



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 01:02 AM EDT

PDB ID : 4TNJ / pdb_00004tnj
Title : RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2014-06-04
Resolution : 4.50 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

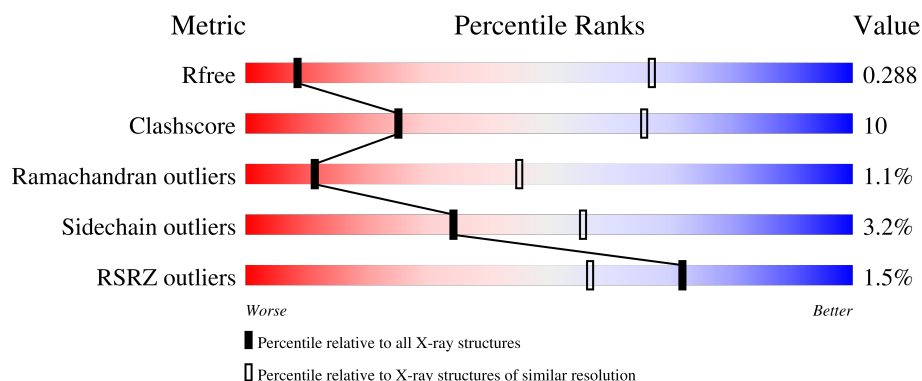
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	

Continued on next page...

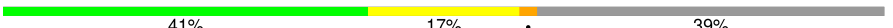
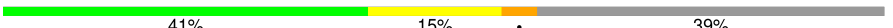
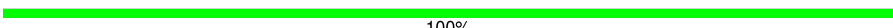
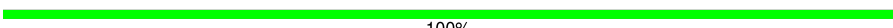
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	344	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	T	32	
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	G	28	
19	Y	28	
20	Z	62	
20	z	62	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 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
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	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			

Continued on next page...

Continued from previous page...

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 Y.

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

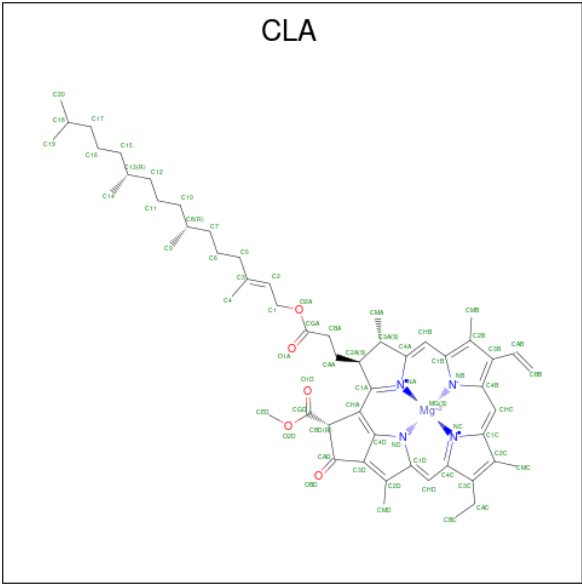
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

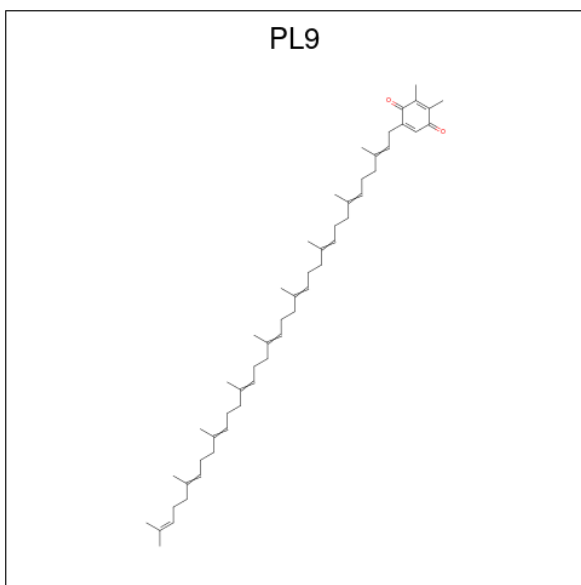
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

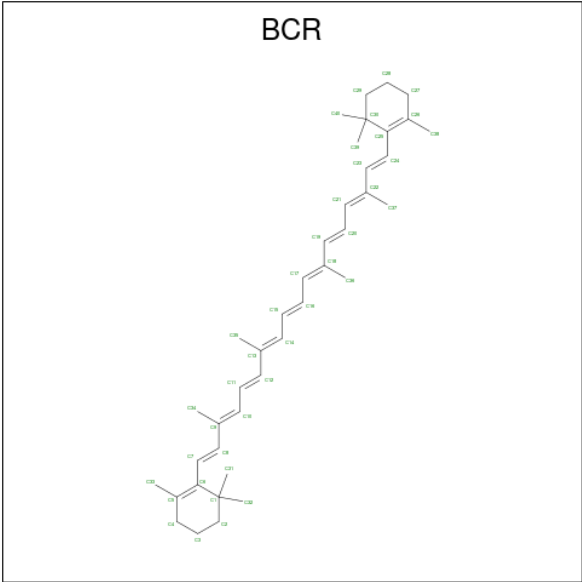
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 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
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



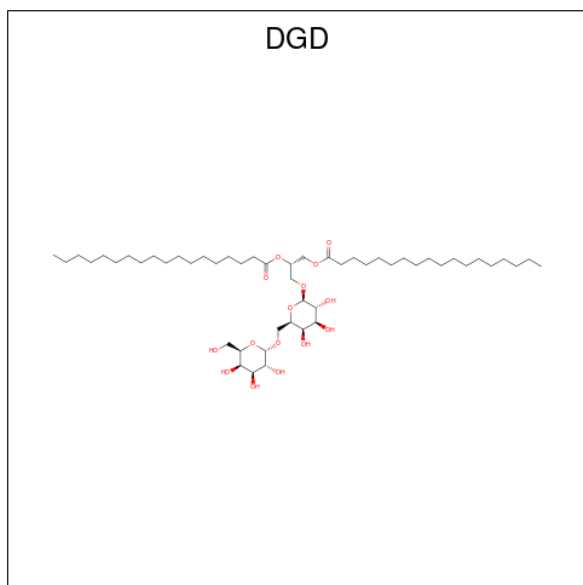
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



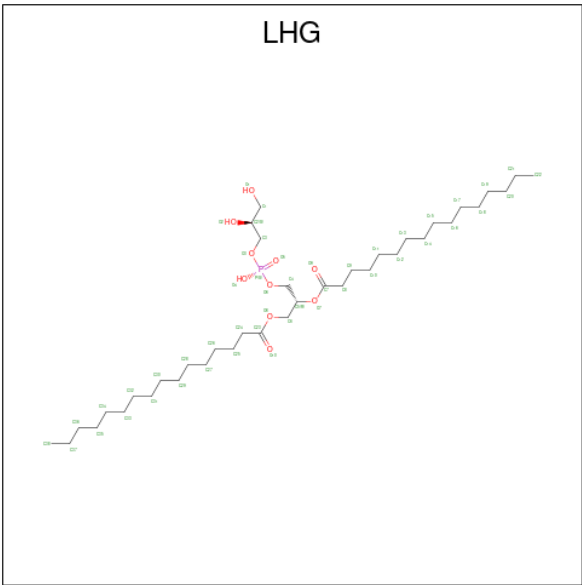
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

Continued on next page...

Continued from previous page...

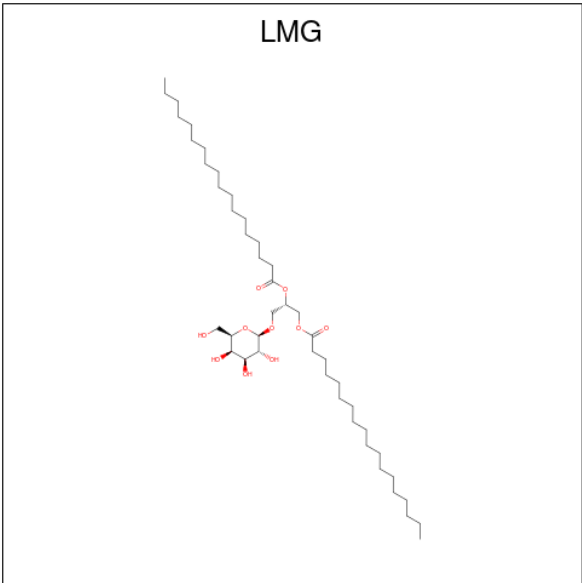
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

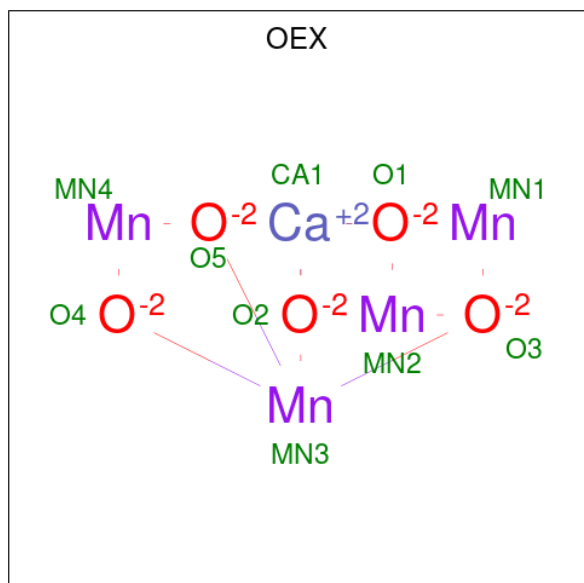


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

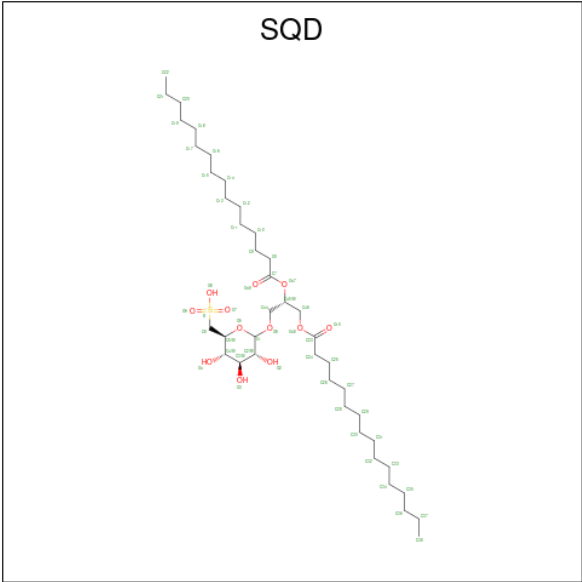
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



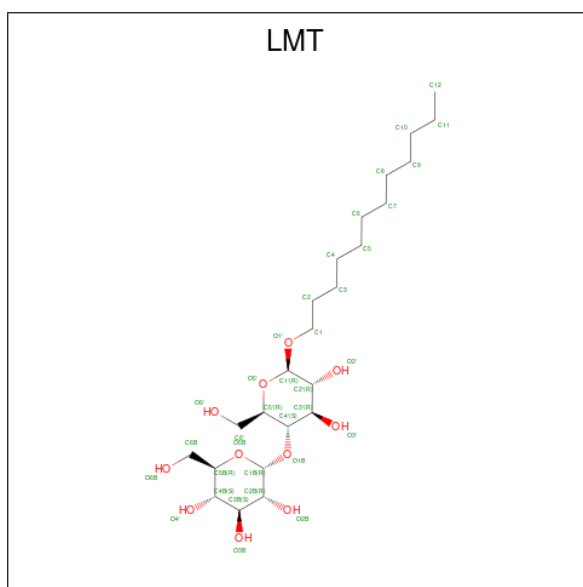
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



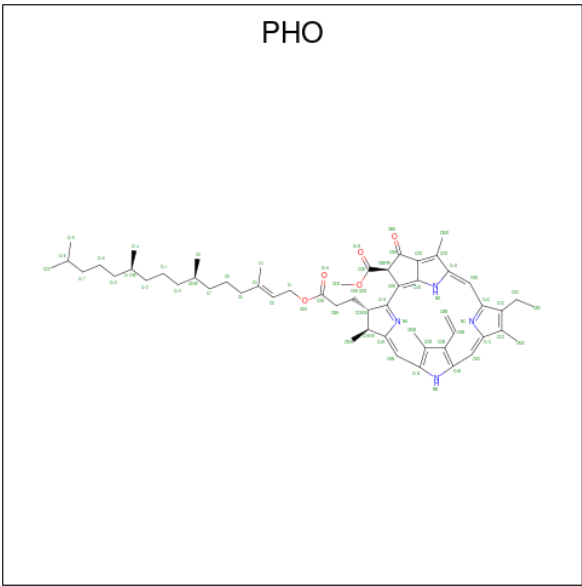
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			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 DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



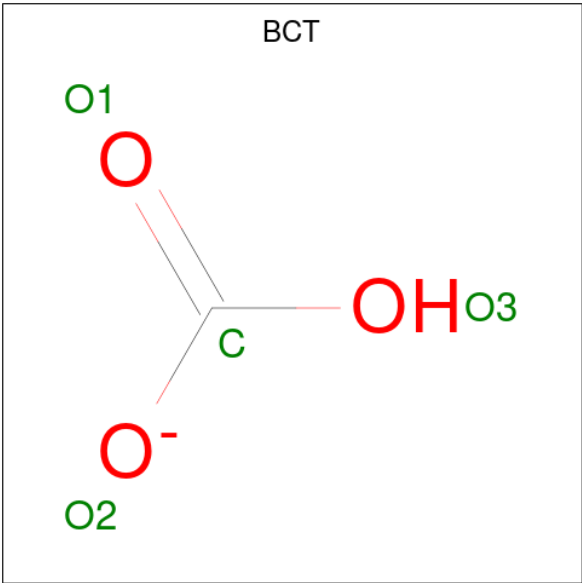
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	D	1	Total 31	C 20	O 11	0	0
31	I	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	b	1	Total 35	C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

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



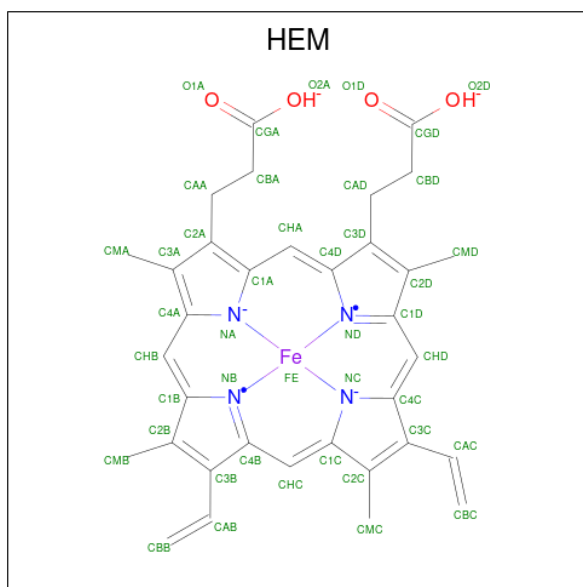
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

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



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

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

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

Continued on next page...

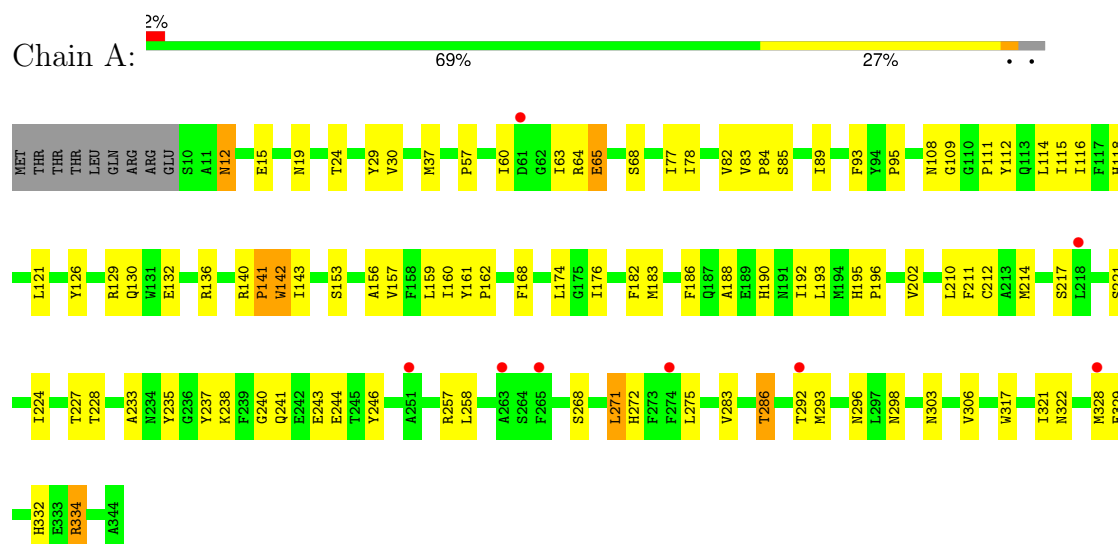
Continued from previous page...

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

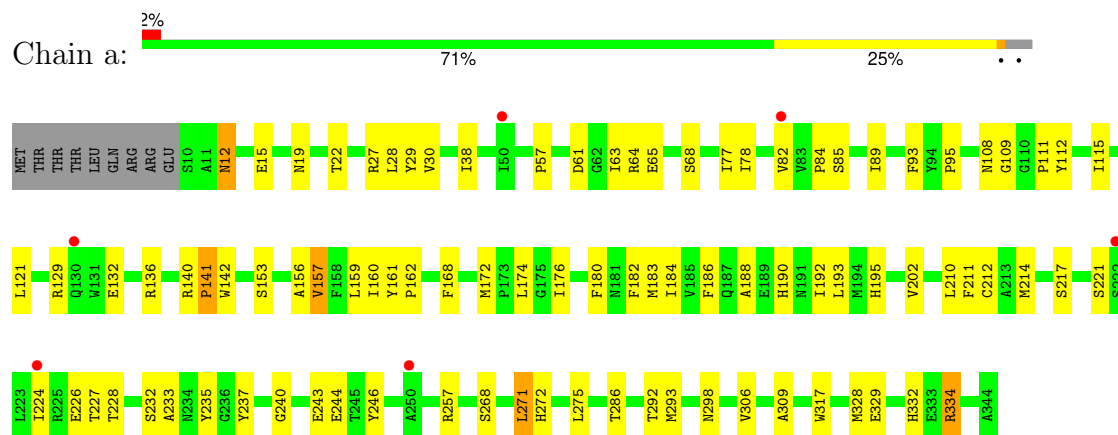
3 Residue-property plots

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

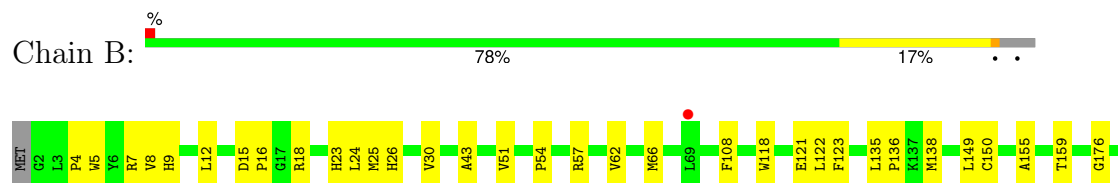
- Molecule 1: Photosystem Q(B) protein 1

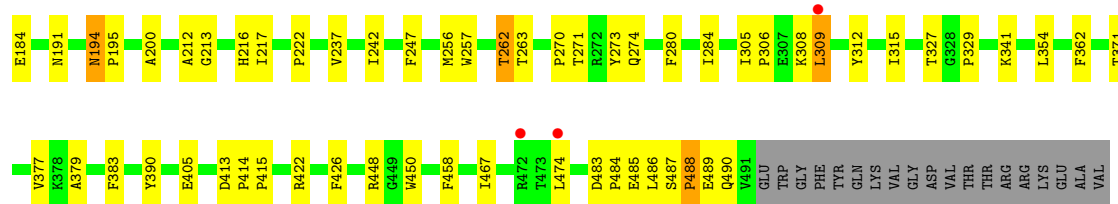


- Molecule 1: Photosystem Q(B) protein 1

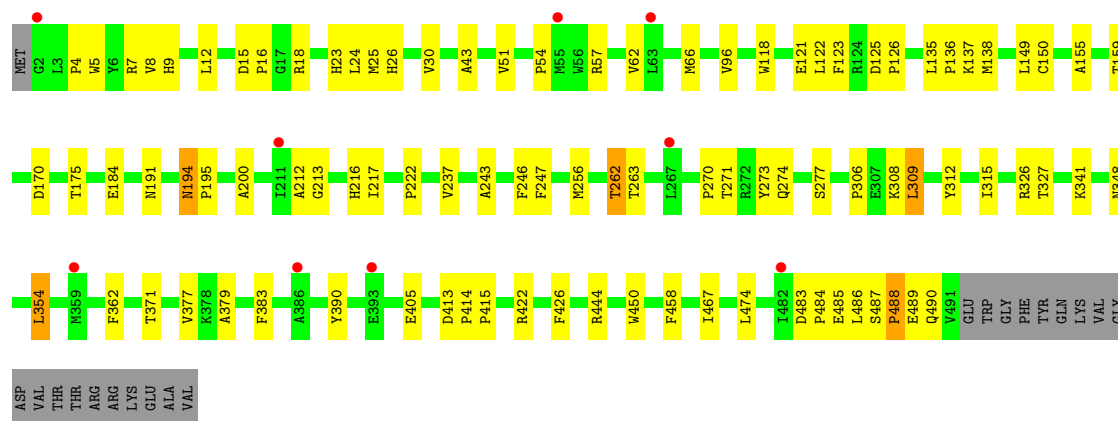
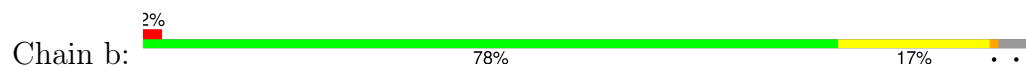


- Molecule 2: Photosystem II core light harvesting protein

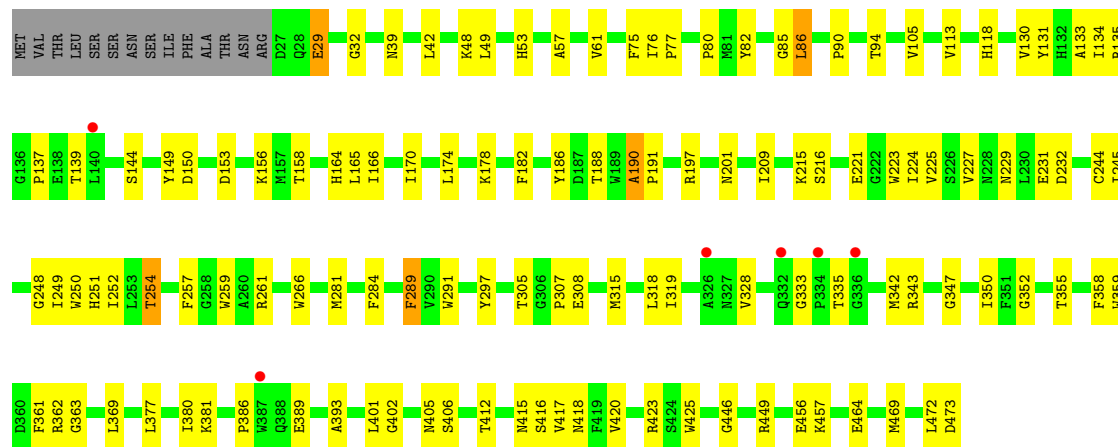




• Molecule 2: Photosystem II core light harvesting protein

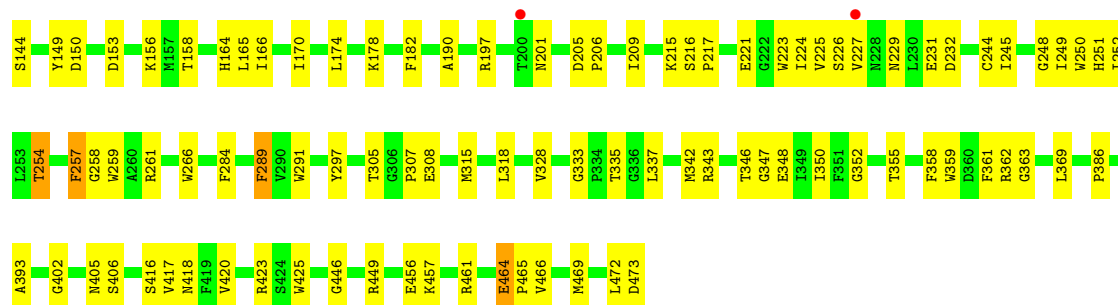


• Molecule 3: Photosystem II CP43 protein

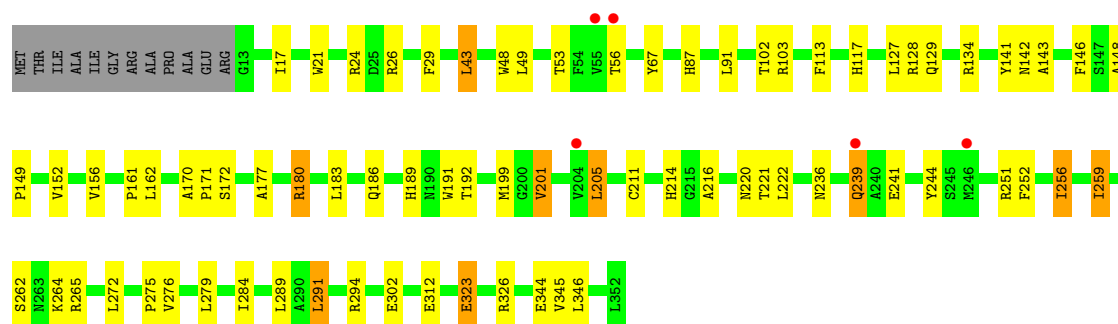
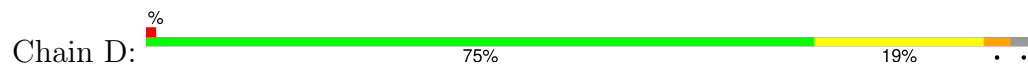


• Molecule 3: Photosystem II CP43 protein

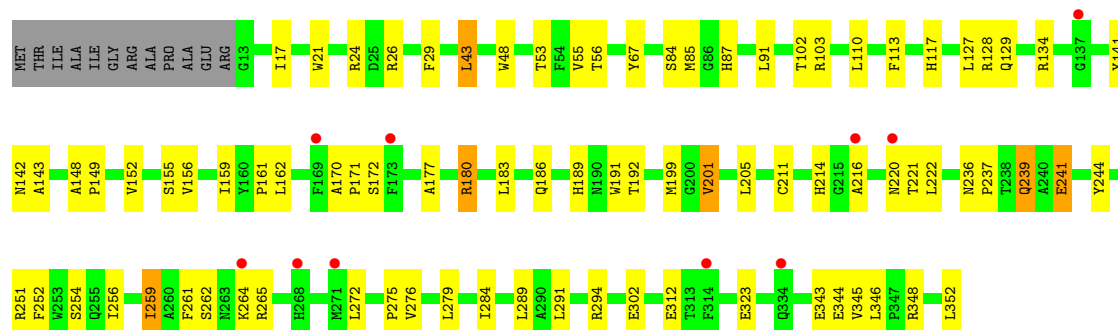




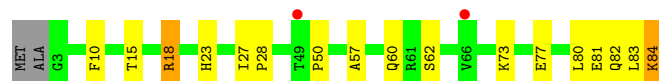
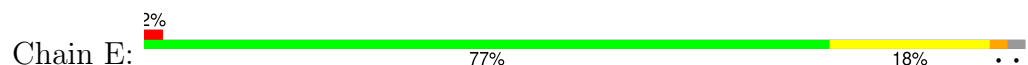
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein

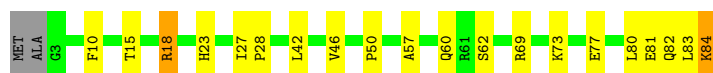


- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

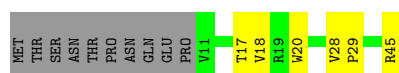




- Molecule 6: Cytochrome b559 subunit beta



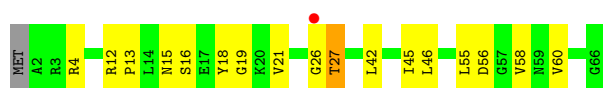
- Molecule 6: Cytochrome b559 subunit beta



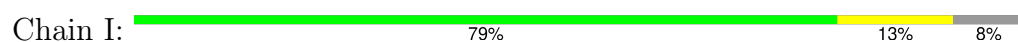
- Molecule 7: Photosystem II reaction center protein H



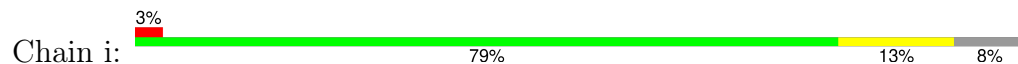
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J



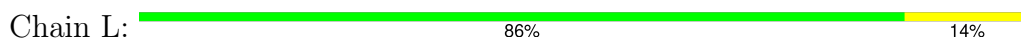
- Molecule 10: Photosystem II reaction center protein K



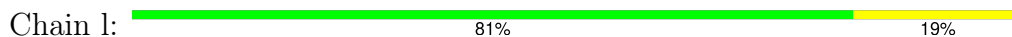
- Molecule 10: Photosystem II reaction center protein K



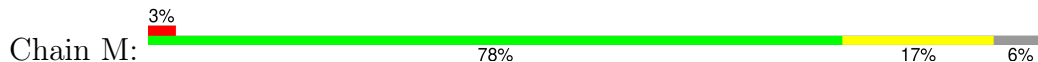
- Molecule 11: Photosystem II reaction center protein L



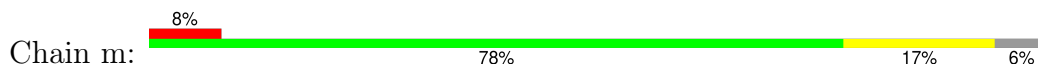
- Molecule 11: Photosystem II reaction center protein L

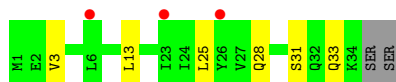


- Molecule 12: Photosystem II reaction center protein M

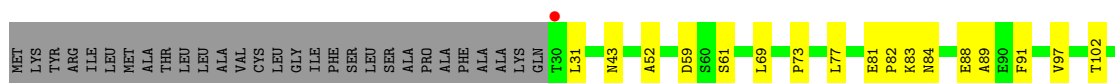


- Molecule 12: Photosystem II reaction center protein M

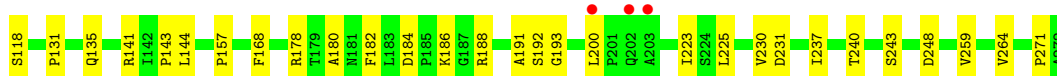
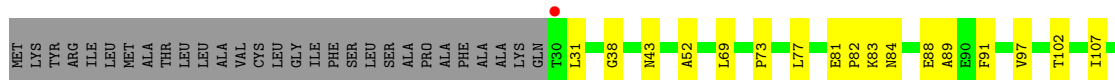




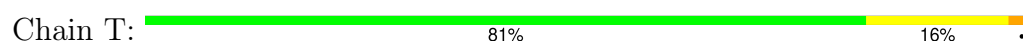
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



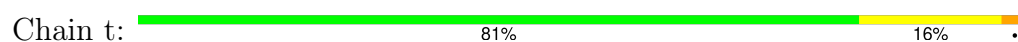
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



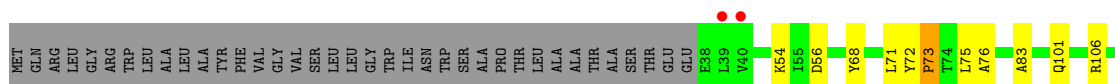
- Molecule 14: Photosystem II reaction center protein T



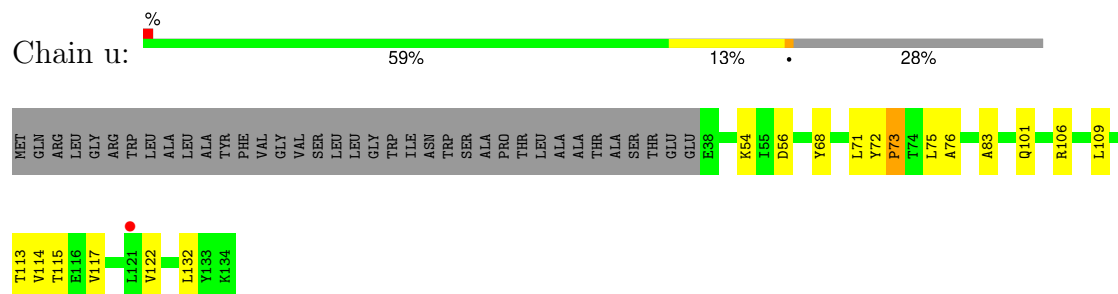
- Molecule 14: Photosystem II reaction center protein T



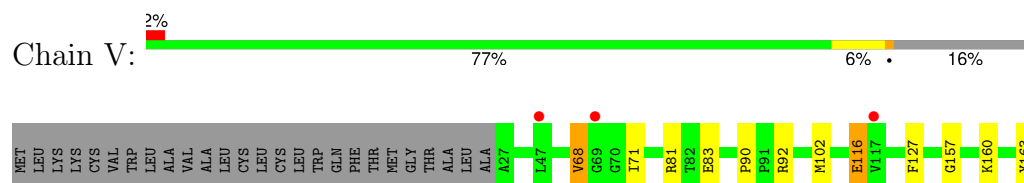
- Molecule 15: Photosystem II 12 kDa extrinsic protein



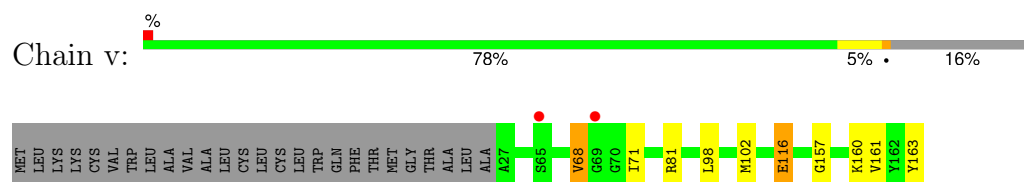
- Molecule 15: Photosystem II 12 kDa extrinsic protein



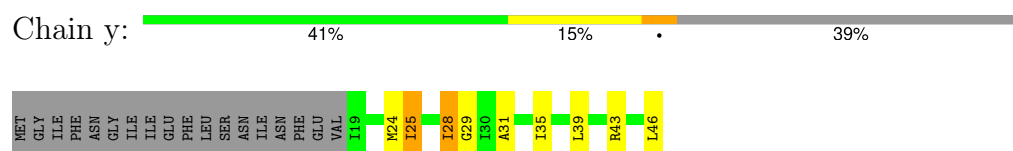
- Molecule 16: Cytochrome c-550



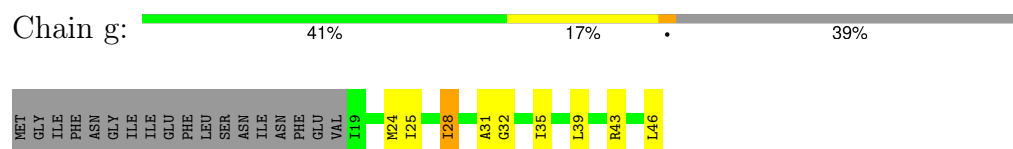
- Molecule 16: Cytochrome c-550



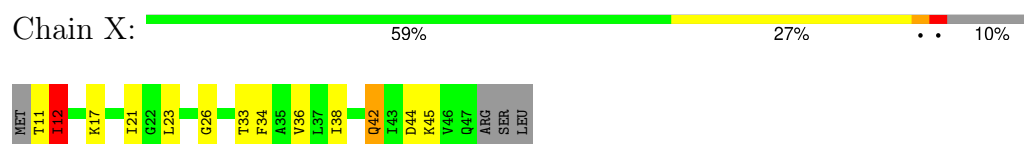
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein





- Molecule 19: Photosystem II reaction center protein Y

Chain Y: 100%

There are no outlier residues recorded for this chain.

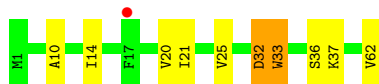
- Molecule 19: Photosystem II reaction center protein Y

Chain G: 100%

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 2% 84% 13%



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 79% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.276 , 0.284 0.280 , 0.288	Depositor DCC
R_{free} test set	2668 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 124.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.30	0/2713	0.78	2/3700 (0.1%)
1	a	0.30	0/2713	0.79	2/3700 (0.1%)
2	B	0.30	0/3986	0.80	8/5433 (0.1%)
2	b	0.30	0/3986	0.81	8/5433 (0.1%)
3	C	0.30	0/3556	0.80	8/4842 (0.2%)
3	c	0.30	0/3556	0.80	8/4842 (0.2%)
4	D	0.29	0/2801	0.76	0/3818
4	d	0.30	0/2801	0.77	0/3818
5	E	0.31	0/685	0.83	0/933
5	e	0.31	0/685	0.84	0/933
6	F	0.34	0/291	0.75	0/397
6	f	0.34	0/291	0.76	0/397
7	H	0.34	0/520	0.73	0/709
7	h	0.33	0/520	0.73	0/709
8	I	0.29	0/293	0.78	0/395
8	i	0.30	0/293	0.78	0/395
9	J	0.29	0/255	0.85	0/346
9	j	0.30	0/255	0.84	0/346
10	K	0.44	0/303	0.86	0/416
10	k	0.45	0/303	0.87	0/416
11	L	0.29	0/311	0.72	0/422
11	l	0.28	0/311	0.72	0/422
12	M	0.30	0/270	0.79	0/367
12	m	0.30	0/270	0.79	0/367
13	O	0.27	0/1876	0.70	0/2548
13	o	0.28	0/1876	0.70	2/2548 (0.1%)
14	T	0.27	0/284	0.76	0/381
14	t	0.27	0/284	0.74	0/381
15	U	0.30	0/785	0.77	0/1064
15	u	0.30	0/785	0.79	0/1064
16	V	0.29	0/1081	0.76	2/1468 (0.1%)
16	v	0.30	0/1081	0.76	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.34	0/202	0.77	0/272
17	y	0.33	0/202	0.77	0/272
18	X	0.38	0/273	0.80	0/370
18	x	0.38	0/273	0.80	0/370
20	Z	0.31	0/490	0.83	0/669
20	z	0.31	0/490	0.85	0/669
All	All	0.30	0/41950	0.78	40/57100 (0.1%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.70	133.21	119.84
2	b	483	ASP	C-N-CA	10.70	133.21	119.84
2	B	483	ASP	CA-C-N	10.56	133.04	119.84
2	B	483	ASP	C-N-CA	10.56	133.04	119.84
3	C	363	GLY	CA-C-N	6.37	125.86	119.24

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	2628	0	2524	77	0
1	a	2628	0	2524	66	0
2	B	3850	0	3718	61	0
2	b	3850	0	3718	61	0
3	C	3444	0	3365	77	0
3	c	3444	0	3365	76	0
4	D	2706	0	2608	60	0
4	d	2706	0	2608	66	0
5	E	666	0	651	11	0
5	e	666	0	651	13	0
6	F	282	0	291	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	4	0
7	H	507	0	521	14	0
7	h	507	0	521	15	0
8	I	286	0	308	3	0
8	i	286	0	308	3	0
9	J	249	0	262	8	0
9	j	249	0	262	7	0
10	K	293	0	305	10	0
10	k	293	0	305	11	0
11	L	304	0	316	4	0
11	l	304	0	316	5	0
12	M	267	0	289	6	0
12	m	267	0	289	6	0
13	O	1845	0	1801	26	0
13	o	1845	0	1801	27	0
14	T	275	0	288	5	0
14	t	275	0	288	5	0
15	U	774	0	773	8	0
15	u	774	0	773	8	0
16	V	1060	0	1068	8	0
16	v	1060	0	1068	8	0
17	g	201	0	226	6	0
17	y	201	0	226	7	0
18	X	270	0	299	9	0
18	x	270	0	299	9	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	9	0
20	z	479	0	516	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	28	0
22	B	975	0	1080	55	0
22	C	845	0	936	33	0
22	D	130	0	144	12	0
22	H	65	0	72	8	0
22	a	260	0	288	27	0
22	b	975	0	1080	46	0
22	c	845	0	936	34	0
22	d	130	0	144	12	0
22	h	65	0	72	11	0
23	A	45	0	61	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D	55	0	80	7	0
23	J	35	0	45	0	0
23	a	45	0	61	3	0
23	d	55	0	80	6	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	12	0
24	C	120	0	168	16	0
24	D	40	0	56	3	0
24	H	40	0	56	2	0
24	J	40	0	56	2	0
24	a	40	0	56	3	0
24	b	160	0	224	10	0
24	c	120	0	168	16	0
24	f	40	0	56	1	0
24	g	40	0	56	5	0
24	j	40	0	56	1	0
24	x	40	0	56	1	0
24	y	40	0	56	8	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	2	0
25	a	56	0	70	3	0
25	b	110	0	136	6	0
25	c	181	0	245	11	0
25	d	63	0	87	1	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	1	0
26	c	37	0	44	2	0
27	A	93	0	126	3	0
27	B	98	0	136	5	0
27	C	93	0	126	4	0
27	D	94	0	128	7	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	1	0
27	a	93	0	126	4	0
27	b	98	0	136	4	0
27	c	93	0	126	4	0
27	d	94	0	128	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	e	44	0	58	1	0
27	i	43	0	56	1	0
27	m	42	0	54	1	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	7	0
30	B	47	0	61	3	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	9	0
30	b	47	0	61	1	0
30	d	43	0	50	3	0
30	f	45	0	54	2	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	184	6	0
31	d	31	0	35	0	0
31	i	35	0	46	1	0
32	D	128	0	148	12	0
32	a	64	0	74	5	0
32	d	64	0	74	7	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	5	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	984	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 10.

The worst 5 of 984 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)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.87
3:c:39:ASN:HB2	22:c:507:CLA:HBA1	1.58	0.86
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.60	0.82
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.61	0.81
3:c:362:ARG:H	25:c:515:DGD:HE4	1.46	0.80

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	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	10	43
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	10	43
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	16	53
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	21	58
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36	71
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36	71
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	41
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	41
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	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%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100

Continued on next page...

Continued from previous page...

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%)	3 (9%)	1 (3%)	3	22
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	43
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	43
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%)	6 (6%)	2 (2%)	5	30
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	30
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	19
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	14
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	14
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
All	All	5138/5618 (92%)	4673 (91%)	410 (8%)	55 (1%)	11	45

5 of 55 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
1	a	12	ASN

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	271/280 (97%)	261 (96%)	10 (4%)	30	51
1	a	271/280 (97%)	260 (96%)	11 (4%)	27	49
2	B	390/407 (96%)	380 (97%)	10 (3%)	40	60
2	b	390/407 (96%)	380 (97%)	10 (3%)	40	60
3	C	347/362 (96%)	336 (97%)	11 (3%)	34	55
3	c	347/362 (96%)	336 (97%)	11 (3%)	34	55
4	D	275/283 (97%)	263 (96%)	12 (4%)	25	47
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	41
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	41
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	41
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	41
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	76
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	76

Continued on next page...

Continued from previous page...

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%)	82 (98%)	2 (2%)	43	63
16	V	116/138 (84%)	114 (98%)	2 (2%)	53	67
16	v	116/138 (84%)	114 (98%)	2 (2%)	53	67
17	g	20/37 (54%)	17 (85%)	3 (15%)	3	14
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	14
18	X	30/34 (88%)	28 (93%)	2 (7%)	15	37
18	x	30/34 (88%)	28 (93%)	2 (7%)	15	37
20	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
20	z	52/52 (100%)	50 (96%)	2 (4%)	29	51
All	All	4244/4594 (92%)	4110 (97%)	134 (3%)	34	55

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	56	ASP
11	l	11	GLU
18	x	12	ILE
7	H	56	ASP
7	H	27	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	44	ASN
13	o	130	GLN
3	c	56	HIS
4	d	117	HIS
13	o	173	ASN

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	$\# Z > 2$
22	CLA	B	610	2	69,73,73	1.23	6 (8%)	82,113,113	1.29	7 (8%)
27	LMG	d	407	-	48,48,55	0.75	0	56,56,63	1.37	4 (7%)
22	CLA	D	405	-	69,73,73	1.20	7 (10%)	82,113,113	1.21	5 (6%)
22	CLA	B	603	2	69,73,73	1.18	8 (11%)	82,113,113	1.34	7 (8%)
22	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
22	CLA	b	607	2	69,73,73	1.19	8 (11%)	82,113,113	1.32	7 (8%)
24	BCR	A	407	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
25	DGD	B	620	-	59,59,67	0.89	1 (1%)	73,73,81	1.34	8 (10%)
32	PHO	D	401	-	58,69,69	2.16	9 (15%)	55,99,99	1.41	6 (10%)
22	CLA	h	101	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	5 (6%)
30	SQD	a	401	-	52,54,54	0.96	3 (5%)	62,65,65	1.49	9 (14%)
22	CLA	C	504	3	69,73,73	1.18	7 (10%)	82,113,113	1.31	5 (6%)
27	LMG	b	628	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	4 (7%)
30	SQD	A	413	-	49,51,54	0.97	2 (4%)	59,62,65	1.66	9 (15%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
23	PL9	a	409	-	45,45,55	1.01	4 (8%)	56,57,69	1.53	10 (17%)
22	CLA	b	610	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
23	PL9	A	406	-	45,45,55	0.97	4 (8%)	56,57,69	1.54	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	b	627	-	36,36,36	1.07	3 (8%)	47,47,47	1.00	2 (4%)
22	CLA	c	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
24	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	B	604	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	C	510	3	69,73,73	1.19	6 (8%)	82,113,113	1.31	6 (7%)
24	BCR	g	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	9 (16%)
32	PHO	D	402	-	58,69,69	2.20	9 (15%)	55,99,99	1.42	5 (9%)
22	CLA	A	402	1	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.27	4 (7%)
30	SQD	a	415	-	49,51,54	0.97	2 (4%)	59,62,65	1.68	9 (15%)
27	LMG	B	624	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	5 (8%)
33	BCT	D	404	21	3,3,3	1.11	0	2,3,3	4.21	2 (100%)
24	BCR	b	622	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
22	CLA	c	507	3	69,73,73	1.19	8 (11%)	82,113,113	1.30	7 (8%)
24	BCR	C	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	9 (16%)
25	DGD	b	624	-	59,59,67	0.90	1 (1%)	73,73,81	1.33	6 (8%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.27	6 (8%)
22	CLA	C	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	c	503	-	69,73,73	1.20	7 (10%)	82,113,113	1.28	5 (6%)
25	DGD	b	601	-	53,53,67	1.05	3 (5%)	67,67,81	1.33	7 (10%)
31	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	C	503	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	4 (4%)
22	CLA	c	505	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	c	508	3	69,73,73	1.19	6 (8%)	82,113,113	1.24	5 (6%)
32	PHO	a	407	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)
31	LMT	B	628	-	36,36,36	1.11	5 (13%)	47,47,47	1.04	1 (2%)
25	DGD	d	408	-	64,64,67	0.91	2 (3%)	78,78,81	1.34	9 (11%)
24	BCR	b	623	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	8 (14%)
24	BCR	H	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	4 (7%)
26	LHG	C	519	-	36,36,48	0.72	2 (5%)	39,42,54	1.28	4 (10%)
25	DGD	c	517	-	67,67,67	0.87	0	81,81,81	1.39	9 (11%)
31	LMT	B	623	-	36,36,36	1.07	3 (8%)	47,47,47	1.01	2 (4%)
22	CLA	C	502	3	69,73,73	1.19	9 (13%)	82,113,113	1.27	5 (6%)
22	CLA	c	510	3	69,73,73	1.20	5 (7%)	82,113,113	1.29	6 (7%)
25	DGD	C	517	-	67,67,67	0.87	0	81,81,81	1.40	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	605	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	5 (6%)
31	LMT	B	627	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)
27	LMG	d	410	-	46,46,55	0.79	1 (2%)	54,54,63	1.31	6 (11%)
24	BCR	C	513	-	41,41,41	1.15	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
31	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	2 (4%)
25	DGD	a	411	-	57,57,67	0.93	1 (1%)	71,71,81	1.39	8 (11%)
23	PL9	d	406	-	55,55,55	1.00	3 (5%)	68,69,69	1.51	13 (19%)
22	CLA	d	405	-	69,73,73	1.19	5 (7%)	82,113,113	1.26	5 (6%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.28	7 (10%)
22	CLA	b	611	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.33	7 (12%)
22	CLA	b	609	2	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
31	LMT	M	102	-	36,36,36	1.12	6 (16%)	47,47,47	1.00	2 (4%)
24	BCR	D	411	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	7 (12%)
24	BCR	c	513	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
25	DGD	C	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.43	13 (16%)
22	CLA	b	615	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
27	LMG	a	413	-	51,51,55	0.74	0	59,59,63	1.35	8 (13%)
34	HEM	v	201	16	50,50,50	1.99	10 (20%)	67,82,82	1.24	4 (5%)
22	CLA	d	404	-	69,73,73	1.20	6 (8%)	82,113,113	1.22	5 (6%)
22	CLA	a	404	1	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
27	LMG	A	415	-	42,42,55	0.83	1 (2%)	50,50,63	1.26	4 (8%)
27	LMG	D	408	-	48,48,55	0.75	0	56,56,63	1.38	4 (7%)
29	OEX	A	412	3,1	0,14,14	-	-	-	-	-
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
32	PHO	d	401	-	58,69,69	2.16	9 (15%)	55,99,99	1.41	7 (12%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	b	619	2	69,73,73	1.19	8 (11%)	82,113,113	1.24	5 (6%)
34	HEM	V	201	16	50,50,50	1.98	10 (20%)	67,82,82	1.21	2 (2%)
24	BCR	f	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	6 (10%)
22	CLA	c	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.27	5 (6%)
22	CLA	a	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	612	2	69,73,73	1.20	7 (10%)	82,113,113	1.22	5 (6%)
23	PL9	J	101	-	35,35,55	0.98	2 (5%)	44,45,69	1.58	8 (18%)
24	BCR	x	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	3 (5%)
22	CLA	a	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
26	LHG	A	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.21	3 (7%)
24	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	7 (12%)
24	BCR	c	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	9 (16%)
22	CLA	b	606	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	7 (8%)
30	SQD	b	602	-	45,47,54	1.02	4 (8%)	55,58,65	1.74	9 (16%)
27	LMG	E	101	-	44,44,55	0.74	0	52,52,63	1.31	5 (9%)
22	CLA	A	405	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
24	BCR	y	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	a	408	1	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
31	LMT	D	410	-	32,32,36	1.15	4 (12%)	43,43,47	1.02	2 (4%)
22	CLA	B	601	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	6 (7%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.40	8 (11%)
22	CLA	b	614	2	69,73,73	1.23	6 (8%)	82,113,113	1.29	6 (7%)
23	PL9	D	407	-	55,55,55	1.02	4 (7%)	68,69,69	1.50	13 (19%)
23	PL9	j	101	-	35,35,55	0.96	2 (5%)	44,45,69	1.58	8 (18%)
24	BCR	C	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	9 (16%)
33	BCT	d	403	21	3,3,3	1.11	0	2,3,3	4.19	2 (100%)
22	CLA	B	613	2	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
31	LMT	b	626	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
22	CLA	c	520	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
24	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	9 (16%)
22	CLA	c	509	3	69,73,73	1.19	8 (11%)	82,113,113	1.23	5 (6%)
22	CLA	C	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
27	LMG	M	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
22	CLA	B	615	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	H	101	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	B	608	2	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	B	612	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
22	CLA	b	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	B	614	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	D	406	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	606	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
31	LMT	I	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	2 (4%)
24	BCR	J	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.58	11 (19%)
24	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.30	7 (12%)
27	LMG	C	522	-	48,48,55	0.76	0	56,56,63	1.32	5 (8%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.33	7 (10%)
22	CLA	A	404	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
27	LMG	a	402	-	42,42,55	0.83	1 (2%)	50,50,63	1.26	4 (8%)
30	SQD	A	414	-	52,54,54	0.96	2 (3%)	62,65,65	1.50	8 (12%)
25	DGD	D	409	-	64,64,67	0.90	0	78,78,81	1.33	9 (11%)
34	HEM	f	101	5,6	50,50,50	1.96	8 (16%)	67,82,82	1.32	4 (5%)
31	LMT	b	604	-	36,36,36	1.11	3 (8%)	47,47,47	1.03	1 (2%)
30	SQD	d	402	-	41,43,54	1.05	3 (7%)	51,54,65	1.73	10 (19%)
22	CLA	C	520	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
31	LMT	B	622	-	36,36,36	1.10	3 (8%)	47,47,47	0.97	1 (2%)
22	CLA	b	617	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
34	HEM	F	101	5,6	50,50,50	1.97	9 (18%)	67,82,82	1.31	4 (5%)
22	CLA	b	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
25	DGD	c	516	-	63,63,67	0.91	2 (3%)	77,77,81	1.43	12 (15%)
22	CLA	B	602	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	C	509	3	69,73,73	1.19	7 (10%)	82,113,113	1.22	5 (6%)
22	CLA	b	616	-	69,73,73	1.18	6 (8%)	82,113,113	1.27	7 (8%)
30	SQD	f	103	-	43,45,54	1.04	3 (6%)	53,56,65	1.56	11 (20%)
30	SQD	D	403	-	41,43,54	1.05	3 (7%)	51,54,65	1.72	10 (19%)
24	BCR	b	620	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	6 (10%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.27	6 (11%)
26	LHG	c	519	-	36,36,48	0.74	2 (5%)	39,42,54	1.29	4 (10%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
24	BCR	j	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.58	12 (21%)
27	LMG	D	412	-	46,46,55	0.78	1 (2%)	54,54,63	1.31	5 (9%)
22	CLA	b	618	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	c	504	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
24	BCR	B	616	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	8 (14%)
22	CLA	C	508	3	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	M	103	-	36,36,36	1.11	4 (11%)	47,47,47	0.99	2 (4%)
22	CLA	c	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	B	607	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
22	CLA	C	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	B	609	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	C	511	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
27	LMG	m	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
27	LMG	A	410	-	51,51,55	0.73	0	59,59,63	1.36	7 (11%)
30	SQD	F	102	-	43,45,54	1.04	3 (6%)	53,56,65	1.57	10 (18%)
31	LMT	d	409	-	32,32,36	1.15	3 (9%)	43,43,47	0.99	2 (4%)
26	LHG	a	412	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	3 (7%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.32	5 (8%)
30	SQD	B	626	-	45,47,54	1.02	4 (8%)	55,58,65	1.71	10 (18%)
24	BCR	a	410	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	C	507	3	69,73,73	1.19	8 (11%)	82,113,113	1.29	7 (8%)
29	OEX	a	414	3,1	0,14,14	-	-	-	-	-
22	CLA	B	605	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	c	501	3	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	610	2	-	12/39/115/115	-
27	LMG	d	407	-	-	20/43/63/70	0/1/1/1
22	CLA	D	405	-	-	14/39/115/115	-
22	CLA	B	603	2	-	7/39/115/115	-
22	CLA	B	611	-	-	10/39/115/115	-
22	CLA	b	607	2	-	7/39/115/115	-
24	BCR	A	407	-	-	3/29/63/63	0/2/2/2
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
32	PHO	D	401	-	-	11/37/103/103	0/5/6/6
22	CLA	h	101	-	-	15/39/115/115	-
30	SQD	a	401	-	-	12/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	504	3	-	17/39/115/115	-
27	LMG	b	628	-	-	24/44/64/70	0/1/1/1
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
27	LMG	c	518	-	-	21/40/60/70	0/1/1/1
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
22	CLA	b	610	-	-	9/39/115/115	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
31	LMT	b	627	-	-	2/21/61/61	0/2/2/2
22	CLA	c	512	3	-	19/39/115/115	-
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	CLA	B	604	2	-	15/39/115/115	-
22	CLA	C	510	3	-	13/39/115/115	-
24	BCR	g	101	-	-	4/29/63/63	0/2/2/2
32	PHO	D	402	-	-	10/37/103/103	0/5/6/6
22	CLA	A	402	1	-	8/39/115/115	-
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
30	SQD	a	415	-	-	17/46/66/69	0/1/1/1
27	LMG	B	624	-	-	25/44/64/70	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
22	CLA	c	507	3	-	13/39/115/115	-
24	BCR	C	514	-	-	4/29/63/63	0/2/2/2
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
22	CLA	C	512	3	-	15/39/115/115	-
22	CLA	c	503	-	-	11/39/115/115	-
25	DGD	b	601	-	-	18/41/81/95	0/2/2/2
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	C	503	3	-	12/39/115/115	-
22	CLA	c	505	3	-	16/39/115/115	-
22	CLA	c	508	3	-	18/39/115/115	-
32	PHO	a	407	-	-	11/37/103/103	0/5/6/6
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
25	DGD	d	408	-	-	35/52/92/95	0/2/2/2
24	BCR	b	623	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
26	LHG	C	519	-	-	16/41/41/53	-
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
31	LMT	B	623	-	-	4/21/61/61	0/2/2/2
22	CLA	C	502	3	-	9/39/115/115	-
22	CLA	c	510	3	-	15/39/115/115	-
25	DGD	C	517	-	-	21/55/95/95	0/2/2/2
22	CLA	b	605	-	-	15/39/115/115	-
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
27	LMG	d	410	-	-	15/41/61/70	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	c	511	-	-	17/39/115/115	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
23	PL9	d	406	-	-	11/53/73/73	0/1/1/1
22	CLA	d	405	-	-	8/39/115/115	-
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
22	CLA	b	611	2	-	13/39/115/115	-
27	LMG	B	621	-	-	15/44/64/70	0/1/1/1
22	CLA	b	609	2	-	17/39/115/115	-
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	BCR	D	411	-	-	5/29/63/63	0/2/2/2
24	BCR	c	513	-	-	6/29/63/63	0/2/2/2
25	DGD	C	516	-	-	19/51/91/95	0/2/2/2
22	CLA	b	615	-	-	10/39/115/115	-
27	LMG	a	413	-	-	26/46/66/70	0/1/1/1
34	HEM	v	201	16	-	5/14/54/54	-
22	CLA	d	404	-	-	11/39/115/115	-
22	CLA	a	404	1	-	8/39/115/115	-
22	CLA	C	505	3	-	16/39/115/115	-
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
32	PHO	d	401	-	-	10/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
22	CLA	b	619	2	-	19/39/115/115	-
34	HEM	V	201	16	-	5/14/54/54	-
24	BCR	f	102	-	-	6/29/63/63	0/2/2/2
22	CLA	c	502	-	-	10/39/115/115	-
22	CLA	a	406	-	-	8/39/115/115	-
22	CLA	b	612	2	-	8/39/115/115	-
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	a	405	-	-	12/39/115/115	-
26	LHG	A	409	-	-	13/43/43/53	-
24	BCR	b	621	-	-	7/29/63/63	0/2/2/2
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
22	CLA	b	606	2	-	13/39/115/115	-
30	SQD	b	602	-	-	14/42/62/69	0/1/1/1
27	LMG	E	101	-	-	18/39/59/70	0/1/1/1
22	CLA	A	405	1	-	8/39/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	a	408	1	-	7/39/115/115	-
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
22	CLA	B	601	-	-	16/39/115/115	-
25	DGD	A	408	-	-	15/45/85/95	0/2/2/2
22	CLA	b	614	2	-	11/39/115/115	-
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
24	BCR	C	521	-	-	5/29/63/63	0/2/2/2
22	CLA	B	613	2	-	13/39/115/115	-
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
22	CLA	c	520	-	-	12/39/115/115	-
24	BCR	c	521	-	-	4/29/63/63	0/2/2/2
22	CLA	c	509	3	-	17/39/115/115	-
22	CLA	C	506	-	-	13/39/115/115	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	615	2	-	19/39/115/115	-
22	CLA	H	101	-	-	15/39/115/115	-
22	CLA	B	608	2	-	8/39/115/115	-
22	CLA	B	612	-	-	16/39/115/115	-
22	CLA	b	613	-	-	18/39/115/115	-
22	CLA	B	614	-	-	9/39/115/115	-
22	CLA	D	406	-	-	8/39/115/115	-
22	CLA	B	606	-	-	10/39/115/115	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
27	LMG	C	522	-	-	19/43/63/70	0/1/1/1
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
22	CLA	A	404	-	-	10/39/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
30	SQD	A	414	-	-	10/49/69/69	0/1/1/1
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
34	HEM	f	101	5,6	-	2/14/54/54	-
31	LMT	b	604	-	-	4/21/61/61	0/2/2/2
30	SQD	d	402	-	-	14/38/58/69	0/1/1/1
22	CLA	C	520	-	-	13/39/115/115	-
31	LMT	B	622	-	-	3/21/61/61	0/2/2/2
22	CLA	b	617	2	-	13/39/115/115	-
34	HEM	F	101	5,6	-	2/14/54/54	-
22	CLA	b	608	2	-	16/39/115/115	-
25	DGD	c	516	-	-	19/51/91/95	0/2/2/2
22	CLA	B	602	2	-	15/39/115/115	-
22	CLA	C	509	3	-	16/39/115/115	-
22	CLA	b	616	-	-	16/39/115/115	-
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
30	SQD	D	403	-	-	14/38/58/69	0/1/1/1
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
27	LMG	i	101	-	-	19/38/58/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	c	519	-	-	17/41/41/53	-
22	CLA	A	403	-	-	13/39/115/115	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
22	CLA	b	618	-	-	9/39/115/115	-
22	CLA	c	504	3	-	17/39/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	C	508	3	-	19/39/115/115	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	c	506	-	-	12/39/115/115	-
22	CLA	B	607	2	-	12/39/115/115	-
22	CLA	C	501	3	-	16/39/115/115	-
22	CLA	B	609	-	-	18/39/115/115	-
22	CLA	C	511	-	-	17/39/115/115	-
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
27	LMG	A	410	-	-	25/46/66/70	0/1/1/1
30	SQD	F	102	-	-	10/40/60/69	0/1/1/1
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
26	LHG	a	412	-	-	11/43/43/53	-
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
22	CLA	C	507	3	-	13/39/115/115	-
22	CLA	B	605	2	-	14/39/115/115	-
22	CLA	c	501	3	-	14/39/115/115	-

The worst 5 of 749 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	402	PHO	C1B-C2B	9.70	1.50	1.39
32	d	401	PHO	C1B-C2B	9.65	1.50	1.39
32	D	401	PHO	C1B-C2B	9.57	1.50	1.39
32	a	407	PHO	C1B-C2B	9.56	1.50	1.39
32	D	402	PHO	C3B-C4B	8.74	1.50	1.41

The worst 5 of 1029 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.16	109.94	106.68
22	c	504	CLA	C4A-NA-C1A	7.08	109.91	106.68
22	C	510	CLA	C4A-NA-C1A	7.06	109.90	106.68
22	B	603	CLA	C4A-NA-C1A	7.02	109.88	106.68
22	B	611	CLA	C4A-NA-C1A	7.02	109.88	106.68

There are no chirality outliers.

5 of 2081 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	404	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

160 monomers are involved in 454 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	610	CLA	3	0
27	d	407	LMG	7	0
22	D	405	CLA	9	0
22	B	603	CLA	2	0
22	B	611	CLA	4	0
22	b	607	CLA	2	0
24	A	407	BCR	2	0
25	B	620	DGD	2	0
32	D	401	PHO	7	0
22	h	101	CLA	11	0
30	a	401	SQD	6	0
22	C	504	CLA	4	0
27	b	628	LMG	1	0
30	A	413	SQD	3	0
27	c	518	LMG	2	0
23	a	409	PL9	3	0
22	b	610	CLA	4	0
23	A	406	PL9	3	0
22	c	512	CLA	3	0
24	B	618	BCR	3	0
22	B	604	CLA	9	0
22	C	510	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	101	BCR	5	0
32	D	402	PHO	5	0
22	A	402	CLA	11	0
27	I	101	LMG	1	0
30	a	415	SQD	3	0
27	B	624	LMG	2	0
24	b	622	BCR	3	0
22	c	507	CLA	4	0
24	C	514	BCR	6	0
25	b	624	DGD	3	0
25	C	515	DGD	3	0
22	C	512	CLA	3	0
22	c	503	CLA	2	0
25	b	601	DGD	3	0
31	b	603	LMT	3	0
22	C	503	CLA	3	0
22	c	505	CLA	1	0
22	c	508	CLA	5	0
32	a	407	PHO	5	0
31	B	628	LMT	2	0
25	d	408	DGD	1	0
24	b	623	BCR	2	0
24	H	102	BCR	2	0
26	C	519	LHG	2	0
25	c	517	DGD	5	0
22	c	510	CLA	4	0
25	C	517	DGD	5	0
31	B	627	LMT	2	0
27	d	410	LMG	1	0
24	C	513	BCR	6	0
24	B	619	BCR	2	0
22	c	511	CLA	2	0
31	i	102	LMT	1	0
25	a	411	DGD	3	0
23	d	406	PL9	6	0
22	d	405	CLA	2	0
25	c	515	DGD	3	0
22	b	611	CLA	7	0
27	B	621	LMG	3	0
22	b	609	CLA	5	0
24	D	411	BCR	3	0
24	c	513	BCR	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	516	DGD	4	0
22	b	615	CLA	4	0
27	a	413	LMG	3	0
34	v	201	HEM	5	0
22	d	404	CLA	10	0
22	a	404	CLA	10	0
22	C	505	CLA	1	0
27	A	415	LMG	1	0
27	D	408	LMG	6	0
27	C	518	LMG	3	0
32	d	401	PHO	7	0
27	b	625	LMG	3	0
22	b	619	CLA	4	0
34	V	201	HEM	5	0
24	f	102	BCR	1	0
22	a	406	CLA	6	0
22	b	612	CLA	5	0
24	x	101	BCR	1	0
22	a	405	CLA	11	0
26	A	409	LHG	3	0
24	b	621	BCR	1	0
24	c	514	BCR	4	0
22	b	606	CLA	9	0
30	b	602	SQD	1	0
27	E	101	LMG	1	0
22	A	405	CLA	1	0
24	y	101	BCR	8	0
22	a	408	CLA	1	0
22	B	601	CLA	1	0
25	A	408	DGD	1	0
22	b	614	CLA	2	0
23	D	407	PL9	7	0
24	C	521	BCR	4	0
22	B	613	CLA	3	0
31	b	626	LMT	1	0
22	c	520	CLA	5	0
24	c	521	BCR	4	0
22	c	509	CLA	3	0
22	C	506	CLA	3	0
27	M	101	LMG	1	0
22	B	615	CLA	4	0
22	H	101	CLA	8	0

Continued on next page...

Continued from previous page...

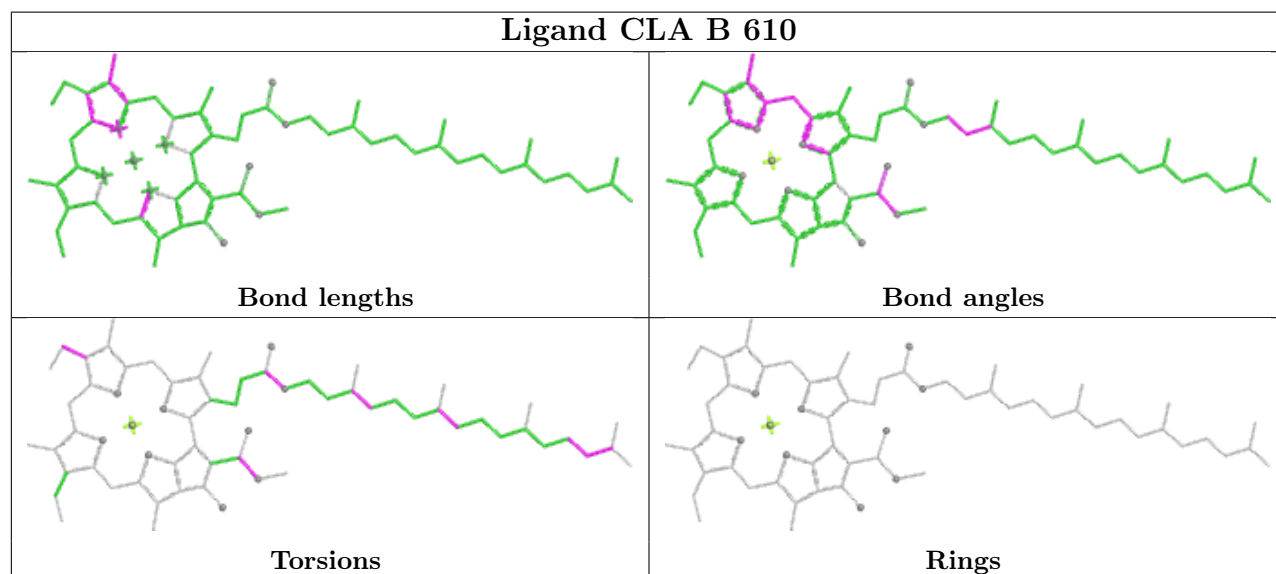
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	608	CLA	6	0
22	B	612	CLA	3	0
22	b	613	CLA	1	0
22	B	614	CLA	1	0
22	D	406	CLA	3	0
22	B	606	CLA	6	0
31	I	102	LMT	1	0
24	J	102	BCR	2	0
24	B	617	BCR	1	0
27	C	522	LMG	1	0
25	B	625	DGD	2	0
22	A	404	CLA	5	0
27	e	101	LMG	1	0
27	a	402	LMG	1	0
30	A	414	SQD	4	0
25	D	409	DGD	2	0
34	f	101	HEM	4	0
31	b	604	LMT	2	0
30	d	402	SQD	3	0
22	C	520	CLA	4	0
31	B	622	LMT	2	0
22	b	617	CLA	2	0
34	F	101	HEM	4	0
22	b	608	CLA	7	0
25	c	516	DGD	3	0
22	B	602	CLA	10	0
22	C	509	CLA	4	0
22	b	616	CLA	2	0
30	f	103	SQD	2	0
30	D	403	SQD	3	0
24	b	620	BCR	5	0
27	i	101	LMG	1	0
26	c	519	LHG	2	0
22	A	403	CLA	13	0
24	j	102	BCR	1	0
27	D	412	LMG	1	0
22	b	618	CLA	2	0
22	c	504	CLA	3	0
24	B	616	BCR	7	0
22	C	508	CLA	1	0
22	c	506	CLA	4	0
22	B	607	CLA	8	0

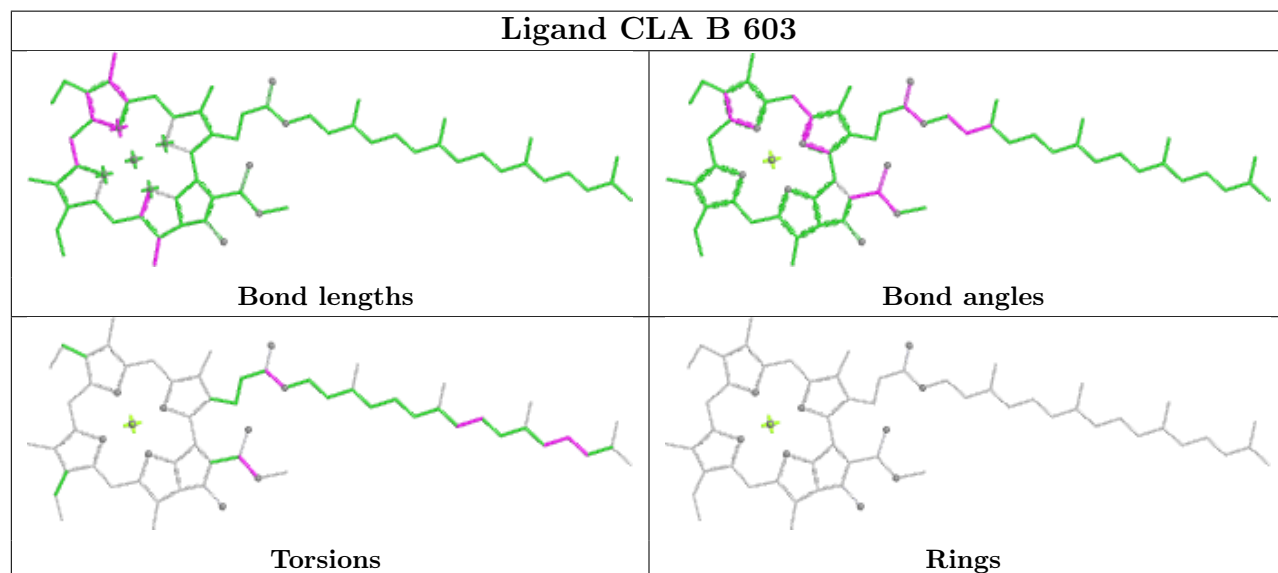
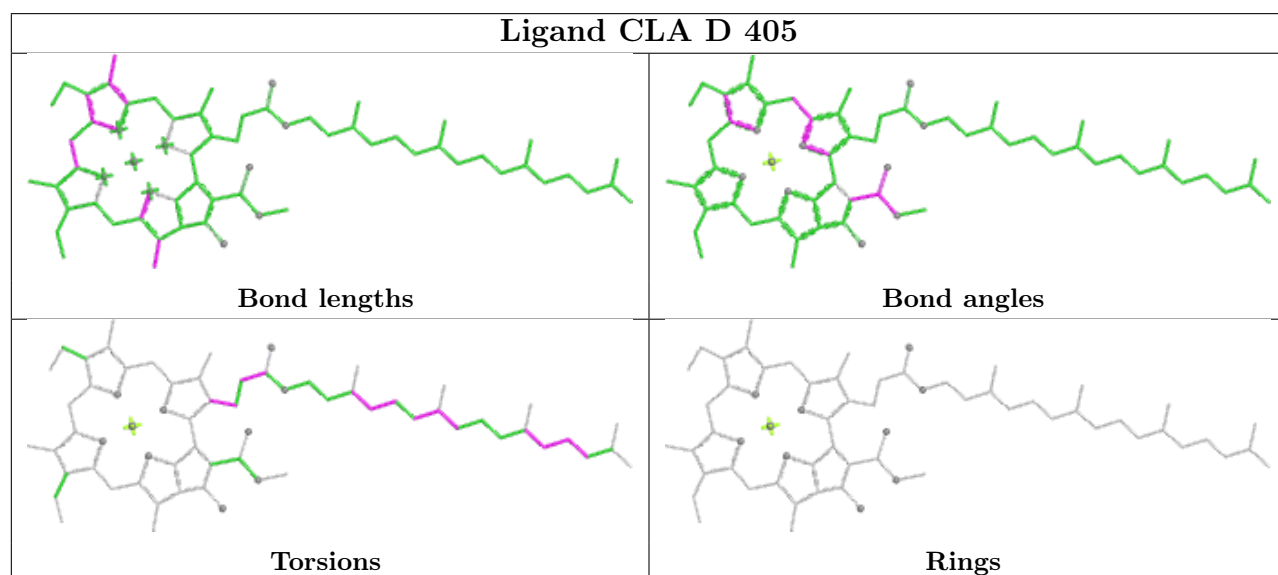
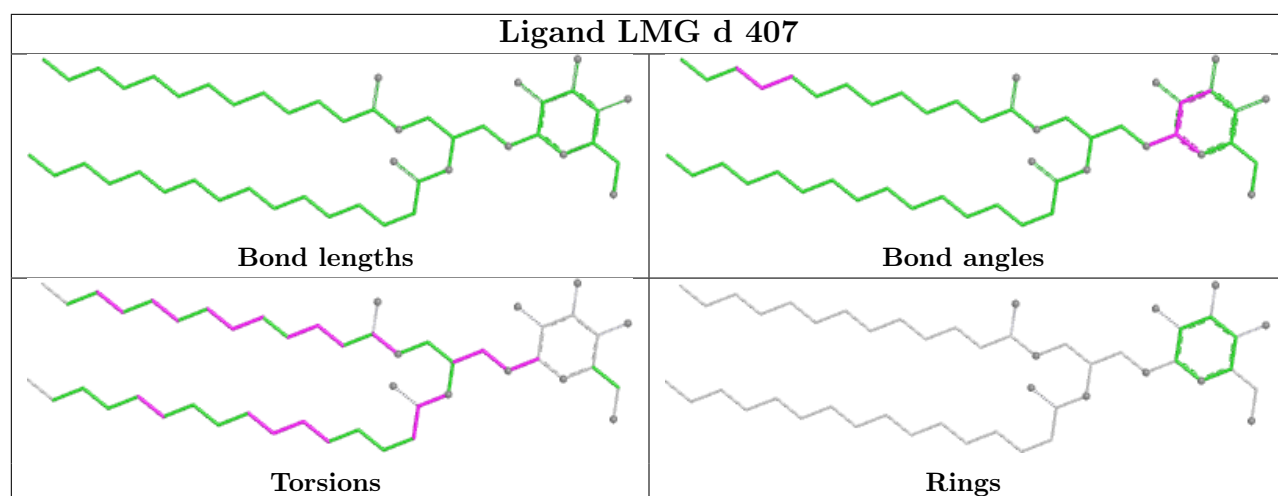
Continued on next page...

