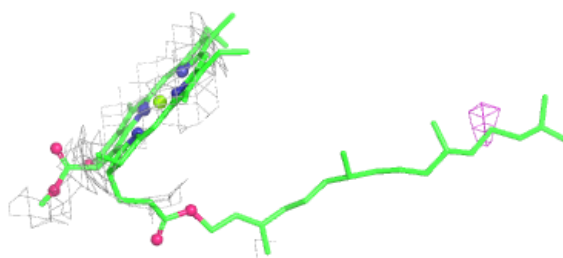
**Electron density around DGD c 518:**

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

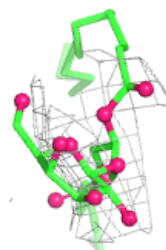
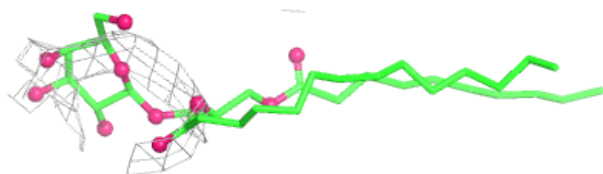
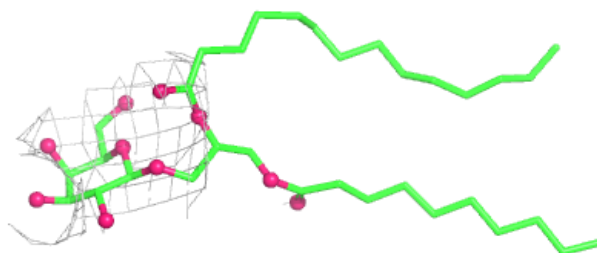


Electron density around CLA C 504:

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

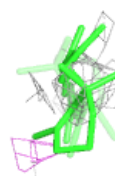
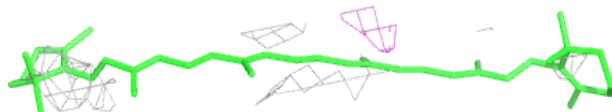
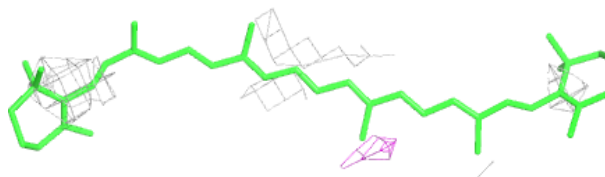
**Electron density around LMG I 101:**

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

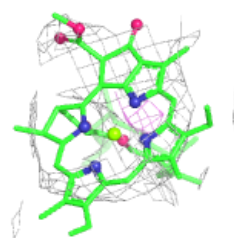
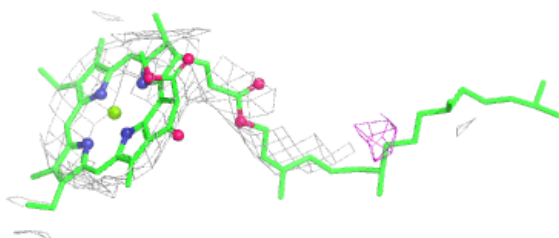
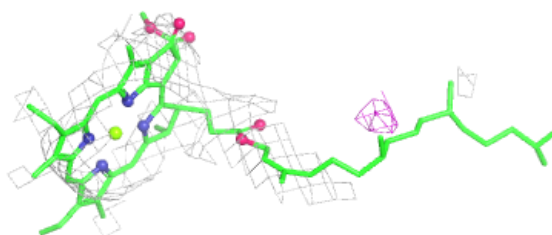


Electron density around BCR y 101:

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

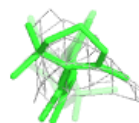
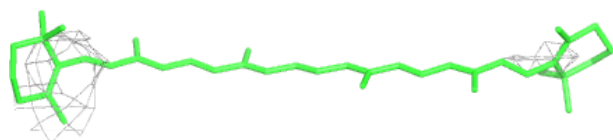
**Electron density around CLA c 502:**

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

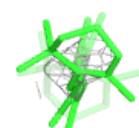
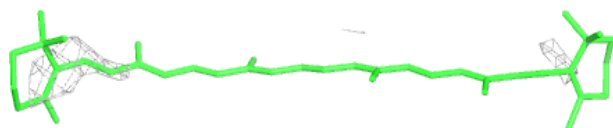
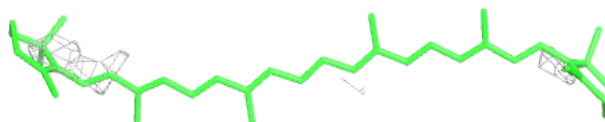


Electron density around BCR C 515:

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

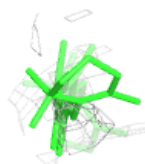
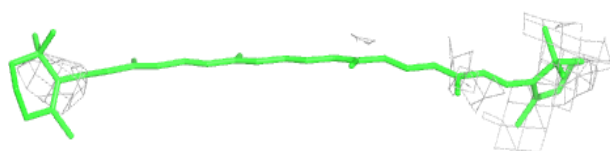
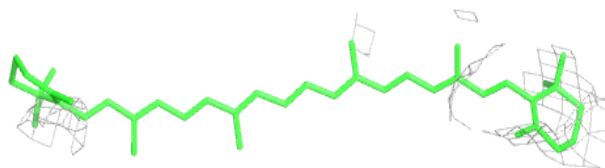
**Electron density around BCR A 410:**

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



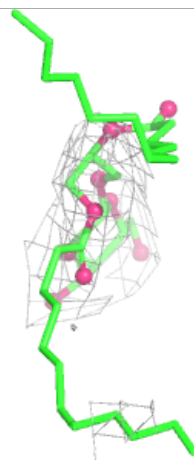
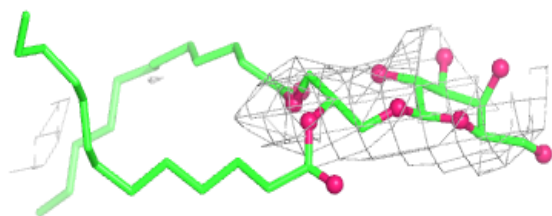
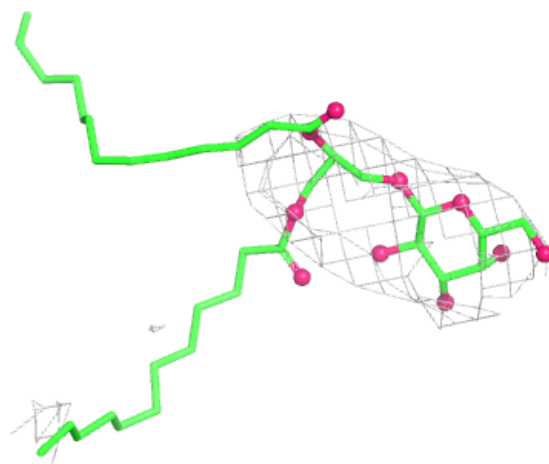
Electron density around BCR B 617:

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



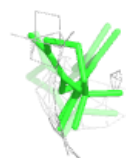
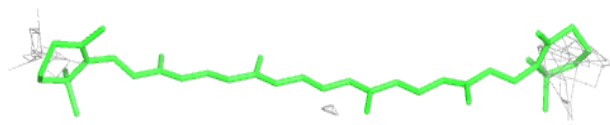
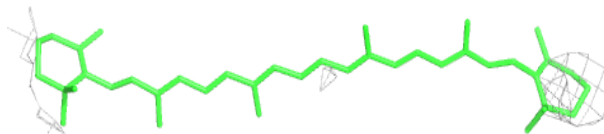
Electron density around LMG e 101:

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

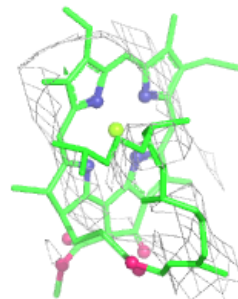
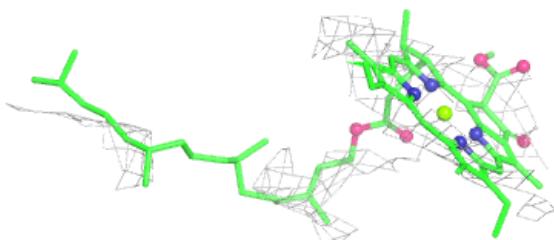
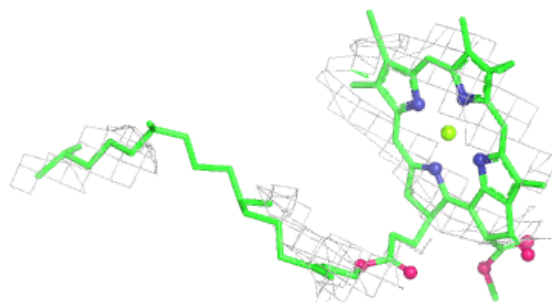


Electron density around BCR c 515:

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

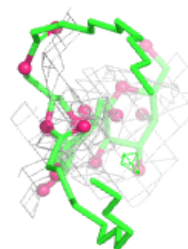
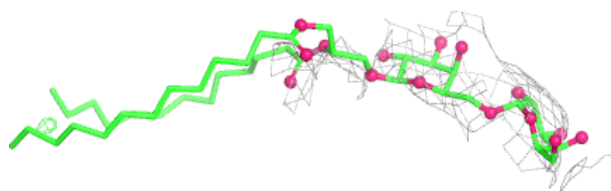
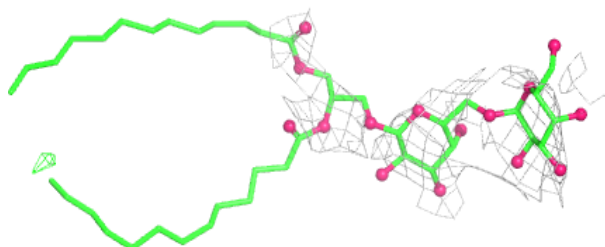
**Electron density around CLA C 511:**

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

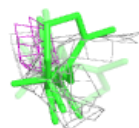
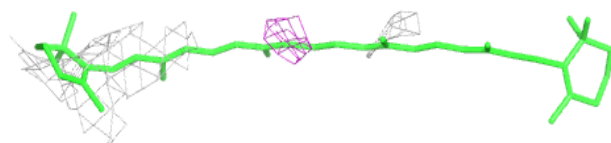
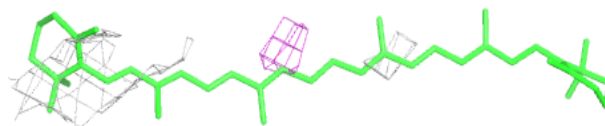


Electron density around DGD a 413:

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

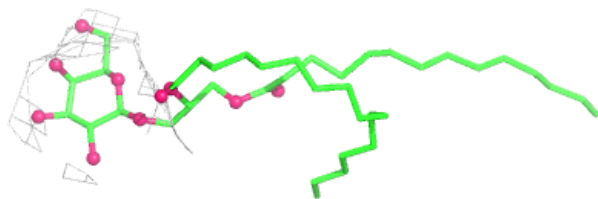
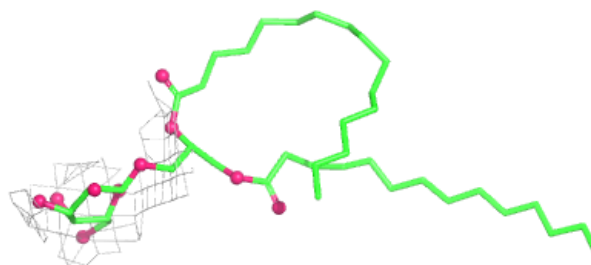
**Electron density around BCR T 101:**

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

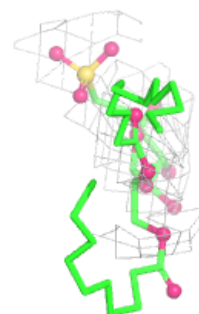
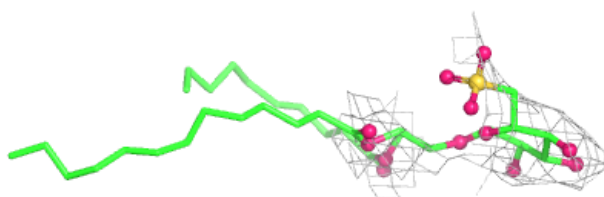


Electron density around LMG b 624:

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

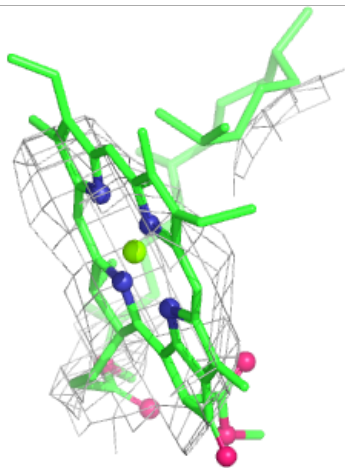
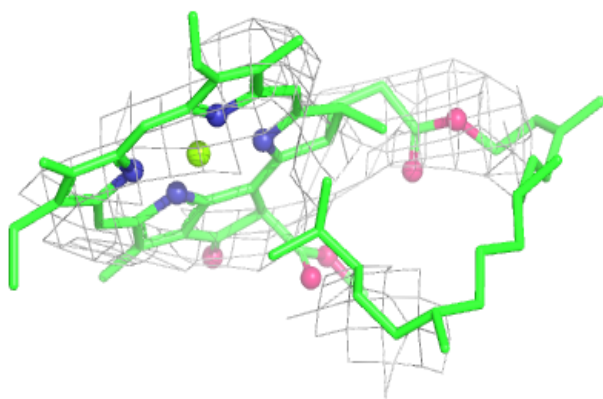
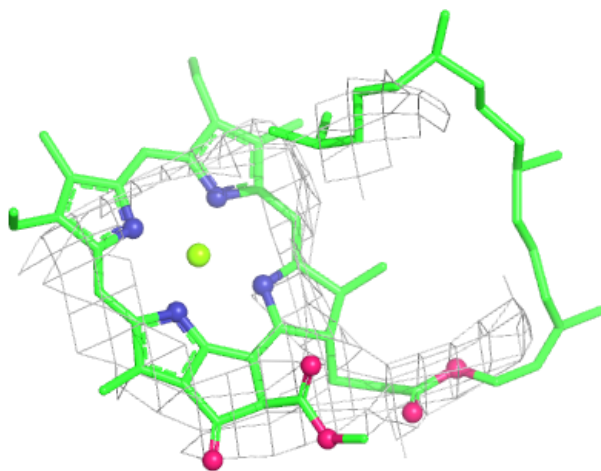
**Electron density around SQD f 102:**

