



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 02:58 AM EDT

PDB ID : 4TNI / pdb_00004tni
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2014-06-04
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

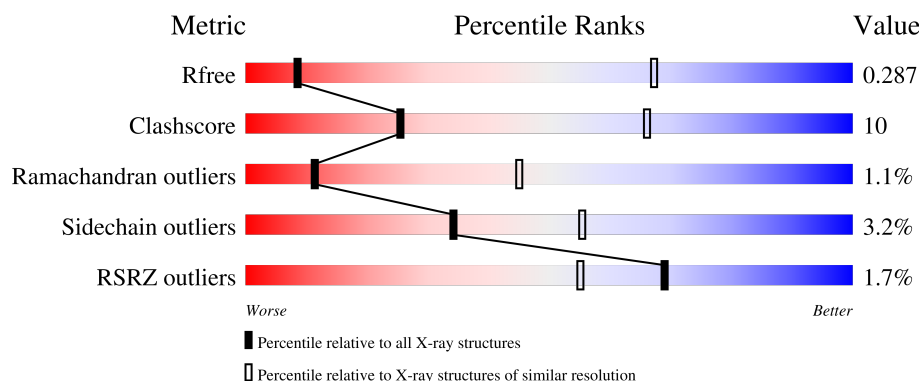
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	

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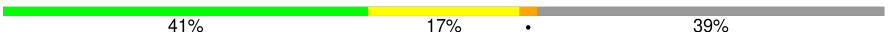
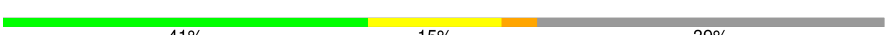
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 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	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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				

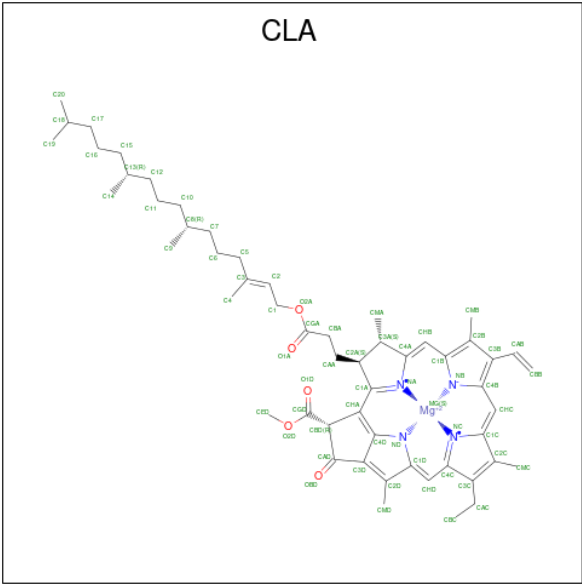
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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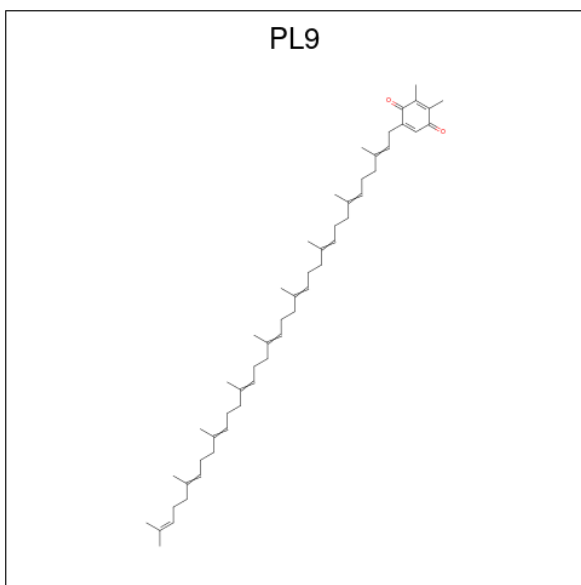
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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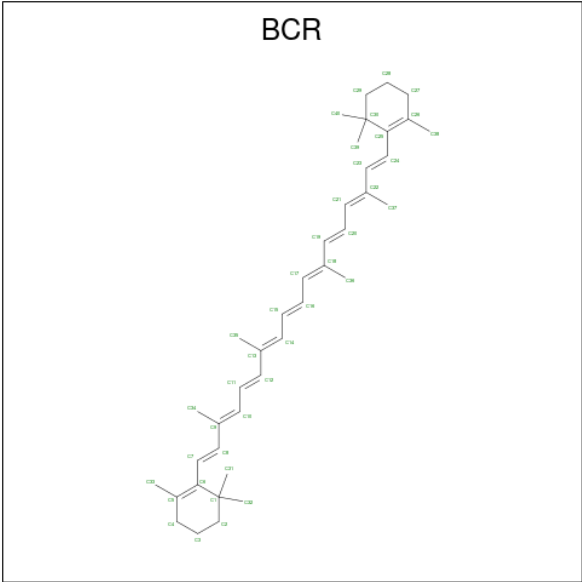
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



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

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



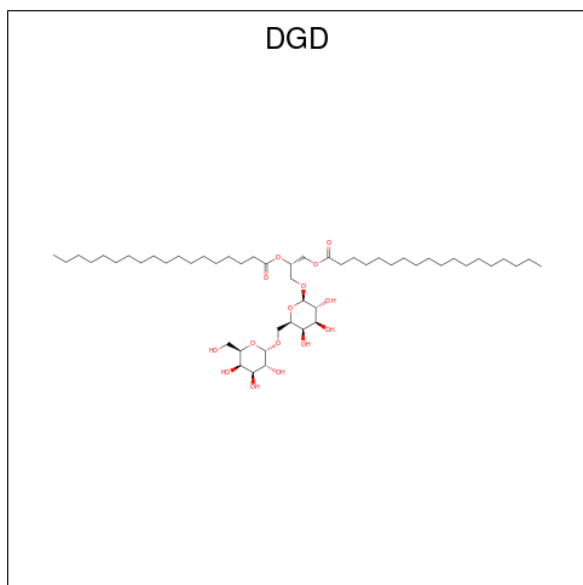
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total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

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

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



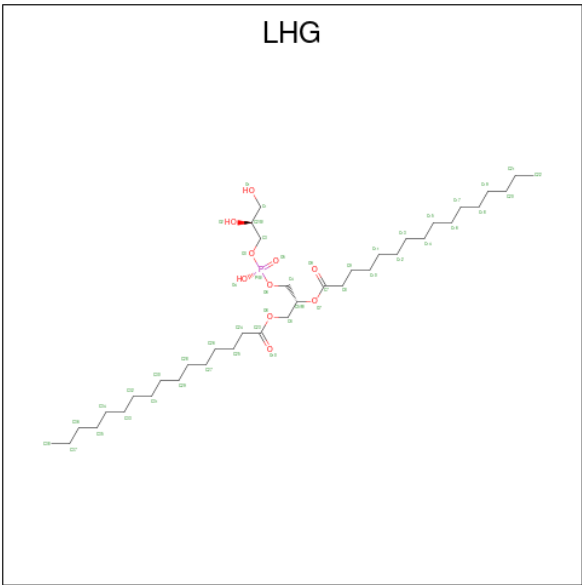
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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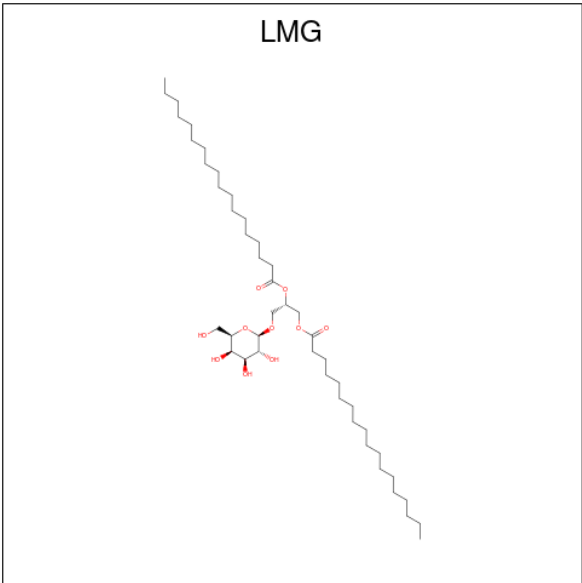
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

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



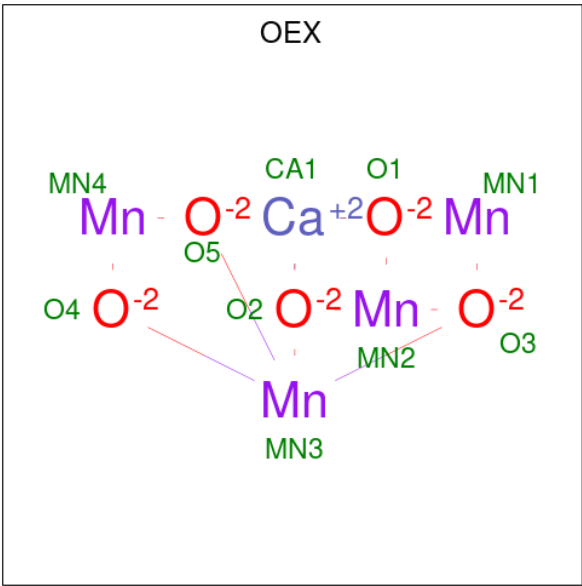
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

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



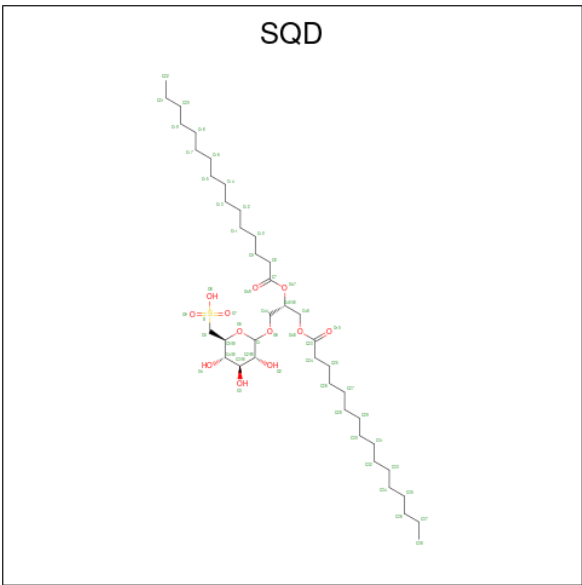
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



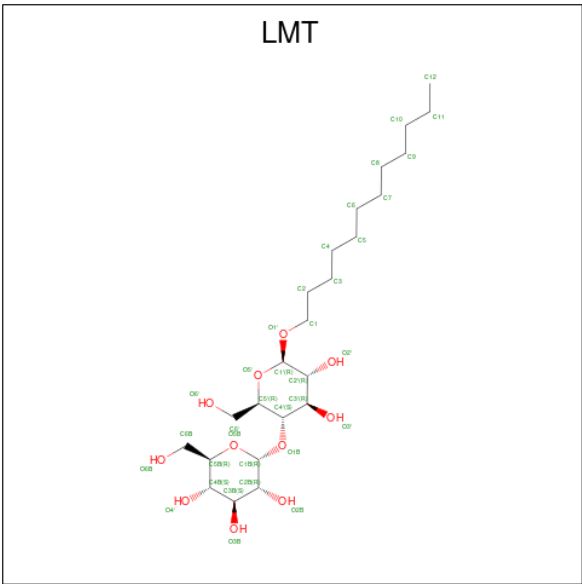
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
28	A	1	10	1	4	5	0	0
28	a	1	10	1	4	5	0	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



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

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



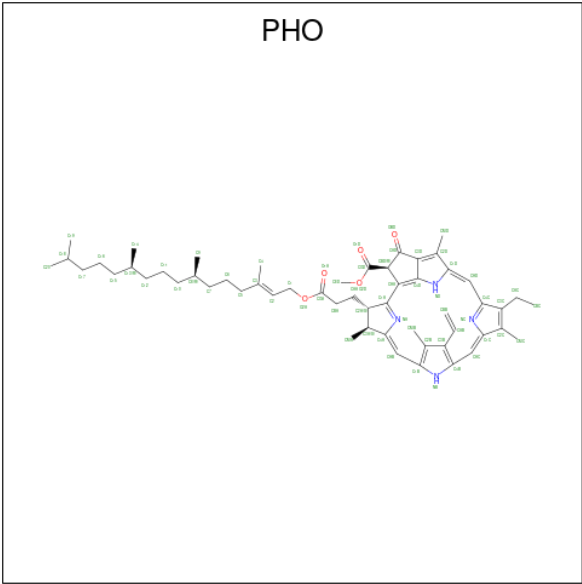
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).

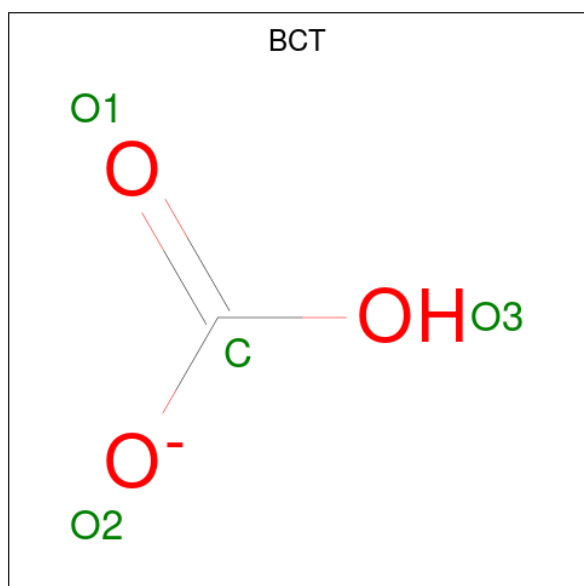


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	D	1	Total	Cl	0	0
			1	1		
32	a	1	Total	Cl	0	0
			1	1		

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



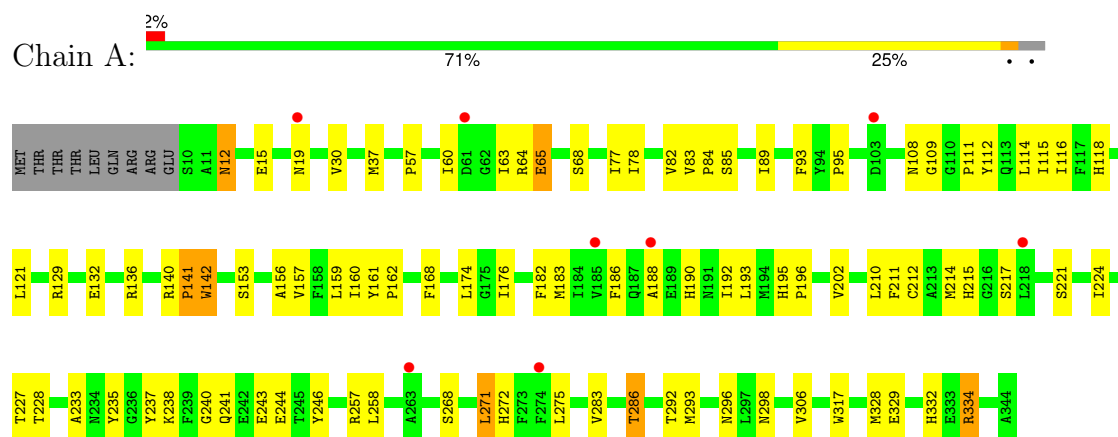
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

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

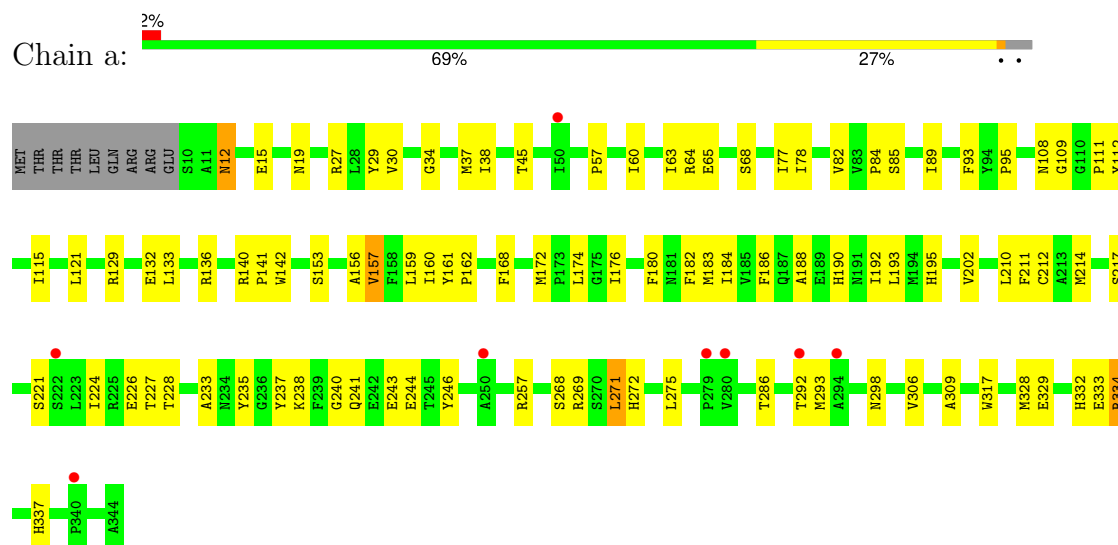
3 Residue-property plots [i](#)

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

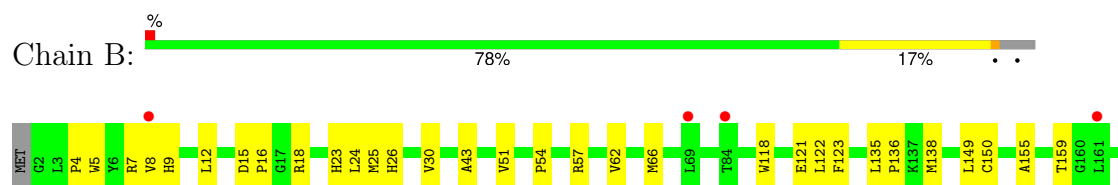
• Molecule 1: Photosystem Q(B) protein 1

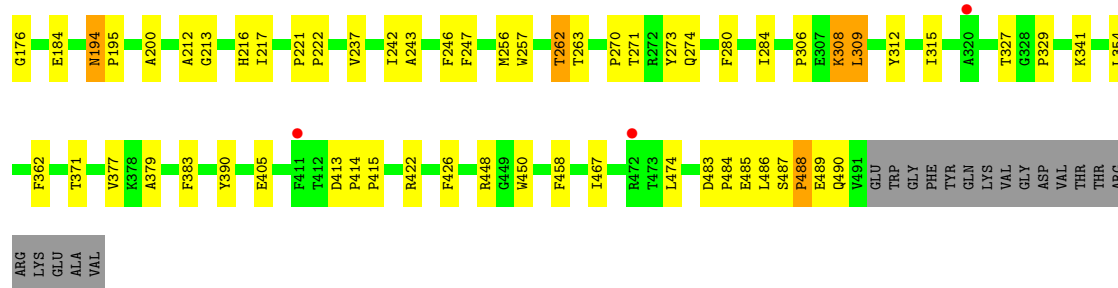


• Molecule 1: Photosystem Q(B) protein 1

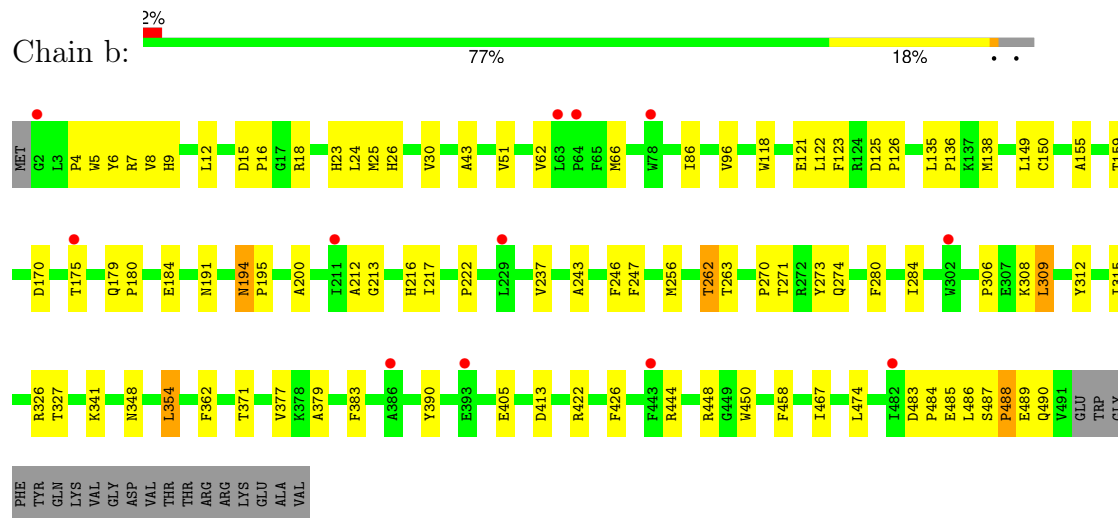


• Molecule 2: Photosystem II core light harvesting protein

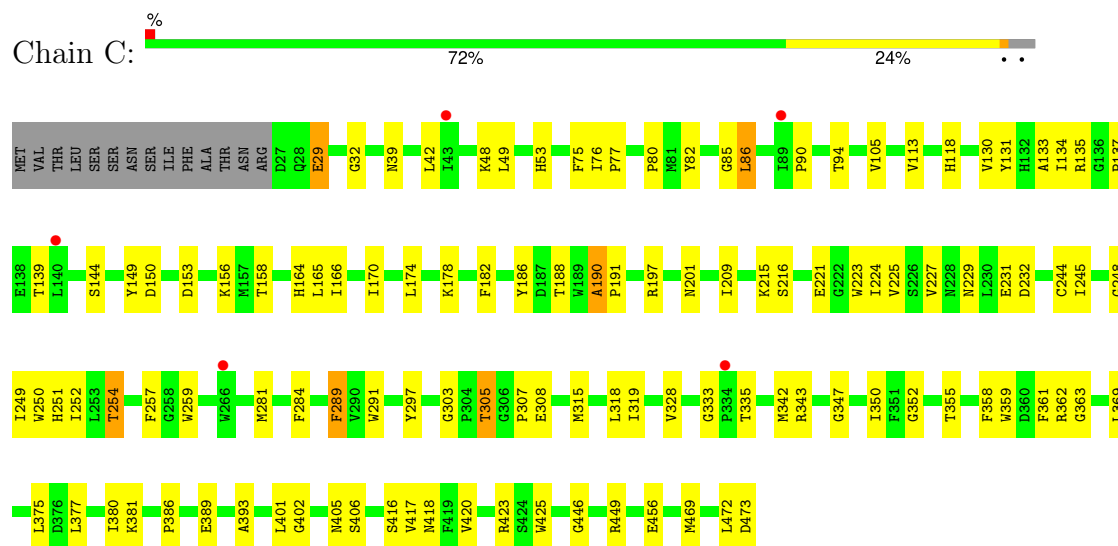




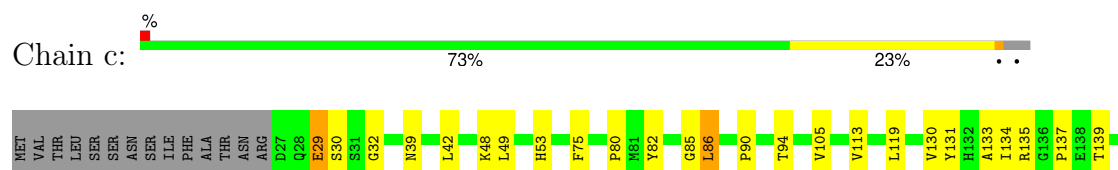
• Molecule 2: Photosystem II core light harvesting protein

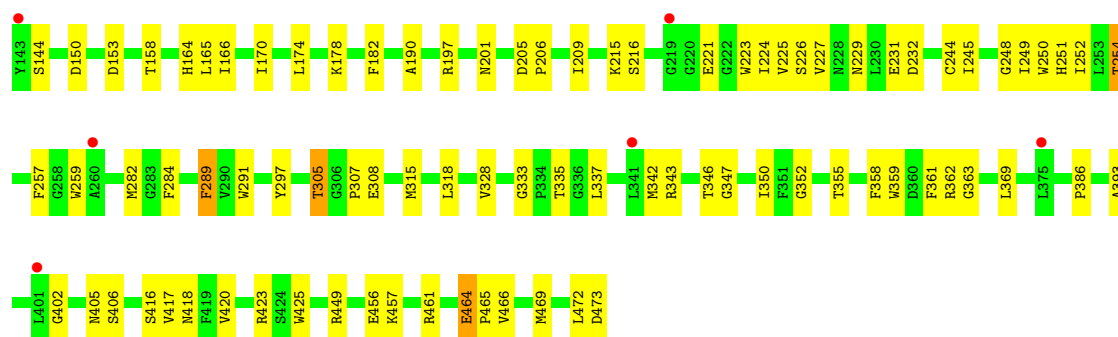


• Molecule 3: Photosystem II CP43 protein

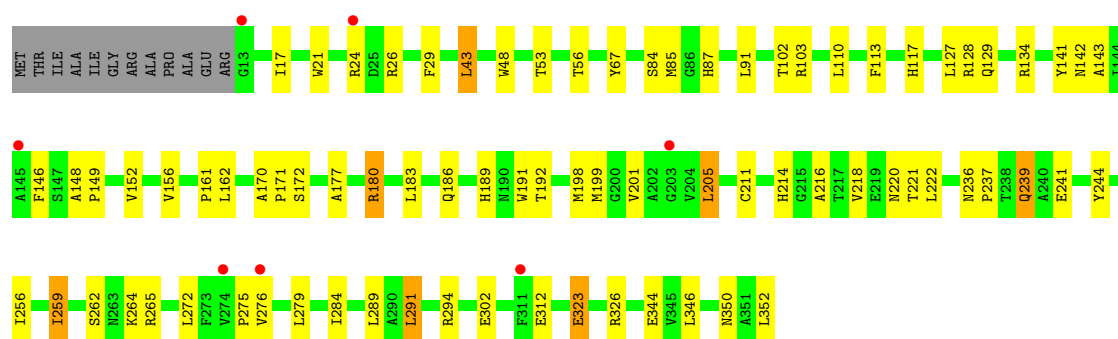
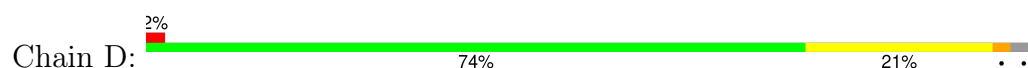


• Molecule 3: Photosystem II CP43 protein

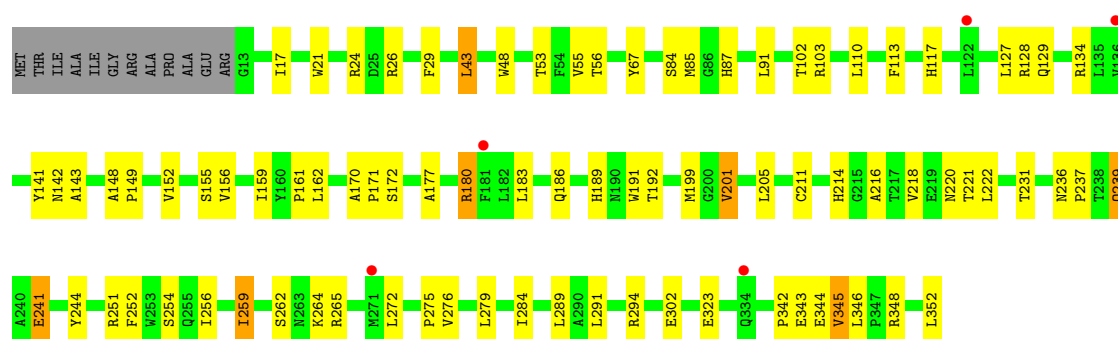




• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha





- Molecule 6: Cytochrome b559 subunit beta



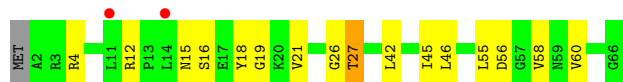
- Molecule 6: Cytochrome b559 subunit beta



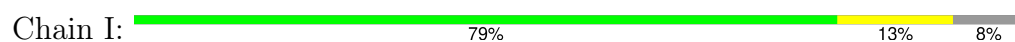
- Molecule 7: Photosystem II reaction center protein H



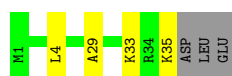
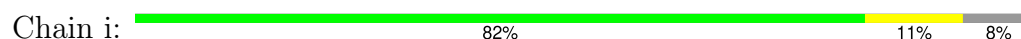
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





• Molecule 9: Photosystem II reaction center protein J



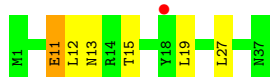
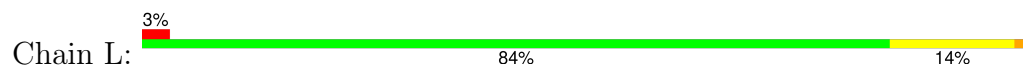
• Molecule 10: Photosystem II reaction center protein K



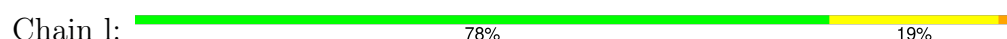
• Molecule 10: Photosystem II reaction center protein K



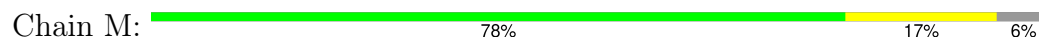
• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L

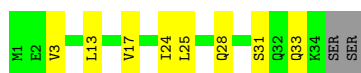


• Molecule 12: Photosystem II reaction center protein M

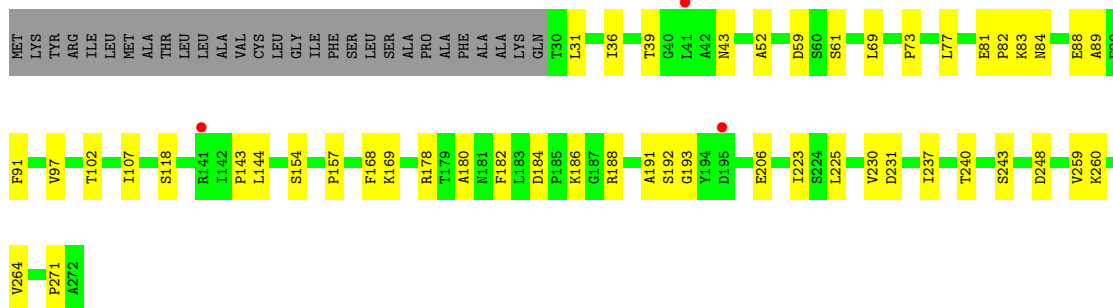


• Molecule 12: Photosystem II reaction center protein M

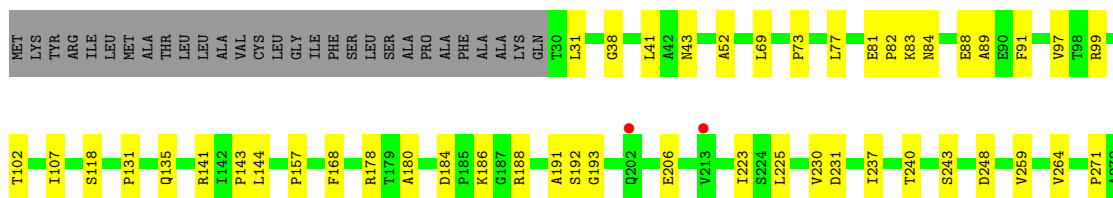




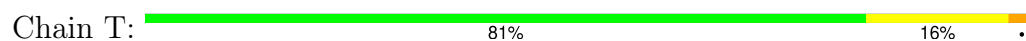
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



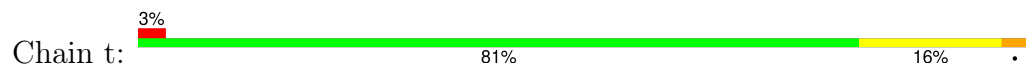
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



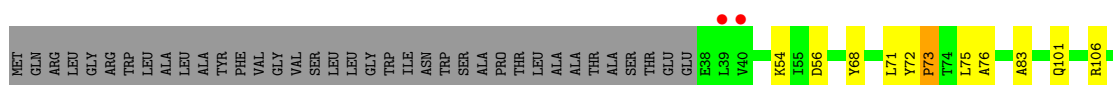
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T

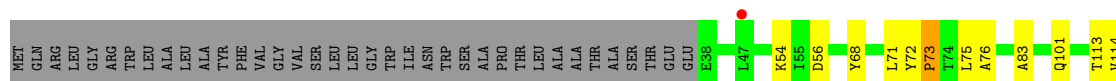


• Molecule 15: Photosystem II 12 kDa extrinsic protein

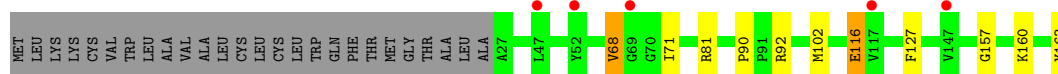
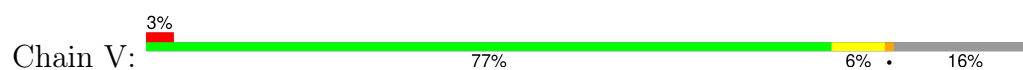




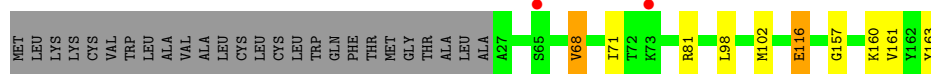
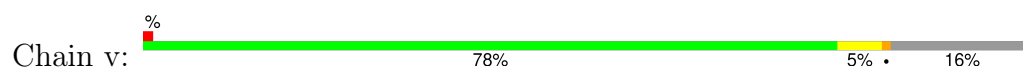
- Molecule 15: Photosystem II 12 kDa extrinsic protein



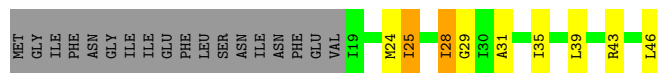
- Molecule 16: Cytochrome c-550



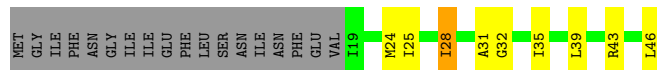
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

Chain x:  61% 24% • • 10%



- Molecule 19: Photosystem II reaction center protein Y

Chain Y:  100%

There are no outlier residues recorded for this chain.

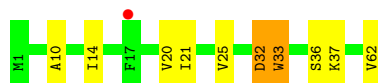
- Molecule 19: Photosystem II reaction center protein Y

Chain G:  100%

There are no outlier residues recorded for this chain.

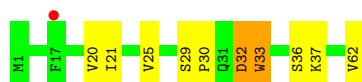
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  2% 84% 13% •



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  2% 84% 13% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.6 (72.96-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.278 , 0.284 0.283 , 0.287	Depositor DCC
R_{free} test set	2522 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 127.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	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)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: FE2, DGD, BCR, LMG, PL9, BCT, LMT, OEX, CL, HEM, CLA, CA, LHG, SQD, PHO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/2713	0.77	2/3700 (0.1%)
1	a	0.30	0/2713	0.78	3/3700 (0.1%)
2	B	0.30	0/3986	0.80	8/5433 (0.1%)
2	b	0.30	0/3986	0.81	8/5433 (0.1%)
3	C	0.30	0/3556	0.79	6/4842 (0.1%)
3	c	0.30	0/3556	0.80	8/4842 (0.2%)
4	D	0.29	0/2801	0.76	0/3818
4	d	0.29	0/2801	0.77	0/3818
5	E	0.31	0/685	0.82	0/933
5	e	0.31	0/685	0.83	0/933
6	F	0.34	0/291	0.74	0/397
6	f	0.34	0/291	0.74	0/397
7	H	0.33	0/520	0.73	0/709
7	h	0.33	0/520	0.73	0/709
8	I	0.29	0/293	0.77	0/395
8	i	0.29	0/293	0.78	0/395
9	J	0.30	0/255	0.84	0/346
9	j	0.30	0/255	0.84	0/346
10	K	0.44	0/303	0.85	0/416
10	k	0.45	0/303	0.86	0/416
11	L	0.28	0/311	0.72	0/422
11	l	0.28	0/311	0.71	0/422
12	M	0.30	0/270	0.77	0/367
12	m	0.33	0/270	0.84	1/367 (0.3%)
13	O	0.27	0/1876	0.71	0/2548
13	o	0.27	0/1876	0.70	0/2548
14	T	0.27	0/284	0.74	0/381
14	t	0.27	0/284	0.73	0/381
15	U	0.30	0/785	0.77	0/1064
15	u	0.30	0/785	0.78	0/1064
16	V	0.29	0/1081	0.75	2/1468 (0.1%)
16	v	0.29	0/1081	0.75	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.32	0/202	0.78	0/272
17	y	0.32	0/202	0.76	0/272
18	X	0.38	0/273	0.79	0/370
18	x	0.37	0/273	0.79	0/370
20	Z	0.31	0/490	0.83	0/669
20	z	0.31	0/490	0.84	0/669
All	All	0.30	0/41950	0.78	38/57100 (0.1%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	483	ASP	CA-C-N	10.64	133.14	119.84
2	b	483	ASP	C-N-CA	10.64	133.14	119.84
2	B	483	ASP	CA-C-N	10.56	133.04	119.84
2	B	483	ASP	C-N-CA	10.56	133.04	119.84
3	c	363	GLY	CA-C-N	6.26	125.75	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	71	0
1	a	2628	0	2524	68	0
2	B	3850	0	3718	59	0
2	b	3850	0	3718	62	0
3	C	3444	0	3365	72	0
3	c	3444	0	3365	71	0
4	D	2706	0	2608	63	0
4	d	2706	0	2608	68	0
5	E	666	0	651	13	0
5	e	666	0	651	15	0
6	F	282	0	291	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	5	0
7	H	507	0	521	13	0
7	h	507	0	521	13	0
8	I	286	0	308	3	0
8	i	286	0	308	2	0
9	J	249	0	262	7	0
9	j	249	0	262	7	0
10	K	293	0	305	11	0
10	k	293	0	305	9	0
11	L	304	0	316	5	0
11	l	304	0	316	6	0
12	M	267	0	289	6	0
12	m	267	0	289	7	0
13	O	1845	0	1801	28	0
13	o	1845	0	1801	29	0
14	T	275	0	288	5	0
14	t	275	0	288	5	0
15	U	774	0	773	8	0
15	u	774	0	773	7	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	8	0
17	g	201	0	226	7	0
17	y	201	0	226	7	0
18	X	270	0	299	10	0
18	x	270	0	299	9	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	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	27	0
22	B	975	0	1080	52	0
22	C	845	0	936	28	0
22	D	130	0	144	10	0
22	H	65	0	72	8	0
22	a	260	0	288	25	0
22	b	975	0	1080	50	0
22	c	845	0	936	32	0
22	d	130	0	144	11	0
22	h	65	0	72	9	0
23	A	45	0	61	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D	55	0	80	8	0
23	J	35	0	45	1	0
23	a	45	0	61	3	0
23	d	55	0	80	6	0
23	j	35	0	45	0	0
24	A	40	0	56	3	0
24	B	160	0	224	11	0
24	C	80	0	112	11	0
24	F	40	0	56	3	0
24	H	40	0	56	3	0
24	J	40	0	56	1	0
24	K	40	0	56	3	0
24	a	40	0	56	2	0
24	b	160	0	224	13	0
24	c	120	0	168	15	0
24	f	40	0	56	2	0
24	g	40	0	56	5	0
24	j	40	0	56	1	0
24	x	40	0	56	1	0
24	y	40	0	56	7	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	11	0
25	D	63	0	87	1	0
25	a	56	0	70	2	0
25	b	110	0	136	4	0
25	c	181	0	245	10	0
25	d	63	0	87	2	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	1	0
26	c	37	0	44	2	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	3	0
27	D	143	0	196	9	0
27	E	44	0	58	1	0
27	I	43	0	56	0	0
27	M	42	0	54	2	0
27	a	93	0	126	3	0
27	b	49	0	68	5	0
27	c	93	0	126	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	d	143	0	196	10	0
27	e	44	0	58	1	0
27	i	43	0	56	1	0
27	m	42	0	54	1	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	105	0	147	8	0
29	B	90	0	111	4	0
29	F	45	0	54	2	0
29	a	105	0	147	8	0
29	b	47	0	61	1	0
29	d	43	0	50	4	0
29	f	45	0	54	3	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	0	0
30	M	70	0	91	0	0
30	b	140	0	183	5	0
30	d	31	0	35	0	0
30	i	35	0	46	1	0
31	D	128	0	148	12	0
31	d	128	0	148	10	0
32	D	1	0	0	0	0
32	a	1	0	0	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	5	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51372	970	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 970 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	1.58	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:c:362:ARG:H	25:c:515:DGD:HE4	1.44	0.81
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.62	0.81

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%)	309 (93%)	20 (6%)	4 (1%)	10	42
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	16	53
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	21	58
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	14	49
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	14	49
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36	71
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36	71
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	41
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9	41
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	22
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	22
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10	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	21
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	30
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5	30
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2	19
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2	19
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	14
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	14
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	35
All	All	5138/5618 (92%)	4675 (91%)	408 (8%)	55 (1%)	11	45

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	261 (96%)	10 (4%)	30	51
1	a	271/280 (97%)	260 (96%)	11 (4%)	27	49
2	B	390/407 (96%)	379 (97%)	11 (3%)	38	59
2	b	390/407 (96%)	380 (97%)	10 (3%)	40	60
3	C	347/362 (96%)	335 (96%)	12 (4%)	32	53
3	c	347/362 (96%)	335 (96%)	12 (4%)	32	53
4	D	275/283 (97%)	265 (96%)	10 (4%)	31	52
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	41
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	41
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	50 (94%)	3 (6%)	18	40
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	40
8	I	32/35 (91%)	31 (97%)	1 (3%)	35	56
8	i	32/35 (91%)	31 (97%)	1 (3%)	35	56
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	48
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	48
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	57
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	57
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	68	76
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	76

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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	67
16	v	116/138 (84%)	114 (98%)	2 (2%)	53	67
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%)	28 (93%)	2 (7%)	15	36
20	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
20	z	52/52 (100%)	50 (96%)	2 (4%)	29	51
All	All	4244/4594 (92%)	4109 (97%)	135 (3%)	34	55

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	27	THR
9	j	7	ARG
17	g	46	LEU
7	H	56	ASP
7	H	27	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	374	ASN
4	d	301	GLN
3	c	44	ASN
3	c	441	HIS
13	o	130	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	605	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	6 (7%)
30	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	2 (4%)
26	LHG	C	519	-	36,36,48	0.72	1 (2%)	39,42,54	1.30	4 (10%)
22	CLA	C	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
30	LMT	M	103	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
33	BCT	d	404	21	3,3,3	1.11	0	2,3,3	4.26	2 (100%)
22	CLA	c	510	3	69,73,73	1.20	5 (7%)	82,113,113	1.28	5 (6%)
22	CLA	d	405	-	69,73,73	1.19	7 (10%)	82,113,113	1.19	6 (7%)
27	LMG	d	412	-	46,46,55	0.77	1 (2%)	54,54,63	1.30	6 (11%)
22	CLA	A	405	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
30	LMT	b	604	-	36,36,36	1.11	4 (11%)	47,47,47	1.05	1 (2%)
29	SQD	B	622	-	41,43,54	1.05	2 (4%)	51,54,65	1.68	11 (21%)
25	DGD	C	517	-	67,67,67	0.86	0	81,81,81	1.40	9 (11%)
27	LMG	a	412	-	51,51,55	0.75	0	59,59,63	1.34	6 (10%)
24	BCR	c	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	9 (16%)
22	CLA	B	613	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	C	509	3	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	C	520	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	611	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	6 (7%)
22	CLA	b	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
24	BCR	y	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.27	8 (14%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.27	4 (7%)
22	CLA	B	612	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
22	CLA	b	619	2	69,73,73	1.18	7 (10%)	82,113,113	1.23	4 (4%)
24	BCR	A	407	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	7 (12%)
25	DGD	b	624	-	59,59,67	0.90	1 (1%)	73,73,81	1.33	7 (9%)
22	CLA	c	504	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	5 (6%)
26	LHG	A	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	3 (7%)
22	CLA	c	508	3	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
27	LMG	i	101	-	43,43,55	0.80	0	51,51,63	1.27	6 (11%)
22	CLA	a	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
24	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	7 (12%)
24	BCR	g	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	8 (14%)
27	LMG	D	408	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	5 (8%)
22	CLA	B	606	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
27	LMG	d	409	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	4 (4%)
23	PL9	j	101	-	35,35,55	0.98	2 (5%)	44,45,69	1.58	9 (20%)
22	CLA	c	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
30	LMT	B	624	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.29	5 (9%)
22	CLA	a	405	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	5 (6%)
30	LMT	B	627	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)
22	CLA	B	604	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
22	CLA	a	404	1	69,73,73	1.19	7 (10%)	82,113,113	1.25	7 (8%)
22	CLA	C	504	3	69,73,73	1.18	7 (10%)	82,113,113	1.31	5 (6%)
27	LMG	d	408	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	5 (8%)
31	PHO	D	402	-	58,69,69	2.20	9 (15%)	55,99,99	1.42	5 (9%)
26	LHG	a	411	-	38,38,48	0.69	1 (2%)	41,44,54	1.23	3 (7%)
28	OEX	A	411	1,3	0,14,14	-	-	-	-	-
22	CLA	C	508	3	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	c	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.28	5 (6%)
25	DGD	C	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.42	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OEX	a	414	1,3	0,14,14	-	-	-		
22	CLA	b	612	2	69,73,73	1.20	6 (8%)	82,113,113	1.22	5 (6%)
22	CLA	b	617	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	C	512	3	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	H	101	-	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	b	610	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
34	HEM	v	201	16	50,50,50	2.00	10 (20%)	67,82,82	1.25	4 (5%)
22	CLA	C	507	3	69,73,73	1.19	8 (11%)	82,113,113	1.29	6 (7%)
31	PHO	D	401	-	58,69,69	2.15	9 (15%)	55,99,99	1.42	6 (10%)
22	CLA	c	509	3	69,73,73	1.19	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
25	DGD	c	517	-	67,67,67	0.87	0	81,81,81	1.39	9 (11%)
30	LMT	d	411	-	32,32,36	1.16	4 (12%)	43,43,47	1.00	2 (4%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	7 (11%)
22	CLA	B	603	2	69,73,73	1.18	8 (11%)	82,113,113	1.35	7 (8%)
27	LMG	D	412	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	6 (11%)
22	CLA	B	605	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
25	DGD	D	410	-	64,64,67	0.91	0	78,78,81	1.32	9 (11%)
23	PL9	J	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.58	8 (18%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
24	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	9 (16%)
31	PHO	d	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)
29	SQD	f	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.57	10 (18%)
22	CLA	C	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
24	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	8 (14%)
29	SQD	a	401	-	52,54,54	0.95	2 (3%)	62,65,65	1.48	9 (14%)
22	CLA	a	407	1	69,73,73	1.18	6 (8%)	82,113,113	1.24	5 (6%)
22	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
34	HEM	F	101	5,6	50,50,50	1.97	9 (18%)	67,82,82	1.32	4 (5%)
27	LMG	a	402	-	42,42,55	0.82	2 (4%)	50,50,63	1.26	5 (10%)
29	SQD	A	412	-	49,51,54	0.96	2 (4%)	59,62,65	1.67	10 (16%)
22	CLA	D	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.20	5 (6%)
22	CLA	b	609	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
24	BCR	B	616	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.32	7 (10%)
22	CLA	A	402	1	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
23	PL9	D	407	-	55,55,55	1.06	4 (7%)	68,69,69	1.50	13 (19%)
22	CLA	c	507	3	69,73,73	1.18	8 (11%)	82,113,113	1.29	7 (8%)
24	BCR	j	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.60	12 (21%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
34	HEM	f	101	5,6	50,50,50	1.97	8 (16%)	67,82,82	1.33	4 (5%)
30	LMT	b	603	-	36,36,36	1.10	4 (11%)	47,47,47	0.96	1 (2%)
22	CLA	c	501	3	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	b	614	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	6 (7%)
22	CLA	b	618	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
22	CLA	b	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
29	SQD	A	413	-	52,54,54	0.95	3 (5%)	62,65,65	1.48	9 (14%)
22	CLA	b	607	2	69,73,73	1.19	8 (11%)	82,113,113	1.33	7 (8%)
22	CLA	B	610	2	69,73,73	1.24	6 (8%)	82,113,113	1.34	6 (7%)
30	LMT	D	411	-	32,32,36	1.16	4 (12%)	43,43,47	1.03	2 (4%)
22	CLA	C	511	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	b	616	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	7 (8%)
24	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	8 (14%)
22	CLA	B	607	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	B	608	2	69,73,73	1.20	7 (10%)	82,113,113	1.25	5 (6%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	c	520	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.41	9 (12%)
29	SQD	a	415	-	49,51,54	0.97	2 (4%)	59,62,65	1.69	10 (16%)
24	BCR	b	622	-	41,41,41	1.13	2 (4%)	56,56,56	1.39	11 (19%)
25	DGD	d	410	-	64,64,67	0.92	2 (3%)	78,78,81	1.34	9 (11%)
22	CLA	B	609	-	69,73,73	1.19	8 (11%)	82,113,113	1.27	5 (6%)
24	BCR	f	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
24	BCR	H	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
24	BCR	F	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	6 (10%)
22	CLA	b	615	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
27	LMG	M	101	-	42,42,55	0.84	1 (2%)	50,50,63	1.23	4 (8%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	9 (16%)
22	CLA	b	606	2	69,73,73	1.18	7 (10%)	82,113,113	1.22	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	5 (6%)
24	BCR	b	623	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	9 (16%)
30	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
24	BCR	b	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
34	HEM	V	201	16	50,50,50	1.98	9 (18%)	67,82,82	1.22	4 (5%)
22	CLA	C	503	3	69,73,73	1.19	8 (11%)	82,113,113	1.26	4 (4%)
30	LMT	b	627	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	2 (4%)
22	CLA	c	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
25	DGD	c	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.42	11 (14%)
22	CLA	d	406	-	69,73,73	1.19	5 (7%)	82,113,113	1.27	5 (6%)
22	CLA	A	404	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
29	SQD	B	626	-	45,47,54	1.01	3 (6%)	55,58,65	1.70	10 (18%)
22	CLA	C	502	3	69,73,73	1.19	9 (13%)	82,113,113	1.26	5 (6%)
24	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
31	PHO	d	401	-	58,69,69	2.15	9 (15%)	55,99,99	1.42	7 (12%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
25	DGD	a	410	-	57,57,67	0.92	1 (1%)	71,71,81	1.40	9 (12%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
22	CLA	B	601	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	6 (7%)
22	CLA	B	615	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
30	LMT	B	628	-	36,36,36	1.12	4 (11%)	47,47,47	1.05	1 (2%)
24	BCR	a	409	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	7 (12%)
33	BCT	D	404	21	3,3,3	1.11	0	2,3,3	4.29	2 (100%)
22	CLA	B	602	2	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
30	LMT	I	102	-	36,36,36	1.09	4 (11%)	47,47,47	1.02	2 (4%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	D	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
23	PL9	A	406	-	45,45,55	1.01	4 (8%)	56,57,69	1.55	10 (17%)
24	BCR	J	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.62	12 (21%)
27	LMG	m	101	-	42,42,55	0.84	0	50,50,63	1.23	4 (8%)
22	CLA	C	510	3	69,73,73	1.18	6 (8%)	82,113,113	1.30	6 (7%)
22	CLA	b	611	2	69,73,73	1.19	8 (11%)	82,113,113	1.24	4 (4%)
24	BCR	x	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
27	LMG	D	409	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	c	503	-	69,73,73	1.20	8 (11%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PL9	a	408	-	45,45,55	1.05	4 (8%)	56,57,69	1.54	10 (17%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.26	6 (8%)
30	LMT	b	626	-	36,36,36	1.11	4 (11%)	47,47,47	0.96	1 (2%)
29	SQD	d	403	-	41,43,54	1.05	2 (4%)	51,54,65	1.70	11 (21%)
29	SQD	b	602	-	45,47,54	1.02	3 (6%)	55,58,65	1.72	10 (18%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	9 (12%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	h	101	-	69,73,73	1.20	8 (11%)	82,113,113	1.24	5 (6%)
23	PL9	d	407	-	55,55,55	1.05	3 (5%)	68,69,69	1.51	12 (17%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.29	4 (7%)
30	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.01	2 (4%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.25	5 (7%)
27	LMG	C	521	-	48,48,55	0.77	1 (2%)	56,56,63	1.30	5 (8%)
24	BCR	C	514	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	9 (16%)
27	LMG	A	414	-	42,42,55	0.83	2 (4%)	50,50,63	1.25	4 (8%)
26	LHG	c	519	-	36,36,48	0.73	2 (5%)	39,42,54	1.30	4 (10%)
24	BCR	K	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	8 (14%)
29	SQD	F	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.57	10 (18%)

