



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 08:20 AM EDT

PDB ID : 4TNK / pdb_00004tnk
Title : RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 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 : 5.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

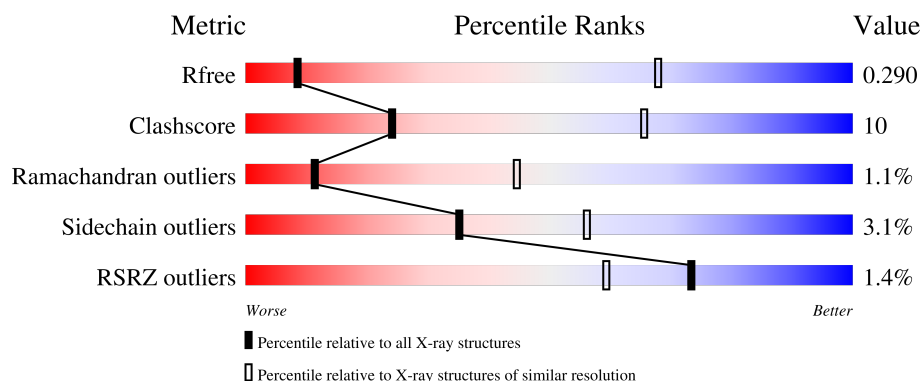
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1011 (6.38-4.00)
Clashscore	190562	1066 (6.38-4.00)
Ramachandran outliers	187476	1004 (6.46-3.94)
Sidechain outliers	187428	1006 (6.46-3.92)
RSRZ outliers	180081	1006 (6.38-4.00)

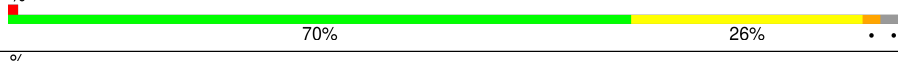
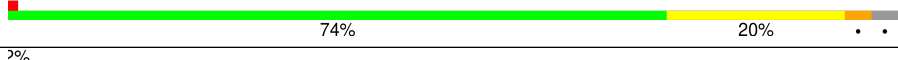
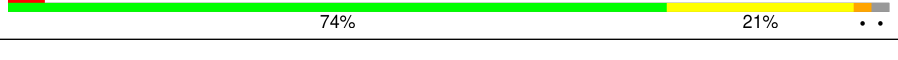
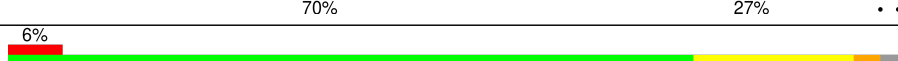
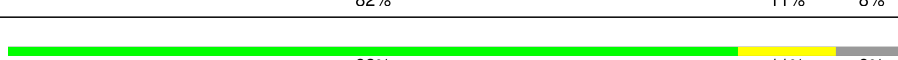
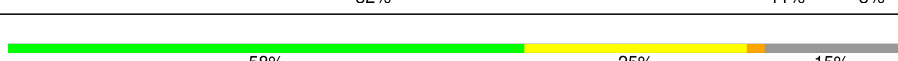
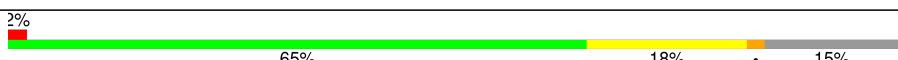
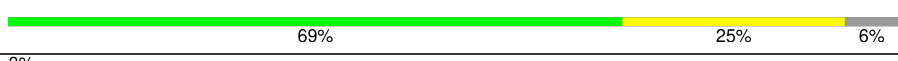
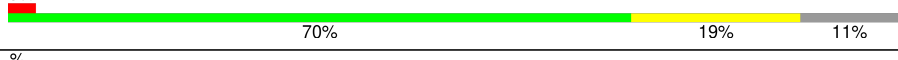
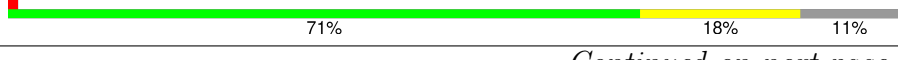
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	71% 25% ..

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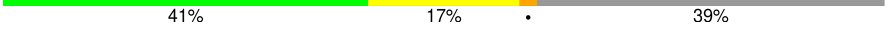
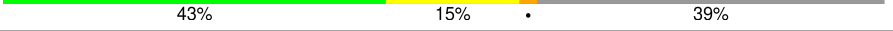
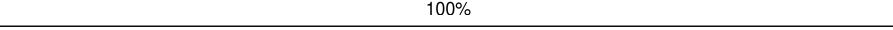
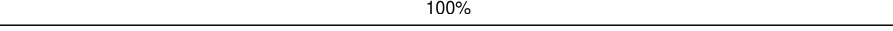
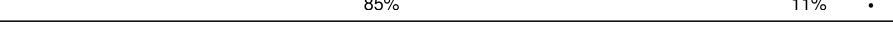
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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

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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	

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Mol	Chain	Length	Quality of chain
14	T	32	 81% 19%
14	t	32	 84% 16%
15	U	134	 61% 10% 28% 2%
15	u	134	 58% 13% 28% 1%
16	V	163	 74% 9% 16% 1%
16	v	163	 72% 10% 16% 1%
17	g	46	 41% 17% 39% 3%
17	y	46	 43% 15% 39% 3%
18	X	41	 61% 24% 10% 2%
18	x	41	 63% 24% 10% 3%
19	G	28	 100%
19	Y	28	 100%
20	Z	62	 77% 19% 4% 0%
20	z	62	 85% 11% 4% 0%

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			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

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

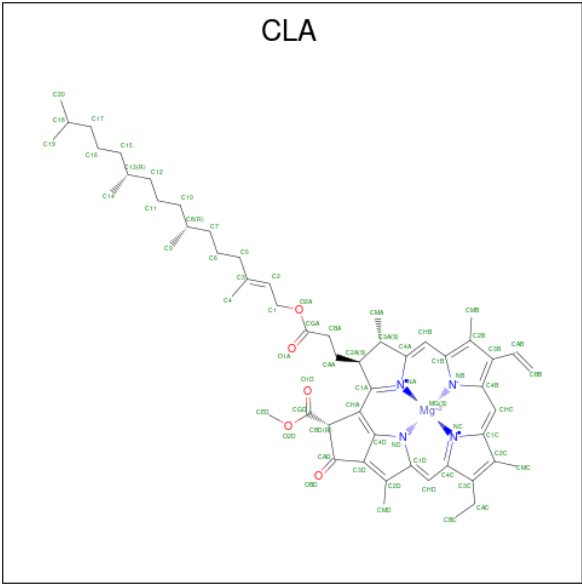
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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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

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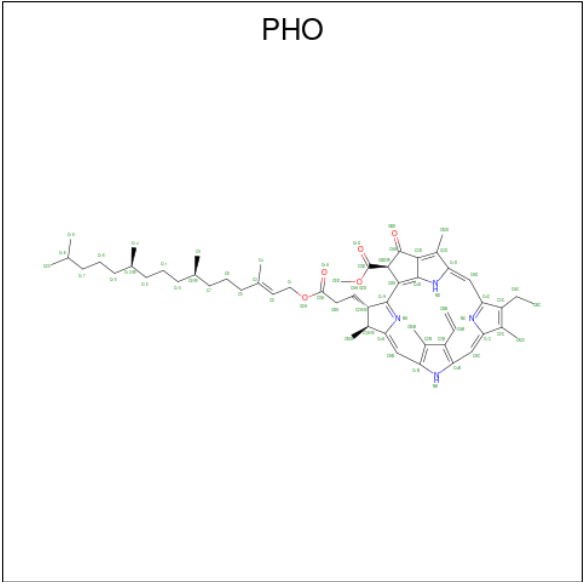
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total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

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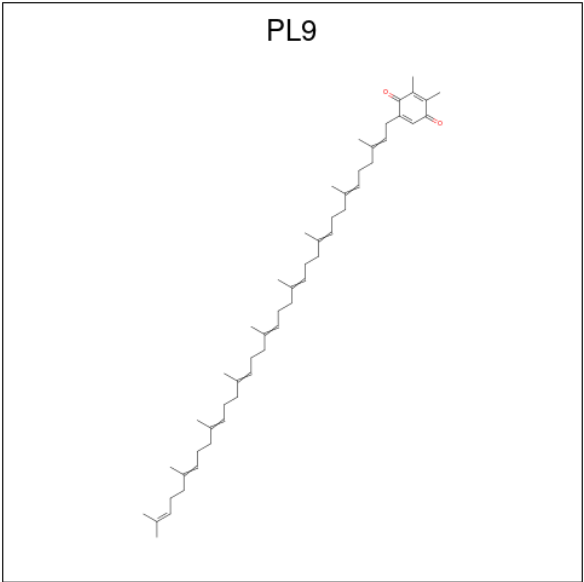
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



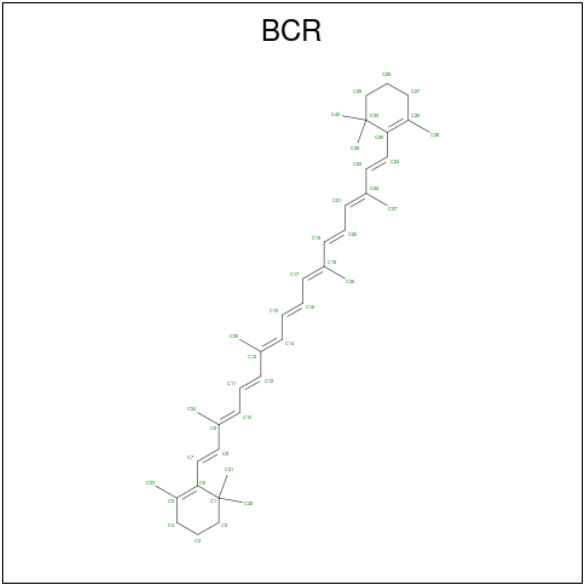
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



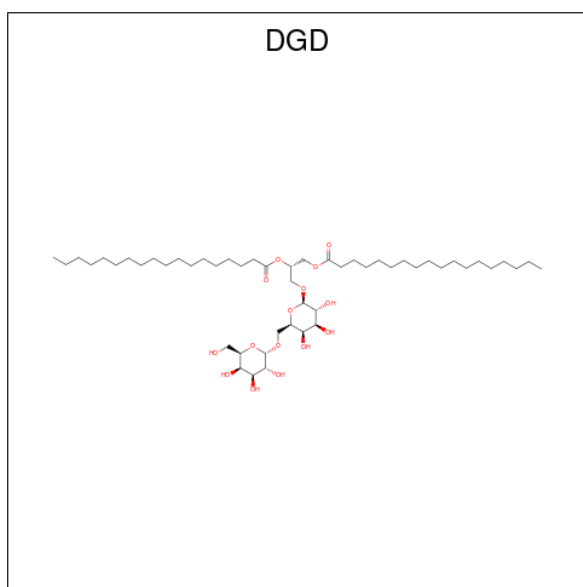
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	B	1	Total	C	0	0
			40	40		
25	C	1	Total	C	0	0
			40	40		

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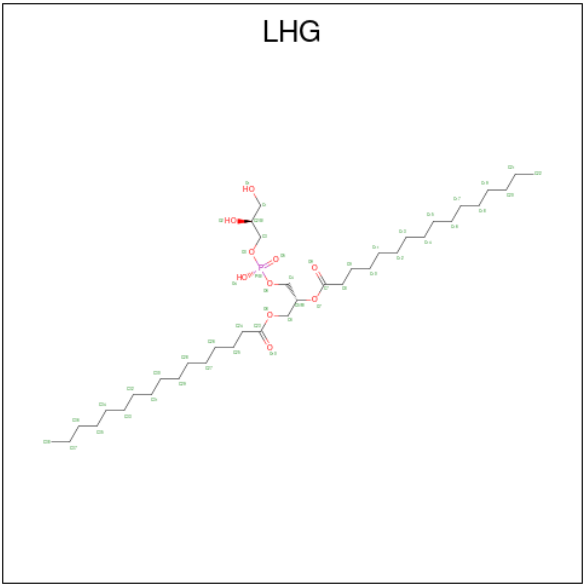
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	i	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	g	1	Total C 40 40	0	0
25	x	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

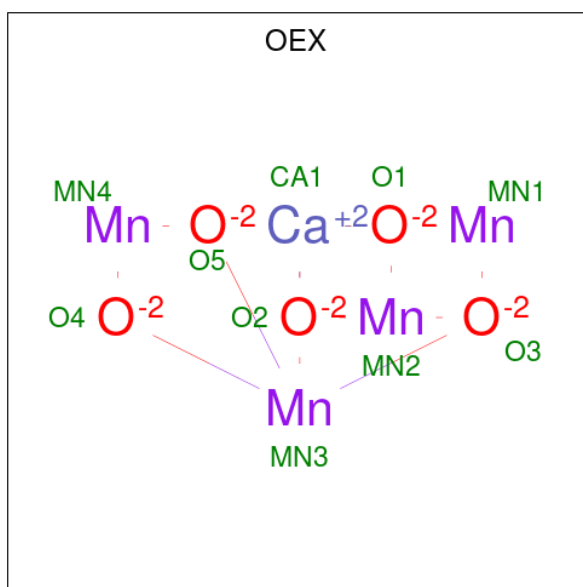


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			39	28	10	1		
27	C	1	Total	C	O	P	0	0
			37	26	10	1		
27	a	1	Total	C	O	P	0	0
			39	28	10	1		
27	c	1	Total	C	O	P	0	0
			37	26	10	1		

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

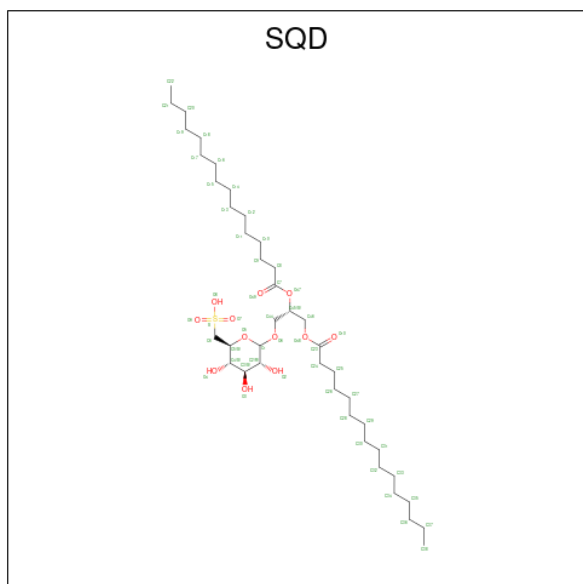
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



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

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



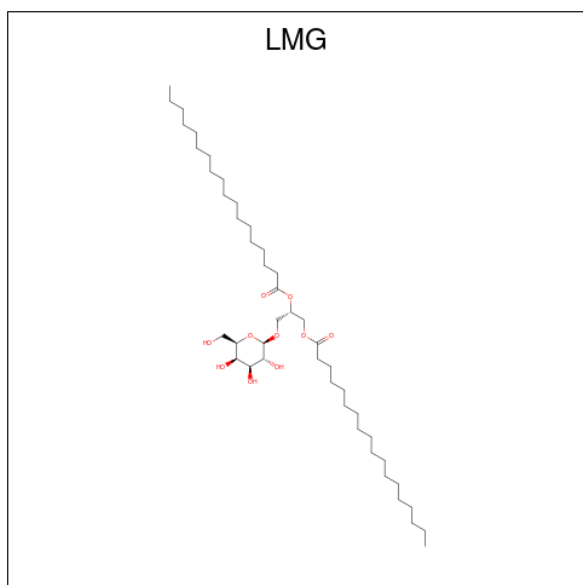
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		

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

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



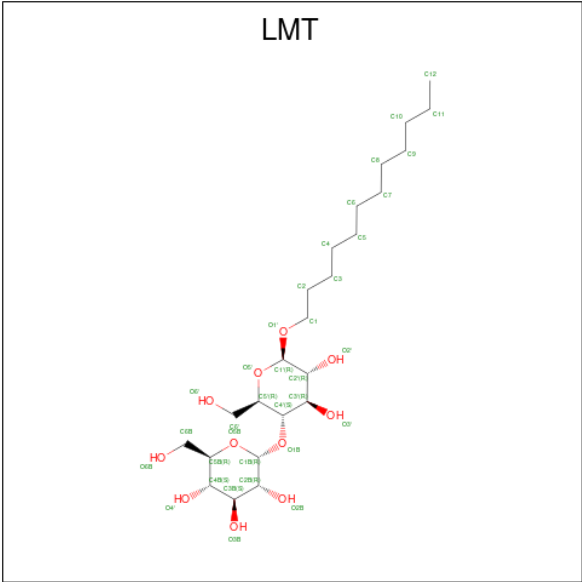
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		

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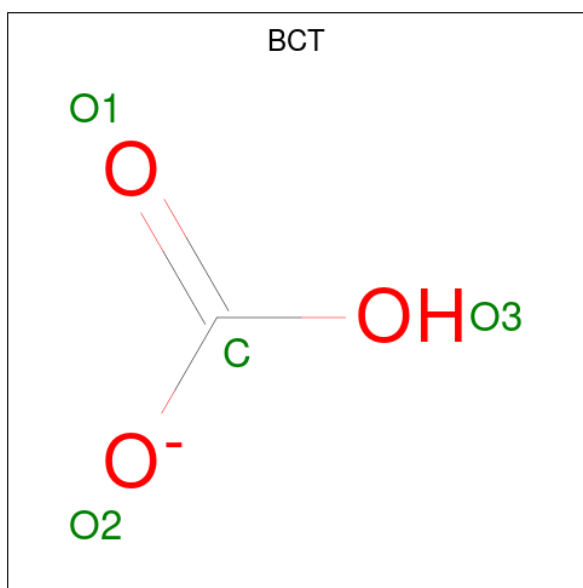
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			45	35	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	E	1	Total	C	O	0	0
			44	34	10		
31	I	1	Total	C	O	0	0
			43	33	10		
31	L	1	Total	C	O	0	0
			51	41	10		
31	M	1	Total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

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



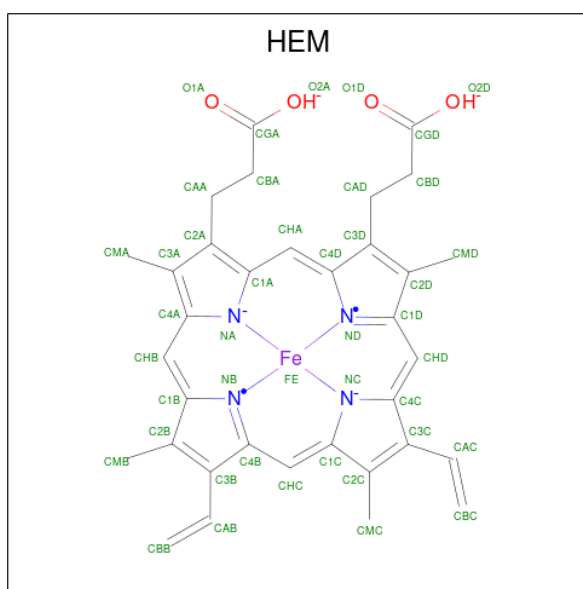
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			31	20	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	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: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

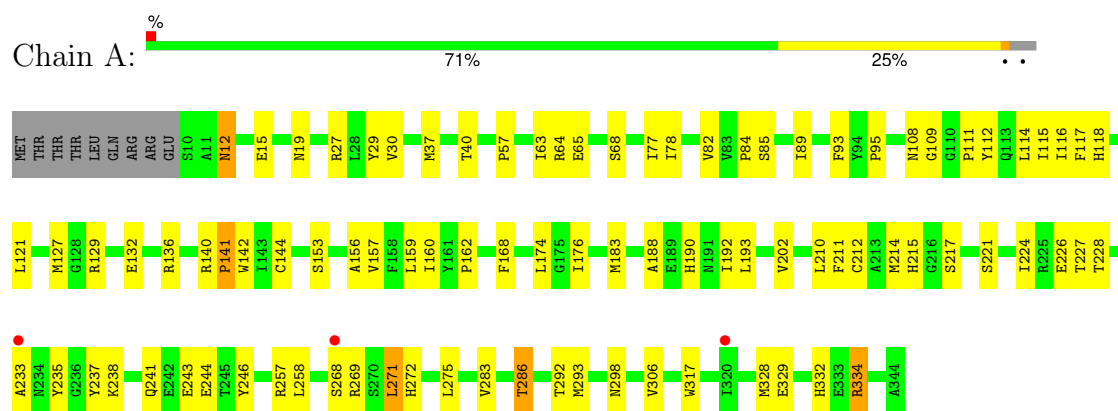
- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

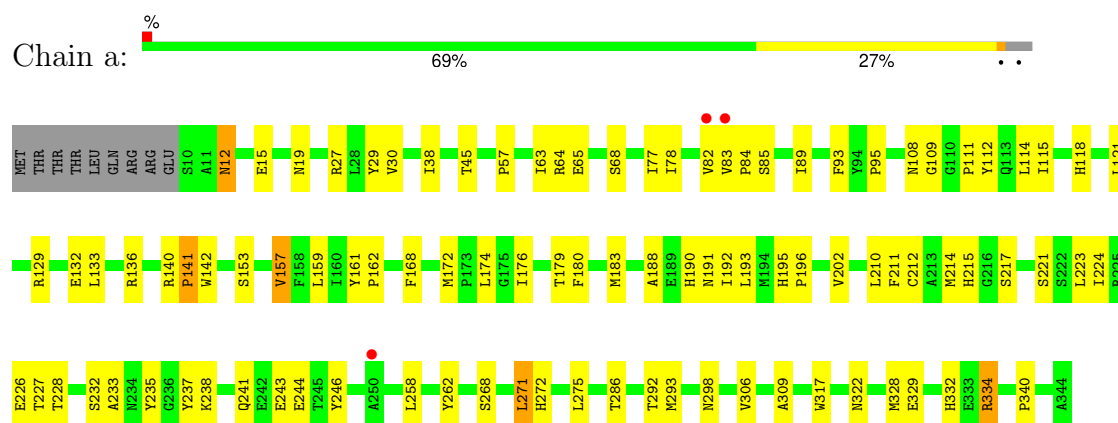
3 Residue-property plots [i](#)

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

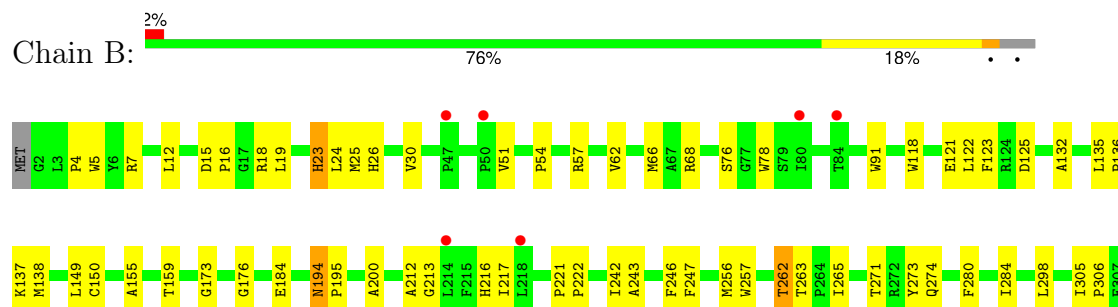
• Molecule 1: Photosystem Q(B) protein 1

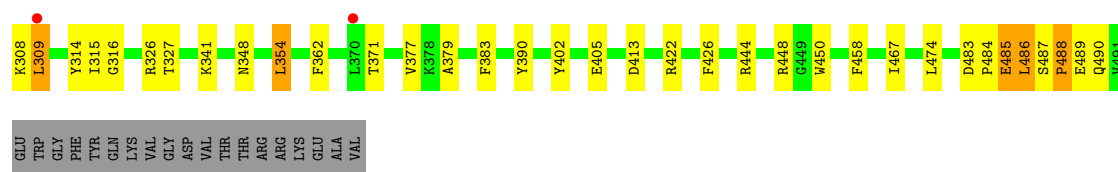


• Molecule 1: Photosystem Q(B) protein 1

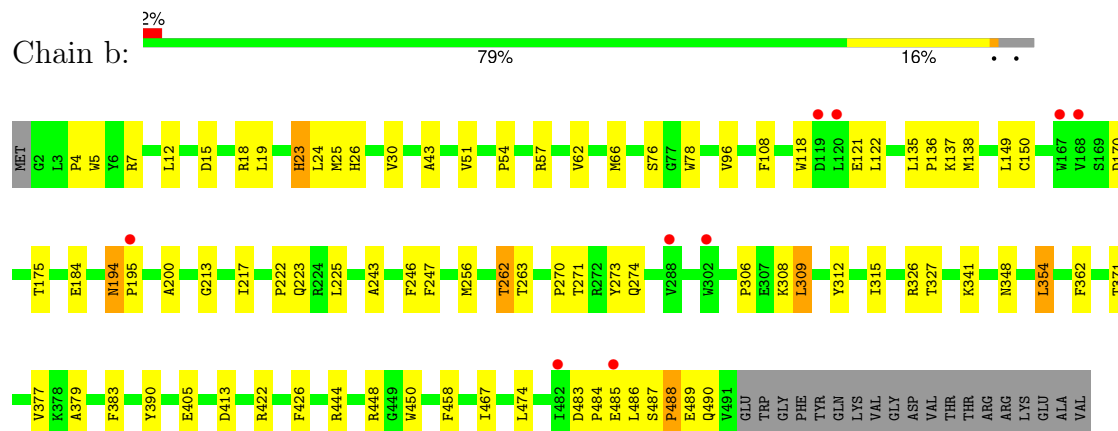


• Molecule 2: Photosystem II core light harvesting protein

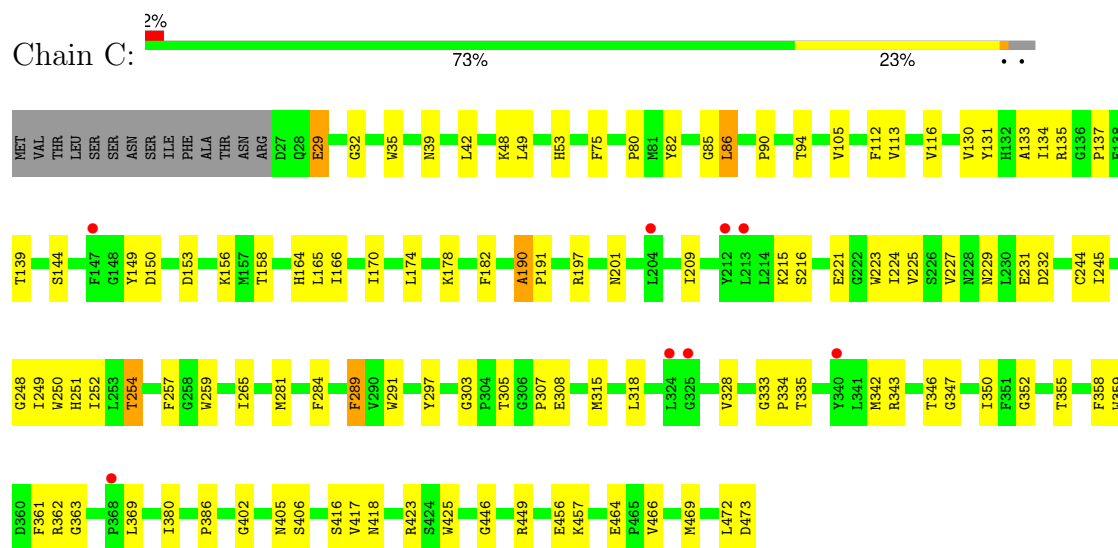




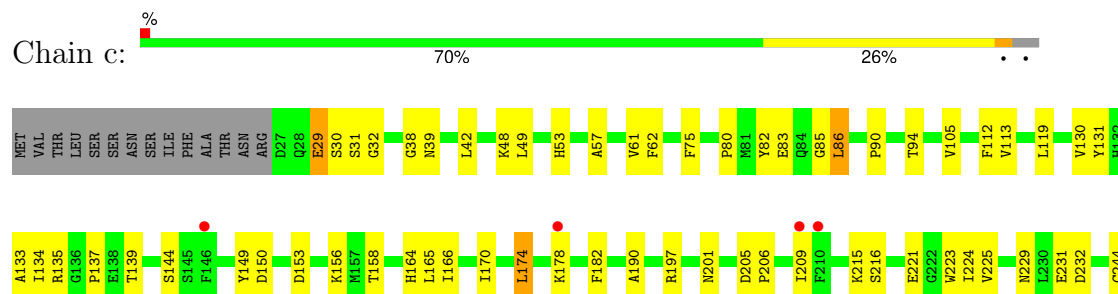
• Molecule 2: Photosystem II core light harvesting protein

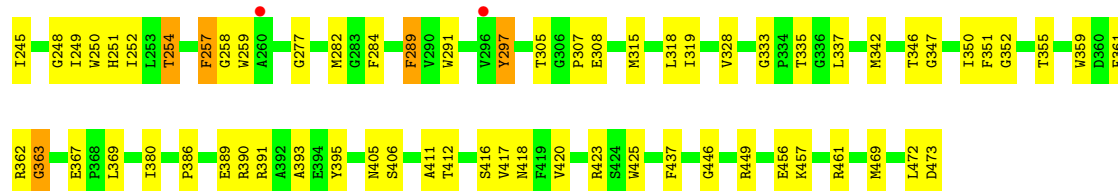


• Molecule 3: Photosystem II CP43 protein

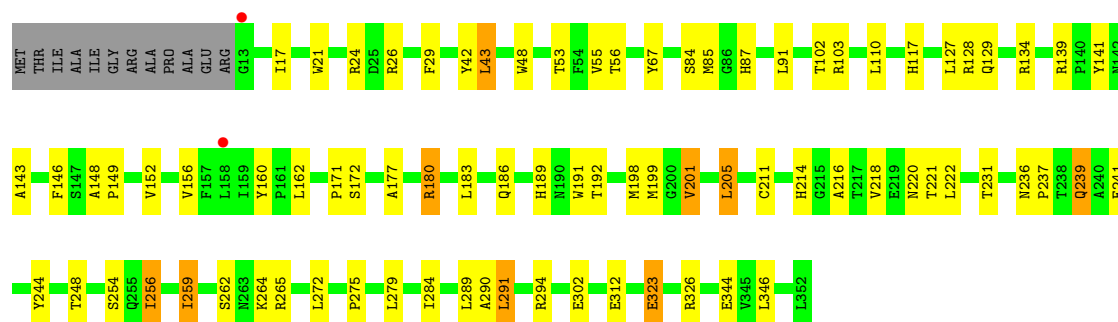
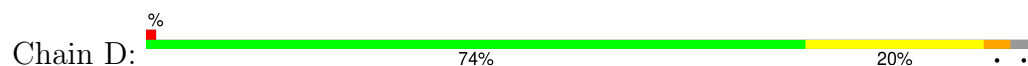


• Molecule 3: Photosystem II CP43 protein

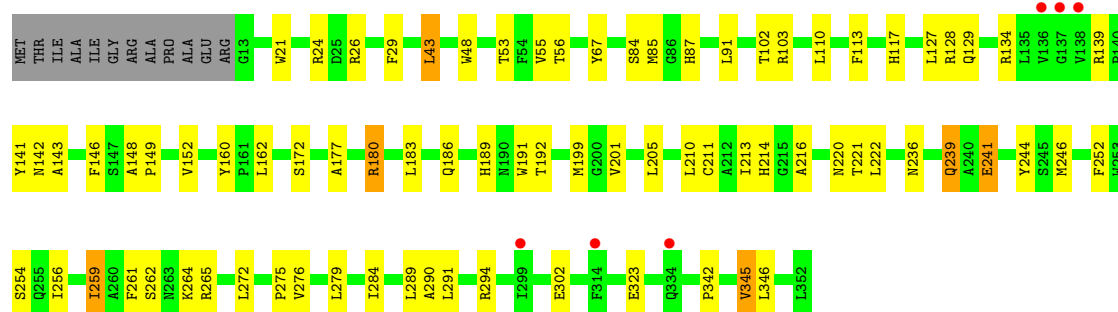
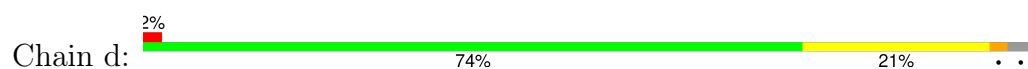




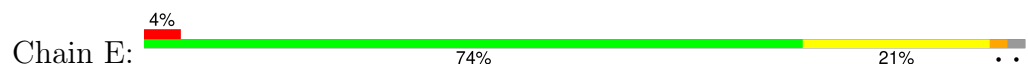
• Molecule 4: Photosystem II D2 protein



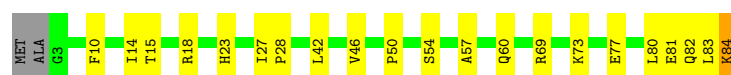
• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

Chain F:  62% 16% 22%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  60% 18% 22%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  5% 70% 27% ..



- Molecule 7: Photosystem II reaction center protein H

Chain h:  6% 77% 18% ..



- Molecule 8: Photosystem II reaction center protein I

Chain I:  82% 11% 8%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  82% 11% 8%

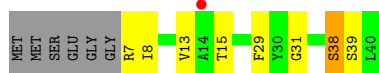


- Molecule 9: Photosystem II reaction center protein J

Chain J:  58% 25% 15%



- Molecule 9: Photosystem II reaction center protein J



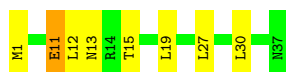
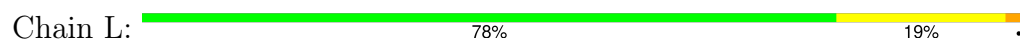
- Molecule 10: Photosystem II reaction center protein K



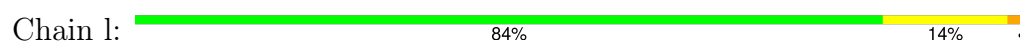
- Molecule 10: Photosystem II reaction center protein K



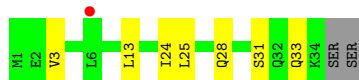
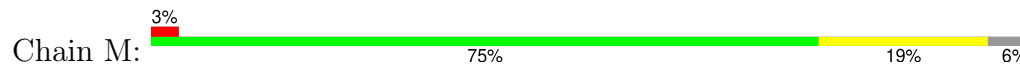
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



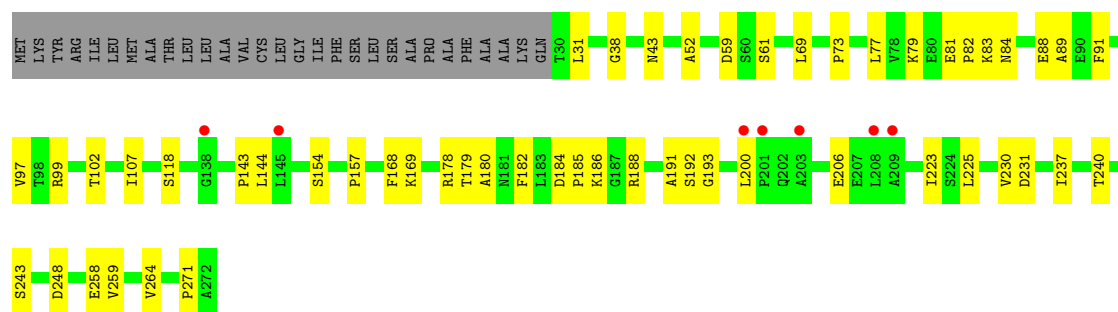
- Molecule 12: Photosystem II reaction center protein M



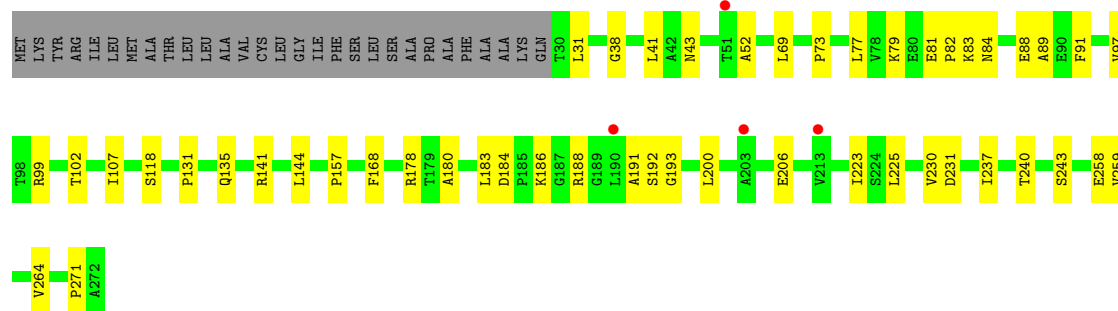
- Molecule 12: Photosystem II reaction center protein M



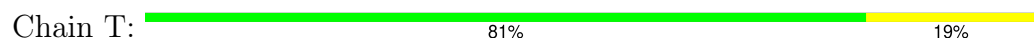
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



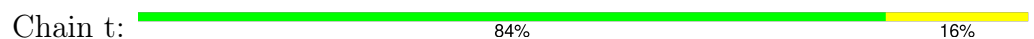
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



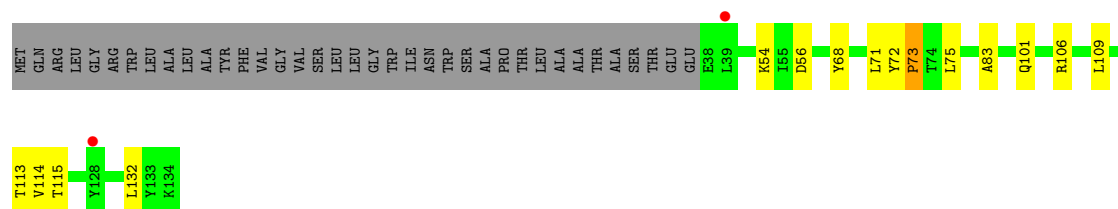
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 

MET GLN ARG LEU ARG TRP LEU ALA ALA ALA TYR PHE VAL GLY SER TRP LEU LEU GLY TRP ILE ASN THR SER ALA PRO THR LEU ALA ALA THR ALA SER THR GLU E38 K54 I55 D56 Y68 L71 Y72 P73 T74 L75 A76 A83 I94 L97 Q101

T113 V114 T115 E116 V117 V122 L132 Y133 K134

- Molecule 16: Cytochrome c-550

Chain V: 

MET LEU LYS CYS VAL TRP LEU VAL VAL LEU CYS LEU TRP PHE THR MET GLY THR ALA LEU ALA A27 L47 Q60 A64 V68 I71 R81 T82 E83 P90 P91 R92 L98 M102 E116 F127 I141 G157 K160

Y163

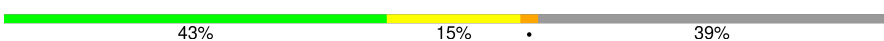
- Molecule 16: Cytochrome c-550

Chain v: 

MET LEU LYS CYS VAL TRP LEU VAL VAL LEU CYS LEU TRP PHE THR MET GLY THR ALA LEU ALA A27 L38 Q60 A64 V68 G69 G70 I71 R81 P90 P91 R92 I95 L98 M102 E116 P119 F127 G157 G158 G159

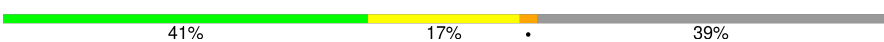
K160 Y161 Y162 Y163

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 

MET GLY ILE PHE ASN GLY ILE ILE ILE GLU PHE LEU LEU SER ASN ASN PHE PHE GLU VAL I119 M24 I25 I28 A31 I35 I39 R43 L46

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g: 

MET GLY ILE PHE ASN GLY ILE ILE ILE GLU PHE LEU LEU SER ASN ASN PHE PHE GLU VAL I119 M24 I25 I28 A31 G32 I35 I39 R43 L46

- Molecule 18: Photosystem II reaction center X protein

Chain X: 



- Molecule 18: Photosystem II reaction center X protein

Chain x: 63% 24% 10%



- 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: 77% 19%



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 85% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.62Å 229.30Å 306.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.41 – 5.20 68.41 – 5.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (68.41-5.20) 97.9 (68.41-5.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.271 , 0.289 0.282 , 0.290	Depositor DCC
R_{free} test set	1753 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	176.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 146.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: LHG, BCR, CL, PHO, BCT, FE2, PL9, DGD, OEX, LMG, SQD, CLA, CA, HEM, LMT

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	0.31	0/2713	0.78	2/3700 (0.1%)
1	a	0.32	0/2713	0.79	2/3700 (0.1%)
2	B	0.31	0/3986	0.81	8/5433 (0.1%)
2	b	0.31	0/3986	0.81	8/5433 (0.1%)
3	C	0.31	0/3556	0.80	8/4842 (0.2%)
3	c	0.31	0/3556	0.81	8/4842 (0.2%)
4	D	0.30	0/2801	0.77	0/3818
4	d	0.30	0/2801	0.77	0/3818
5	E	0.32	0/685	0.84	0/933
5	e	0.33	0/685	0.84	0/933
6	F	0.35	0/291	0.74	0/397
6	f	0.35	0/291	0.76	0/397
7	H	0.33	0/520	0.72	0/709
7	h	0.34	0/520	0.74	0/709
8	I	0.31	0/293	0.78	0/395
8	i	0.30	0/293	0.80	0/395
9	J	0.29	0/255	0.86	0/346
9	j	0.32	0/255	0.84	0/346
10	K	0.44	0/303	0.84	0/416
10	k	0.44	0/303	0.88	0/416
11	L	0.29	0/311	0.71	0/422
11	l	0.29	0/311	0.72	0/422
12	M	0.33	0/270	0.86	0/367
12	m	0.34	0/270	0.87	1/367 (0.3%)
13	O	0.29	0/1876	0.72	2/2548 (0.1%)
13	o	0.28	0/1876	0.72	2/2548 (0.1%)
14	T	0.28	0/284	0.73	0/381
14	t	0.29	0/284	0.74	0/381
15	U	0.30	0/785	0.78	0/1064
15	u	0.30	0/785	0.79	0/1064
16	V	0.30	0/1081	0.76	2/1468 (0.1%)
16	v	0.30	0/1081	0.75	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.35	0/202	0.77	0/272
17	y	0.34	0/202	0.77	0/272
18	X	0.41	0/273	0.82	0/370
18	x	0.39	0/273	0.81	0/370
20	Z	0.32	0/490	0.83	0/669
20	z	0.32	0/490	0.86	0/669
All	All	0.31	0/41950	0.79	43/57100 (0.1%)

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	483	ASP	CA-C-N	10.68	133.19	119.84
2	B	483	ASP	C-N-CA	10.68	133.19	119.84
2	b	483	ASP	CA-C-N	10.42	132.86	119.84
2	b	483	ASP	C-N-CA	10.42	132.86	119.84
3	c	190	ALA	CA-C-N	6.30	125.79	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	68	0
1	a	2628	0	2524	73	0
2	B	3850	0	3718	68	0
2	b	3850	0	3718	57	0
3	C	3444	0	3365	74	0
3	c	3444	0	3365	86	0
4	D	2706	0	2608	72	0
4	d	2706	0	2608	60	0
5	E	666	0	651	13	0
5	e	666	0	651	14	0
6	F	282	0	291	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	7	0
7	H	507	0	521	16	0
7	h	507	0	521	14	0
8	I	286	0	308	3	0
8	i	286	0	308	2	0
9	J	249	0	262	8	0
9	j	249	0	262	7	0
10	K	293	0	305	11	0
10	k	293	0	305	13	0
11	L	304	0	316	7	0
11	l	304	0	316	5	0
12	M	267	0	289	7	0
12	m	267	0	289	7	0
13	O	1845	0	1801	30	0
13	o	1845	0	1801	30	0
14	T	275	0	288	4	0
14	t	275	0	288	3	0
15	U	774	0	773	6	0
15	u	774	0	773	9	0
16	V	1060	0	1068	10	0
16	v	1060	0	1068	14	0
17	g	201	0	226	7	0
17	y	201	0	226	5	0
18	X	270	0	299	9	0
18	x	270	0	299	8	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	12	0
20	z	479	0	516	9	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	56	0
22	C	845	0	936	31	0
22	D	130	0	144	13	0
22	H	65	0	72	11	0
22	a	260	0	288	24	0
22	b	1040	0	1152	59	0
22	c	845	0	936	34	0
22	d	130	0	144	11	0
23	A	64	0	74	6	0
23	D	64	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d	128	0	148	11	0
24	A	45	0	61	5	0
24	D	55	0	80	9	0
24	J	35	0	45	0	0
24	a	45	0	61	4	0
24	d	55	0	80	6	0
24	j	35	0	45	0	0
25	A	40	0	56	4	0
25	B	160	0	224	14	0
25	C	80	0	112	10	0
25	F	40	0	56	1	0
25	H	40	0	56	2	0
25	J	40	0	56	3	0
25	K	40	0	56	5	0
25	b	160	0	224	10	0
25	c	120	0	168	16	0
25	f	40	0	56	3	0
25	g	40	0	56	11	0
25	i	40	0	56	2	0
25	j	40	0	56	2	0
25	x	40	0	56	1	0
25	y	40	0	56	6	0
26	A	56	0	70	1	0
26	B	110	0	136	4	0
26	C	181	0	245	11	0
26	D	63	0	87	2	0
26	a	56	0	70	2	0
26	b	110	0	136	5	0
26	c	181	0	245	14	0
26	d	63	0	87	3	0
27	A	39	0	51	2	0
27	C	37	0	44	3	0
27	a	39	0	51	1	0
27	c	37	0	44	2	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	6	0
30	B	90	0	111	3	0
30	F	45	0	54	3	0
30	a	105	0	147	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	47	0	61	2	0
30	d	43	0	50	3	0
30	f	45	0	54	3	0
31	B	98	0	136	5	0
31	C	93	0	126	3	0
31	D	94	0	128	8	0
31	E	44	0	58	1	0
31	I	43	0	56	1	0
31	L	51	0	72	2	0
31	M	42	0	54	2	0
31	a	42	0	54	0	0
31	b	91	0	122	5	0
31	c	93	0	126	3	0
31	d	143	0	196	10	0
31	e	44	0	58	2	0
31	i	43	0	56	0	0
31	l	51	0	72	2	0
31	m	42	0	54	3	0
32	B	140	0	184	3	0
32	D	31	0	35	0	0
32	I	35	0	46	1	0
32	M	70	0	92	0	0
32	b	140	0	184	6	0
32	d	31	0	35	0	0
32	i	35	0	46	0	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	3	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	1012	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 1012 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	1.55	0.87
3:c:39:ASN:HB2	22:c:507:CLA:HBA1	1.57	0.84
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.83
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.60	0.83
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.60	0.82

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%)	311 (93%)	18 (5%)	4 (1%)	10	42
1	a	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	10	42
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	16	52
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%)	316 (94%)	21 (6%)	1 (0%)	36	71
4	d	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	36	71
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	40
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	40
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%)	27 (82%)	6 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	21
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	21
10	K	35/46 (76%)	32 (91%)	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%)	207 (86%)	31 (13%)	3 (1%)	10	42
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	42
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	20
14	t	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	3	20
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	28
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	28
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	18
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	18
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	13
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	13
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	34
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	34
All	All	5138/5618 (92%)	4677 (91%)	406 (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
13	O	52	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	260 (96%)	11 (4%)	27	48
1	a	271/280 (97%)	260 (96%)	11 (4%)	27	48
2	B	390/407 (96%)	380 (97%)	10 (3%)	40	61
2	b	390/407 (96%)	379 (97%)	11 (3%)	38	59
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%)	264 (96%)	11 (4%)	28	49
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	40
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	40
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%)	51 (96%)	2 (4%)	29	50
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	50
8	I	32/35 (91%)	31 (97%)	1 (3%)	35	56
8	i	32/35 (91%)	31 (97%)	1 (3%)	35	56
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	48
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	48
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	58
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	58
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	68	77
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	29/29 (100%)	28 (97%)	1 (3%)	32	54
14	t	29/29 (100%)	28 (97%)	1 (3%)	32	54
15	U	84/112 (75%)	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	68
16	v	116/138 (84%)	114 (98%)	2 (2%)	53	68
17	g	20/37 (54%)	17 (85%)	3 (15%)	3	13
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	13
18	X	30/34 (88%)	28 (93%)	2 (7%)	15	36
18	x	30/34 (88%)	29 (97%)	1 (3%)	33	55
20	Z	52/52 (100%)	50 (96%)	2 (4%)	29	50
20	z	52/52 (100%)	50 (96%)	2 (4%)	29	50
All	All	4244/4594 (92%)	4112 (97%)	132 (3%)	35	56

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	60	VAL
13	o	31	LEU
20	z	33	TRP
7	H	60	VAL
7	H	27	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	56	HIS
4	d	301	GLN
4	d	117	HIS
4	d	239	GLN
12	m	32	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	B	613	2	69,73,73	1.17	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	b	612	2	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	c	507	3	69,73,73	1.19	7 (10%)	82,113,113	1.32	7 (8%)
25	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	8 (14%)
31	LMG	l	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.33	7 (11%)
22	CLA	A	402	1	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
32	LMT	b	604	-	36,36,36	1.11	5 (13%)	47,47,47	1.05	1 (2%)
22	CLA	c	510	3	69,73,73	1.21	5 (7%)	82,113,113	1.27	6 (7%)
22	CLA	c	509	3	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	c	508	3	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	a	405	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
31	LMG	i	102	-	43,43,55	0.83	0	51,51,63	1.25	4 (7%)
22	CLA	C	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
22	CLA	C	519	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	b	609	2	69,73,73	1.19	6 (8%)	82,113,113	1.29	4 (4%)
26	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.33	7 (10%)
25	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	9 (16%)
22	CLA	c	512	3	69,73,73	1.20	6 (8%)	82,113,113	1.26	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	506	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
22	CLA	b	616	-	69,73,73	1.17	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	b	617	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	7 (8%)
25	BCR	B	616	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	8 (14%)
22	CLA	b	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.34	7 (8%)
30	SQD	a	412	-	49,51,54	0.96	3 (6%)	59,62,65	1.70	11 (18%)
31	LMG	I	101	-	43,43,55	0.84	1 (2%)	51,51,63	1.26	4 (7%)
27	LHG	A	410	-	38,38,48	0.71	1 (2%)	41,44,54	1.23	3 (7%)
22	CLA	c	502	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	4 (4%)
31	LMG	C	521	-	48,48,55	0.76	0	56,56,63	1.31	5 (8%)
22	CLA	c	520	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
31	LMG	D	409	-	46,46,55	0.79	1 (2%)	54,54,63	1.32	6 (11%)
31	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.30	4 (7%)
25	BCR	K	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	B	612	-	69,73,73	1.17	6 (8%)	82,113,113	1.26	8 (9%)
22	CLA	a	404	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
32	LMT	B	629	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	1 (2%)
24	PL9	J	101	-	35,35,55	1.02	3 (8%)	44,45,69	1.64	9 (20%)
25	BCR	F	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	7 (12%)
32	LMT	i	103	-	36,36,36	1.07	4 (11%)	47,47,47	1.03	2 (4%)
22	CLA	B	603	2	69,73,73	1.20	7 (10%)	82,113,113	1.34	7 (8%)
22	CLA	C	504	3	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
32	LMT	D	408	-	32,32,36	1.15	3 (9%)	43,43,47	1.04	2 (4%)
22	CLA	B	609	-	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
23	PHO	D	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.41	5 (9%)
26	DGD	D	407	-	64,64,67	0.97	3 (4%)	78,78,81	1.33	8 (10%)
24	PL9	A	407	-	45,45,55	1.00	4 (8%)	56,57,69	1.54	10 (17%)
22	CLA	c	503	-	69,73,73	1.20	7 (10%)	82,113,113	1.31	5 (6%)
22	CLA	C	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
22	CLA	D	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
32	LMT	B	628	-	36,36,36	1.10	4 (11%)	47,47,47	1.02	1 (2%)
22	CLA	A	406	1	69,73,73	1.19	6 (8%)	82,113,113	1.23	4 (4%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	5 (6%)
31	LMG	D	406	-	48,48,55	0.76	0	56,56,63	1.39	4 (7%)
31	LMG	d	412	-	46,46,55	0.80	1 (2%)	54,54,63	1.30	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DGD	d	410	-	64,64,67	0.95	2 (3%)	78,78,81	1.36	9 (11%)
25	BCR	H	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	6 (10%)
34	HEM	F	101	6,5	50,50,50	1.93	8 (16%)	67,82,82	1.26	5 (7%)
32	LMT	M	103	-	36,36,36	1.11	4 (11%)	47,47,47	1.01	2 (4%)
22	CLA	d	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	5 (6%)
30	SQD	A	413	-	49,51,54	0.96	3 (6%)	59,62,65	1.71	10 (16%)
32	LMT	B	624	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
22	CLA	B	607	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	b	614	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
24	PL9	D	405	-	55,55,55	1.14	4 (7%)	68,69,69	1.52	14 (20%)
23	PHO	A	405	-	58,69,69	2.15	9 (15%)	55,99,99	1.39	6 (10%)
31	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.29	4 (7%)
22	CLA	C	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	6 (7%)
23	PHO	d	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.41	5 (9%)
25	BCR	C	513	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	8 (14%)
32	LMT	M	102	-	36,36,36	1.12	4 (11%)	47,47,47	1.03	2 (4%)
23	PHO	d	401	-	58,69,69	2.12	11 (18%)	55,99,99	1.43	6 (10%)
31	LMG	m	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
30	SQD	B	627	-	45,47,54	1.01	3 (6%)	55,58,65	1.76	10 (18%)
26	DGD	c	516	-	63,63,67	0.93	2 (3%)	77,77,81	1.42	11 (14%)
22	CLA	B	615	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
22	CLA	B	605	2	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
31	LMG	C	517	-	45,45,55	0.76	0	53,53,63	1.31	6 (11%)
22	CLA	B	610	2	69,73,73	1.24	6 (8%)	82,113,113	1.39	8 (9%)
30	SQD	f	103	-	43,45,54	1.02	2 (4%)	53,56,65	1.62	11 (20%)
25	BCR	i	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
26	DGD	c	517	-	67,67,67	0.89	0	81,81,81	1.39	8 (9%)
29	OEX	a	411	1,3	0,14,14	-	-	-	-	-
31	LMG	b	626	-	49,49,55	0.80	1 (2%)	57,57,63	1.33	7 (12%)
22	CLA	b	610	2	69,73,73	1.17	5 (7%)	82,113,113	1.29	5 (6%)
33	BCT	D	402	21	3,3,3	1.10	0	2,3,3	4.37	2 (100%)
22	CLA	B	608	2	69,73,73	1.21	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	a	403	1	69,73,73	1.19	7 (10%)	82,113,113	1.29	5 (6%)
27	LHG	C	518	-	36,36,48	0.72	1 (2%)	39,42,54	1.31	4 (10%)
22	CLA	d	406	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DGD	C	515	-	63,63,67	0.92	2 (3%)	77,77,81	1.41	11 (14%)
31	LMG	a	402	-	42,42,55	0.87	2 (4%)	50,50,63	1.23	4 (8%)
22	CLA	c	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.29	5 (6%)
22	CLA	b	607	-	69,73,73	1.19	6 (8%)	82,113,113	1.21	7 (8%)
22	CLA	b	618	2	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	c	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	B	601	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	5 (6%)
25	BCR	g	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	8 (14%)
22	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	6 (7%)
22	CLA	b	605	-	69,73,73	1.21	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	C	510	3	69,73,73	1.19	5 (7%)	82,113,113	1.32	5 (6%)
29	OEX	A	412	1,3	0,14,14	-	-	-	-	-
27	LHG	a	409	-	38,38,48	0.69	1 (2%)	41,44,54	1.24	3 (7%)
22	CLA	B	604	2	69,73,73	1.18	7 (10%)	82,113,113	1.30	4 (4%)
22	CLA	C	509	3	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
22	CLA	D	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.21	5 (6%)
22	CLA	B	606	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
22	CLA	C	507	3	69,73,73	1.19	6 (8%)	82,113,113	1.32	7 (8%)
22	CLA	C	508	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
31	LMG	L	101	-	51,51,55	0.76	0	59,59,63	1.35	5 (8%)
32	LMT	b	629	-	36,36,36	1.08	3 (8%)	47,47,47	1.04	2 (4%)
22	CLA	C	503	-	69,73,73	1.19	6 (8%)	82,113,113	1.31	5 (6%)
31	LMG	B	621	-	49,49,55	0.78	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	H	101	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	5 (6%)
25	BCR	A	408	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	7 (12%)
26	DGD	A	409	-	57,57,67	0.96	0	71,71,81	1.43	8 (11%)
26	DGD	c	515	-	54,54,67	0.96	1 (1%)	68,68,81	1.29	5 (7%)
26	DGD	B	620	-	59,59,67	0.94	1 (1%)	73,73,81	1.35	7 (9%)
22	CLA	C	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
22	CLA	a	406	1	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
32	LMT	I	102	-	36,36,36	1.09	4 (11%)	47,47,47	1.06	2 (4%)
25	BCR	b	623	-	41,41,41	1.14	2 (4%)	56,56,56	1.42	11 (19%)
30	SQD	A	414	-	52,54,54	0.95	4 (7%)	62,65,65	1.50	9 (14%)
22	CLA	c	504	3	69,73,73	1.18	8 (11%)	82,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	c	519	-	36,36,48	0.77	2 (5%)	39,42,54	1.30	4 (10%)
34	HEM	v	201	16	50,50,50	2.01	11 (22%)	67,82,82	1.26	3 (4%)
22	CLA	b	613	2	69,73,73	1.20	7 (10%)	82,113,113	1.23	5 (6%)
25	BCR	b	622	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	10 (17%)
30	SQD	a	401	-	52,54,54	0.95	3 (5%)	62,65,65	1.51	10 (16%)
22	CLA	b	620	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
30	SQD	F	103	-	43,45,54	1.04	2 (4%)	53,56,65	1.62	11 (20%)
31	LMG	d	409	-	48,48,55	0.77	0	56,56,63	1.41	5 (8%)
25	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
25	BCR	J	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.61	13 (23%)
33	BCT	d	404	21	3,3,3	1.11	0	2,3,3	4.40	2 (100%)
22	CLA	b	606	-	69,73,73	1.19	8 (11%)	82,113,113	1.23	4 (4%)
32	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	1 (2%)
25	BCR	y	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	8 (14%)
22	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
34	HEM	V	201	16	50,50,50	1.94	9 (18%)	67,82,82	1.16	1 (1%)
30	SQD	d	403	-	41,43,54	1.05	2 (4%)	51,54,65	1.70	11 (21%)
25	BCR	C	520	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	9 (16%)
30	SQD	b	602	-	45,47,54	1.02	3 (6%)	55,58,65	1.78	10 (18%)
25	BCR	B	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.43	10 (17%)
22	CLA	c	506	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
25	BCR	c	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.37	10 (17%)
22	CLA	B	602	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
30	SQD	B	622	-	41,43,54	1.05	2 (4%)	51,54,65	1.74	11 (21%)
22	CLA	b	615	2	69,73,73	1.24	6 (8%)	82,113,113	1.36	7 (8%)
24	PL9	d	407	-	55,55,55	1.08	5 (9%)	68,69,69	1.52	12 (17%)
25	BCR	x	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
31	LMG	b	627	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
24	PL9	j	101	-	35,35,55	1.06	2 (5%)	44,45,69	1.60	9 (20%)
25	BCR	c	514	-	41,41,41	1.12	3 (7%)	56,56,56	1.32	8 (14%)
26	DGD	a	408	-	57,57,67	0.96	0	71,71,81	1.39	9 (12%)
26	DGD	b	625	-	59,59,67	0.92	1 (1%)	73,73,81	1.37	8 (10%)
32	LMT	B	623	-	36,36,36	1.11	4 (11%)	47,47,47	1.02	1 (2%)
25	BCR	j	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.55	13 (23%)
25	BCR	f	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	404	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
25	BCR	b	624	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	9 (16%)
26	DGD	B	626	-	53,53,67	1.05	3 (5%)	67,67,81	1.32	7 (10%)
26	DGD	C	514	-	54,54,67	0.97	2 (3%)	68,68,81	1.26	4 (5%)
31	LMG	M	101	-	42,42,55	0.86	0	50,50,63	1.23	4 (8%)
31	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
34	HEM	f	101	6,5	50,50,50	1.92	8 (16%)	67,82,82	1.32	5 (7%)
26	DGD	C	516	-	67,67,67	0.87	0	81,81,81	1.42	9 (11%)
22	CLA	b	619	-	69,73,73	1.18	6 (8%)	82,113,113	1.27	5 (6%)
25	BCR	b	621	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	7 (12%)
24	PL9	a	407	-	45,45,55	1.03	3 (6%)	56,57,69	1.56	11 (19%)
32	LMT	b	628	-	36,36,36	1.10	4 (11%)	47,47,47	1.01	1 (2%)
31	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.30	6 (11%)
31	LMG	B	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.34	7 (12%)
22	CLA	b	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	5 (6%)
31	LMG	d	408	-	49,49,55	0.77	1 (2%)	57,57,63	1.34	7 (12%)
32	LMT	d	411	-	32,32,36	1.15	5 (15%)	43,43,47	1.03	2 (4%)
22	CLA	C	505	3	69,73,73	1.18	7 (10%)	82,113,113	1.27	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	613	2	-	14/39/115/115	-
22	CLA	b	612	2	-	13/39/115/115	-
22	CLA	c	507	3	-	12/39/115/115	-
25	BCR	c	521	-	-	4/29/63/63	0/2/2/2
31	LMG	l	101	-	-	27/46/66/70	0/1/1/1
22	CLA	A	402	1	-	7/39/115/115	-
32	LMT	b	604	-	-	5/21/61/61	0/2/2/2
22	CLA	c	510	3	-	13/39/115/115	-
22	CLA	c	509	3	-	15/39/115/115	-
22	CLA	c	508	3	-	18/39/115/115	-
22	CLA	a	405	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	i	102	-	-	18/38/58/70	0/1/1/1
22	CLA	C	501	3	-	15/39/115/115	-
22	CLA	C	519	-	-	13/39/115/115	-
22	CLA	b	609	2	-	15/39/115/115	-
26	DGD	b	601	-	-	18/41/81/95	0/2/2/2
25	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	c	512	3	-	16/39/115/115	-
22	CLA	C	506	-	-	11/39/115/115	-
22	CLA	b	616	-	-	10/39/115/115	-
22	CLA	b	617	-	-	15/39/115/115	-
25	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	b	608	2	-	5/39/115/115	-
30	SQD	a	412	-	-	20/46/66/69	0/1/1/1
31	LMG	I	101	-	-	20/38/58/70	0/1/1/1
27	LHG	A	410	-	-	11/43/43/53	-
22	CLA	c	502	-	-	10/39/115/115	-
31	LMG	C	521	-	-	20/43/63/70	0/1/1/1
22	CLA	c	520	-	-	12/39/115/115	-
31	LMG	D	409	-	-	15/41/61/70	0/1/1/1
31	LMG	E	101	-	-	16/39/59/70	0/1/1/1
25	BCR	K	101	-	-	5/29/63/63	0/2/2/2
22	CLA	B	612	-	-	15/39/115/115	-
22	CLA	a	404	-	-	14/39/115/115	-
32	LMT	B	629	-	-	4/21/61/61	0/2/2/2
24	PL9	J	101	-	-	9/29/49/73	0/1/1/1
25	BCR	F	102	-	-	4/29/63/63	0/2/2/2
32	LMT	i	103	-	-	4/21/61/61	0/2/2/2
22	CLA	B	603	2	-	10/39/115/115	-
22	CLA	C	504	3	-	17/39/115/115	-
32	LMT	D	408	-	-	2/17/57/61	0/2/2/2
22	CLA	B	609	-	-	19/39/115/115	-
23	PHO	D	401	-	-	9/37/103/103	0/5/6/6
26	DGD	D	407	-	-	36/52/92/95	0/2/2/2
24	PL9	A	407	-	-	19/41/61/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	503	-	-	13/39/115/115	-
22	CLA	C	511	-	-	17/39/115/115	-
22	CLA	D	404	-	-	6/39/115/115	-
32	LMT	B	628	-	-	2/21/61/61	0/2/2/2
22	CLA	A	406	1	-	8/39/115/115	-
22	CLA	A	403	-	-	13/39/115/115	-
31	LMG	D	406	-	-	22/43/63/70	0/1/1/1
31	LMG	d	412	-	-	15/41/61/70	0/1/1/1
26	DGD	d	410	-	-	36/52/92/95	0/2/2/2
25	BCR	H	102	-	-	7/29/63/63	0/2/2/2
34	HEM	F	101	6,5	-	2/14/54/54	-
32	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	d	405	-	-	12/39/115/115	-
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
32	LMT	B	624	-	-	3/21/61/61	0/2/2/2
22	CLA	B	607	2	-	12/39/115/115	-
22	CLA	b	614	-	-	18/39/115/115	-
24	PL9	D	405	-	-	12/53/73/73	0/1/1/1
23	PHO	A	405	-	-	10/37/103/103	0/5/6/6
31	LMG	e	101	-	-	20/39/59/70	0/1/1/1
22	CLA	C	502	-	-	10/39/115/115	-
23	PHO	d	402	-	-	13/37/103/103	0/5/6/6
25	BCR	C	513	-	-	4/29/63/63	0/2/2/2
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
23	PHO	d	401	-	-	8/37/103/103	0/5/6/6
31	LMG	m	101	-	-	17/37/57/70	0/1/1/1
30	SQD	B	627	-	-	15/42/62/69	0/1/1/1
26	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	B	615	2	-	19/39/115/115	-
22	CLA	B	605	2	-	18/39/115/115	-
31	LMG	C	517	-	-	22/40/60/70	0/1/1/1
22	CLA	B	610	2	-	11/39/115/115	-
30	SQD	f	103	-	-	10/40/60/69	0/1/1/1
25	BCR	i	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	c	517	-	-	21/55/95/95	0/2/2/2
31	LMG	b	626	-	-	14/44/64/70	0/1/1/1
22	CLA	b	610	2	-	14/39/115/115	-
22	CLA	B	608	2	-	10/39/115/115	-
22	CLA	a	403	1	-	8/39/115/115	-
27	LHG	C	518	-	-	14/41/41/53	-
22	CLA	d	406	-	-	8/39/115/115	-
26	DGD	C	515	-	-	20/51/91/95	0/2/2/2
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
22	CLA	c	505	3	-	15/39/115/115	-
22	CLA	b	607	-	-	13/39/115/115	-
22	CLA	b	618	2	-	13/39/115/115	-
22	CLA	c	501	3	-	14/39/115/115	-
22	CLA	B	601	-	-	15/39/115/115	-
25	BCR	g	101	-	-	5/29/63/63	0/2/2/2
22	CLA	B	611	-	-	9/39/115/115	-
22	CLA	b	605	-	-	15/39/115/115	-
22	CLA	c	511	-	-	17/39/115/115	-
22	CLA	C	510	3	-	15/39/115/115	-
27	LHG	a	409	-	-	10/43/43/53	-
22	CLA	B	604	2	-	16/39/115/115	-
22	CLA	C	509	3	-	12/39/115/115	-
22	CLA	D	403	-	-	12/39/115/115	-
22	CLA	B	606	-	-	10/39/115/115	-
22	CLA	C	507	3	-	13/39/115/115	-
22	CLA	C	508	-	-	18/39/115/115	-
31	LMG	L	101	-	-	27/46/66/70	0/1/1/1
32	LMT	b	629	-	-	3/21/61/61	0/2/2/2
22	CLA	C	503	-	-	12/39/115/115	-
31	LMG	B	621	-	-	15/44/64/70	0/1/1/1
22	CLA	H	101	-	-	15/39/115/115	-
25	BCR	A	408	-	-	4/29/63/63	0/2/2/2
26	DGD	A	409	-	-	16/45/85/95	0/2/2/2
26	DGD	c	515	-	-	19/42/82/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DGD	B	620	-	-	18/47/87/95	0/2/2/2
22	CLA	C	512	3	-	16/39/115/115	-
22	CLA	a	406	1	-	9/39/115/115	-
32	LMT	I	102	-	-	3/21/61/61	0/2/2/2
25	BCR	b	623	-	-	0/29/63/63	0/2/2/2
30	SQD	A	414	-	-	14/49/69/69	0/1/1/1
22	CLA	c	504	3	-	20/39/115/115	-
27	LHG	c	519	-	-	16/41/41/53	-
34	HEM	v	201	16	-	5/14/54/54	-
22	CLA	b	613	2	-	10/39/115/115	-
25	BCR	b	622	-	-	6/29/63/63	0/2/2/2
30	SQD	a	401	-	-	14/49/69/69	0/1/1/1
22	CLA	b	620	2	-	19/39/115/115	-
30	SQD	F	103	-	-	11/40/60/69	0/1/1/1
31	LMG	d	409	-	-	21/43/63/70	0/1/1/1
25	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	BCR	J	102	-	-	6/29/63/63	0/2/2/2
22	CLA	b	606	-	-	14/39/115/115	-
32	LMT	b	603	-	-	3/21/61/61	0/2/2/2
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	B	614	-	-	10/39/115/115	-
34	HEM	V	201	16	-	5/14/54/54	-
30	SQD	d	403	-	-	17/38/58/69	0/1/1/1
25	BCR	C	520	-	-	3/29/63/63	0/2/2/2
30	SQD	b	602	-	-	14/42/62/69	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	CLA	c	506	-	-	10/39/115/115	-
25	BCR	c	513	-	-	5/29/63/63	0/2/2/2
22	CLA	B	602	-	-	13/39/115/115	-
30	SQD	B	622	-	-	15/38/58/69	0/1/1/1
22	CLA	b	615	2	-	13/39/115/115	-
24	PL9	d	407	-	-	11/53/73/73	0/1/1/1
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
31	LMG	b	627	-	-	15/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PL9	j	101	-	-	8/29/49/73	0/1/1/1
25	BCR	c	514	-	-	4/29/63/63	0/2/2/2
26	DGD	a	408	-	-	14/45/85/95	0/2/2/2
26	DGD	b	625	-	-	18/47/87/95	0/2/2/2
32	LMT	B	623	-	-	2/21/61/61	0/2/2/2
25	BCR	j	102	-	-	7/29/63/63	0/2/2/2
25	BCR	f	102	-	-	4/29/63/63	0/2/2/2
22	CLA	A	404	-	-	10/39/115/115	-
25	BCR	b	624	-	-	5/29/63/63	0/2/2/2
26	DGD	B	626	-	-	18/41/81/95	0/2/2/2
26	DGD	C	514	-	-	18/42/82/95	0/2/2/2
31	LMG	M	101	-	-	17/37/57/70	0/1/1/1
31	LMG	c	522	-	-	19/43/63/70	0/1/1/1
34	HEM	f	101	6,5	-	2/14/54/54	-
26	DGD	C	516	-	-	21/55/95/95	0/2/2/2
22	CLA	b	619	-	-	10/39/115/115	-
25	BCR	b	621	-	-	2/29/63/63	0/2/2/2
24	PL9	a	407	-	-	18/41/61/73	0/1/1/1
32	LMT	b	628	-	-	3/21/61/61	0/2/2/2
31	LMG	c	518	-	-	22/40/60/70	0/1/1/1
31	LMG	B	625	-	-	24/44/64/70	0/1/1/1
22	CLA	b	611	-	-	10/39/115/115	-
31	LMG	d	408	-	-	25/44/64/70	0/1/1/1
32	LMT	d	411	-	-	1/17/57/61	0/2/2/2
22	CLA	C	505	3	-	16/39/115/115	-

The worst 5 of 750 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	401	PHO	C1B-C2B	9.54	1.50	1.39
23	A	405	PHO	C1B-C2B	9.52	1.50	1.39
23	d	402	PHO	C1B-C2B	9.50	1.49	1.39
23	d	401	PHO	C1B-C2B	9.32	1.49	1.39
23	D	401	PHO	C3B-C4B	8.81	1.50	1.41

The worst 5 of 1047 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.55	110.12	106.68
22	B	611	CLA	C4A-NA-C1A	7.50	110.10	106.68
22	B	605	CLA	C4A-NA-C1A	7.34	110.03	106.68
22	b	608	CLA	C4A-NA-C1A	7.30	110.01	106.68
22	C	501	CLA	C4A-NA-C1A	7.18	109.96	106.68

There are no chirality outliers.

5 of 2097 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.