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



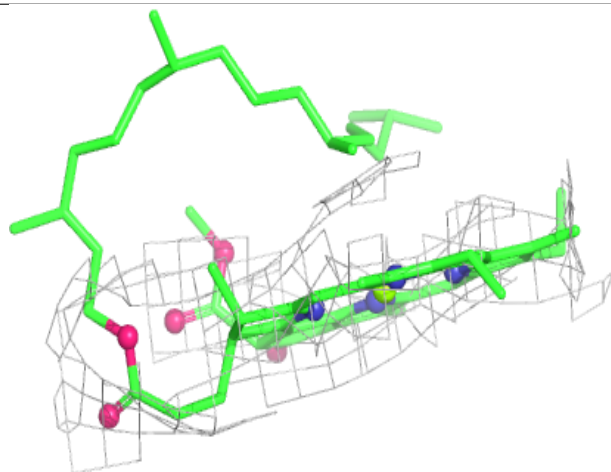
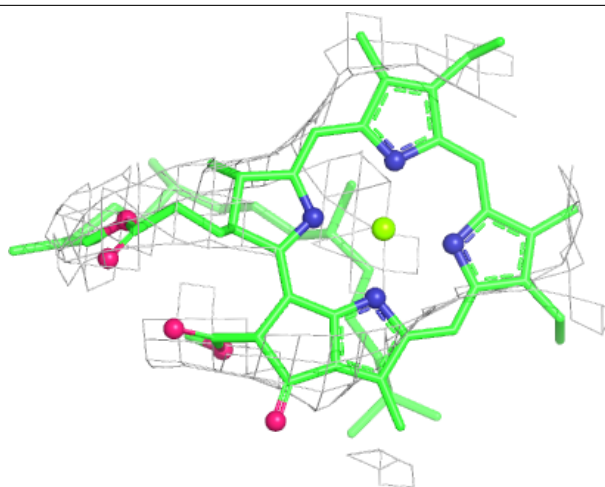
Electron density around CLA b 619:

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



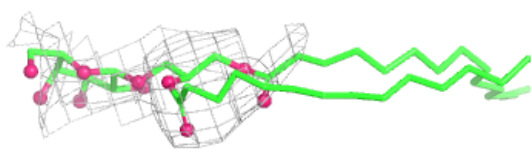
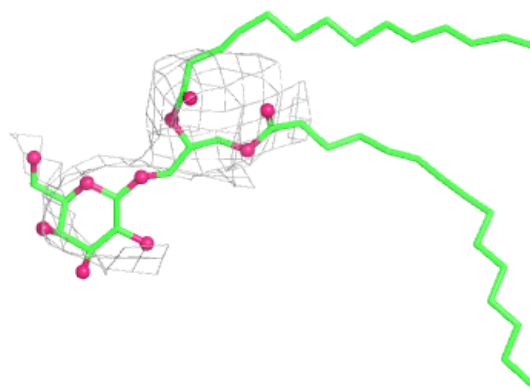
Electron density around CLA C 510:

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

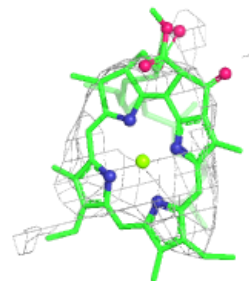
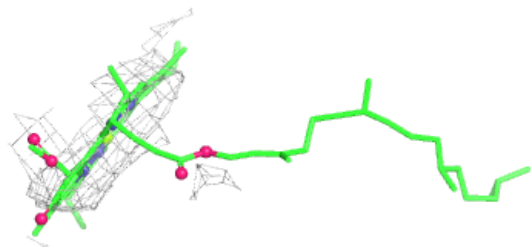


Electron density around LMG C 520:

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

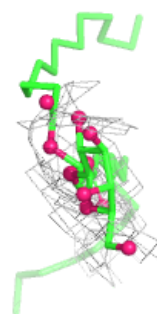
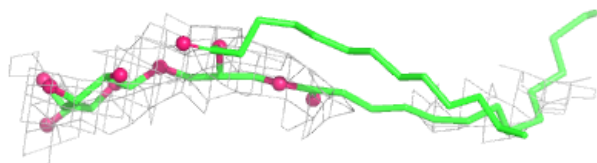
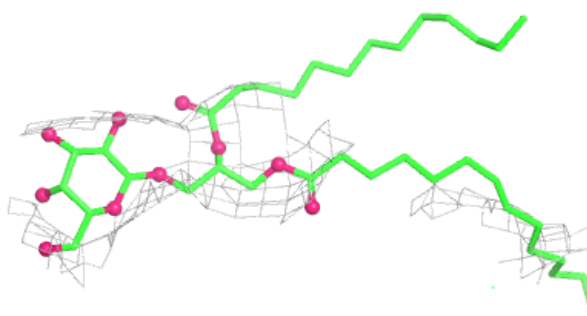
**Electron density around CLA a 409:**

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

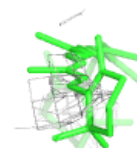
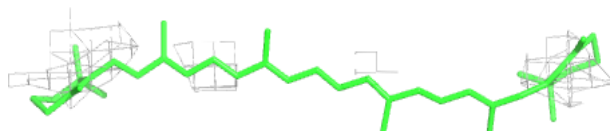
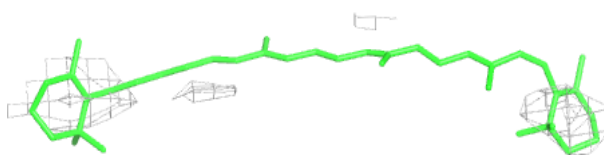


Electron density around LMG D 406:

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

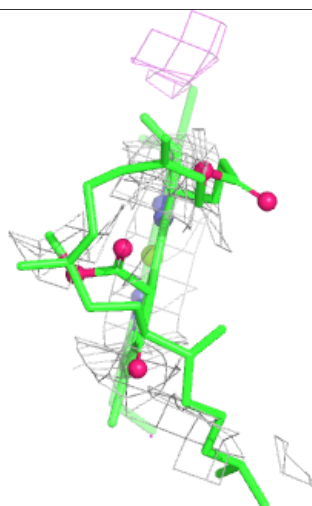
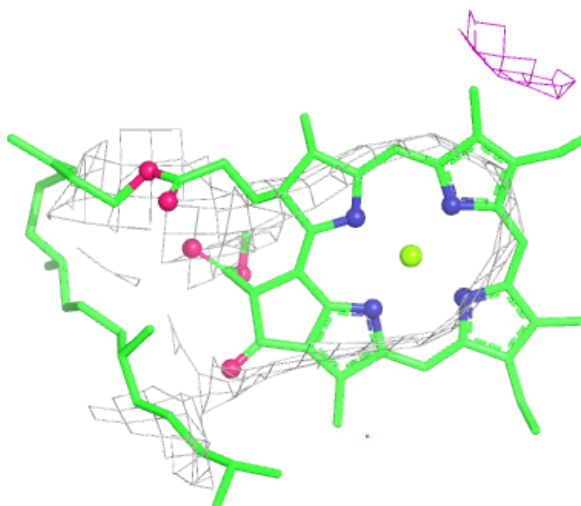
**Electron density around BCR C 514:**

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



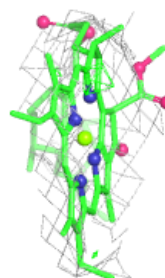
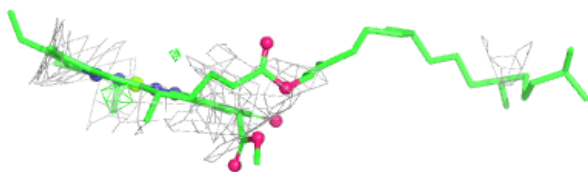
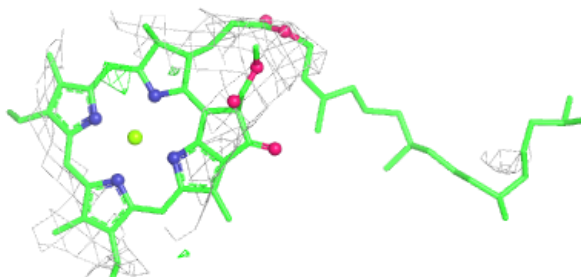
Electron density around CLA B 610:

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

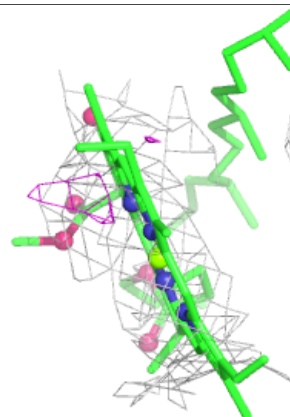
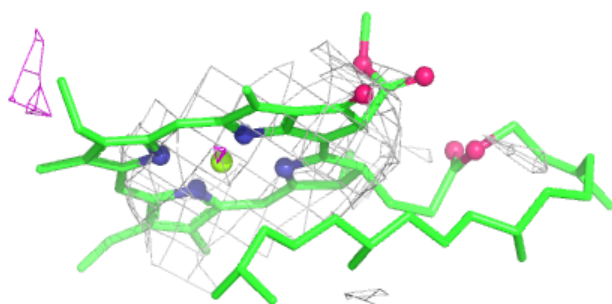
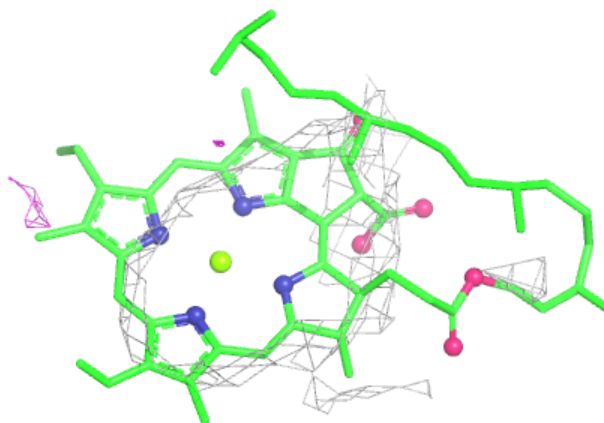


Electron density around CLA b 606:

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

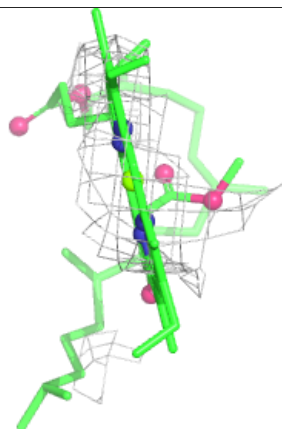
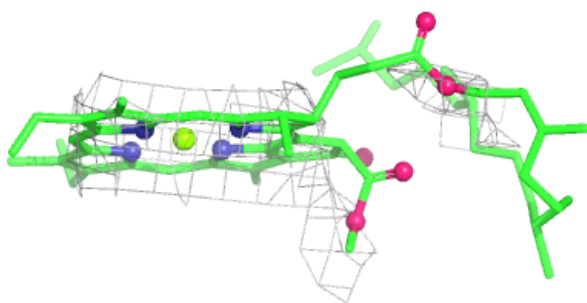
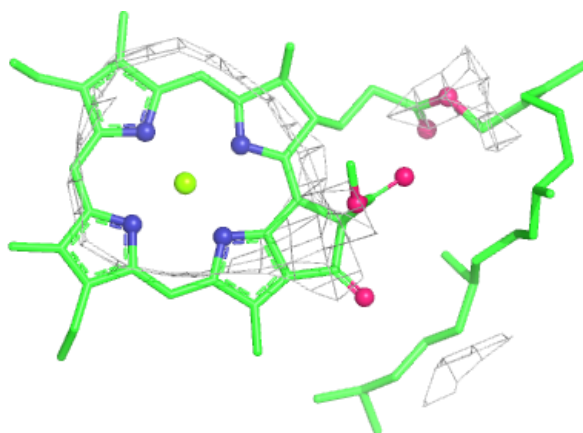
**Electron density around CLA C 509:**

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

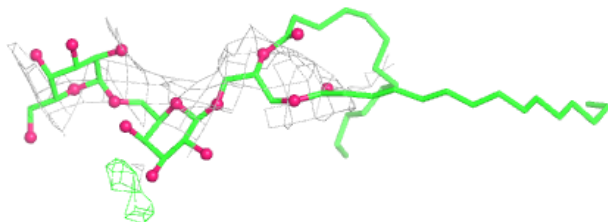


Electron density around CLA b 614:

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

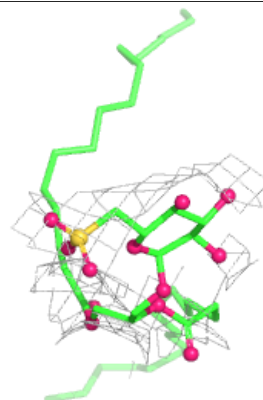
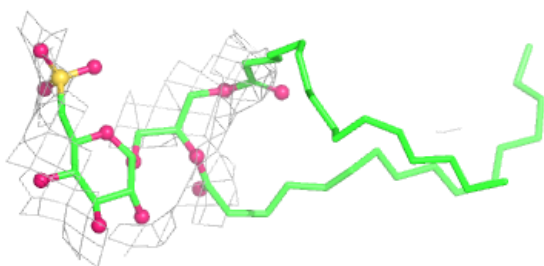
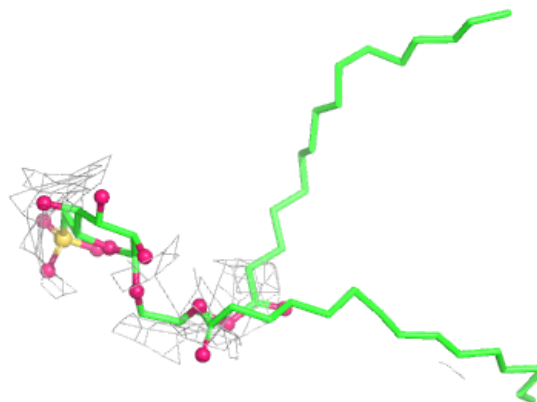
**Electron density around DGD b 623:**

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

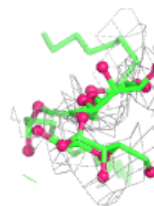
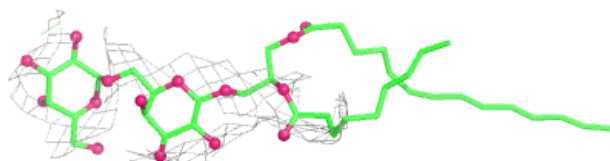
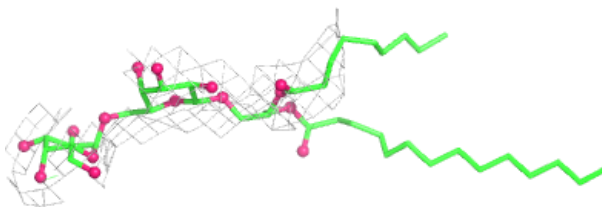


Electron density around SQD A 417:

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

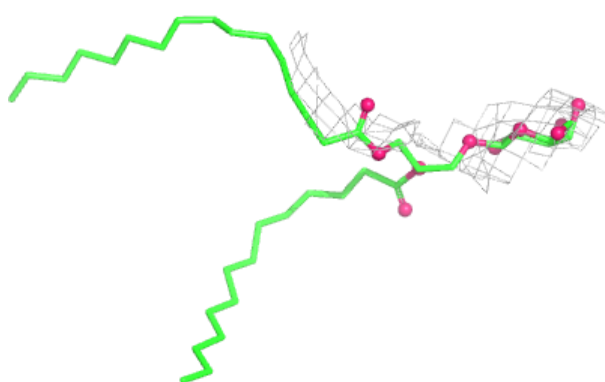
**Electron density around DGD c 516:**

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

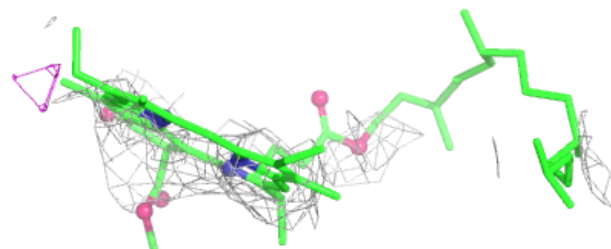
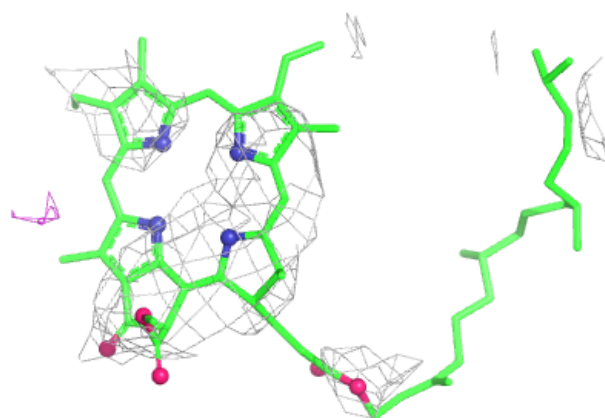


Electron density around LMG B 623:

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

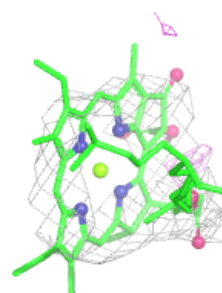
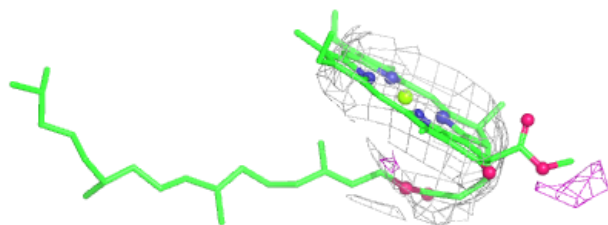
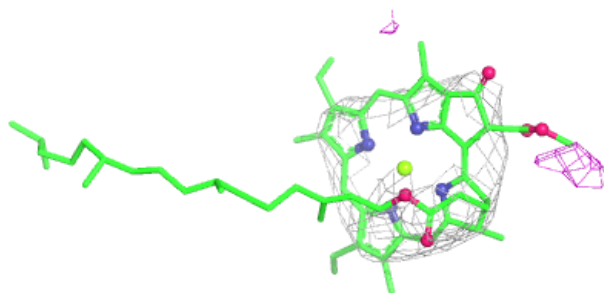
**Electron density around PHO A 406:**

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

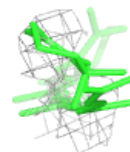
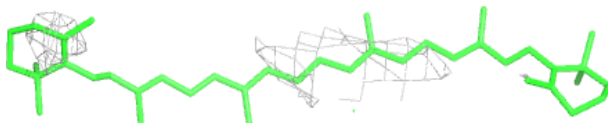
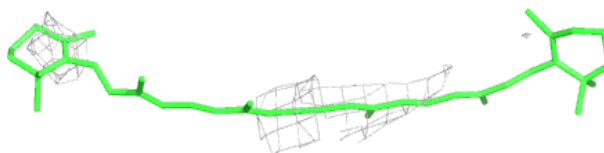


Electron density around CLA B 608:

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

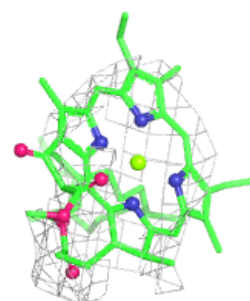
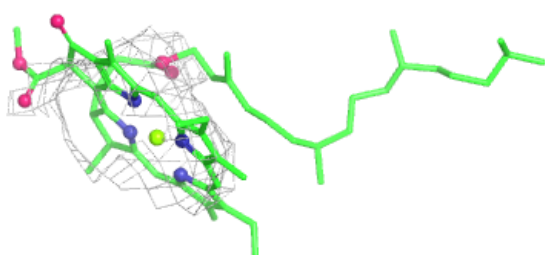
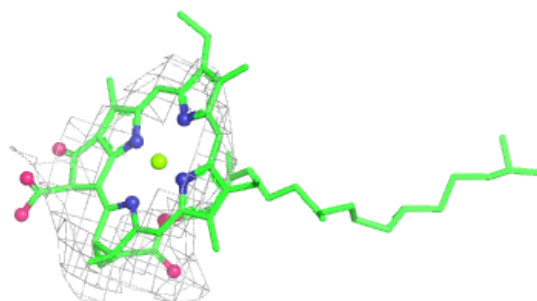
**Electron density around BCR D 405:**

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

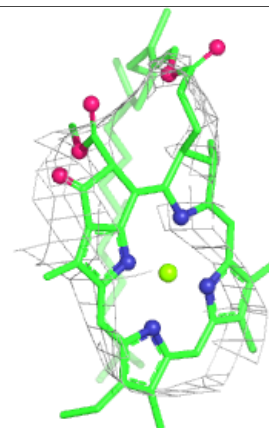
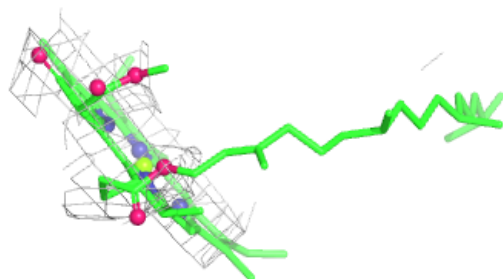
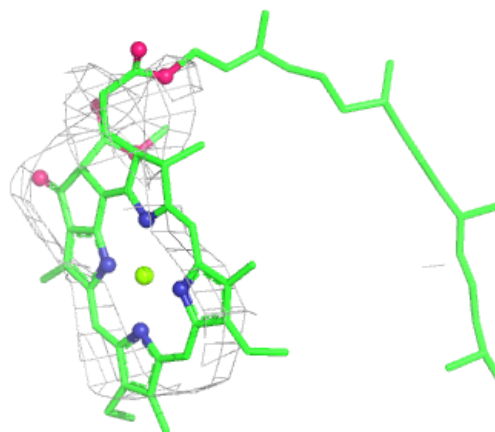


Electron density around CLA C 505:

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

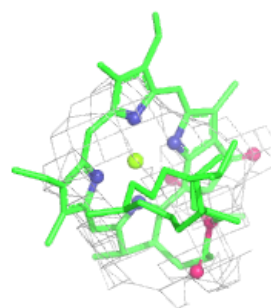
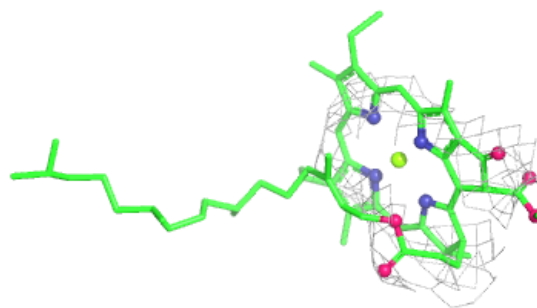
**Electron density around CLA c 507:**

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

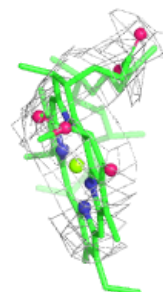
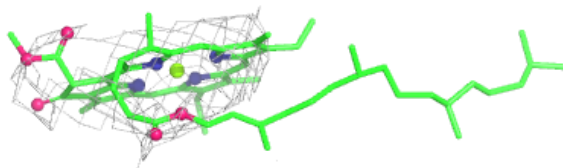
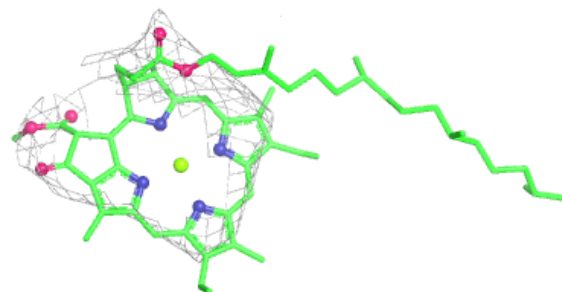


Electron density around CLA c 505:

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

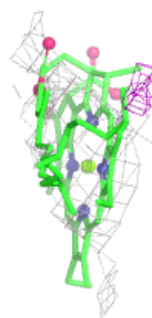
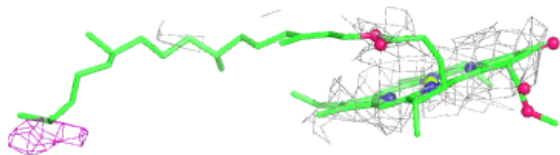
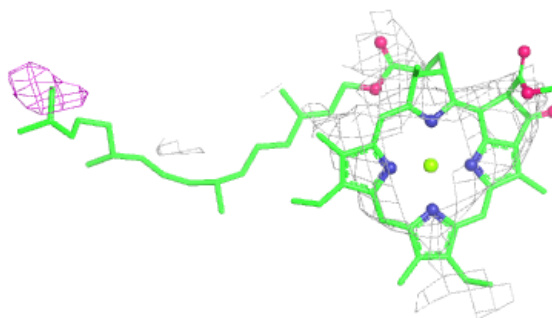
**Electron density around CLA C 501:**

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

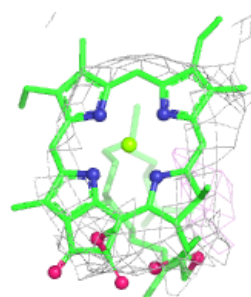
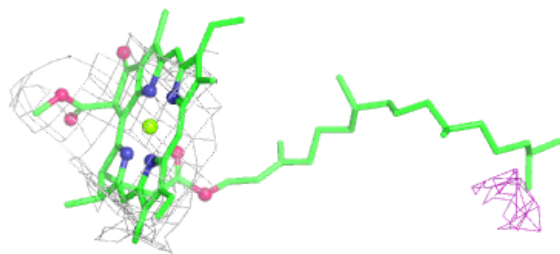
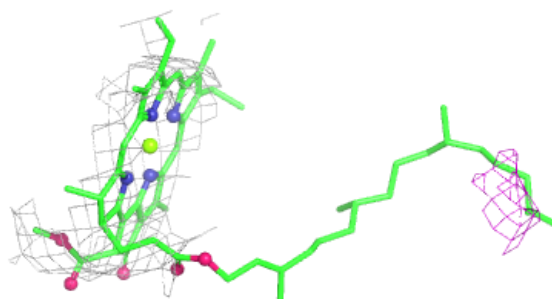


Electron density around CLA b 607:

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

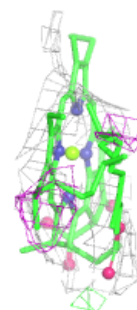
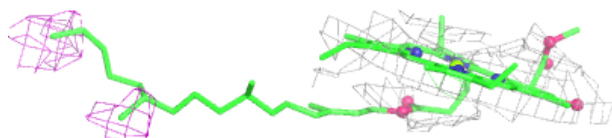
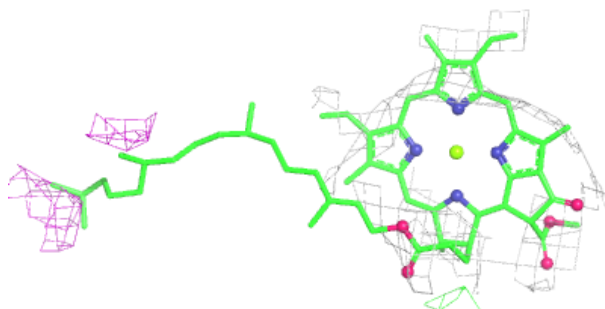
**Electron density around CLA c 508:**

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

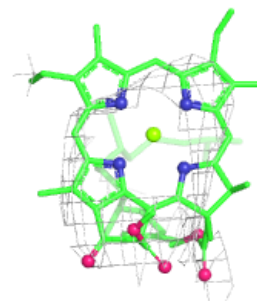
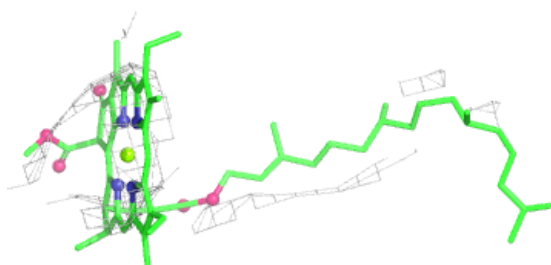


Electron density around CLA B 603:

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

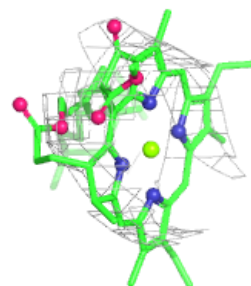
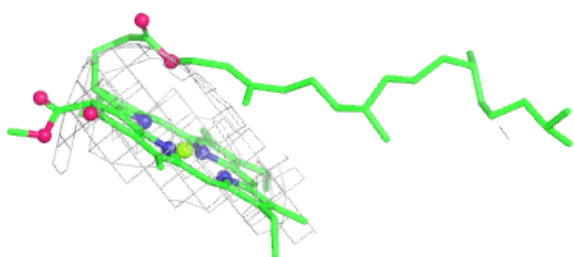
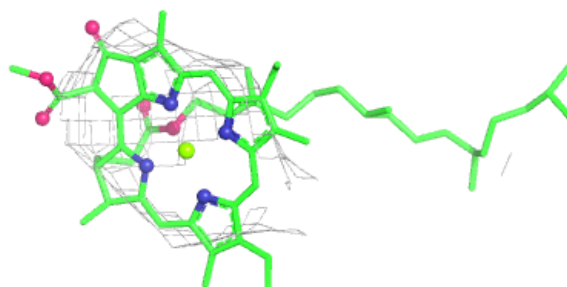
**Electron density around CLA B 605:**

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

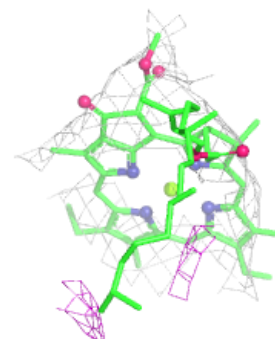
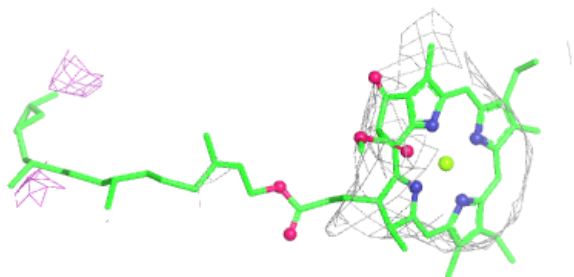
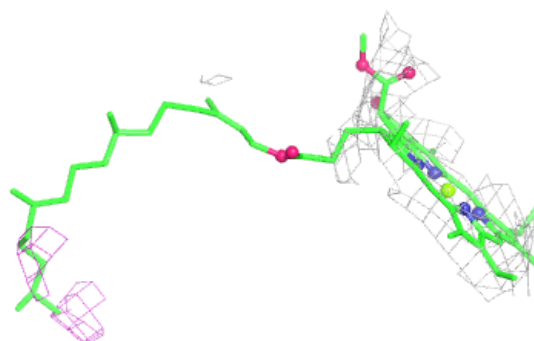