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	605	-	-	15/39/115/115	-
30	LMT	i	102	-	-	3/21/61/61	0/2/2/2
26	LHG	C	519	-	-	17/41/41/53	-
22	CLA	C	501	3	-	16/39/115/115	-
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	c	510	3	-	15/39/115/115	-
22	CLA	d	405	-	-	12/39/115/115	-
27	LMG	d	412	-	-	16/41/61/70	0/1/1/1
22	CLA	A	405	1	-	8/39/115/115	-
30	LMT	b	604	-	-	5/21/61/61	0/2/2/2
29	SQD	B	622	-	-	14/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	C	517	-	-	21/55/95/95	0/2/2/2
27	LMG	a	412	-	-	26/46/66/70	0/1/1/1
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	B	613	2	-	12/39/115/115	-
22	CLA	C	509	3	-	15/39/115/115	-
22	CLA	C	520	-	-	13/39/115/115	-
22	CLA	B	611	-	-	9/39/115/115	-
22	CLA	b	608	2	-	15/39/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
22	CLA	B	612	-	-	15/39/115/115	-
22	CLA	b	619	2	-	19/39/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
22	CLA	c	504	3	-	18/39/115/115	-
26	LHG	A	409	-	-	12/43/43/53	-
22	CLA	c	508	3	-	16/39/115/115	-
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
22	CLA	a	406	-	-	8/39/115/115	-
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
24	BCR	g	101	-	-	4/29/63/63	0/2/2/2
27	LMG	D	408	-	-	25/44/64/70	0/1/1/1
22	CLA	B	606	-	-	9/39/115/115	-
27	LMG	d	409	-	-	20/43/63/70	0/1/1/1
22	CLA	C	505	3	-	16/39/115/115	-
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
22	CLA	c	512	3	-	17/39/115/115	-
30	LMT	B	624	-	-	4/21/61/61	0/2/2/2
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
22	CLA	a	405	-	-	13/39/115/115	-
30	LMT	B	627	-	-	3/21/61/61	0/2/2/2
22	CLA	B	604	2	-	15/39/115/115	-
22	CLA	a	404	1	-	8/39/115/115	-
22	CLA	C	504	3	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	d	408	-	-	23/44/64/70	0/1/1/1
31	PHO	D	402	-	-	11/37/103/103	0/5/6/6
26	LHG	a	411	-	-	11/43/43/53	-
22	CLA	C	508	3	-	17/39/115/115	-
22	CLA	c	505	3	-	16/39/115/115	-
25	DGD	C	516	-	-	19/51/91/95	0/2/2/2
22	CLA	b	612	2	-	9/39/115/115	-
22	CLA	b	617	2	-	13/39/115/115	-
22	CLA	C	512	3	-	15/39/115/115	-
22	CLA	H	101	-	-	15/39/115/115	-
22	CLA	b	610	-	-	9/39/115/115	-
34	HEM	v	201	16	-	5/14/54/54	-
22	CLA	C	507	3	-	13/39/115/115	-
31	PHO	D	401	-	-	10/37/103/103	0/5/6/6
22	CLA	c	509	3	-	17/39/115/115	-
22	CLA	A	403	-	-	13/39/115/115	-
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
22	CLA	B	603	2	-	9/39/115/115	-
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
22	CLA	B	605	2	-	14/39/115/115	-
25	DGD	D	410	-	-	34/52/92/95	0/2/2/2
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
24	BCR	b	621	-	-	7/29/63/63	0/2/2/2
31	PHO	d	402	-	-	11/37/103/103	0/5/6/6
29	SQD	f	103	-	-	12/40/60/69	0/1/1/1
22	CLA	C	506	-	-	12/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
29	SQD	a	401	-	-	14/49/69/69	0/1/1/1
22	CLA	a	407	1	-	8/39/115/115	-
22	CLA	B	614	-	-	9/39/115/115	-
34	HEM	F	101	5,6	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
29	SQD	A	412	-	-	18/46/66/69	0/1/1/1
22	CLA	D	405	-	-	14/39/115/115	-
22	CLA	b	609	2	-	16/39/115/115	-
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
22	CLA	A	402	1	-	8/39/115/115	-
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	c	507	3	-	13/39/115/115	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
34	HEM	f	101	5,6	-	2/14/54/54	-
30	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	c	501	3	-	14/39/115/115	-
22	CLA	b	614	2	-	11/39/115/115	-
22	CLA	b	618	-	-	9/39/115/115	-
22	CLA	b	613	-	-	18/39/115/115	-
29	SQD	A	413	-	-	12/49/69/69	0/1/1/1
22	CLA	b	607	2	-	7/39/115/115	-
22	CLA	B	610	2	-	13/39/115/115	-
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
22	CLA	C	511	-	-	17/39/115/115	-
22	CLA	b	616	-	-	15/39/115/115	-
24	BCR	c	521	-	-	3/29/63/63	0/2/2/2
22	CLA	B	607	2	-	12/39/115/115	-
22	CLA	B	608	2	-	8/39/115/115	-
27	LMG	B	621	-	-	15/44/64/70	0/1/1/1
22	CLA	c	520	-	-	13/39/115/115	-
25	DGD	A	408	-	-	13/45/85/95	0/2/2/2
29	SQD	a	415	-	-	18/46/66/69	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
25	DGD	d	410	-	-	35/52/92/95	0/2/2/2
22	CLA	B	609	-	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	f	102	-	-	6/29/63/63	0/2/2/2
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
24	BCR	F	102	-	-	5/29/63/63	0/2/2/2
22	CLA	b	615	-	-	10/39/115/115	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
24	BCR	C	513	-	-	4/29/63/63	0/2/2/2
22	CLA	b	606	2	-	14/39/115/115	-
22	CLA	c	502	-	-	9/39/115/115	-
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
30	LMT	B	623	-	-	3/21/61/61	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
34	HEM	V	201	16	-	5/14/54/54	-
22	CLA	C	503	3	-	12/39/115/115	-
30	LMT	b	627	-	-	3/21/61/61	0/2/2/2
22	CLA	c	506	-	-	12/39/115/115	-
25	DGD	c	516	-	-	19/51/91/95	0/2/2/2
22	CLA	d	406	-	-	8/39/115/115	-
22	CLA	A	404	-	-	10/39/115/115	-
29	SQD	B	626	-	-	14/42/62/69	0/1/1/1
22	CLA	C	502	3	-	9/39/115/115	-
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	PHO	d	401	-	-	10/37/103/103	0/5/6/6
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
25	DGD	a	410	-	-	15/45/85/95	0/2/2/2
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
22	CLA	B	601	-	-	18/39/115/115	-
22	CLA	B	615	2	-	19/39/115/115	-
30	LMT	B	628	-	-	5/21/61/61	0/2/2/2
24	BCR	a	409	-	-	4/29/63/63	0/2/2/2
22	CLA	B	602	2	-	15/39/115/115	-
30	LMT	I	102	-	-	3/21/61/61	0/2/2/2
24	BCR	c	513	-	-	4/29/63/63	0/2/2/2
22	CLA	D	406	-	-	8/39/115/115	-
23	PL9	A	406	-	-	19/41/61/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
22	CLA	C	510	3	-	14/39/115/115	-
22	CLA	b	611	2	-	12/39/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
27	LMG	D	409	-	-	21/43/63/70	0/1/1/1
22	CLA	c	503	-	-	11/39/115/115	-
23	PL9	a	408	-	-	18/41/61/73	0/1/1/1
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
30	LMT	b	626	-	-	2/21/61/61	0/2/2/2
29	SQD	d	403	-	-	14/38/58/69	0/1/1/1
29	SQD	b	602	-	-	13/42/62/69	0/1/1/1
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
22	CLA	c	511	-	-	17/39/115/115	-
22	CLA	h	101	-	-	15/39/115/115	-
23	PL9	d	407	-	-	12/53/73/73	0/1/1/1
27	LMG	E	101	-	-	19/39/59/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
27	LMG	C	521	-	-	20/43/63/70	0/1/1/1
24	BCR	C	514	-	-	4/29/63/63	0/2/2/2
27	LMG	A	414	-	-	15/37/57/70	0/1/1/1
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	K	102	-	-	5/29/63/63	0/2/2/2
29	SQD	F	103	-	-	11/40/60/69	0/1/1/1

The worst 5 of 752 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	402	PHO	C1B-C2B	9.76	1.50	1.39
31	d	401	PHO	C1B-C2B	9.67	1.50	1.39
31	d	402	PHO	C1B-C2B	9.57	1.50	1.39
31	D	401	PHO	C1B-C2B	9.55	1.50	1.39
31	D	402	PHO	C3B-C4B	8.71	1.50	1.41

The worst 5 of 1031 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.27	110.00	106.68
22	B	611	CLA	C4A-NA-C1A	7.25	109.99	106.68
22	c	504	CLA	C4A-NA-C1A	7.17	109.95	106.68
22	B	603	CLA	C4A-NA-C1A	7.15	109.94	106.68
22	b	615	CLA	C4A-NA-C1A	7.01	109.88	106.68

There are no chirality outliers.

5 of 2091 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 440 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	i	102	LMT	1	0
26	C	519	LHG	2	0
22	C	501	CLA	2	0
22	c	510	CLA	4	0
22	d	405	CLA	8	0
27	d	412	LMG	1	0
22	A	405	CLA	1	0
30	b	604	LMT	2	0
29	B	622	SQD	3	0
25	C	517	DGD	5	0
27	a	412	LMG	2	0
24	c	514	BCR	4	0
22	B	613	CLA	3	0
22	C	509	CLA	4	0
22	C	520	CLA	2	0
22	B	611	CLA	4	0
22	b	608	CLA	7	0
24	y	101	BCR	7	0
22	B	612	CLA	3	0
22	b	619	CLA	4	0
24	A	407	BCR	3	0
25	b	624	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	504	CLA	3	0
26	A	409	LHG	3	0
22	c	508	CLA	3	0
27	i	101	LMG	1	0
22	a	406	CLA	6	0
24	B	617	BCR	2	0
24	g	101	BCR	5	0
27	D	408	LMG	2	0
22	B	606	CLA	6	0
27	d	409	LMG	6	0
22	C	505	CLA	1	0
22	c	512	CLA	3	0
27	e	101	LMG	1	0
22	a	405	CLA	9	0
30	B	627	LMT	2	0
22	B	604	CLA	6	0
22	a	404	CLA	10	0
22	C	504	CLA	4	0
27	d	408	LMG	3	0
31	D	402	PHO	5	0
26	a	411	LHG	1	0
22	C	508	CLA	1	0
22	c	505	CLA	1	0
25	C	516	DGD	3	0
22	b	612	CLA	5	0
22	b	617	CLA	2	0
22	C	512	CLA	3	0
22	H	101	CLA	8	0
22	b	610	CLA	6	0
34	v	201	HEM	5	0
22	C	507	CLA	4	0
31	D	401	PHO	7	0
22	c	509	CLA	3	0
22	A	403	CLA	14	0
25	c	517	DGD	5	0
27	A	410	LMG	2	0
22	B	603	CLA	2	0
27	D	412	LMG	1	0
22	B	605	CLA	7	0
25	D	410	DGD	1	0
23	J	101	PL9	1	0
27	b	625	LMG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	621	BCR	1	0
31	d	402	PHO	4	0
29	f	103	SQD	3	0
22	C	506	CLA	3	0
24	B	619	BCR	1	0
29	a	401	SQD	5	0
22	a	407	CLA	1	0
22	B	614	CLA	1	0
34	F	101	HEM	4	0
27	a	402	LMG	1	0
29	A	412	SQD	4	0
22	D	405	CLA	8	0
22	b	609	CLA	5	0
25	B	625	DGD	2	0
24	B	616	BCR	5	0
25	b	601	DGD	2	0
22	A	402	CLA	10	0
23	D	407	PL9	8	0
22	c	507	CLA	4	0
24	j	102	BCR	1	0
27	C	518	LMG	3	0
34	f	101	HEM	4	0
30	b	603	LMT	2	0
22	c	501	CLA	4	0
22	b	614	CLA	2	0
22	b	618	CLA	2	0
22	b	613	CLA	1	0
29	A	413	SQD	4	0
22	b	607	CLA	2	0
22	B	610	CLA	3	0
22	C	511	CLA	1	0
22	b	616	CLA	3	0
24	c	521	BCR	4	0
22	B	607	CLA	7	0
22	B	608	CLA	5	0
27	B	621	LMG	3	0
22	c	520	CLA	4	0
25	A	408	DGD	1	0
29	a	415	SQD	3	0
24	b	622	BCR	3	0
25	d	410	DGD	2	0
24	f	102	BCR	2	0

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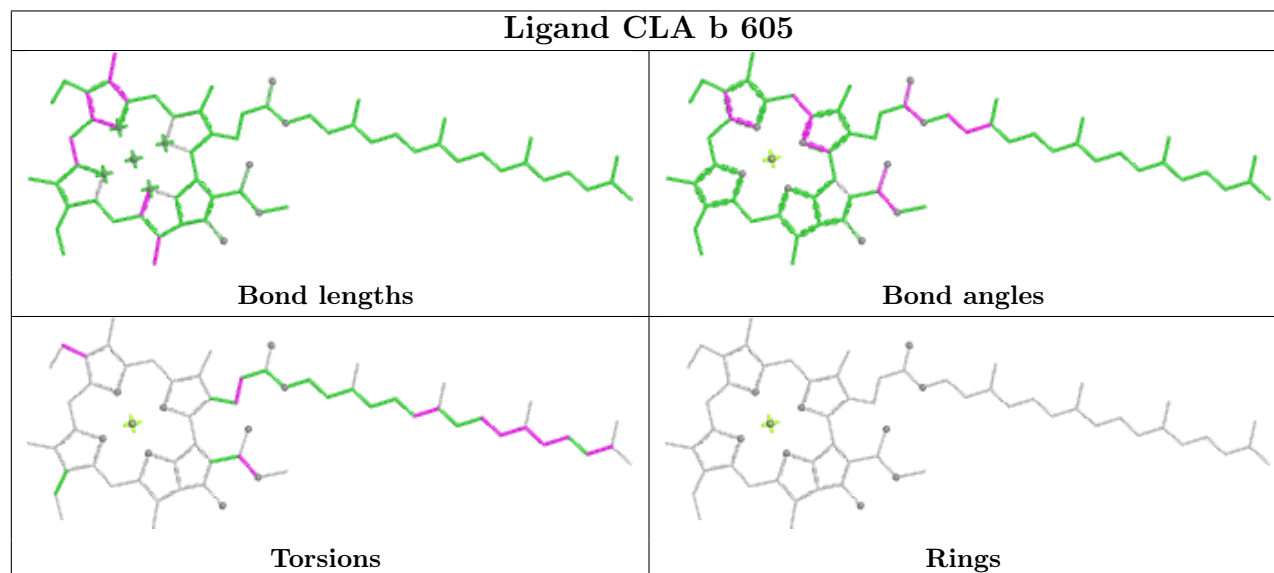
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	H	102	BCR	3	0
24	F	102	BCR	3	0
22	b	615	CLA	4	0
27	M	101	LMG	2	0
24	C	513	BCR	5	0
22	b	606	CLA	9	0
24	b	623	BCR	4	0
30	B	623	LMT	2	0
24	b	620	BCR	6	0
34	V	201	HEM	5	0
22	C	503	CLA	3	0
22	c	506	CLA	4	0
25	c	516	DGD	2	0
22	d	406	CLA	3	0
22	A	404	CLA	4	0
29	B	626	SQD	1	0
24	B	618	BCR	4	0
31	d	401	PHO	6	0
27	c	522	LMG	1	0
25	a	410	DGD	2	0
27	c	518	LMG	2	0
22	B	601	CLA	1	0
22	B	615	CLA	4	0
30	B	628	LMT	2	0
24	a	409	BCR	2	0
22	B	602	CLA	10	0
24	c	513	BCR	7	0
22	D	406	CLA	2	0
23	A	406	PL9	4	0
24	J	102	BCR	1	0
27	m	101	LMG	1	0
22	C	510	CLA	5	0
22	b	611	CLA	8	0
24	x	101	BCR	1	0
27	D	409	LMG	6	0
22	c	503	CLA	2	0
23	a	408	PL9	3	0
25	c	515	DGD	3	0
30	b	626	LMT	1	0
29	d	403	SQD	4	0
29	b	602	SQD	1	0
25	B	620	DGD	2	0

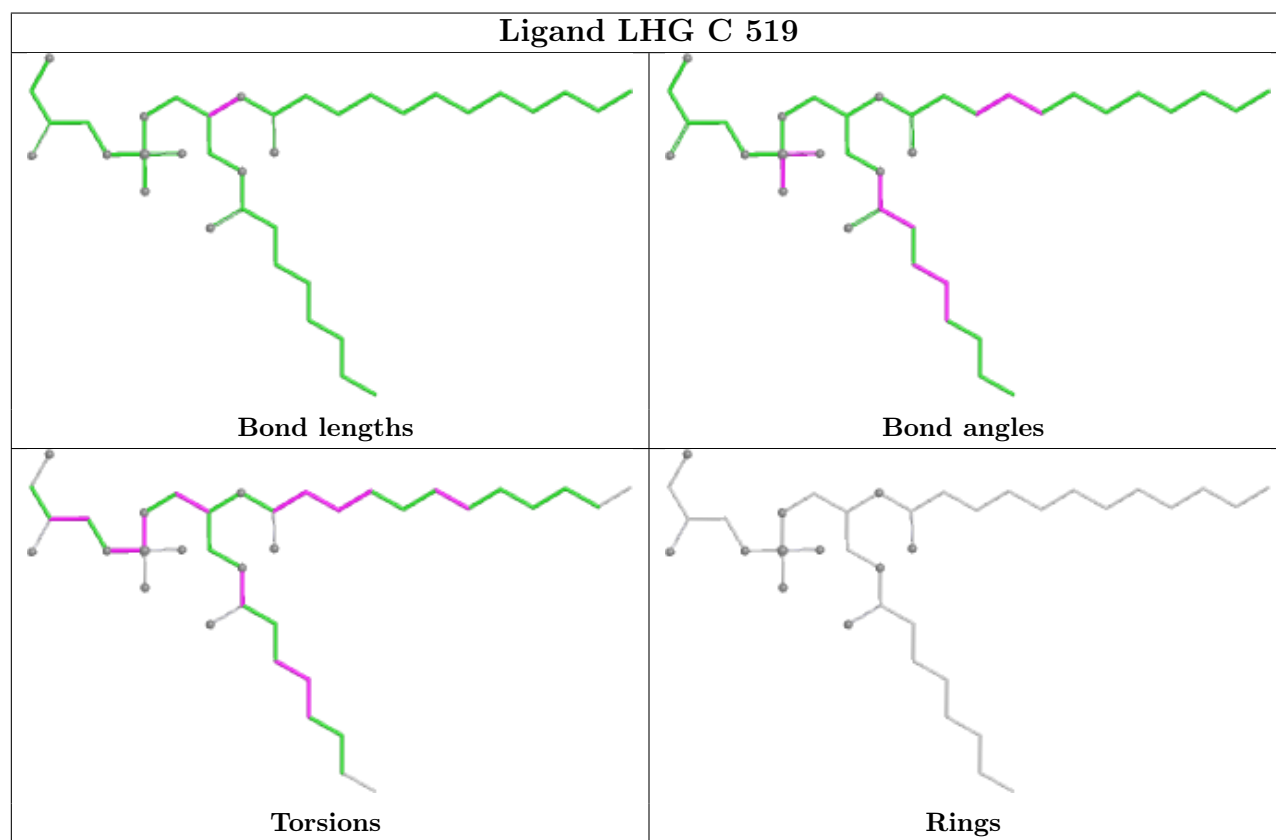
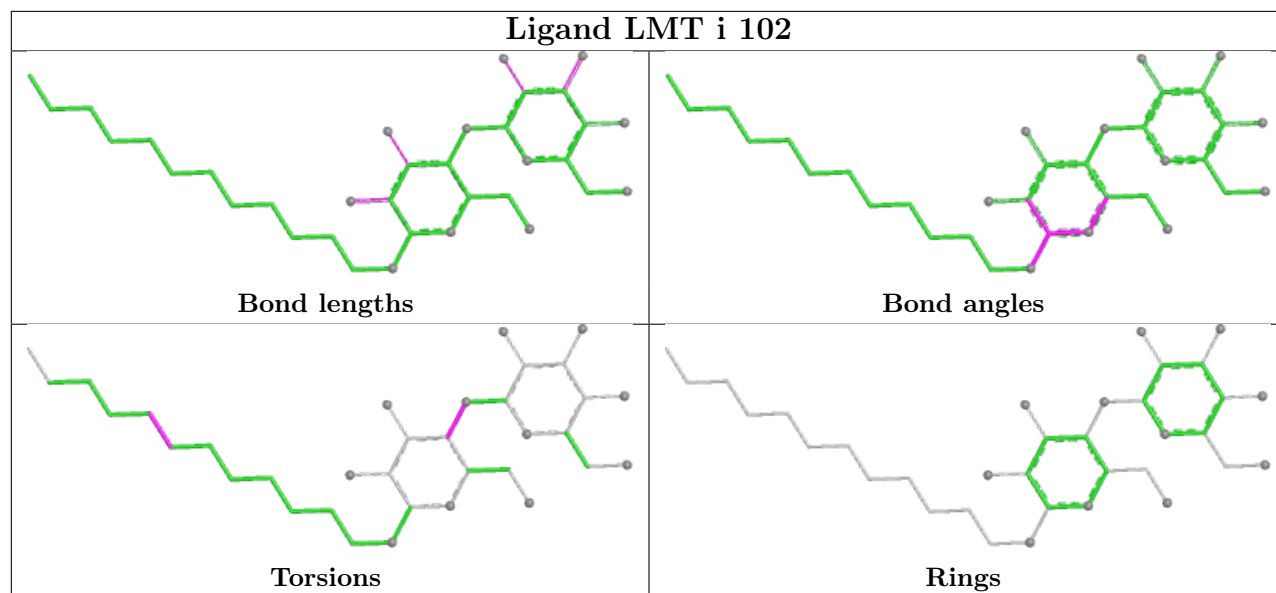
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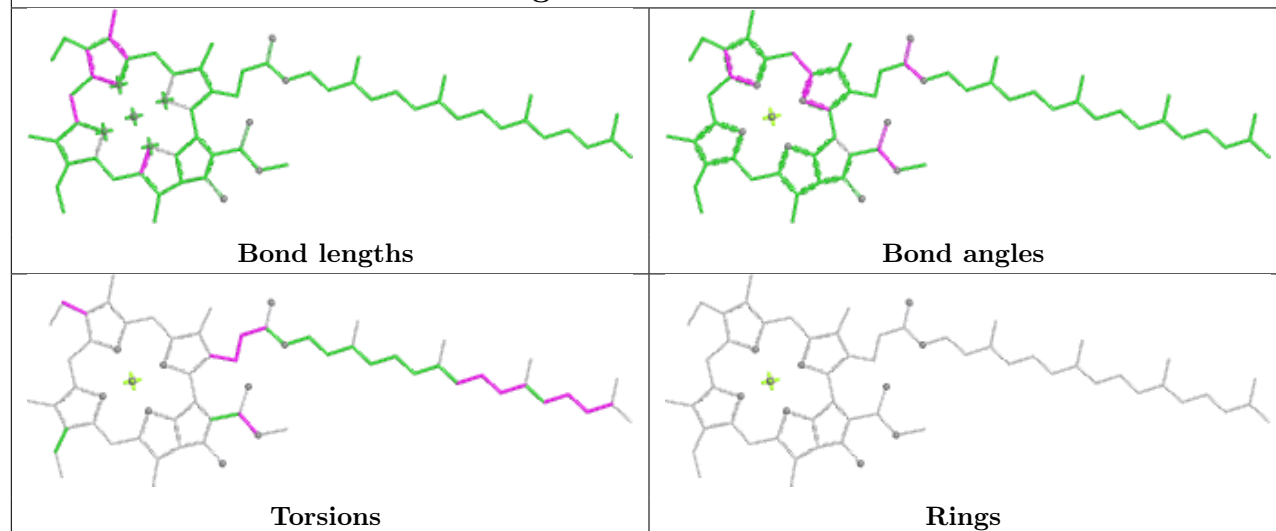
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	511	CLA	2	0
22	h	101	CLA	9	0
23	d	407	PL9	6	0
27	E	101	LMG	1	0
25	C	515	DGD	3	0
24	C	514	BCR	6	0
27	A	414	LMG	1	0
26	c	519	LHG	2	0
24	K	102	BCR	3	0
29	F	103	SQD	2	0

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.

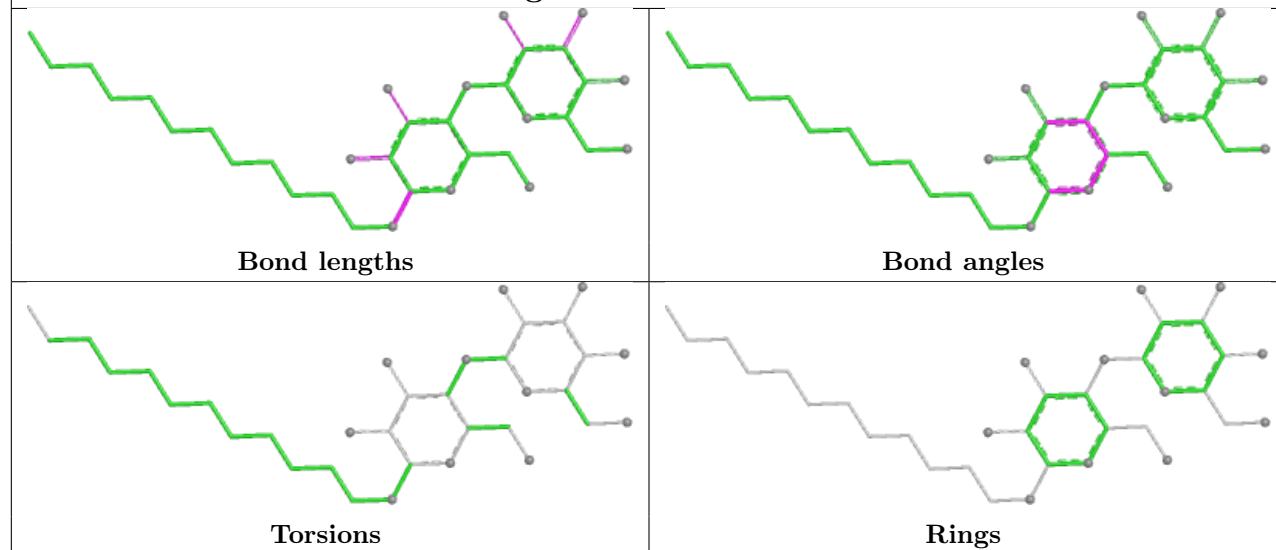




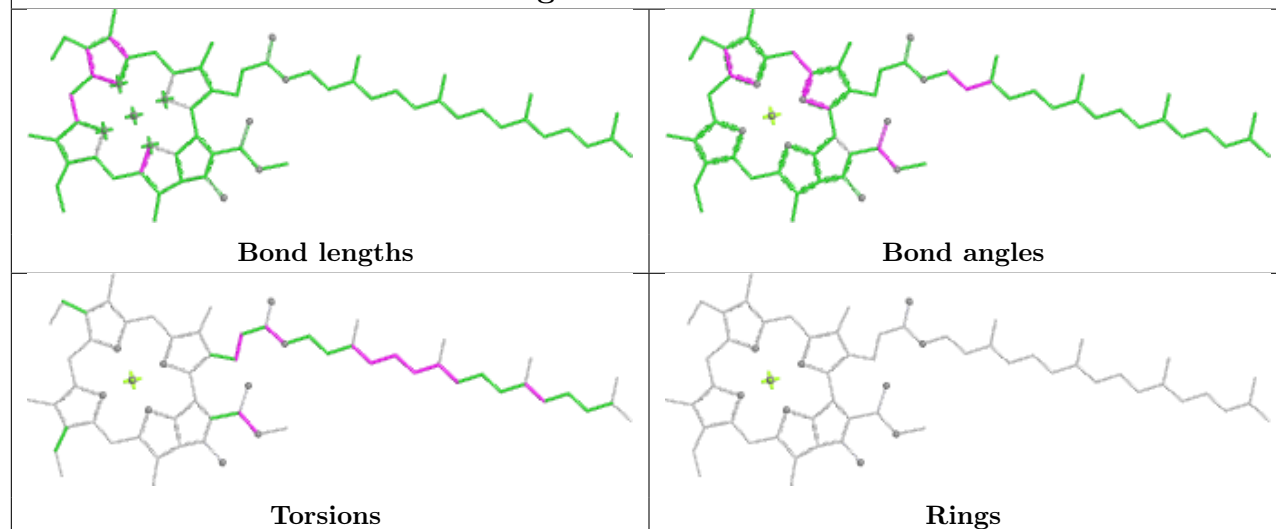
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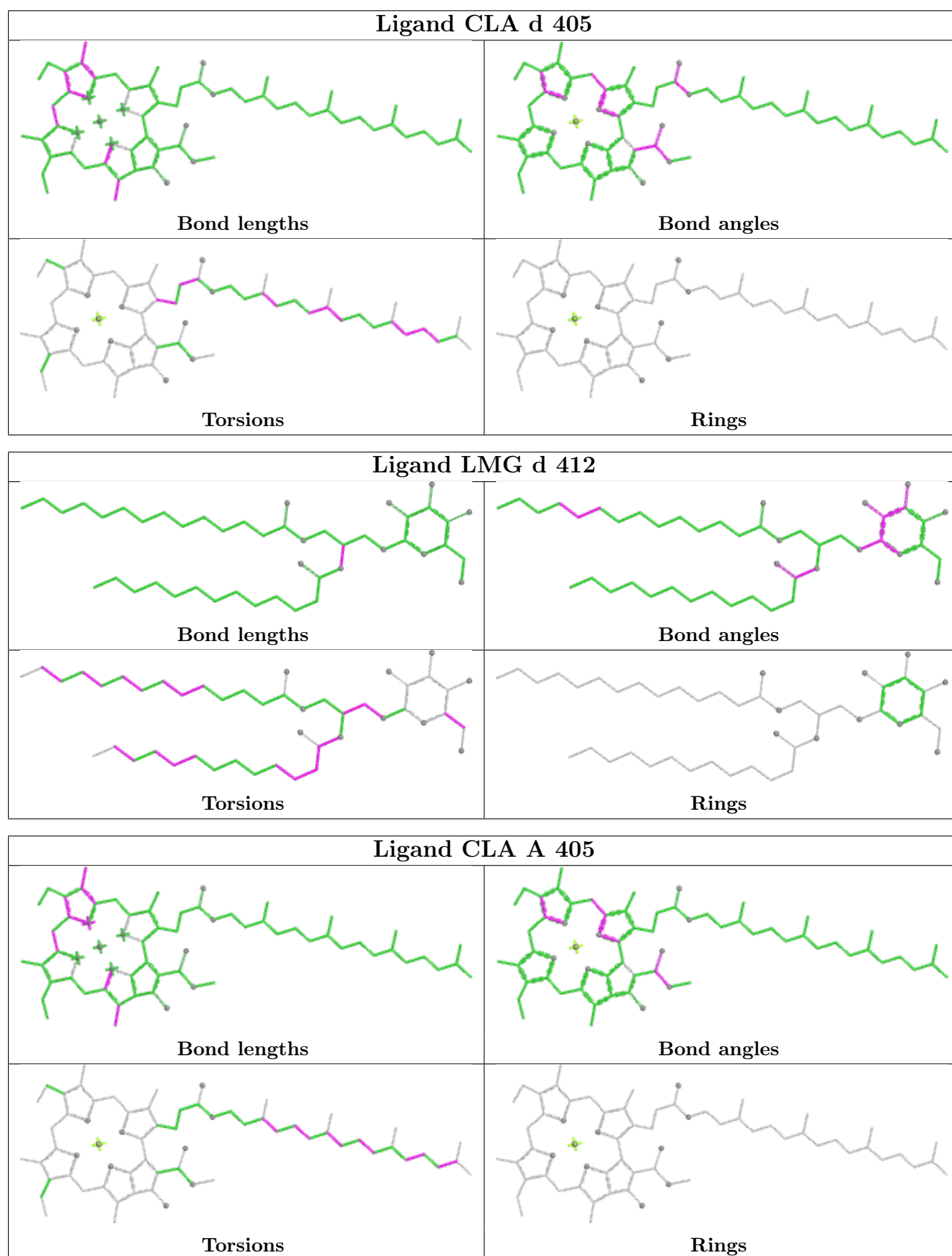


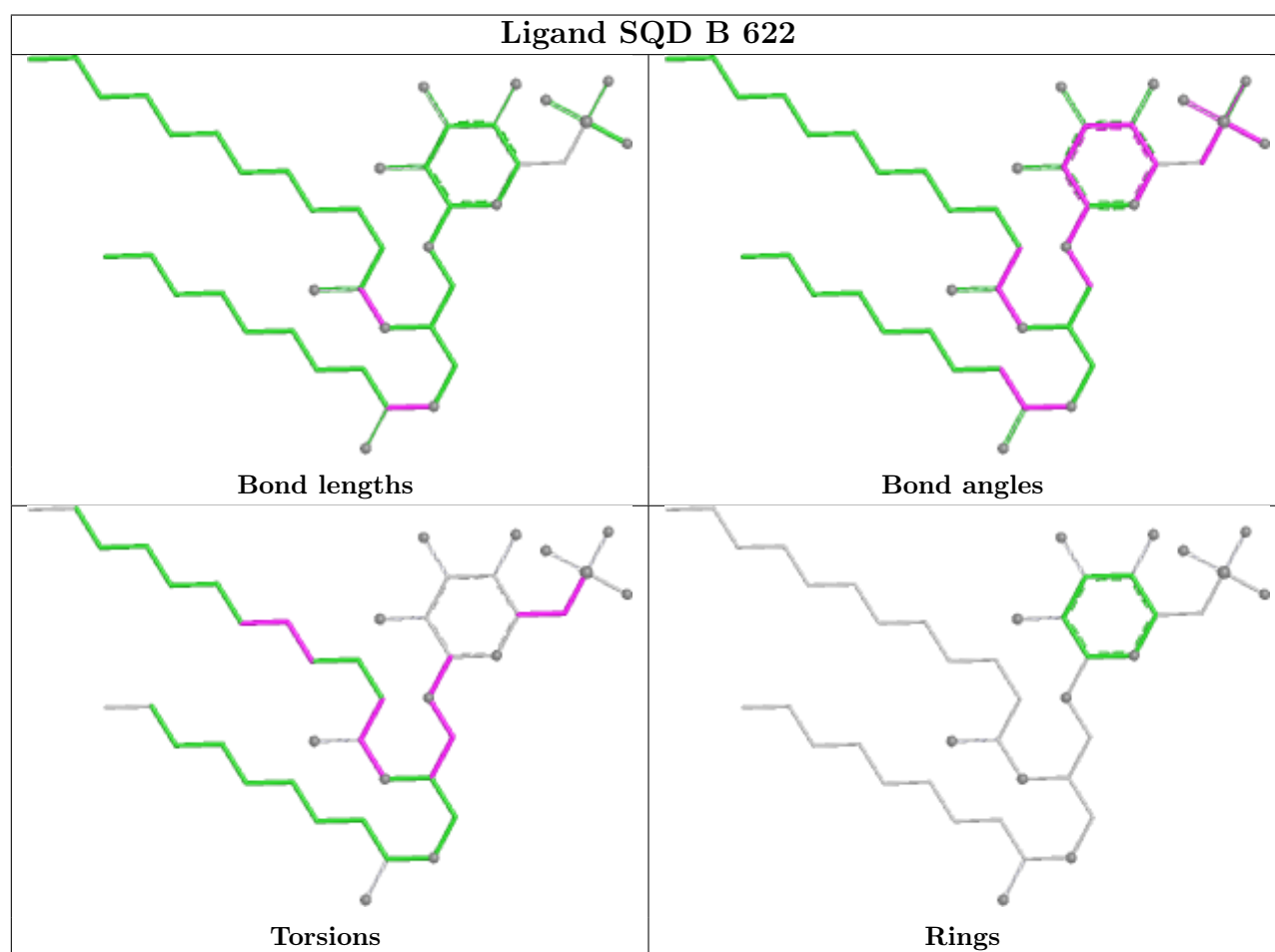
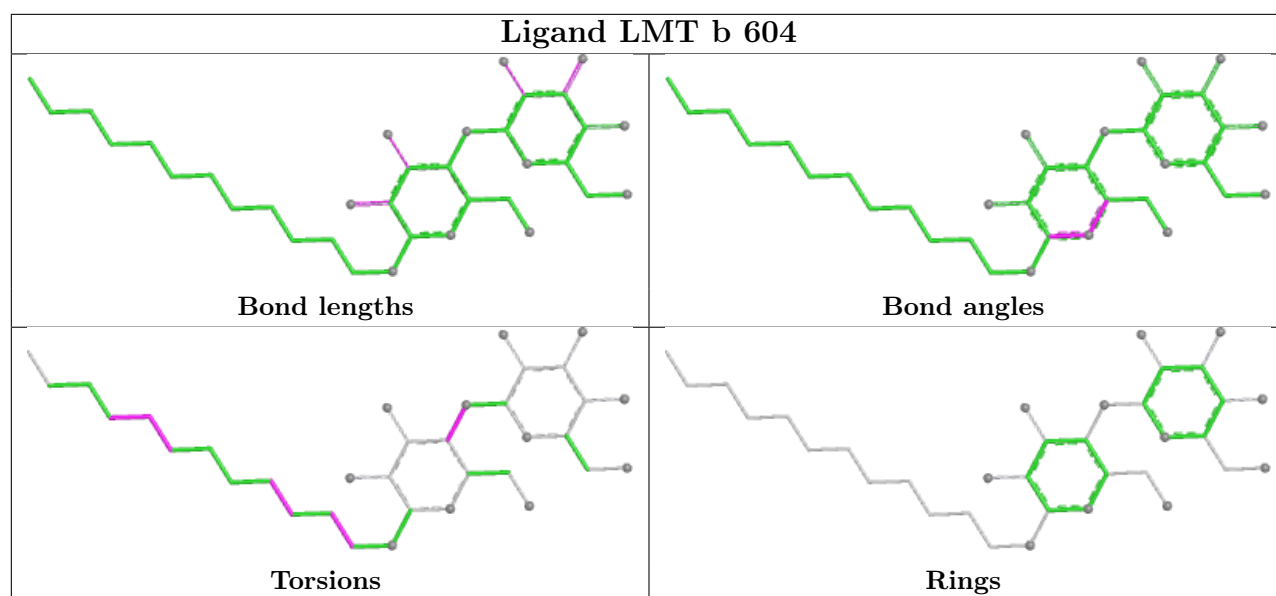
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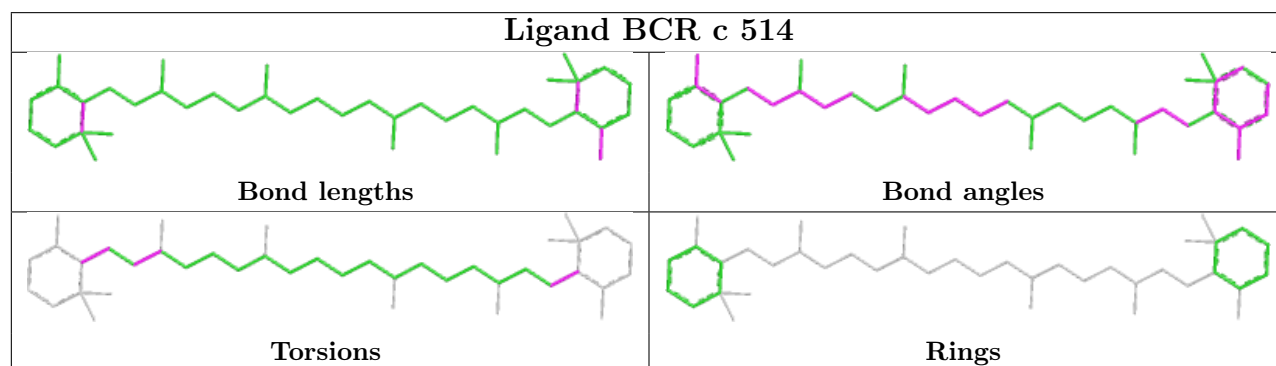
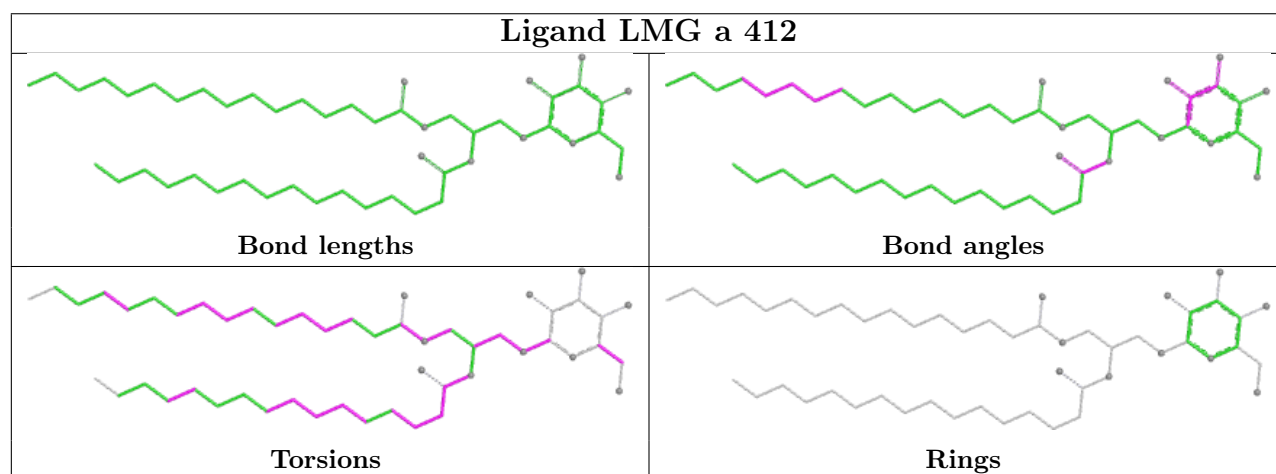
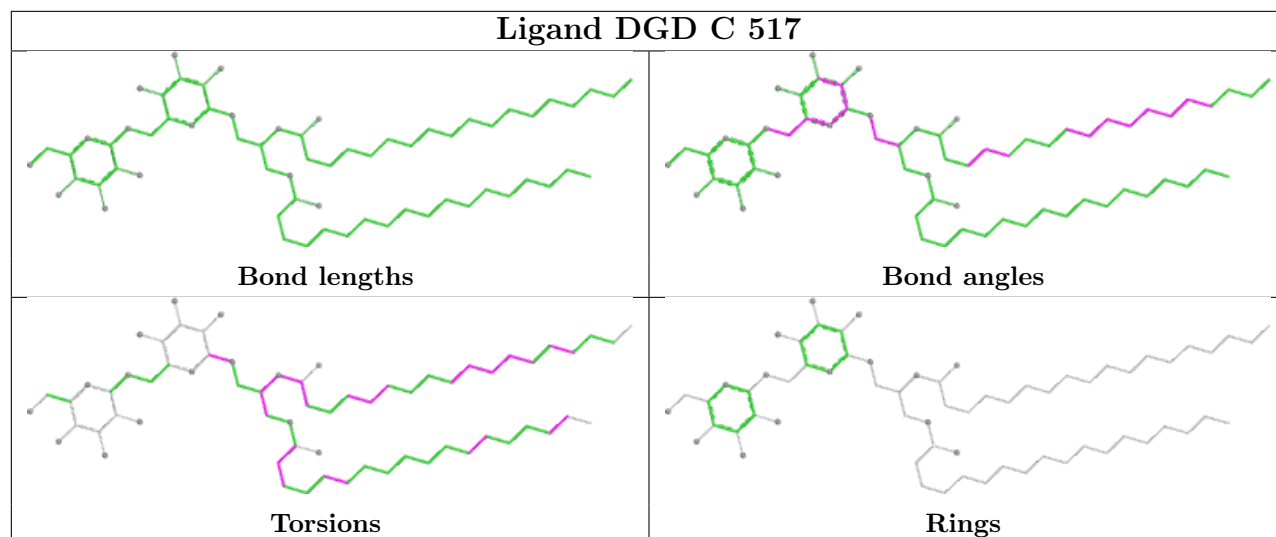