158 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	613	CLA	4	0
22	b	612	CLA	8	0
22	c	507	CLA	5	0
25	c	521	BCR	4	0
31	l	101	LMG	2	0
22	A	402	CLA	9	0
32	b	604	LMT	1	0
22	c	510	CLA	4	0
22	c	509	CLA	3	0
22	c	508	CLA	3	0
22	a	405	CLA	5	0
22	C	501	CLA	3	0
22	C	519	CLA	3	0
22	b	609	CLA	7	0
26	b	601	DGD	4	0
25	B	617	BCR	2	0
22	c	512	CLA	2	0
22	C	506	CLA	4	0
22	b	616	CLA	4	0
22	b	617	CLA	3	0
25	B	616	BCR	7	0
22	b	608	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	412	SQD	4	0
31	I	101	LMG	1	0
27	A	410	LHG	2	0
22	c	502	CLA	1	0
31	C	521	LMG	1	0
22	c	520	CLA	5	0
31	D	409	LMG	1	0
31	E	101	LMG	1	0
25	K	101	BCR	5	0
22	B	612	CLA	2	0
22	a	404	CLA	10	0
25	F	102	BCR	1	0
22	B	603	CLA	5	0
22	C	504	CLA	3	0
22	B	609	CLA	1	0
23	D	401	PHO	6	0
26	D	407	DGD	2	0
24	A	407	PL9	5	0
22	c	503	CLA	2	0
22	C	511	CLA	1	0
22	D	404	CLA	2	0
32	B	628	LMT	1	0
22	A	406	CLA	2	0
22	A	403	CLA	12	0
31	D	406	LMG	7	0
31	d	412	LMG	1	0
26	d	410	DGD	3	0
25	H	102	BCR	2	0
34	F	101	HEM	4	0
22	d	405	CLA	9	0
30	A	413	SQD	3	0
32	B	624	LMT	1	0
22	B	607	CLA	7	0
22	b	614	CLA	1	0
24	D	405	PL9	9	0
23	A	405	PHO	6	0
31	e	101	LMG	2	0
23	d	402	PHO	5	0
25	C	513	BCR	5	0
23	d	401	PHO	6	0
31	m	101	LMG	3	0
30	B	627	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	516	DGD	5	0
22	B	615	CLA	4	0
22	B	605	CLA	5	0
31	C	517	LMG	2	0
22	B	610	CLA	3	0
30	f	103	SQD	3	0
25	i	101	BCR	2	0
26	c	517	DGD	6	0
31	b	626	LMG	4	0
22	b	610	CLA	4	0
22	B	608	CLA	5	0
22	a	403	CLA	8	0
27	C	518	LHG	3	0
22	d	406	CLA	2	0
26	C	515	DGD	3	0
22	c	505	CLA	1	0
22	b	607	CLA	10	0
22	b	618	CLA	3	0
22	c	501	CLA	4	0
22	B	601	CLA	1	0
25	g	101	BCR	11	0
22	B	611	CLA	3	0
22	C	510	CLA	5	0
27	a	409	LHG	1	0
22	B	604	CLA	9	0
22	C	509	CLA	4	0
22	D	403	CLA	11	0
22	B	606	CLA	6	0
22	C	507	CLA	4	0
22	C	508	CLA	1	0
31	L	101	LMG	2	0
22	C	503	CLA	2	0
31	B	621	LMG	3	0
22	H	101	CLA	11	0
25	A	408	BCR	4	0
26	A	409	DGD	1	0
26	c	515	DGD	3	0
26	B	620	DGD	3	0
22	C	512	CLA	3	0
22	a	406	CLA	2	0
32	I	102	LMT	1	0
25	b	623	BCR	2	0

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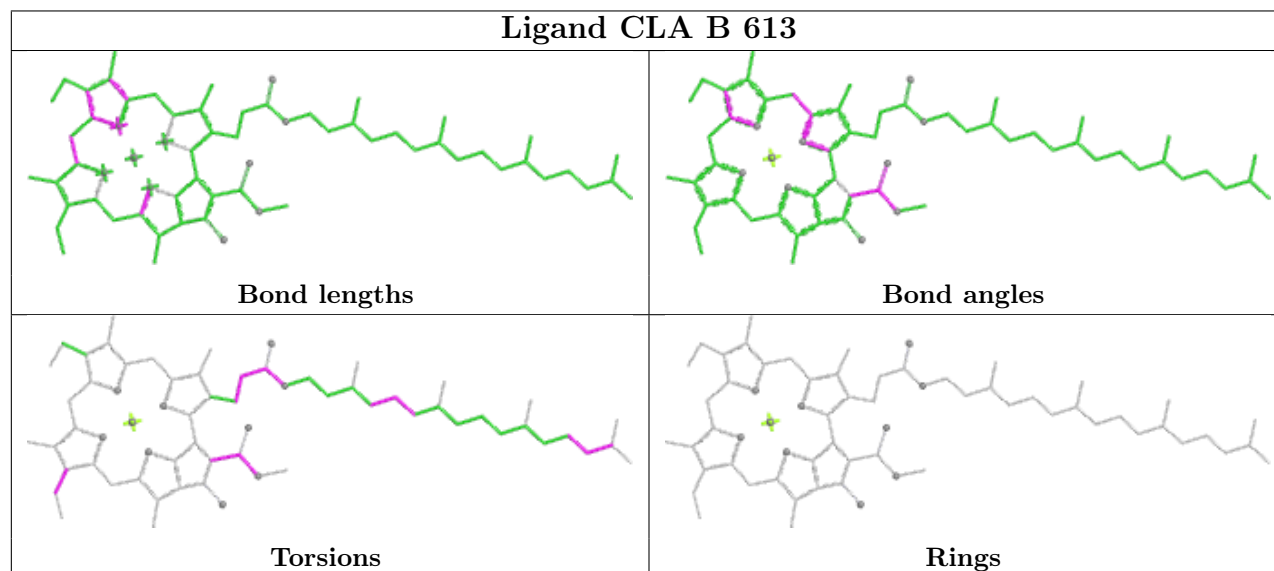
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	414	SQD	3	0
22	c	504	CLA	4	0
27	c	519	LHG	2	0
34	v	201	HEM	5	0
22	b	613	CLA	6	0
25	b	622	BCR	1	0
30	a	401	SQD	4	0
22	b	620	CLA	4	0
30	F	103	SQD	3	0
31	d	409	LMG	7	0
25	B	619	BCR	2	0
25	J	102	BCR	3	0
22	b	606	CLA	8	0
32	b	603	LMT	4	0
25	y	101	BCR	6	0
22	B	614	CLA	3	0
34	V	201	HEM	3	0
30	d	403	SQD	3	0
25	C	520	BCR	5	0
30	b	602	SQD	2	0
25	B	618	BCR	4	0
22	c	506	CLA	4	0
25	c	513	BCR	8	0
22	B	602	CLA	10	0
30	B	622	SQD	2	0
22	b	615	CLA	2	0
24	d	407	PL9	6	0
25	x	101	BCR	1	0
31	b	627	LMG	1	0
25	c	514	BCR	4	0
26	a	408	DGD	2	0
26	b	625	DGD	1	0
32	B	623	LMT	1	0
25	j	102	BCR	2	0
25	f	102	BCR	3	0
22	A	404	CLA	6	0
25	b	624	BCR	4	0
26	B	626	DGD	1	0
26	C	514	DGD	3	0
31	M	101	LMG	2	0
31	c	522	LMG	1	0
34	f	101	HEM	4	0

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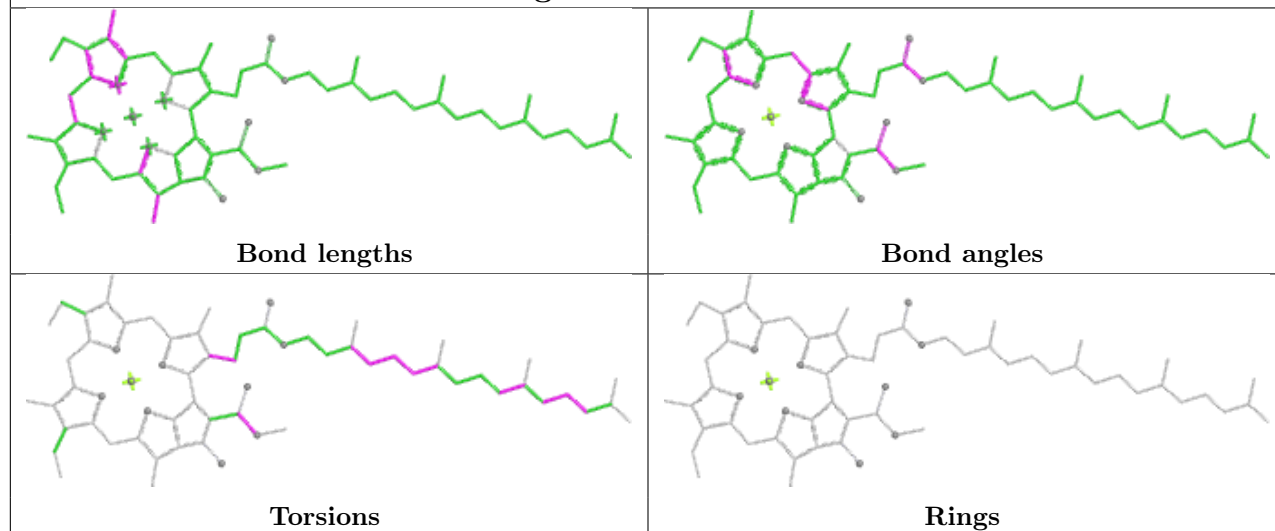
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	516	DGD	5	0
22	b	619	CLA	1	0
25	b	621	BCR	4	0
24	a	407	PL9	4	0
32	b	628	LMT	1	0
31	c	518	LMG	2	0
31	B	625	LMG	2	0
22	b	611	CLA	6	0
31	d	408	LMG	2	0
22	C	505	CLA	2	0

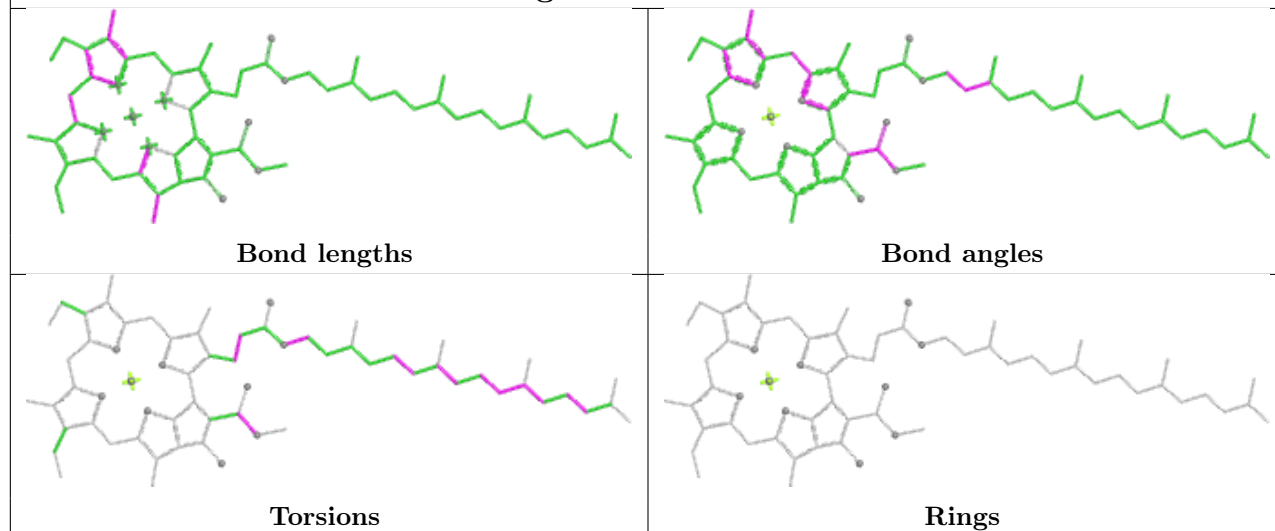
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



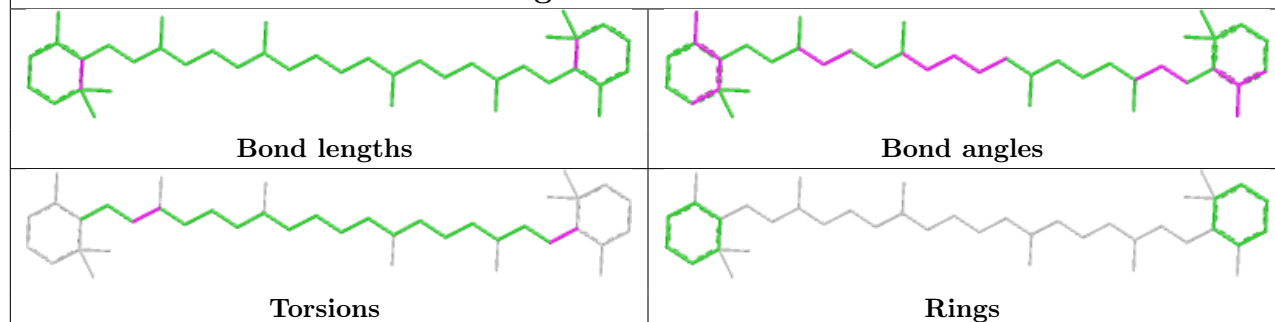
Ligand CLA b 612

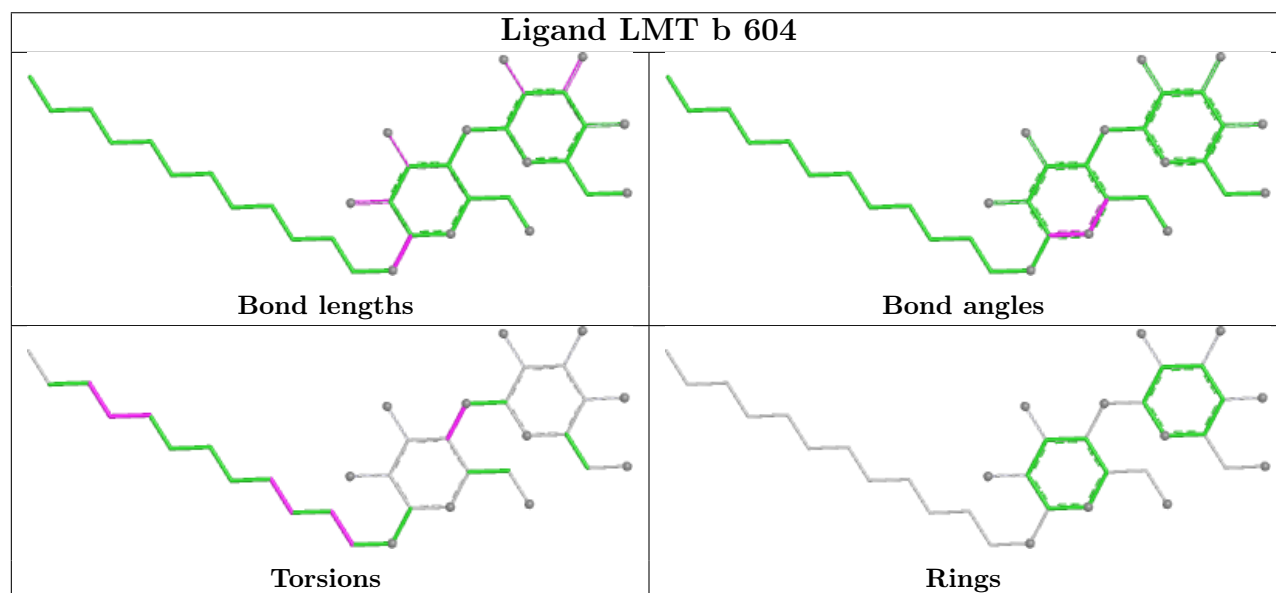
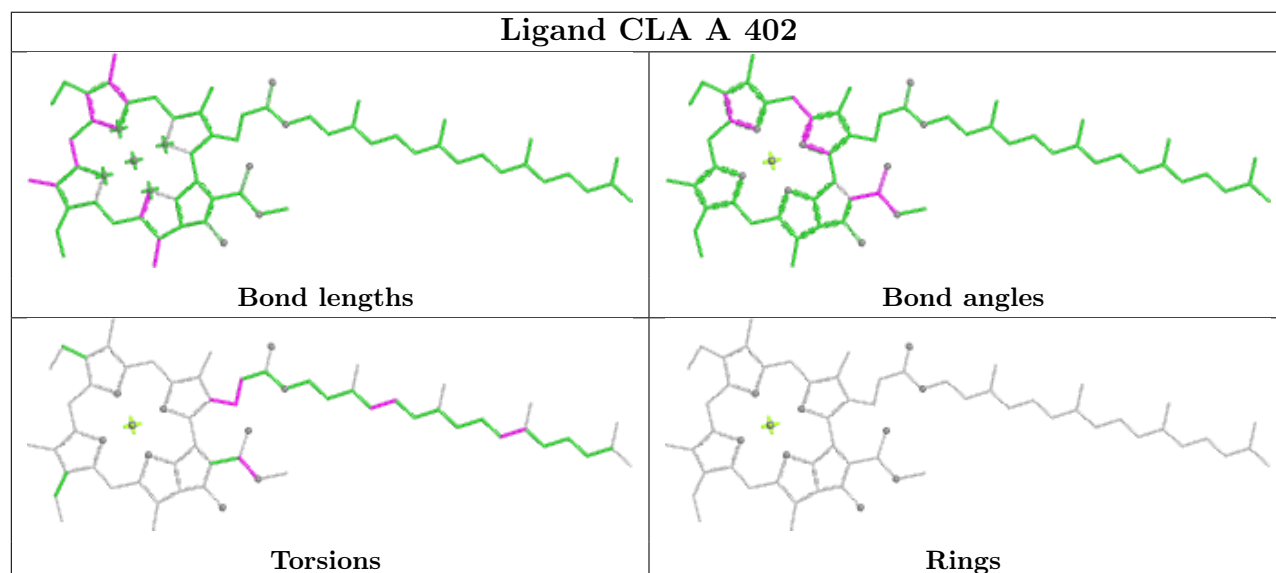
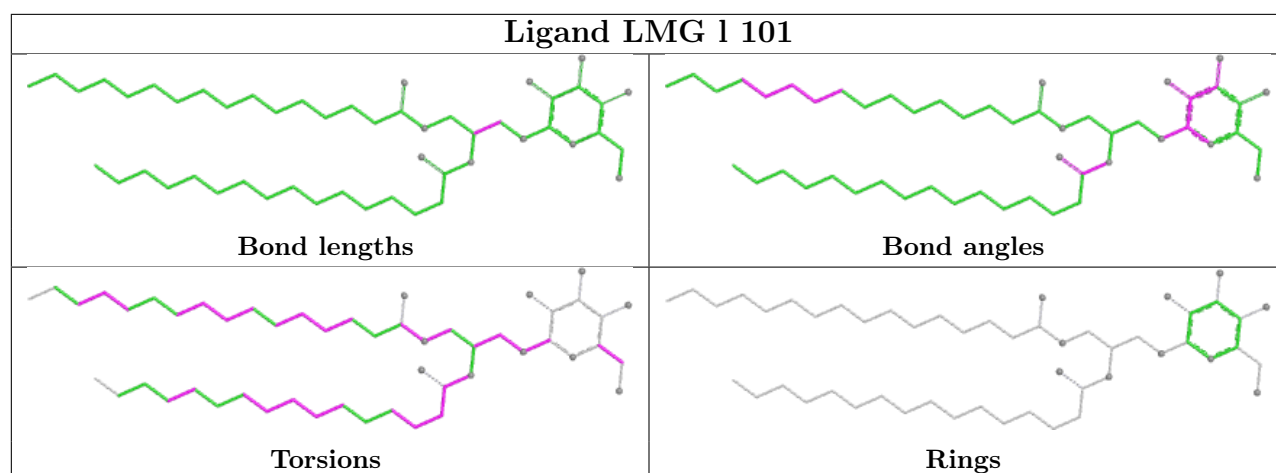


Ligand CLA c 507

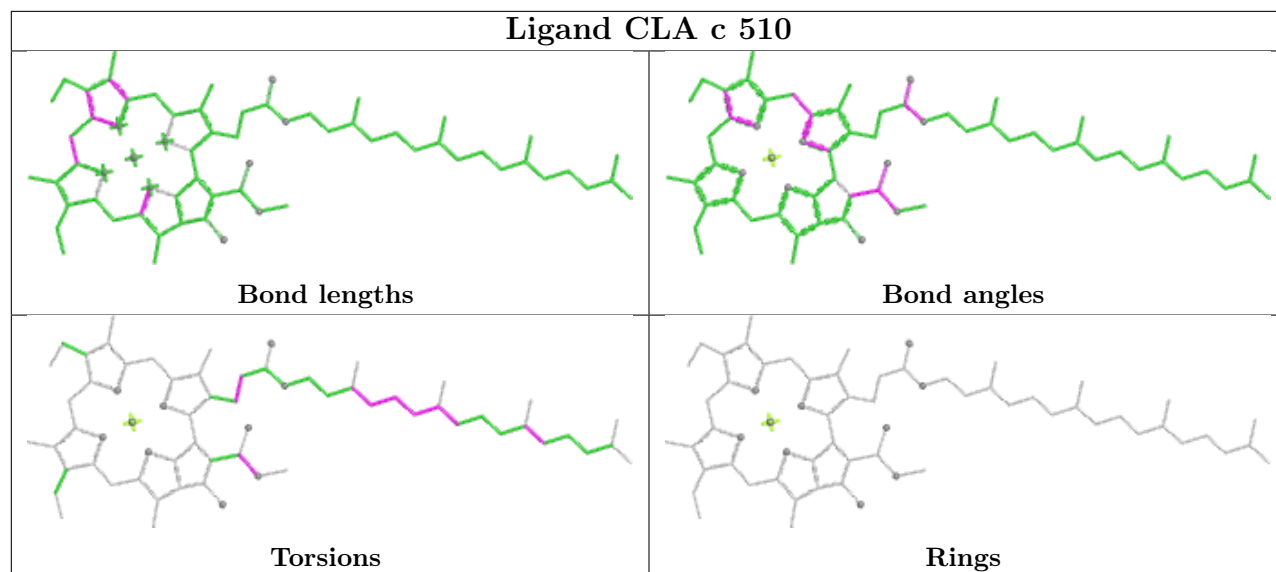


Ligand BCR c 521

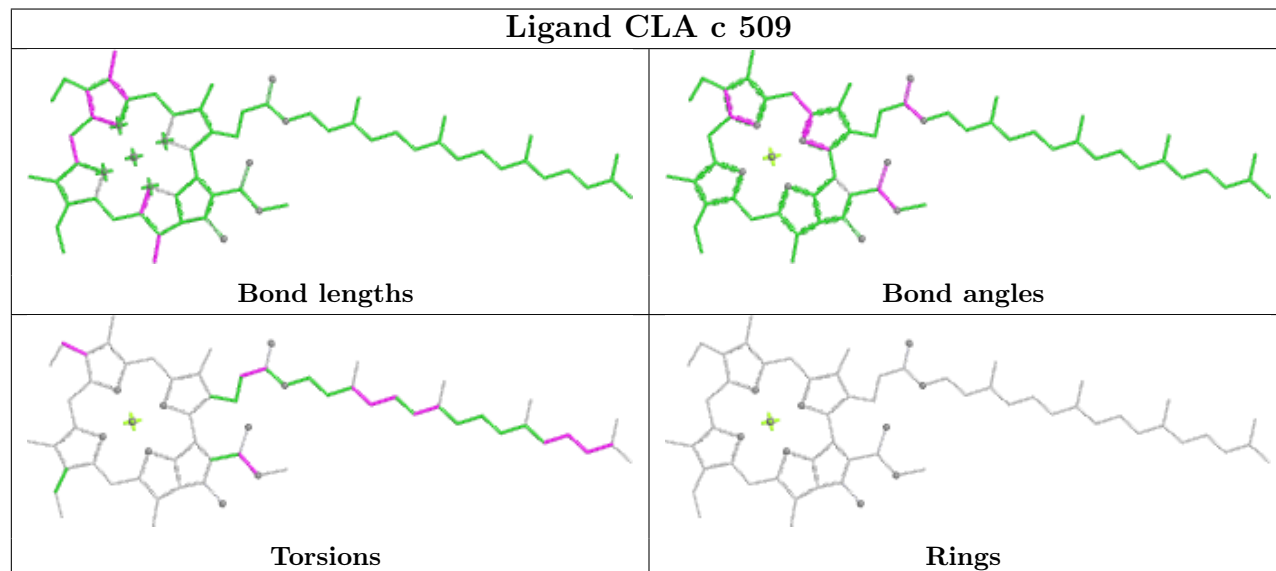




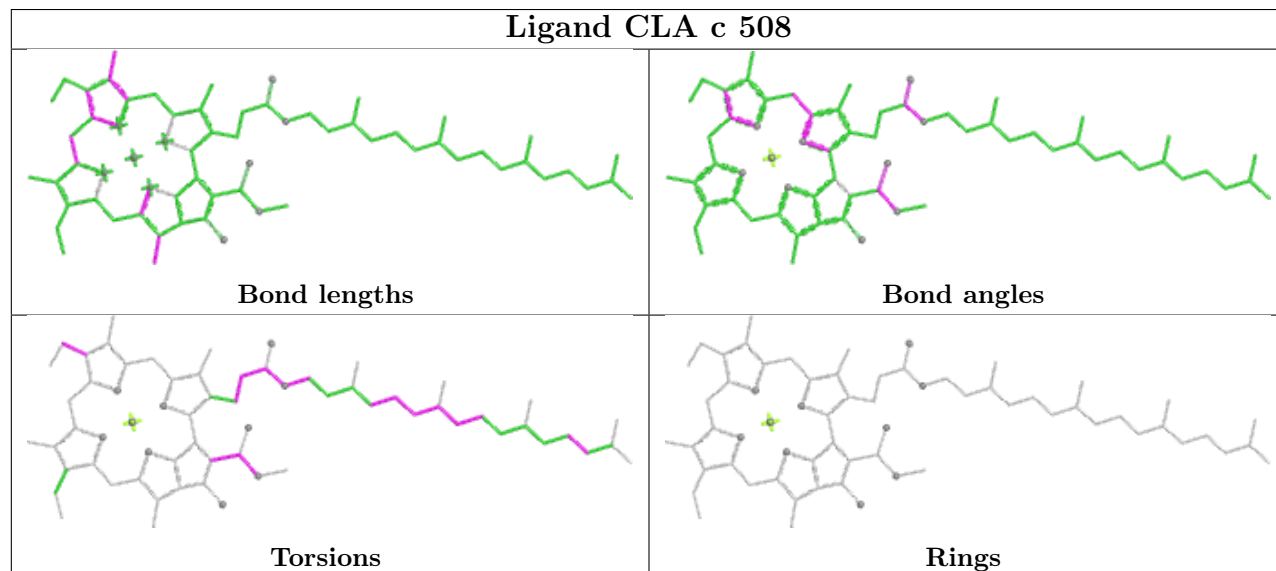
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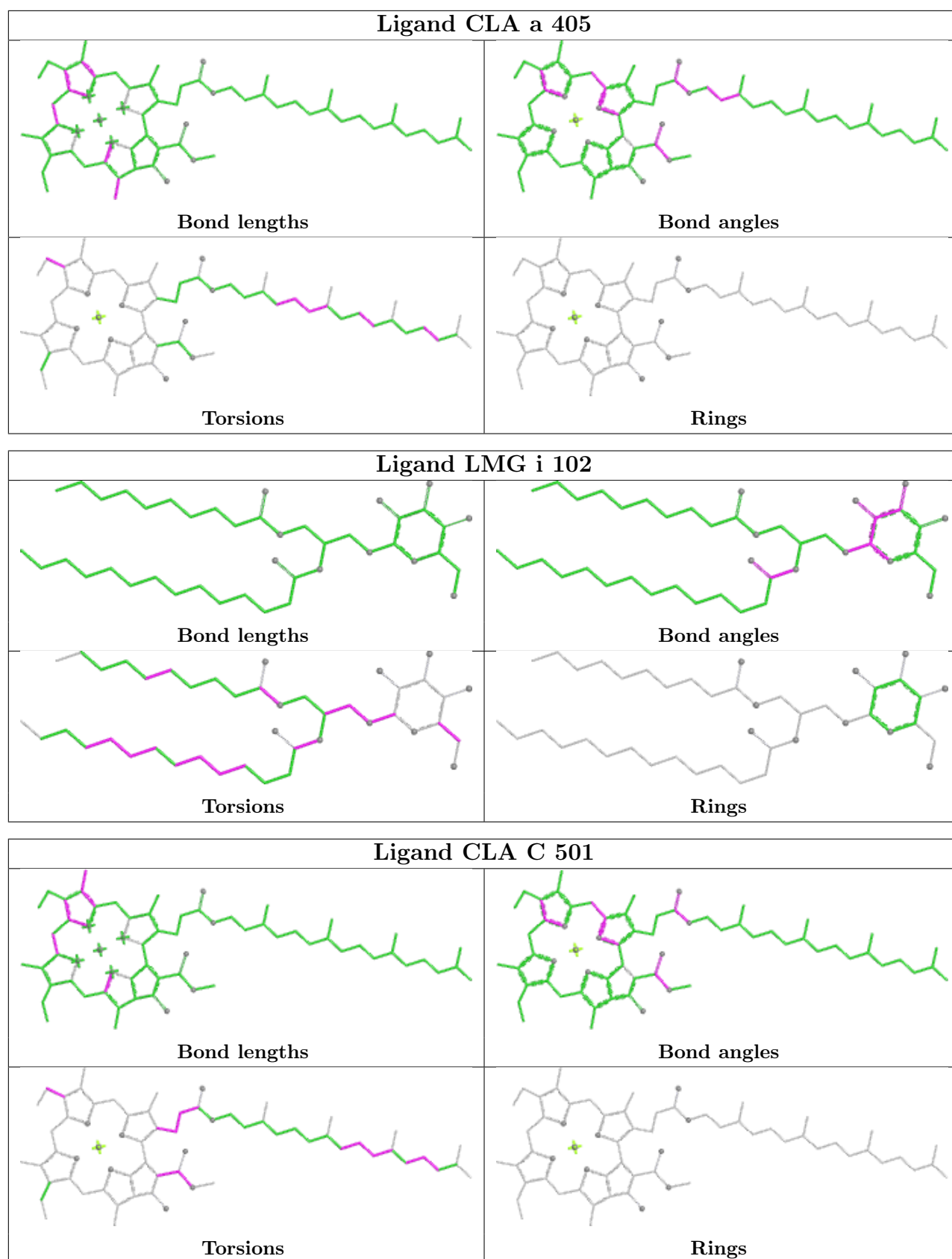


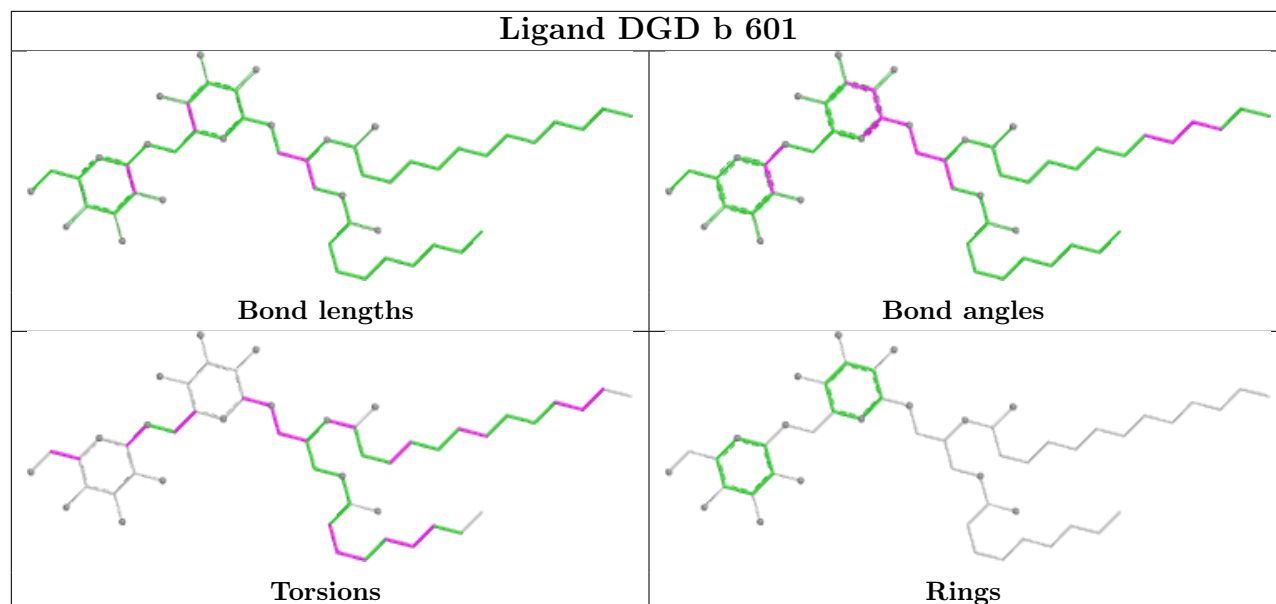
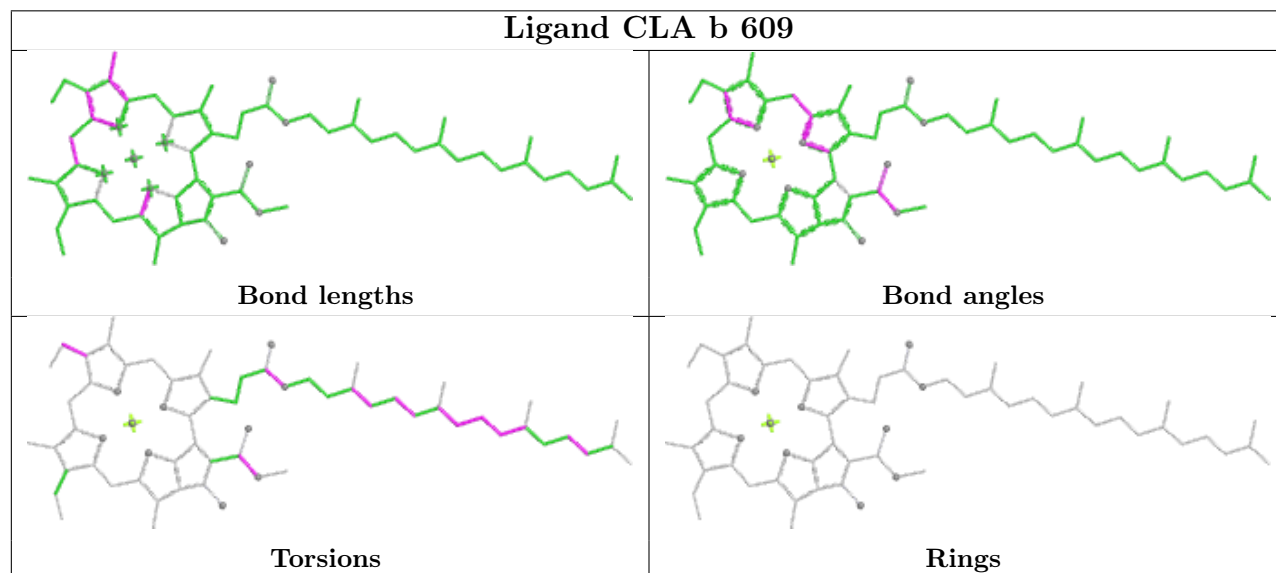
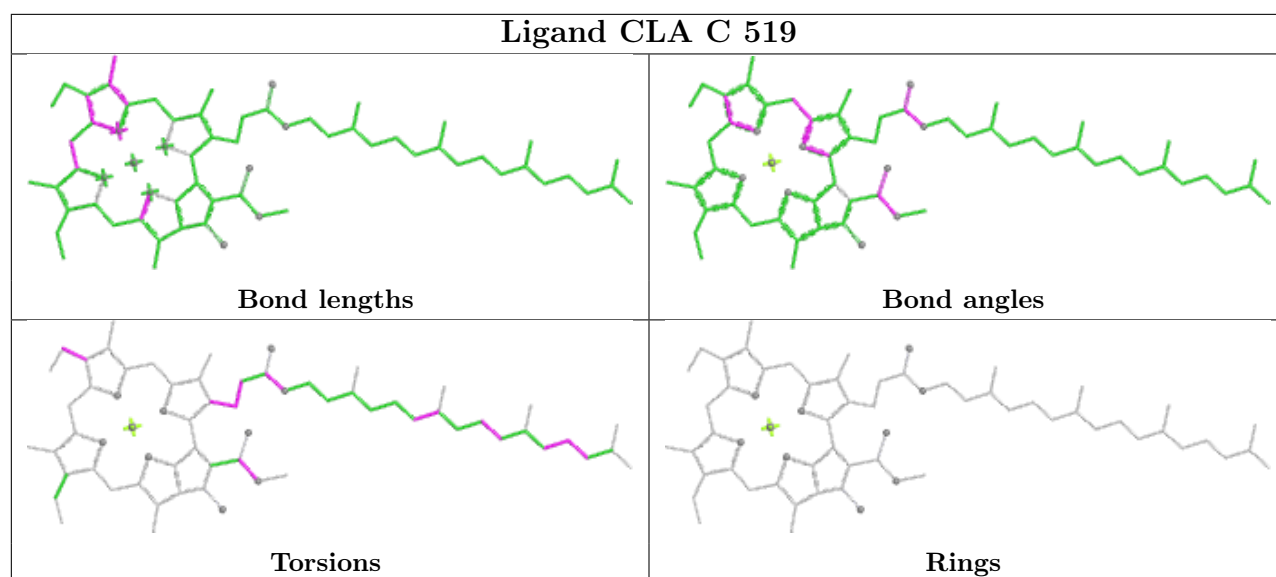
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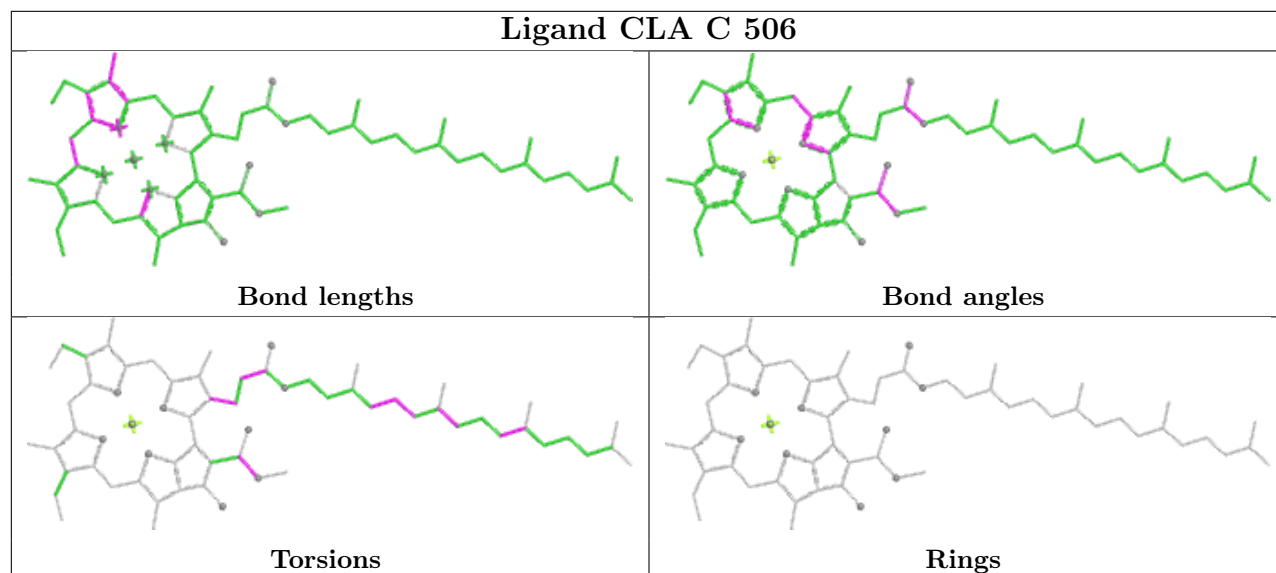
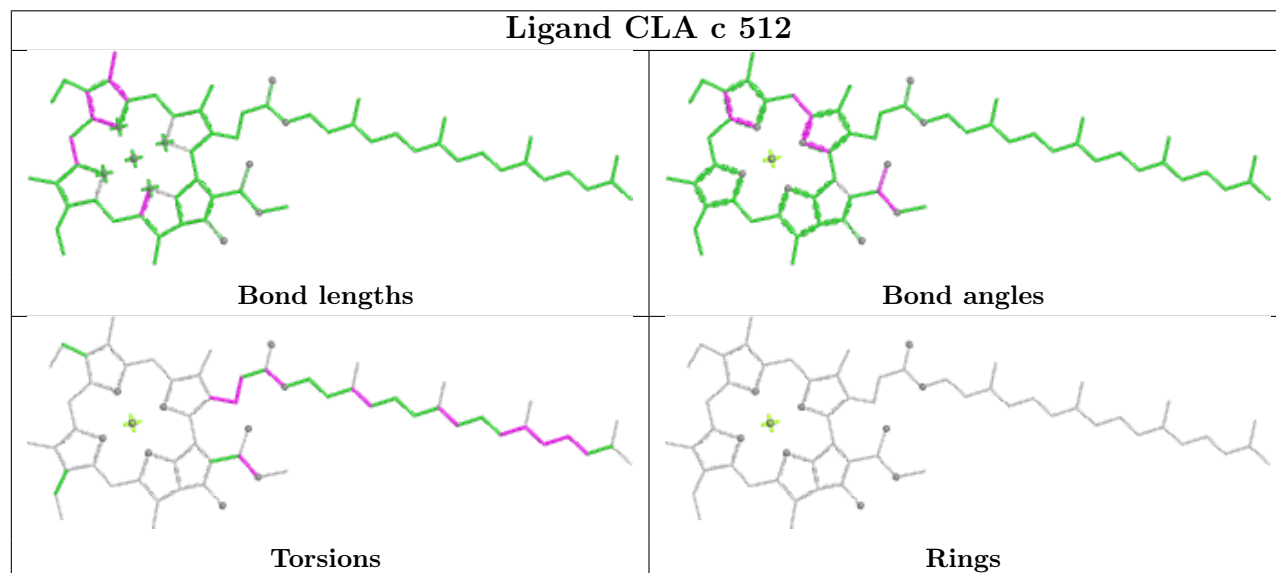
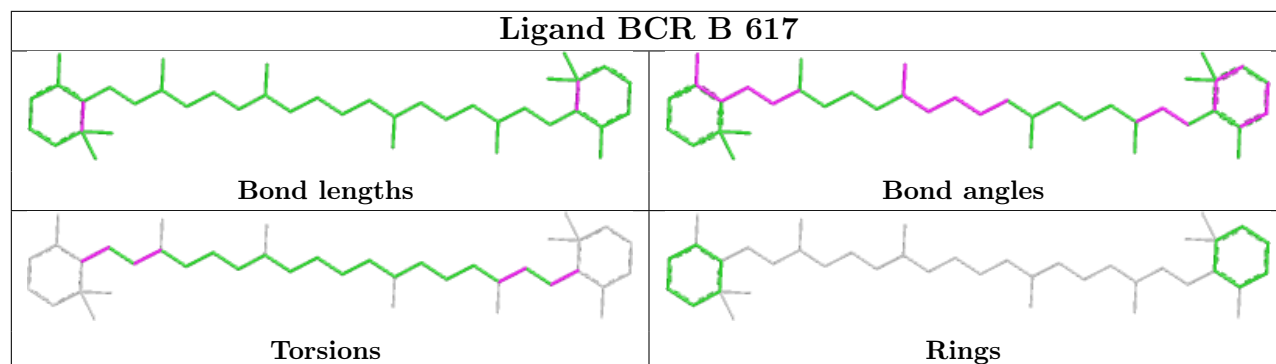


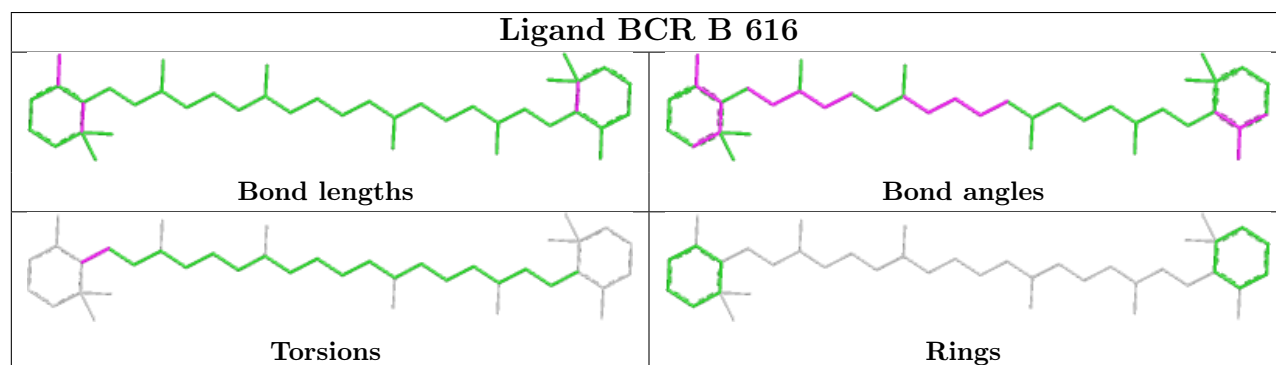
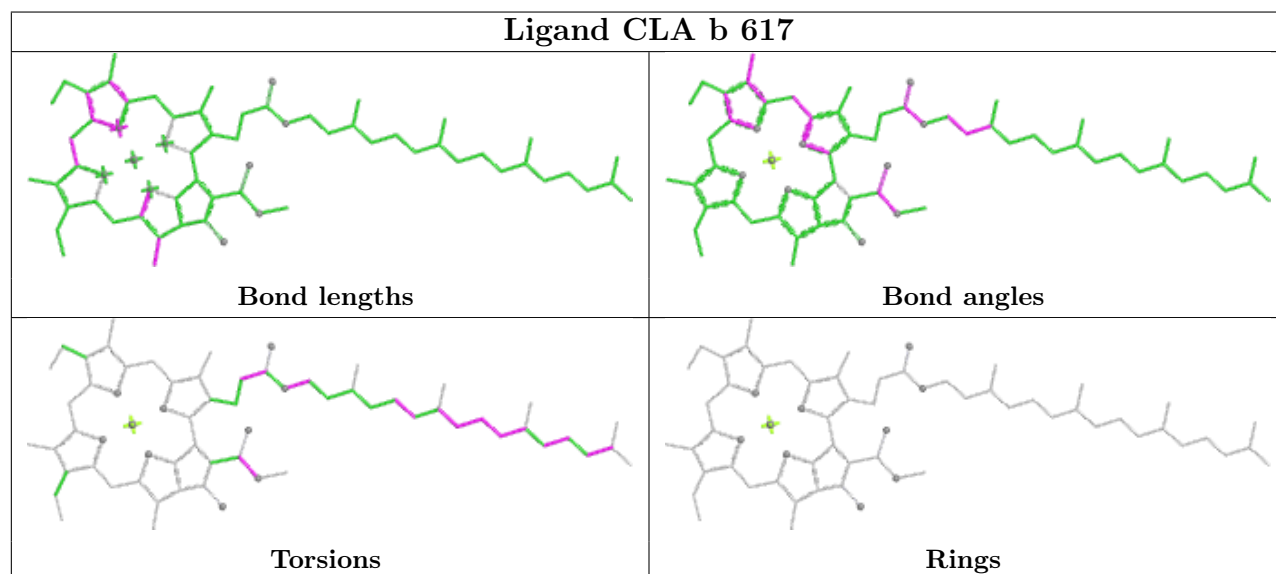
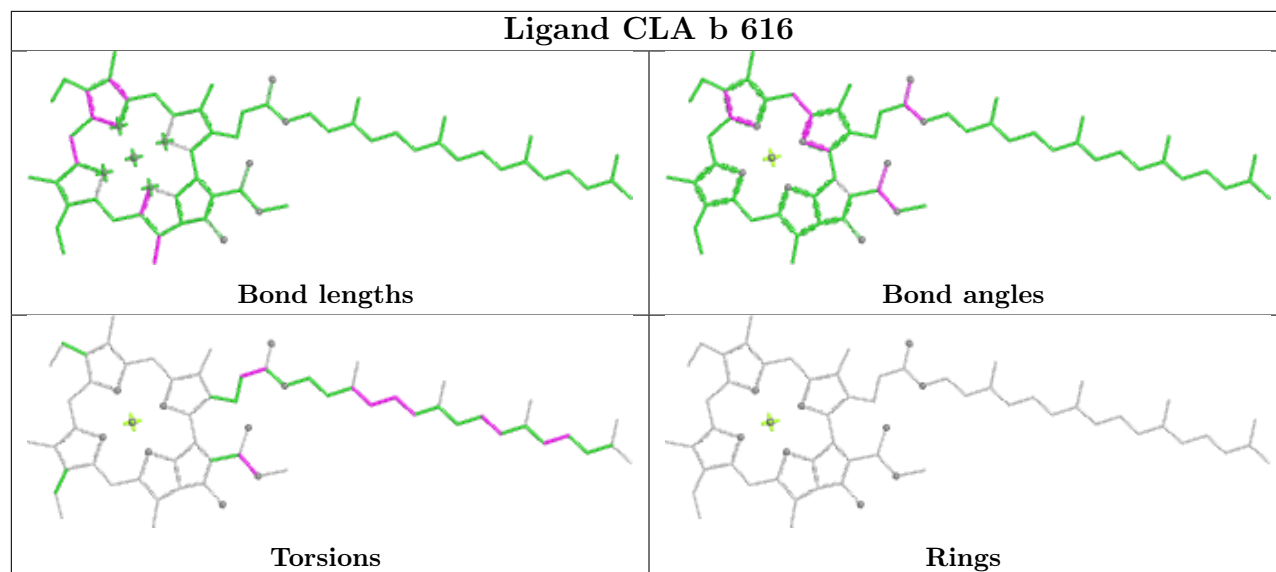
Ligand CLA c 508



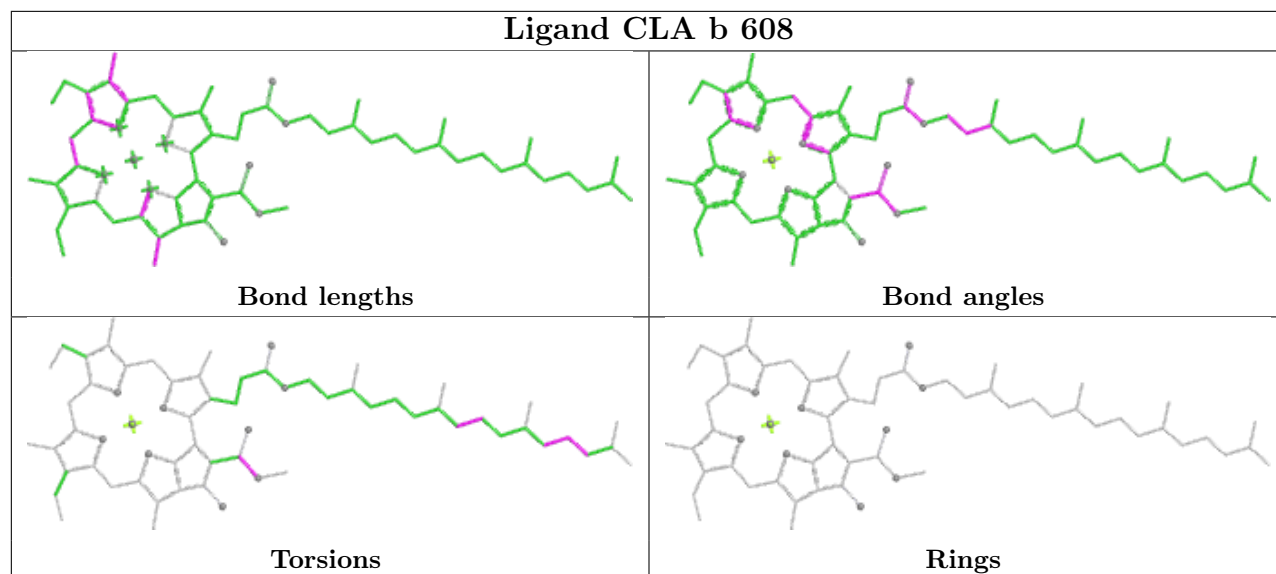




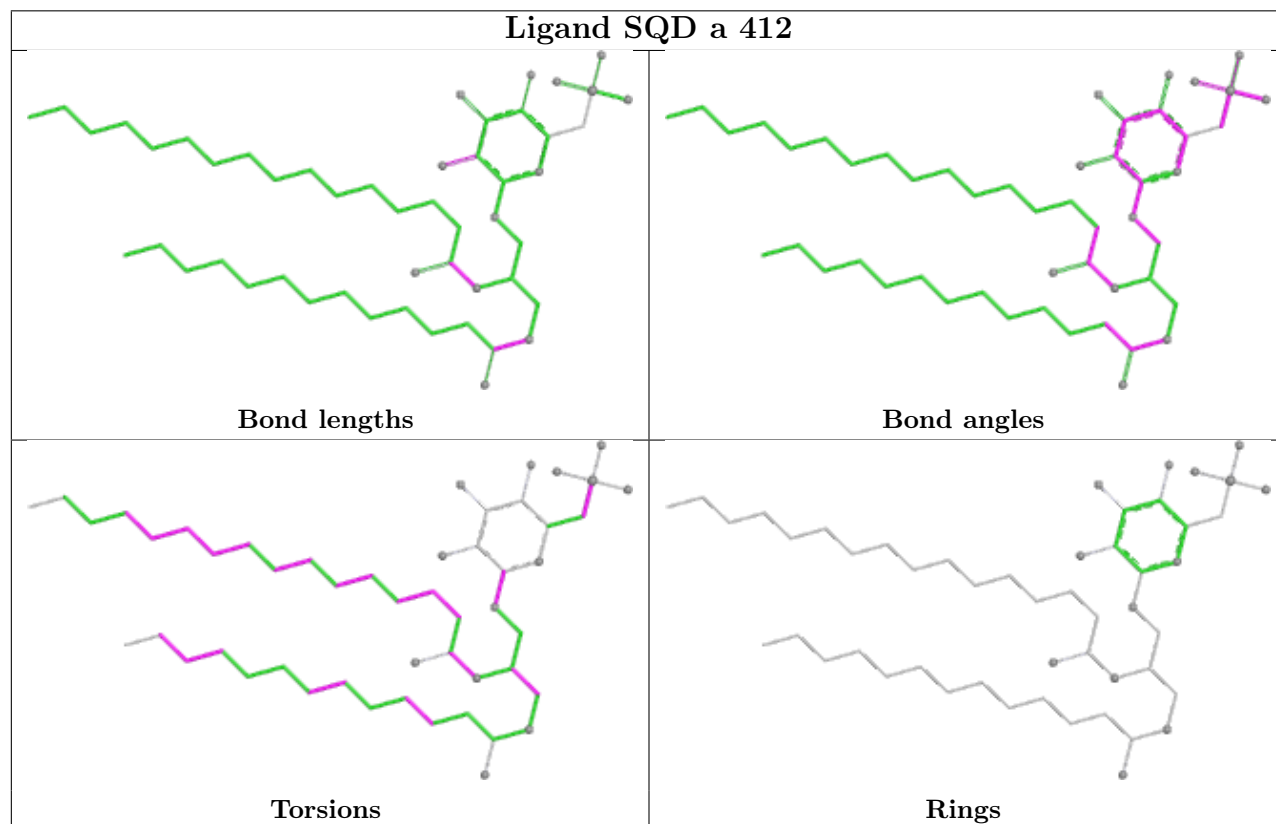


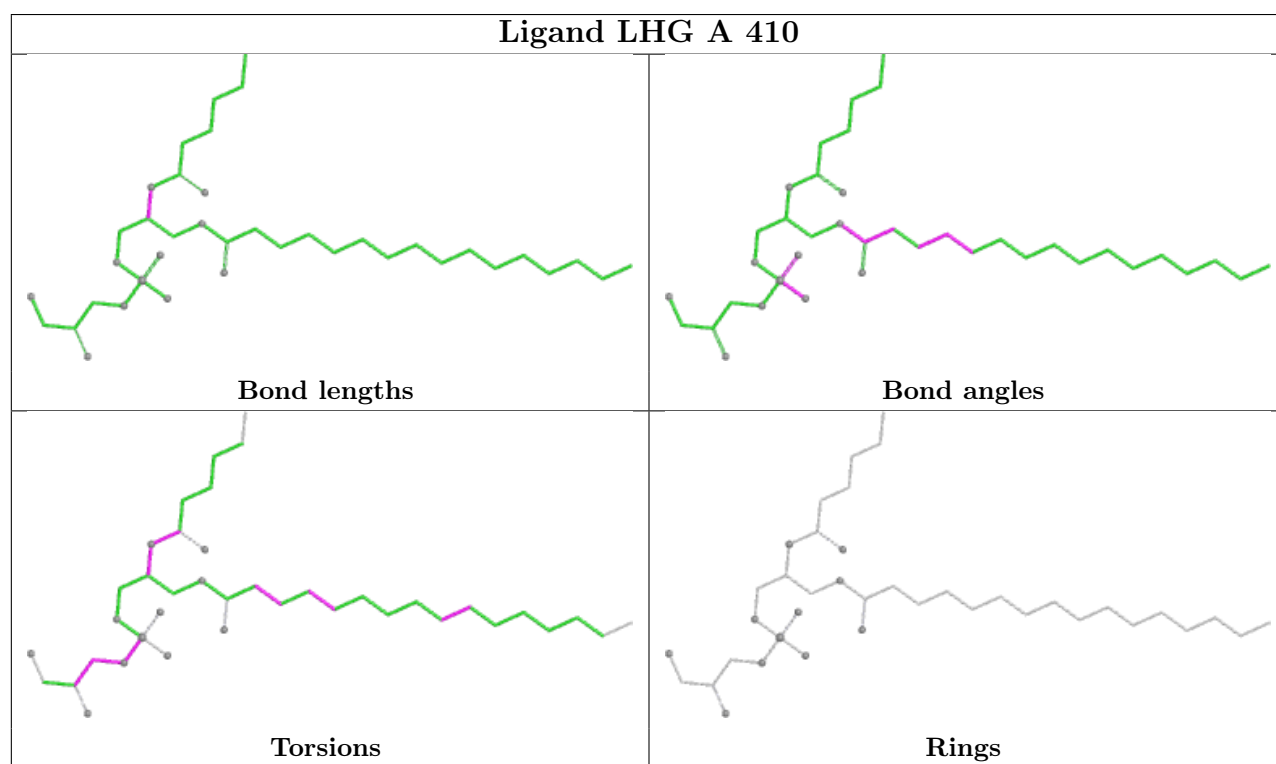
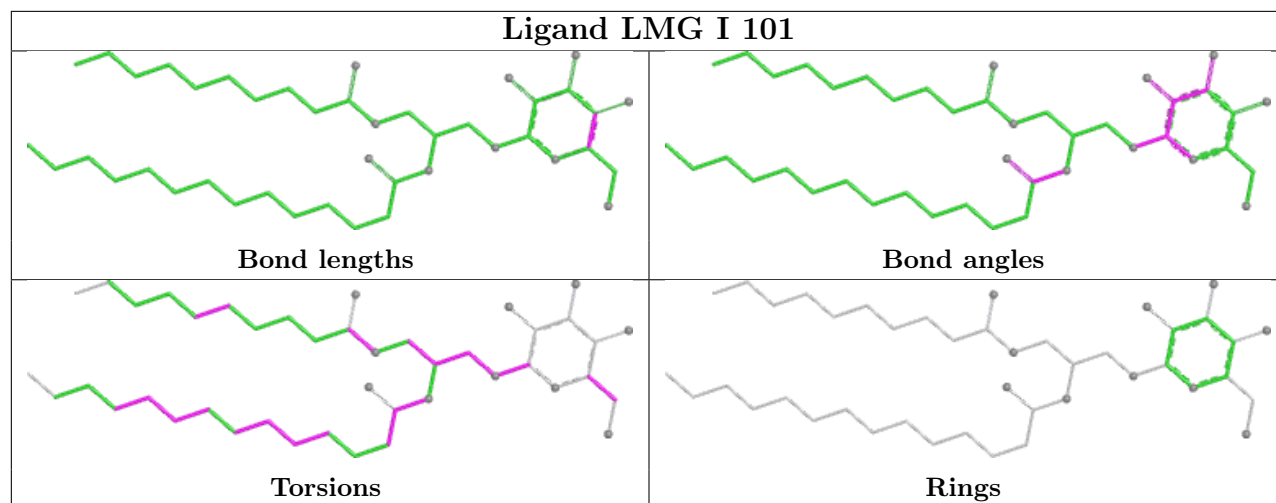


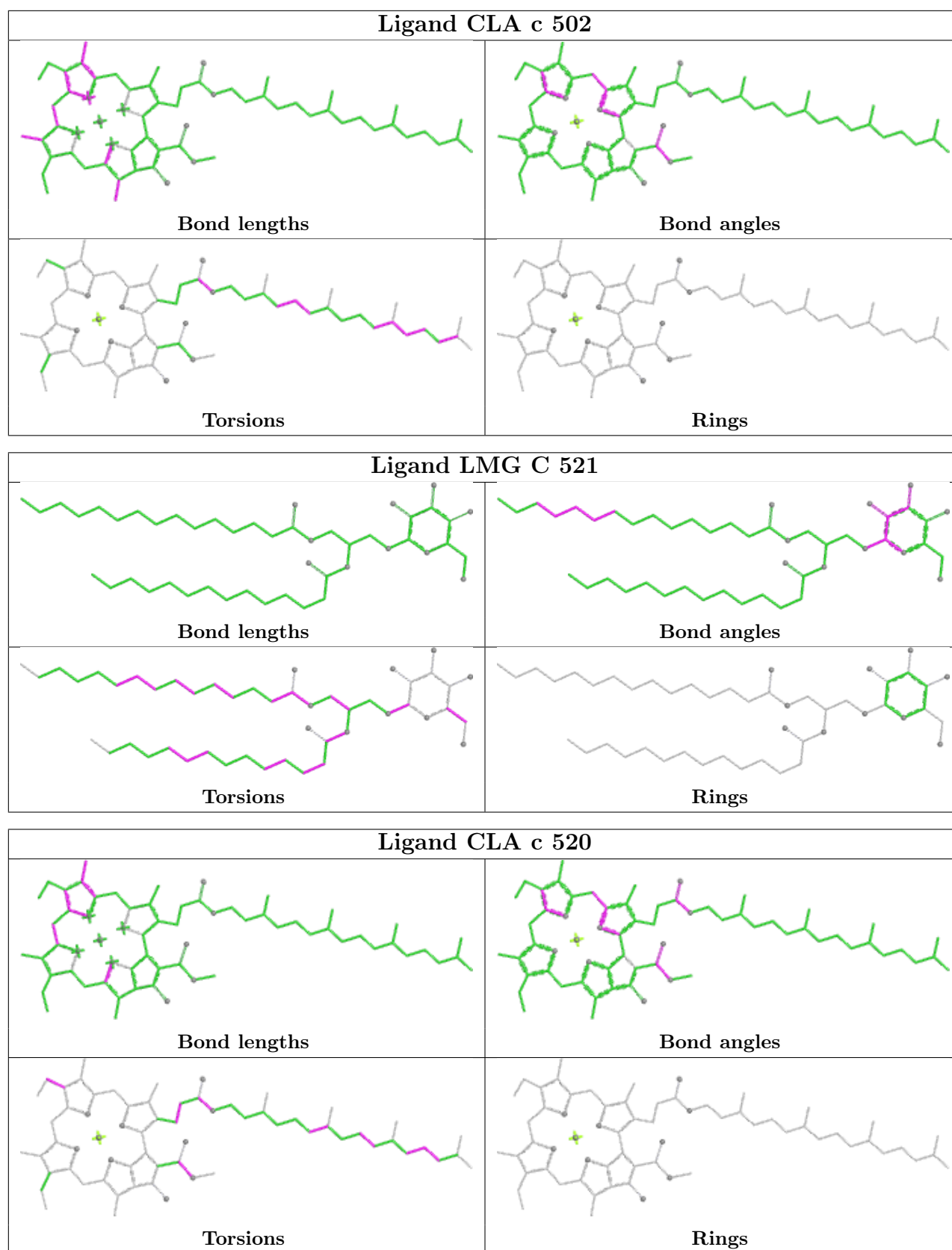
Ligand CLA b 608

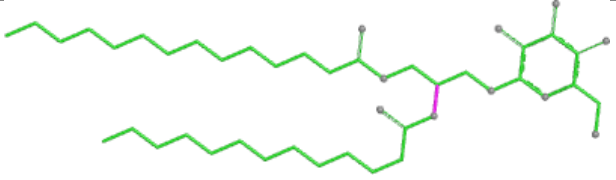
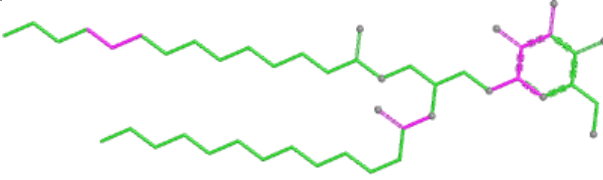
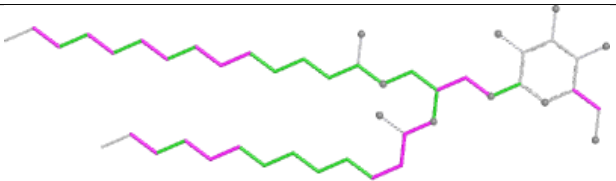
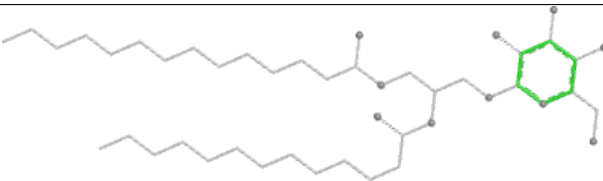


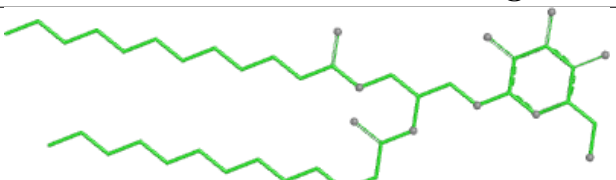
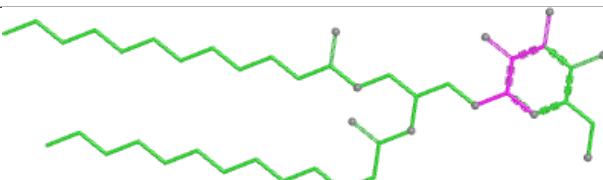
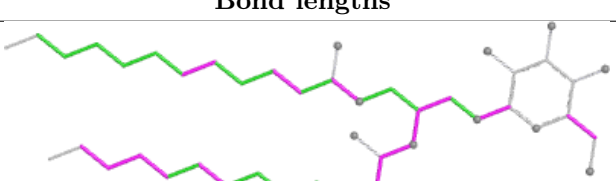
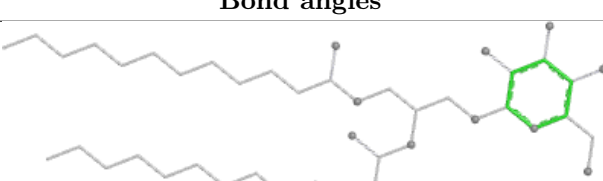
Ligand SQD a 412

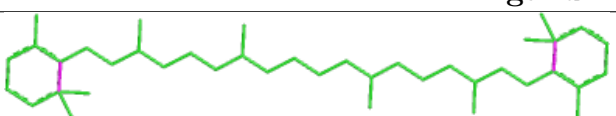
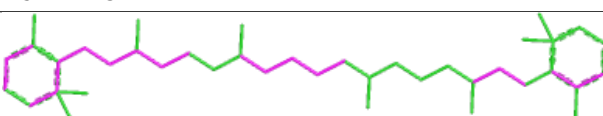
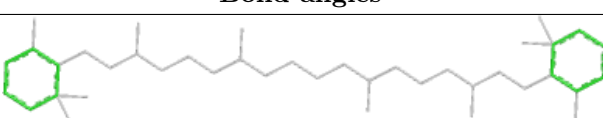


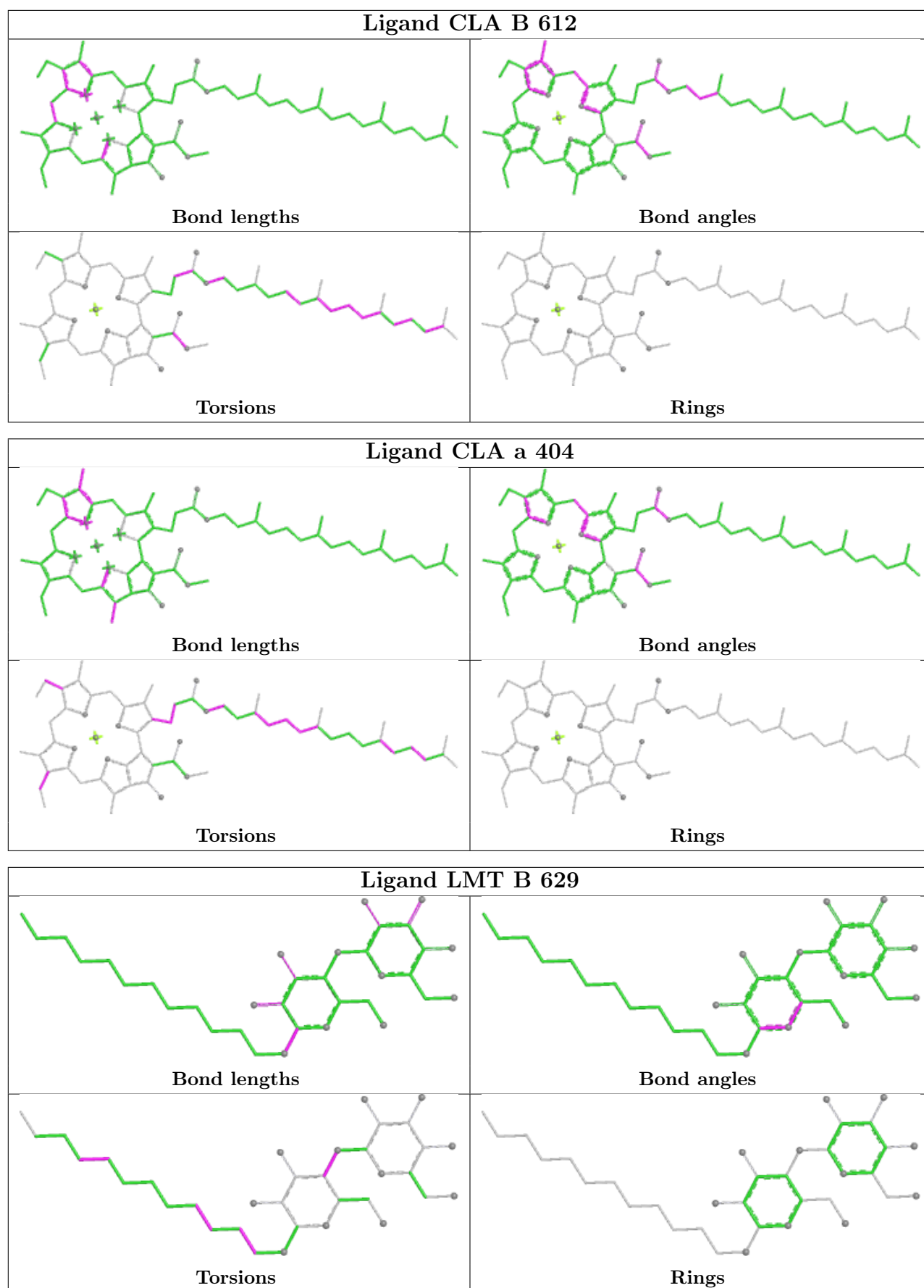


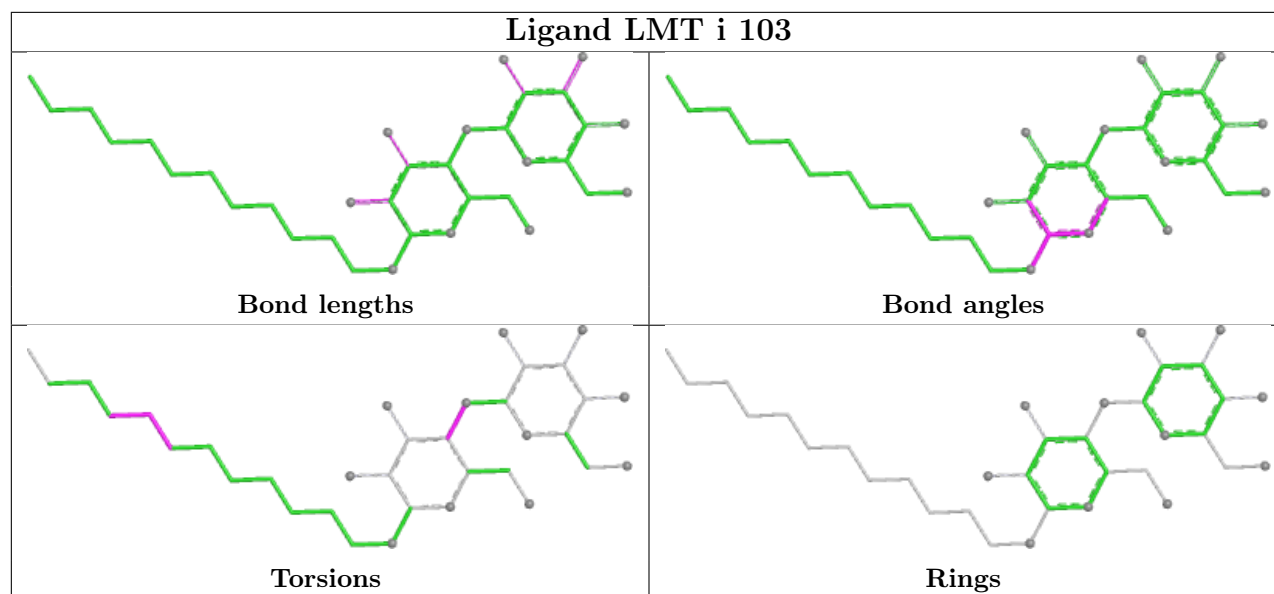
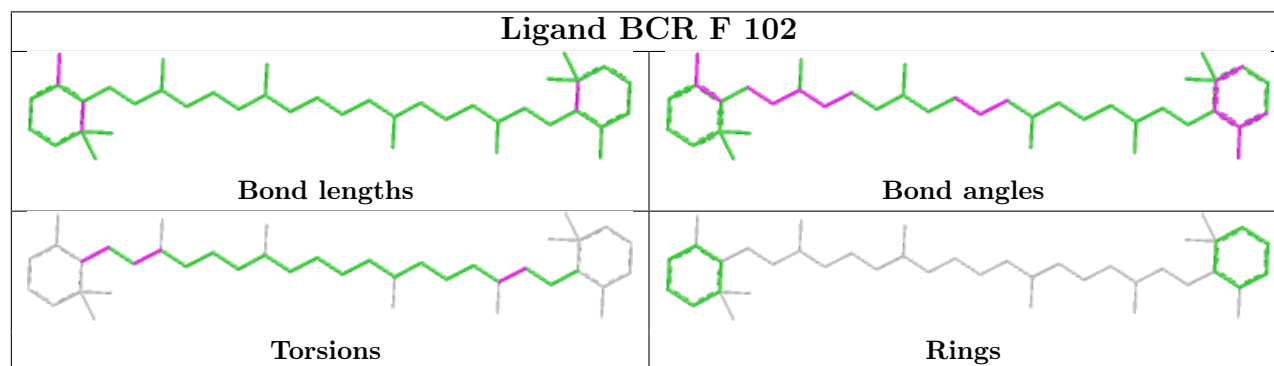
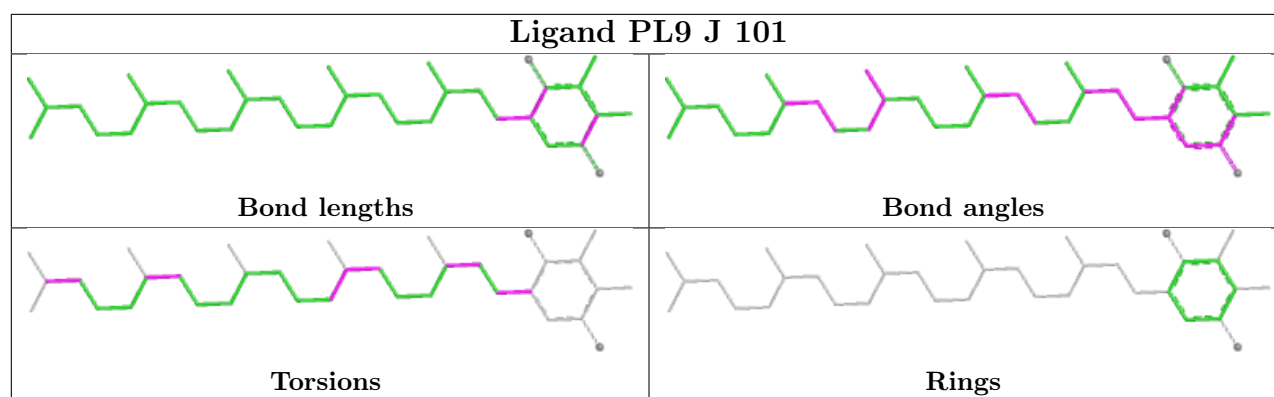


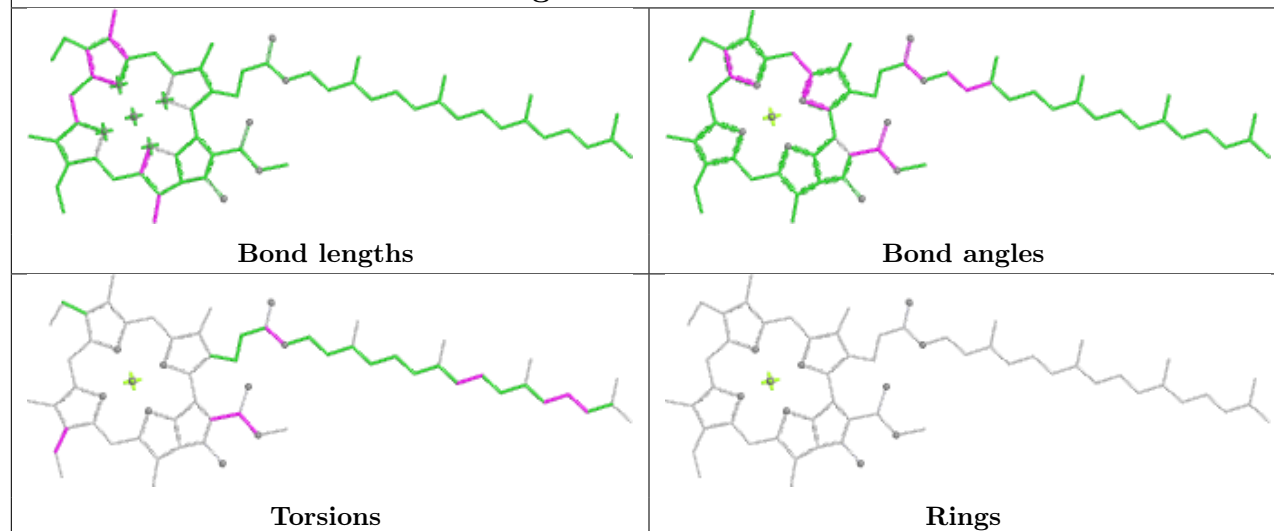
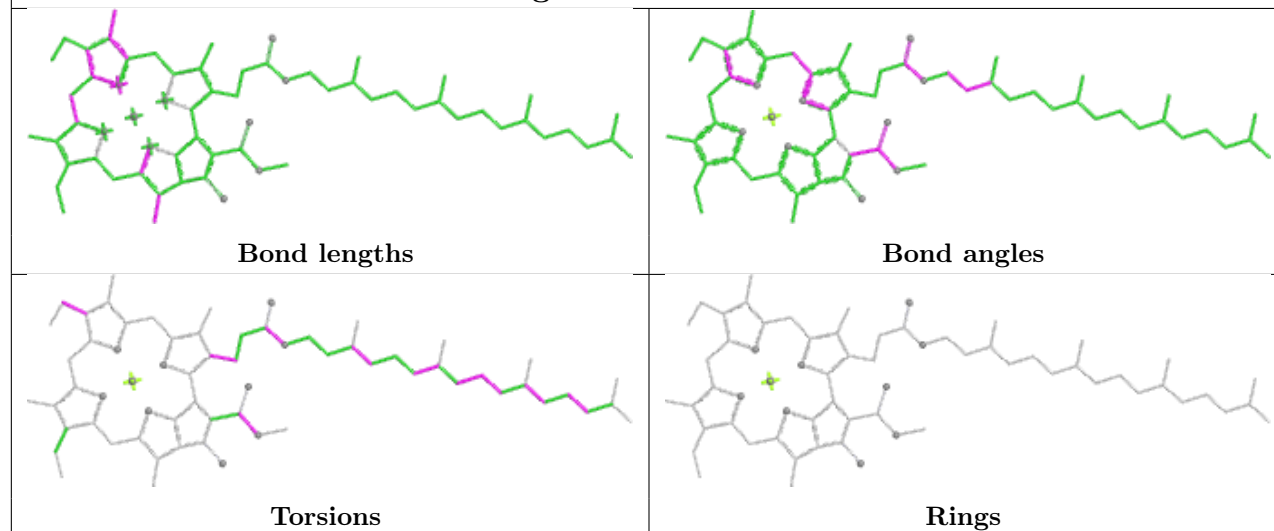
Ligand LMG D 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