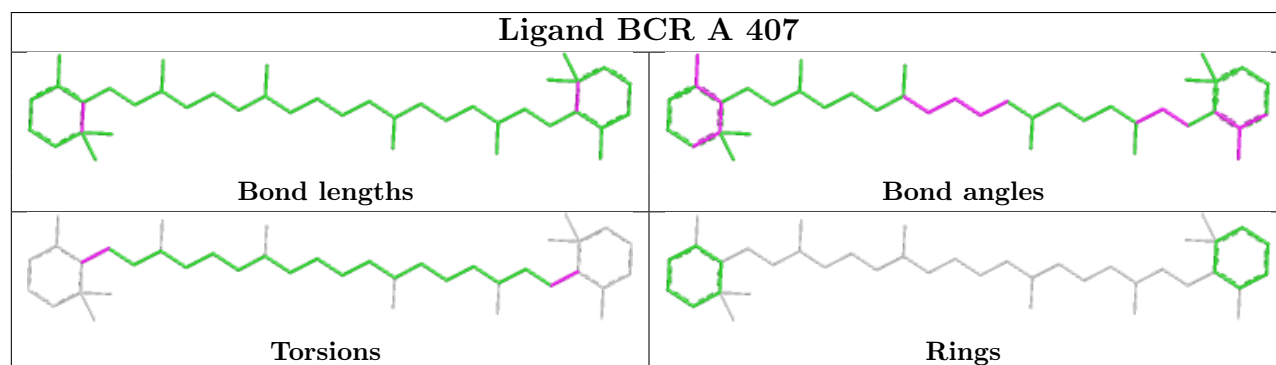
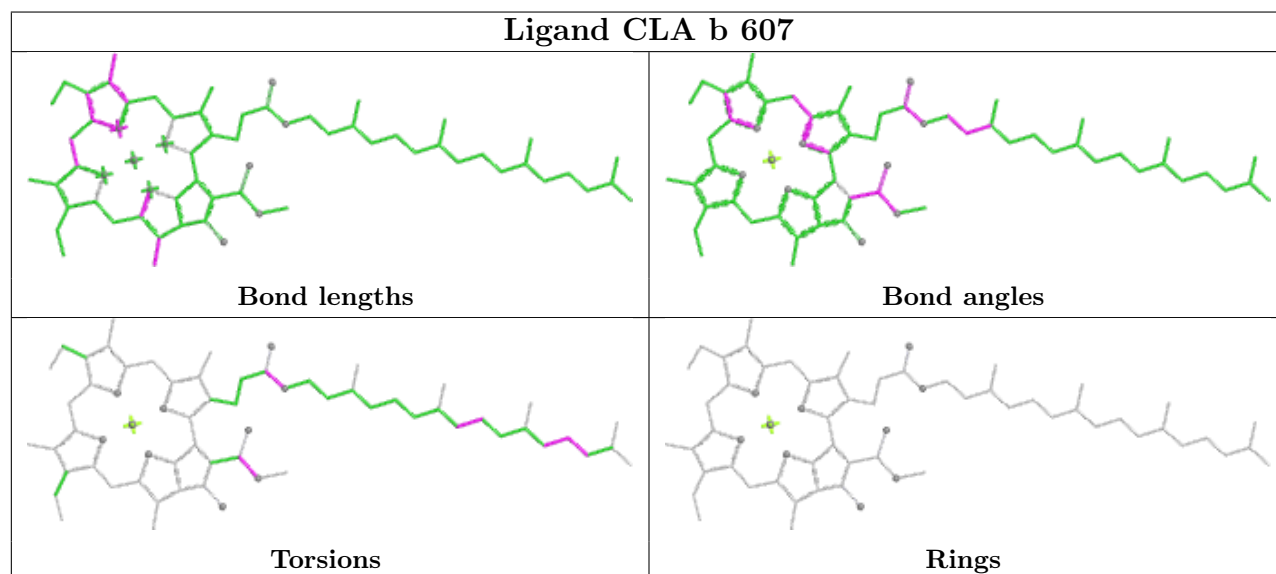
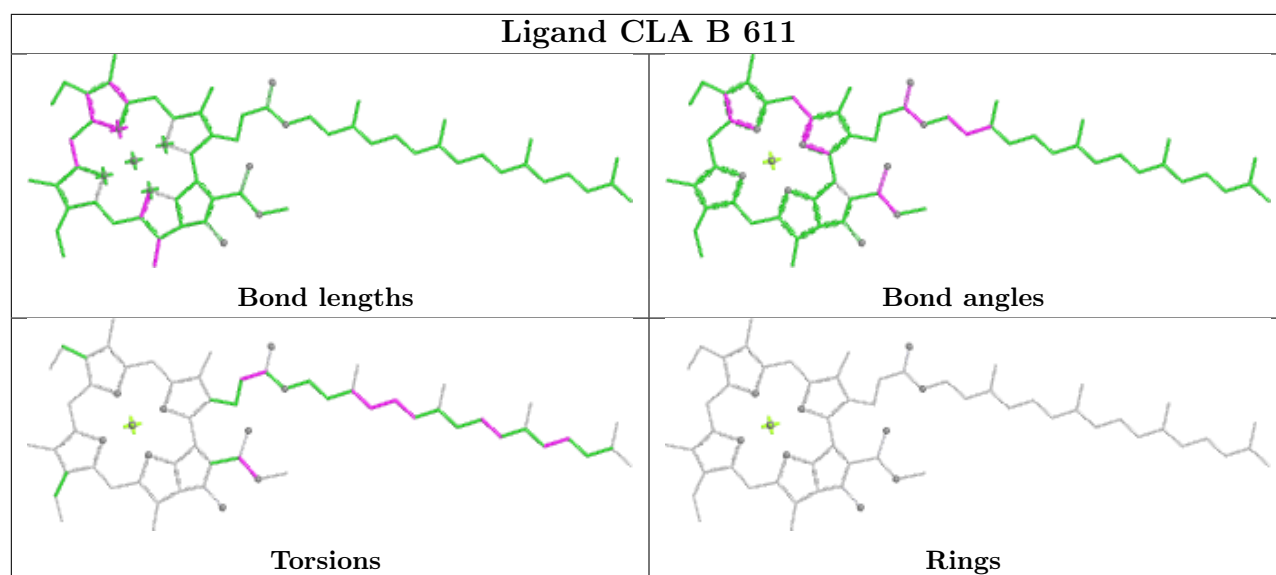
Continued from previous page...

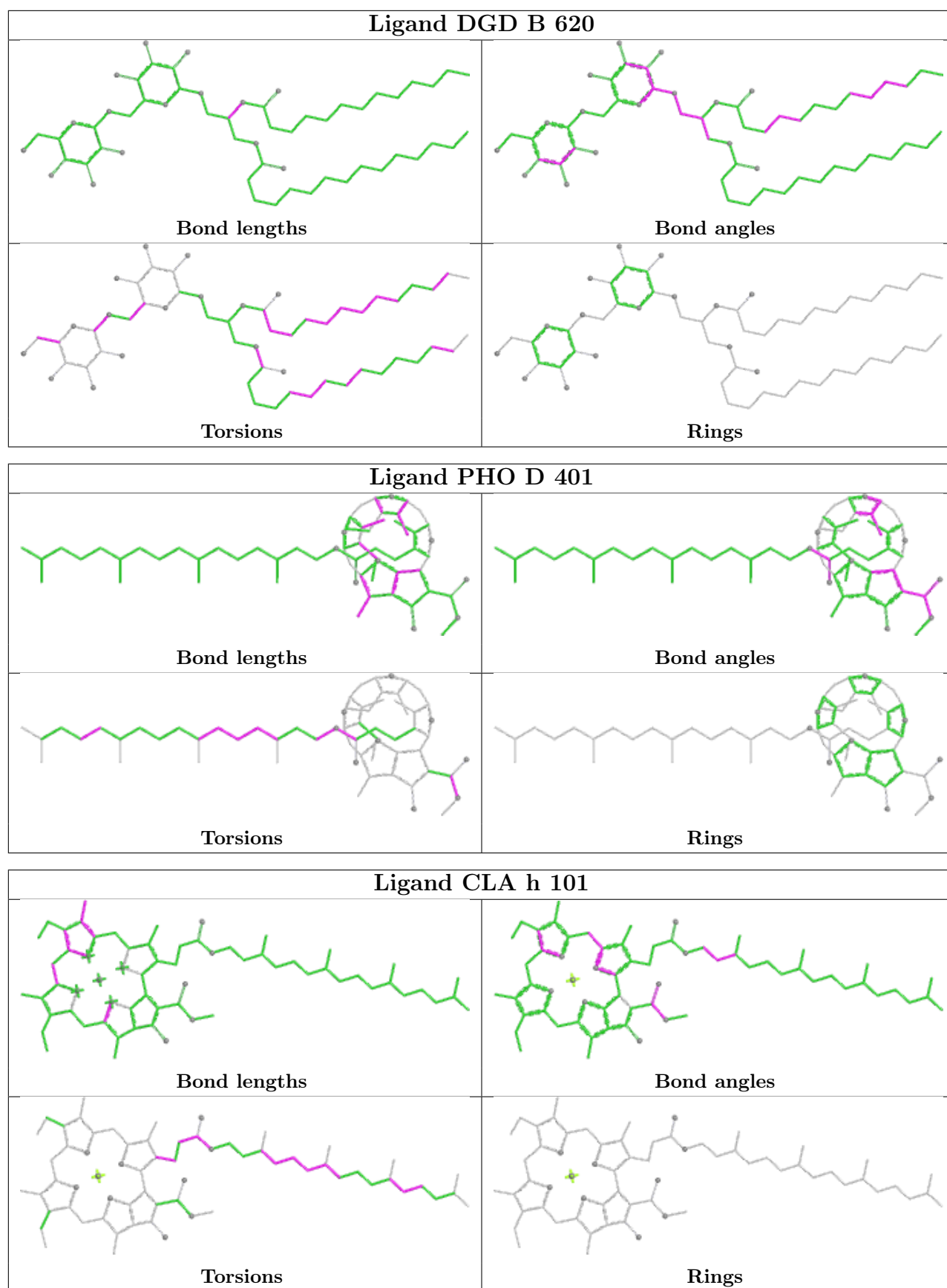
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	501	CLA	3	0
22	C	511	CLA	1	0
27	m	101	LMG	1	0
27	A	410	LMG	2	0
30	F	102	SQD	2	0
26	a	412	LHG	1	0
27	c	522	LMG	2	0
30	B	626	SQD	3	0
24	a	410	BCR	3	0
22	C	507	CLA	4	0
22	B	605	CLA	6	0
22	c	501	CLA	3	0

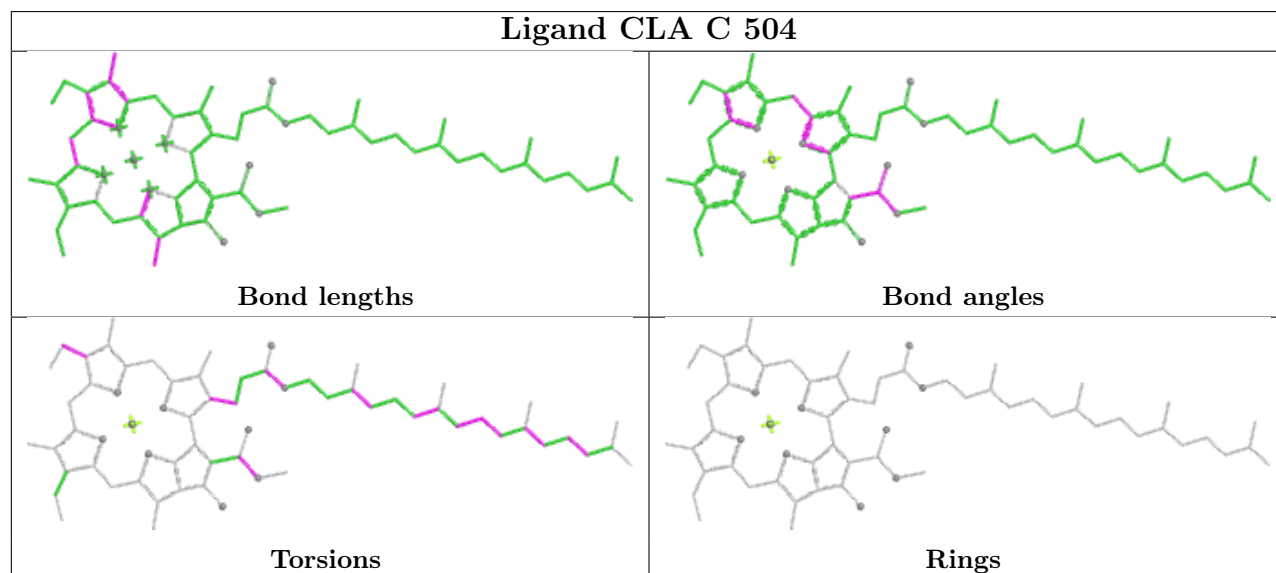
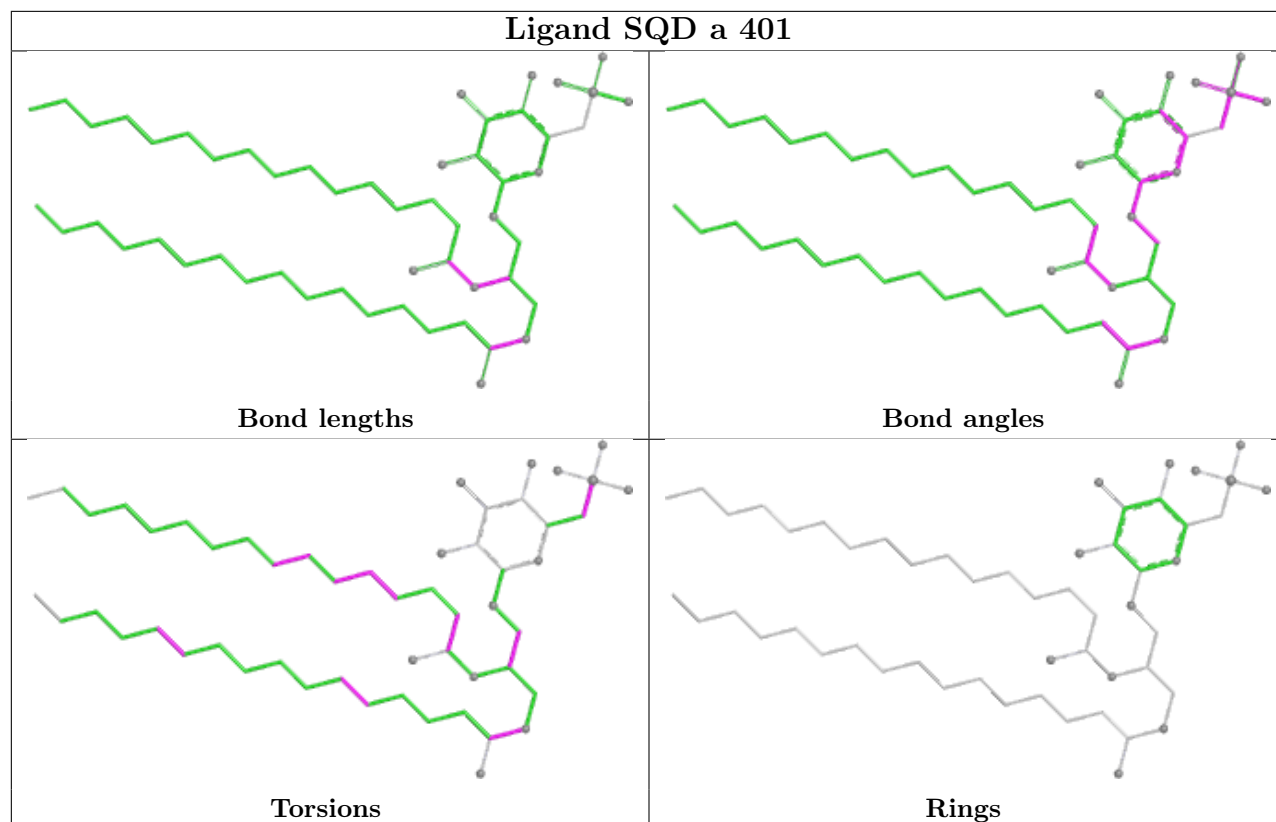
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

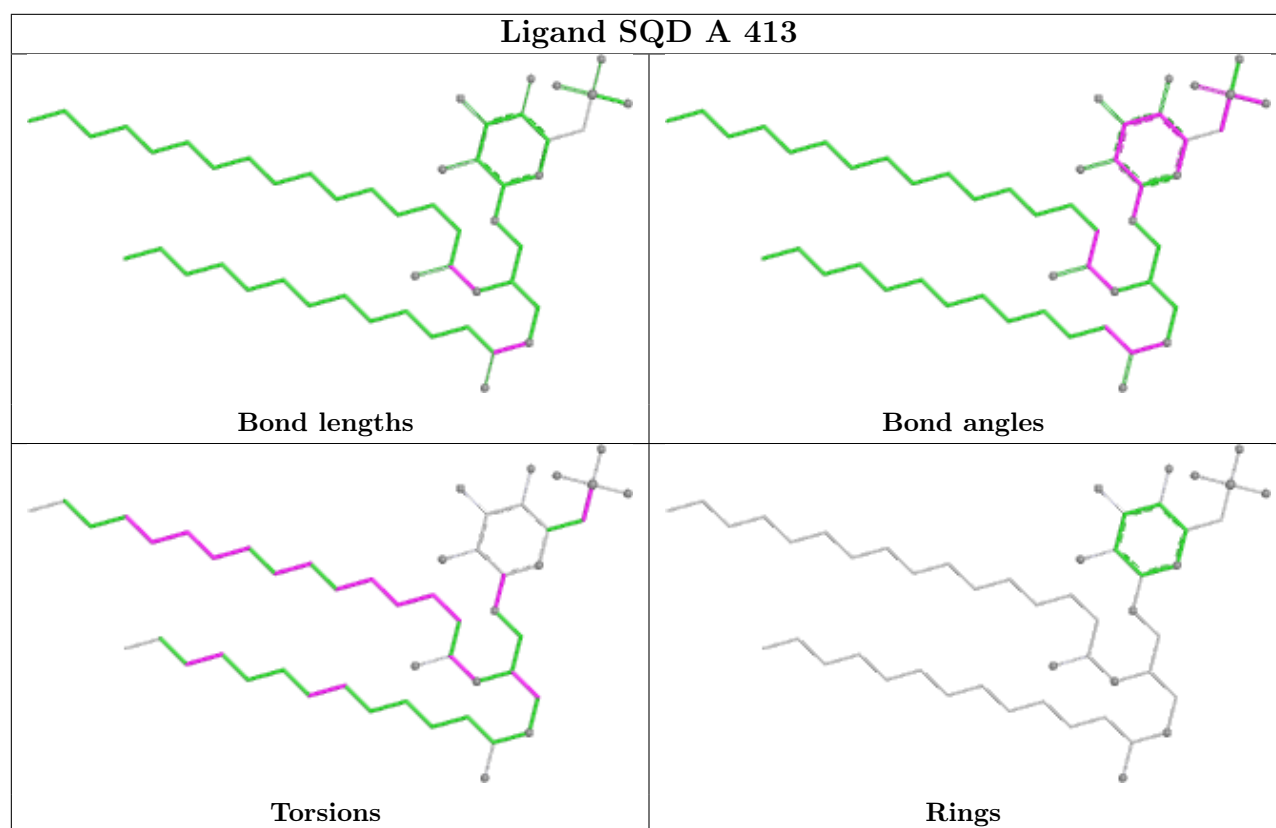
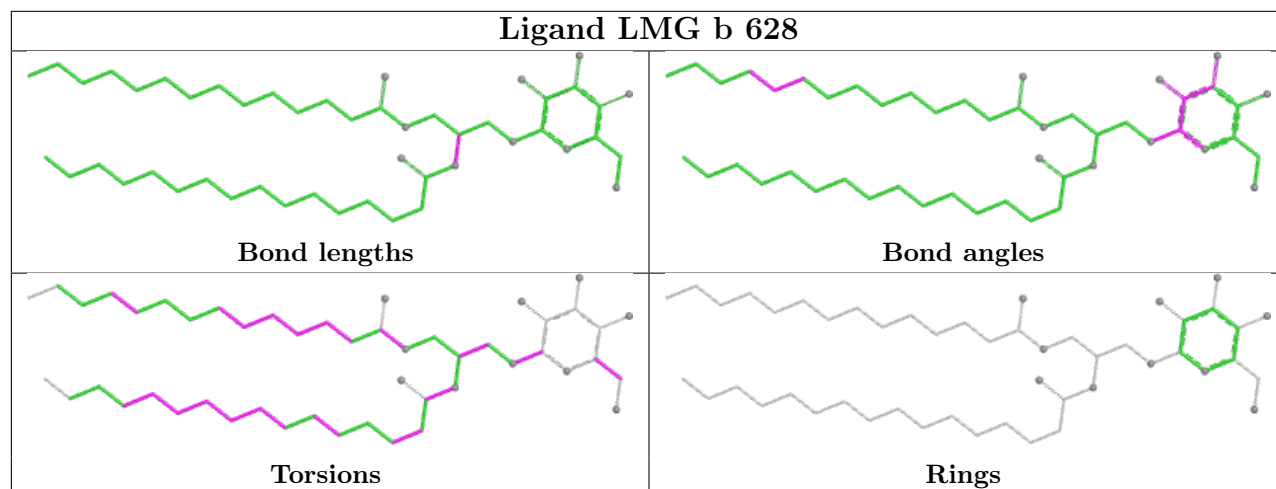


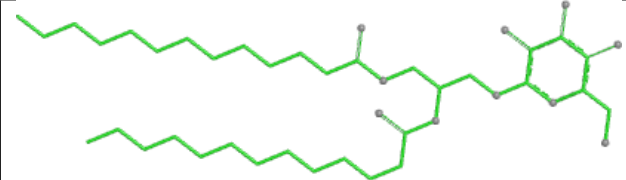
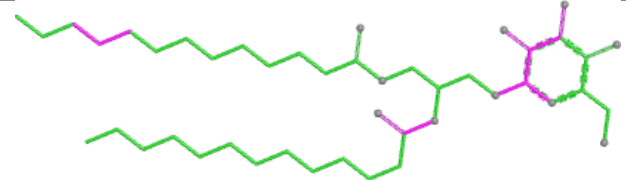
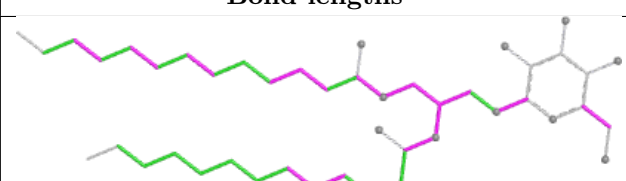
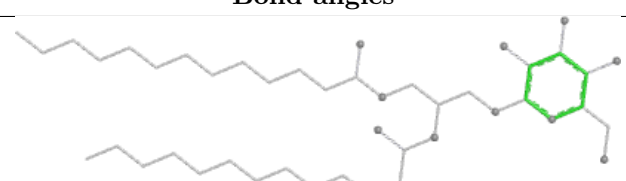


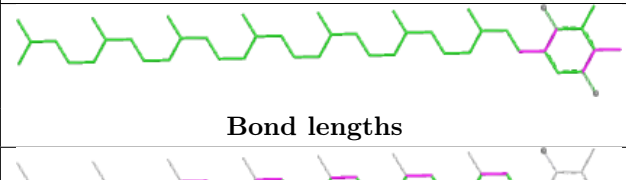
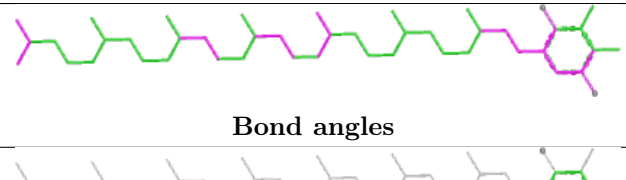
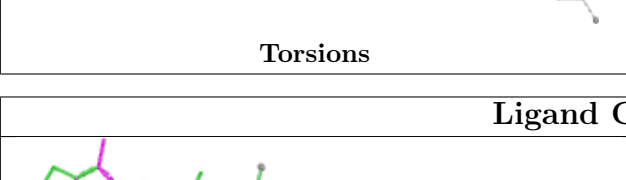
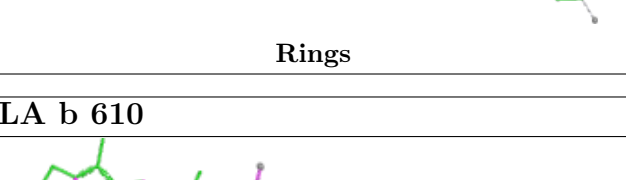


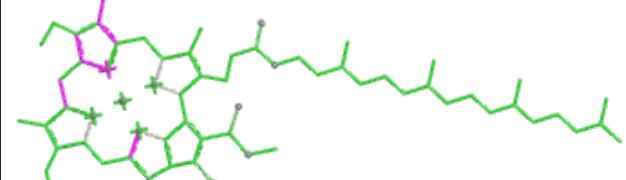
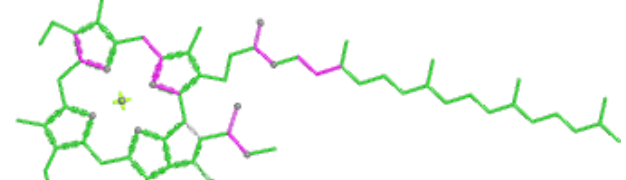
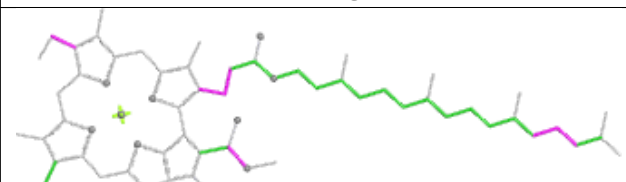
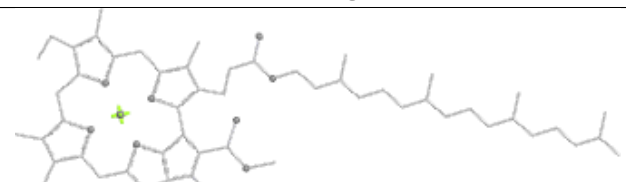


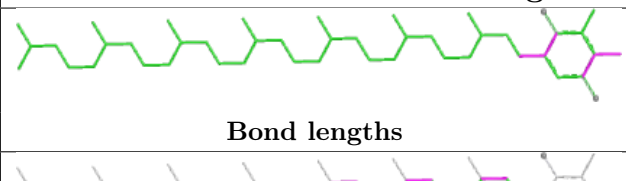
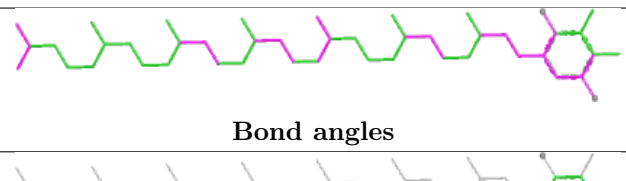


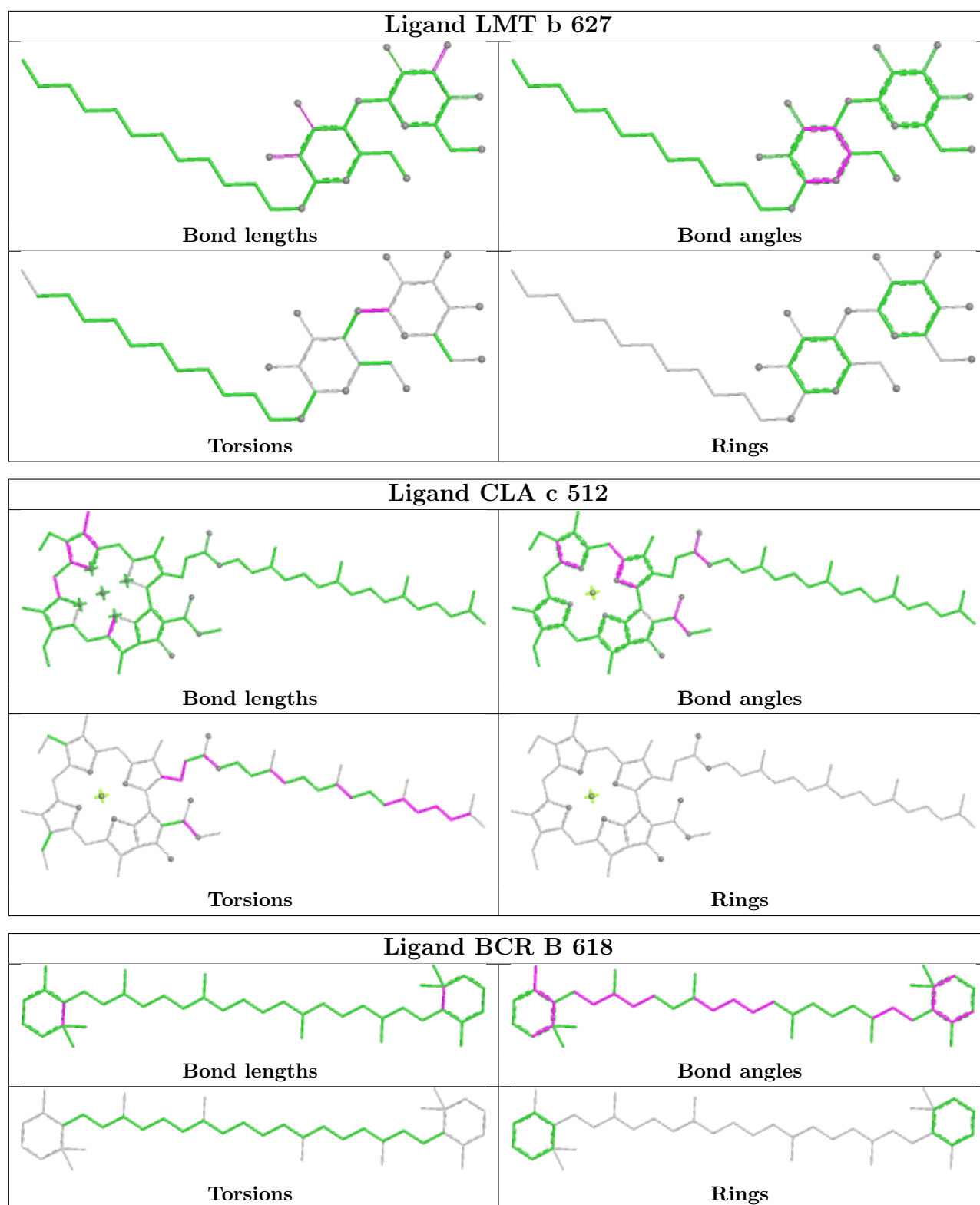


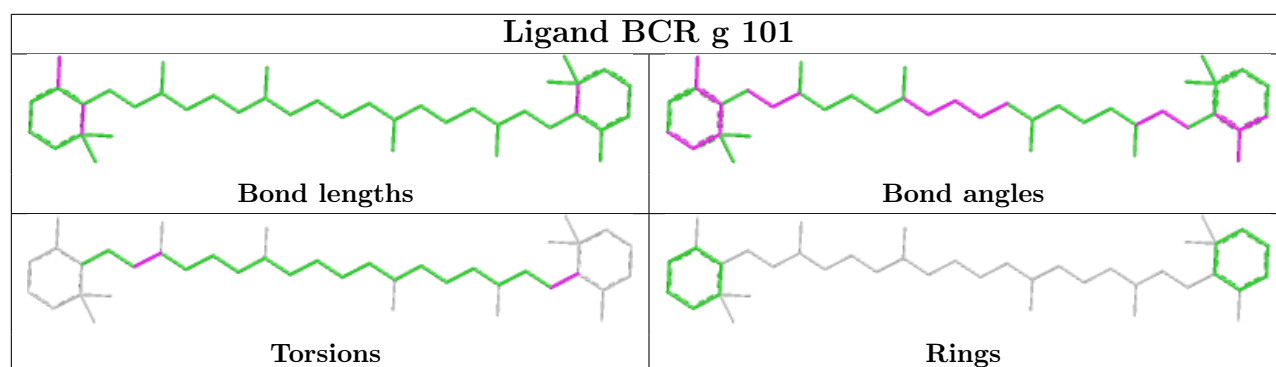
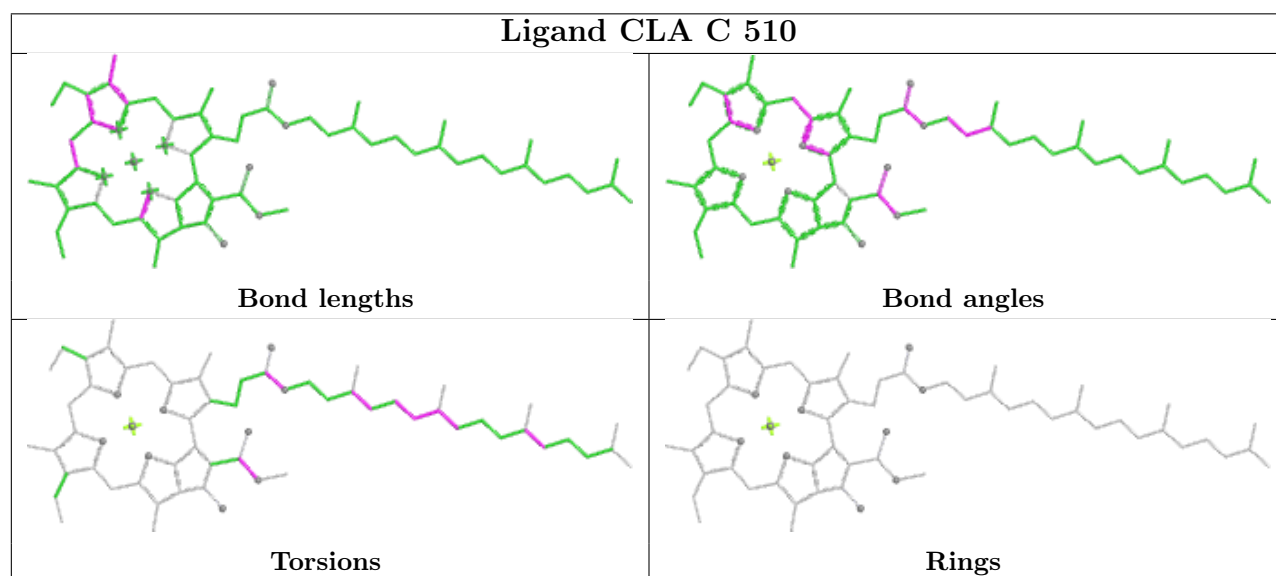
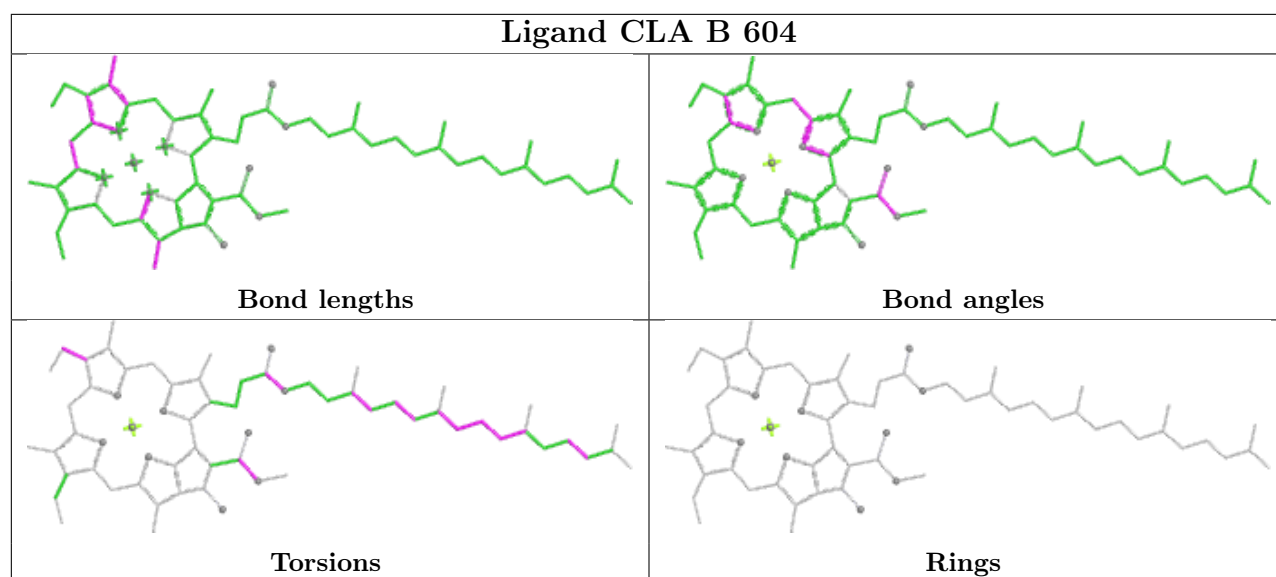
Ligand LMG c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

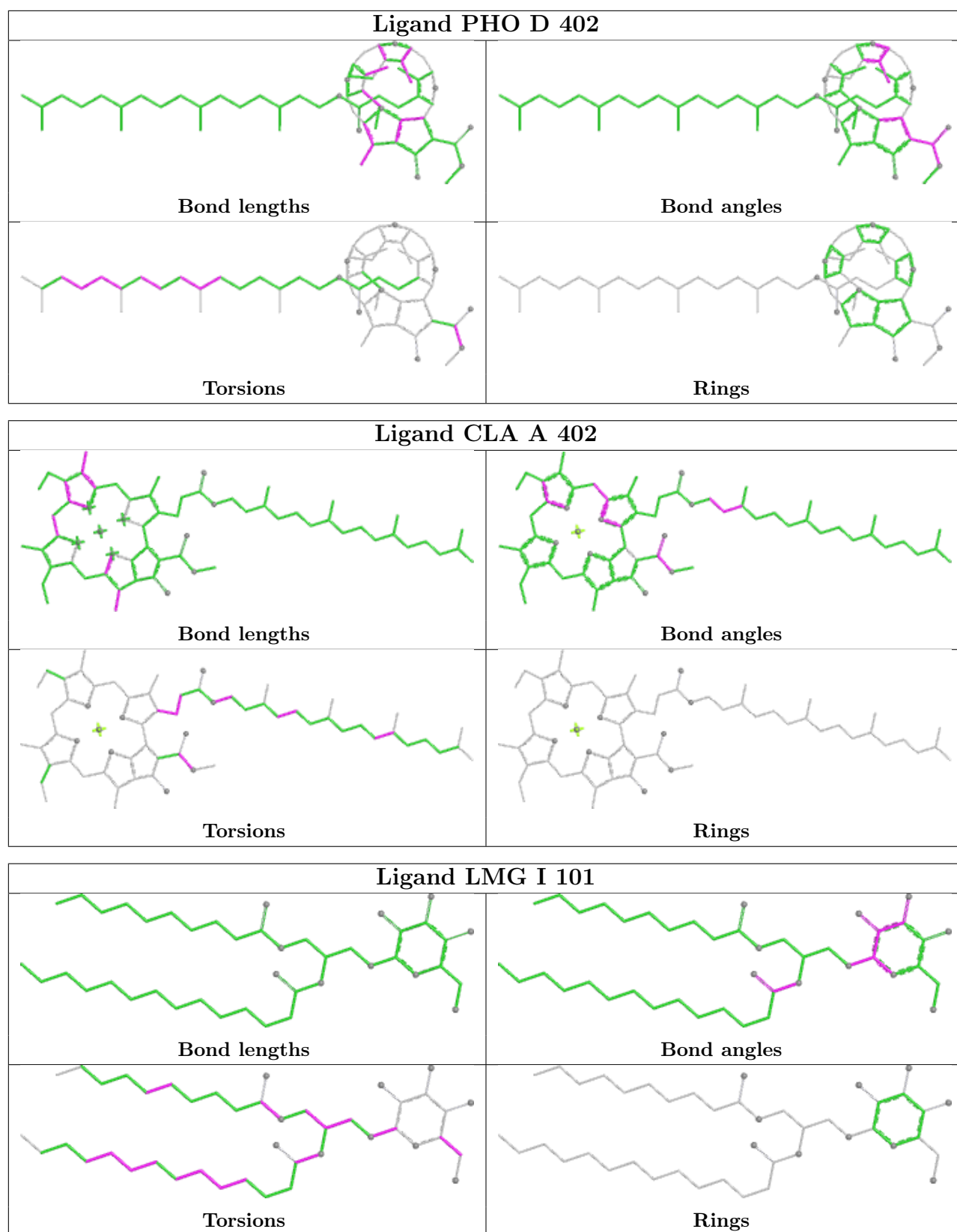
Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

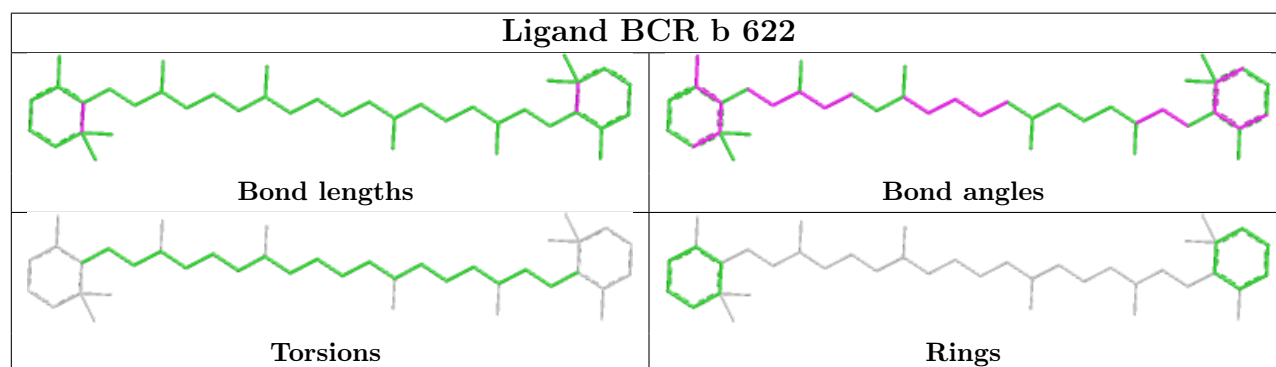
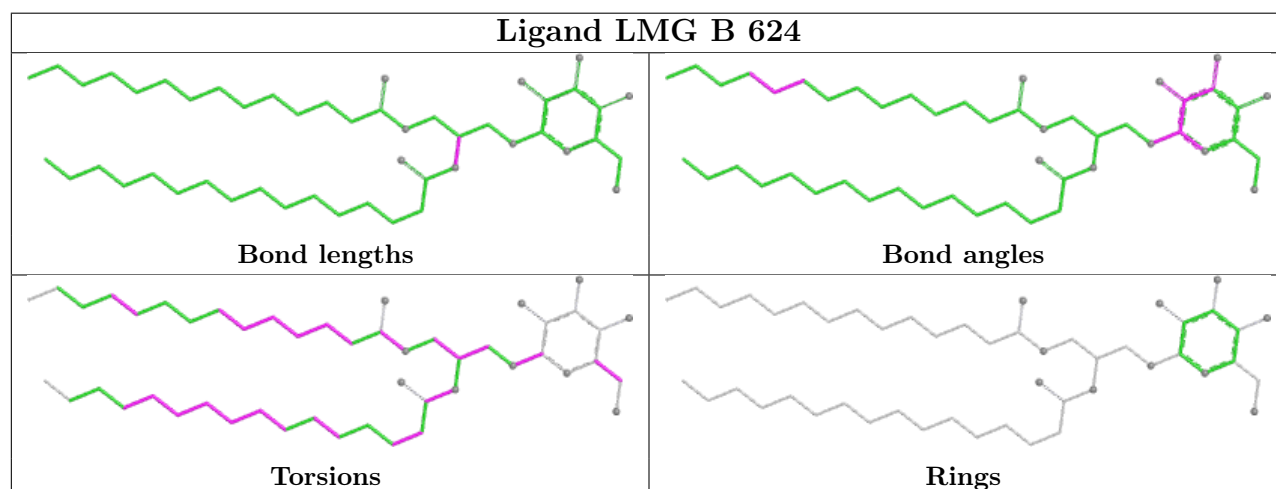
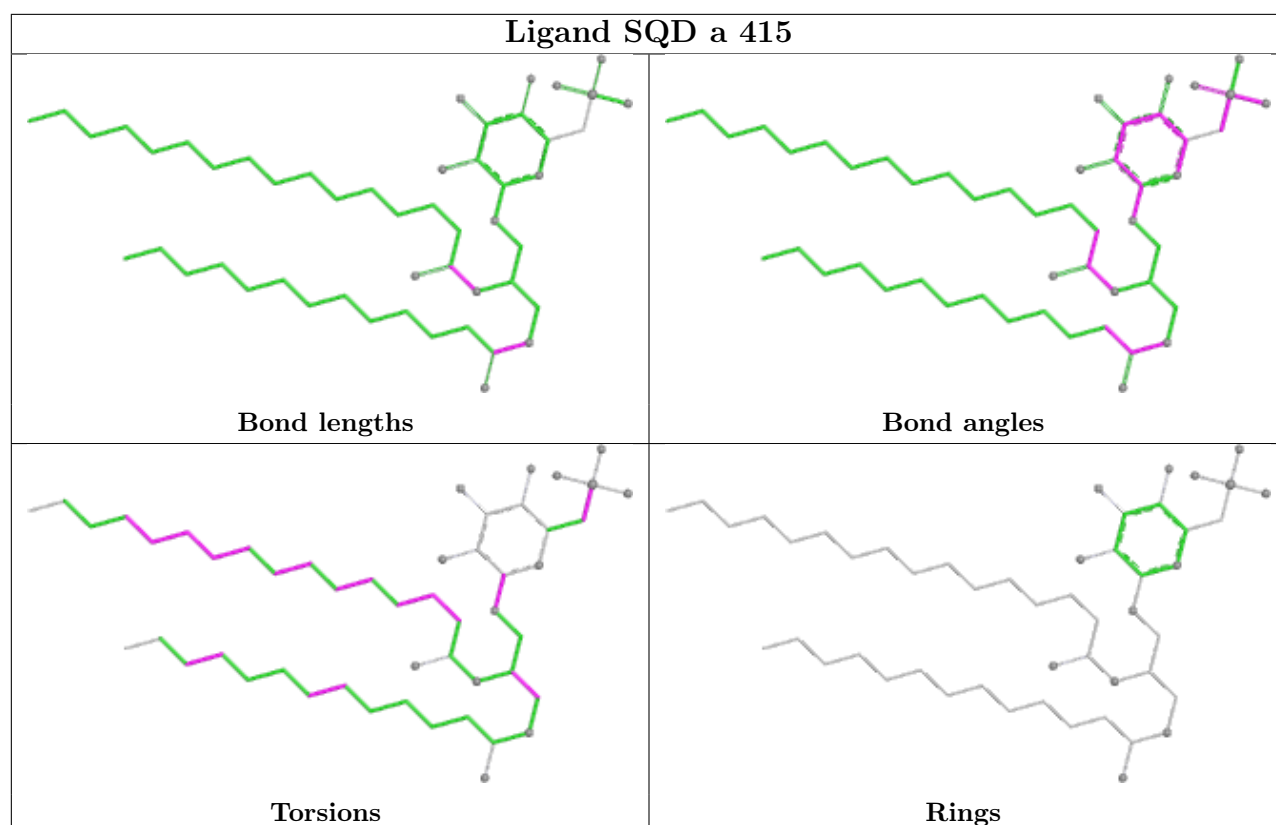
Ligand CLA b 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

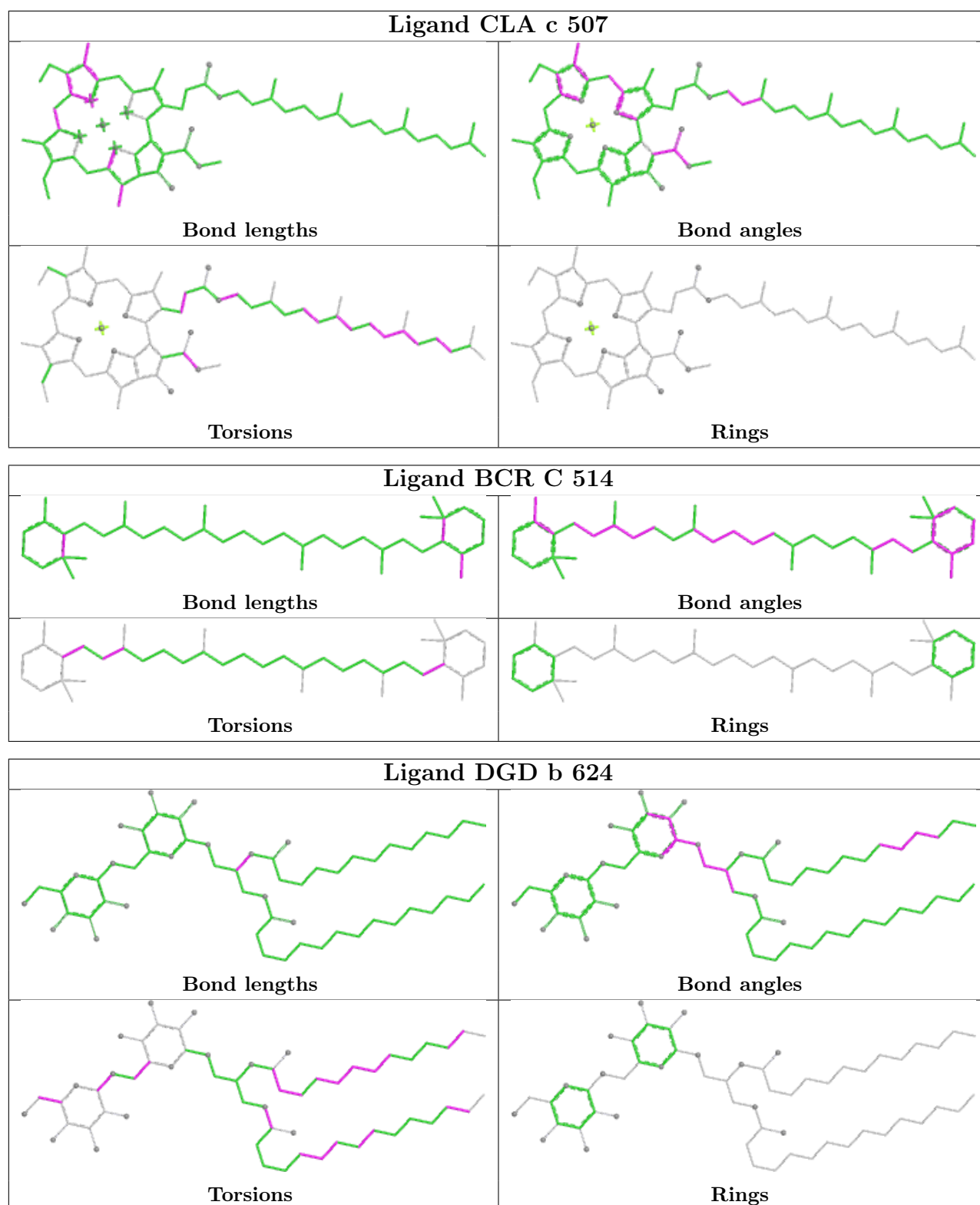
Ligand PL9 A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

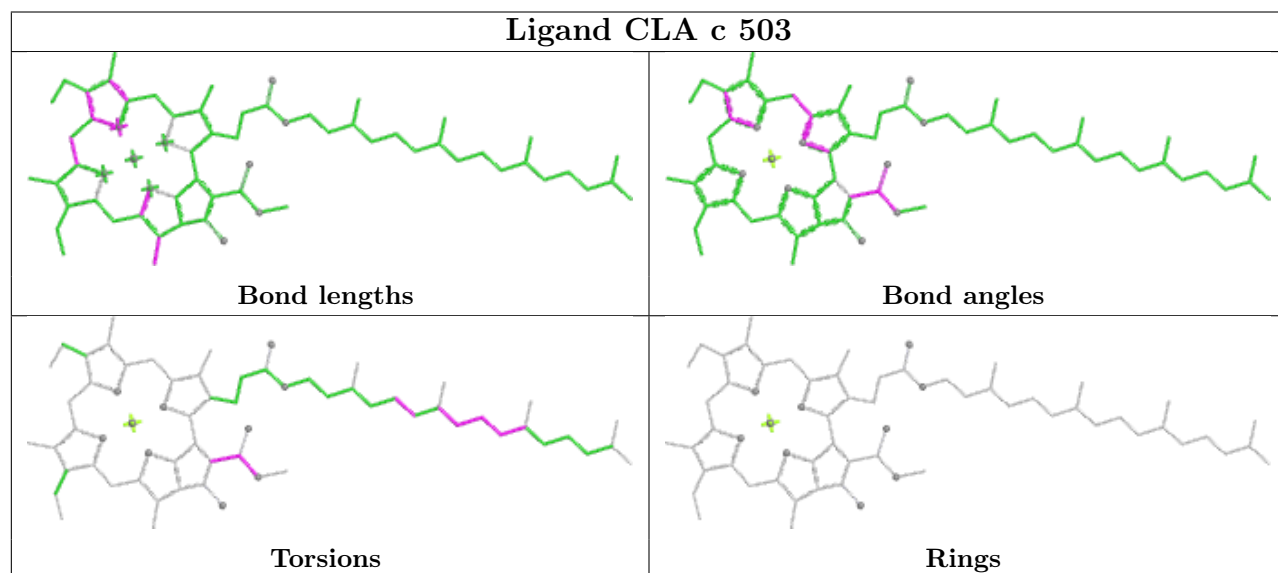
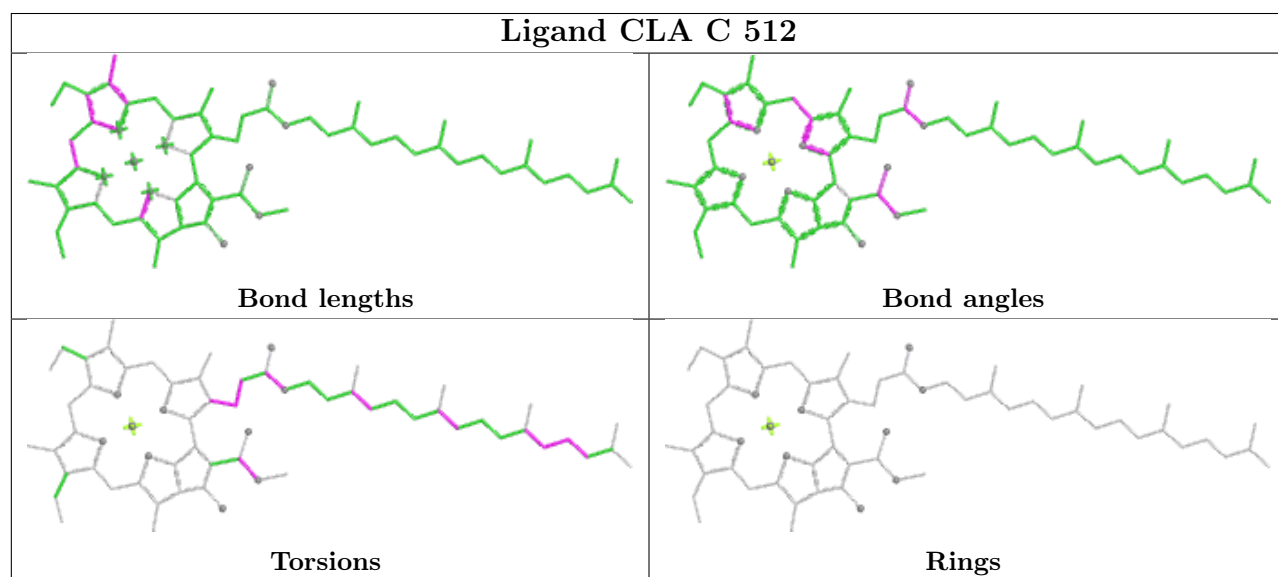
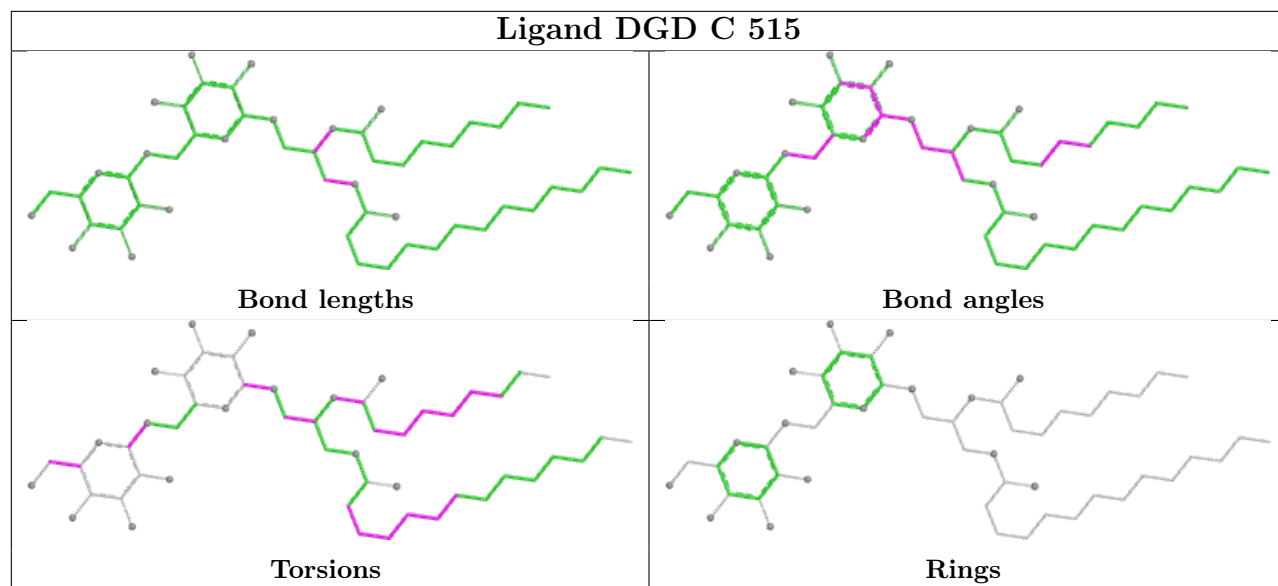


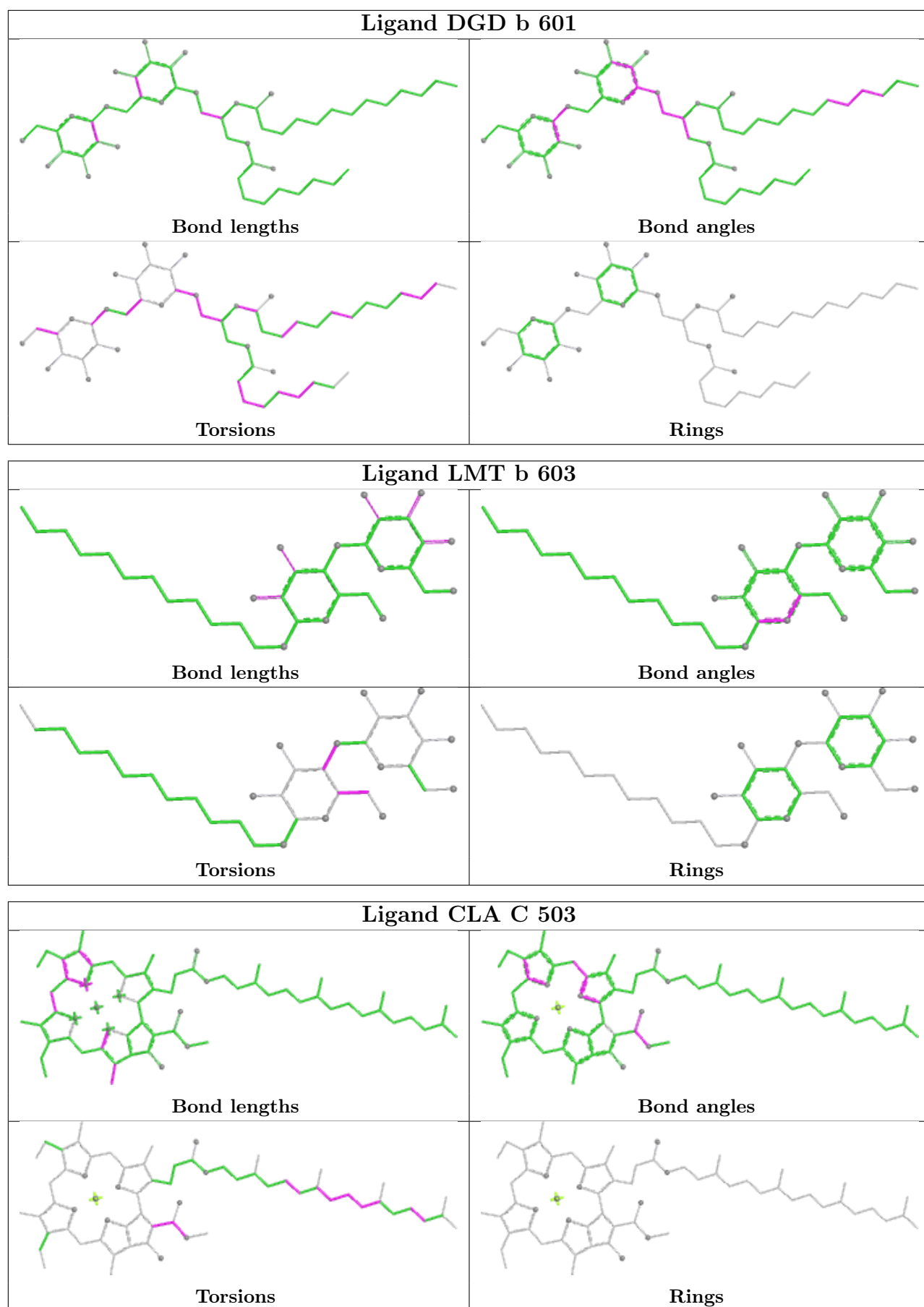




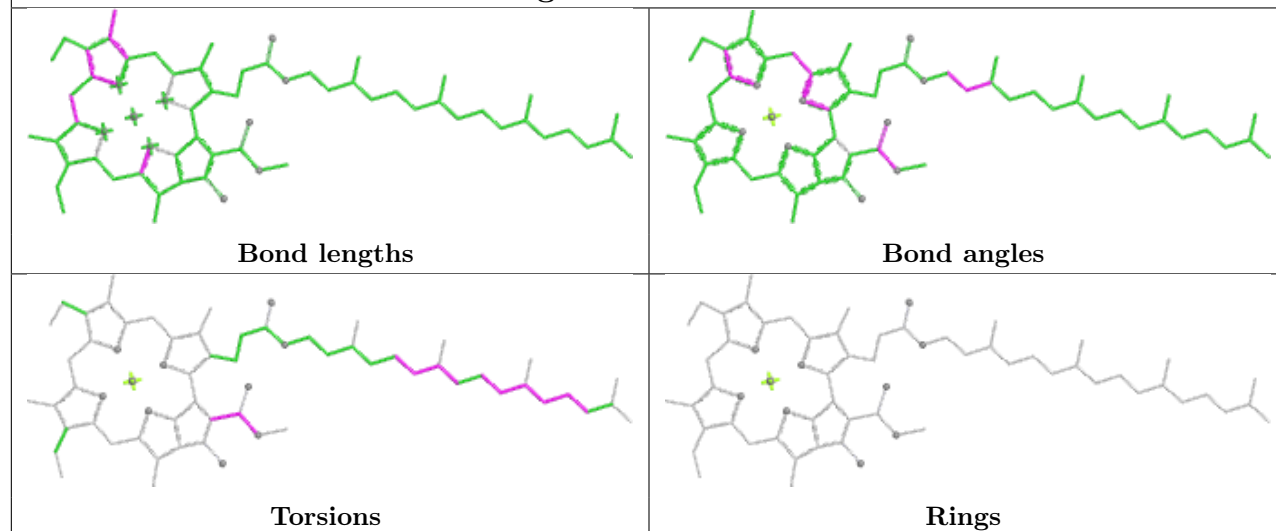




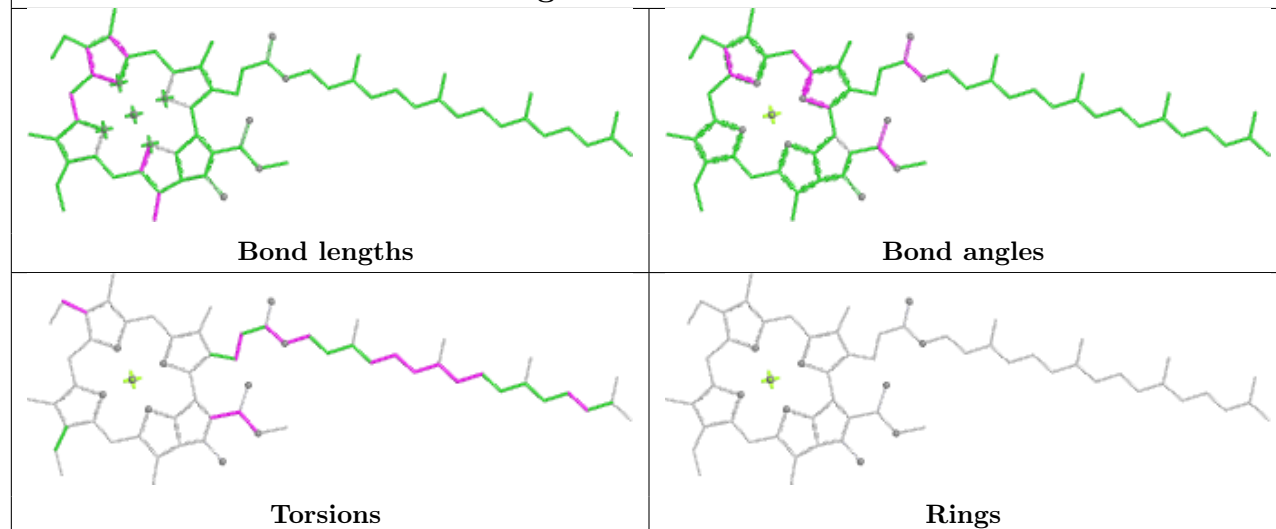




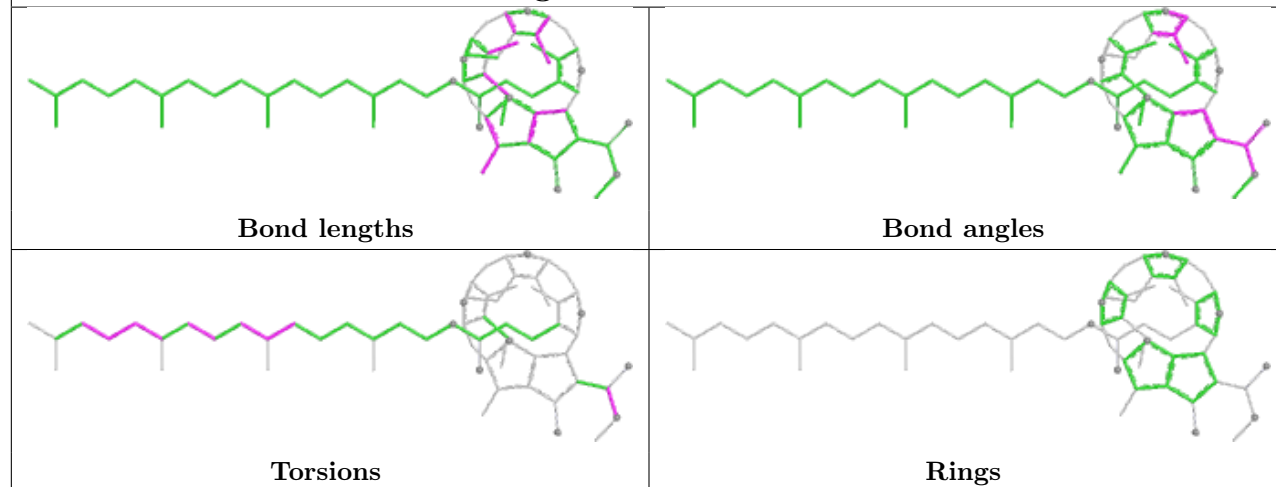
Ligand CLA c 505

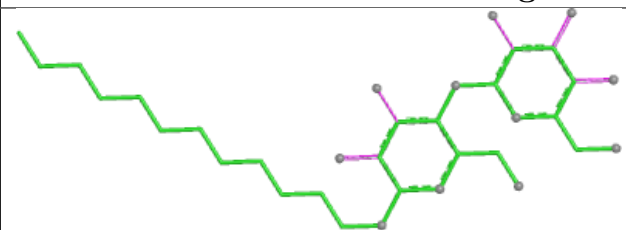
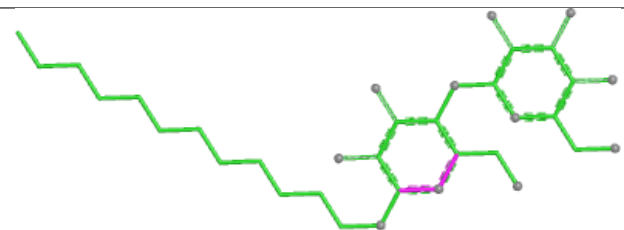
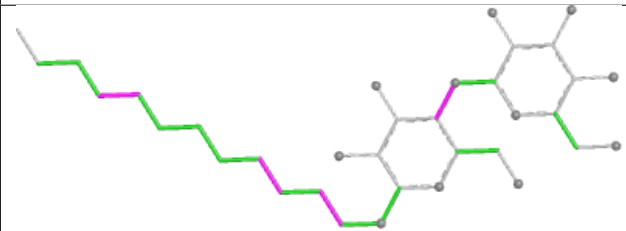
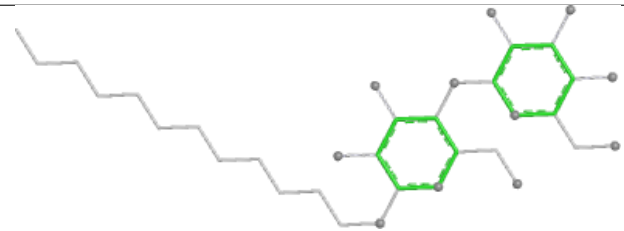
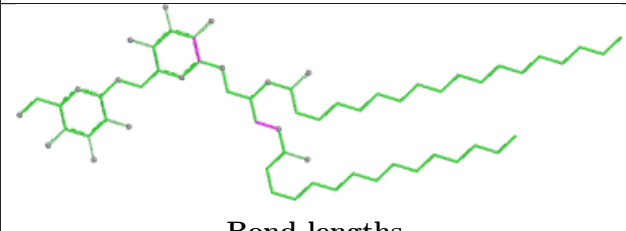
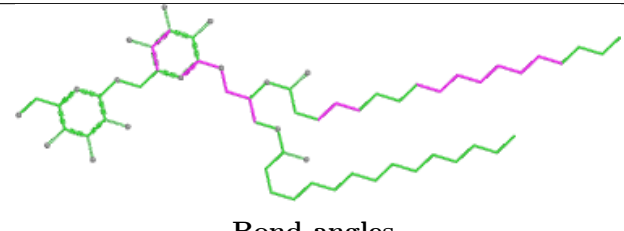
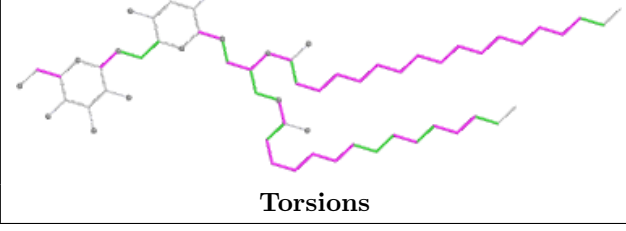
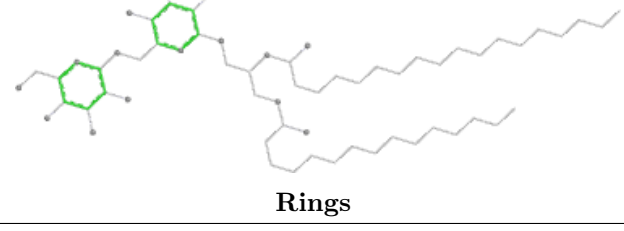
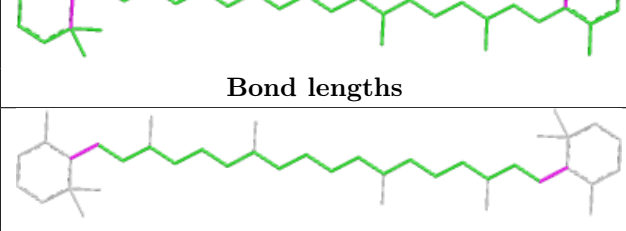
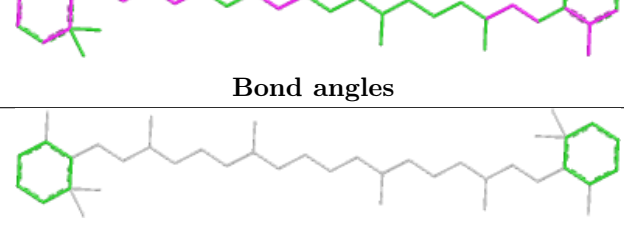


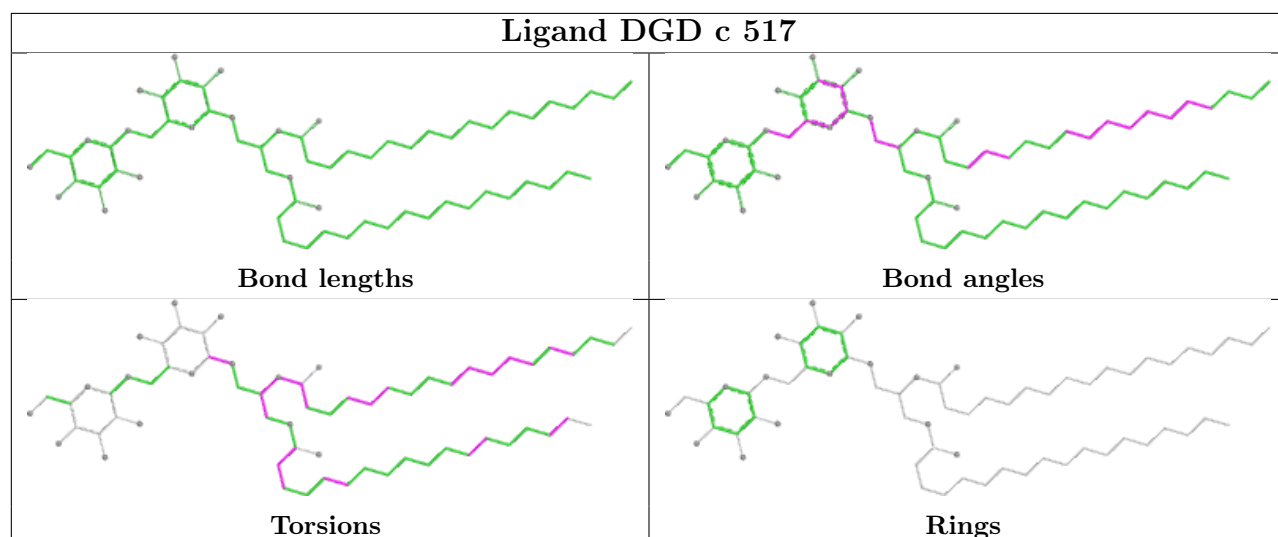
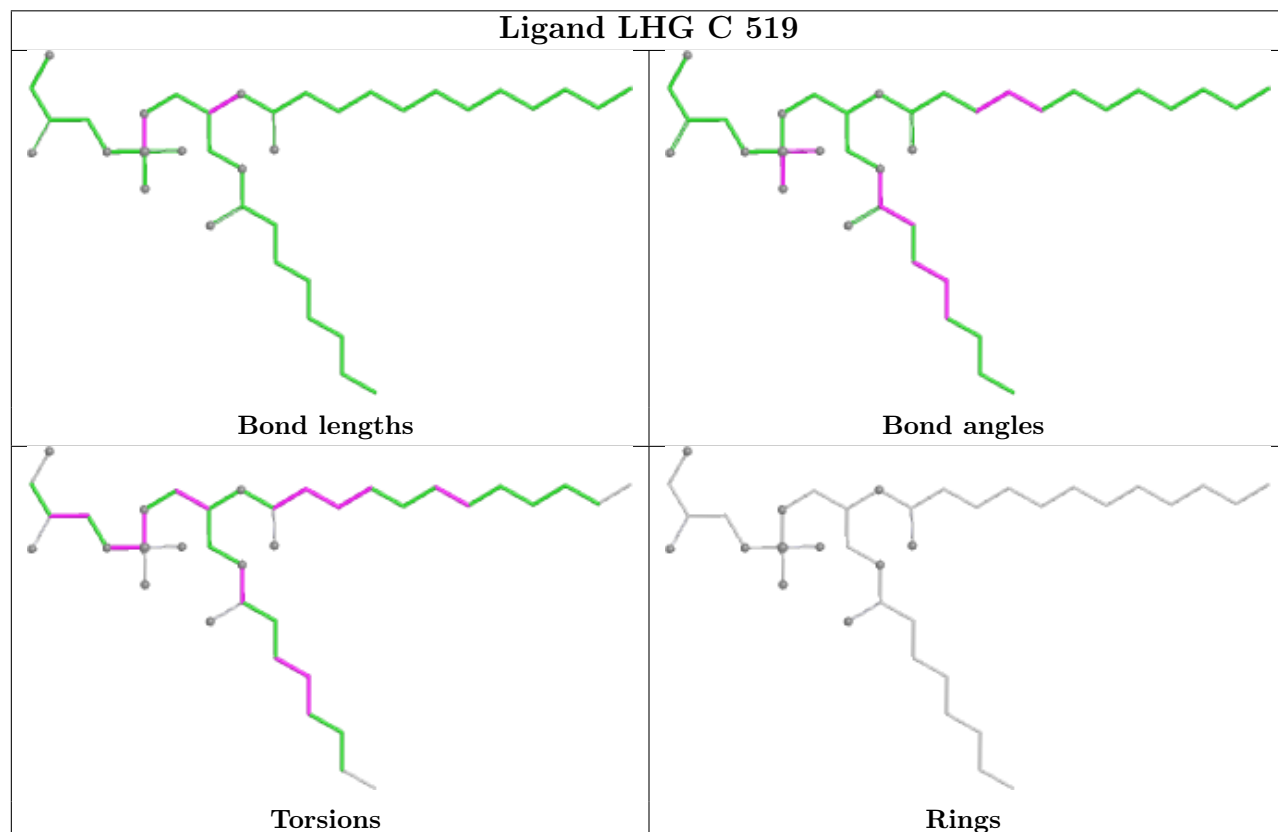
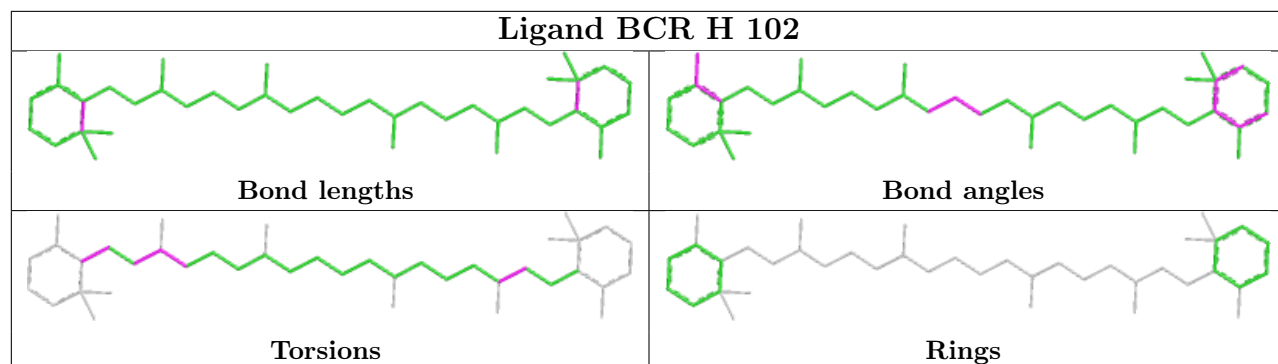
Ligand CLA c 508