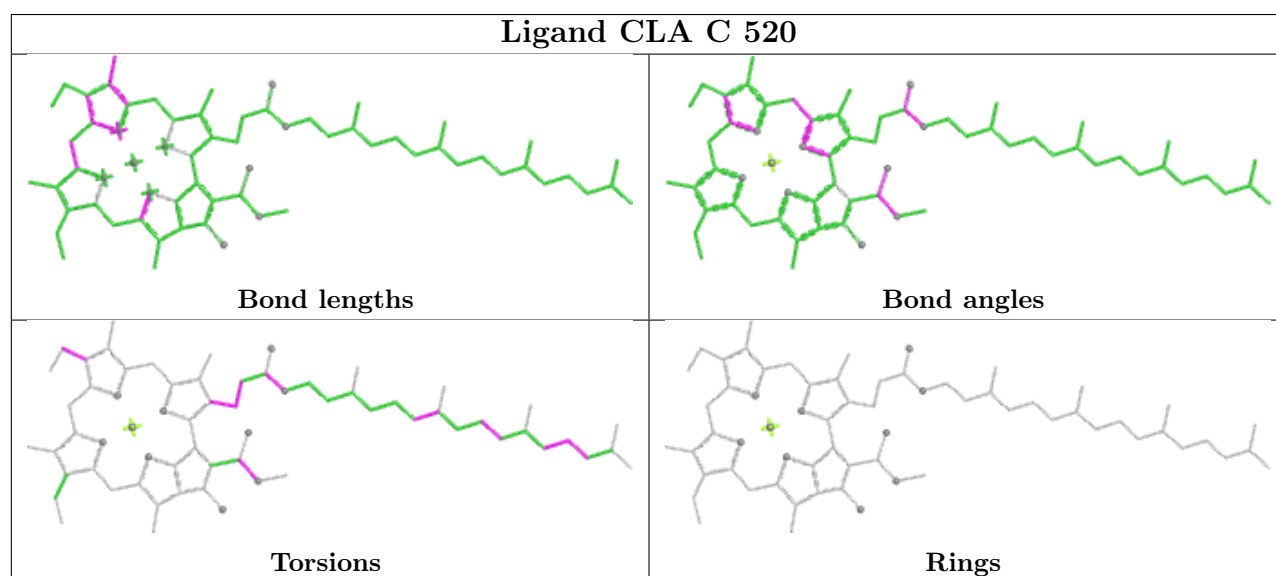
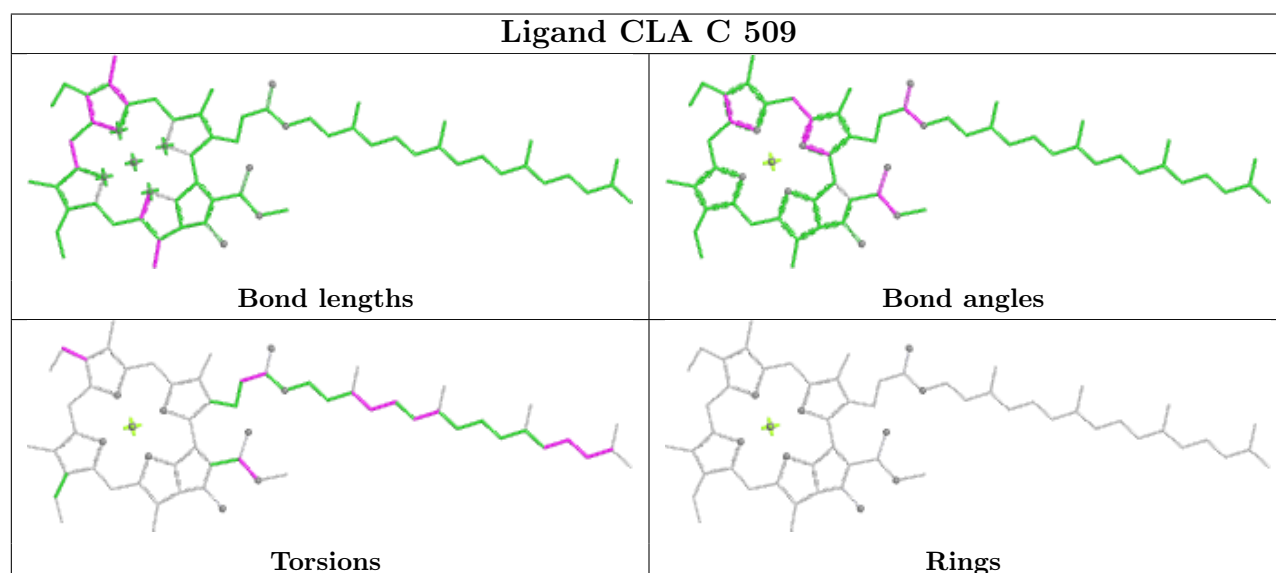
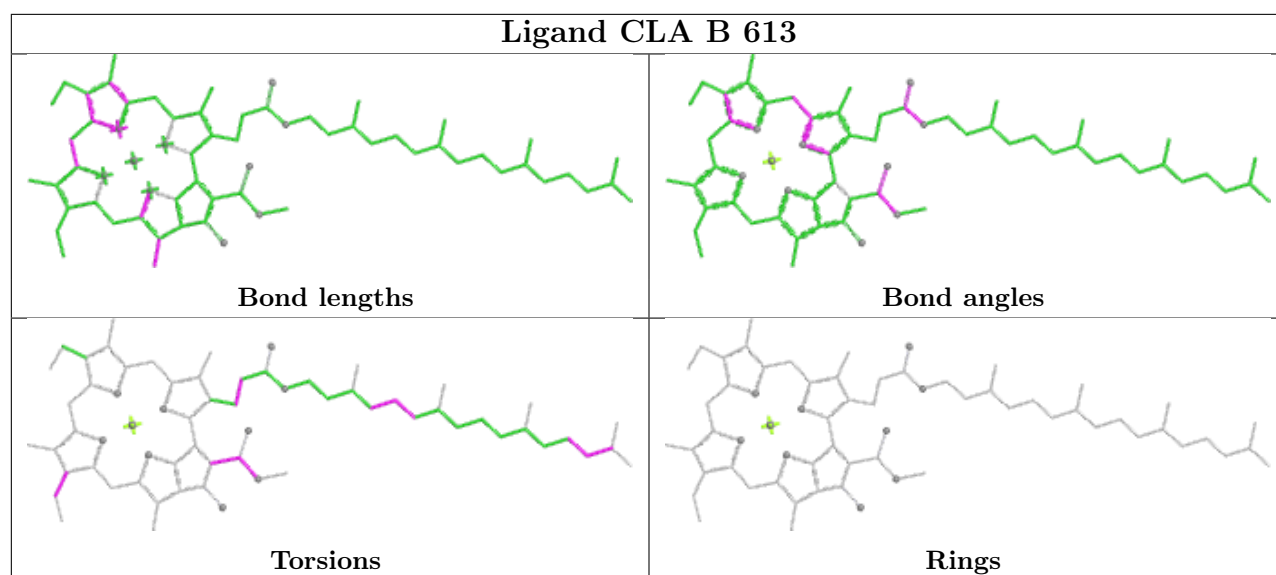
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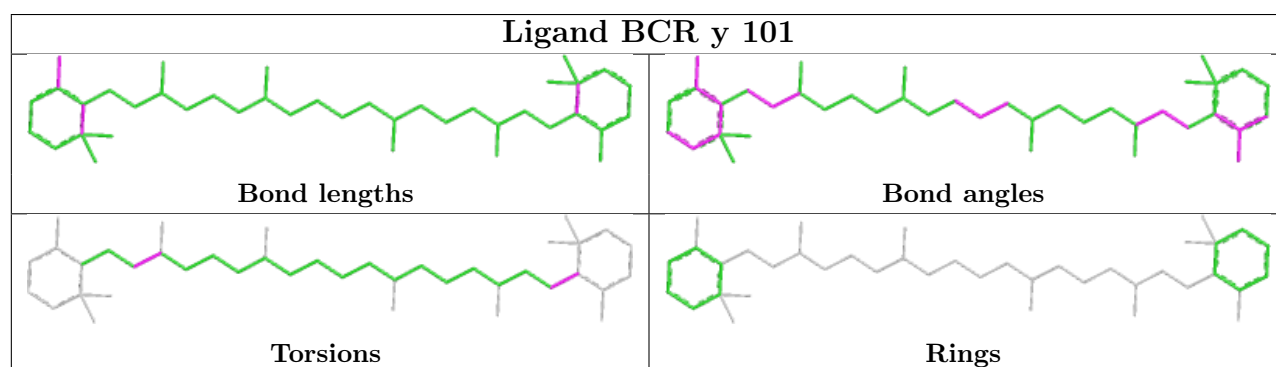
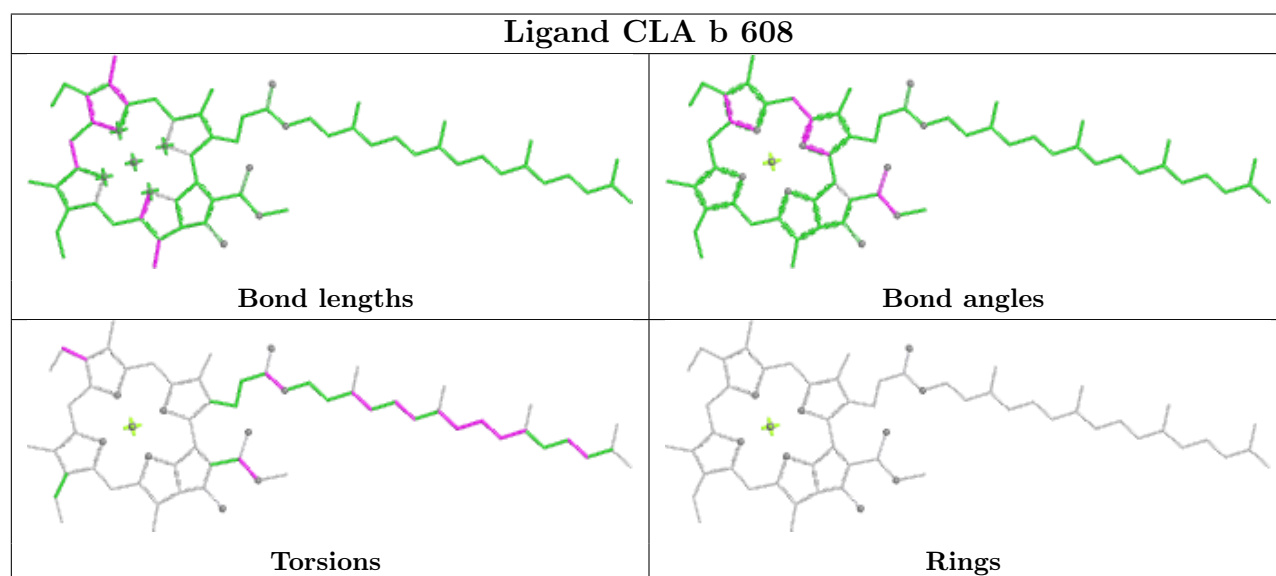
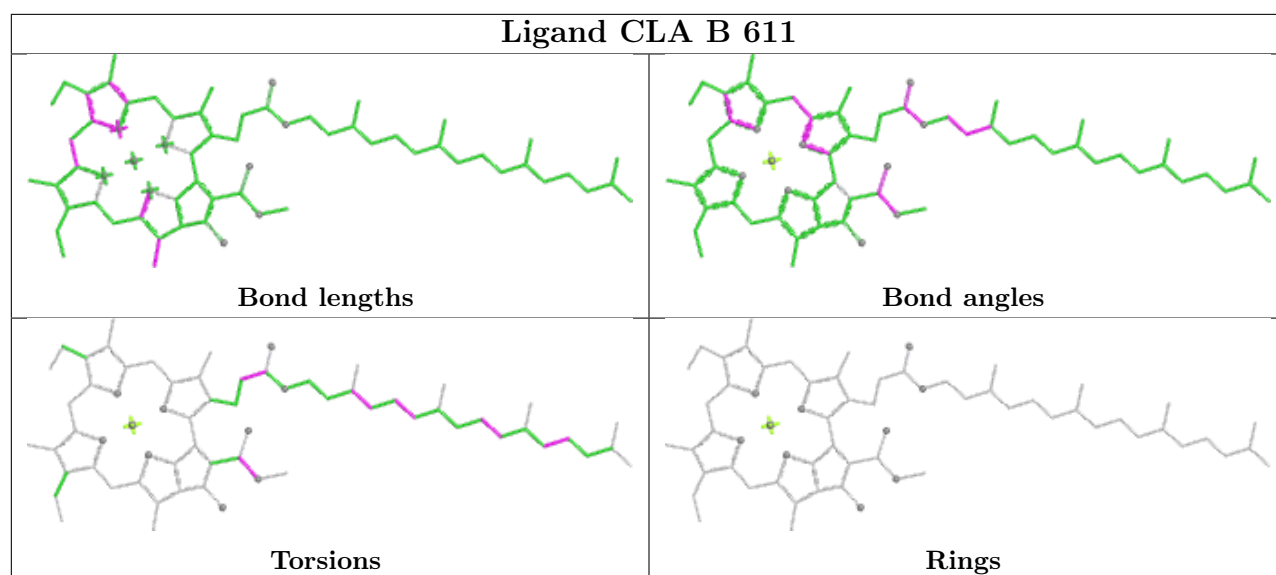


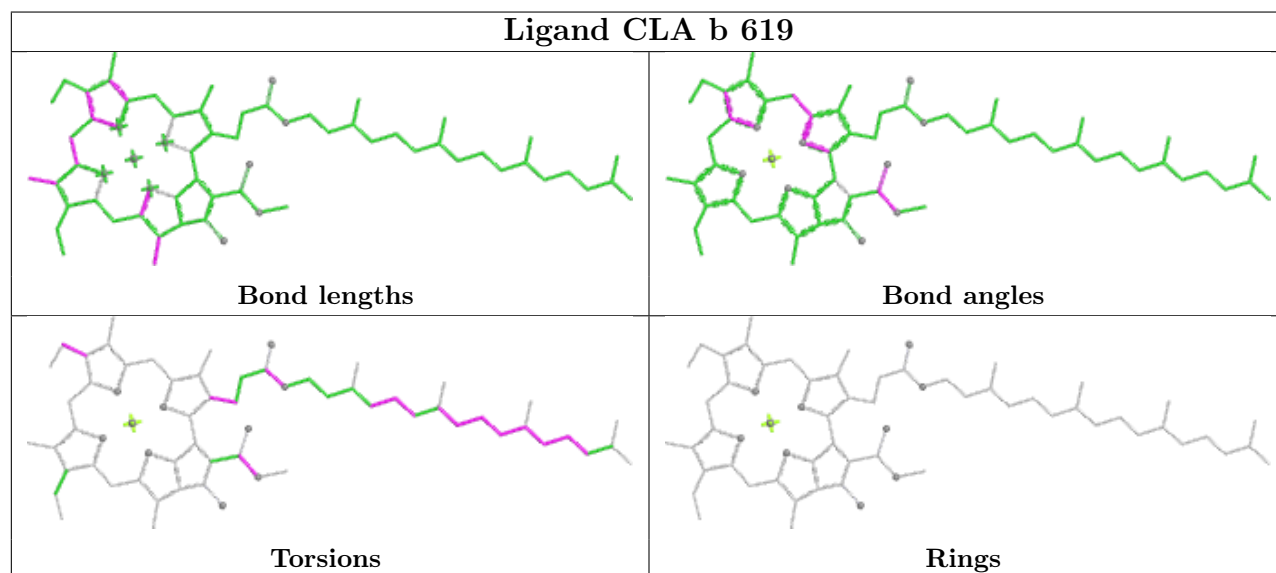
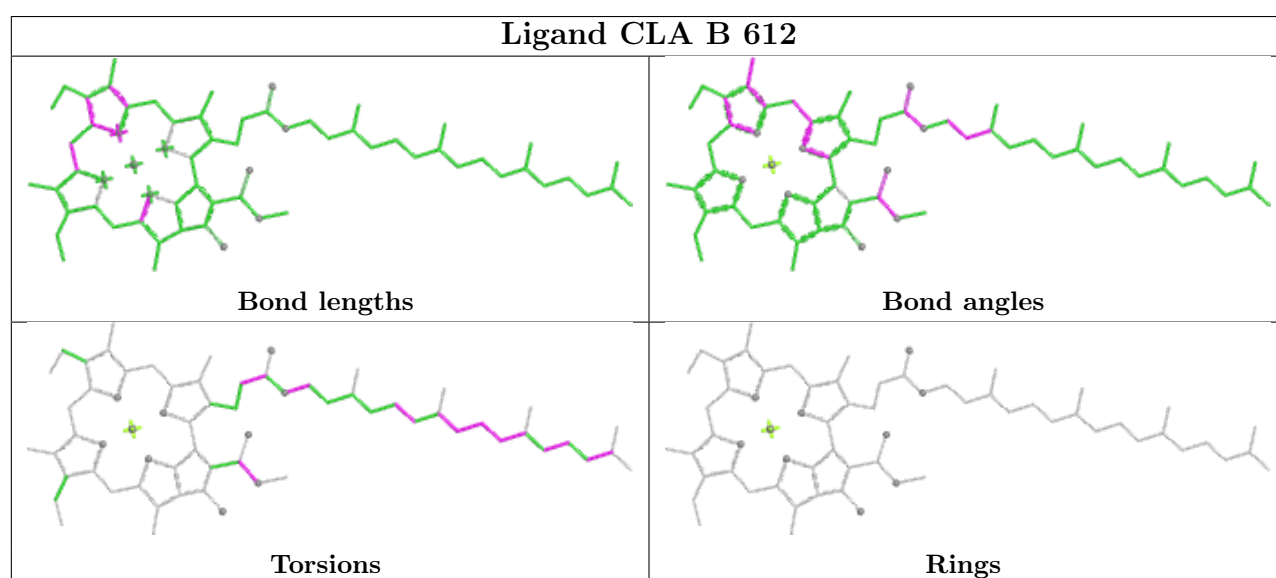
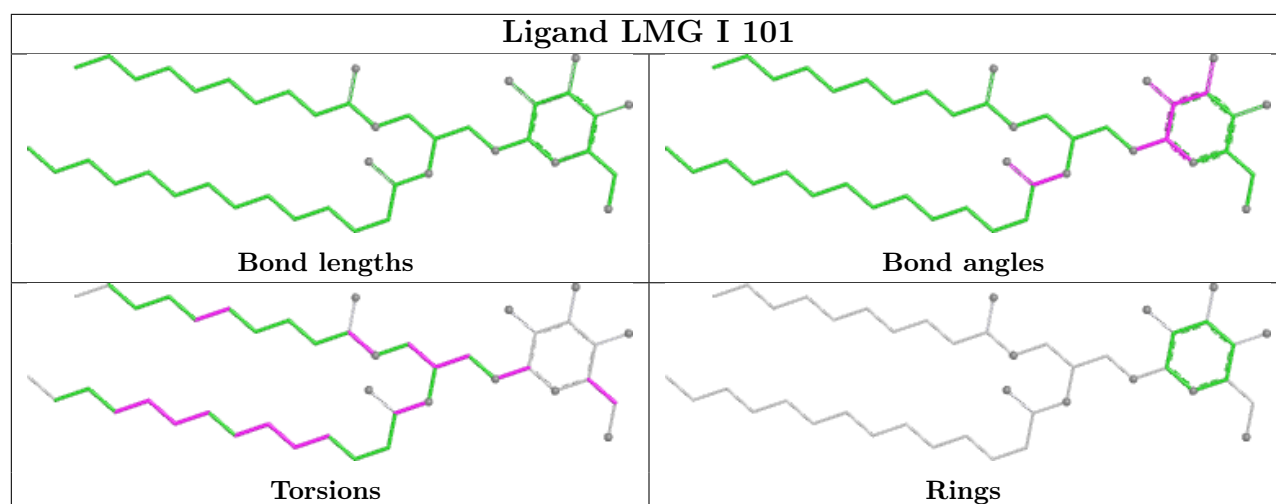


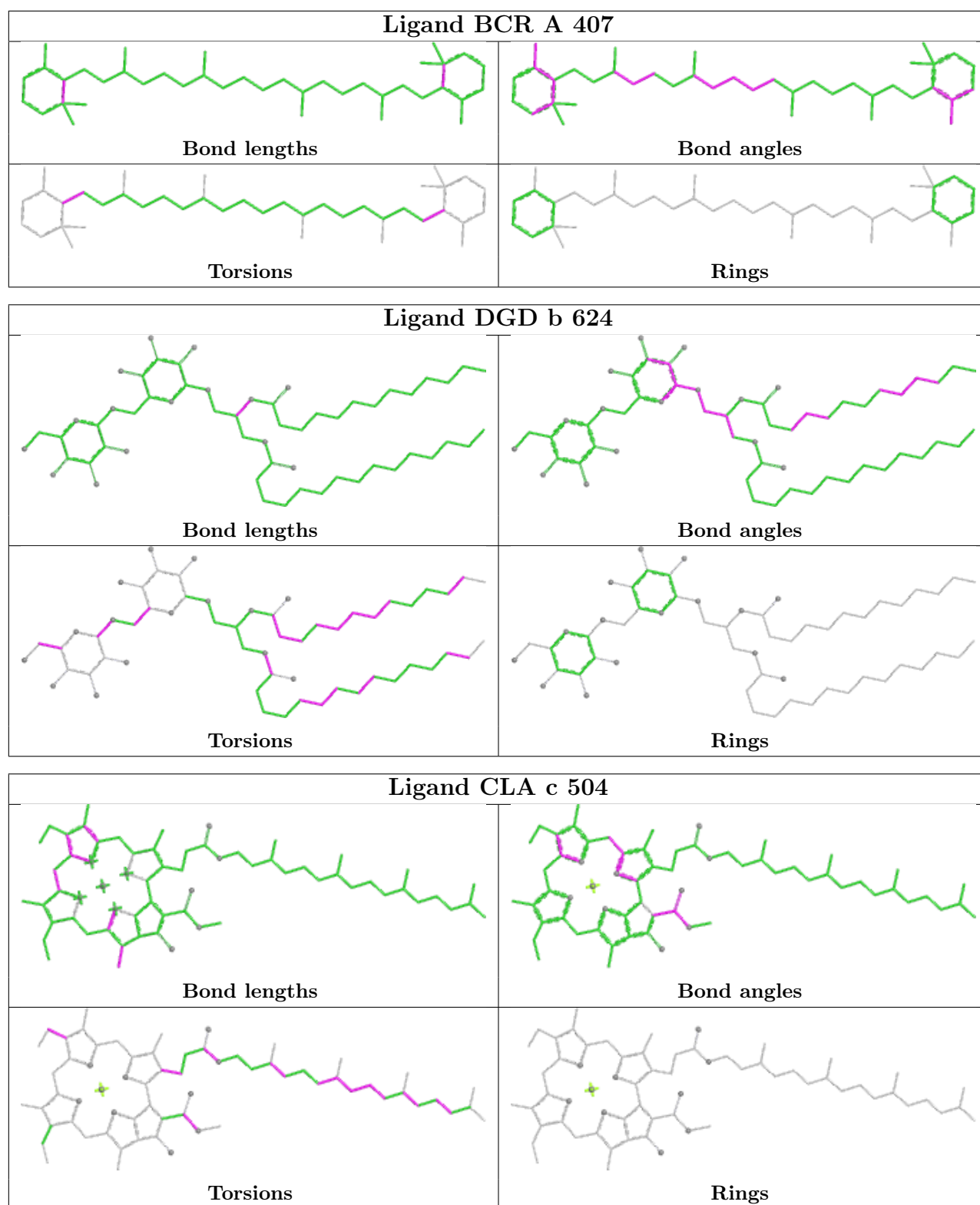


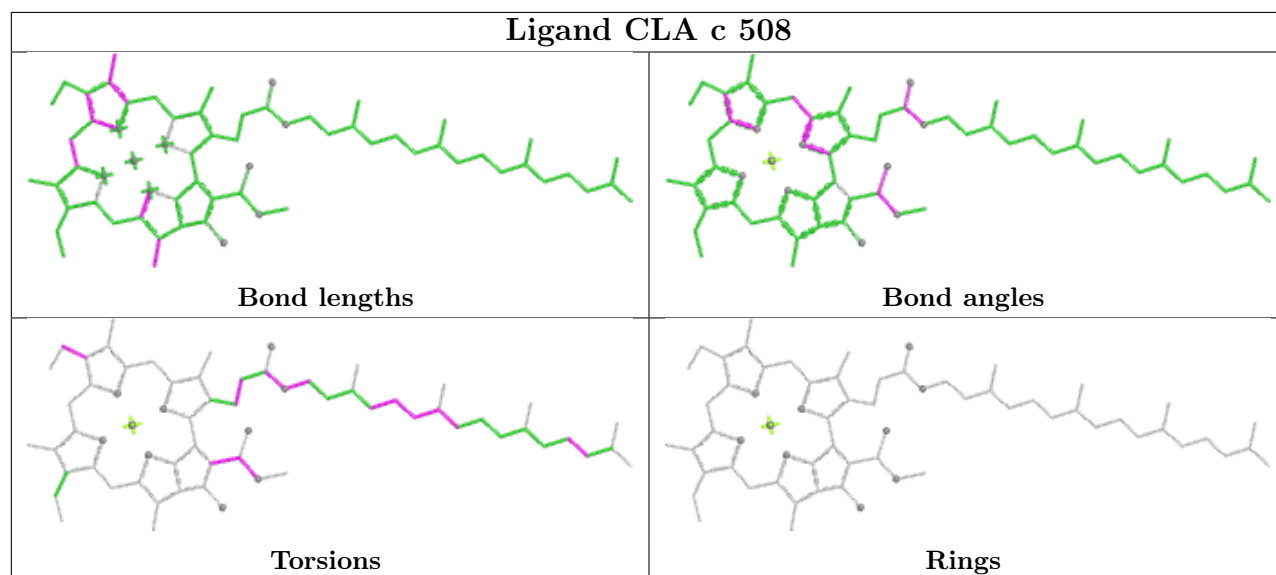
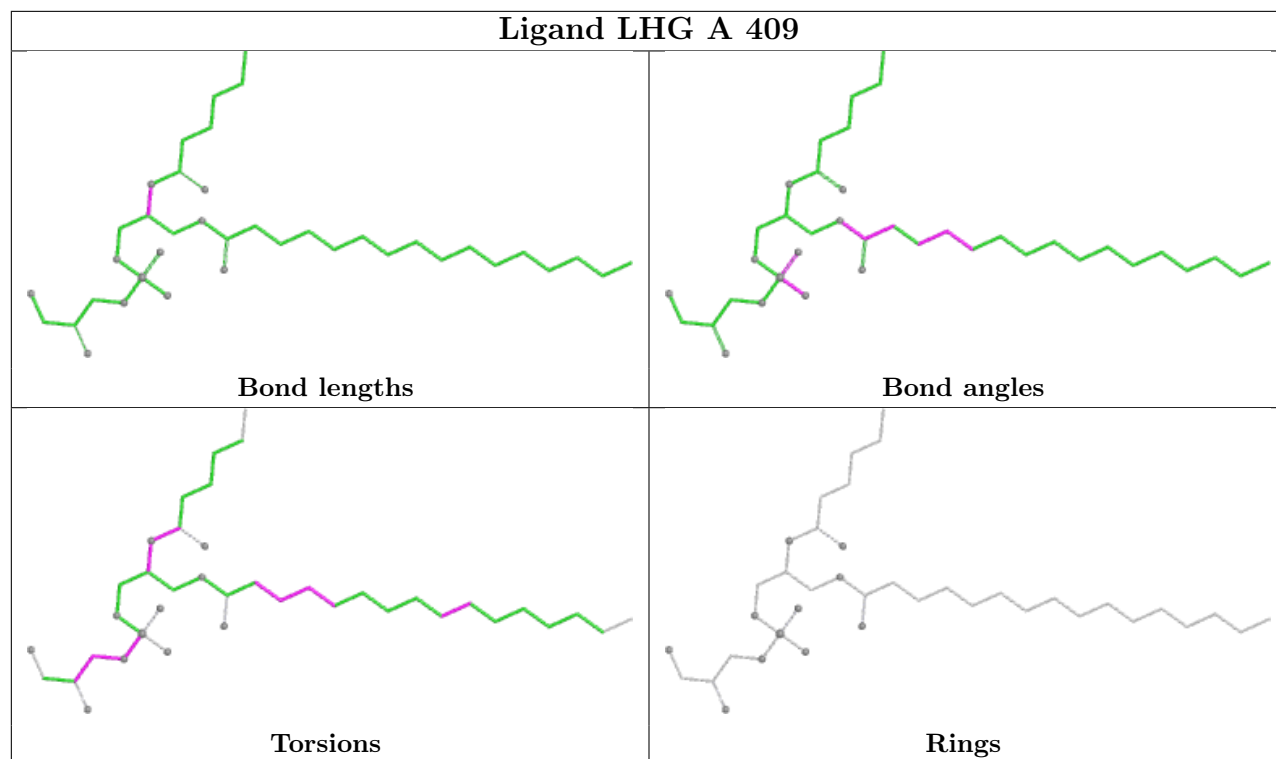


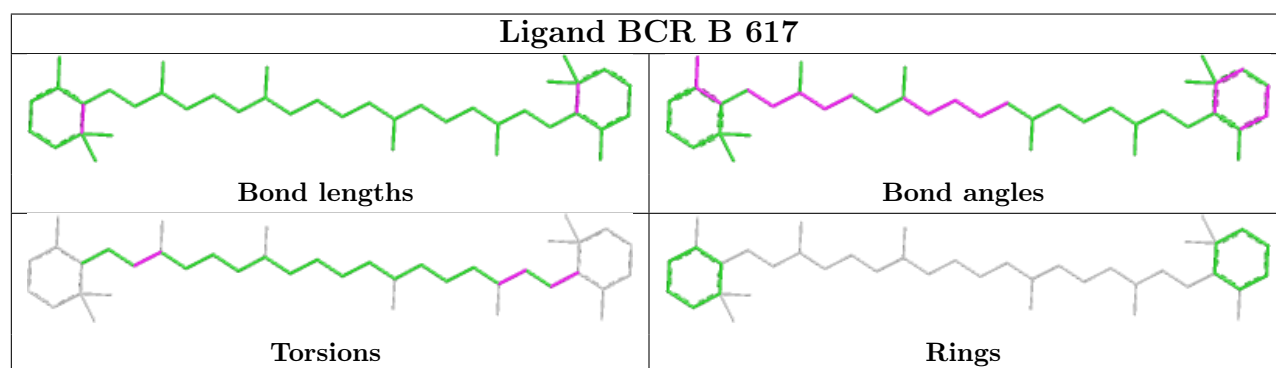
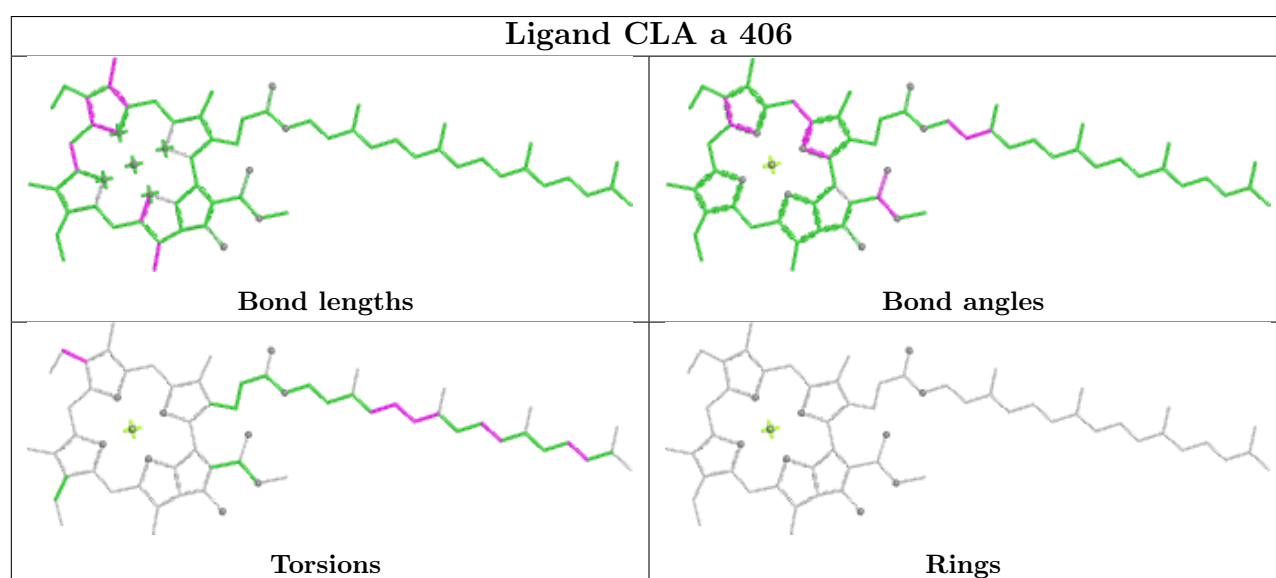
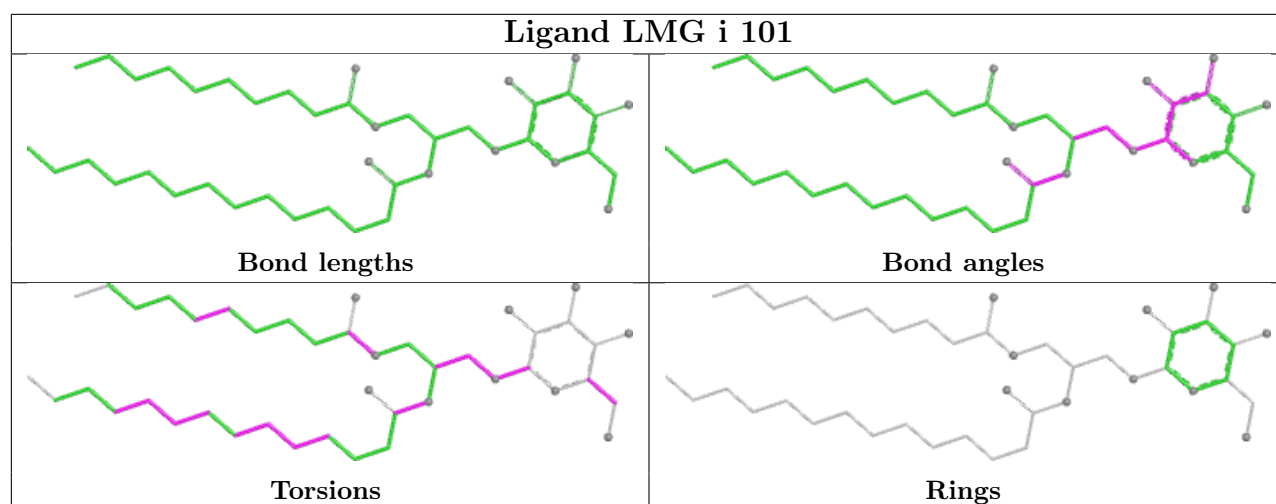


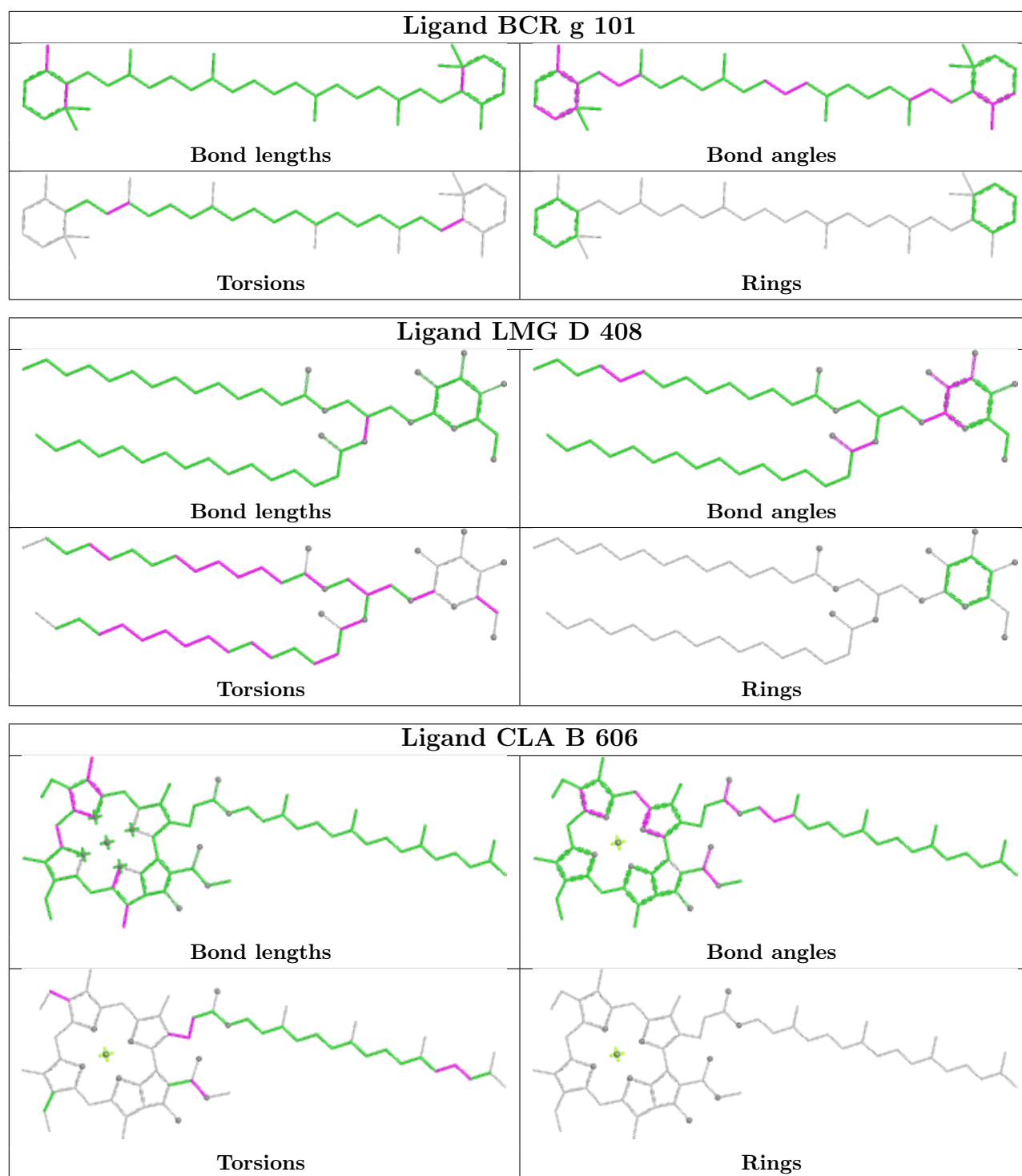


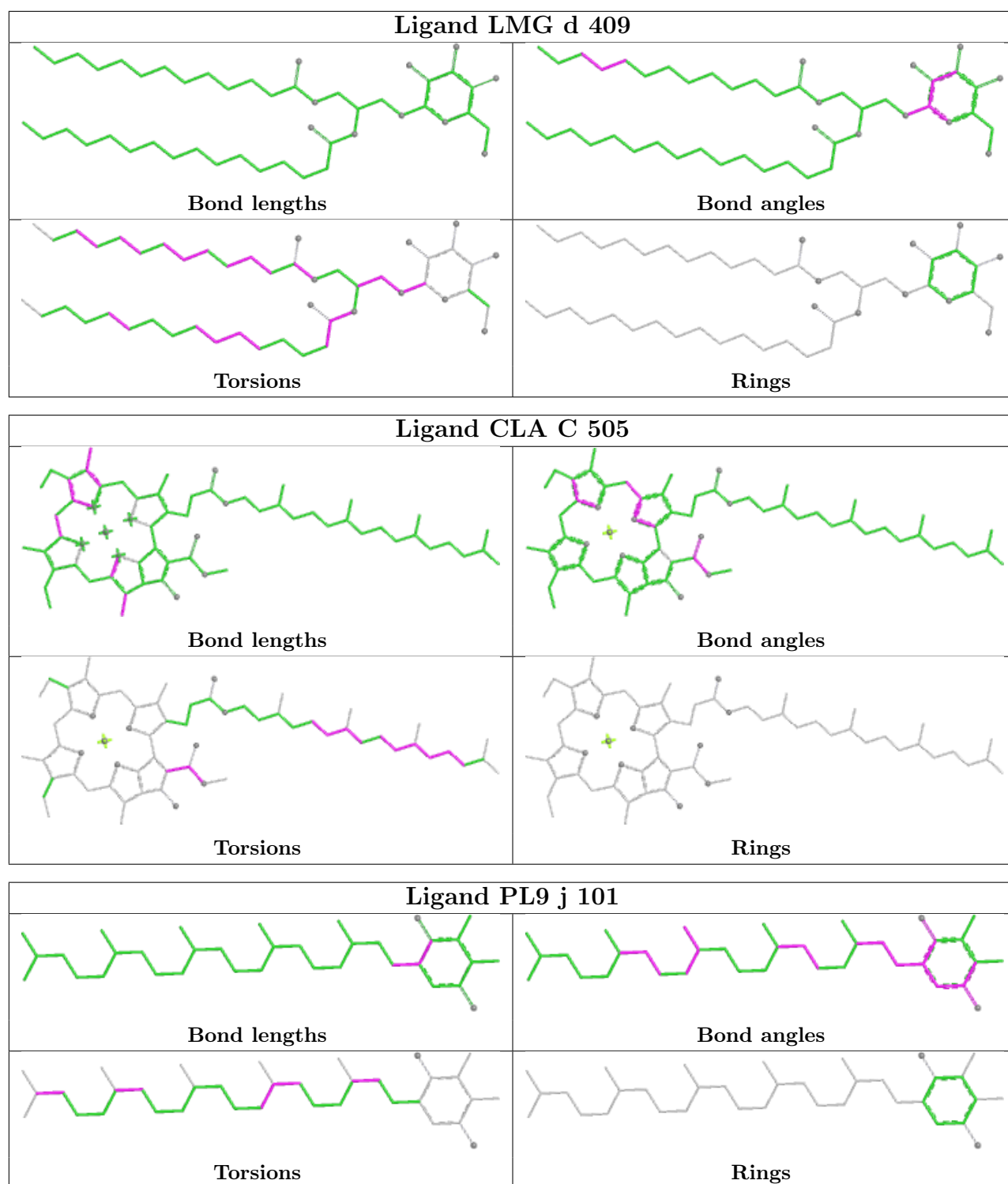


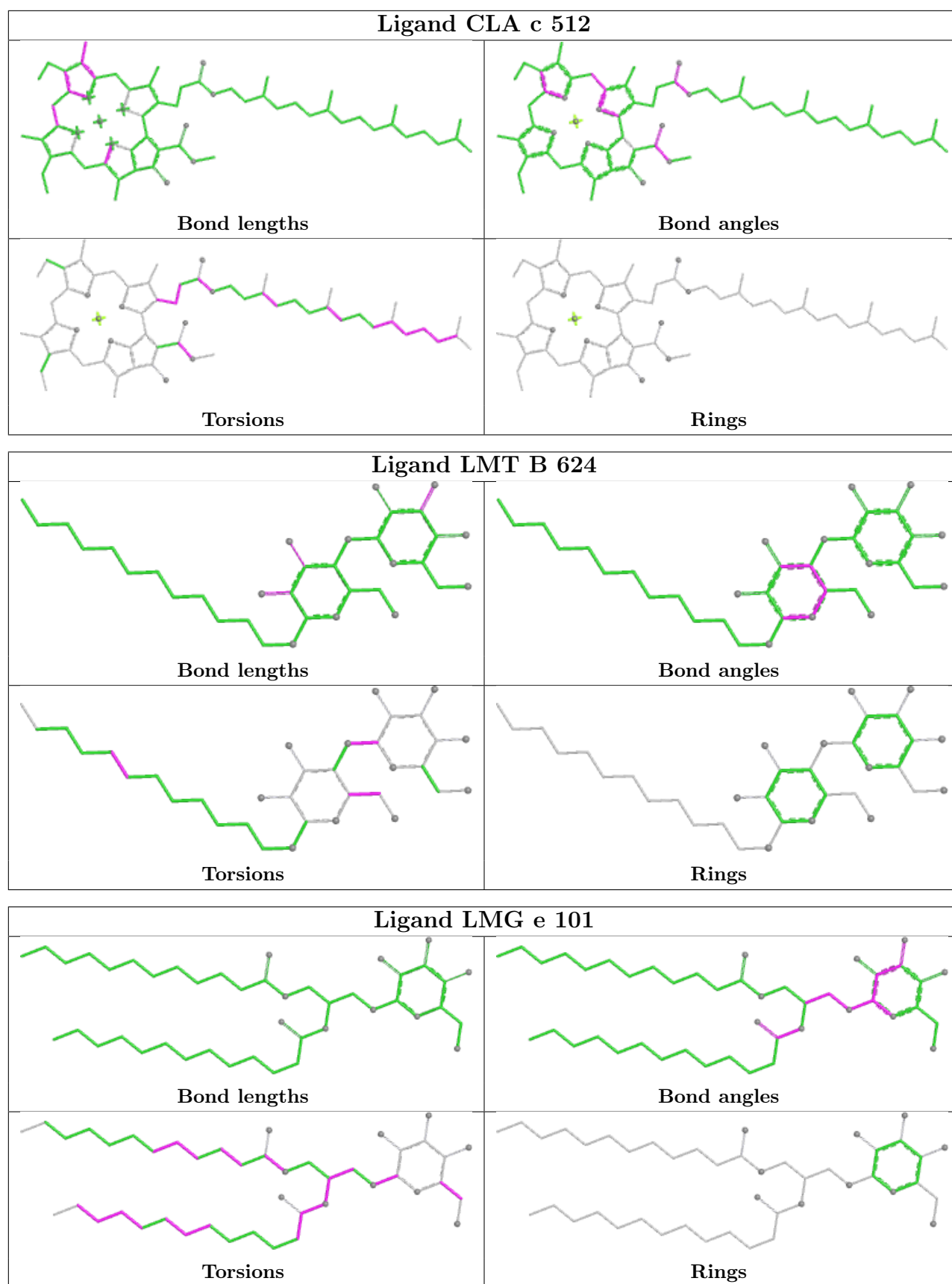




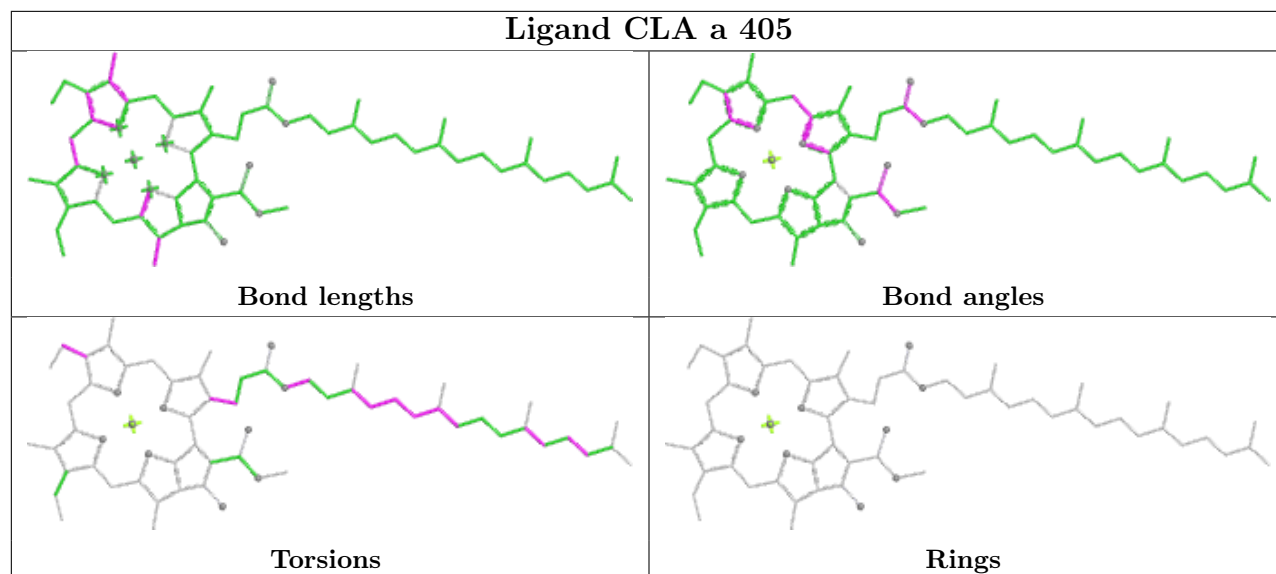




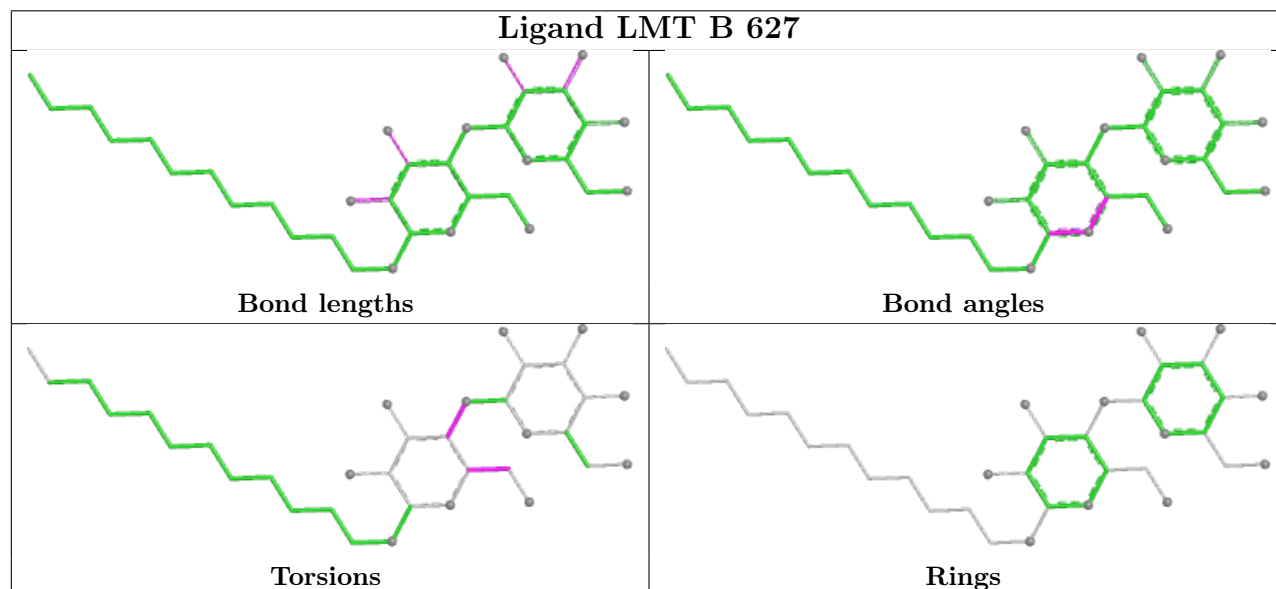




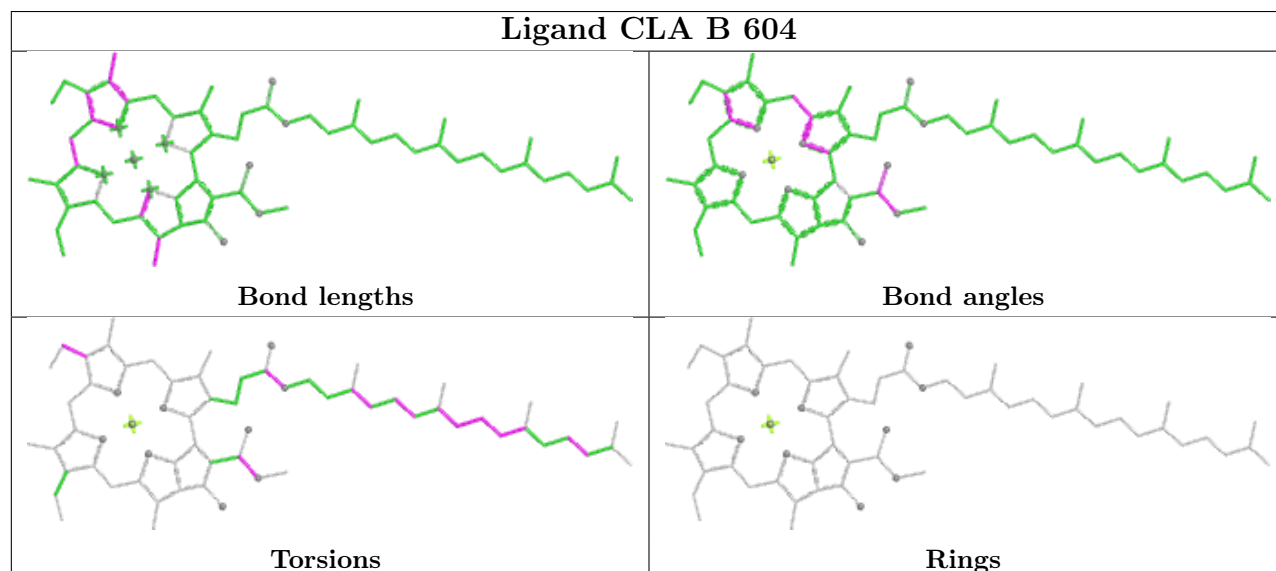
Ligand CLA a 405

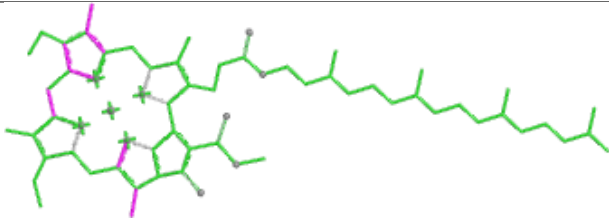
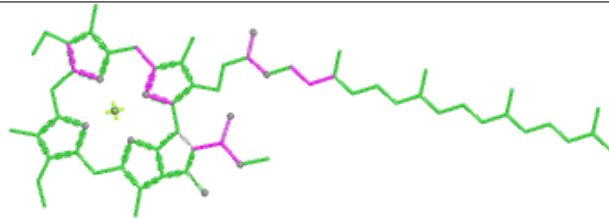
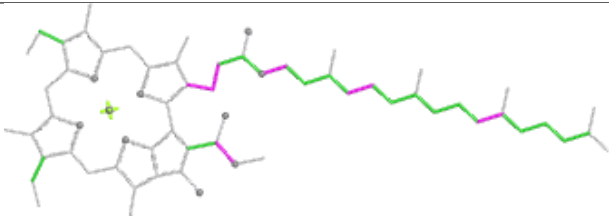
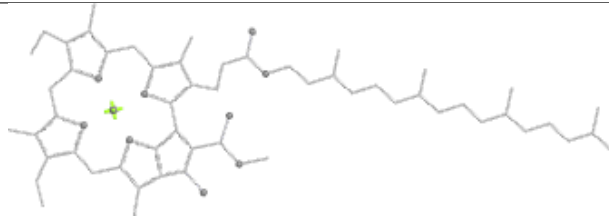