Electron density around CLA B 614:

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

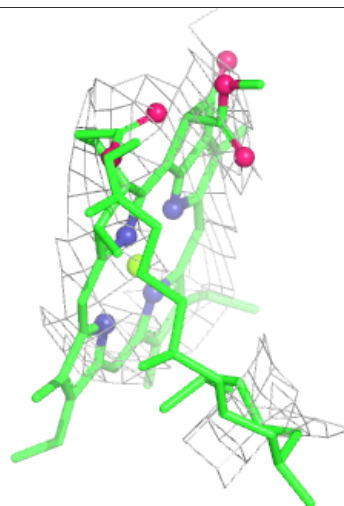
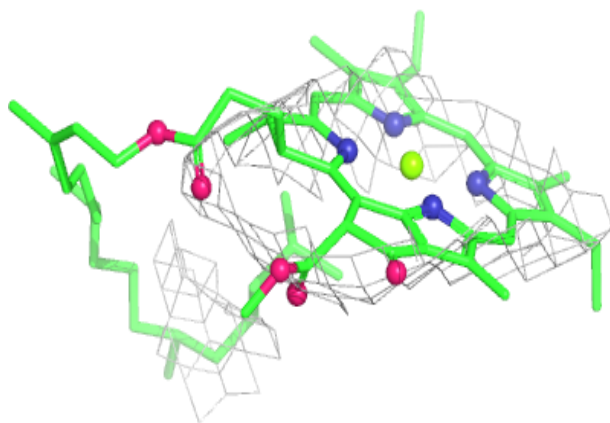
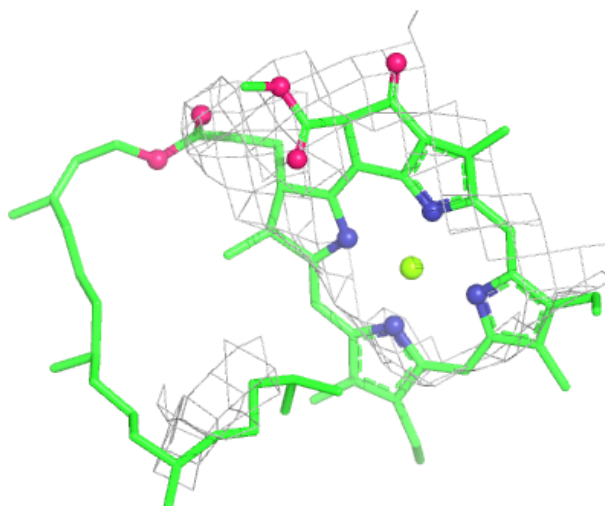
**Electron density around CLA d 402:**

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



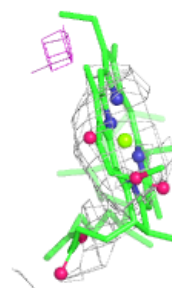
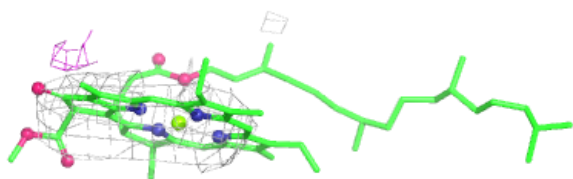
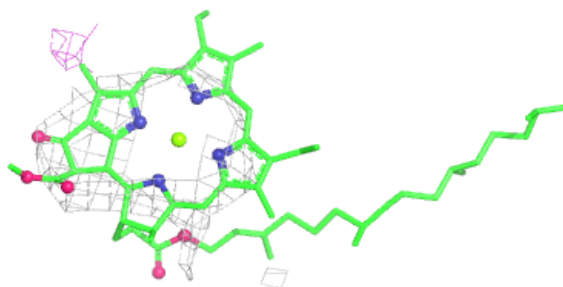
Electron density around CLA B 615:

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

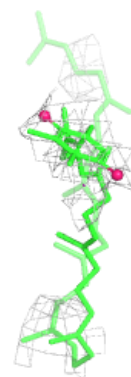
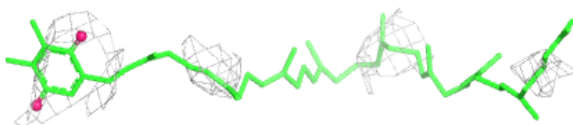
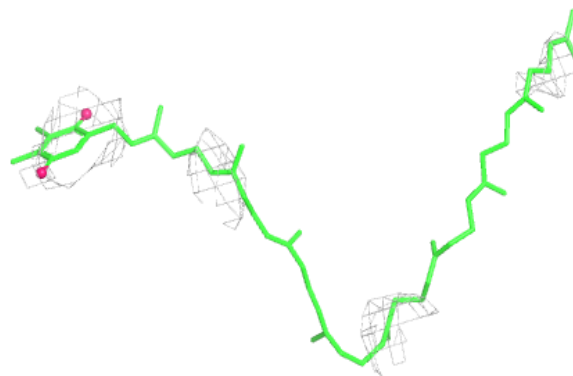


Electron density around CLA c 501:

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

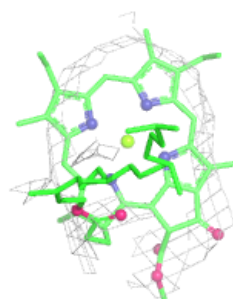
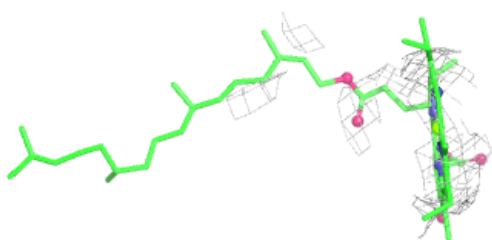
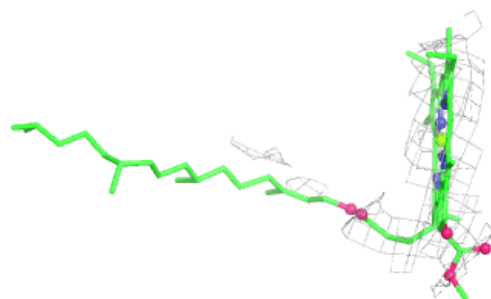
**Electron density around PL9 D 404:**

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

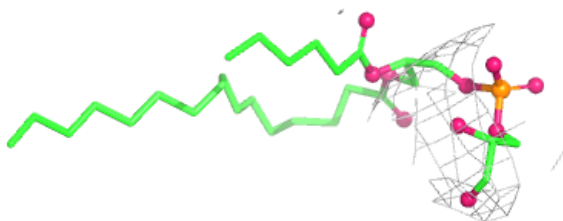


Electron density around CLA B 606:

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

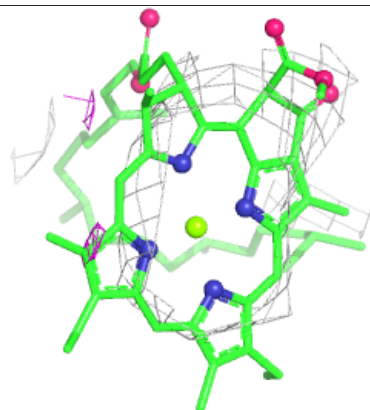
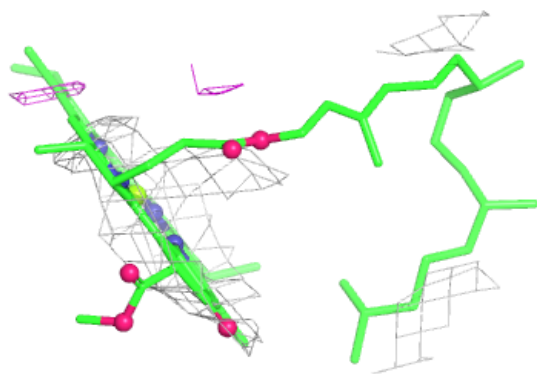
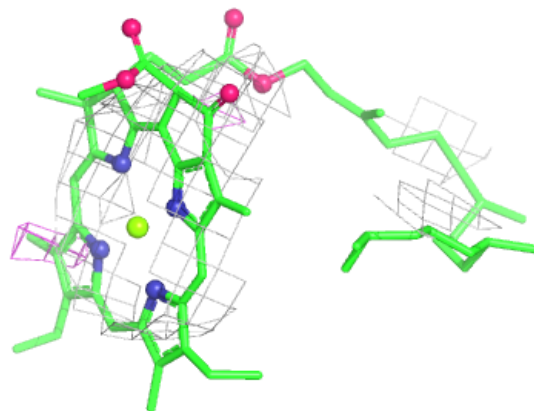
**Electron density around LHG A 412:**

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

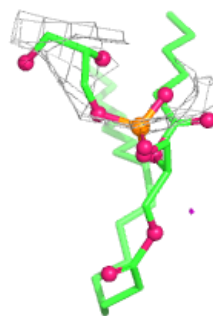
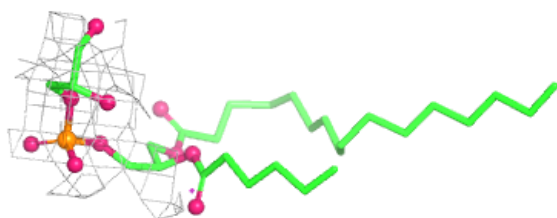
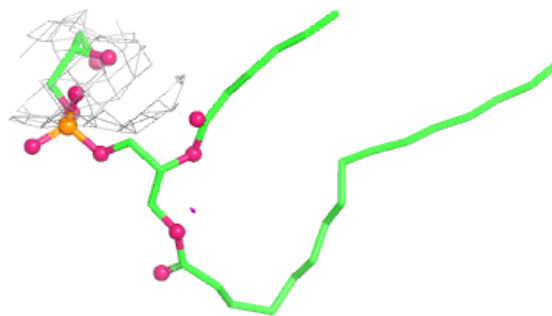


Electron density around CLA c 503:

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

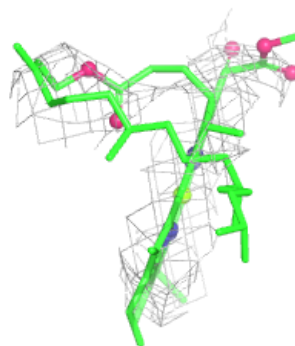
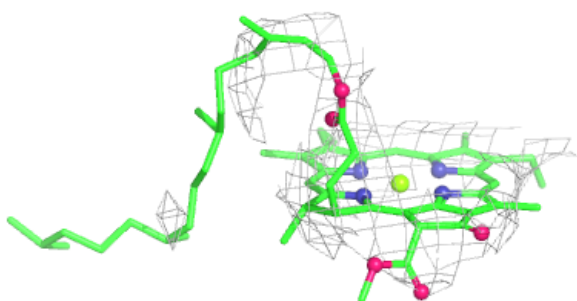
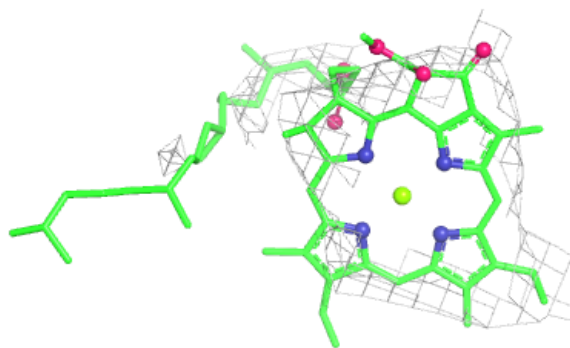
**Electron density around LHG a 414:**

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

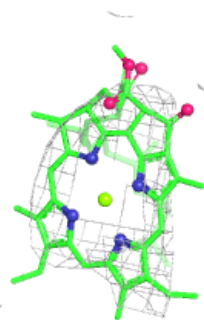
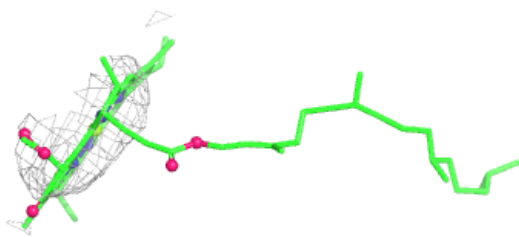
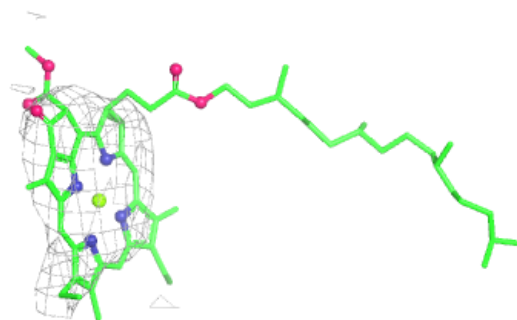


Electron density around CLA a 405:

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

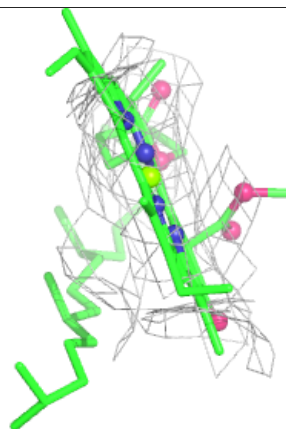
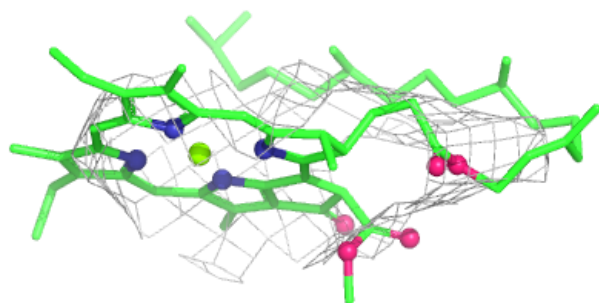
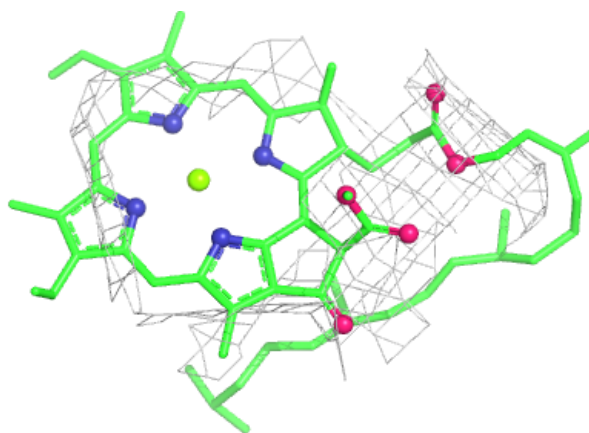
**Electron density around CLA A 407:**