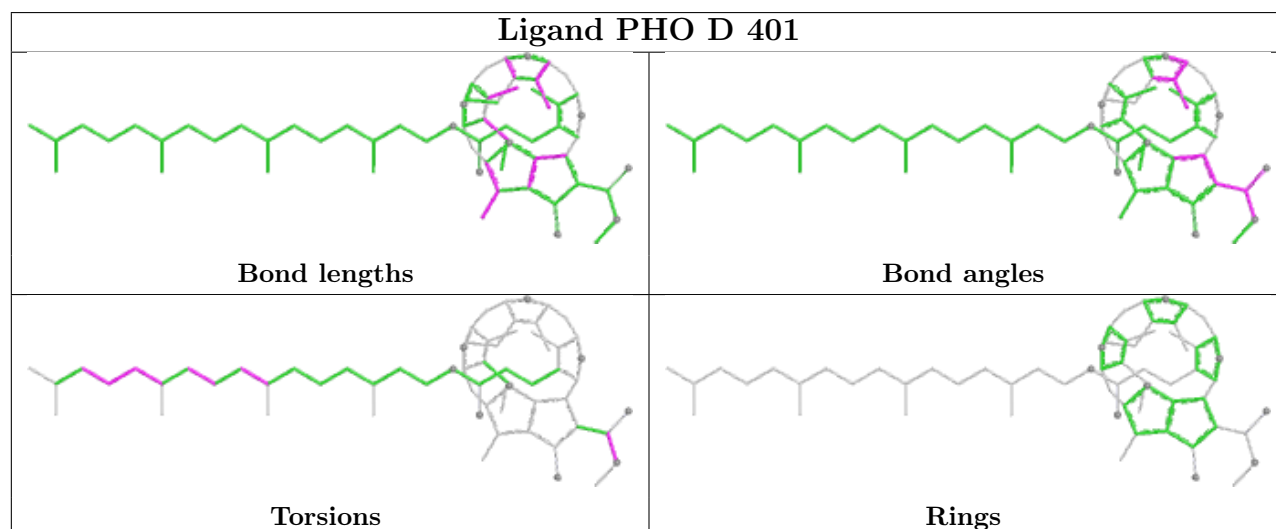
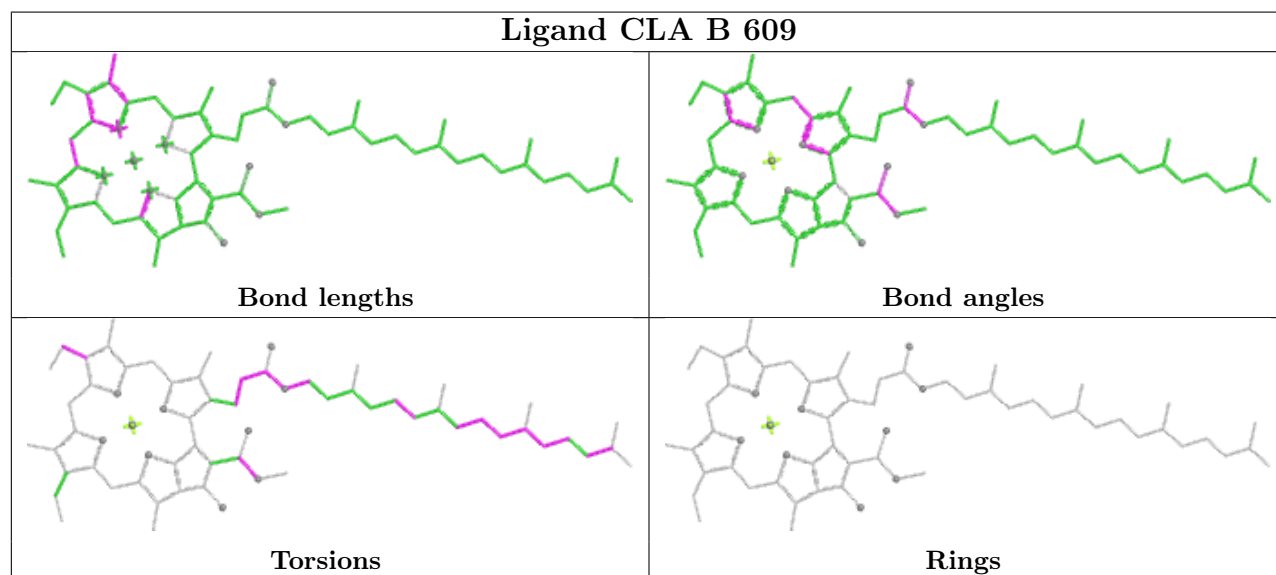
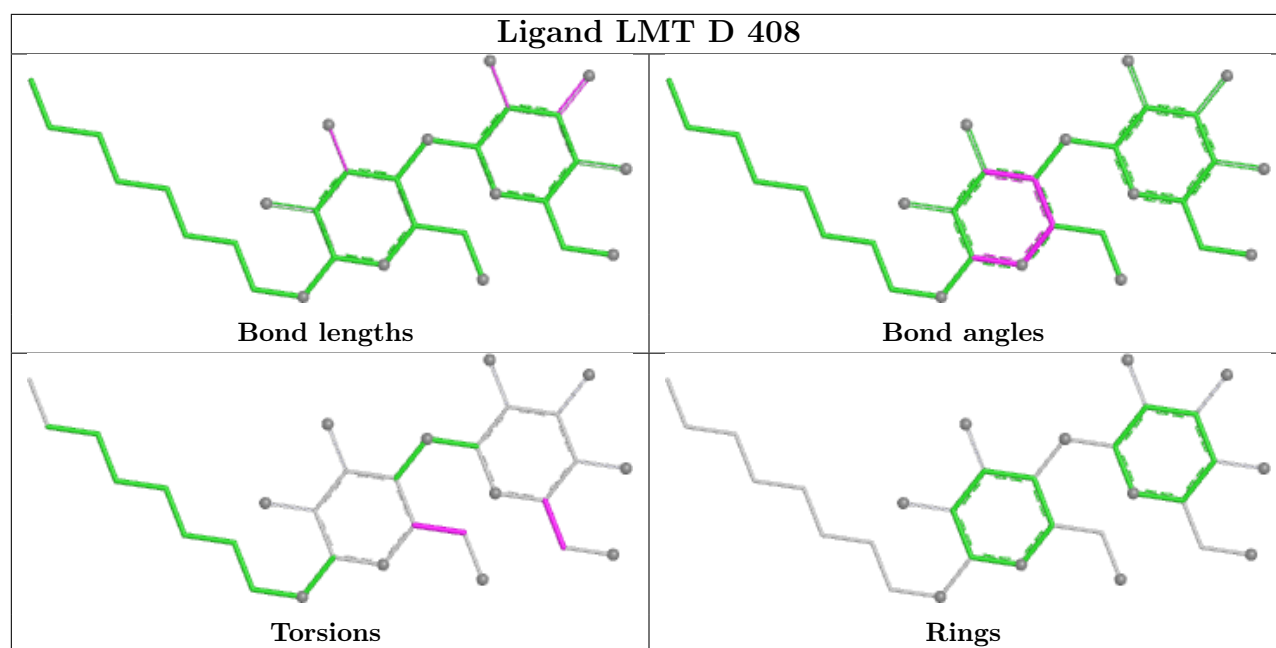
Ligand LMG E 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

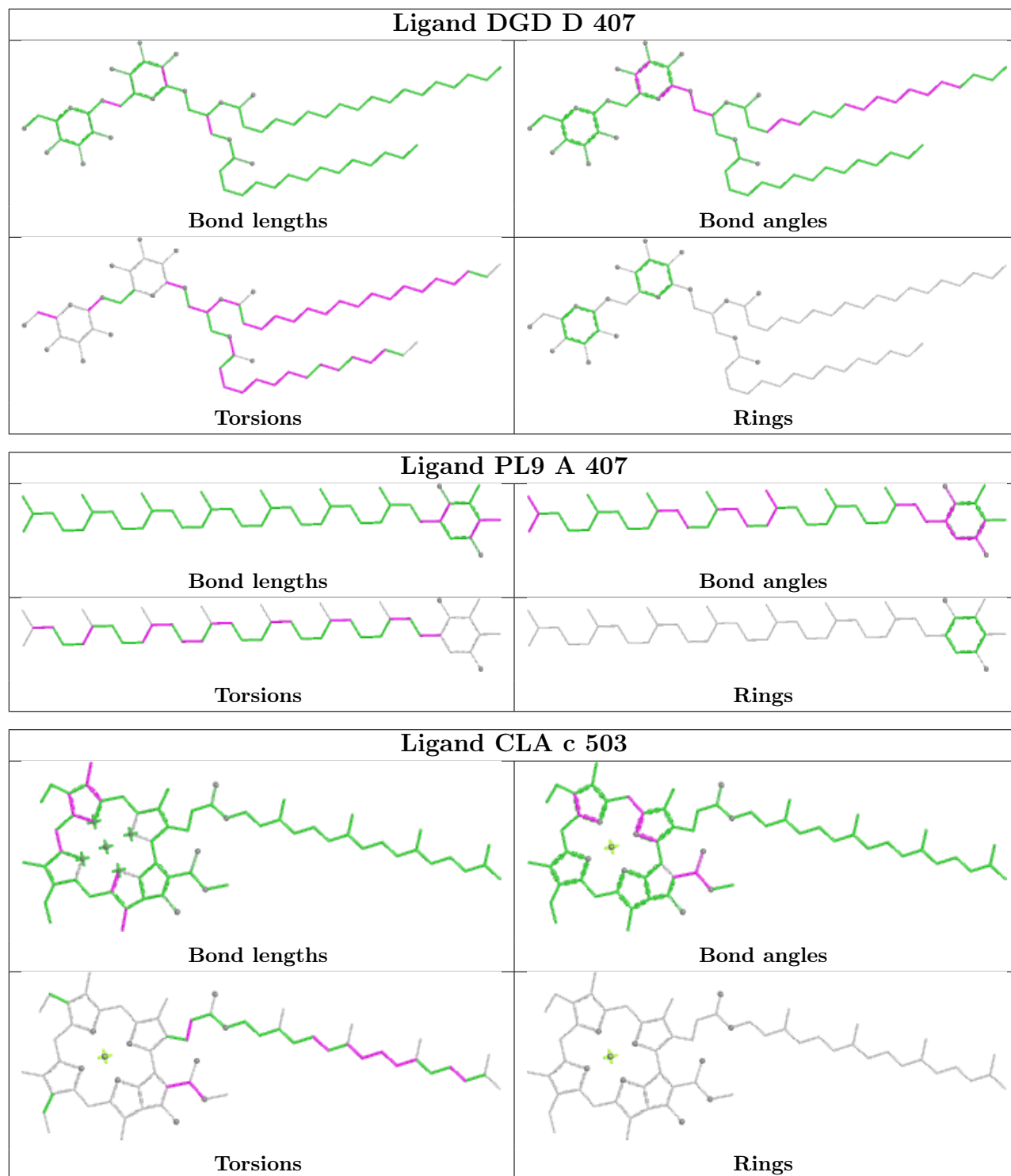
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

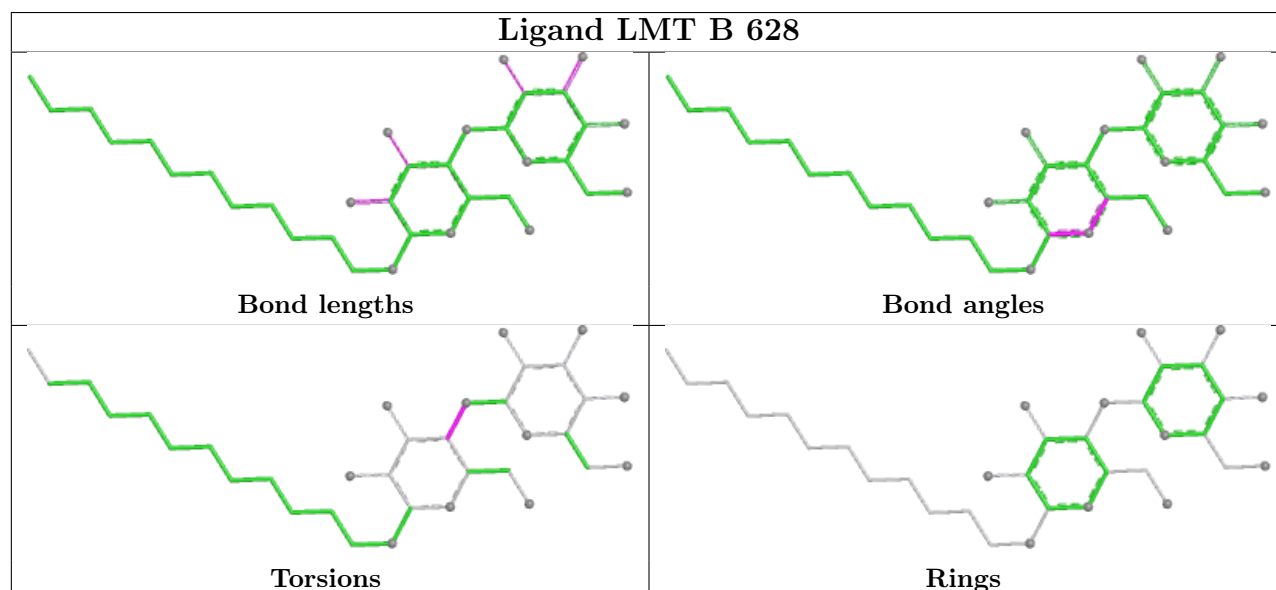
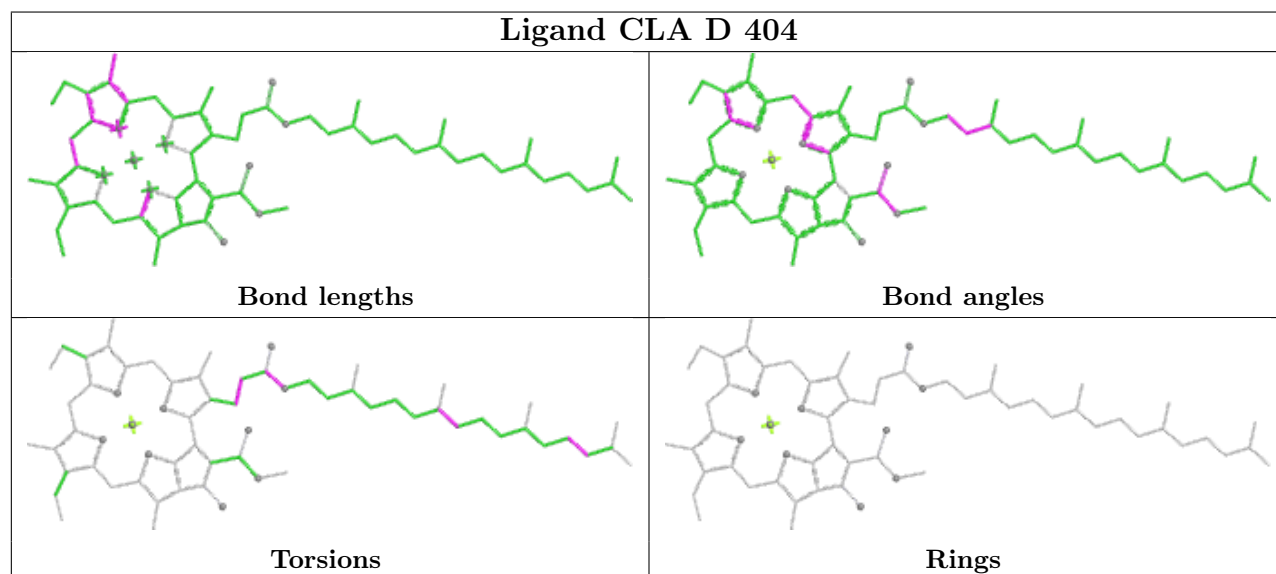
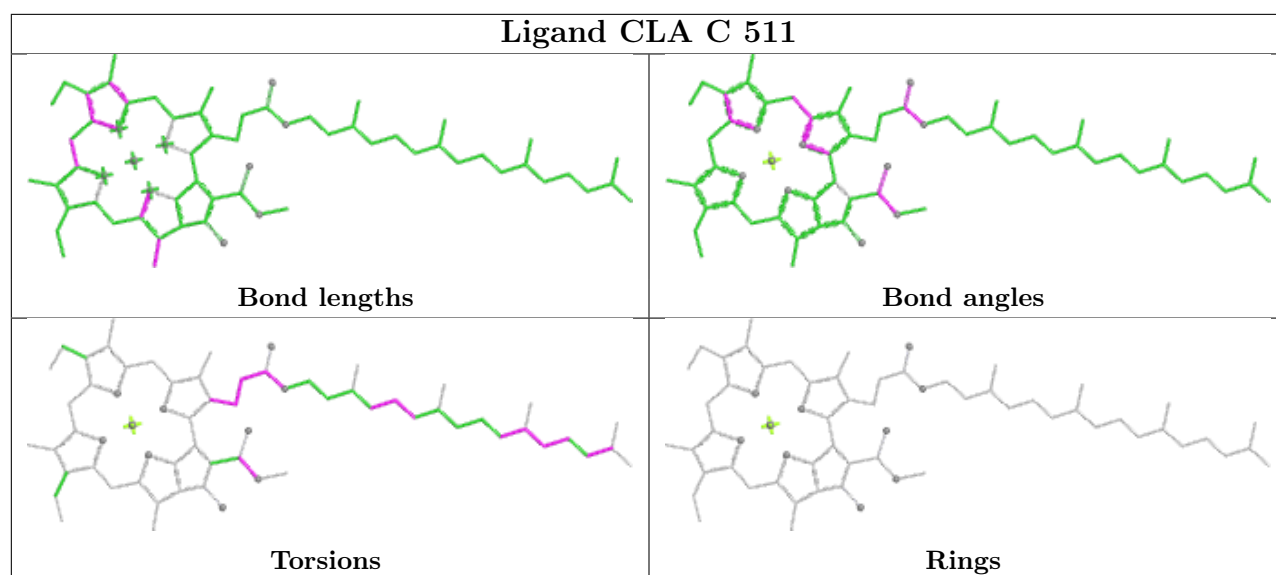


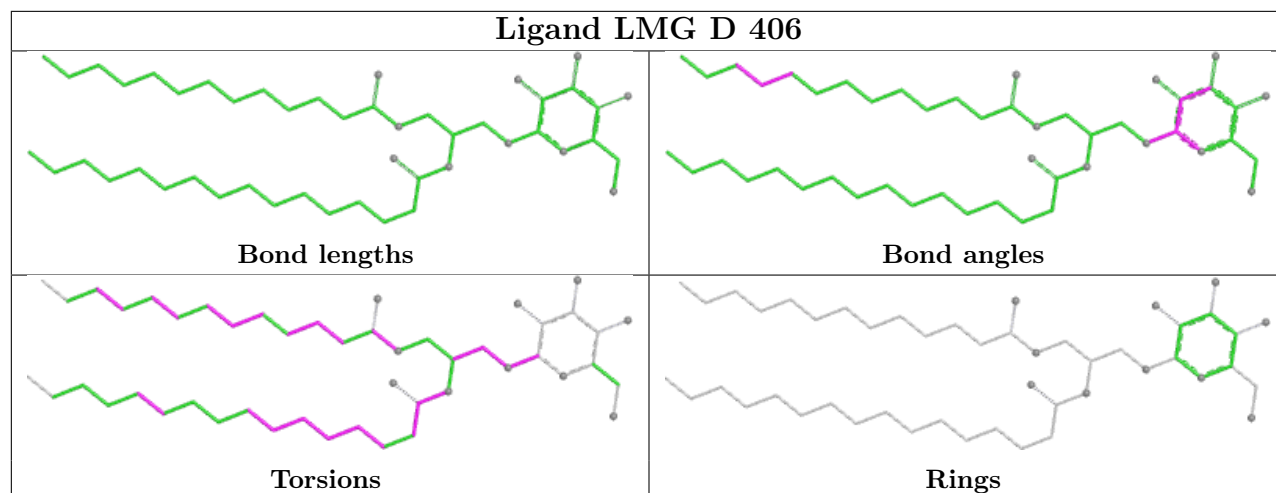
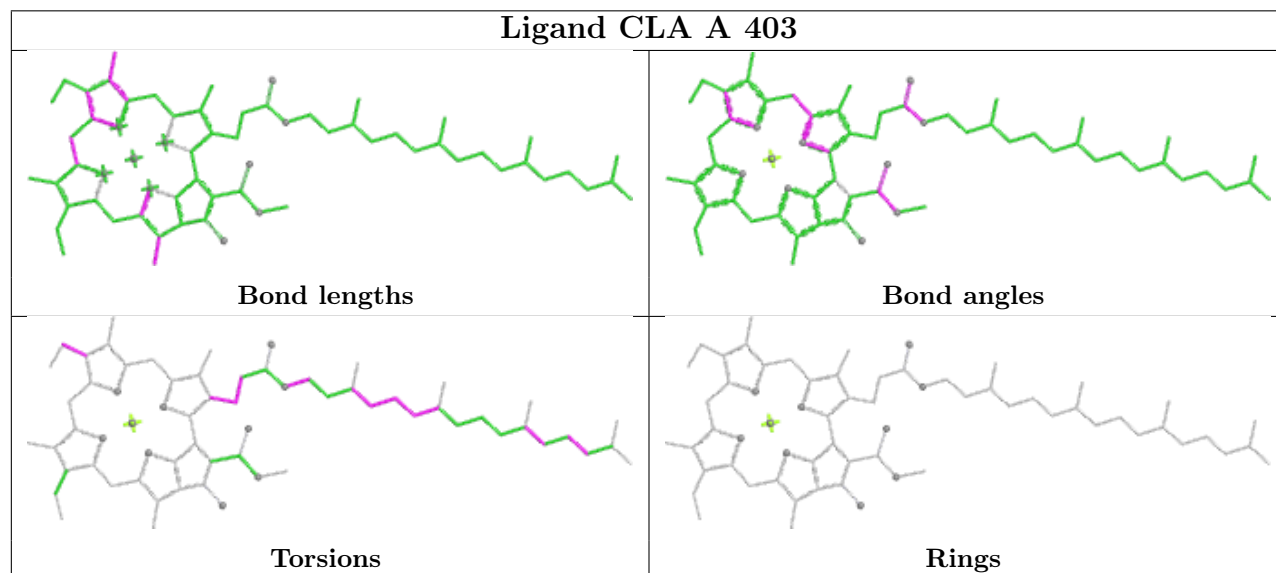
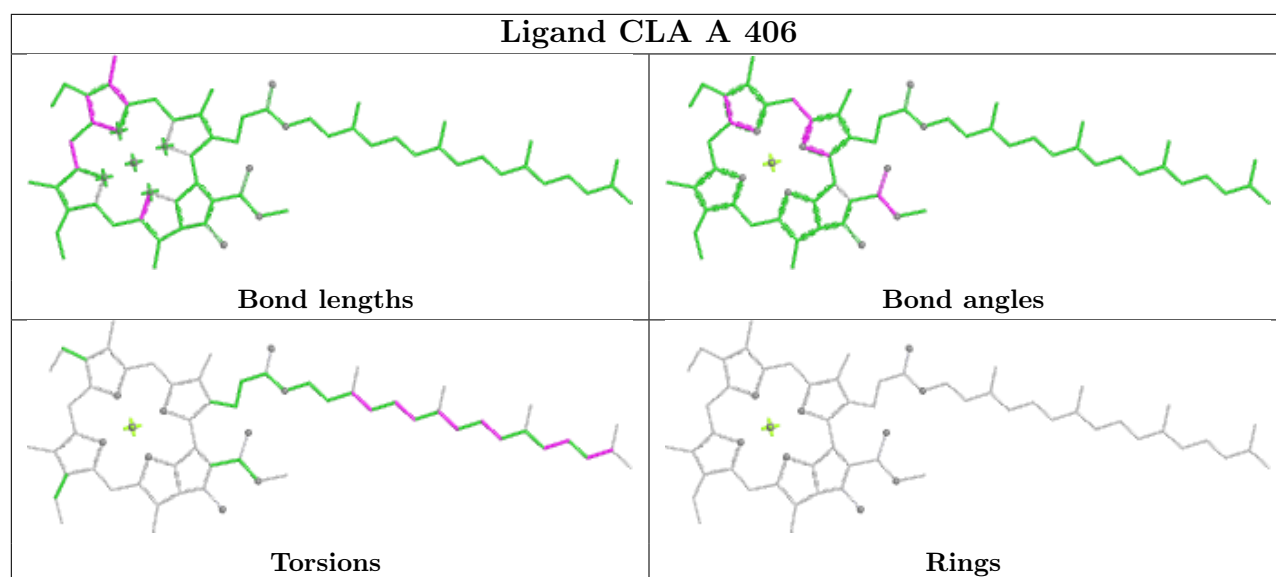


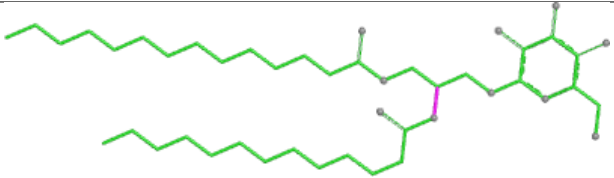
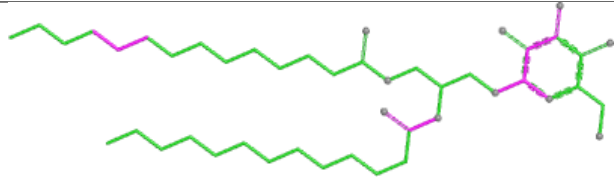
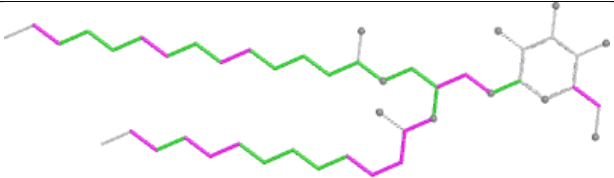
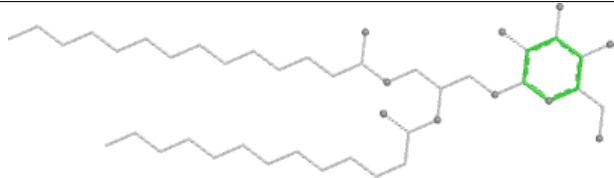
Ligand CLA B 603**Ligand CLA C 504**

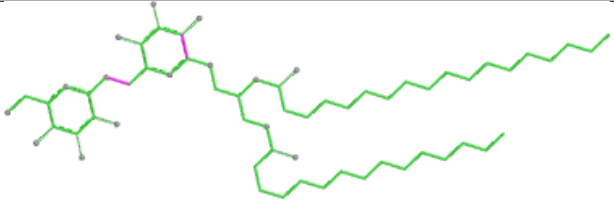
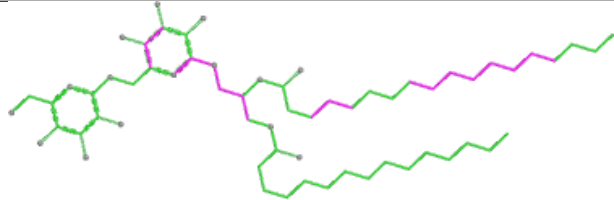
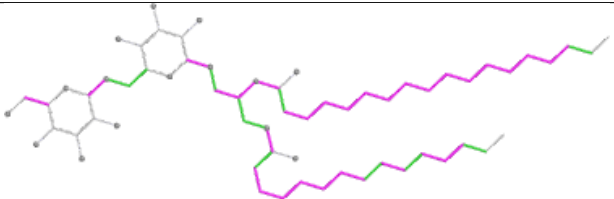
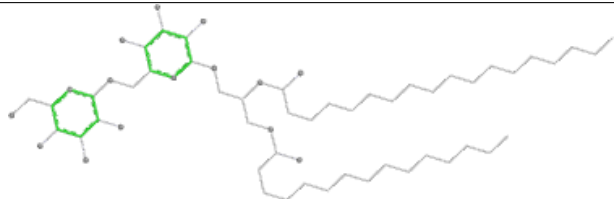


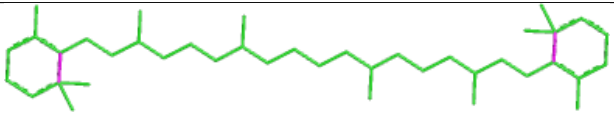
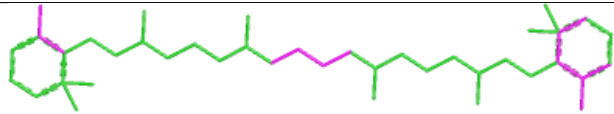
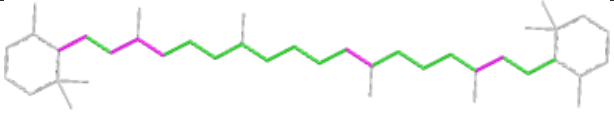
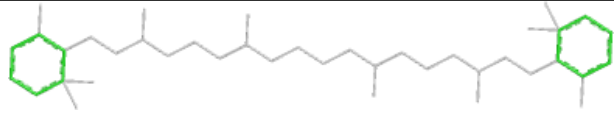


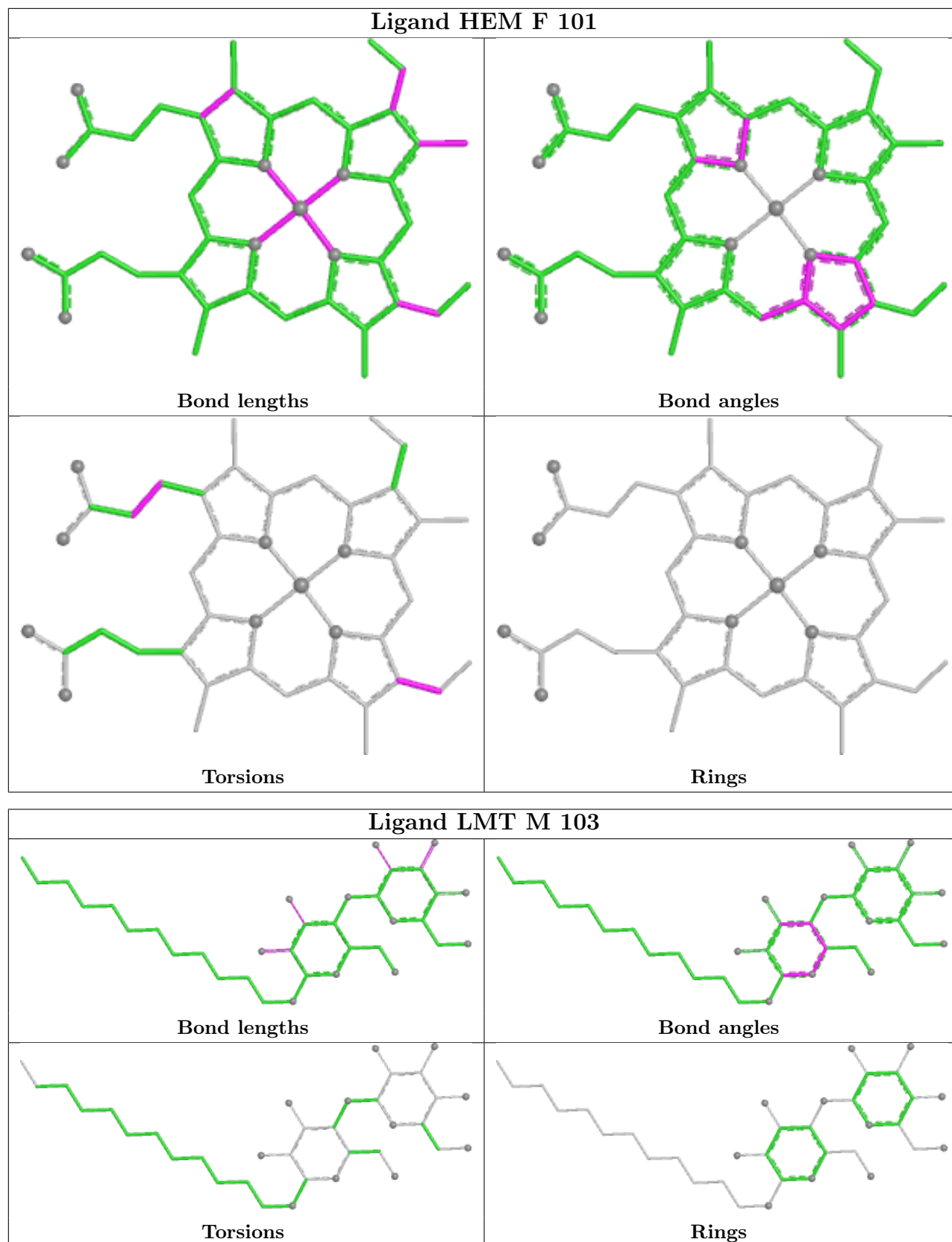


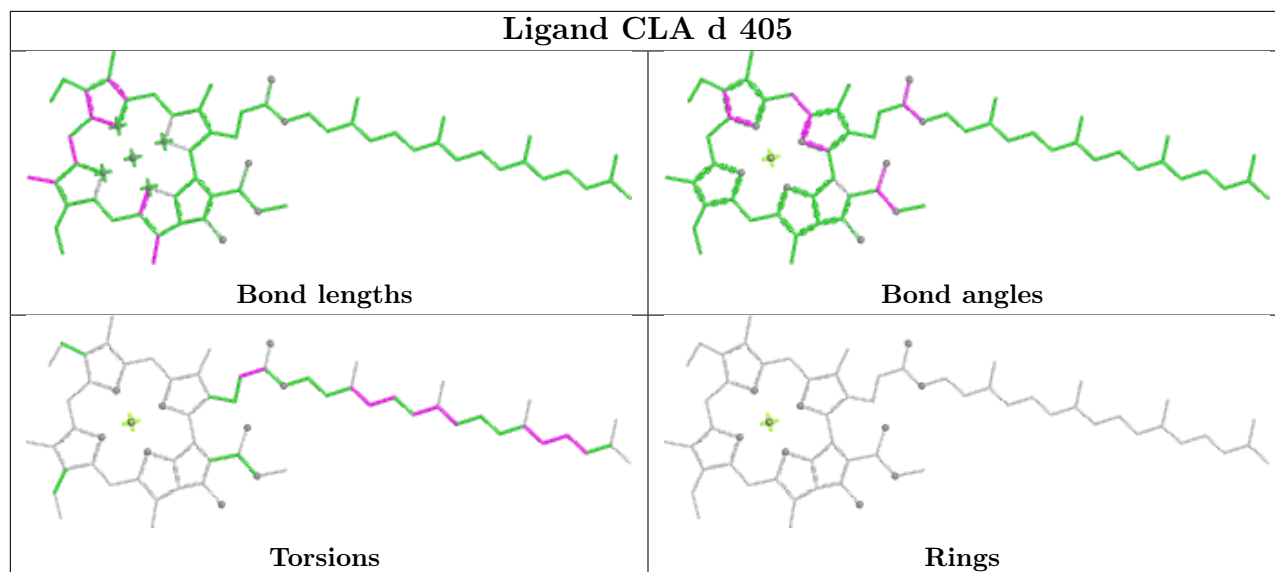
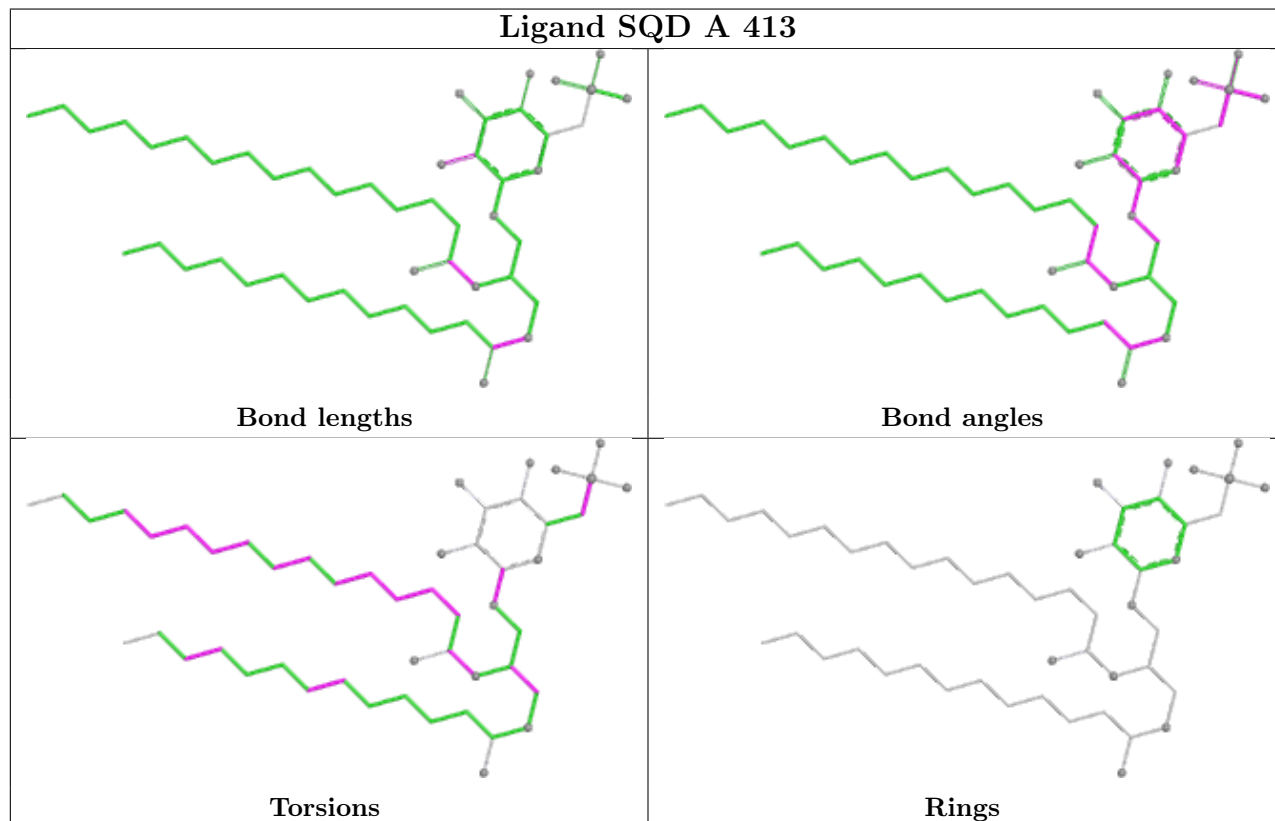


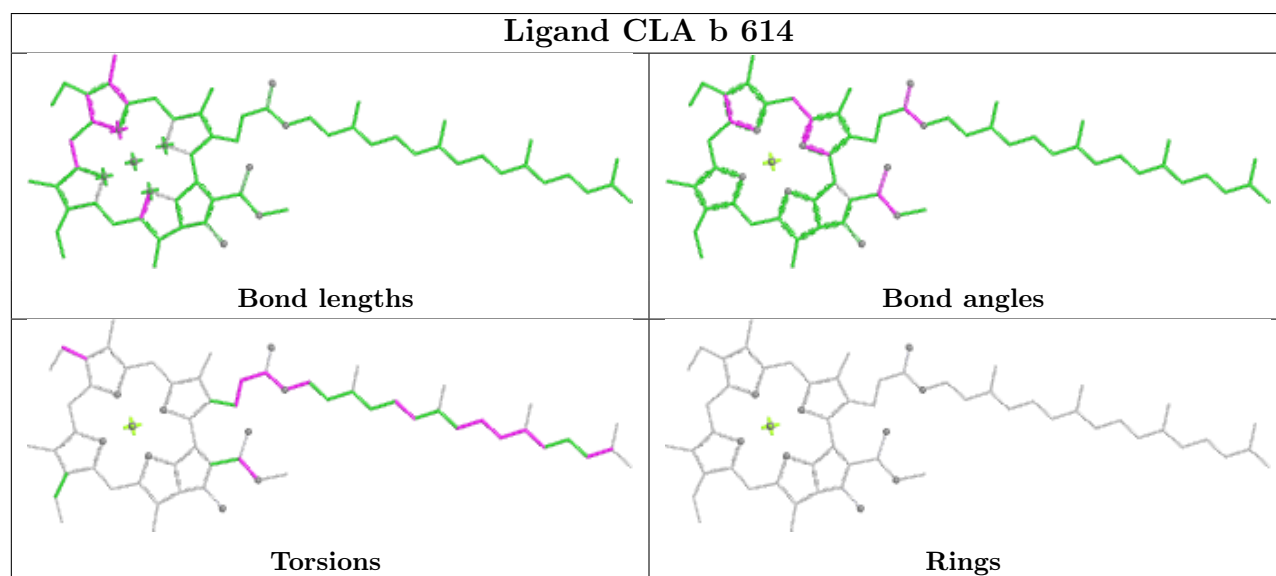
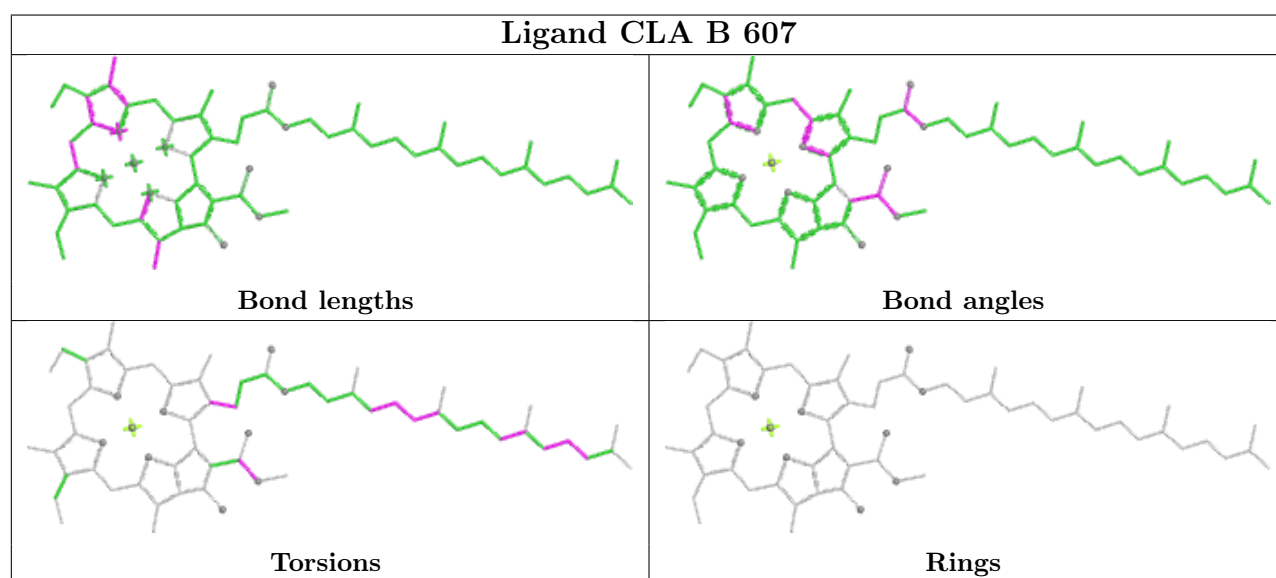
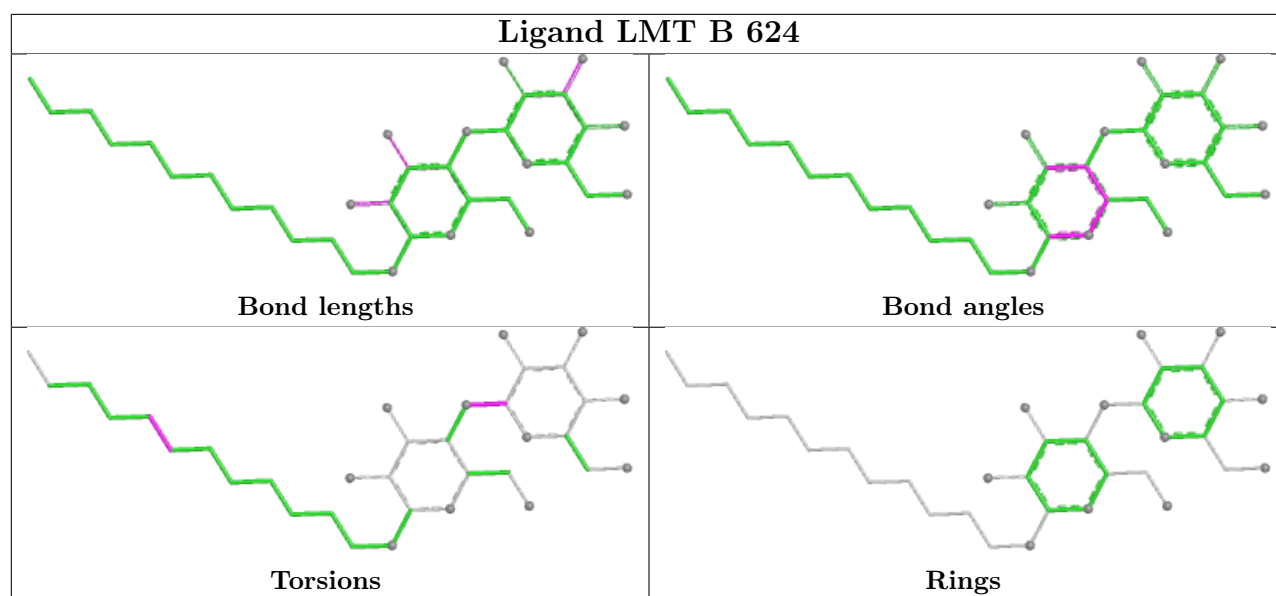
Ligand LMG d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

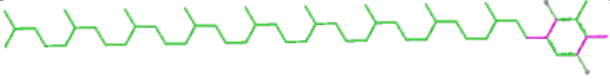
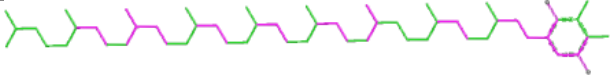
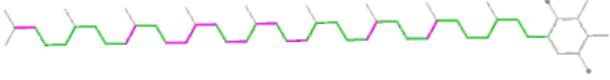
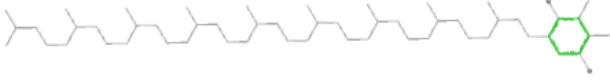
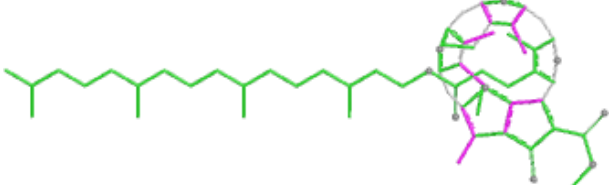
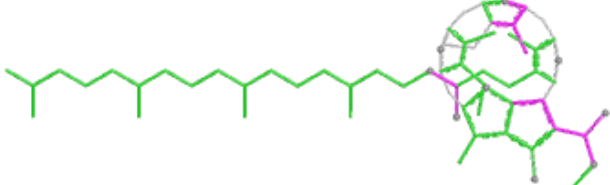
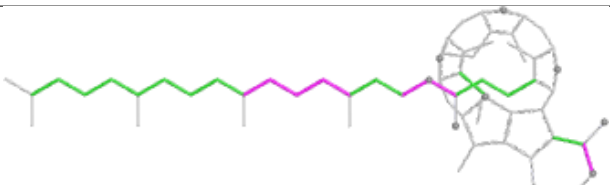
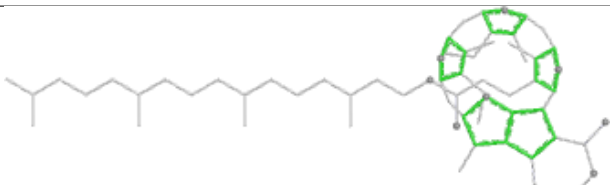
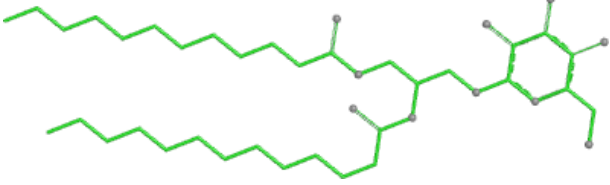
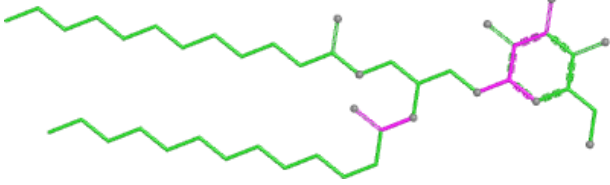
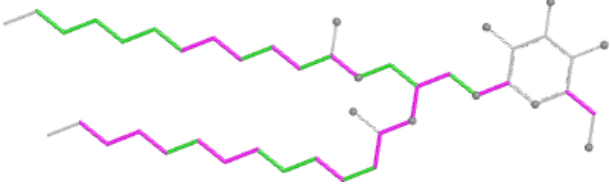
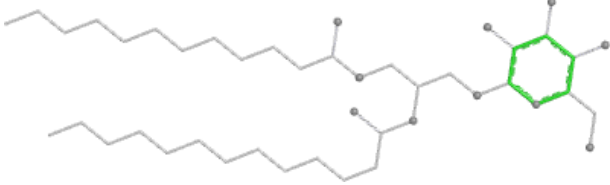
Ligand DGD d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

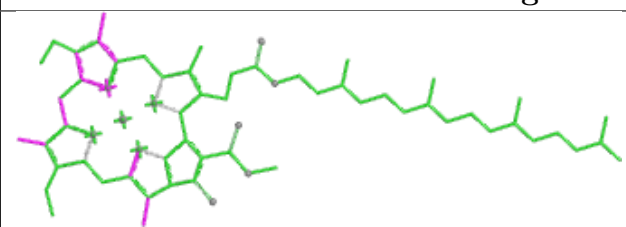
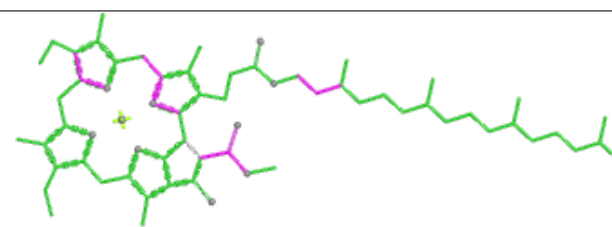
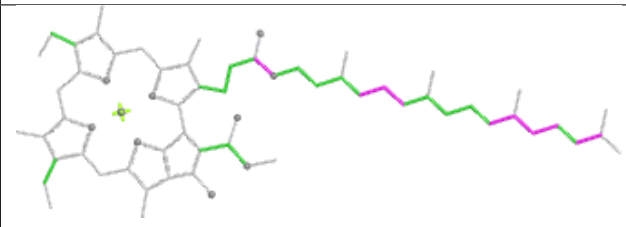
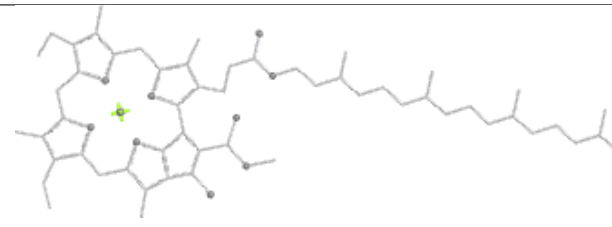
Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

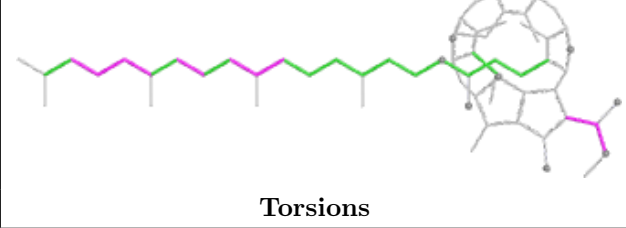
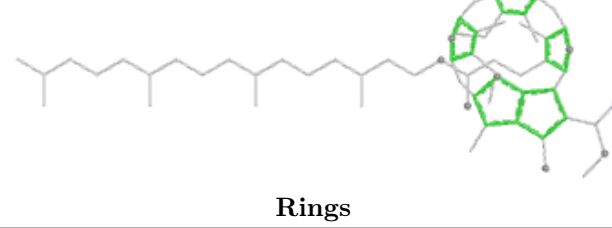


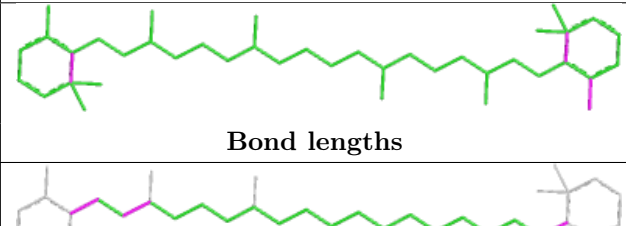
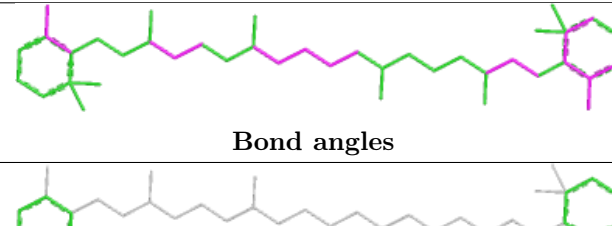
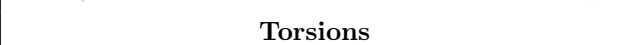
Ligand CLA d 405**Ligand SQD A 413**

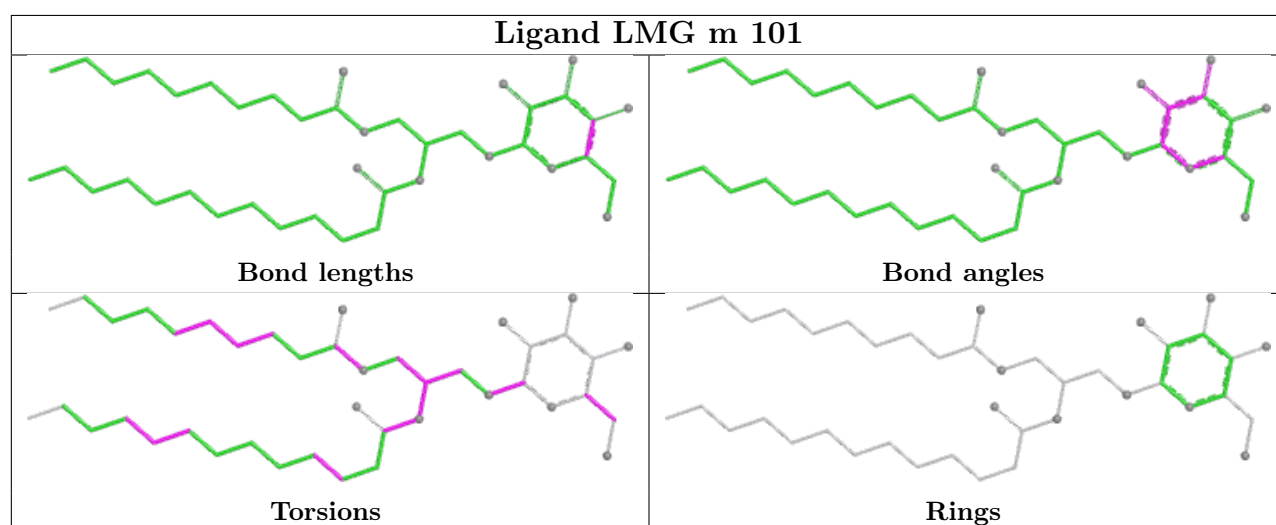
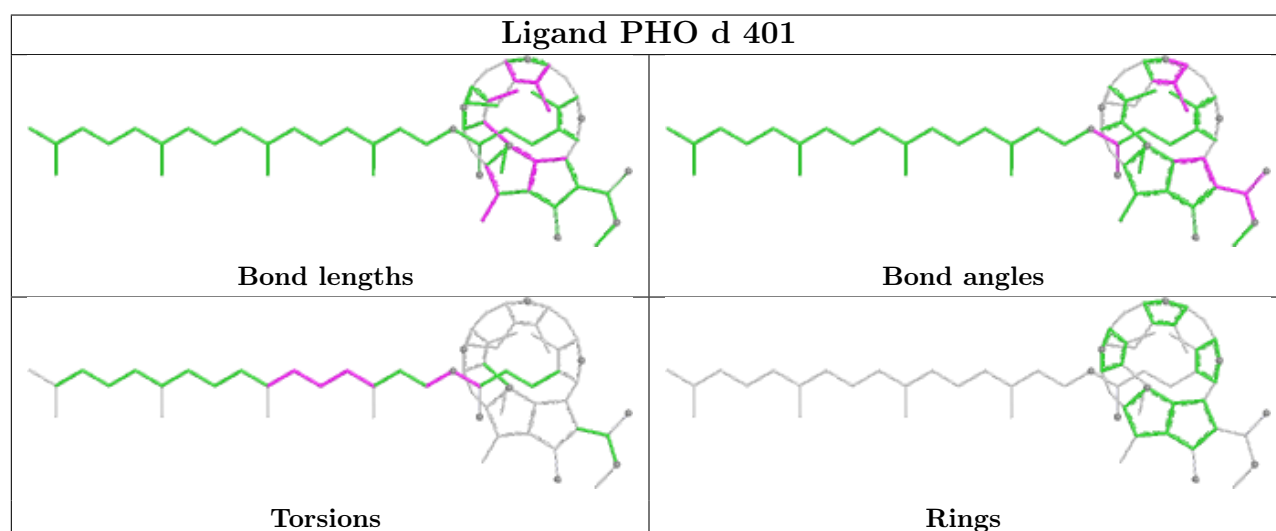
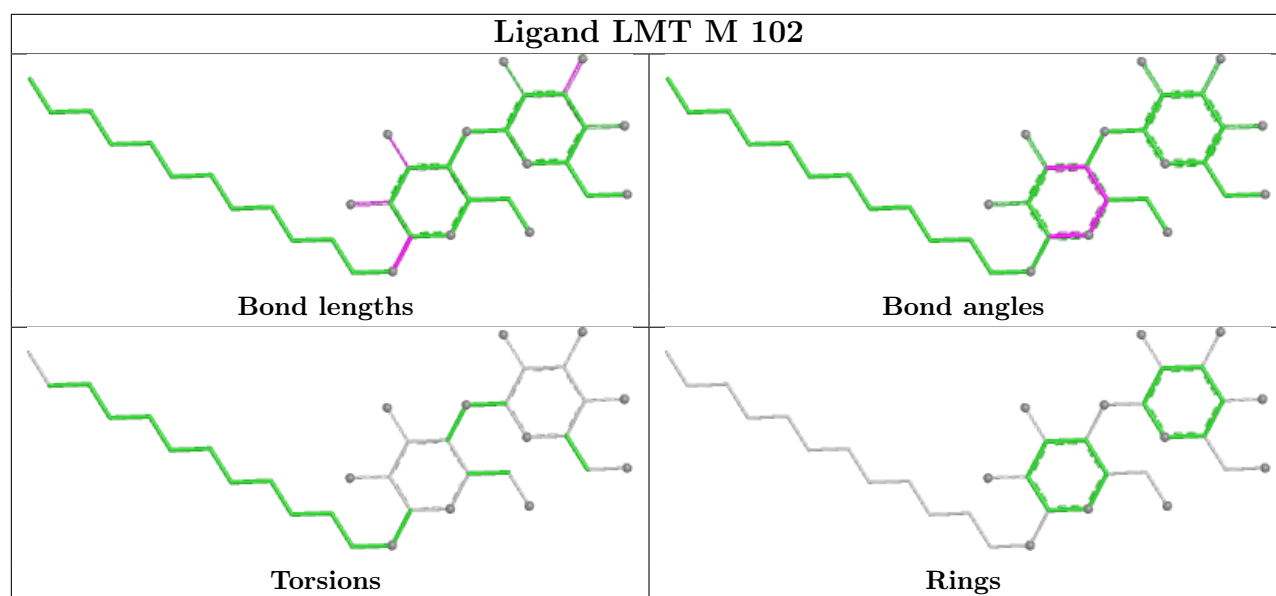


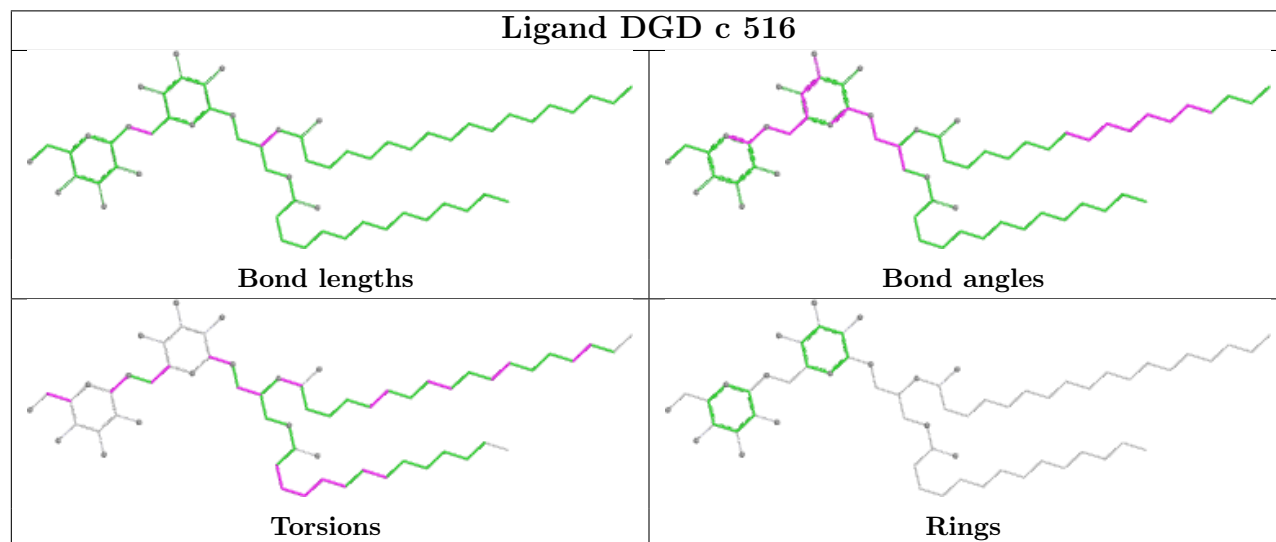
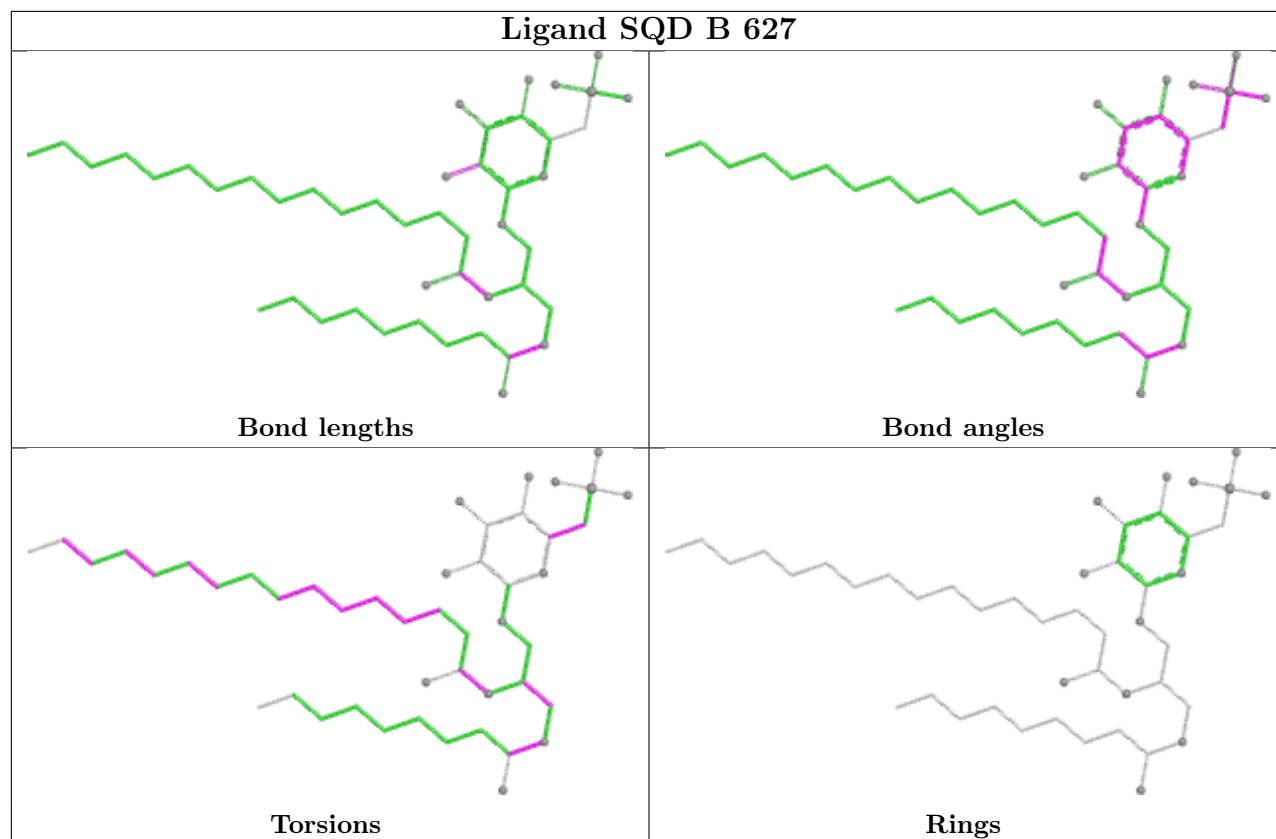
Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

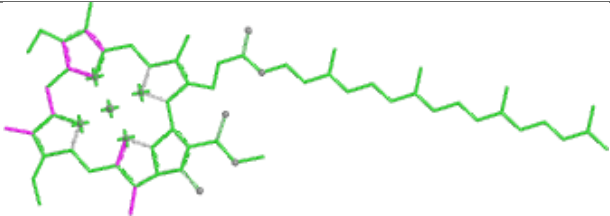
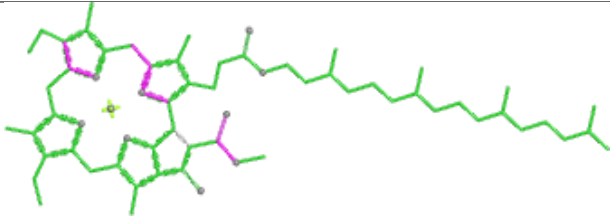
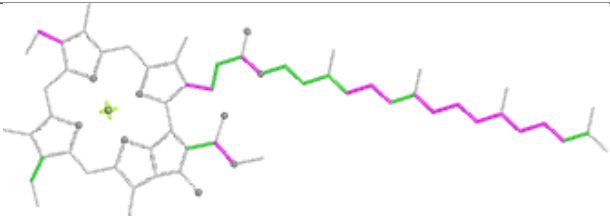
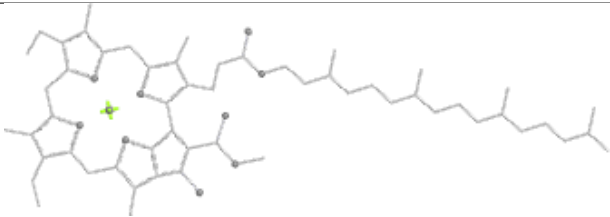
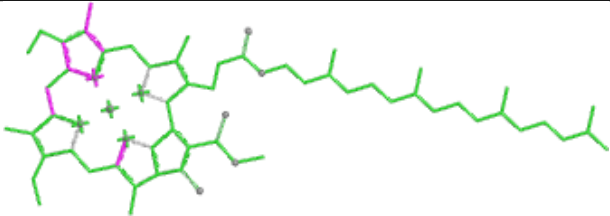
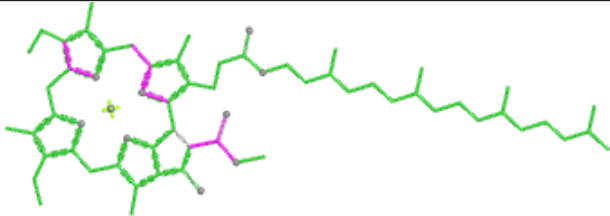
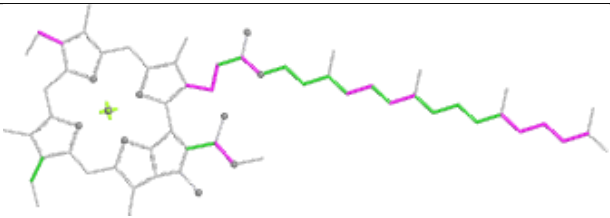
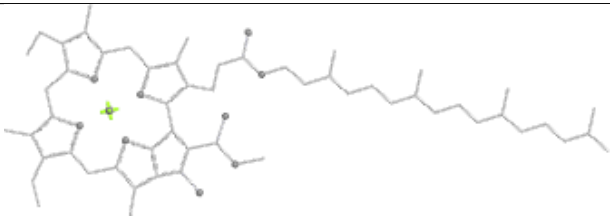
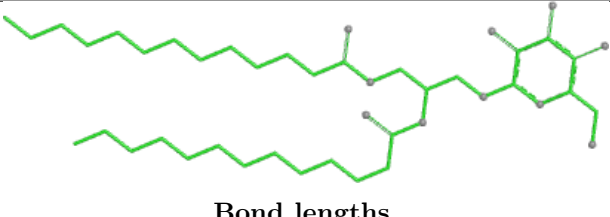
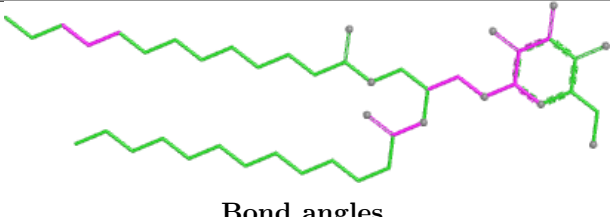
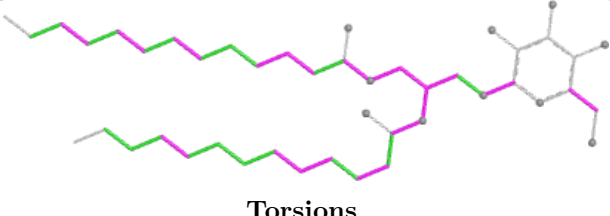
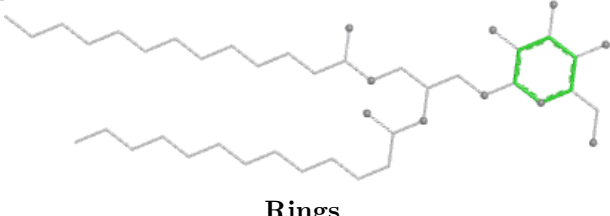
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

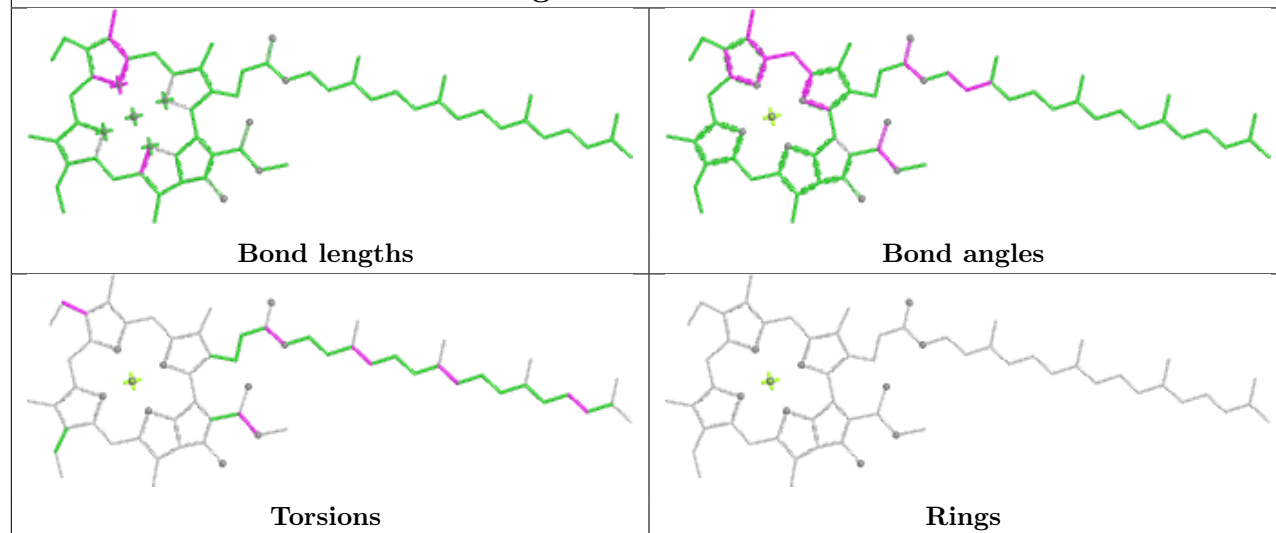
Ligand BCR C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings



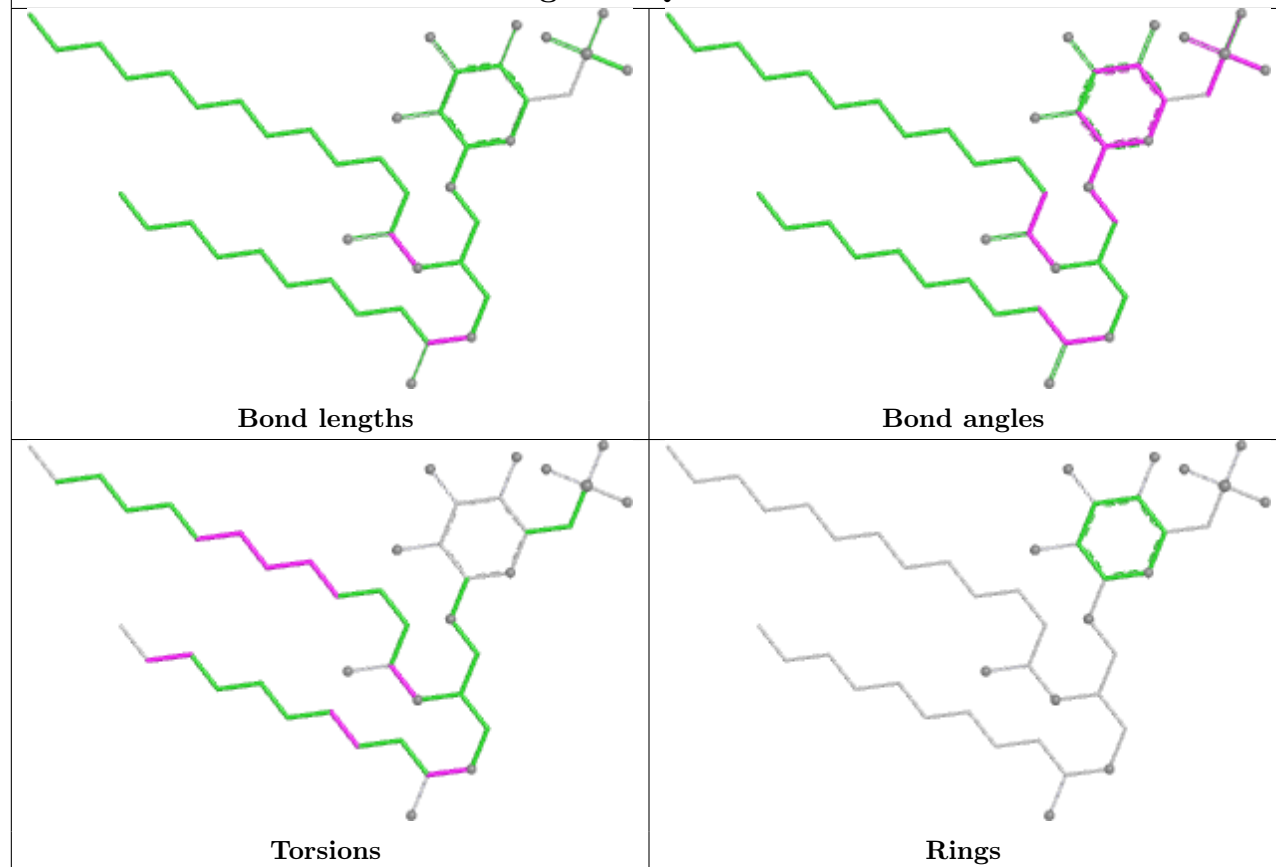


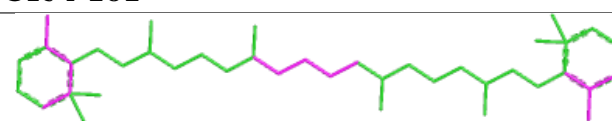
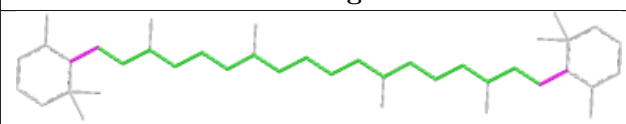
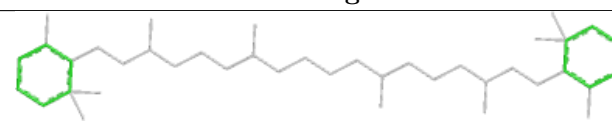
Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

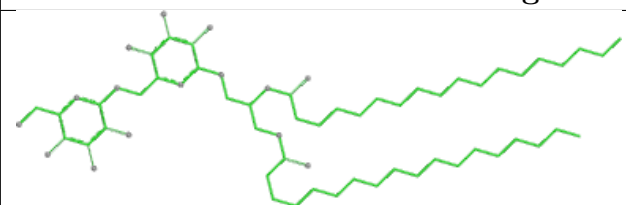
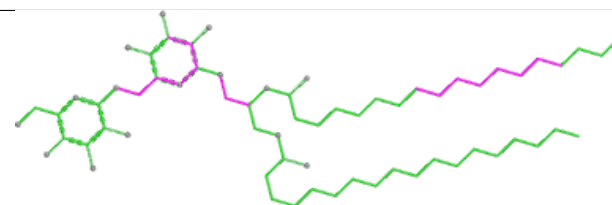
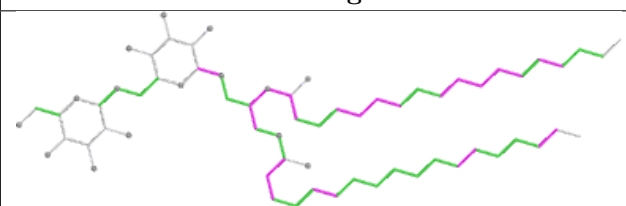
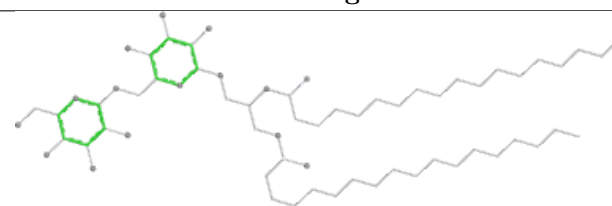
Ligand CLA B 610

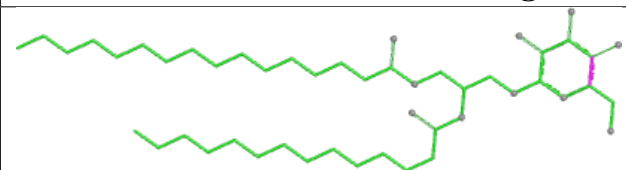
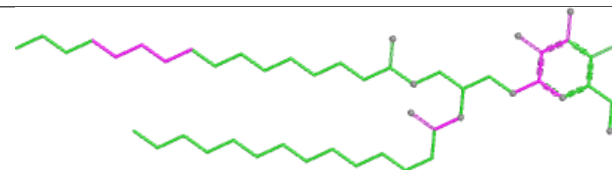
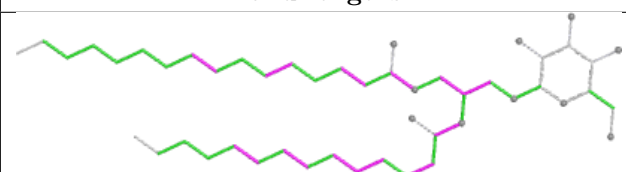
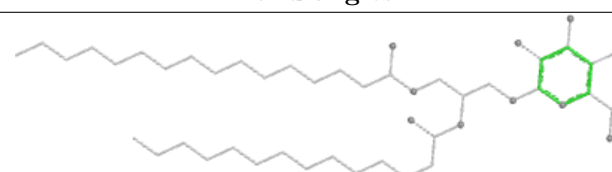