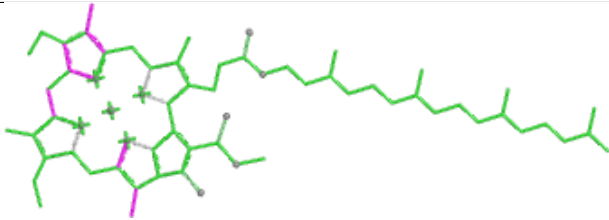
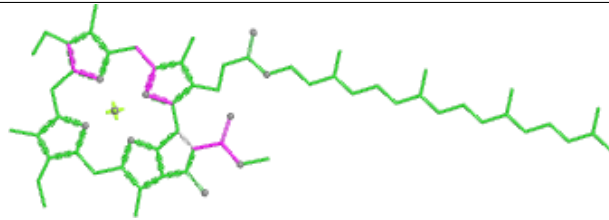
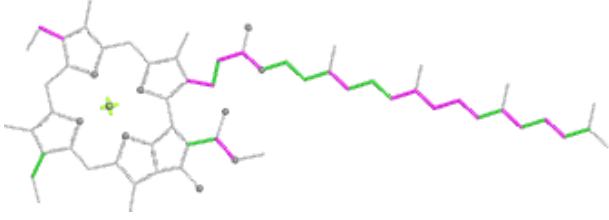
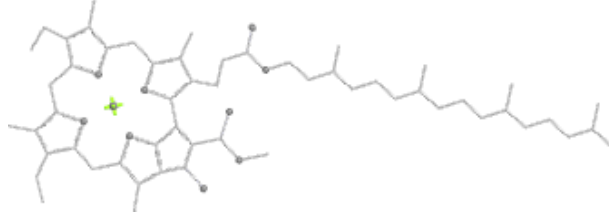
Ligand LMT B 627

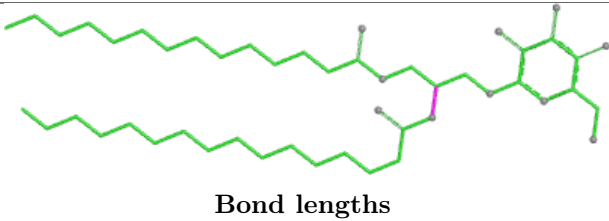
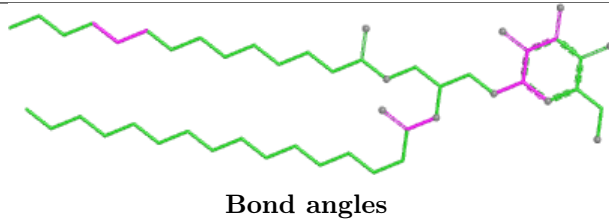
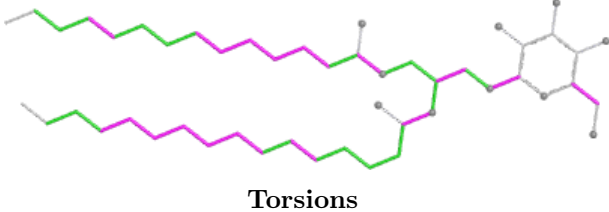
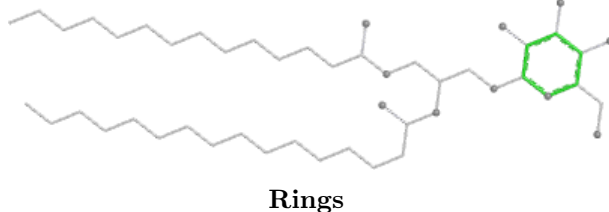


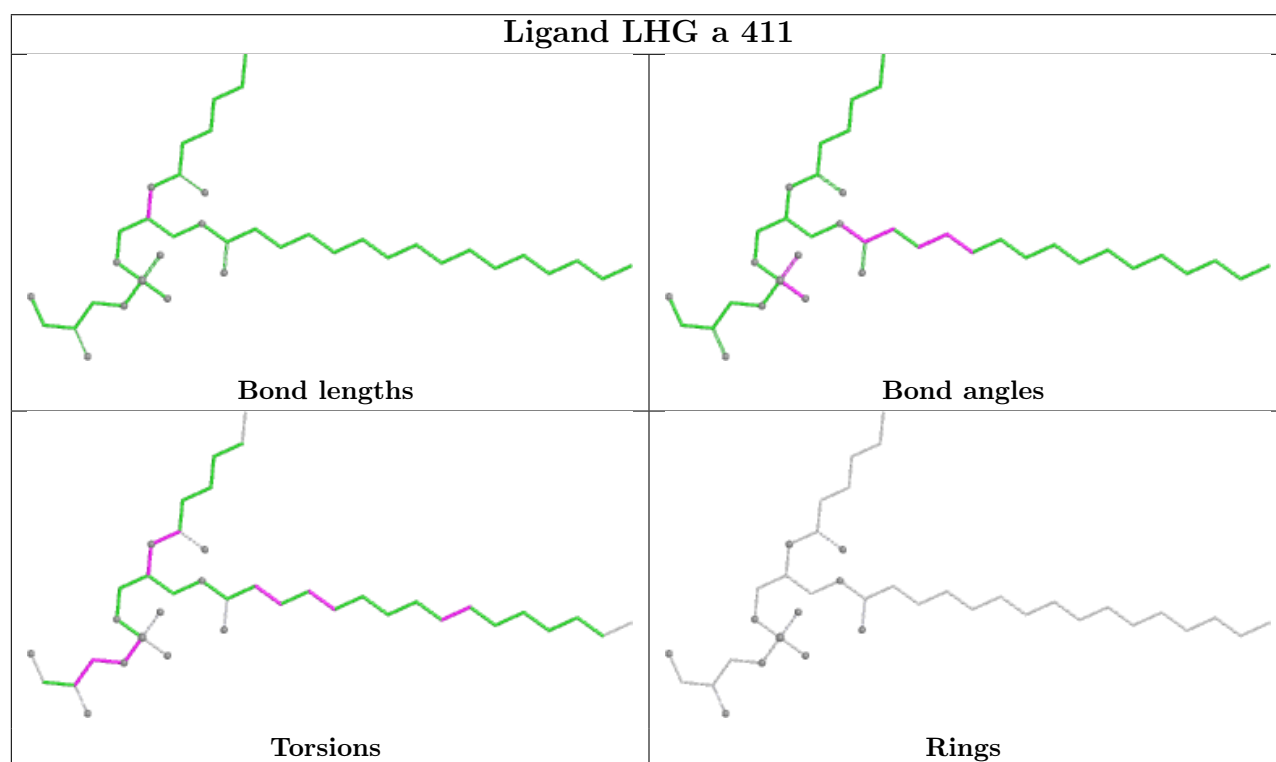
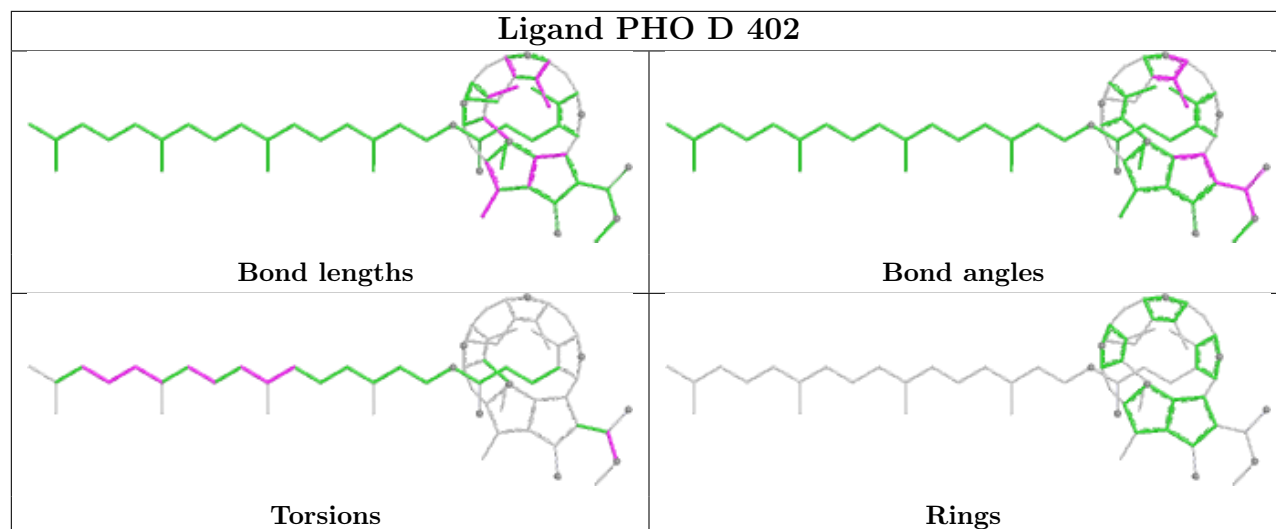
Ligand CLA B 604

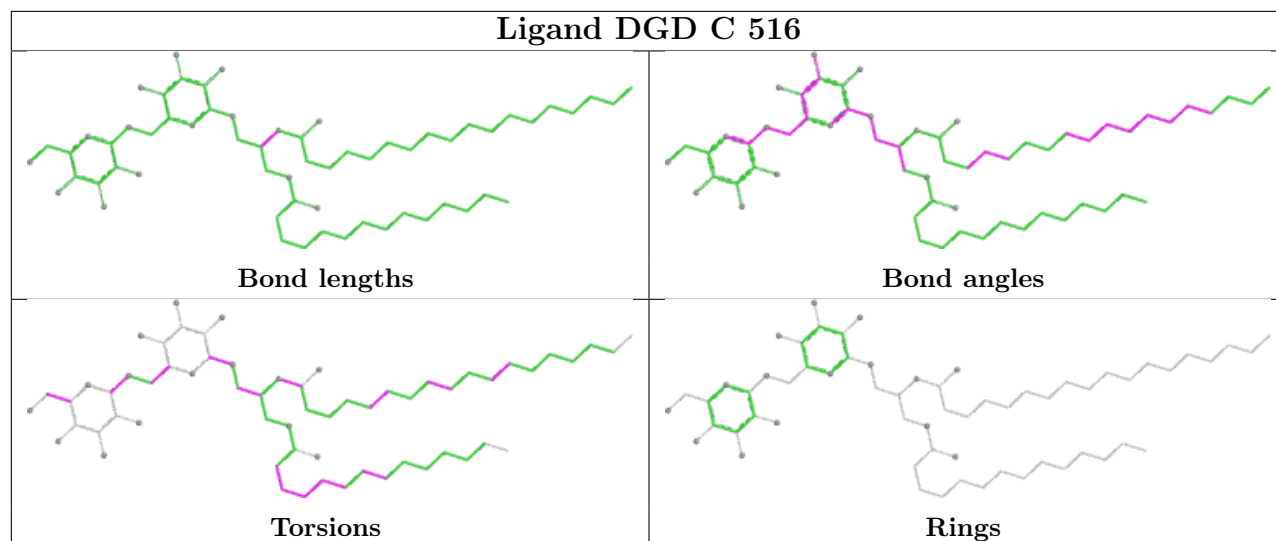
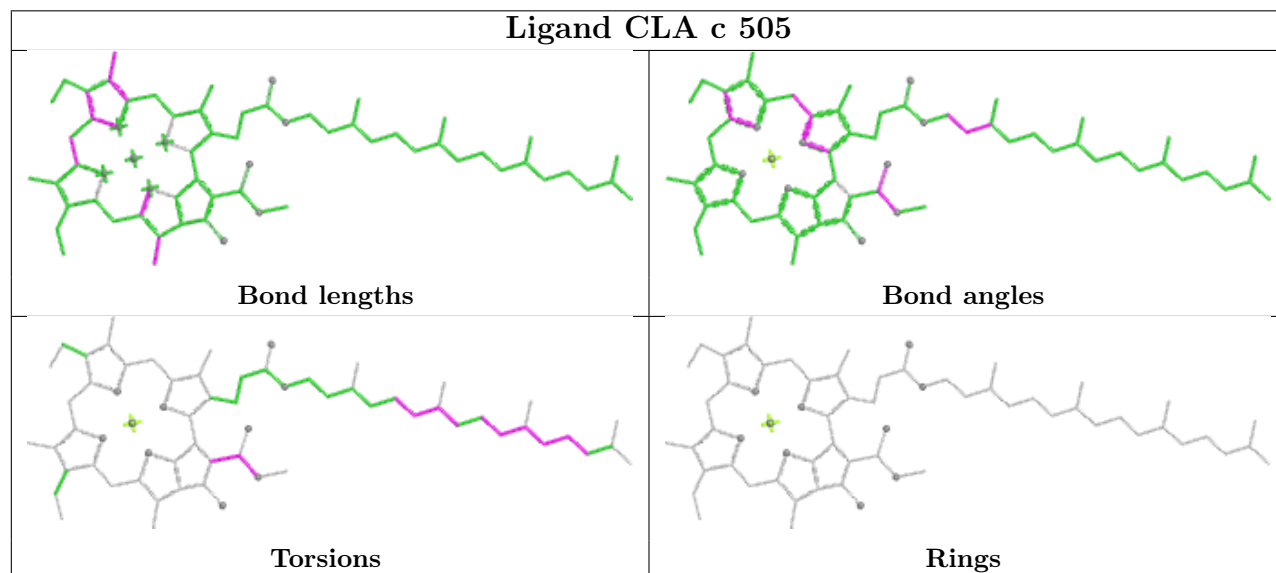
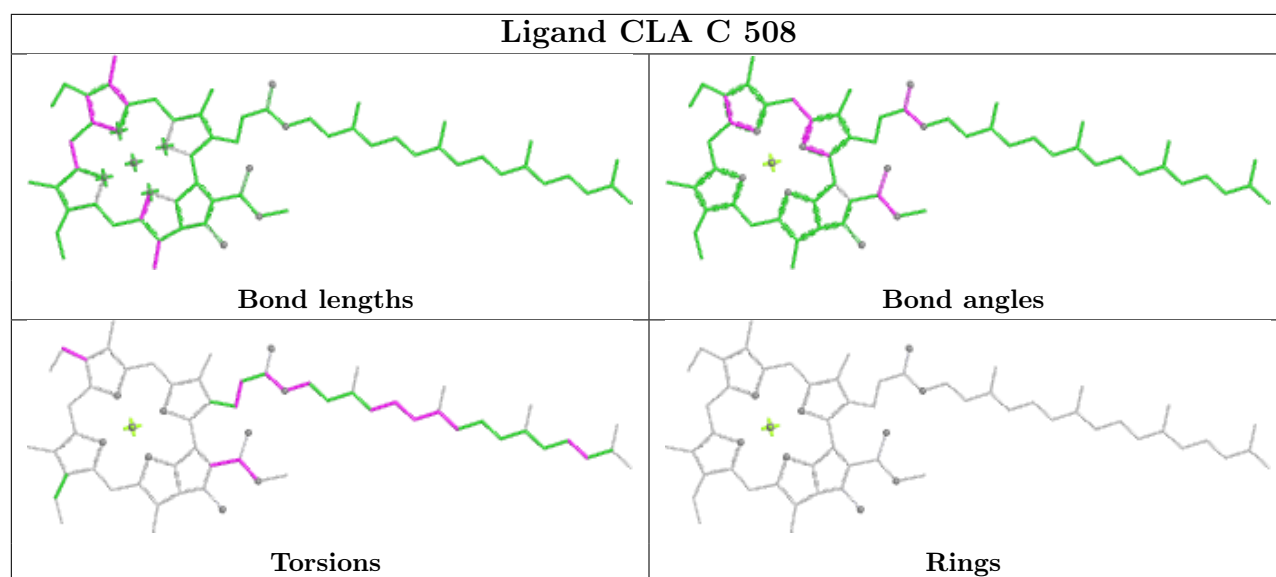


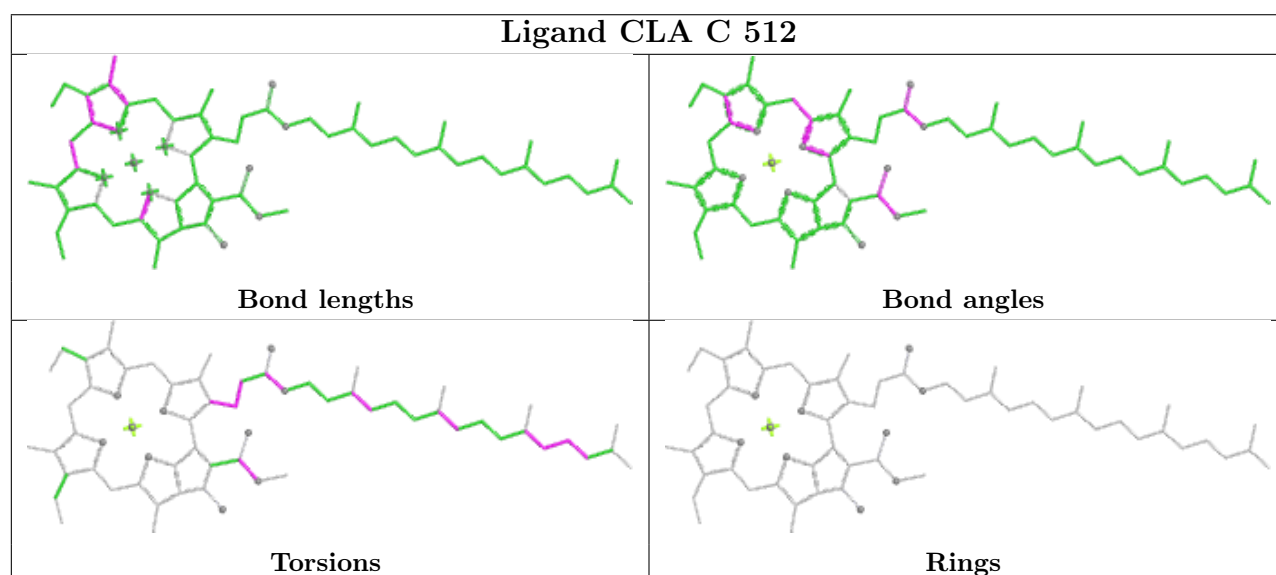
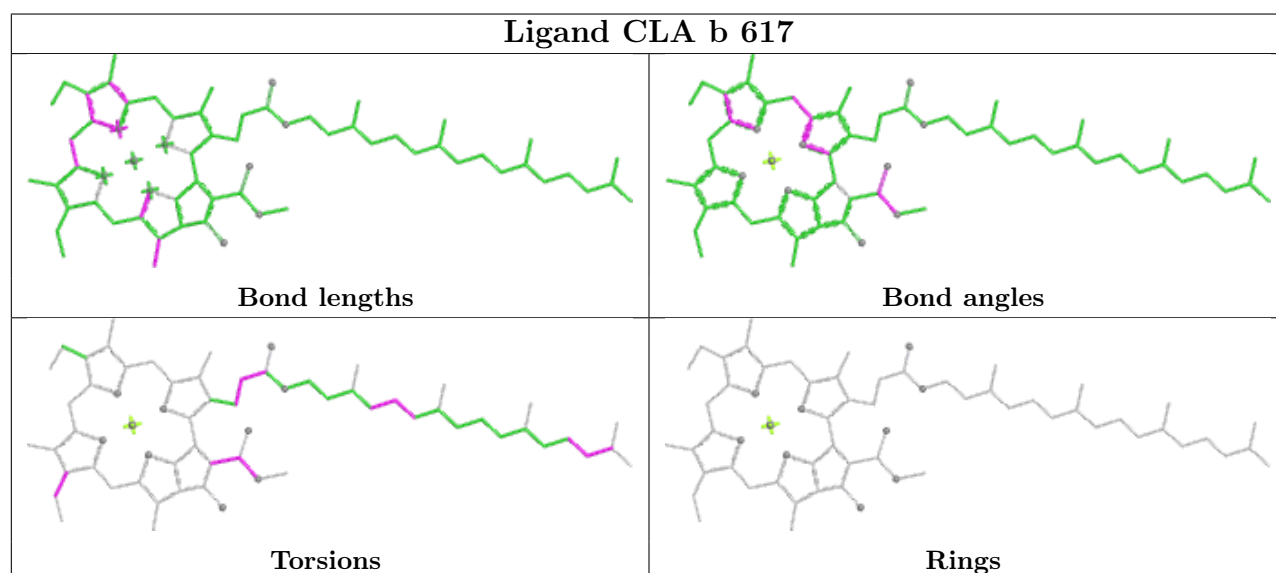
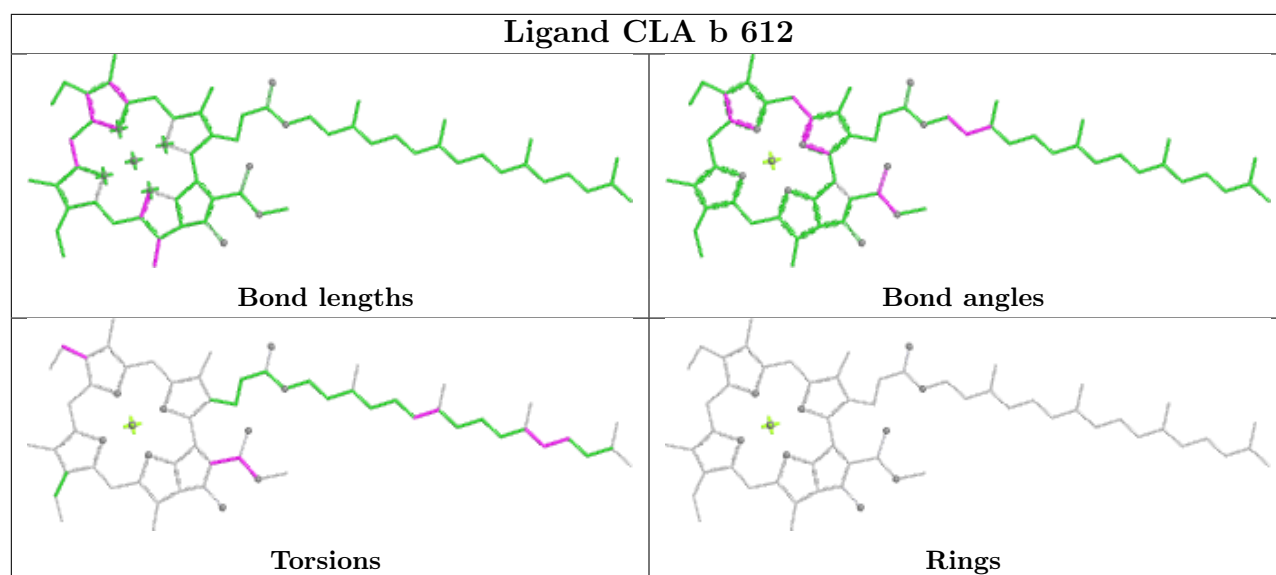
Ligand CLA a 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

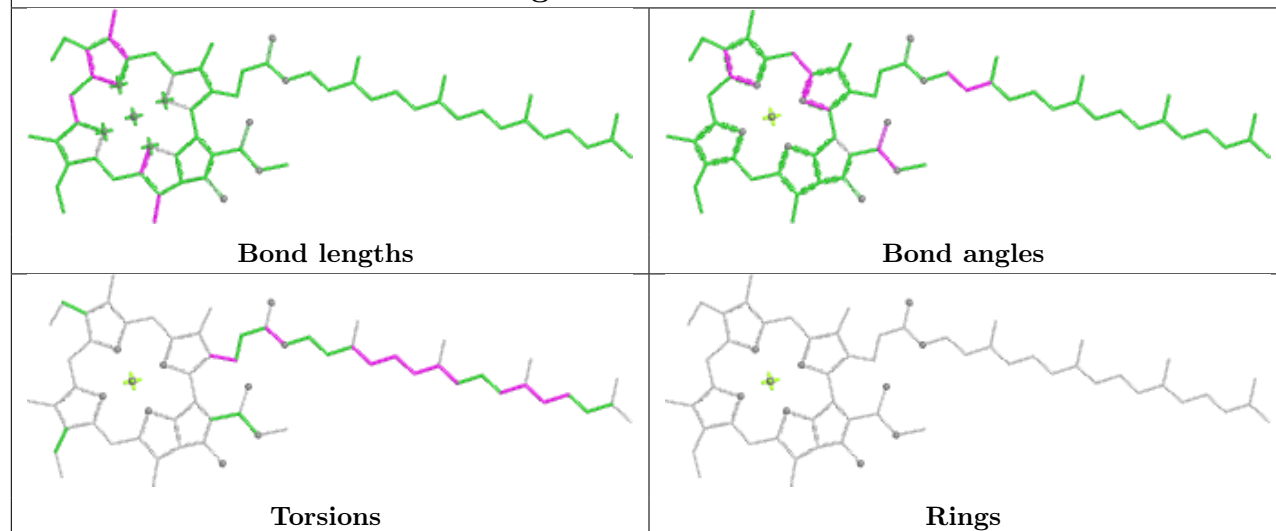
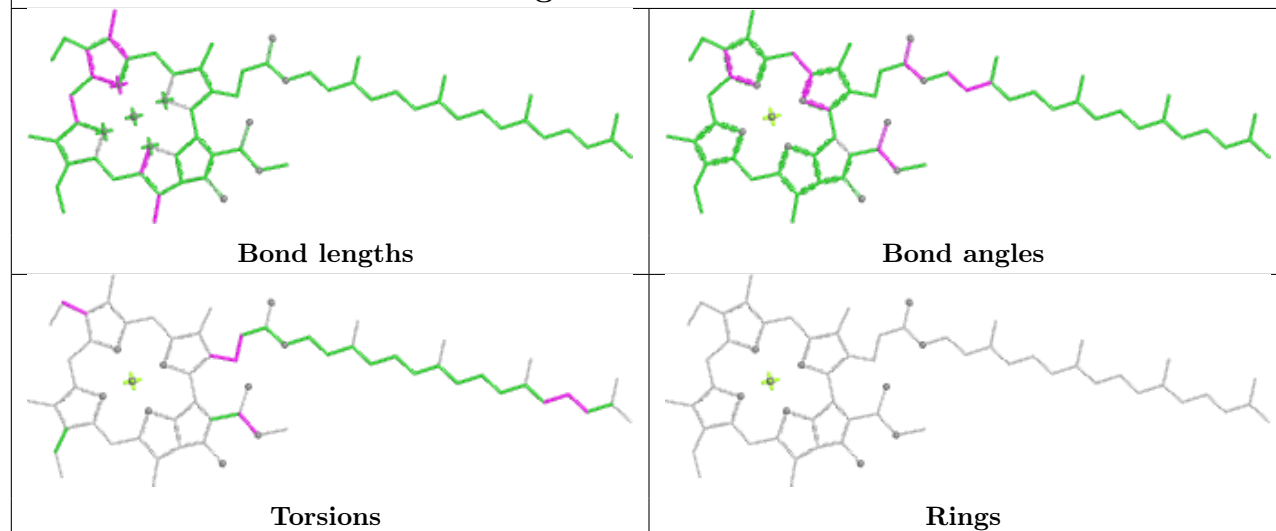
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

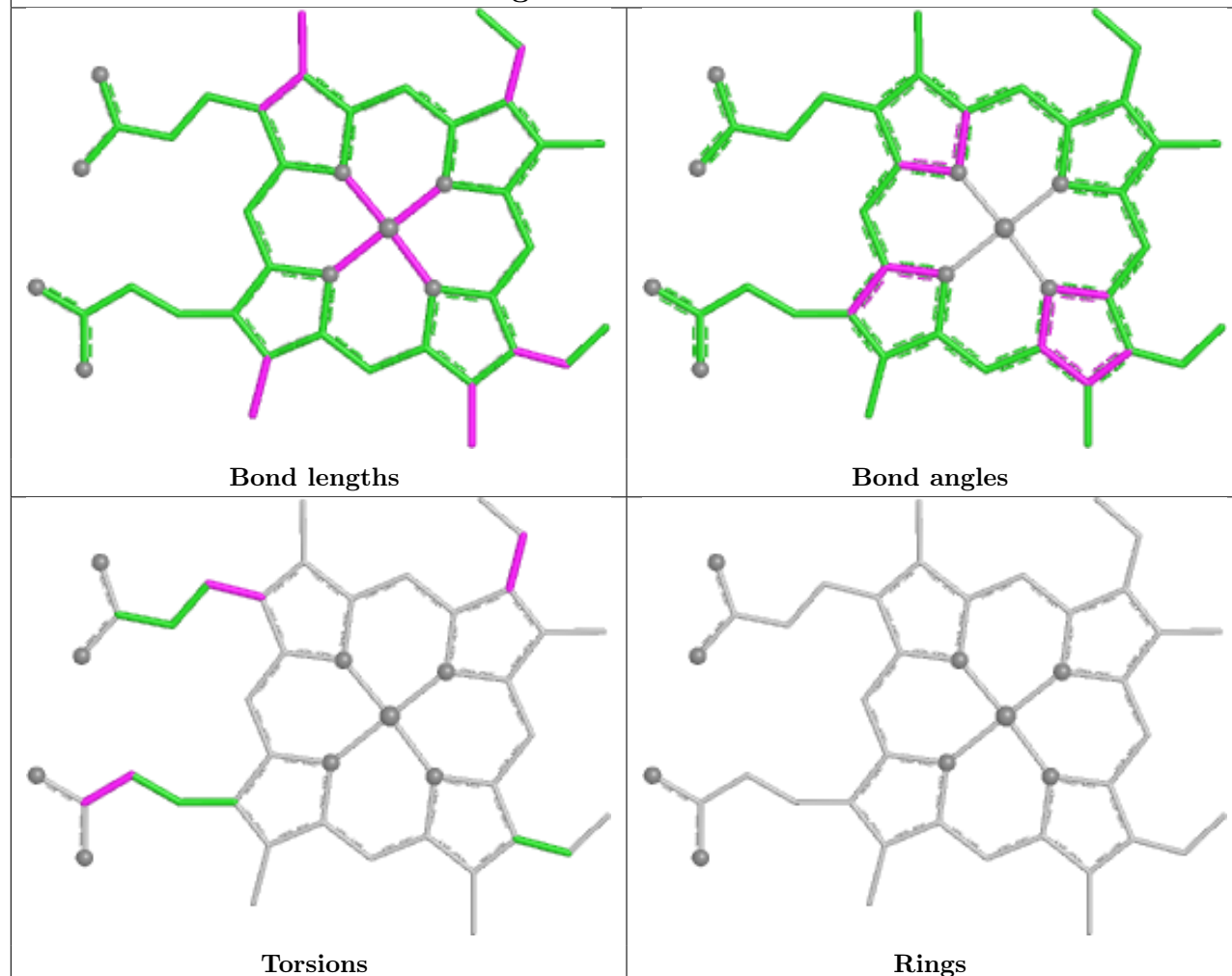




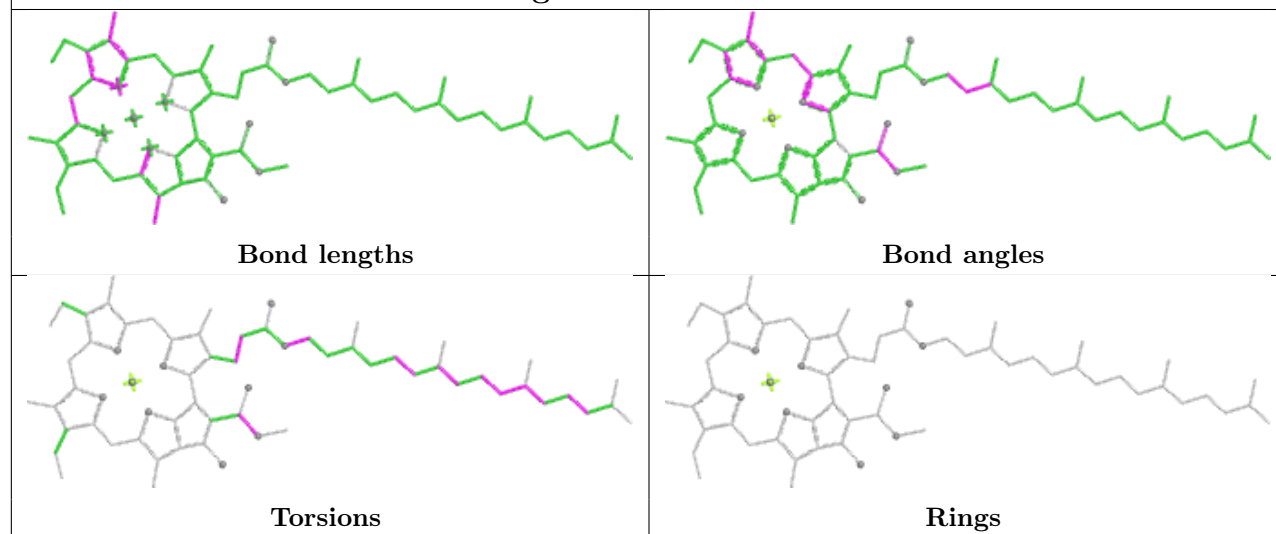


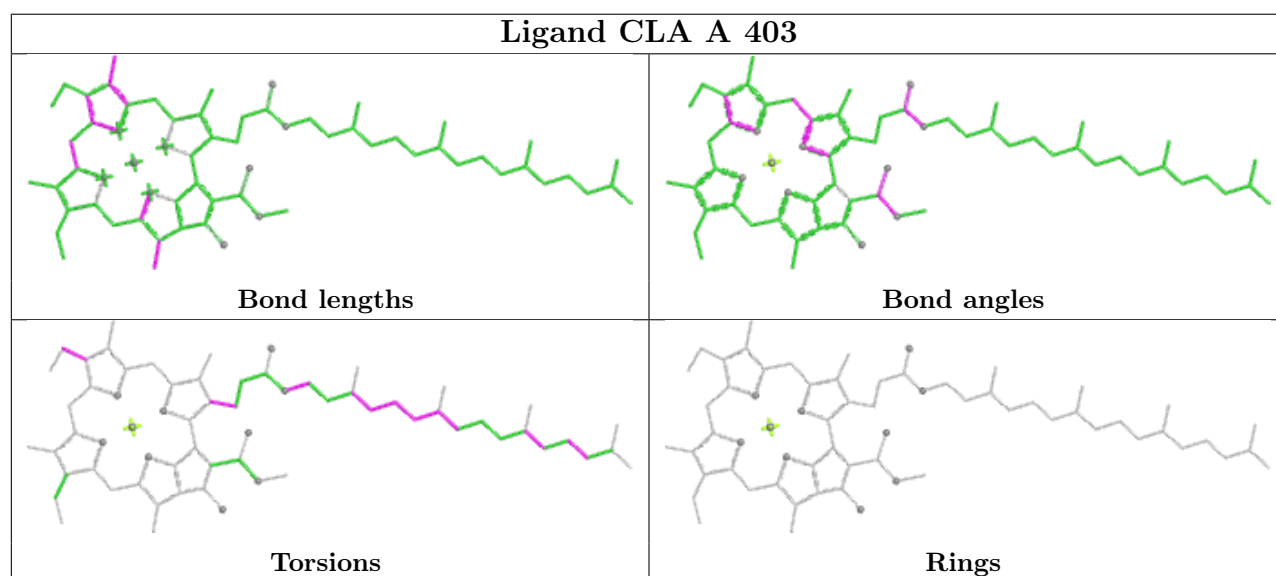
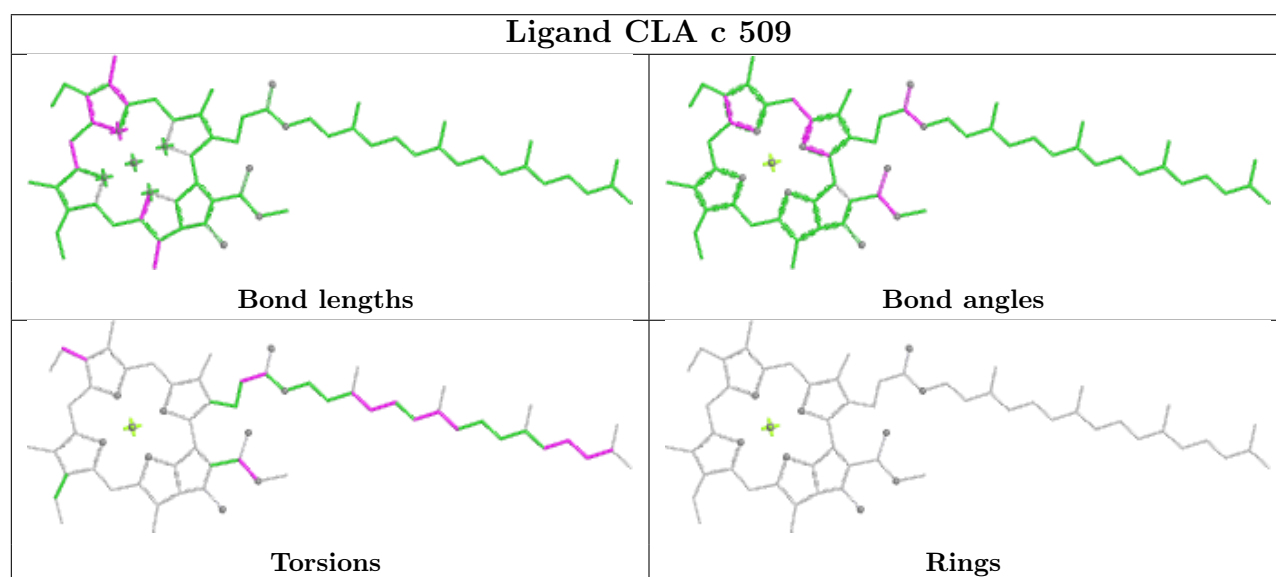
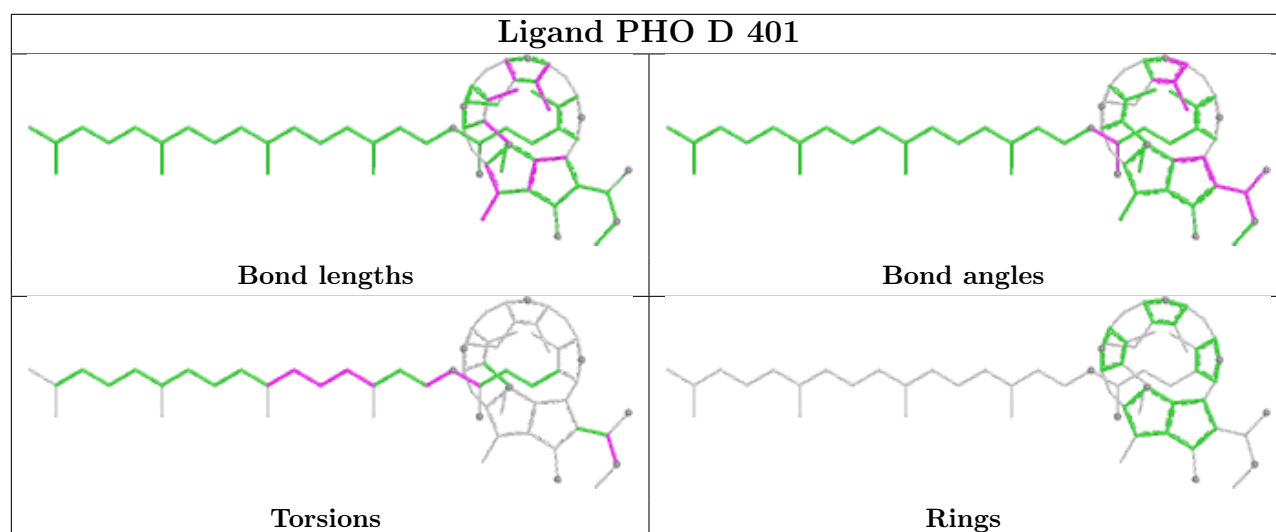
Ligand CLA H 101**Ligand CLA b 610**

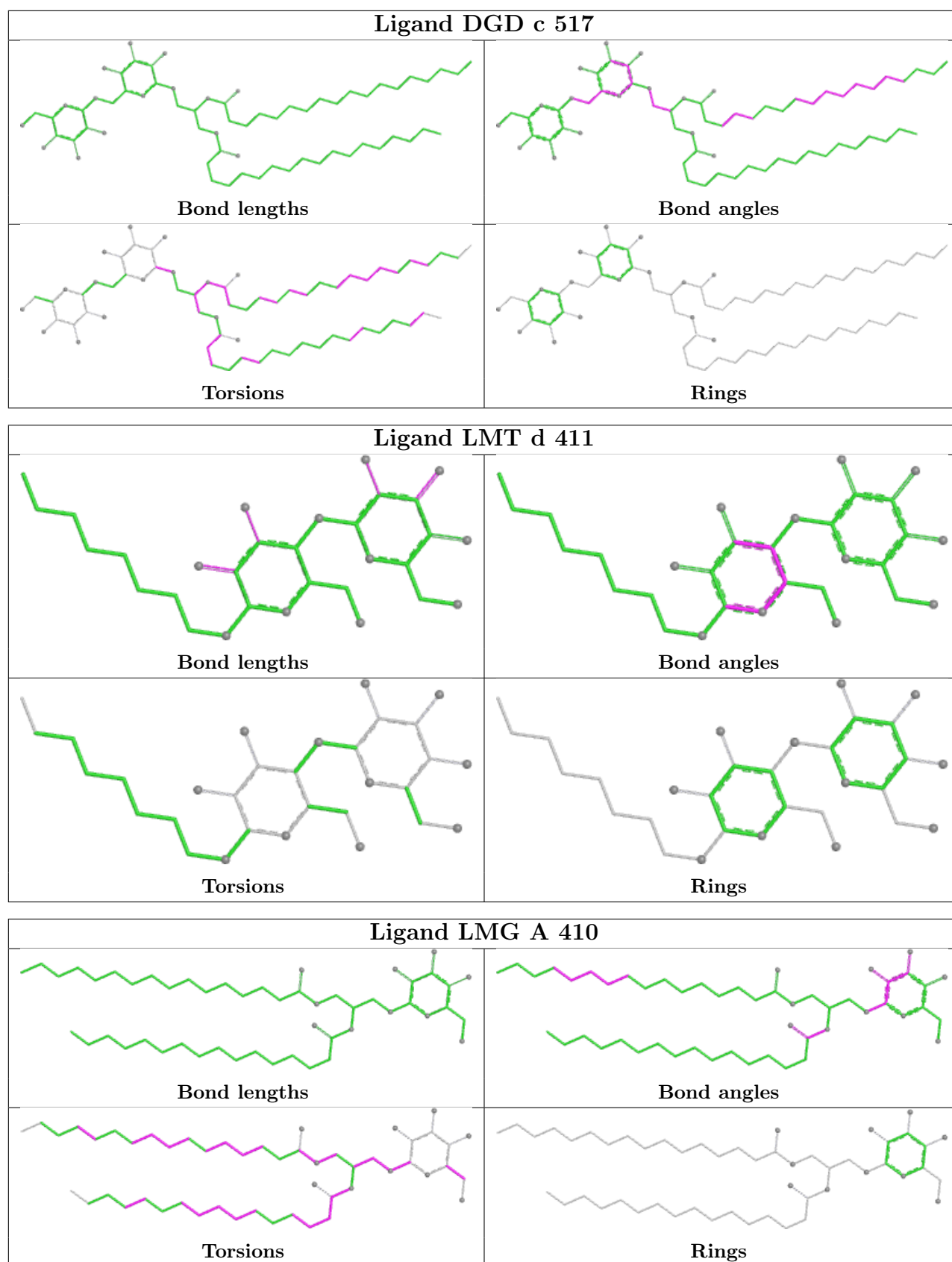
Ligand HEM v 201

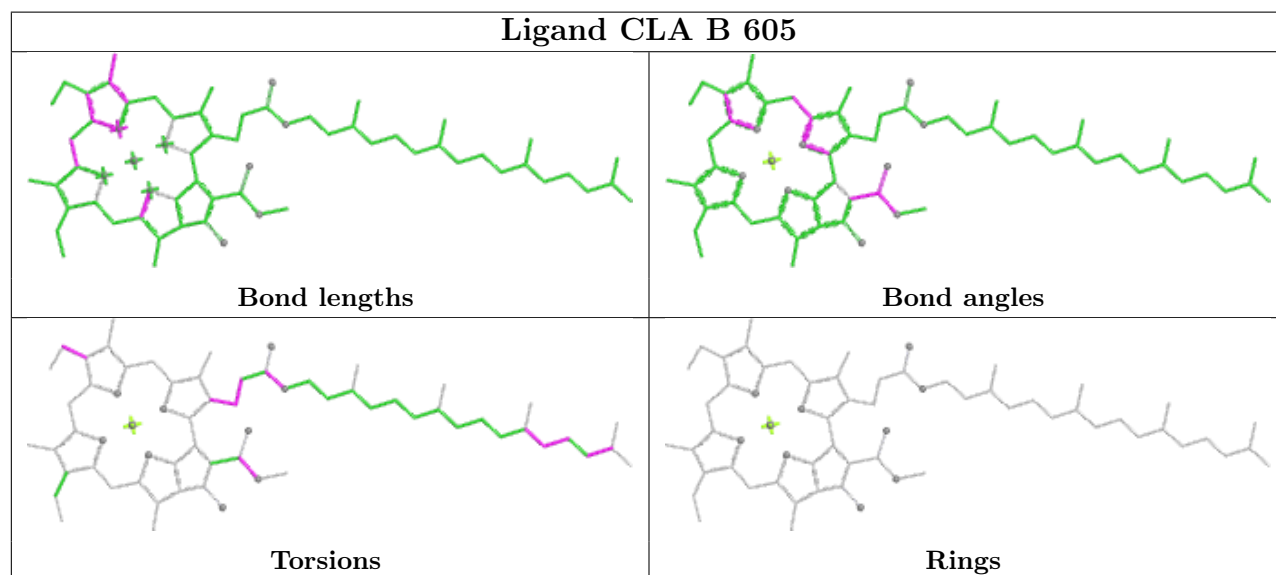
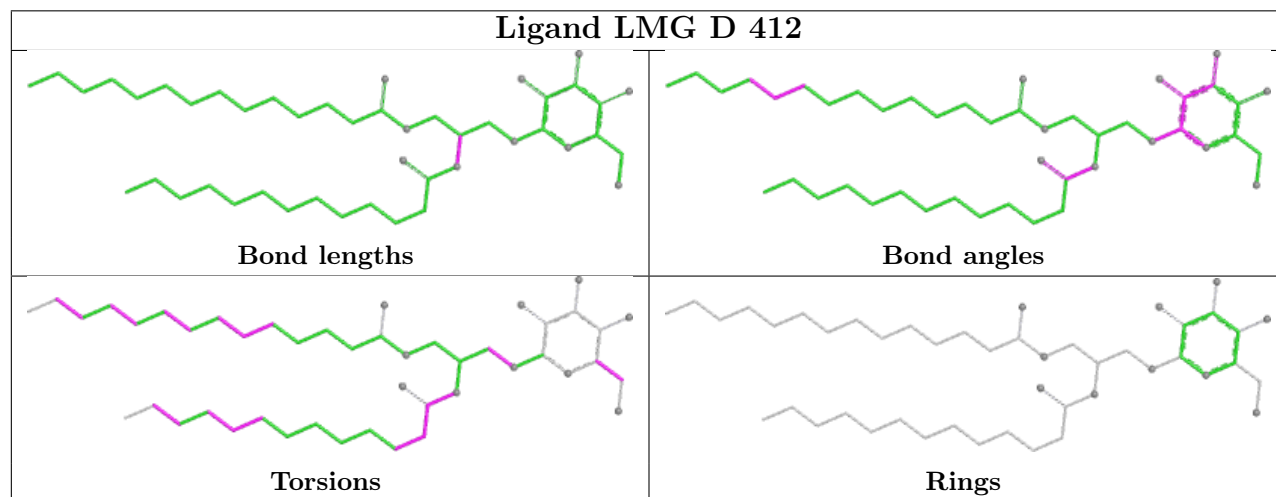
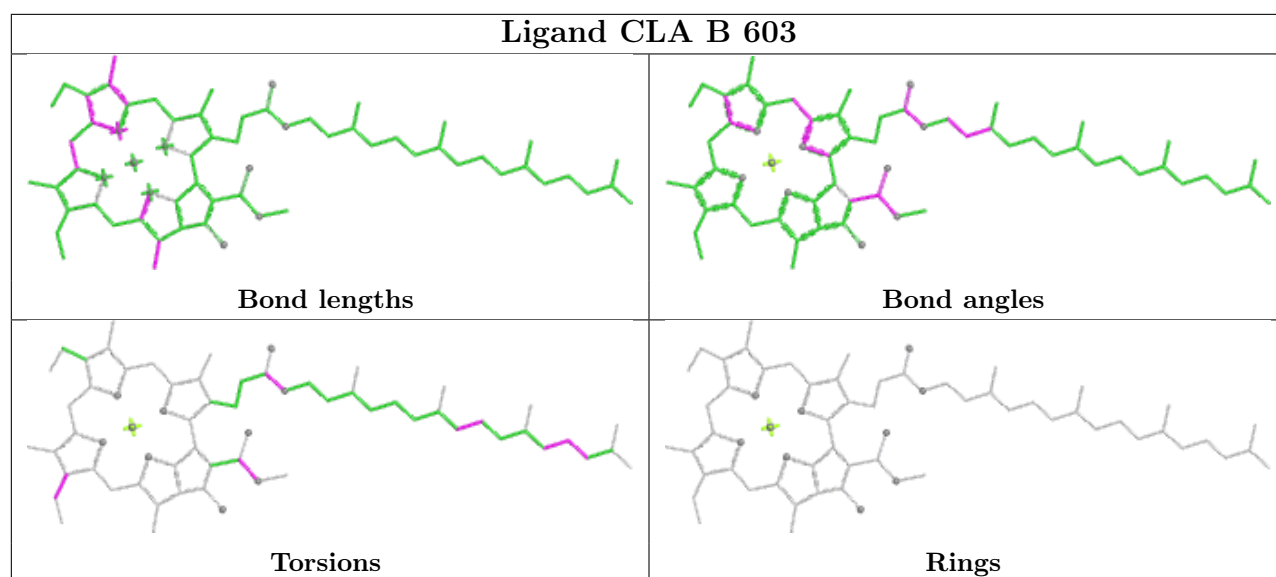


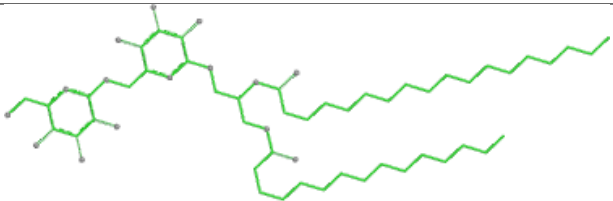
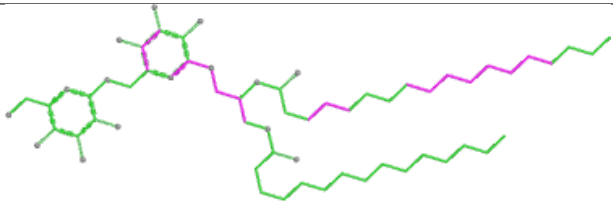
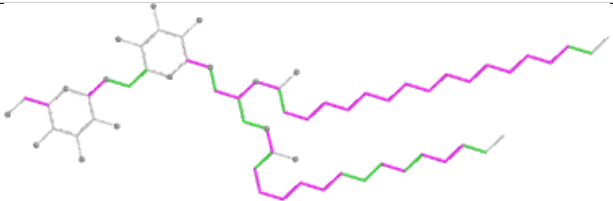
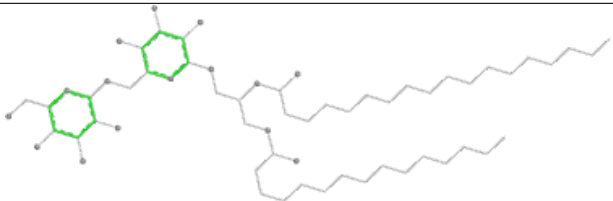
Ligand CLA C 507