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

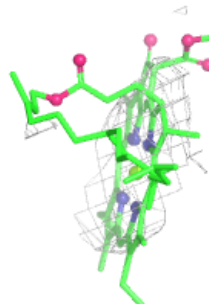
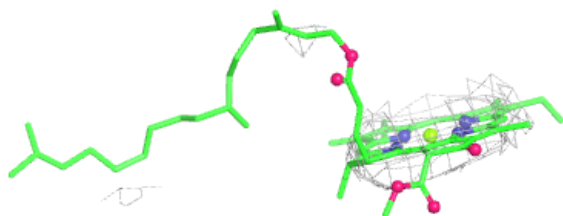
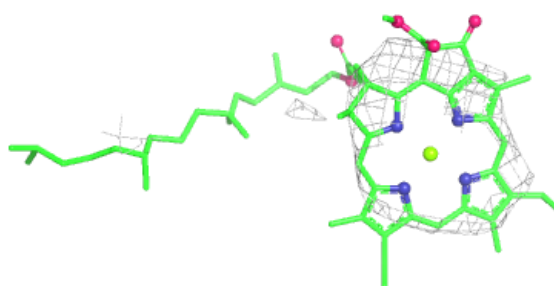


Electron density around CLA c 509:

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

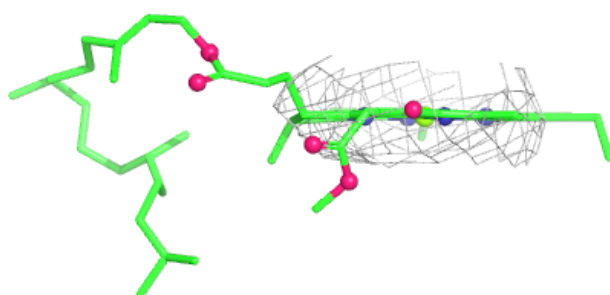
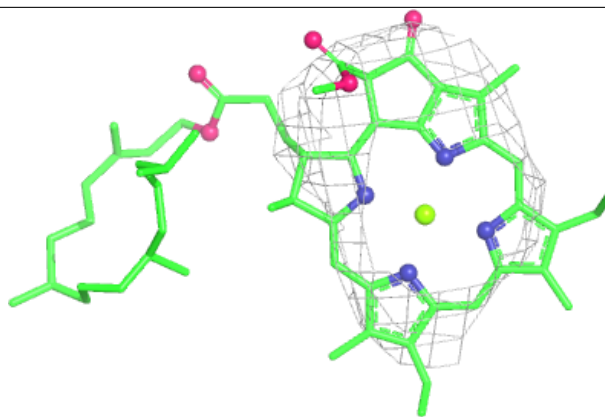
**Electron density around CLA A 405:**

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

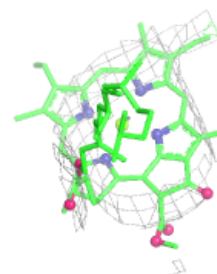
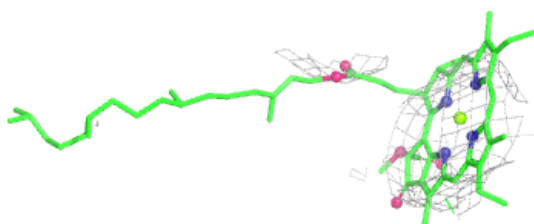
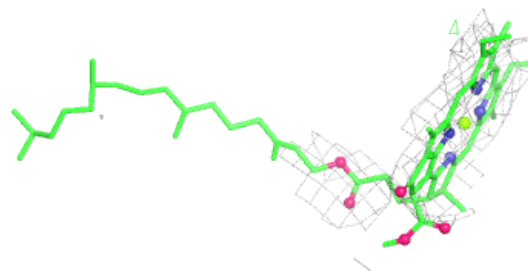


Electron density around CLA C 512:

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

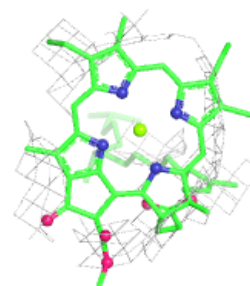
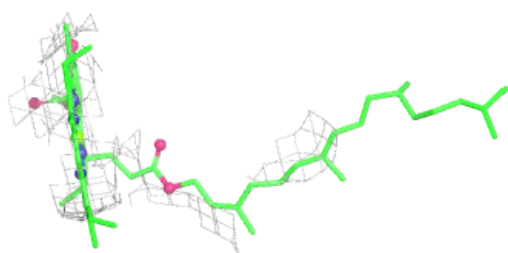
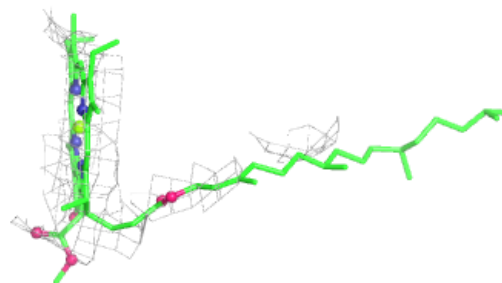
**Electron density around CLA B 604:**

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

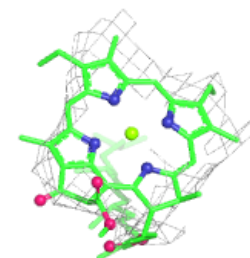
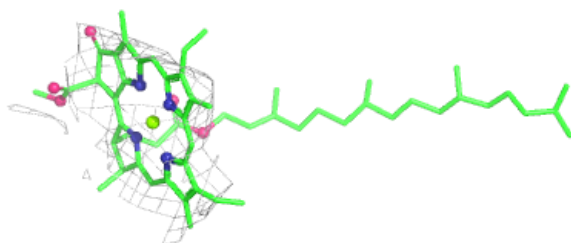
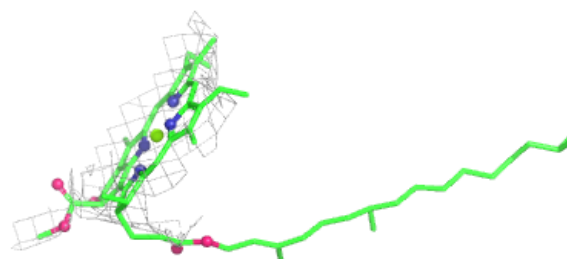


Electron density around CLA b 610:

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

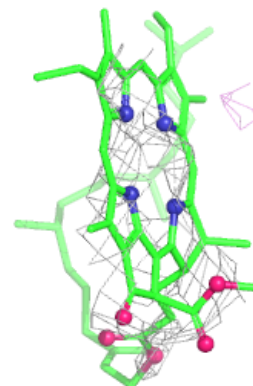
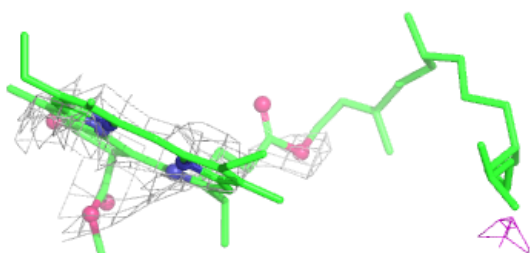
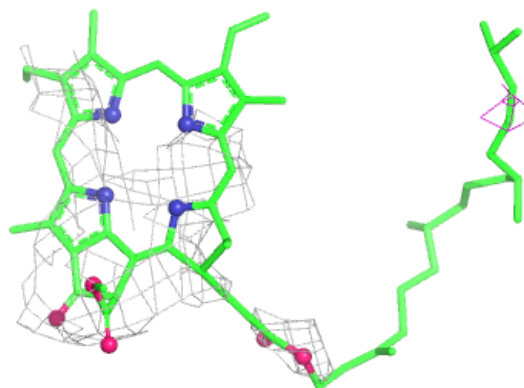
**Electron density around CLA b 611:**

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

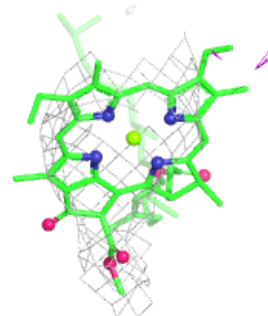
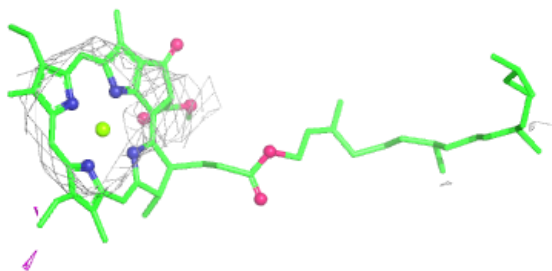
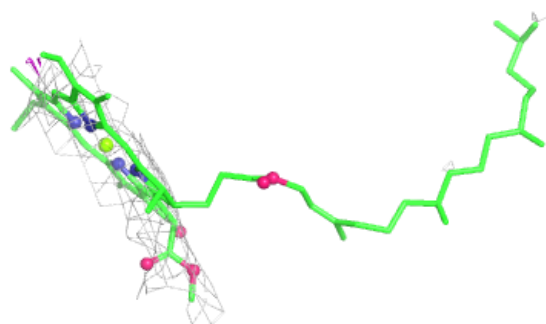


Electron density around PHO a 408:

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

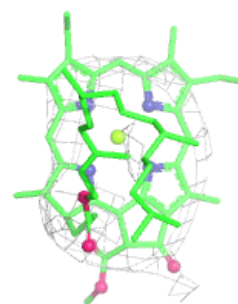
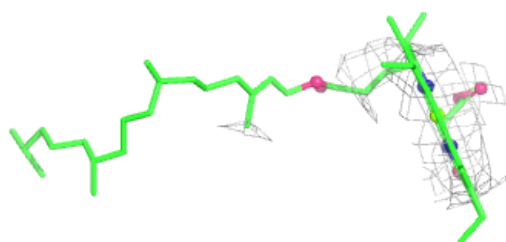
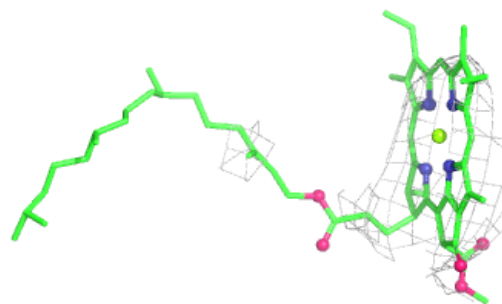
**Electron density around CLA D 401:**

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

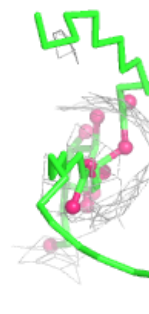
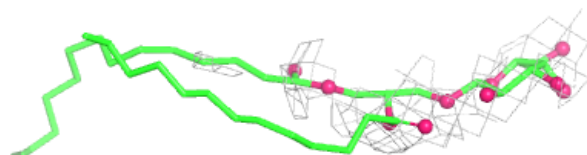
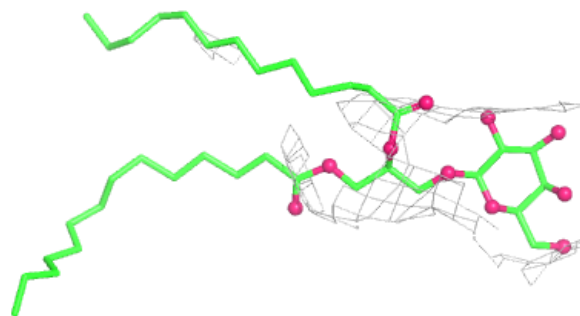


Electron density around CLA d 403:

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

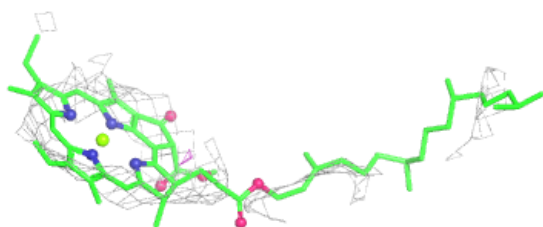
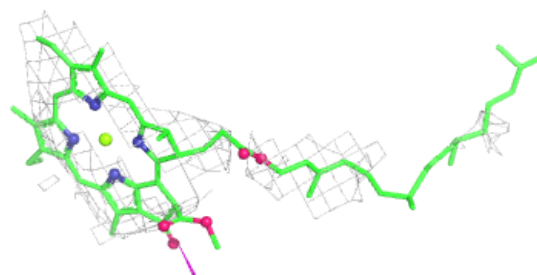
**Electron density around LMG d 406:**

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

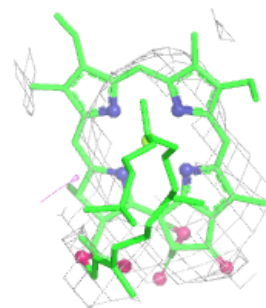
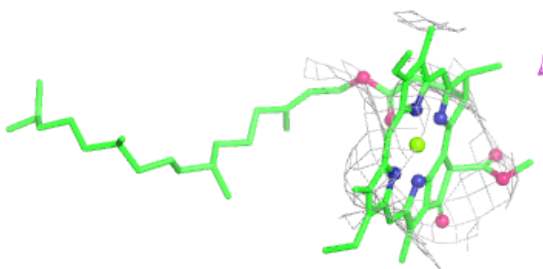
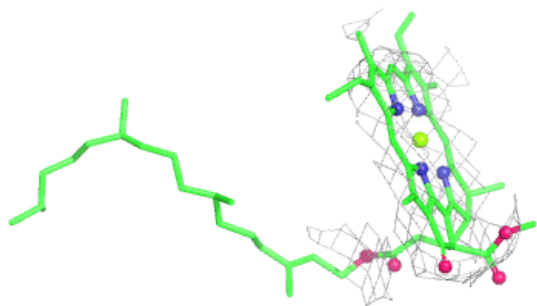


Electron density around CLA a 404:

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

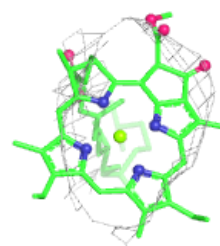
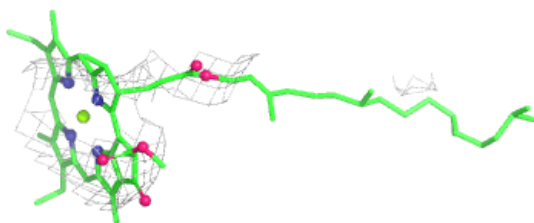
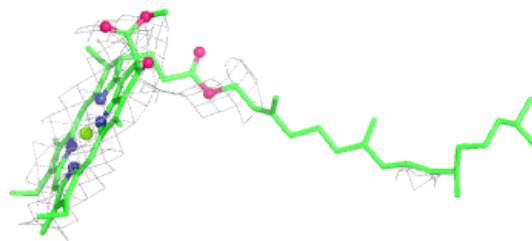
**Electron density around CLA C 508:**