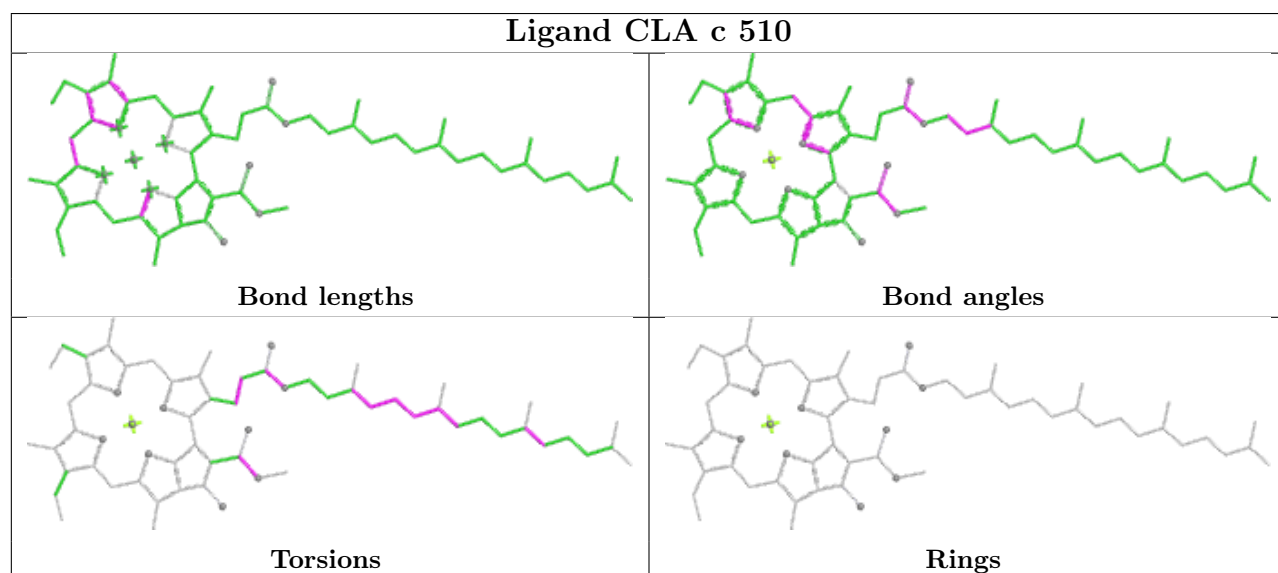
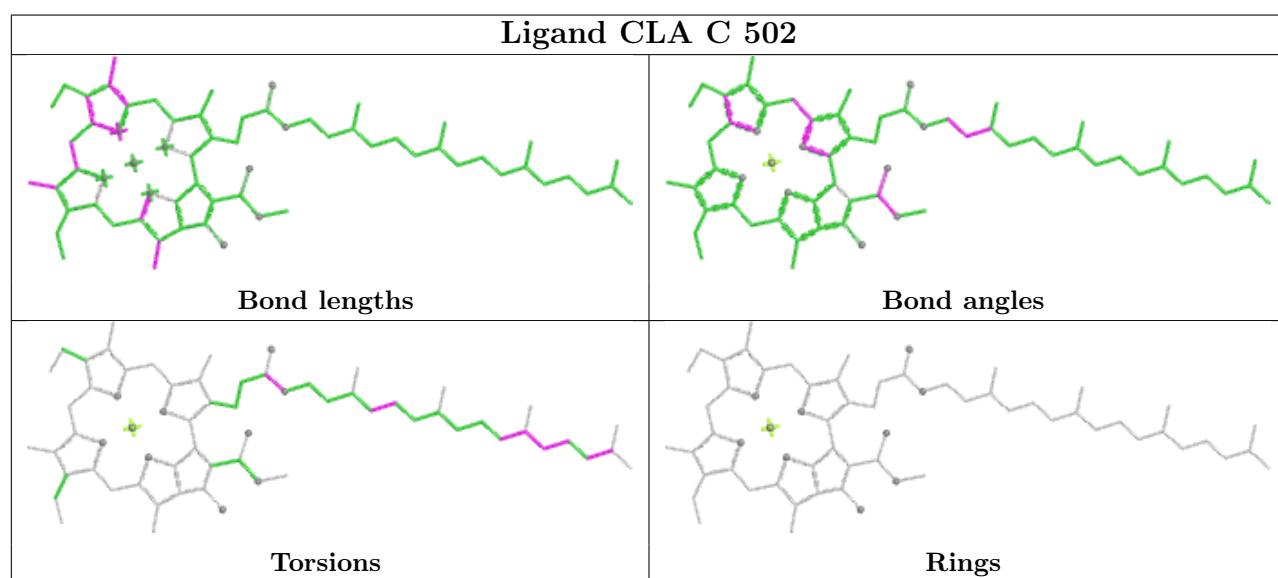
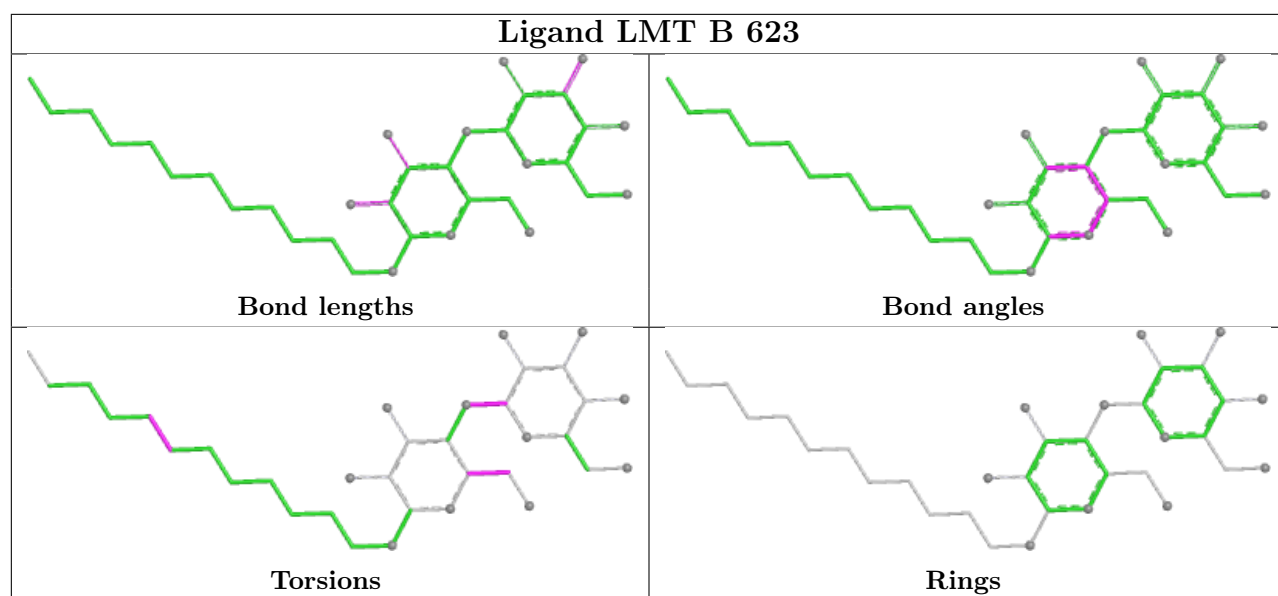


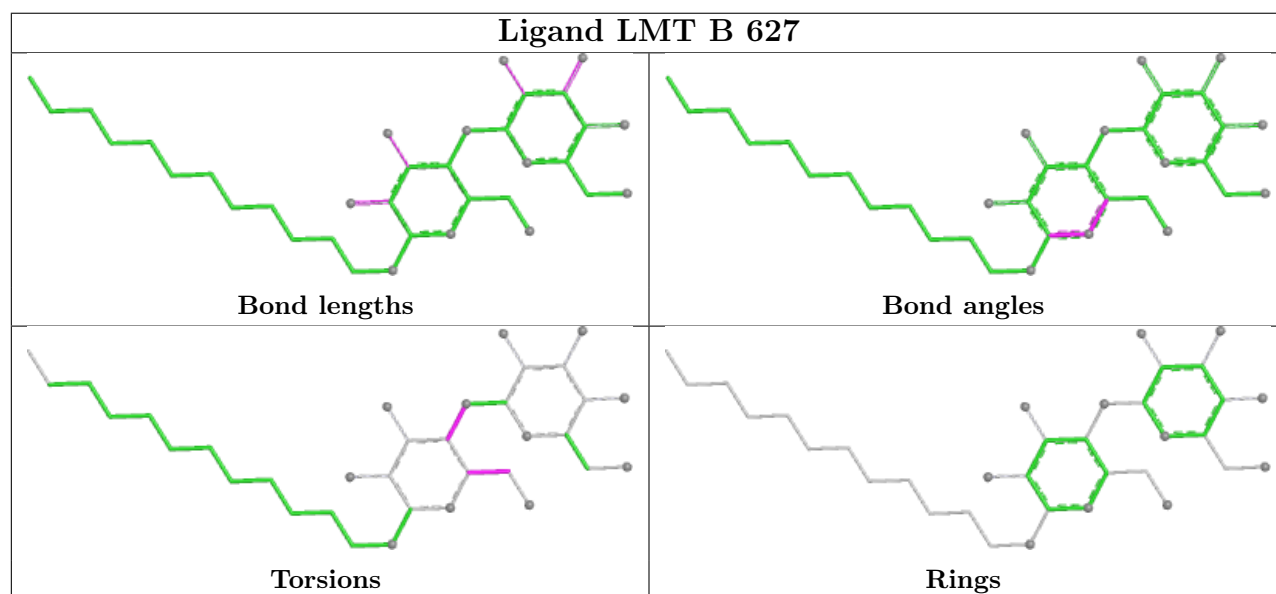
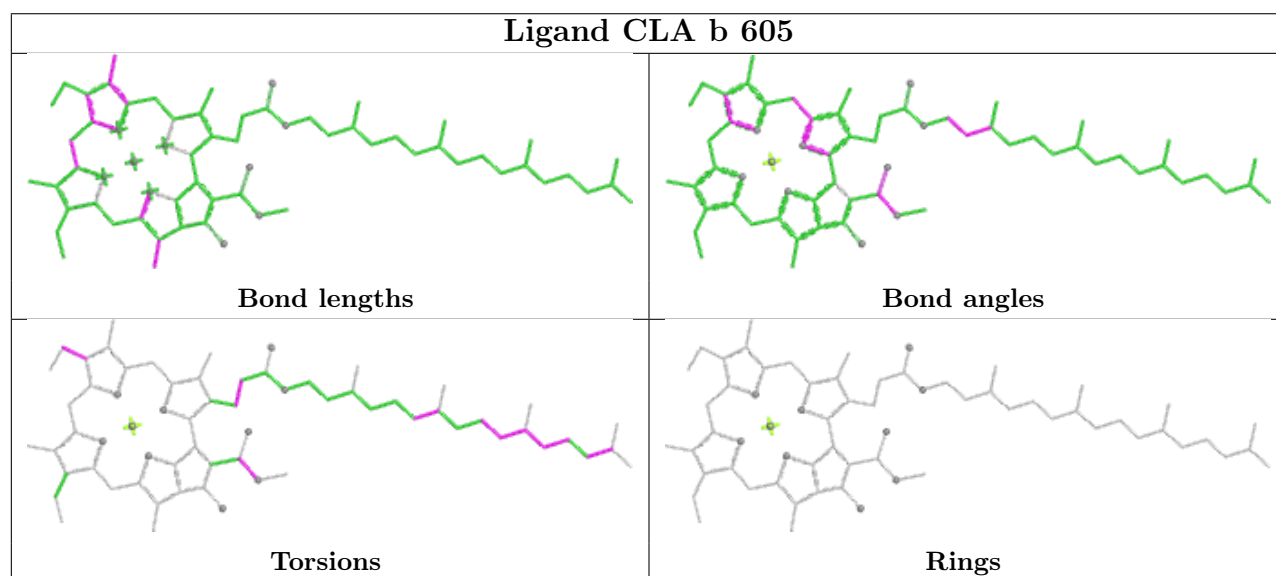
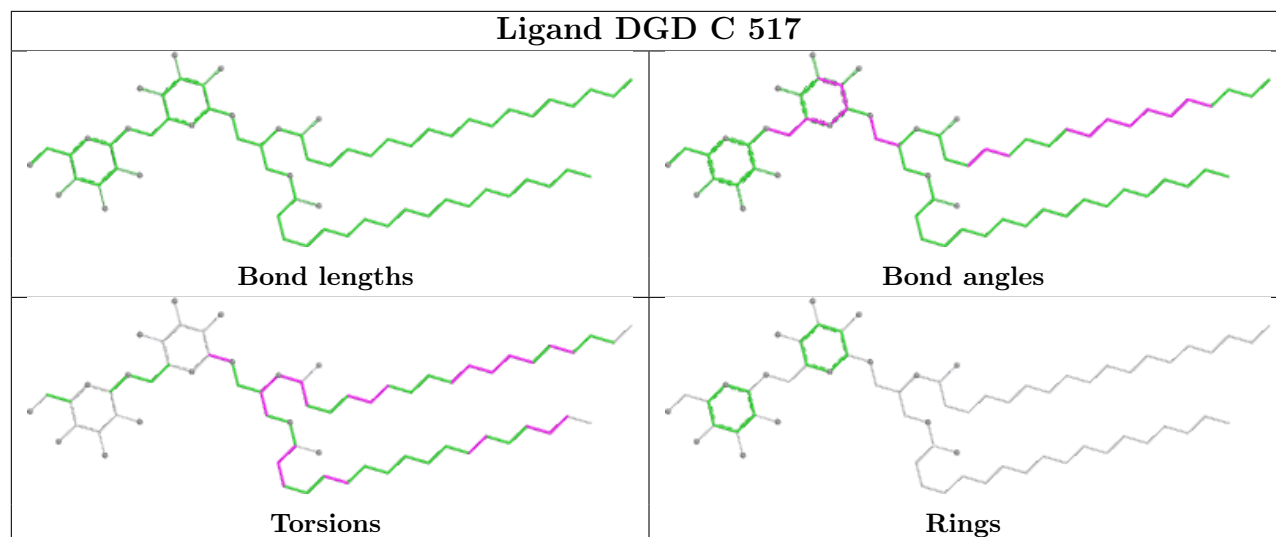
Ligand PHO a 407

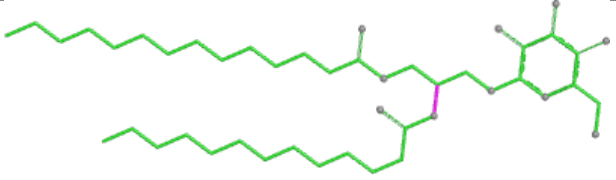
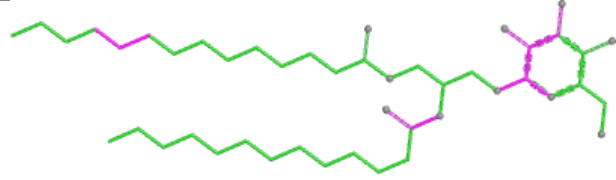
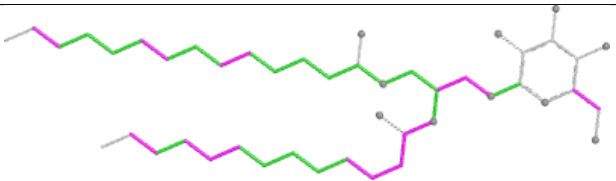
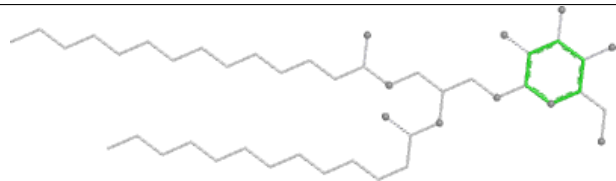


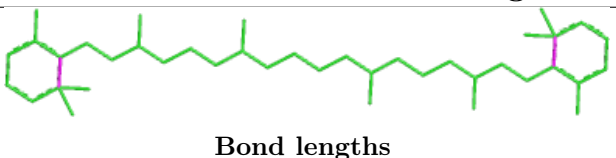
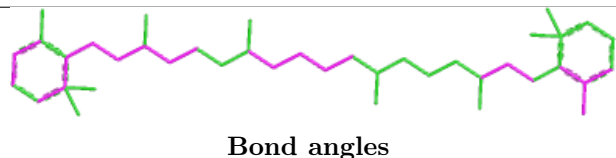
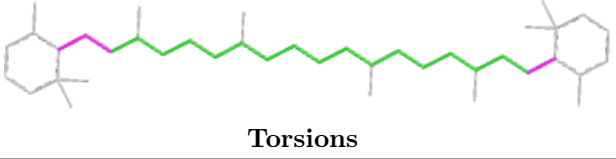
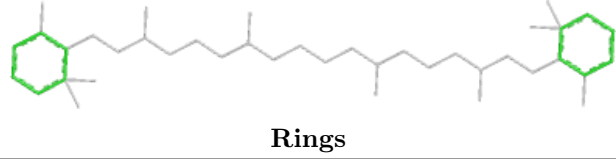
Ligand LMT B 628	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

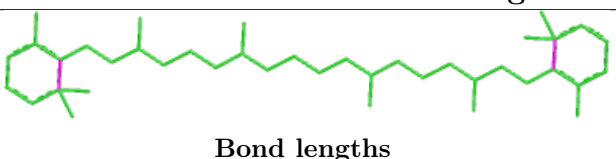
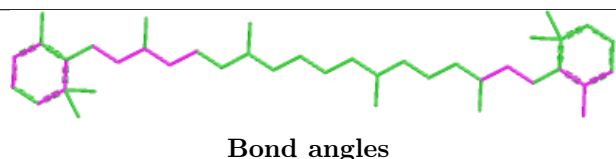
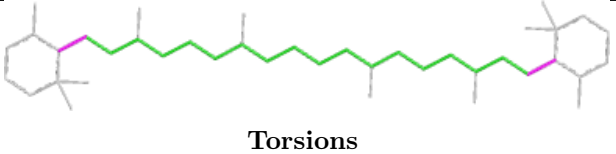
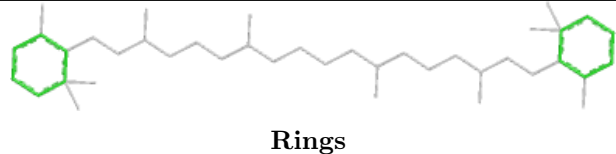


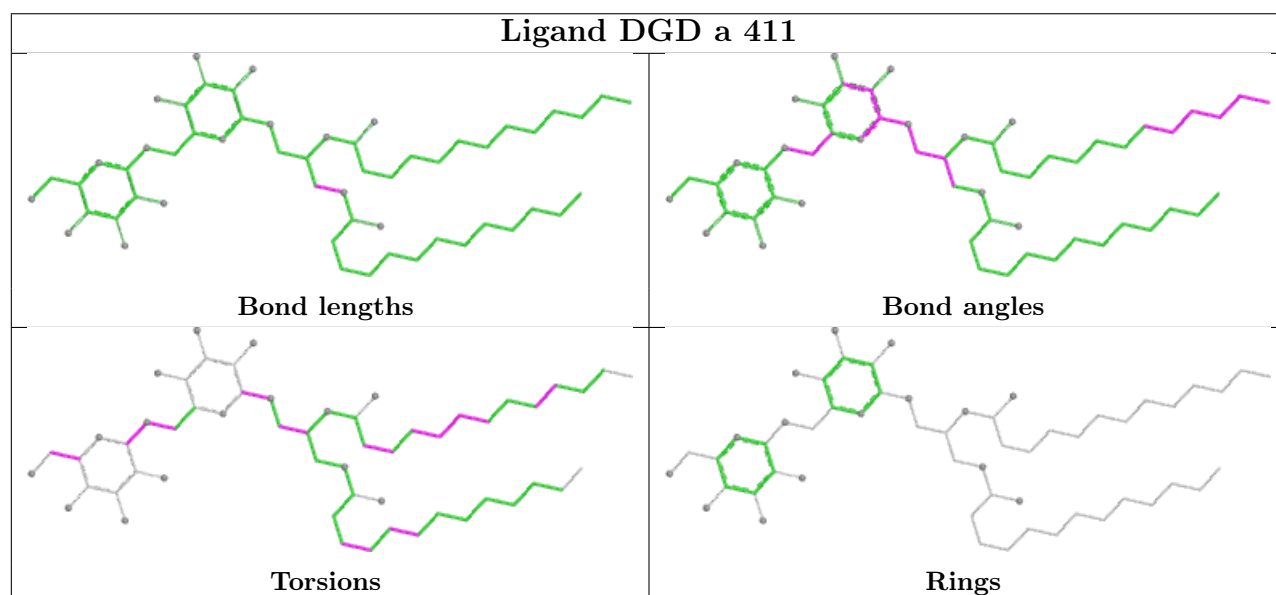
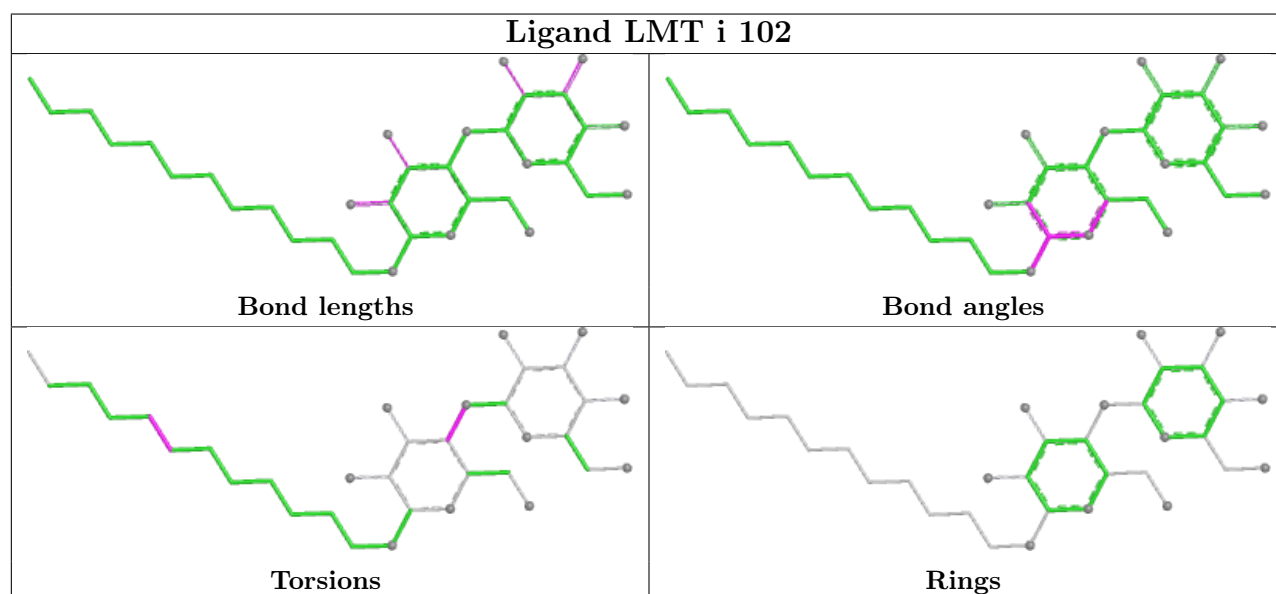
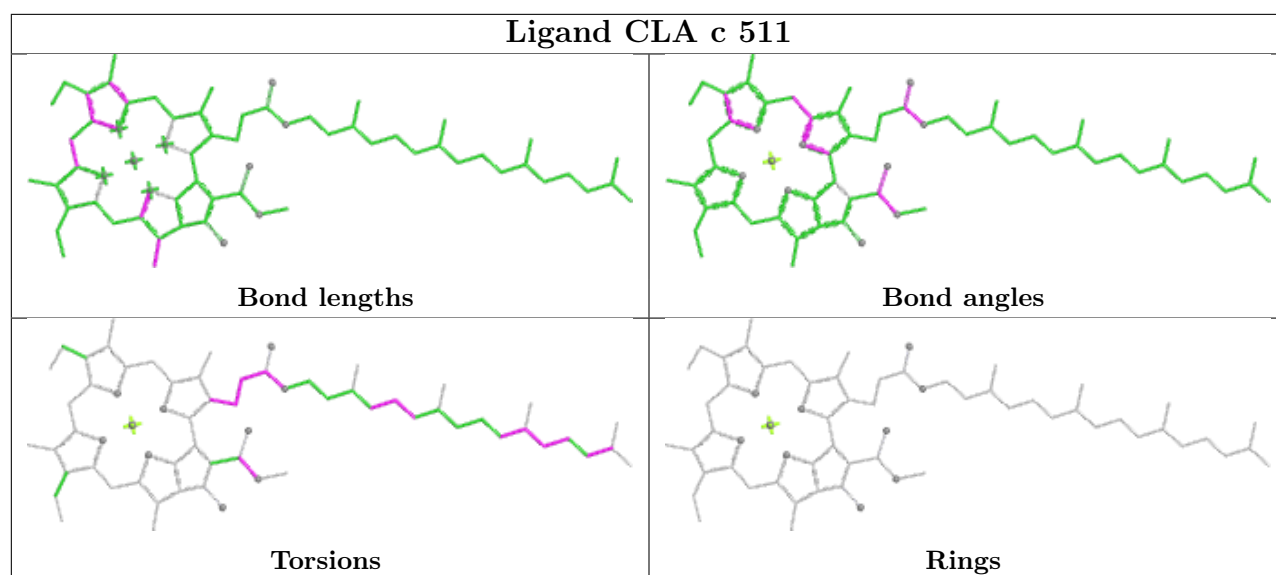


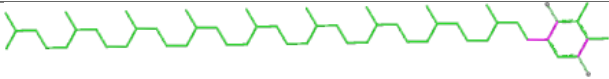
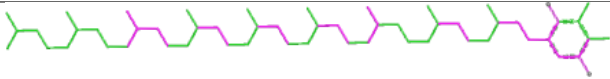
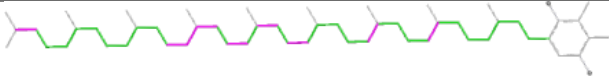
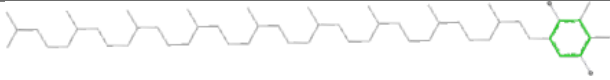


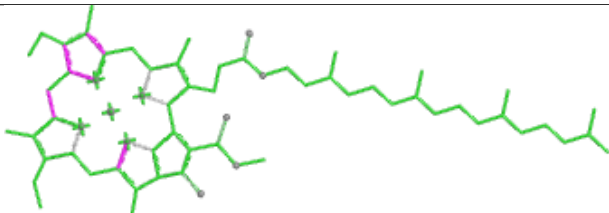
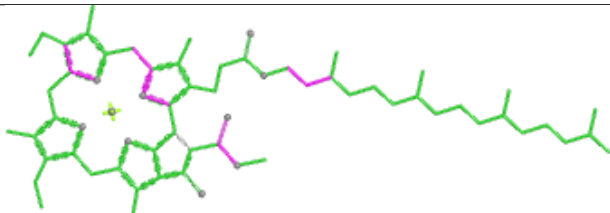
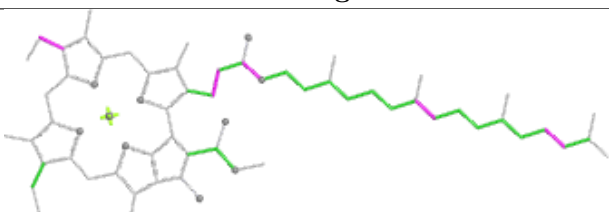
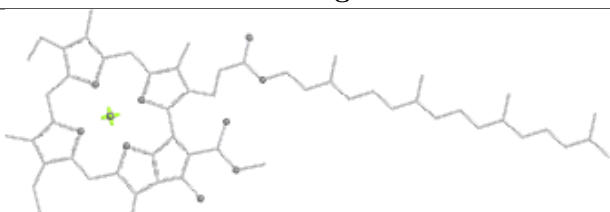
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

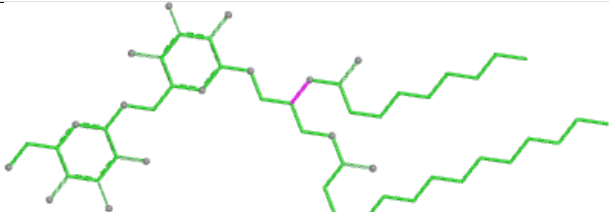
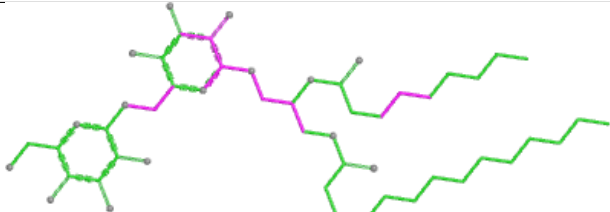
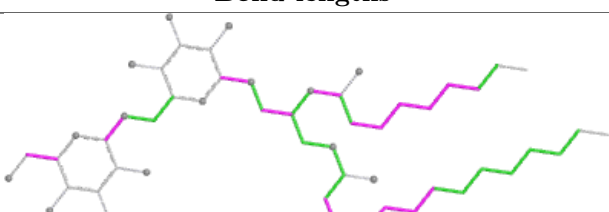
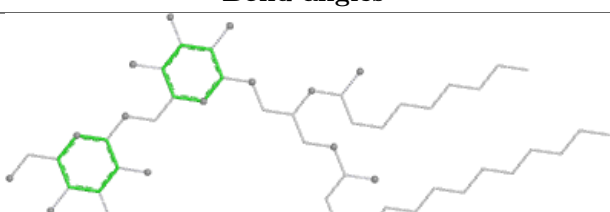
Ligand BCR C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

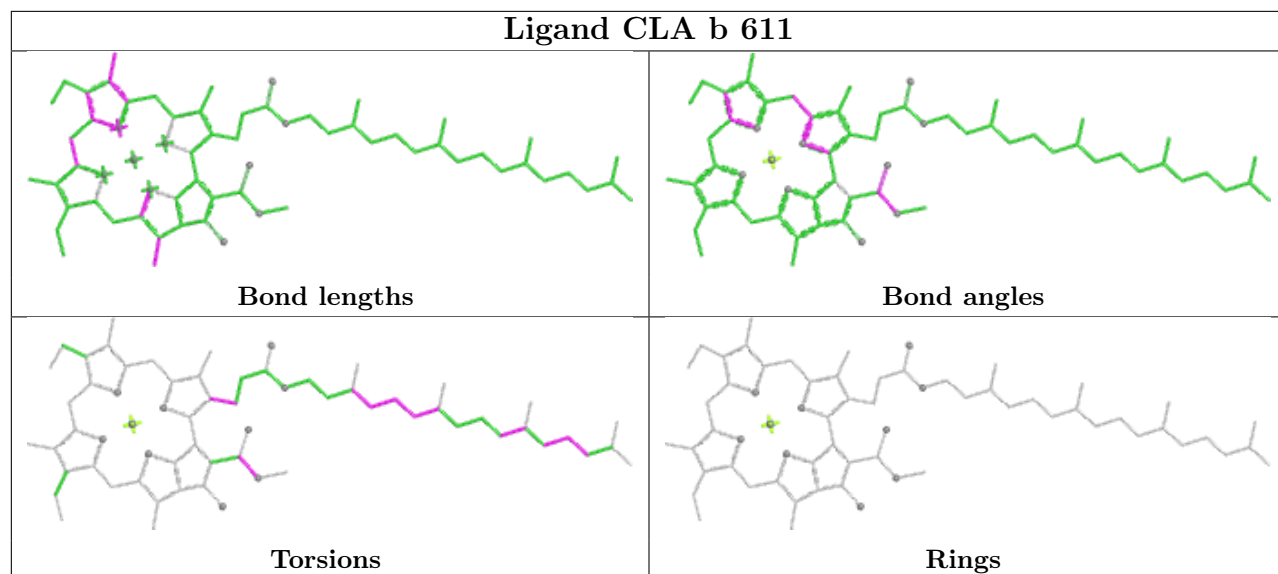


Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

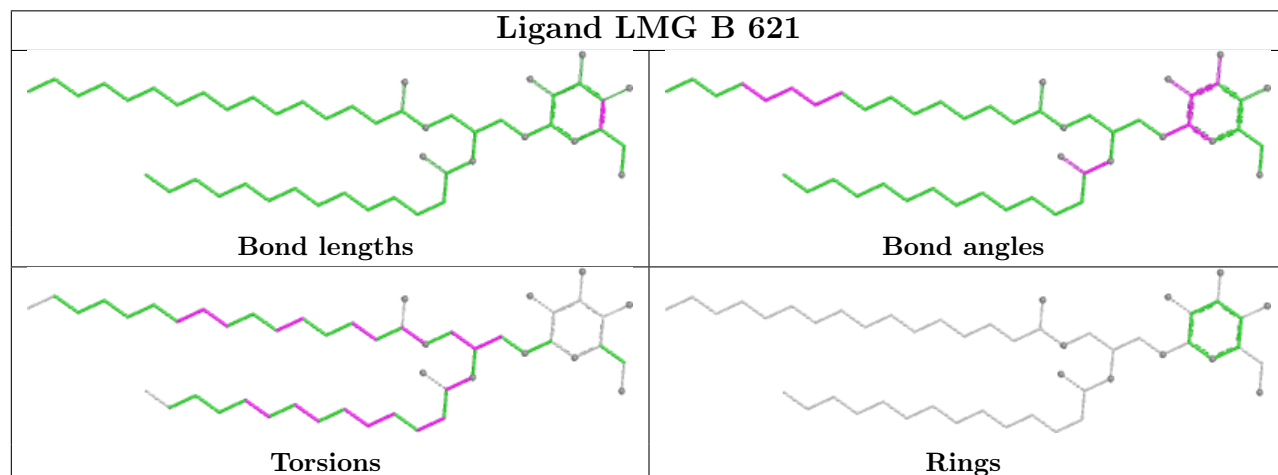
Ligand CLA d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

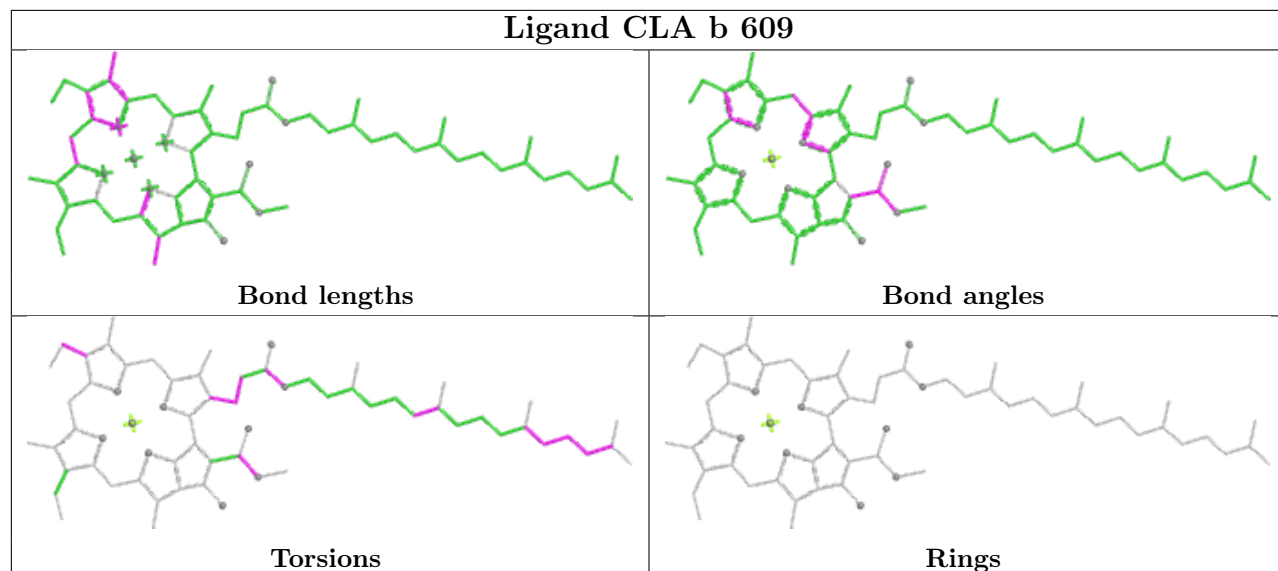
Ligand CLA b 611

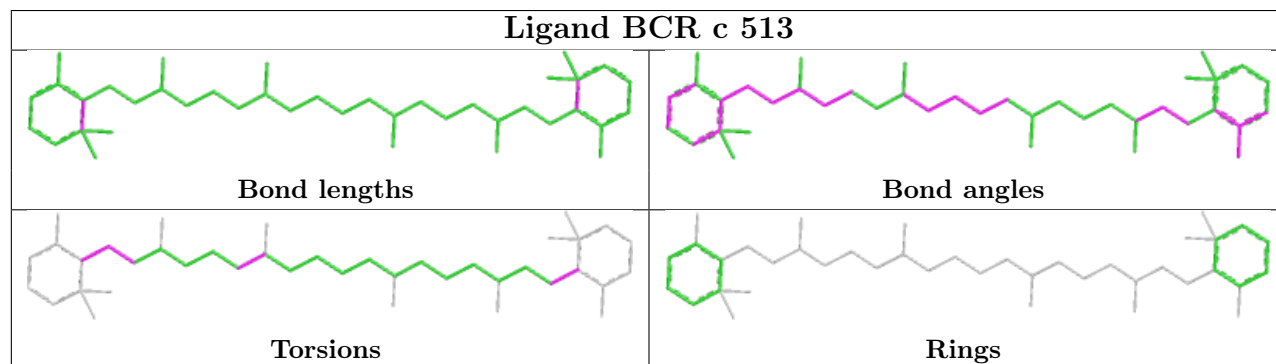
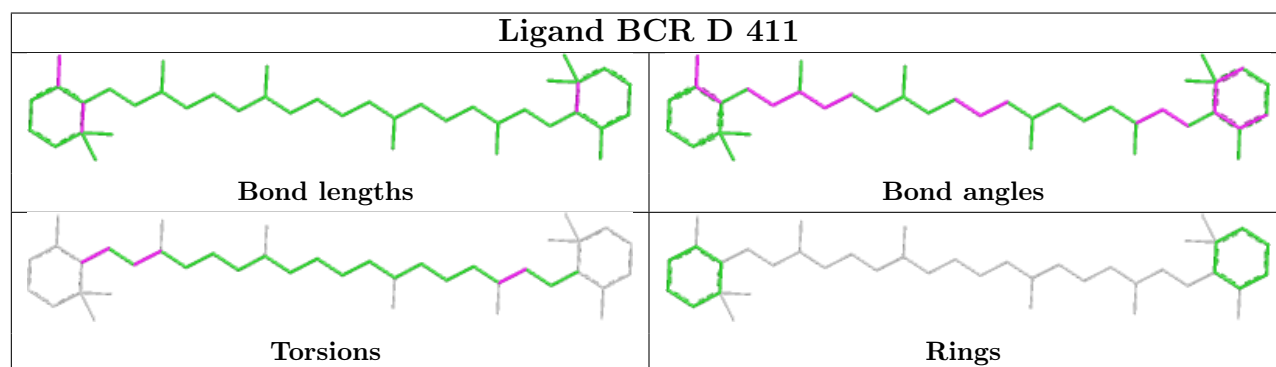
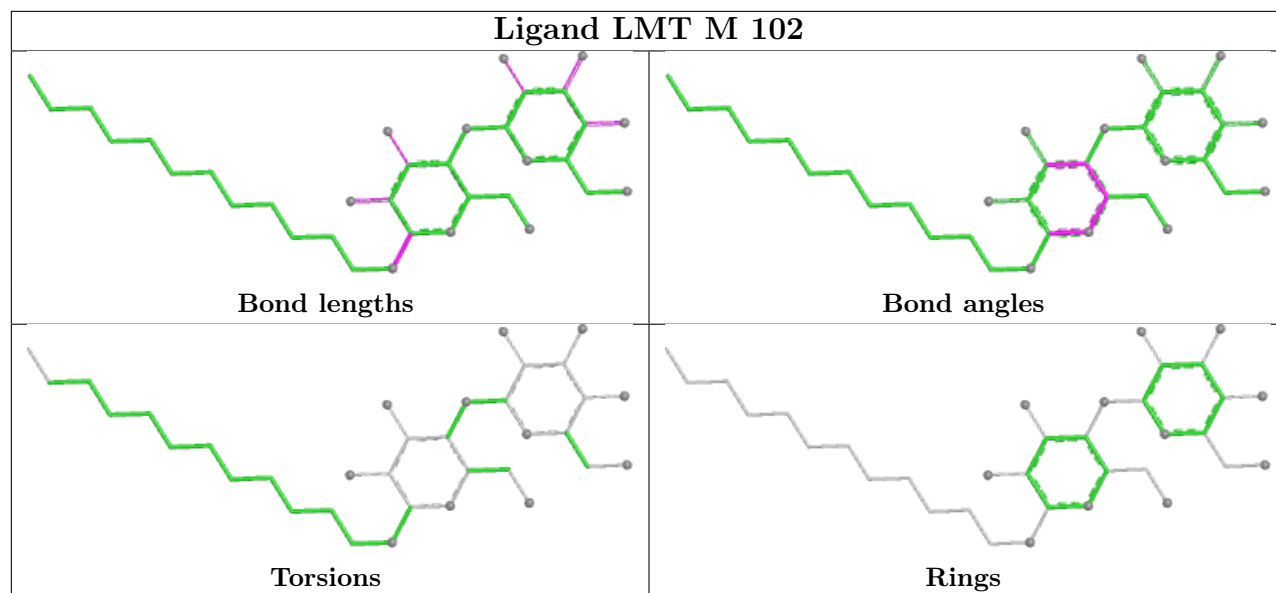


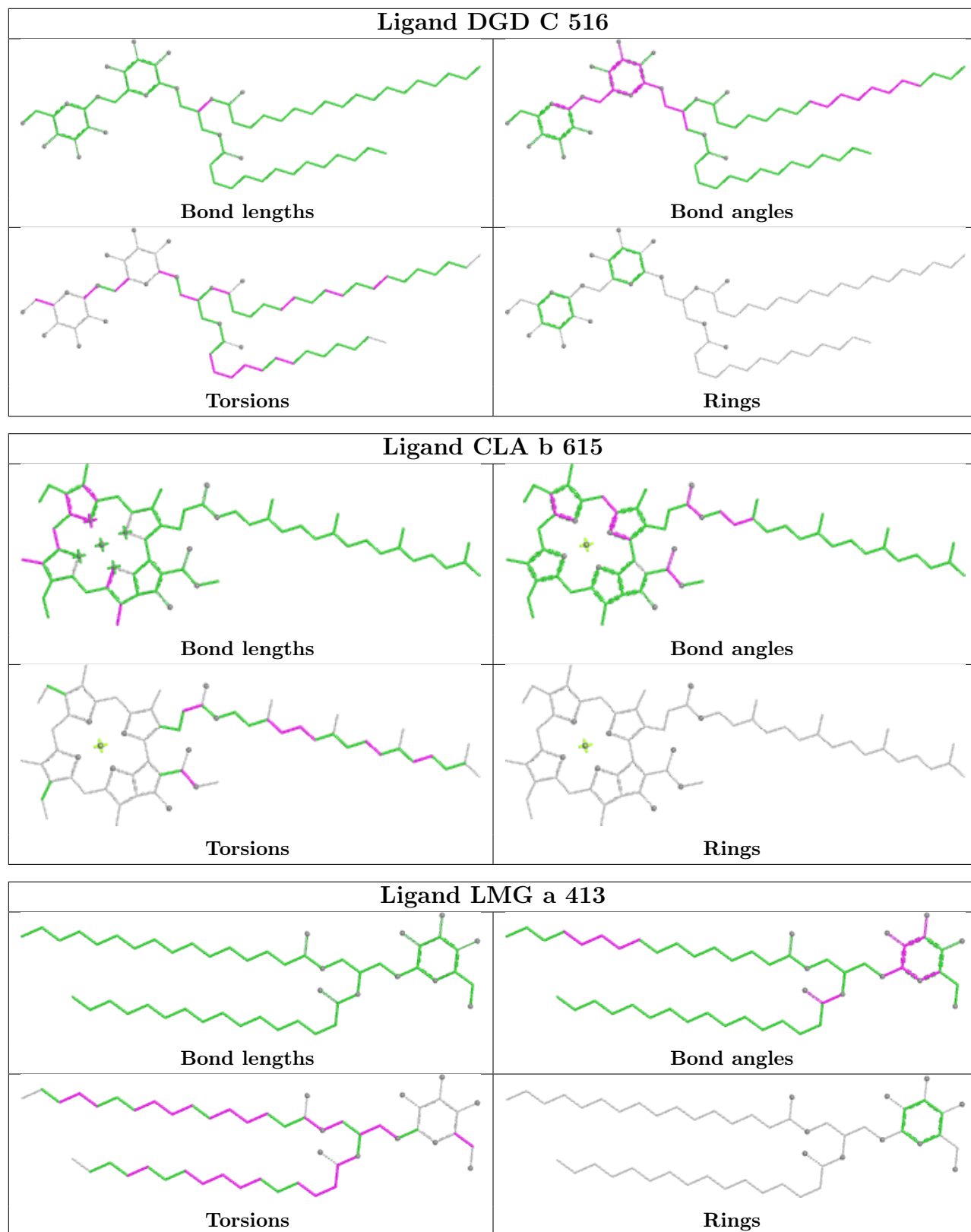
Ligand LMG B 621

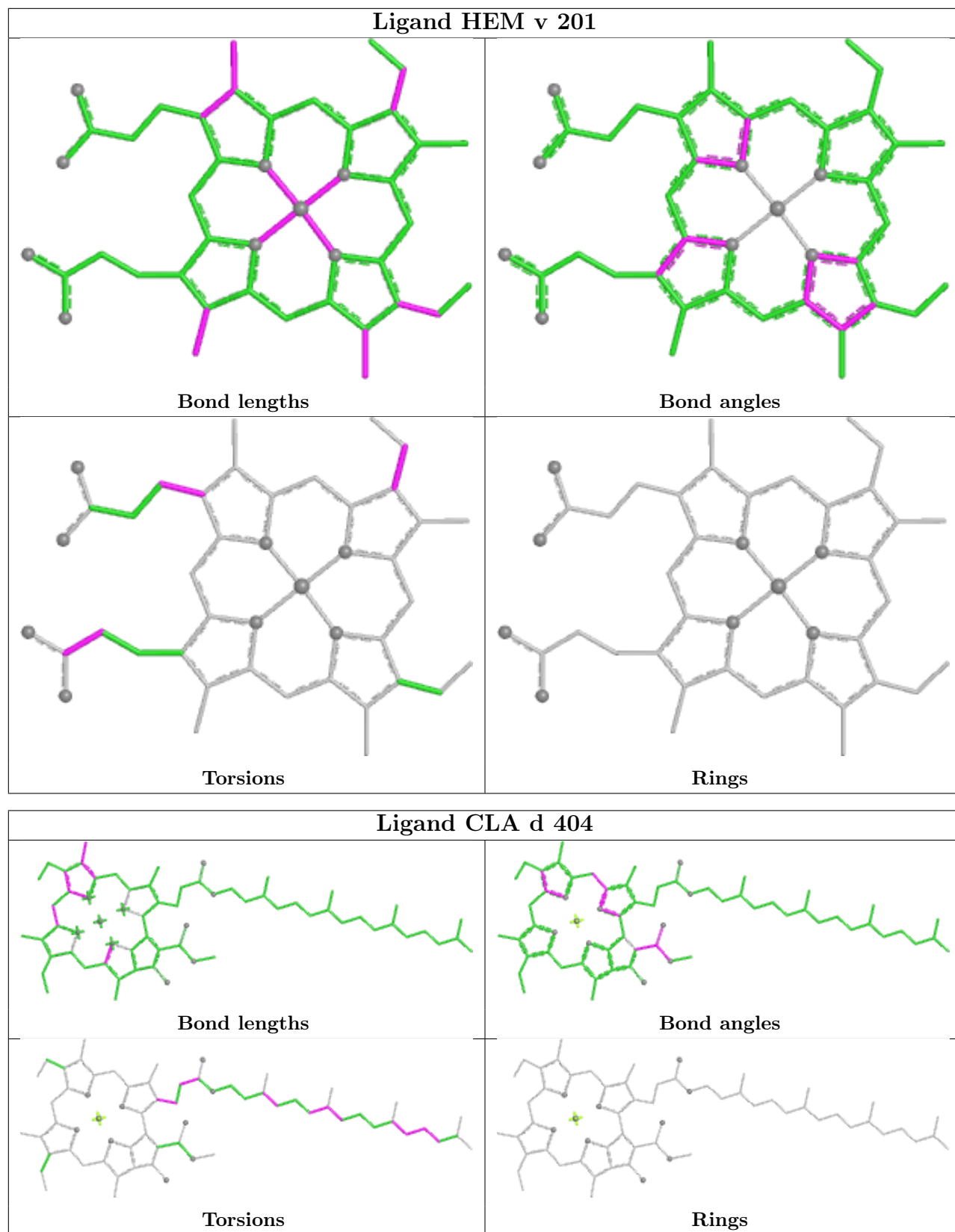


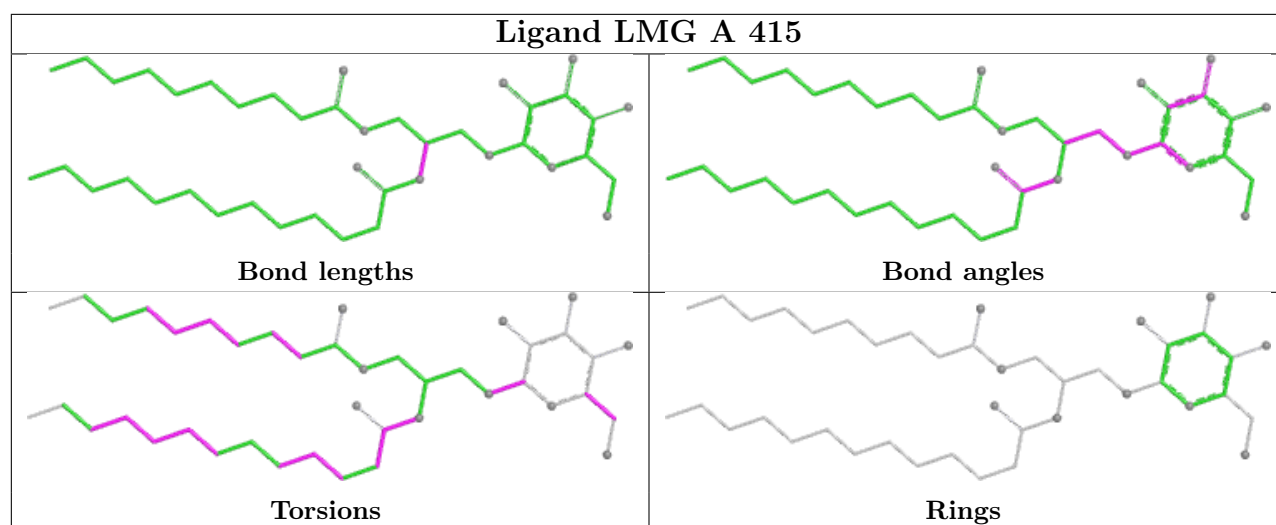
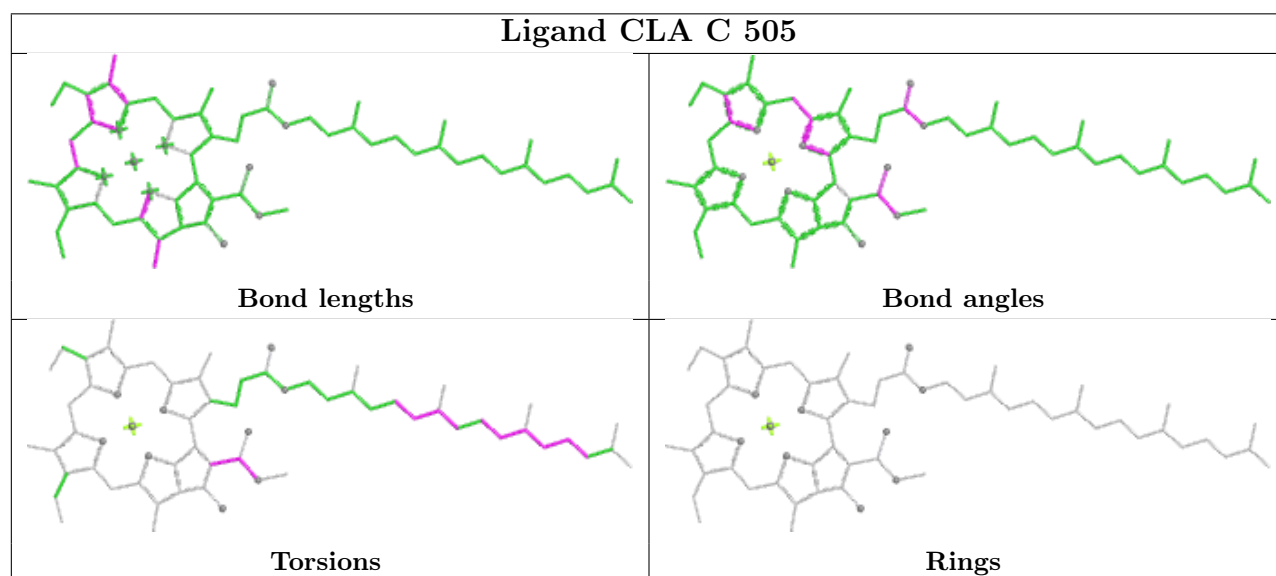
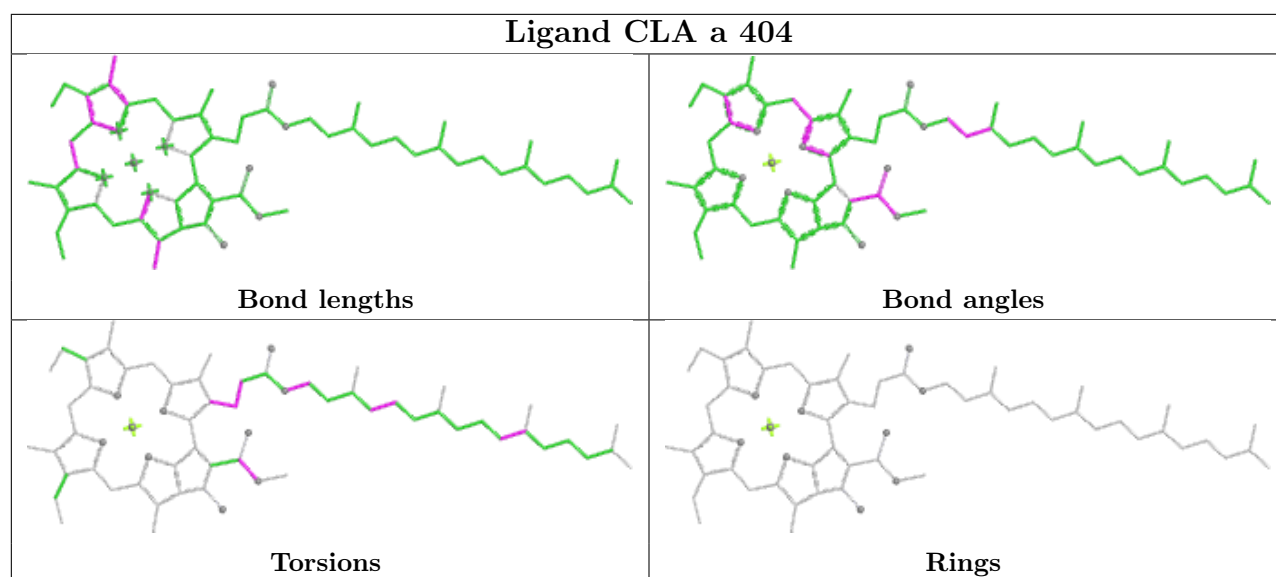
Ligand CLA b 609

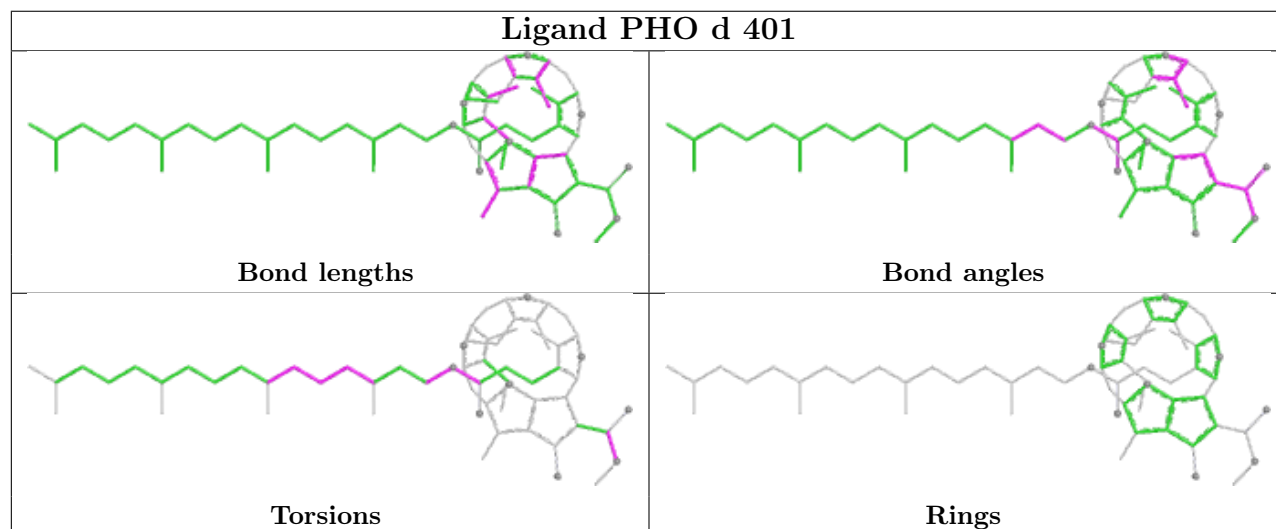
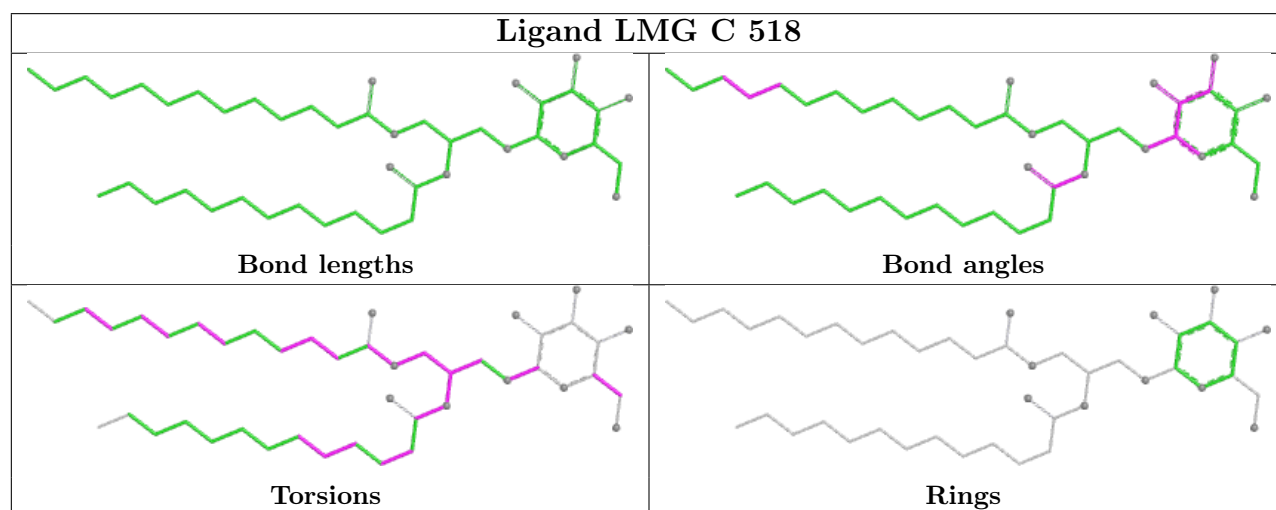
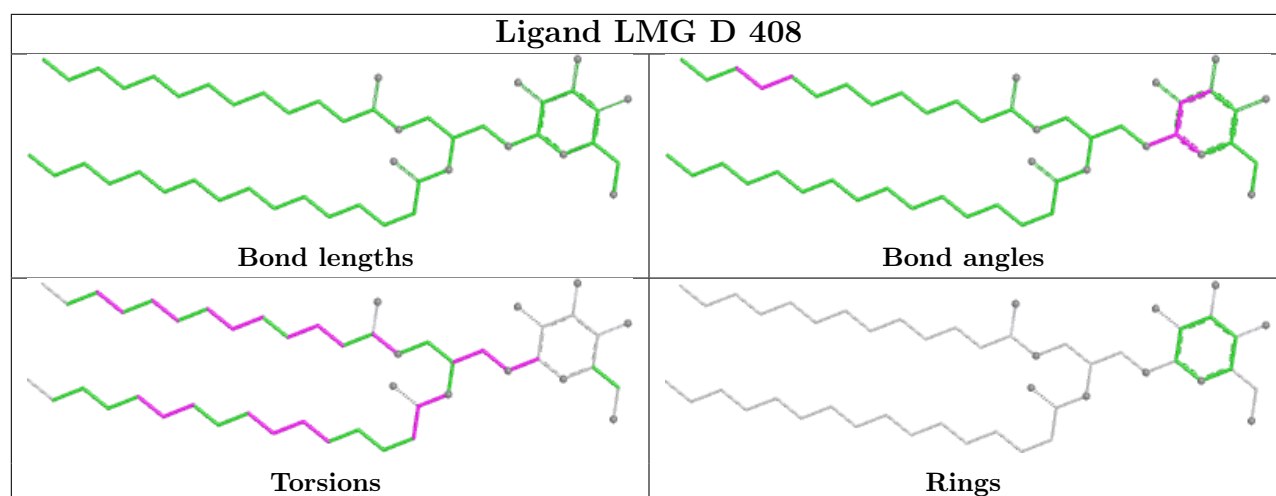


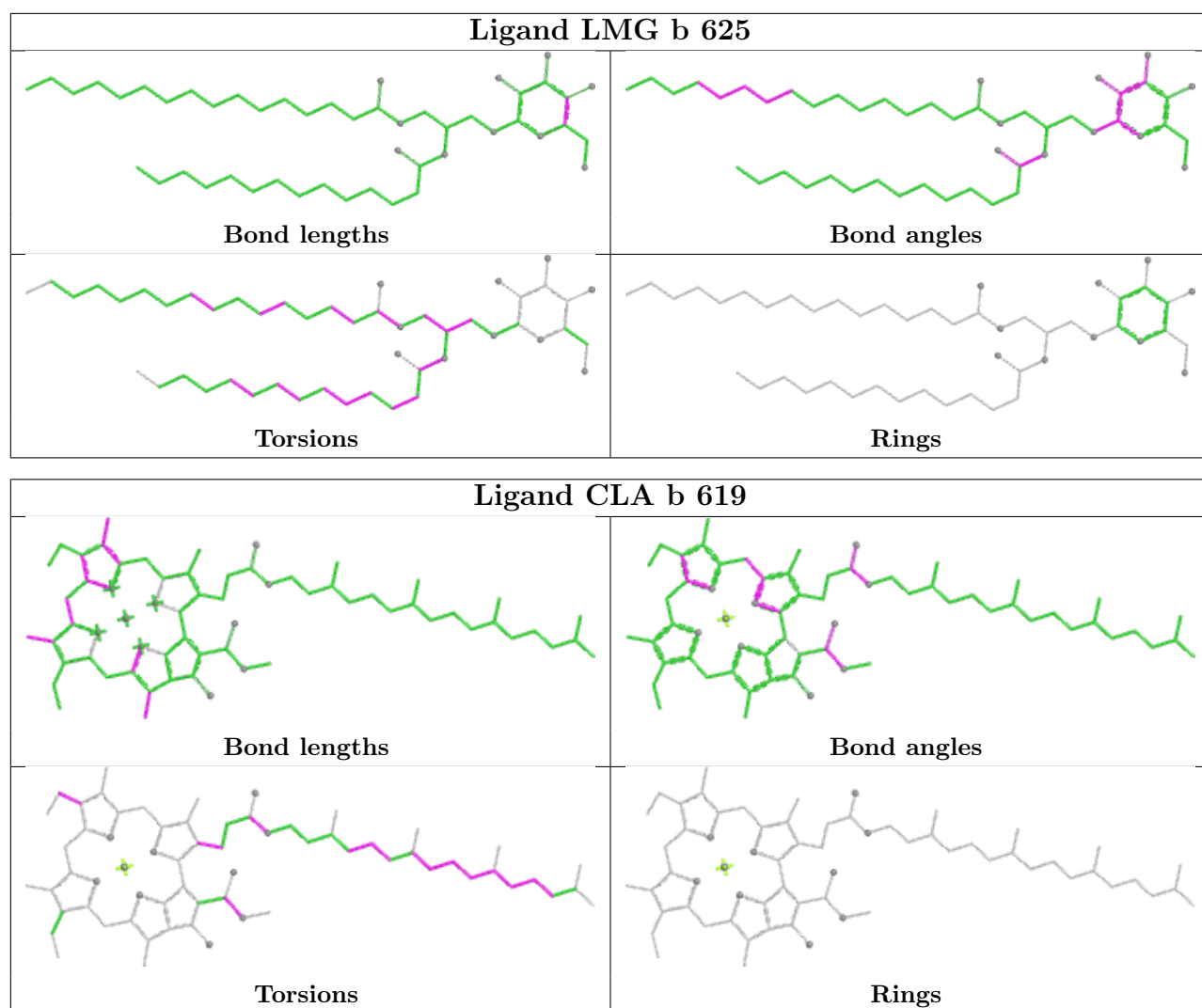


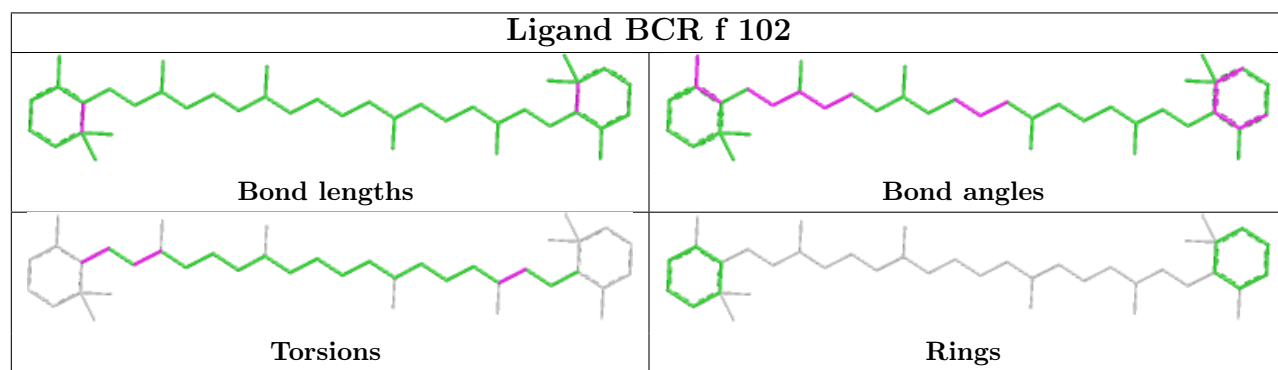
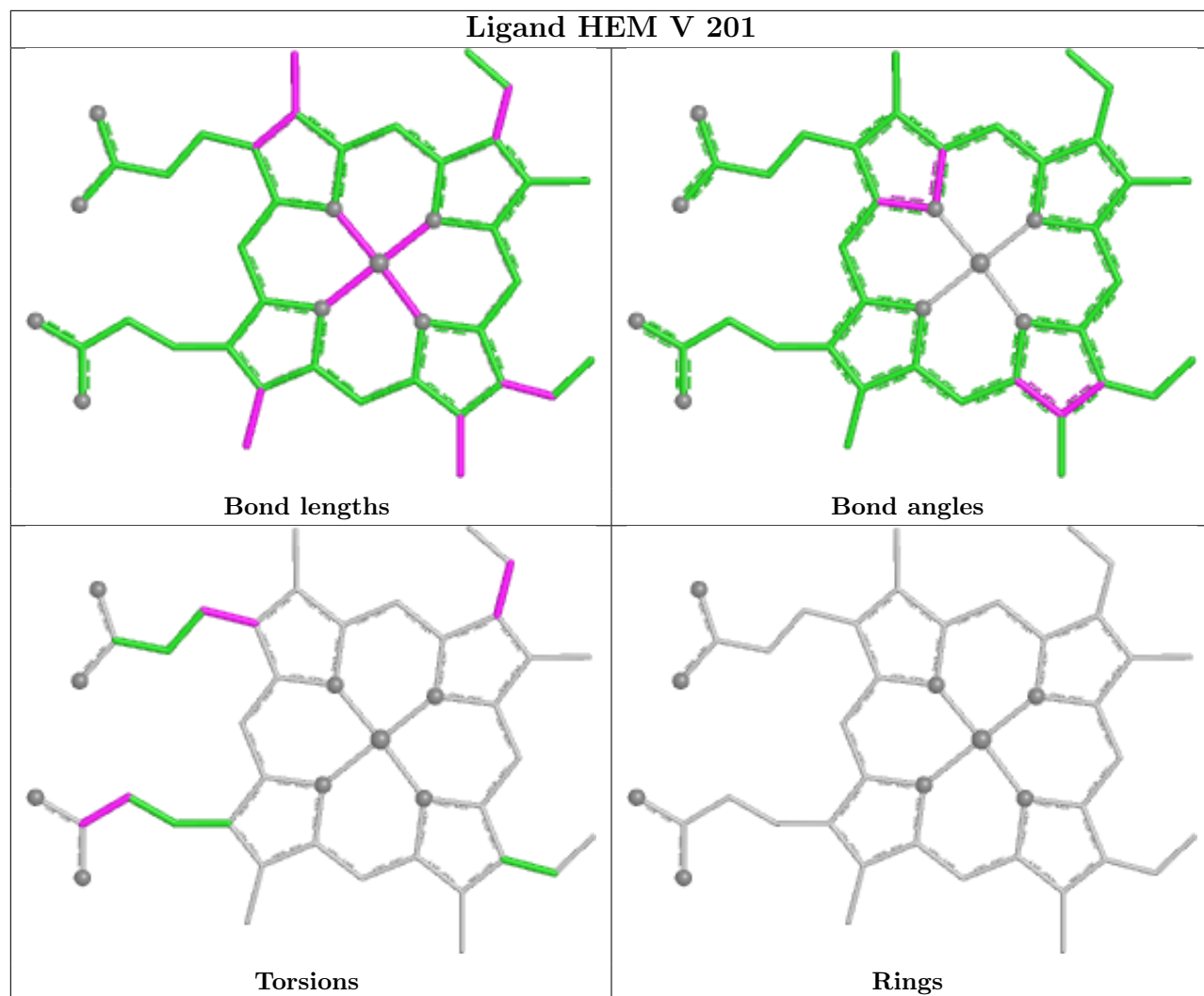


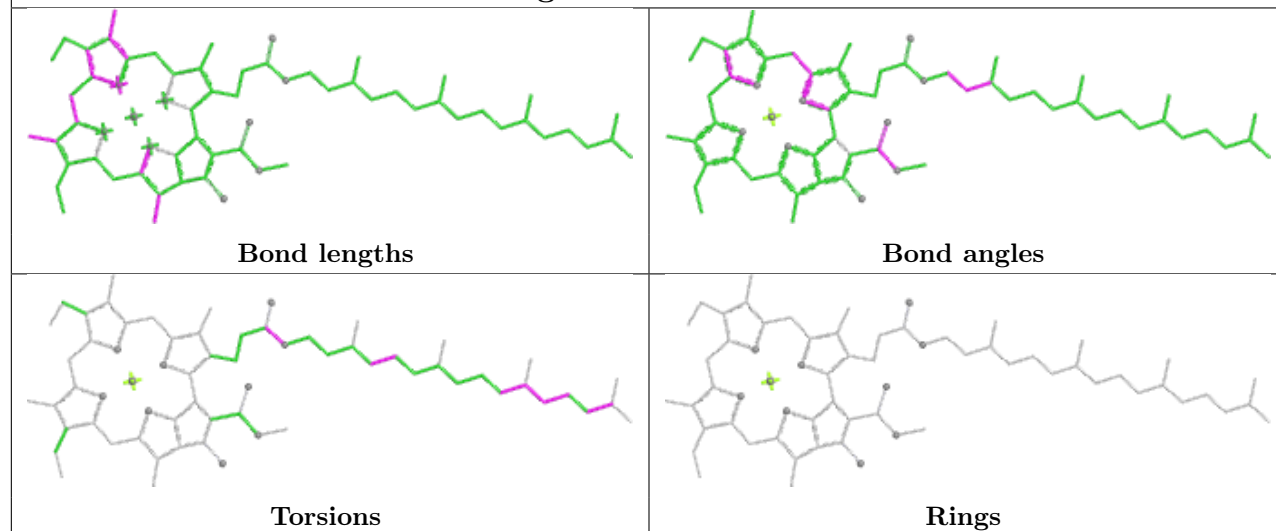
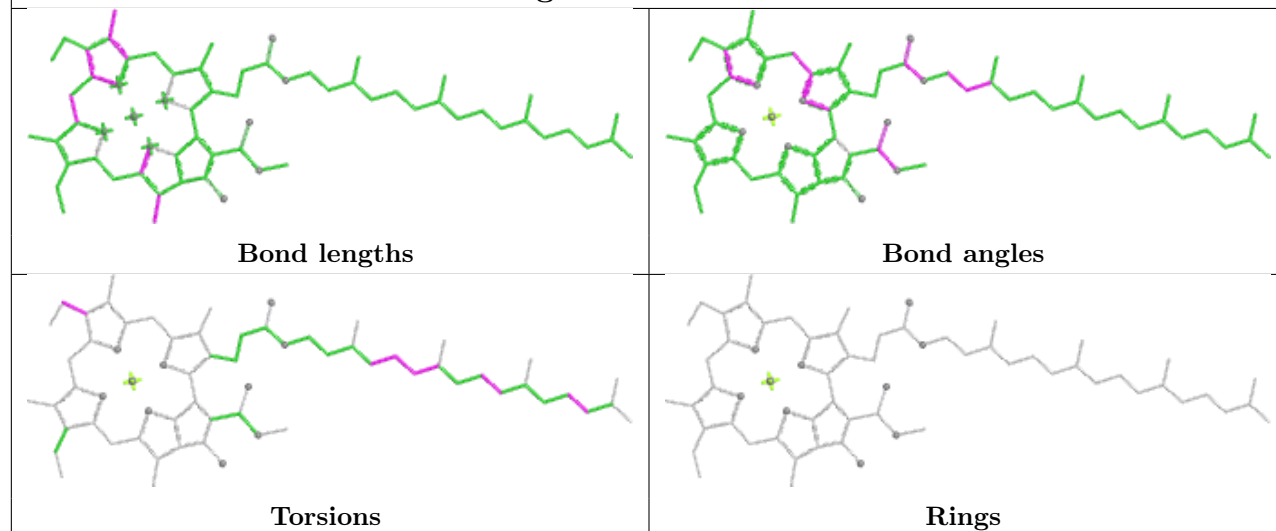
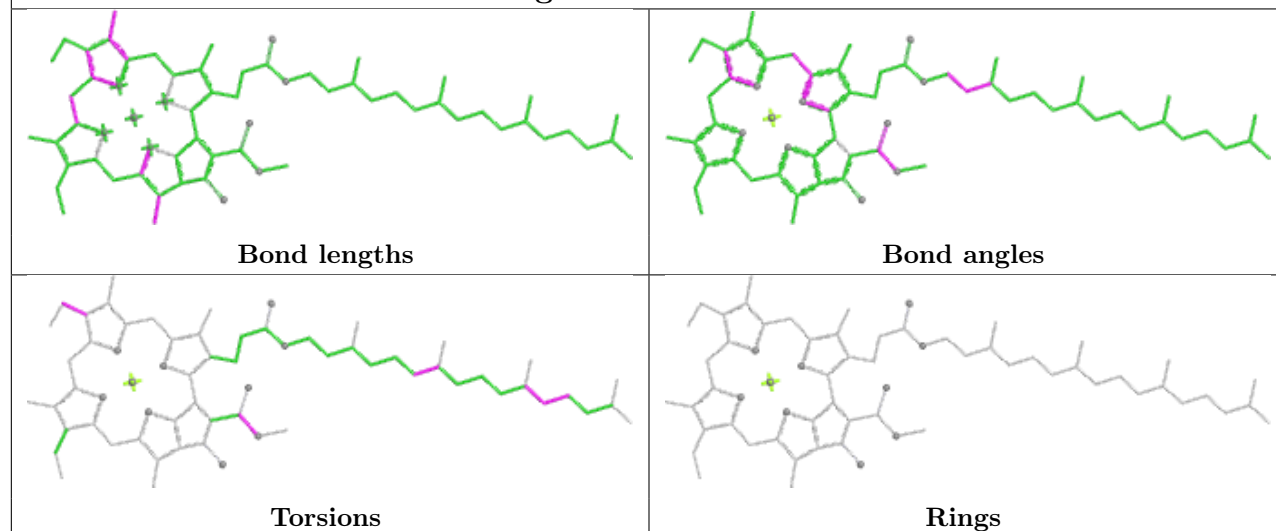