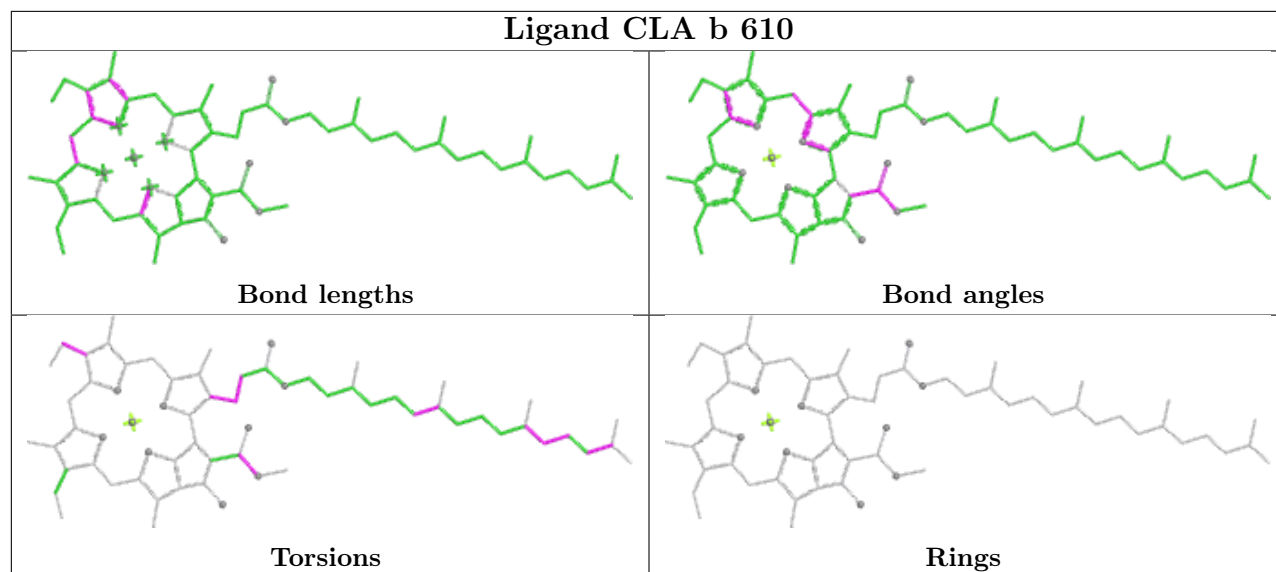
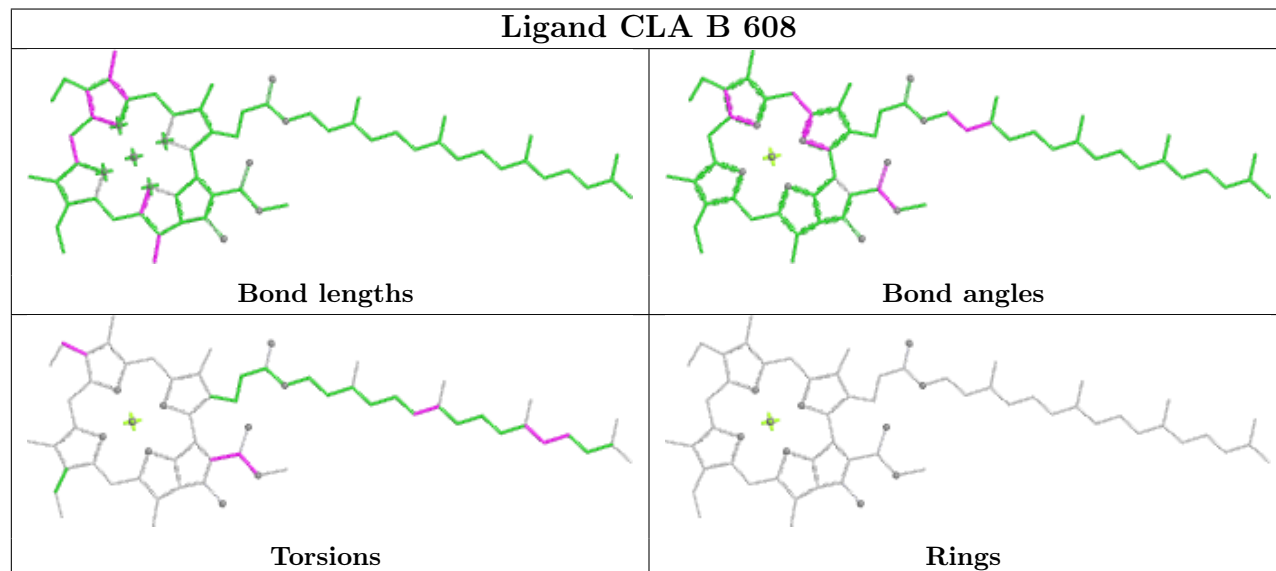
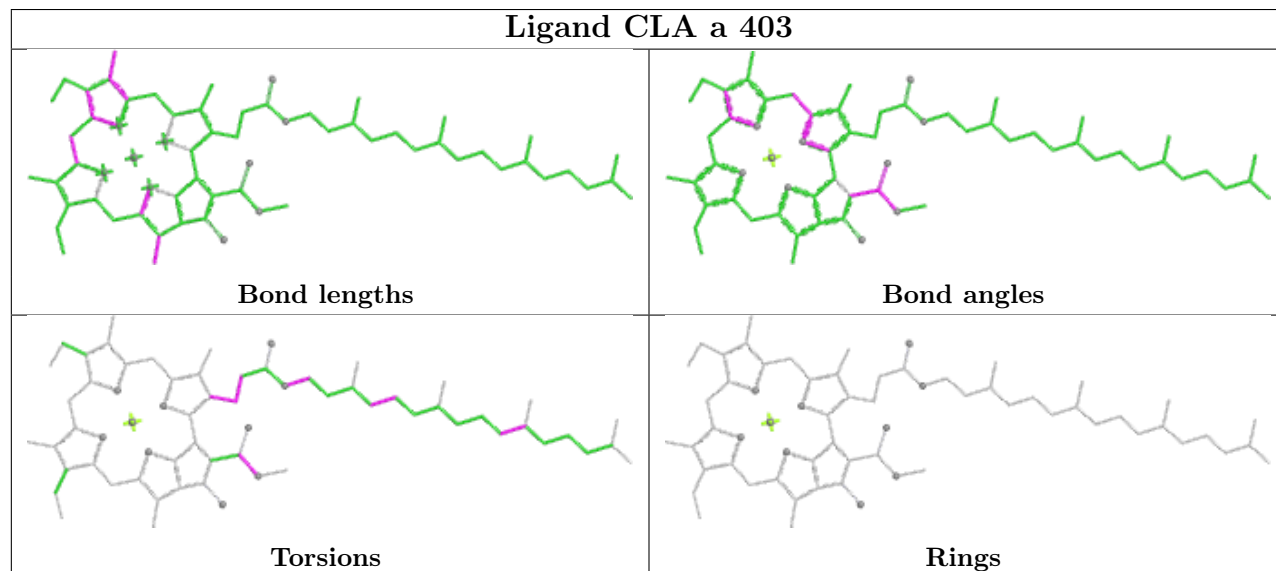
Ligand SQD f 103

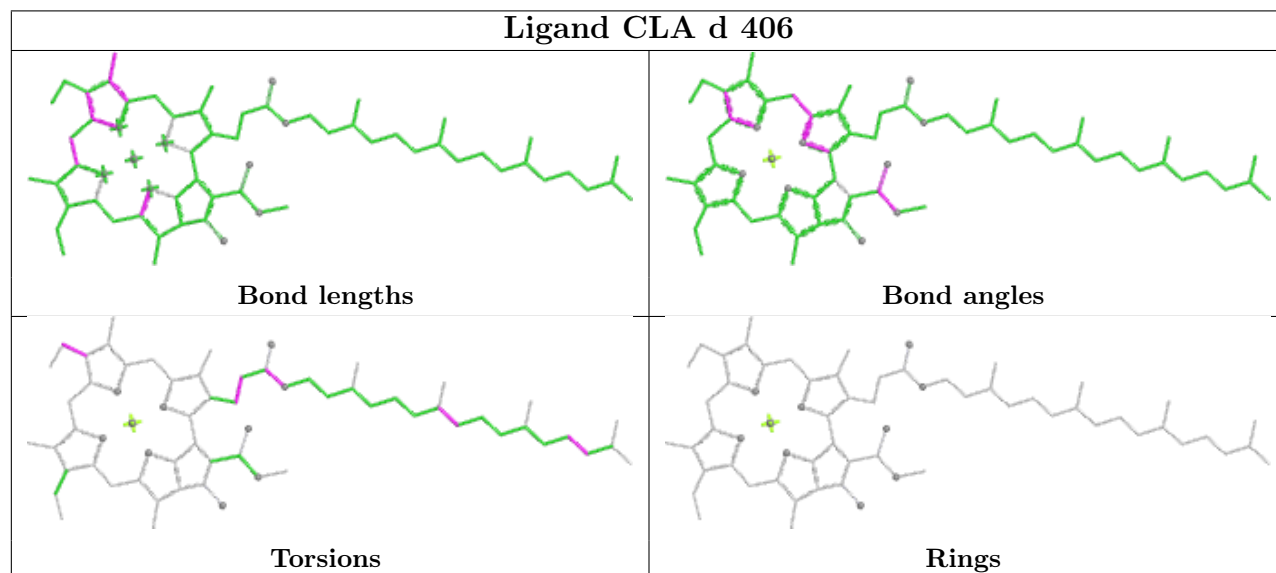
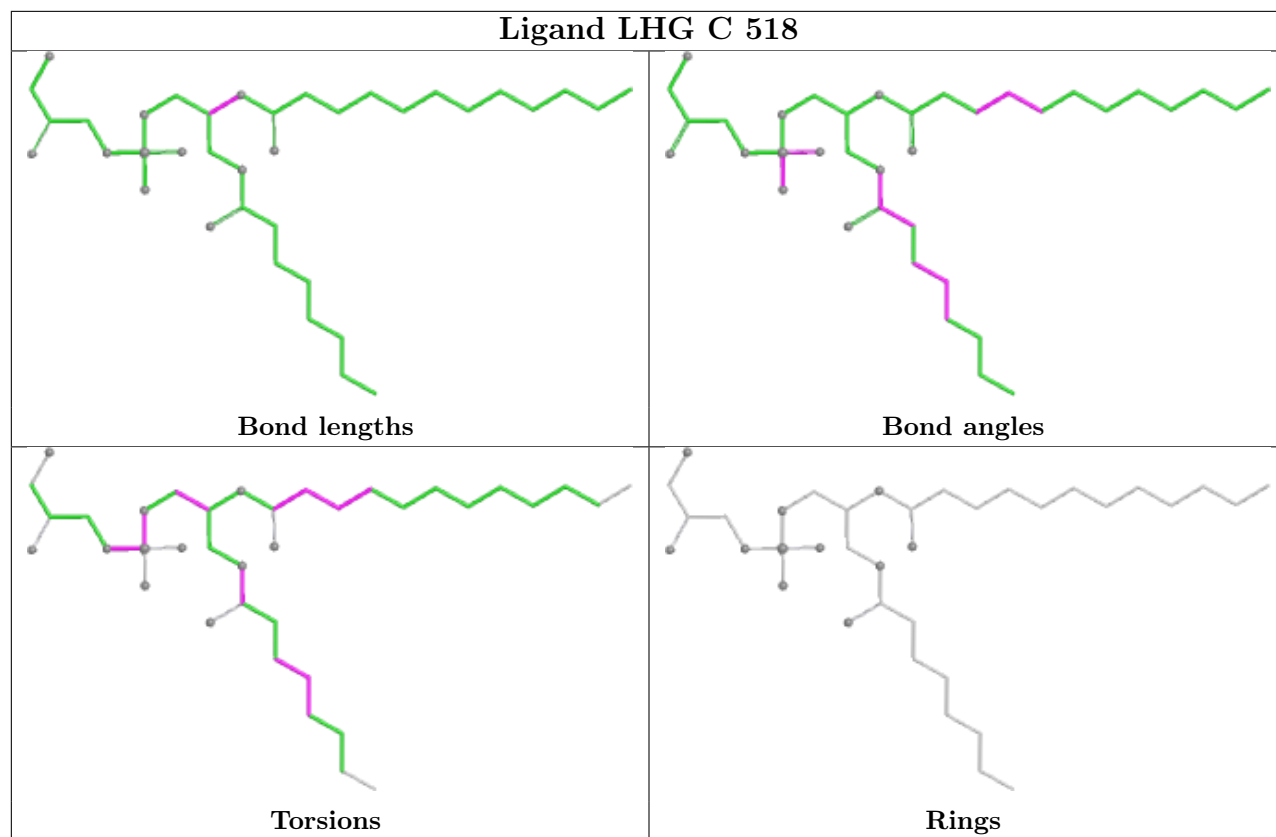


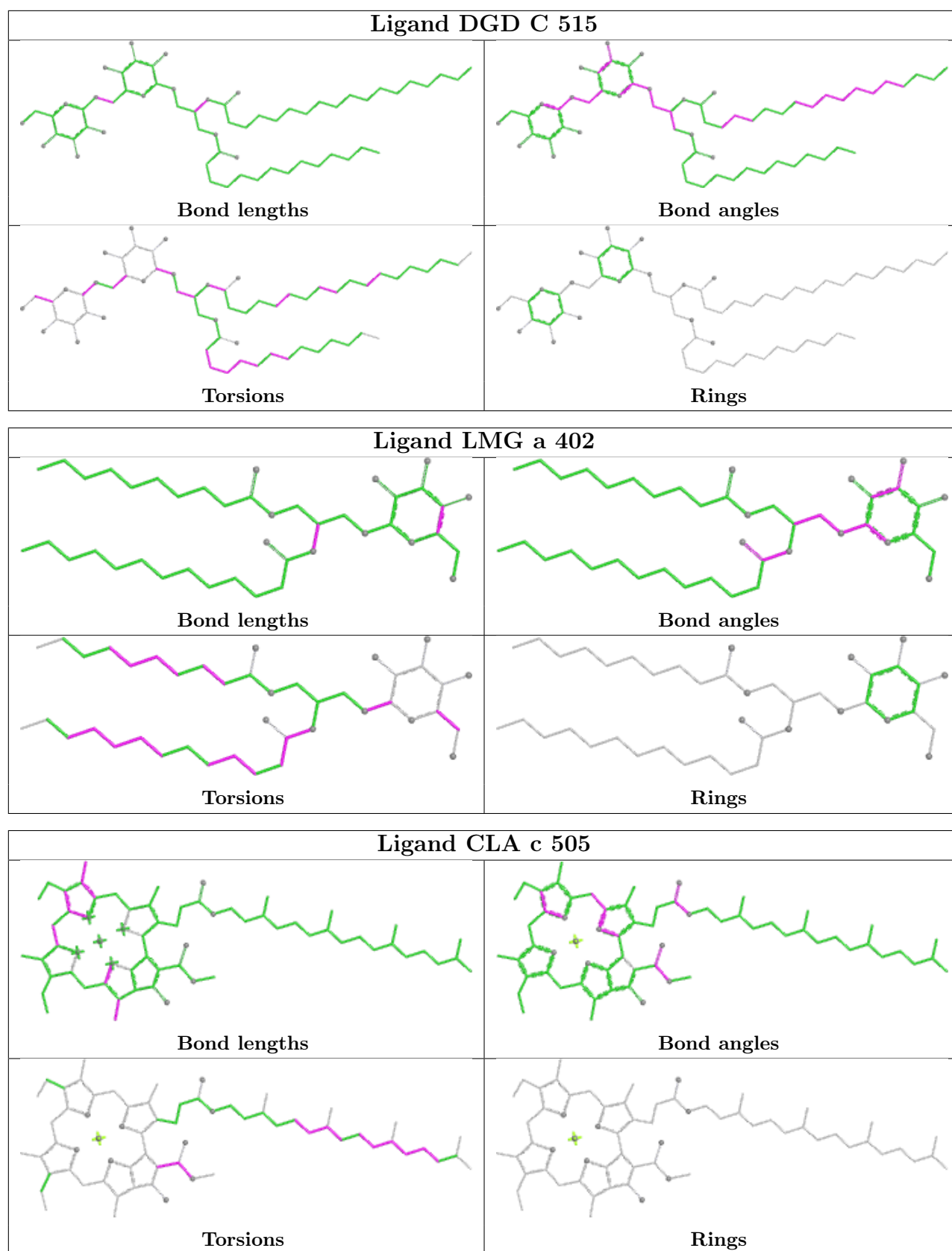
Ligand BCR i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

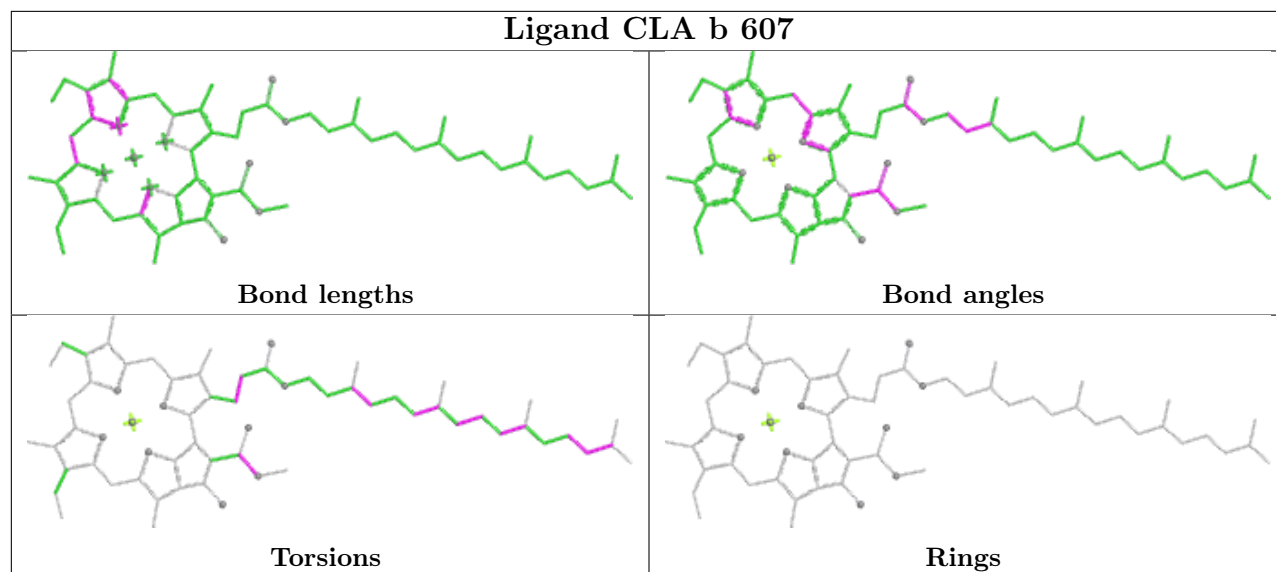
Ligand LMG b 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 610**Ligand CLA B 608****Ligand CLA a 403**

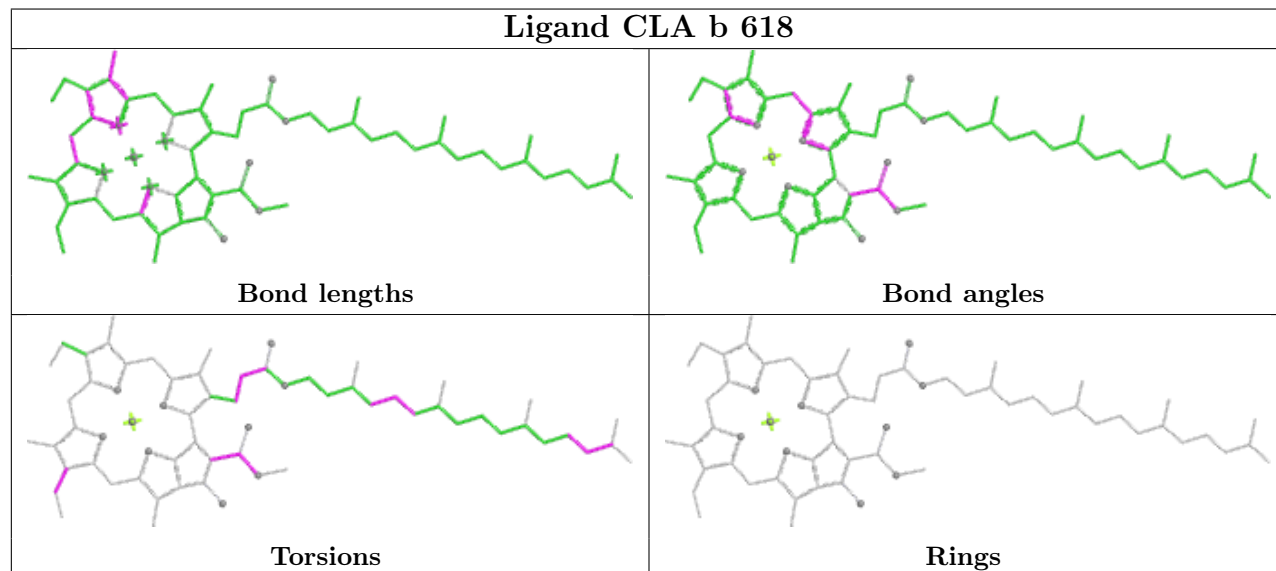




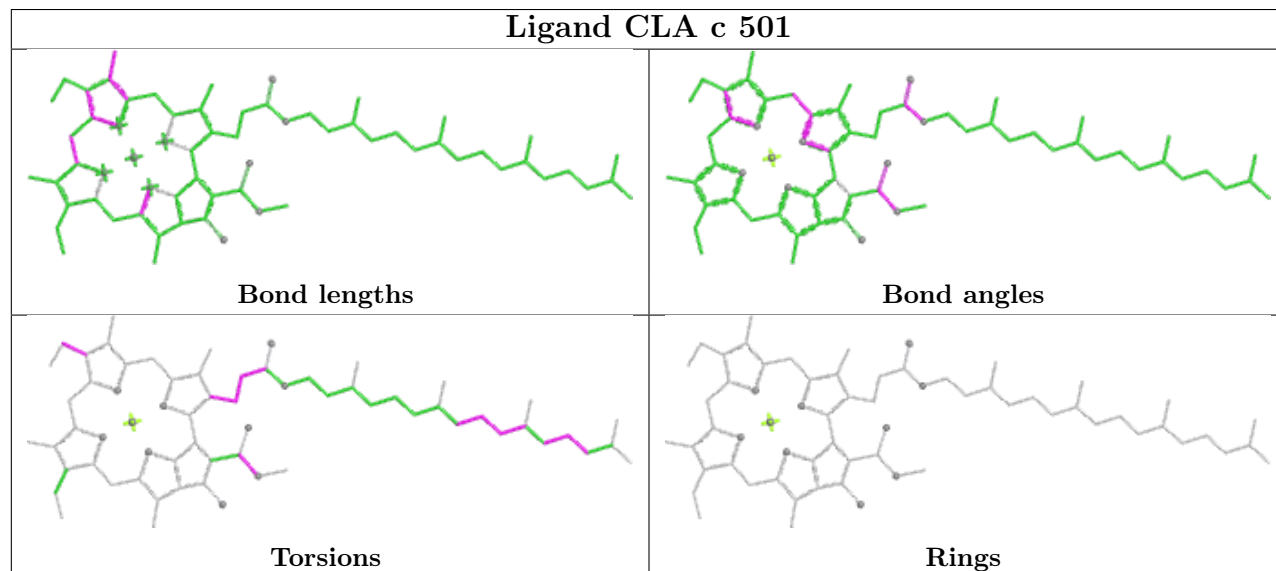
Ligand CLA b 607

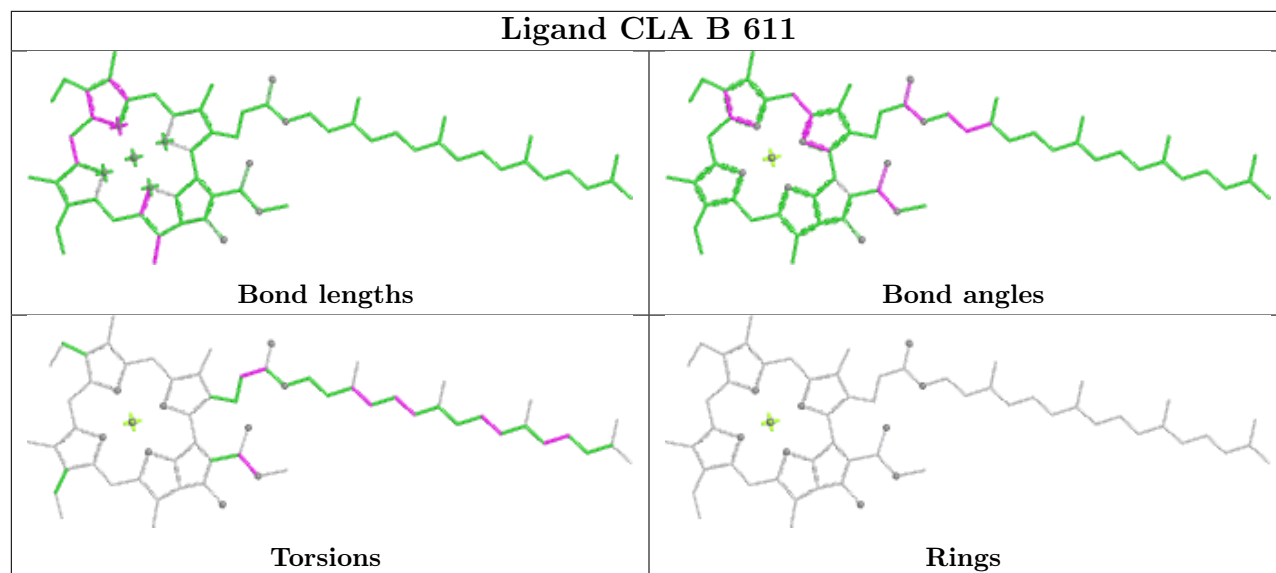
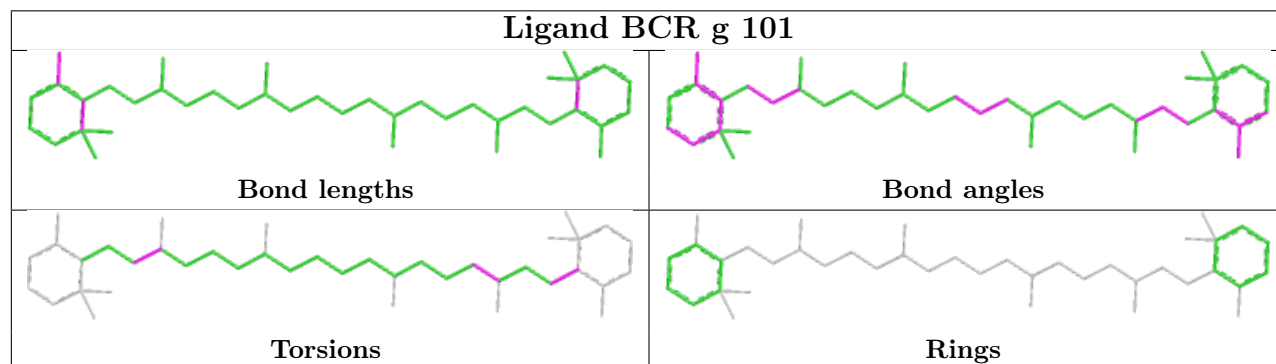
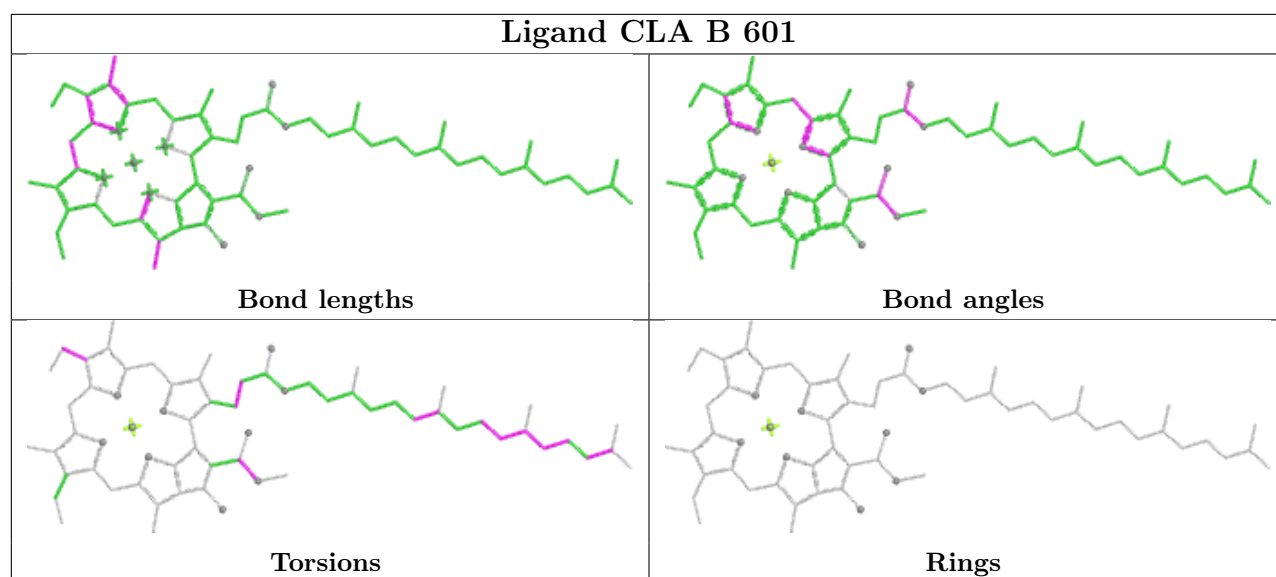


Ligand CLA b 618

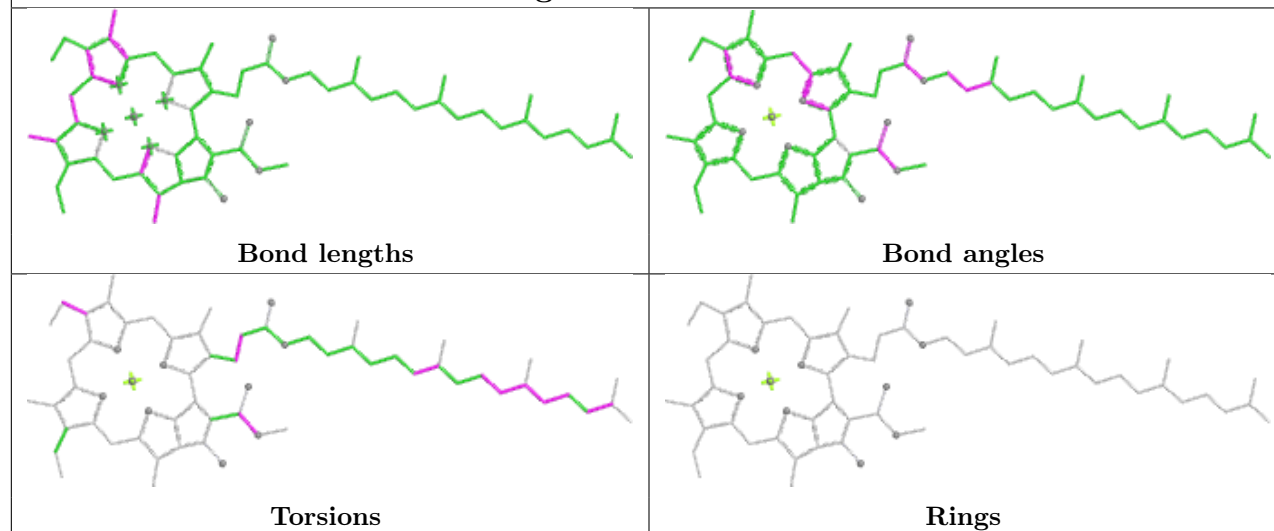


Ligand CLA c 501

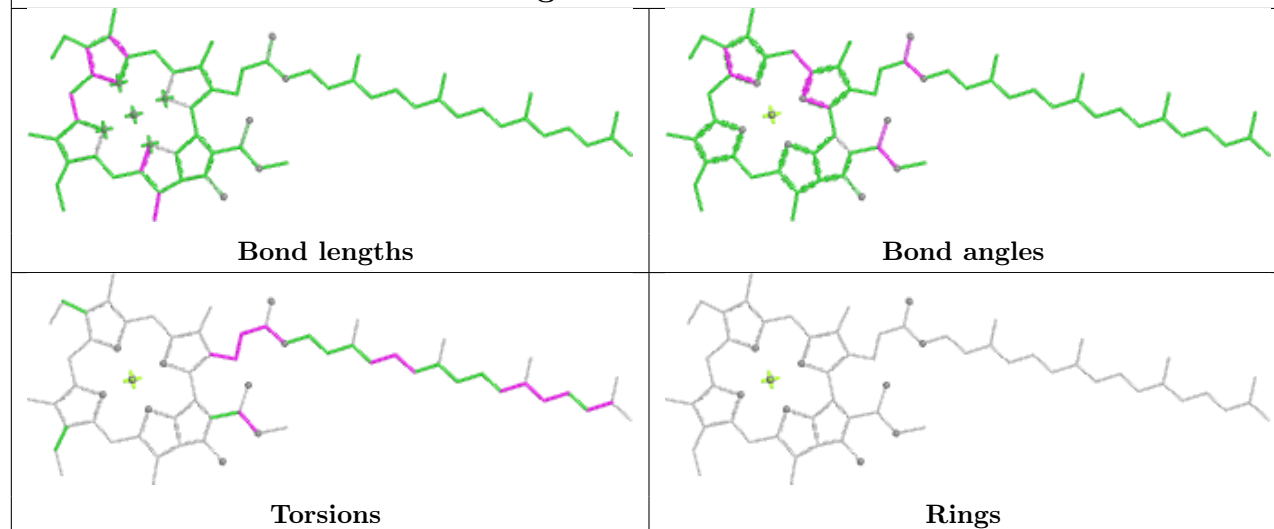




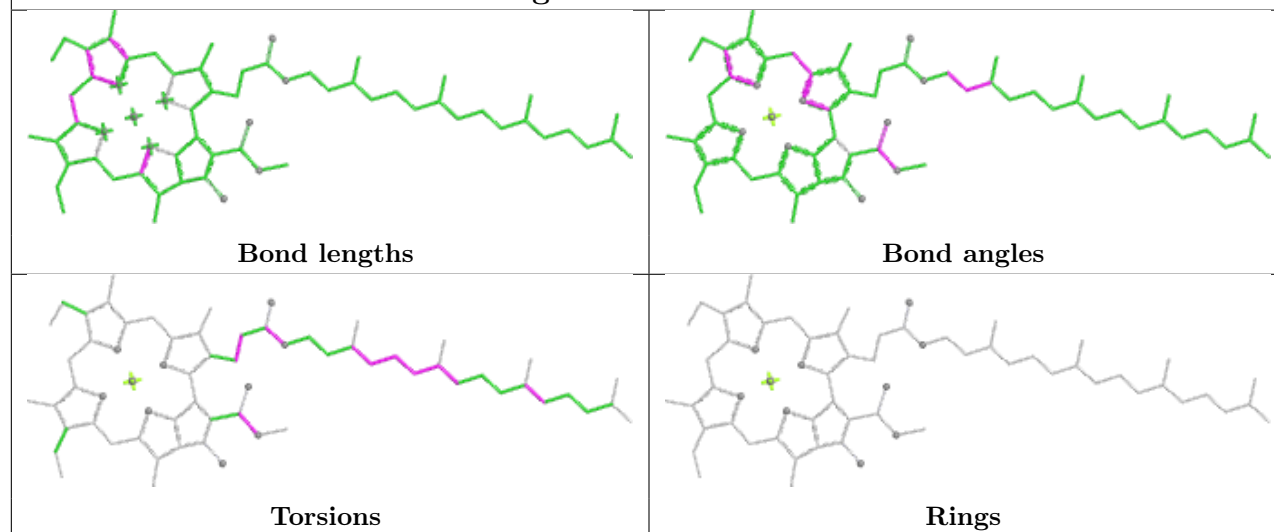
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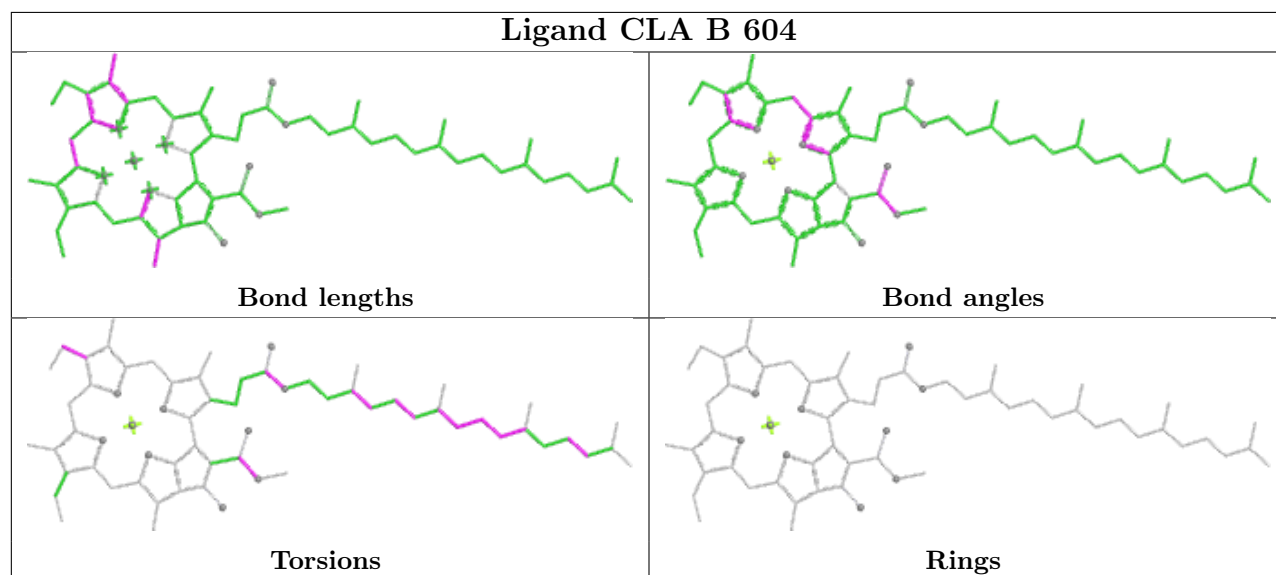
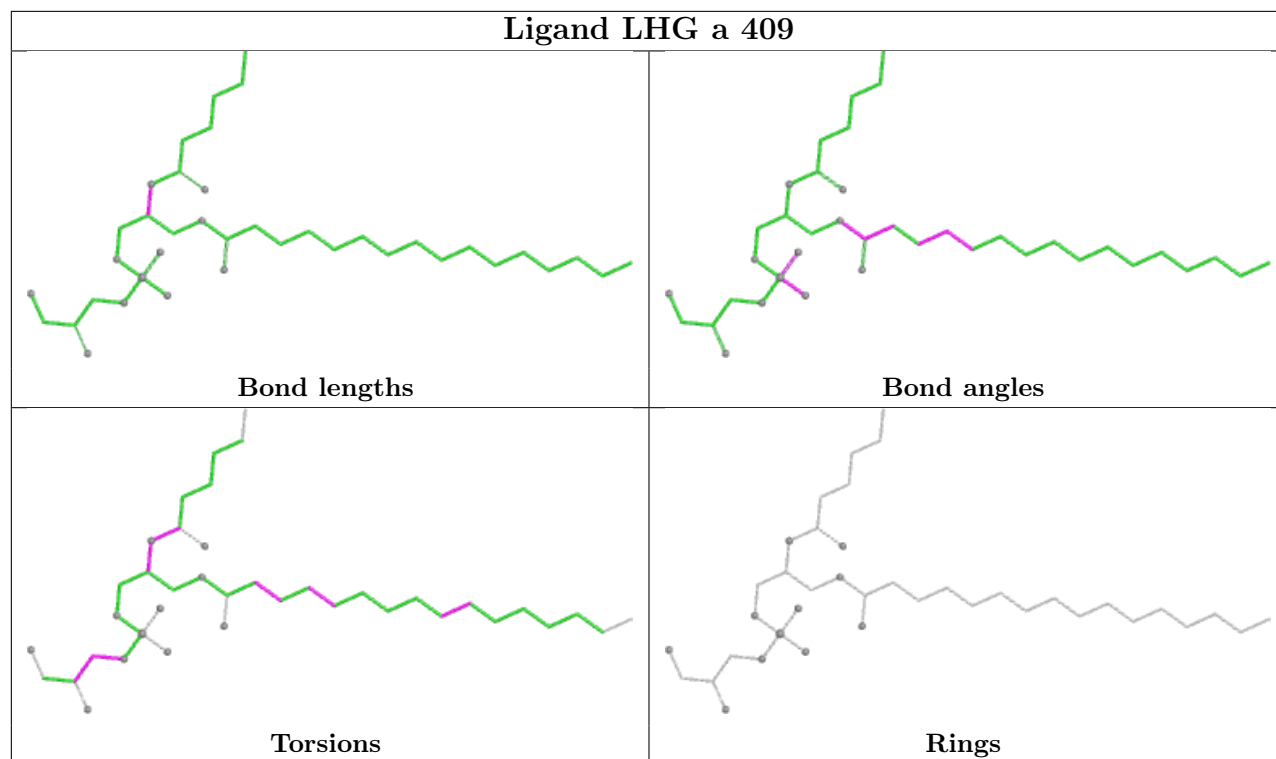


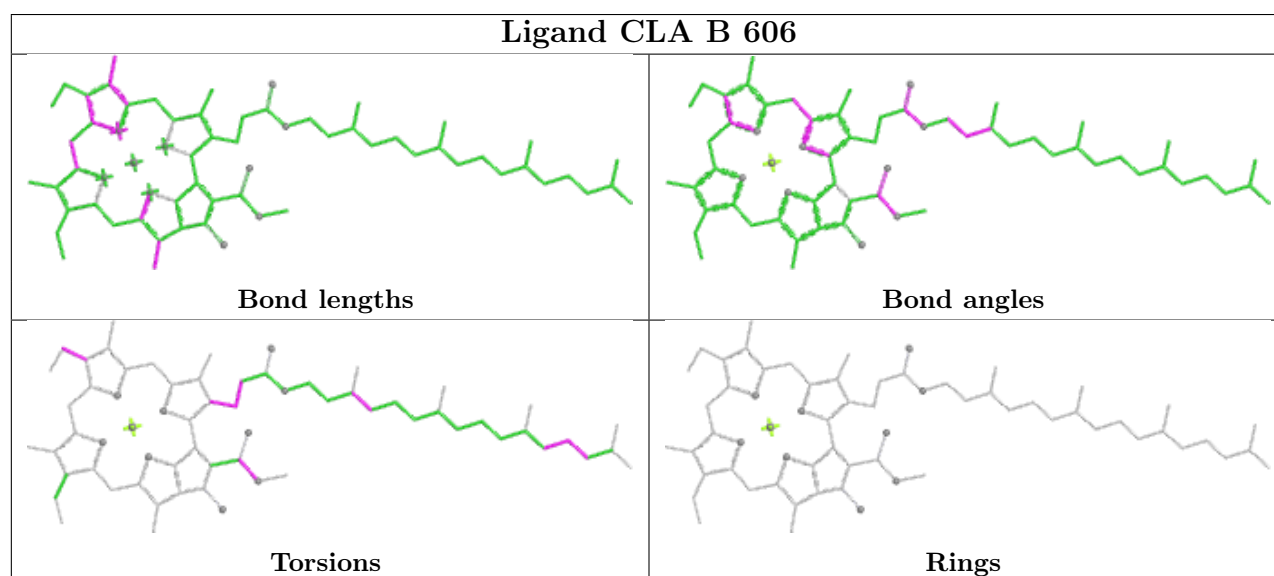
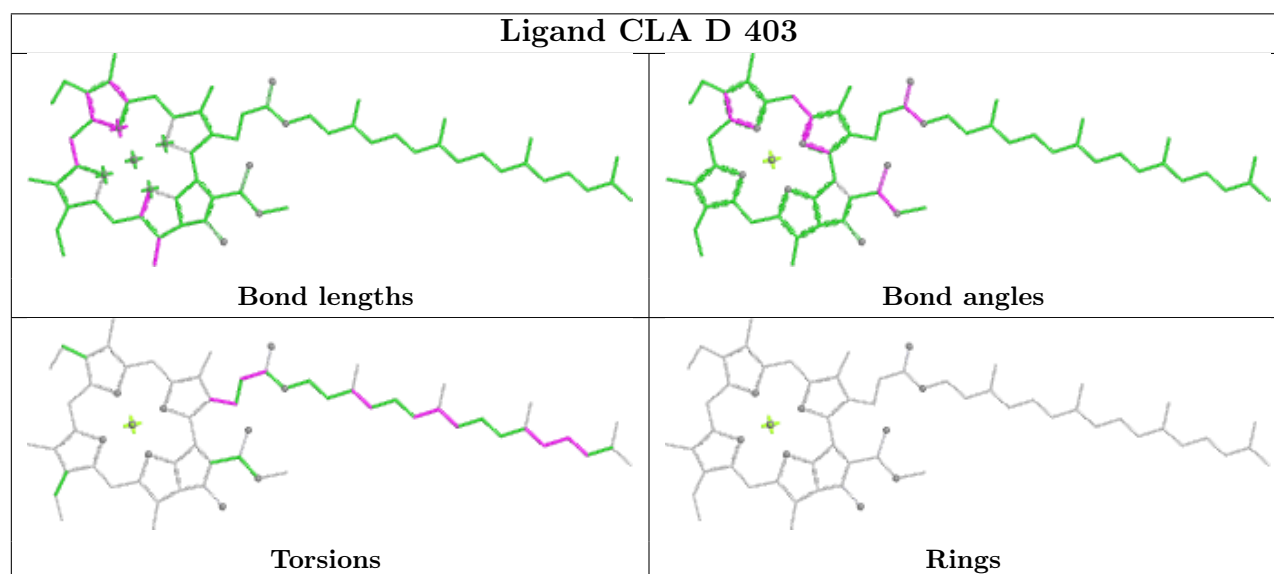
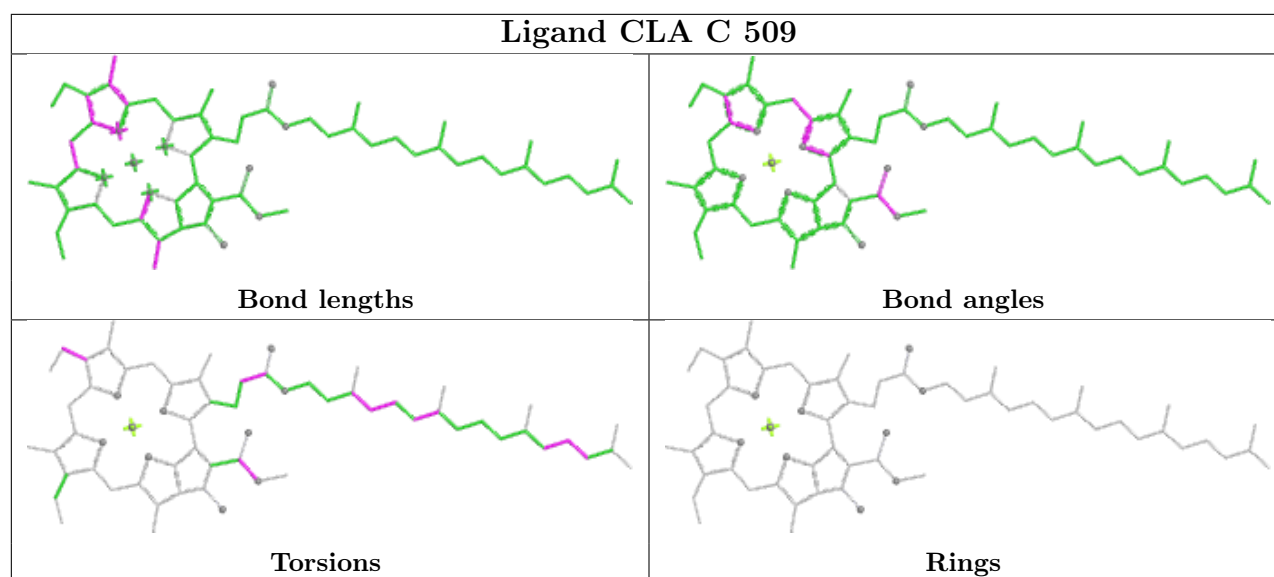
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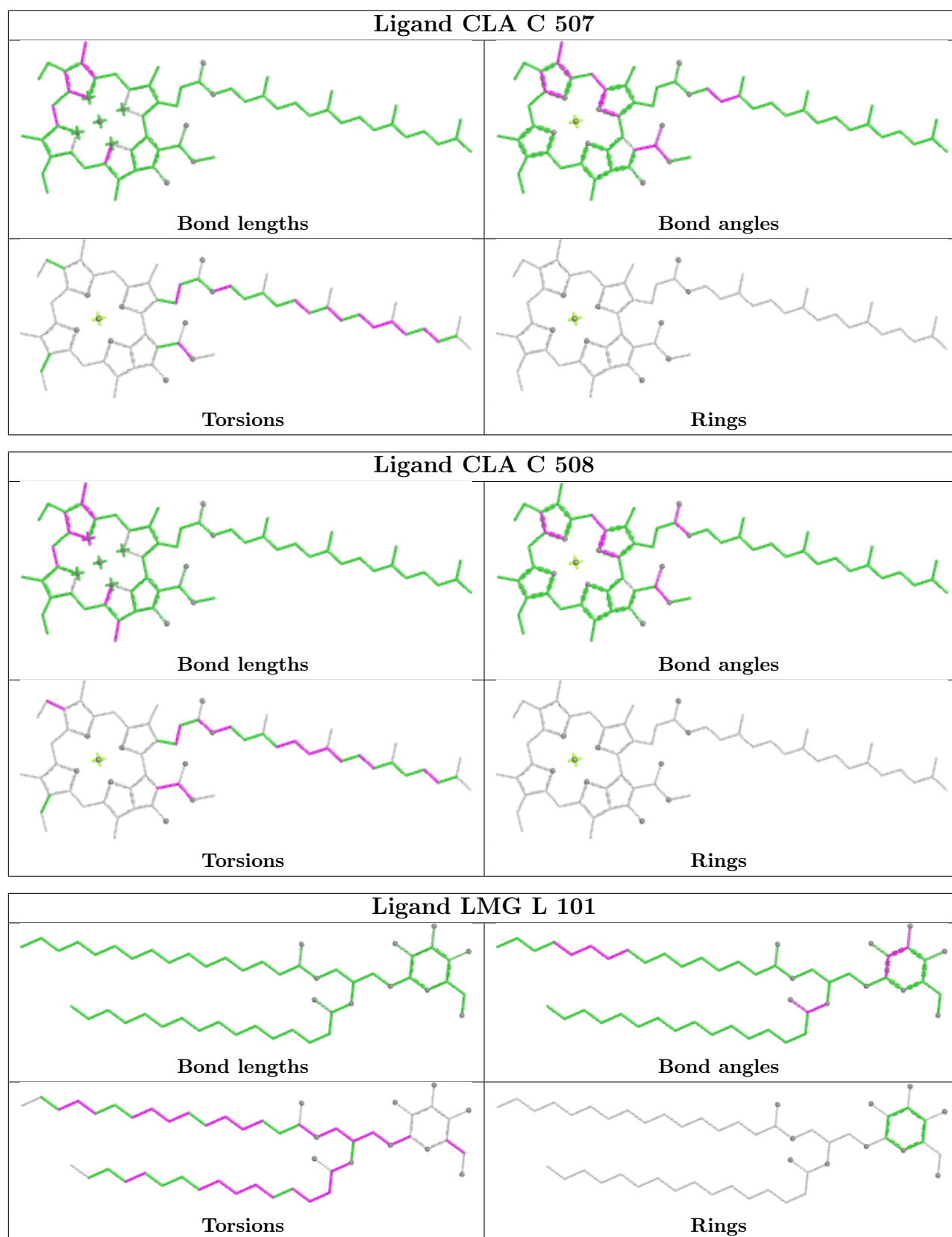


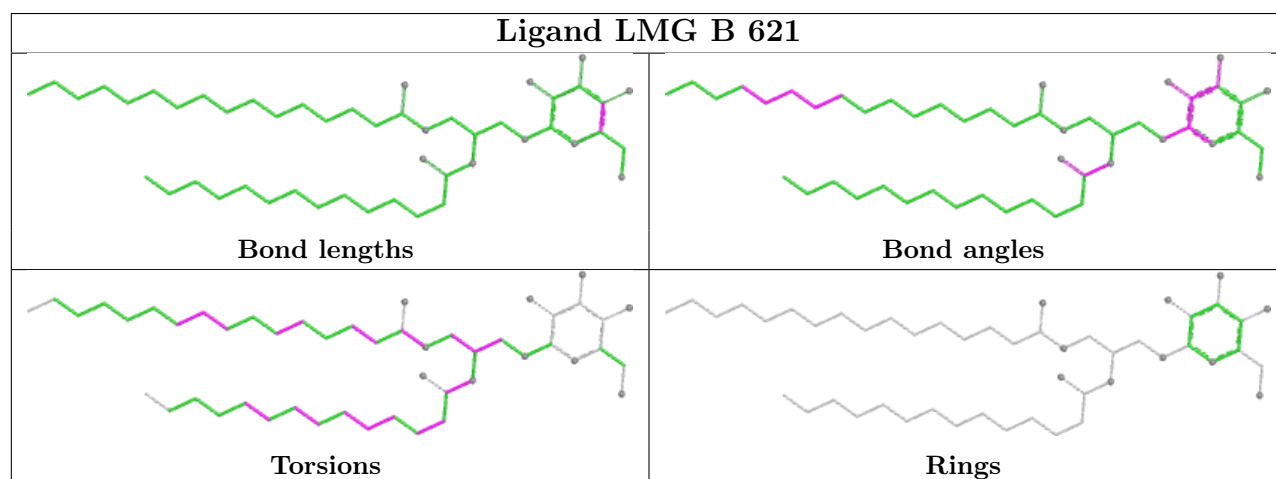
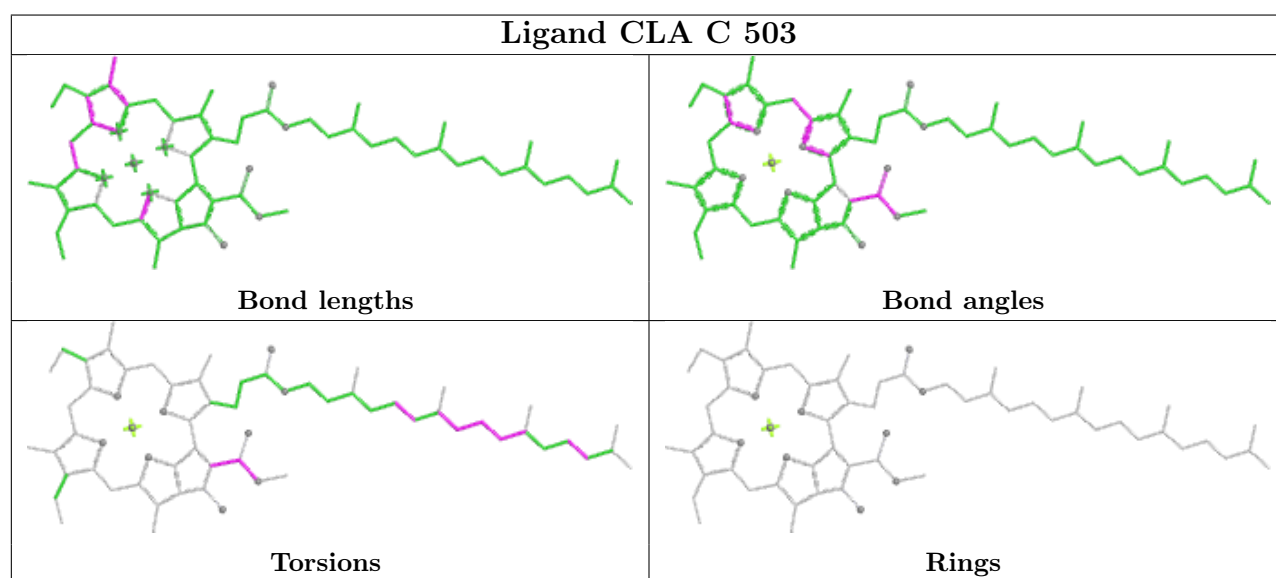
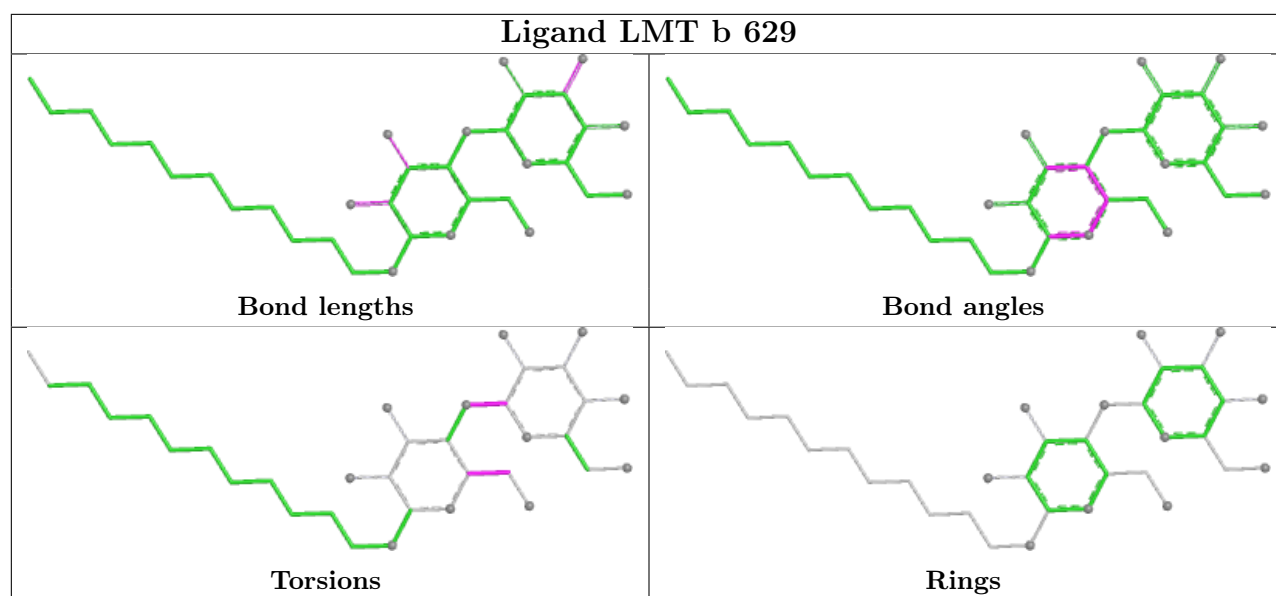
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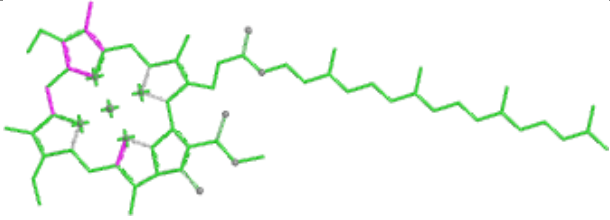
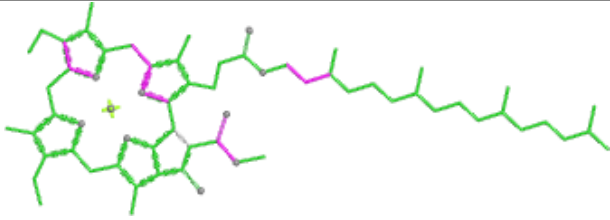
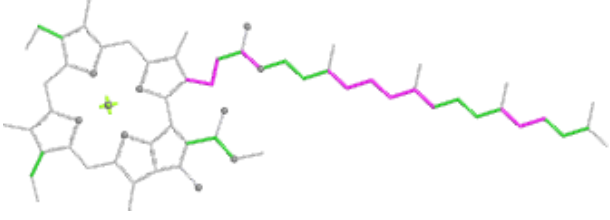
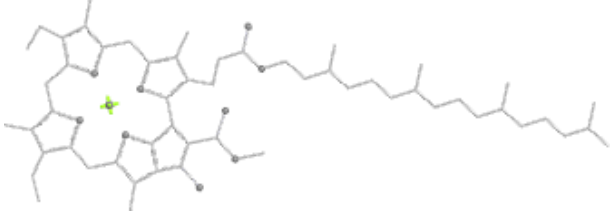
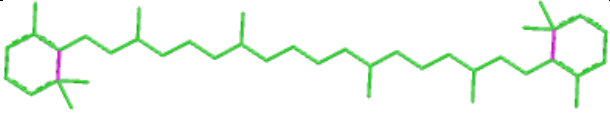
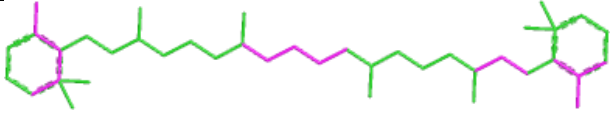
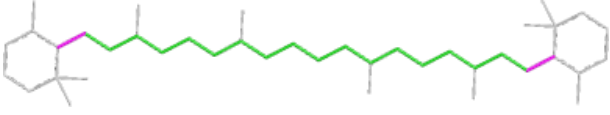
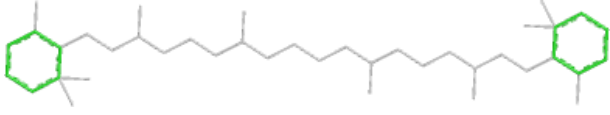
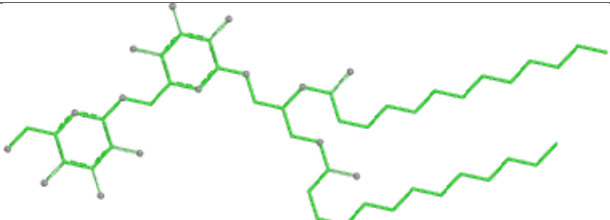
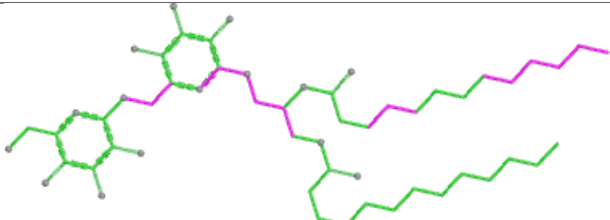
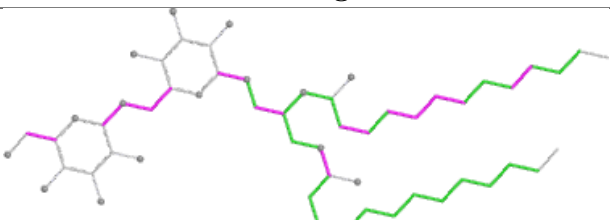
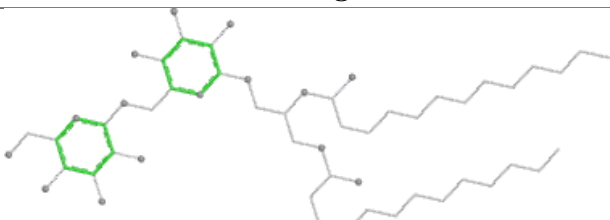


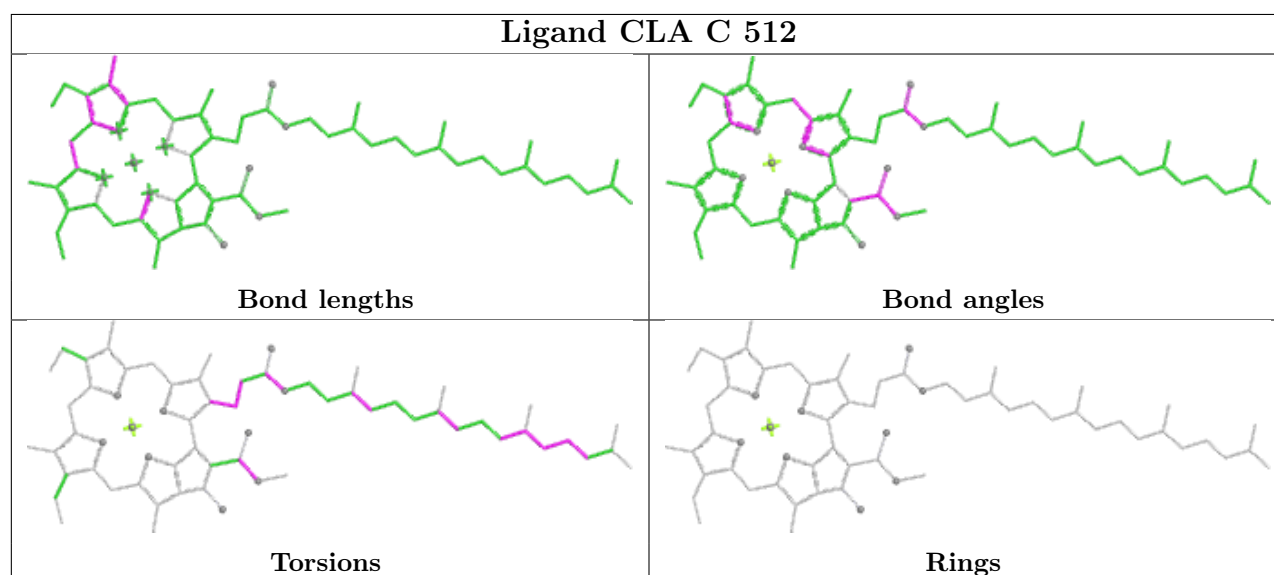
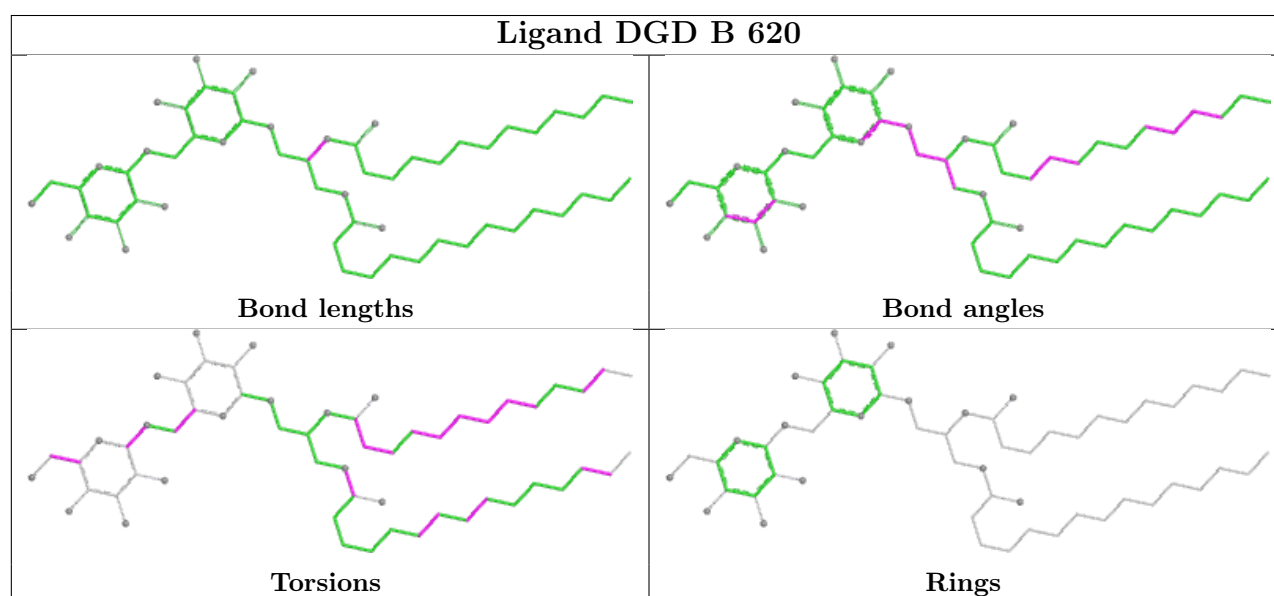
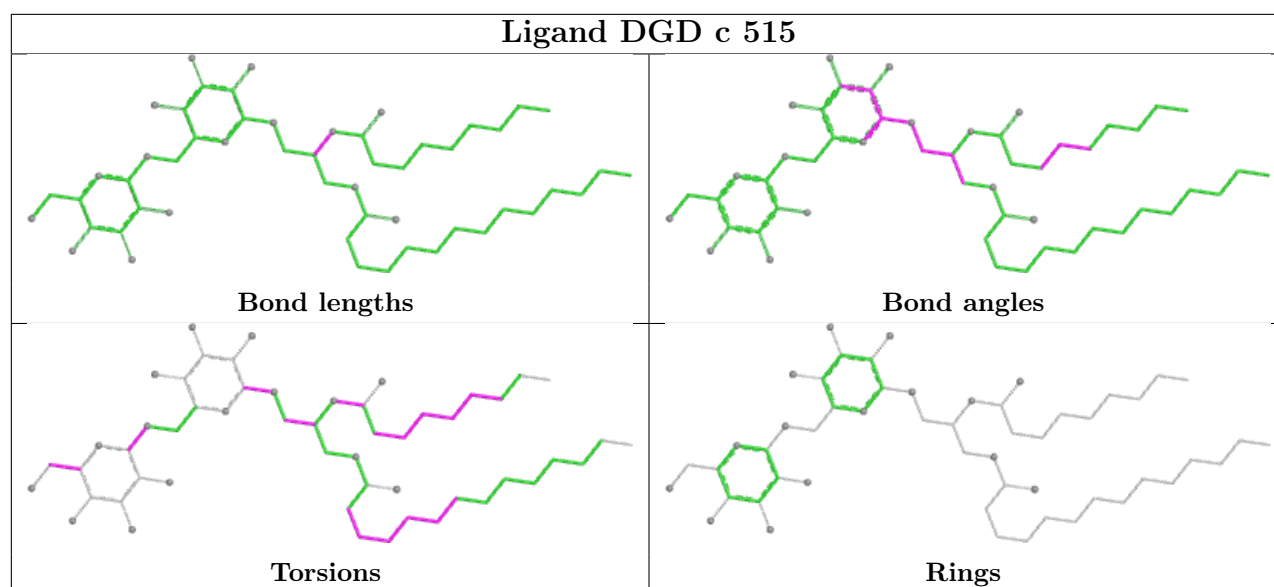




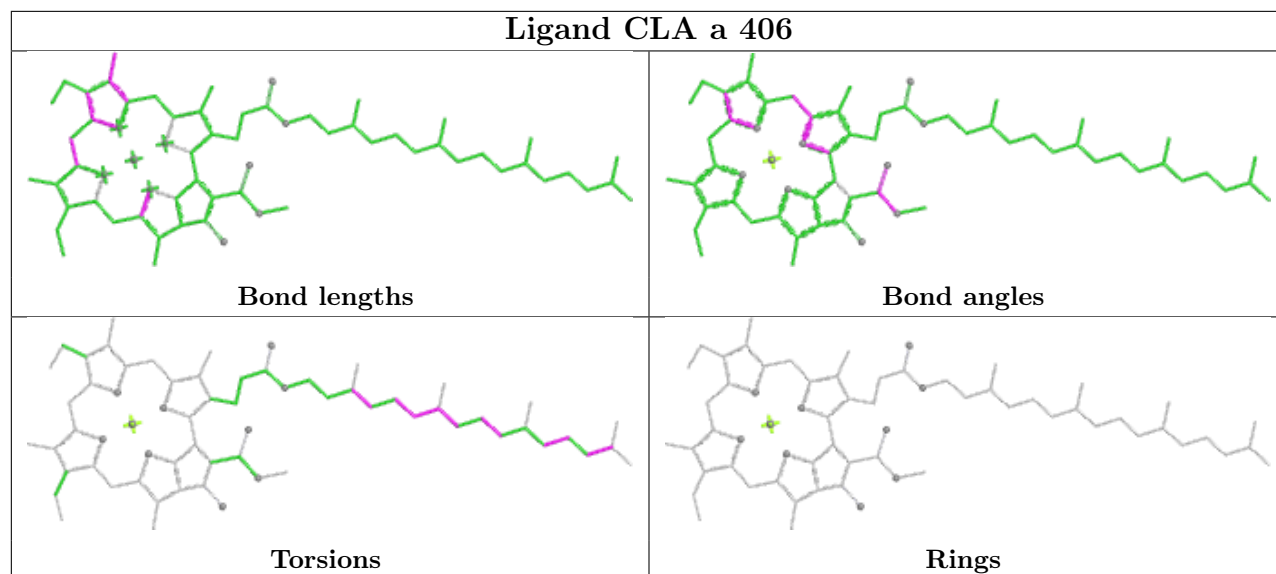




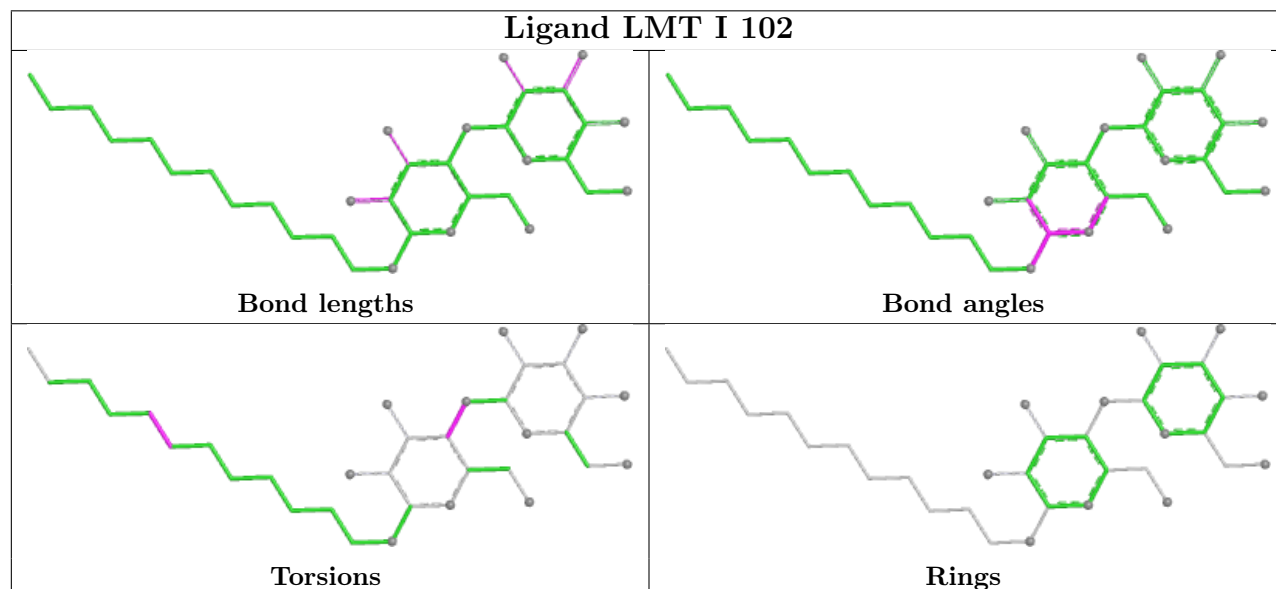
Ligand CLA H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings



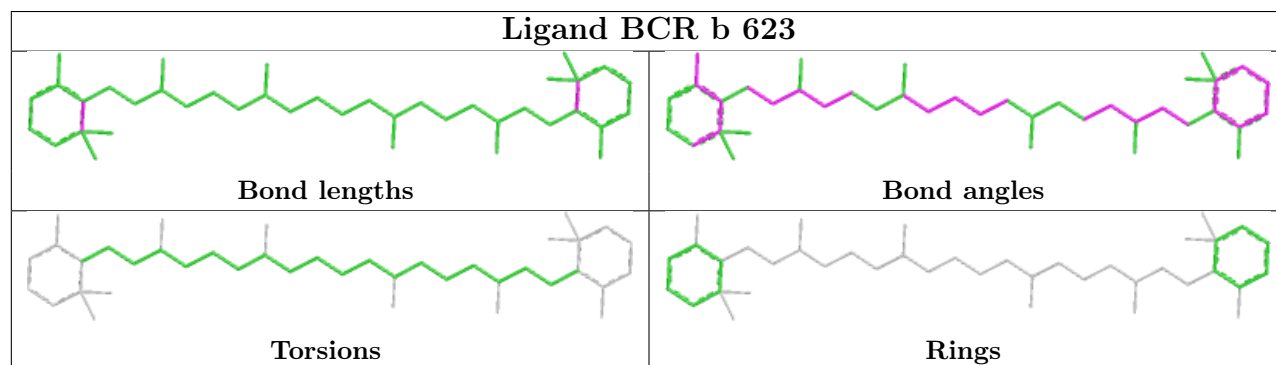
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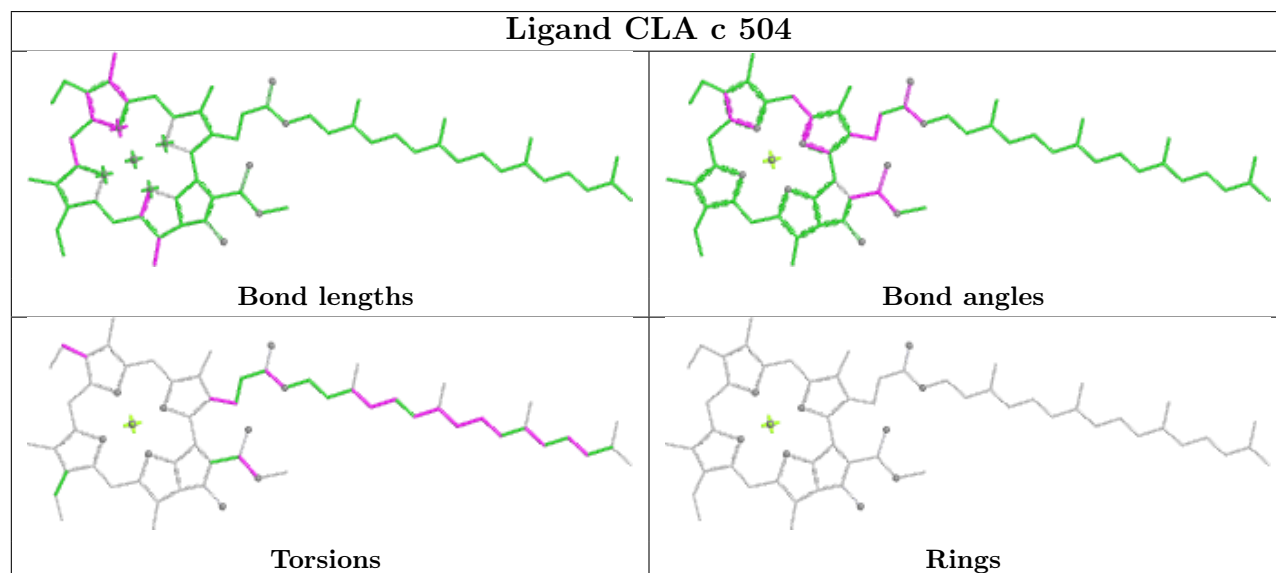
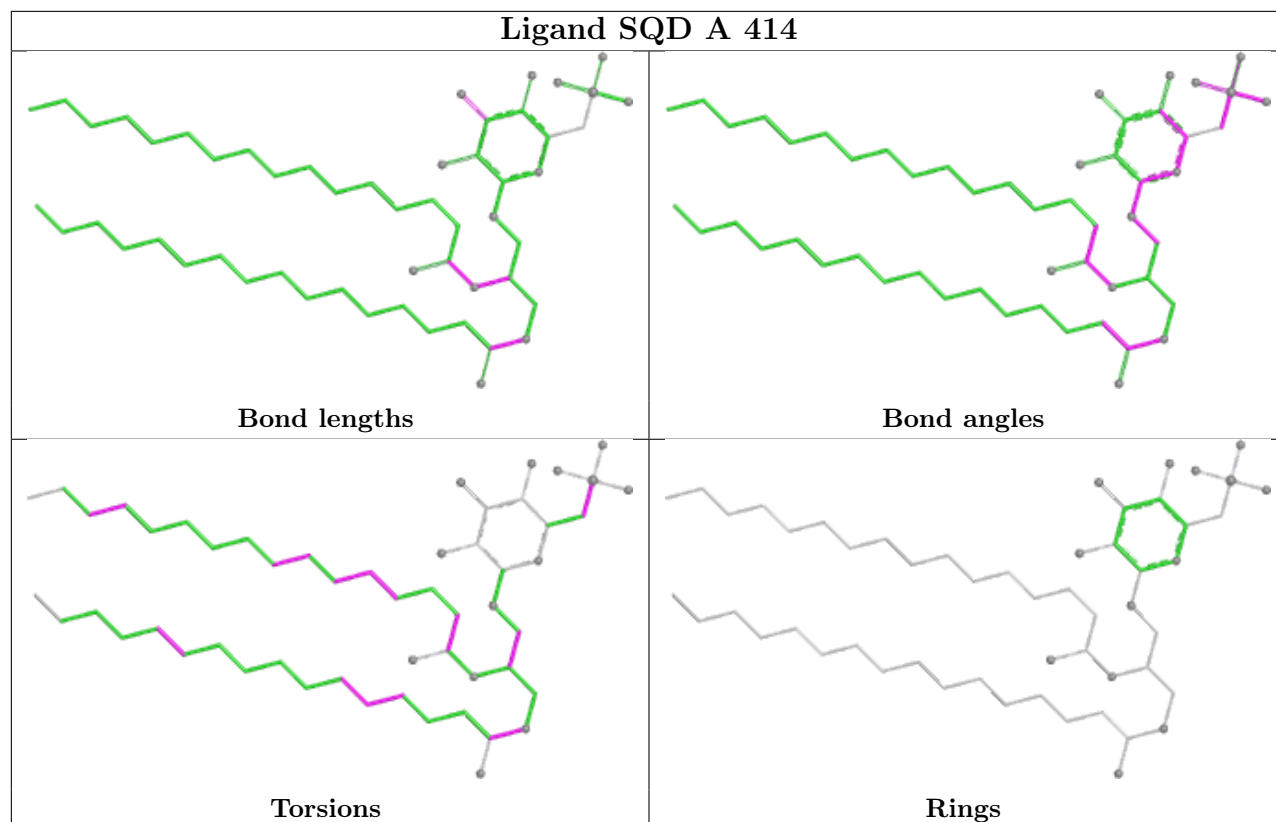