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

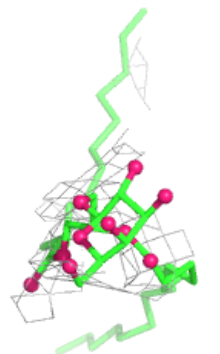
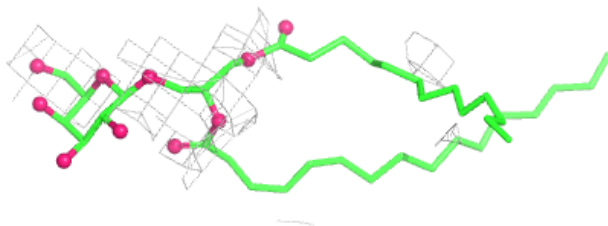
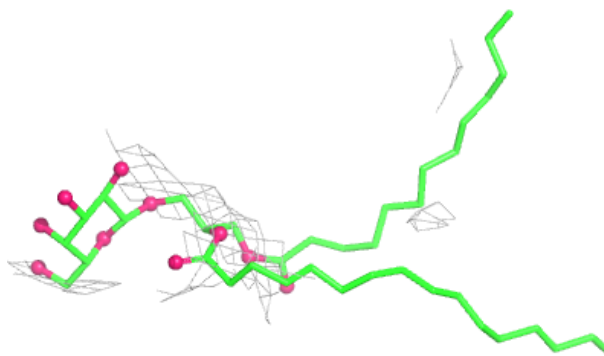


Electron density around CLA b 608:

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

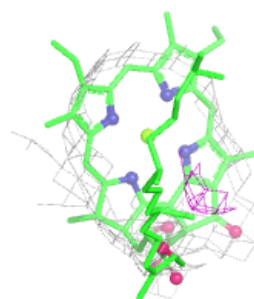
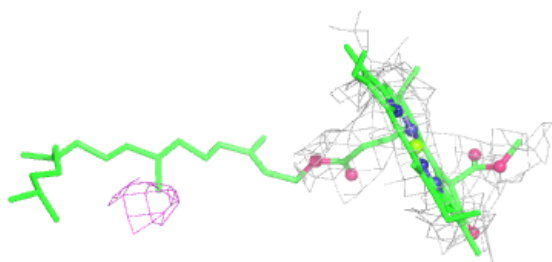
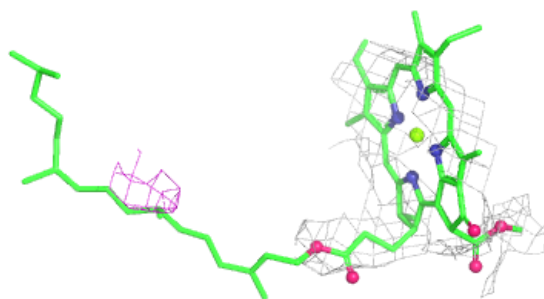
**Electron density around LMG D 407:**

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

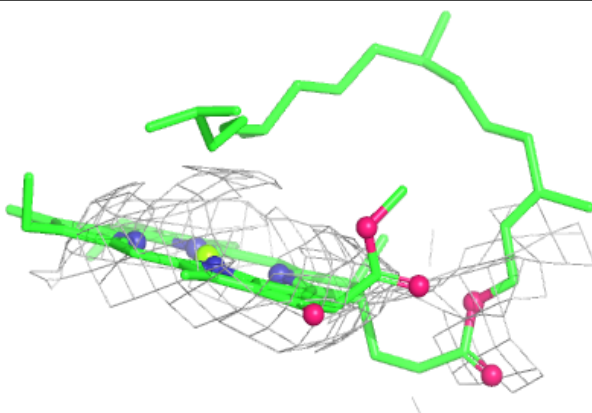
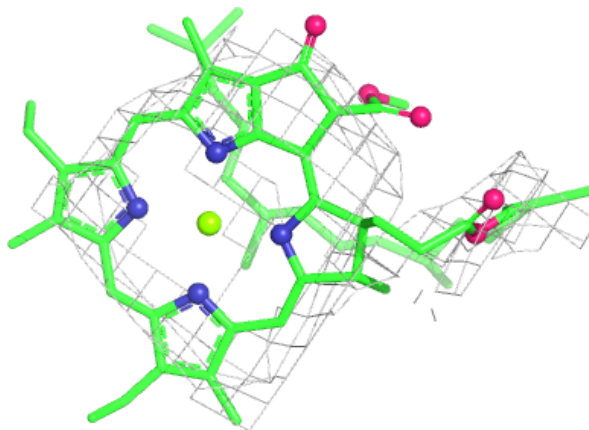


Electron density around CLA B 609:

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

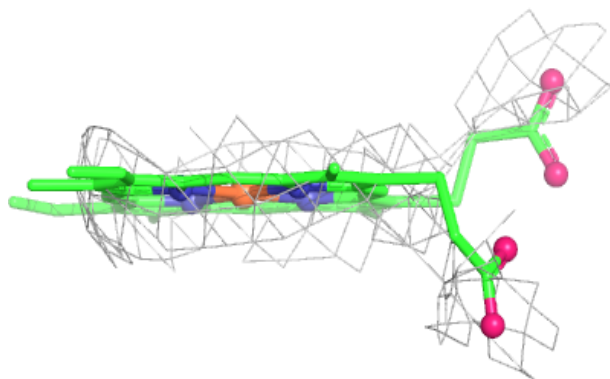
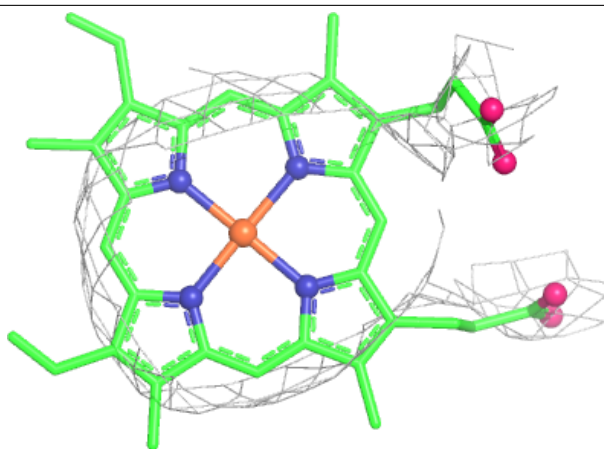
**Electron density around CLA c 510:**

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



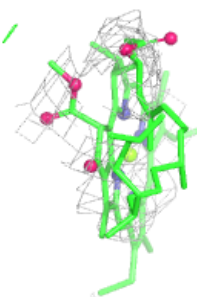
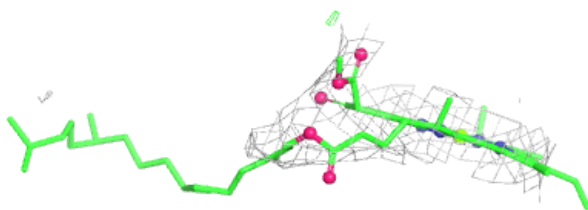
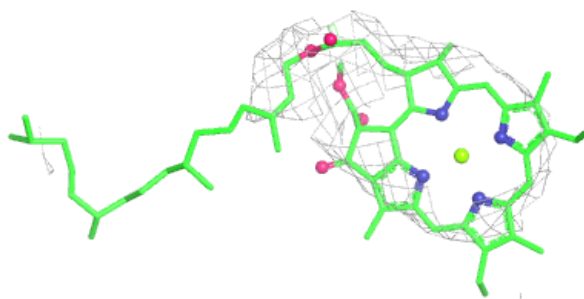
Electron density around HEM f 101:

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

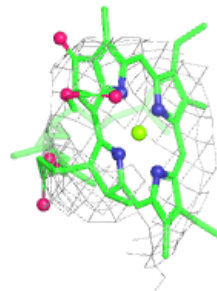
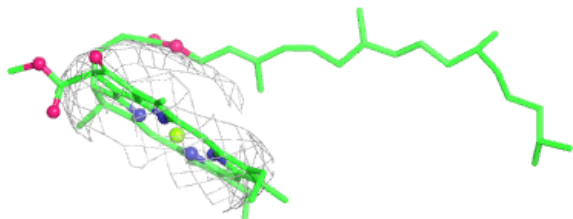
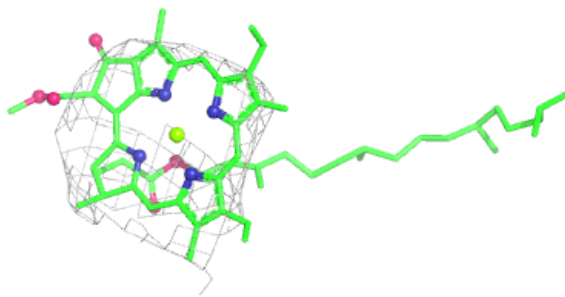


Electron density around CLA B 602:

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

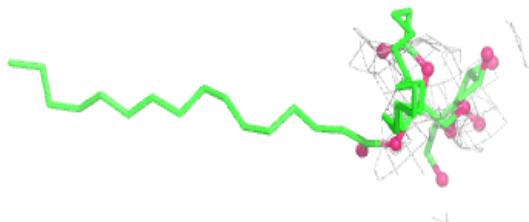
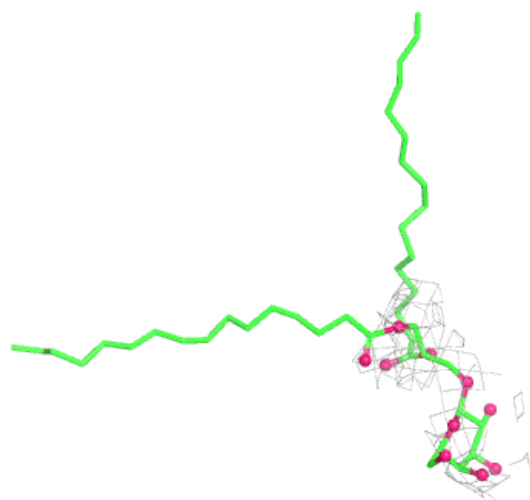
**Electron density around CLA b 612:**

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



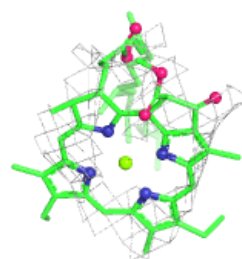
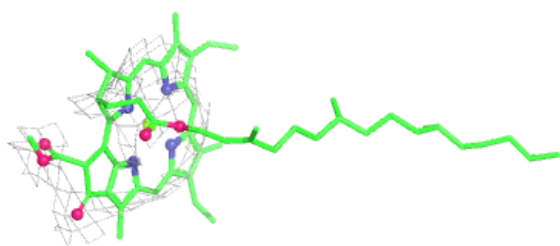
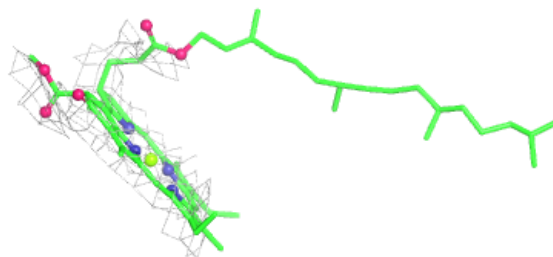
Electron density around LMG A 414:

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

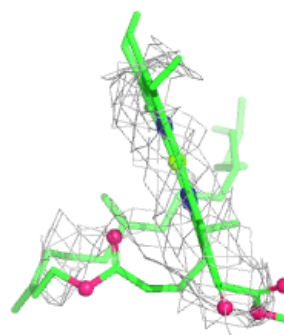
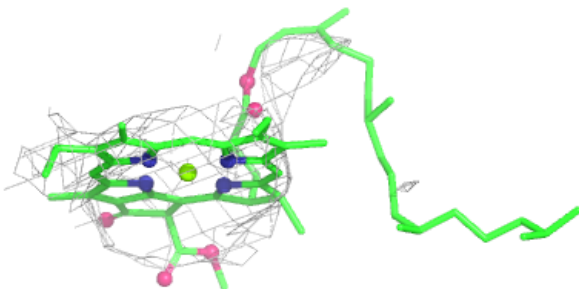
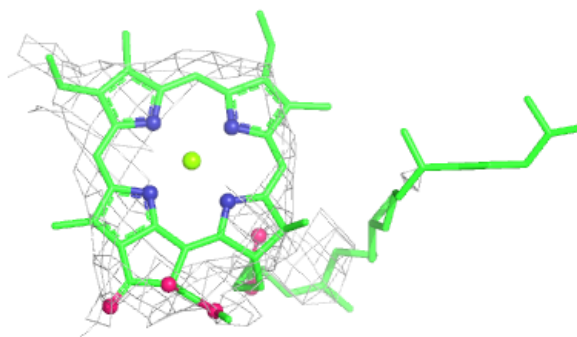


Electron density around CLA c 504:

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

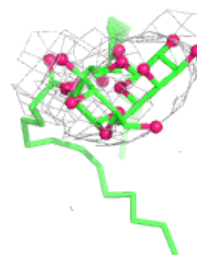
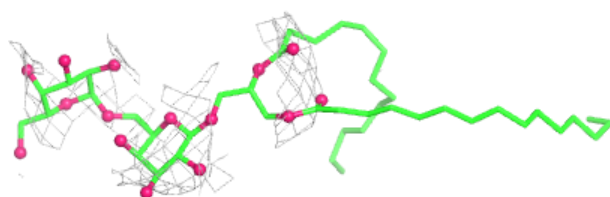
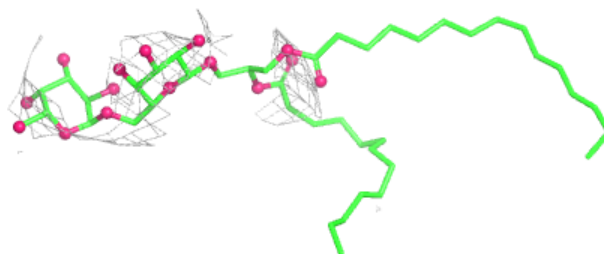
**Electron density around CLA A 404:**

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

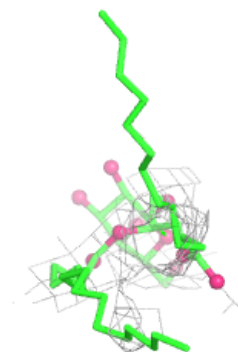
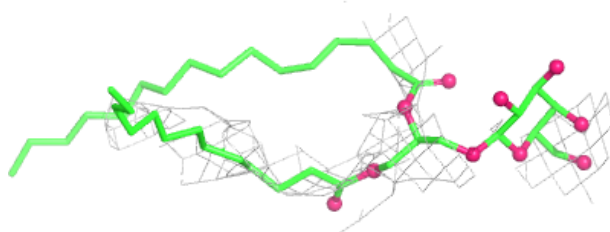


Electron density around DGD B 621:

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

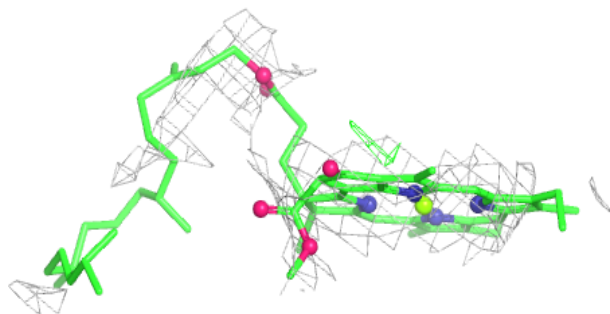
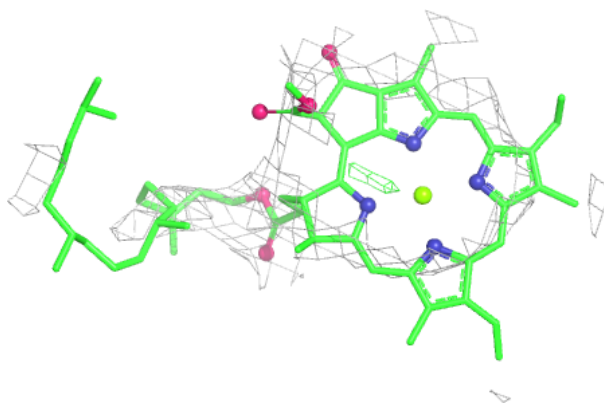
**Electron density around LMG d 407:**