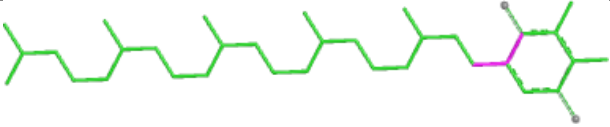
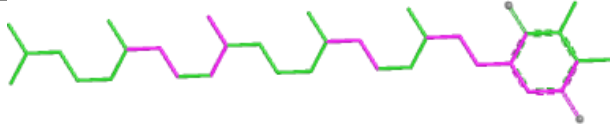
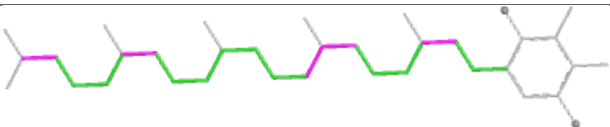
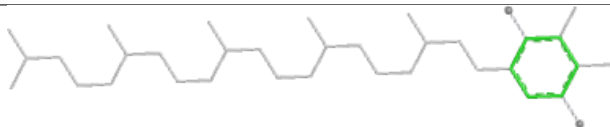
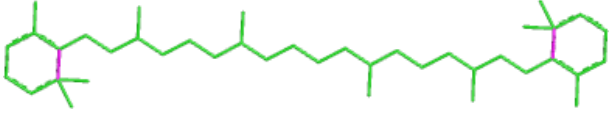
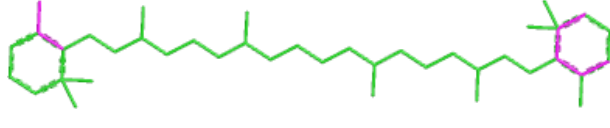
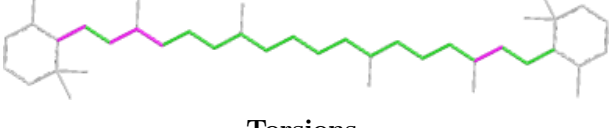
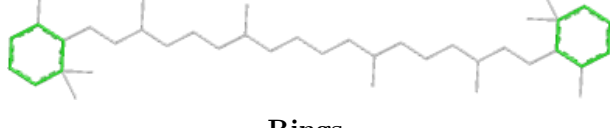
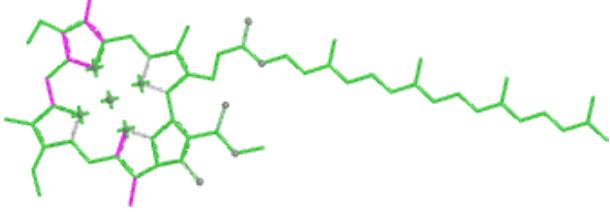
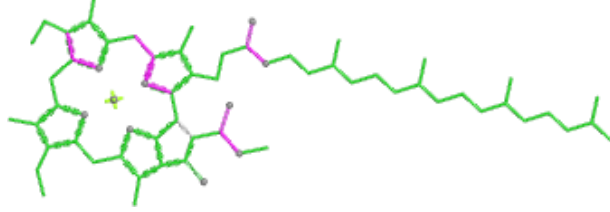
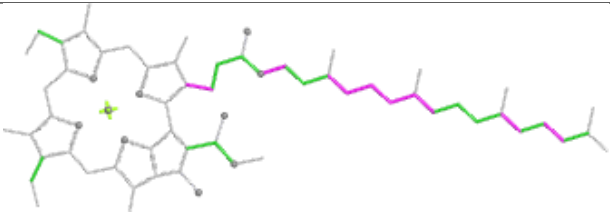
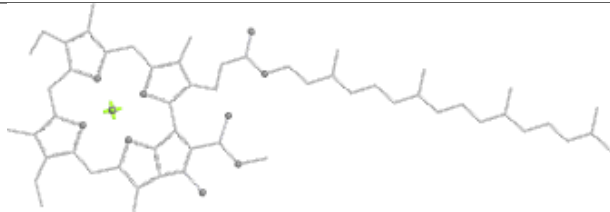


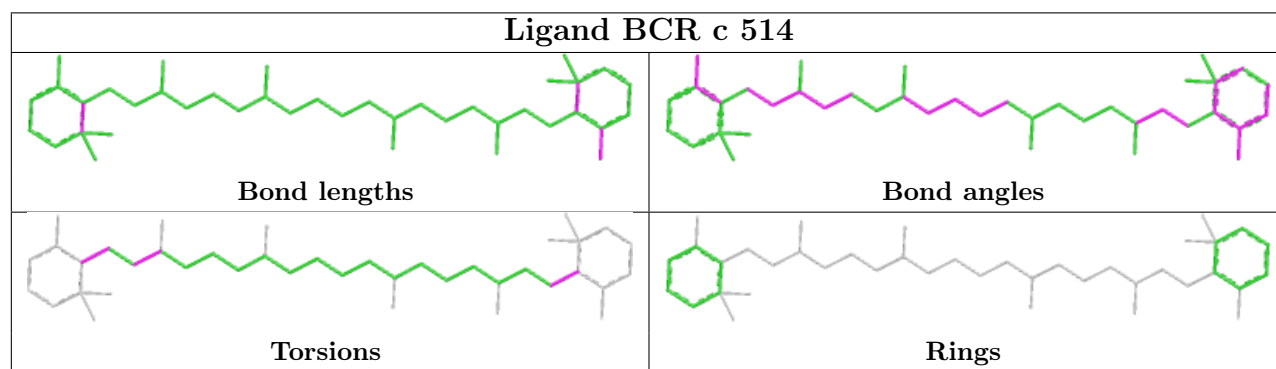
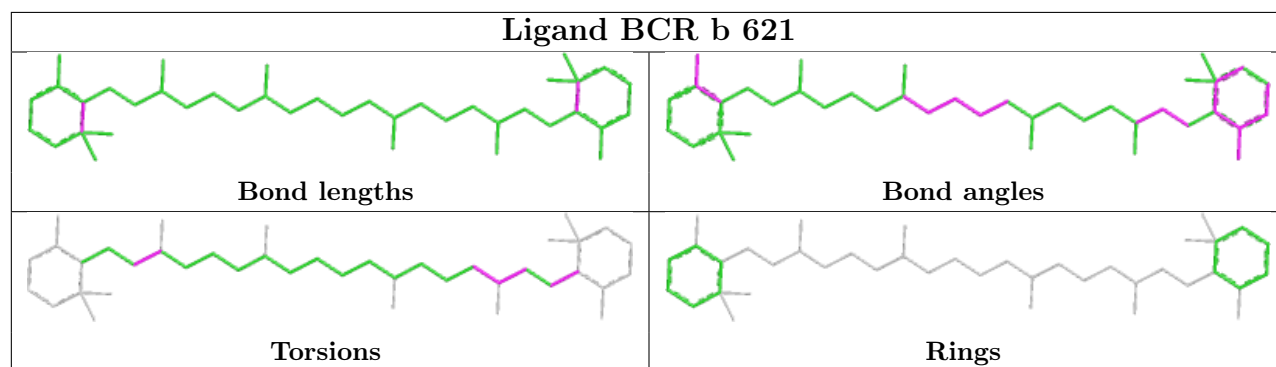
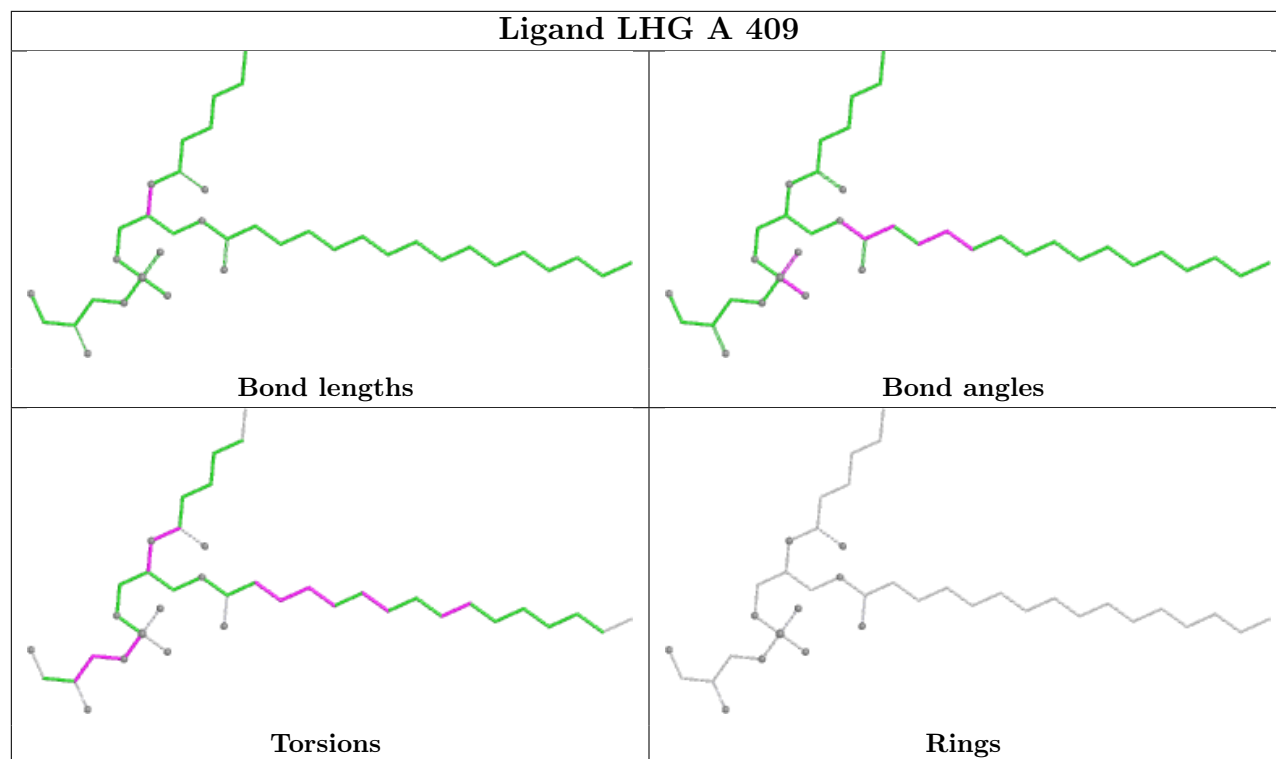


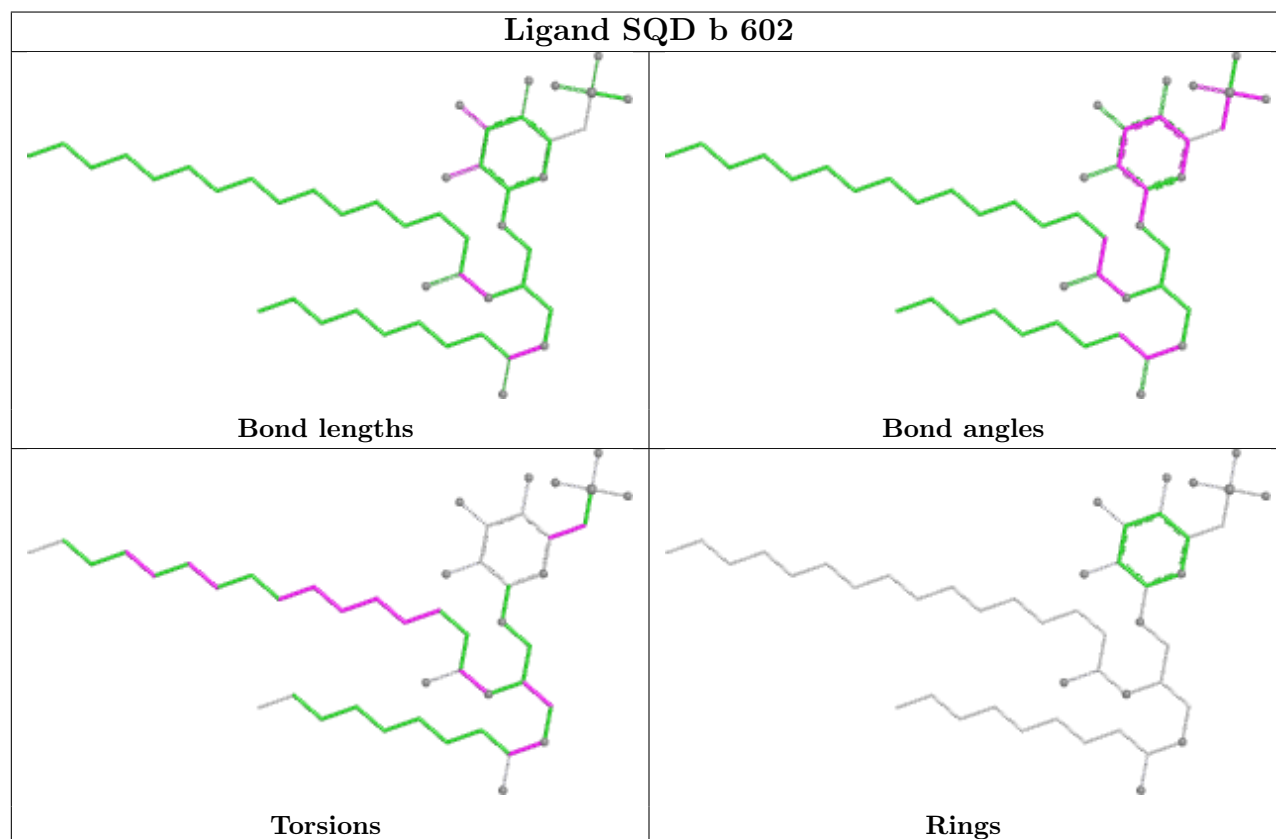
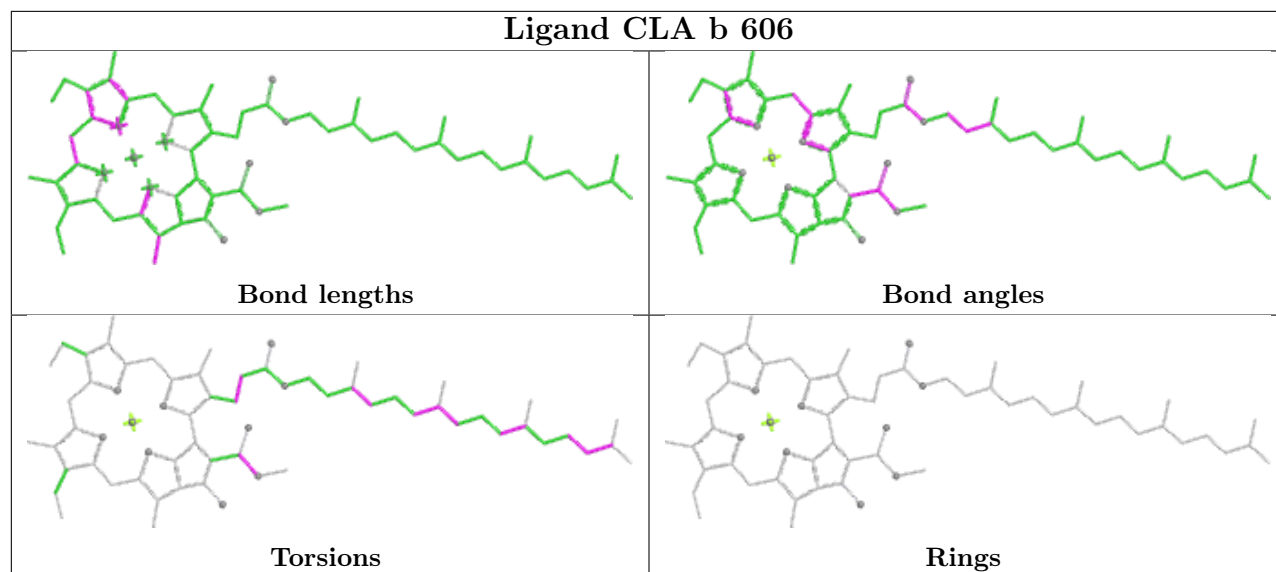


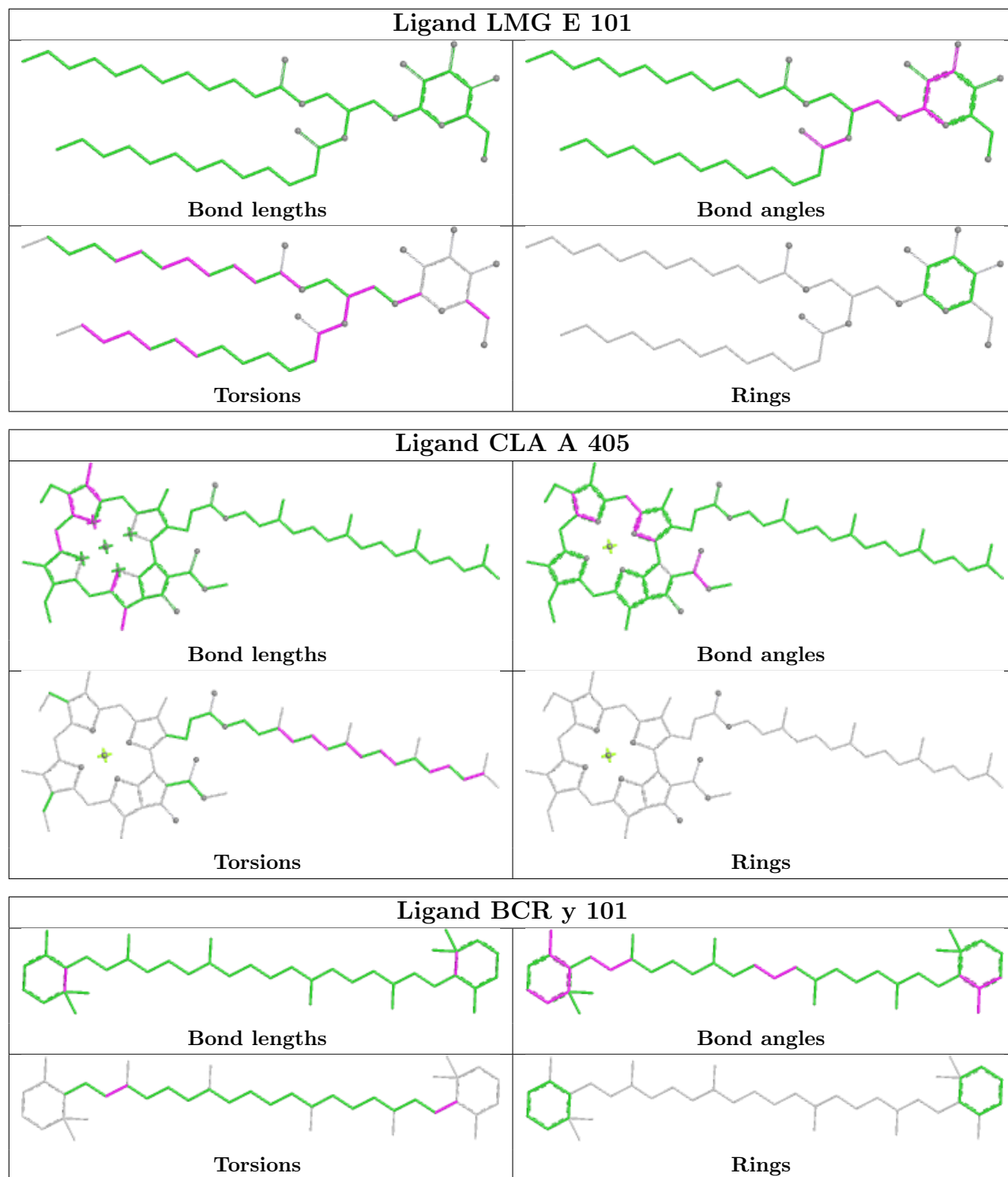


Ligand CLA c 502**Ligand CLA a 406****Ligand CLA b 612**

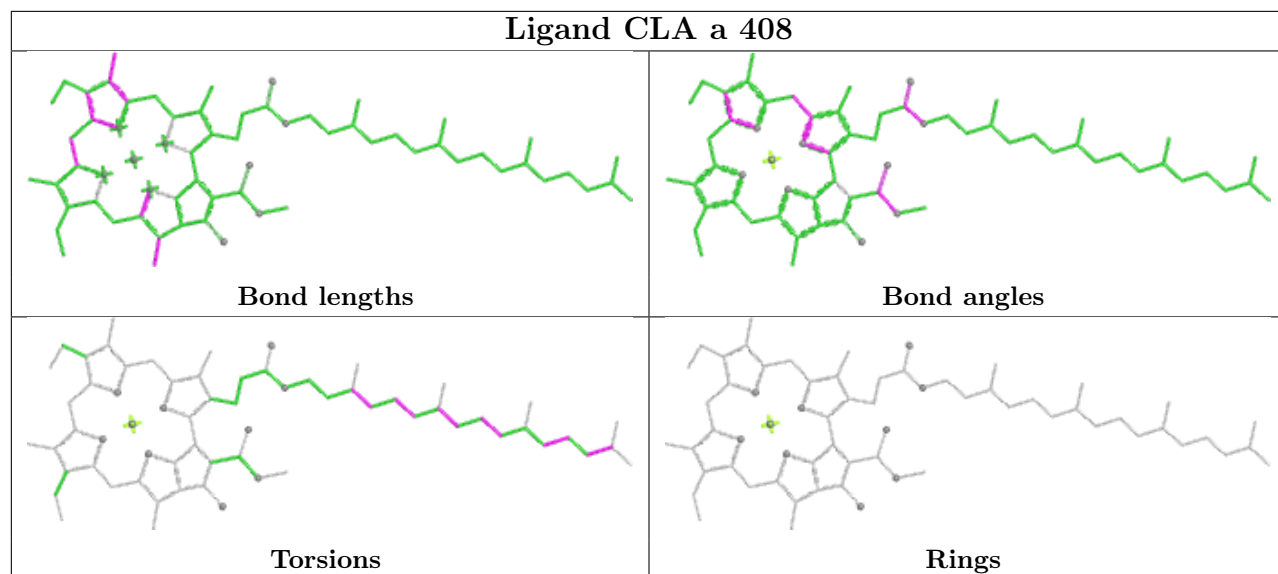
Ligand PL9 J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 405	
 Bond lengths	 Bond angles
 Torsions	 Rings



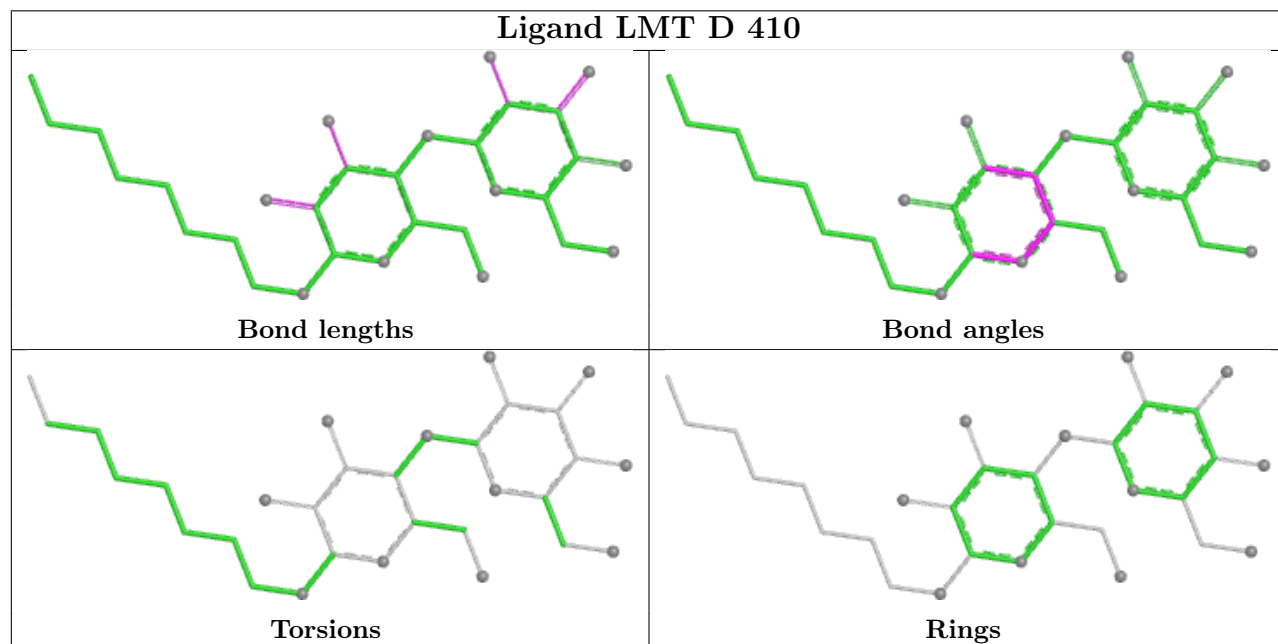


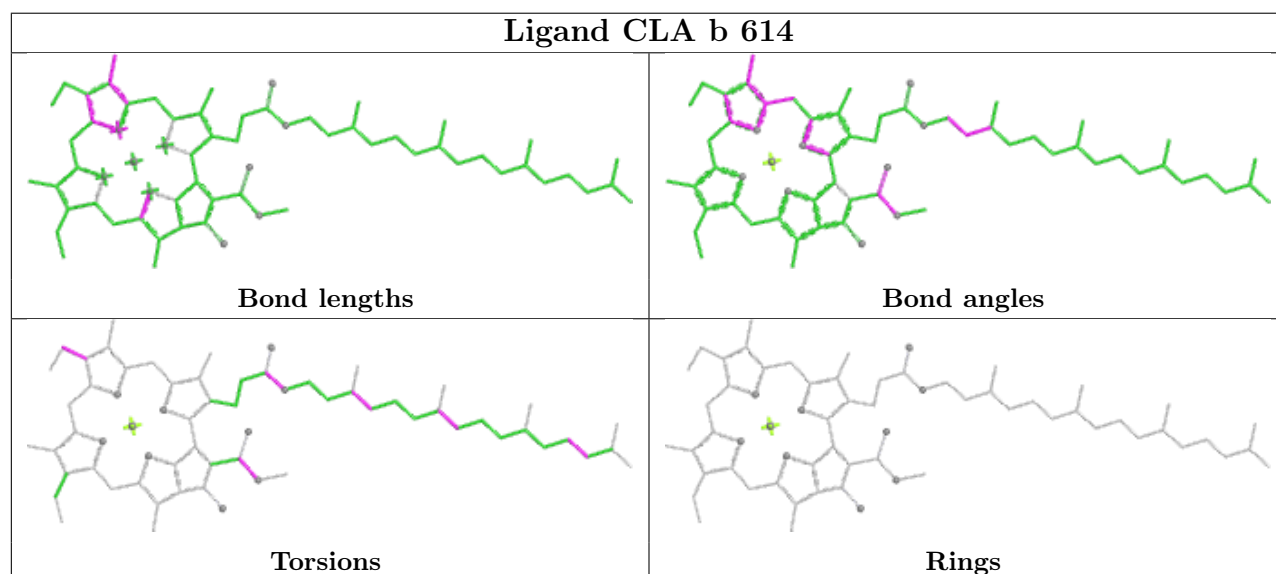
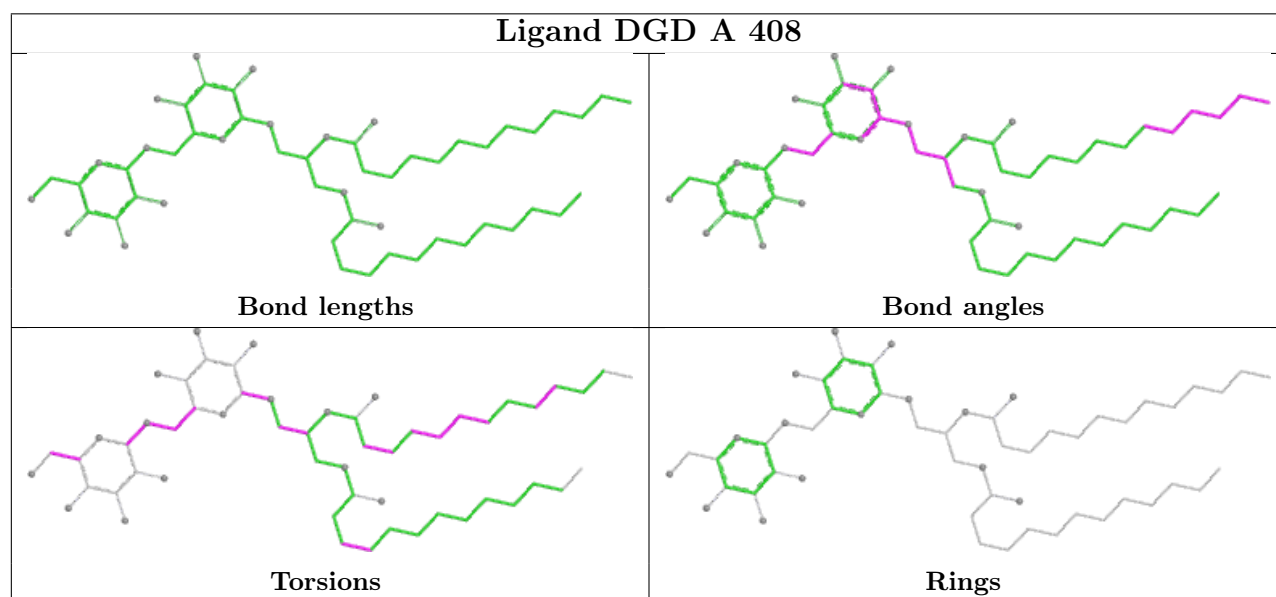
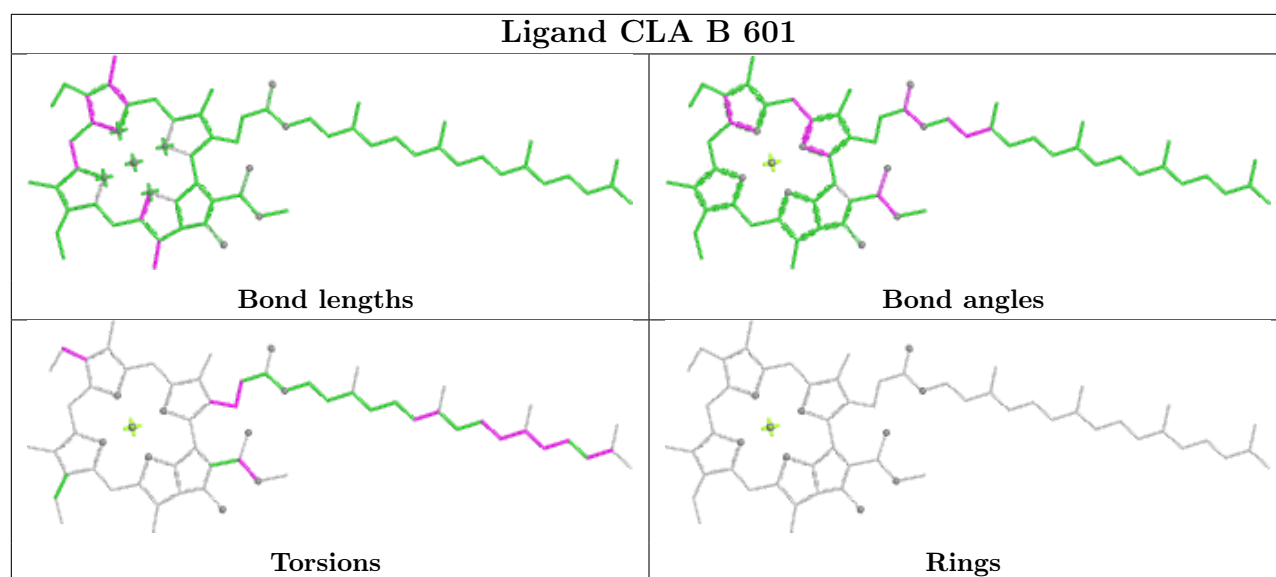


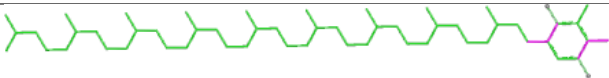
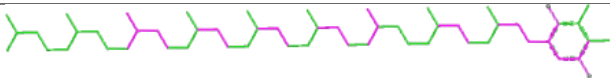
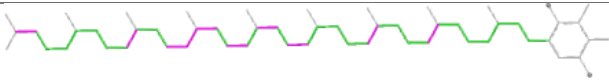
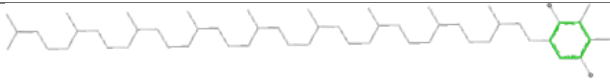
Ligand CLA a 408

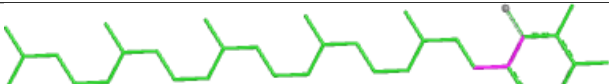
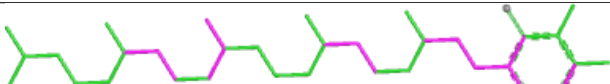
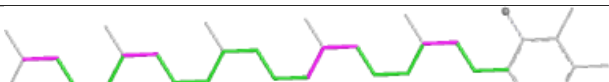
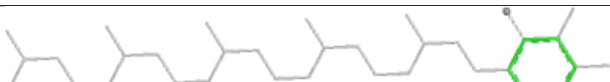


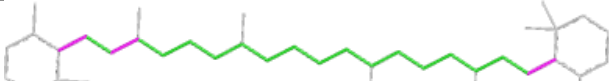
Ligand LMT D 410

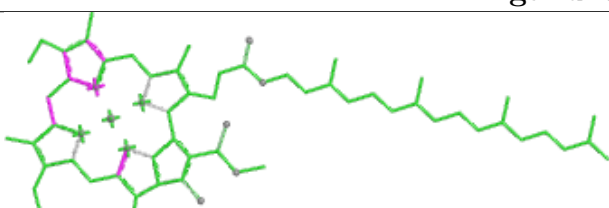
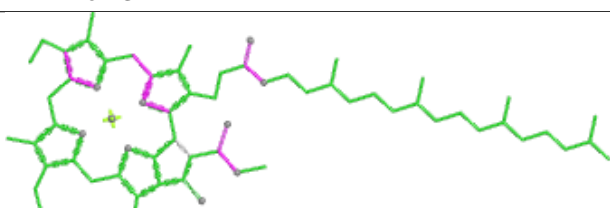
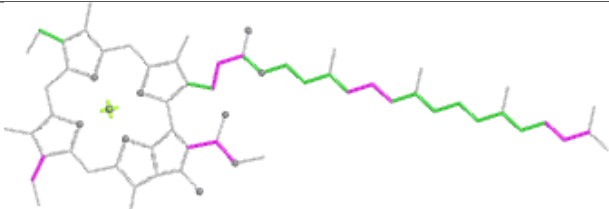
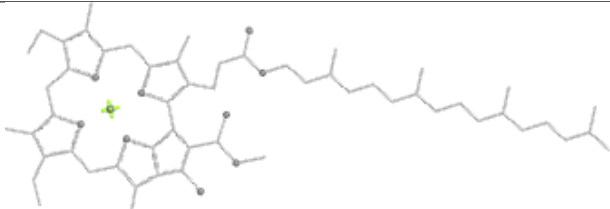


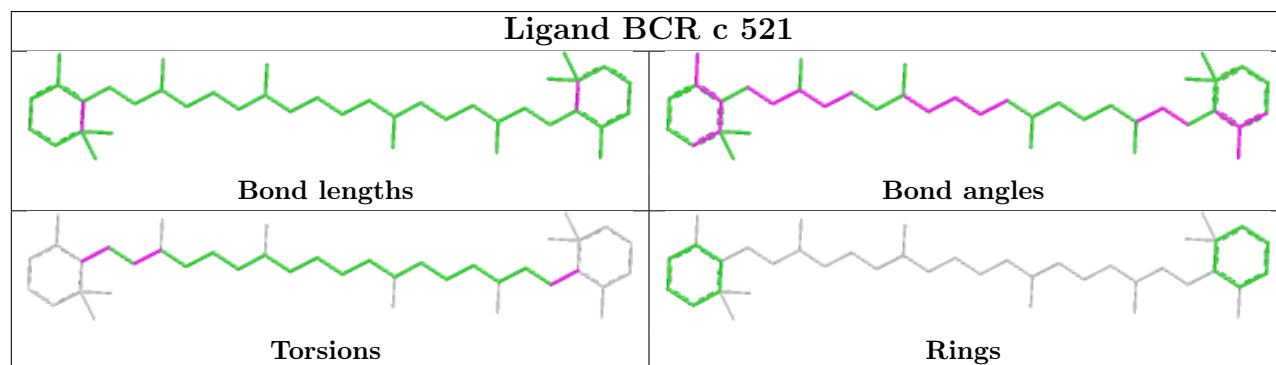
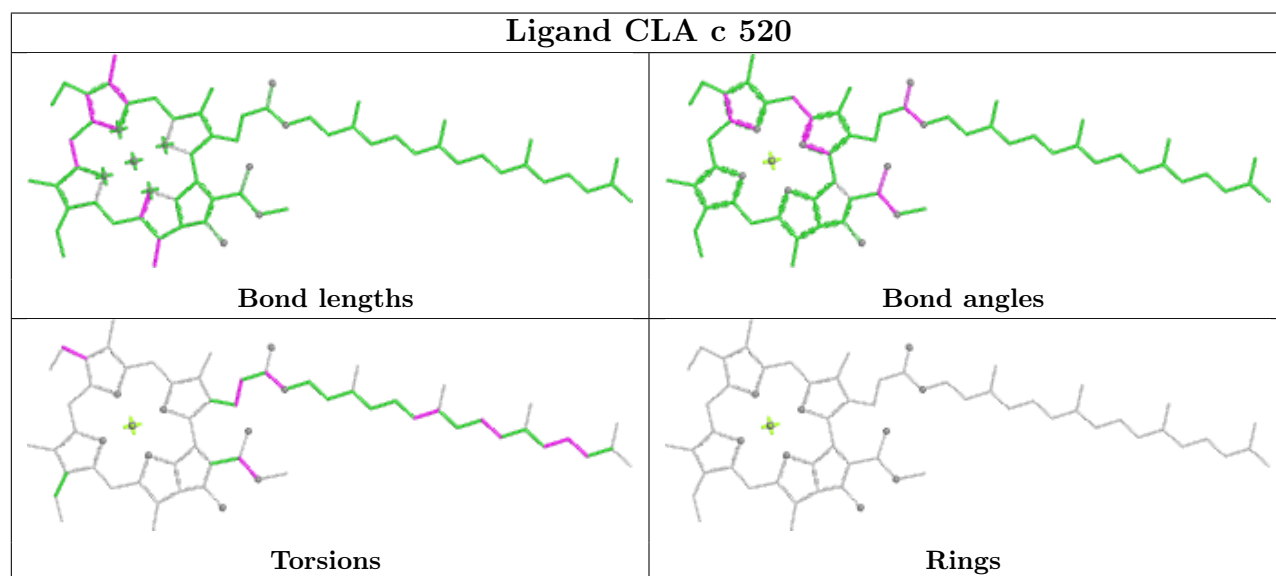
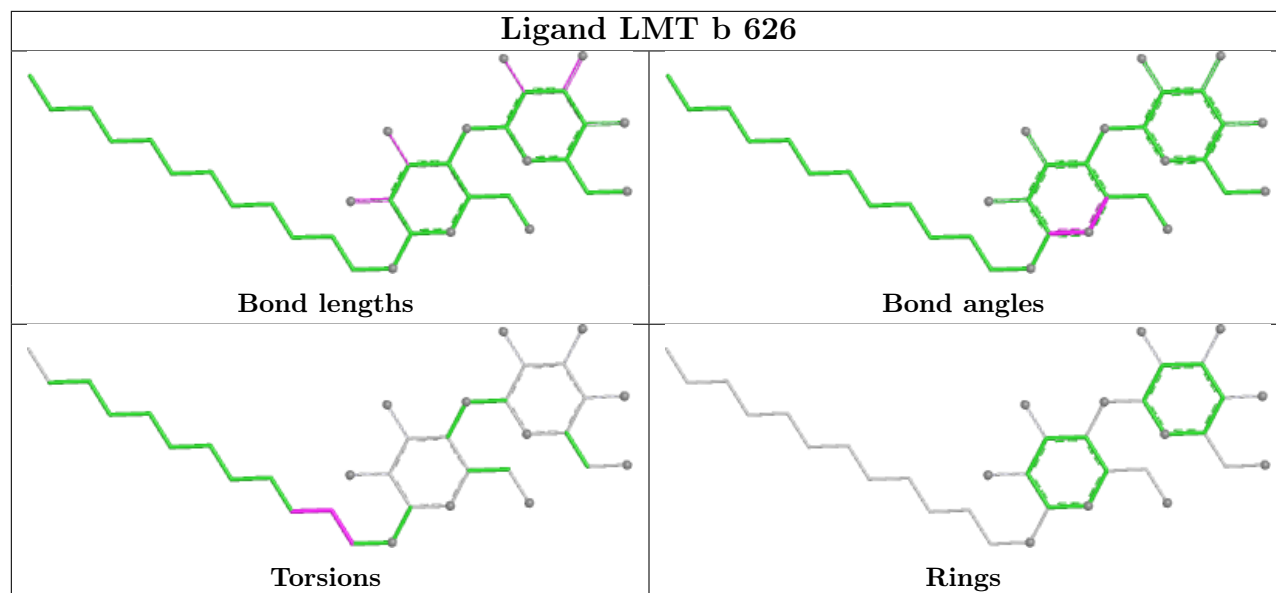


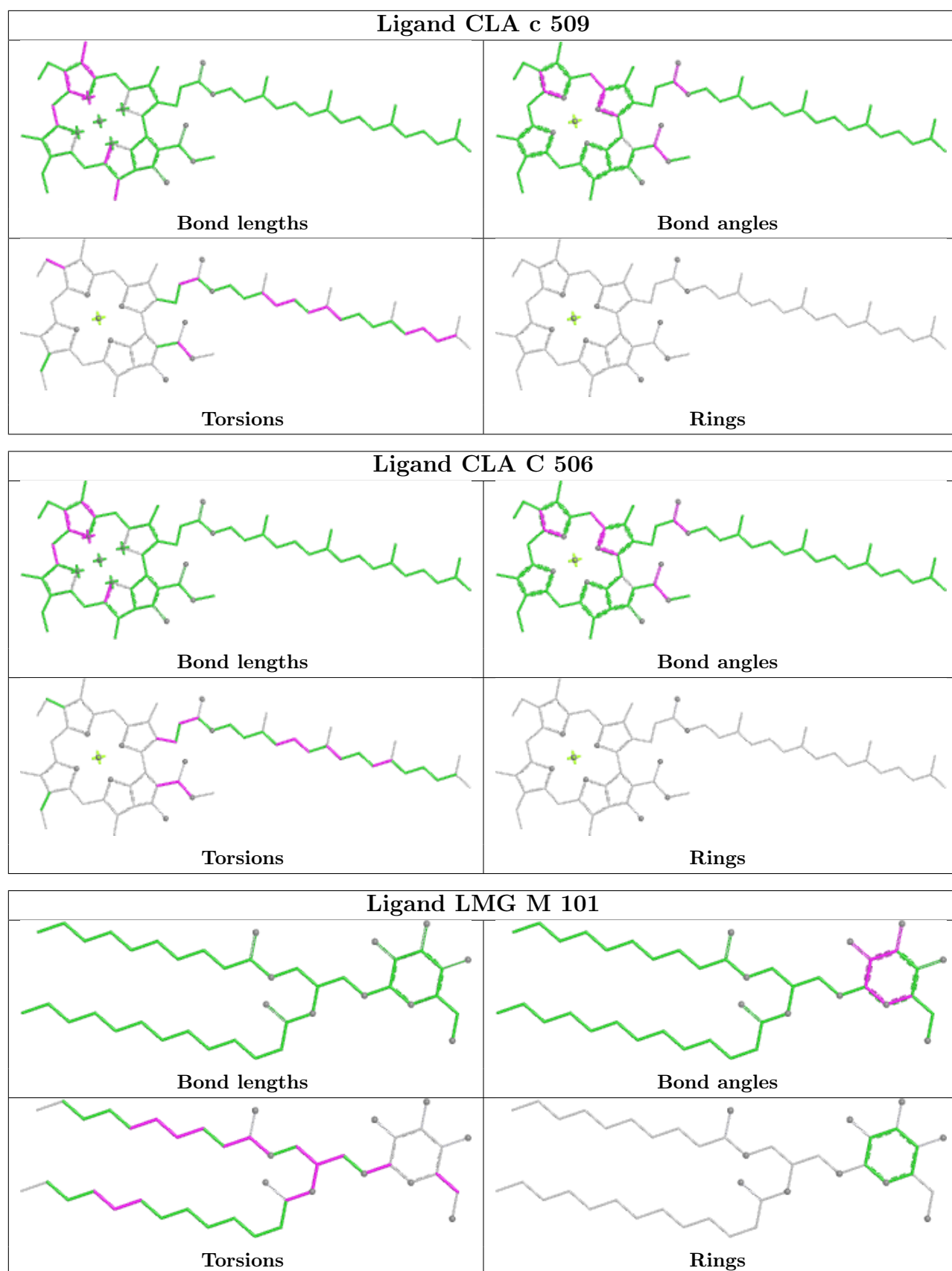
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

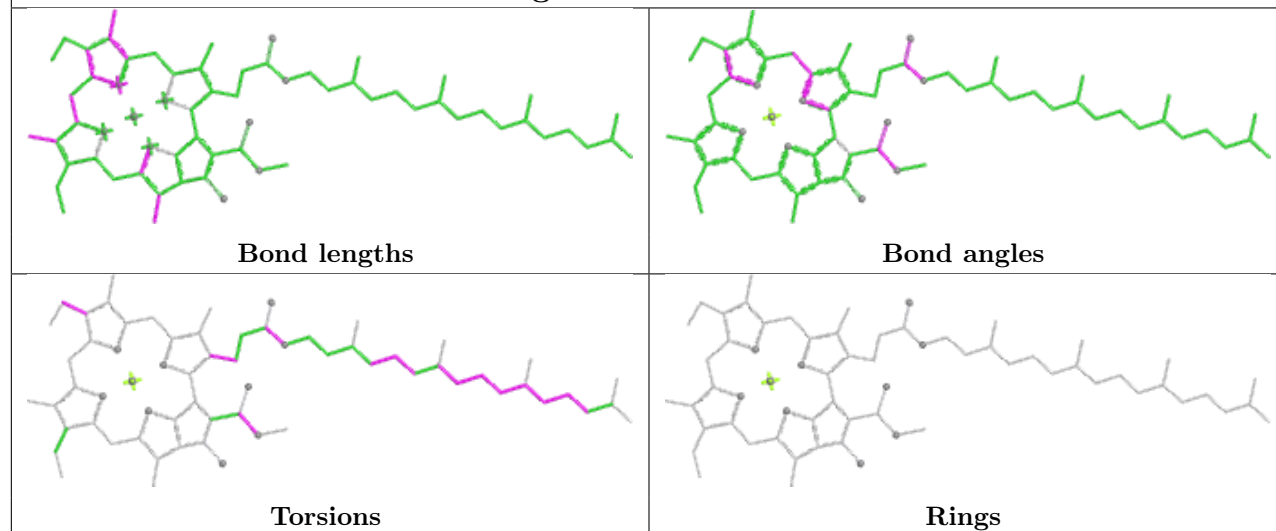
Ligand BCR C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

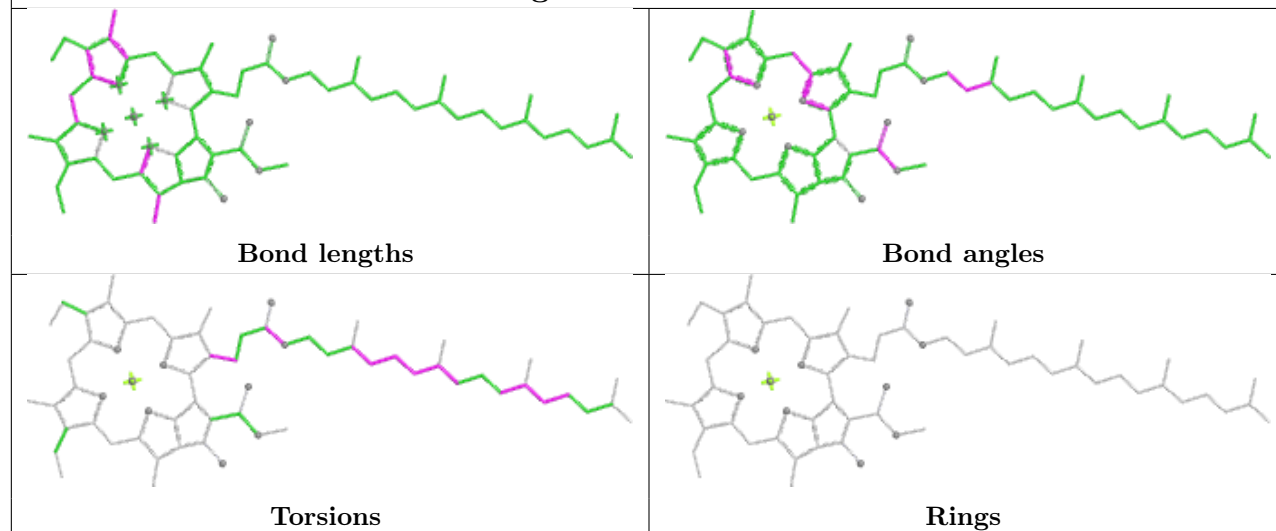




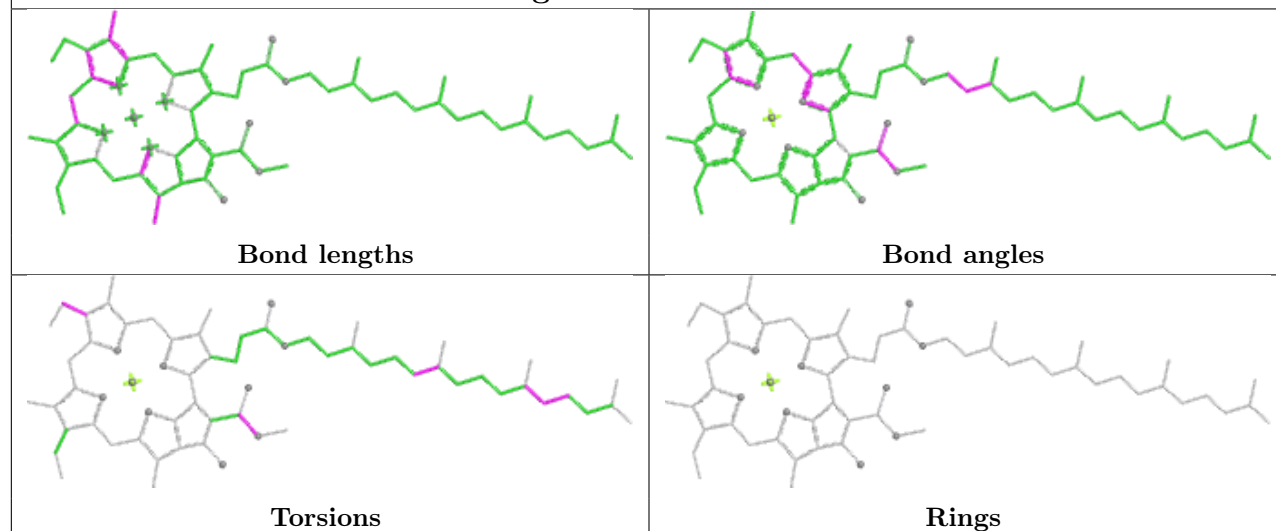
Ligand CLA B 615

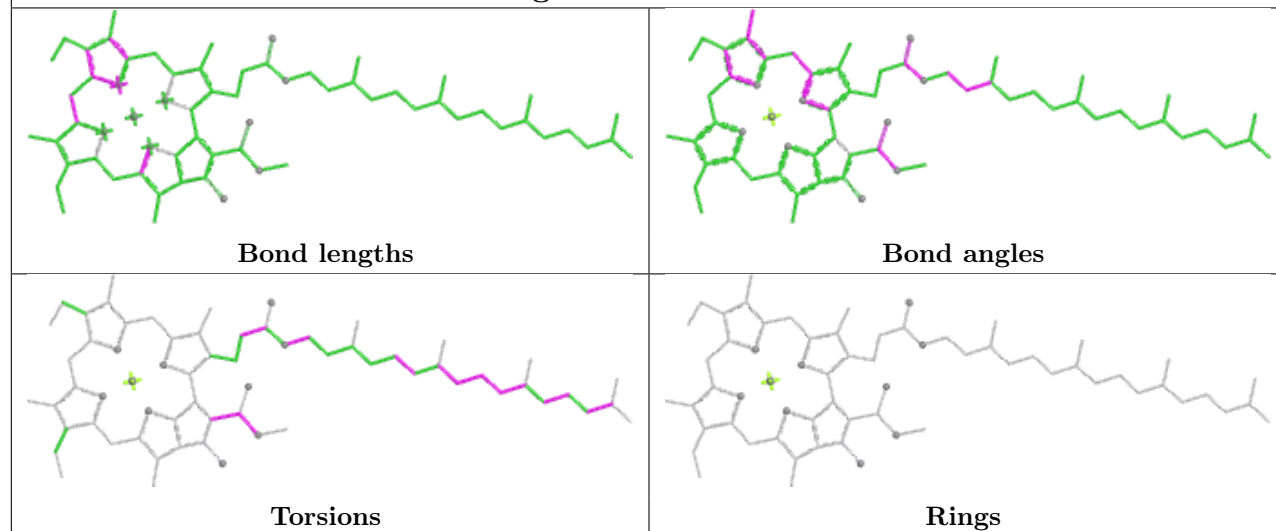
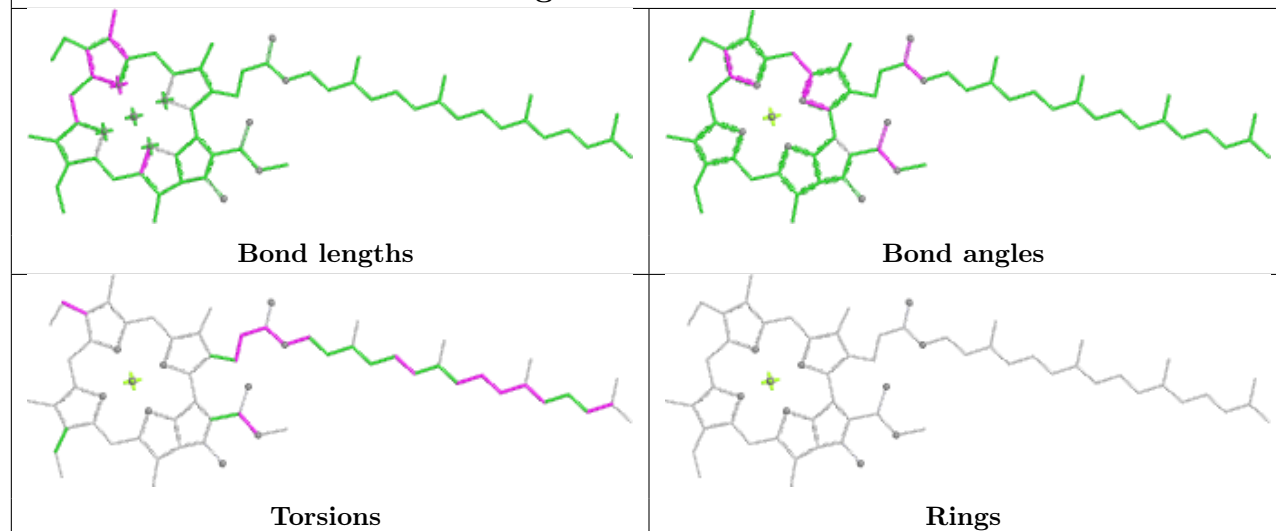
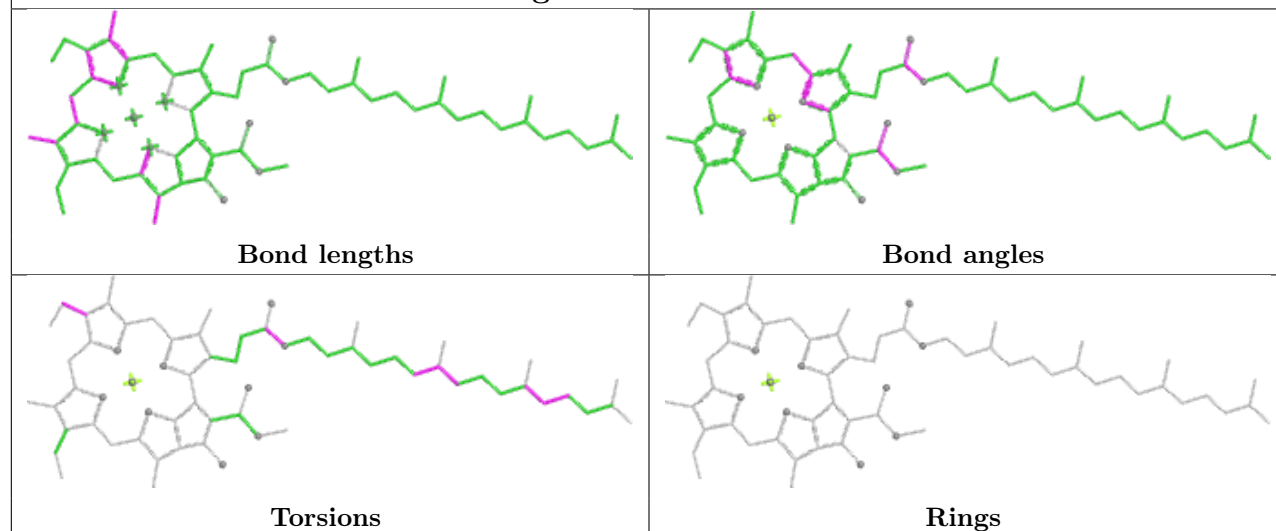


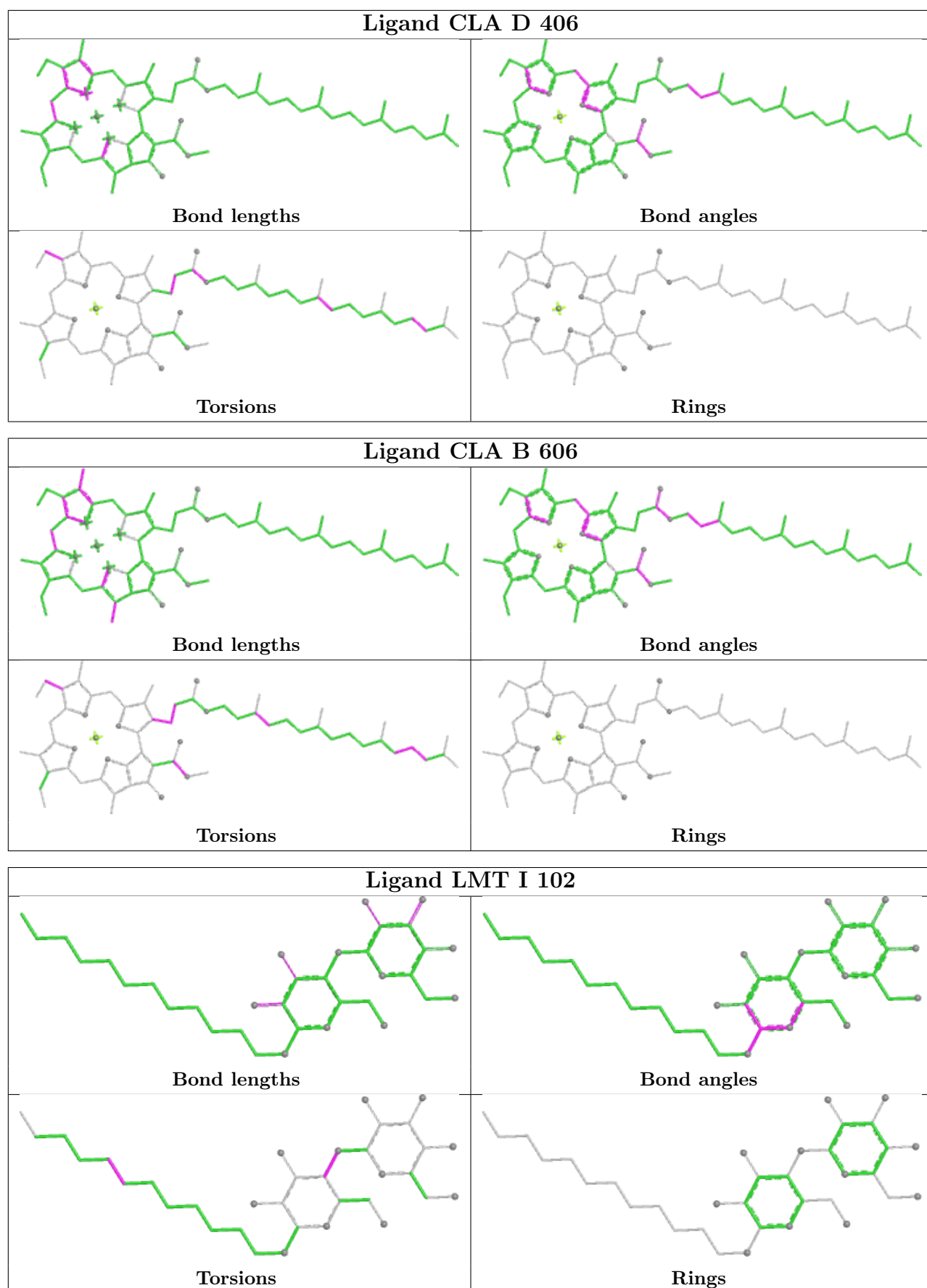
Ligand CLA H 101

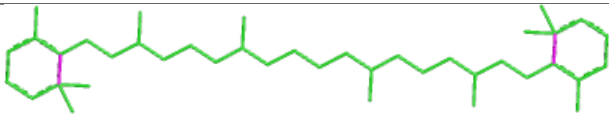
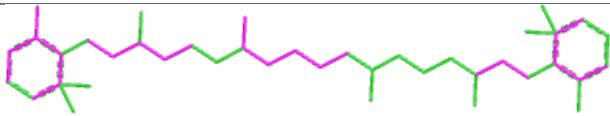
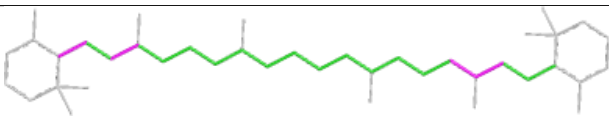
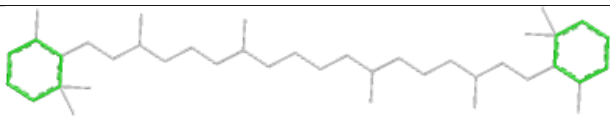


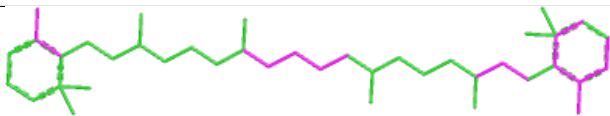
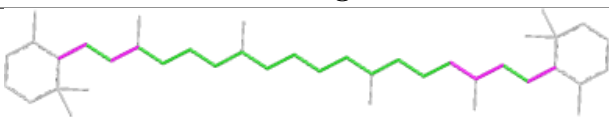
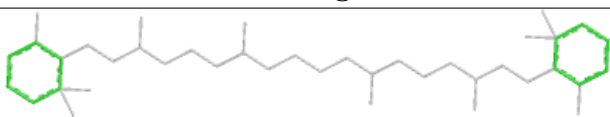
Ligand CLA B 608

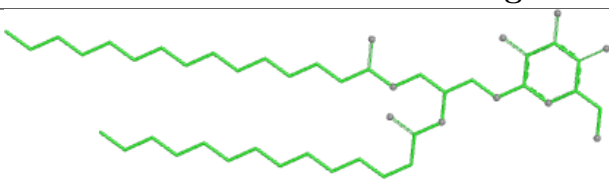
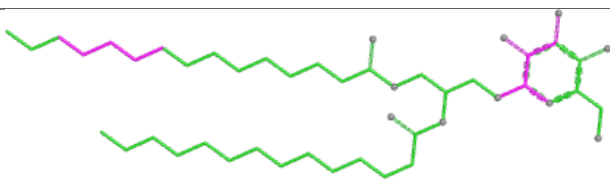
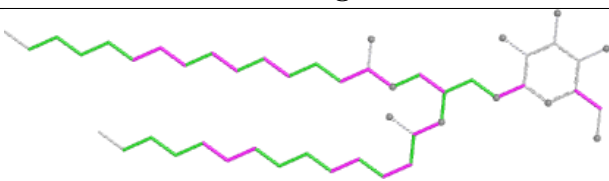
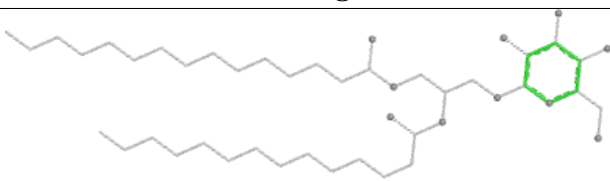


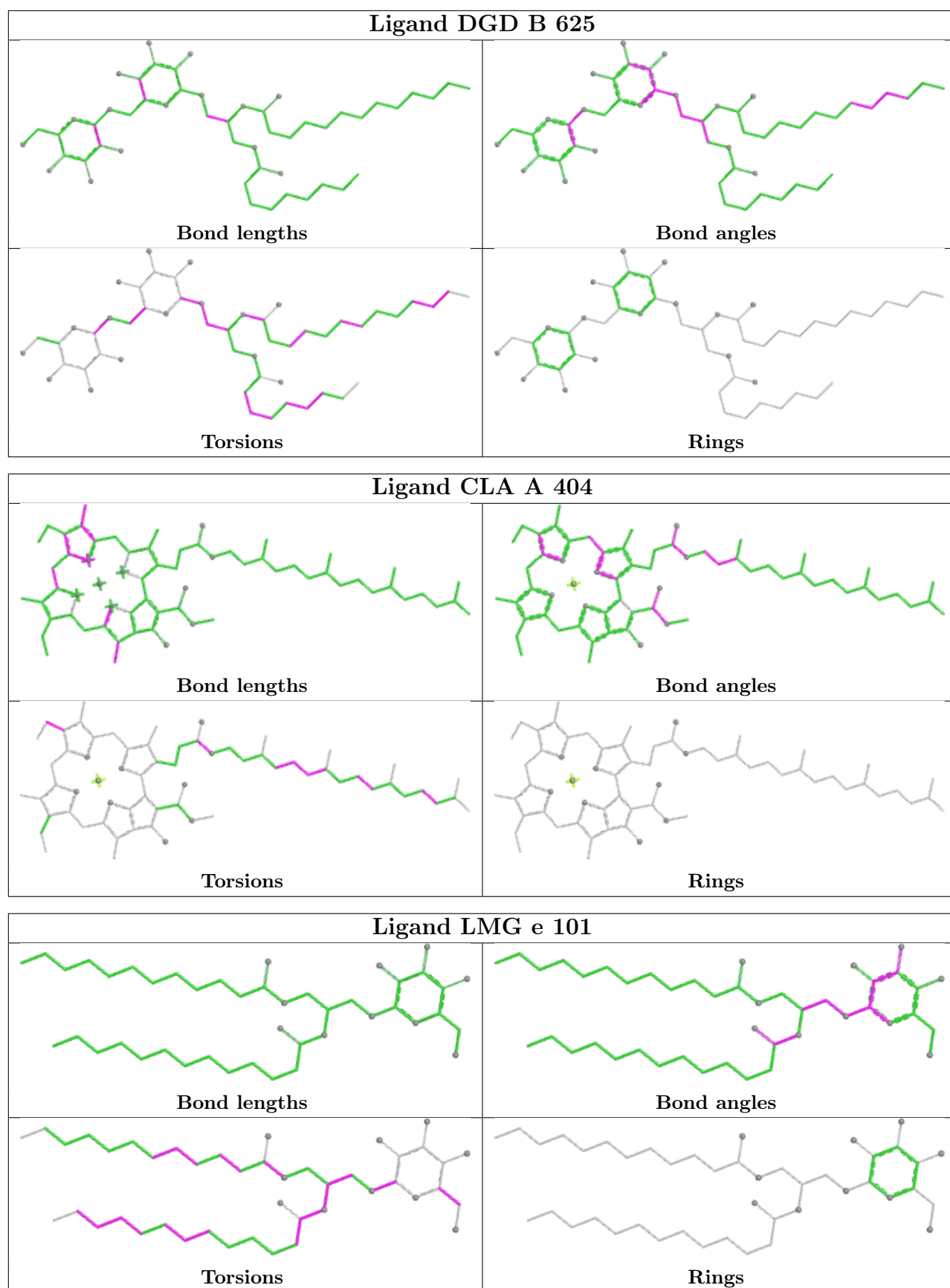
Ligand CLA B 612**Ligand CLA b 613****Ligand CLA B 614**

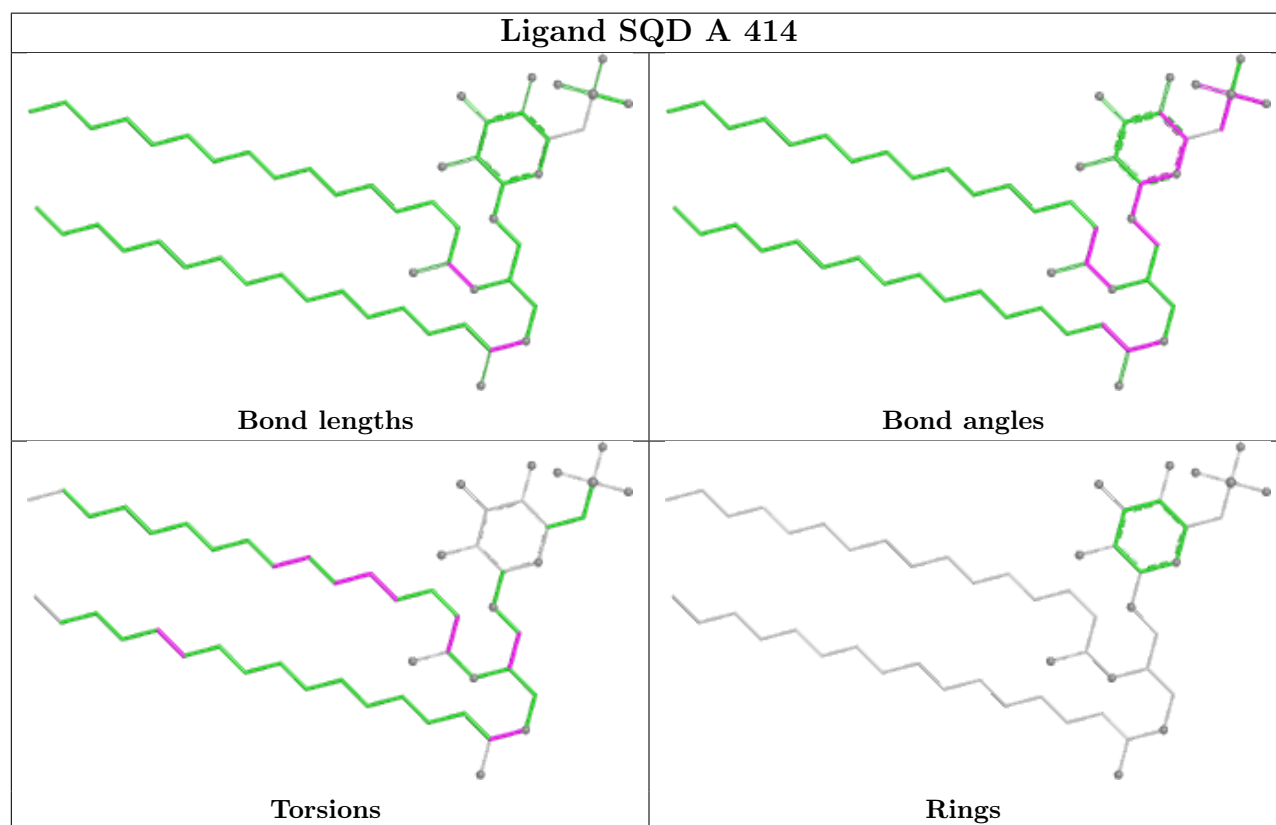
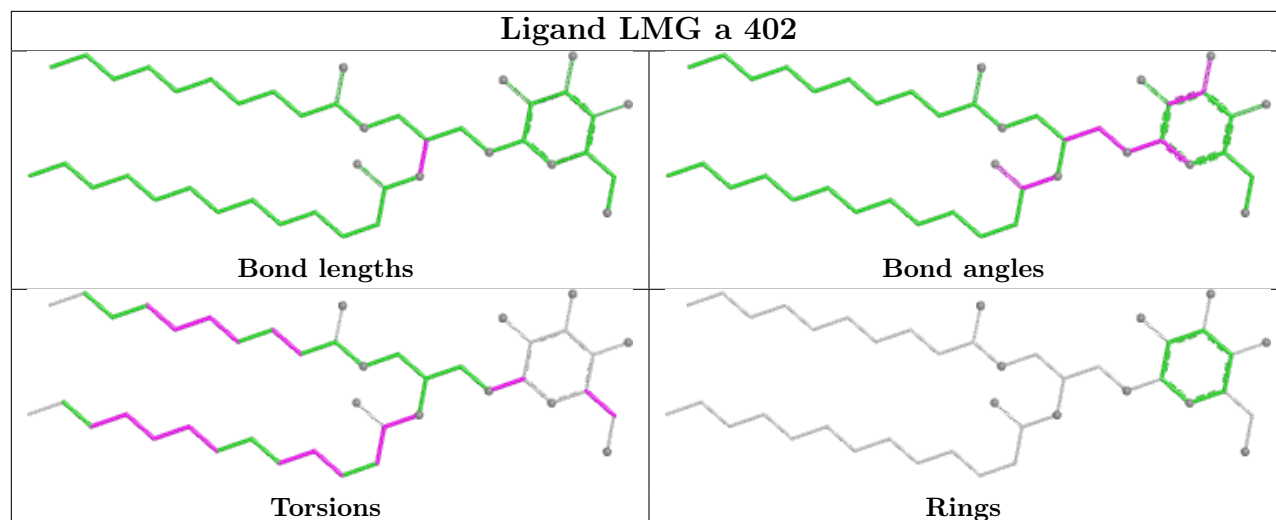