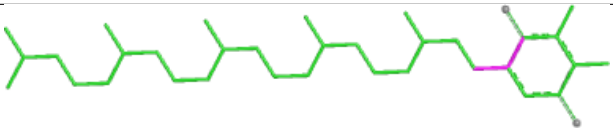
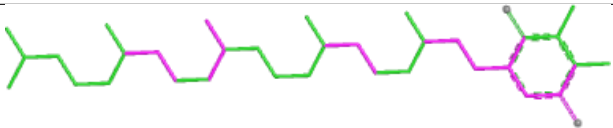
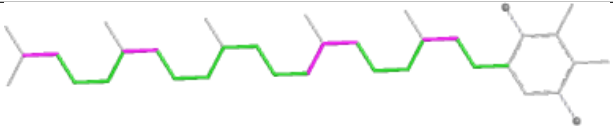
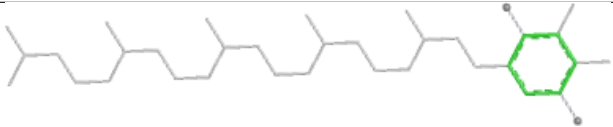


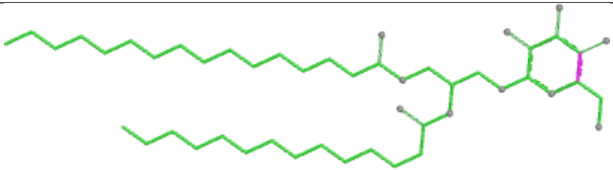
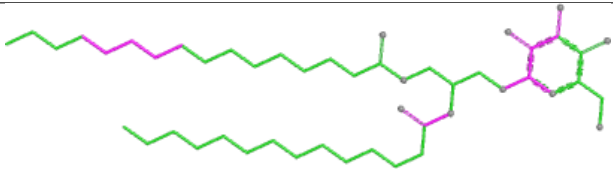
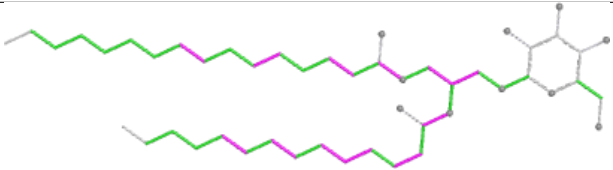
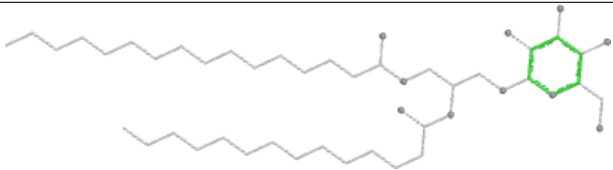


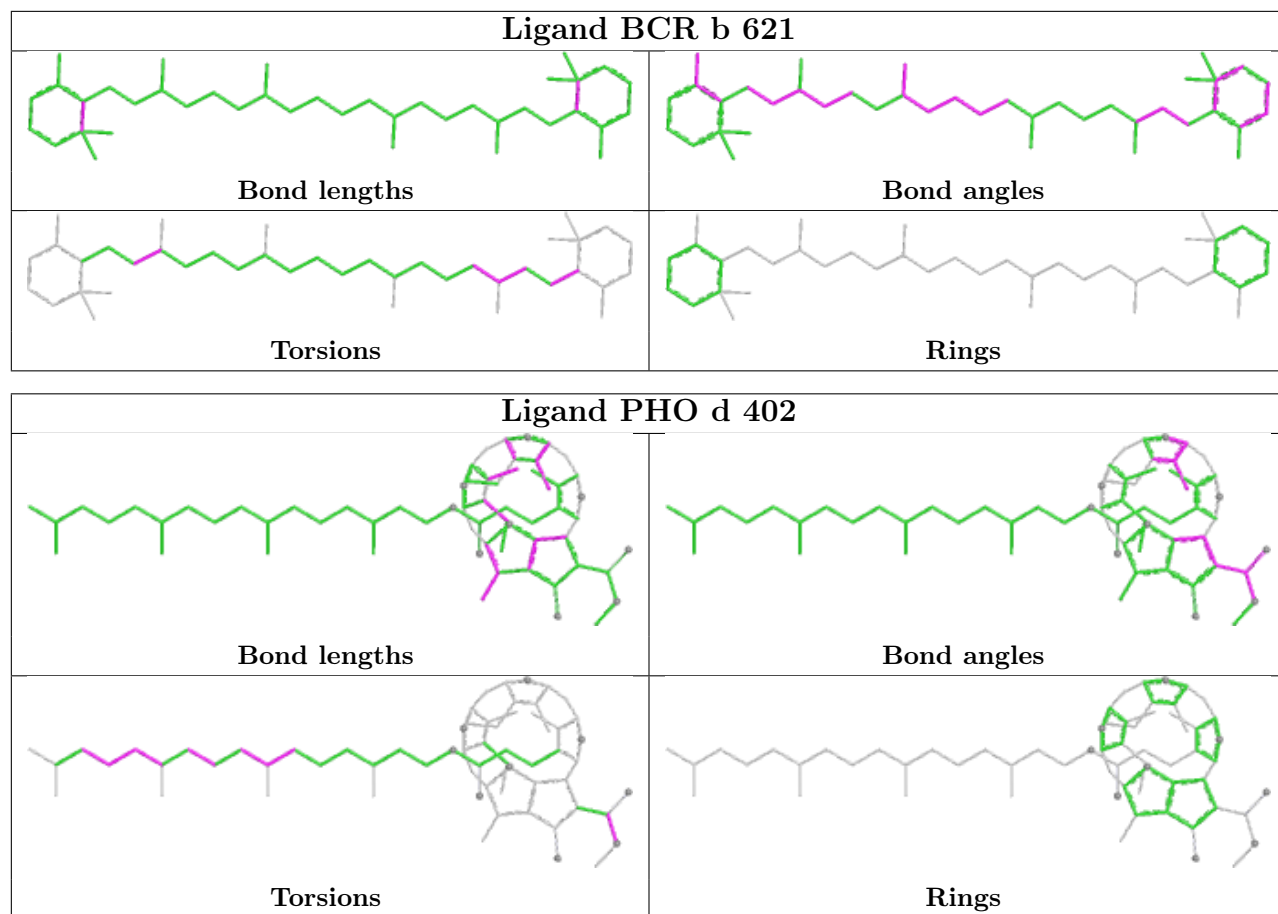


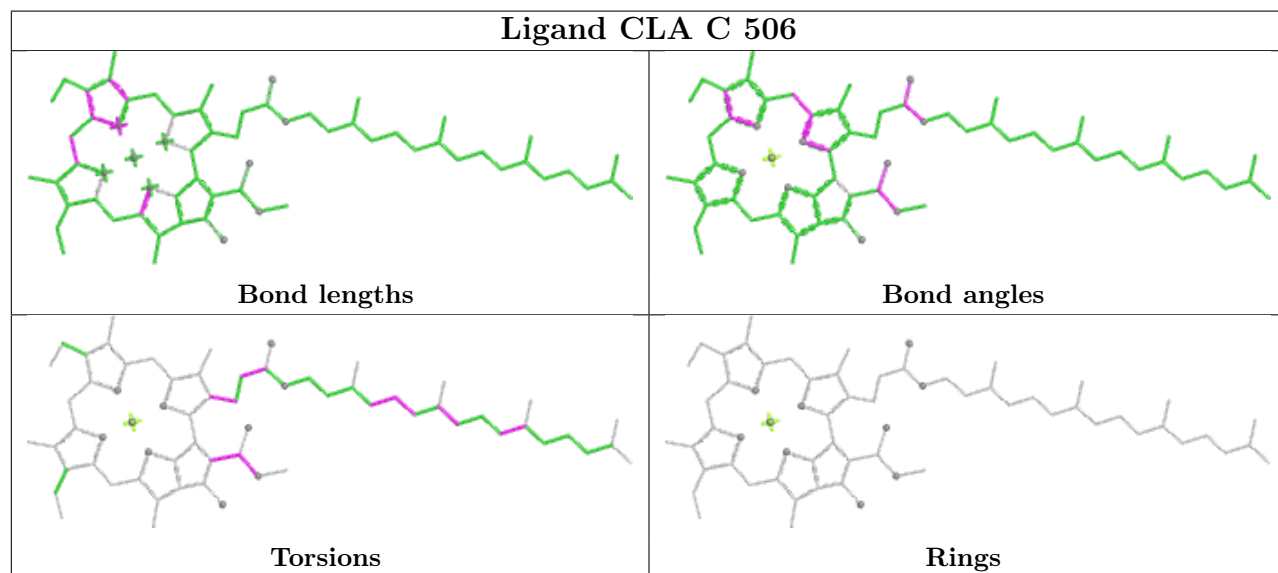
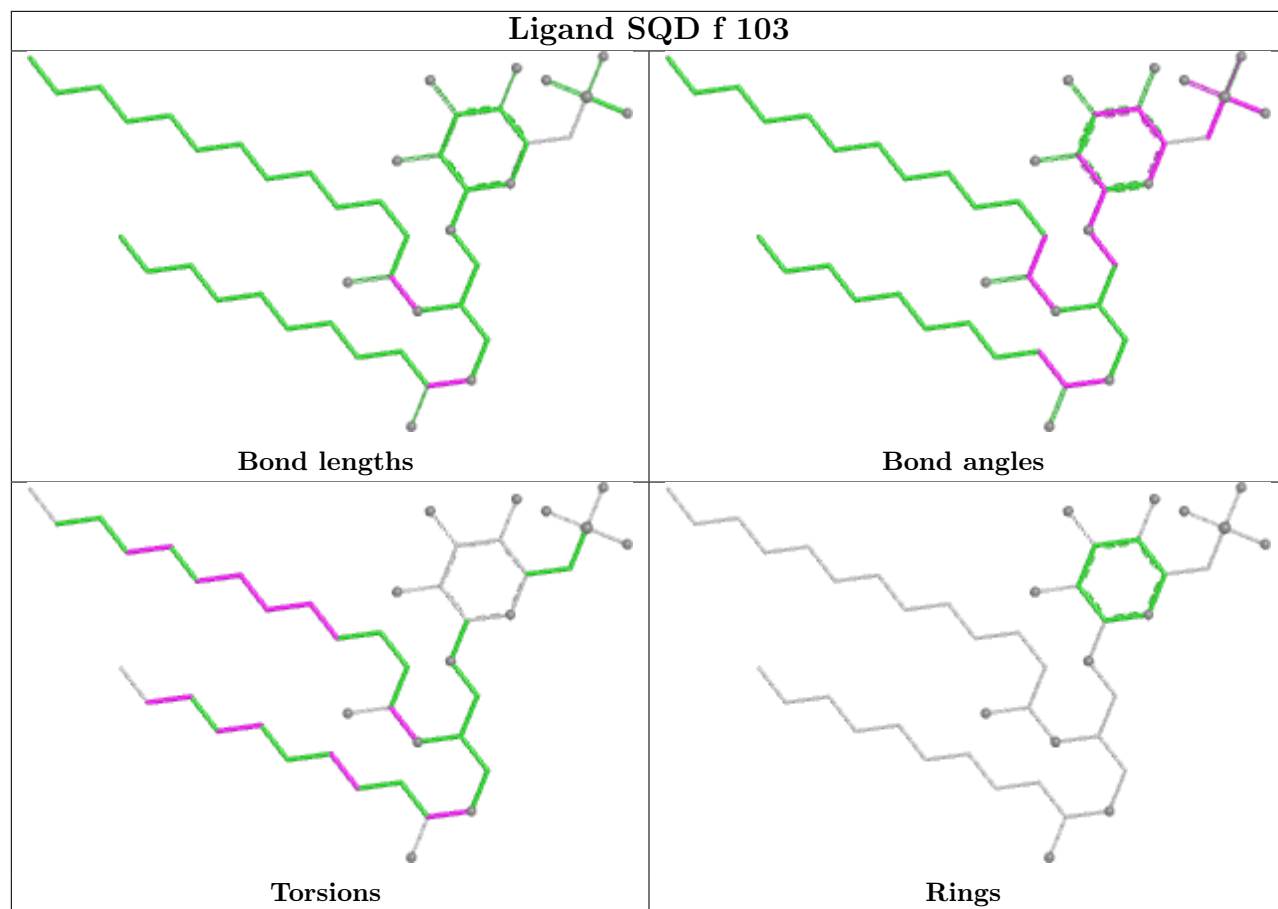


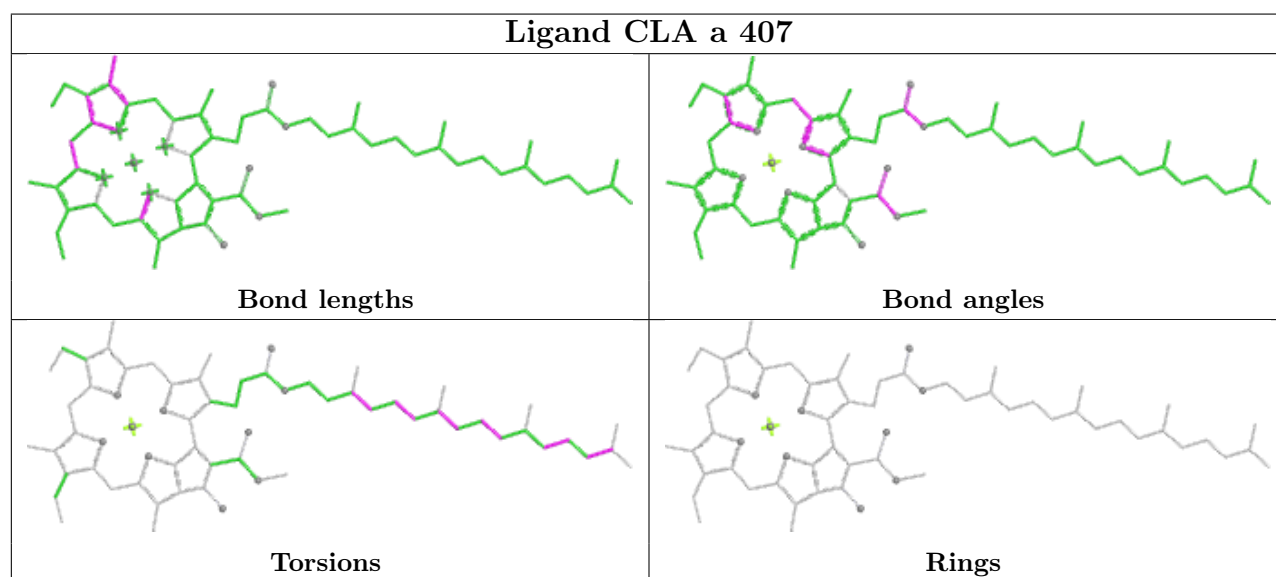
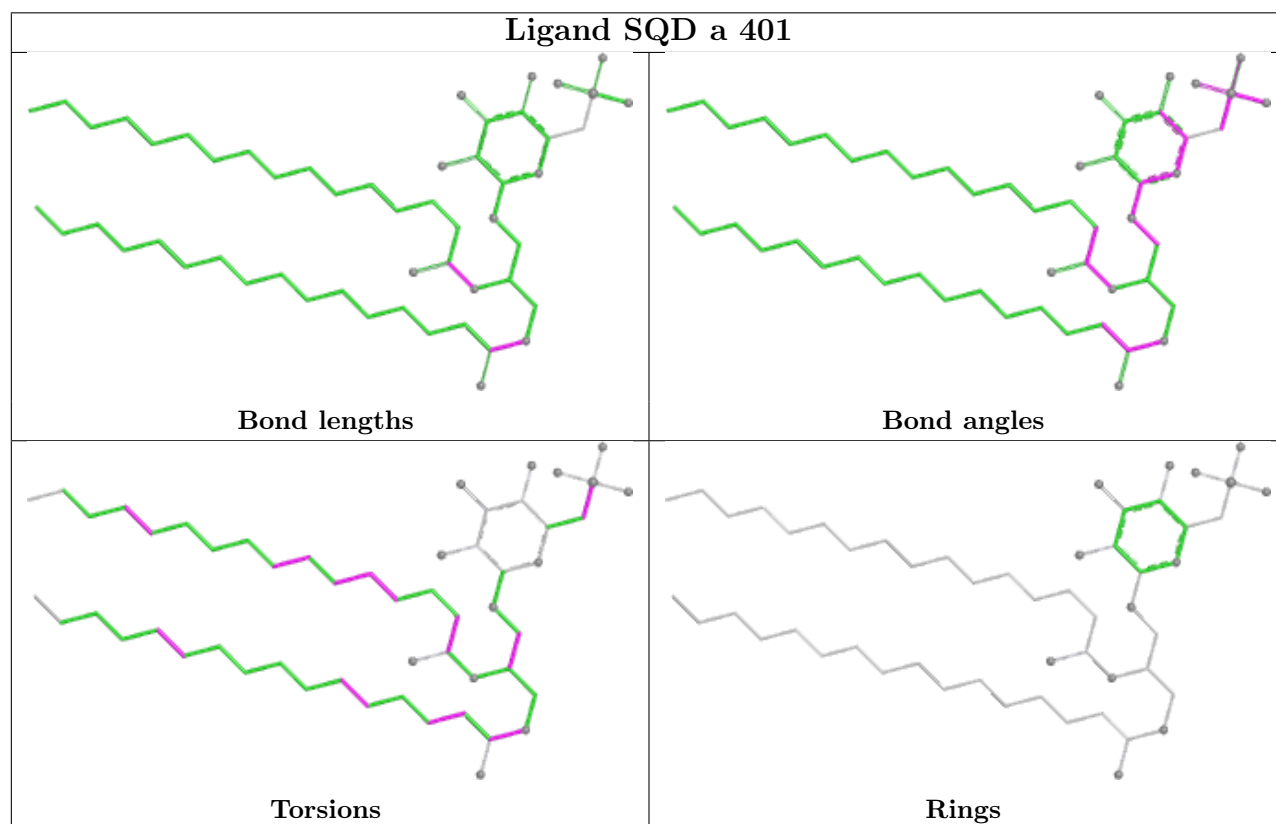
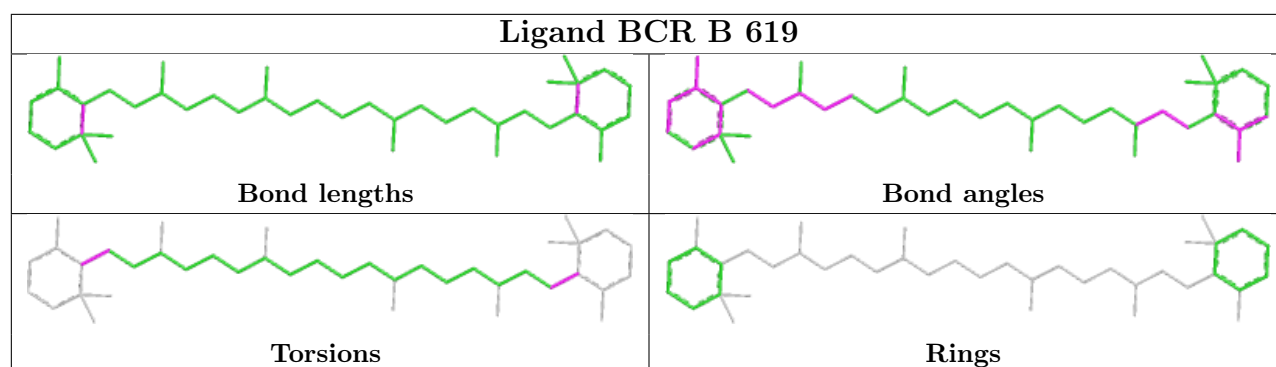
Ligand DGD D 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

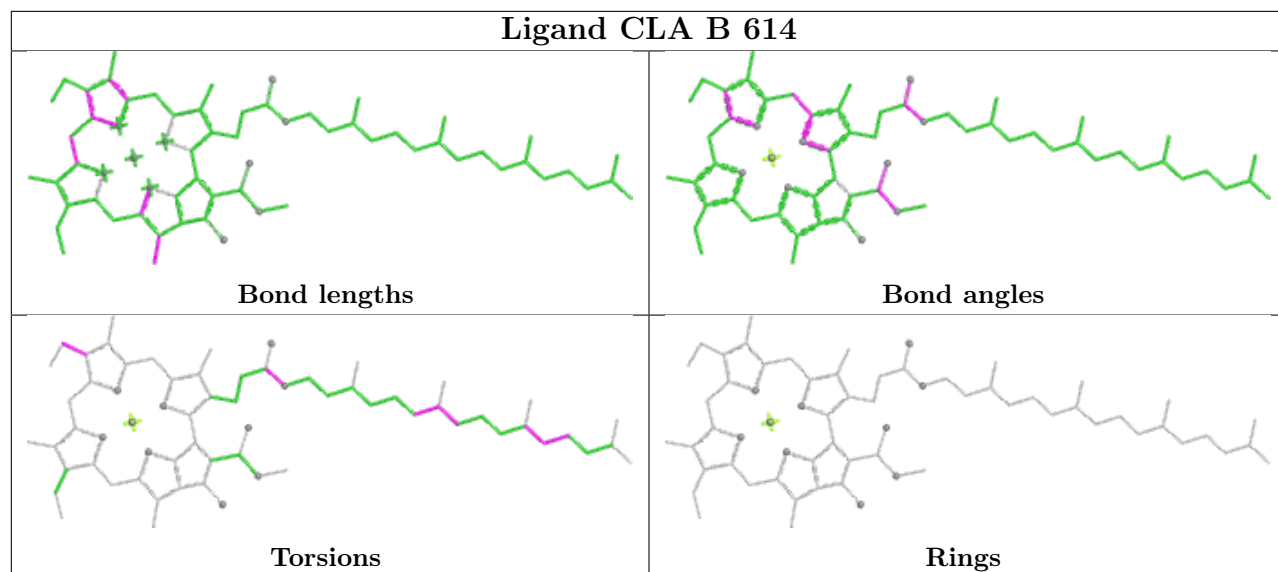
Ligand LMG b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings



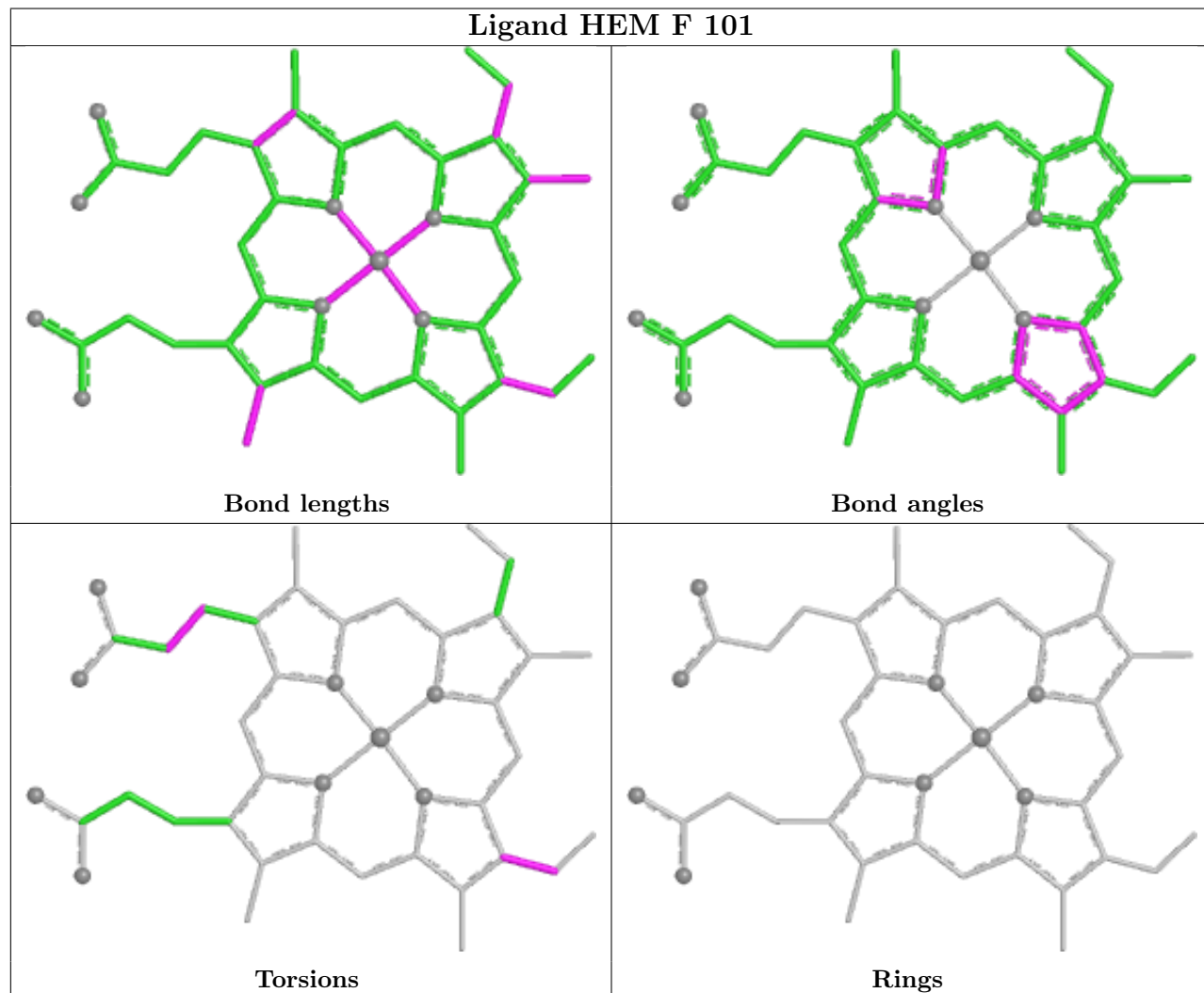


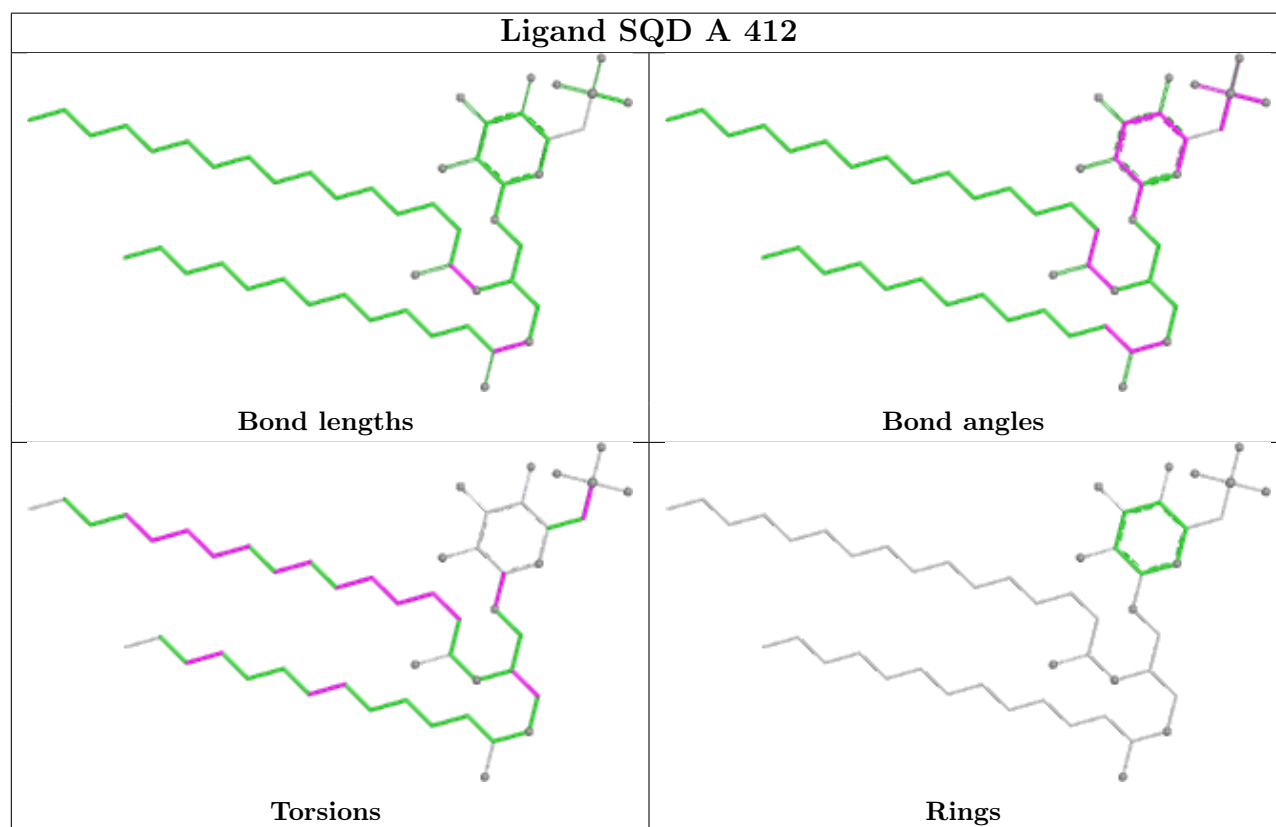
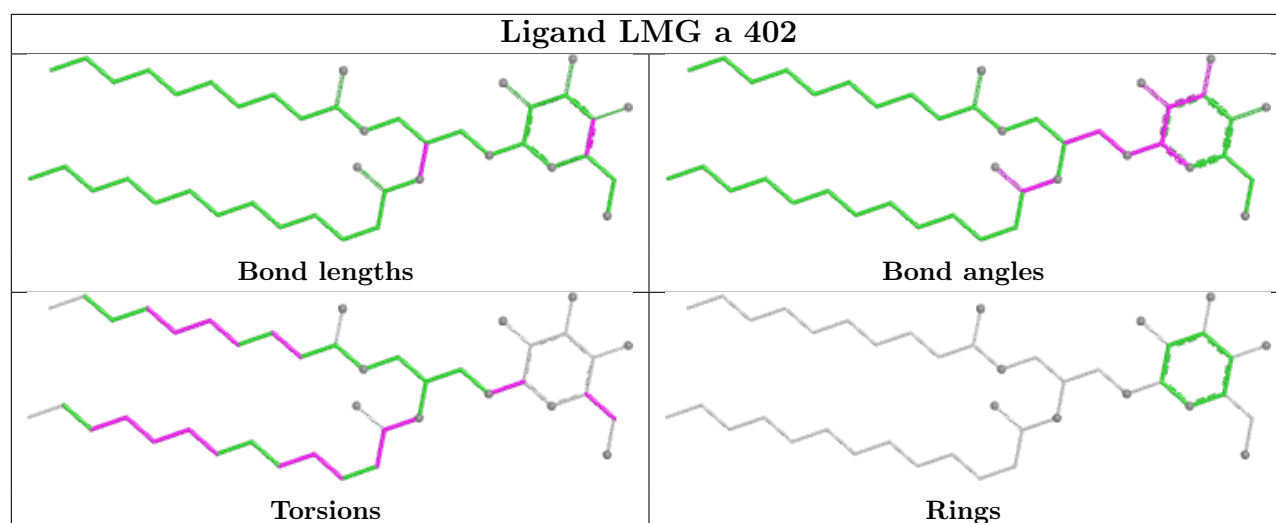


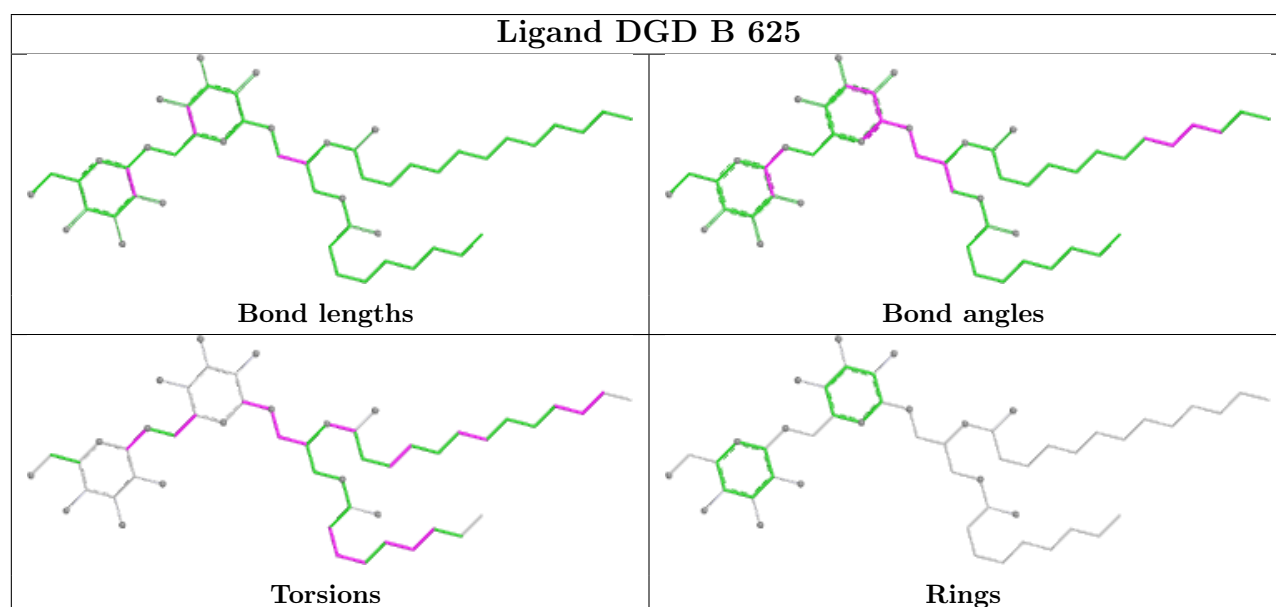
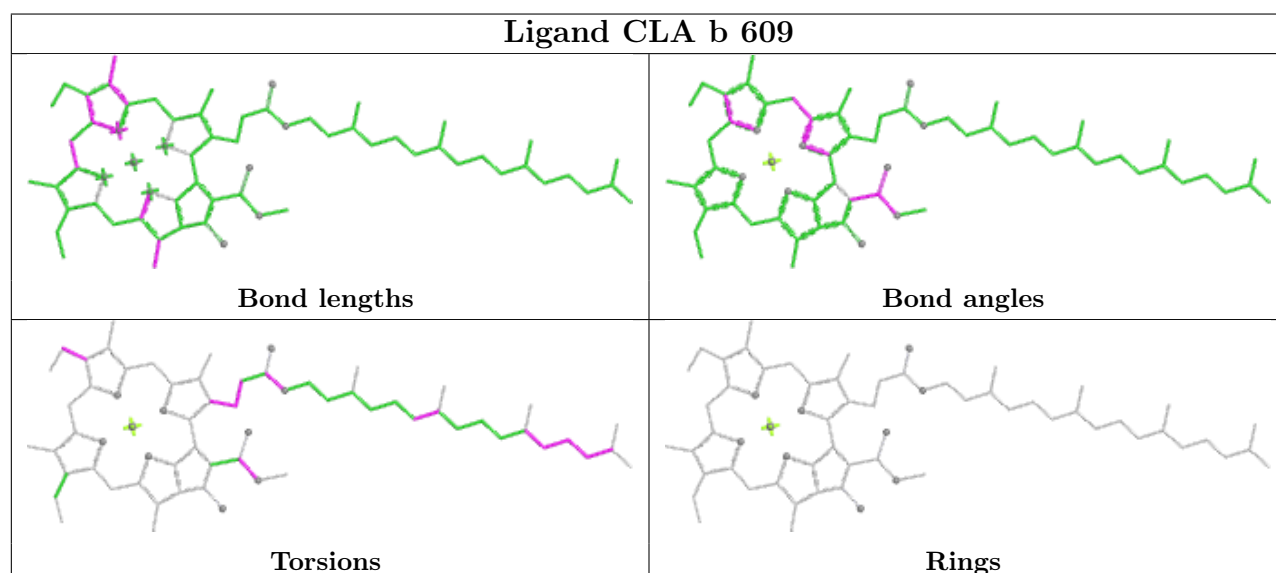
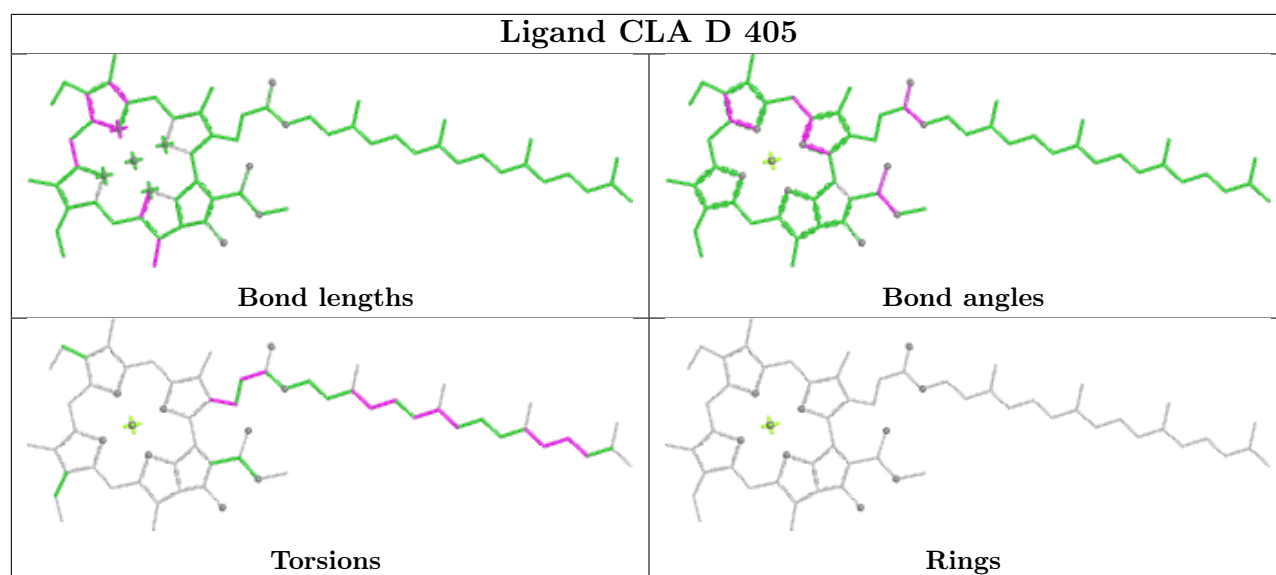
Ligand CLA B 614

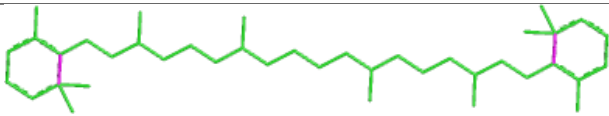
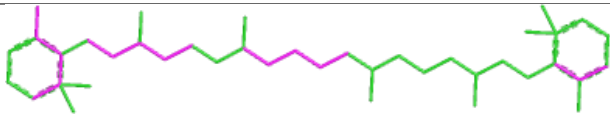
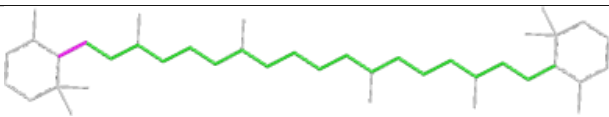
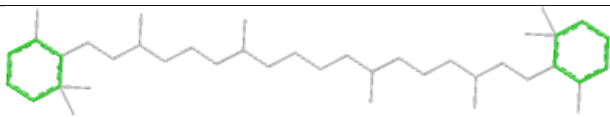


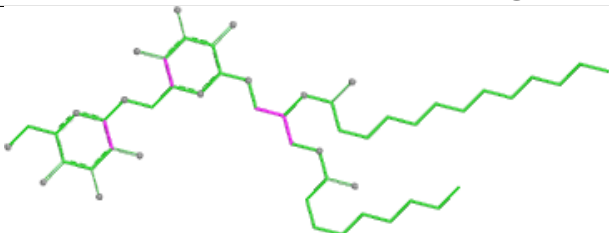
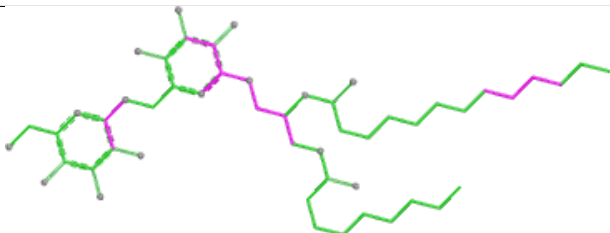
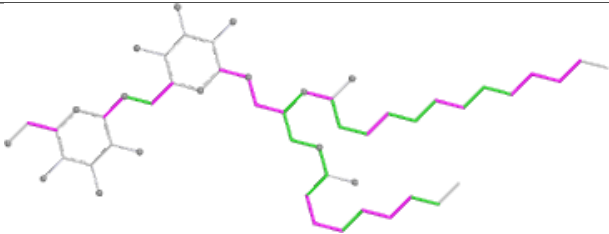
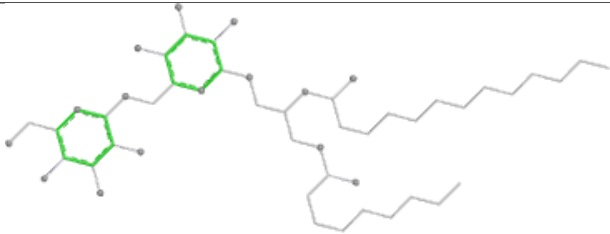
Ligand HEM F 101

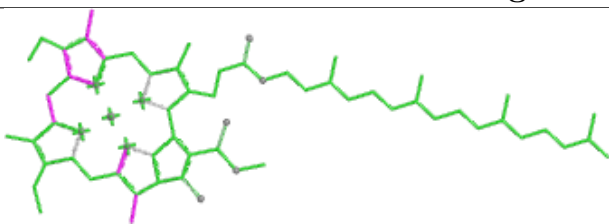
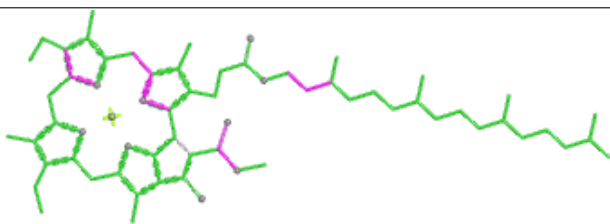
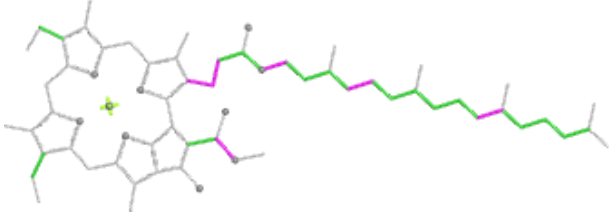
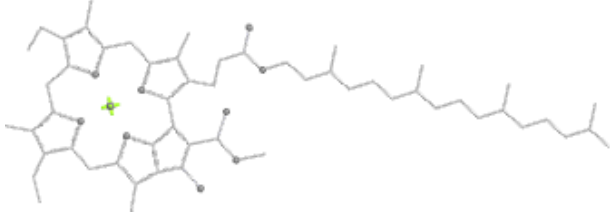


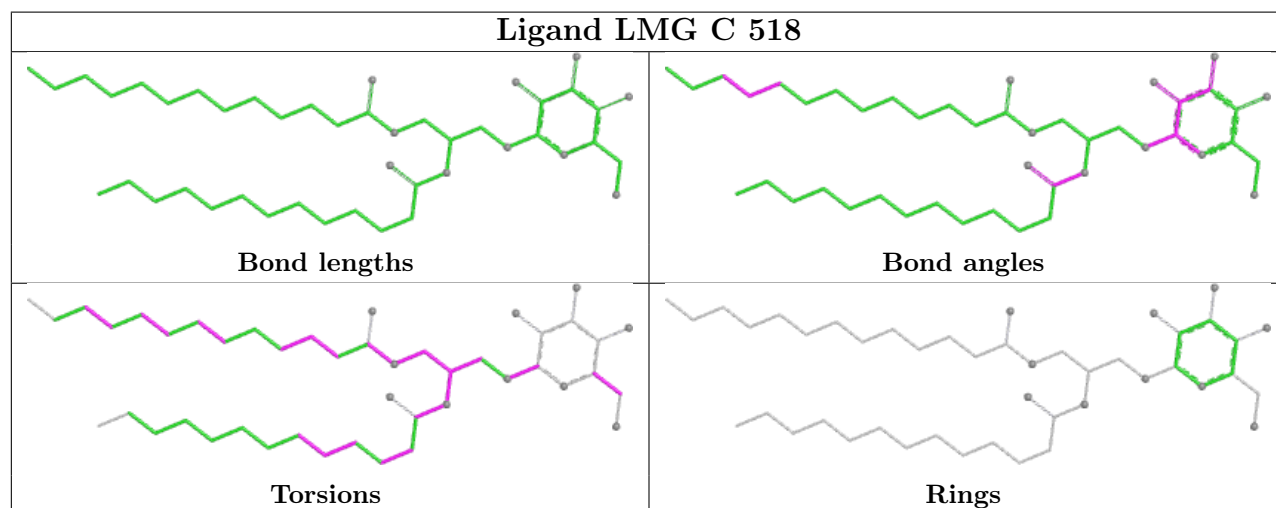
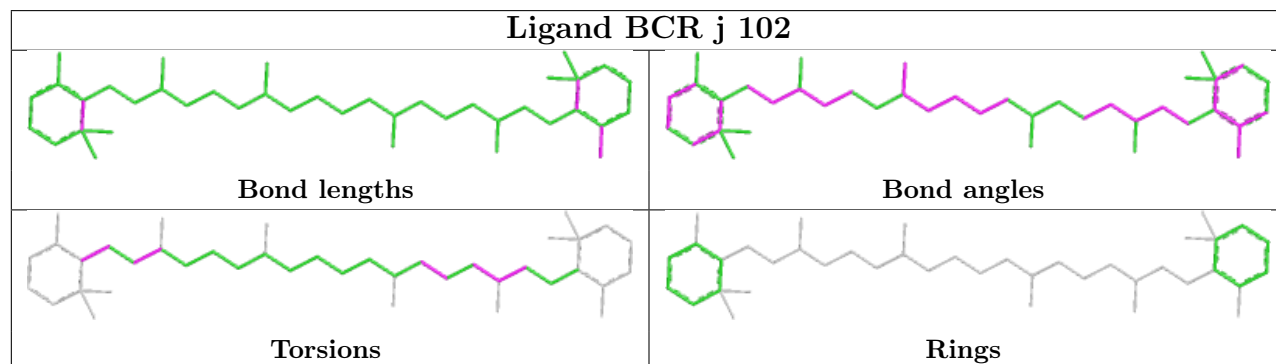
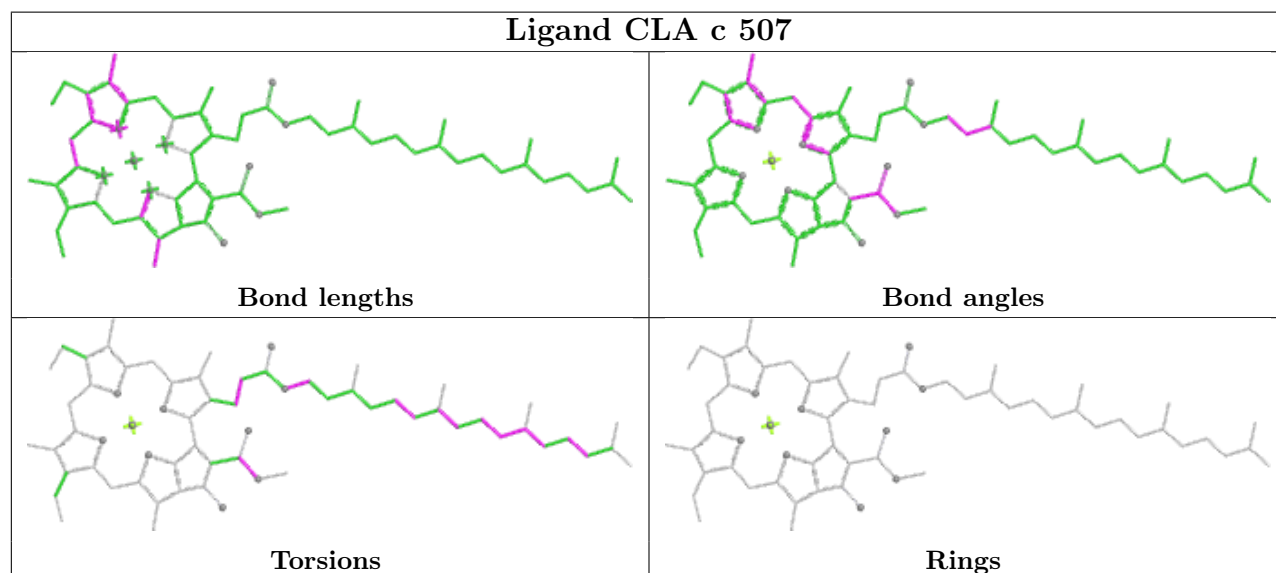
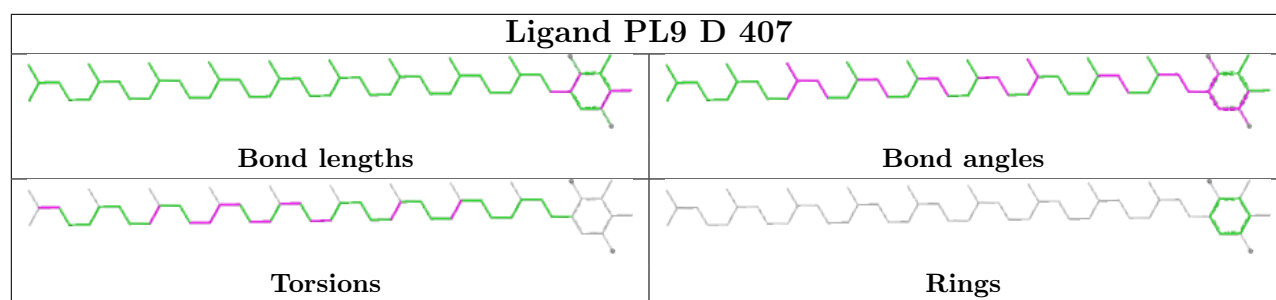