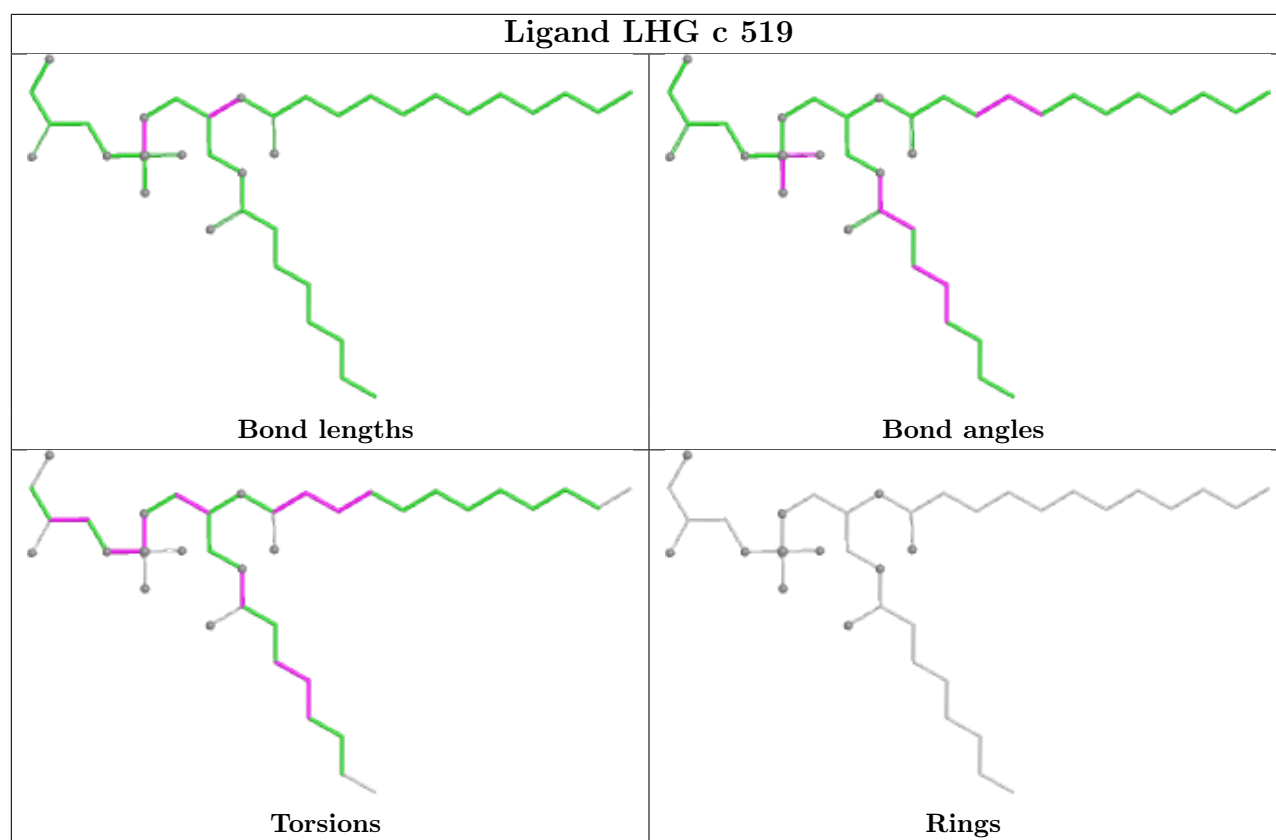
Ligand LMT I 102



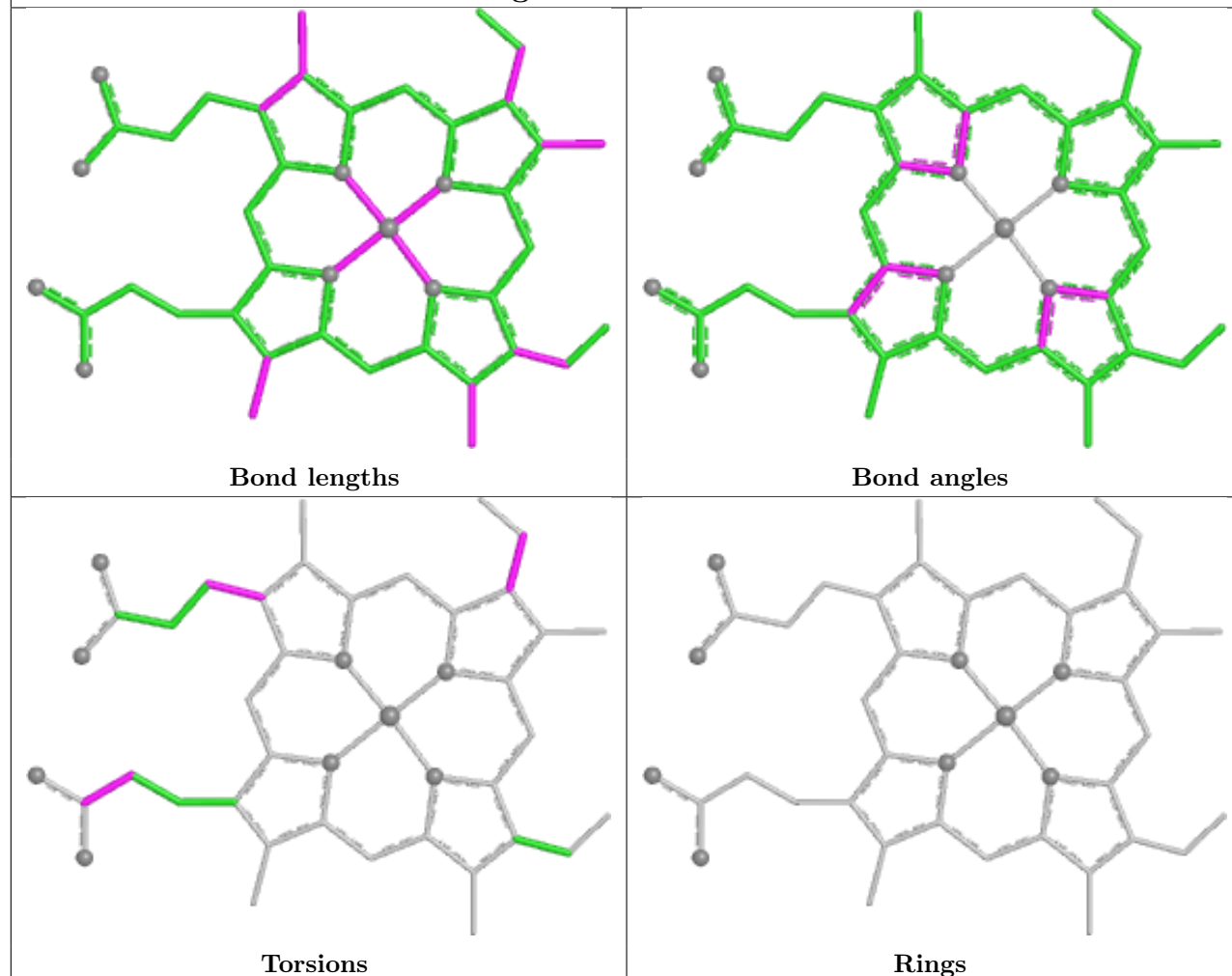
Ligand BCR b 623



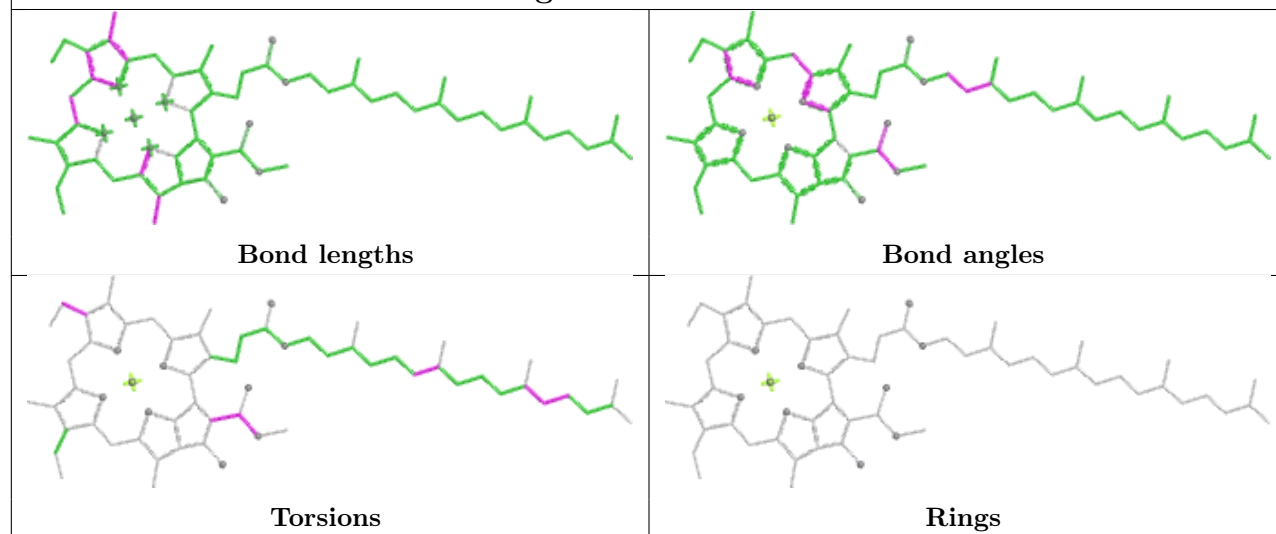


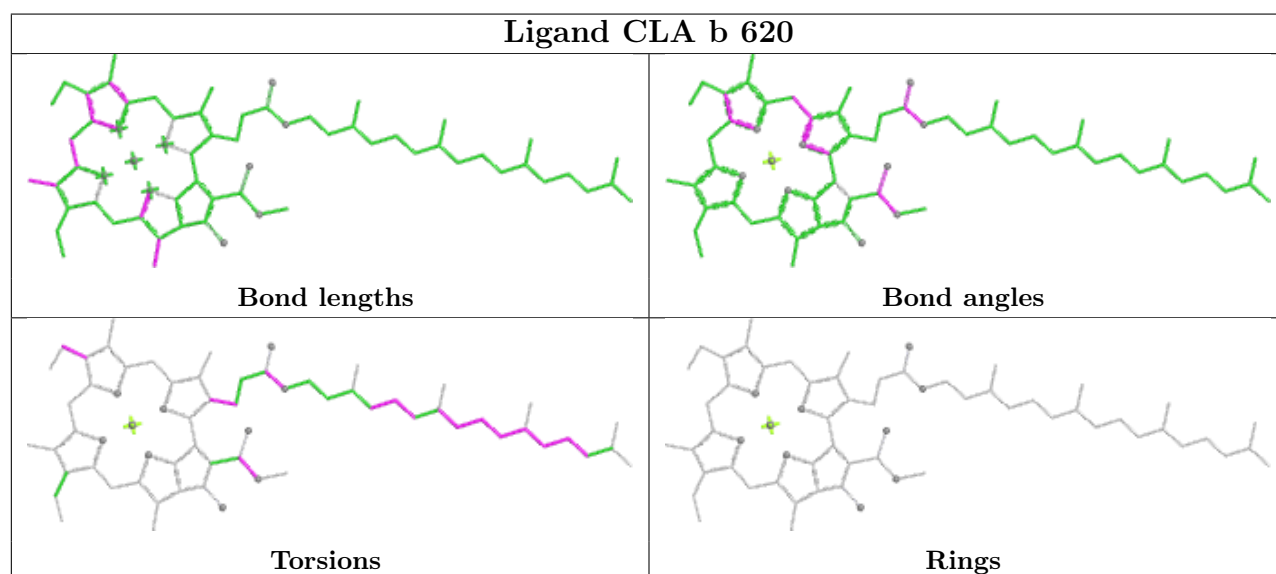
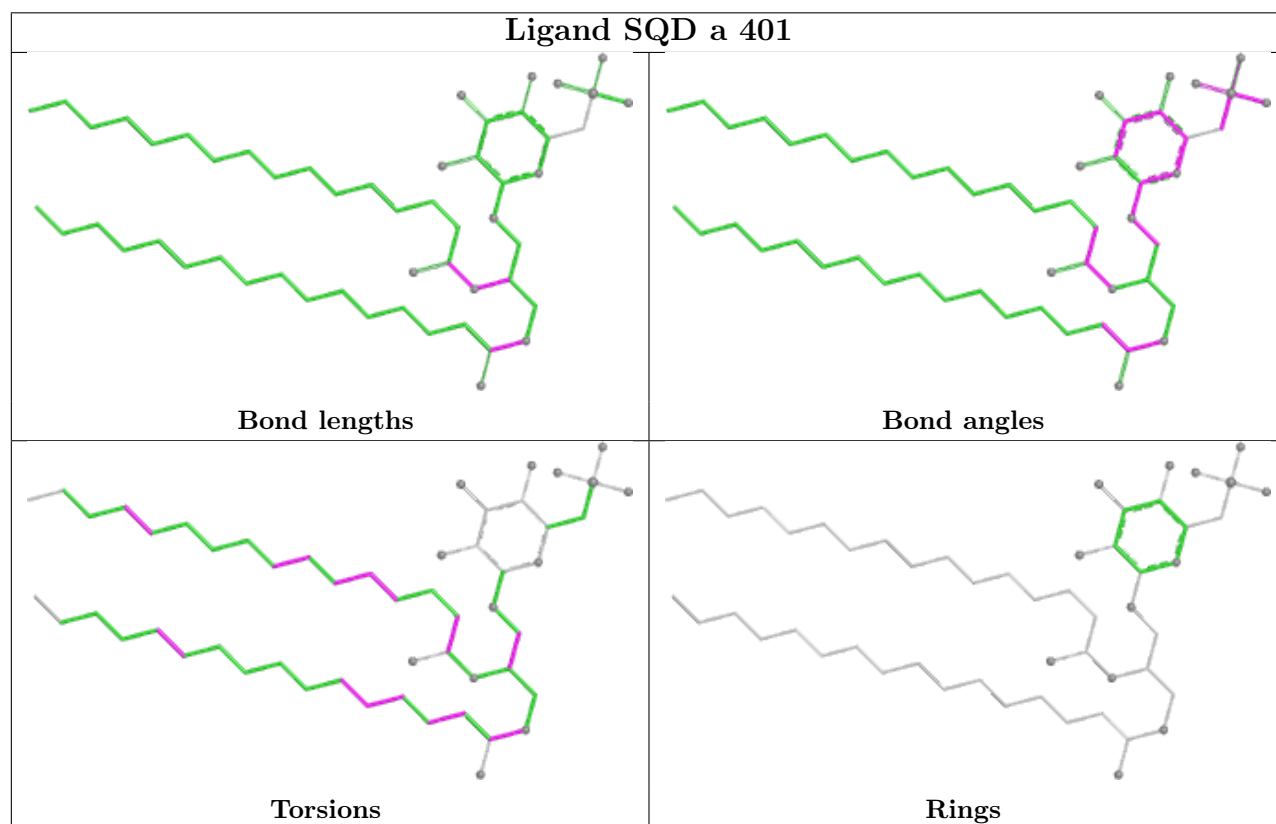
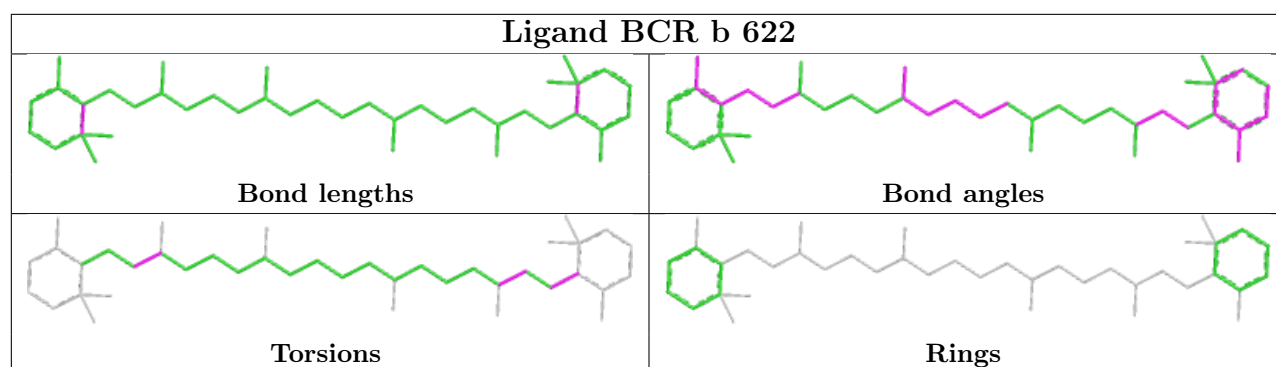


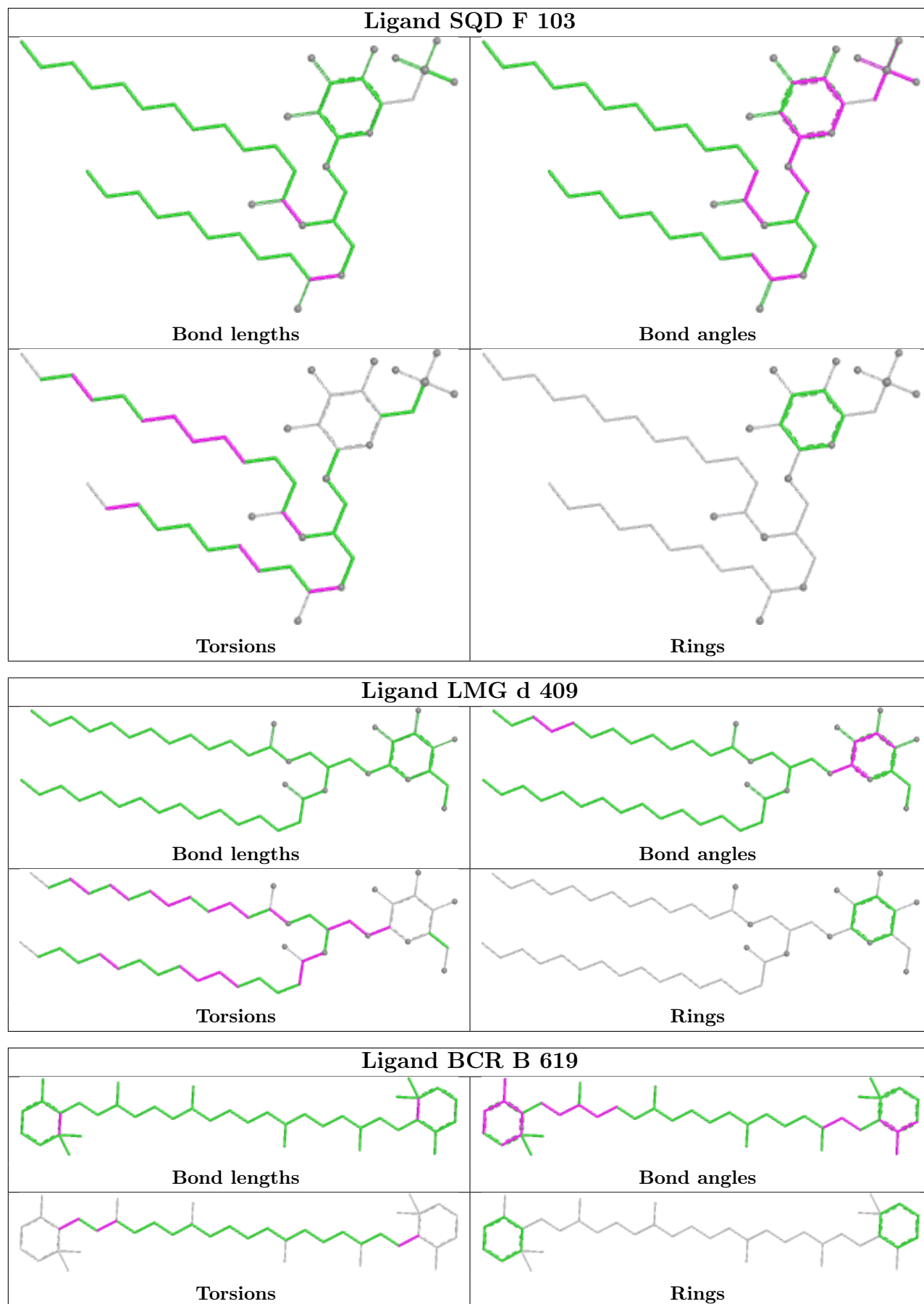
Ligand HEM v 201

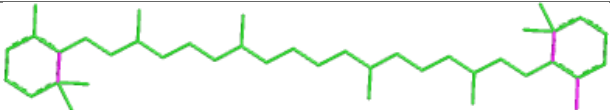
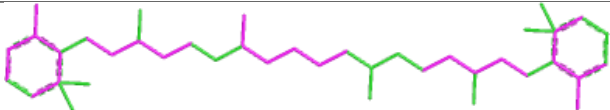
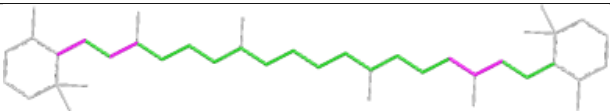
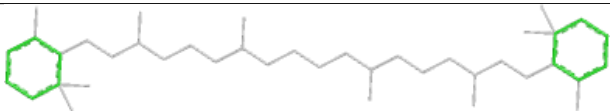
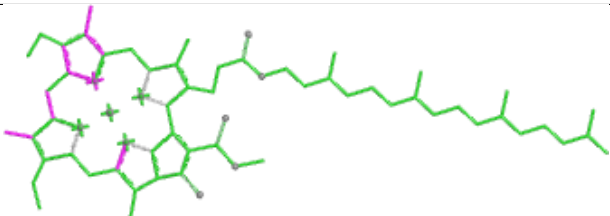
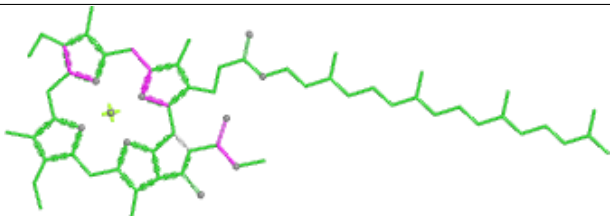
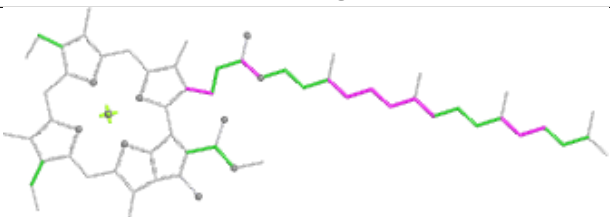
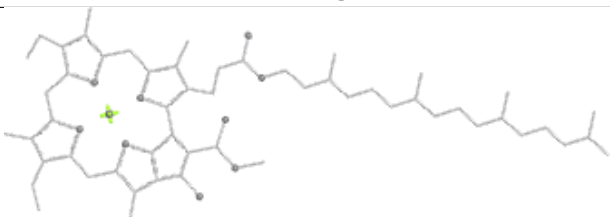
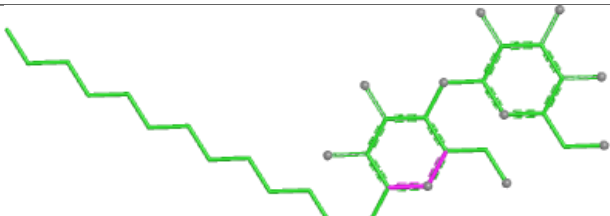
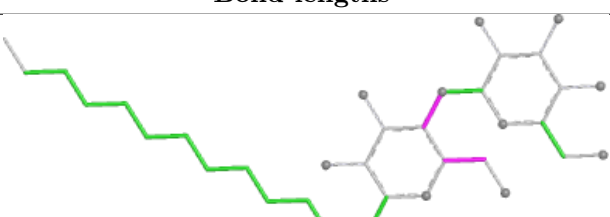
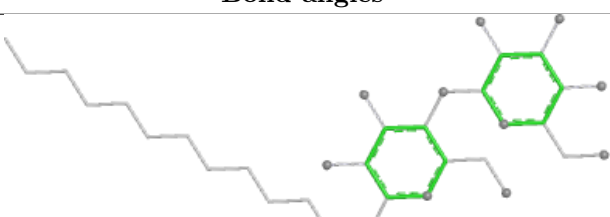


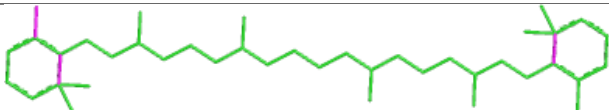
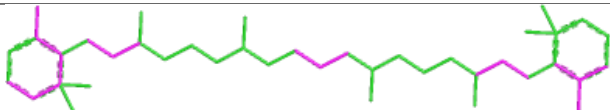
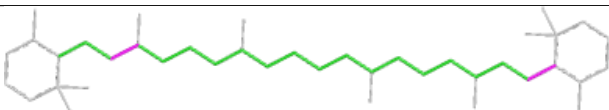
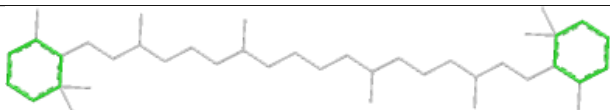
Ligand CLA b 613

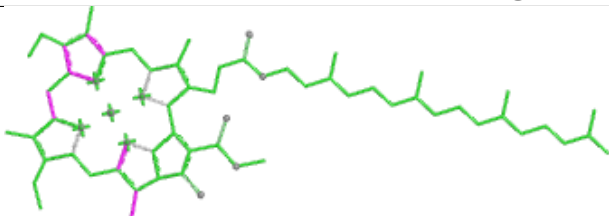
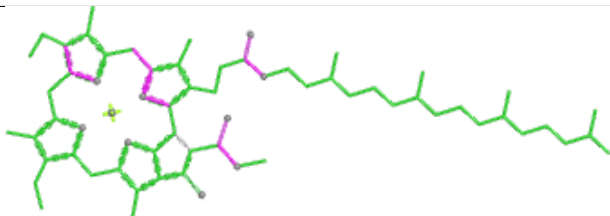
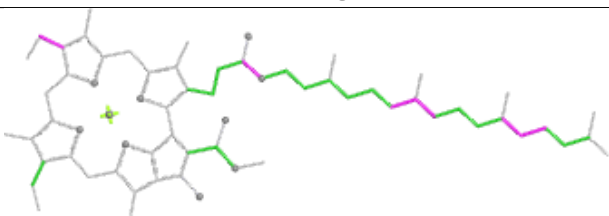
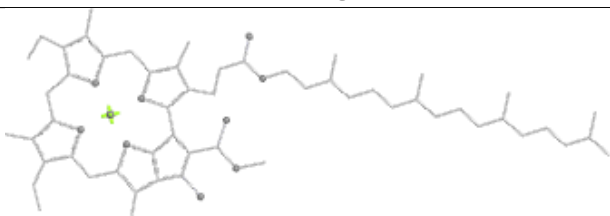




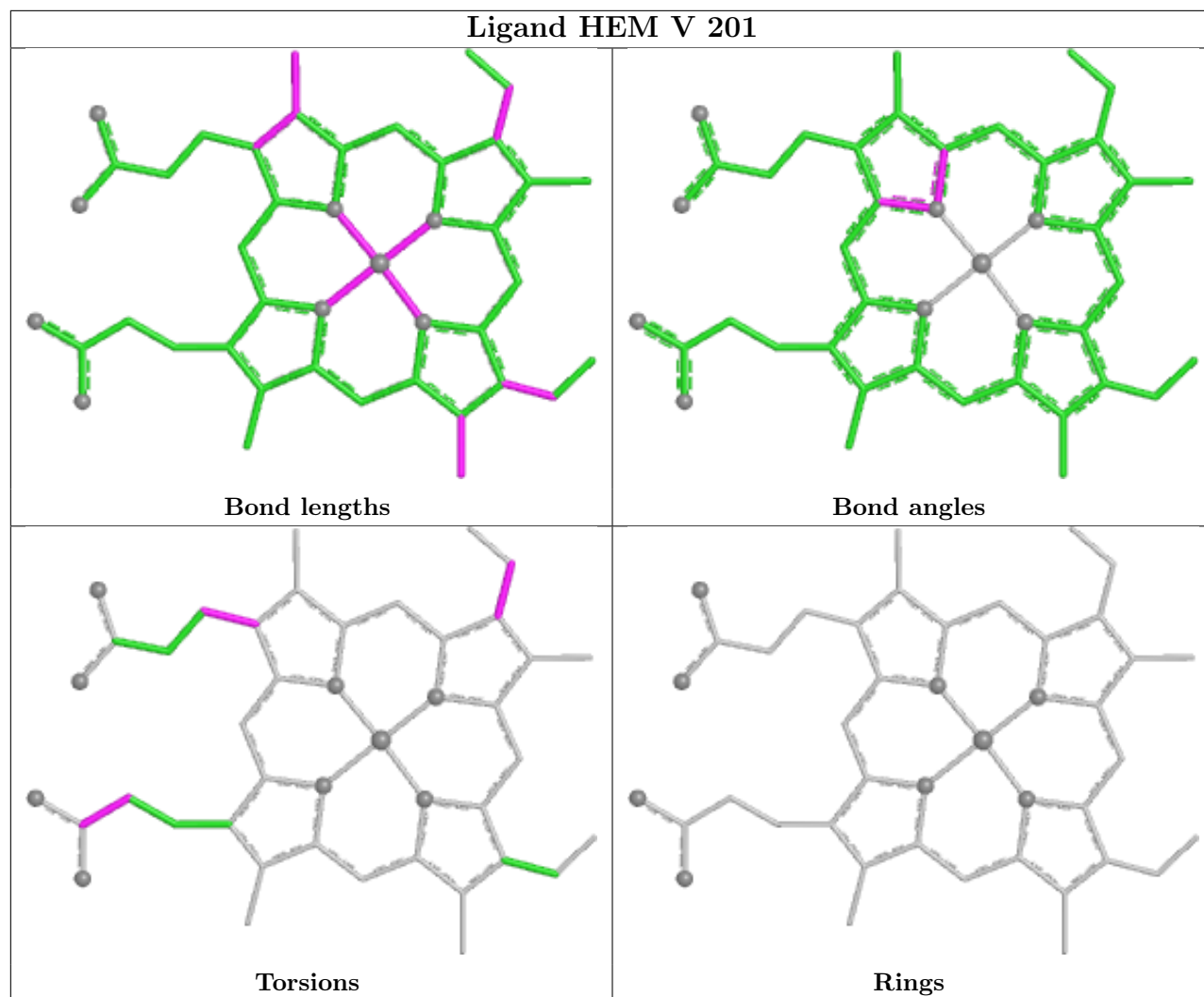


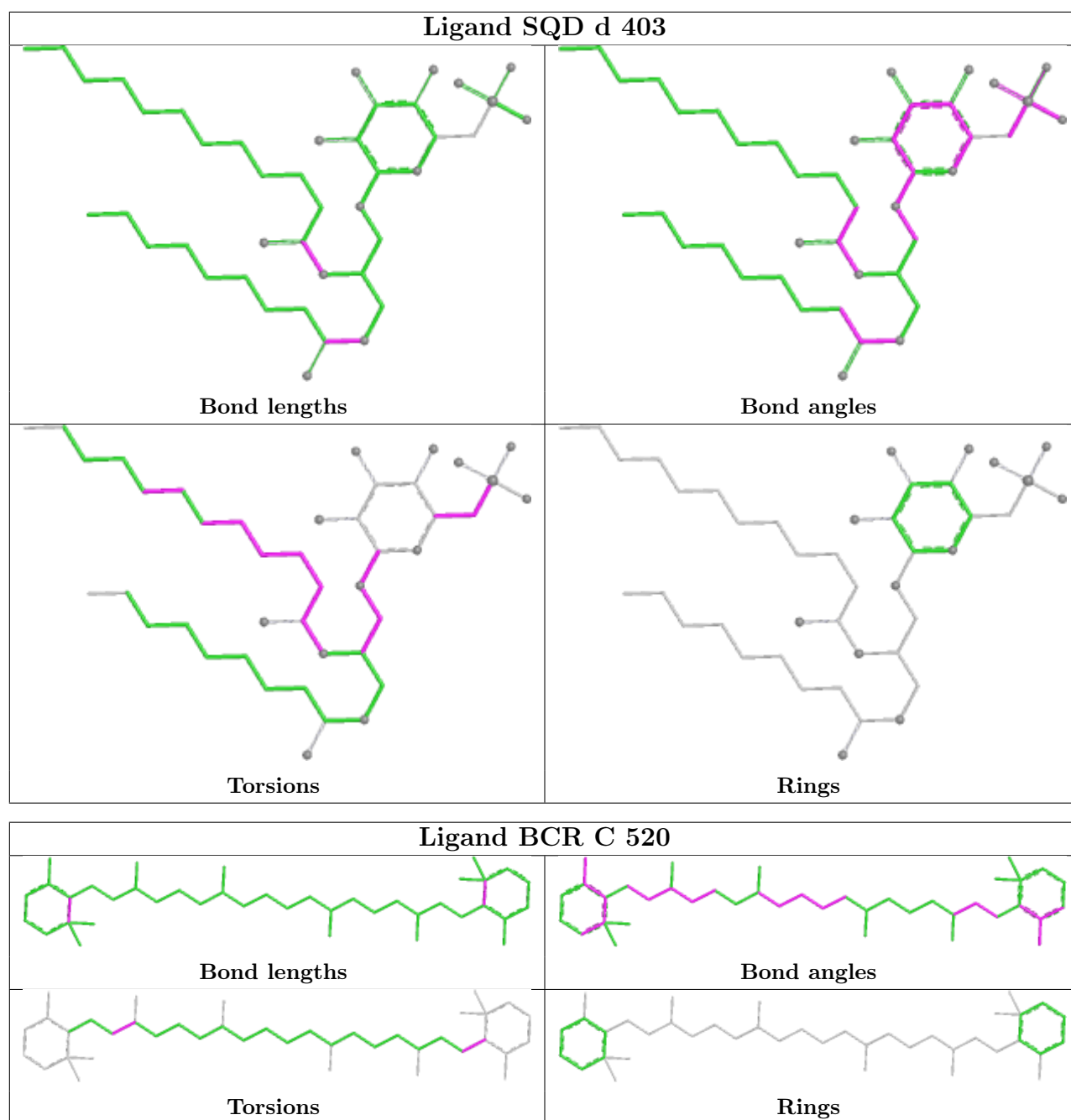
Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

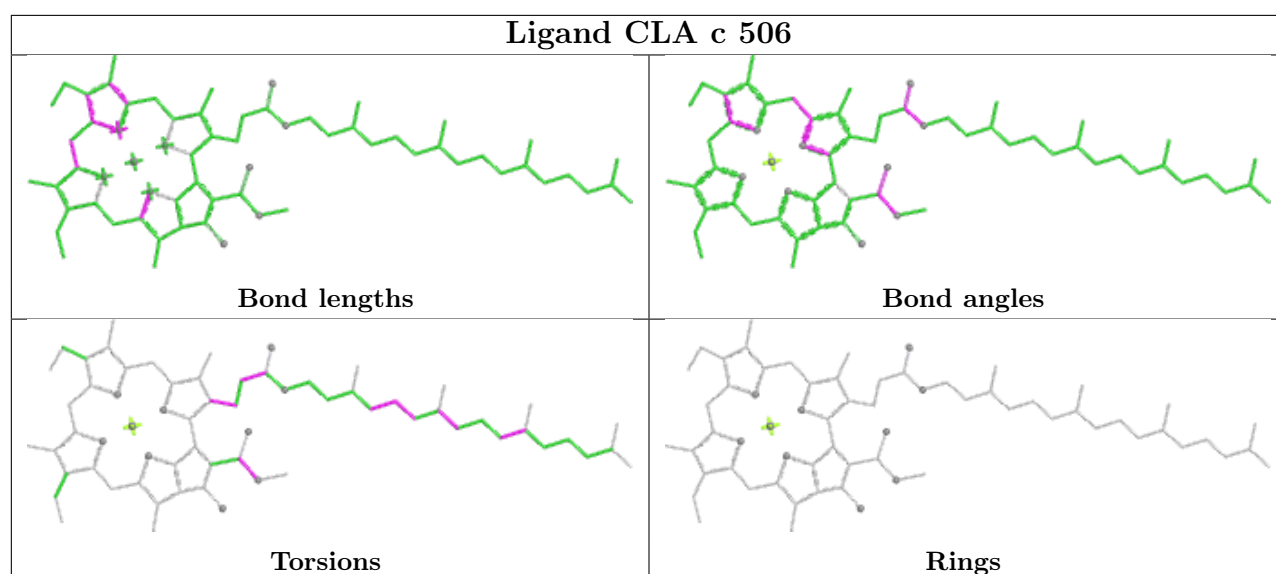
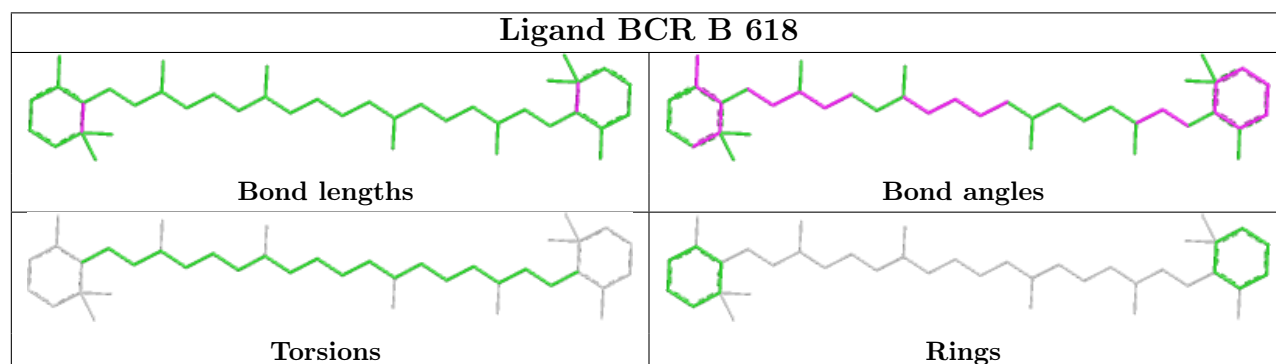
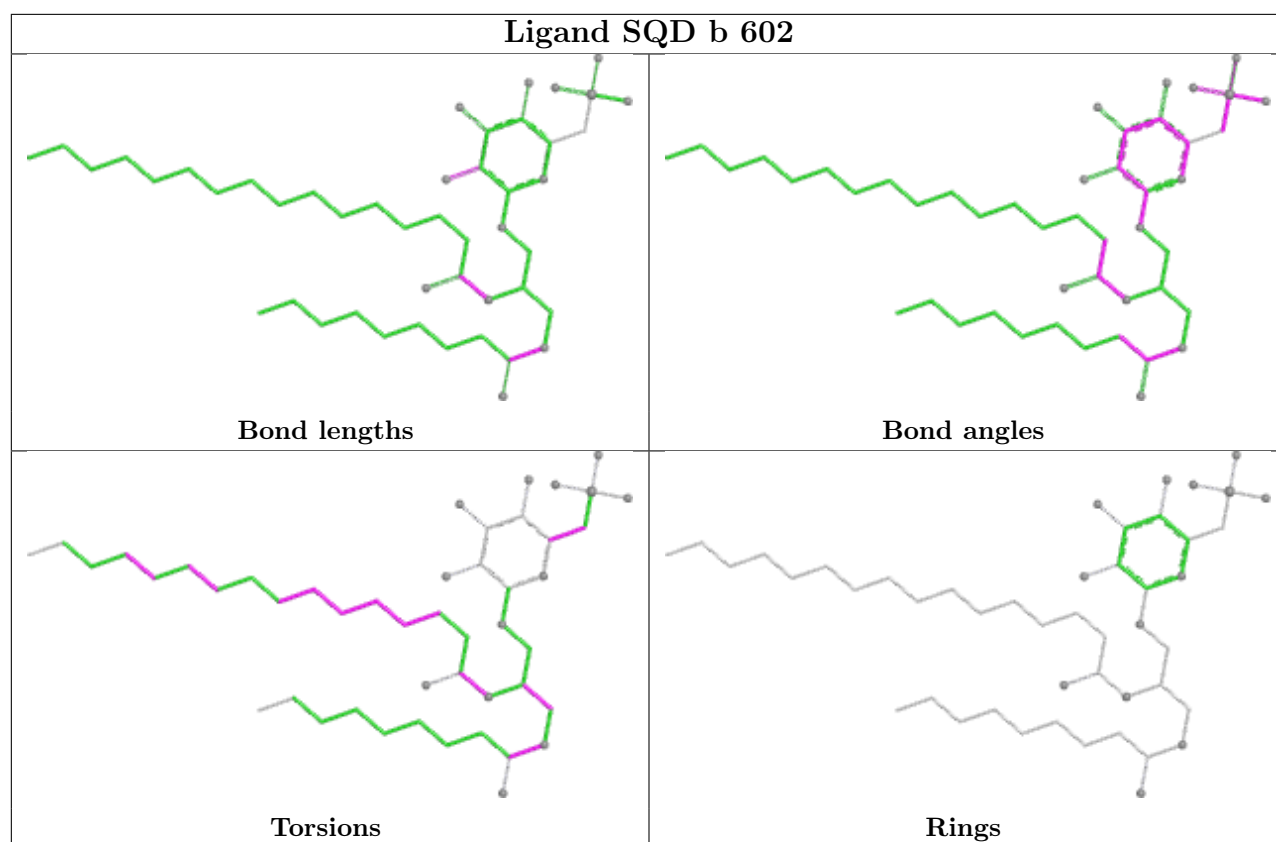
Ligand BCR y 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

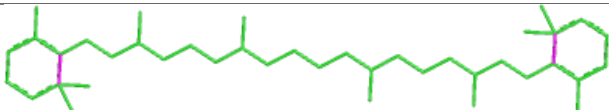
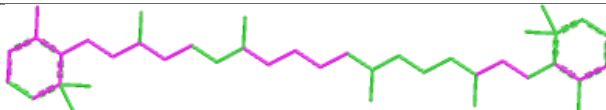
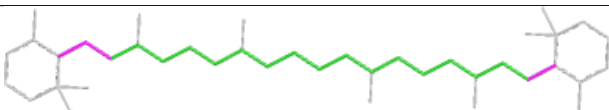
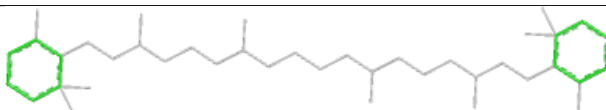
Ligand CLA B 614	
	Bond lengths
	Bond angles
	Torsions
	Rings

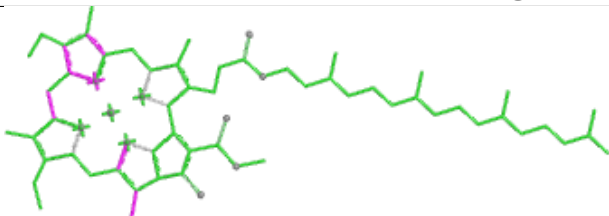
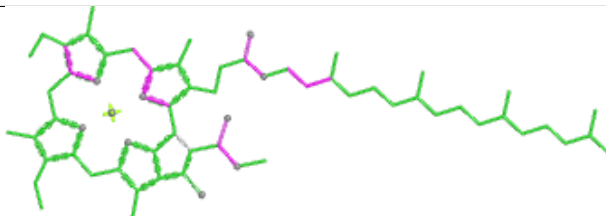
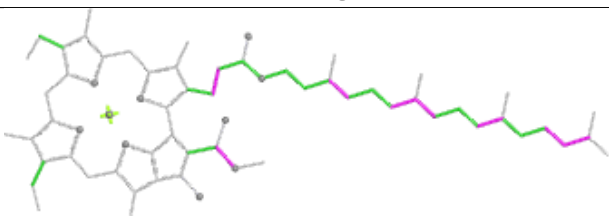
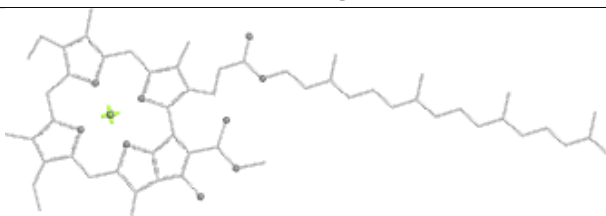
Ligand HEM V 201



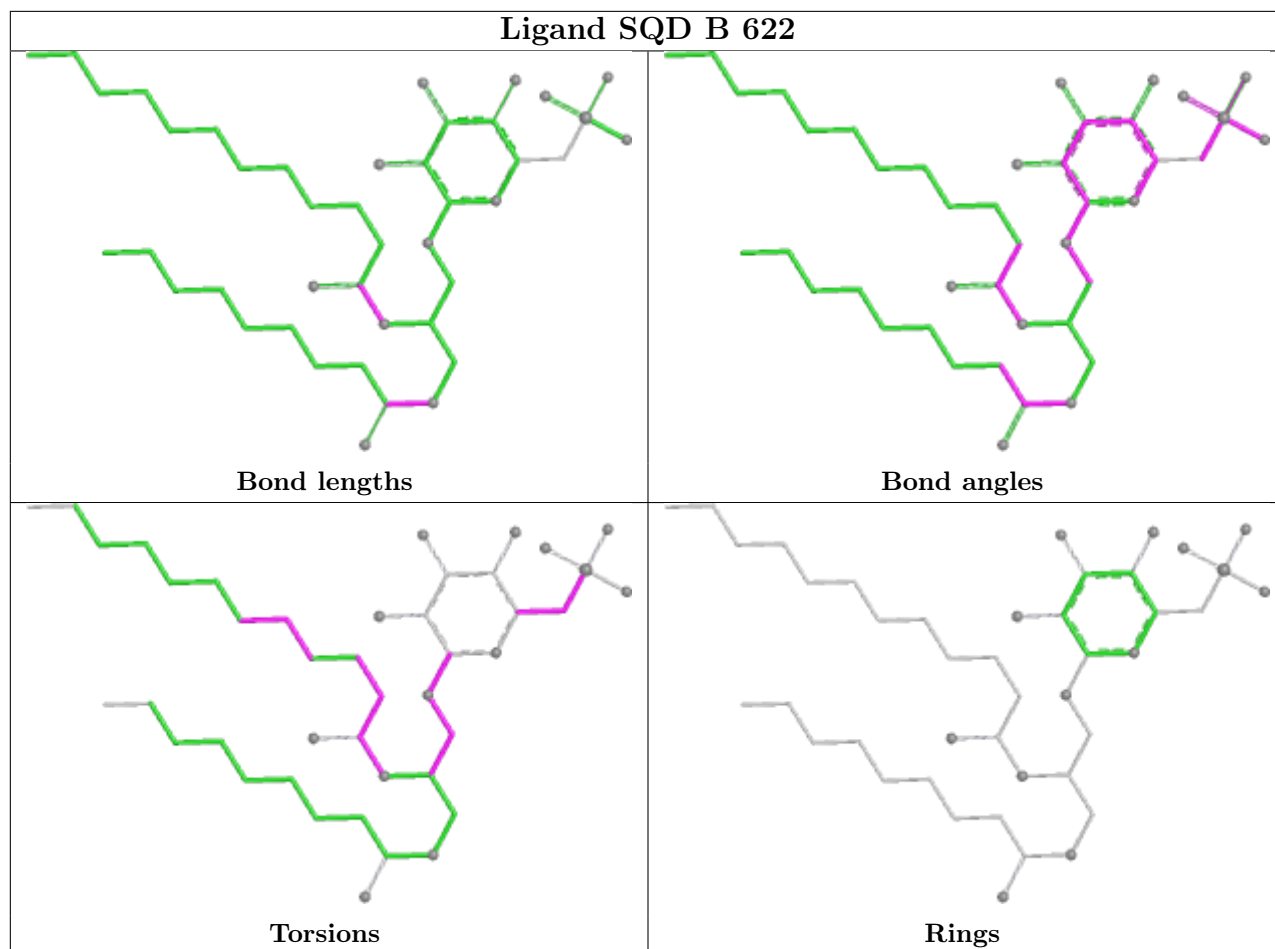




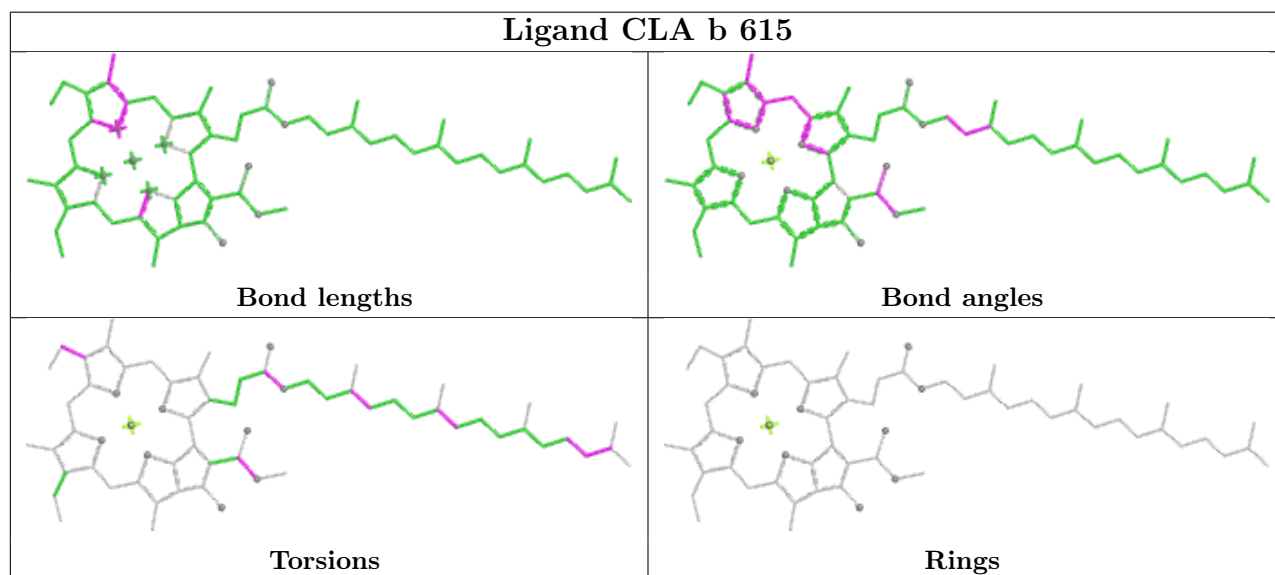
Ligand BCR c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

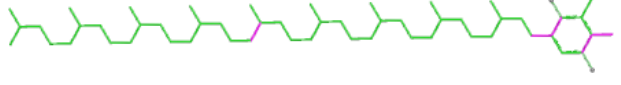
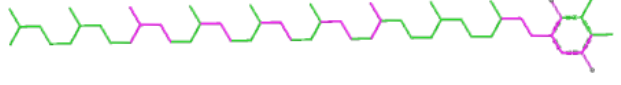
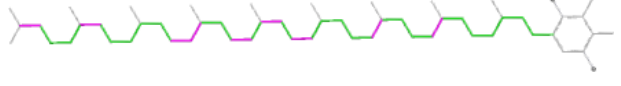
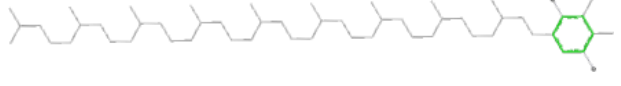
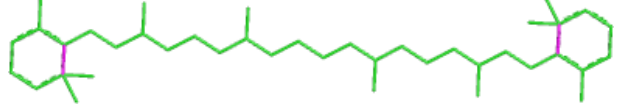
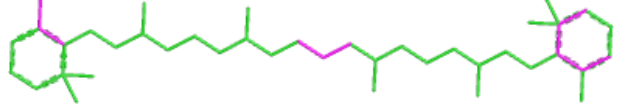
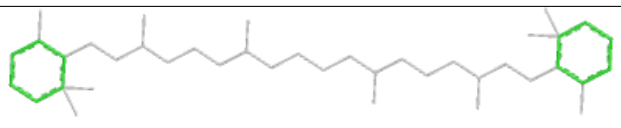
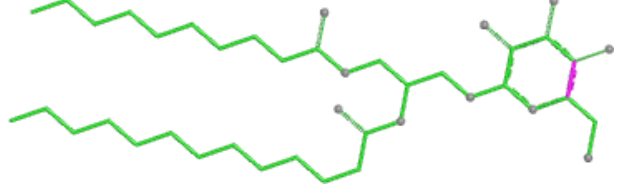
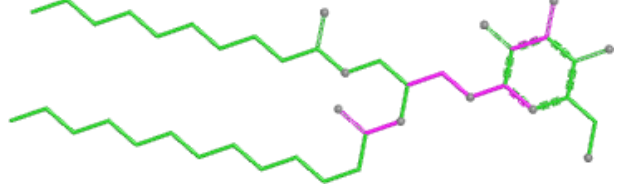
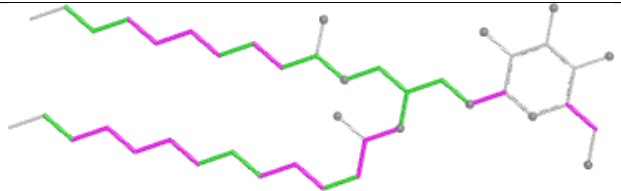
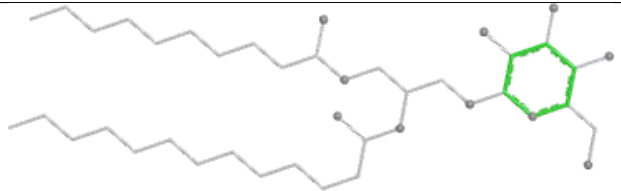
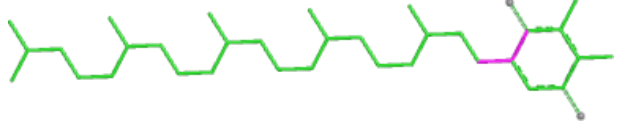
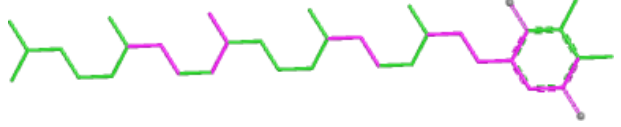
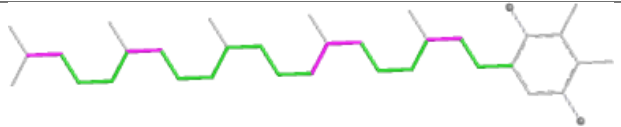
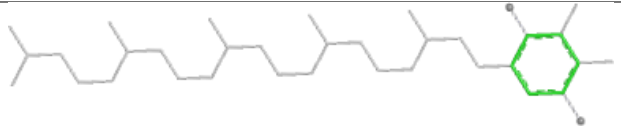
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

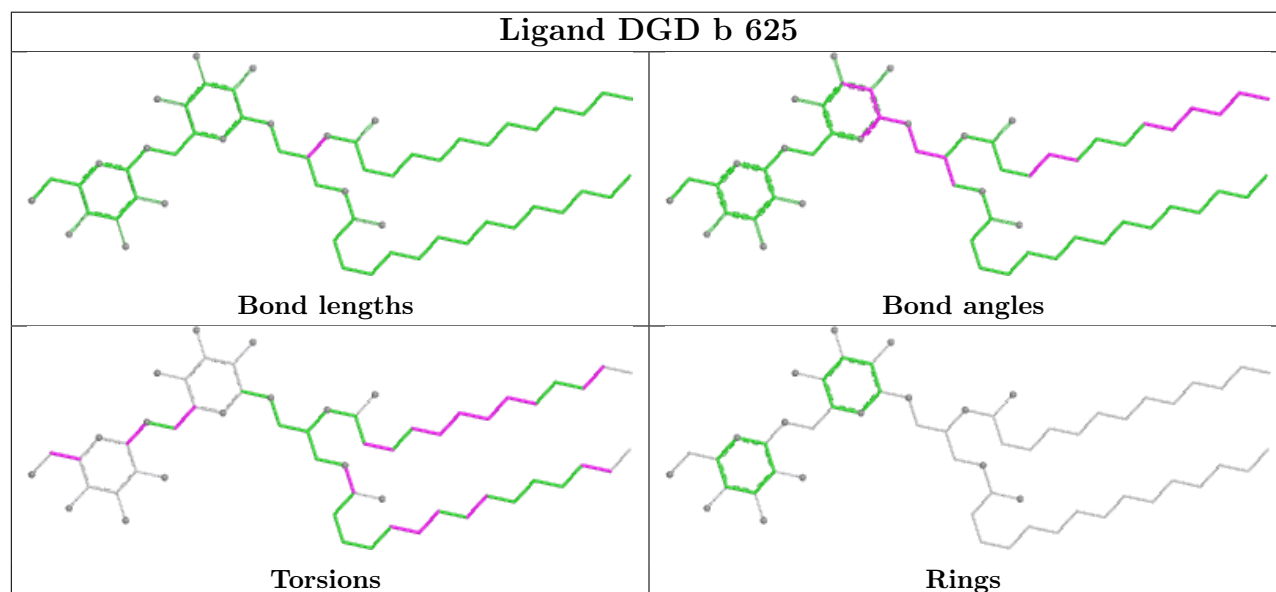
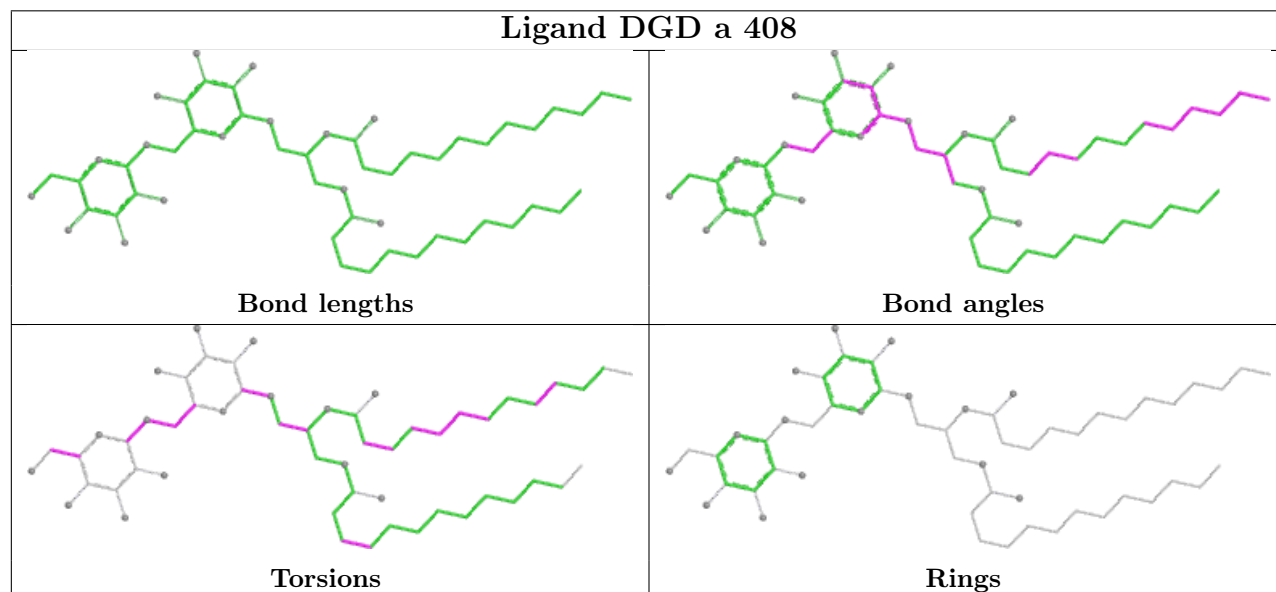
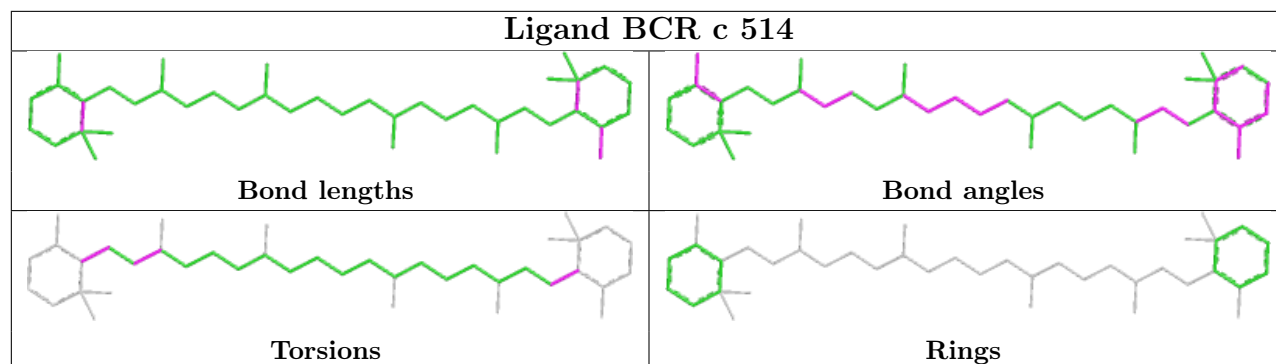
Ligand SQD B 622

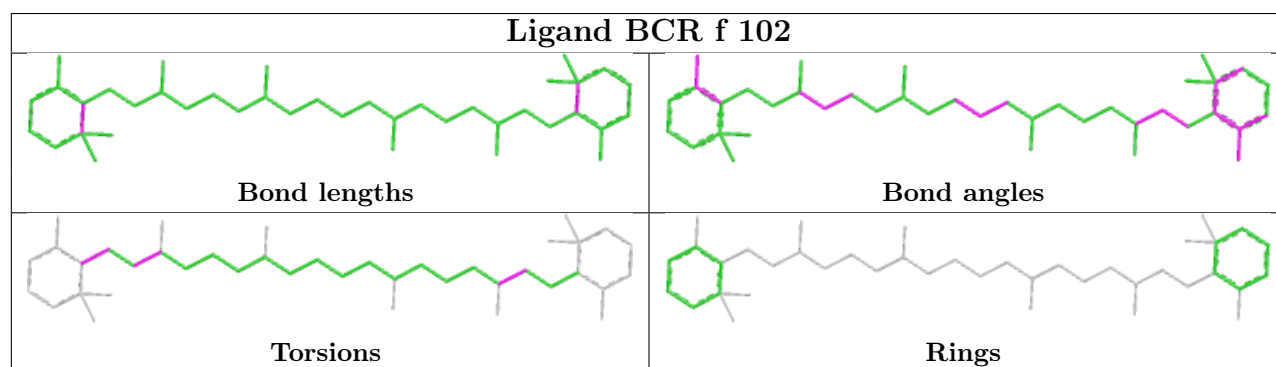
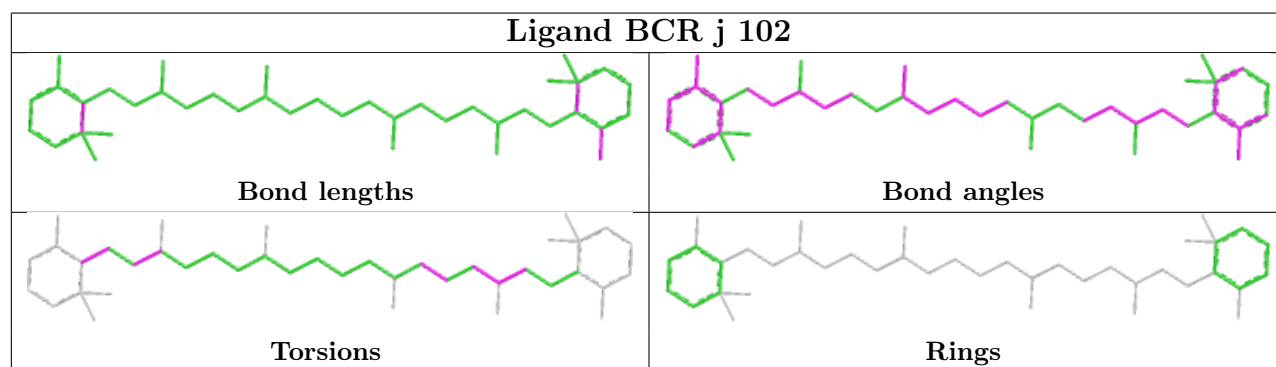
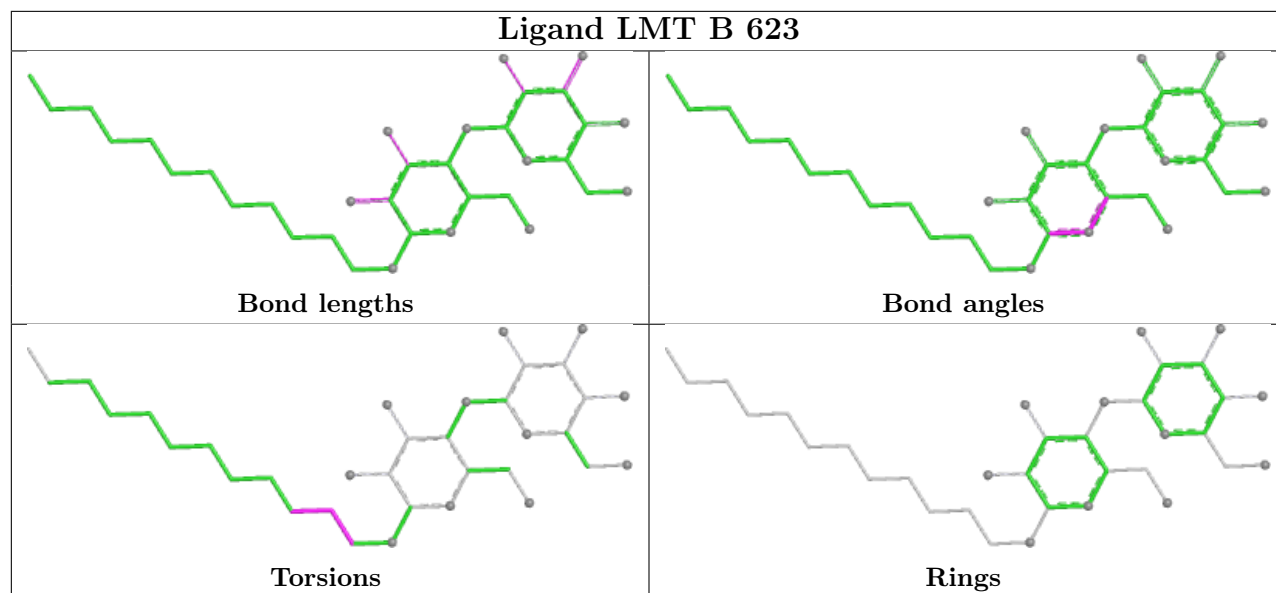


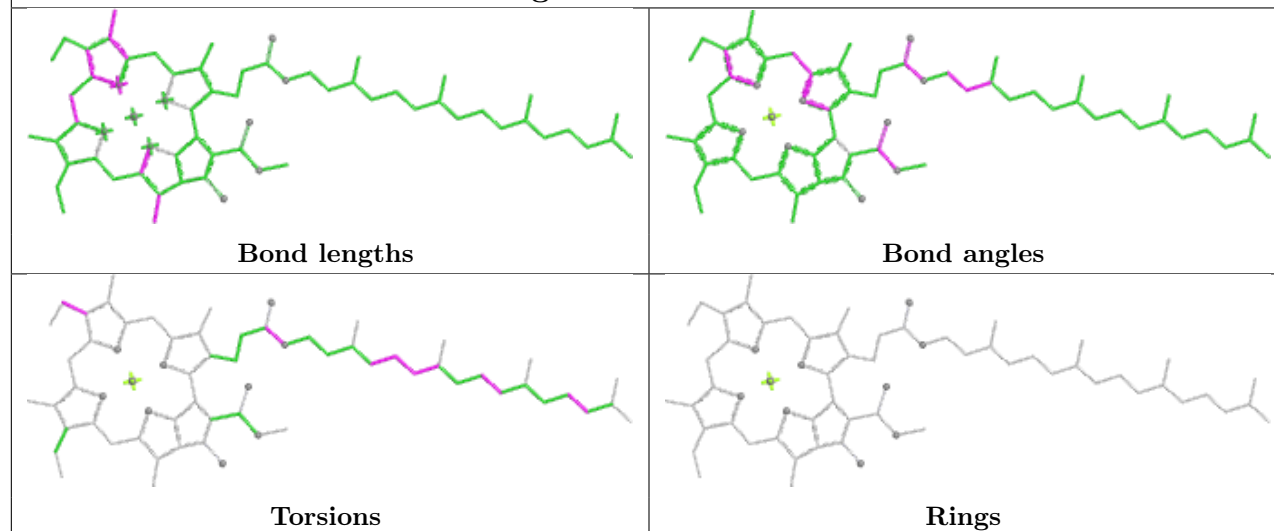
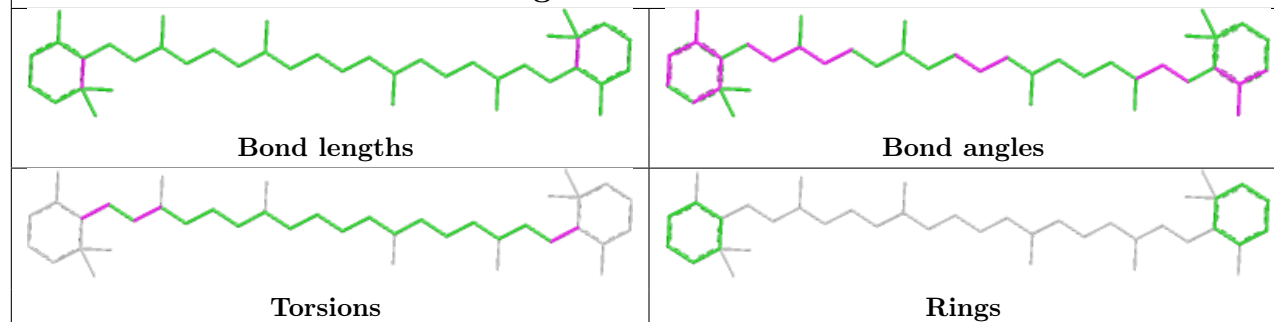
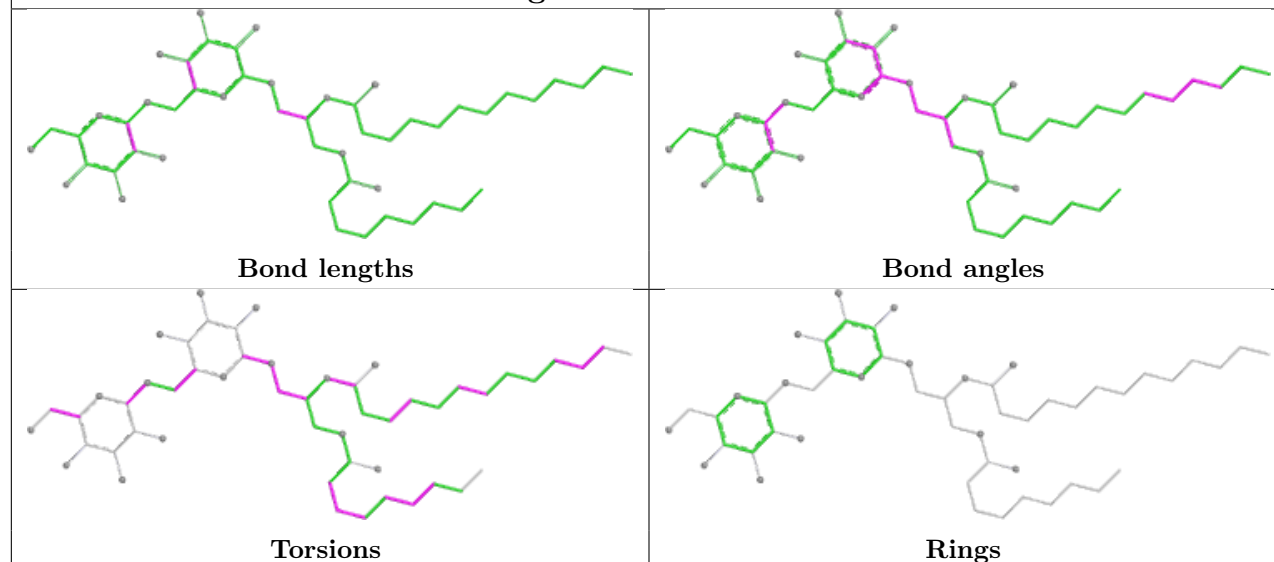
Ligand CLA b 615

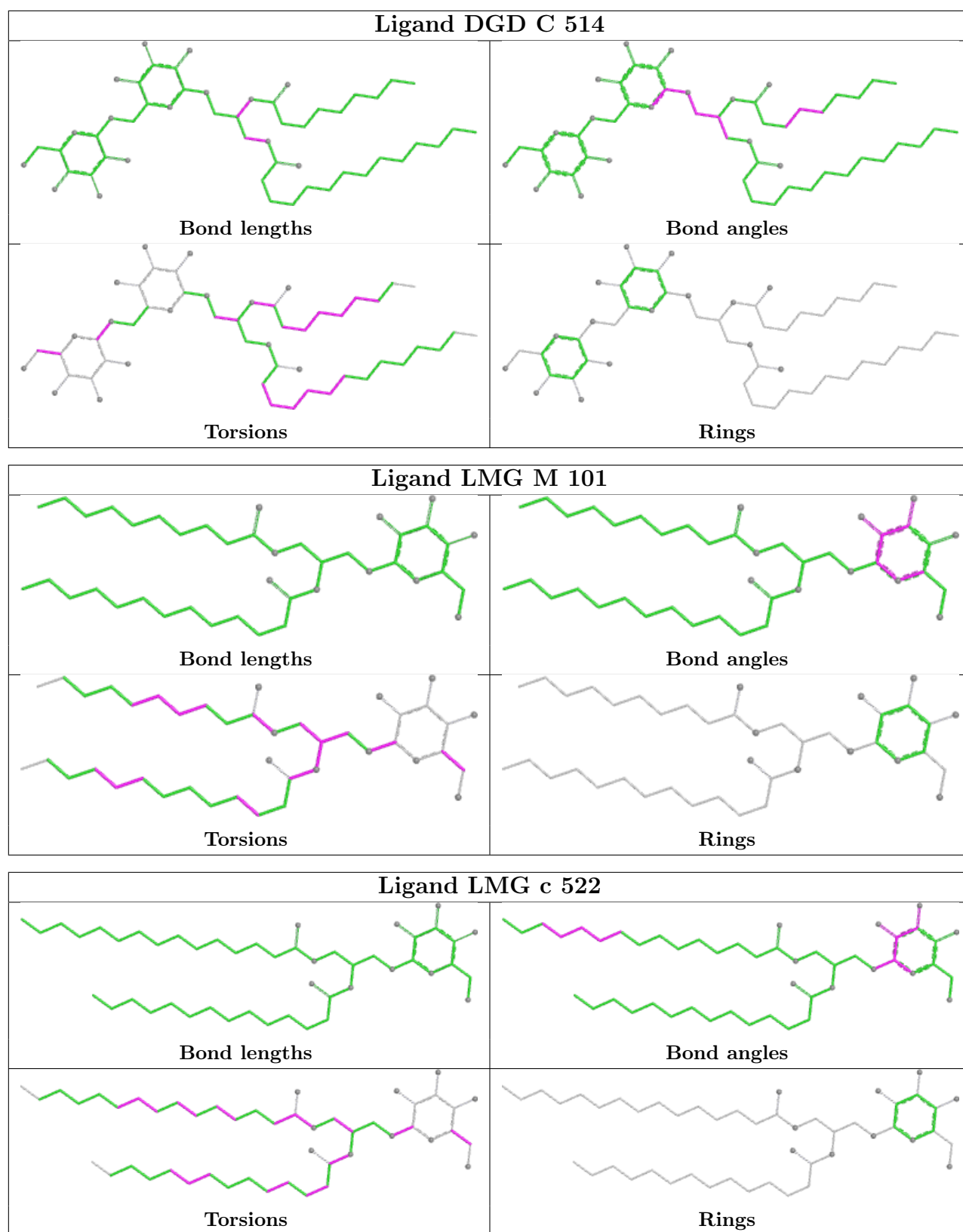


Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 627	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