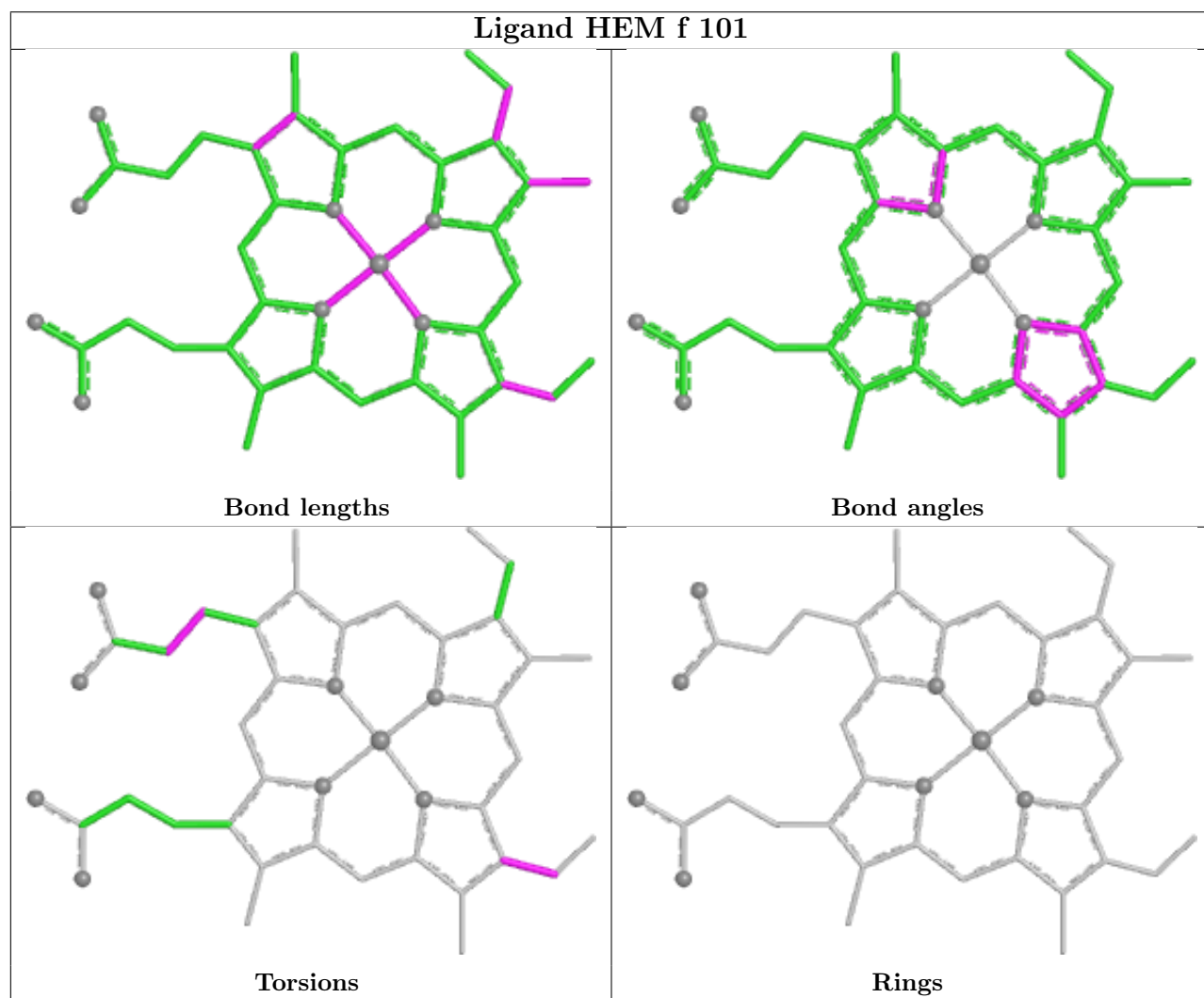
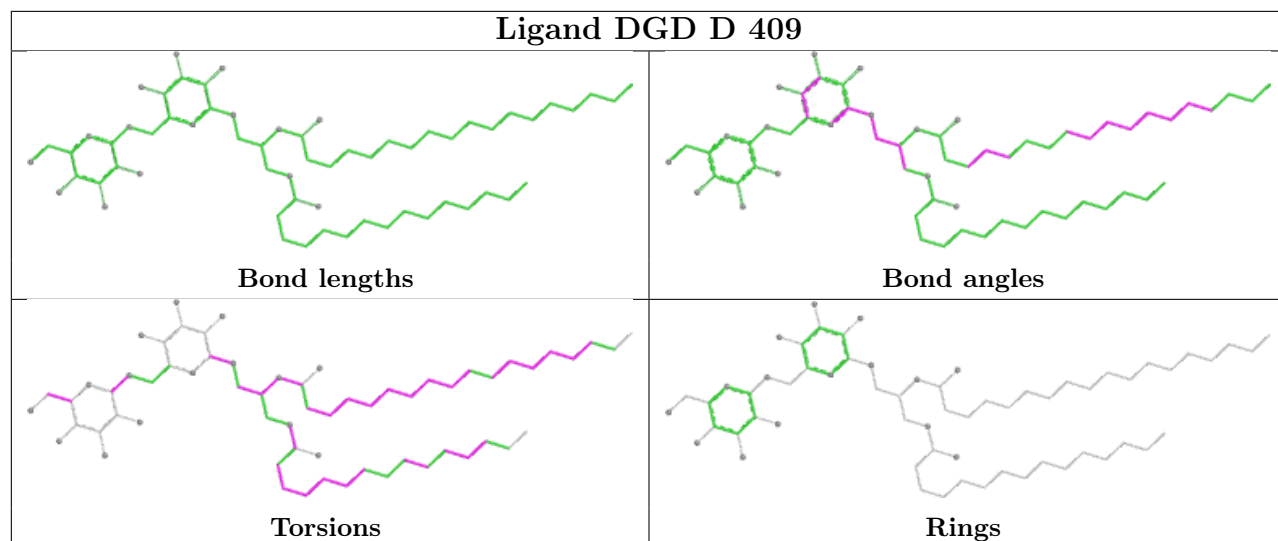
Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

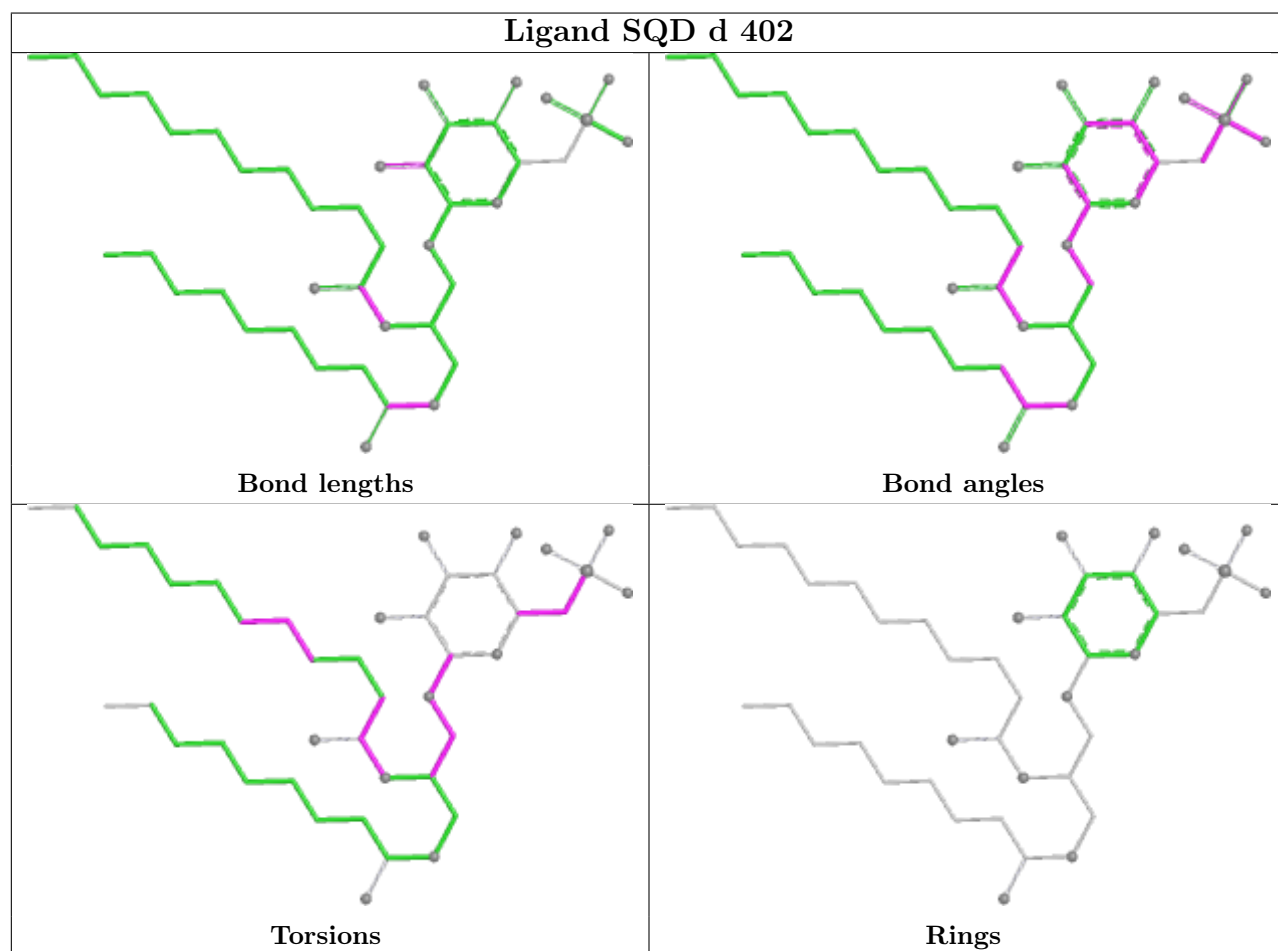
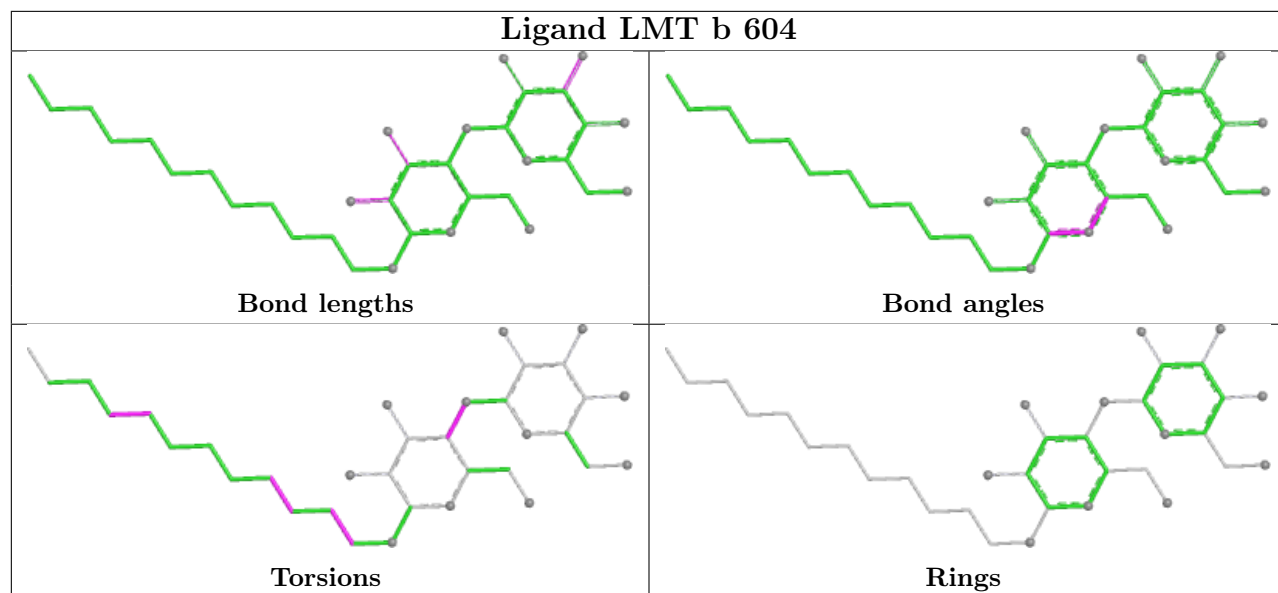
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

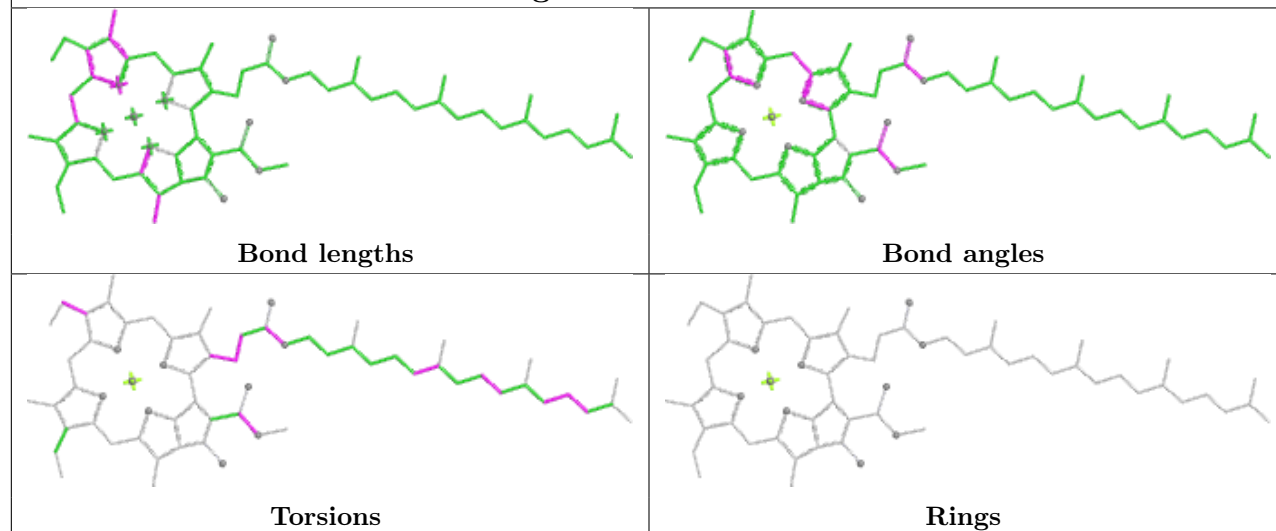




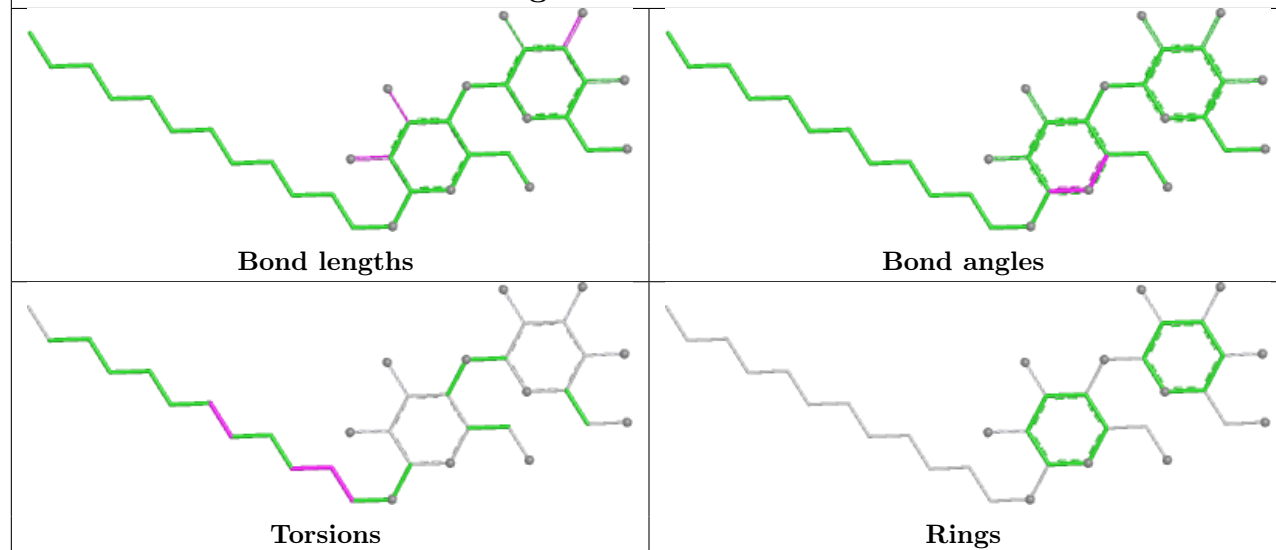




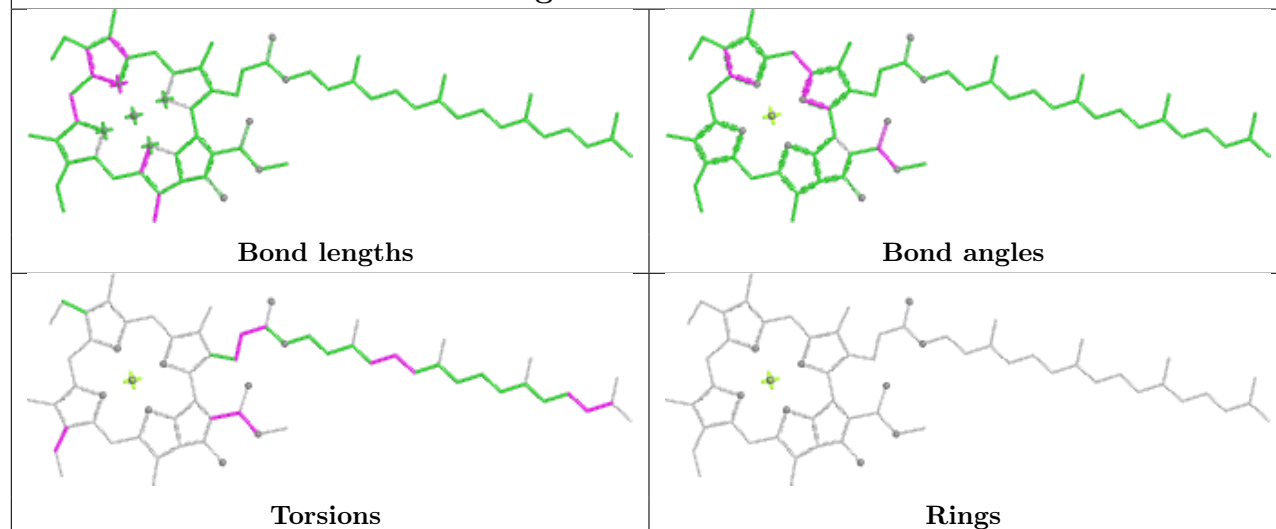
Ligand CLA C 520

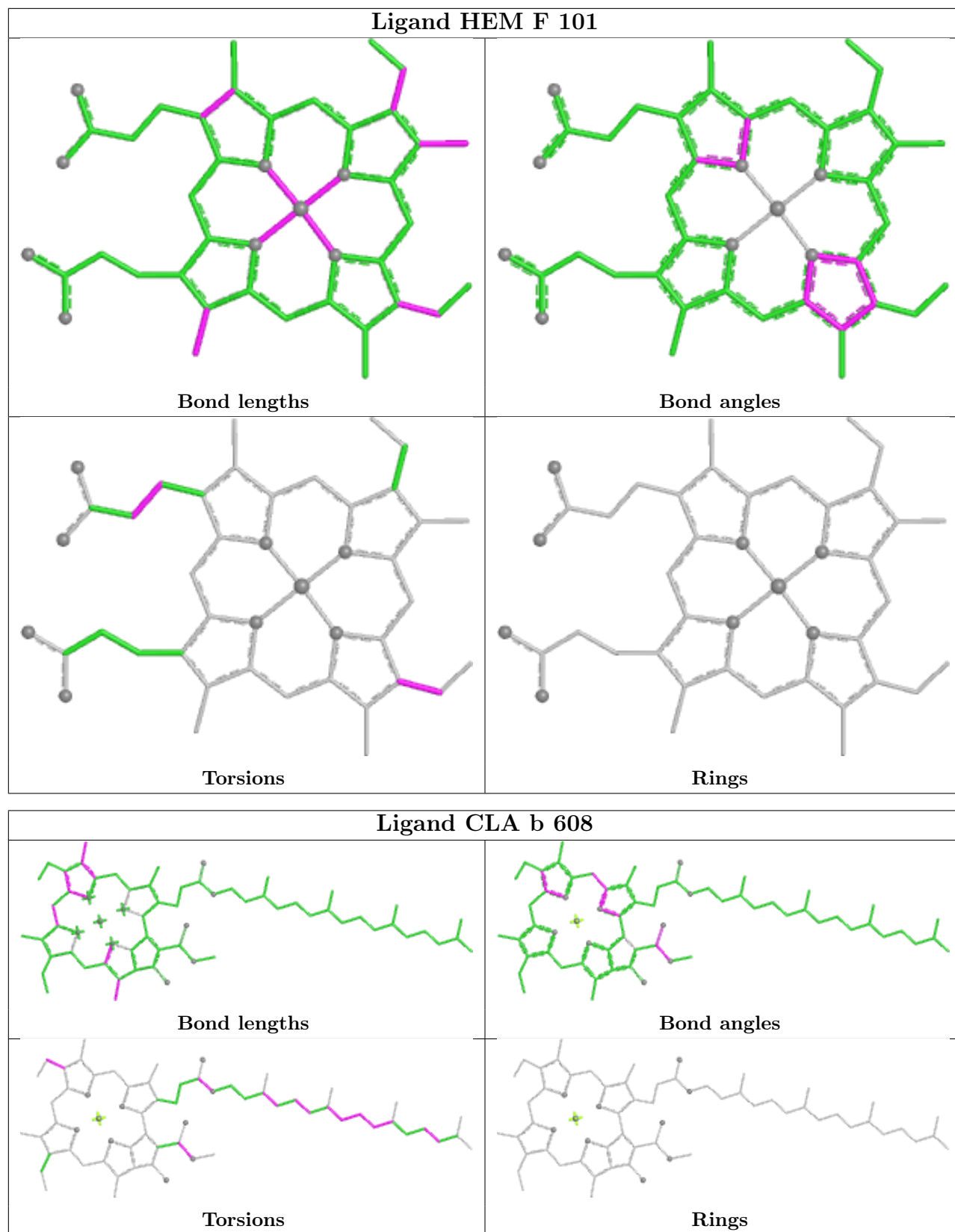


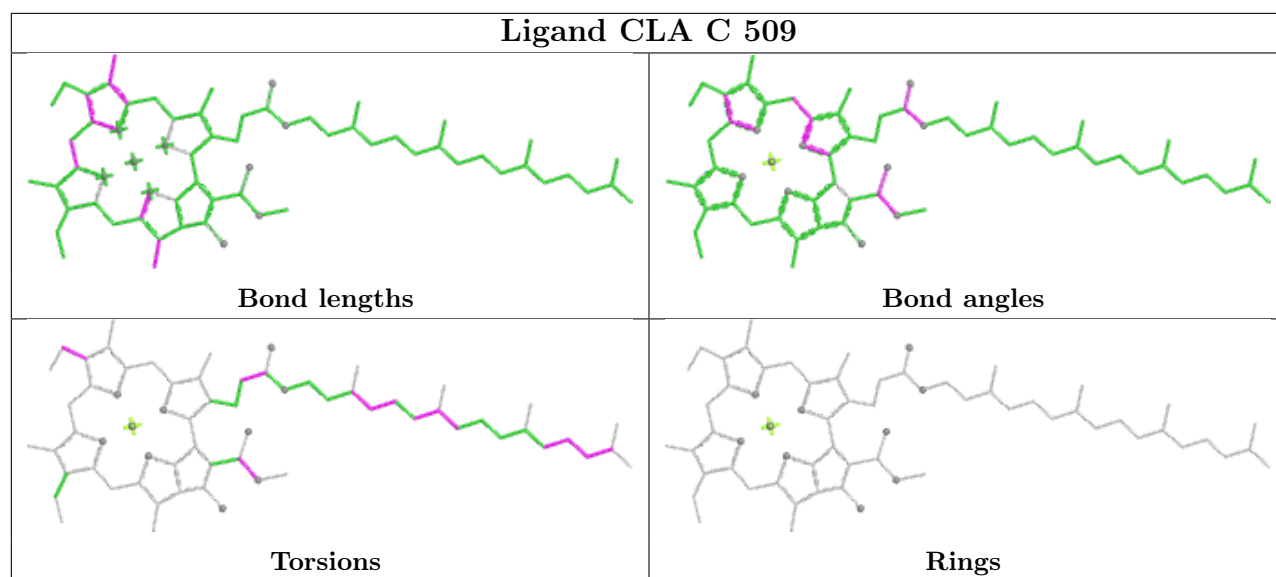
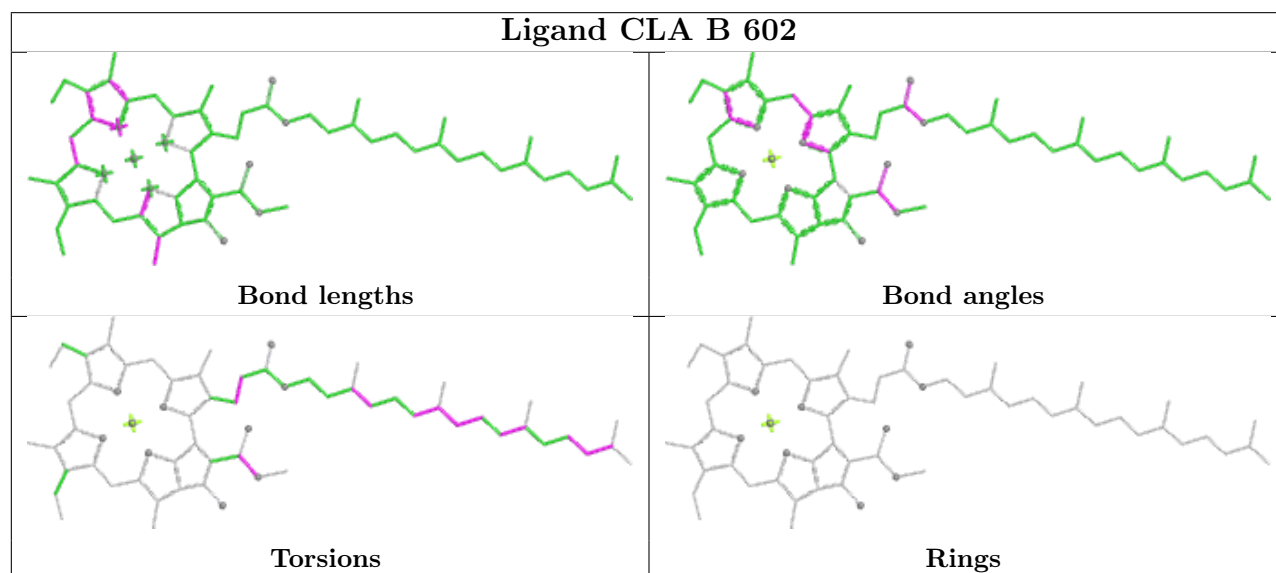
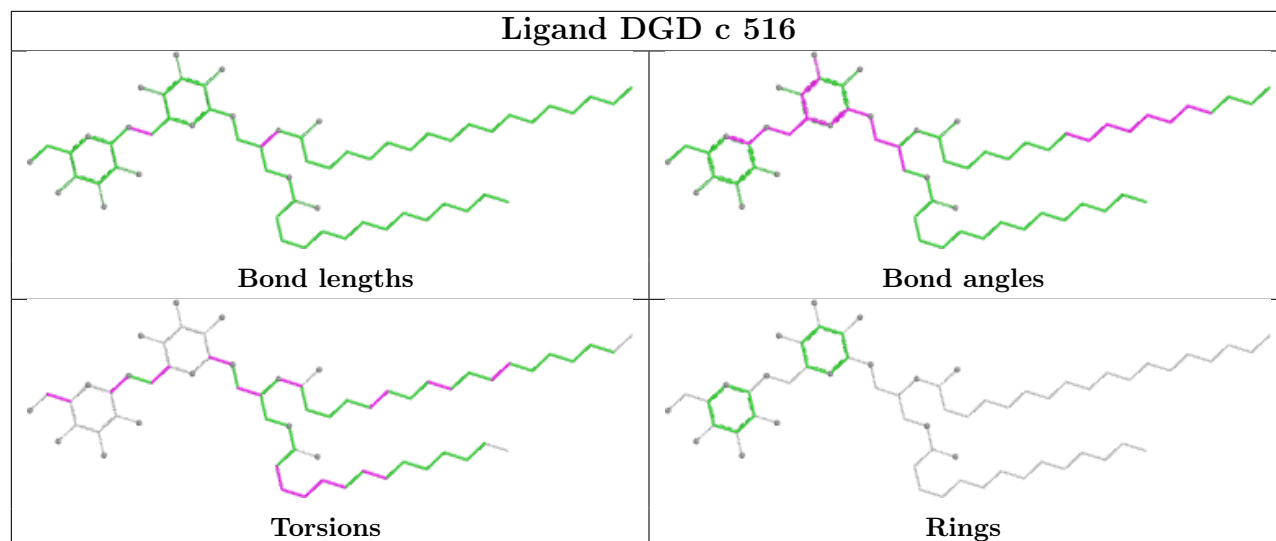
Ligand LMT B 622

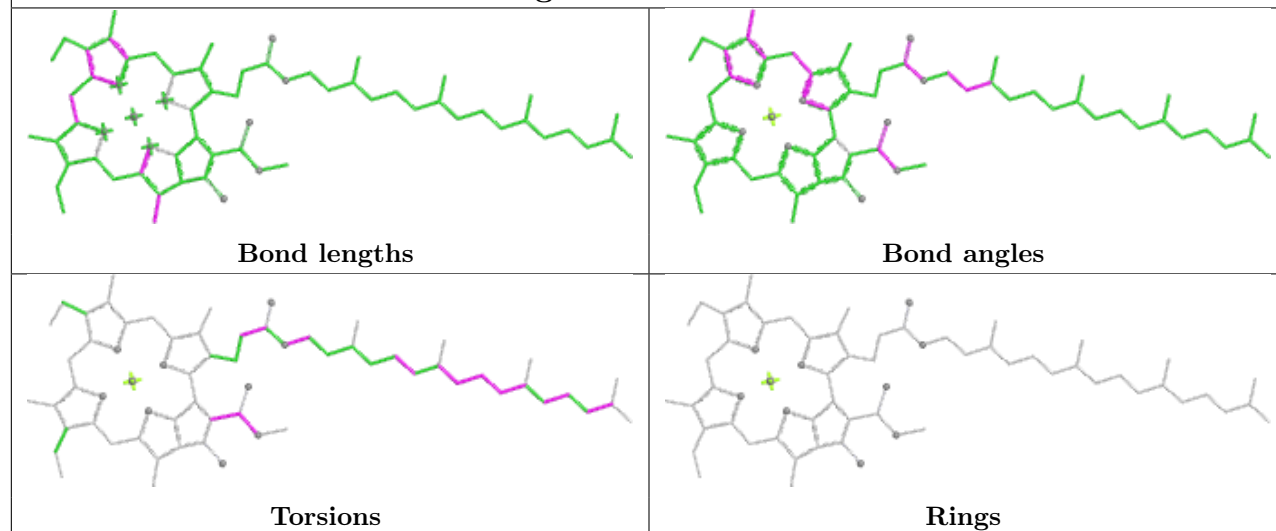
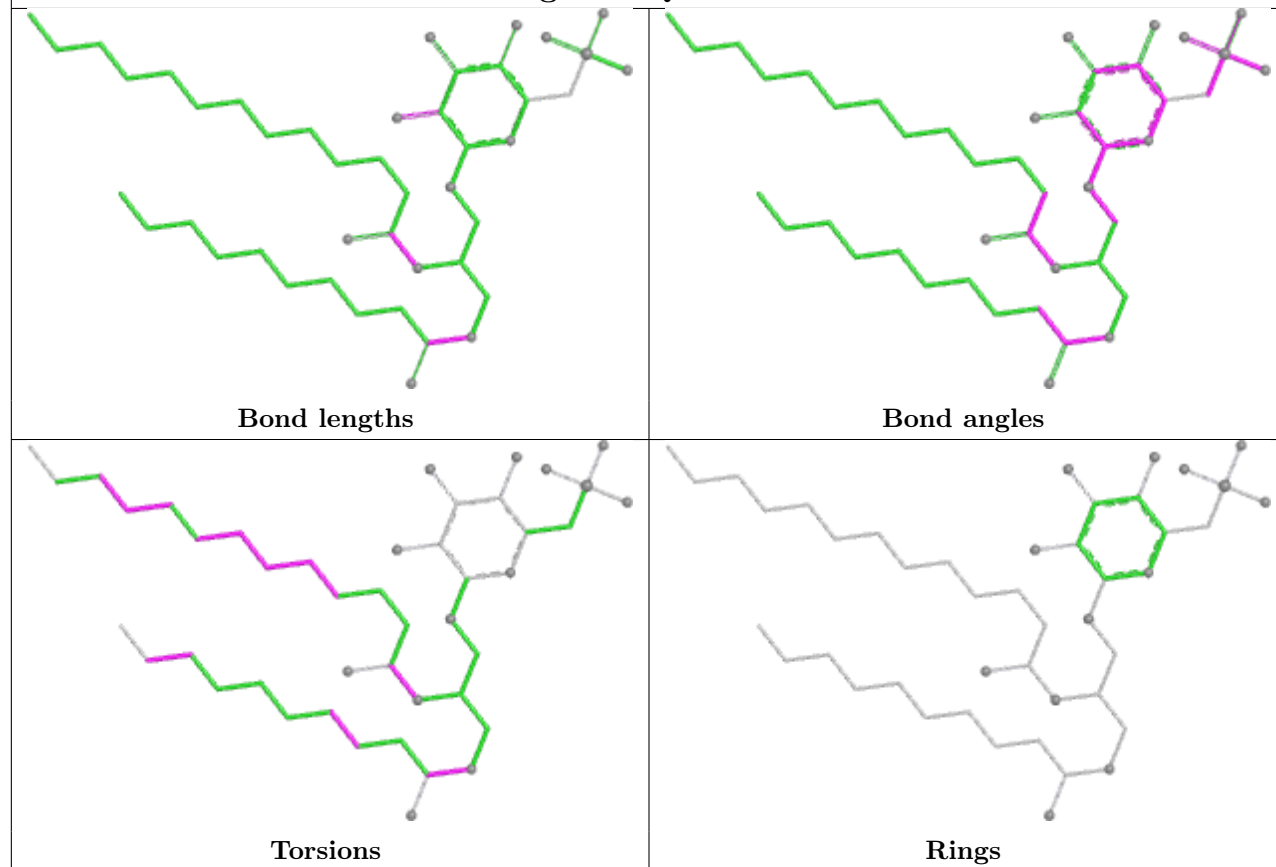


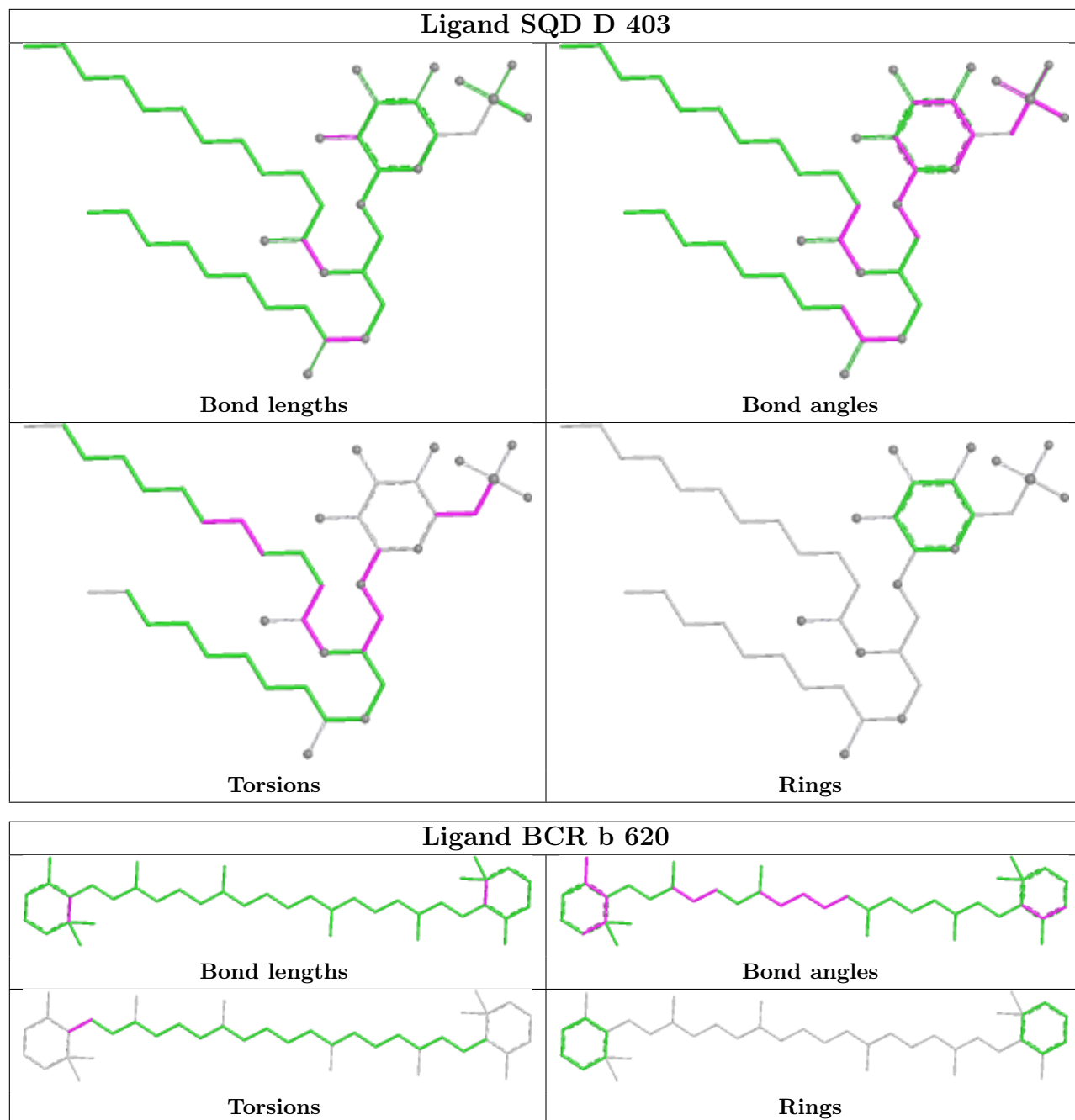
Ligand CLA b 617

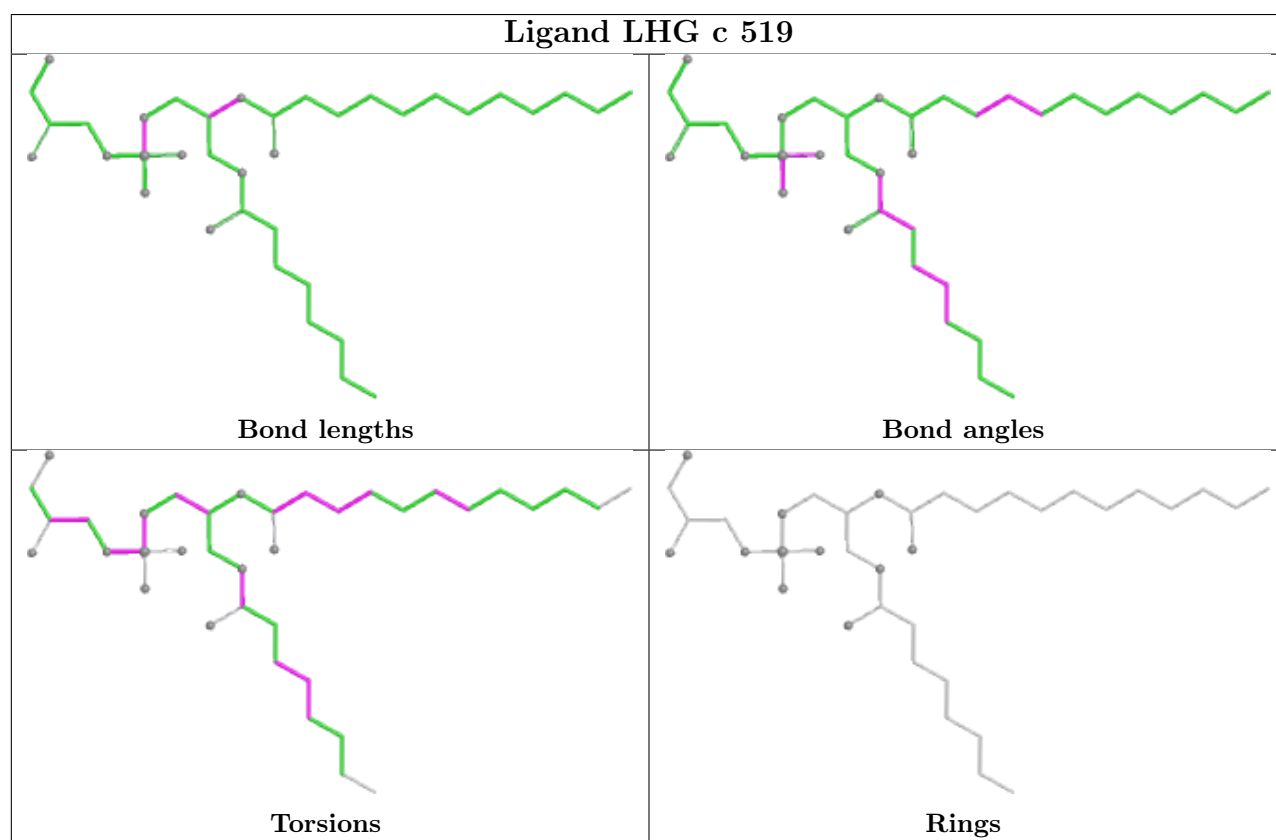
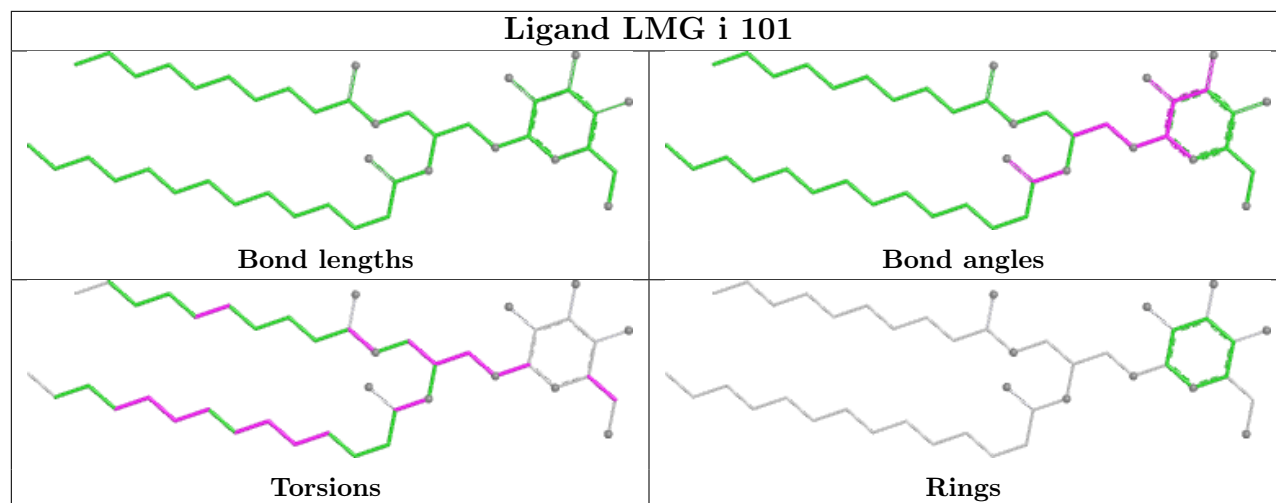


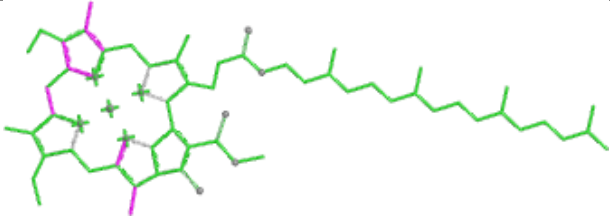
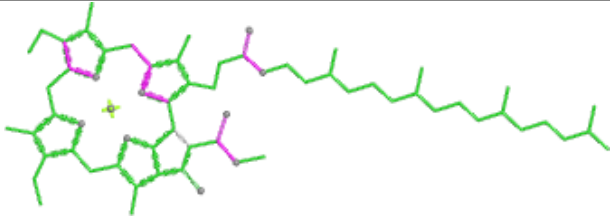
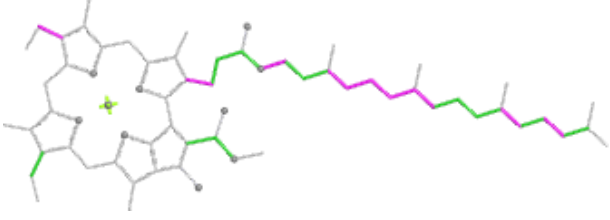
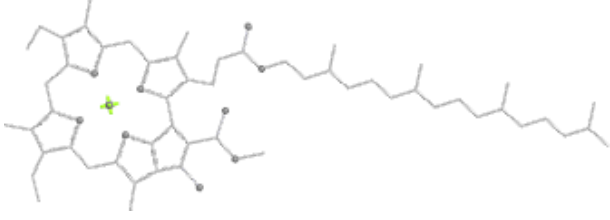
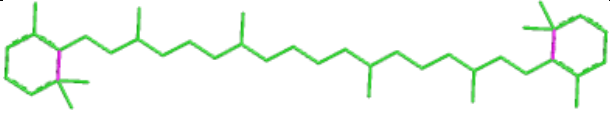
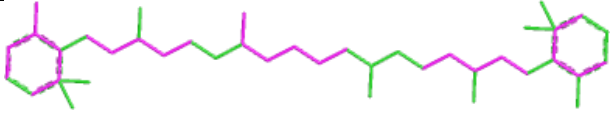
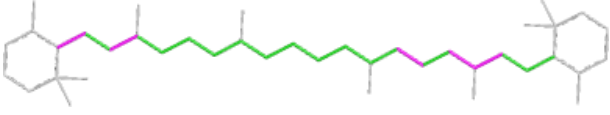
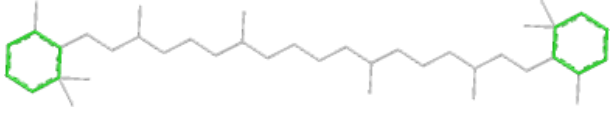
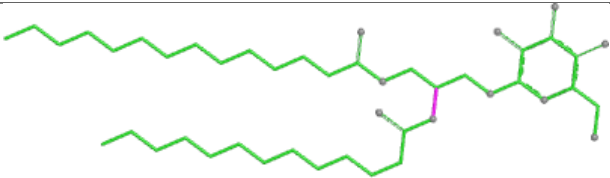
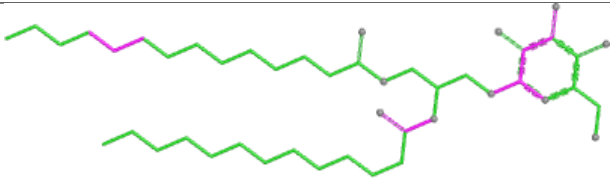
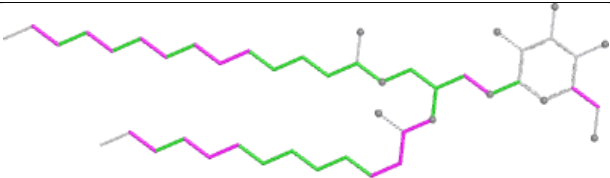
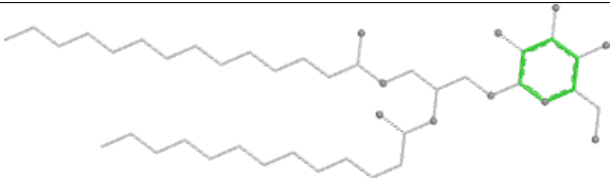


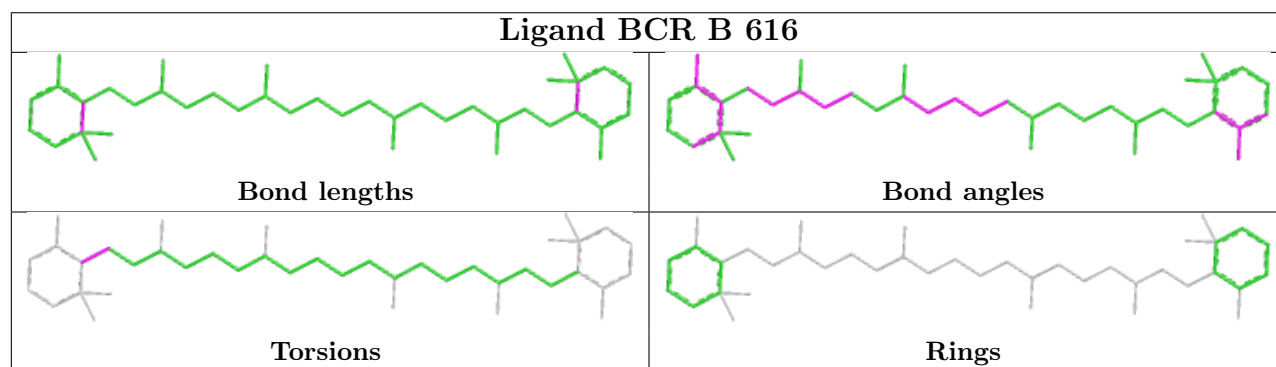
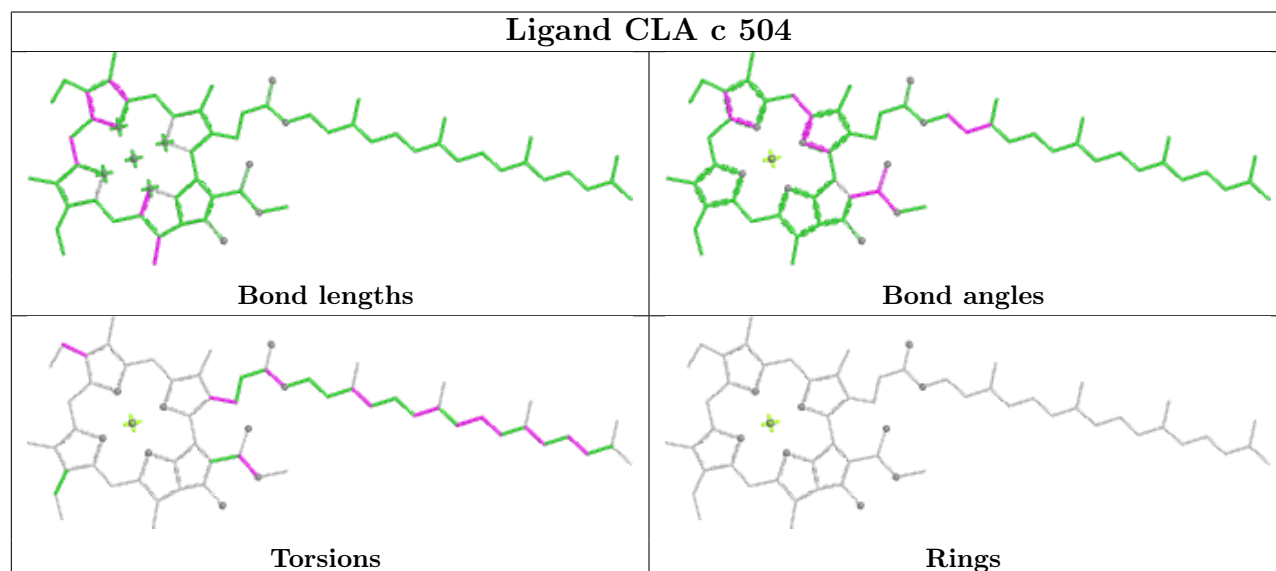
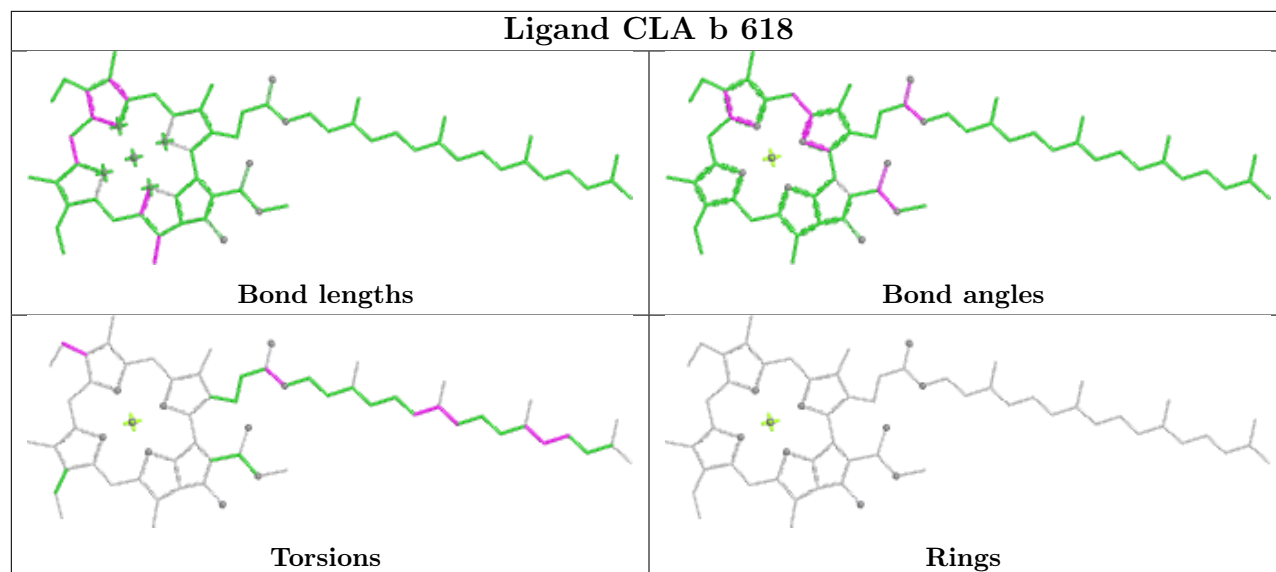


Ligand CLA b 616**Ligand SQD f 103**

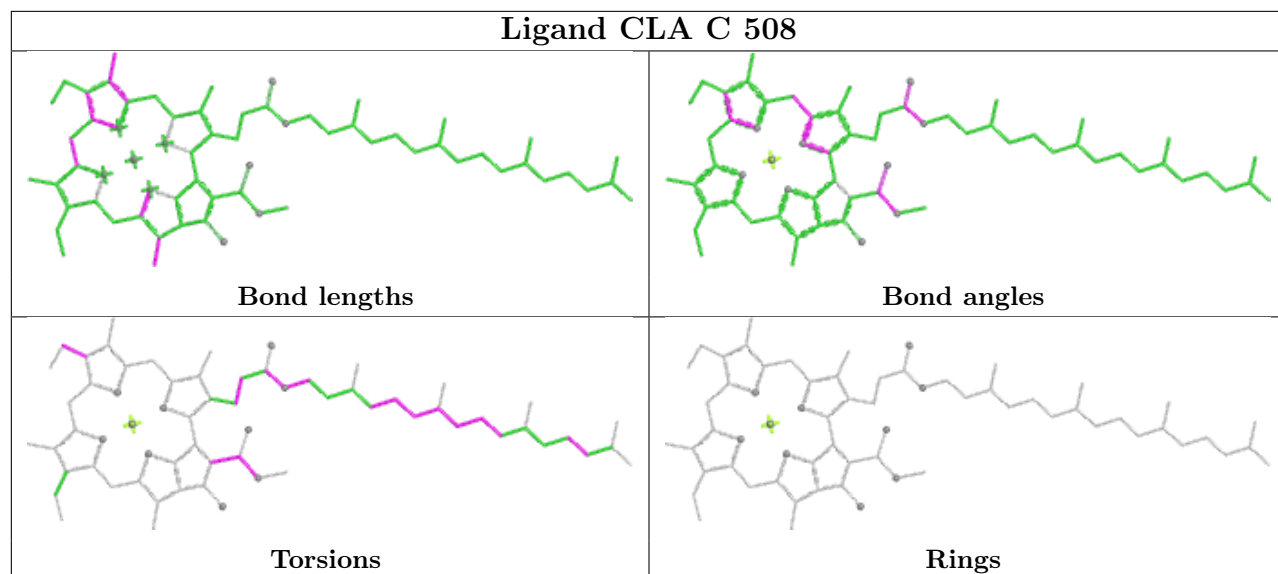




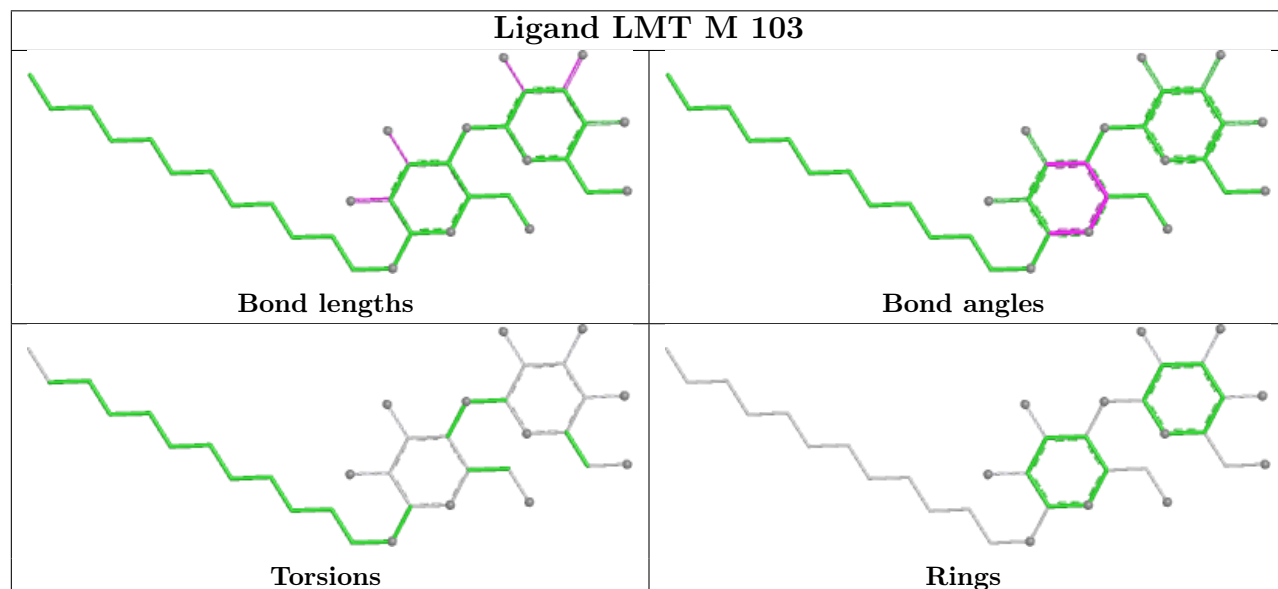
Ligand CLA A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR j 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings



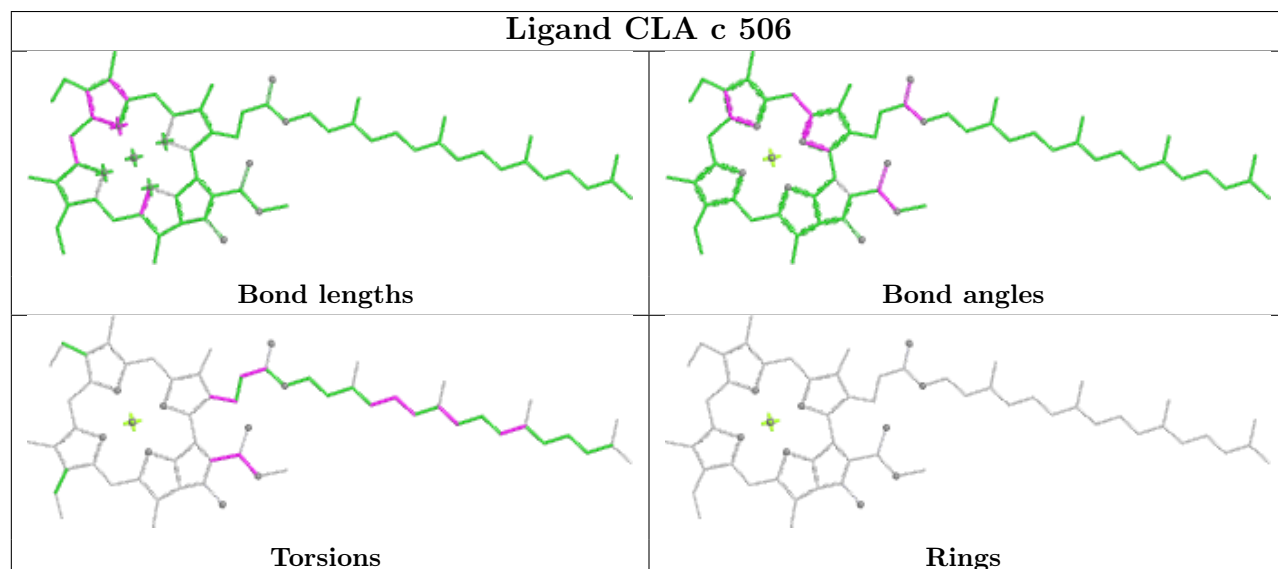
Ligand CLA C 508



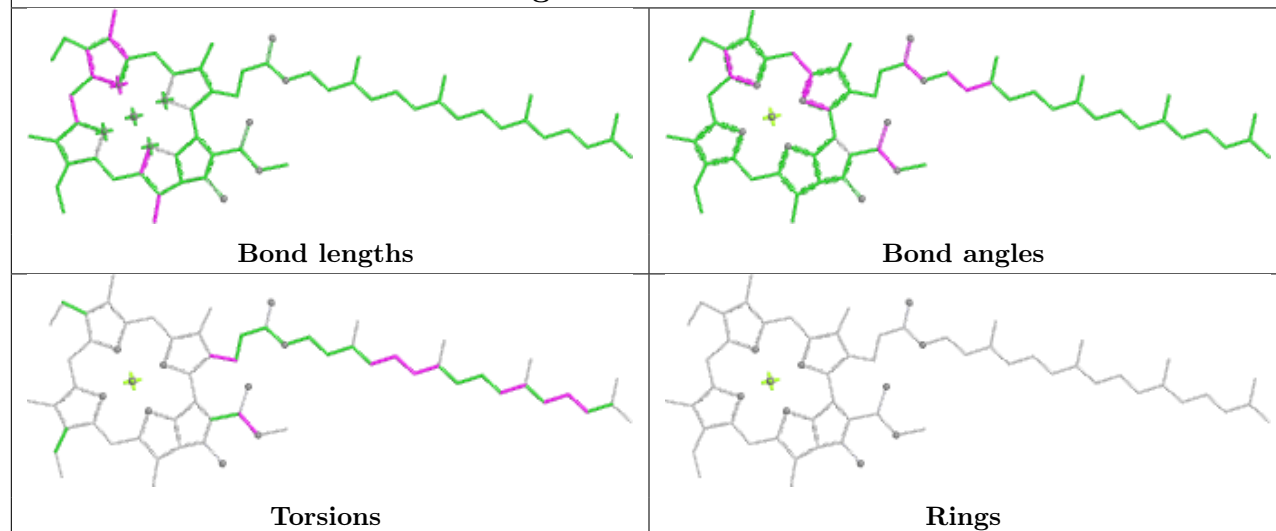
Ligand LMT M 103



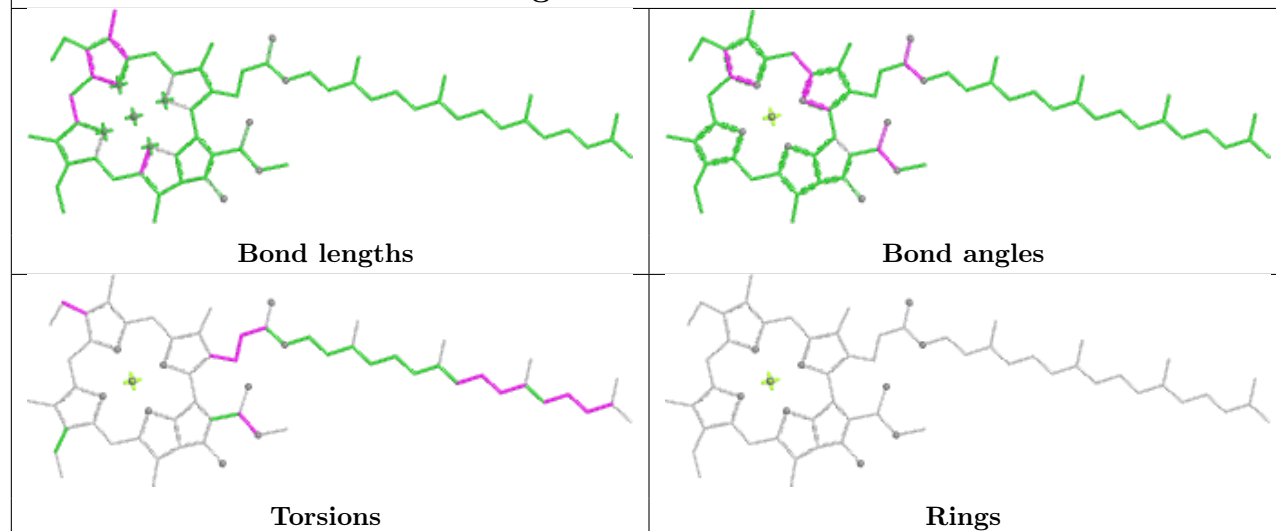
Ligand CLA c 506



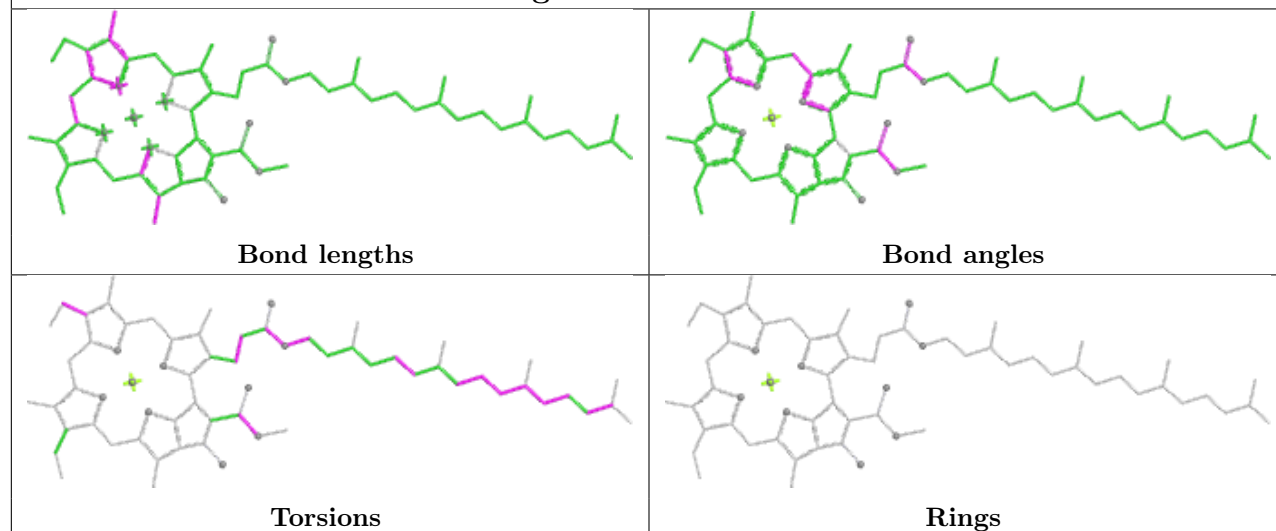
Ligand CLA B 607

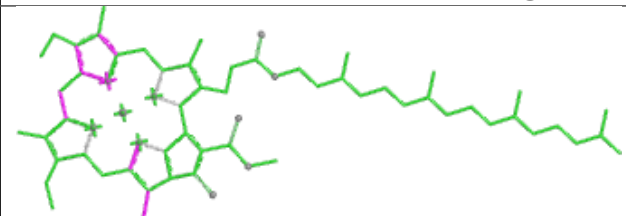
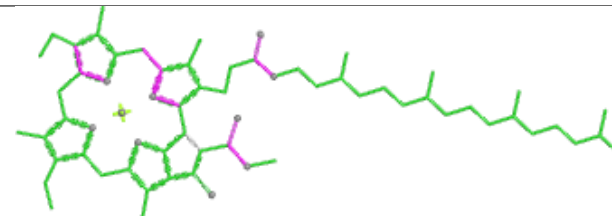
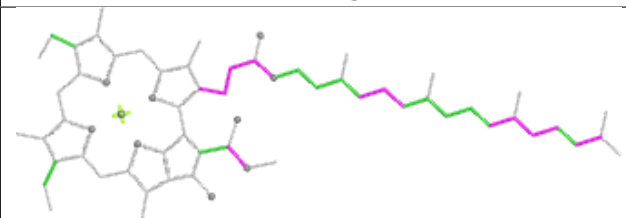
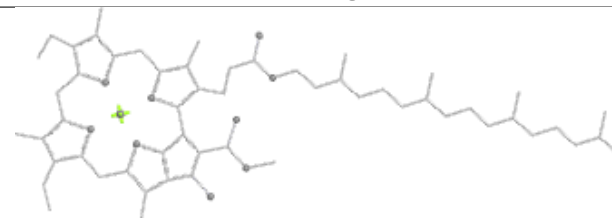


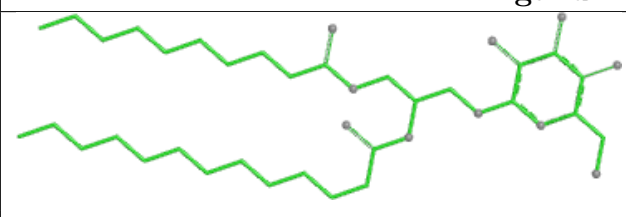
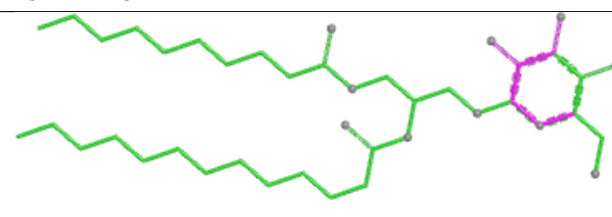
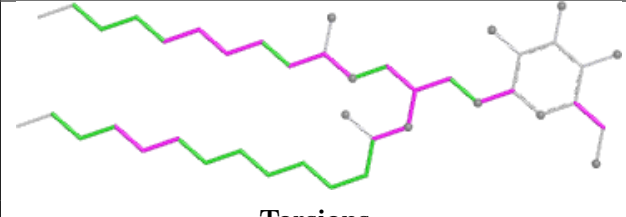
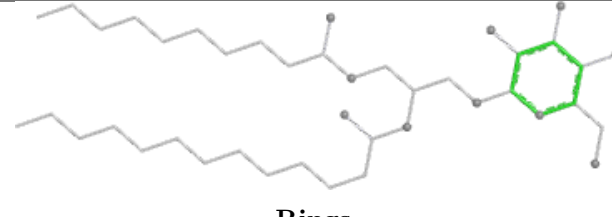
Ligand CLA C 501

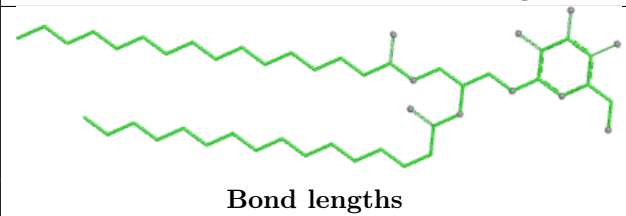
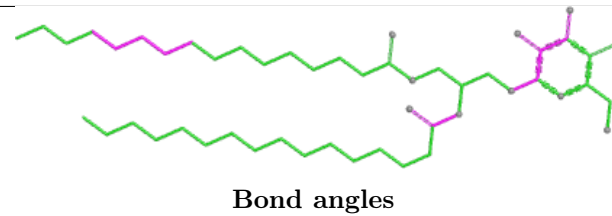
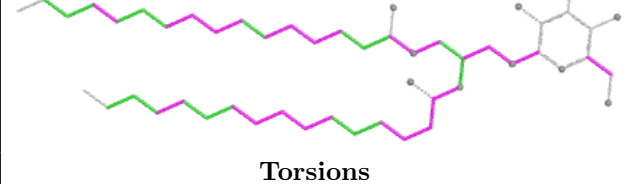
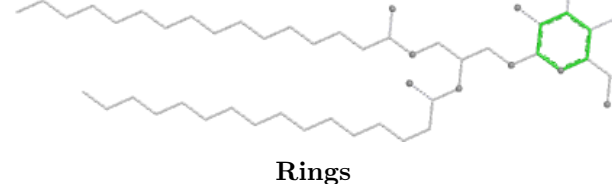


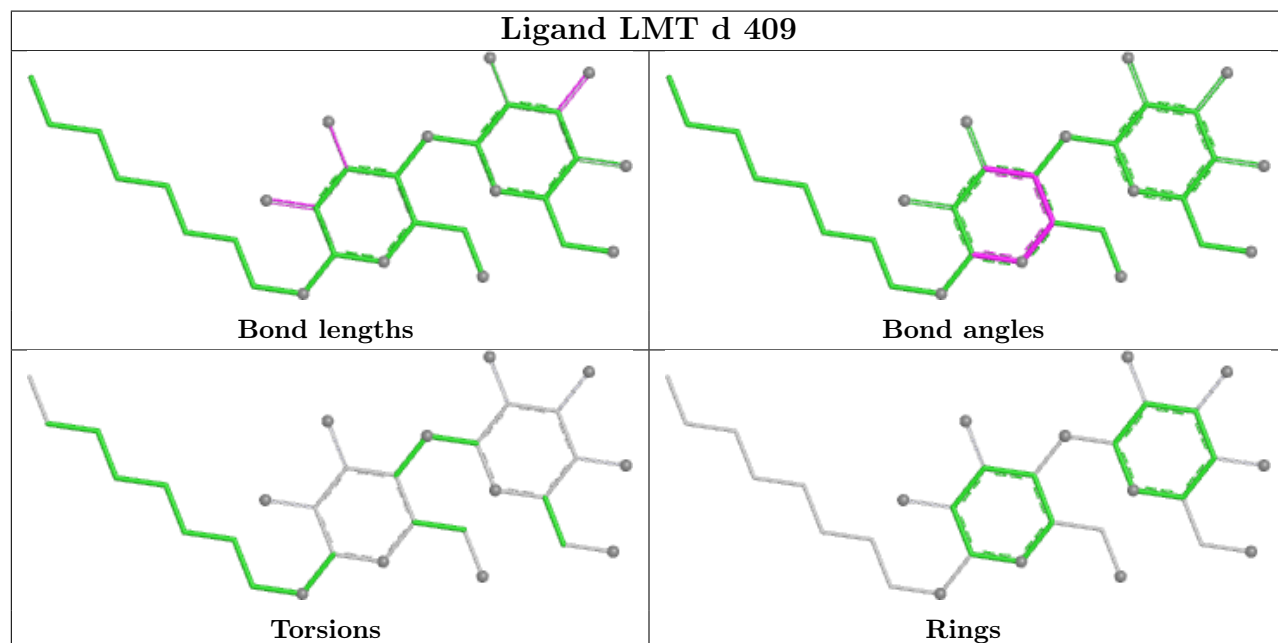
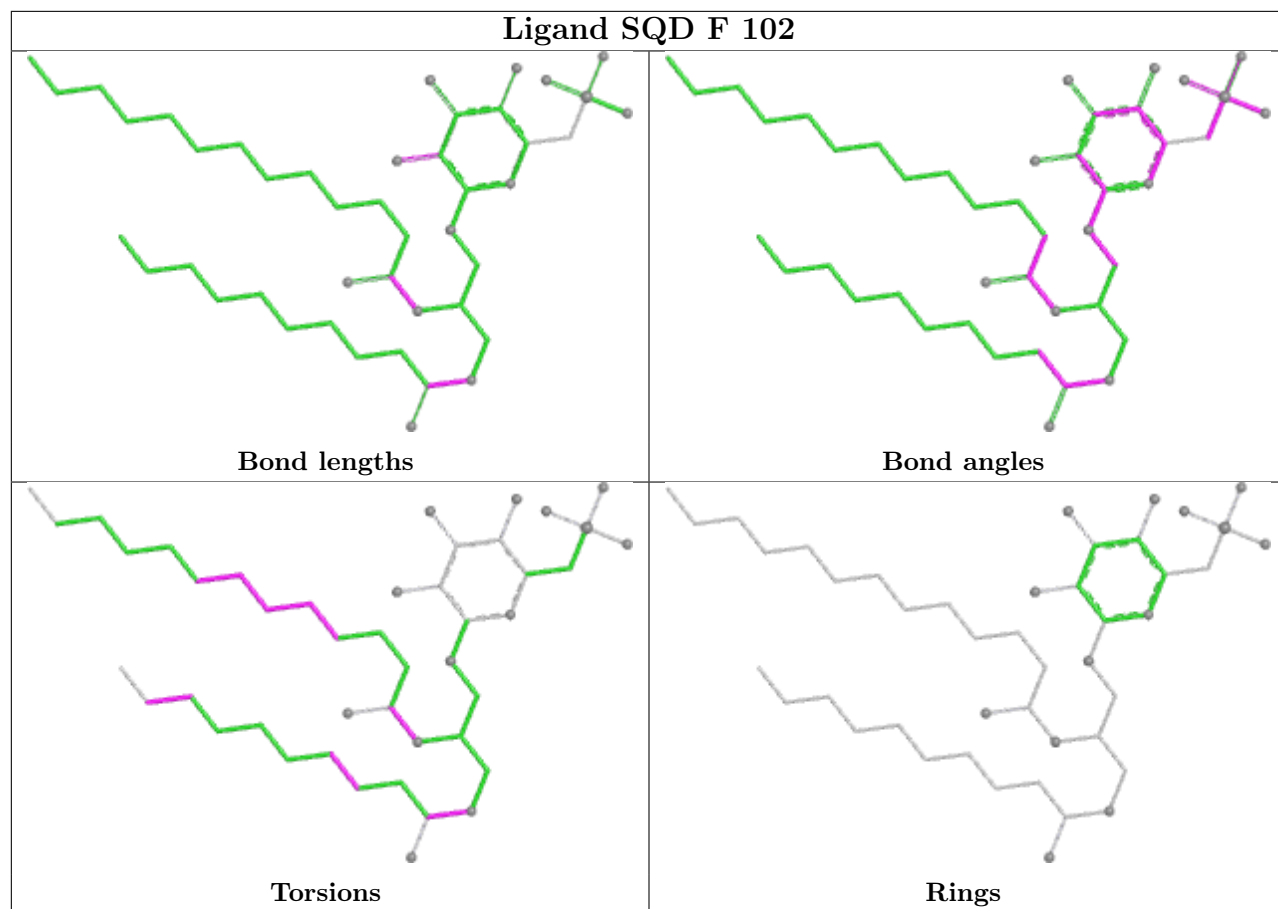
Ligand CLA B 609