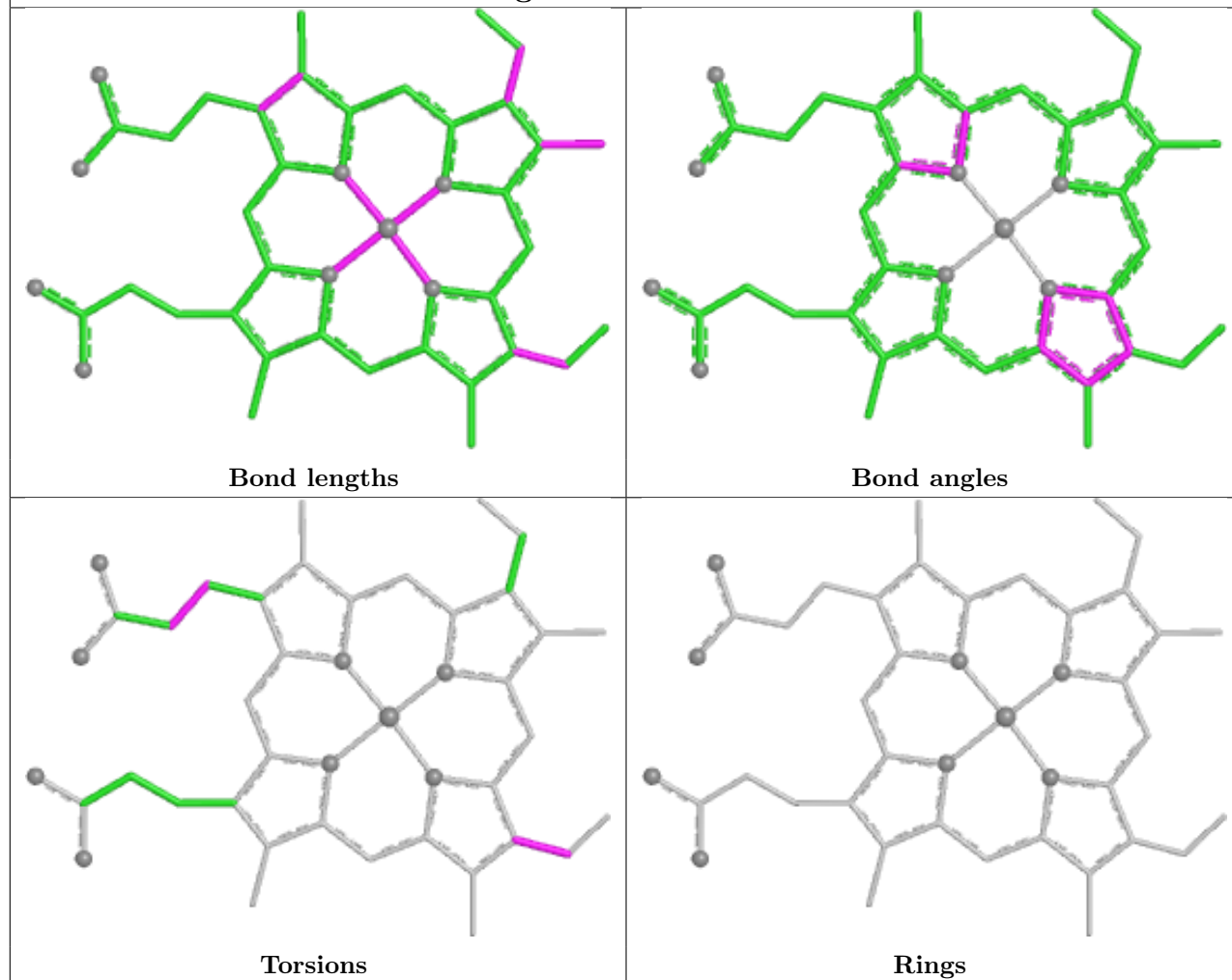
Ligand BCR B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD b 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

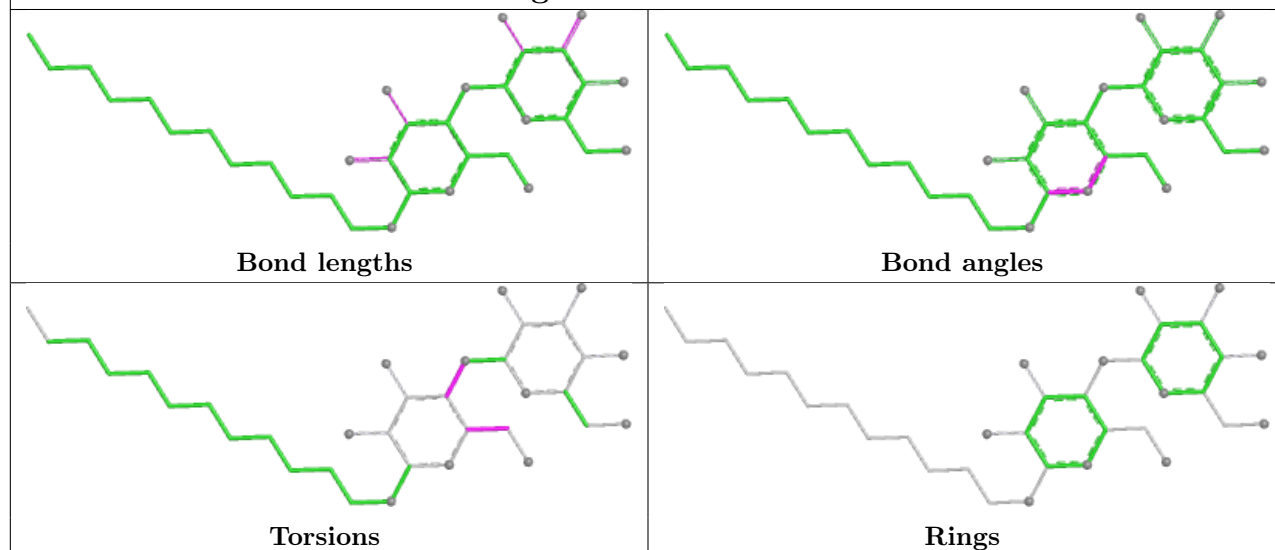
Ligand CLA A 402	
	
Bond lengths	Bond angles
	
Torsions	Rings



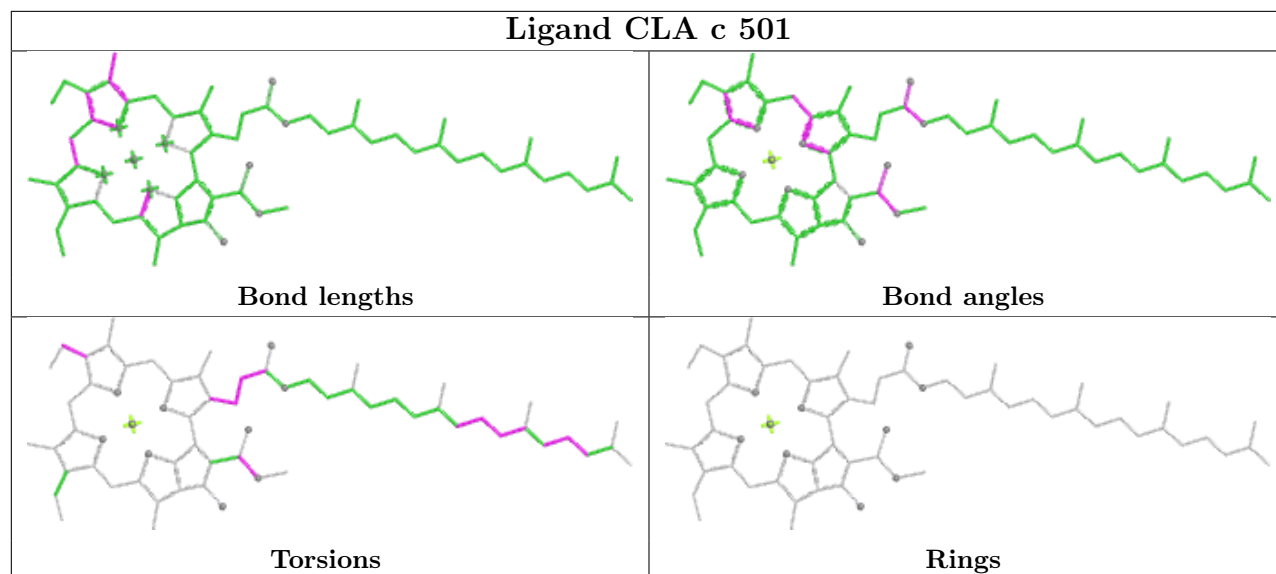
Ligand HEM f 101



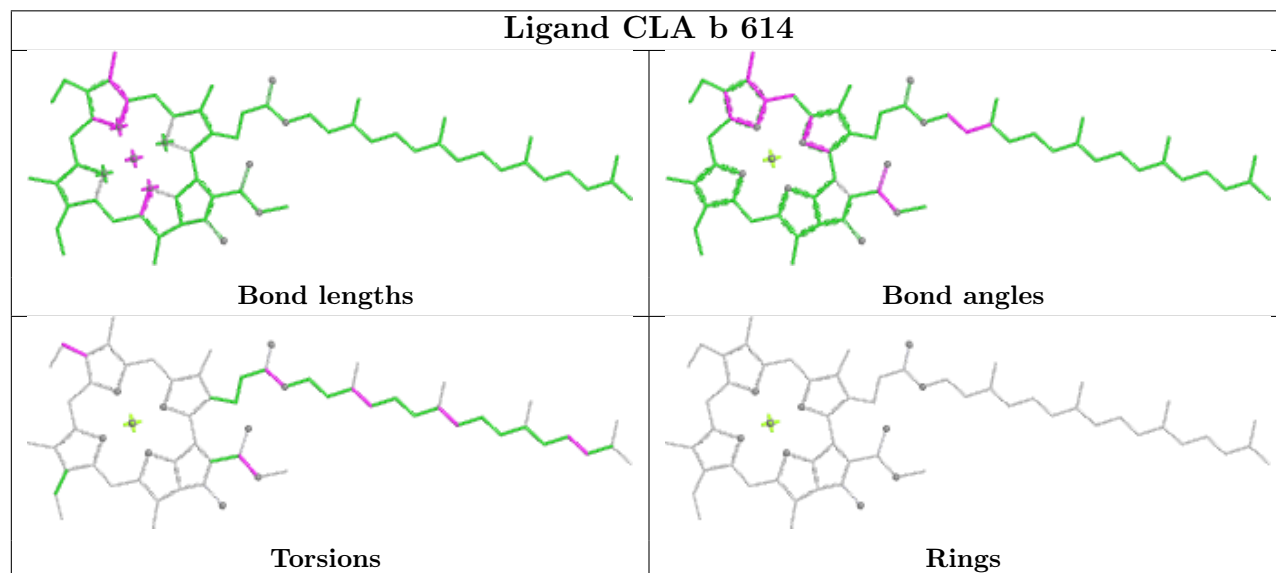
Ligand LMT b 603



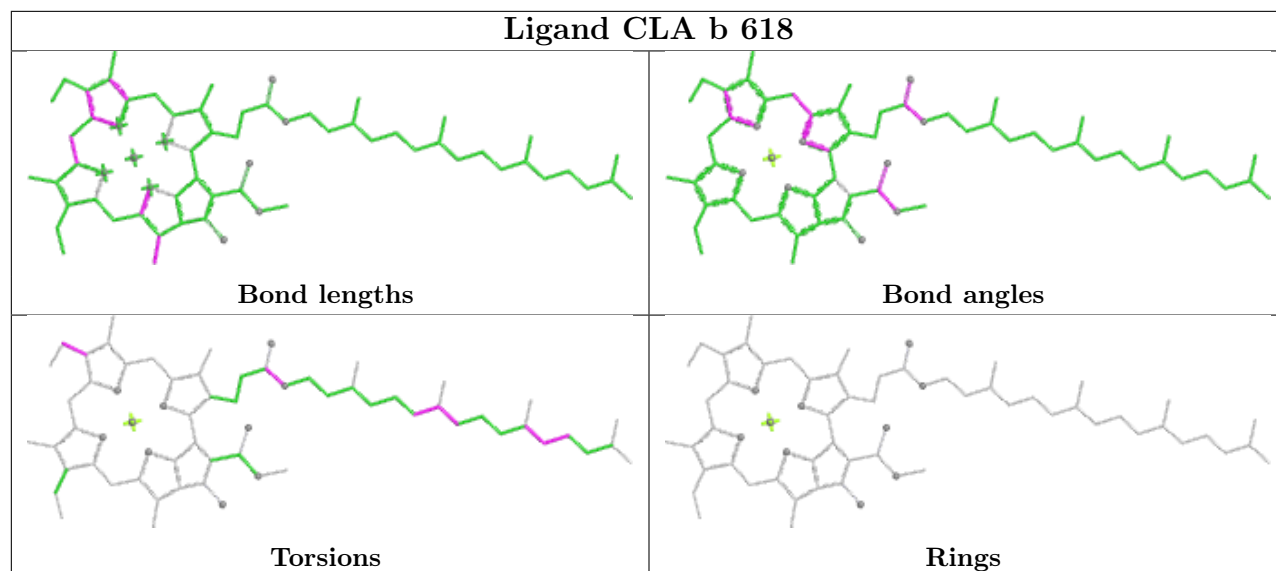
Ligand CLA c 501



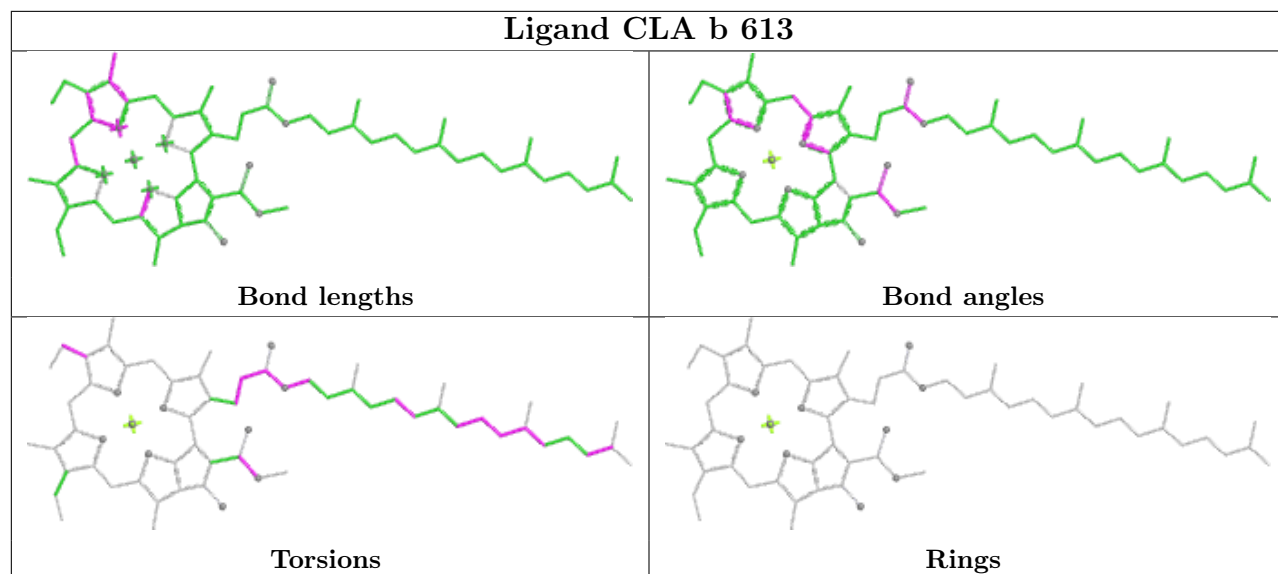
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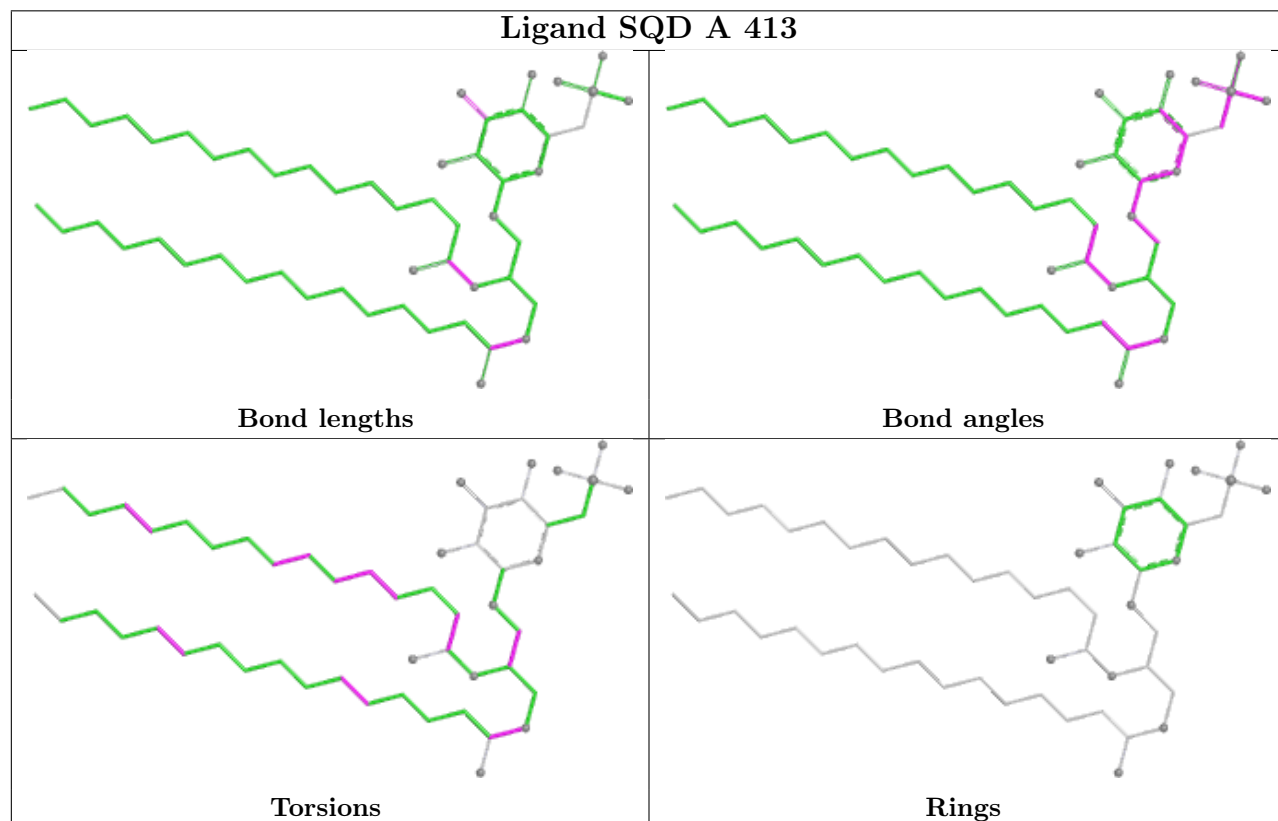
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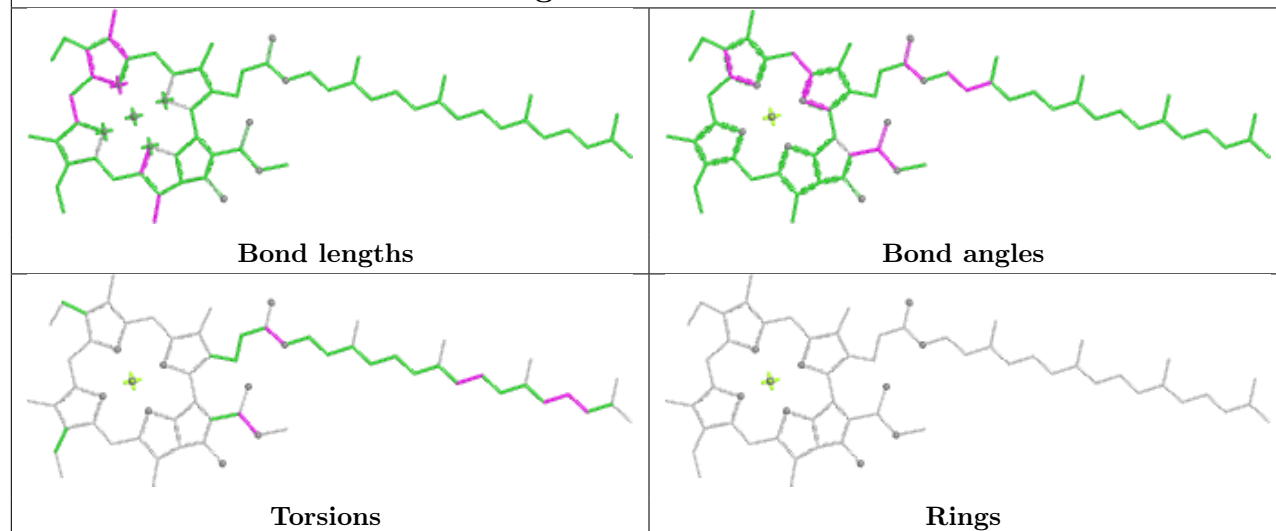
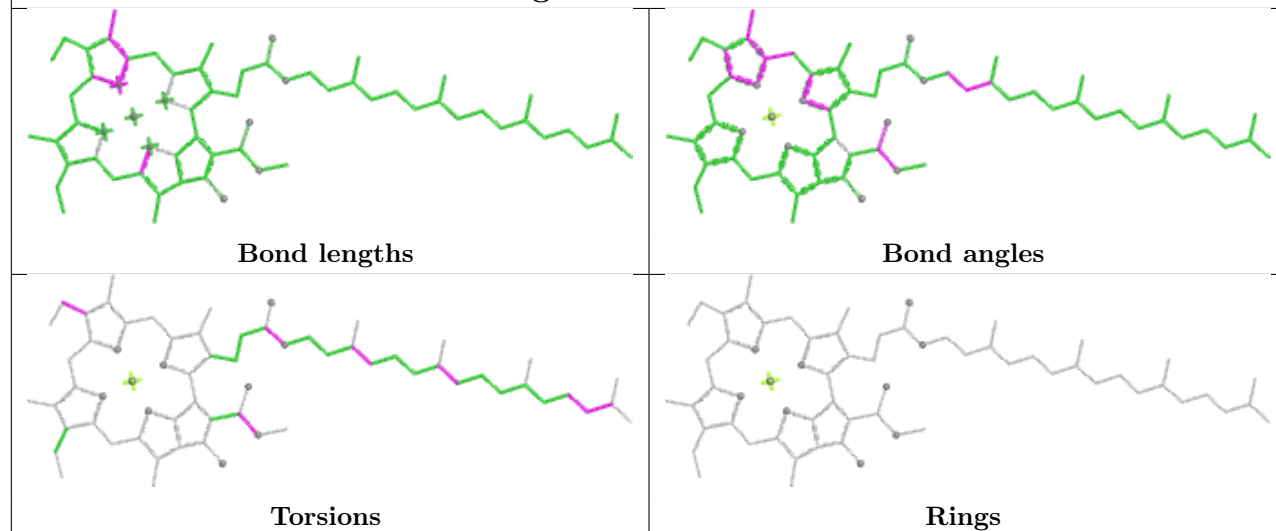


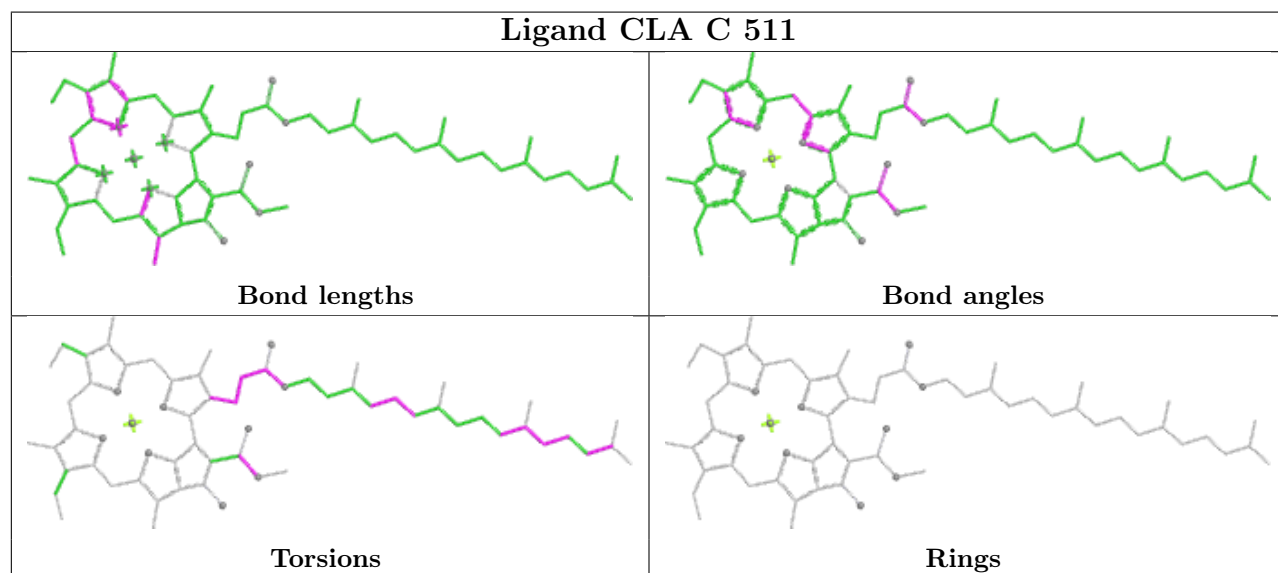
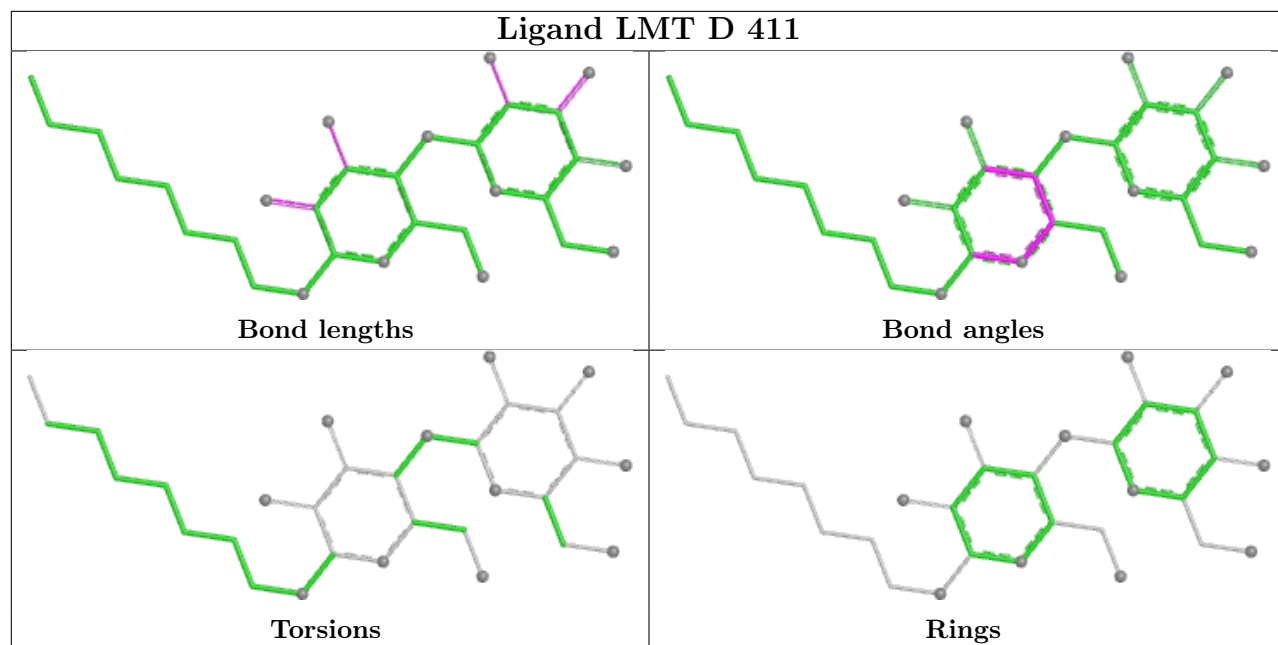
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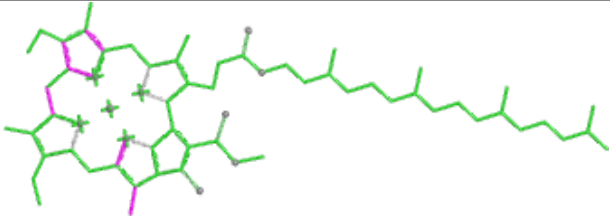
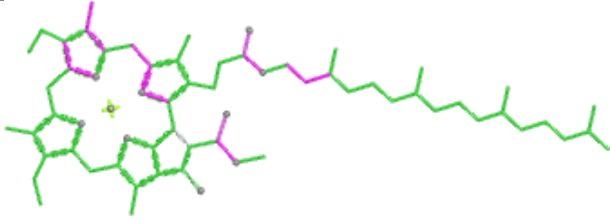
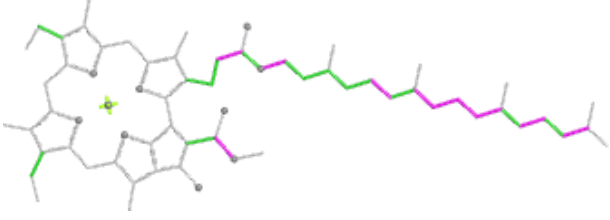
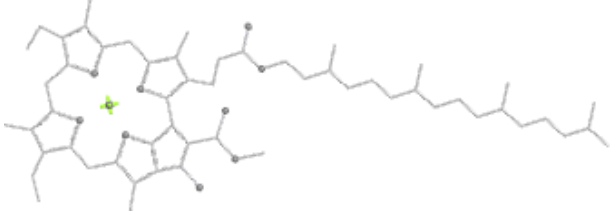
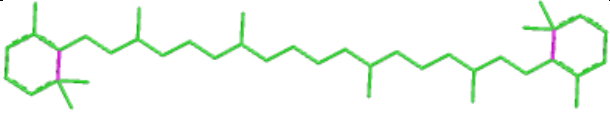
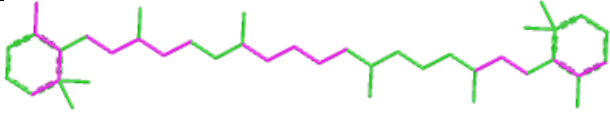
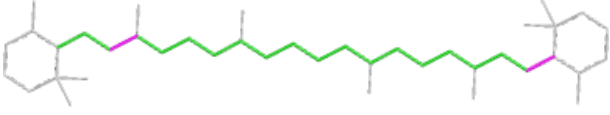
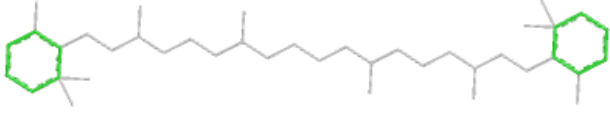
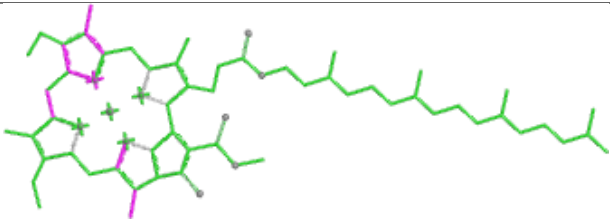
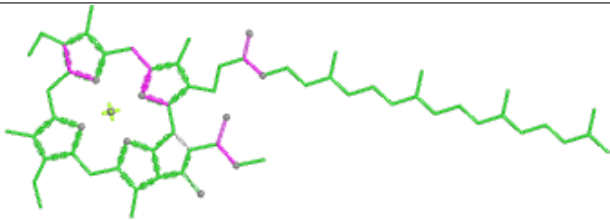
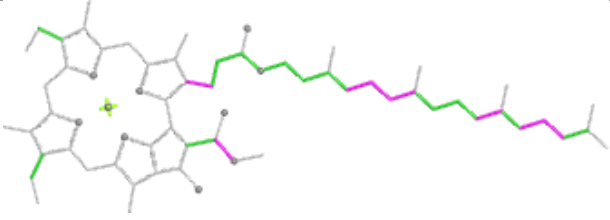
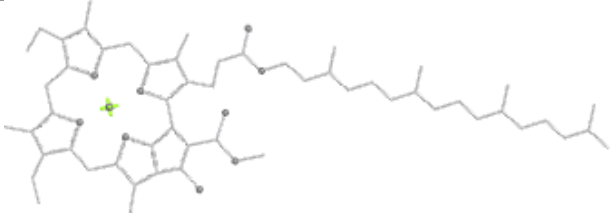


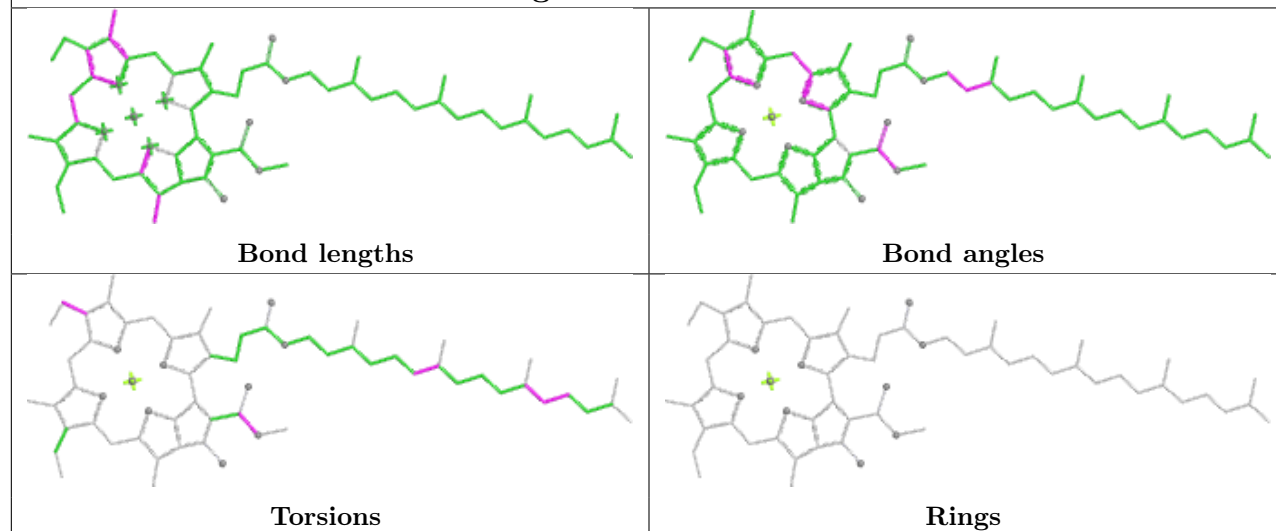
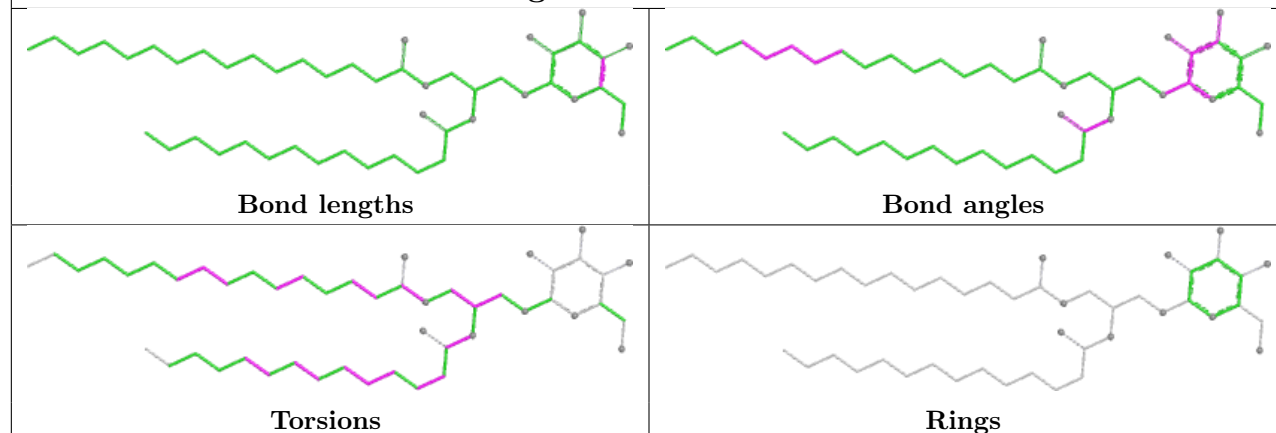
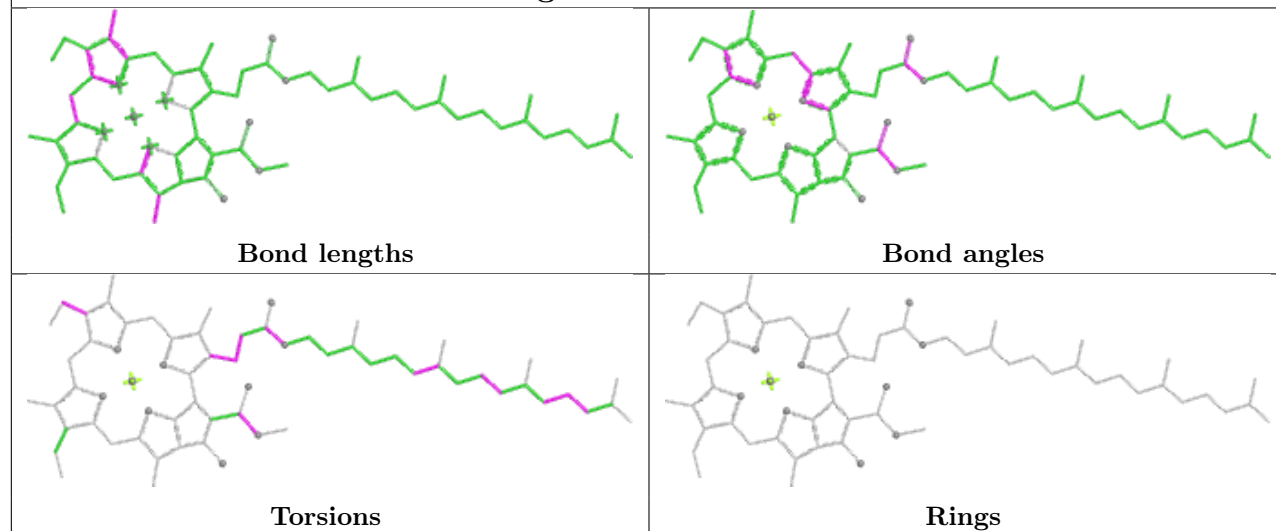
Ligand SQD A 413

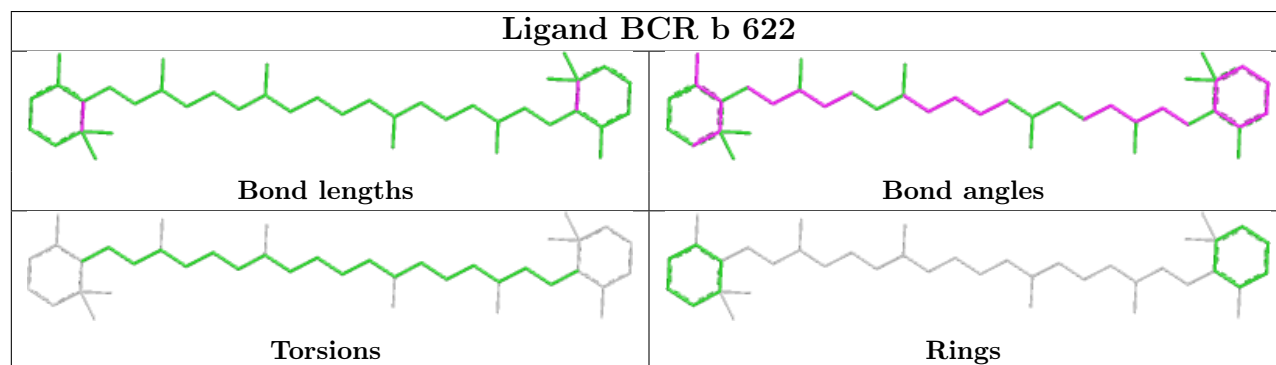
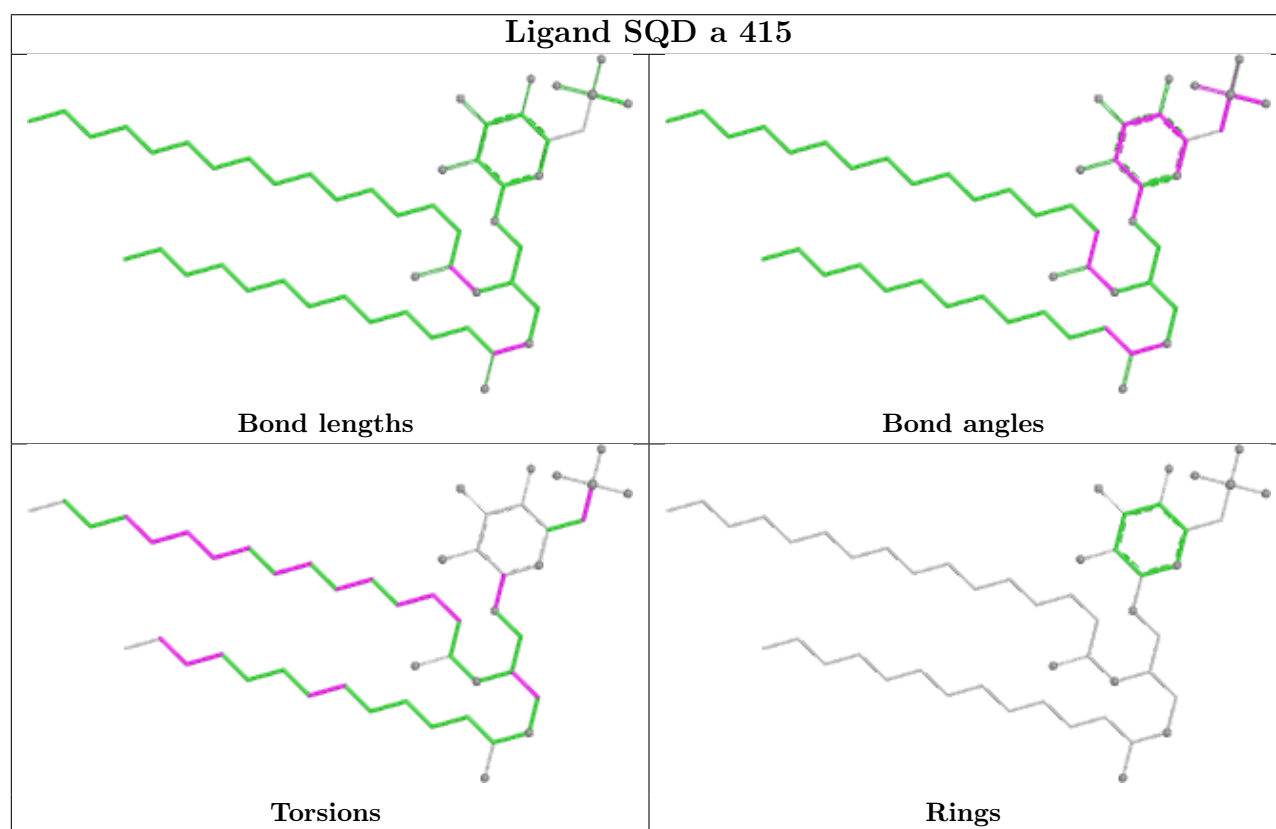
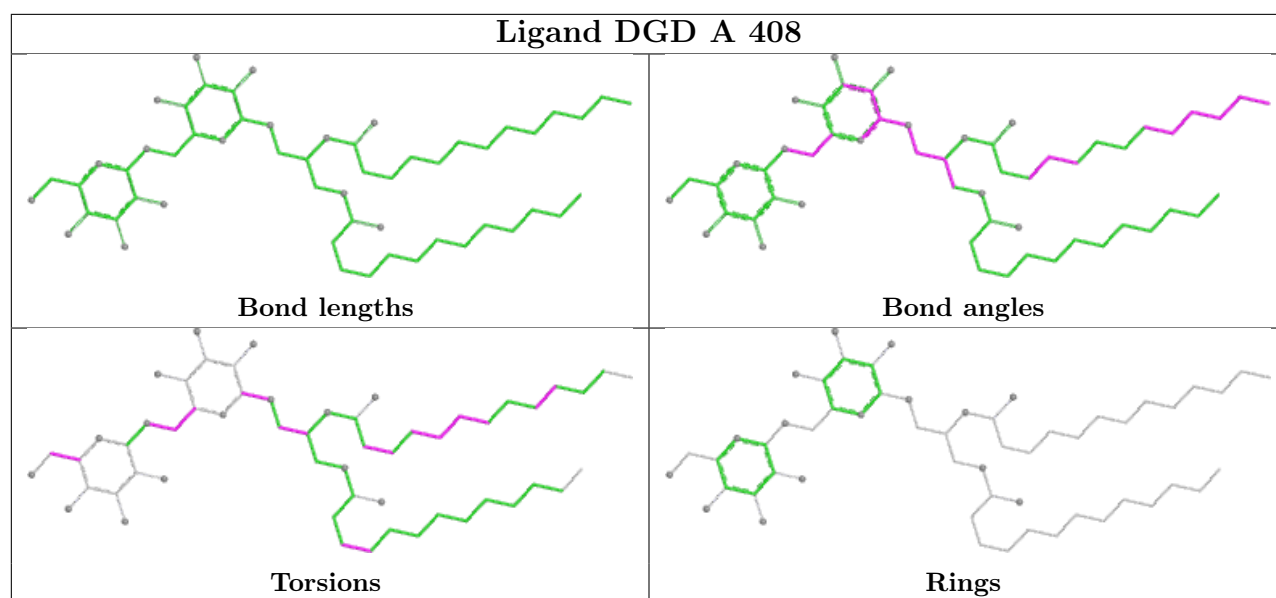


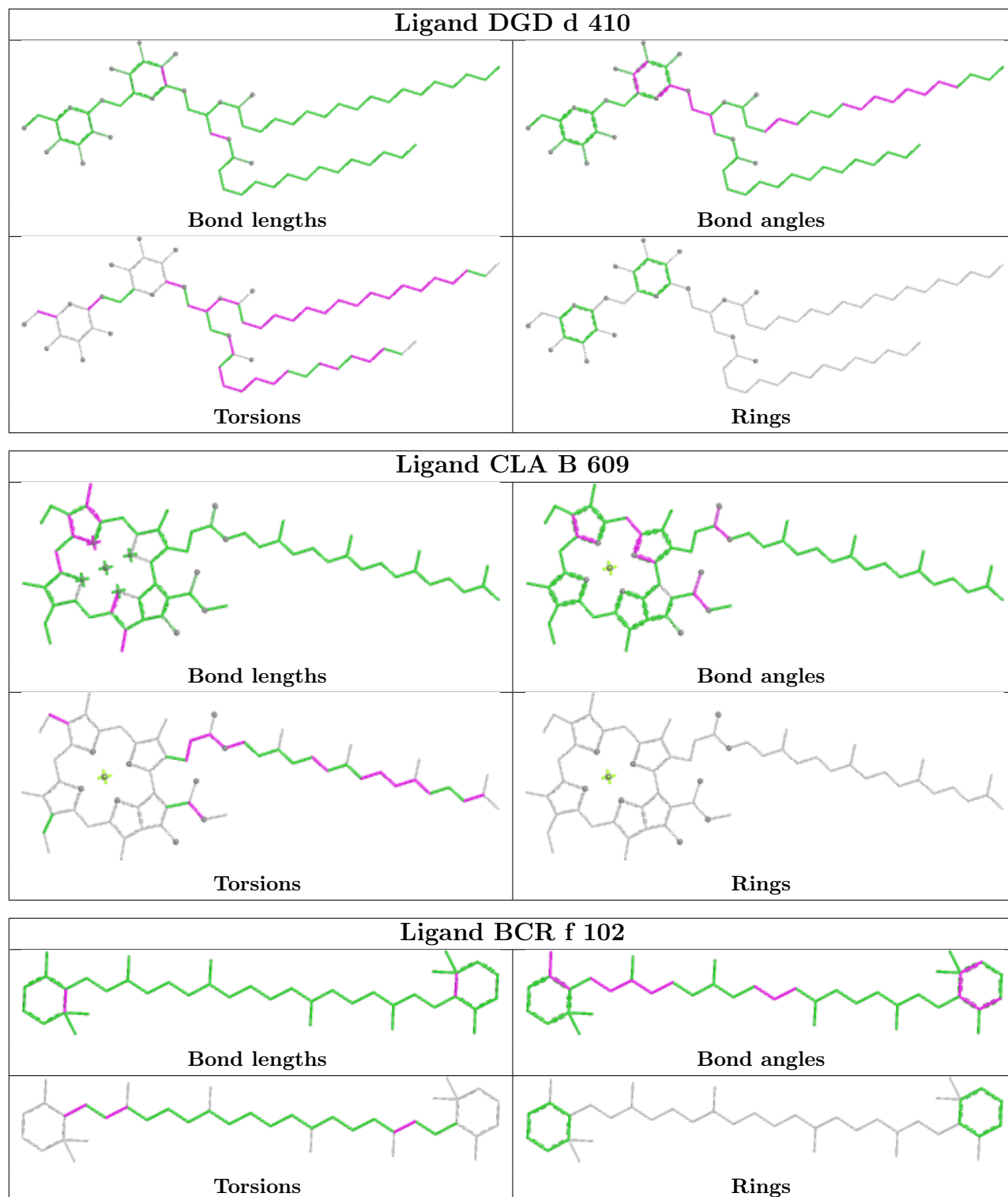
Ligand CLA b 607**Ligand CLA B 610**

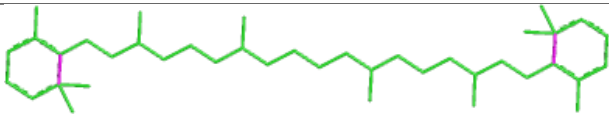
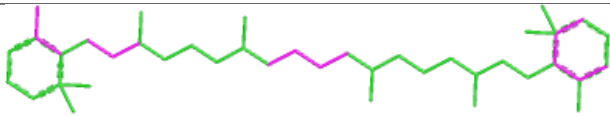
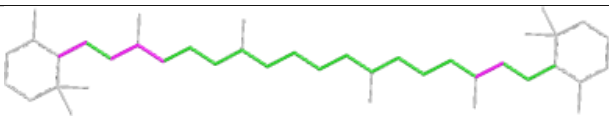
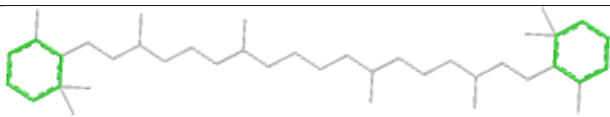


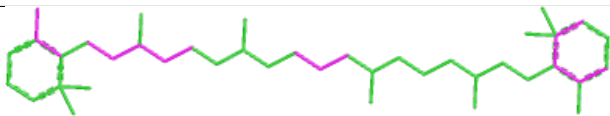
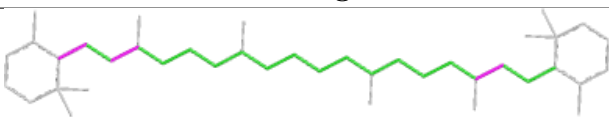
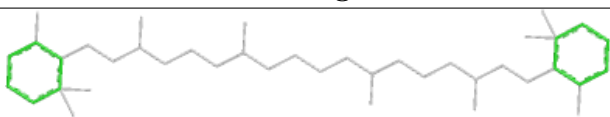
Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