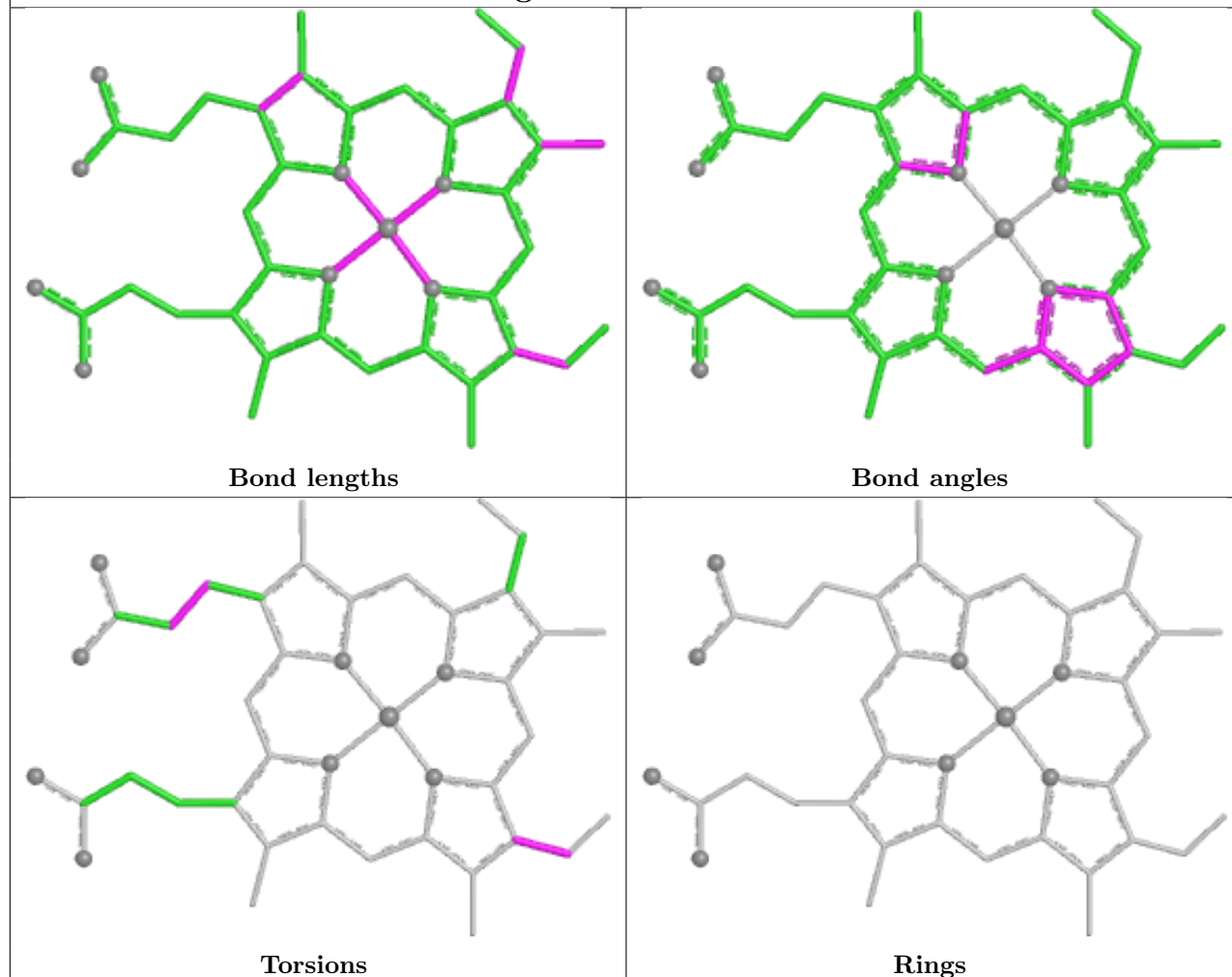




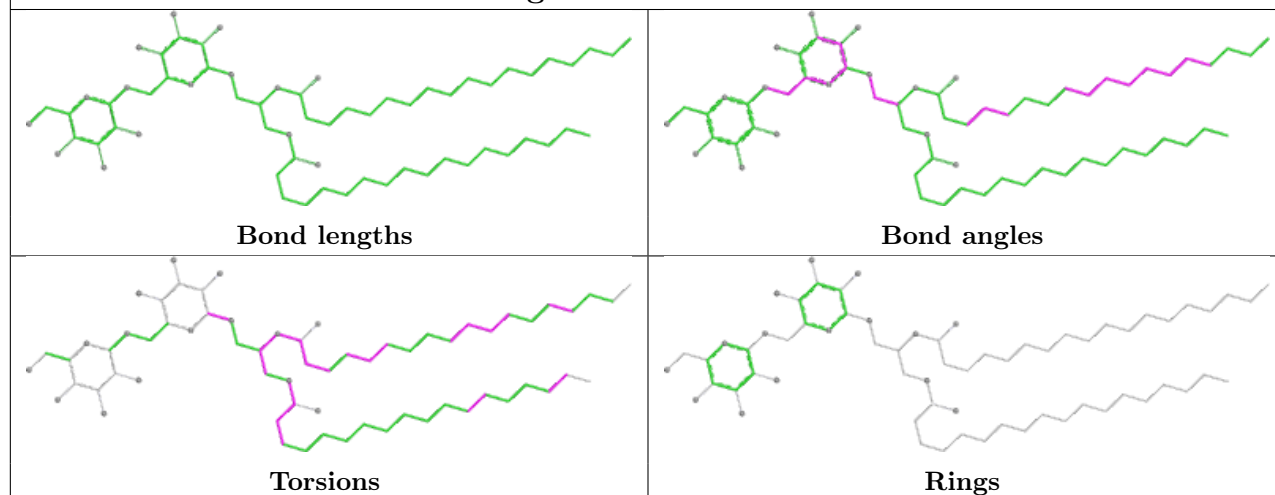
Ligand CLA A 404**Ligand BCR b 624****Ligand DGD B 626**

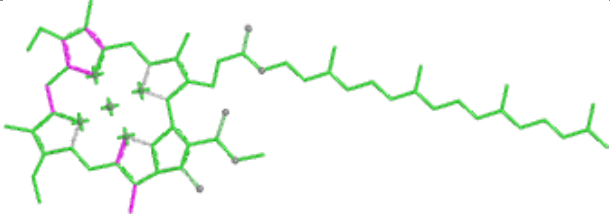
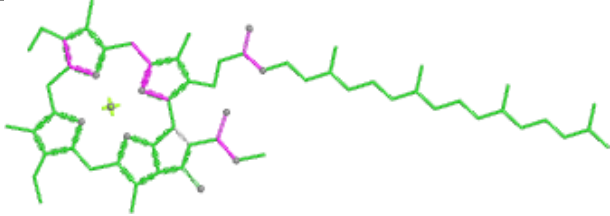
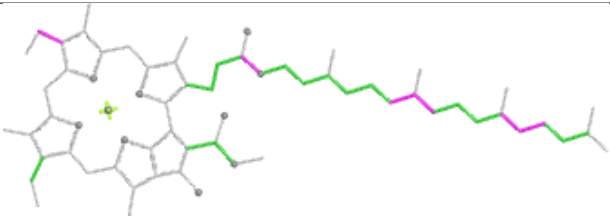
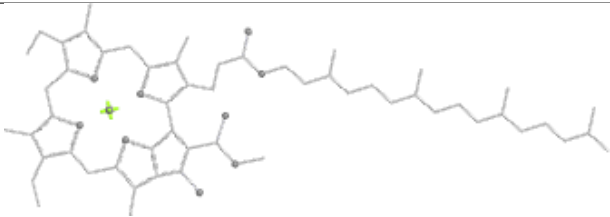
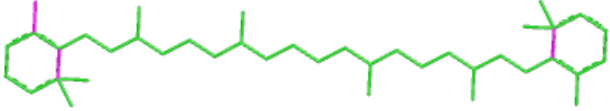
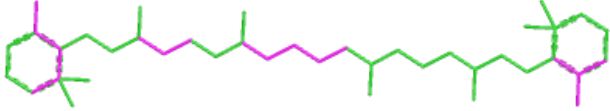
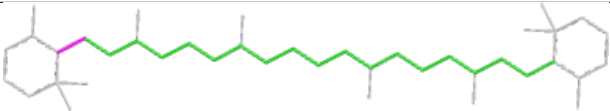
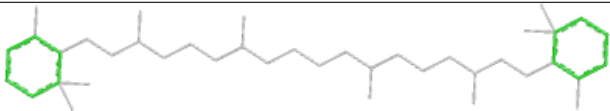
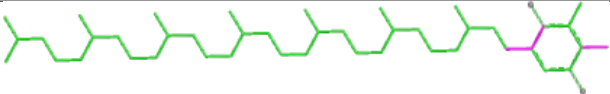
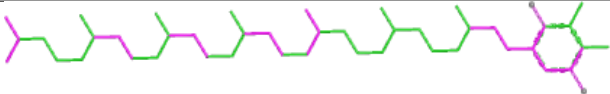
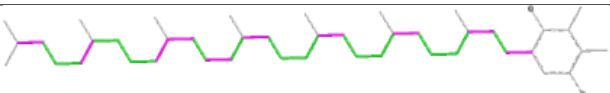
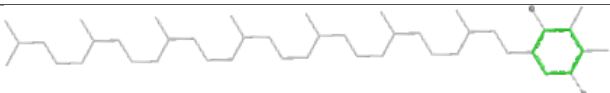


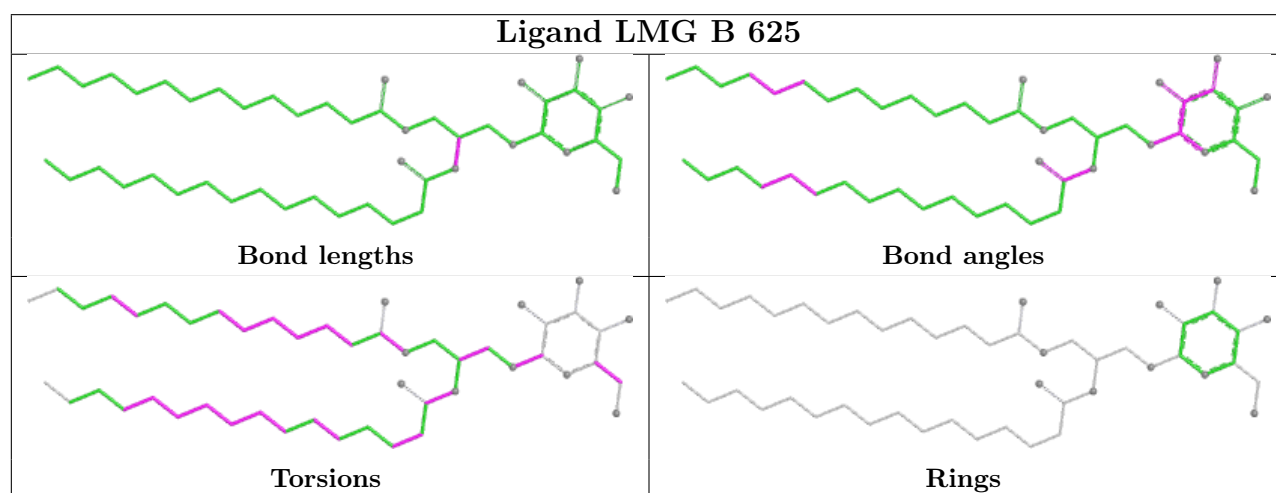
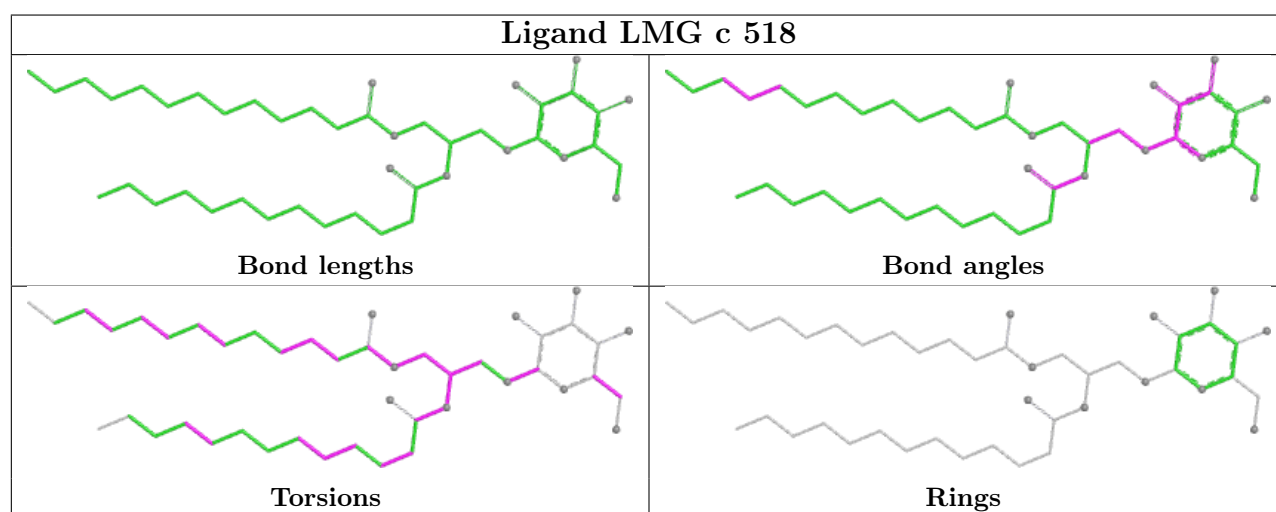
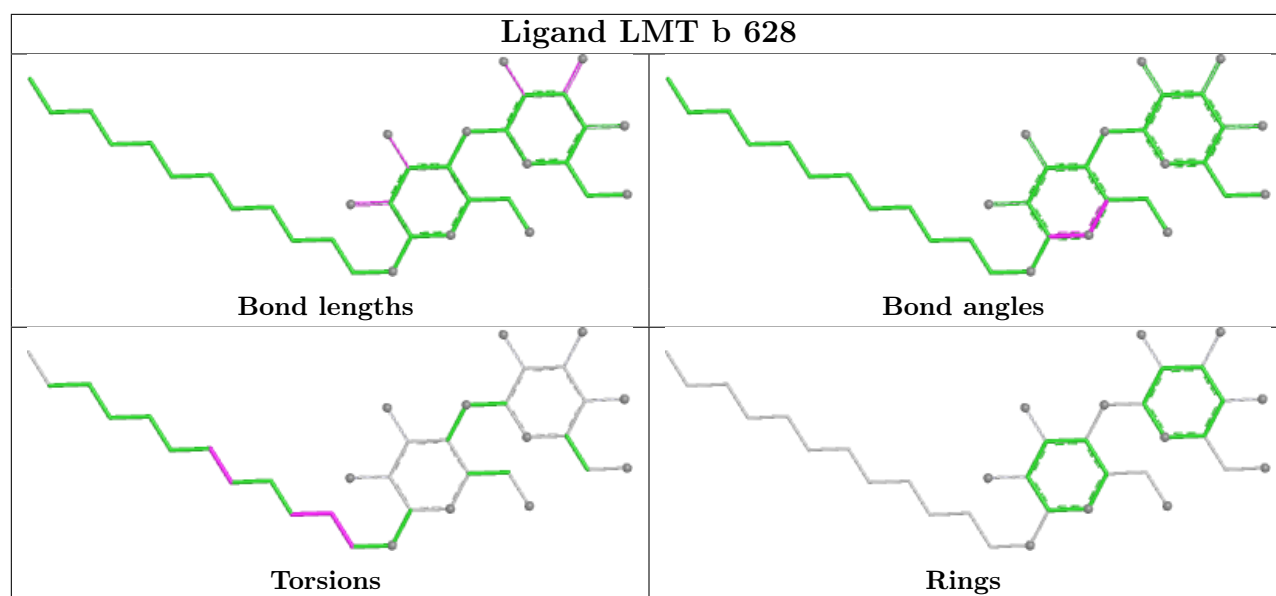
Ligand HEM f 101

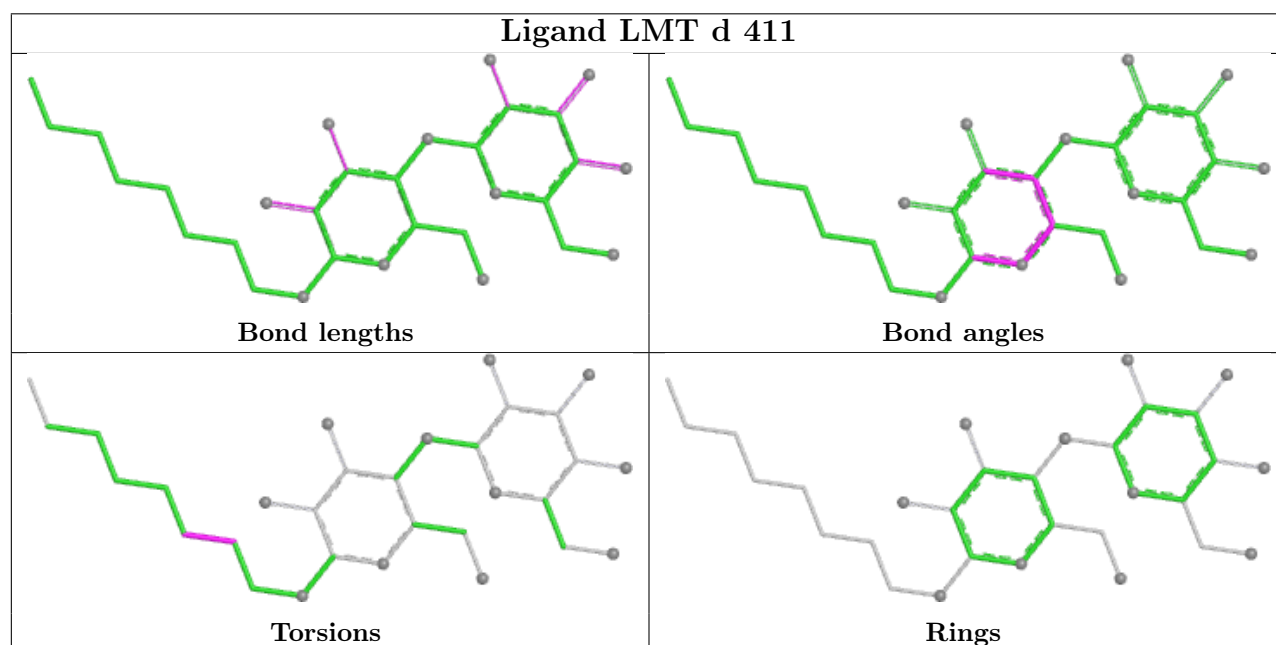
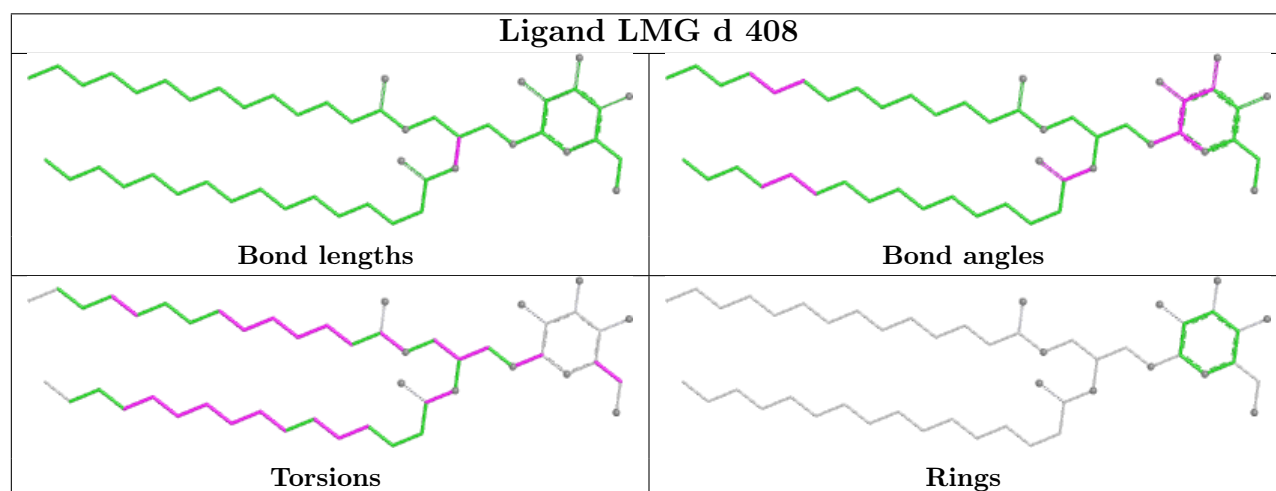
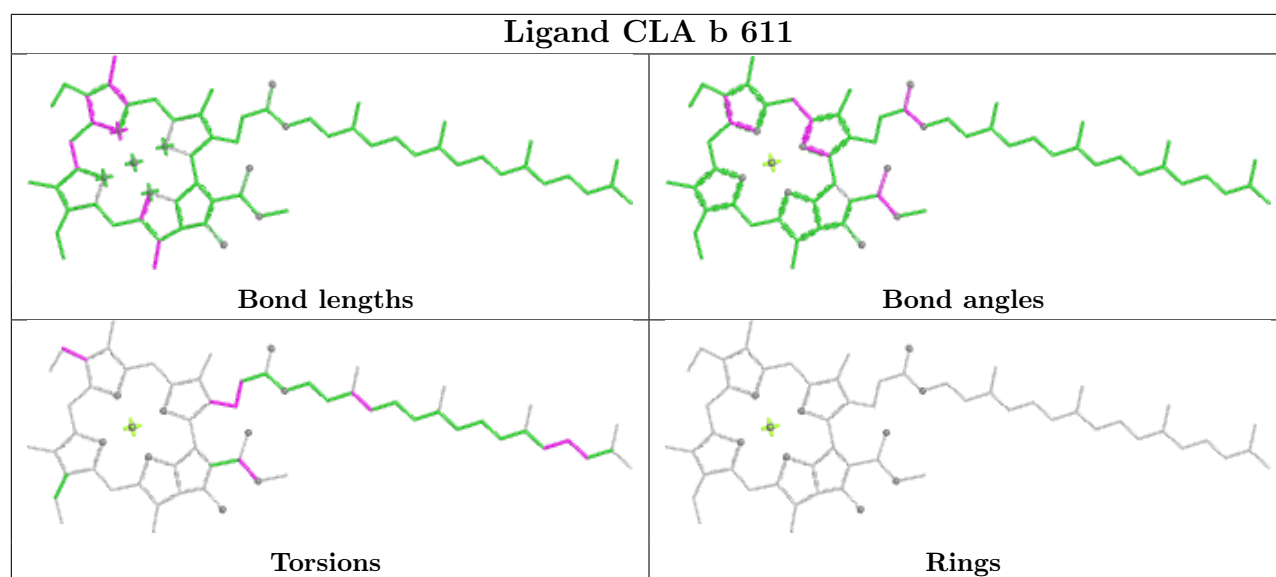


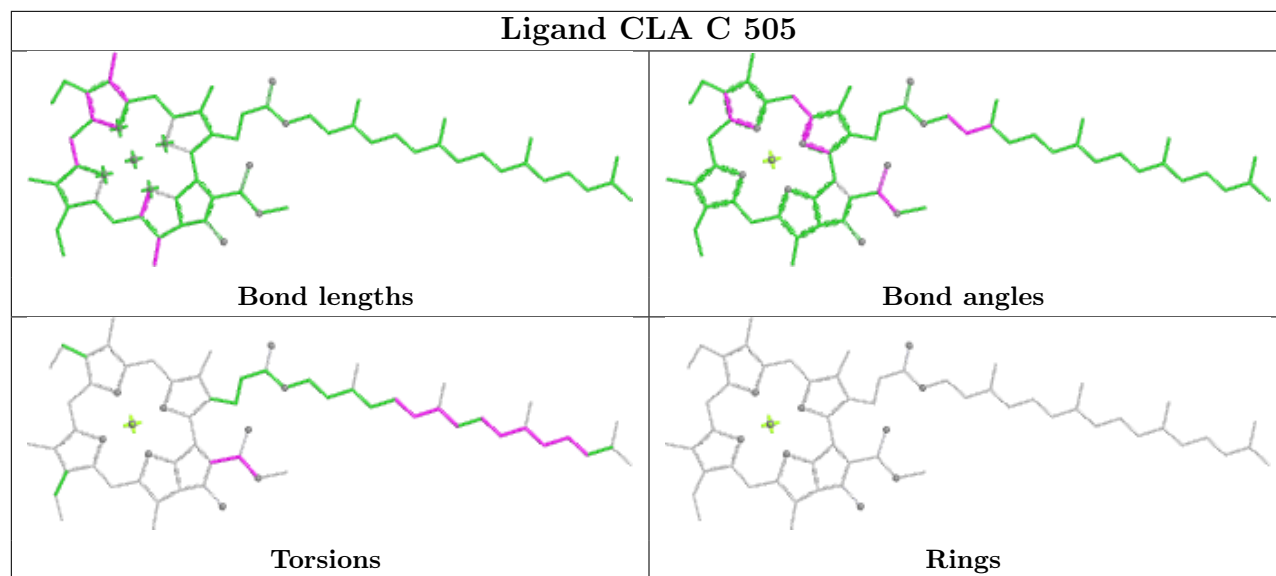
Ligand DGD C 516



Ligand CLA b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 407	
 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%)	-0.19	3 (0%) 81 67	206, 208, 208, 209	0
1	a	335/344 (97%)	-0.26	3 (0%) 81 67	206, 208, 209, 209	0
2	B	490/510 (96%)	-0.20	8 (1%) 70 57	206, 207, 209, 210	0
2	b	490/510 (96%)	-0.20	9 (1%) 67 55	206, 208, 209, 210	0
3	C	447/461 (96%)	-0.18	8 (1%) 67 55	206, 208, 209, 209	0
3	c	447/461 (96%)	-0.19	6 (1%) 75 61	205, 208, 209, 210	0
4	D	340/352 (96%)	-0.24	2 (0%) 85 73	205, 207, 208, 210	0
4	d	340/352 (96%)	-0.28	6 (1%) 67 55	206, 208, 209, 209	0
5	E	82/84 (97%)	-0.16	3 (3%) 45 40	206, 208, 209, 209	0
5	e	82/84 (97%)	-0.20	0 100 100	207, 208, 209, 209	0
6	F	35/45 (77%)	-0.24	0 100 100	207, 207, 208, 209	0
6	f	35/45 (77%)	-0.35	0 100 100	207, 208, 209, 209	0
7	H	65/66 (98%)	0.29	3 (4%) 37 35	206, 208, 209, 209	0
7	h	65/66 (98%)	0.28	4 (6%) 26 29	206, 208, 209, 209	0
8	I	35/38 (92%)	-0.27	0 100 100	207, 208, 209, 209	0
8	i	35/38 (92%)	-0.33	0 100 100	206, 207, 209, 210	0
9	J	34/40 (85%)	-0.25	0 100 100	207, 208, 208, 209	0
9	j	34/40 (85%)	-0.22	1 (2%) 53 44	206, 208, 209, 209	0
10	K	37/46 (80%)	-0.30	2 (5%) 31 31	207, 208, 209, 209	0
10	k	37/46 (80%)	-0.33	0 100 100	207, 208, 209, 209	0
11	L	37/37 (100%)	-0.32	0 100 100	207, 208, 209, 209	0
11	l	37/37 (100%)	-0.42	0 100 100	206, 208, 209, 210	0
12	M	34/36 (94%)	-0.10	1 (2%) 53 44	206, 207, 208, 209	0
12	m	34/36 (94%)	-0.27	0 100 100	207, 207, 208, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	-0.08	7 (2%) 53 44	205, 208, 209, 210	0
13	o	243/272 (89%)	-0.11	4 (1%) 70 57	206, 208, 209, 210	0
14	T	32/32 (100%)	-0.27	0 100 100	206, 208, 208, 209	0
14	t	32/32 (100%)	-0.18	0 100 100	206, 207, 209, 209	0
15	U	97/134 (72%)	-0.30	2 (2%) 63 51	206, 207, 208, 209	0
15	u	97/134 (72%)	-0.01	0 100 100	206, 207, 208, 209	0
16	V	137/163 (84%)	-0.05	1 (0%) 84 71	206, 207, 208, 209	0
16	v	137/163 (84%)	-0.15	1 (0%) 84 71	206, 208, 209, 209	0
17	g	28/46 (60%)	0.14	0 100 100	207, 208, 209, 209	0
17	y	28/46 (60%)	-0.31	0 100 100	206, 208, 209, 209	0
18	X	37/41 (90%)	0.03	1 (2%) 56 46	206, 208, 209, 210	0
18	x	37/41 (90%)	-0.04	0 100 100	207, 208, 208, 209	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.42	0 100 100	206, 207, 208, 209	0
20	z	62/62 (100%)	-0.22	0 100 100	207, 208, 209, 210	0
All	All	5214/5674 (91%)	-0.18	75 (1%) 73 59	205, 208, 209, 210	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	250	ALA	5.2
2	B	218	LEU	4.9
3	C	324	LEU	4.8
2	B	214	LEU	4.4
2	B	50	PRO	4.2

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
32	LMT	I	102	35/35	0.49	0.17	206,208,210,210	0
32	LMT	d	411	31/35	0.51	0.16	206,209,210,211	0
22	CLA	b	620	65/65	0.61	0.16	206,208,209,210	0
32	LMT	D	408	31/35	0.61	0.14	207,208,210,210	0
22	CLA	B	601	65/65	0.65	0.17	205,208,209,209	0
35	CA	O	301	1/1	0.65	0.11	208,208,208,208	0
22	CLA	b	605	65/65	0.66	0.21	206,208,210,210	0
32	LMT	b	629	35/35	0.67	0.14	206,208,209,210	0
32	LMT	b	628	35/35	0.68	0.13	206,208,210,210	0
32	LMT	B	628	35/35	0.68	0.13	206,208,210,211	0
32	LMT	i	103	35/35	0.69	0.15	206,209,210,210	0
32	LMT	M	102	35/35	0.71	0.19	205,208,209,209	0
31	LMG	I	101	43/55	0.72	0.20	205,208,210,211	0
25	BCR	H	102	40/40	0.73	0.22	206,207,209,210	0
32	LMT	b	603	35/35	0.74	0.13	206,208,210,210	0
30	SQD	B	627	47/54	0.77	0.14	206,208,210,212	0
26	DGD	B	626	52/66	0.77	0.18	206,208,210,211	0
31	LMG	C	517	45/55	0.78	0.17	206,207,209,210	0
27	LHG	c	519	37/49	0.78	0.17	204,207,210,213	0
25	BCR	j	102	40/40	0.79	0.25	206,208,209,210	0
31	LMG	b	627	42/55	0.79	0.21	204,207,211,211	0
26	DGD	d	410	63/66	0.80	0.18	206,208,210,211	0
26	DGD	C	516	66/66	0.80	0.20	205,207,208,208	0
26	DGD	b	601	52/66	0.81	0.17	204,208,209,210	0
35	CA	K	102	1/1	0.81	0.12	210,210,210,210	0
31	LMG	e	101	44/55	0.81	0.22	205,208,209,211	0
32	LMT	b	604	35/35	0.82	0.13	207,208,210,210	0
27	LHG	C	518	37/49	0.83	0.12	205,208,210,211	0
22	CLA	C	512	65/65	0.83	0.15	205,207,209,211	0
32	LMT	B	623	35/35	0.83	0.10	206,208,210,210	0
26	DGD	a	408	56/66	0.83	0.18	206,208,210,211	0
32	LMT	B	629	35/35	0.83	0.14	206,208,209,210	0
26	DGD	A	409	56/66	0.83	0.20	206,208,210,211	0
22	CLA	C	506	65/65	0.83	0.16	206,207,208,209	0
31	LMG	b	626	49/55	0.83	0.18	205,207,209,209	0
32	LMT	B	624	35/35	0.84	0.14	206,207,211,212	0
31	LMG	i	102	43/55	0.84	0.16	205,207,209,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	DGD	D	407	63/66	0.85	0.17	206,208,209,210	0
25	BCR	b	624	40/40	0.85	0.14	205,206,207,208	0
25	BCR	c	521	40/40	0.85	0.20	206,208,209,209	0
31	LMG	B	621	49/55	0.85	0.16	206,207,208,209	0
24	PL9	A	407	45/55	0.85	0.23	206,207,208,210	0
31	LMG	m	101	42/55	0.85	0.20	205,207,209,210	0
31	LMG	E	101	44/55	0.85	0.16	204,208,209,210	0
25	BCR	g	101	40/40	0.86	0.16	205,207,208,209	0
22	CLA	c	512	65/65	0.86	0.15	206,207,209,210	0
24	PL9	d	407	55/55	0.86	0.15	205,207,208,208	0
31	LMG	a	402	42/55	0.86	0.18	204,207,209,210	0
25	BCR	J	102	40/40	0.87	0.23	205,207,209,209	0
27	LHG	a	409	39/49	0.87	0.16	206,207,209,209	0
22	CLA	C	508	65/65	0.87	0.14	205,207,208,209	0
30	SQD	A	413	51/54	0.87	0.16	204,207,209,209	0
26	DGD	b	625	58/66	0.87	0.17	206,207,208,209	0
24	PL9	J	101	35/55	0.87	0.21	206,207,210,210	0
35	CA	k	101	1/1	0.87	0.05	208,208,208,208	0
22	CLA	b	607	65/65	0.88	0.13	205,207,208,208	0
30	SQD	b	602	47/54	0.88	0.14	205,208,209,212	0
26	DGD	C	515	62/66	0.88	0.12	205,207,209,210	0
22	CLA	a	405	65/65	0.88	0.18	205,207,209,209	0
33	BCT	d	404	4/4	0.88	0.17	206,207,208,208	0
25	BCR	b	621	40/40	0.88	0.22	206,207,208,208	0
25	BCR	C	513	40/40	0.88	0.18	205,207,208,208	0
26	DGD	B	620	58/66	0.88	0.16	205,207,209,209	0
35	CA	o	301	1/1	0.88	0.08	209,209,209,209	0
30	SQD	d	403	43/54	0.89	0.13	205,208,209,209	0
25	BCR	B	616	40/40	0.89	0.15	205,207,208,209	0
25	BCR	i	101	40/40	0.89	0.22	206,207,208,208	0
22	CLA	a	406	65/65	0.89	0.14	206,208,208,209	0
26	DGD	c	516	62/66	0.89	0.13	206,208,208,209	0
31	LMG	M	101	42/55	0.89	0.14	205,208,209,210	0
25	BCR	C	520	40/40	0.89	0.19	206,207,209,210	0
23	PHO	A	405	64/64	0.89	0.12	205,207,208,209	0
22	CLA	b	619	65/65	0.89	0.12	206,208,209,209	0
22	CLA	C	511	65/65	0.89	0.14	206,207,208,209	0
25	BCR	b	622	40/40	0.89	0.15	205,207,208,208	0
30	SQD	A	414	54/54	0.89	0.15	205,207,209,210	0
30	SQD	B	622	43/54	0.89	0.17	205,208,209,212	0
22	CLA	c	510	65/65	0.89	0.10	206,208,209,211	0
25	BCR	c	514	40/40	0.89	0.18	206,208,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PL9	j	101	35/55	0.90	0.20	205,208,209,210	0
22	CLA	B	615	65/65	0.90	0.12	206,207,209,209	0
31	LMG	c	518	45/55	0.90	0.13	206,208,209,210	0
31	LMG	C	521	48/55	0.90	0.16	206,207,208,209	0
27	LHG	A	410	39/49	0.90	0.16	206,207,209,210	0
22	CLA	A	406	65/65	0.90	0.13	206,208,209,209	0
23	PHO	d	401	64/64	0.90	0.11	206,207,208,208	0
25	BCR	b	623	40/40	0.90	0.17	205,206,207,207	0
32	LMT	M	103	35/35	0.91	0.11	206,208,209,209	0
31	LMG	c	522	48/55	0.91	0.17	205,207,209,210	0
24	PL9	a	407	45/55	0.91	0.18	205,207,208,209	0
22	CLA	b	606	65/65	0.91	0.17	205,207,209,210	0
31	LMG	D	406	48/55	0.91	0.14	204,207,208,209	0
22	CLA	D	404	65/65	0.91	0.14	205,207,208,208	0
30	SQD	F	103	45/54	0.91	0.16	205,208,209,210	0
30	SQD	a	401	54/54	0.91	0.14	205,208,210,213	0
30	SQD	a	412	51/54	0.91	0.16	205,207,208,209	0
22	CLA	c	508	65/65	0.91	0.11	205,208,209,209	0
25	BCR	y	101	40/40	0.91	0.17	206,207,208,208	0
25	BCR	B	619	40/40	0.91	0.13	205,207,208,208	0
25	BCR	F	102	40/40	0.92	0.17	205,207,208,208	0
25	BCR	x	101	40/40	0.92	0.14	206,207,209,209	0
22	CLA	C	505	65/65	0.92	0.14	206,207,209,210	0
22	CLA	C	519	65/65	0.92	0.13	205,207,209,209	0
22	CLA	c	502	65/65	0.92	0.13	206,207,208,209	0
22	CLA	c	503	65/65	0.92	0.10	206,207,208,209	0
22	CLA	c	505	65/65	0.92	0.15	205,207,208,209	0
22	CLA	C	509	65/65	0.92	0.11	205,207,208,208	0
25	BCR	A	408	40/40	0.92	0.16	206,207,208,208	0
22	CLA	A	404	65/65	0.92	0.15	204,207,208,209	0
22	CLA	c	511	65/65	0.92	0.13	206,208,209,209	0
31	LMG	d	408	49/55	0.92	0.13	205,207,208,209	0
22	CLA	b	610	65/65	0.92	0.11	206,207,209,209	0
26	DGD	c	517	66/66	0.92	0.12	206,207,209,209	0
30	SQD	f	103	45/54	0.92	0.14	205,208,210,210	0
22	CLA	b	614	65/65	0.92	0.12	206,207,209,210	0
31	LMG	B	625	49/55	0.92	0.14	205,207,208,208	0
22	CLA	b	611	65/65	0.93	0.12	206,207,208,209	0
22	CLA	a	404	65/65	0.93	0.14	204,207,208,208	0
31	LMG	d	409	48/55	0.93	0.12	206,207,209,210	0
22	CLA	C	510	65/65	0.93	0.09	206,207,209,209	0
26	DGD	c	515	53/66	0.93	0.14	205,207,209,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	I	101	51/55	0.93	0.12	206,207,209,209	0
22	CLA	B	609	65/65	0.93	0.10	206,207,209,210	0
22	CLA	B	613	65/65	0.93	0.11	206,207,208,209	0
22	CLA	B	607	65/65	0.93	0.10	206,207,208,209	0
26	DGD	C	514	53/66	0.93	0.14	205,206,208,209	0
24	PL9	D	405	55/55	0.93	0.12	205,207,208,208	0
22	CLA	D	403	65/65	0.93	0.10	205,207,208,208	0
22	CLA	C	501	65/65	0.93	0.12	206,208,209,209	0
28	CL	a	410	1/1	0.94	0.21	205,205,205,205	0
22	CLA	C	507	65/65	0.94	0.14	206,207,208,208	0
31	LMG	L	101	51/55	0.94	0.13	205,207,208,209	0
22	CLA	c	506	65/65	0.94	0.10	206,208,209,209	0
22	CLA	B	610	65/65	0.94	0.10	205,207,208,208	0
22	CLA	b	616	65/65	0.94	0.08	206,207,208,209	0
25	BCR	c	513	40/40	0.94	0.11	206,207,208,209	0
22	CLA	b	618	65/65	0.94	0.13	206,207,209,210	0
21	FE2	A	401	1/1	0.94	0.11	209,209,209,209	0
25	BCR	f	102	40/40	0.94	0.14	206,207,208,209	0
22	CLA	d	405	65/65	0.94	0.15	205,207,208,208	0
22	CLA	b	608	65/65	0.94	0.10	205,207,208,209	0
23	PHO	D	401	64/64	0.94	0.09	205,207,208,209	0
22	CLA	c	501	65/65	0.94	0.09	206,207,209,209	0
23	PHO	d	402	64/64	0.94	0.09	206,207,209,209	0
22	CLA	b	609	65/65	0.94	0.09	206,207,208,209	0
22	CLA	B	605	65/65	0.94	0.10	206,207,208,209	0
22	CLA	C	502	65/65	0.95	0.14	206,207,208,208	0
22	CLA	c	520	65/65	0.95	0.12	206,207,208,209	0
22	CLA	b	612	65/65	0.95	0.10	205,207,209,209	0
22	CLA	d	406	65/65	0.95	0.11	206,207,209,209	0
22	CLA	b	613	65/65	0.95	0.10	205,207,208,209	0
25	BCR	B	617	40/40	0.95	0.11	205,207,208,209	0
31	LMG	d	412	46/55	0.95	0.12	205,207,208,209	0
22	CLA	H	101	65/65	0.95	0.15	206,207,208,209	0
22	CLA	a	403	65/65	0.95	0.09	205,207,208,210	0
31	LMG	D	409	46/55	0.95	0.12	205,207,208,209	0
33	BCT	D	402	4/4	0.95	0.06	208,208,208,208	0
22	CLA	C	503	65/65	0.95	0.12	206,207,208,209	0
22	CLA	c	509	65/65	0.95	0.08	206,207,209,209	0
22	CLA	B	608	65/65	0.95	0.10	205,207,209,210	0
22	CLA	B	614	65/65	0.95	0.10	205,207,208,209	0
25	BCR	K	101	40/40	0.95	0.10	206,207,208,209	0
22	CLA	B	612	65/65	0.96	0.12	203,207,208,209	0

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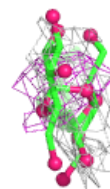
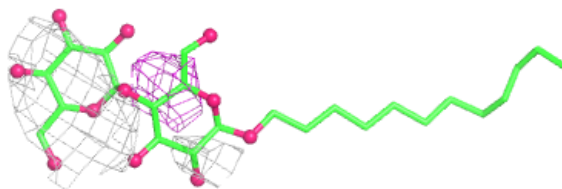
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	A	403	65/65	0.96	0.10	205,207,208,208	0
22	CLA	B	606	65/65	0.96	0.12	205,207,208,209	0
22	CLA	A	402	65/65	0.96	0.11	206,207,208,209	0
22	CLA	B	602	65/65	0.96	0.10	205,207,208,209	0
22	CLA	c	504	65/65	0.96	0.11	205,207,208,209	0
22	CLA	B	603	65/65	0.96	0.09	205,207,208,208	0
22	CLA	B	604	65/65	0.96	0.09	206,207,208,209	0
25	BCR	B	618	40/40	0.96	0.13	205,206,208,208	0
34	HEM	V	201	43/43	0.96	0.14	201,207,208,209	0
34	HEM	f	101	43/43	0.96	0.09	206,207,209,209	0
34	HEM	v	201	43/43	0.96	0.10	206,207,208,209	0
22	CLA	c	507	65/65	0.96	0.10	206,207,209,209	0
22	CLA	C	504	65/65	0.96	0.11	205,207,208,209	0
28	CL	A	411	1/1	0.96	0.06	204,204,204,204	0
22	CLA	B	611	65/65	0.96	0.10	205,207,208,208	0
34	HEM	F	101	43/43	0.97	0.08	206,207,208,210	0
22	CLA	b	615	65/65	0.97	0.09	205,207,208,209	0
21	FE2	a	413	1/1	0.97	0.05	206,206,206,206	0
22	CLA	b	617	65/65	0.97	0.10	206,207,208,209	0
29	OEX	a	411	10/10	0.98	0.07	200,204,205,206	0
29	OEX	A	412	10/10	0.99	0.07	197,202,205,206	0

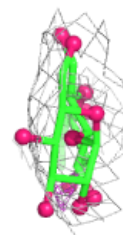
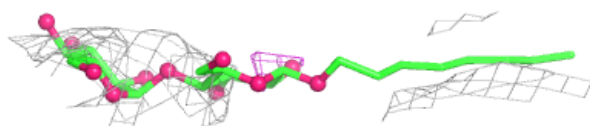
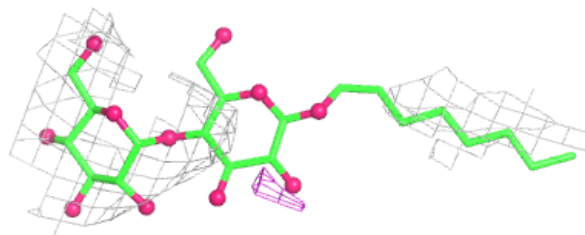
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

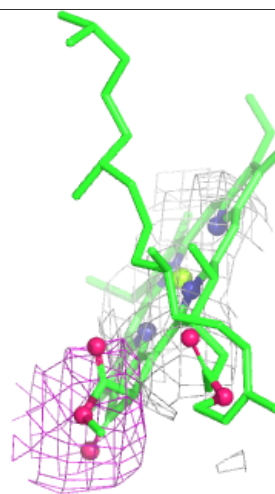
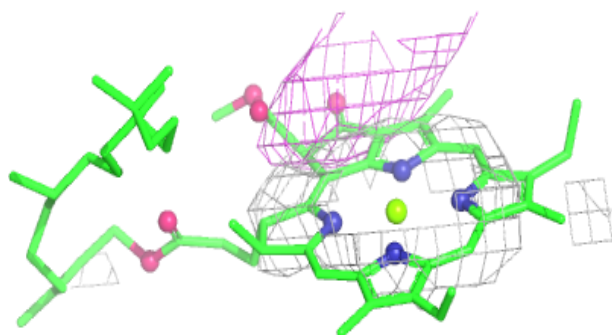
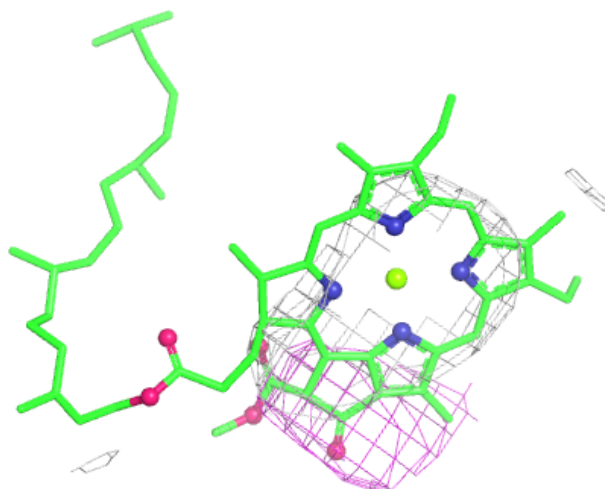
**Electron density around LMT d 411:**

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



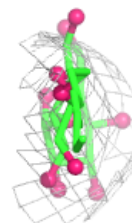
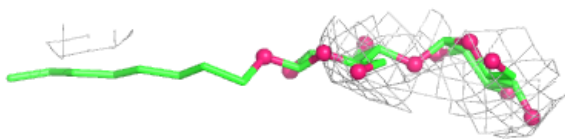
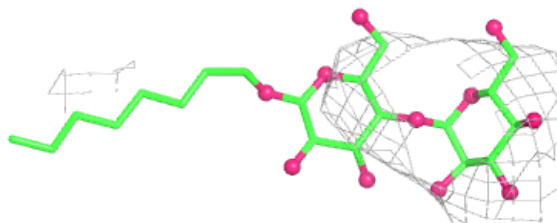
Electron density around CLA b 620:

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



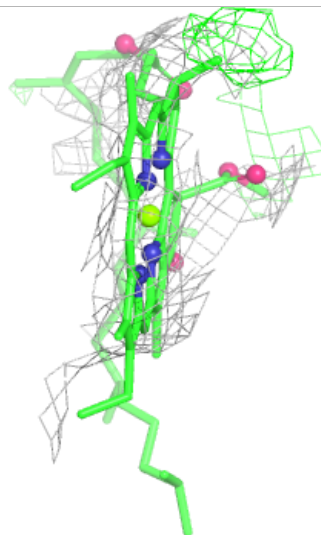
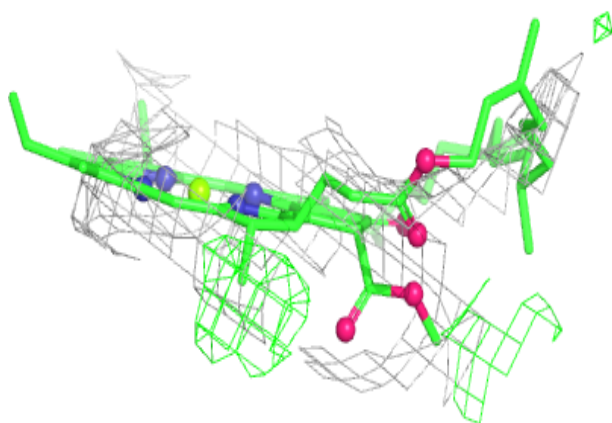
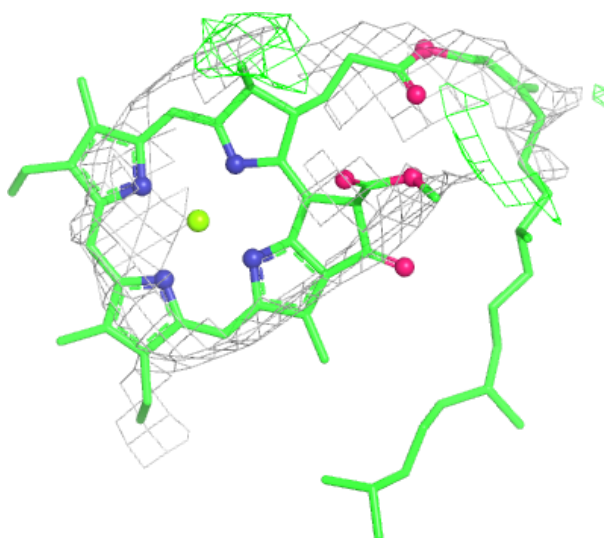
Electron density around LMT D 408:

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



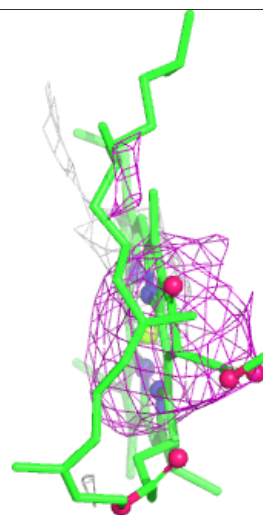
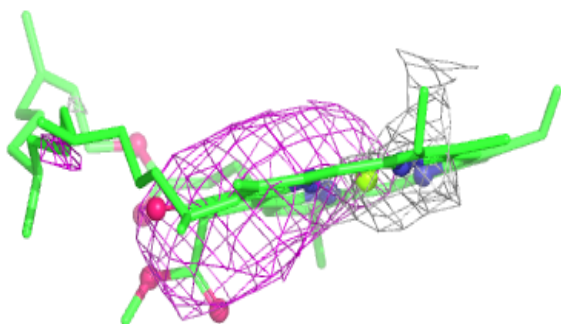
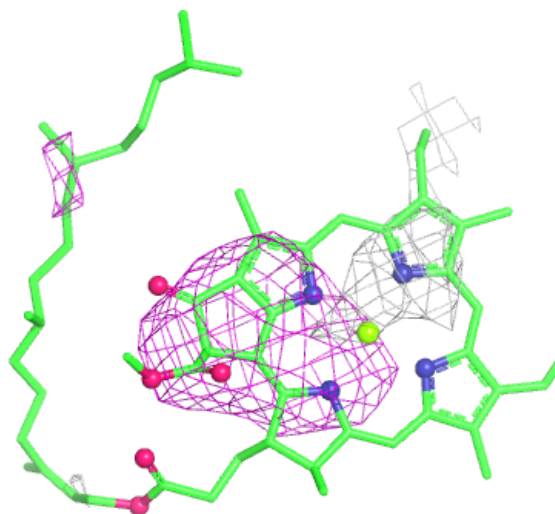
Electron density around CLA B 601:

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



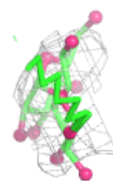
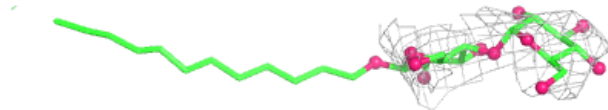
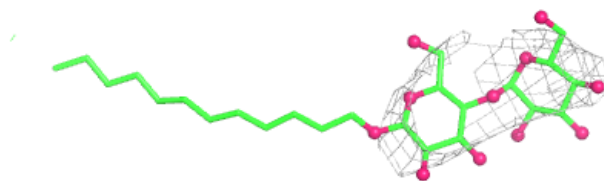
Electron density around CLA b 605:

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

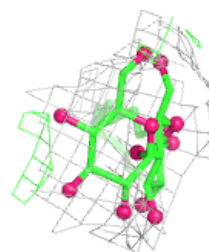
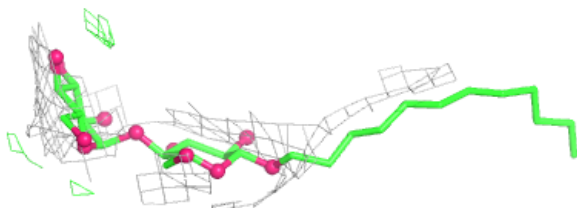
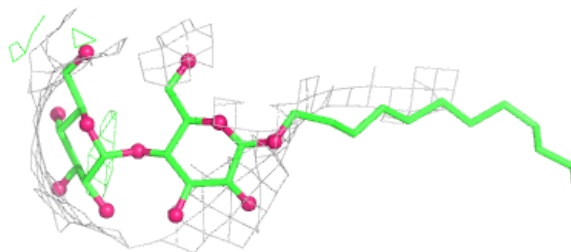


Electron density around LMT b 629:

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

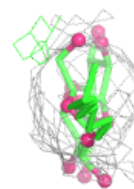
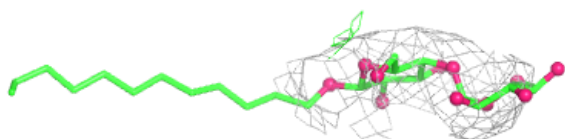
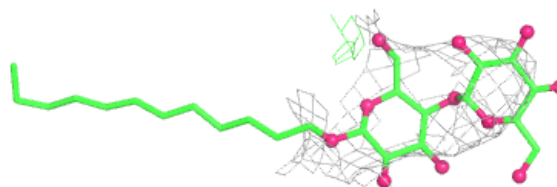
**Electron density around LMT b 628:**

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

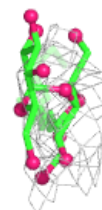
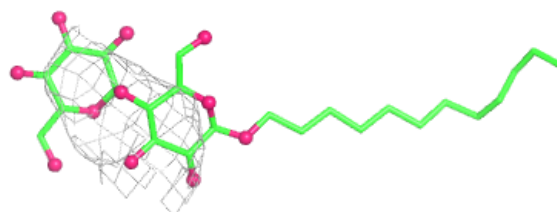


Electron density around LMT B 628:

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

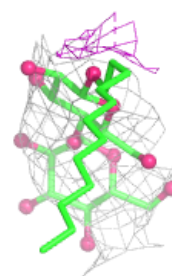
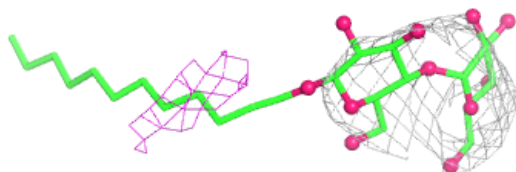
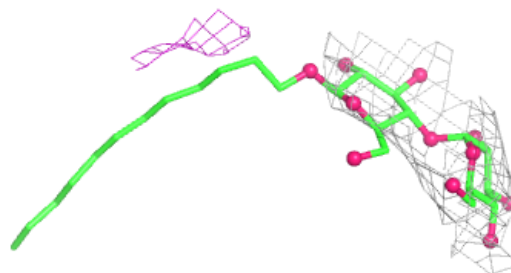
**Electron density around LMT i 103:**

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

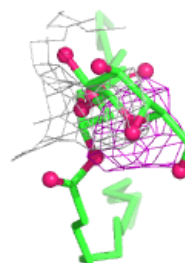
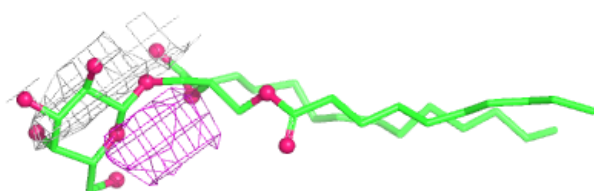
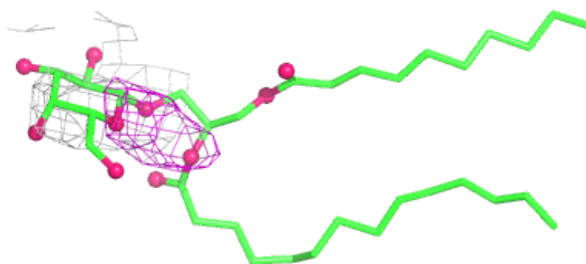


Electron density around LMT M 102:

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

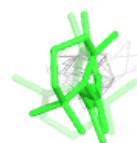
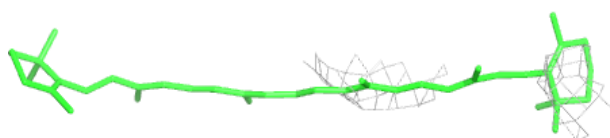
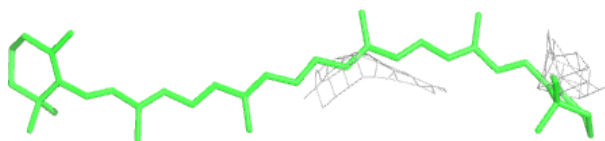
**Electron density around LMG I 101:**

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

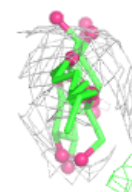
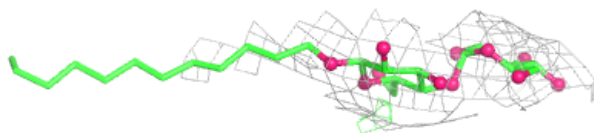
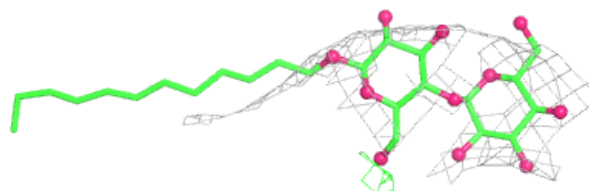


Electron density around BCR H 102:

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

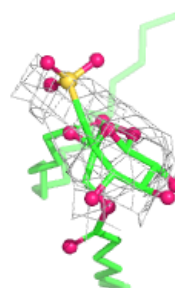
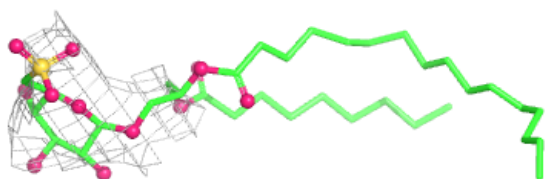
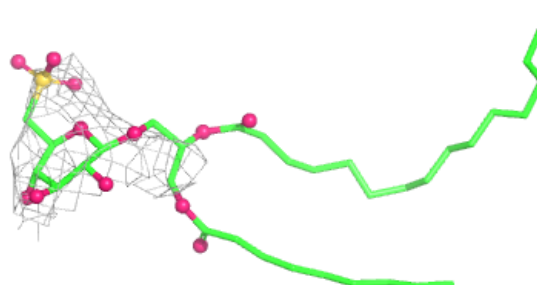
**Electron density around LMT b 603:**

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

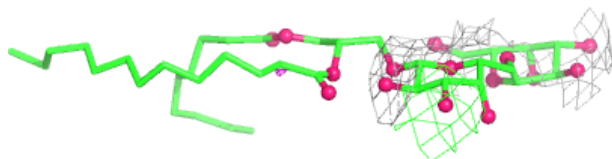
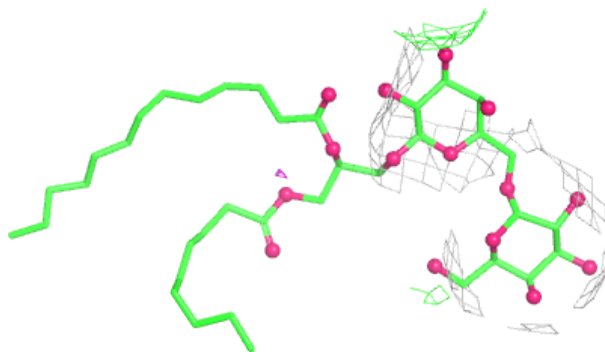


Electron density around SQD B 627:

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

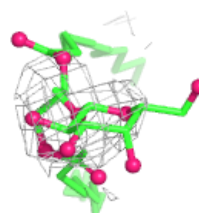
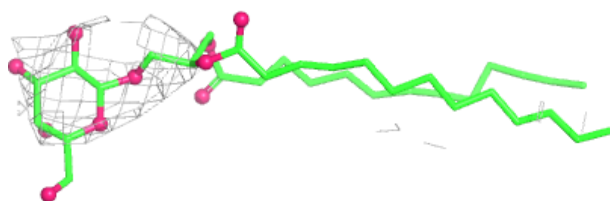
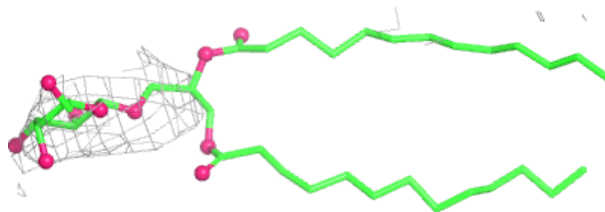
**Electron density around DGD B 626:**

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

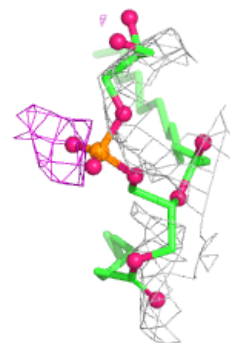
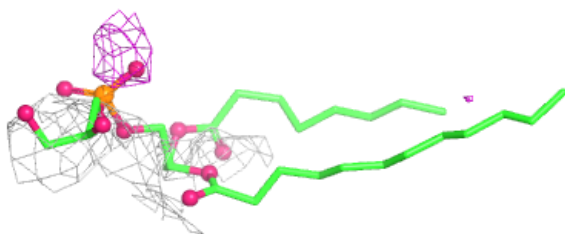
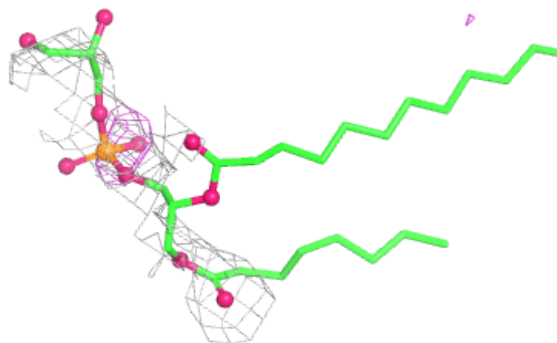


Electron density around LMG C 517:

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

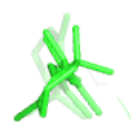
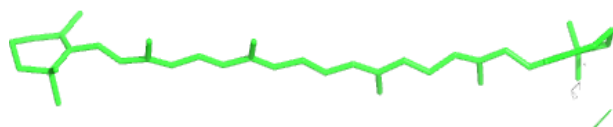
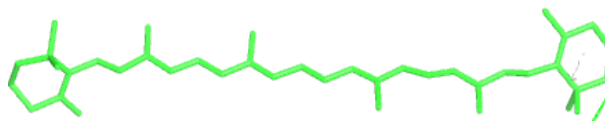
**Electron density around LHG c 519:**

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

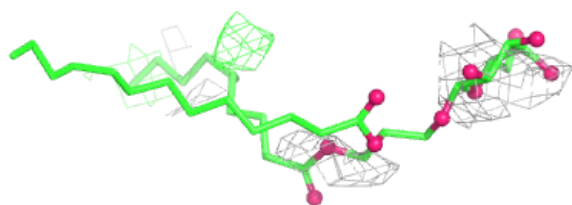
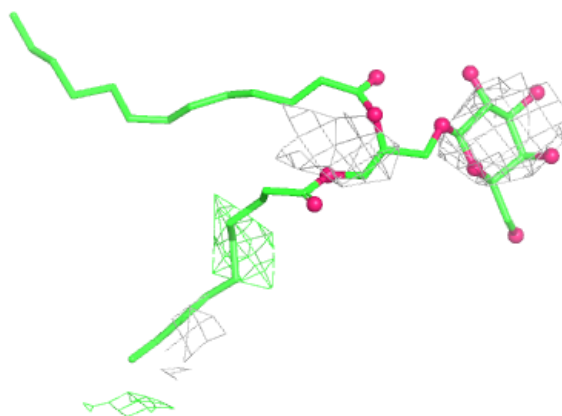


Electron density around BCR j 102:

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

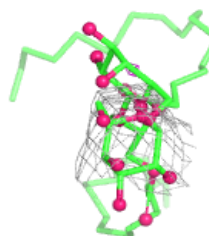
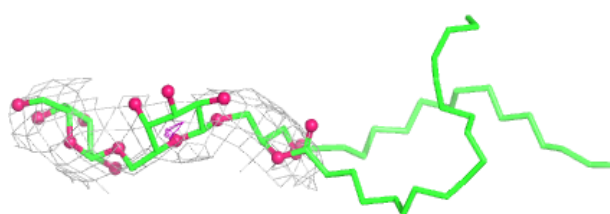
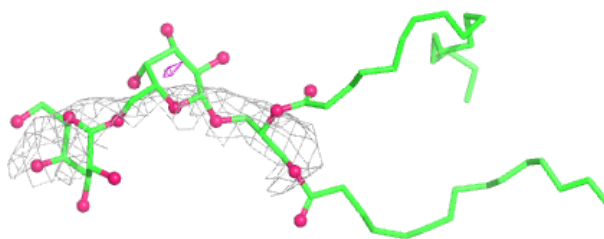
**Electron density around LMG b 627:**

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

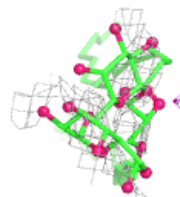
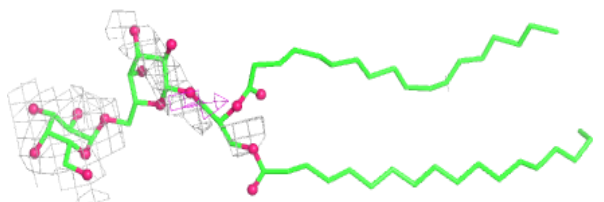


Electron density around DGD d 410:

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

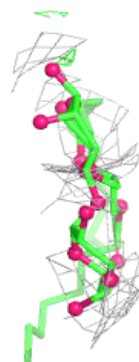
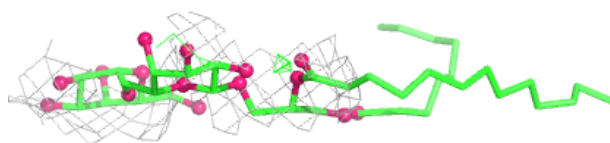
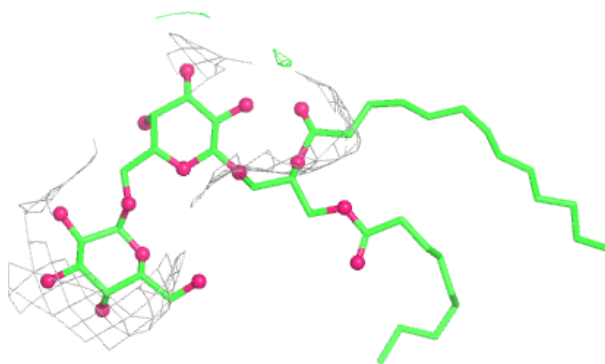
**Electron density around DGD C 516:**

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

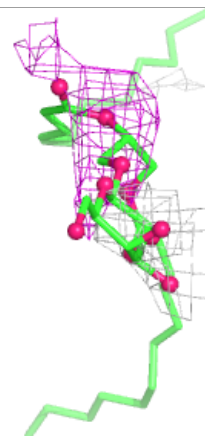
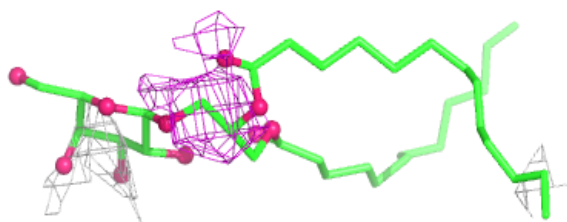
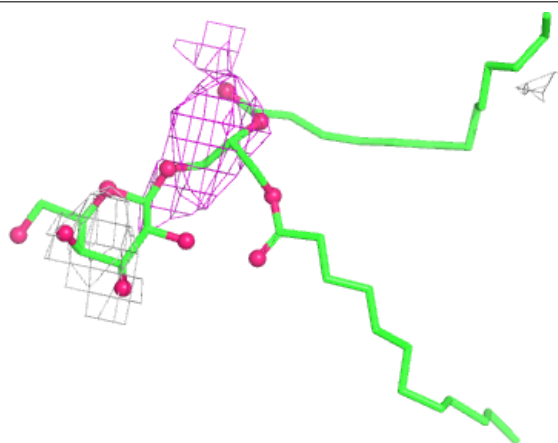


Electron density around DGD b 601:

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

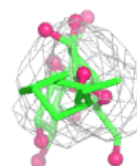
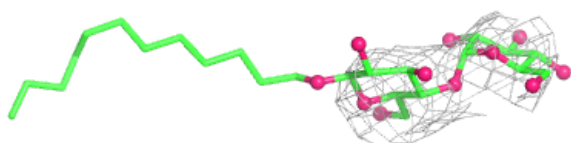
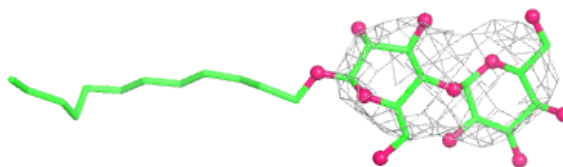
**Electron density around LMG e 101:**

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

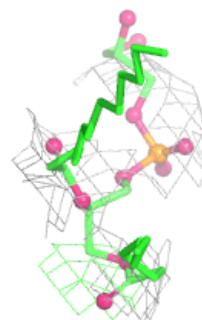
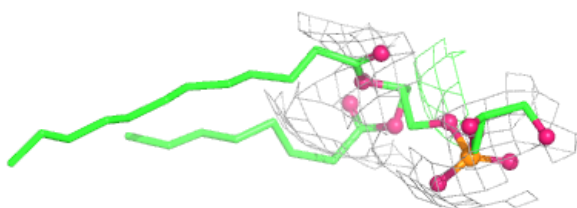


Electron density around LMT b 604:

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

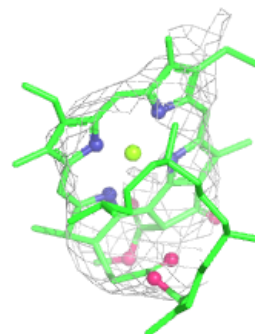
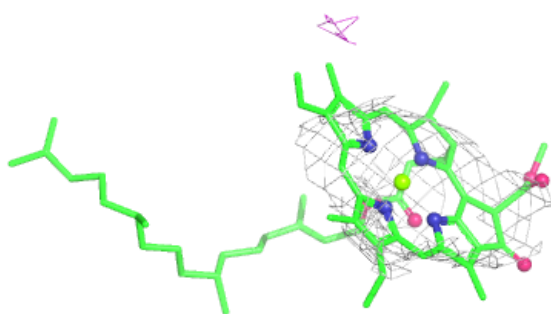
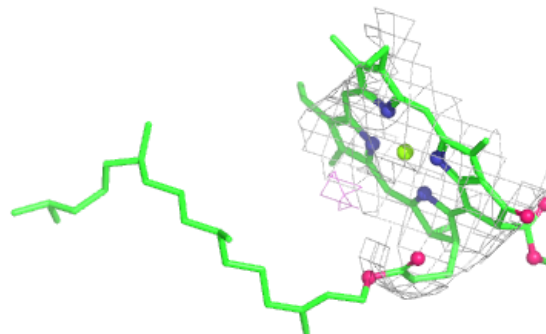
**Electron density around LHG C 518:**

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

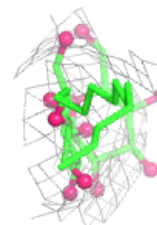
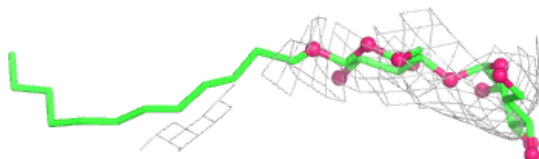
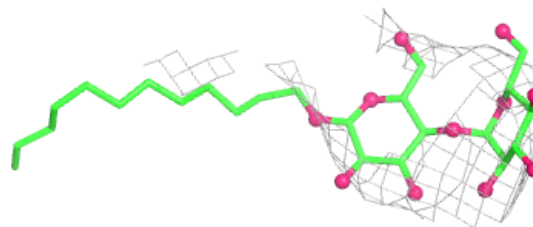


Electron density around CLA C 512:

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

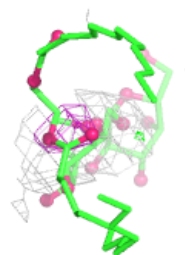
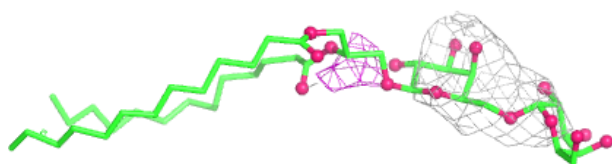
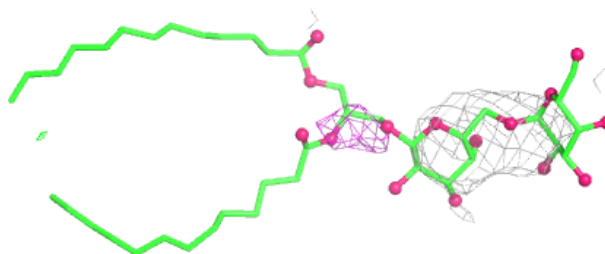
**Electron density around LMT B 623:**

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

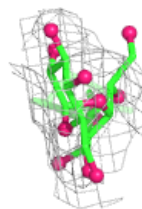
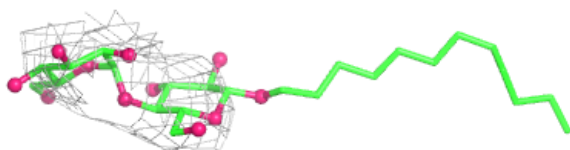
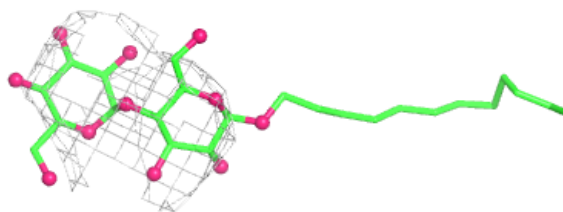


Electron density around DGD a 408:

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

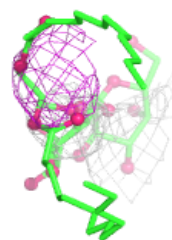
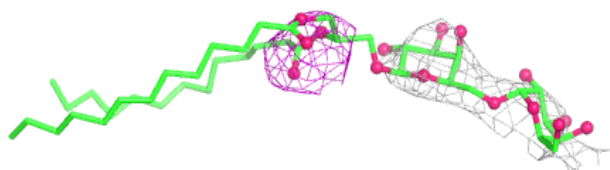
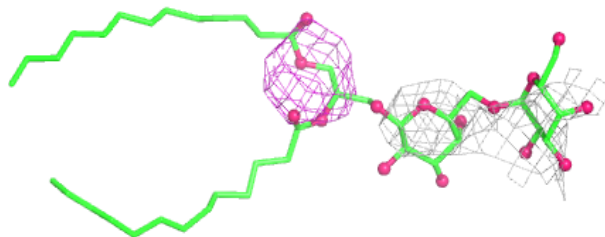
**Electron density around LMT B 629:**

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

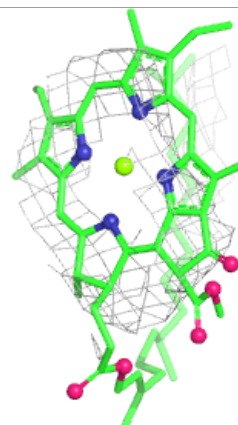
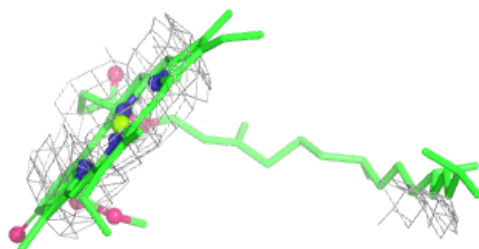
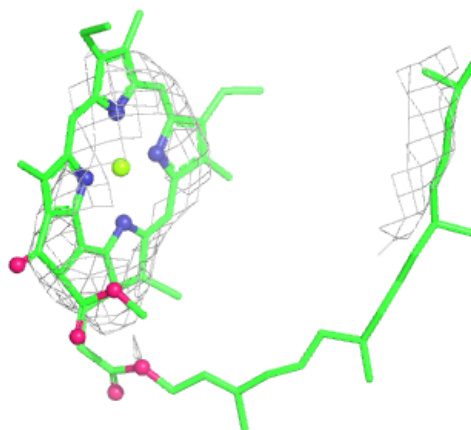


Electron density around DGD A 409:

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

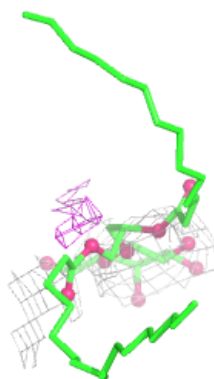
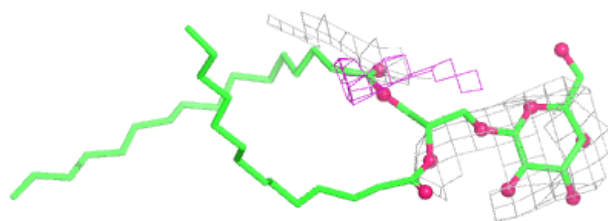
**Electron density around CLA C 506:**

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

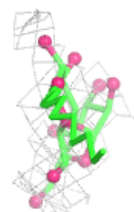
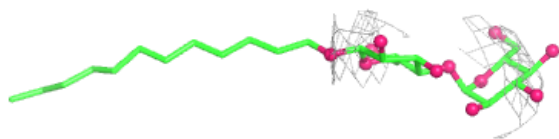
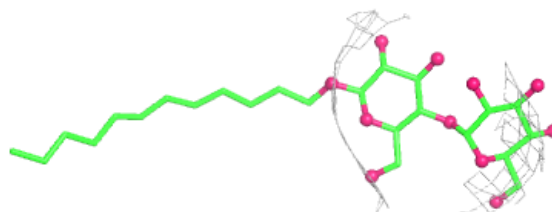


Electron density around LMG b 626:

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

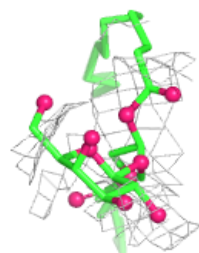
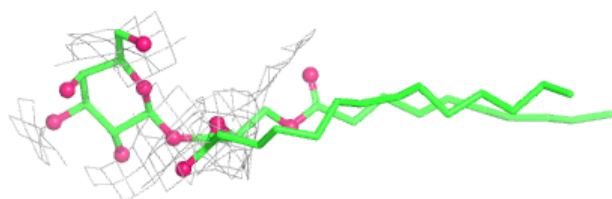
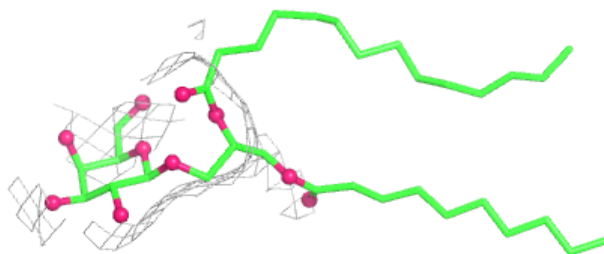
**Electron density around LMT B 624:**