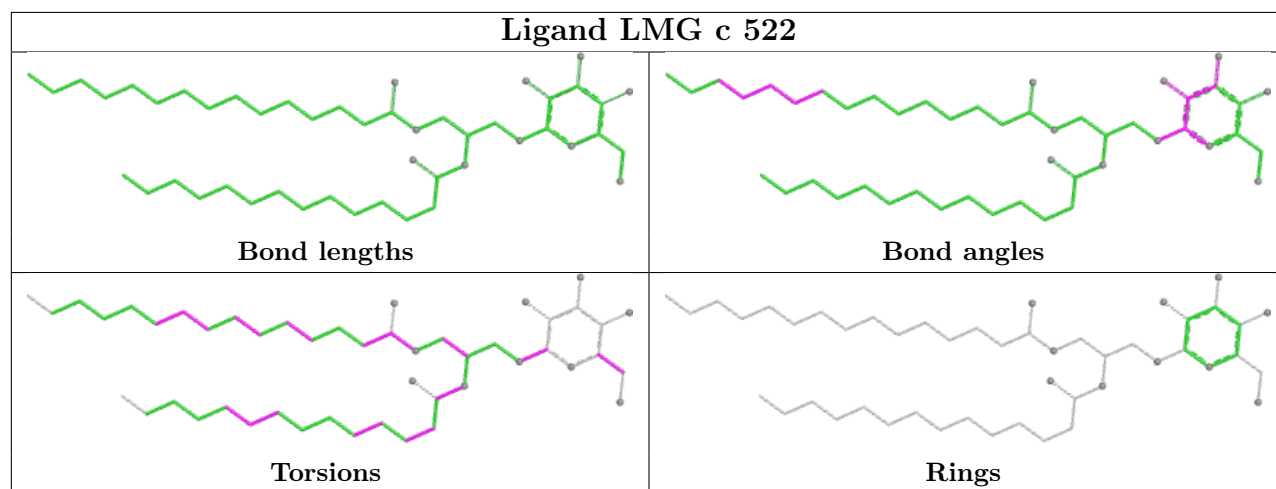
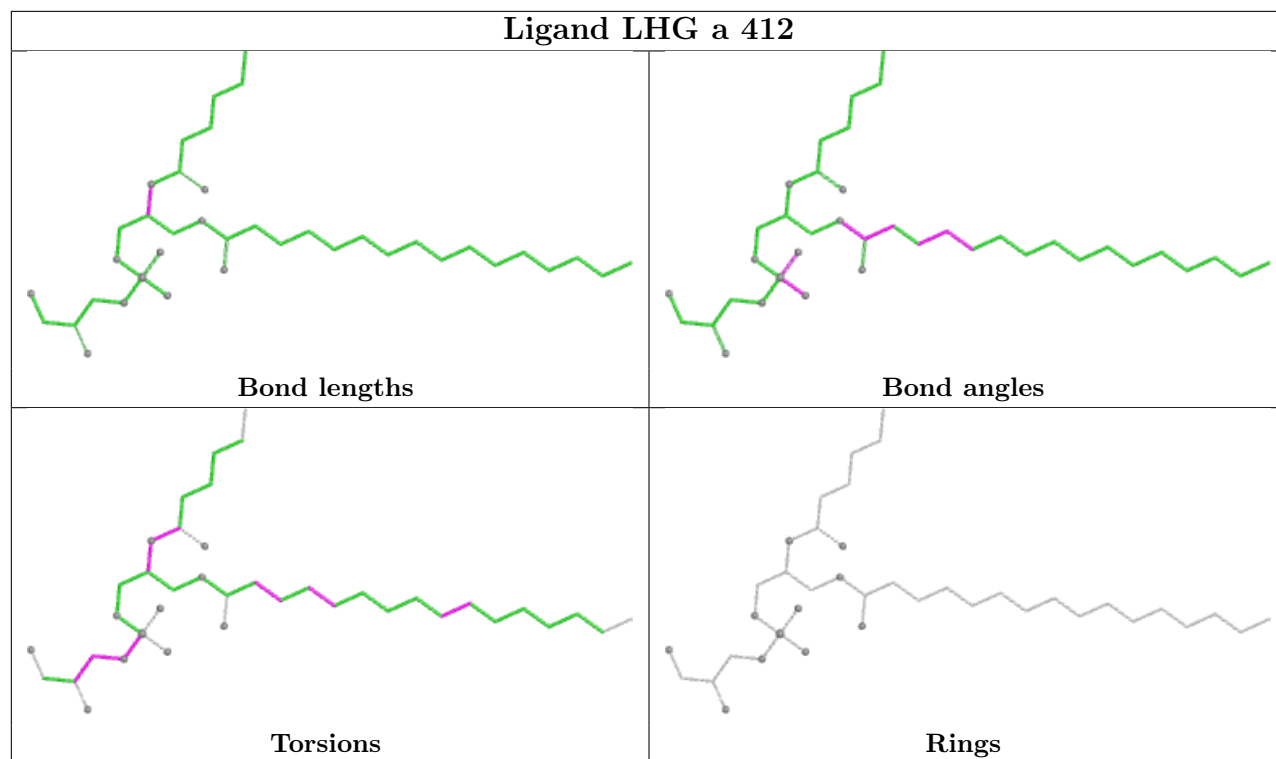


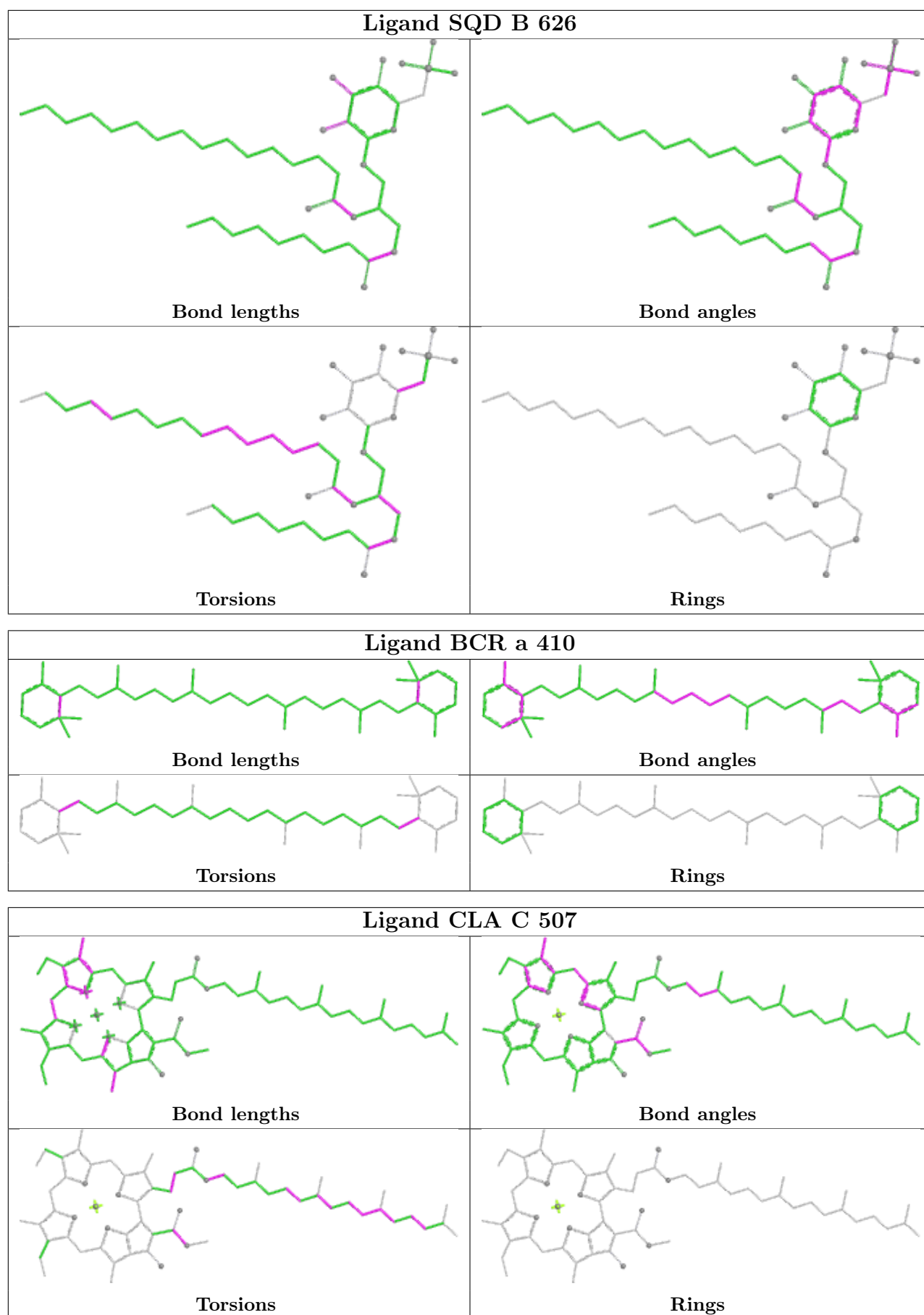
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

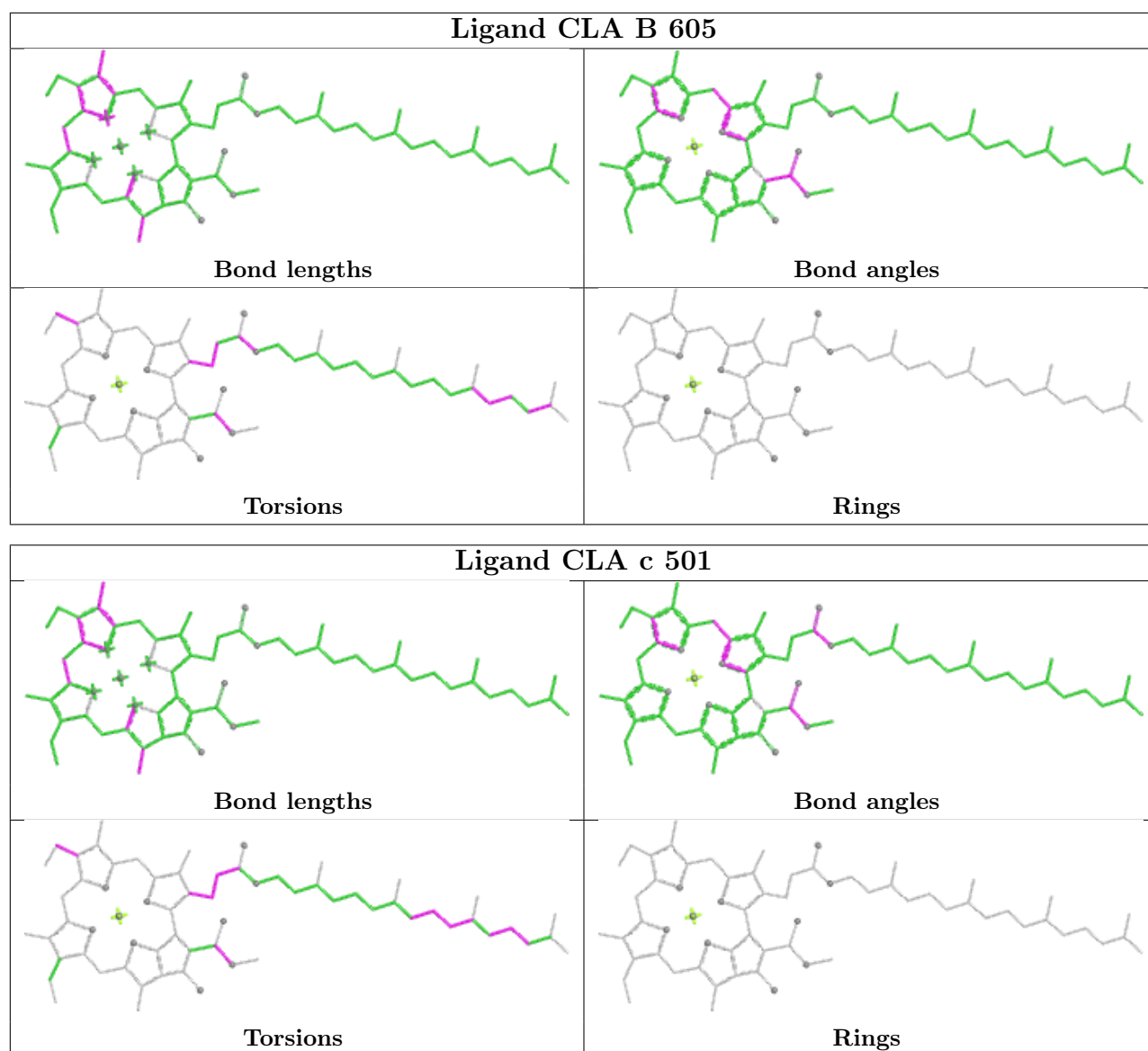
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 410	
	
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	335/344 (97%)	0.12	8 (2%) 59 47	172, 174, 175, 176	0
1	a	335/344 (97%)	0.03	6 (1%) 67 53	172, 174, 175, 176	0
2	B	490/510 (96%)	-0.02	4 (0%) 82 69	172, 174, 175, 176	0
2	b	490/510 (96%)	0.00	9 (1%) 67 53	172, 174, 175, 176	0
3	C	447/461 (96%)	0.04	6 (1%) 75 60	172, 174, 175, 176	0
3	c	447/461 (96%)	-0.10	2 (0%) 88 77	173, 174, 175, 176	0
4	D	340/352 (96%)	0.08	5 (1%) 72 57	171, 174, 175, 176	0
4	d	340/352 (96%)	-0.01	10 (2%) 53 42	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.03	2 (2%) 59 47	172, 174, 175, 175	0
5	e	82/84 (97%)	-0.21	0 100 100	173, 174, 175, 177	0
6	F	35/45 (77%)	0.12	2 (5%) 29 29	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.21	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.13	0 100 100	173, 174, 175, 176	0
7	h	65/66 (98%)	0.15	1 (1%) 72 57	173, 174, 175, 176	0
8	I	35/38 (92%)	-0.17	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	0.05	1 (2%) 53 42	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.14	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	0.06	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.05	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	-0.08	0 100 100	174, 174, 175, 176	0
11	L	37/37 (100%)	0.09	0 100 100	172, 174, 175, 175	0
11	l	37/37 (100%)	0.11	0 100 100	173, 174, 175, 176	0
12	M	34/36 (94%)	0.13	1 (2%) 53 42	172, 174, 174, 176	0
12	m	34/36 (94%)	0.27	3 (8%) 15 19	173, 173, 174, 175	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.09	5 (2%) 63 50	172, 174, 175, 176	0
13	o	243/272 (89%)	0.06	4 (1%) 70 55	172, 174, 175, 176	0
14	T	32/32 (100%)	0.01	0 100 100	173, 174, 176, 176	0
14	t	32/32 (100%)	0.15	0 100 100	173, 174, 175, 176	0
15	U	97/134 (72%)	0.26	4 (4%) 41 36	172, 174, 174, 175	0
15	u	97/134 (72%)	0.19	1 (1%) 79 64	173, 174, 175, 175	0
16	V	137/163 (84%)	0.18	3 (2%) 62 49	172, 174, 175, 175	0
16	v	137/163 (84%)	0.06	2 (1%) 72 57	173, 174, 175, 176	0
17	g	28/46 (60%)	0.21	0 100 100	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.11	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	-0.02	0 100 100	173, 174, 175, 176	0
18	x	37/41 (90%)	0.13	0 100 100	173, 174, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.17	1 (1%) 70 55	173, 174, 175, 176	0
20	z	62/62 (100%)	-0.12	0 100 100	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.03	80 (1%) 72 57	171, 174, 175, 177	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	309	LEU	4.9
15	U	39	LEU	4.8
13	O	195	ASP	4.6
15	U	40	VAL	4.5
1	A	265	PHE	4.4

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
31	LMT	b	627	35/35	0.44	0.19	173,175,177,177	0
31	LMT	I	102	35/35	0.51	0.18	173,175,176,178	0
31	LMT	d	409	31/35	0.52	0.18	172,175,177,177	0
22	CLA	b	605	65/65	0.55	0.22	172,175,176,176	0
22	CLA	B	601	65/65	0.57	0.20	172,175,176,177	0
31	LMT	b	626	35/35	0.58	0.17	172,175,176,177	0
31	LMT	D	410	31/35	0.59	0.15	174,175,176,176	0
31	LMT	i	102	35/35	0.63	0.17	173,175,176,177	0
31	LMT	B	622	35/35	0.64	0.16	171,175,177,177	0
22	CLA	b	619	65/65	0.69	0.18	172,174,175,175	0
27	LMG	C	518	45/55	0.70	0.19	171,174,175,175	0
24	BCR	j	102	40/40	0.72	0.29	173,175,177,178	0
25	DGD	D	409	63/66	0.72	0.21	172,174,176,178	0
33	BCT	d	403	4/4	0.72	0.29	174,174,175,176	0
35	CA	o	301	1/1	0.72	0.14	180,180,180,180	0
24	BCR	J	102	40/40	0.73	0.28	172,174,176,177	0
31	LMT	B	627	35/35	0.73	0.14	172,175,177,177	0
31	LMT	B	628	35/35	0.75	0.18	172,174,177,178	0
35	CA	O	301	1/1	0.76	0.12	177,177,177,177	0
22	CLA	C	506	65/65	0.76	0.20	172,174,175,175	0
25	DGD	d	408	63/66	0.77	0.20	172,175,177,178	0
25	DGD	B	625	52/66	0.77	0.18	172,175,177,177	0
30	SQD	B	626	47/54	0.77	0.16	170,174,176,178	0
31	LMT	b	604	35/35	0.78	0.22	172,174,176,176	0
27	LMG	I	101	43/55	0.78	0.18	172,174,177,177	0
31	LMT	B	623	35/35	0.78	0.14	173,174,177,177	0
22	CLA	c	512	65/65	0.78	0.15	172,174,176,176	0
25	DGD	C	516	62/66	0.80	0.16	171,174,175,176	0
26	LHG	C	519	37/49	0.80	0.17	172,174,179,183	0
27	LMG	a	402	42/55	0.80	0.23	171,174,176,176	0
27	LMG	c	518	45/55	0.80	0.15	172,174,176,176	0
30	SQD	A	413	51/54	0.80	0.19	172,174,175,176	0
27	LMG	b	625	49/55	0.81	0.21	172,174,175,175	0
23	PL9	A	406	45/55	0.81	0.26	172,174,175,175	0
31	LMT	M	102	35/35	0.81	0.19	172,174,175,175	0
31	LMT	b	603	35/35	0.81	0.12	172,174,175,176	0
30	SQD	a	401	54/54	0.82	0.19	172,174,176,178	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SQD	d	402	43/54	0.82	0.17	172,174,176,178	0
27	LMG	M	101	42/55	0.82	0.19	173,174,176,176	0
25	DGD	b	601	52/66	0.83	0.18	172,174,176,177	0
25	DGD	c	516	62/66	0.83	0.21	172,174,175,175	0
24	BCR	H	102	40/40	0.83	0.21	173,174,175,176	0
27	LMG	i	101	43/55	0.84	0.16	172,174,177,178	0
25	DGD	C	517	66/66	0.84	0.17	172,173,174,175	0
23	PL9	J	101	35/55	0.84	0.25	172,175,176,176	0
27	LMG	A	415	42/55	0.85	0.21	171,174,176,177	0
30	SQD	F	102	45/54	0.85	0.19	172,175,177,178	0
27	LMG	a	413	51/55	0.85	0.21	172,173,175,176	0
25	DGD	c	517	66/66	0.85	0.21	172,173,175,176	0
27	LMG	E	101	44/55	0.86	0.19	170,174,176,177	0
27	LMG	c	522	48/55	0.86	0.23	172,174,175,176	0
27	LMG	e	101	44/55	0.86	0.17	171,174,175,176	0
22	CLA	c	506	65/65	0.86	0.16	173,174,175,175	0
26	LHG	c	519	37/49	0.86	0.16	172,174,178,181	0
24	BCR	c	521	40/40	0.87	0.16	172,174,175,175	0
30	SQD	b	602	47/54	0.87	0.15	171,174,176,178	0
27	LMG	m	101	42/55	0.87	0.19	170,174,175,175	0
24	BCR	a	410	40/40	0.87	0.20	172,173,174,175	0
31	LMT	M	103	35/35	0.87	0.17	172,173,175,176	0
25	DGD	A	408	56/66	0.87	0.17	172,174,175,176	0
24	BCR	c	514	40/40	0.87	0.22	172,173,175,175	0
27	LMG	D	408	48/55	0.88	0.17	170,173,175,175	0
22	CLA	C	504	65/65	0.88	0.18	171,173,175,175	0
22	CLA	c	501	65/65	0.88	0.15	172,174,175,175	0
25	DGD	b	624	58/66	0.88	0.20	171,173,174,175	0
30	SQD	a	415	51/54	0.88	0.17	173,174,175,176	0
23	PL9	j	101	35/55	0.88	0.25	173,175,175,176	0
24	BCR	x	101	40/40	0.88	0.18	173,174,175,175	0
28	CL	A	411	1/1	0.88	0.13	172,172,172,172	0
22	CLA	C	512	65/65	0.89	0.12	172,174,176,177	0
24	BCR	B	619	40/40	0.89	0.16	172,173,174,175	0
24	BCR	C	521	40/40	0.89	0.18	172,174,175,176	0
22	CLA	c	505	65/65	0.89	0.15	172,174,175,175	0
22	CLA	C	505	65/65	0.89	0.16	172,174,175,176	0
22	CLA	b	606	65/65	0.89	0.15	172,173,174,174	0
27	LMG	C	522	48/55	0.89	0.18	172,174,174,175	0
25	DGD	a	411	56/66	0.89	0.16	173,174,175,176	0
22	CLA	h	101	65/65	0.89	0.19	171,174,175,175	0
22	CLA	b	609	65/65	0.89	0.14	172,174,175,175	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CA	k	101	1/1	0.89	0.08	172,172,172,172	0
22	CLA	B	605	65/65	0.89	0.13	172,173,175,176	0
22	CLA	A	405	65/65	0.90	0.14	172,174,175,176	0
27	LMG	B	621	49/55	0.90	0.16	172,173,174,174	0
24	BCR	g	101	40/40	0.90	0.15	173,174,175,175	0
22	CLA	b	618	65/65	0.90	0.13	172,174,175,175	0
22	CLA	C	520	65/65	0.90	0.16	172,174,175,176	0
22	CLA	D	405	65/65	0.90	0.15	172,173,174,175	0
25	DGD	C	515	53/66	0.90	0.17	172,173,174,174	0
24	BCR	A	407	40/40	0.90	0.19	171,173,174,174	0
24	BCR	B	616	40/40	0.90	0.15	172,173,174,175	0
22	CLA	c	502	65/65	0.90	0.14	173,174,175,175	0
22	CLA	c	503	65/65	0.90	0.13	172,174,175,175	0
22	CLA	a	408	65/65	0.90	0.15	173,174,175,175	0
22	CLA	C	507	65/65	0.90	0.16	173,174,175,177	0
25	DGD	c	515	53/66	0.90	0.18	171,174,175,177	0
22	CLA	c	510	65/65	0.90	0.12	173,174,175,176	0
24	BCR	b	621	40/40	0.90	0.18	171,173,174,174	0
24	BCR	b	622	40/40	0.90	0.24	171,172,173,173	0
26	LHG	A	409	39/49	0.90	0.17	172,173,175,176	0
32	PHO	D	401	64/64	0.90	0.17	171,173,174,175	0
32	PHO	D	402	64/64	0.90	0.15	171,173,175,175	0
30	SQD	A	414	54/54	0.90	0.15	171,174,176,179	0
22	CLA	c	511	65/65	0.90	0.14	172,174,175,176	0
30	SQD	D	403	43/54	0.90	0.14	172,174,177,180	0
22	CLA	C	510	65/65	0.90	0.14	172,173,175,175	0
22	CLA	B	607	65/65	0.91	0.15	172,174,174,175	0
27	LMG	d	407	48/55	0.91	0.16	171,173,175,175	0
24	BCR	b	620	40/40	0.91	0.21	172,173,174,175	0
22	CLA	C	508	65/65	0.91	0.13	172,174,175,175	0
35	CA	K	101	1/1	0.91	0.13	177,177,177,177	0
22	CLA	a	406	65/65	0.91	0.16	172,174,175,176	0
24	BCR	y	101	40/40	0.91	0.15	173,173,174,175	0
27	LMG	A	410	51/55	0.91	0.17	171,173,174,175	0
23	PL9	d	406	55/55	0.92	0.16	172,173,175,175	0
22	CLA	c	508	65/65	0.92	0.11	172,174,175,175	0
24	BCR	b	623	40/40	0.92	0.13	171,173,174,174	0
24	BCR	c	513	40/40	0.92	0.16	172,173,175,175	0
22	CLA	B	615	65/65	0.92	0.13	172,174,175,175	0
22	CLA	B	604	65/65	0.92	0.11	172,173,175,175	0
24	BCR	B	617	40/40	0.92	0.18	172,173,174,174	0
22	CLA	A	404	65/65	0.92	0.17	170,173,174,175	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	LHG	a	412	39/49	0.92	0.17	171,174,176,177	0
24	BCR	C	513	40/40	0.92	0.15	172,173,174,174	0
24	BCR	C	514	40/40	0.92	0.15	172,173,175,175	0
25	DGD	B	620	58/66	0.92	0.17	171,173,175,176	0
22	CLA	c	520	65/65	0.92	0.15	173,174,174,175	0
27	LMG	B	624	49/55	0.92	0.18	171,173,174,175	0
22	CLA	B	602	65/65	0.92	0.14	171,173,174,175	0
22	CLA	B	613	65/65	0.92	0.14	172,174,174,175	0
23	PL9	D	407	55/55	0.92	0.18	171,173,174,175	0
27	LMG	D	412	46/55	0.92	0.15	172,174,175,175	0
22	CLA	a	405	65/65	0.92	0.17	170,172,174,175	0
23	PL9	a	409	45/55	0.92	0.17	171,173,174,175	0
30	SQD	f	103	45/54	0.92	0.14	172,174,176,178	0
27	LMG	d	410	46/55	0.93	0.15	172,173,175,175	0
22	CLA	C	509	65/65	0.93	0.13	173,173,174,174	0
22	CLA	c	504	65/65	0.93	0.14	172,174,175,175	0
22	CLA	H	101	65/65	0.93	0.14	172,174,175,175	0
22	CLA	b	612	65/65	0.93	0.12	171,174,175,176	0
22	CLA	b	613	65/65	0.93	0.12	172,174,175,175	0
24	BCR	f	102	40/40	0.93	0.17	171,173,175,175	0
32	PHO	a	407	64/64	0.93	0.12	173,174,175,175	0
32	PHO	d	401	64/64	0.93	0.14	172,173,174,174	0
22	CLA	C	503	65/65	0.93	0.13	172,174,175,176	0
22	CLA	C	511	65/65	0.93	0.13	172,174,175,175	0
22	CLA	B	609	65/65	0.93	0.13	172,174,175,175	0
22	CLA	B	610	65/65	0.93	0.12	172,174,174,175	0
22	CLA	d	405	65/65	0.93	0.13	172,174,175,175	0
22	CLA	b	617	65/65	0.94	0.17	173,173,175,176	0
22	CLA	b	607	65/65	0.94	0.12	172,173,175,176	0
22	CLA	c	507	65/65	0.94	0.12	172,174,175,176	0
22	CLA	b	608	65/65	0.94	0.13	172,173,175,176	0
22	CLA	B	603	65/65	0.94	0.11	171,173,175,175	0
22	CLA	b	610	65/65	0.94	0.14	172,173,175,175	0
22	CLA	A	402	65/65	0.94	0.14	172,173,174,175	0
22	CLA	D	406	65/65	0.94	0.13	172,174,175,176	0
27	LMG	b	628	49/55	0.94	0.17	172,174,175,175	0
22	CLA	d	404	65/65	0.94	0.13	172,173,174,174	0
22	CLA	A	403	65/65	0.95	0.13	171,173,174,175	0
22	CLA	B	611	65/65	0.95	0.10	171,173,174,174	0
22	CLA	b	611	65/65	0.95	0.11	172,174,175,175	0
22	CLA	B	608	65/65	0.95	0.13	172,174,175,175	0
22	CLA	B	614	65/65	0.95	0.10	172,174,175,175	0

Continued on next page...

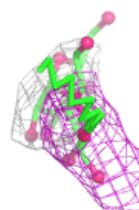
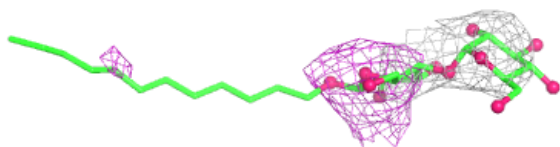
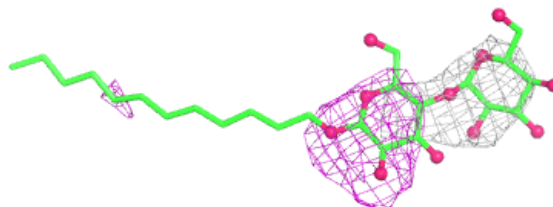
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	B	618	40/40	0.95	0.16	171,172,174,174	0
22	CLA	b	615	65/65	0.95	0.10	172,173,174,175	0
29	OEX	A	412	10/10	0.95	0.10	165,169,172,173	0
29	OEX	a	414	10/10	0.95	0.11	168,171,173,177	0
22	CLA	B	606	65/65	0.95	0.13	172,173,174,175	0
34	HEM	F	101	43/43	0.95	0.11	173,174,175,176	0
34	HEM	V	201	43/43	0.95	0.17	172,173,175,175	0
34	HEM	f	101	43/43	0.95	0.12	173,174,175,175	0
22	CLA	C	501	65/65	0.95	0.11	172,174,174,175	0
22	CLA	c	509	65/65	0.95	0.09	172,173,175,175	0
24	BCR	D	411	40/40	0.95	0.14	171,173,174,175	0
22	CLA	C	502	65/65	0.95	0.15	173,174,174,175	0
22	CLA	b	614	65/65	0.96	0.12	172,173,174,175	0
34	HEM	v	201	43/43	0.96	0.12	171,174,175,175	0
33	BCT	D	404	4/4	0.96	0.05	173,174,174,174	0
22	CLA	B	612	65/65	0.96	0.13	171,173,175,175	0
28	CL	a	416	1/1	0.96	0.16	173,173,173,173	0
22	CLA	a	404	65/65	0.96	0.12	172,173,174,176	0
22	CLA	b	616	65/65	0.97	0.13	171,173,174,175	0
21	FE2	A	401	1/1	0.97	0.10	170,170,170,170	0
21	FE2	a	403	1/1	0.97	0.12	175,175,175,175	0

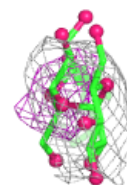
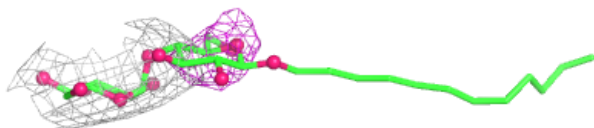
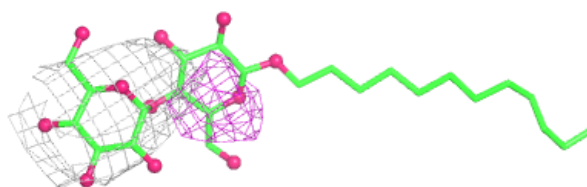
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

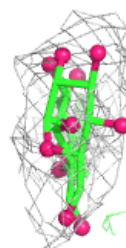
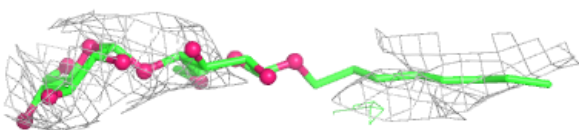
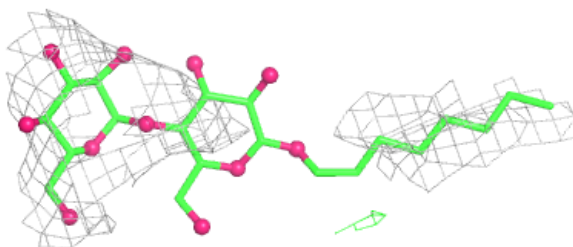
**Electron density around LMT I 102:**

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



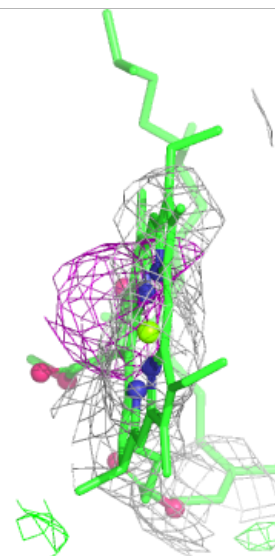
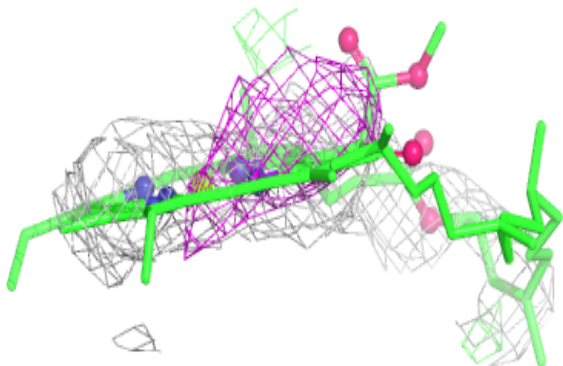
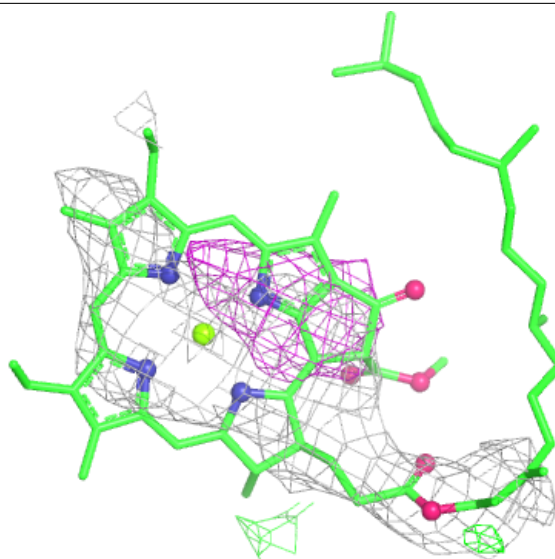
Electron density around LMT d 409:

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



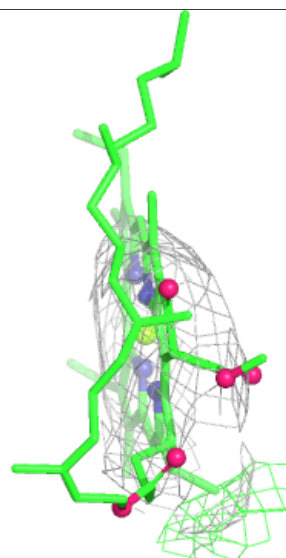
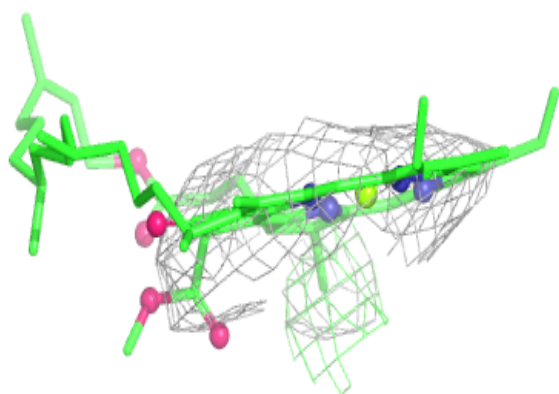
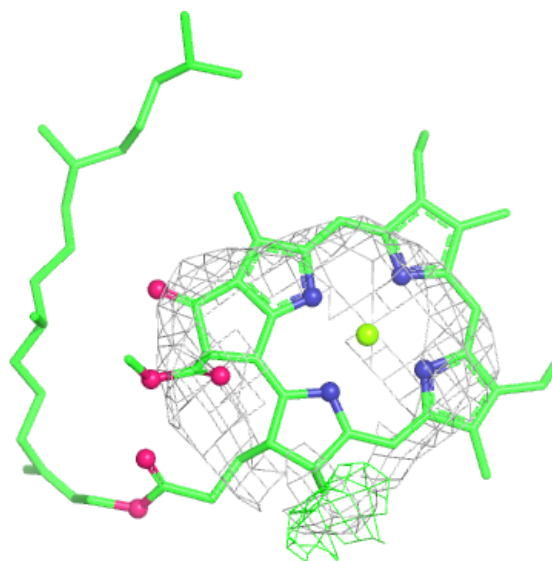
Electron density around CLA b 605:

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



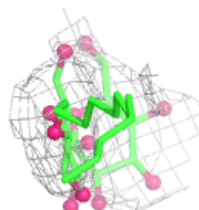
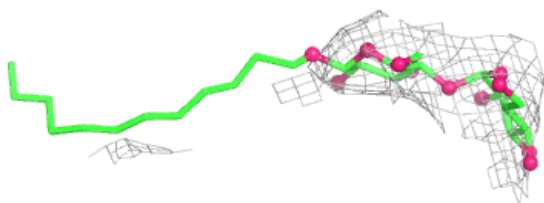
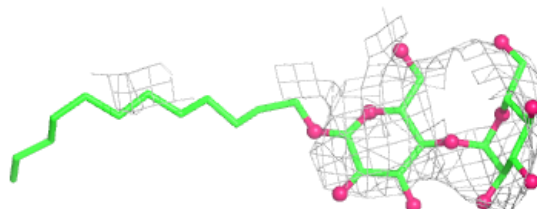
Electron density around CLA B 601:

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

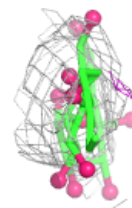
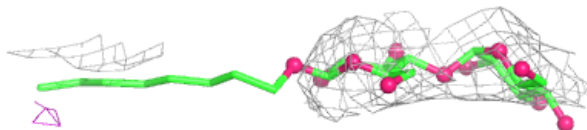
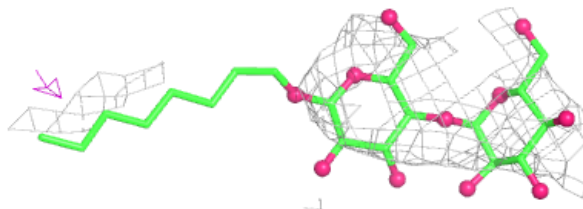


Electron density around LMT b 626:

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

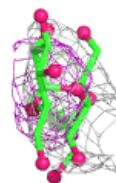
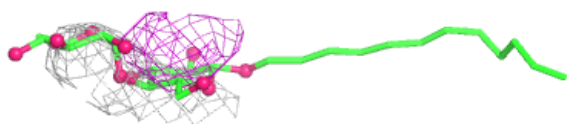
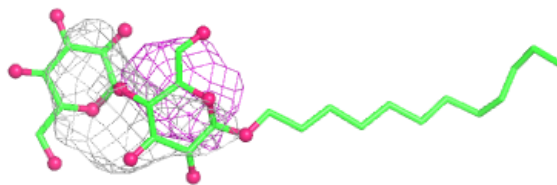
**Electron density around LMT D 410:**

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

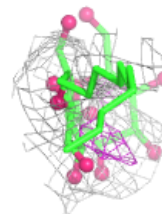
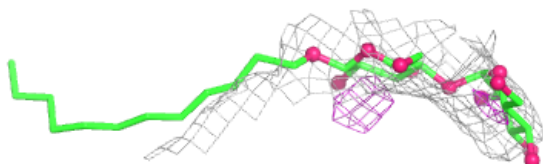
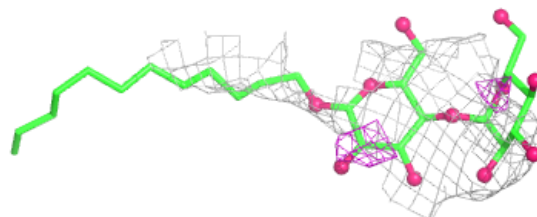


Electron density around LMT i 102:

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

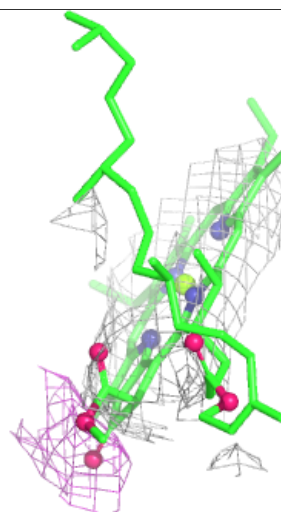
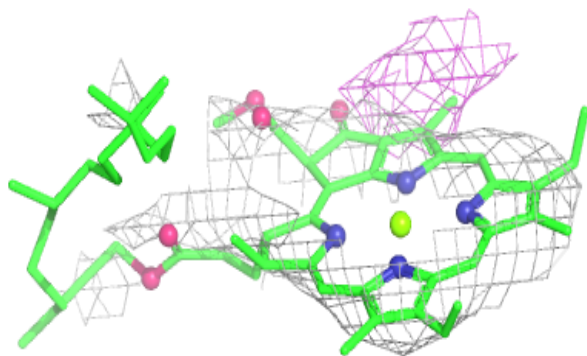
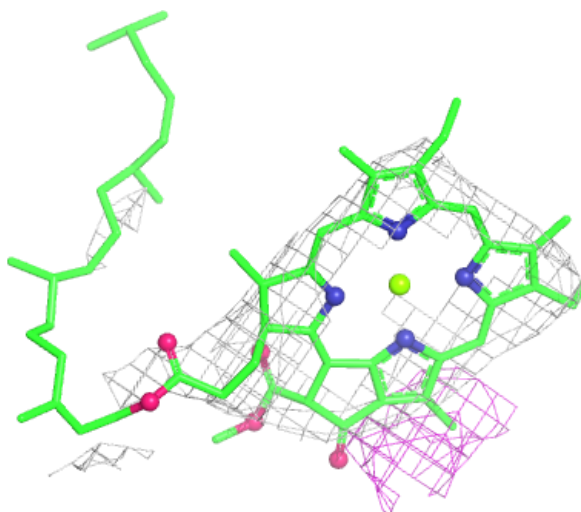
**Electron density around LMT B 622:**

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



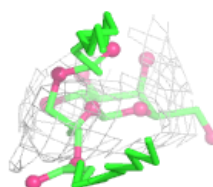
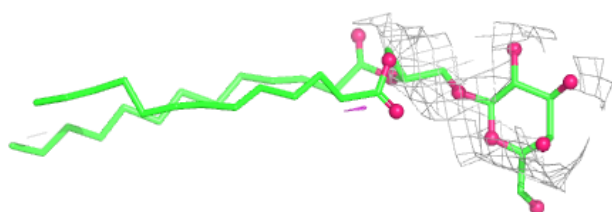
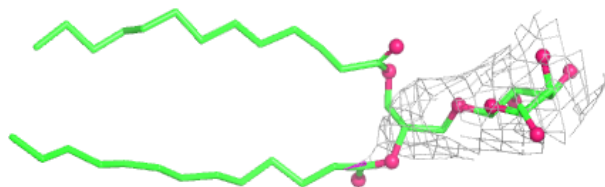
Electron density around CLA b 619:

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

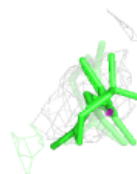
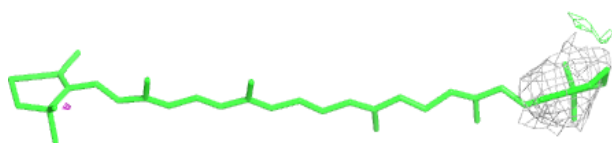
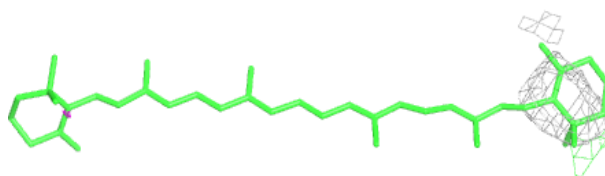


Electron density around LMG C 518:

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

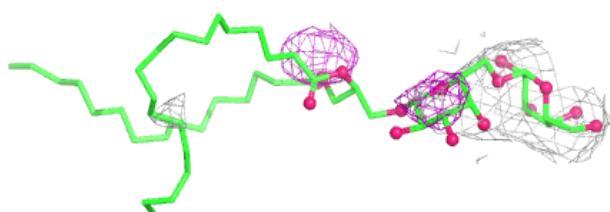
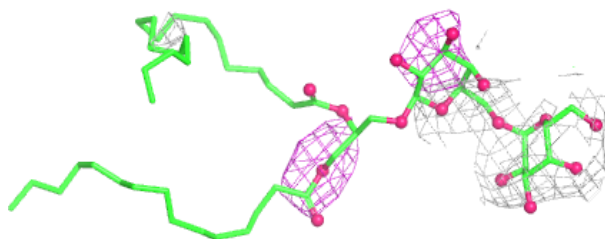
**Electron density around BCR j 102:**

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

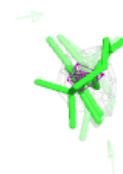
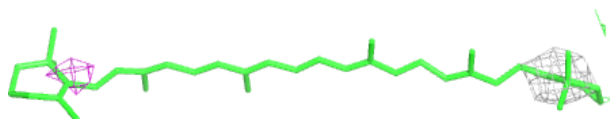
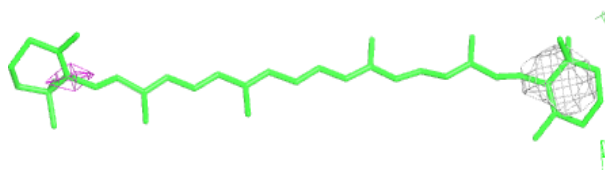


Electron density around DGD D 409:

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

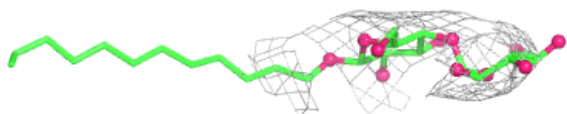
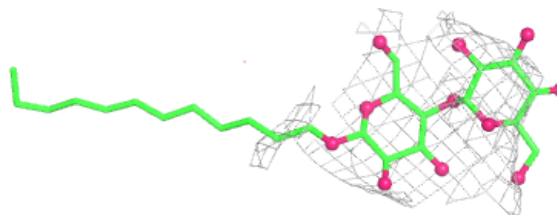
**Electron density around BCR J 102:**

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

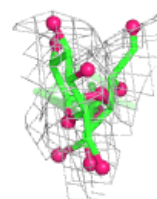
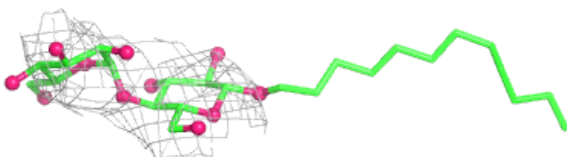
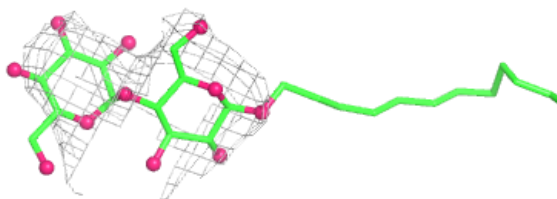


Electron density around LMT B 627:

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

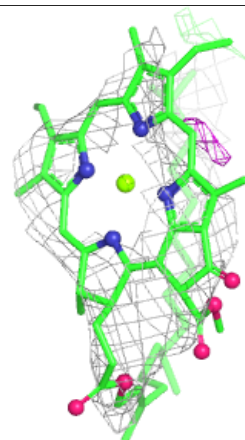
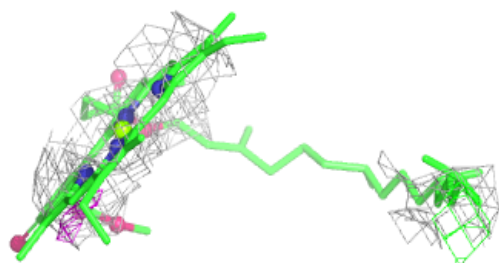
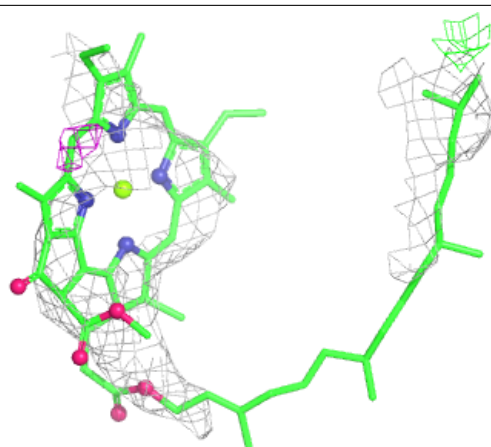
**Electron density around LMT B 628:**

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

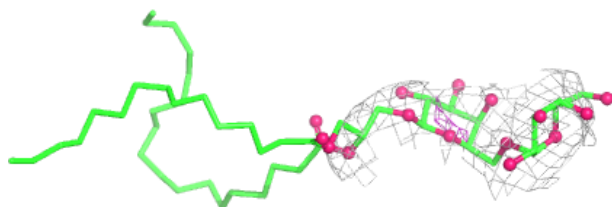
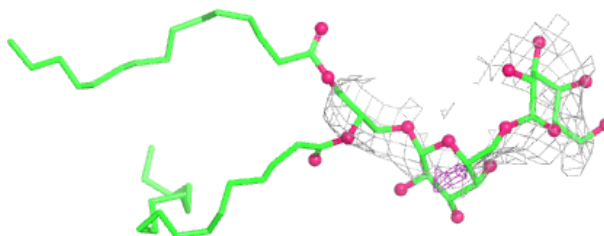


Electron density around CLA C 506:

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

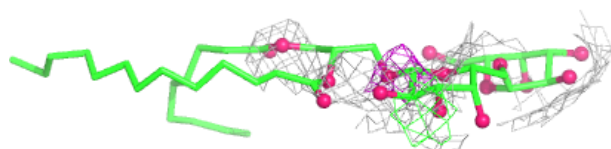
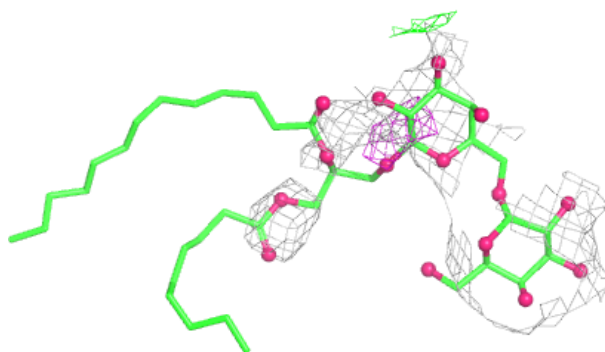
**Electron density around DGD d 408:**

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

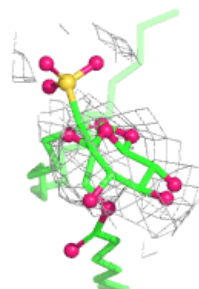
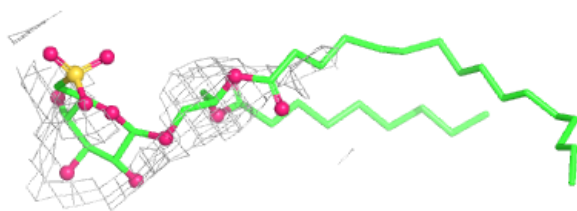
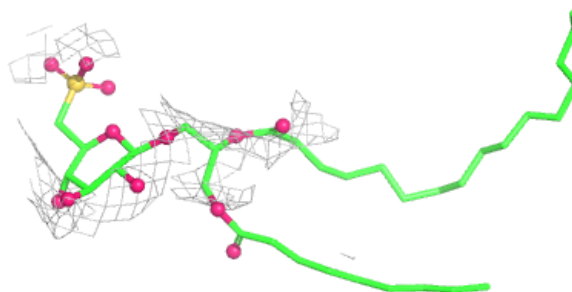


Electron density around DGD B 625:

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

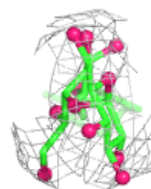
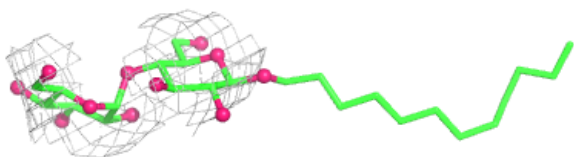
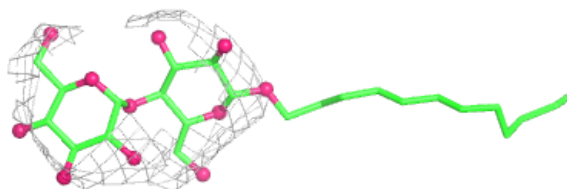
**Electron density around SQD B 626:**

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

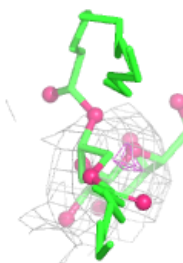
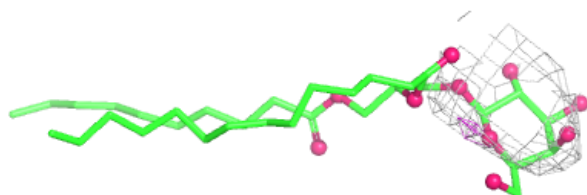
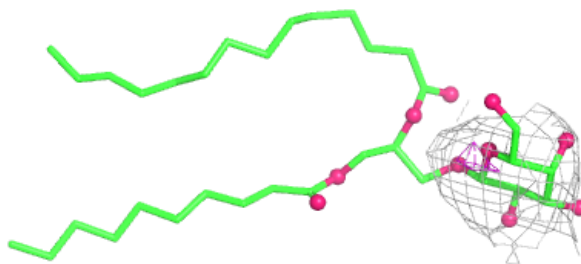


Electron density around LMT b 604:

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

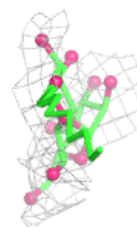
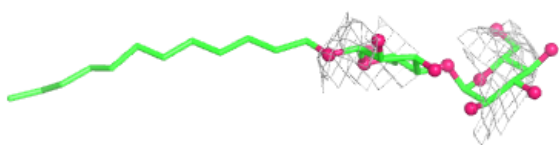
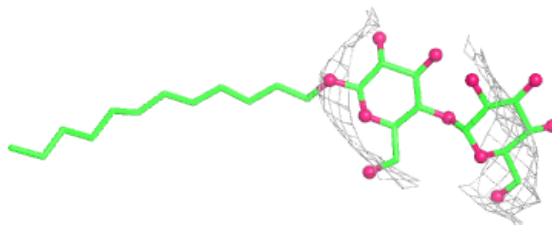
**Electron density around LMG I 101:**

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

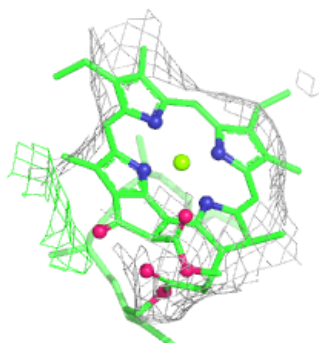
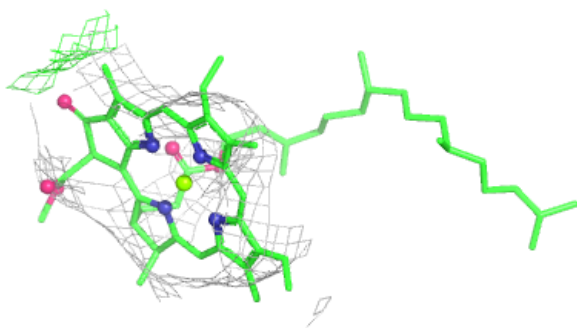
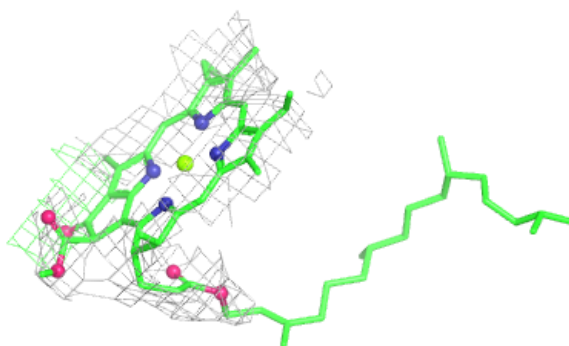


Electron density around LMT B 623:

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

**Electron density around 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)

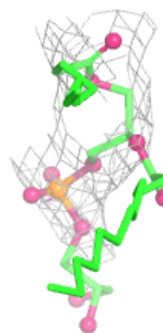
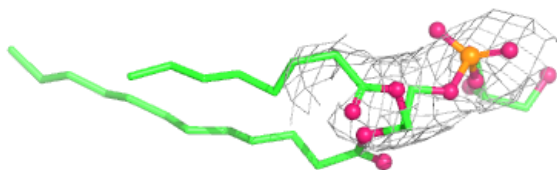
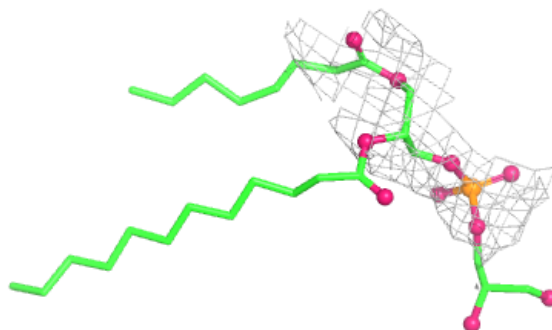


Electron density around DGD C 516:

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

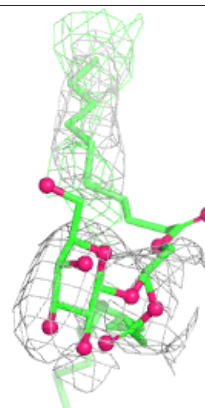
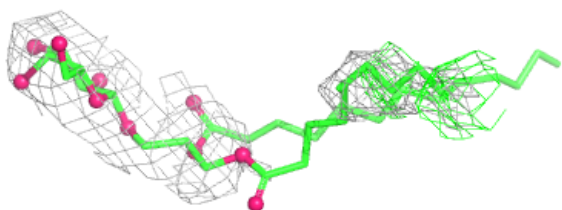
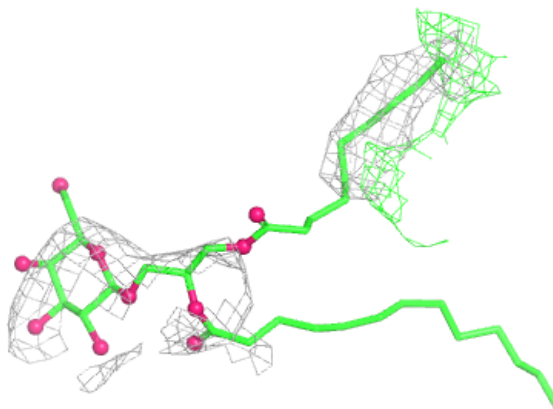
**Electron density around LHG C 519:**

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

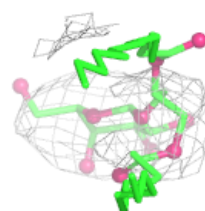
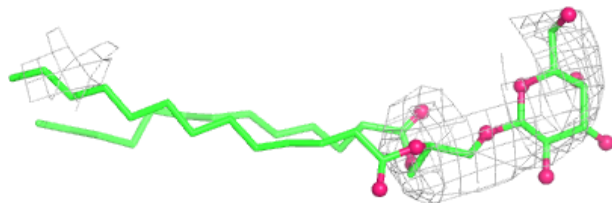
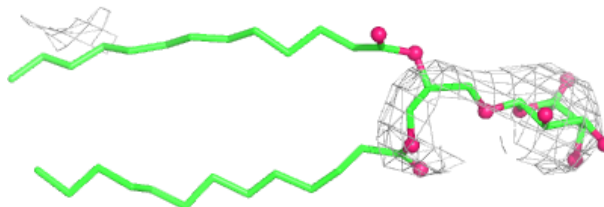


Electron density around LMG a 402:

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

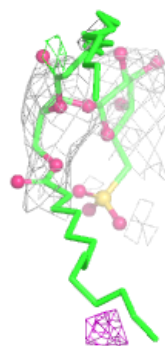
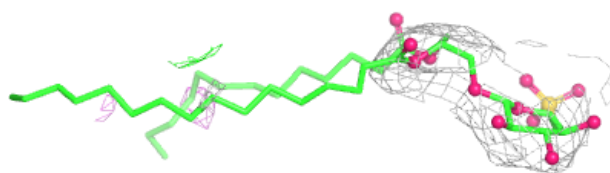
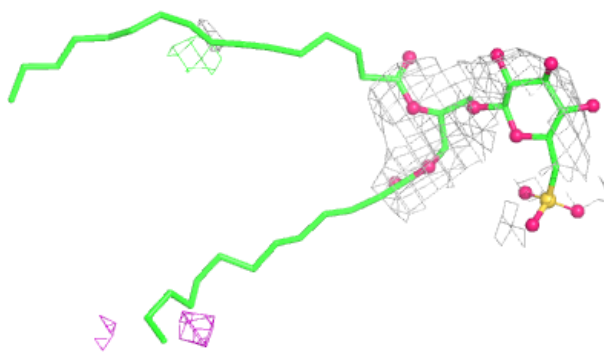
**Electron density around LMG c 518:**

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

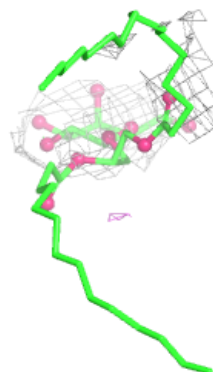
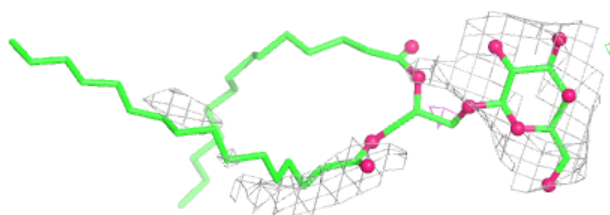


Electron density around SQD A 413:

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

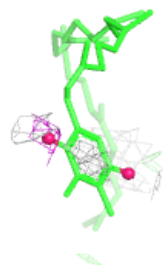
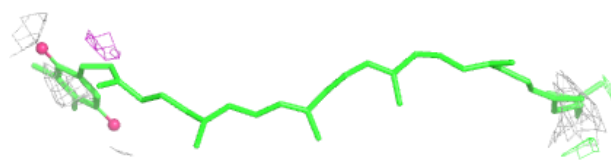
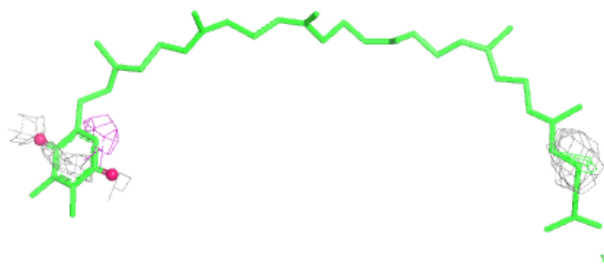
**Electron density around LMG b 625:**

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

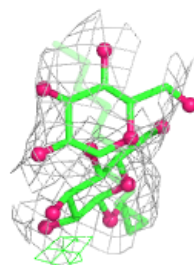
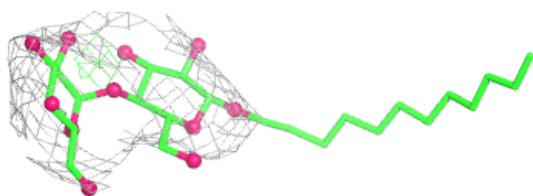


Electron density around PL9 A 406:

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

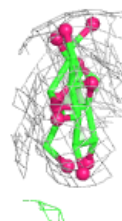
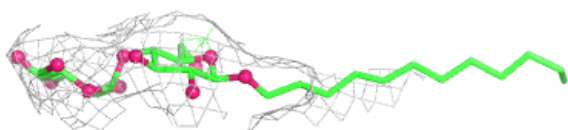
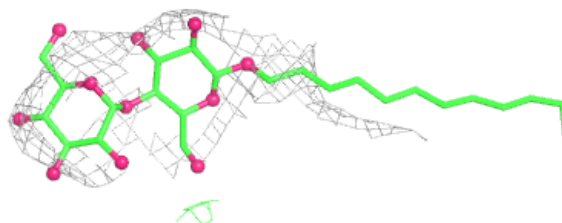
**Electron density around LMT M 102:**

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

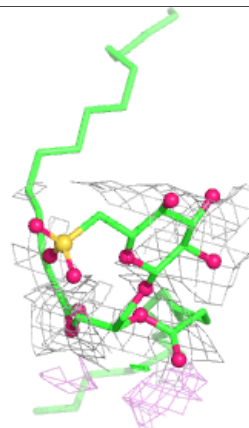
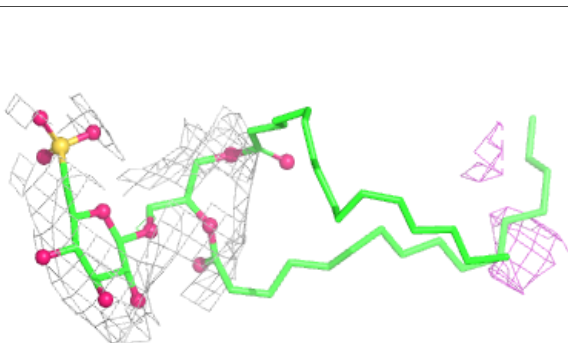
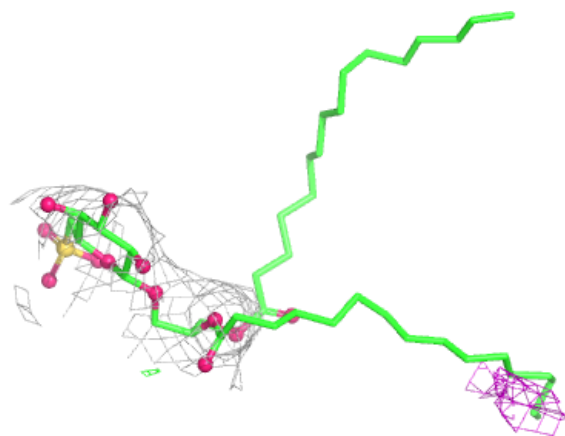


Electron density around LMT b 603:

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

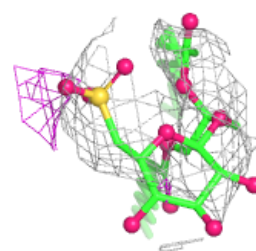
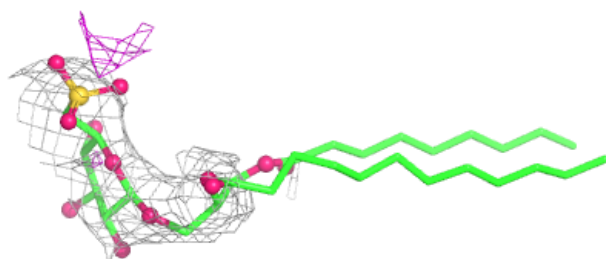
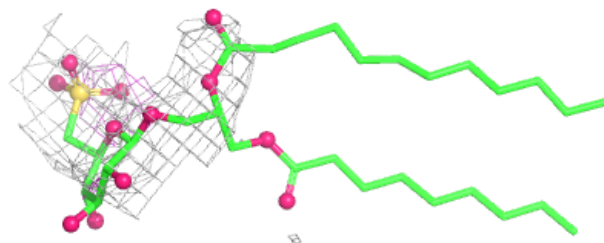
**Electron density around SQD a 401:**

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

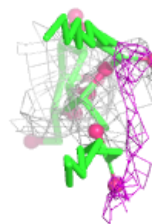
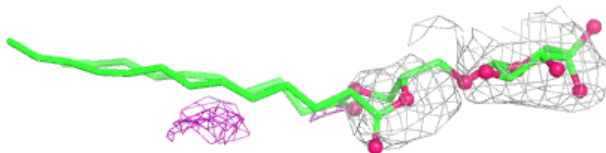
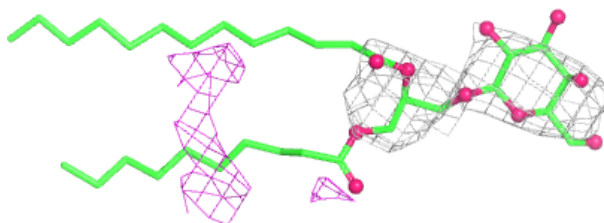


Electron density around SQD d 402:

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

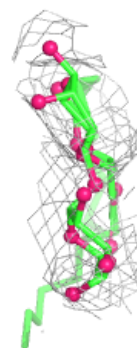
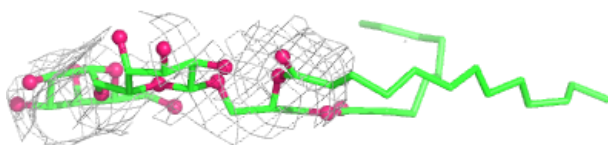
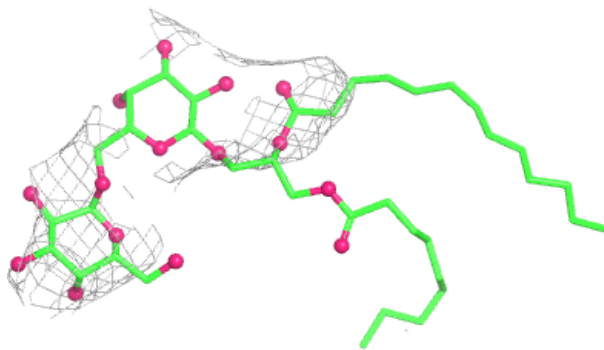
**Electron density around LMG M 101:**

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

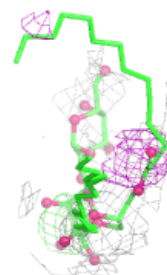
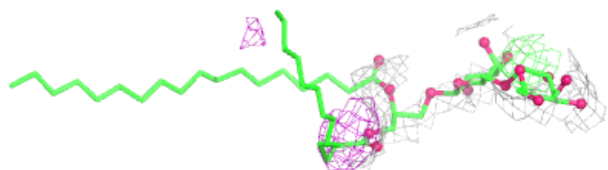


Electron density around DGD b 601:

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

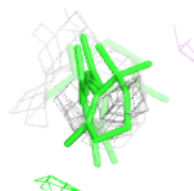
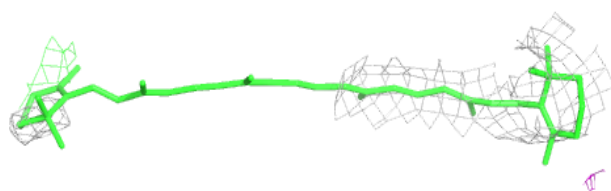
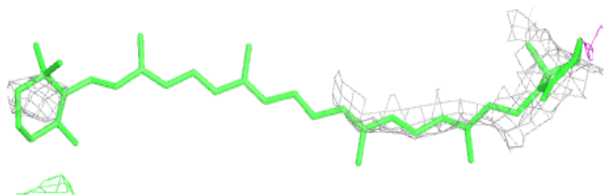
**Electron density around DGD c 516:**

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

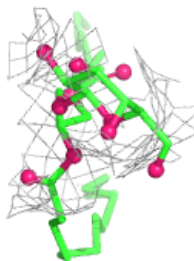
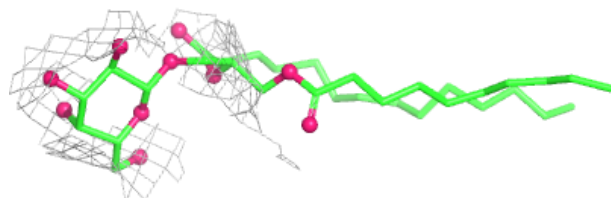
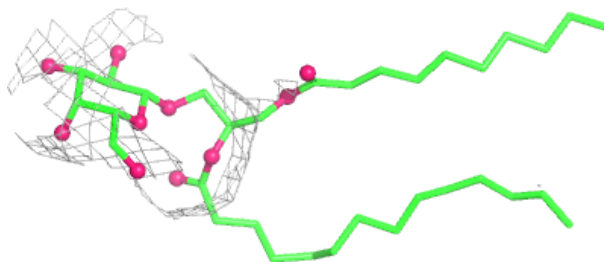


Electron density around BCR H 102:

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

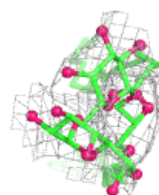
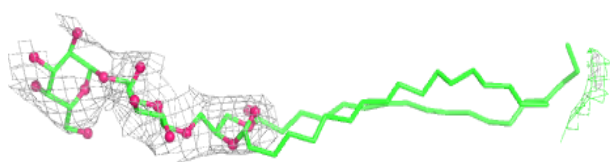
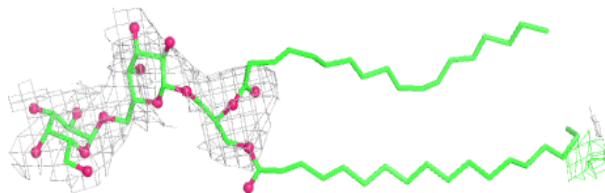
**Electron density around LMG i 101:**

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

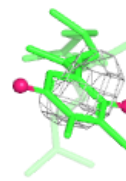
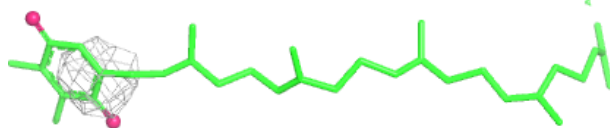
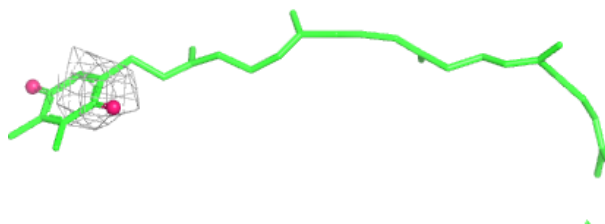


Electron density around DGD C 517:

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

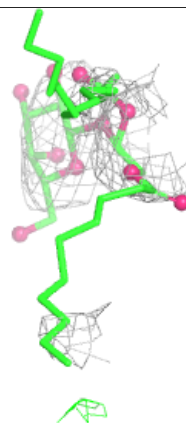
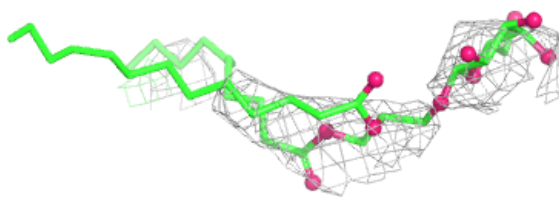
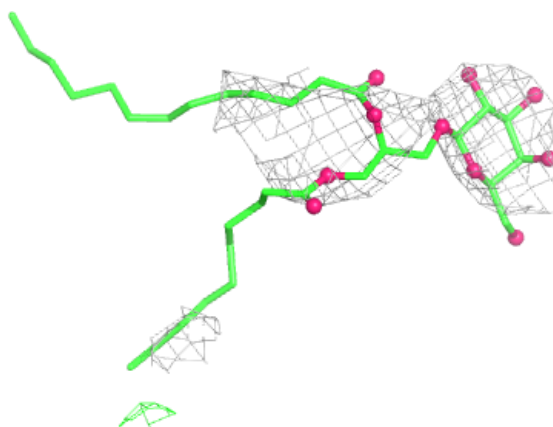
**Electron density around PL9 J 101:**