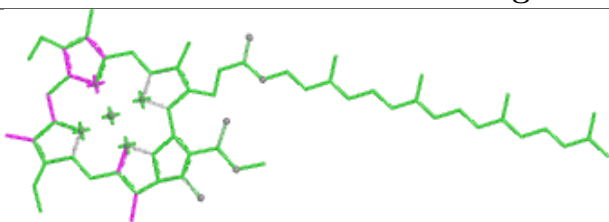
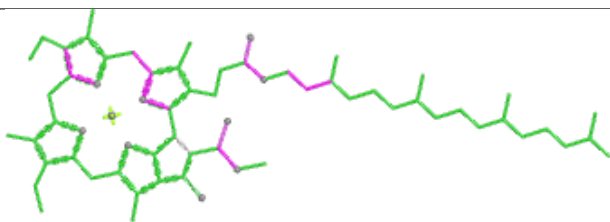
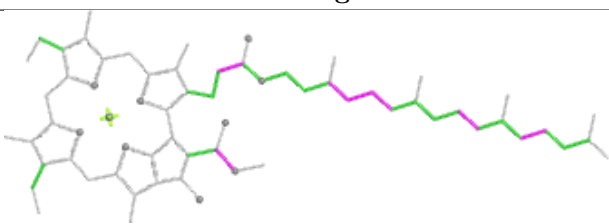
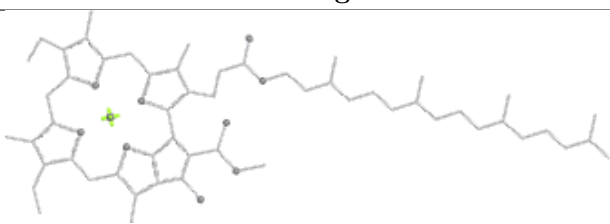
Ligand CLA B 608**Ligand LMG B 621****Ligand CLA c 520**

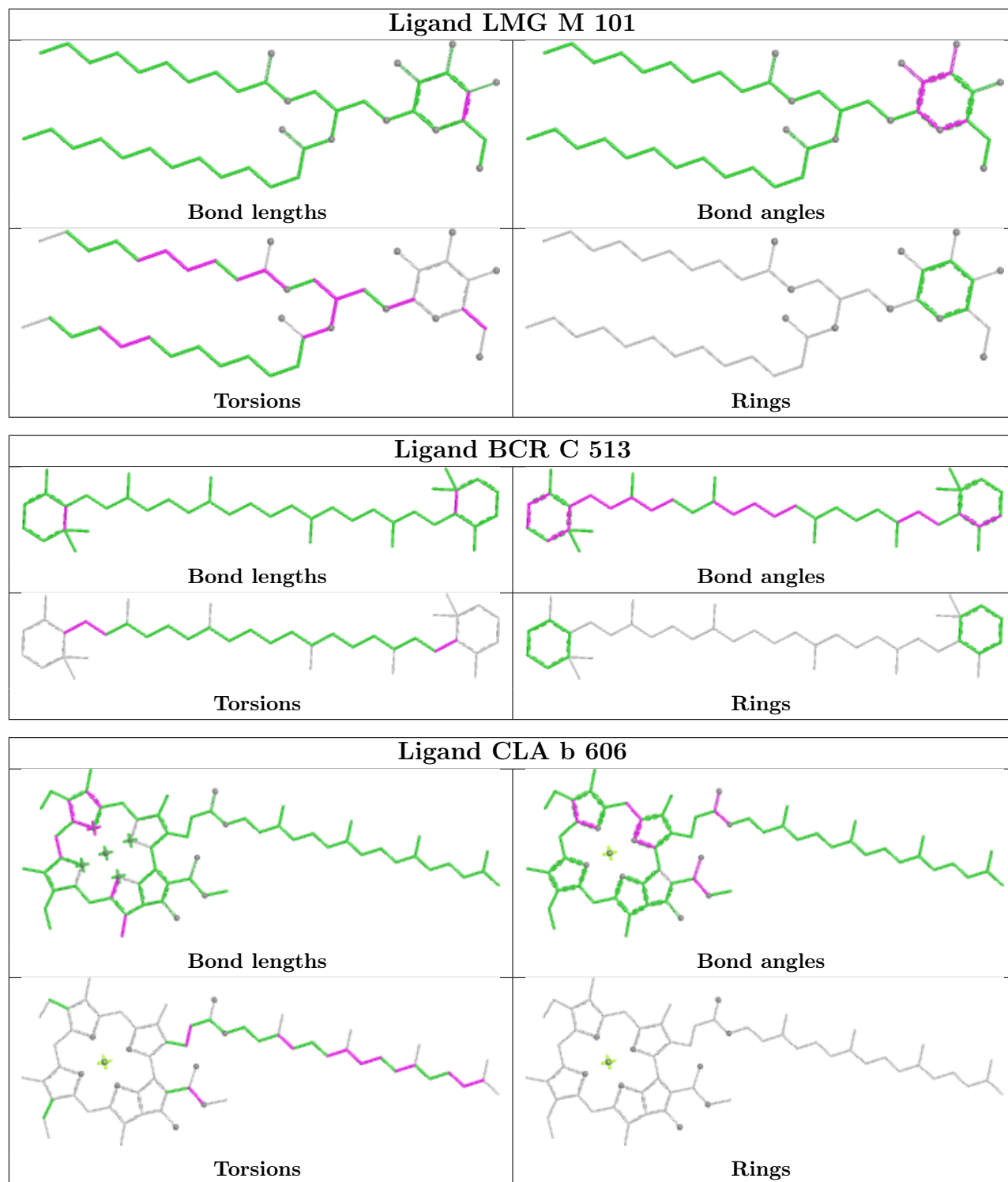


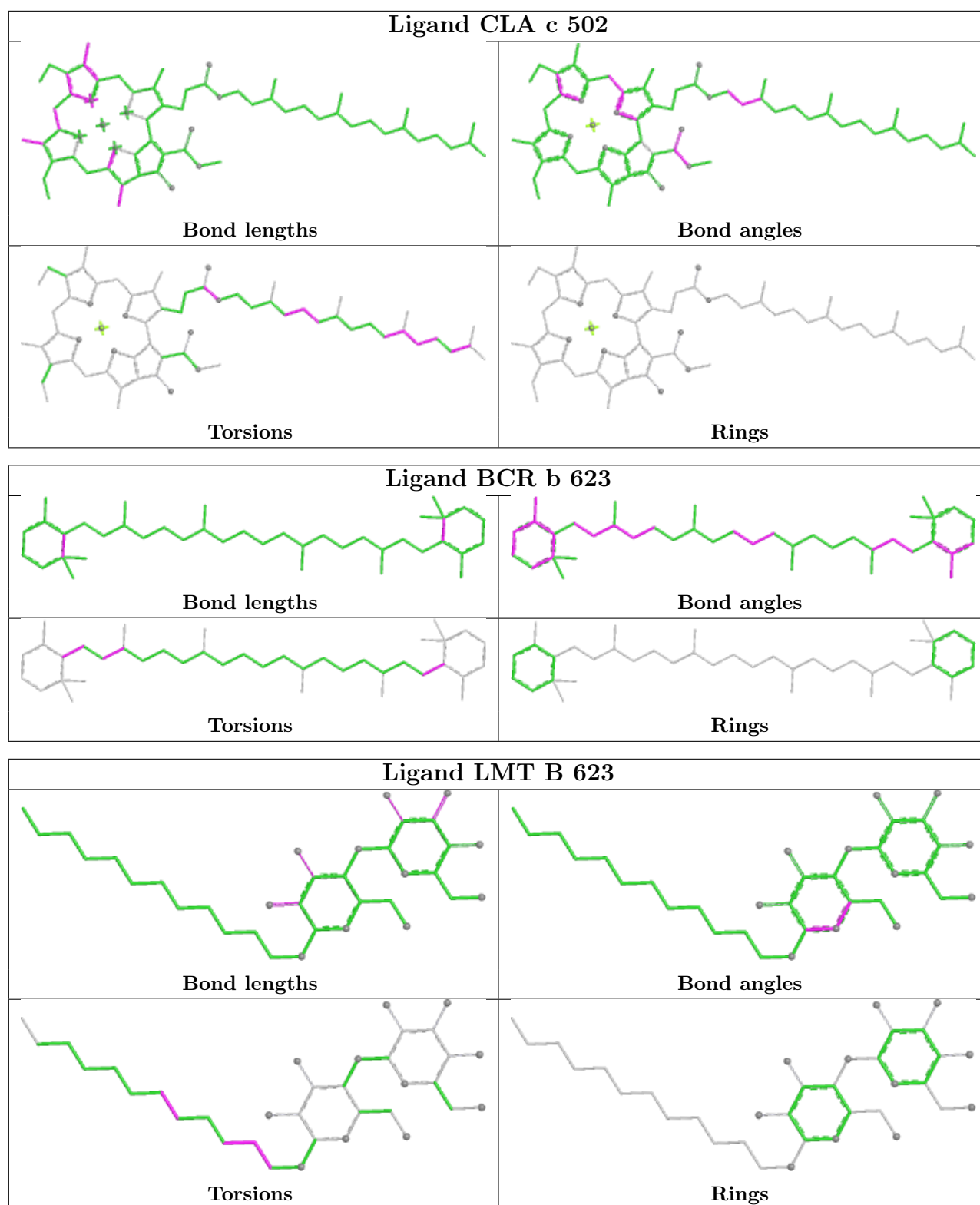


Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

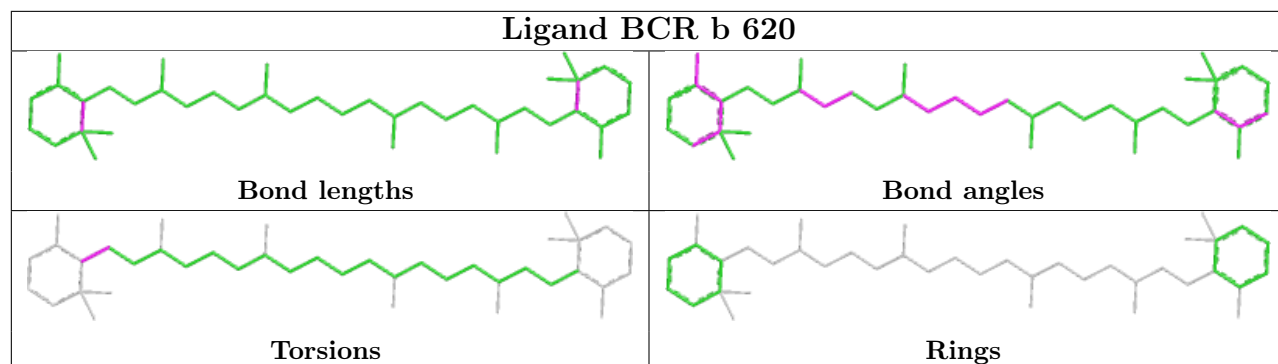
Ligand BCR F 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

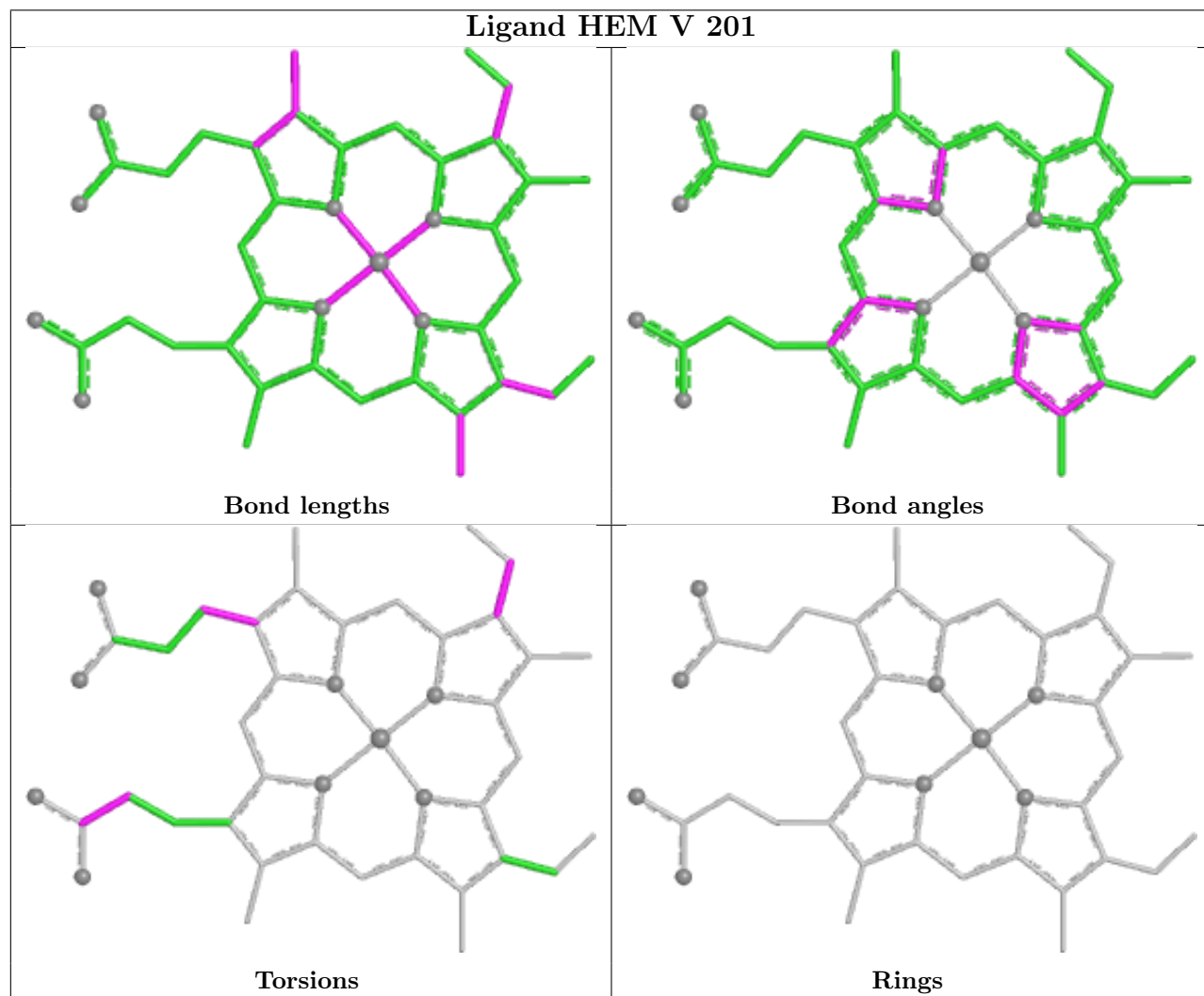


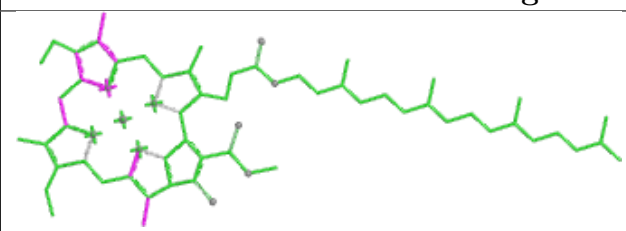
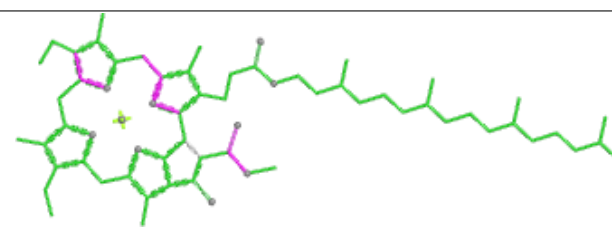
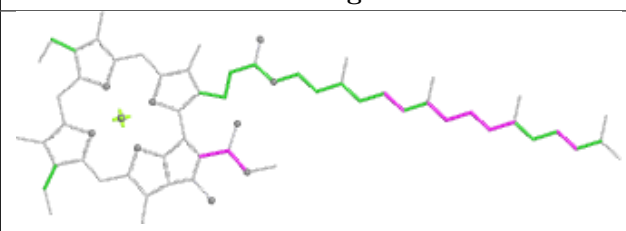
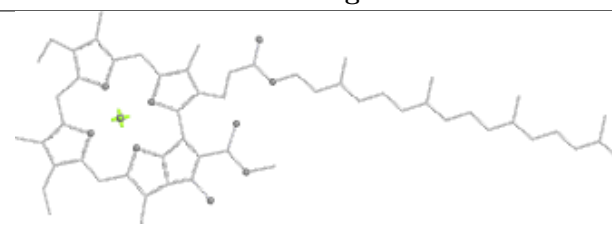


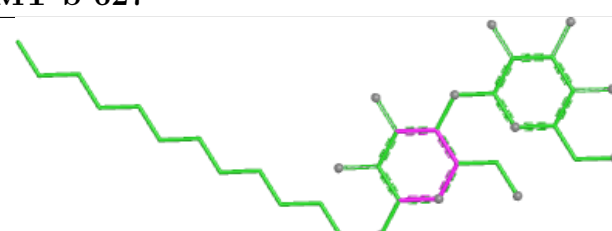
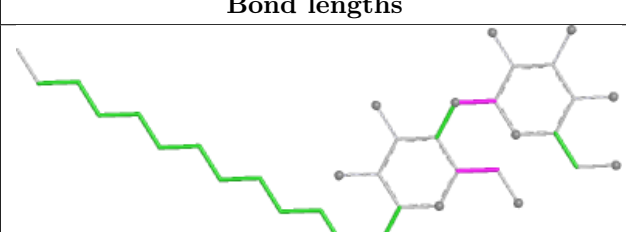
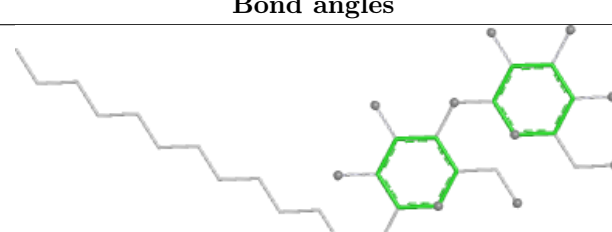
Ligand BCR b 620

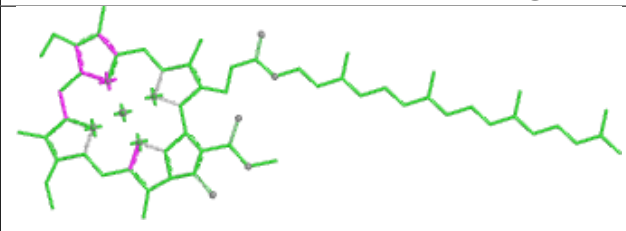
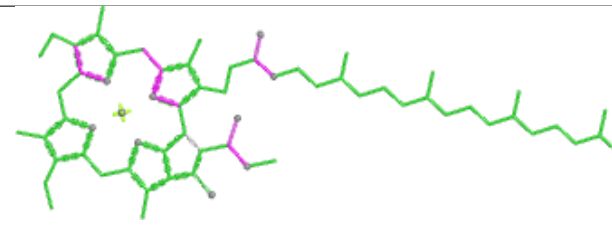
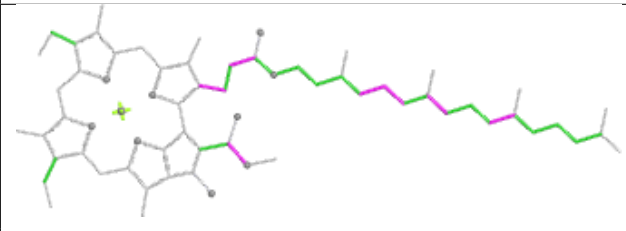
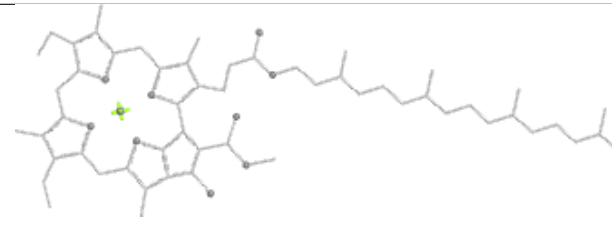


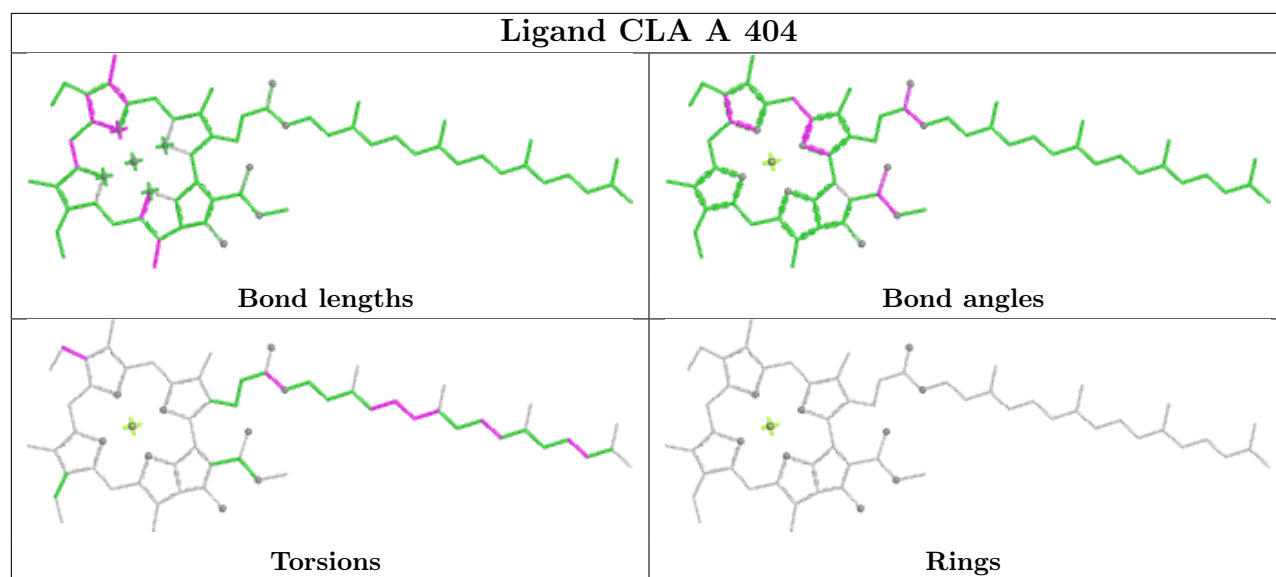
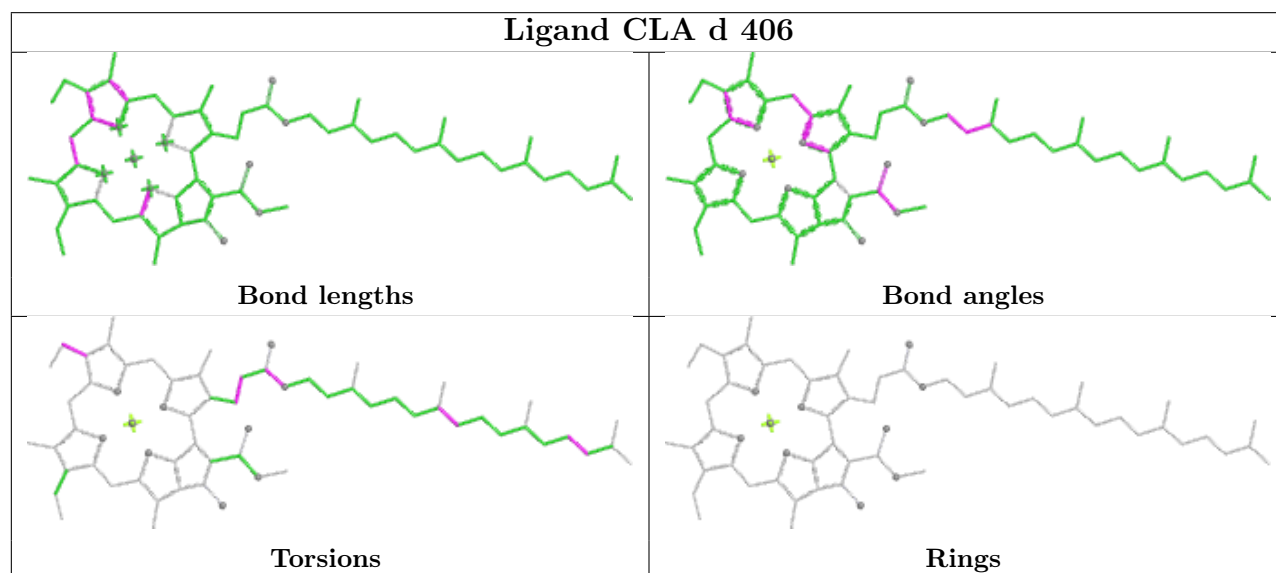
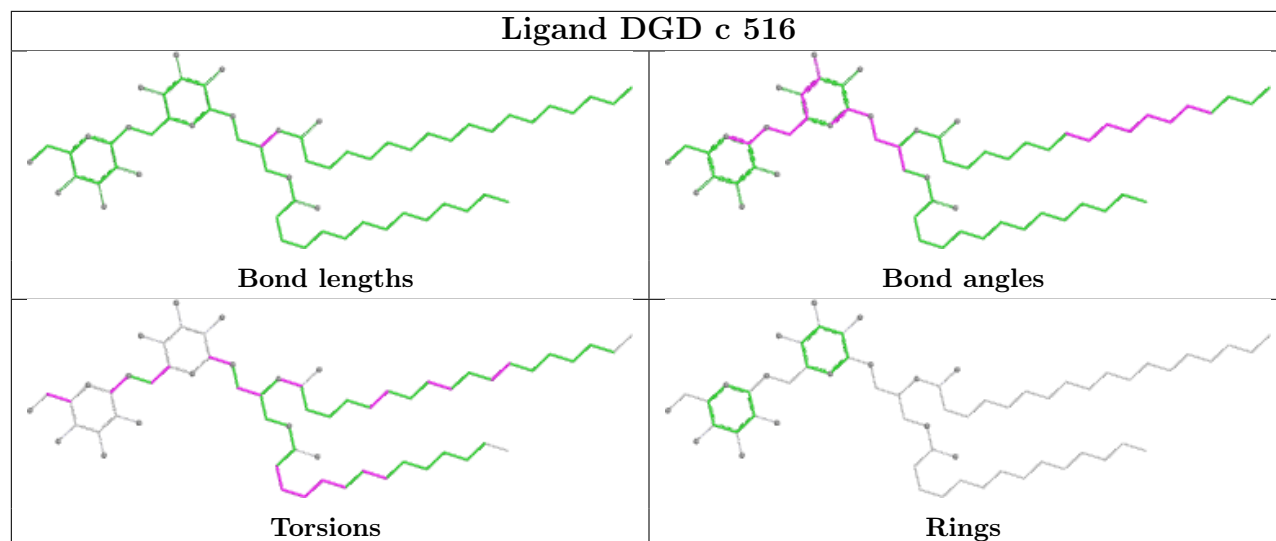
Ligand HEM V 201

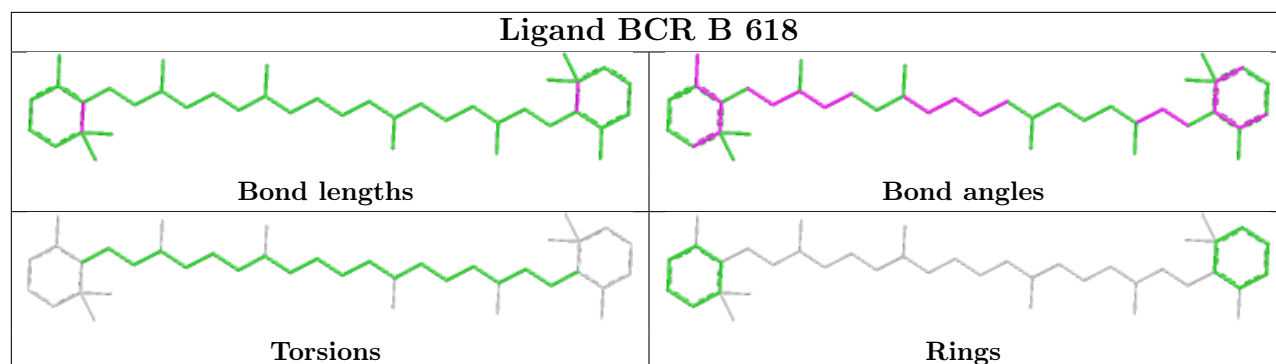
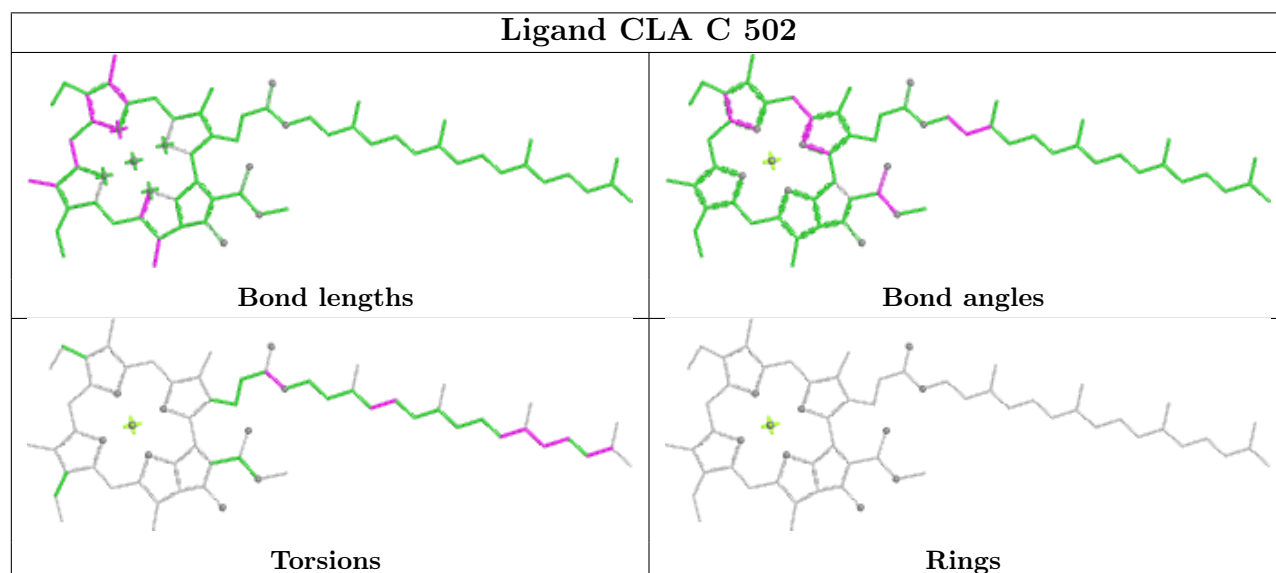
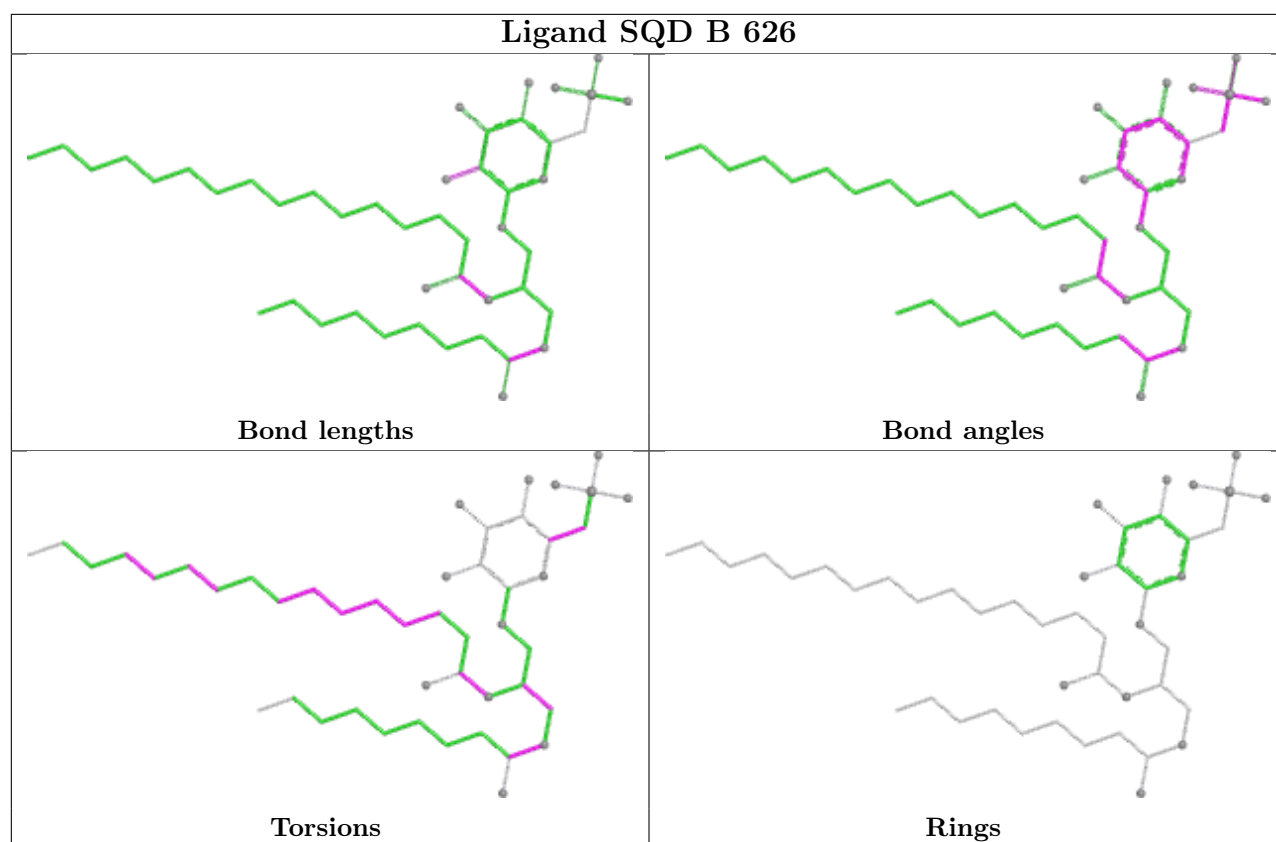


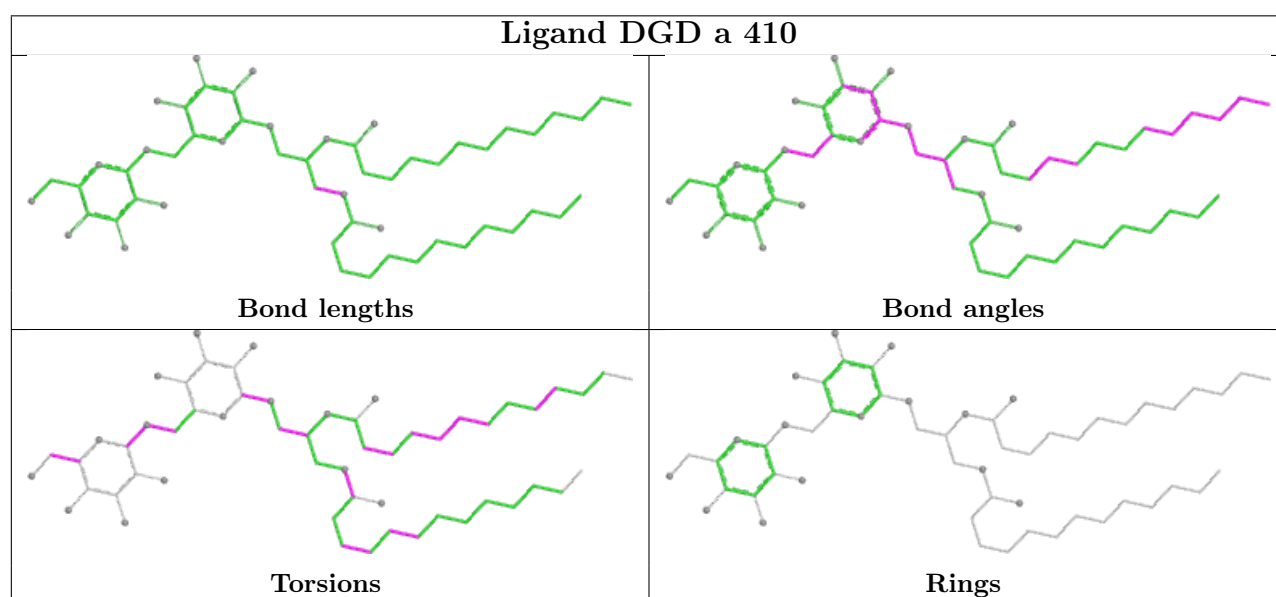
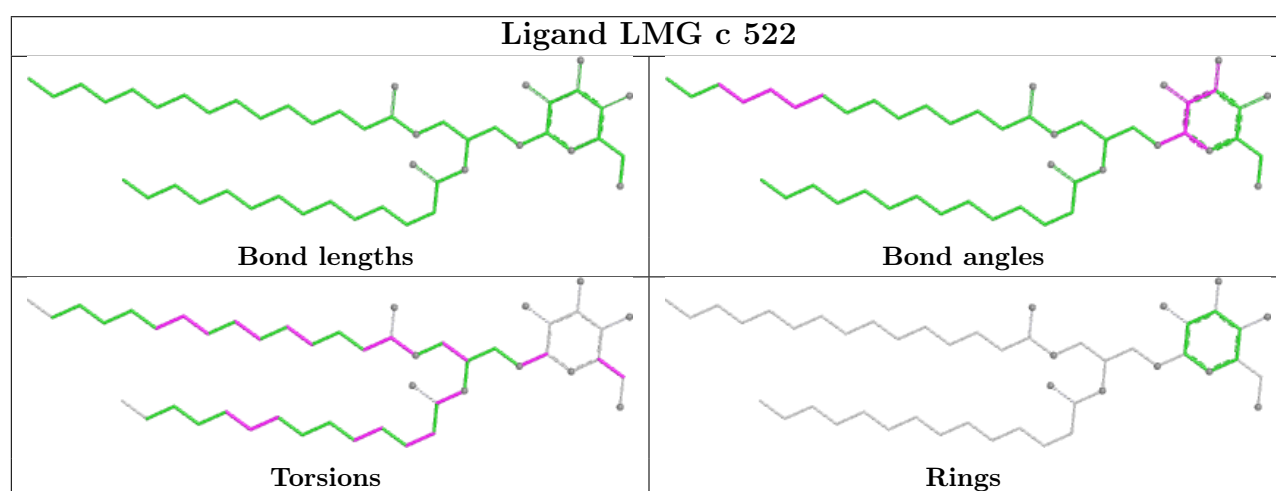
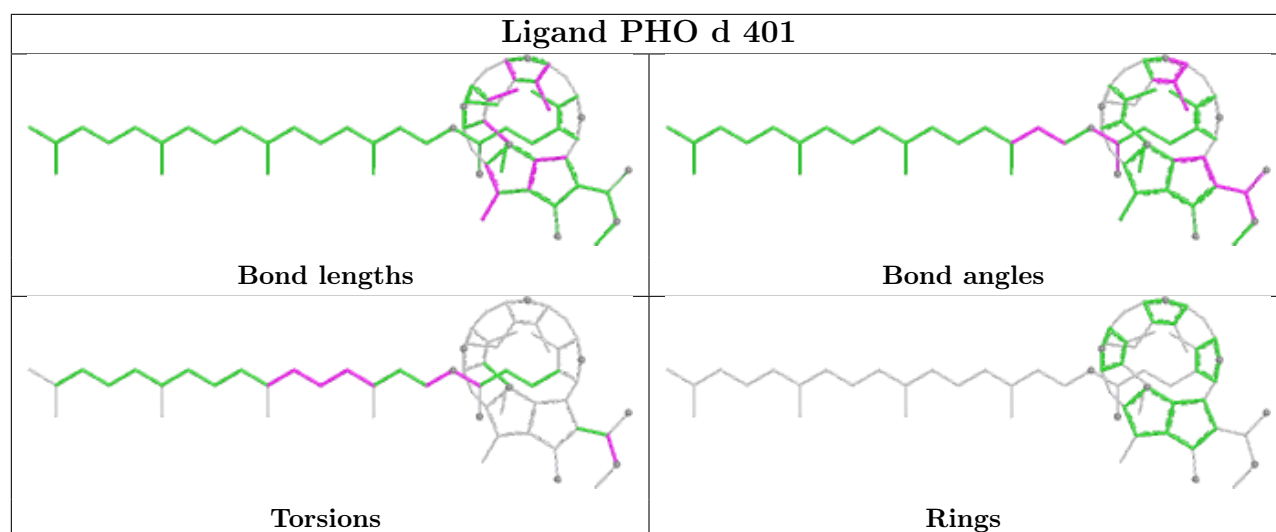
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

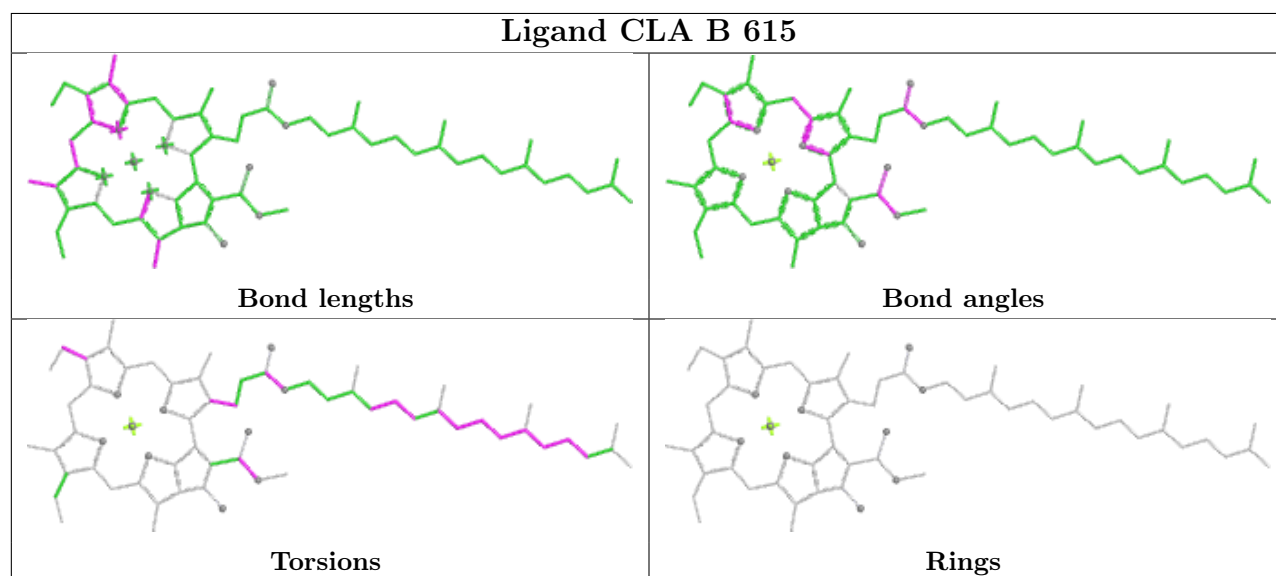
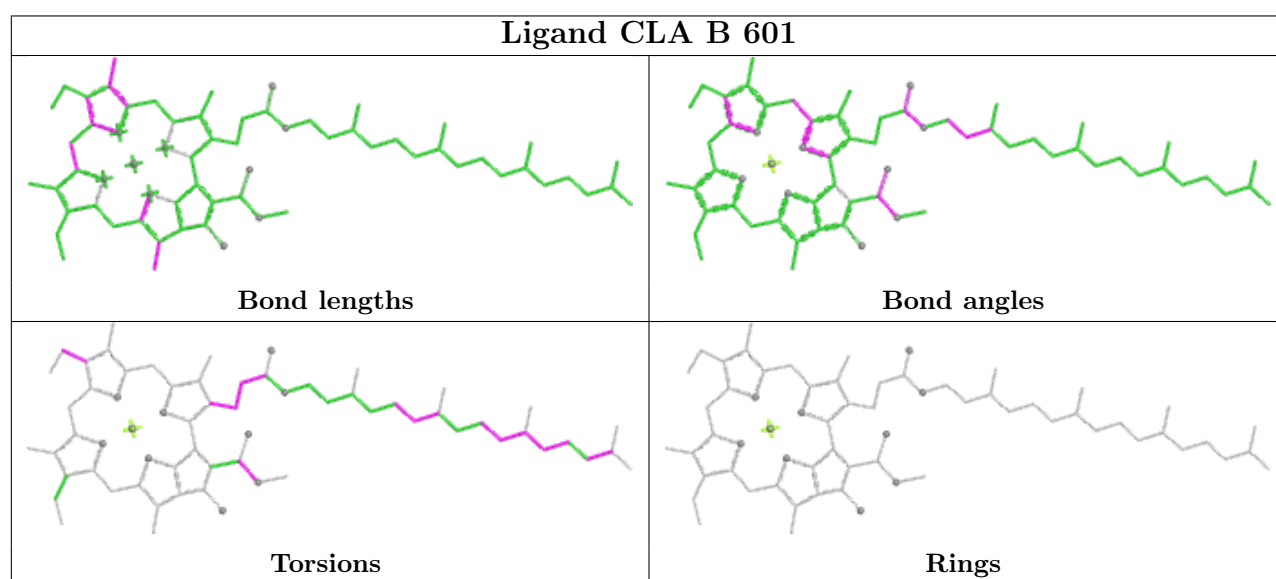
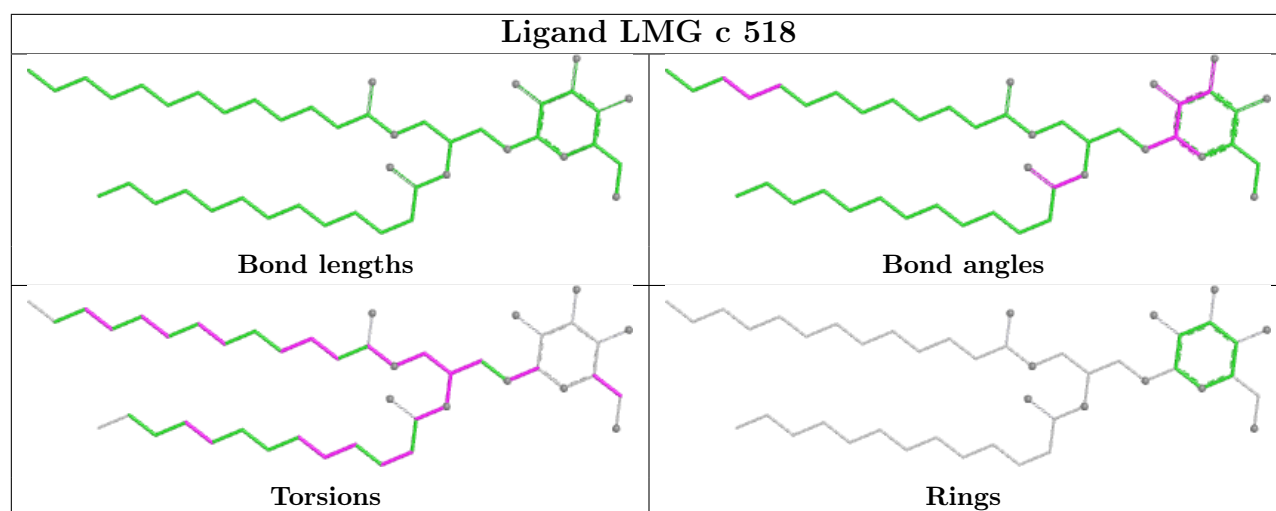
Ligand LMT b 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

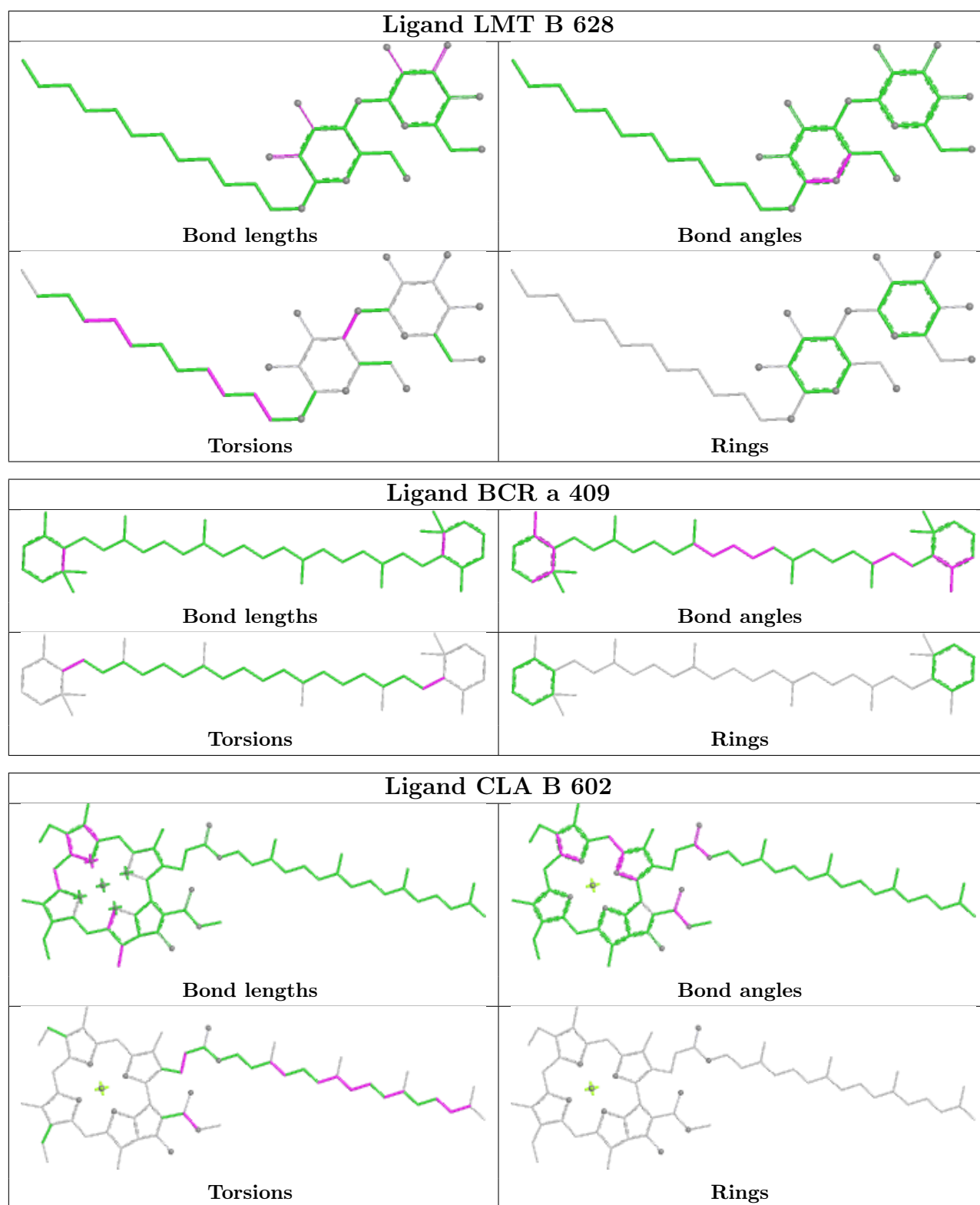
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