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

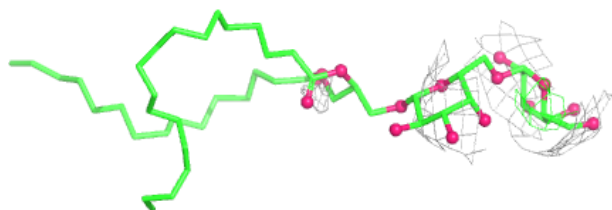
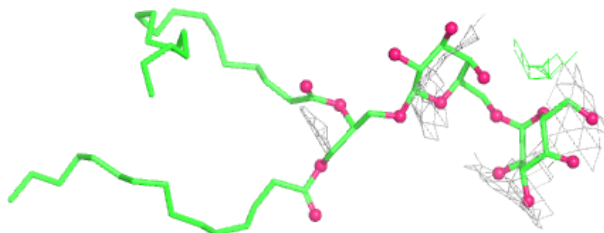


Electron density around LMG i 102:

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

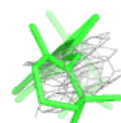
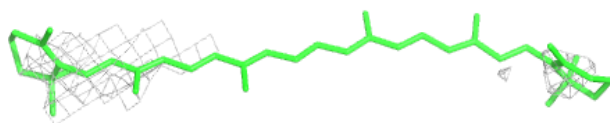
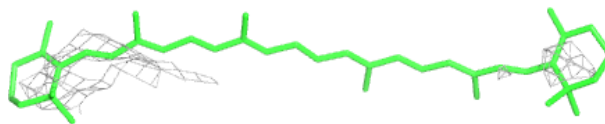
**Electron density around DGD D 407:**

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

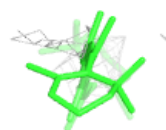
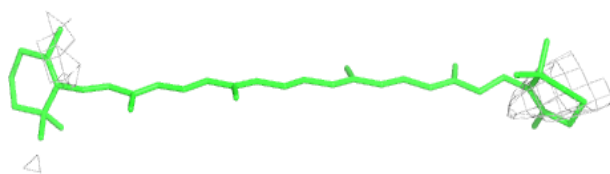
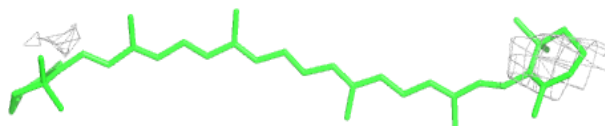


Electron density around BCR b 624:

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

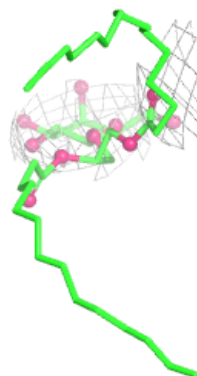
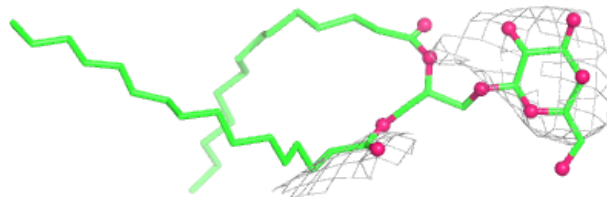
**Electron density around BCR c 521:**

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

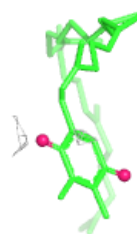
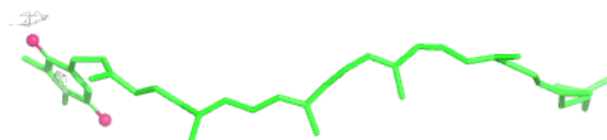
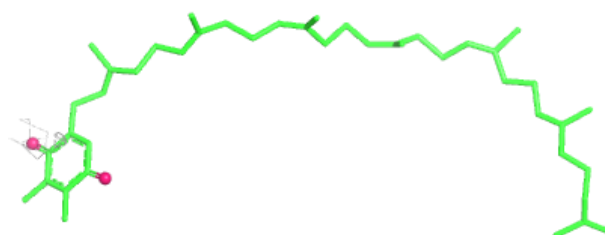


Electron density around LMG B 621:

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

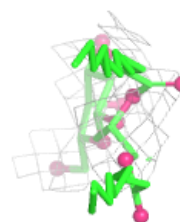
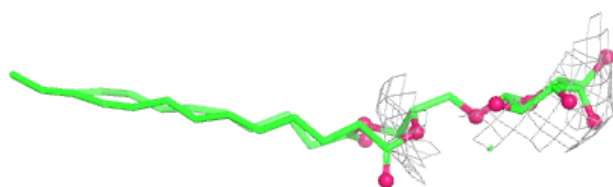
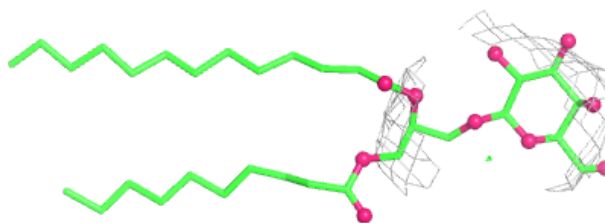
**Electron density around PL9 A 407:**

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

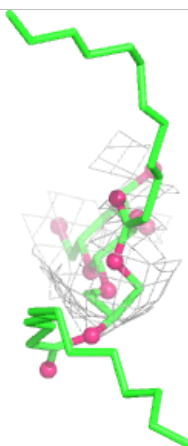
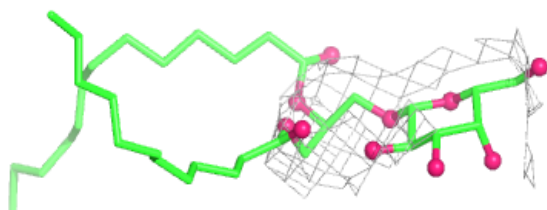


Electron density around LMG m 101:

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

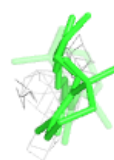
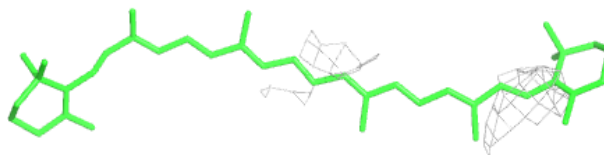
**Electron density around LMG E 101:**

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

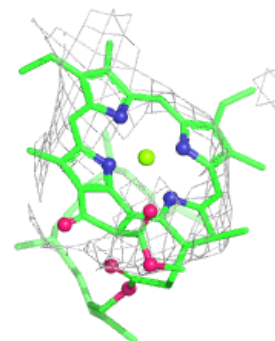
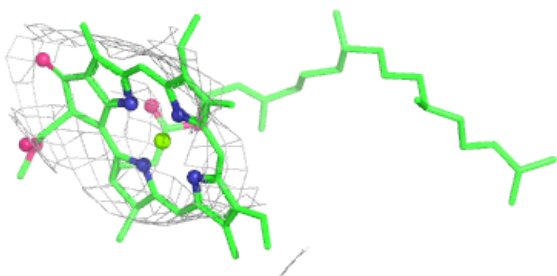
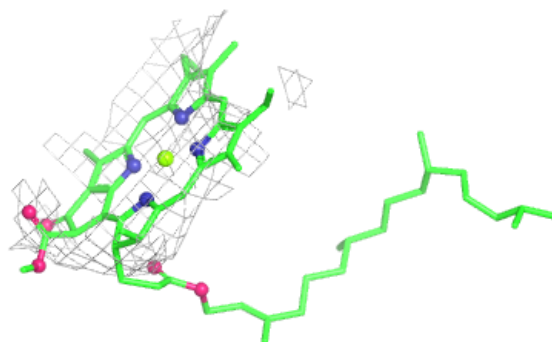


Electron density around BCR g 101:

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

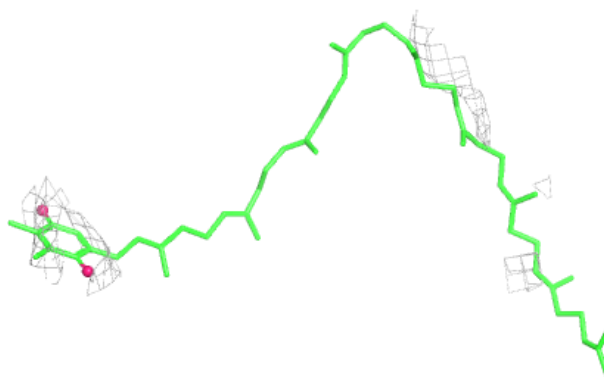
**Electron density around CLA c 512:**

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

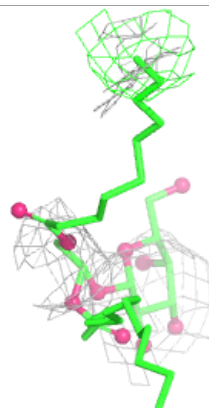
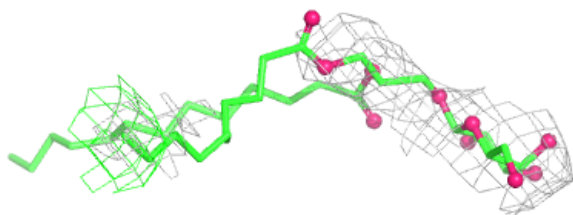
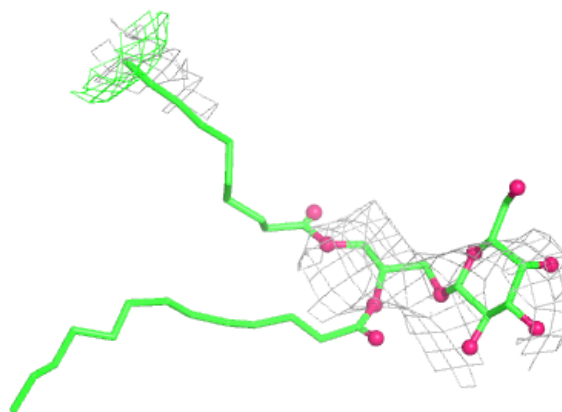


Electron density around PL9 d 407:

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

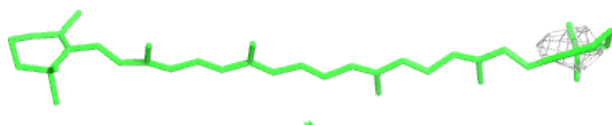
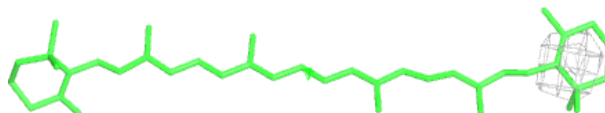
**Electron density around LMG a 402:**

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

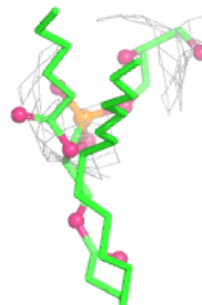
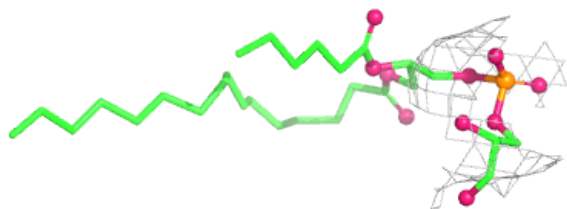
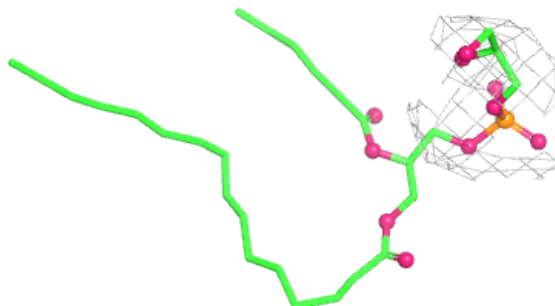


Electron density around BCR J 102:

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

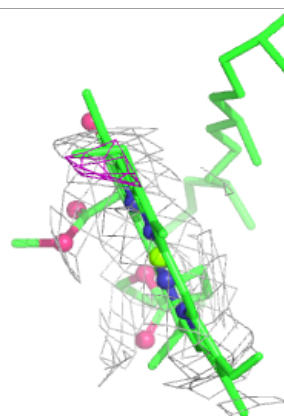
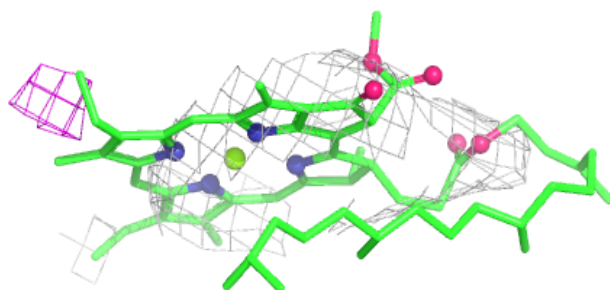
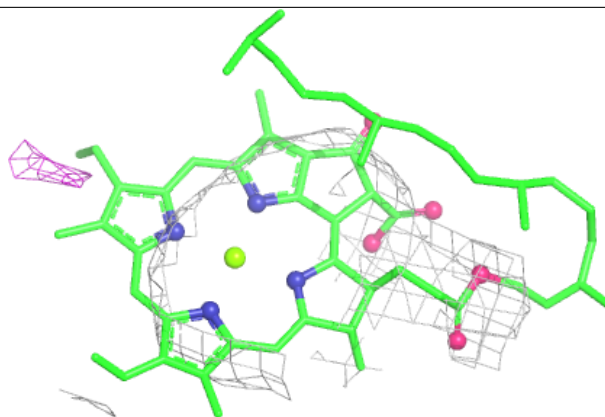
**Electron density around LHG a 409:**

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

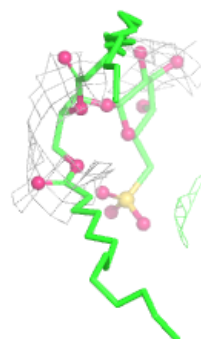
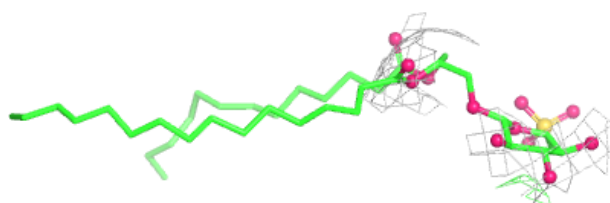
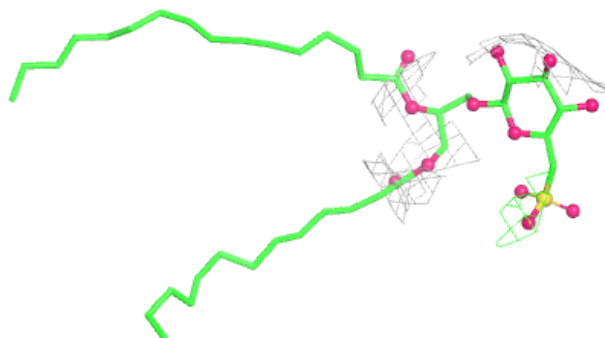


Electron density around CLA C 508:

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

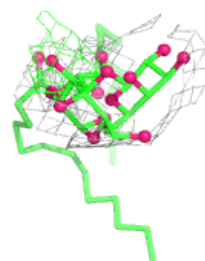
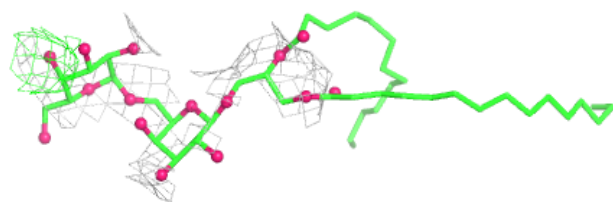
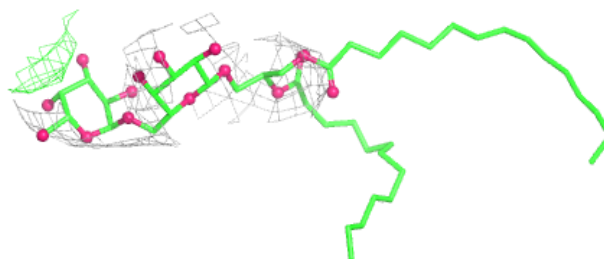
**Electron density around SQD A 413:**

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

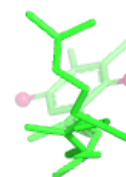
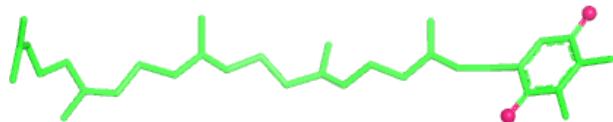
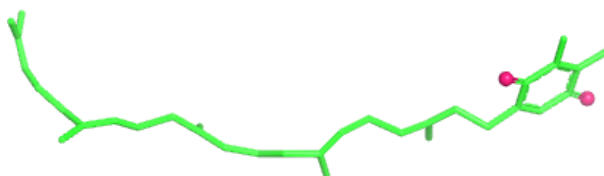


Electron density around DGD b 625:

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

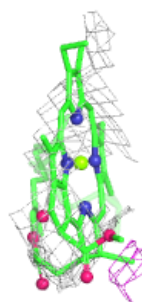
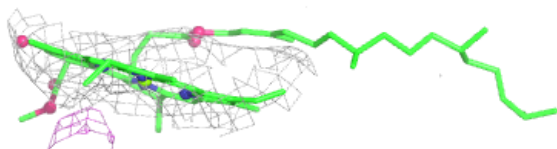
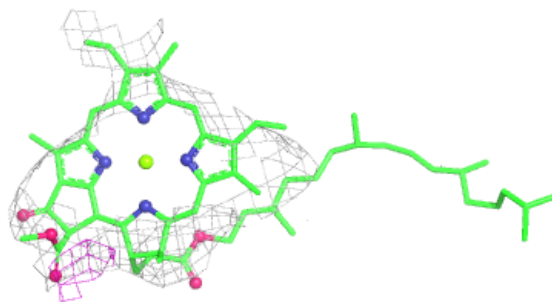
**Electron density around PL9 J 101:**

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

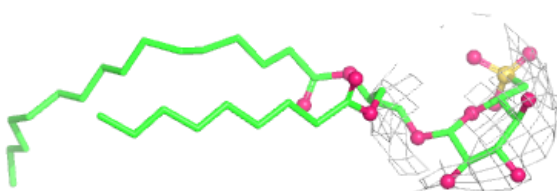
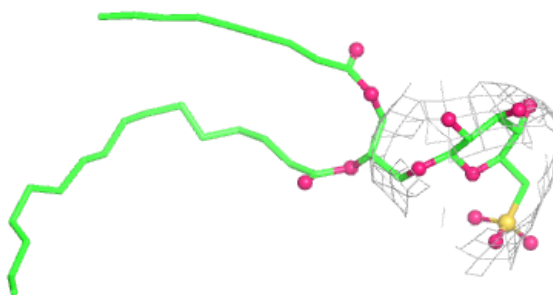


Electron density around CLA b 607:

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

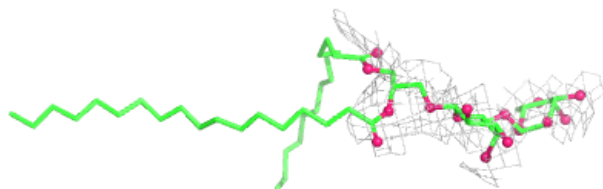
**Electron density around SQD b 602:**

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

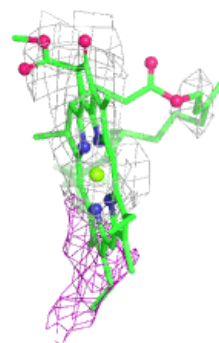
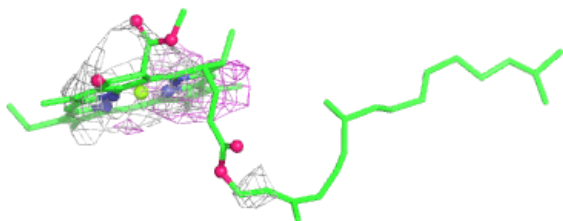
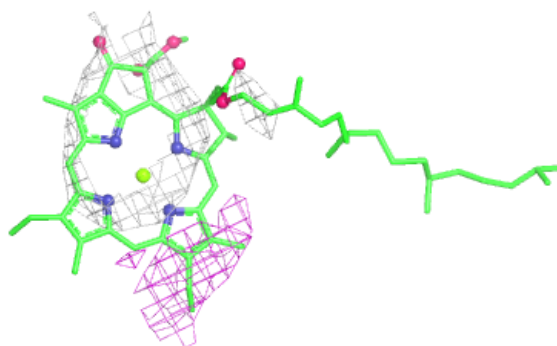


Electron density around DGD C 515:

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

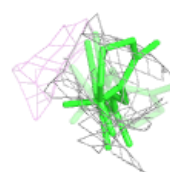
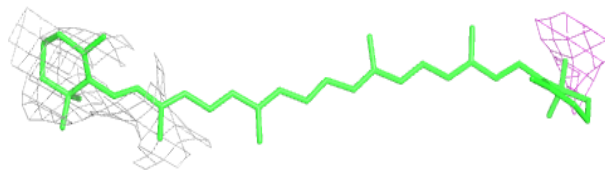
**Electron density around CLA a 405:**

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

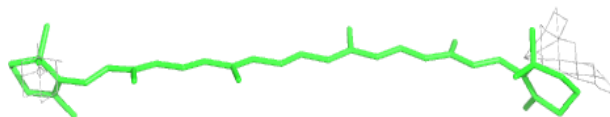
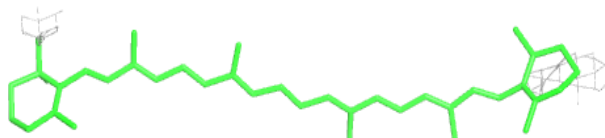


Electron density around BCR b 621:

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

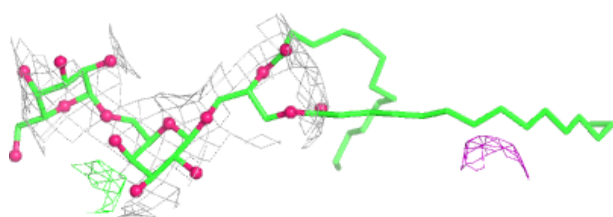
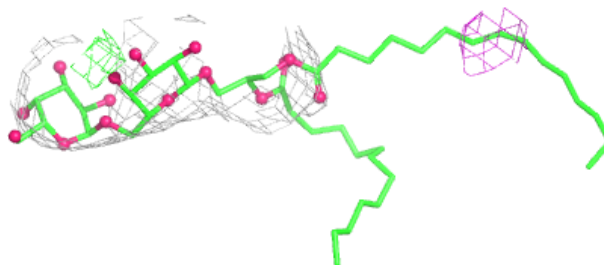
**Electron density around BCR C 513:**

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

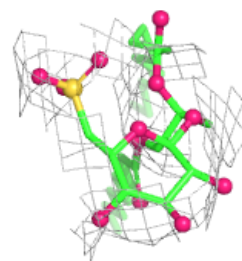
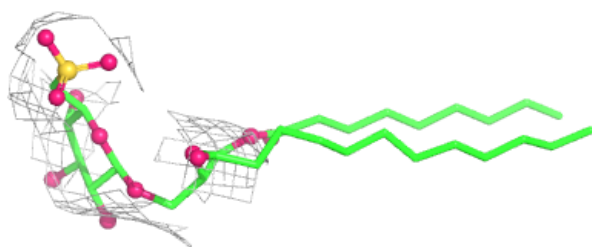
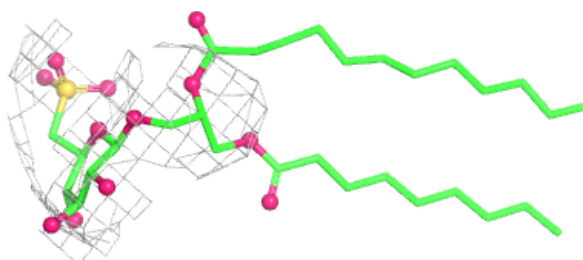


Electron density around DGD B 620:

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

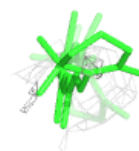
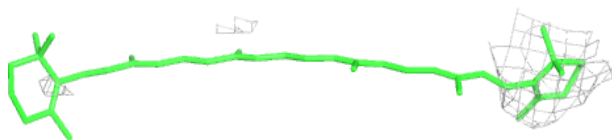
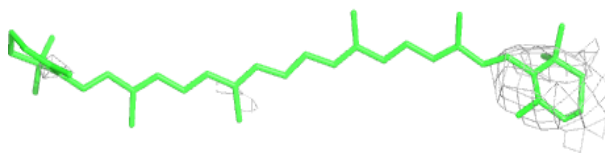
**Electron density around SQD d 403:**

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

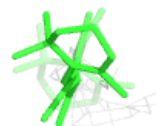
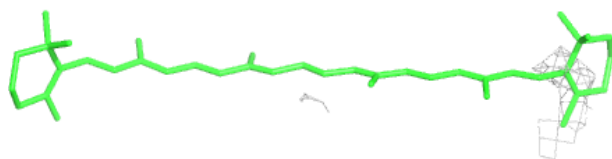
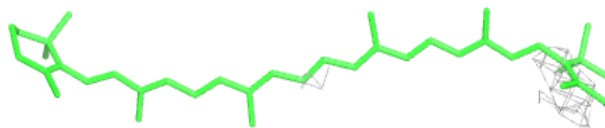


Electron density around BCR B 616:

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

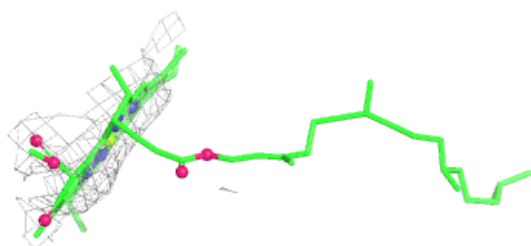
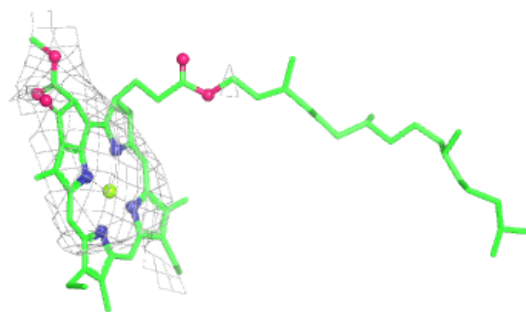
**Electron density around BCR i 101:**

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

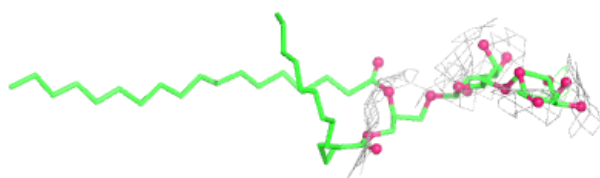


Electron density around CLA a 406:

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

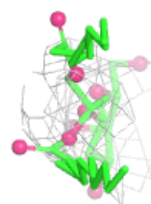
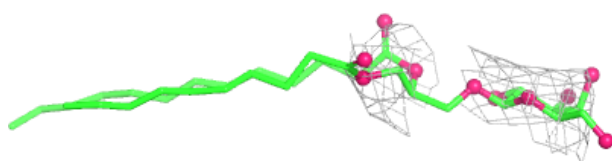
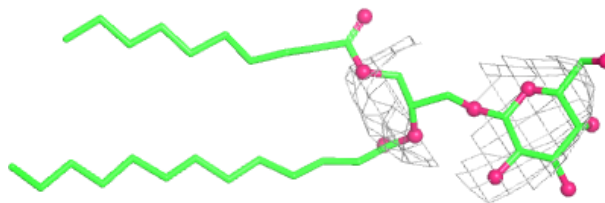
**Electron density around DGD c 516:**

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

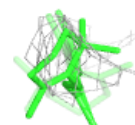
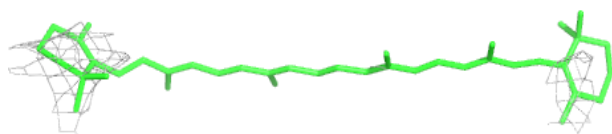
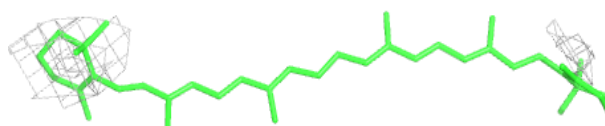


Electron density around LMG M 101:

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

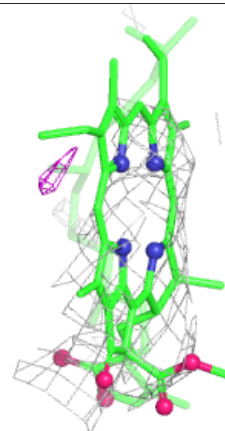
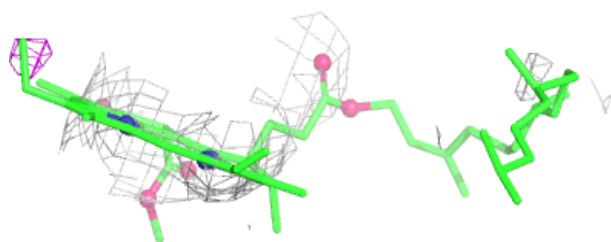
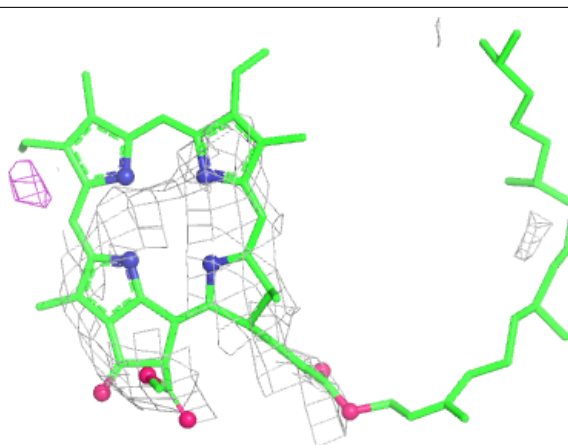
**Electron density around BCR C 520:**

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



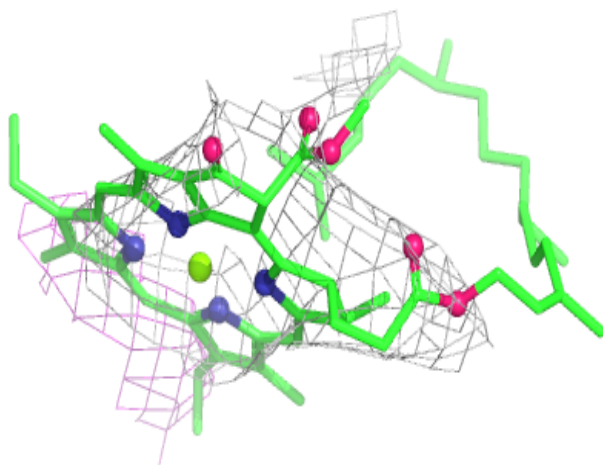
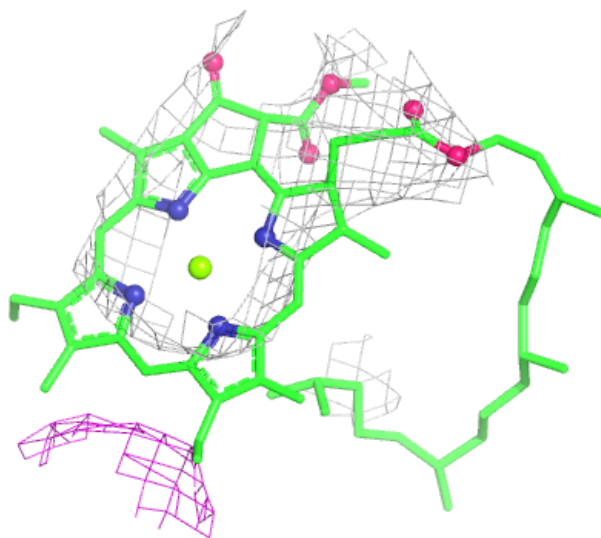
Electron density around PHO A 405:

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



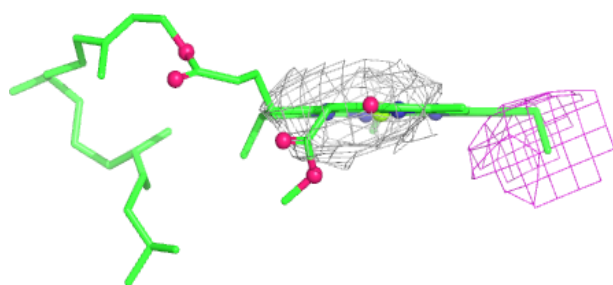
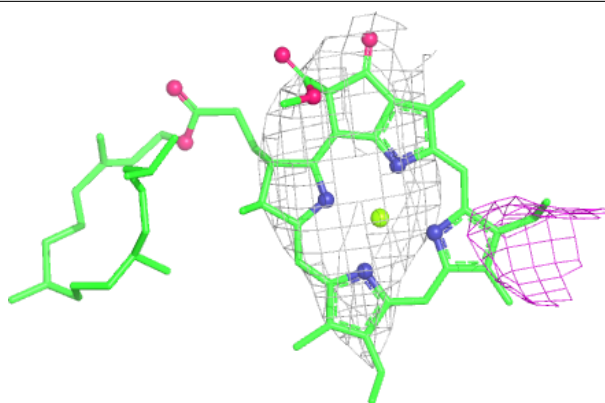
Electron density around CLA b 619:

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

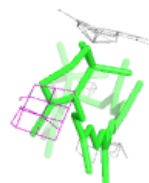
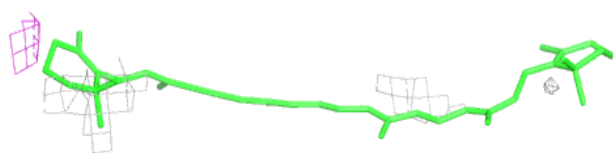
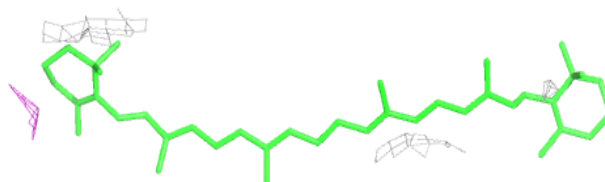


Electron density around CLA C 511:

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

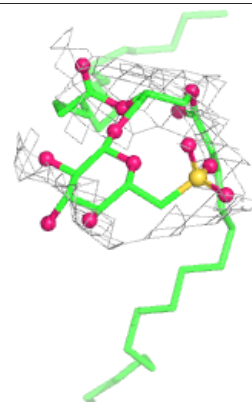
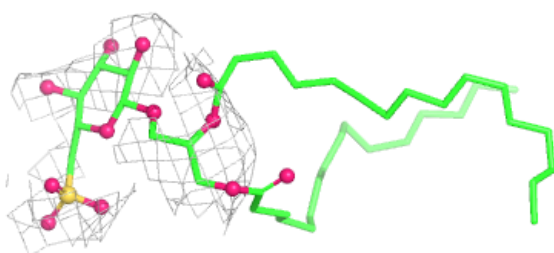
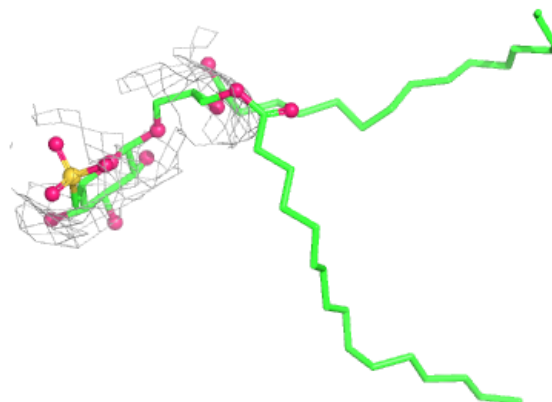
**Electron density around BCR b 622:**

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

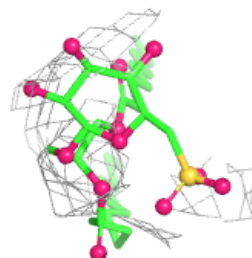
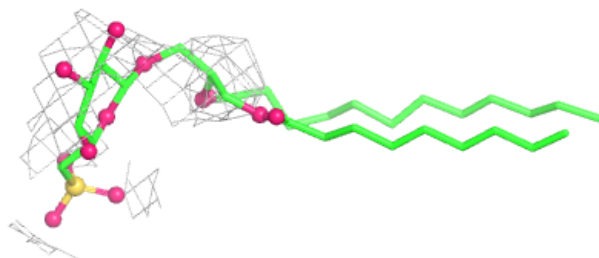
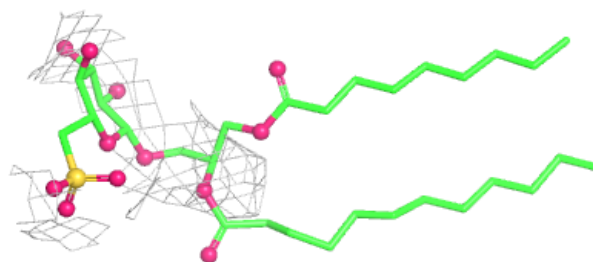


Electron density around SQD A 414:

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

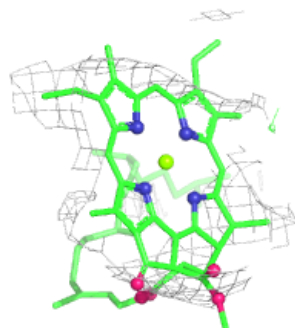
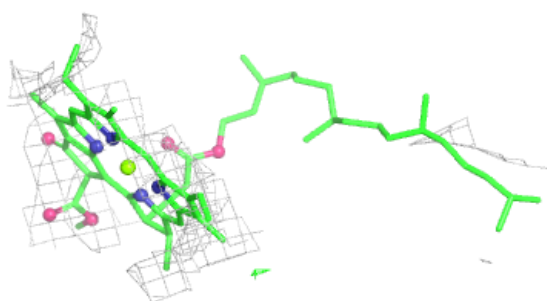
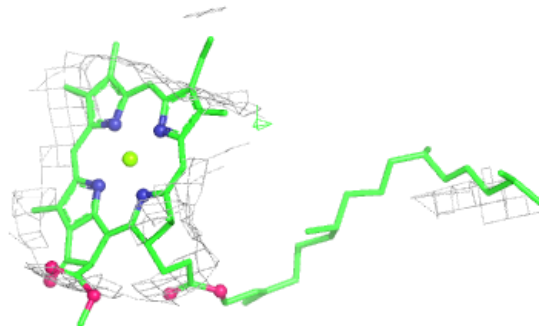
**Electron density around SQD B 622:**

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

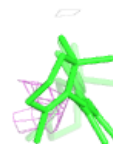
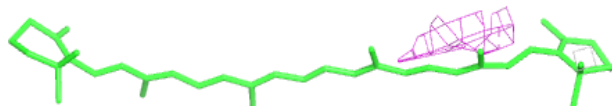
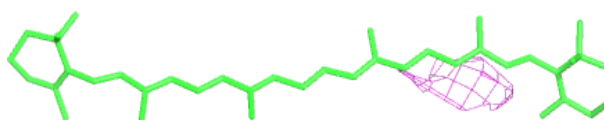


Electron density around CLA c 510:

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

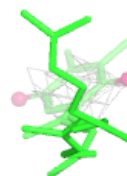
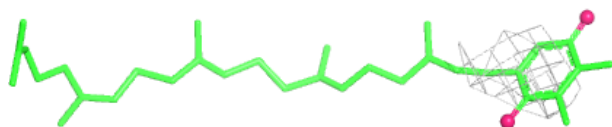
**Electron density around BCR c 514:**

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



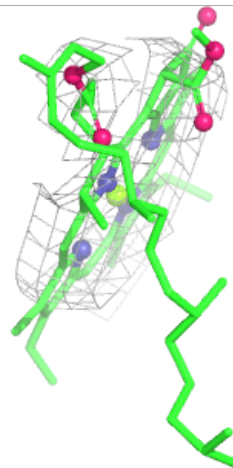
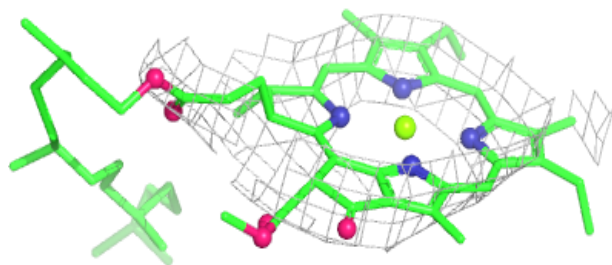
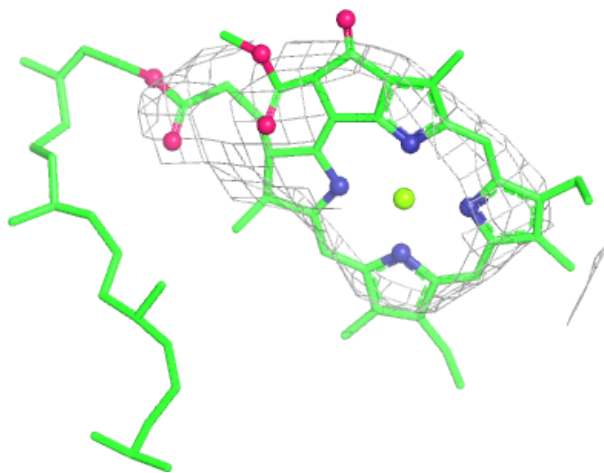
Electron density around PL9 j 101:

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



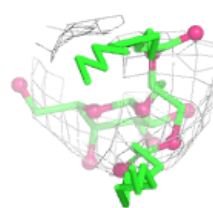
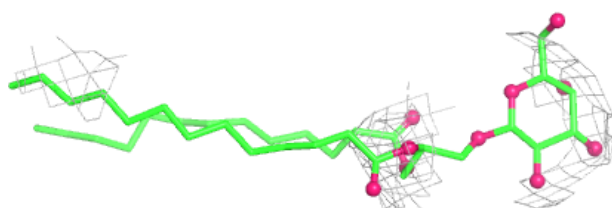
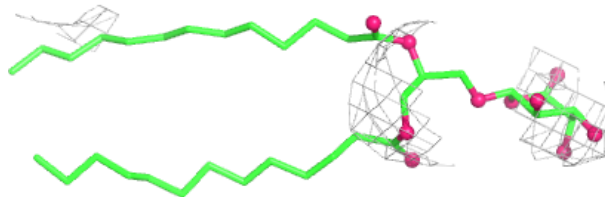
Electron density around CLA B 615:

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

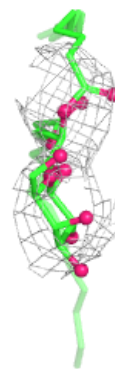
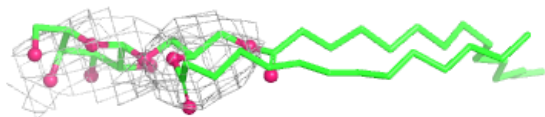
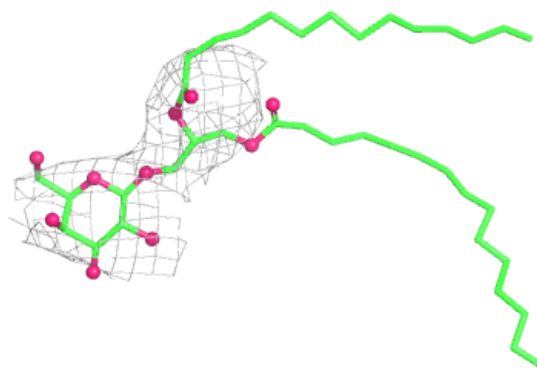


Electron density around LMG c 518:

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

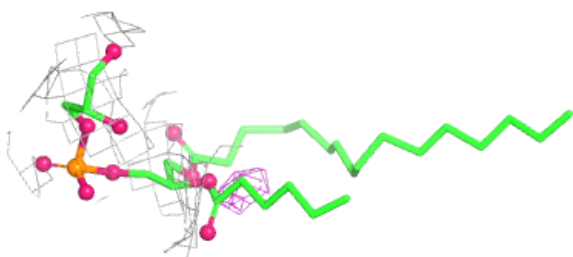
**Electron density around LMG C 521:**

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

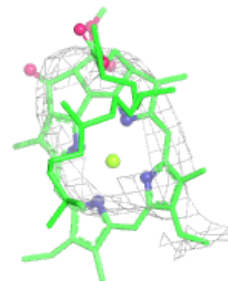
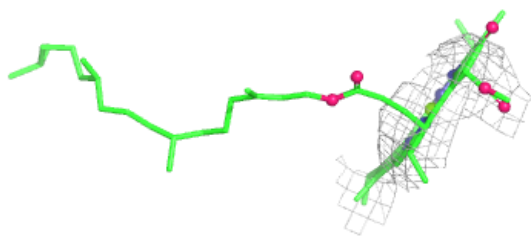
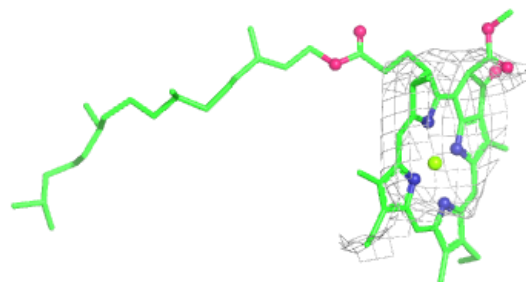


Electron density around LHG A 410:

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

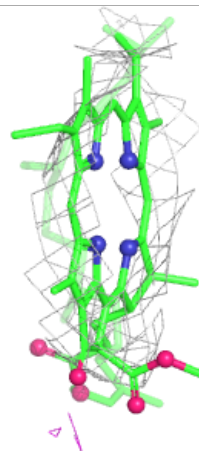
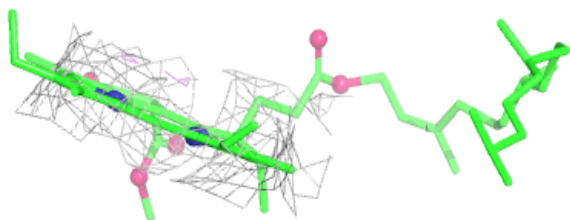
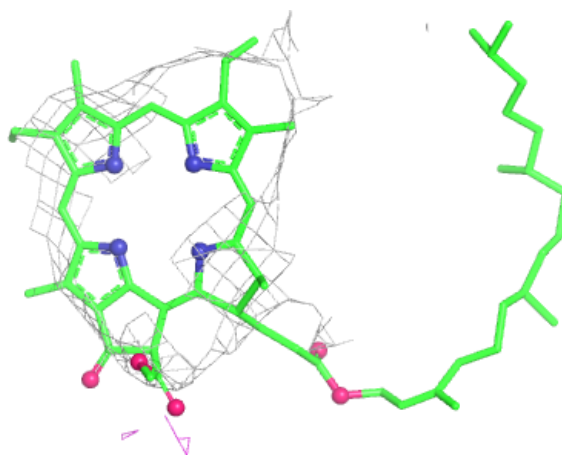
**Electron density around CLA A 406:**

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



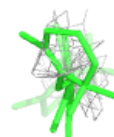
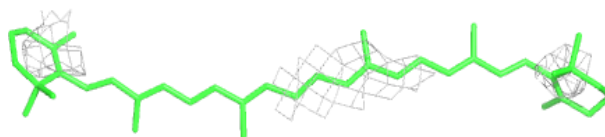
Electron density around PHO d 401:

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

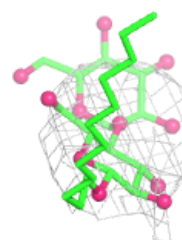
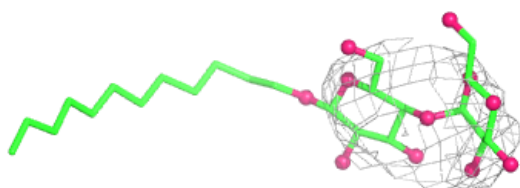
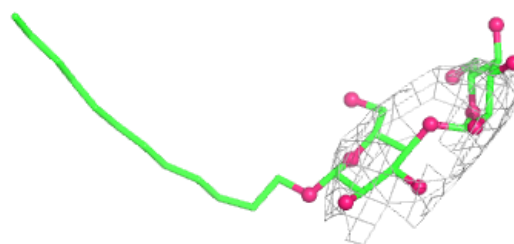


Electron density around BCR b 623:

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

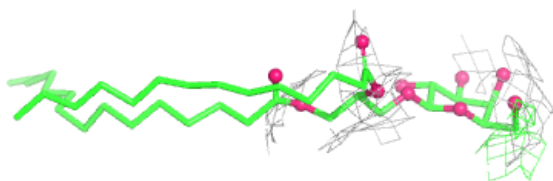
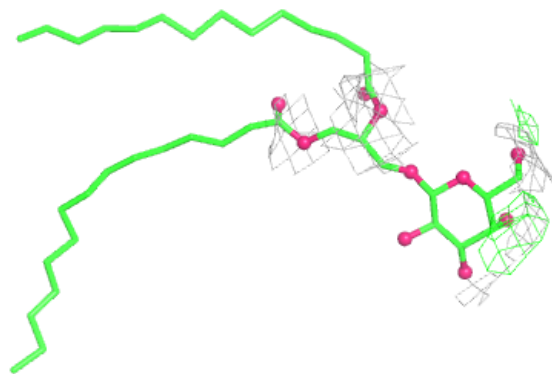
**Electron density around LMT M 103:**

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

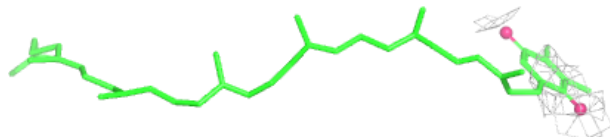
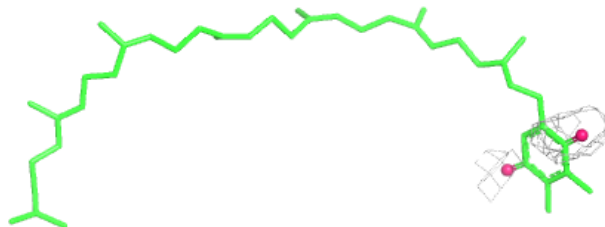


Electron density around LMG c 522:

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

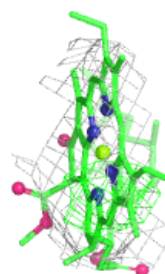
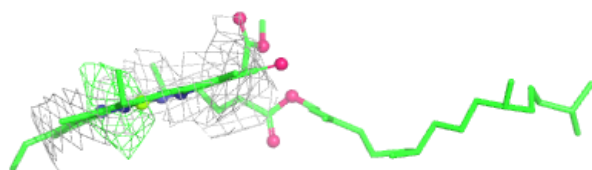
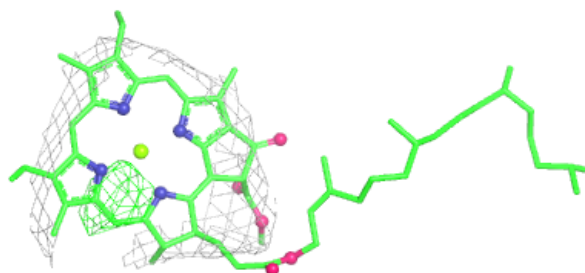
**Electron density around PL9 a 407:**

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

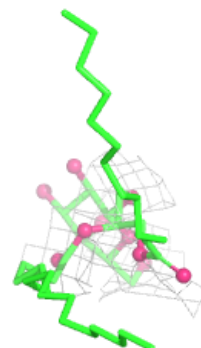
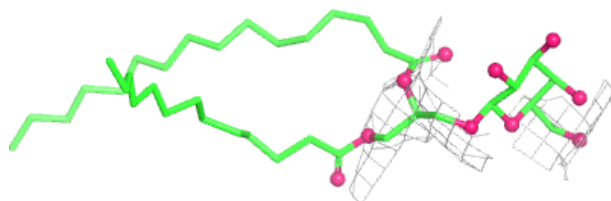
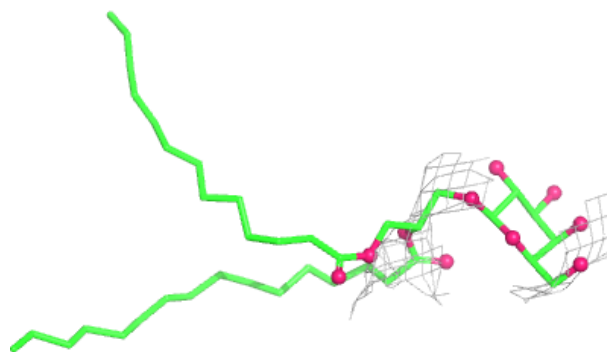


Electron density around CLA b 606:

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

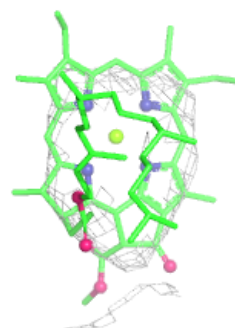
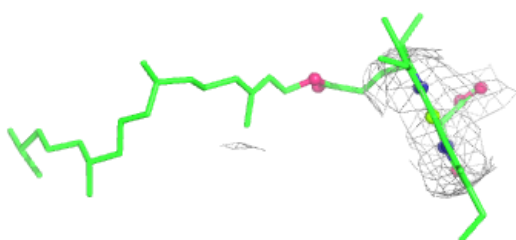
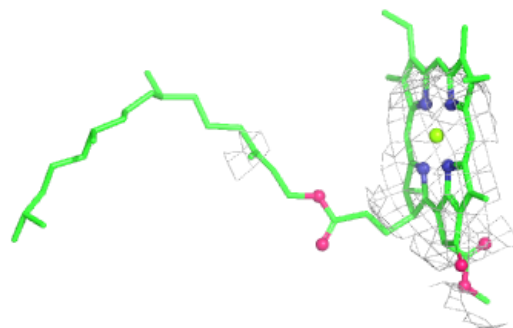
**Electron density around LMG D 406:**

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

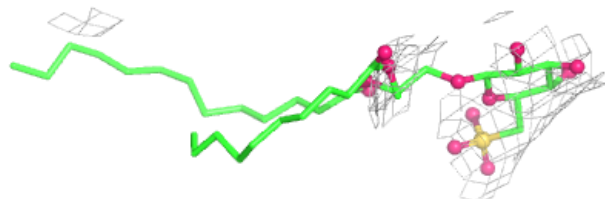


Electron density around CLA D 404:

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

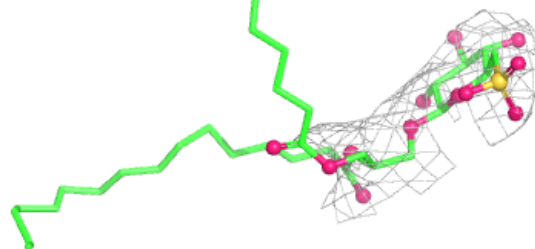
**Electron density around SQD F 103:**

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

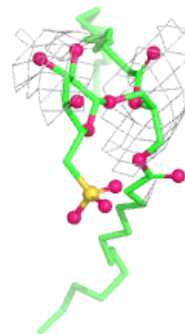
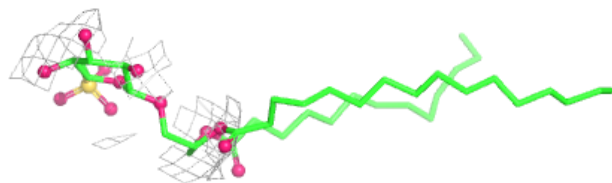


Electron density around SQD a 401:

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

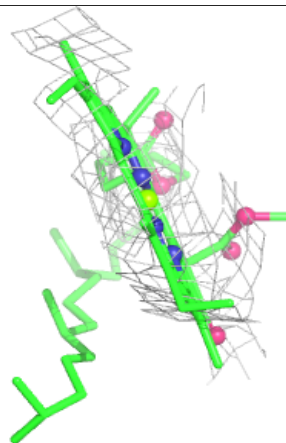
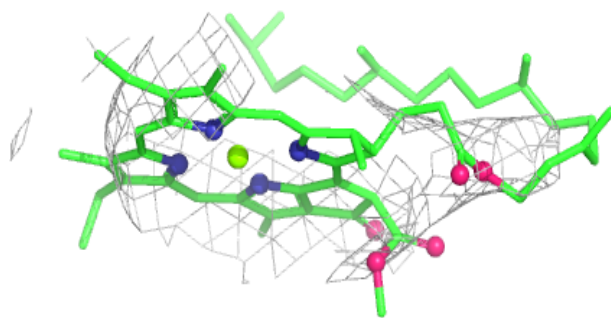
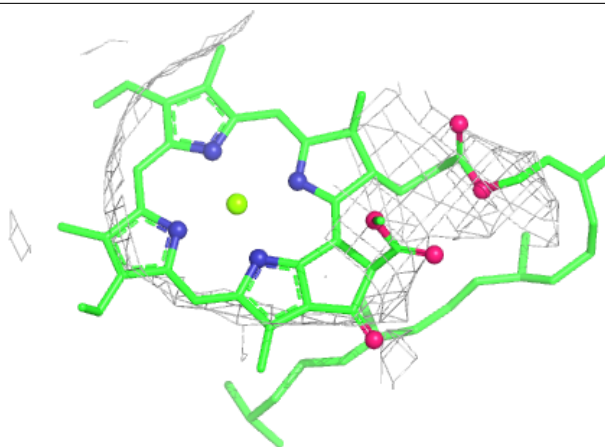
**Electron density around SQD a 412:**

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

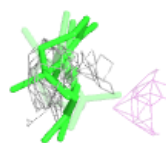
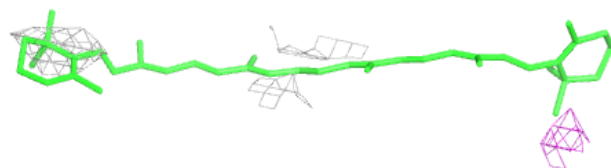


Electron density around CLA c 508:

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

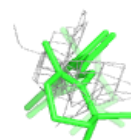
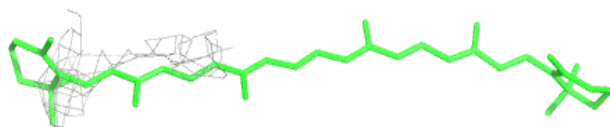
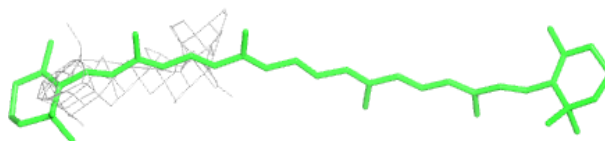
**Electron density around BCR y 101:**

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

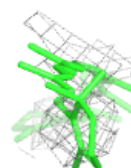
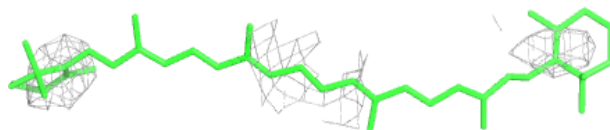
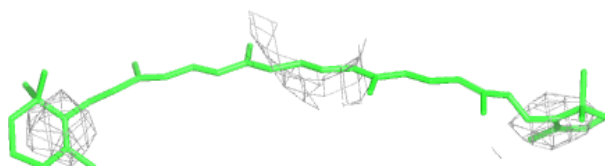


Electron density around BCR B 619:

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

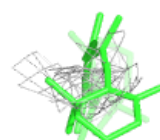
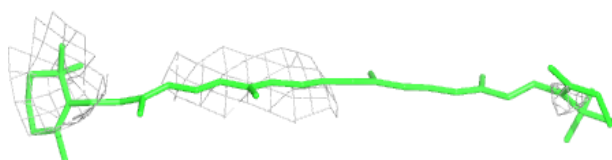
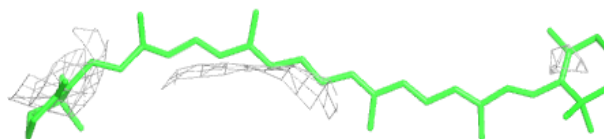
**Electron density around BCR F 102:**

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

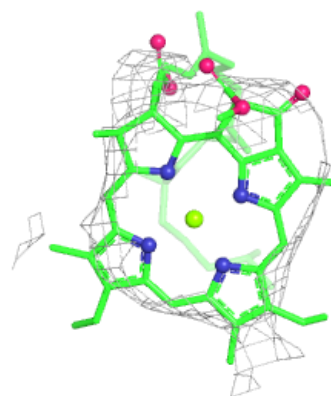
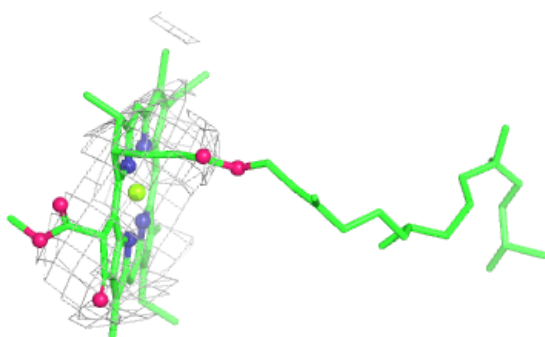
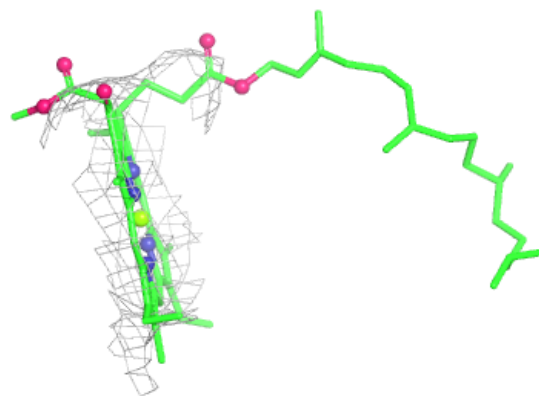


Electron density around BCR x 101:

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

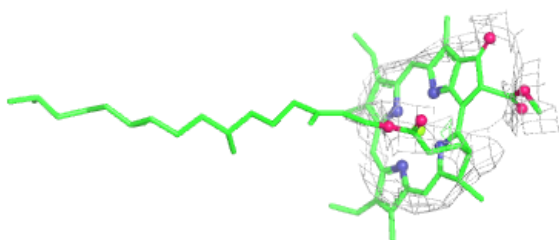
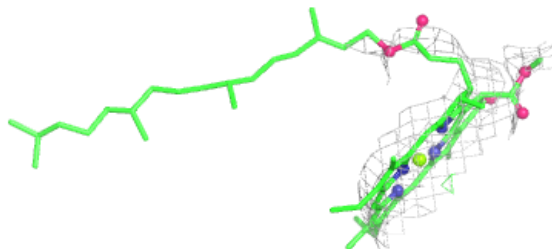
**Electron density around CLA C 505:**

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

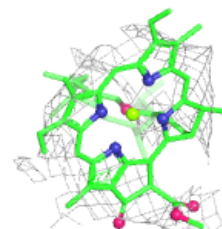
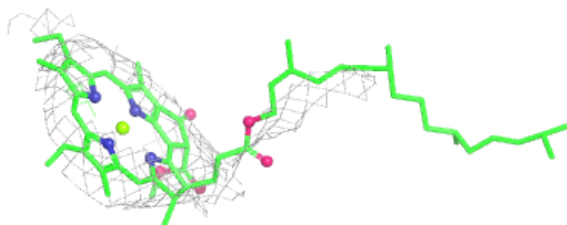
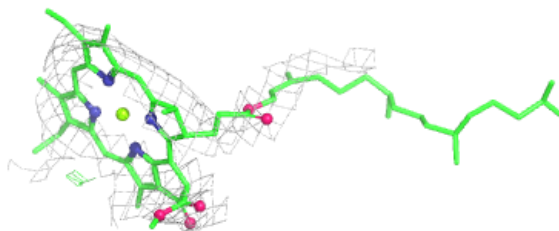


Electron density around CLA C 519:

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

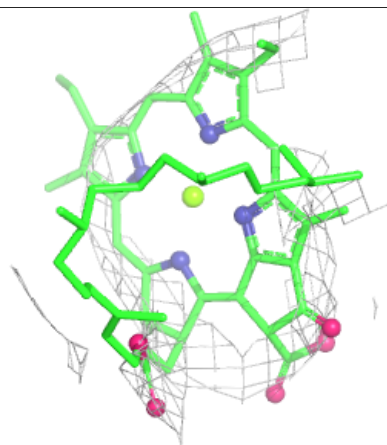
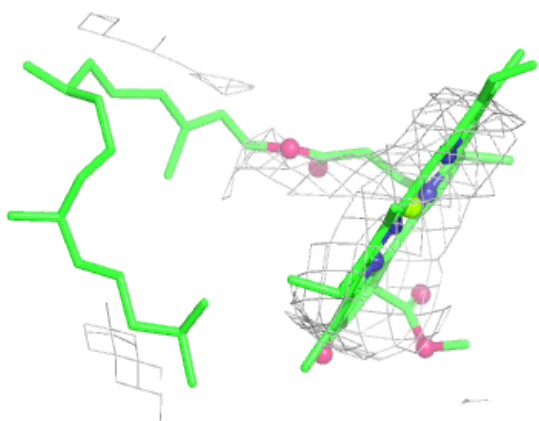
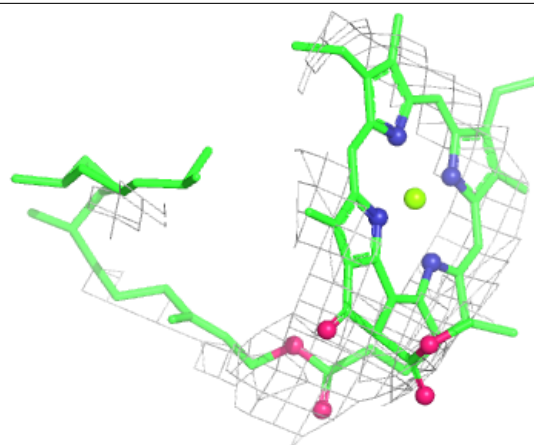
**Electron density around CLA c 502:**

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



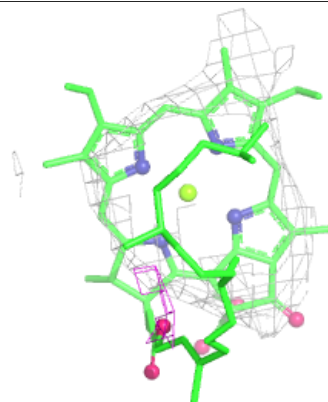
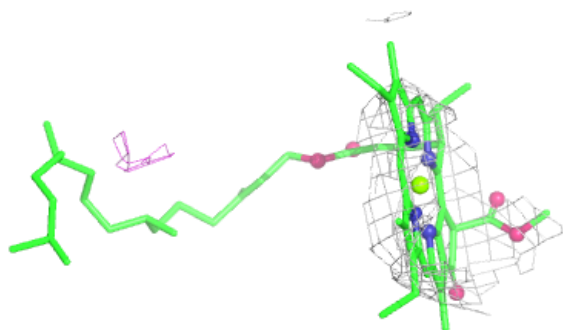
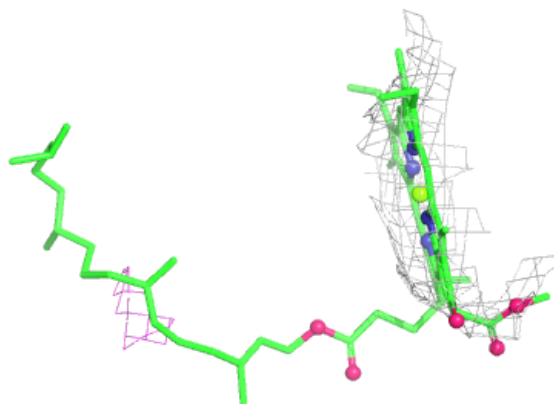
Electron density around CLA c 503:

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



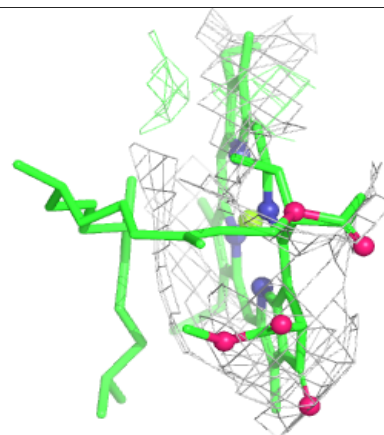
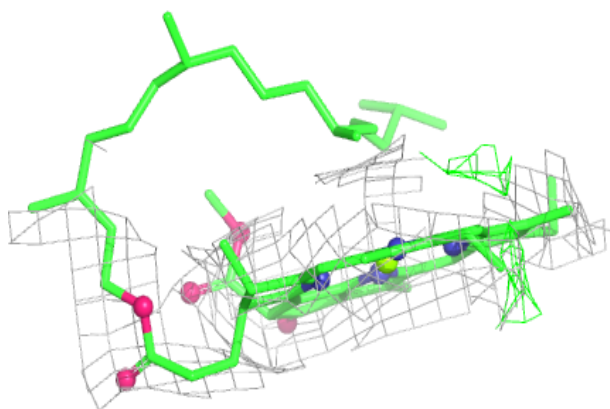
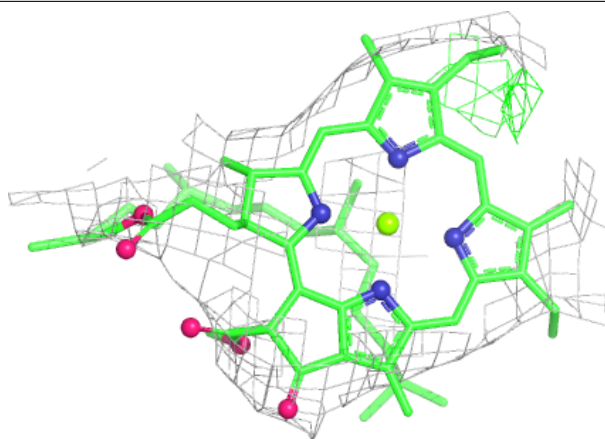
Electron density around CLA c 505:

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

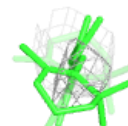
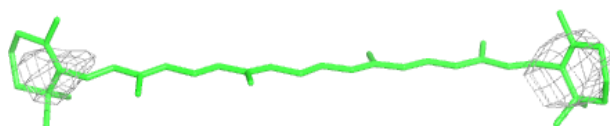
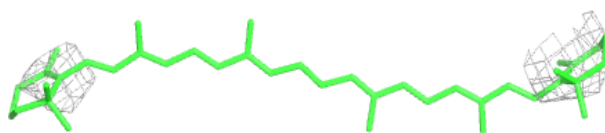


Electron density around CLA C 509:

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

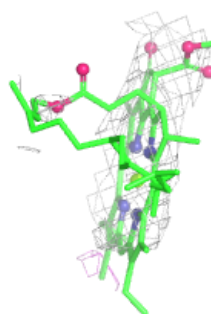
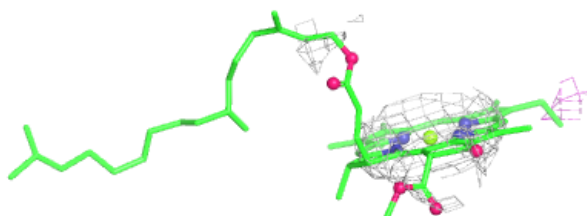
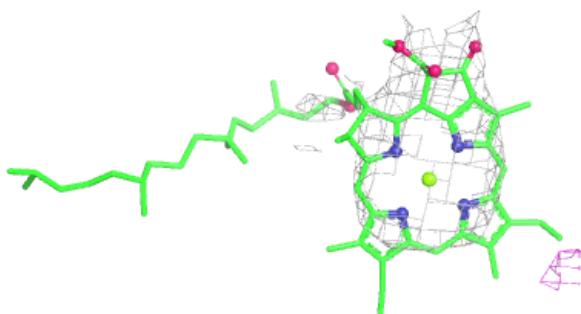
**Electron density around BCR A 408:**

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



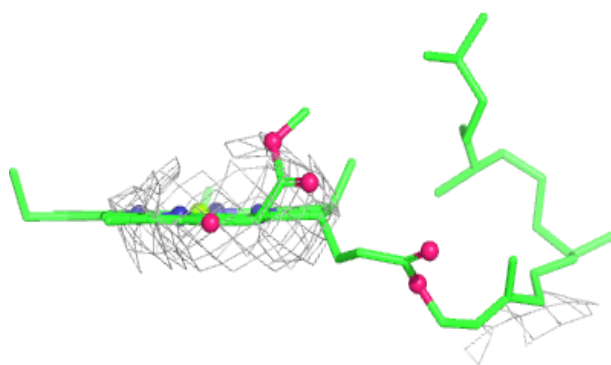
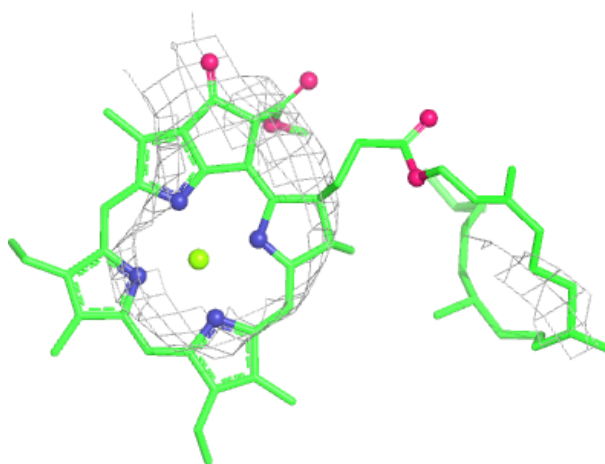
Electron density around CLA A 404:

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



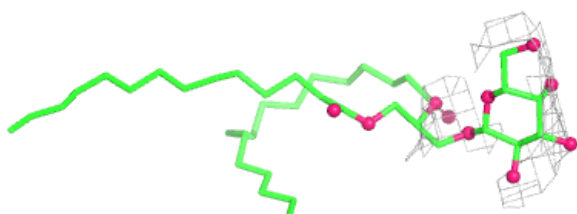
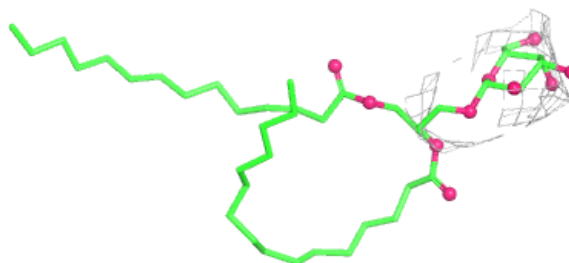
Electron density around CLA c 511:

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

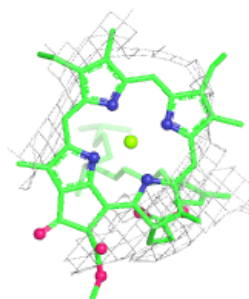
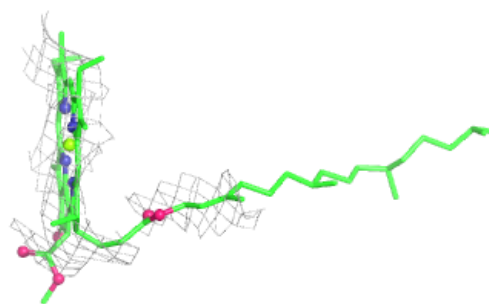


Electron density around LMG d 408:

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

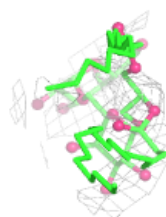
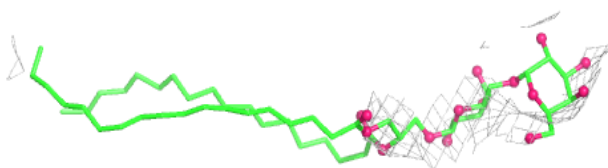
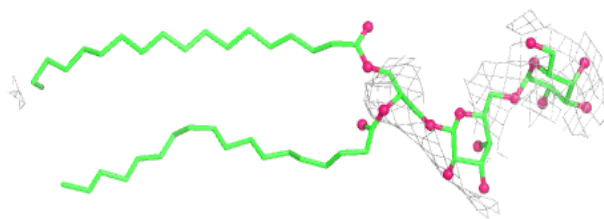
**Electron density around CLA b 610:**

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

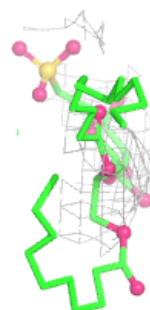
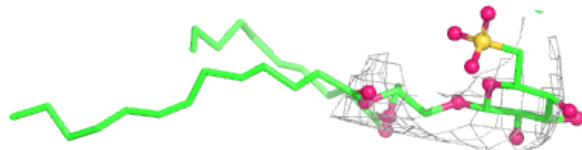
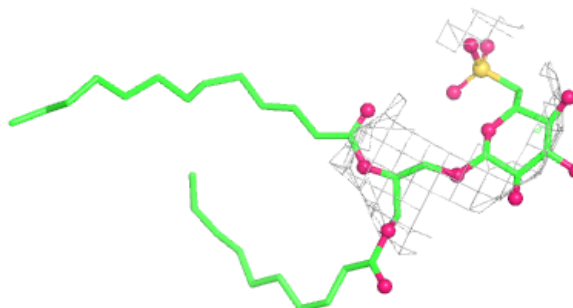


Electron density around DGD c 517:

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

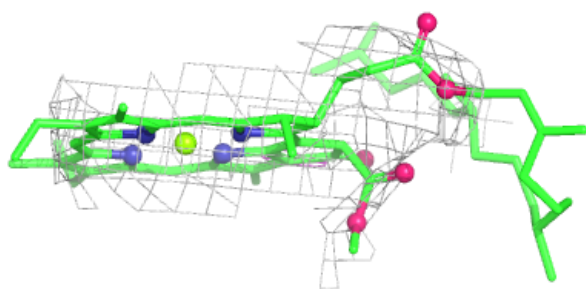
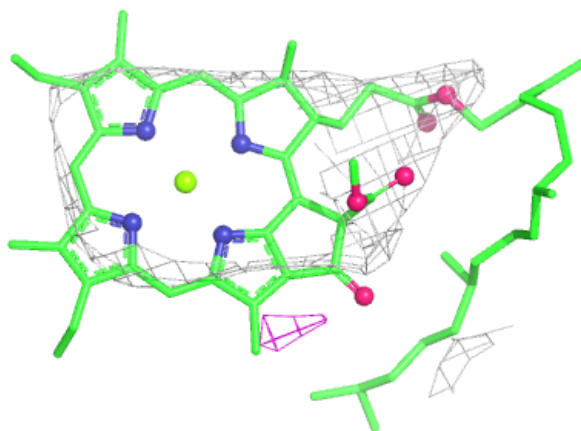
**Electron density around SQD f 103:**

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

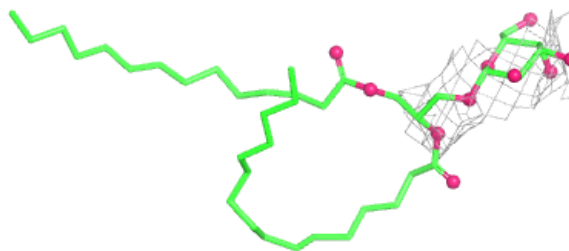


Electron density around CLA b 614:

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

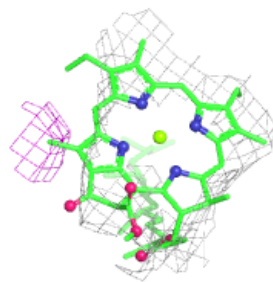
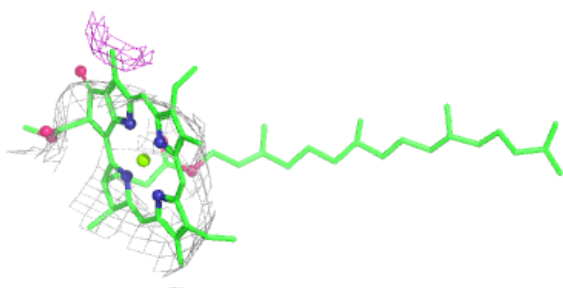
**Electron density around LMG B 625:**

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

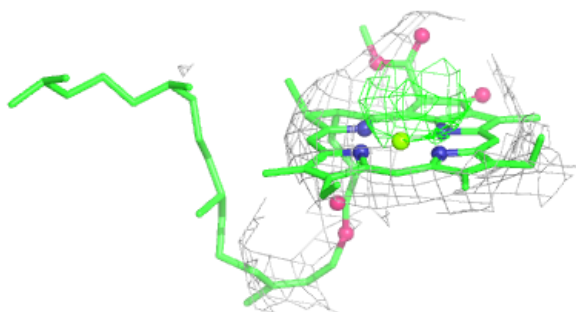
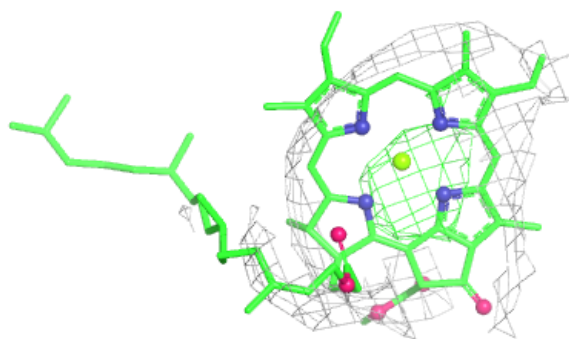


Electron density around CLA b 611:

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

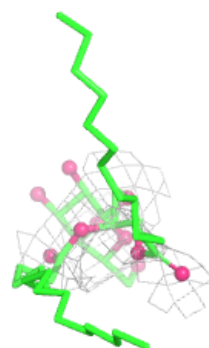
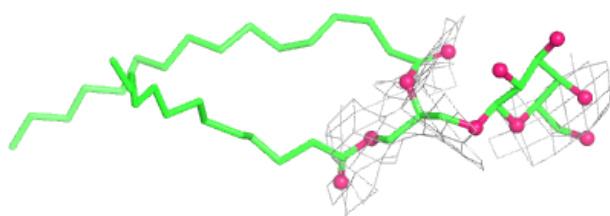
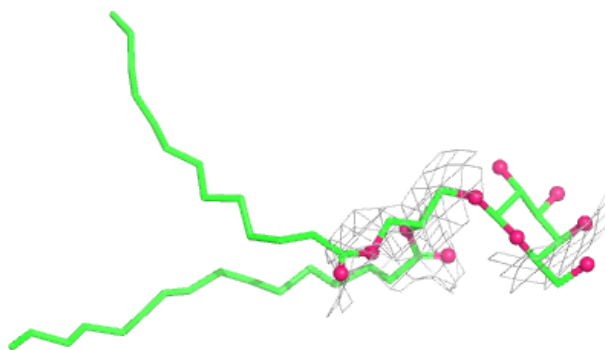
**Electron density around CLA a 404:**

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

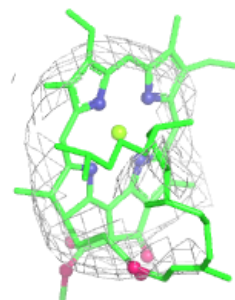
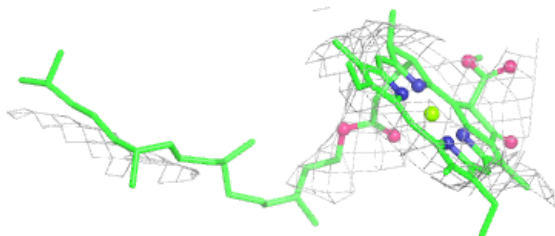
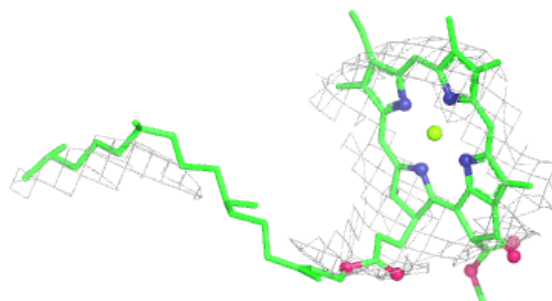


Electron density around LMG d 409:

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

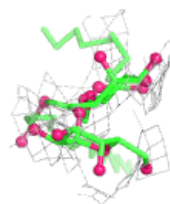
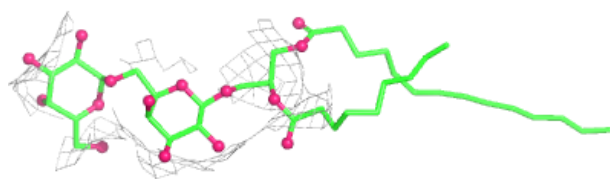
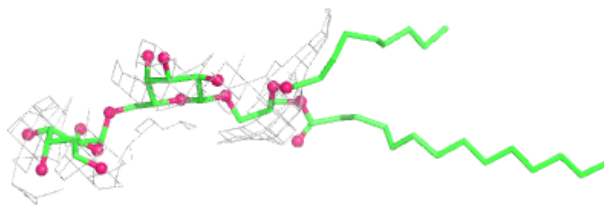
**Electron density around CLA C 510:**

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



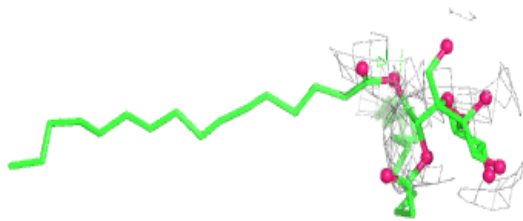
Electron density around DGD c 515:

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



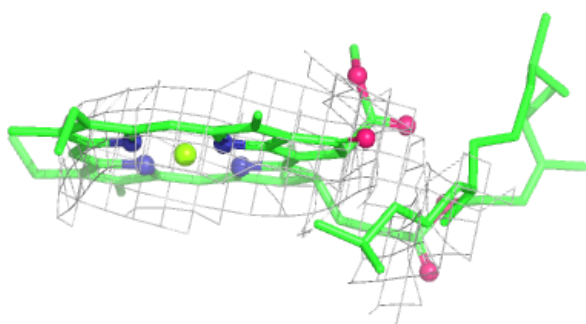
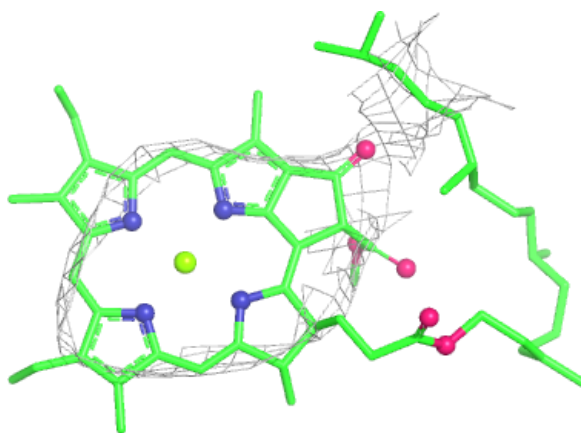
Electron density around LMG 1 101:

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

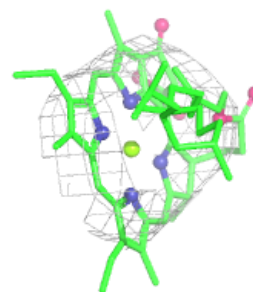
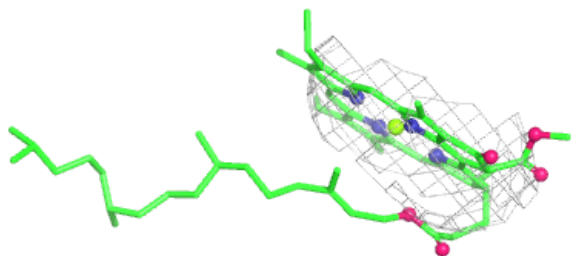
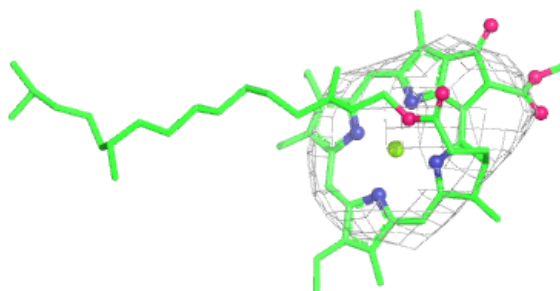


Electron density around CLA B 609:

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

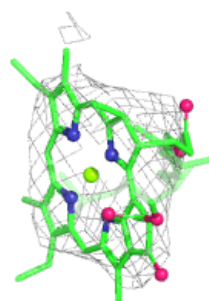
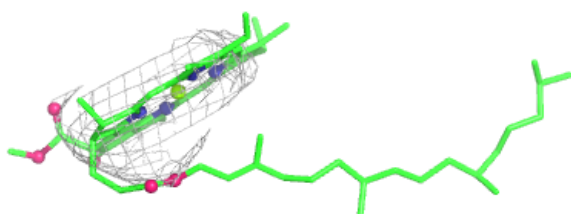
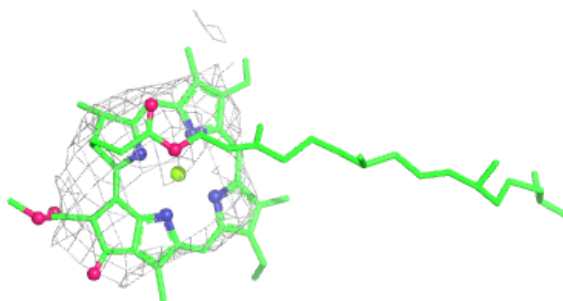
**Electron density around CLA B 613:**

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

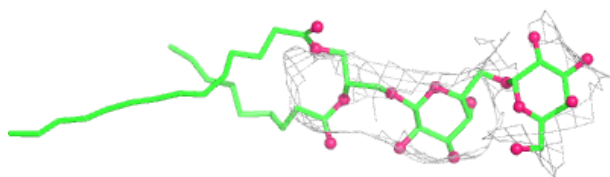
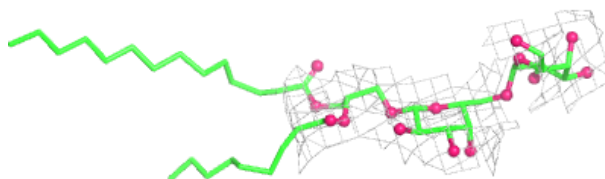


Electron density around CLA B 607:

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

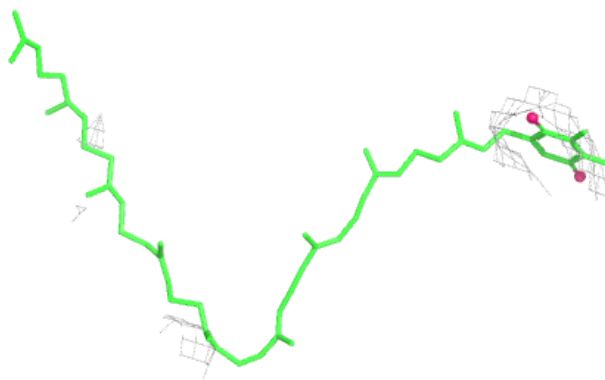
**Electron density around DGD C 514:**

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

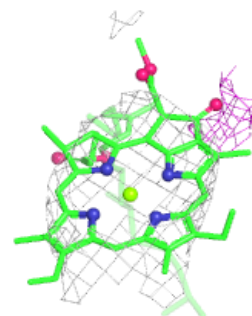
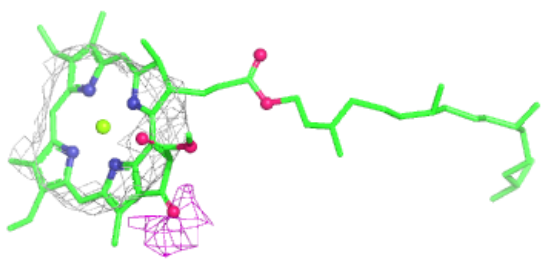
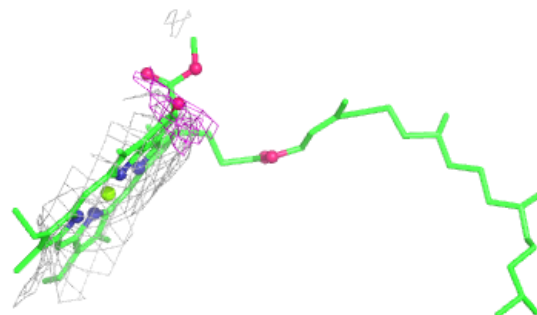


Electron density around PL9 D 405:

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

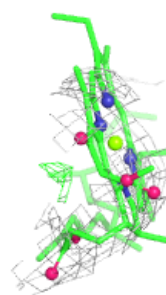
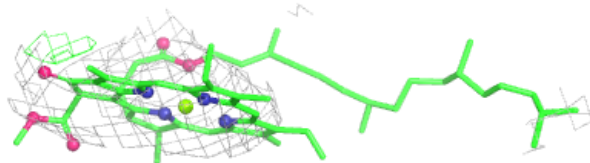
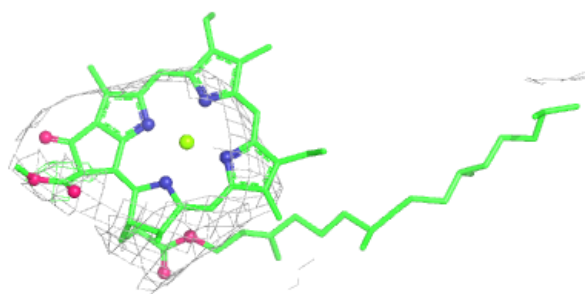
**Electron density around CLA D 403:**

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

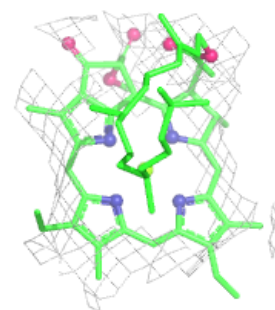
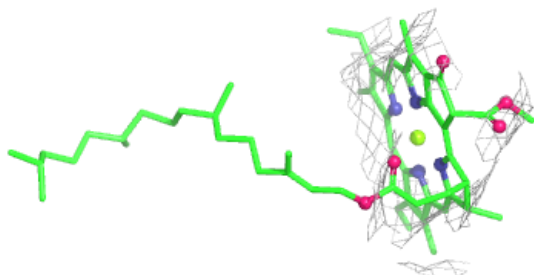
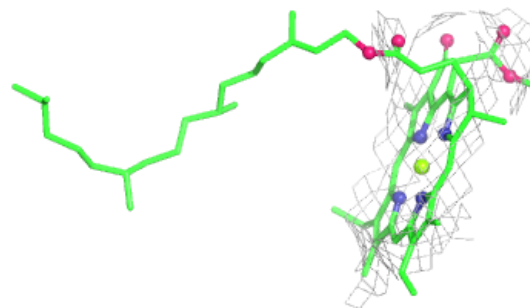


Electron density around CLA C 501:

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

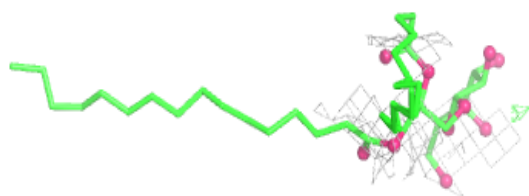
**Electron density around CLA C 507:**

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



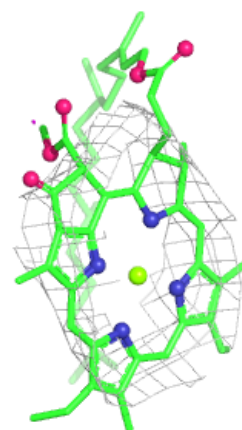
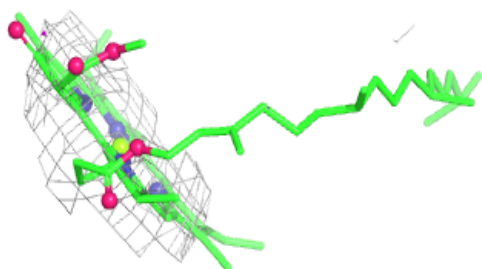
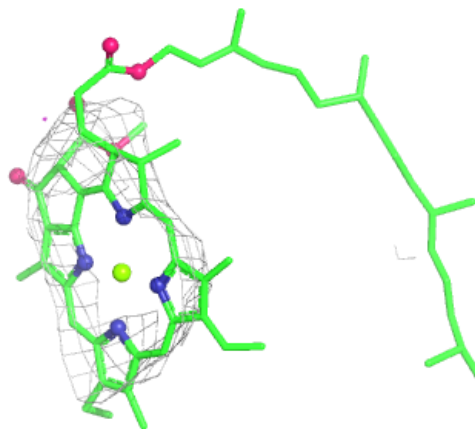
Electron density around LMG L 101:

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



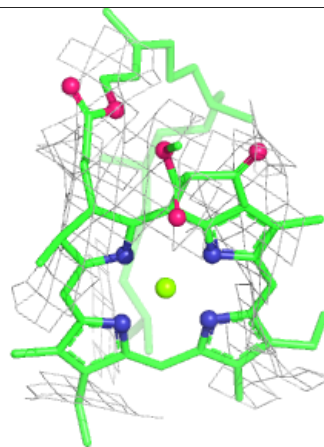
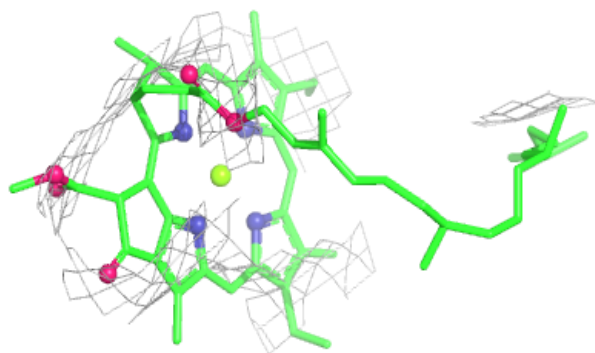
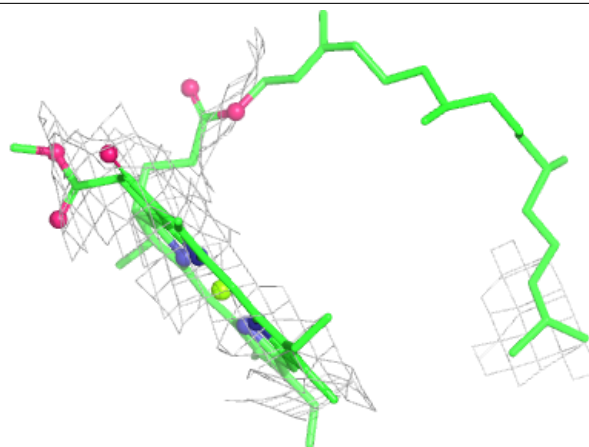
Electron density around CLA c 506:

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

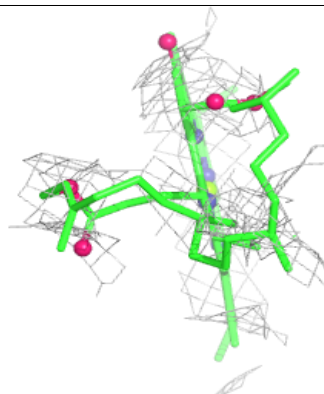
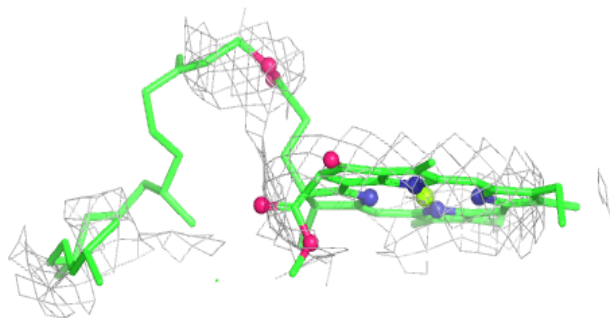
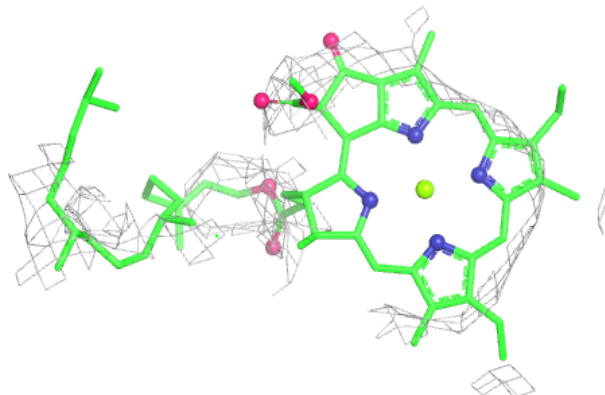


Electron density around CLA B 610:

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

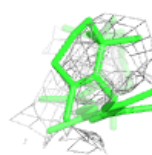
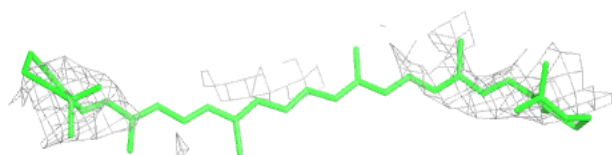
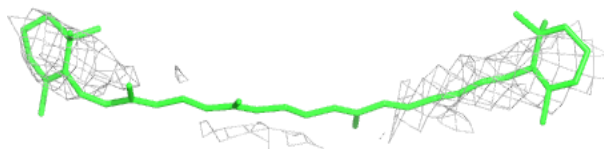
**Electron density around CLA b 616:**

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

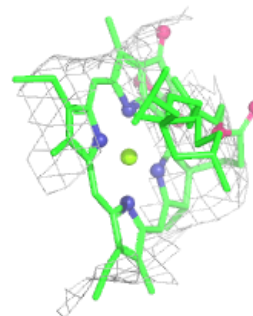
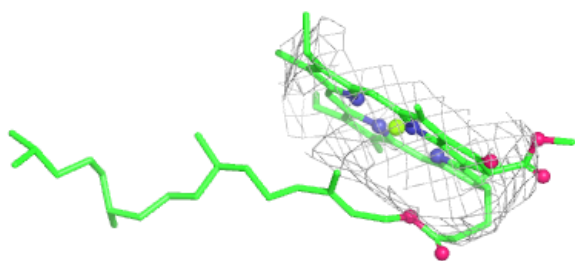
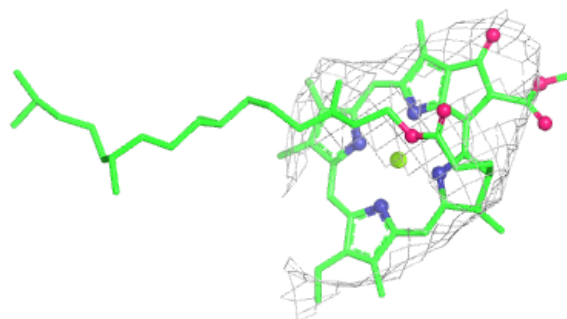


Electron density around BCR c 513:

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

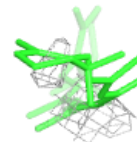
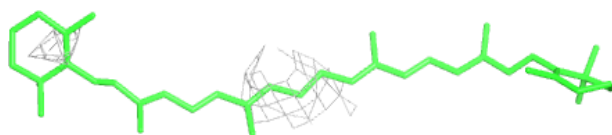
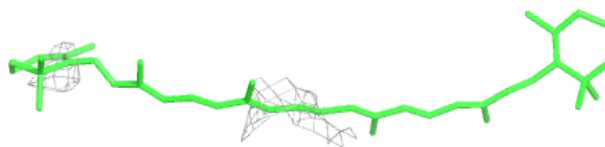
**Electron density around CLA b 618:**

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

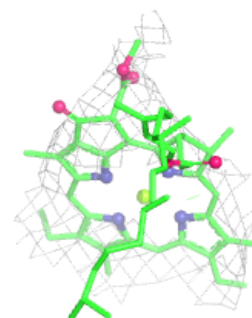
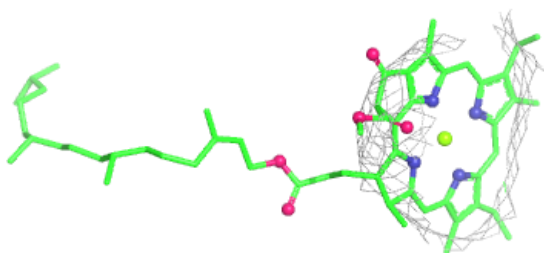
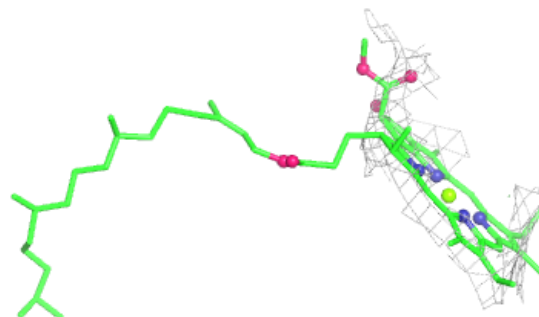


Electron density around BCR f 102:

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

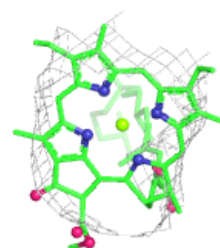
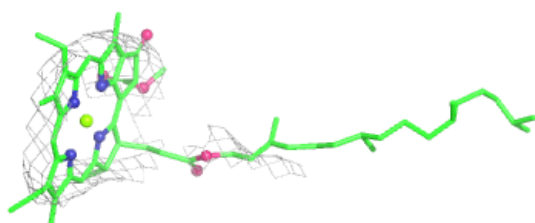
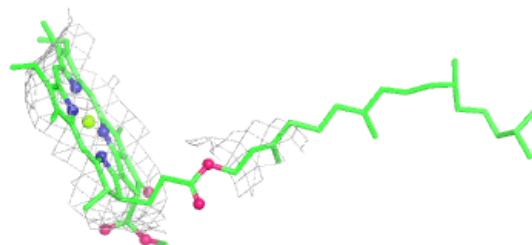
**Electron density around CLA d 405:**

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

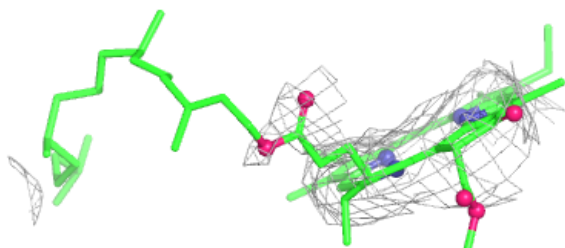
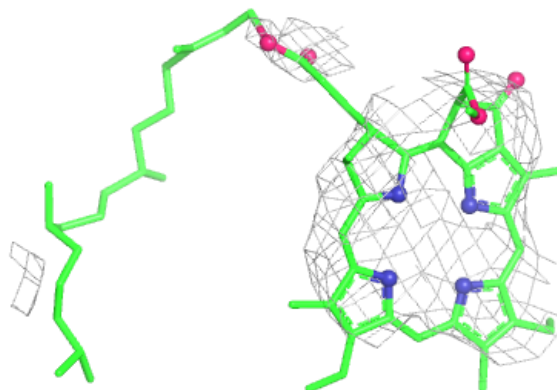


Electron density around CLA b 608:

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

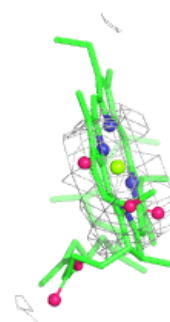
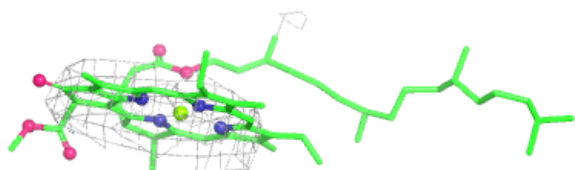
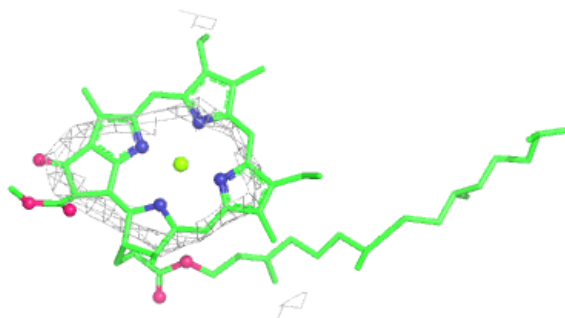
**Electron density around PHO D 401:**

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

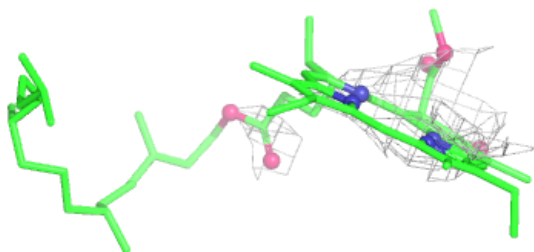
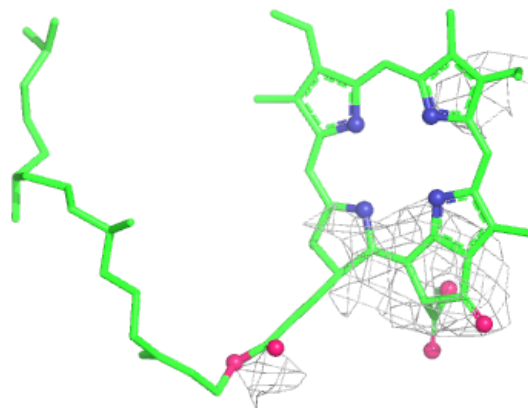


Electron density around CLA c 501:

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

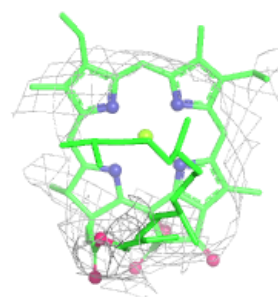
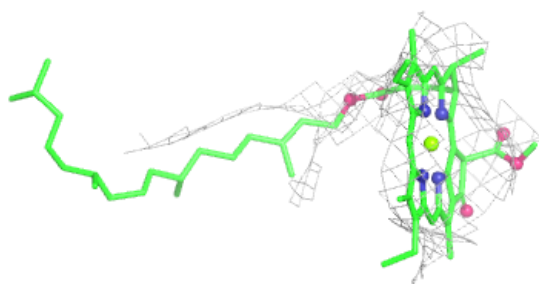
**Electron density around PHO d 402:**

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

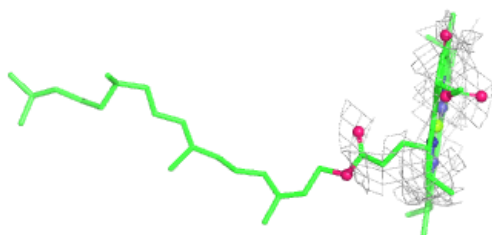
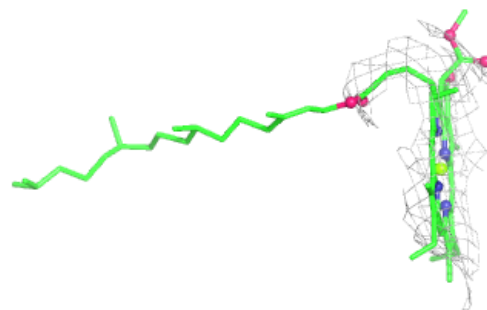


Electron density around CLA b 609:

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

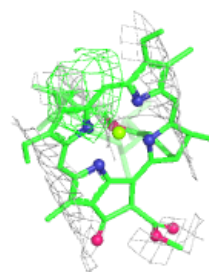
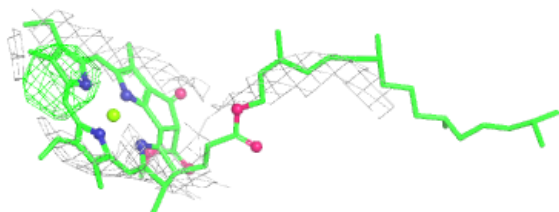
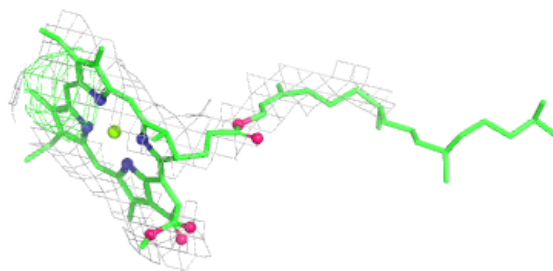
**Electron density around CLA B 605:**

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

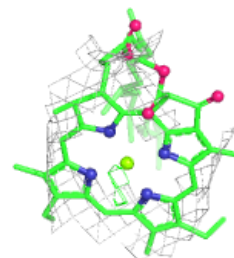
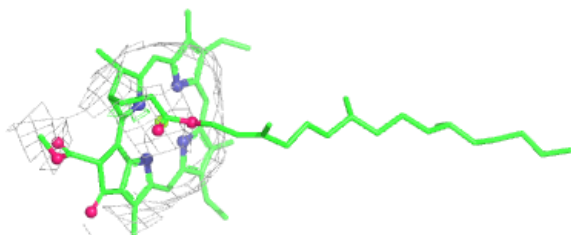
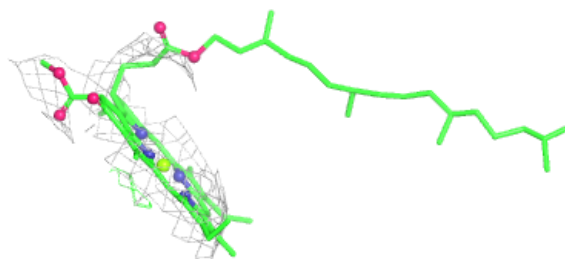


Electron density around CLA C 502:

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

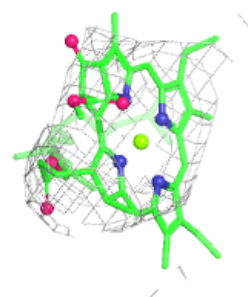
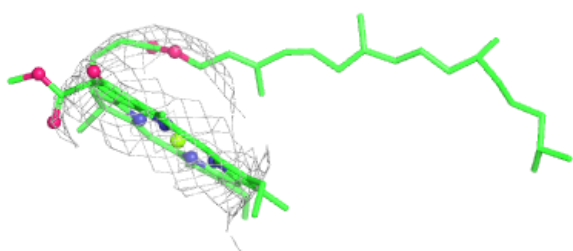
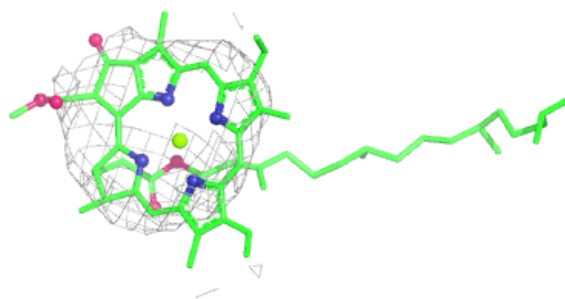
**Electron density around CLA c 520:**

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

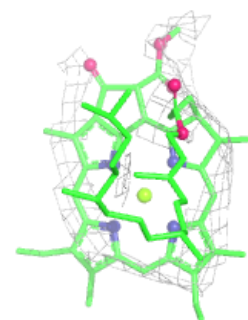
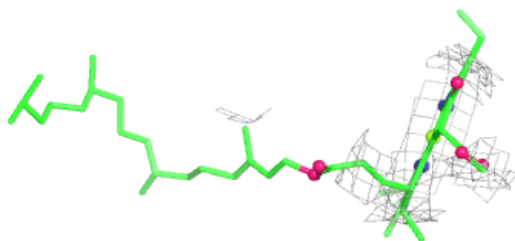
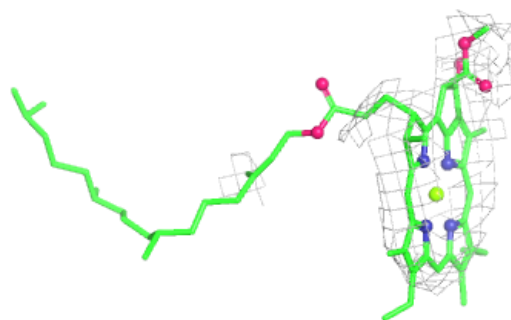


Electron density around CLA b 612:

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

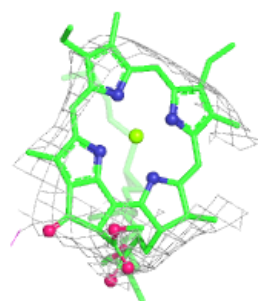
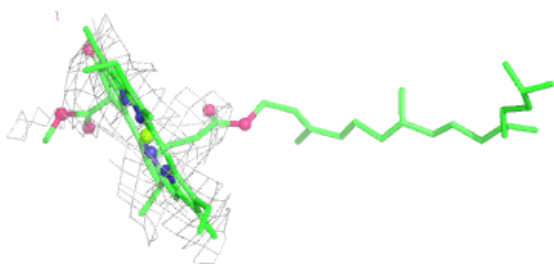
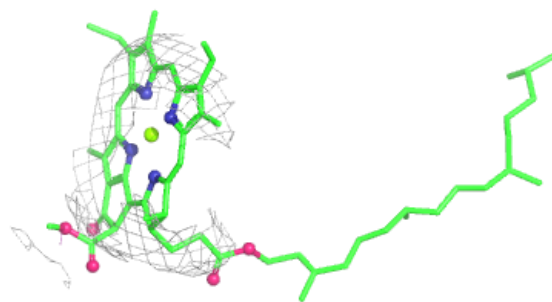
**Electron density around CLA d 406:**

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

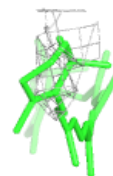
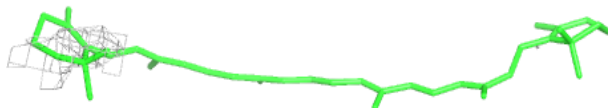
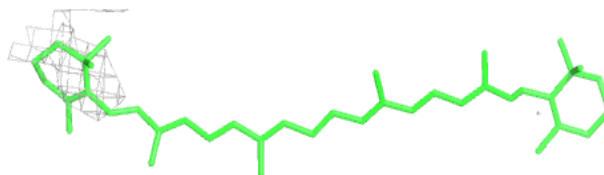


Electron density around CLA b 613:

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

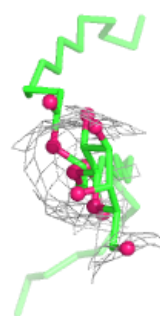
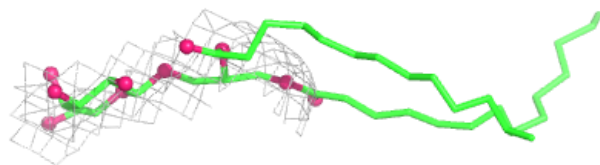
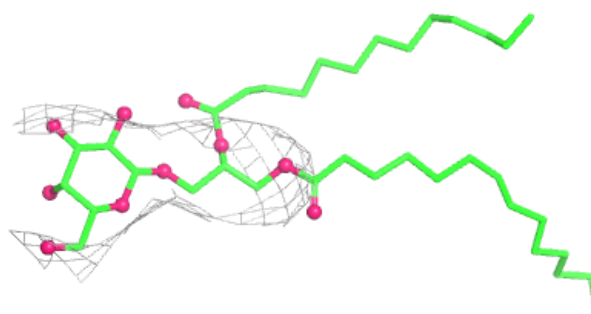
**Electron density around BCR B 617:**

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

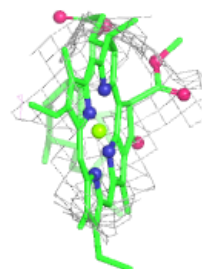
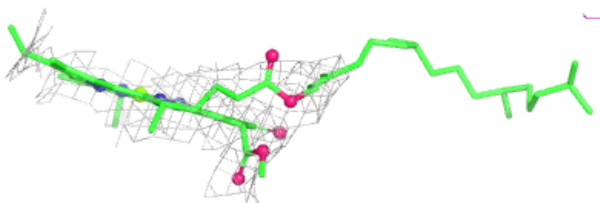


Electron density around LMG d 412:

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

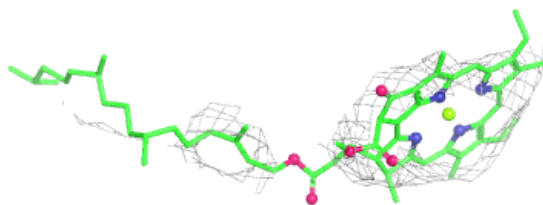
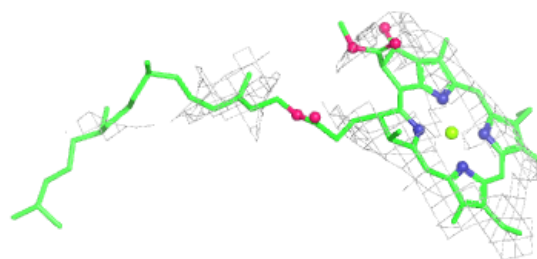
**Electron density around CLA H 101:**

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

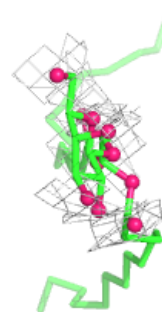
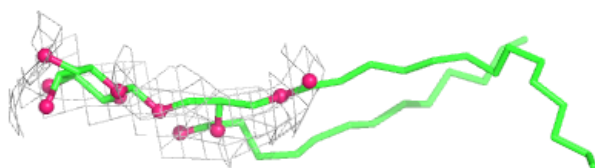
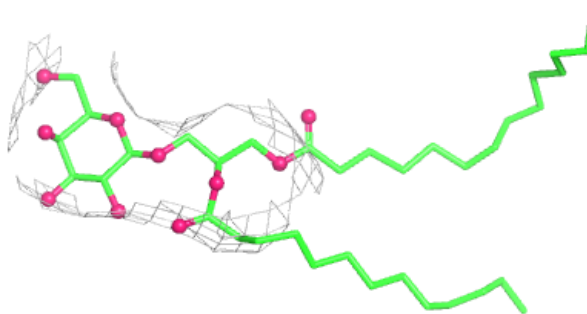


Electron density around CLA a 403:

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

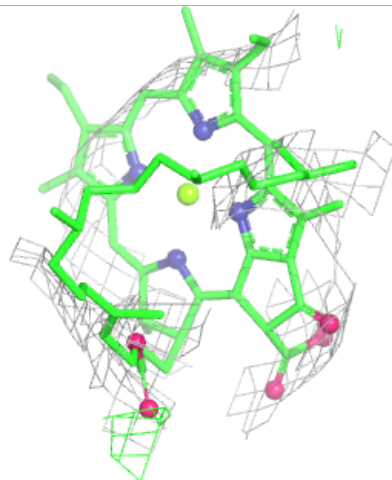
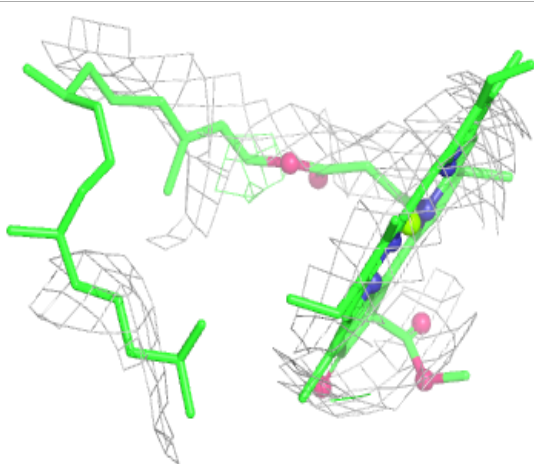
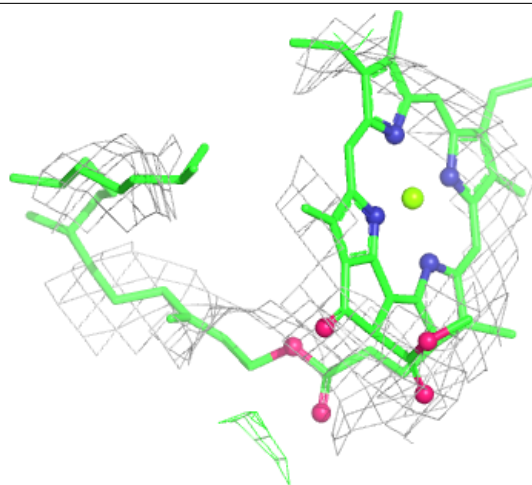
**Electron density around LMG D 409:**

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



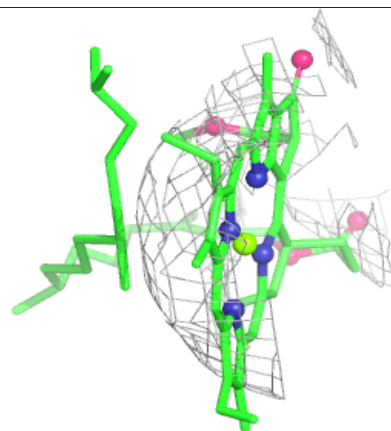
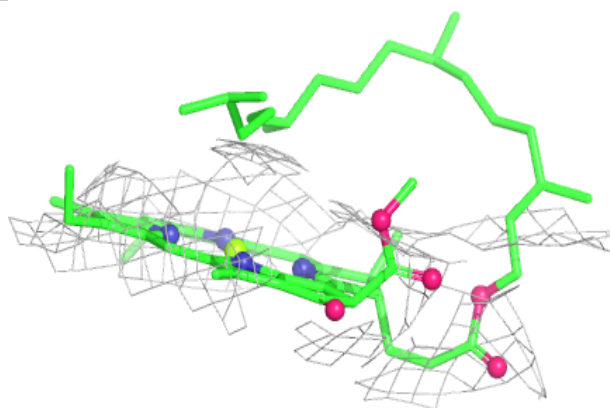
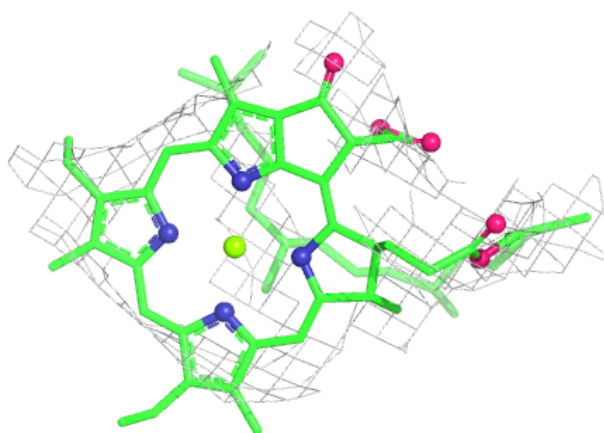
Electron density around CLA C 503:

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

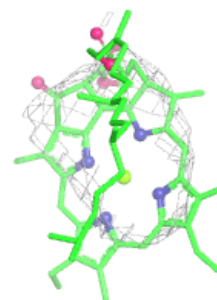
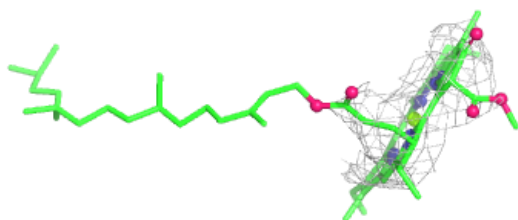
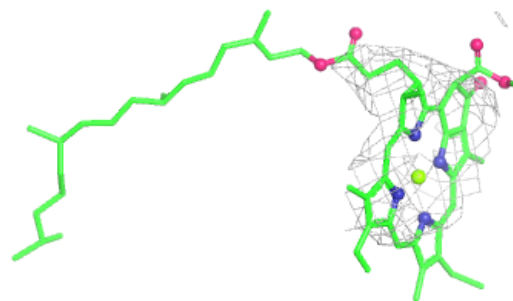


Electron density around CLA c 509:

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

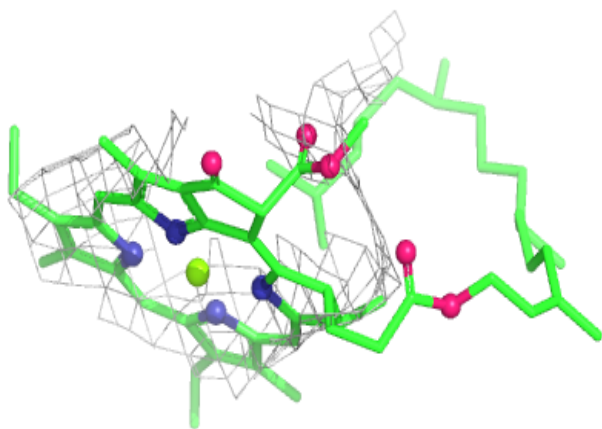
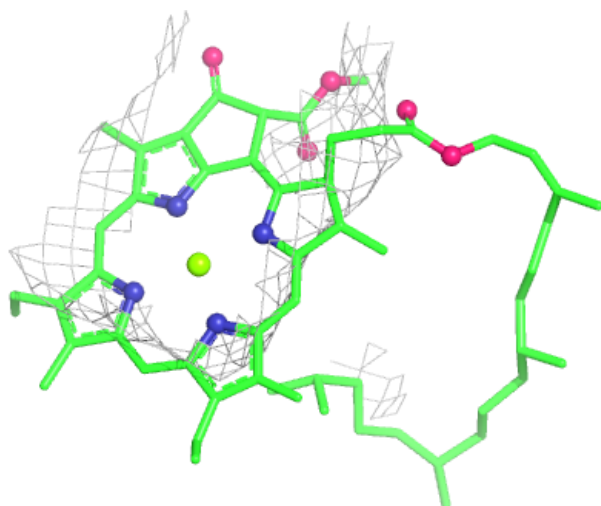
**Electron density around CLA B 608:**

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



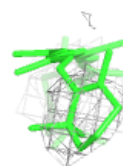
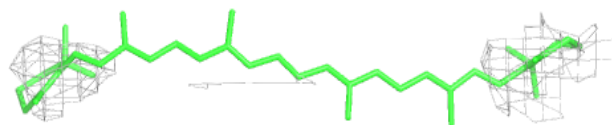
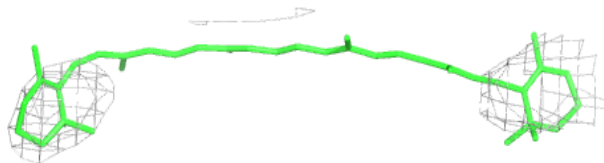
Electron density around CLA B 614:

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



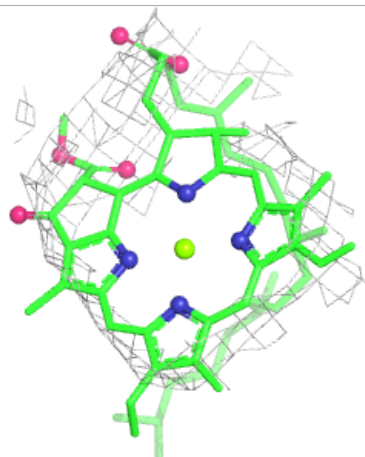
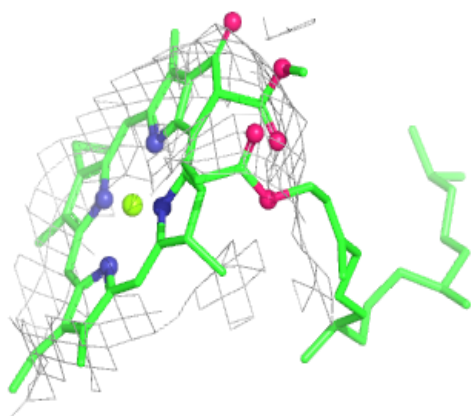
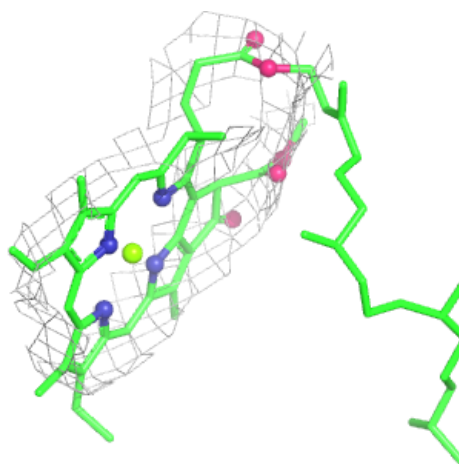
Electron density around BCR K 101:

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



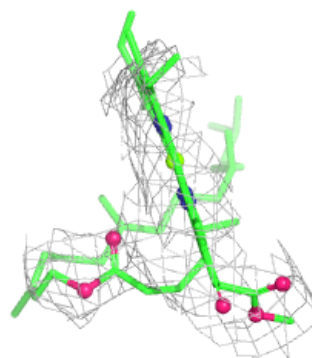
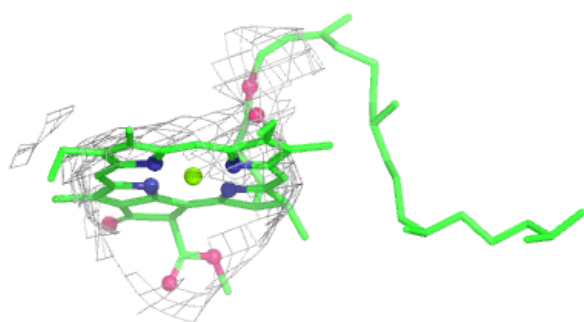
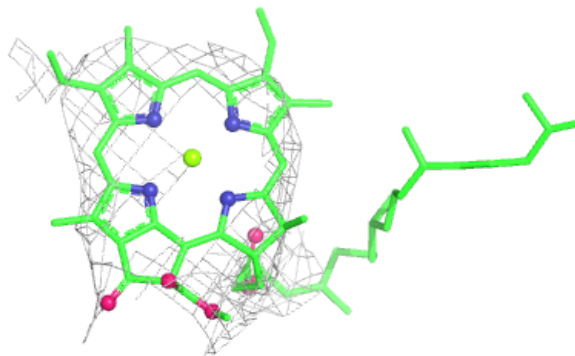
Electron density around CLA B 612:

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

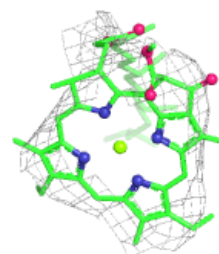
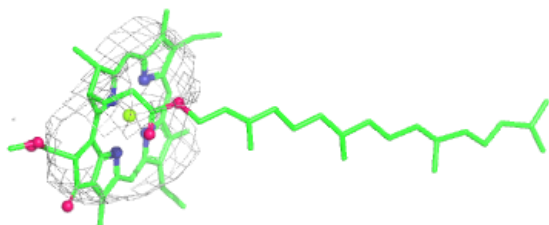
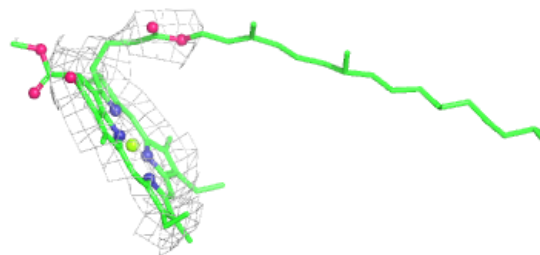


Electron density around CLA A 403:

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

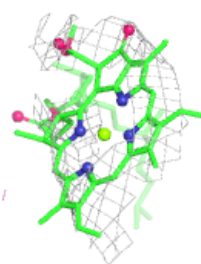
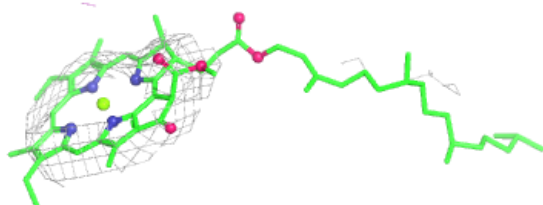
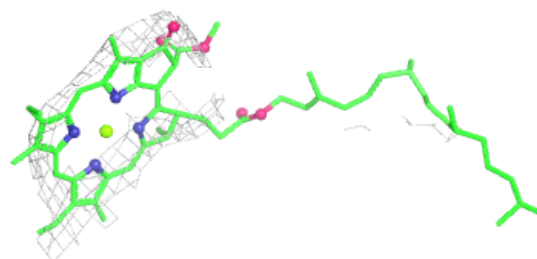
**Electron density around CLA B 606:**

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

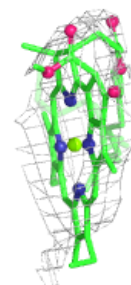
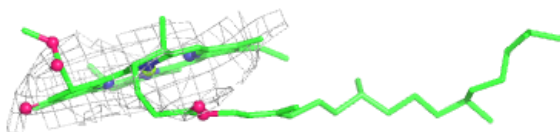
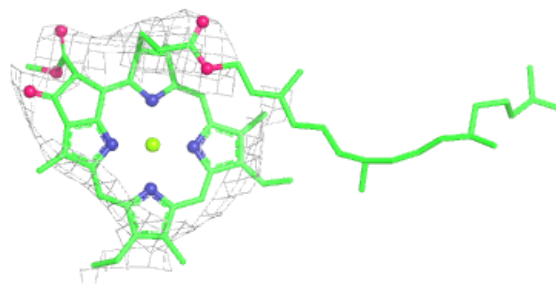


Electron density around CLA A 402:

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

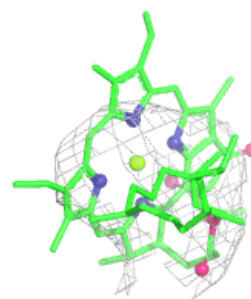
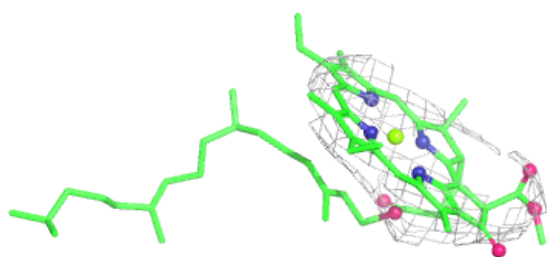
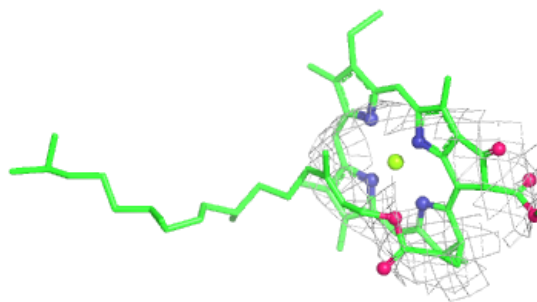
**Electron density around CLA B 602:**

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

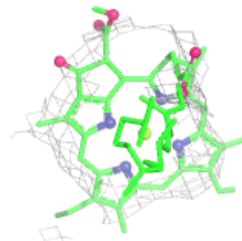
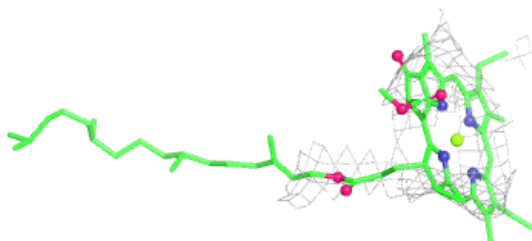
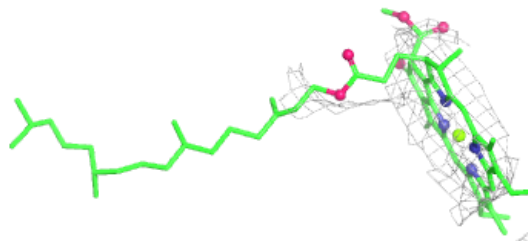


Electron density around CLA c 504:

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

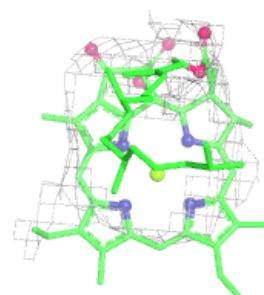
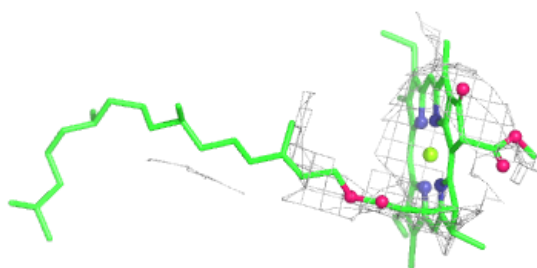
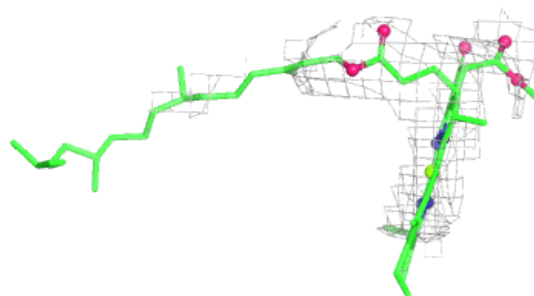
**Electron density around CLA B 603:**

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

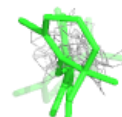
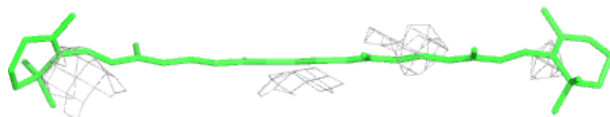
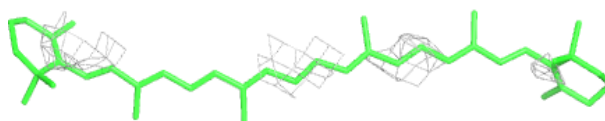


Electron density around CLA B 604:

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

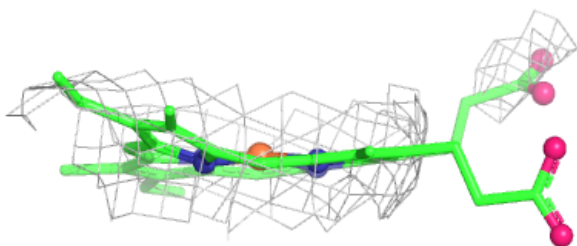
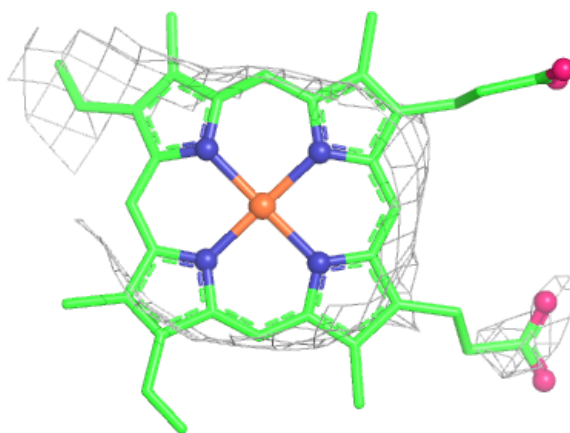
**Electron density around BCR B 618:**

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



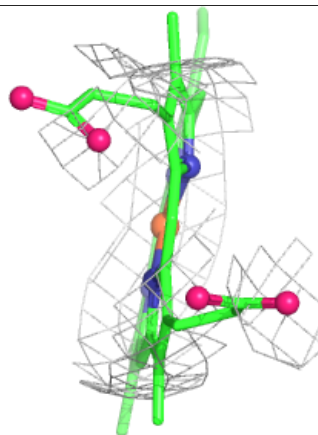
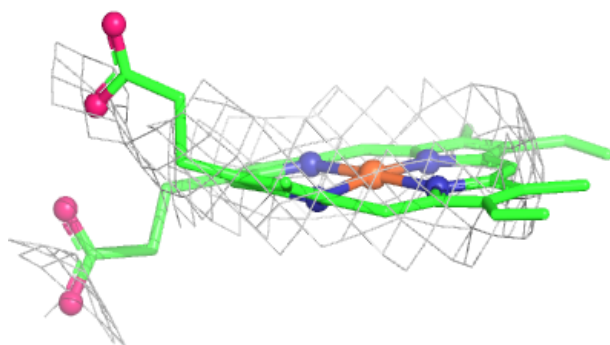
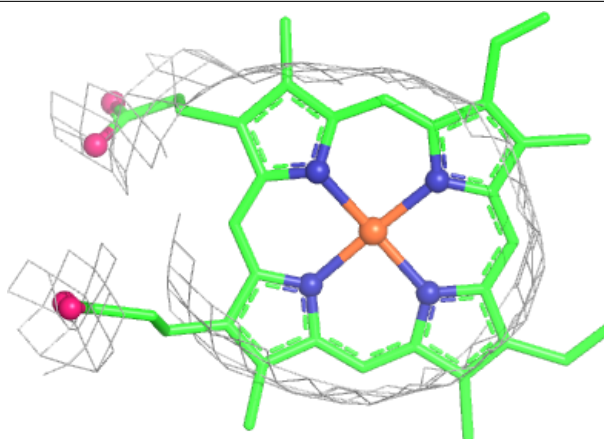
Electron density around HEM V 201:

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



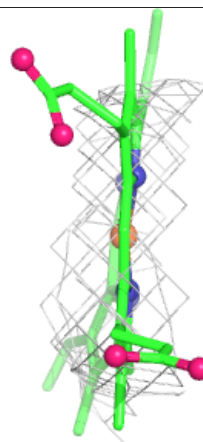
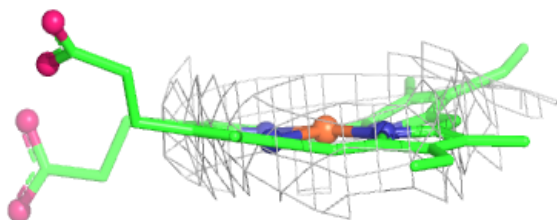
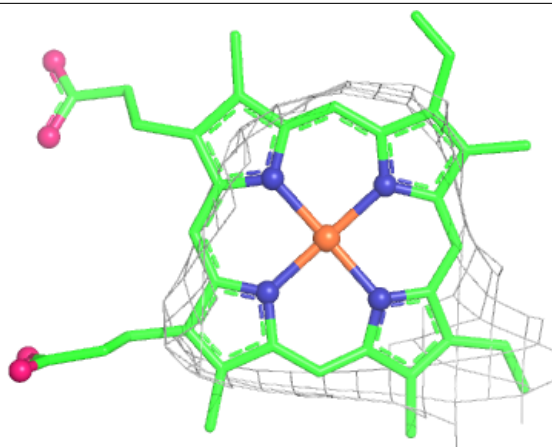
Electron density around HEM f 101:

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



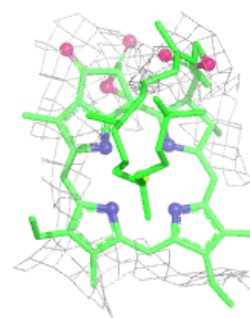
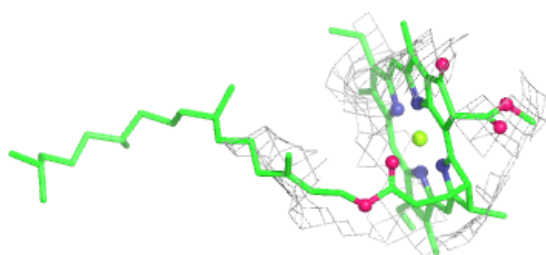
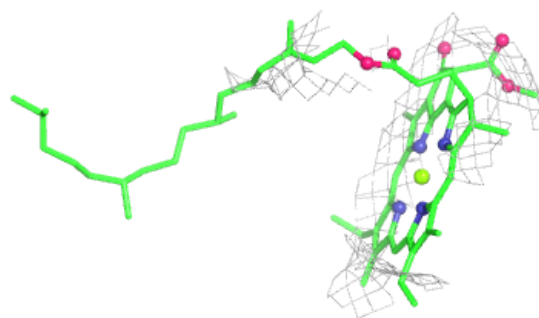
Electron density around HEM v 201:

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

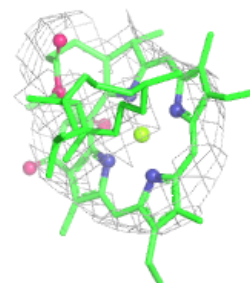
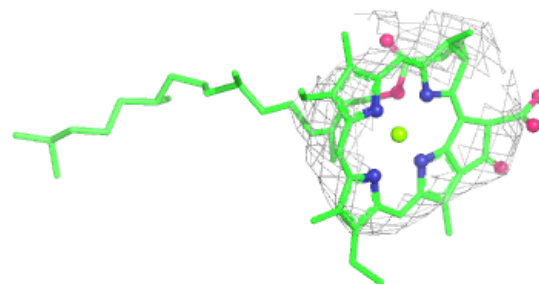


Electron density around CLA c 507:

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

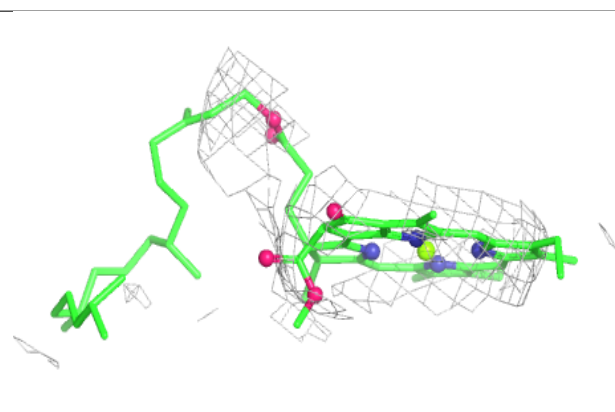
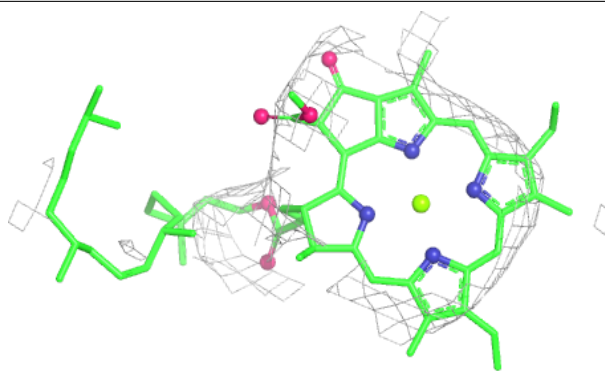
**Electron density around CLA C 504:**

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

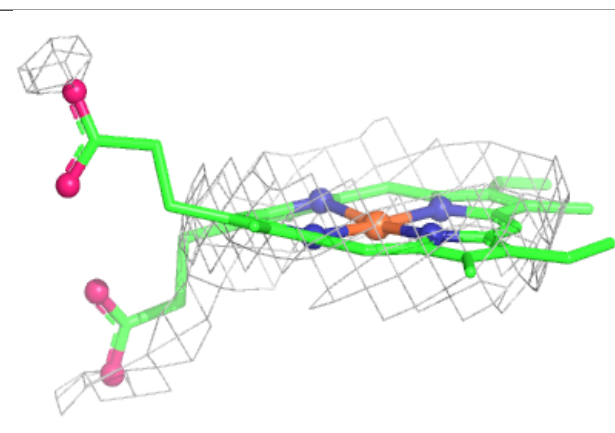
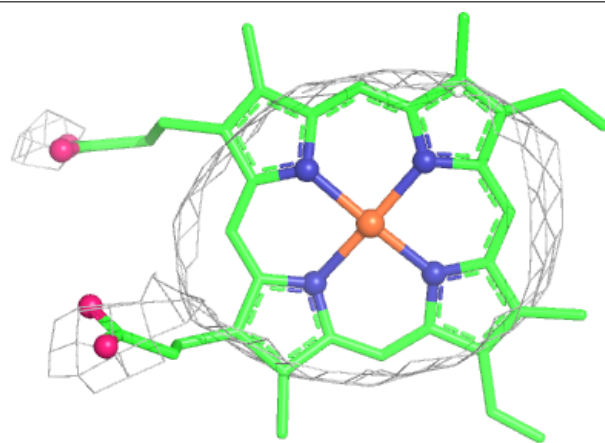


Electron density around CLA B 611:

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

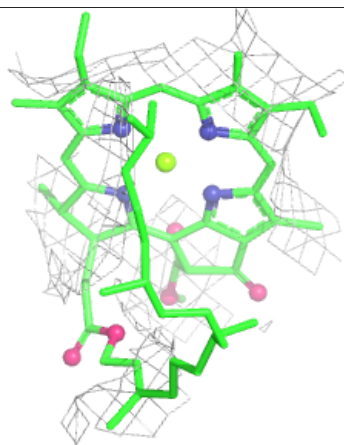
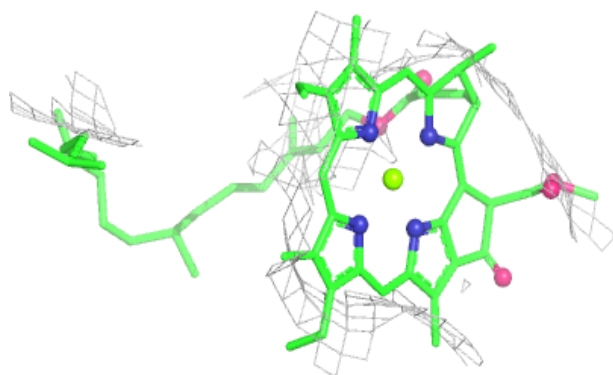
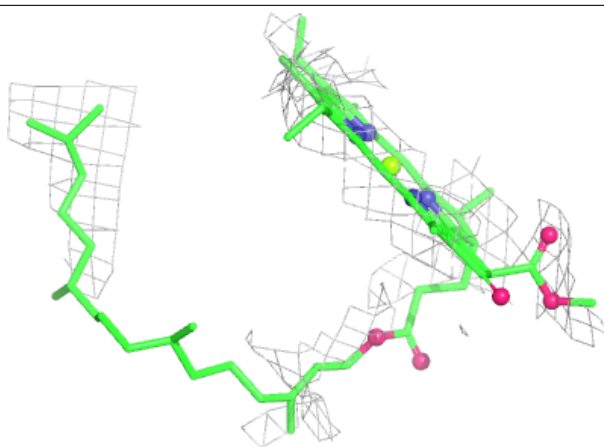
**Electron density around HEM F 101:**

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



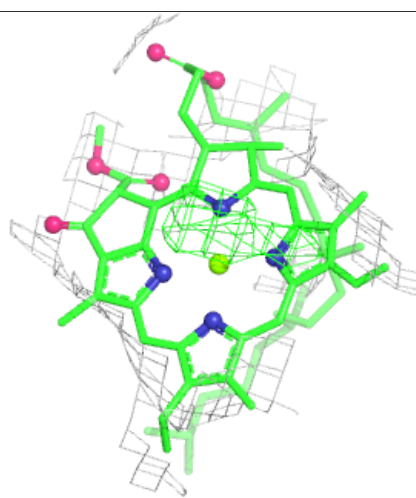
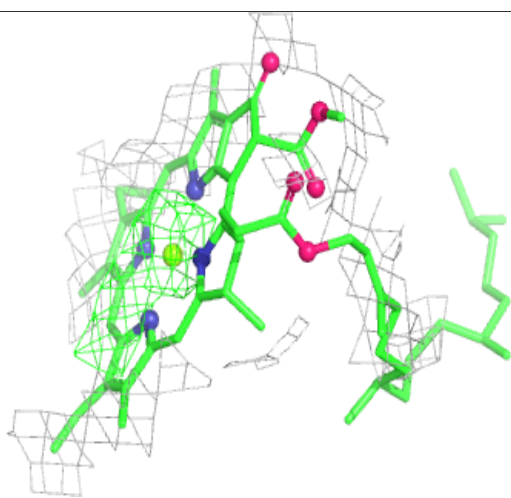
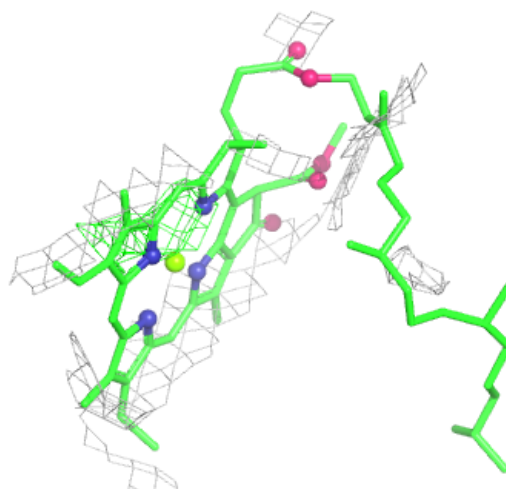
Electron density around CLA b 615:

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



Electron density around CLA b 617:

$2mF_o-DF_c$ (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.