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

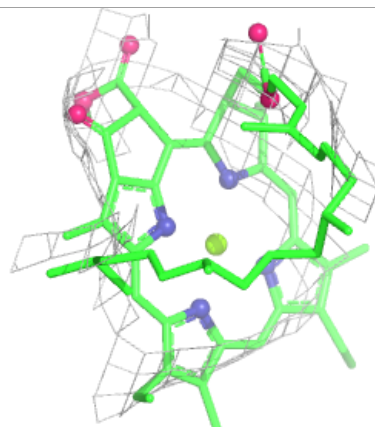
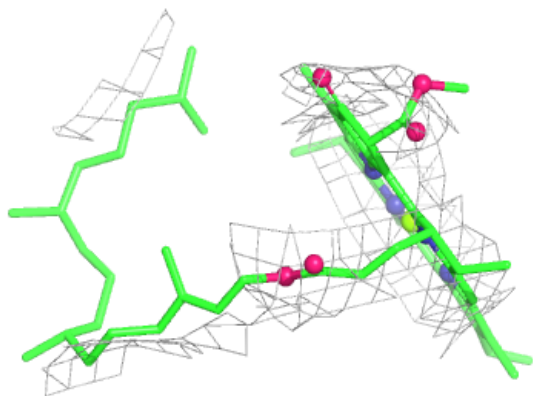
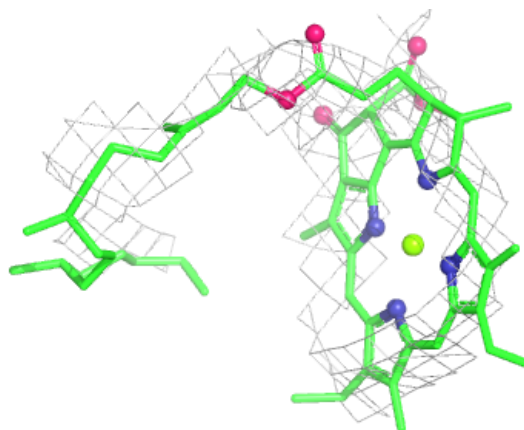


Electron density around CLA B 612:

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

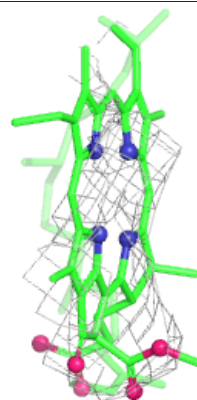
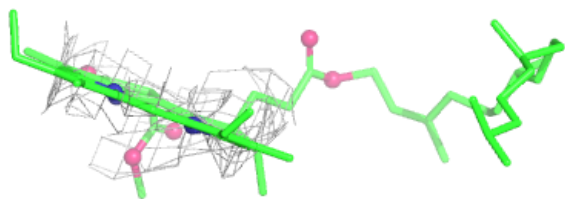
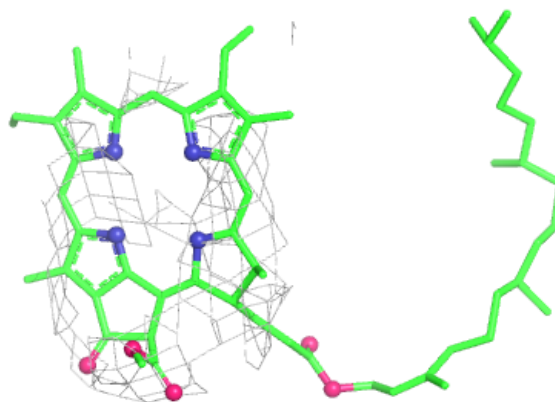
**Electron density around CLA C 503:**

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

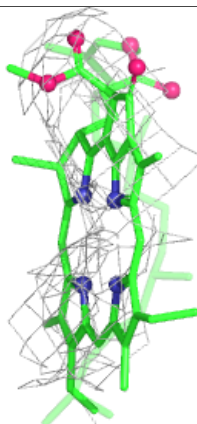
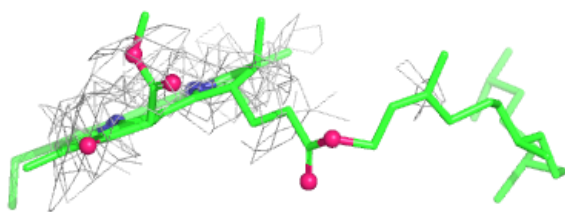
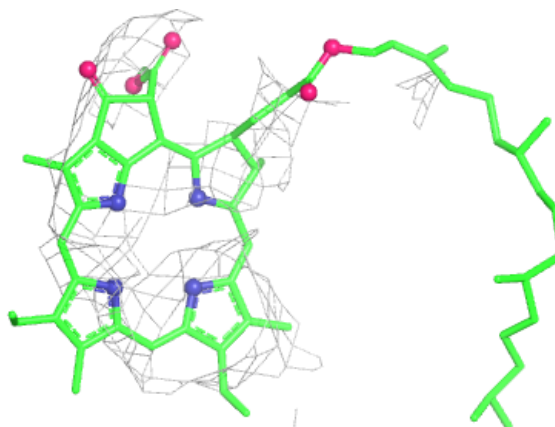


Electron density around PHO D 402:

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

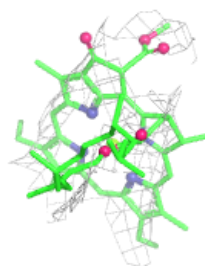
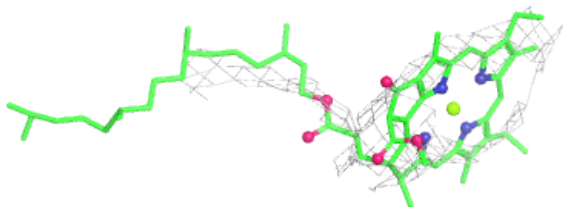
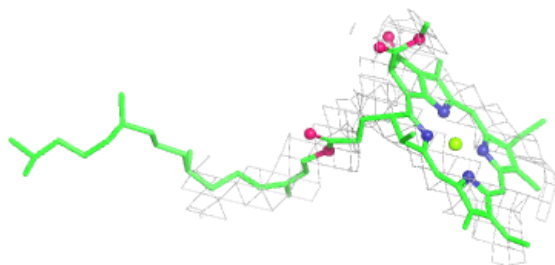
**Electron density around PHO a 407:**

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

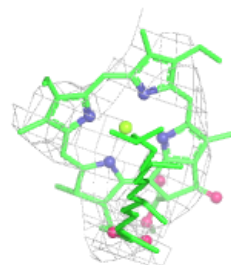
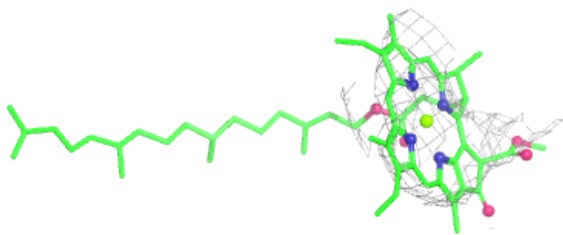
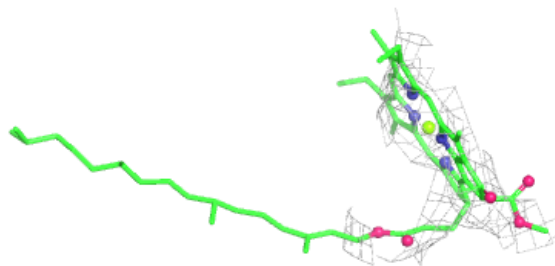


Electron density around CLA C 502:

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

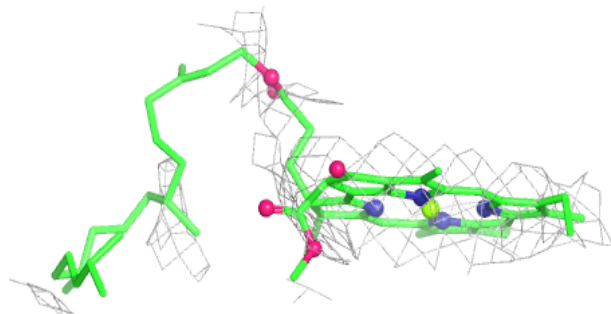
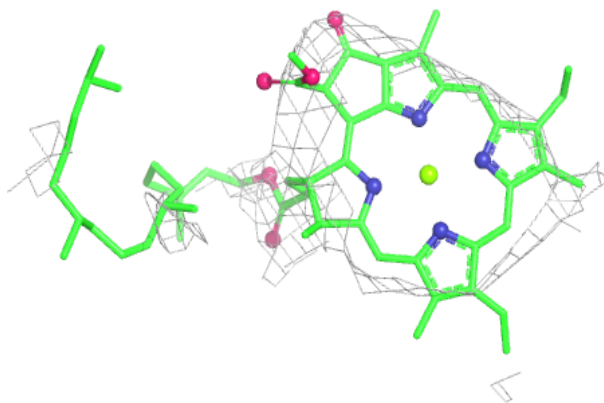
**Electron density around CLA B 607:**

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



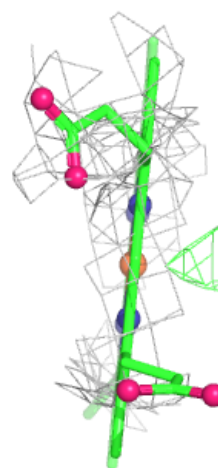
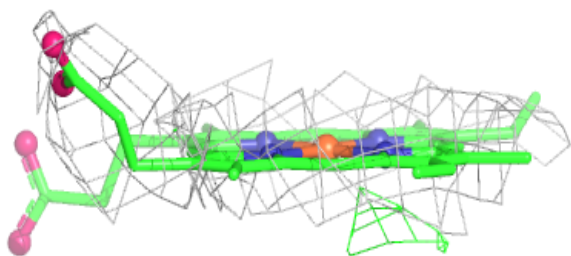
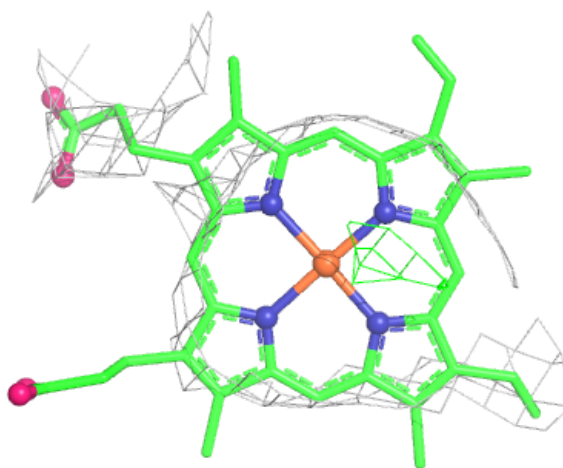
Electron density around CLA b 616:

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



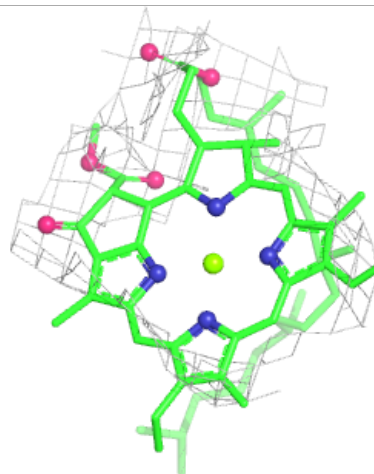
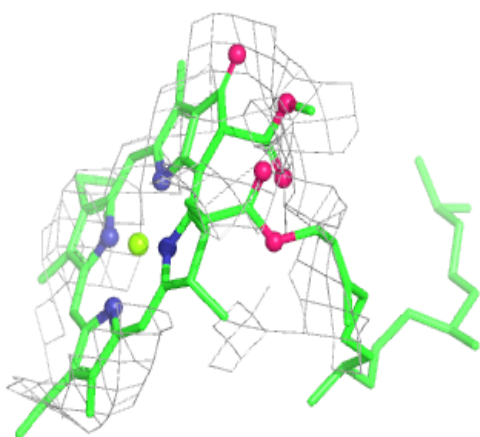
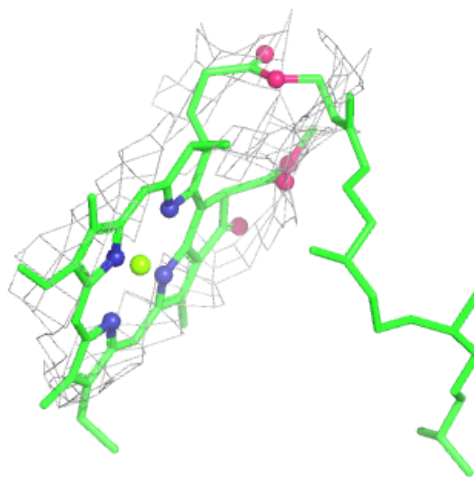
Electron density around HEM V 201:

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



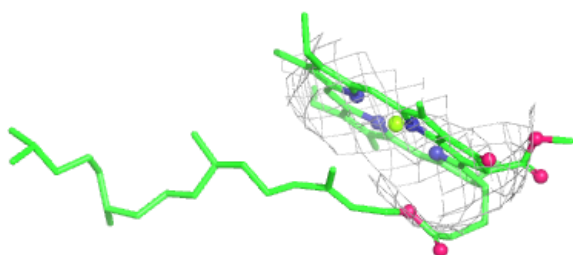
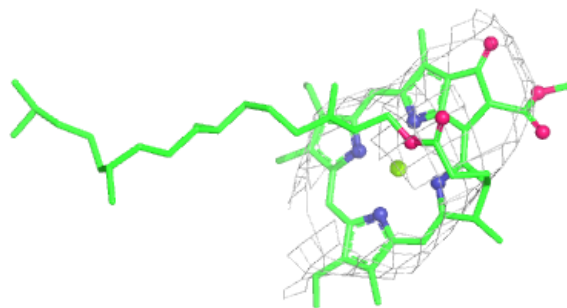
Electron density around CLA b 617:

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



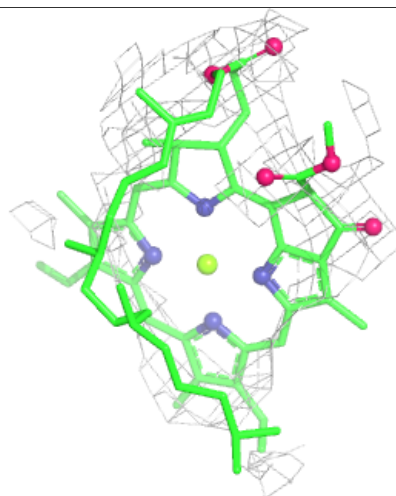
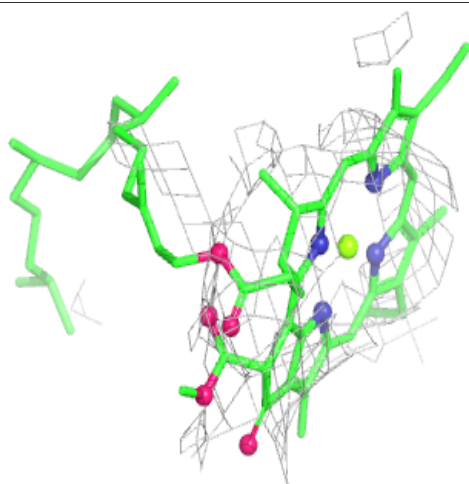
Electron density around CLA b 618:

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



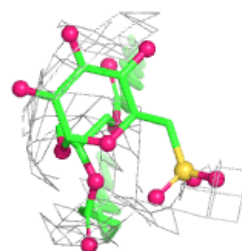
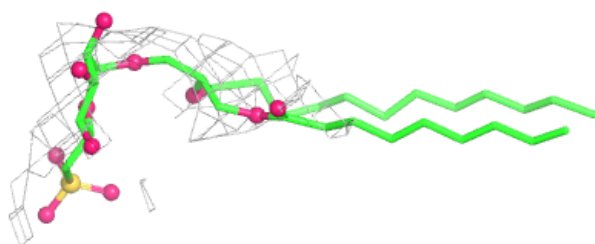
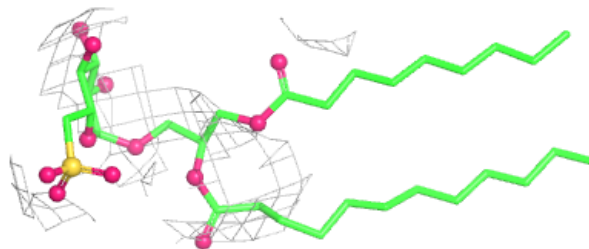
Electron density around CLA B 613:

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



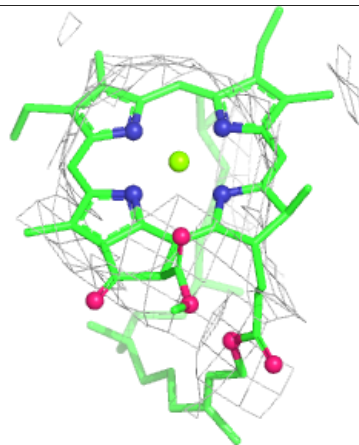
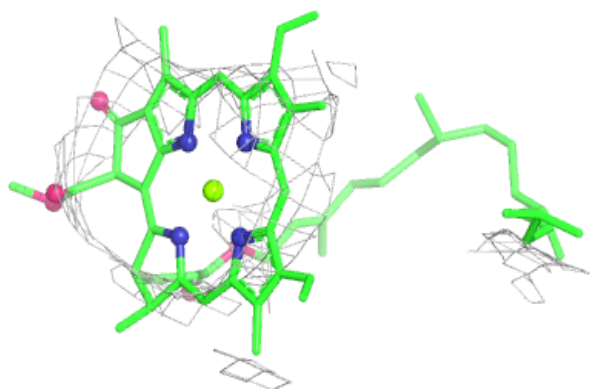
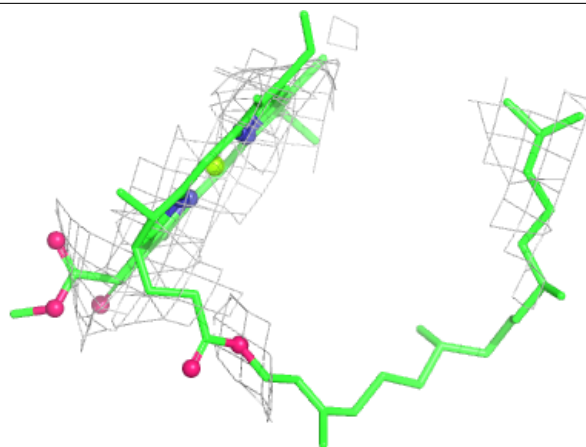
Electron density around SQD D 408:

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



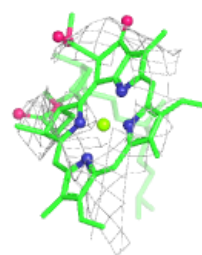
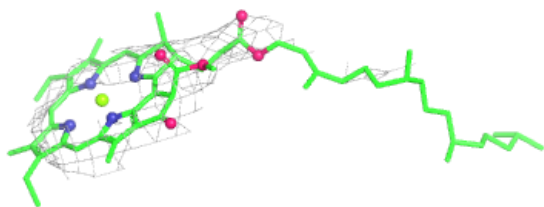
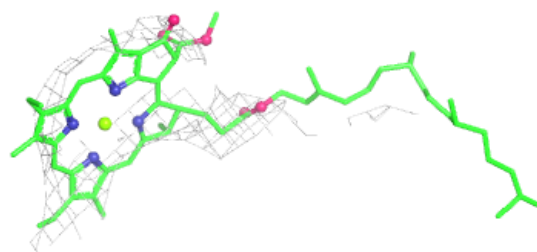
Electron density around CLA B 611:

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

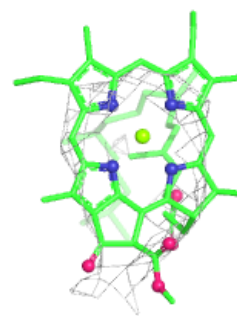
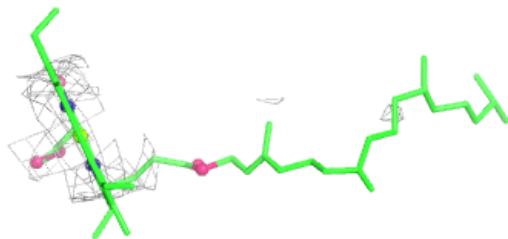
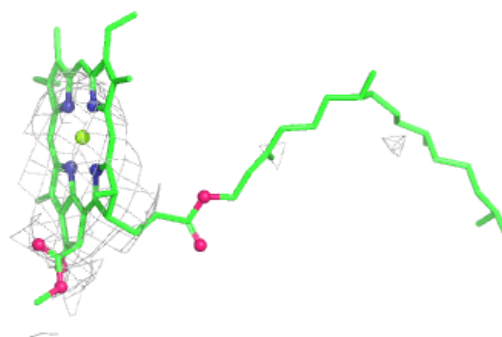


Electron density around CLA A 403:

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

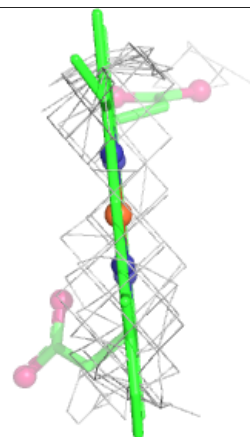
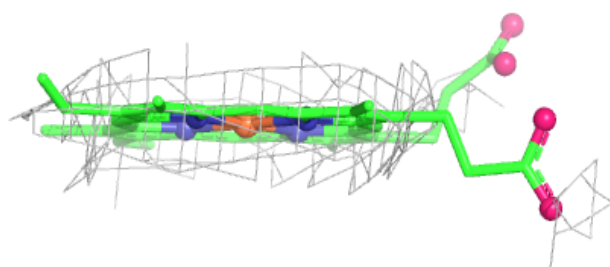
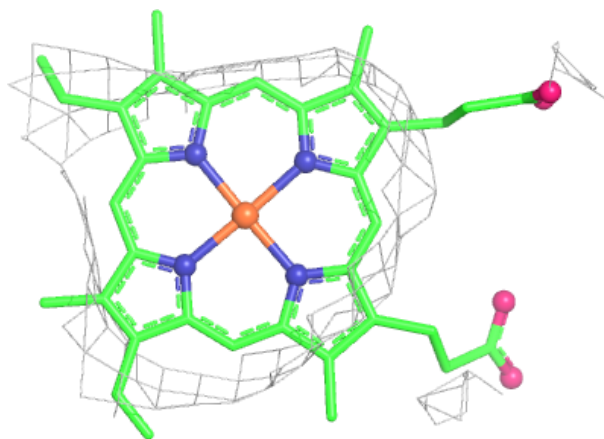
**Electron density around CLA D 403:**

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



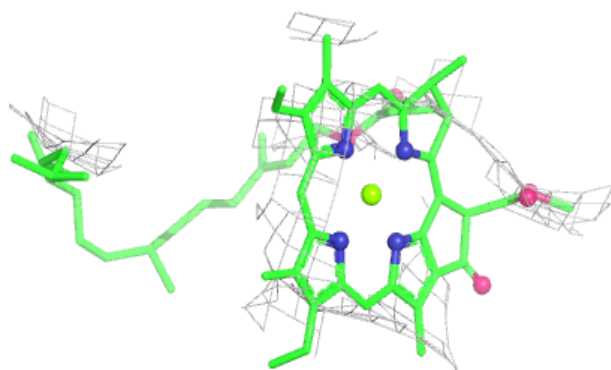
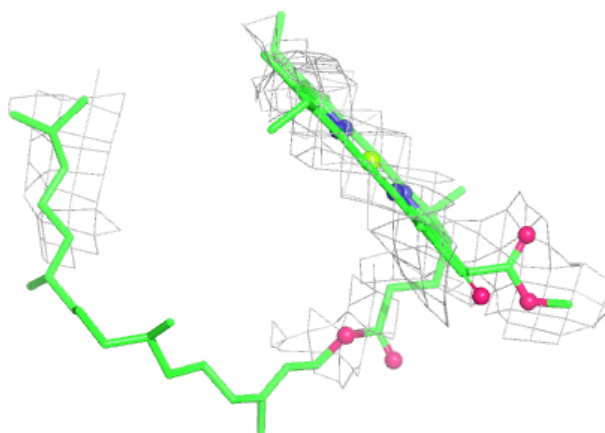
Electron density around HEM v 201:

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

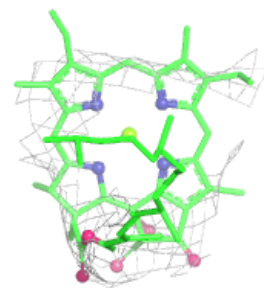
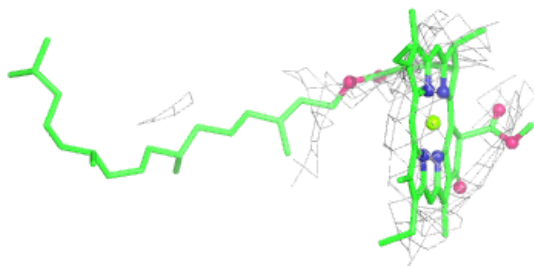
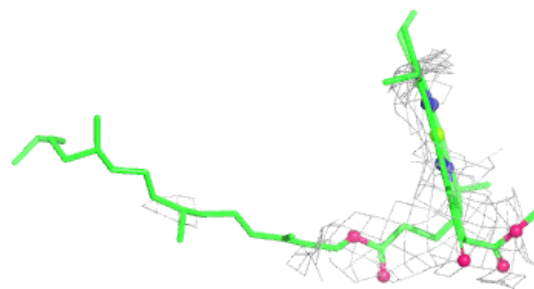


Electron density around CLA b 615:

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

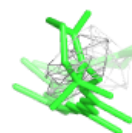
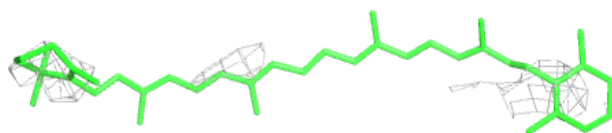
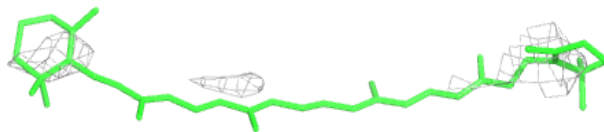
**Electron density around CLA b 609:**

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



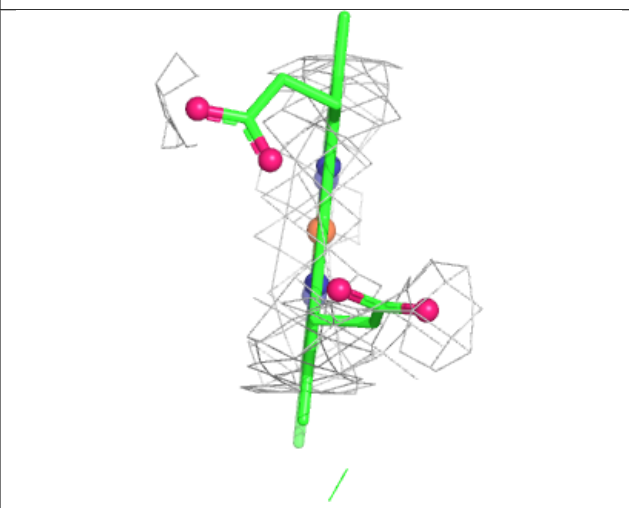
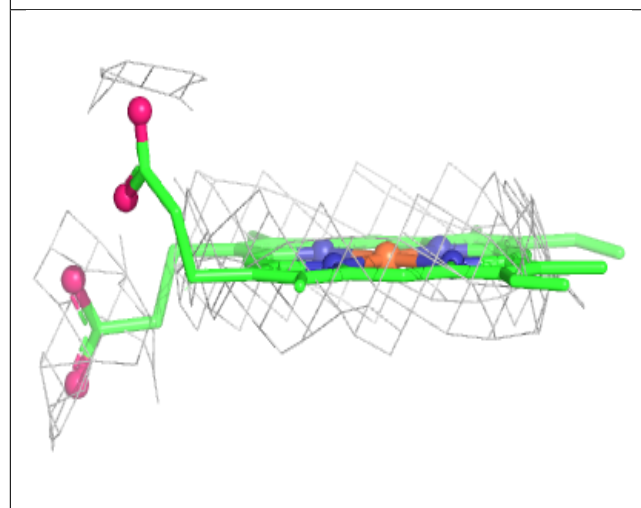
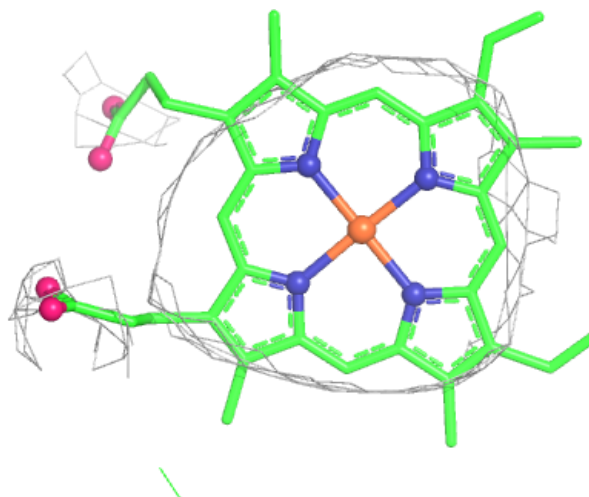
Electron density around BCR d 405:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.