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

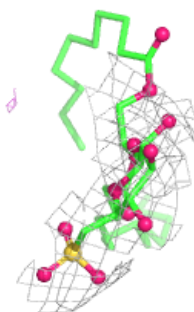
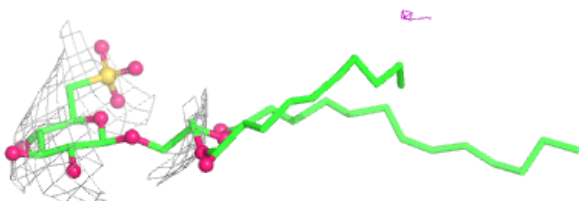
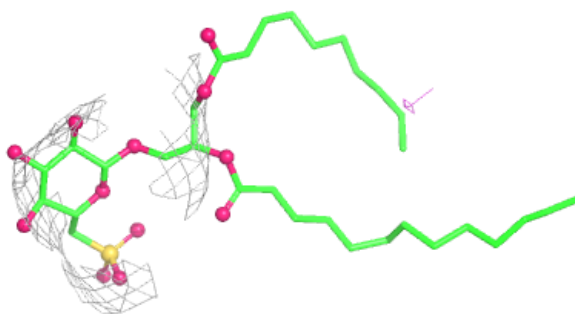


Electron density around LMG A 415:

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

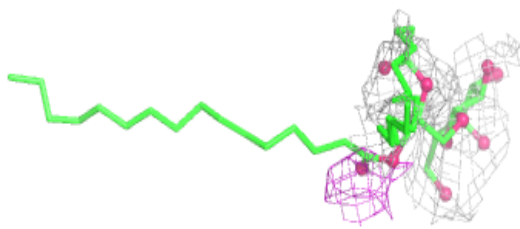
**Electron density around SQD F 102:**

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



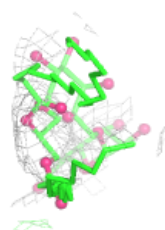
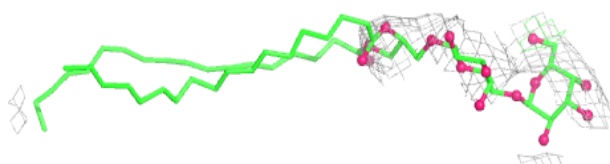
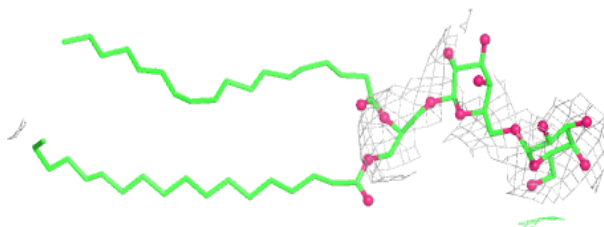
Electron density around LMG a 413:

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

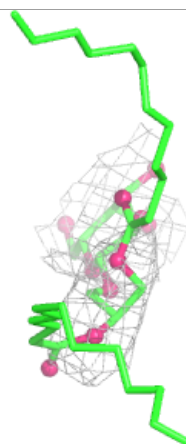
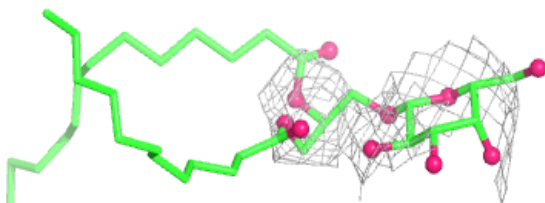
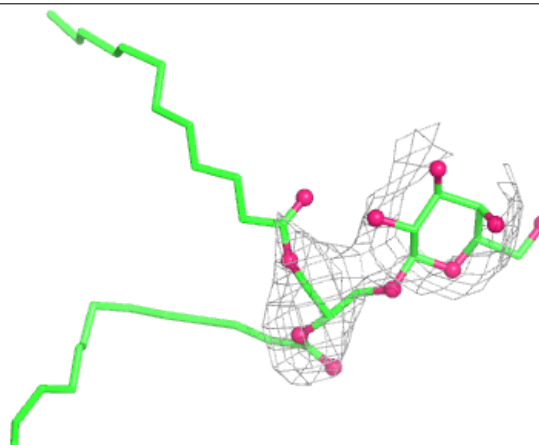


Electron density around DGD c 517:

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

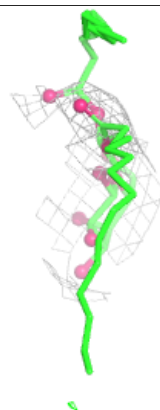
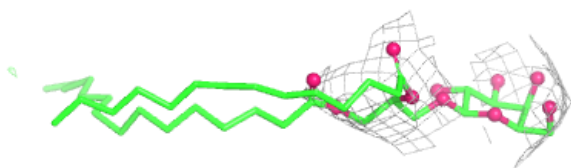
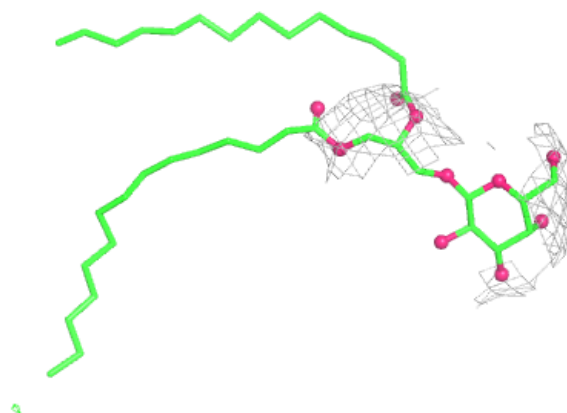
**Electron density around LMG E 101:**

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



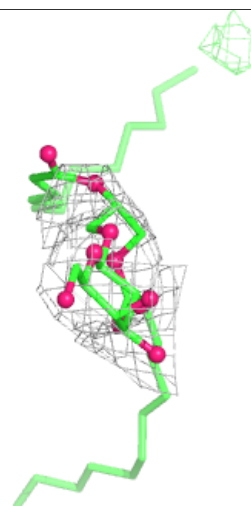
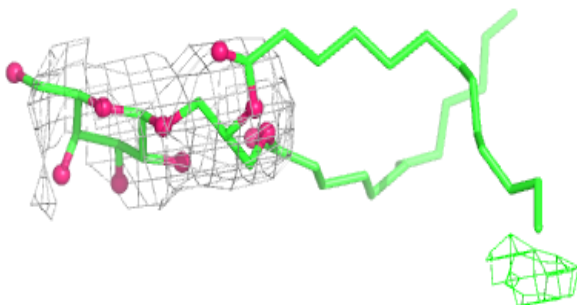
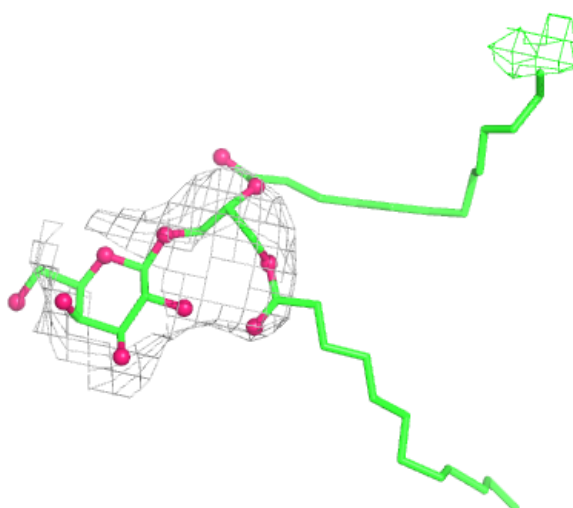
Electron density around LMG c 522:

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



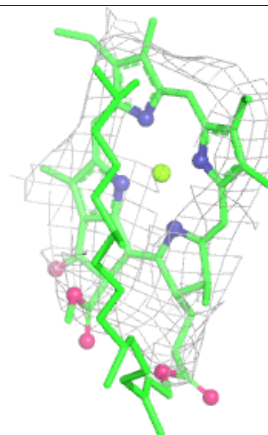
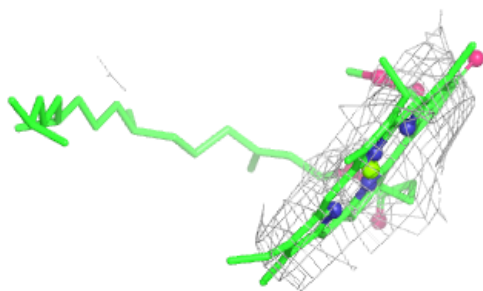
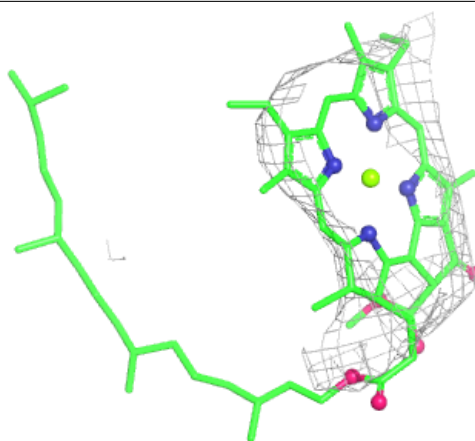
Electron density around LMG e 101:

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



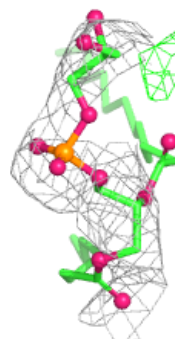
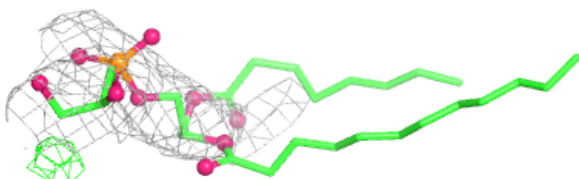
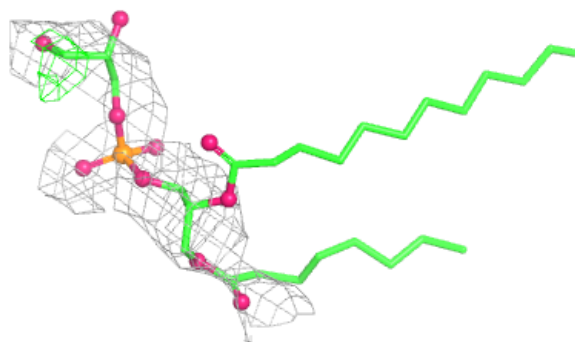
Electron density around CLA c 506:

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

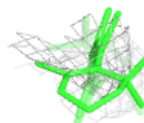
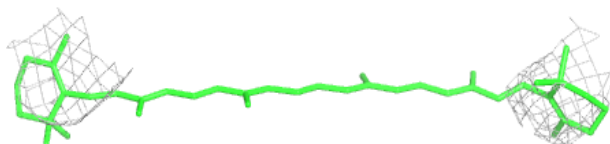
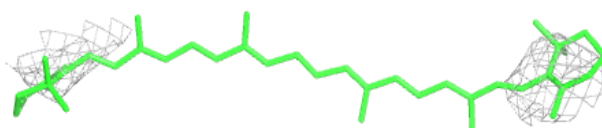


Electron density around LHG c 519:

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

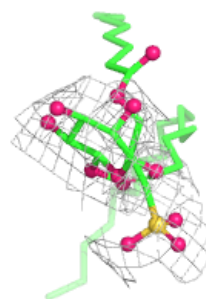
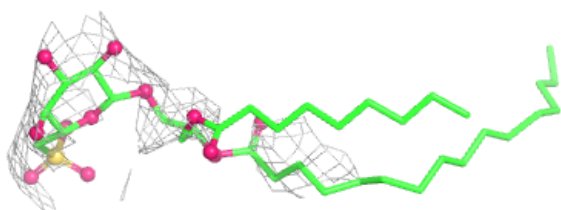
**Electron density around BCR c 521:**

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

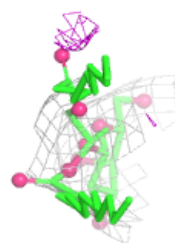
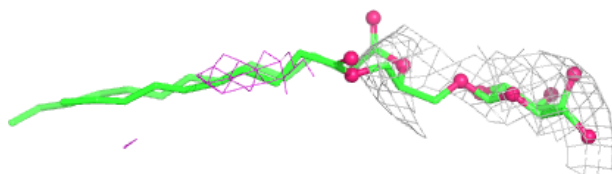
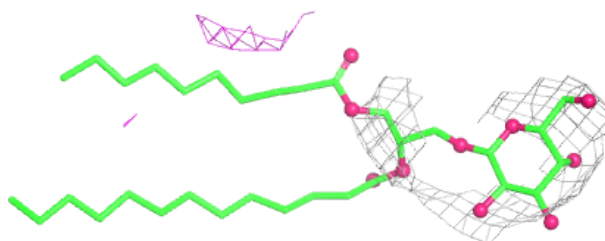


Electron density around SQD b 602:

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

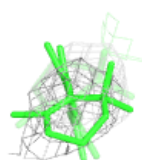
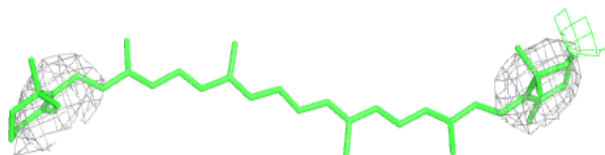
**Electron density around LMG m 101:**

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

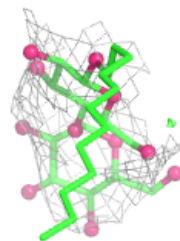
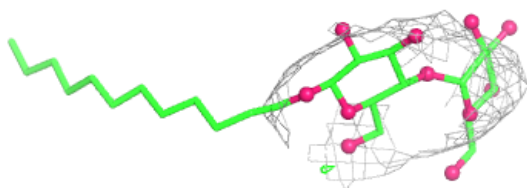


Electron density around BCR a 410:

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

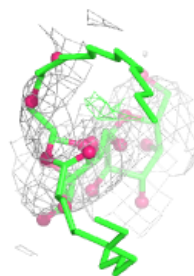
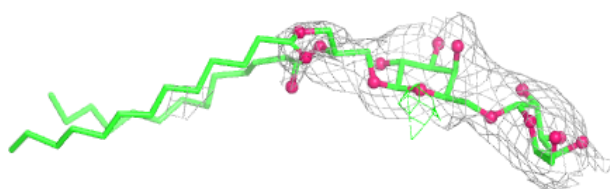
**Electron density around LMT M 103:**

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

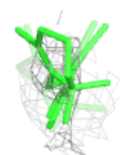
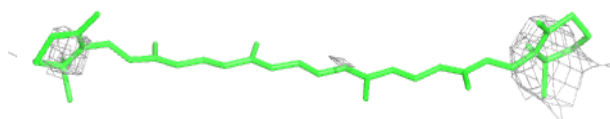
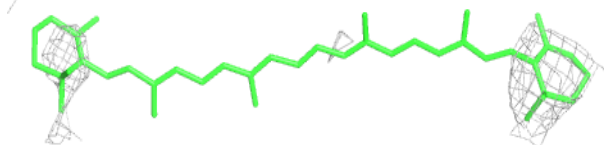


Electron density around DGD A 408:

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

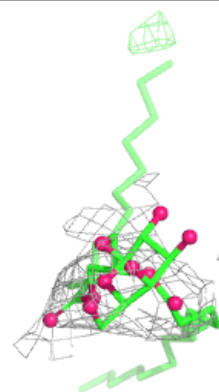
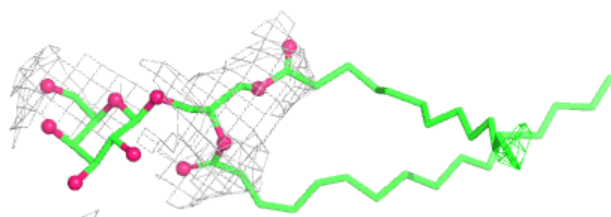
**Electron density around BCR c 514:**

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

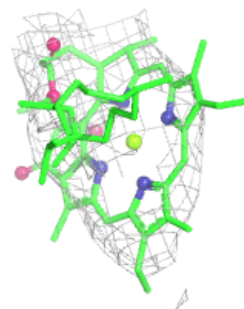
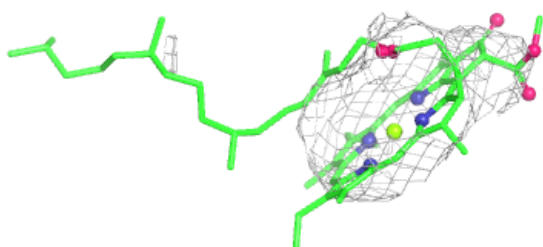
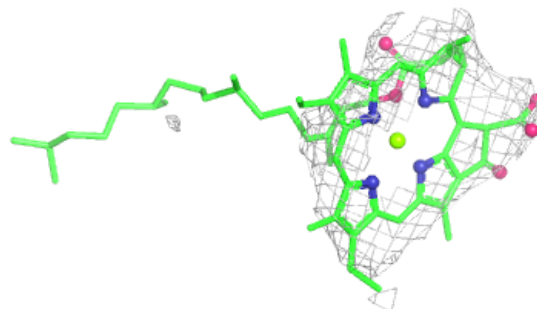


Electron density around LMG D 408:

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

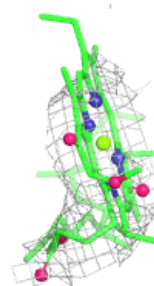
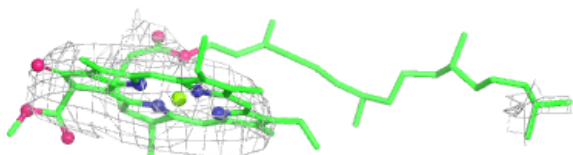
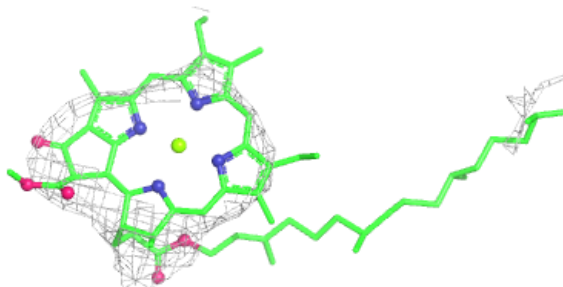
**Electron density around CLA C 504:**

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

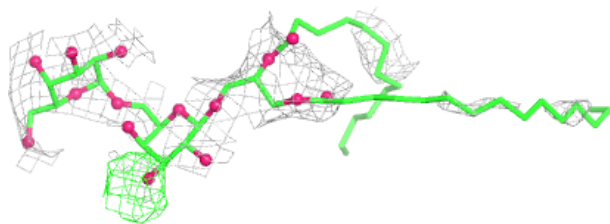


Electron density around CLA c 501:

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

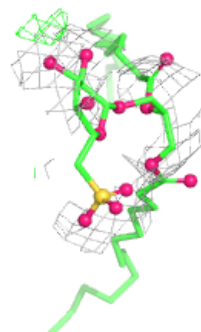
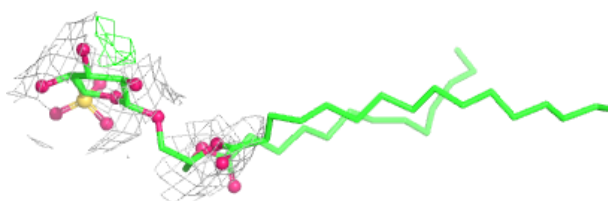
**Electron density around DGD b 624:**

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

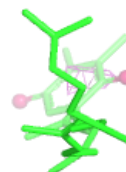
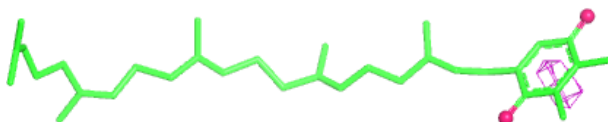
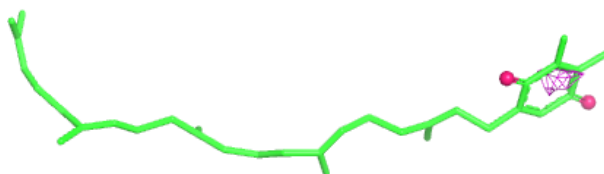


Electron density around SQD a 415:

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

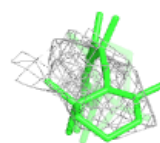
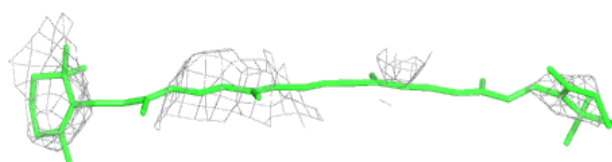
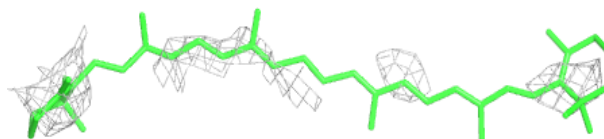
**Electron density around PL9 j 101:**

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

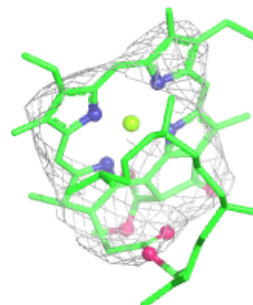
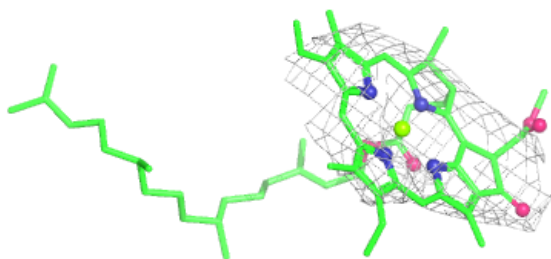
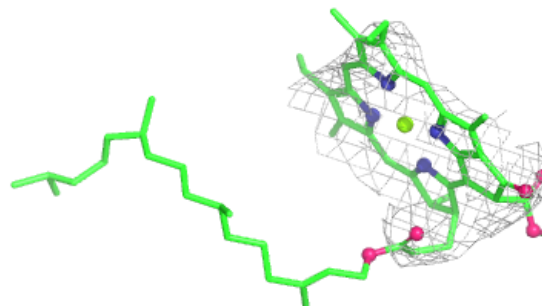


Electron density around BCR x 101:

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

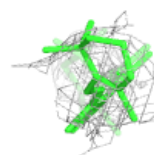
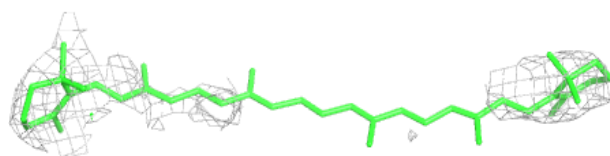
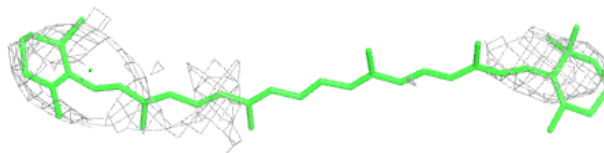
**Electron density around CLA C 512:**

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

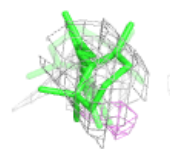
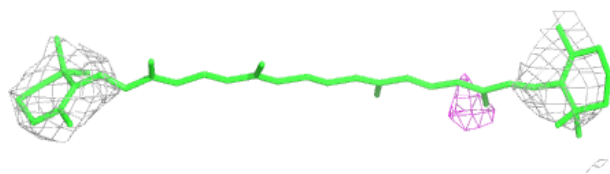
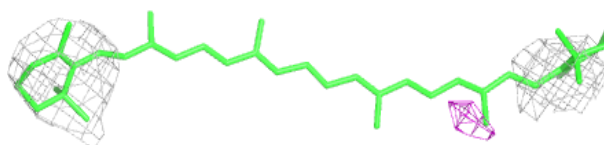


Electron density around BCR B 619:

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

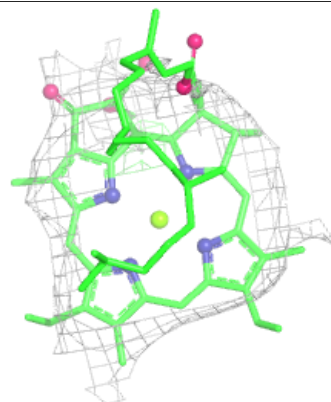
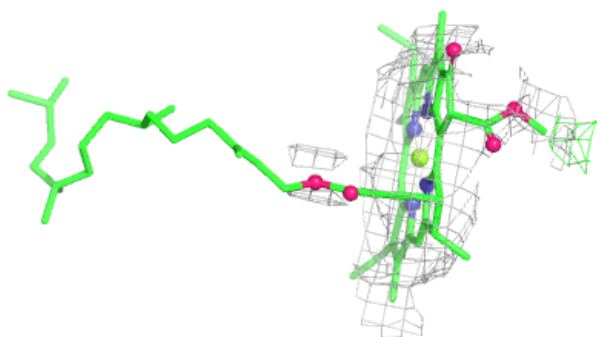
**Electron density around BCR C 521:**

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

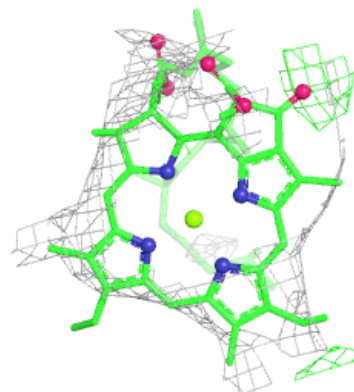
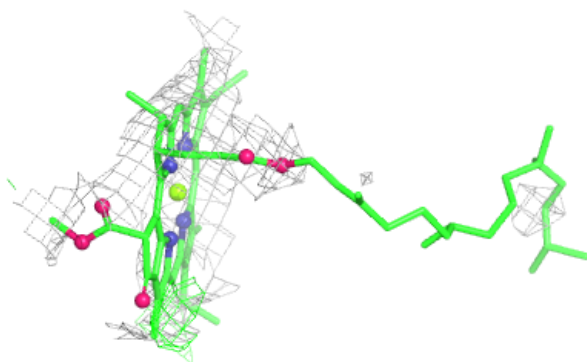
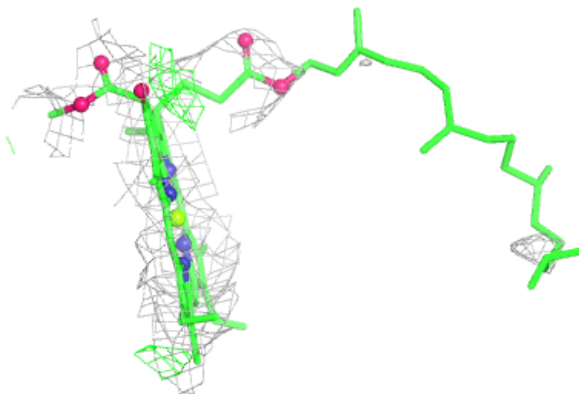


Electron density around CLA c 505:

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

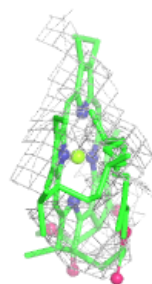
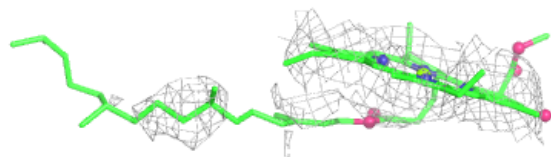
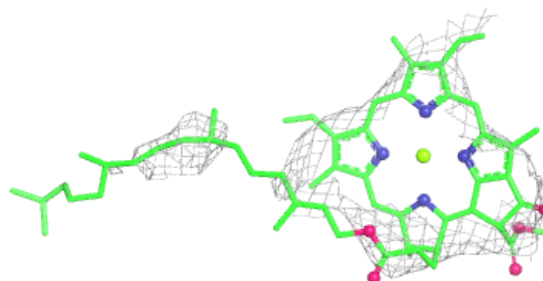
**Electron density around CLA C 505:**

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

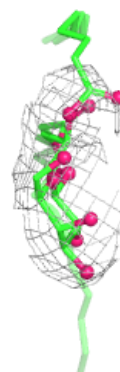
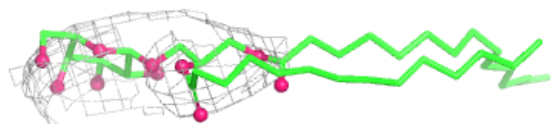
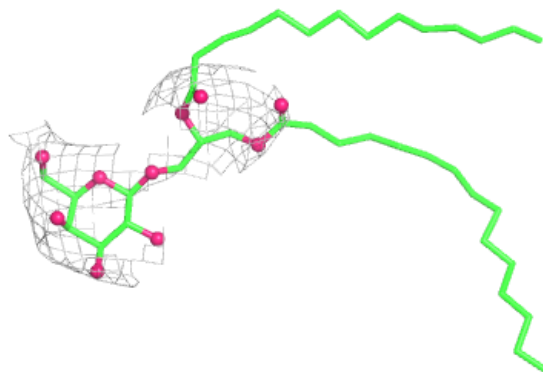


Electron density around CLA b 606:

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

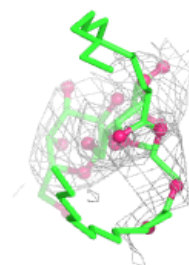
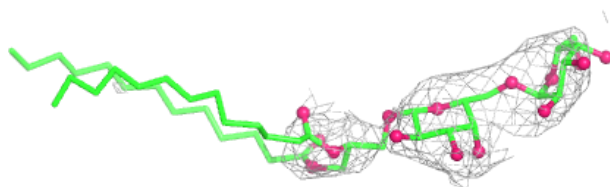
**Electron density around LMG C 522:**

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

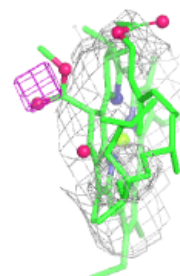
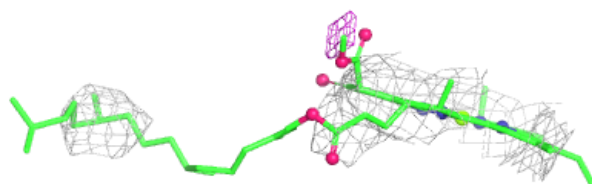
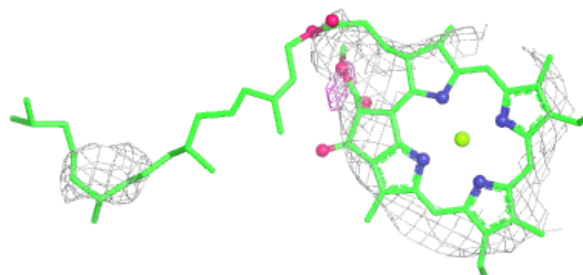


Electron density around DGD a 411:

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

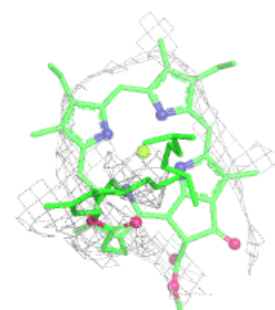
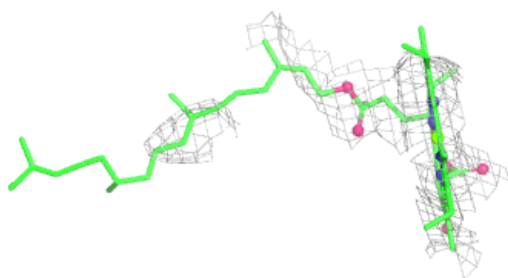
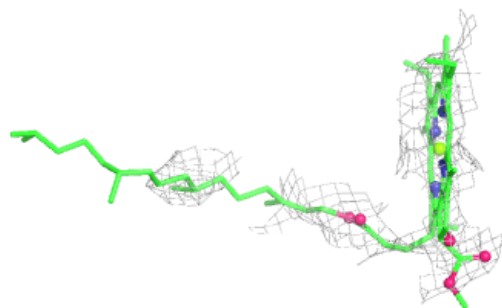
**Electron density around CLA h 101:**

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

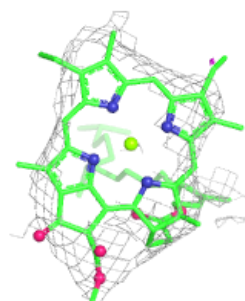
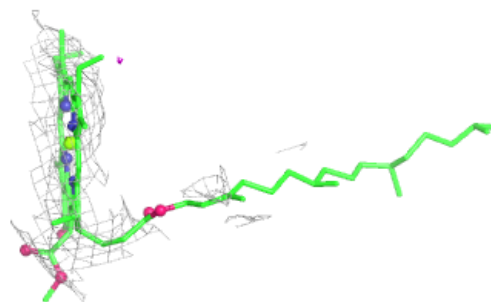


Electron density around CLA b 609:

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

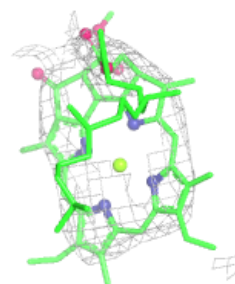
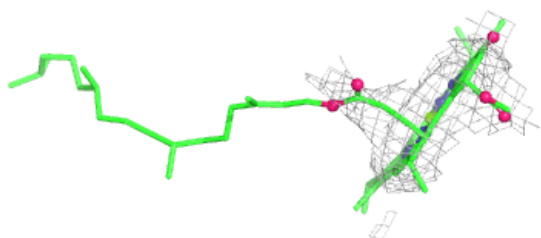
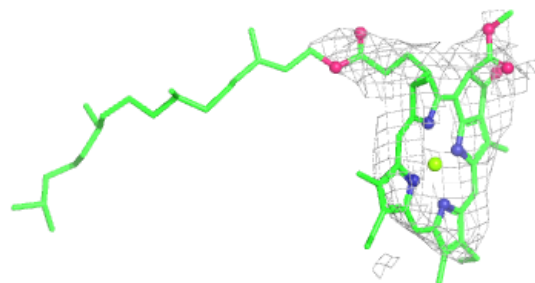
**Electron density around CLA B 605:**

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

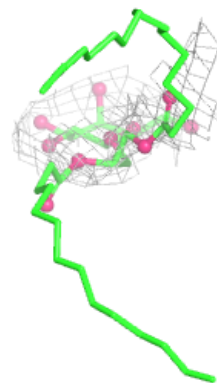
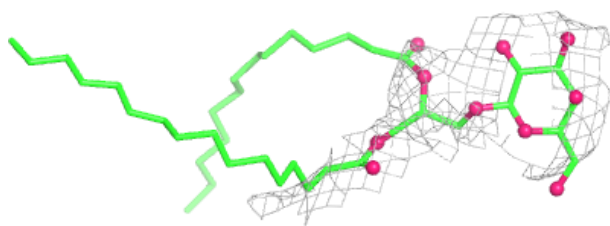
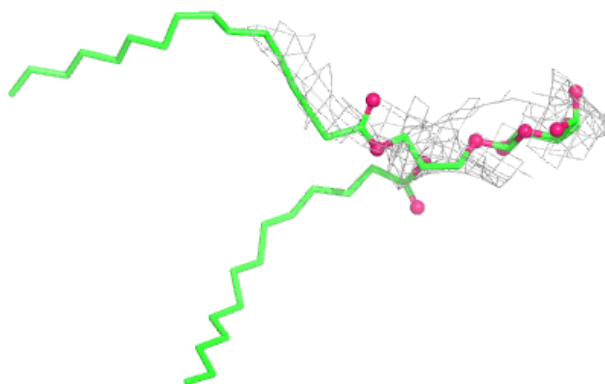


Electron density around CLA A 405:

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

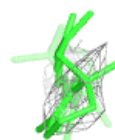
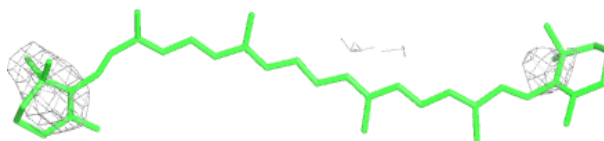
**Electron density around LMG B 621:**

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



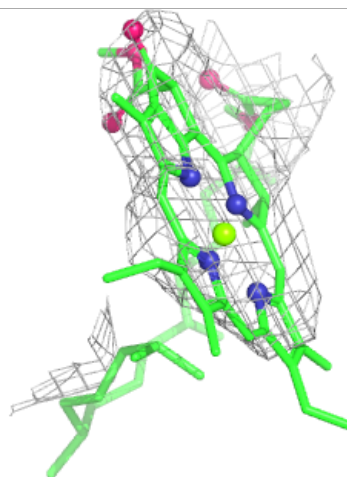
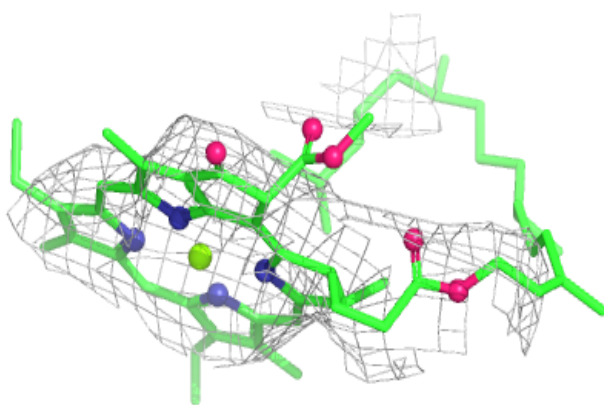
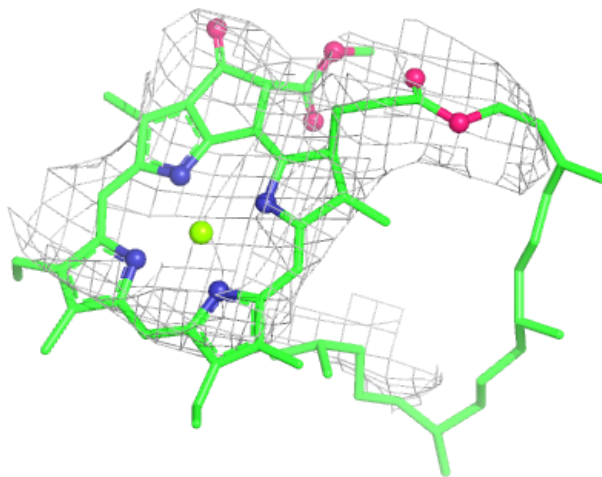
Electron density around BCR g 101:

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



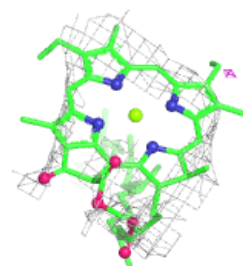
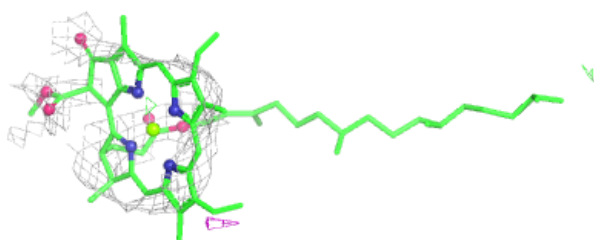
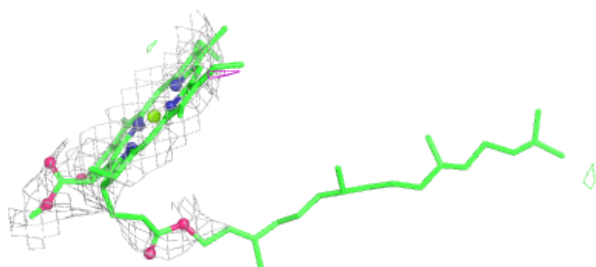
Electron density around CLA b 618:

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

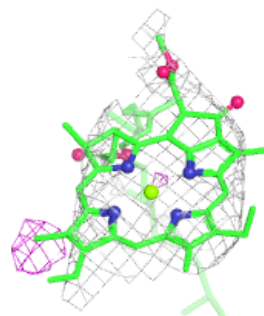
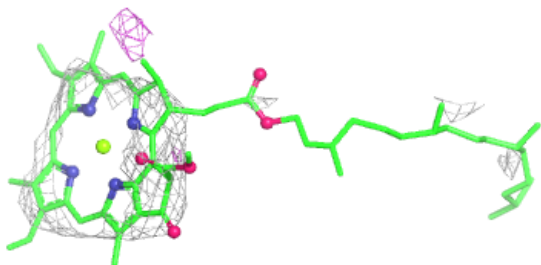
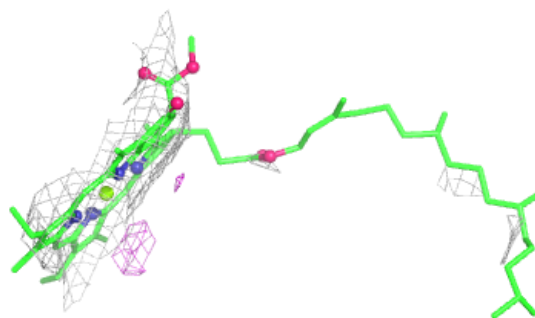


Electron density around CLA C 520:

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

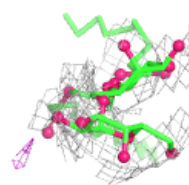
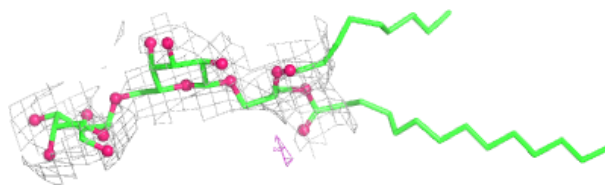
**Electron density around CLA D 405:**

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

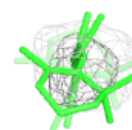
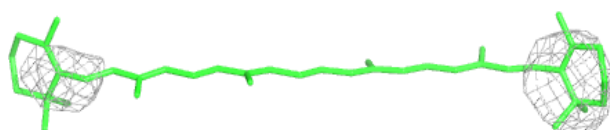
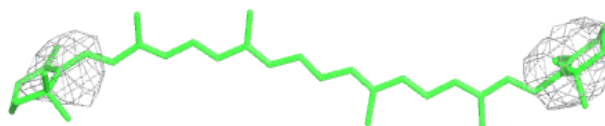


Electron density around DGD C 515:

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

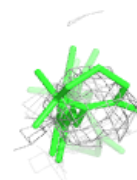
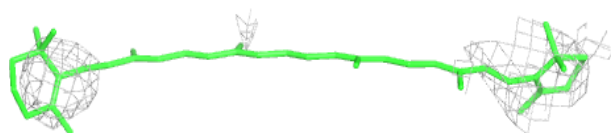
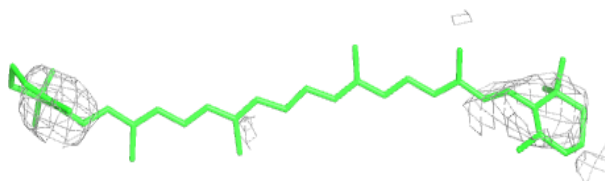
**Electron density around BCR A 407:**

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

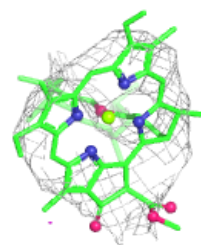
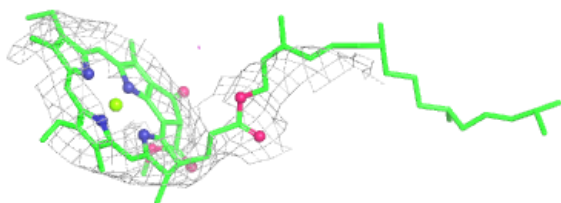


Electron density around BCR B 616:

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

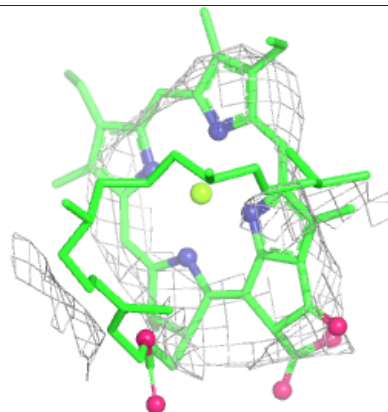
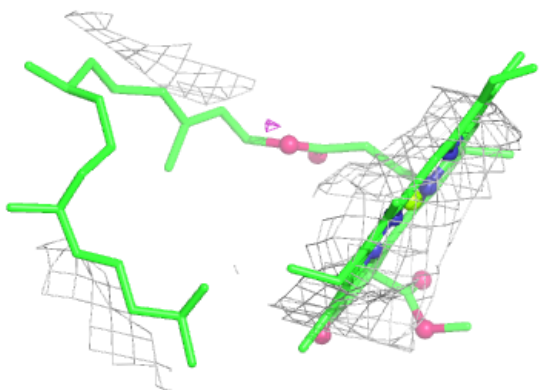
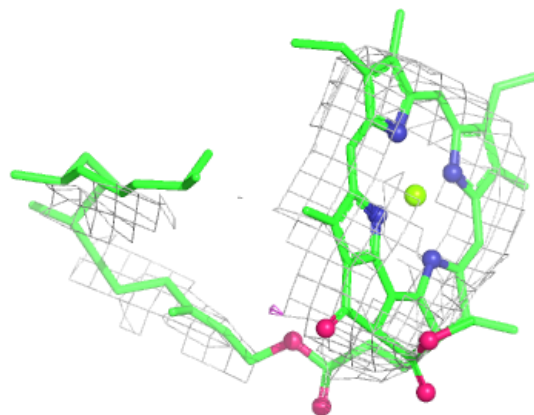
**Electron density around CLA c 502:**

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

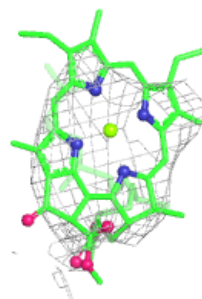
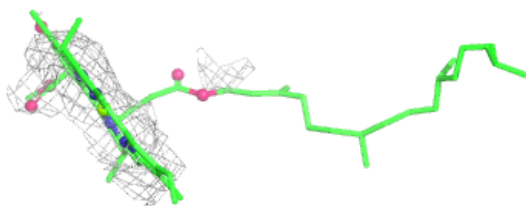
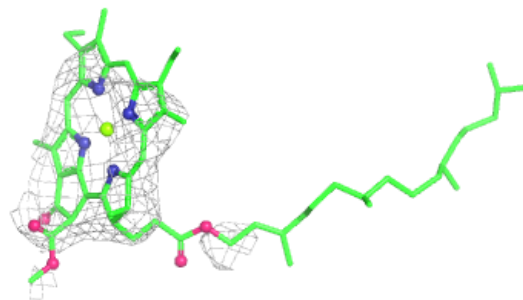


Electron density around CLA c 503:

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

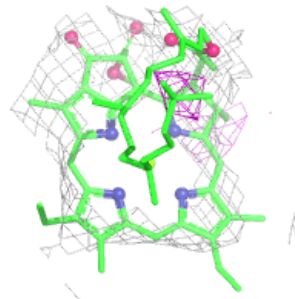
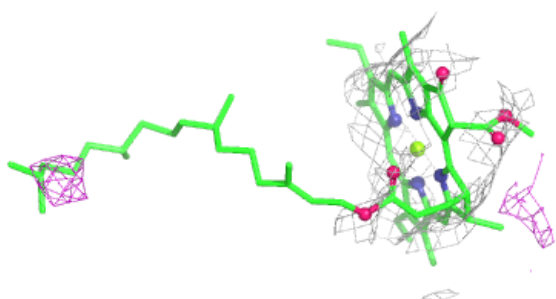
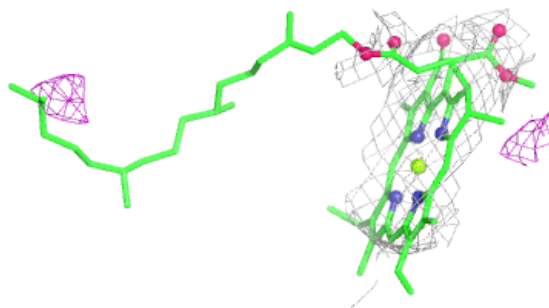
**Electron density around CLA a 408:**

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

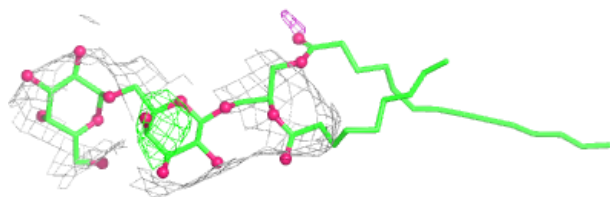
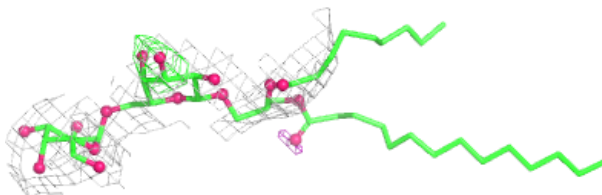


Electron density around CLA C 507:

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

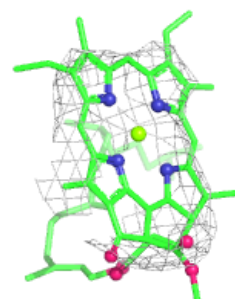
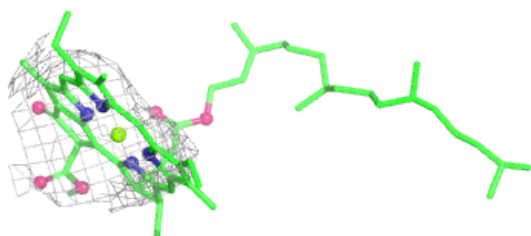
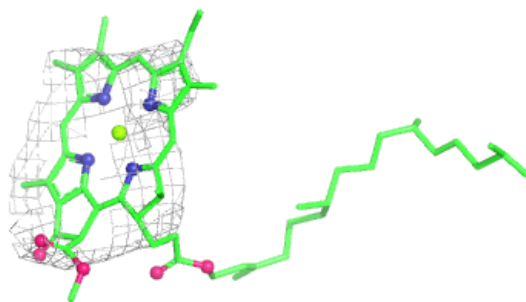
**Electron density around DGD c 515:**

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

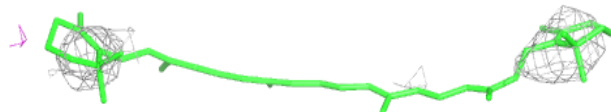
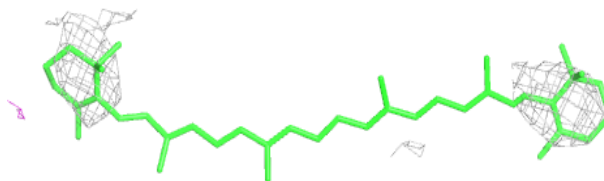


Electron density around CLA c 510:

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

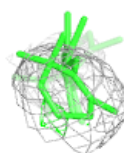
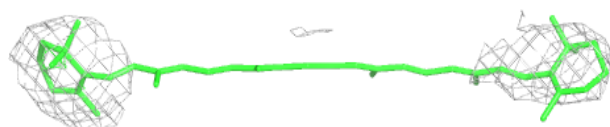
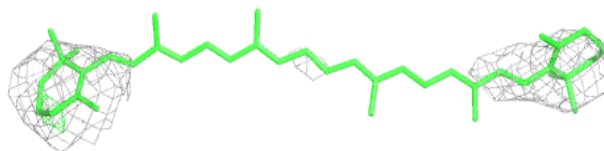
**Electron density around BCR b 621:**

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

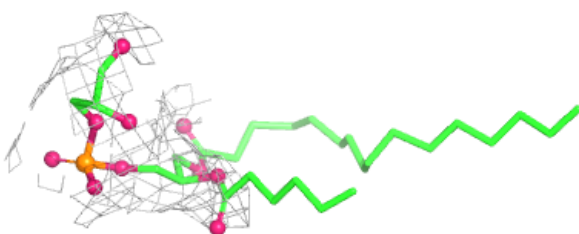
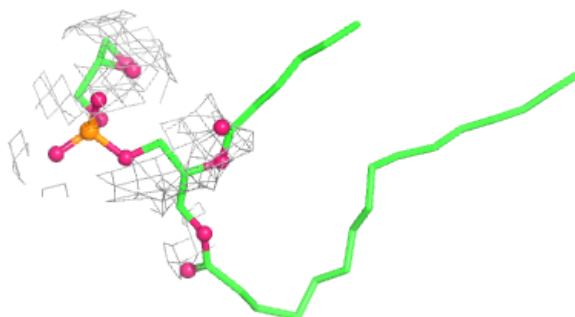


Electron density around BCR b 622:

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

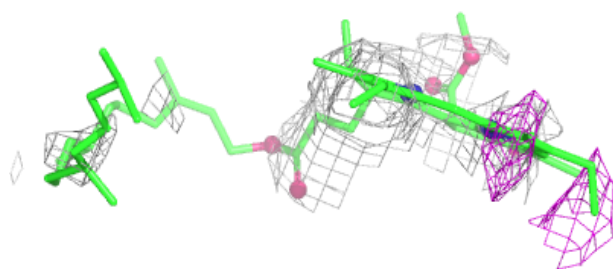
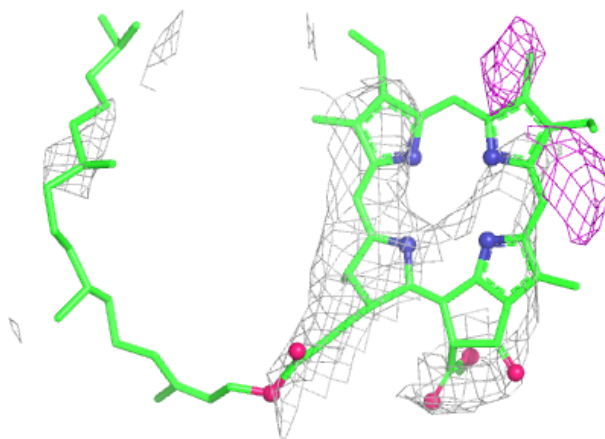
**Electron density around LHG A 409:**

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



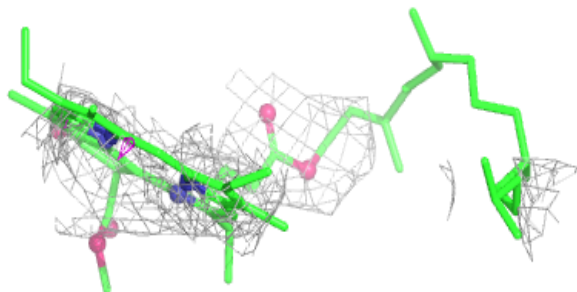
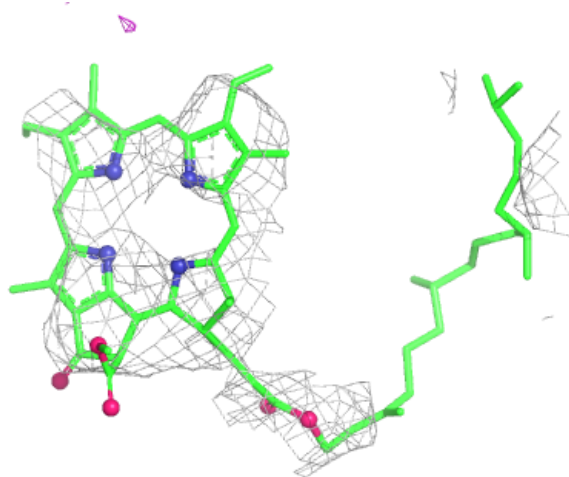
Electron density around PHO D 401:

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



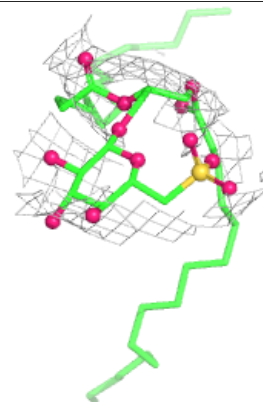
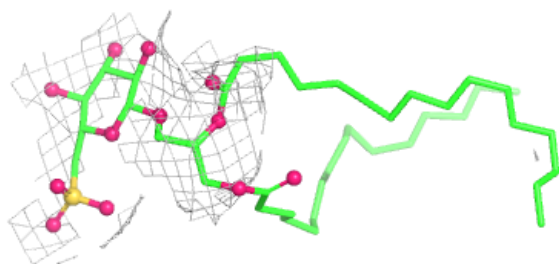
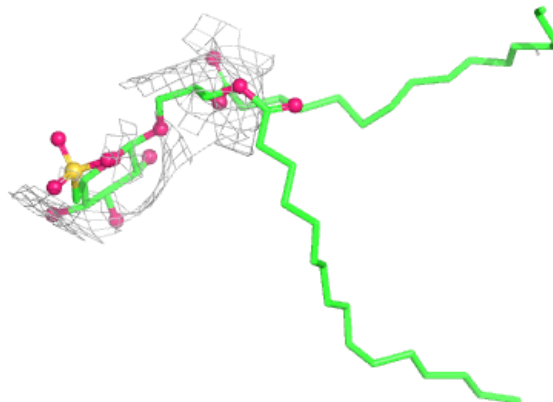
Electron density around PHO D 402:

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



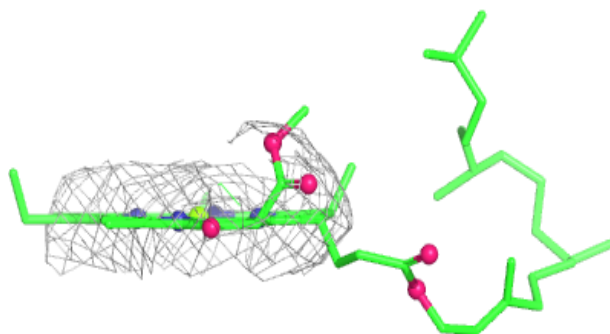
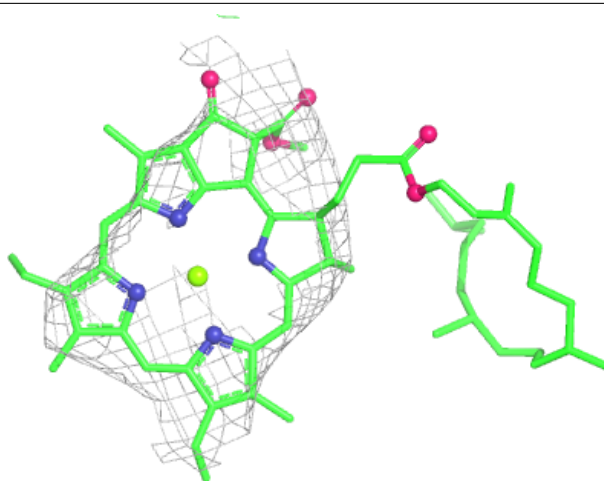
Electron density around SQD A 414:

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



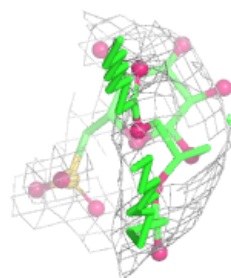
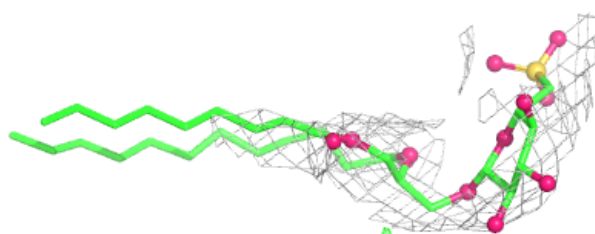
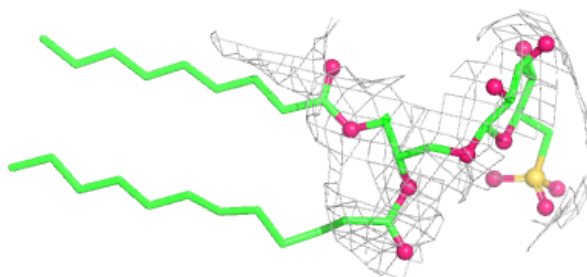
Electron density around CLA c 511:

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

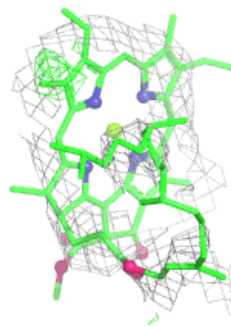
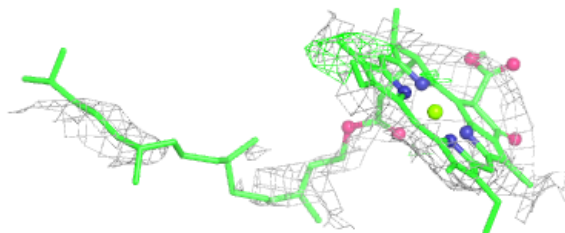


Electron density around SQD D 403:

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

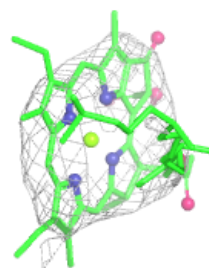
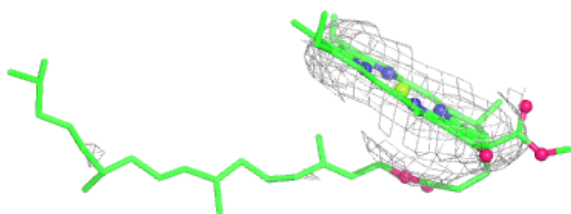
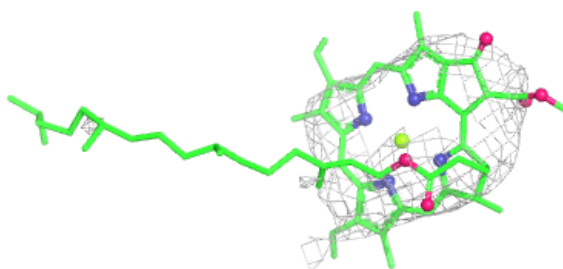
**Electron density around CLA C 510:**

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

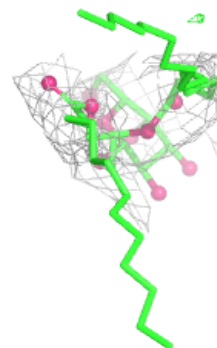
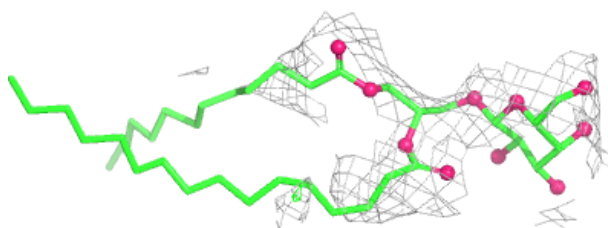
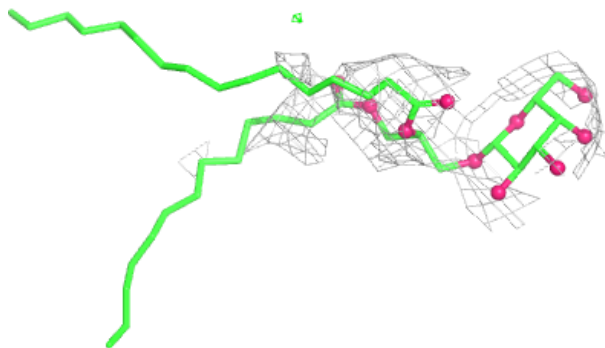


Electron density around CLA B 607:

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

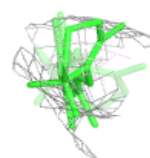
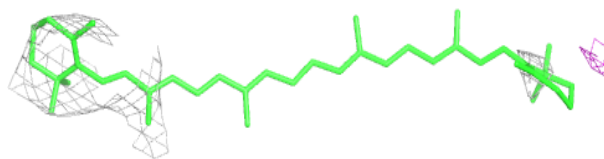
**Electron density around LMG d 407:**

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



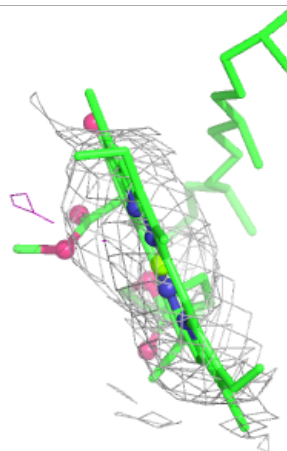
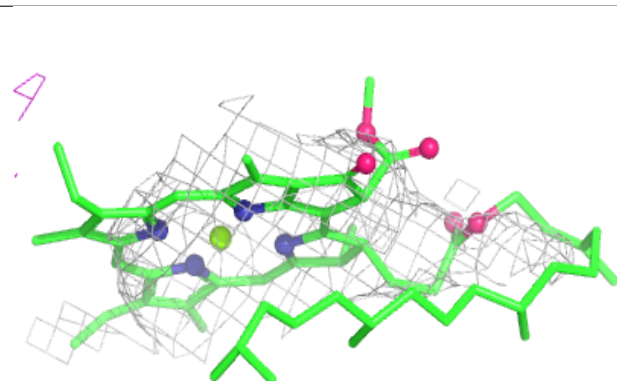
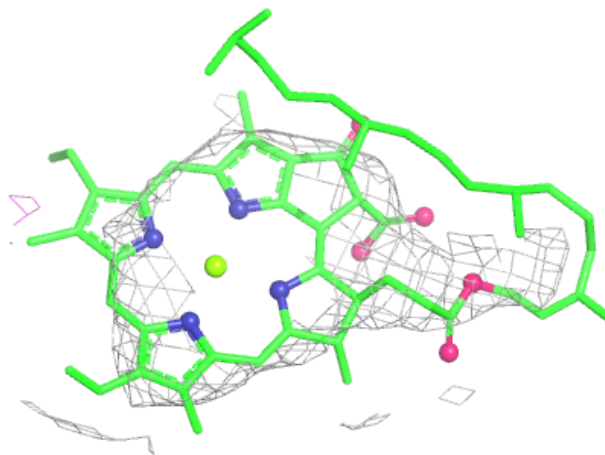
Electron density around BCR b 620:

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



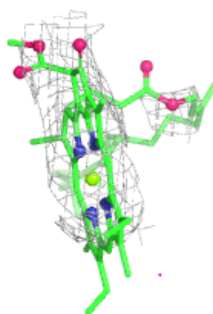
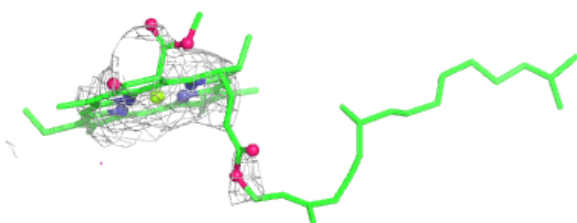
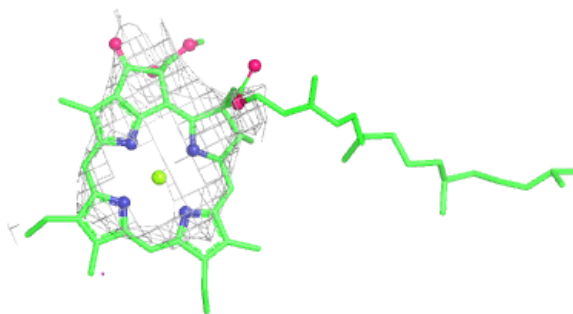
Electron density around CLA C 508:

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

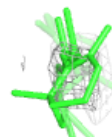
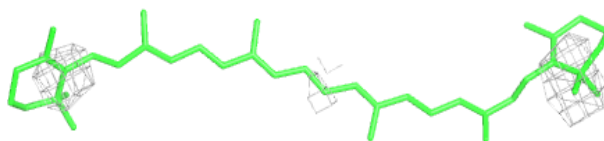


Electron density around CLA a 406:

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

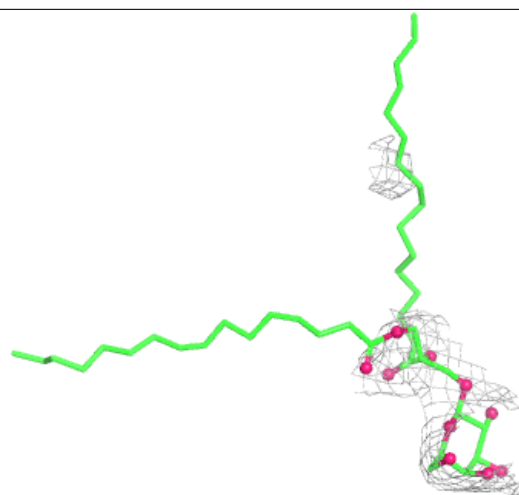
**Electron density around BCR y 101:**

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



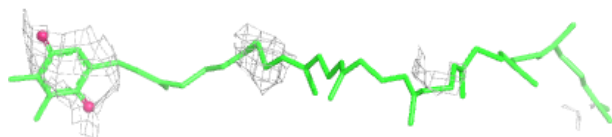
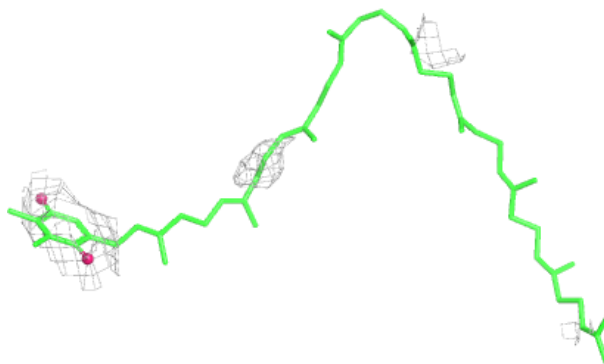
Electron density around LMG A 410:

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

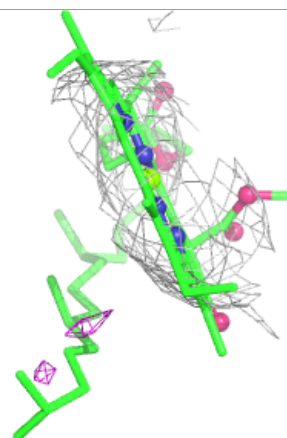
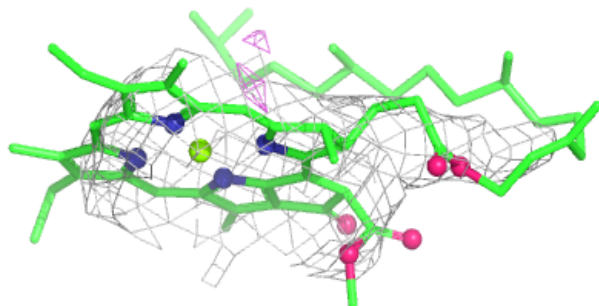
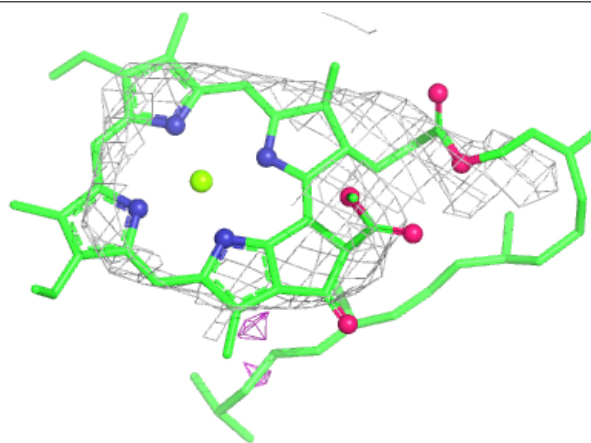


Electron density around PL9 d 406:

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

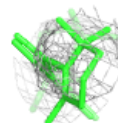
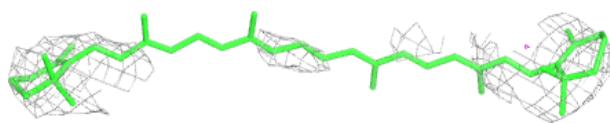
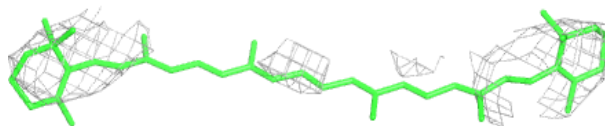
**Electron density around CLA c 508:**

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

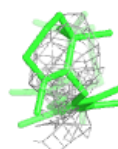
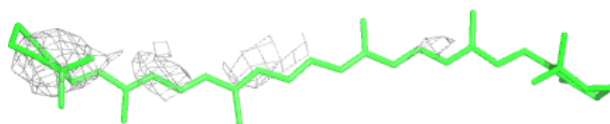
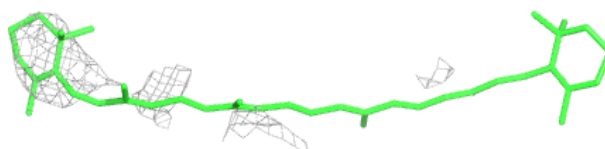


Electron density around BCR b 623:

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

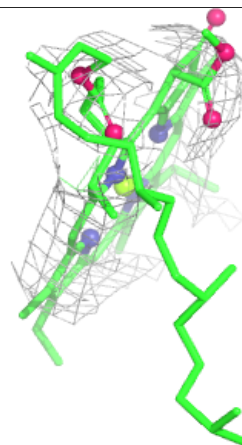
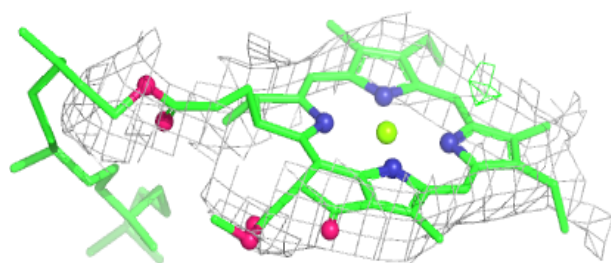
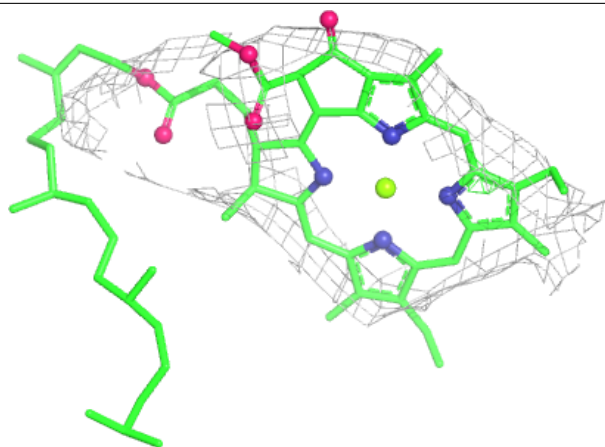
**Electron density around BCR c 513:**

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



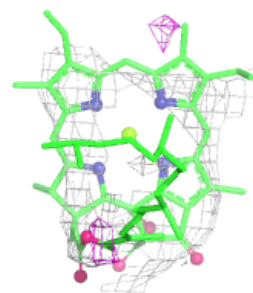
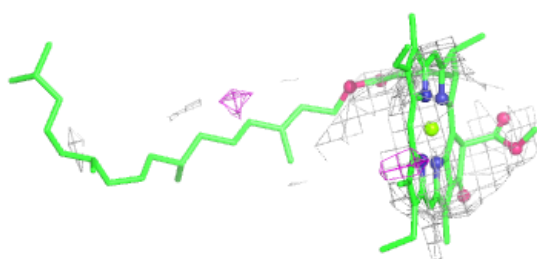
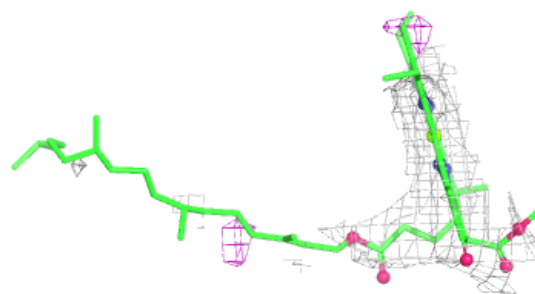
Electron density around CLA B 615:

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

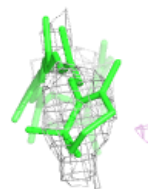
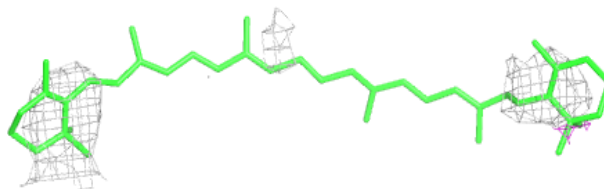


Electron density around CLA B 604:

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

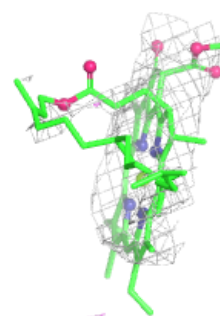
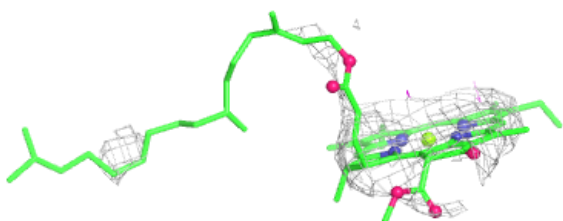
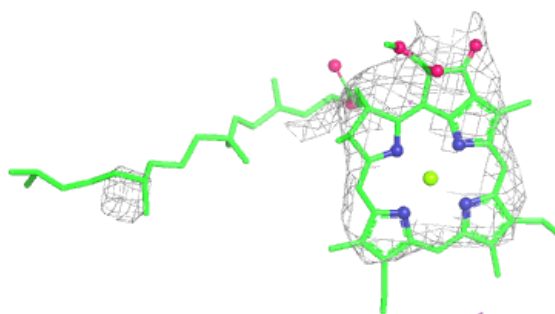
**Electron density around BCR B 617:**

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

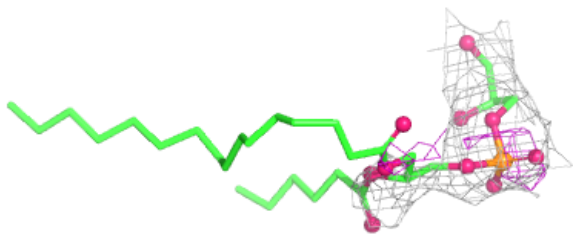
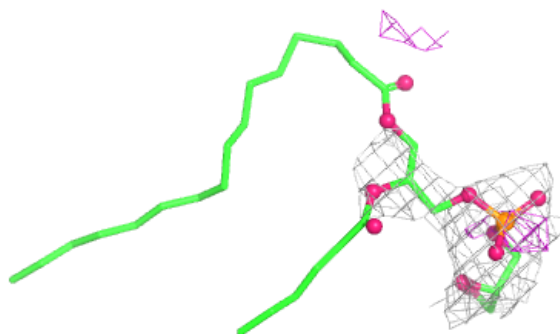


Electron density around CLA A 404:

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

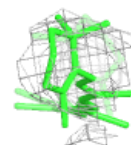
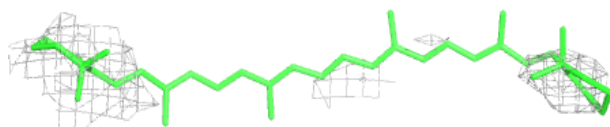
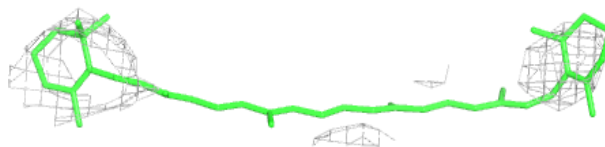
**Electron density around LHG a 412:**

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

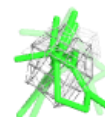
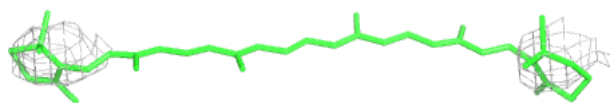
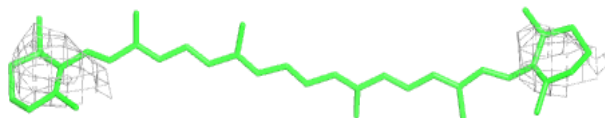


Electron density around BCR C 513:

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

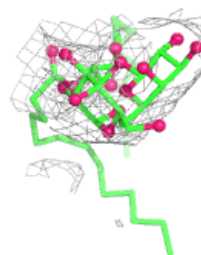
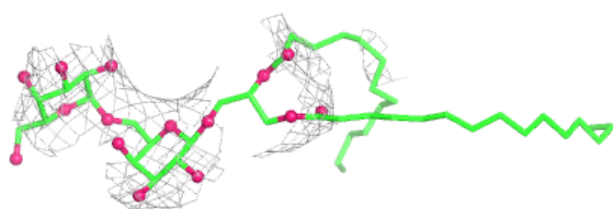
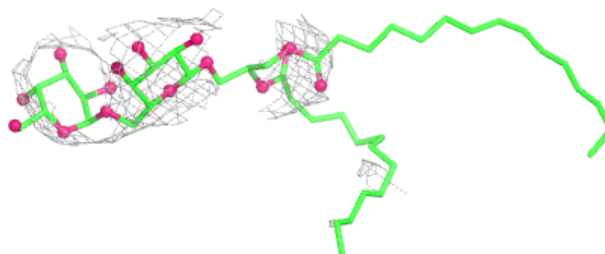
**Electron density around BCR C 514:**

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

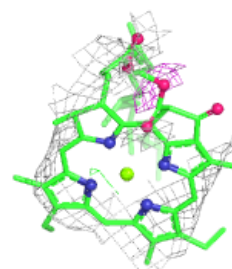
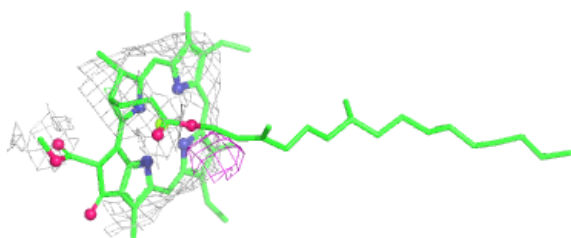
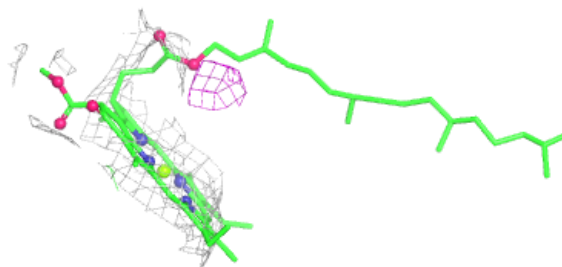


Electron density around DGD B 620:

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

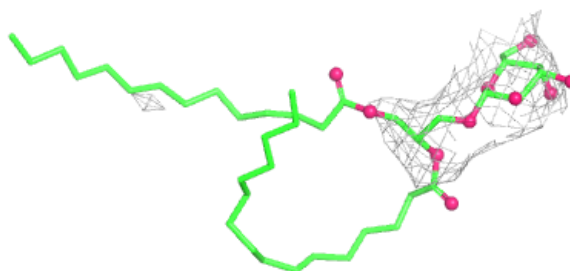
**Electron density around CLA c 520:**

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

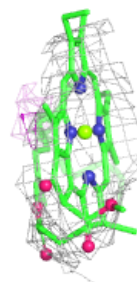
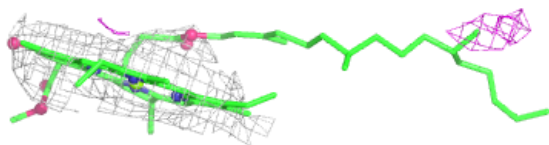
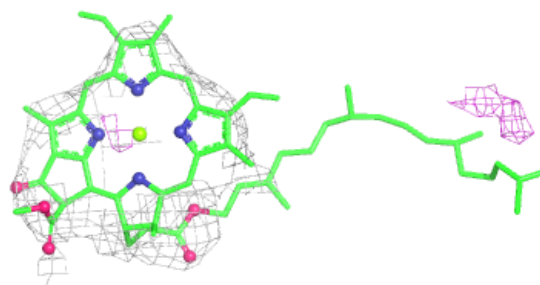


Electron density around LMG B 624:

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

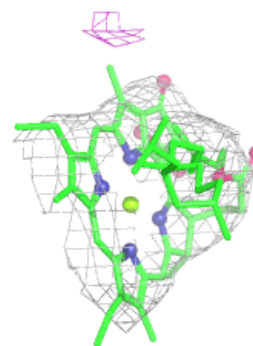
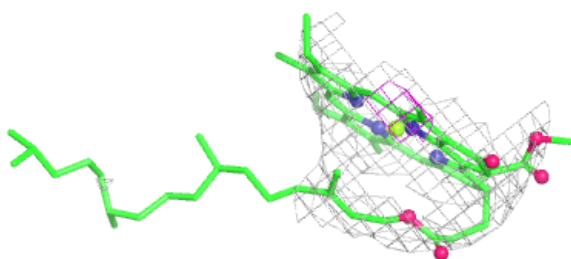
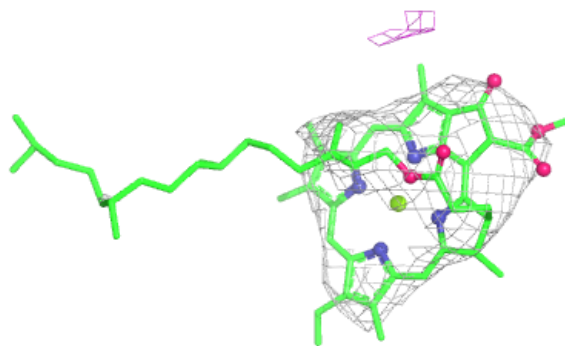
**Electron density around CLA B 602:**

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

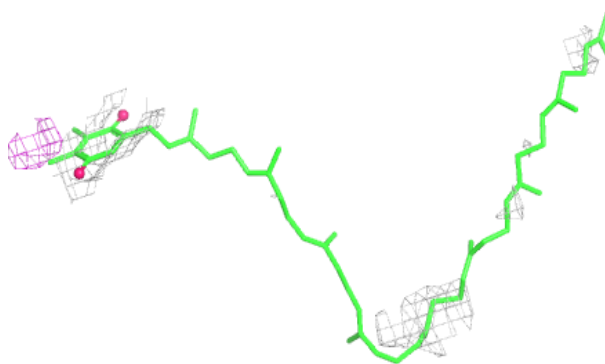


Electron density around CLA B 613:

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

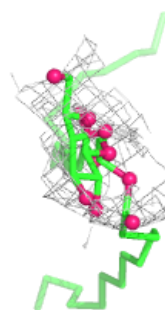
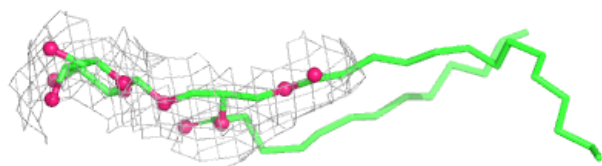
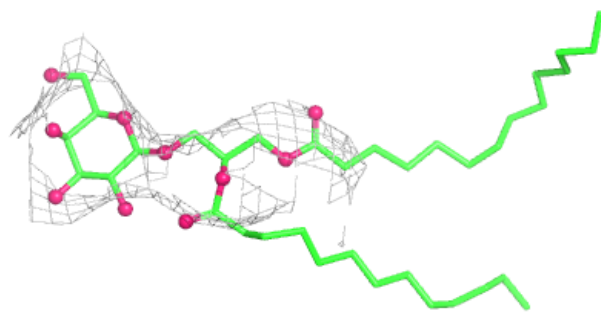
**Electron density around PL9 D 407:**

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

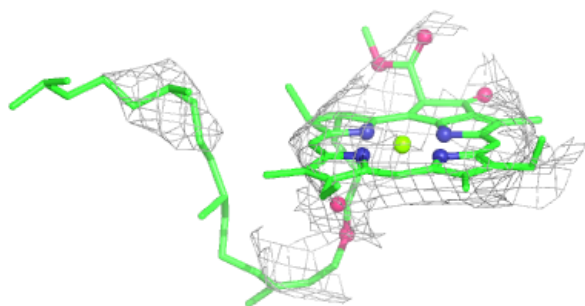
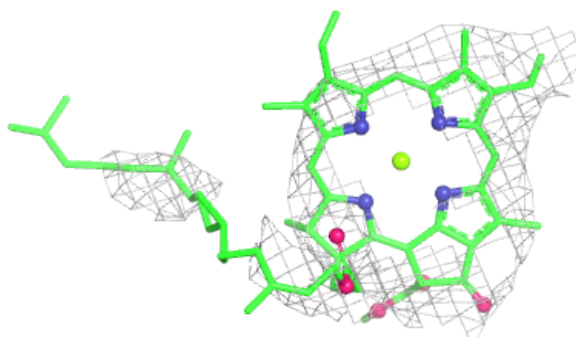


Electron density around LMG D 412:

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

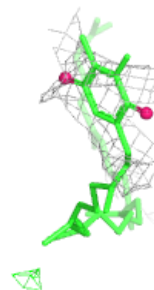
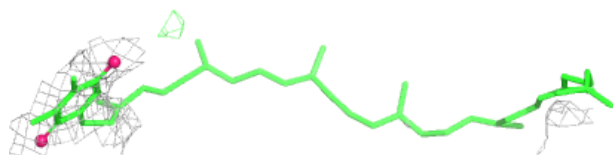
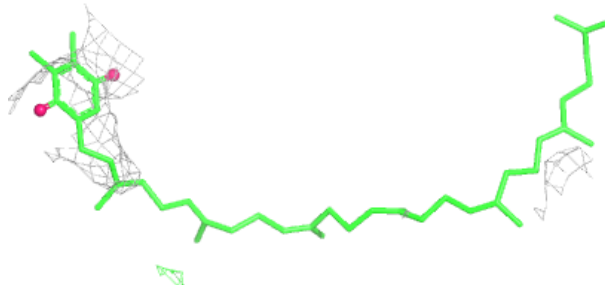
**Electron density around CLA a 405:**

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

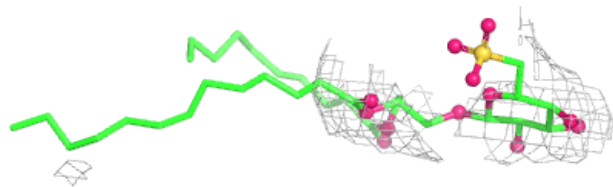
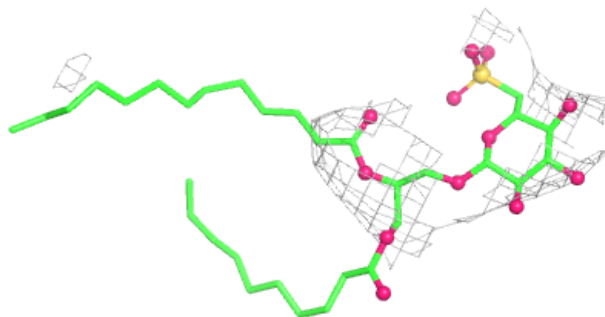


Electron density around PL9 a 409:

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

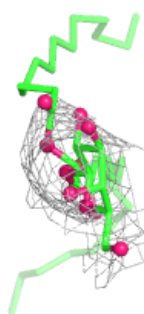
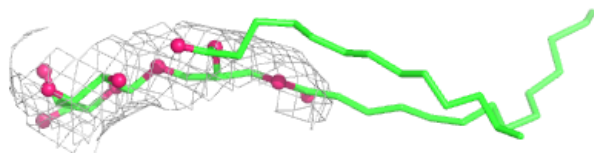
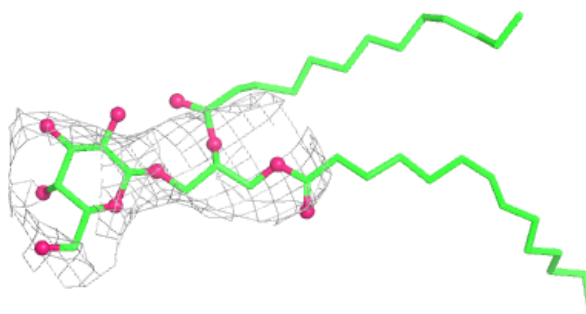
**Electron density around SQD f 103:**

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



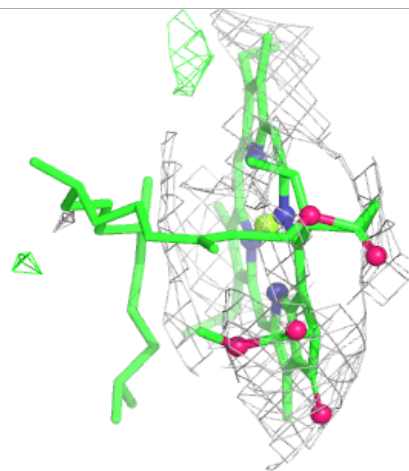
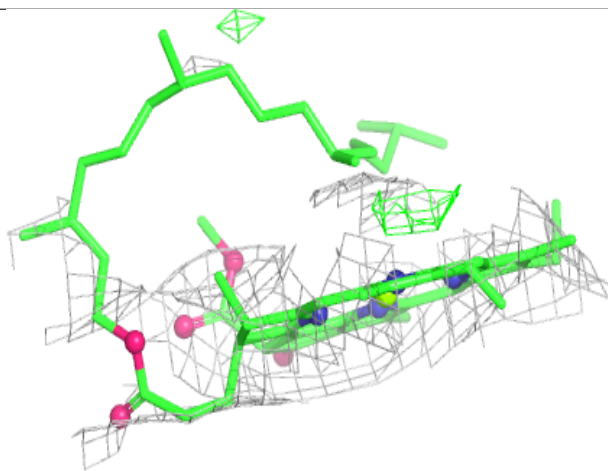
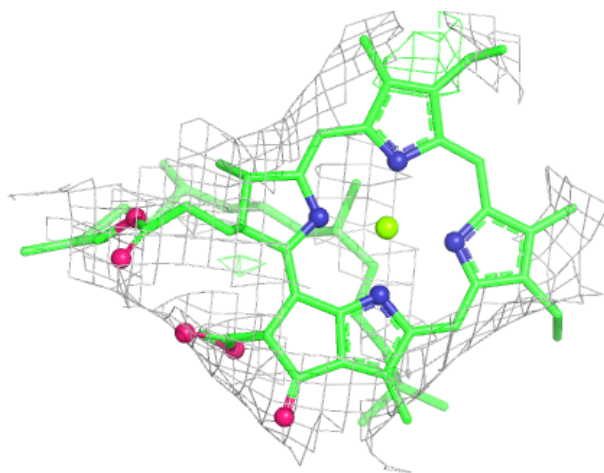
Electron density around LMG d 410:

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



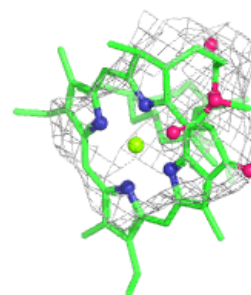
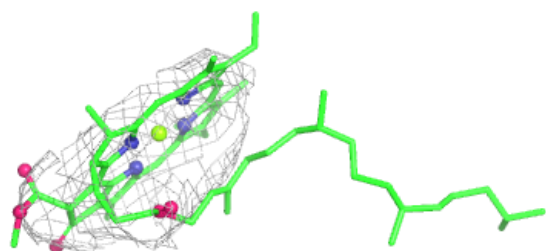
Electron density around CLA C 509:

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

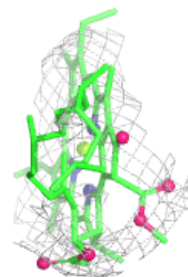
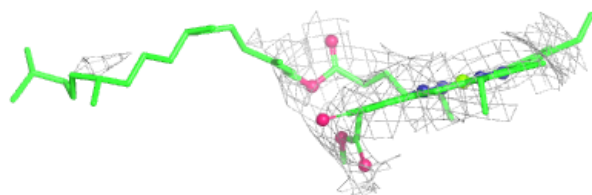
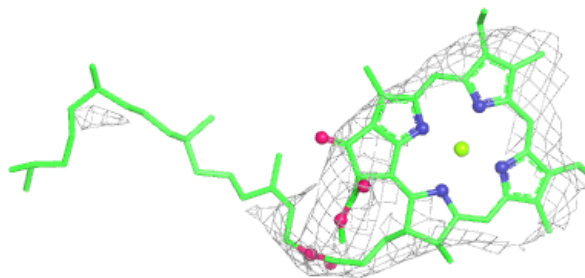


Electron density around CLA c 504:

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

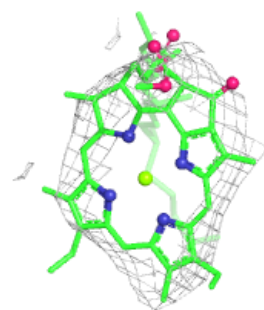
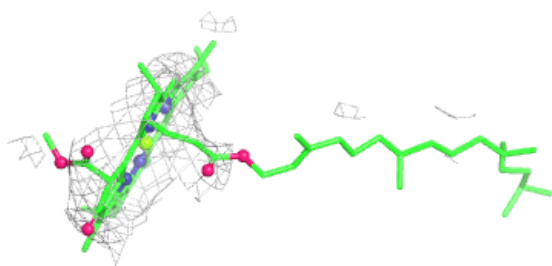
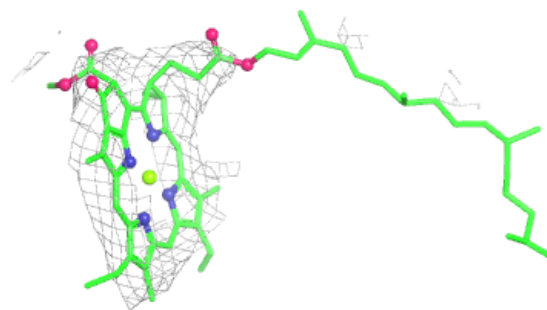
**Electron density around CLA H 101:**

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

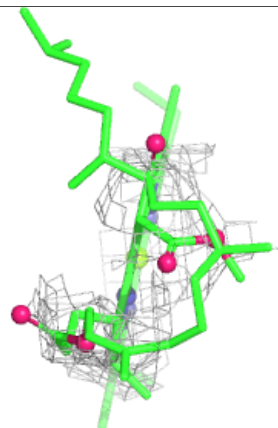
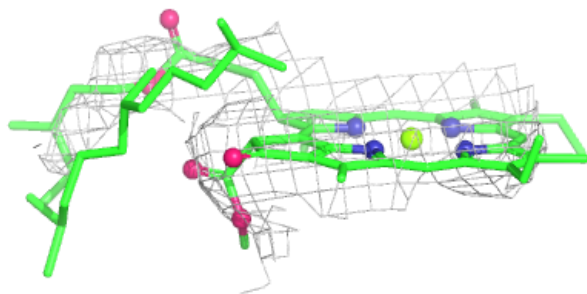
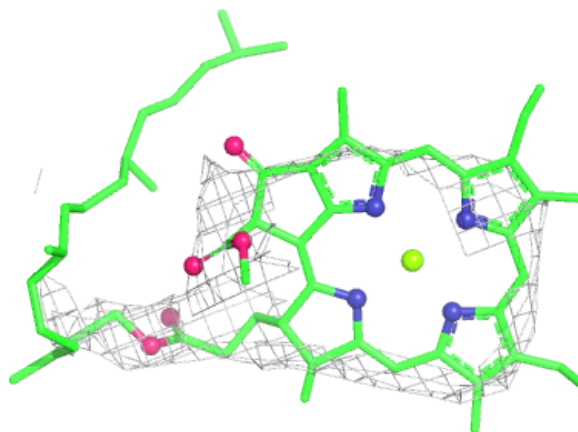


Electron density around CLA b 612:

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

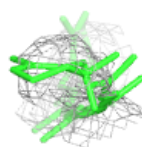
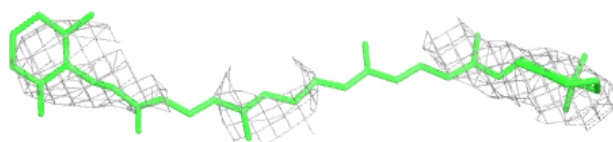
**Electron density around CLA b 613:**

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

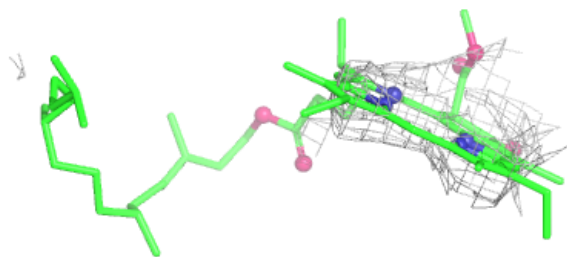
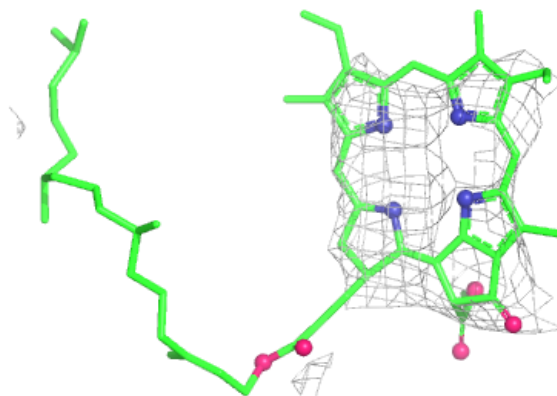


Electron density around BCR f 102:

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

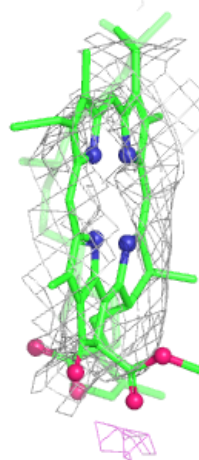
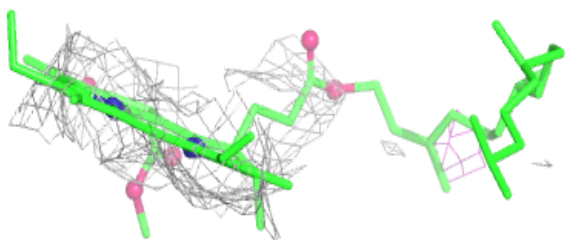
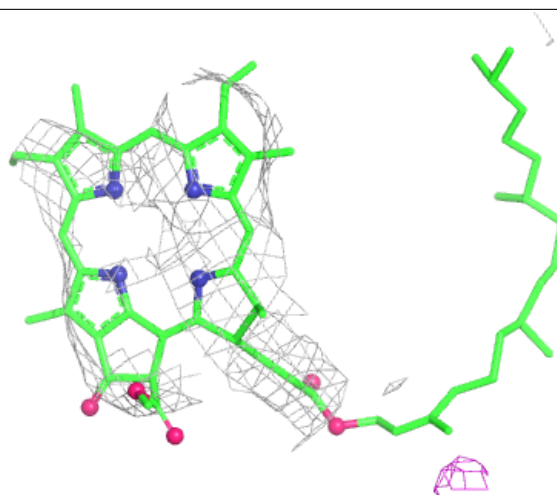
**Electron density around PHO a 407:**

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



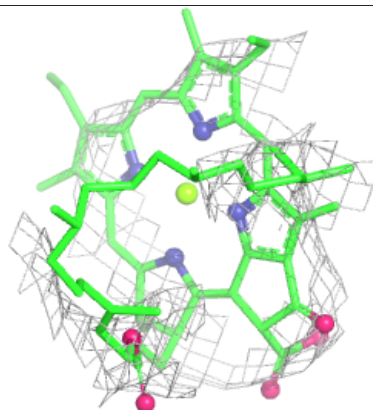
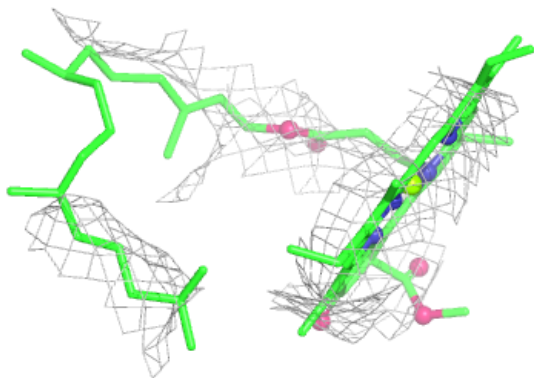
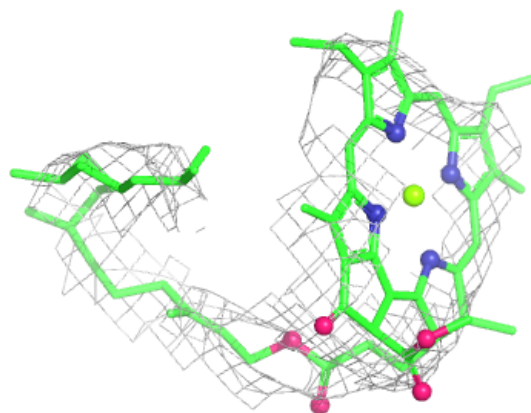
Electron density around PHO d 401:

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



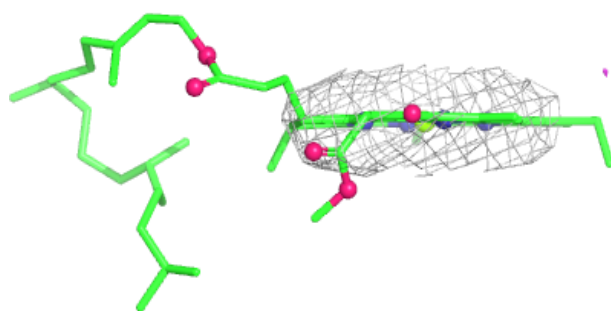
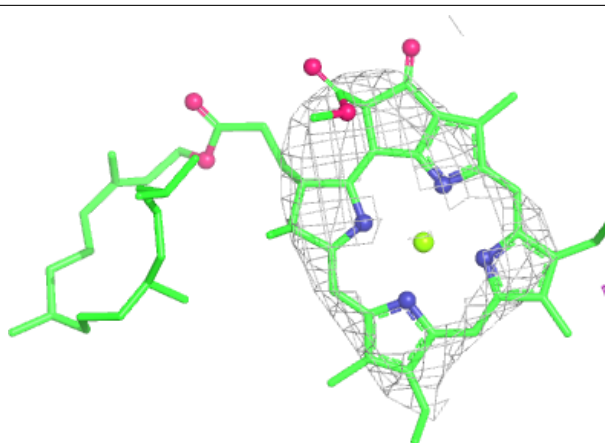
Electron density around CLA C 503:

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



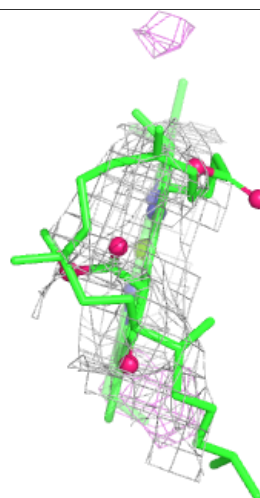
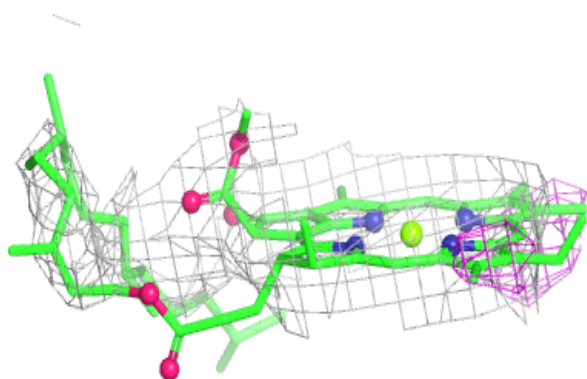
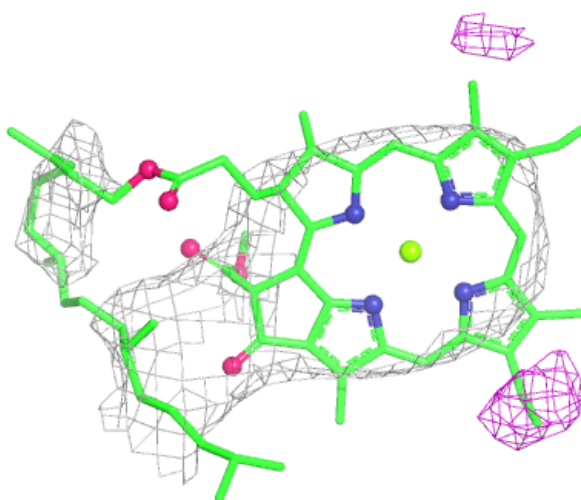
Electron density around CLA C 511:

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



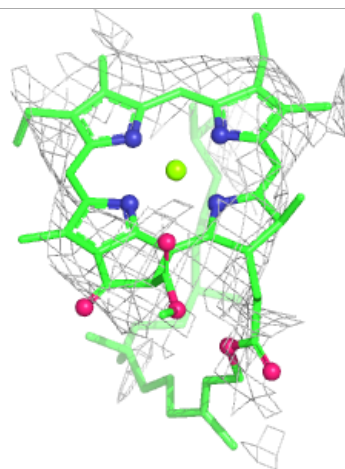
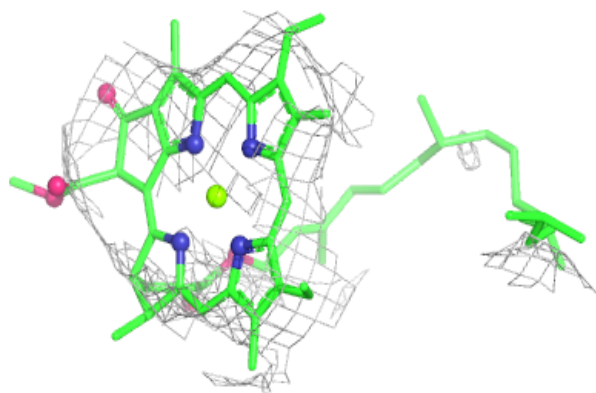
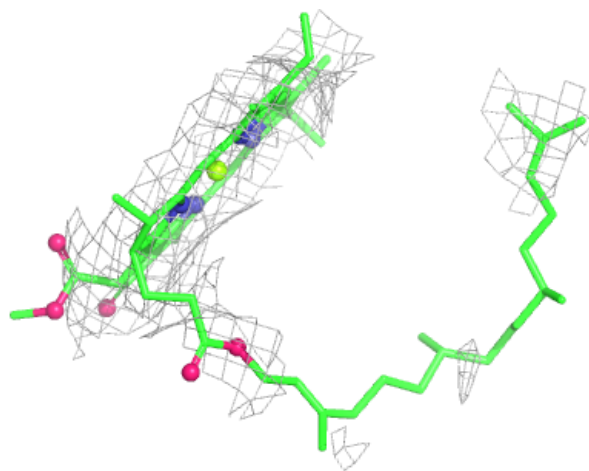
Electron density around CLA B 609:

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



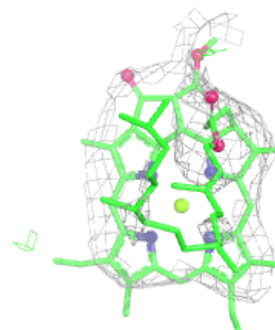
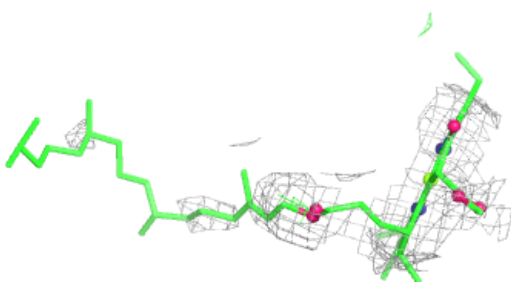
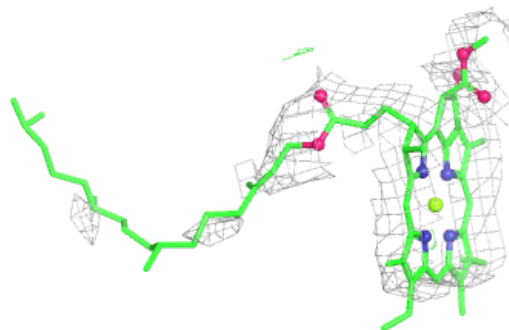
Electron density around CLA B 610:

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

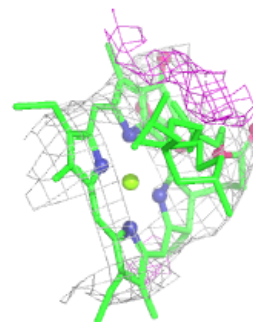
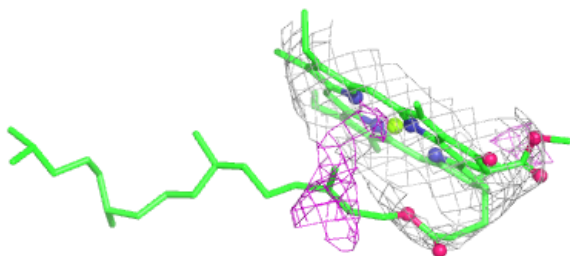
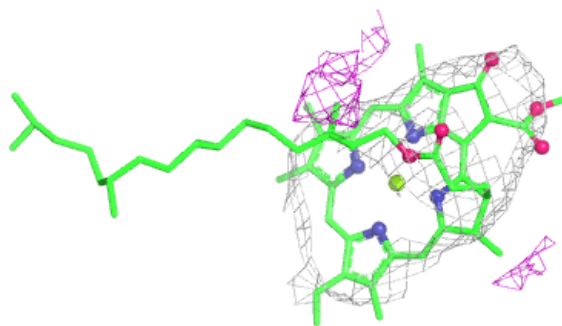


Electron density around CLA d 405:

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

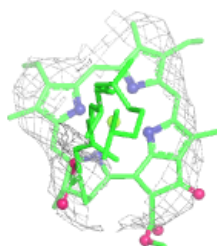
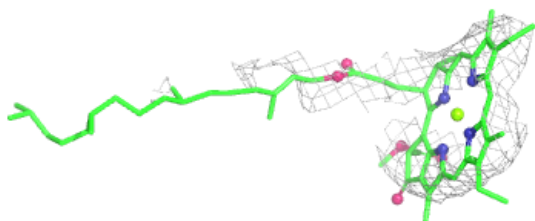
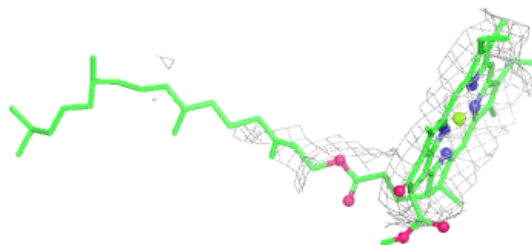
**Electron density around CLA b 617:**

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

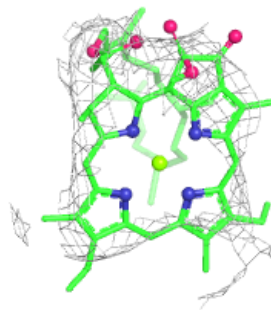
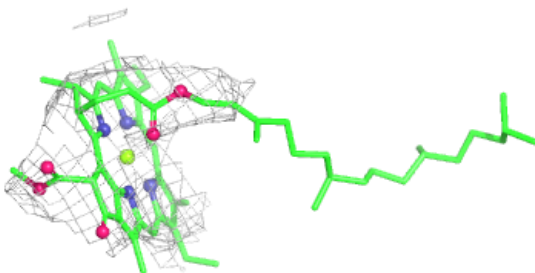
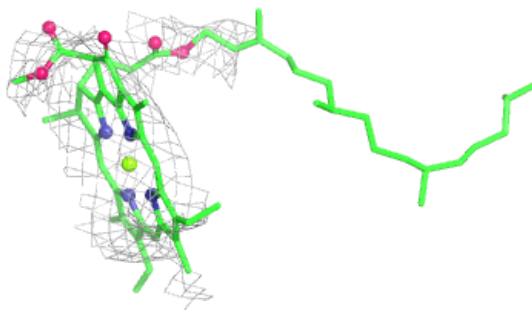


Electron density around CLA b 607:

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

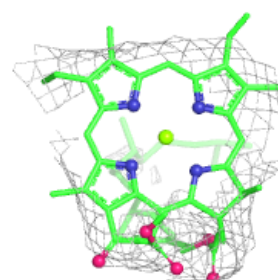
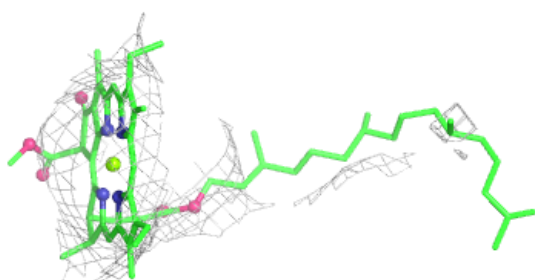
**Electron density around CLA c 507:**

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

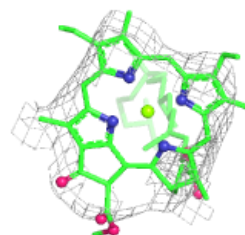
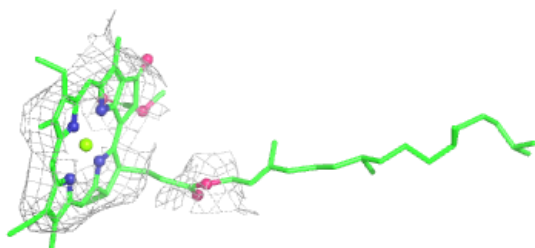
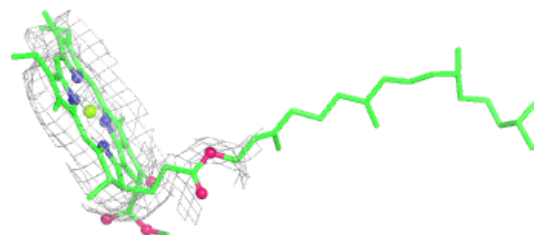


Electron density around CLA b 608:

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

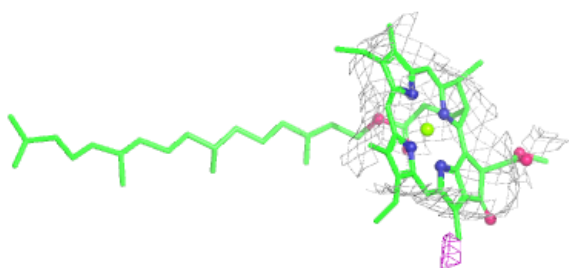
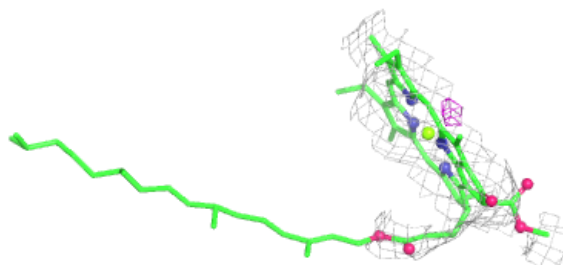
**Electron density around CLA B 603:**

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

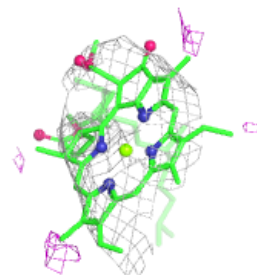
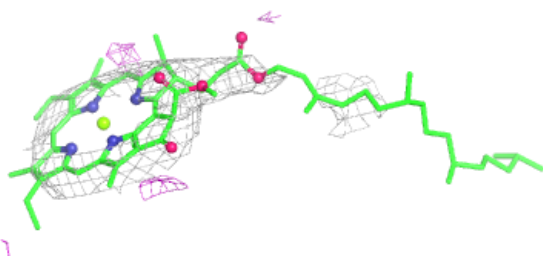
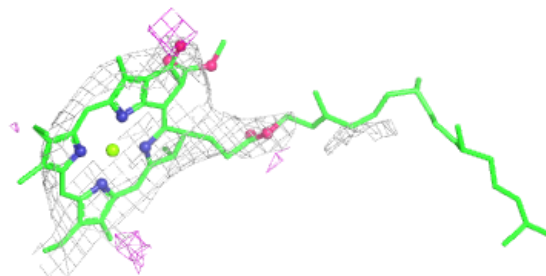


Electron density around CLA b 610:

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

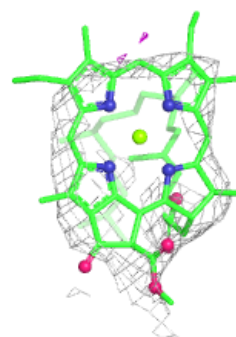
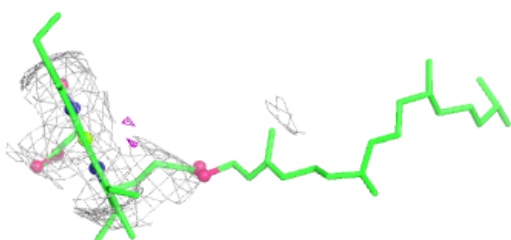
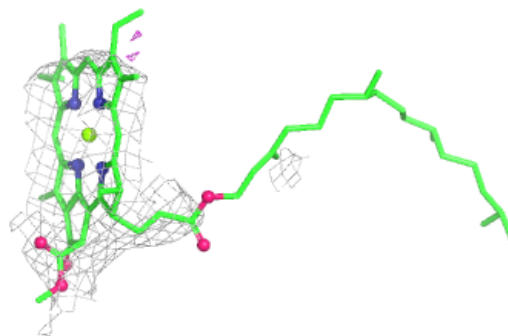
**Electron density around CLA A 402:**

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

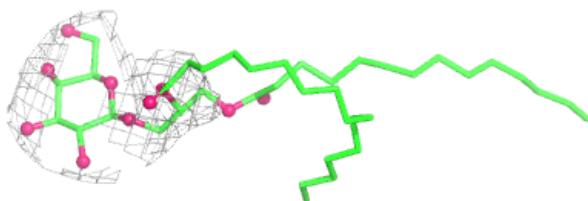
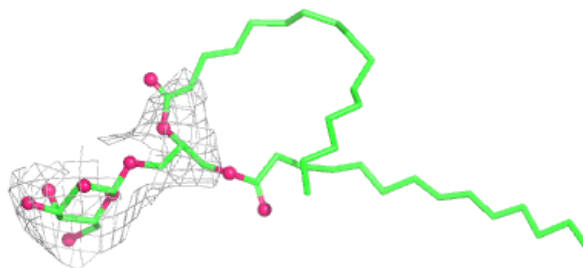


Electron density around CLA D 406:

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

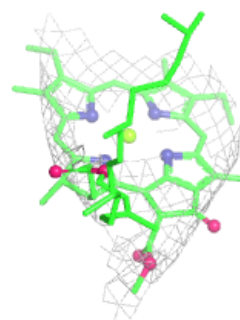
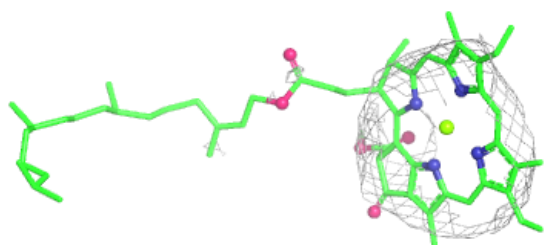
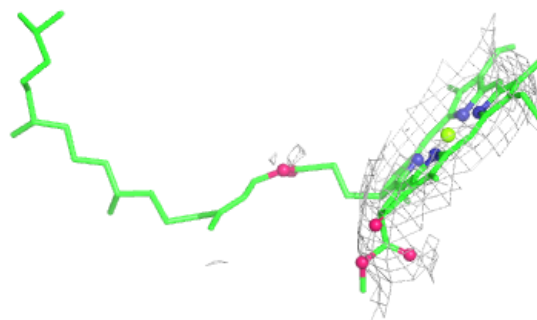
**Electron density around LMG b 628:**

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

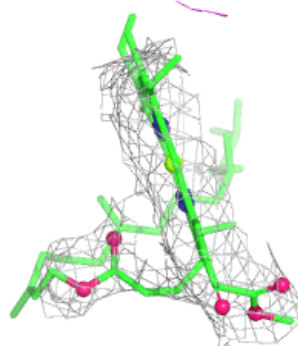
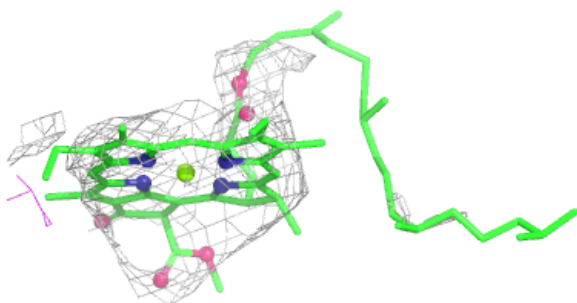
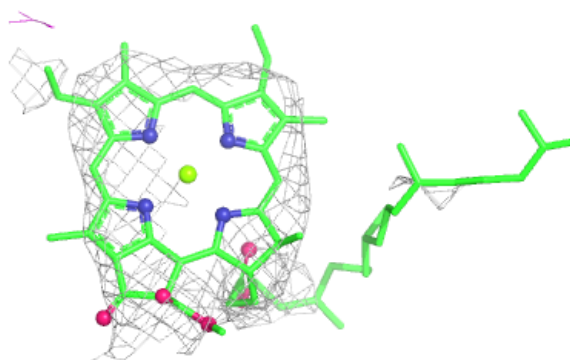


Electron density around CLA d 404:

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

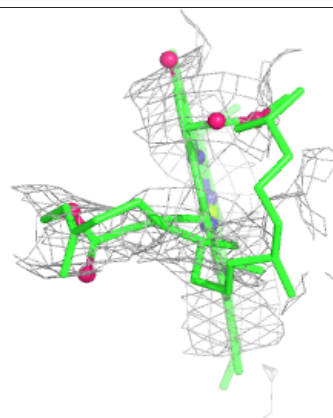
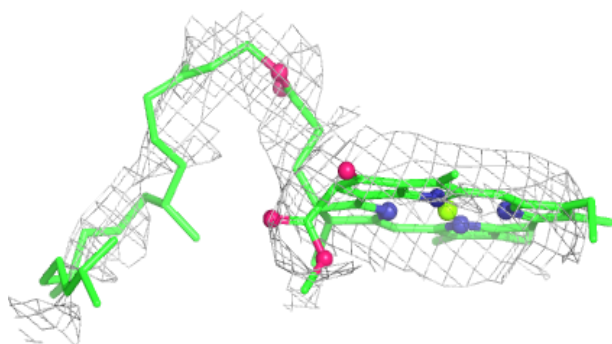
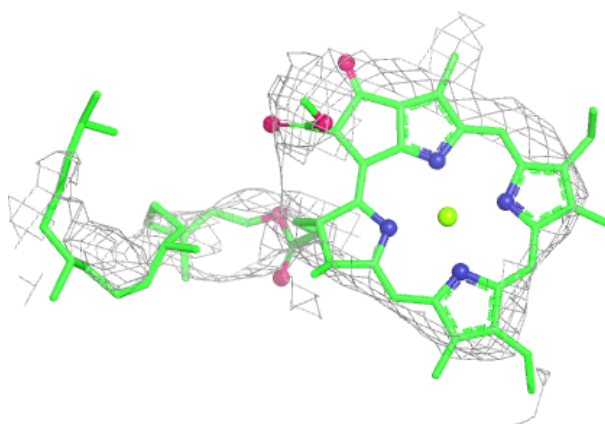
**Electron density around CLA A 403:**

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

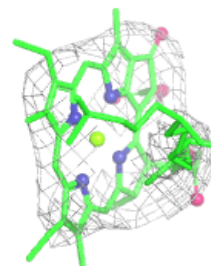
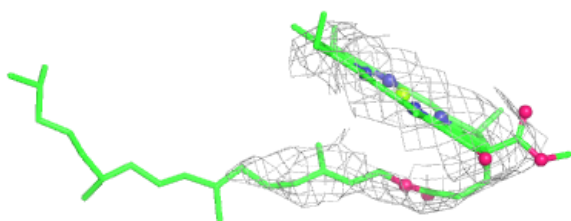


Electron density around CLA B 611:

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

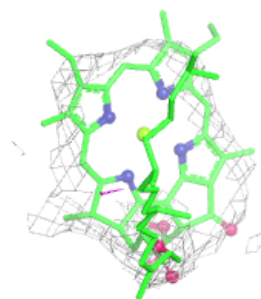
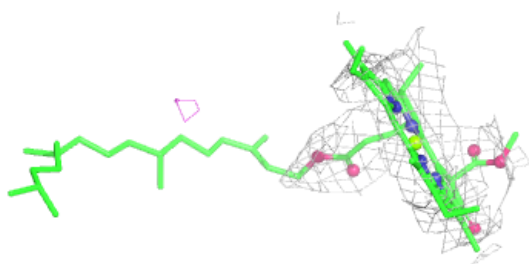
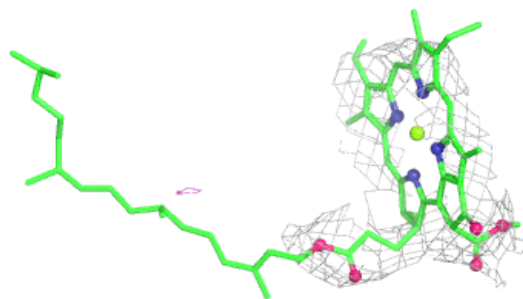
**Electron density around CLA b 611:**

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



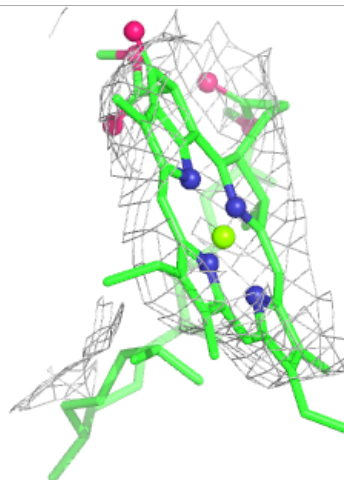
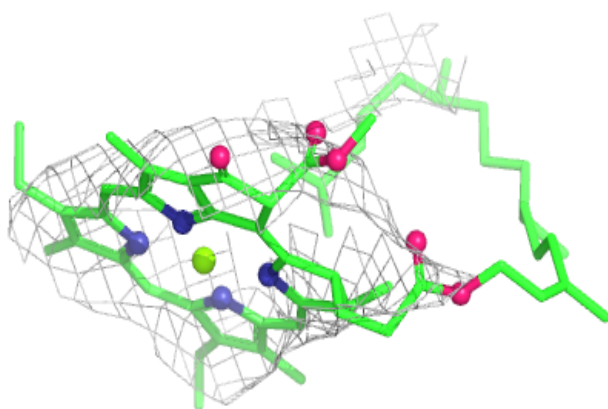
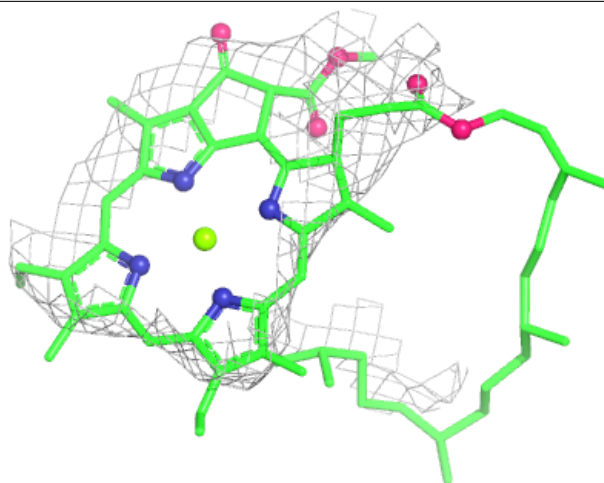
Electron density around CLA B 608:

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



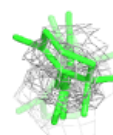
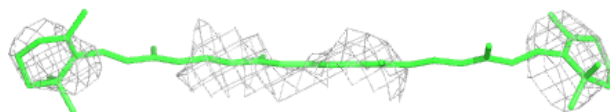
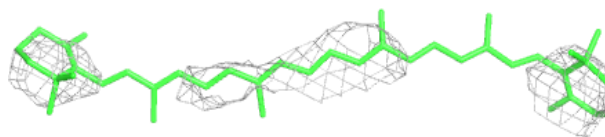
Electron density around CLA B 614:

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

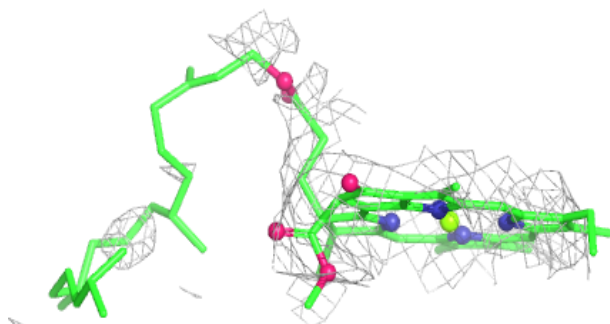
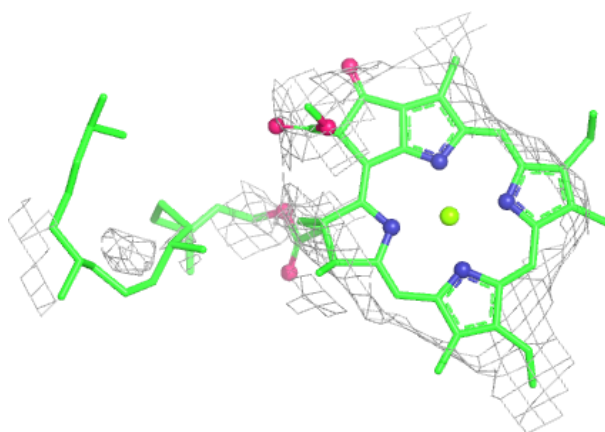


Electron density around BCR B 618:

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

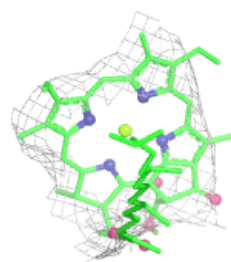
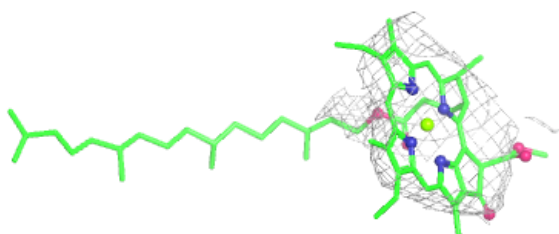
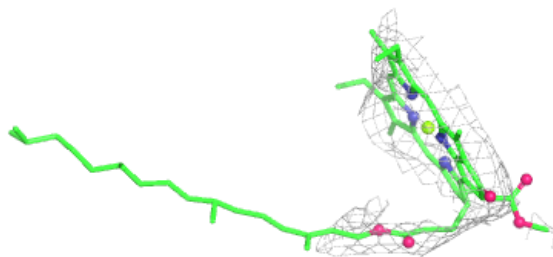
**Electron density around CLA b 615:**

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



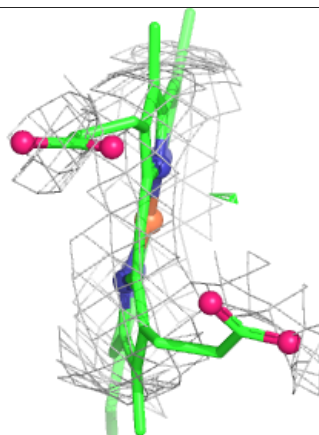
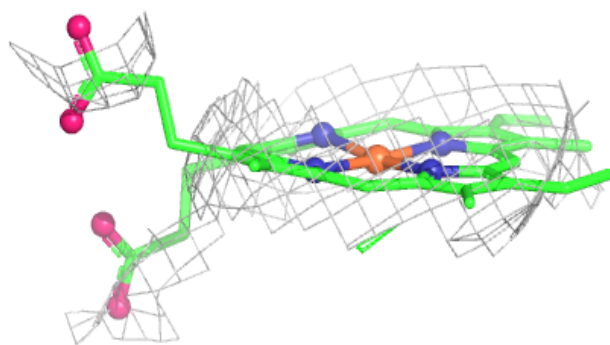
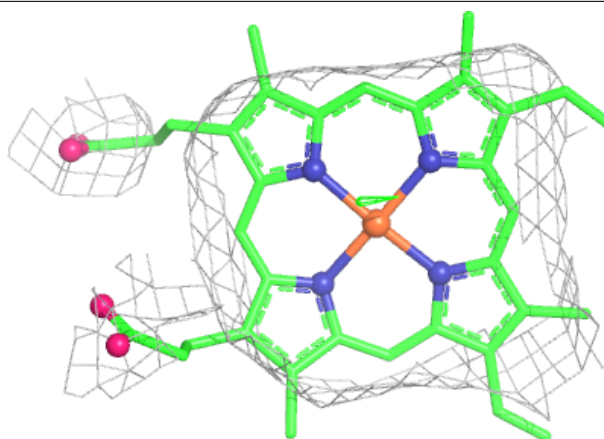
Electron density around CLA B 606:

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



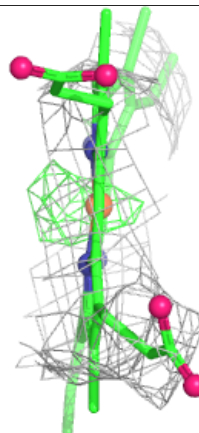
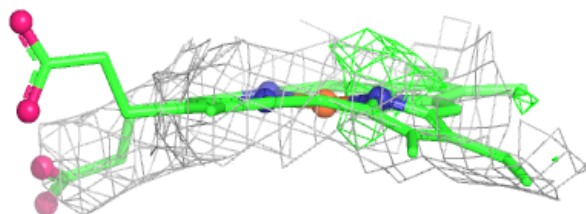
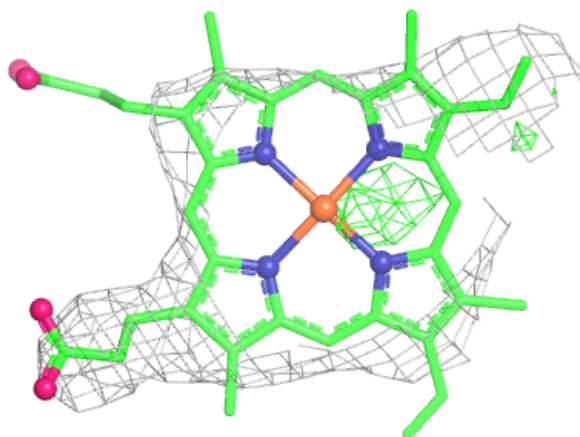
Electron density around HEM F 101:

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

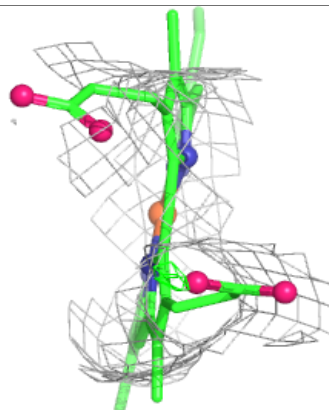
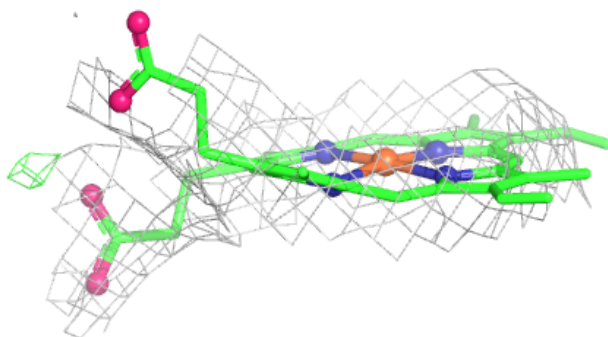
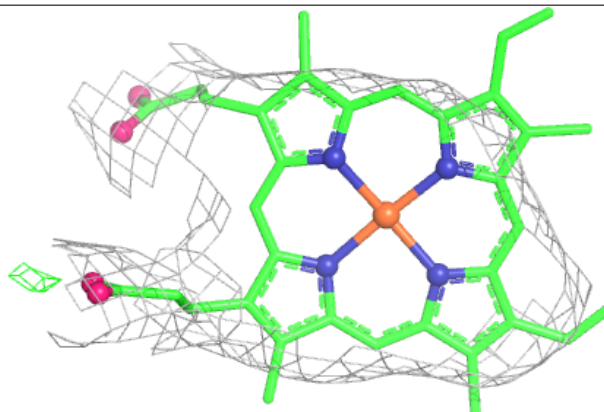


Electron density around HEM V 201:

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

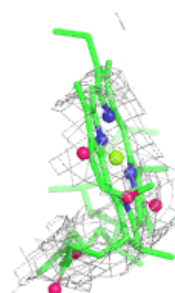
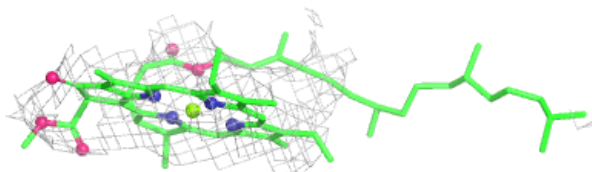
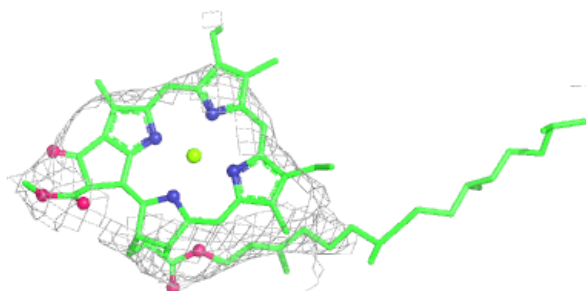
**Electron density around HEM f 101:**

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

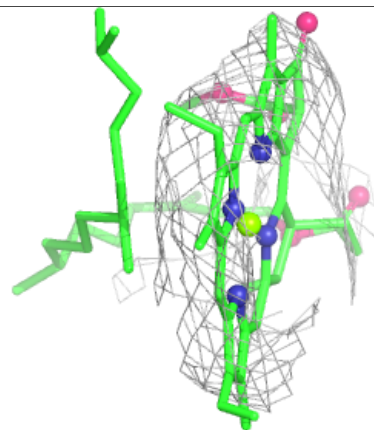
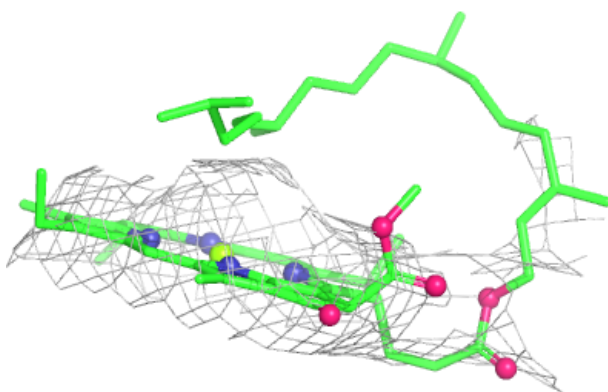
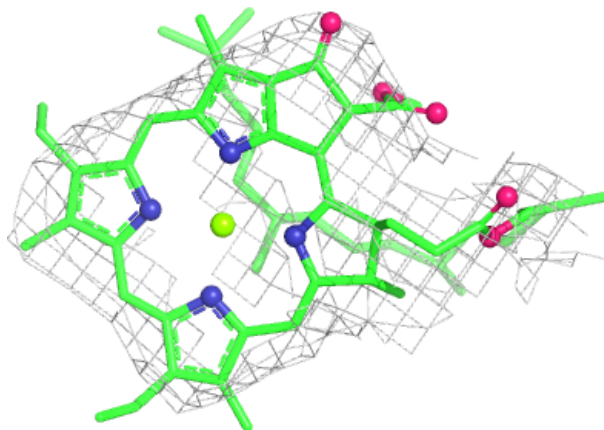


Electron density around CLA C 501:

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

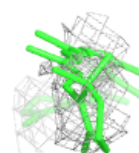
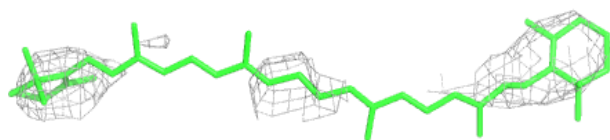
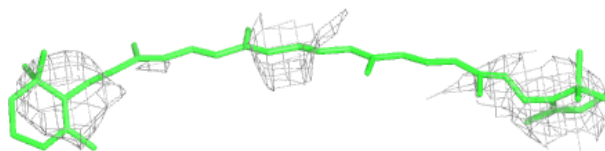
**Electron density around CLA c 509:**

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

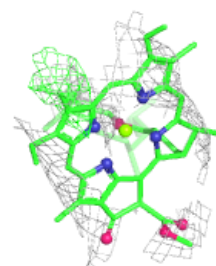
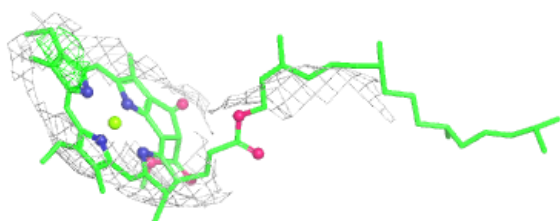


Electron density around BCR D 411:

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

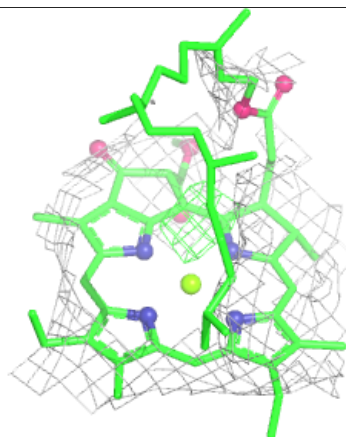
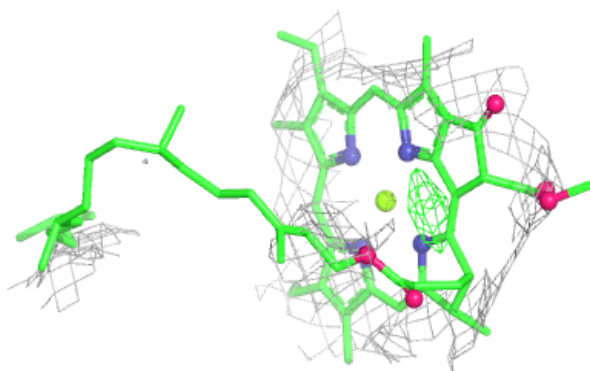
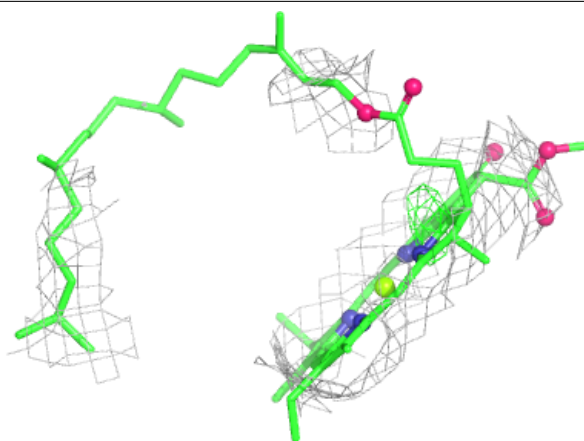
**Electron density around CLA C 502:**

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



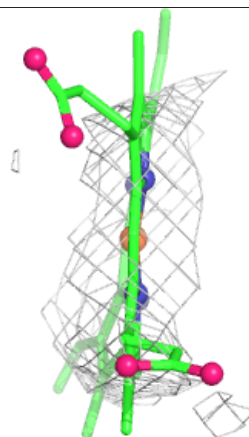
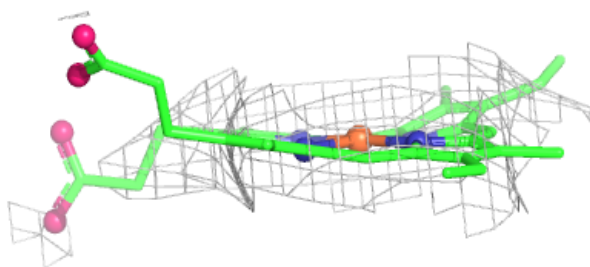
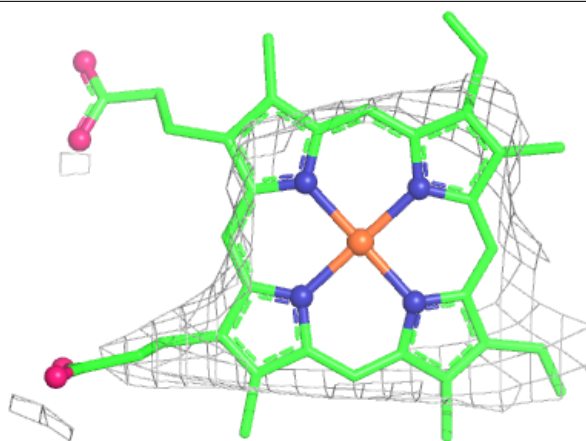
Electron density around CLA b 614:

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



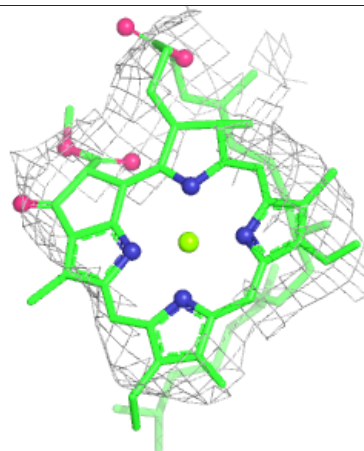
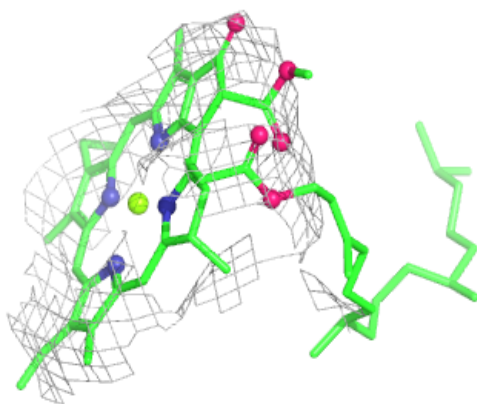
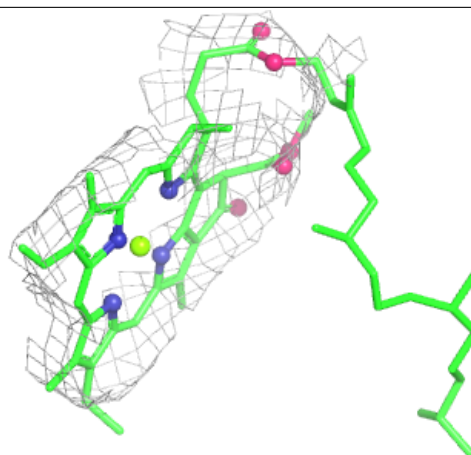
Electron density around HEM v 201:

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



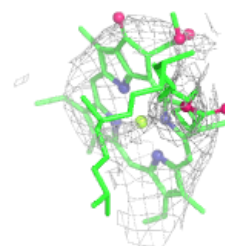
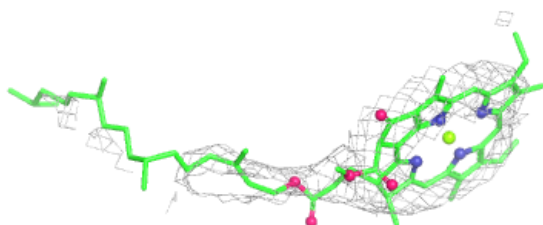
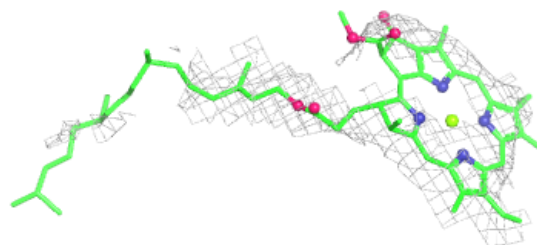
Electron density around CLA B 612:

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



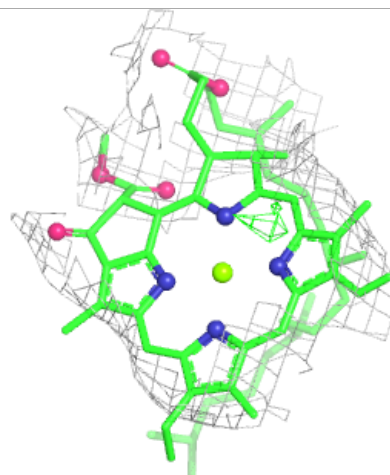
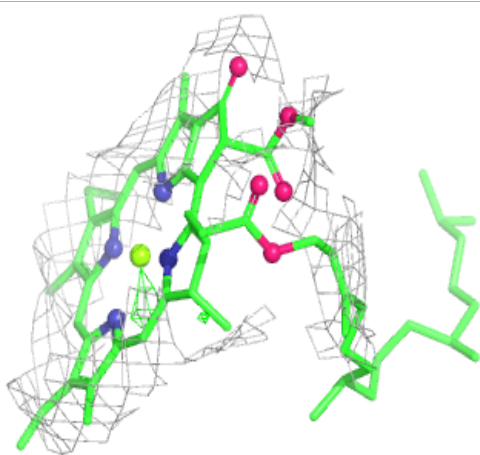
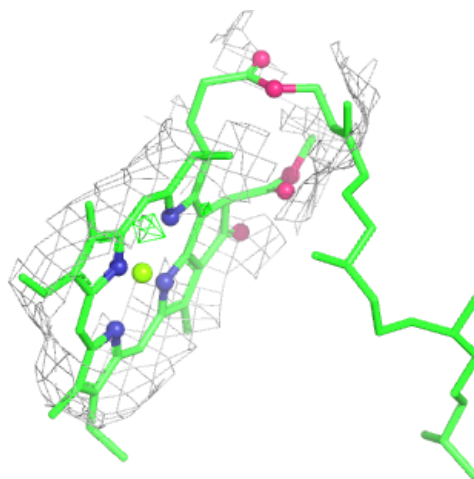
Electron density around CLA a 404:

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



Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.