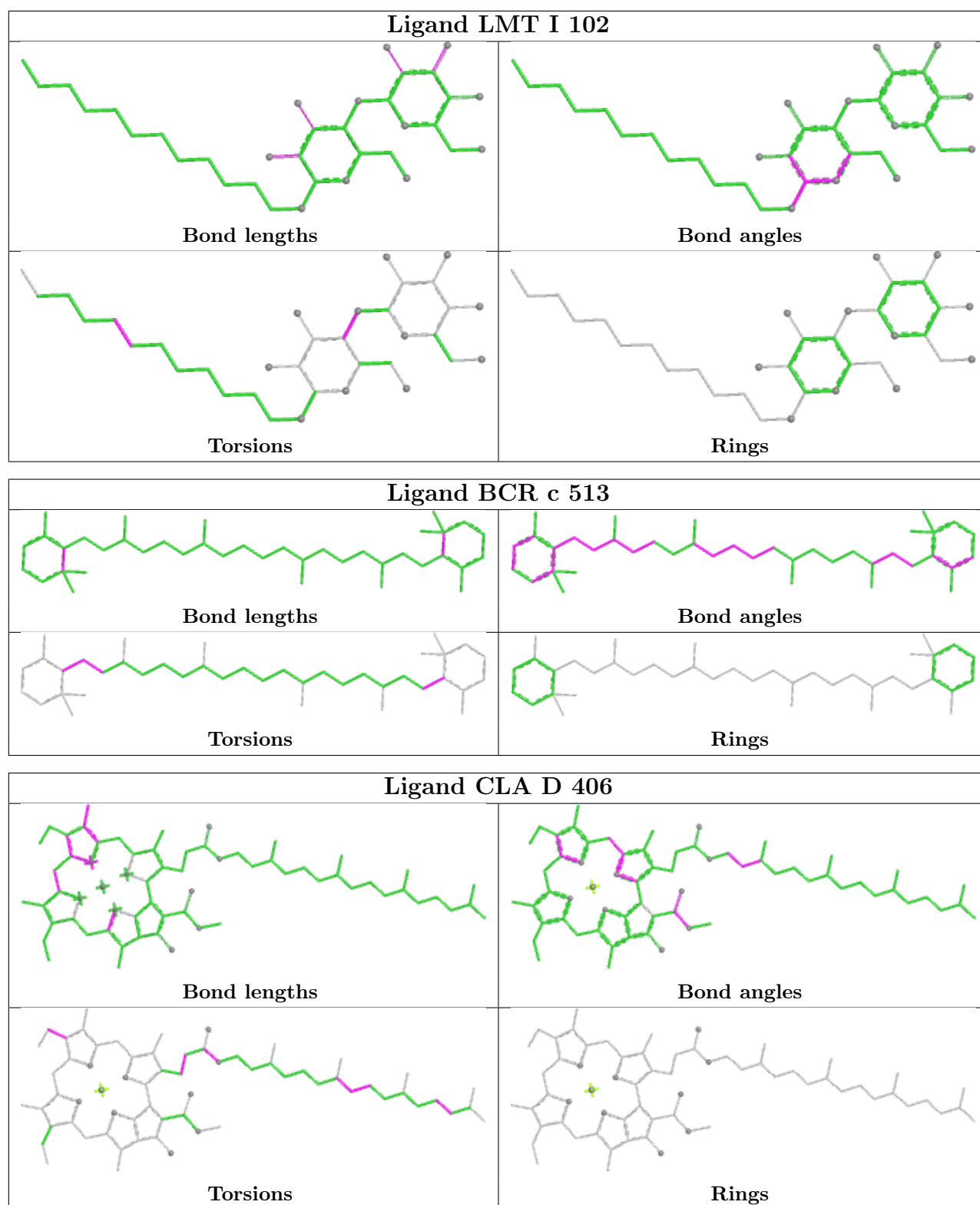


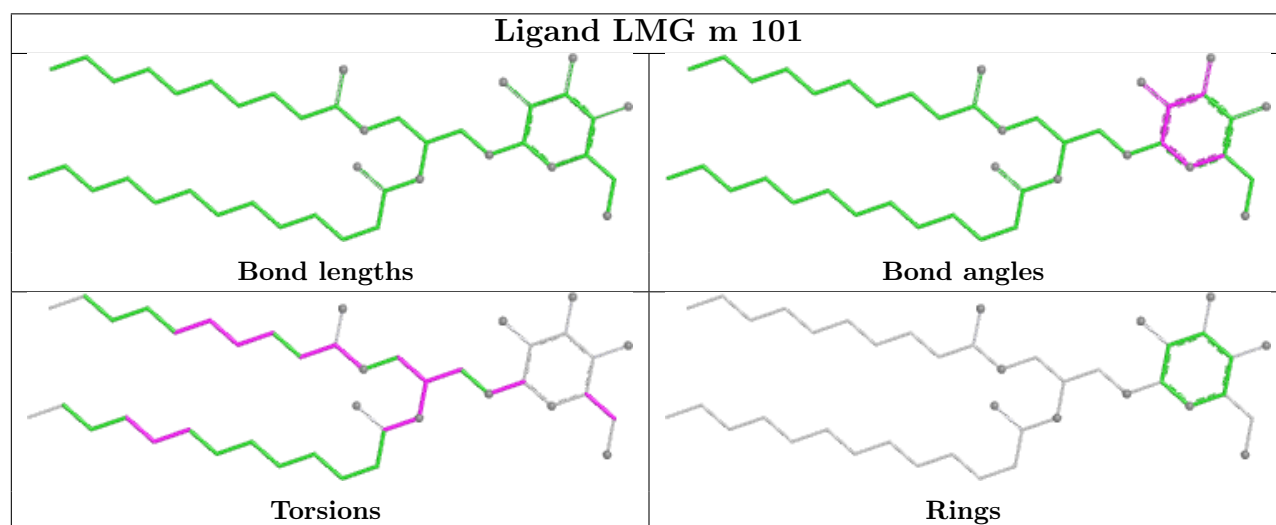
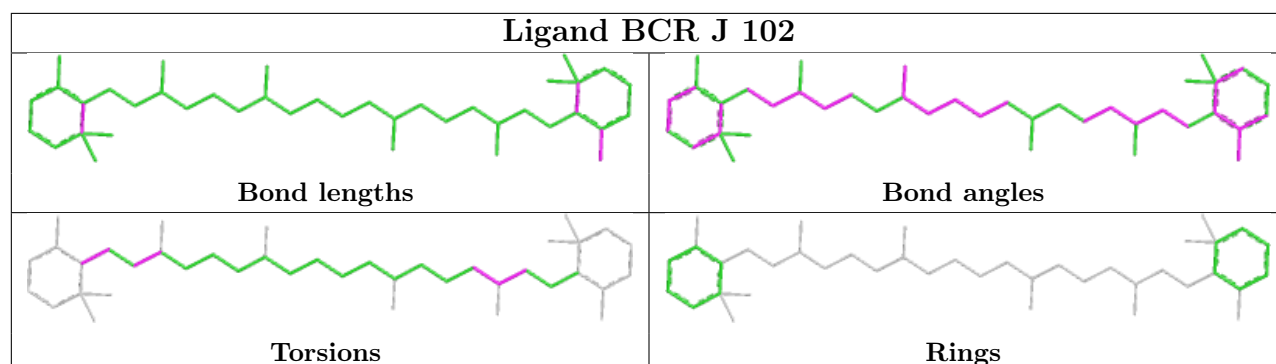
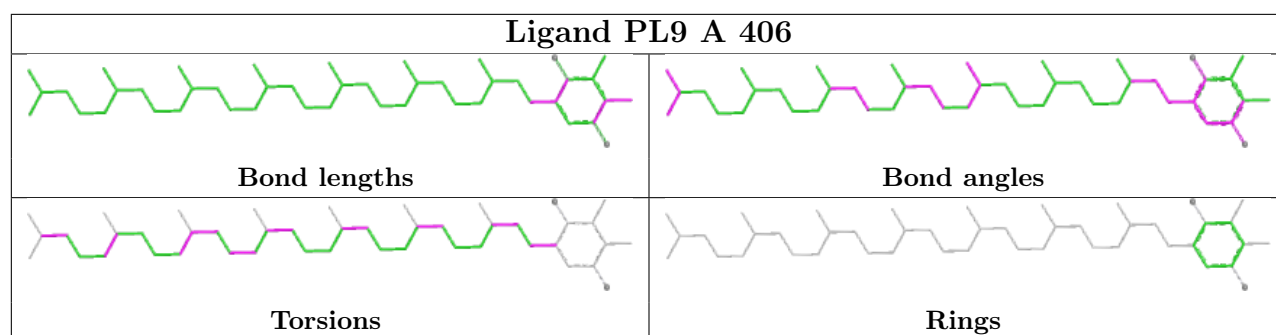


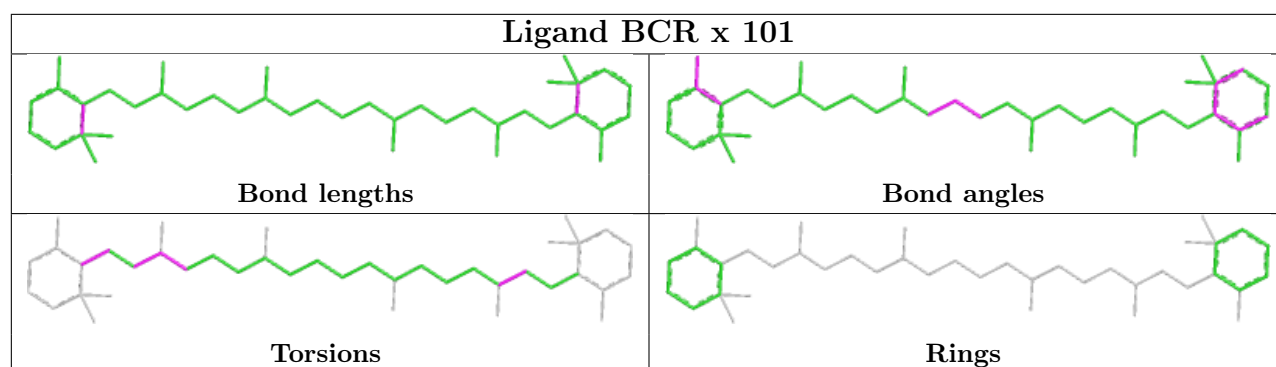
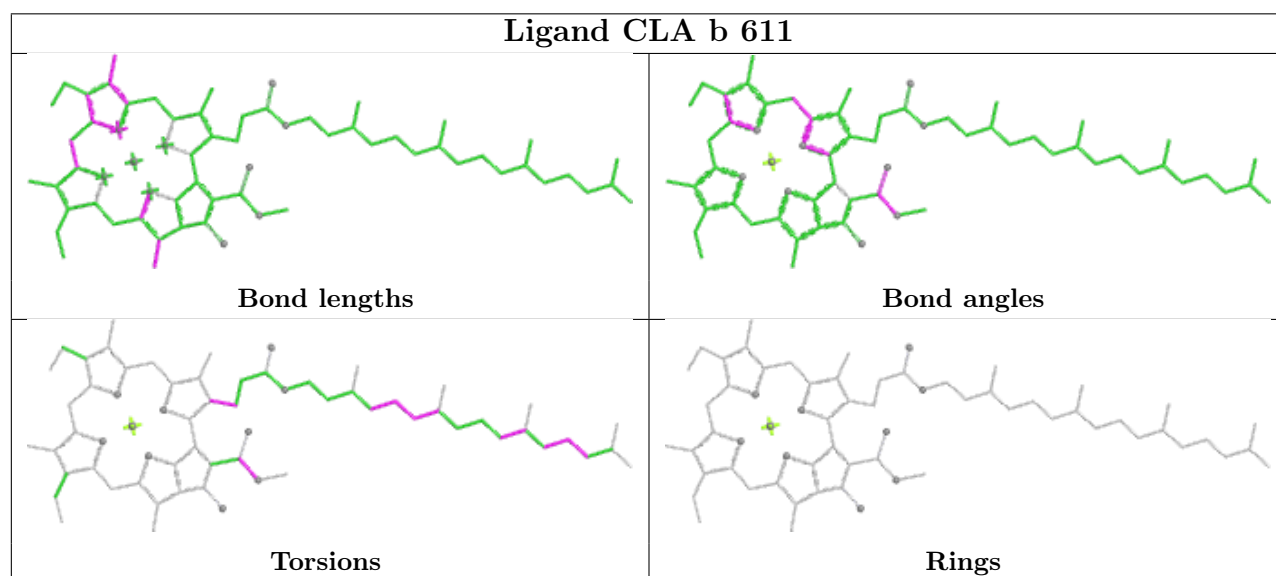
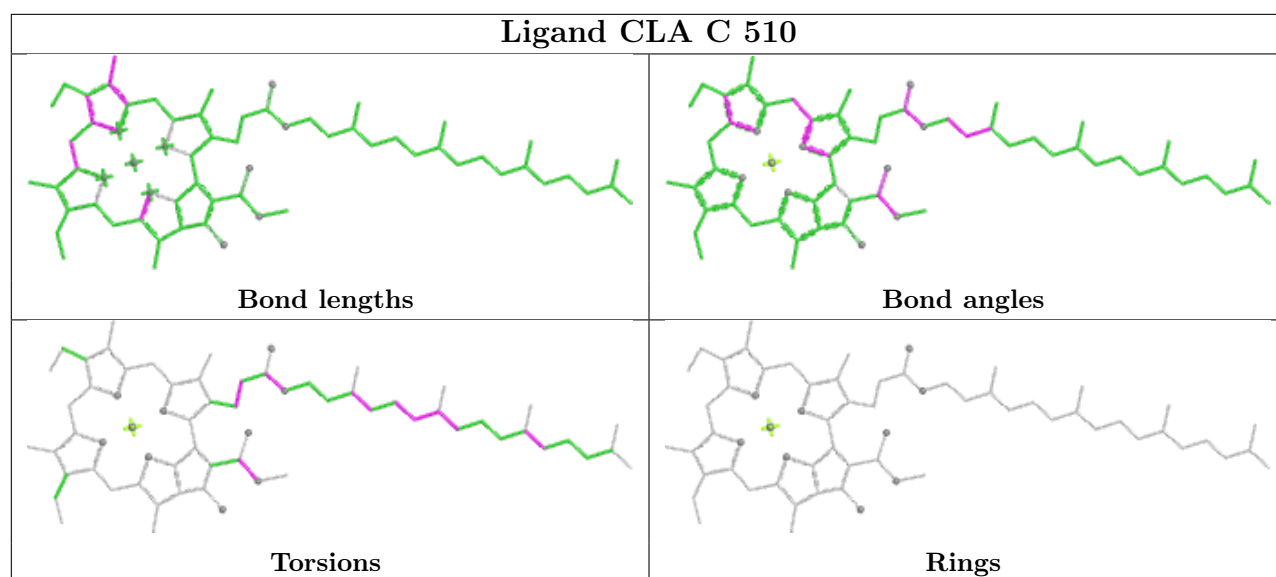


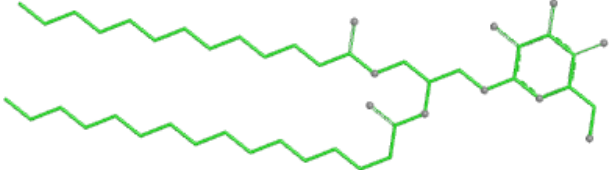
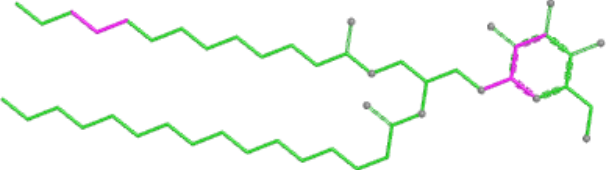
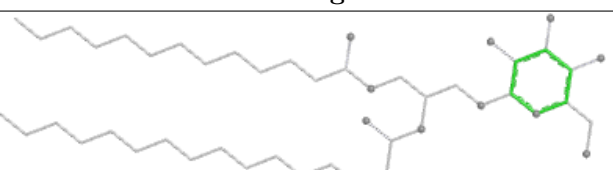
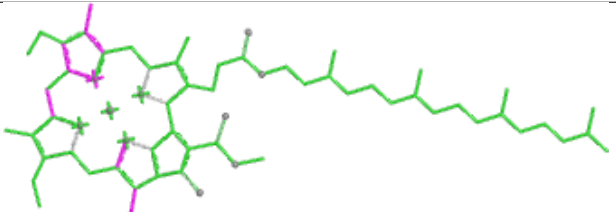
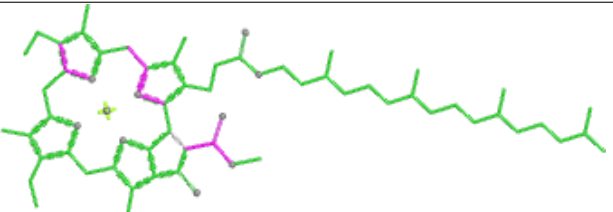
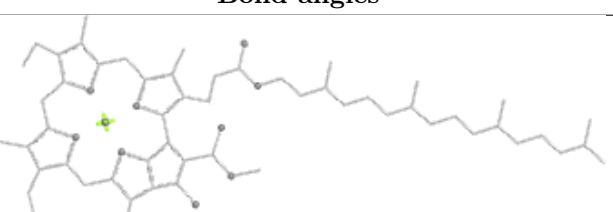
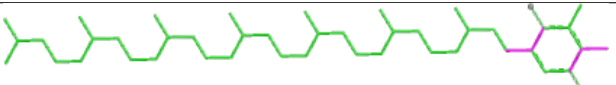
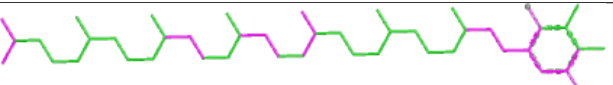
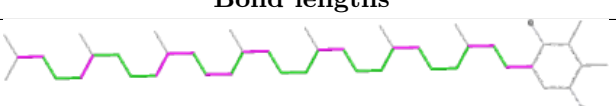
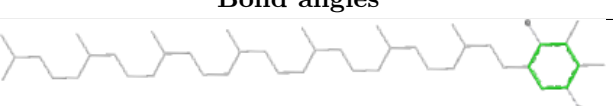


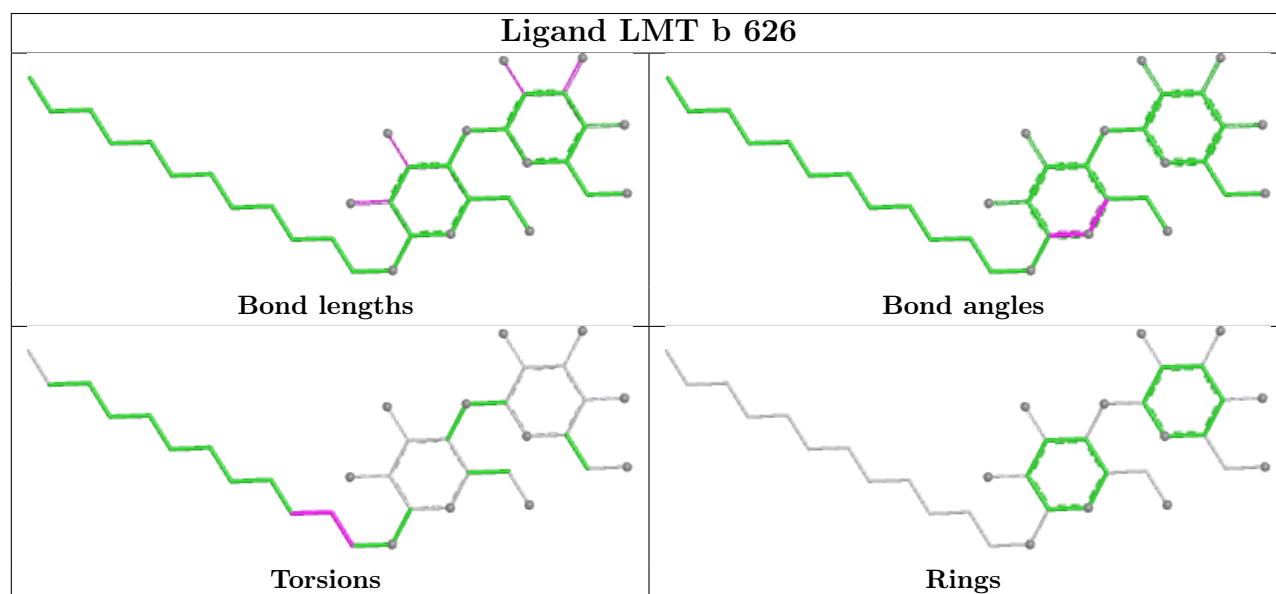
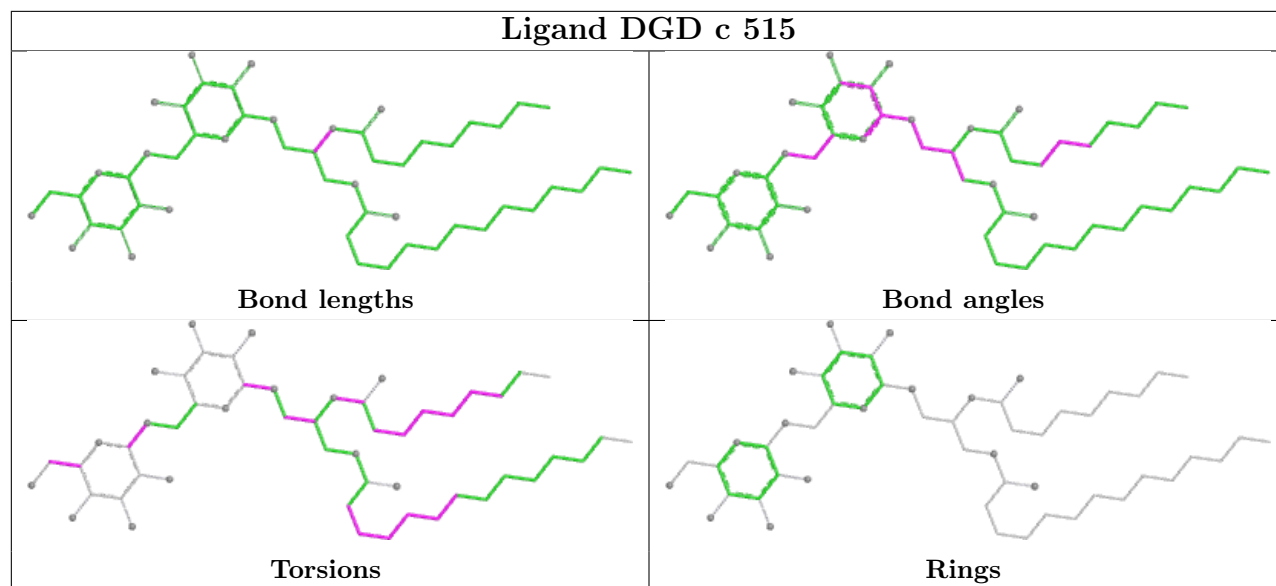




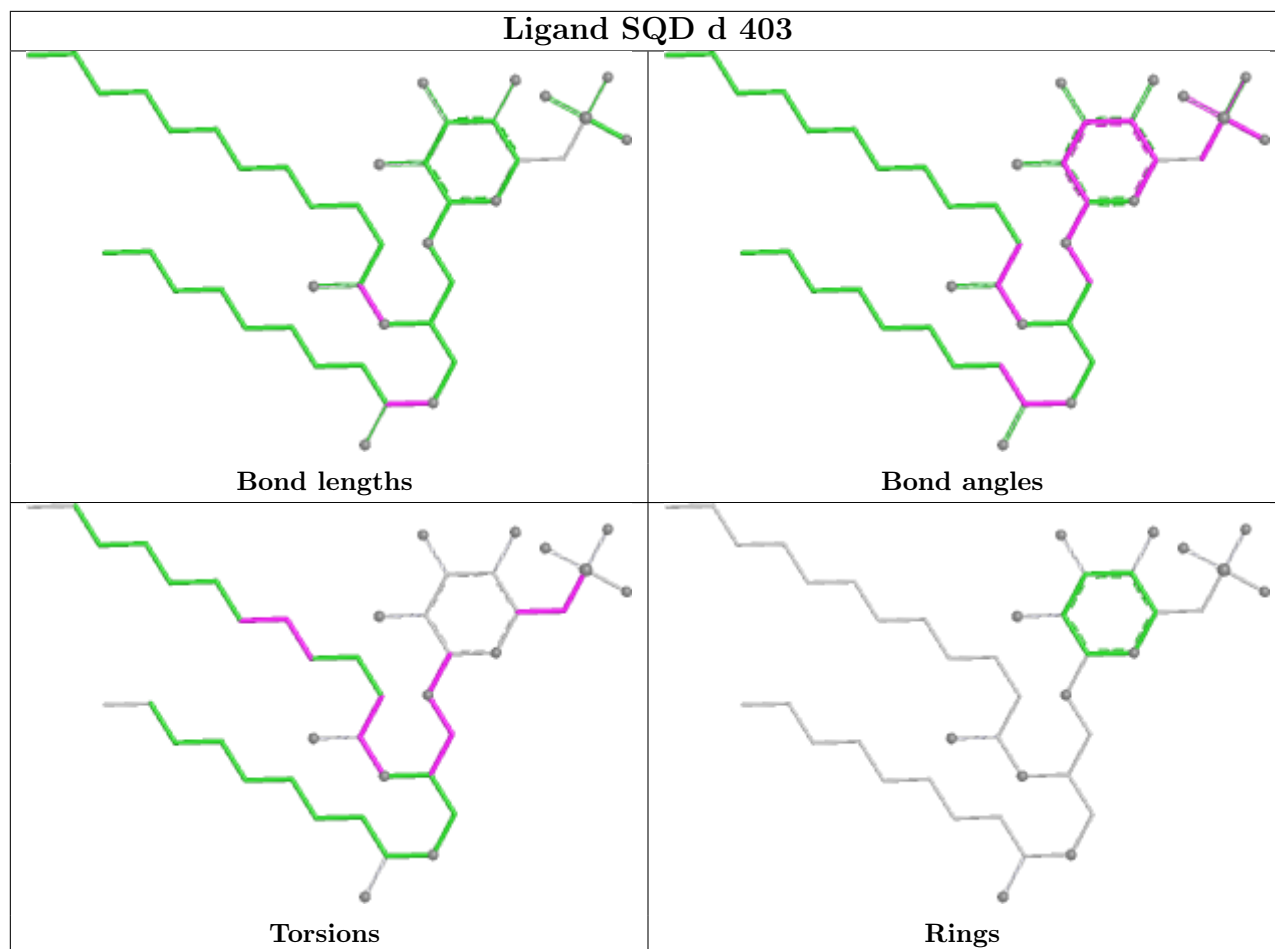




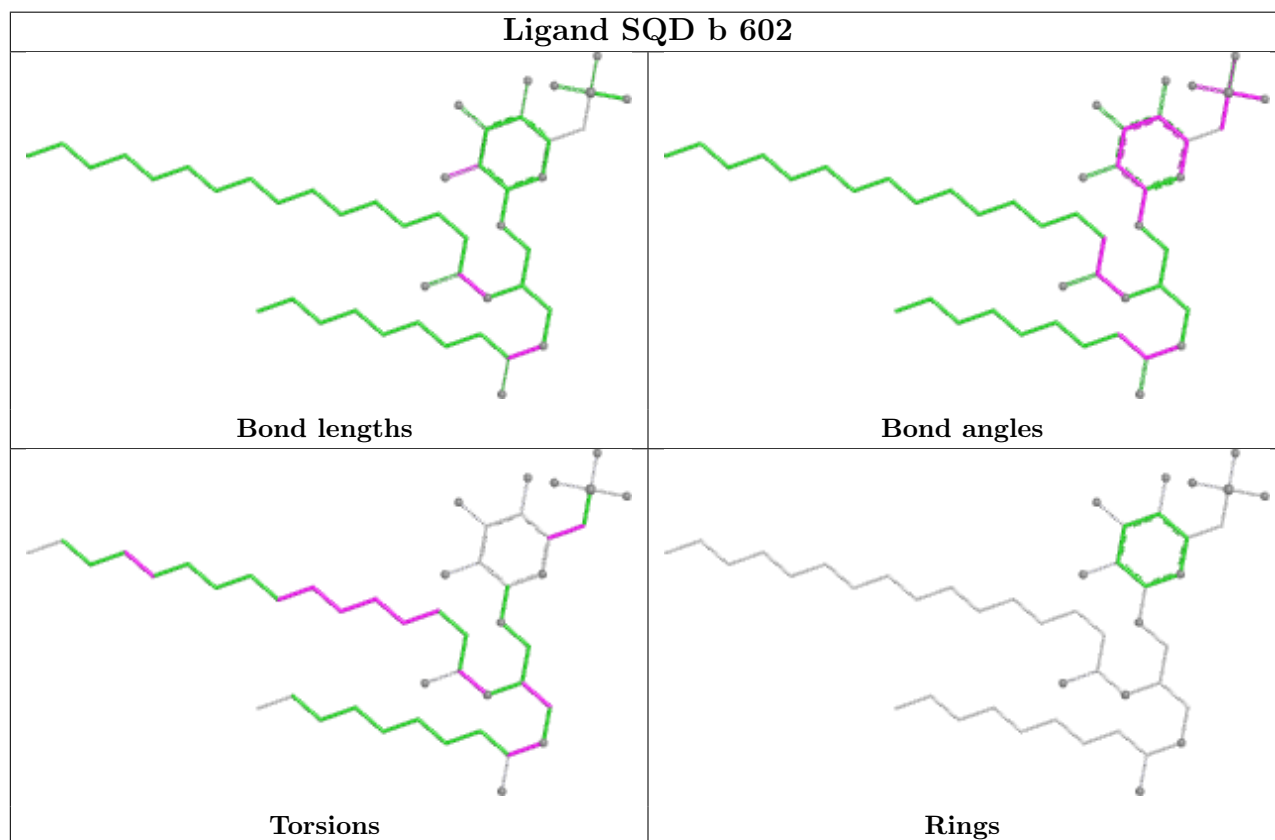
Ligand LMG D 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 503	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

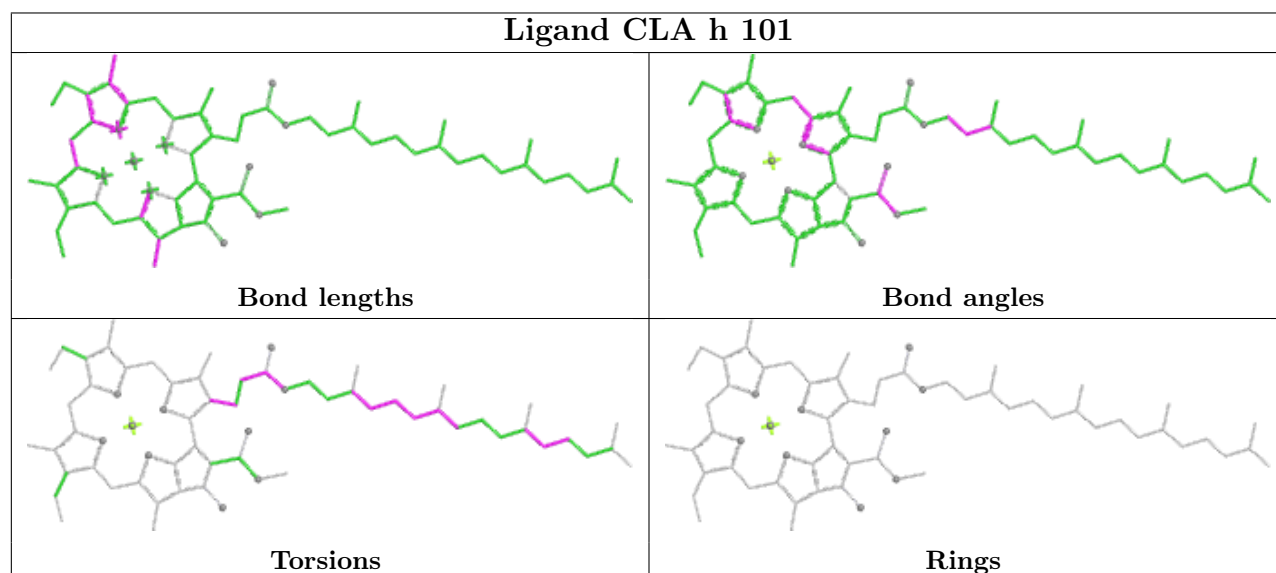
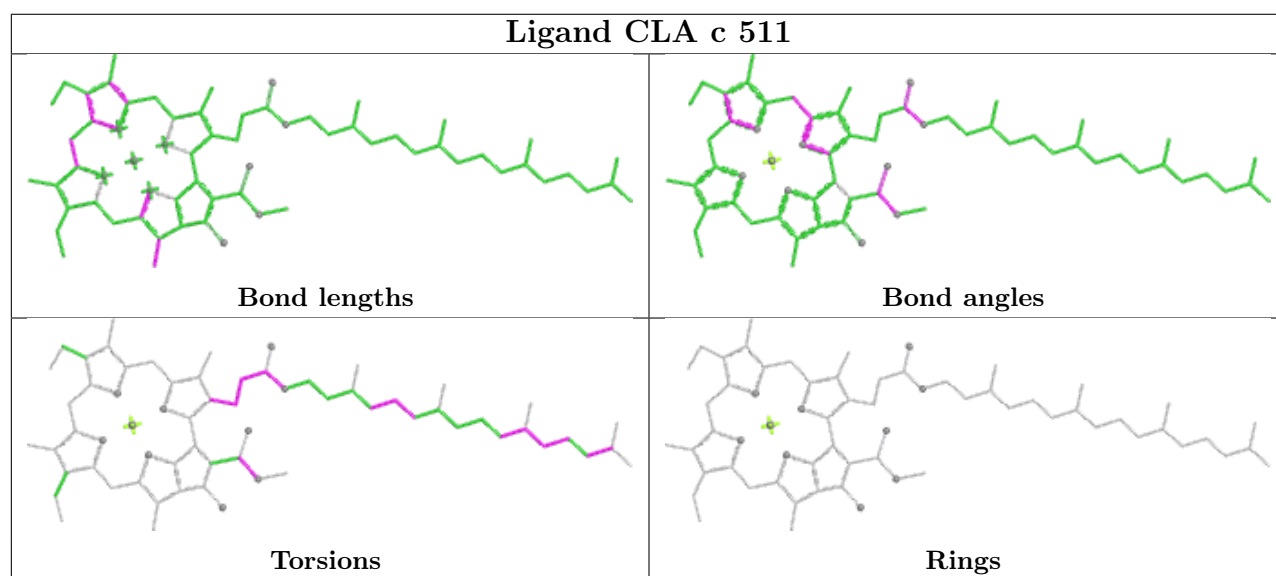
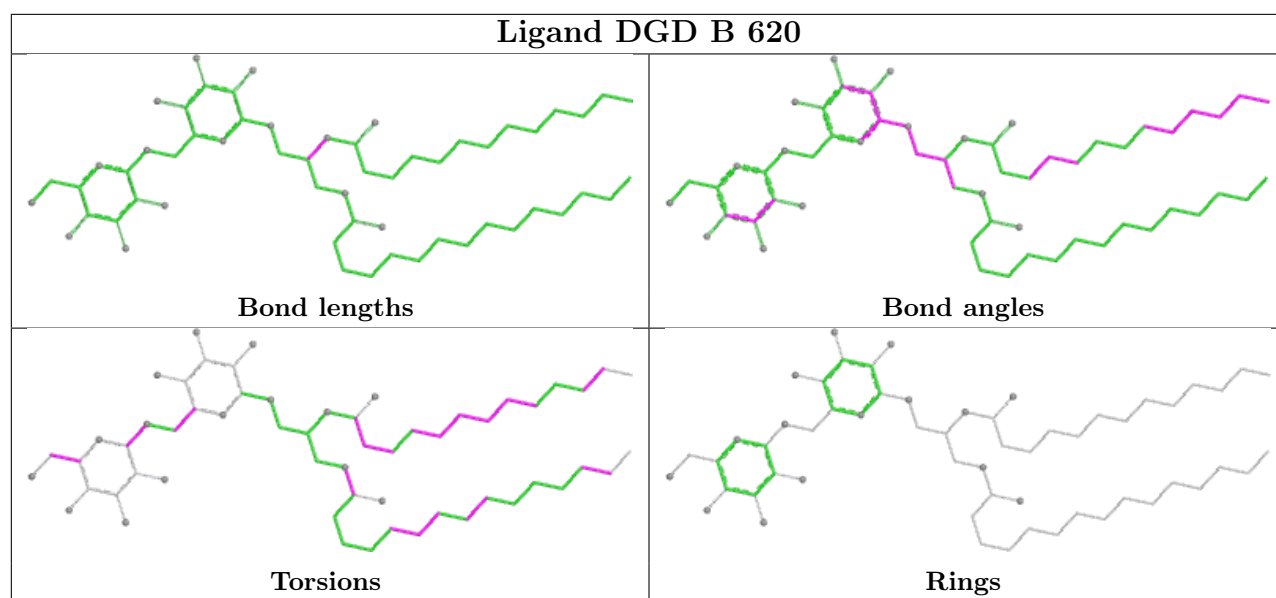


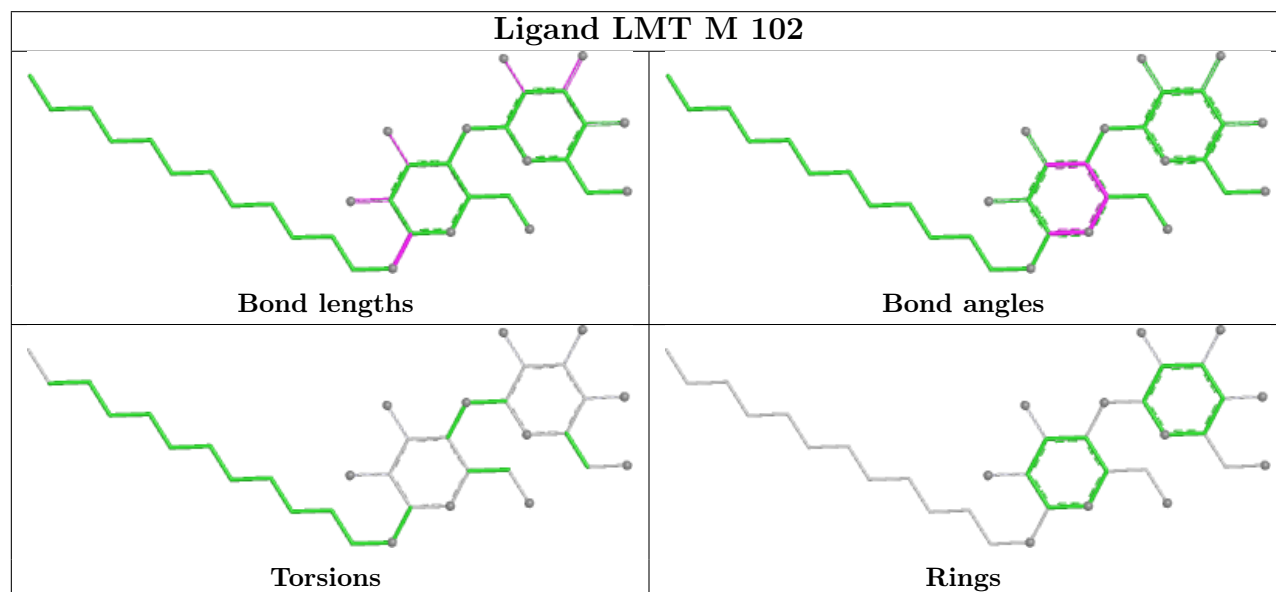
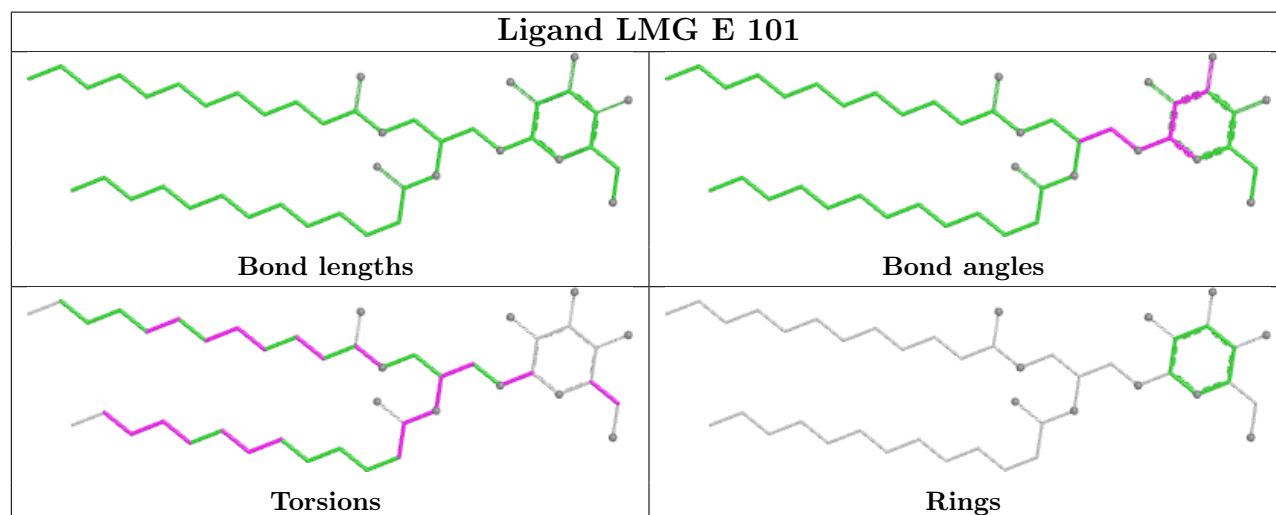
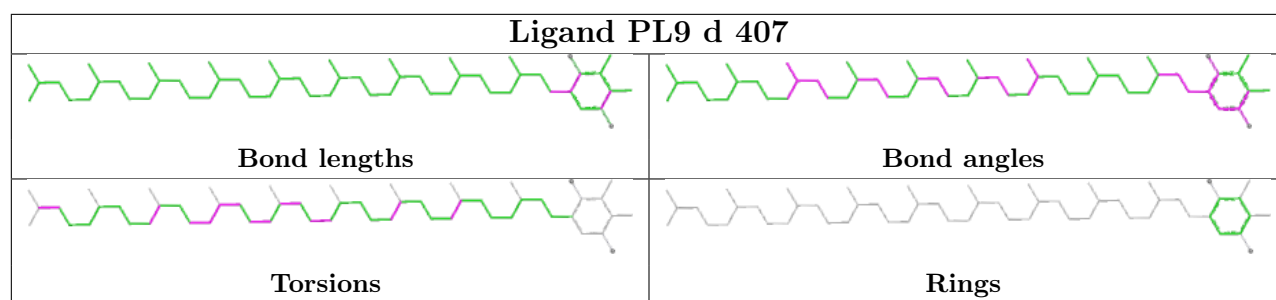
Ligand SQD d 403

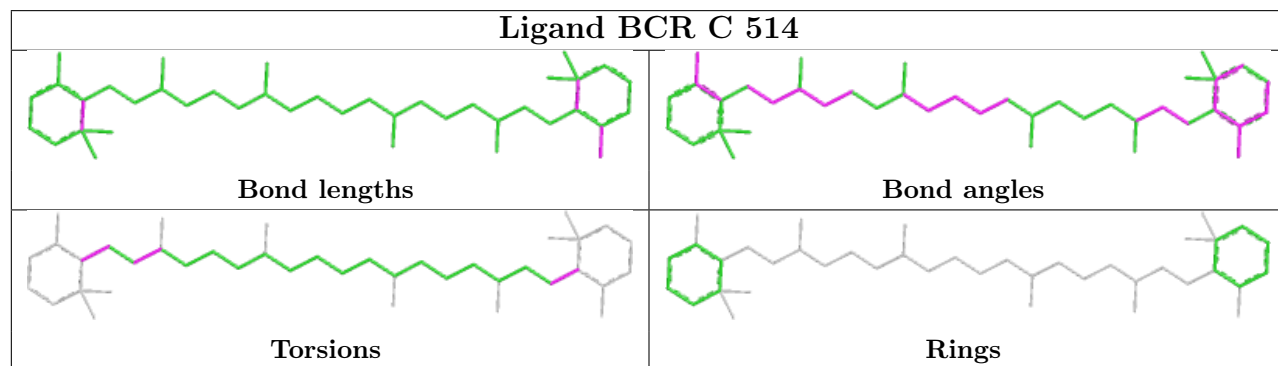
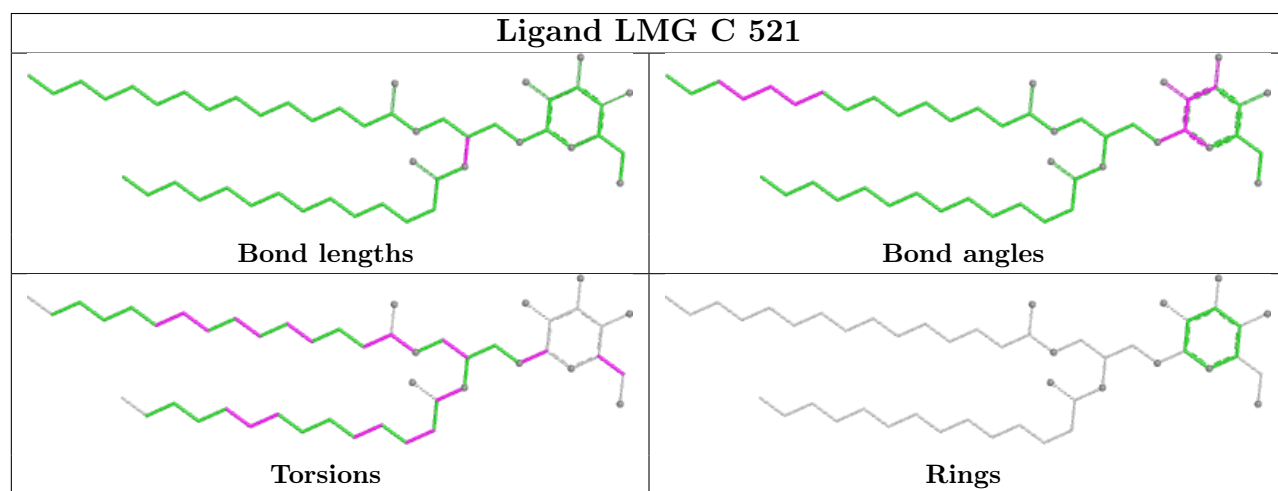
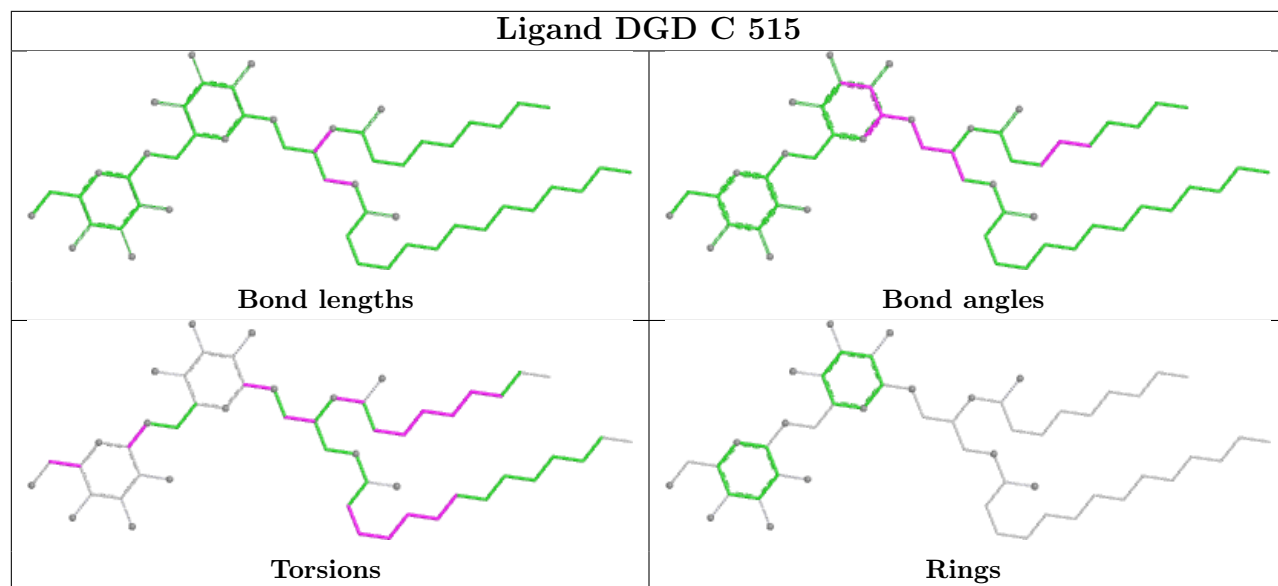


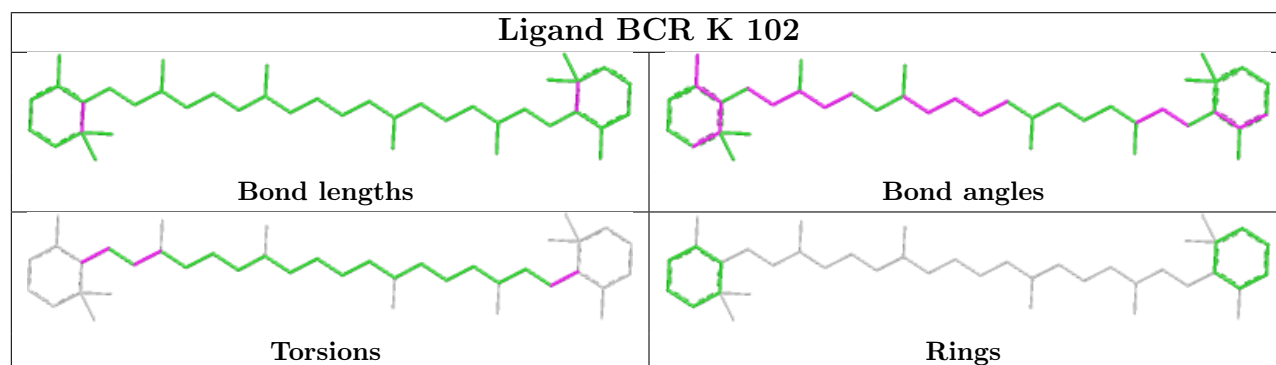
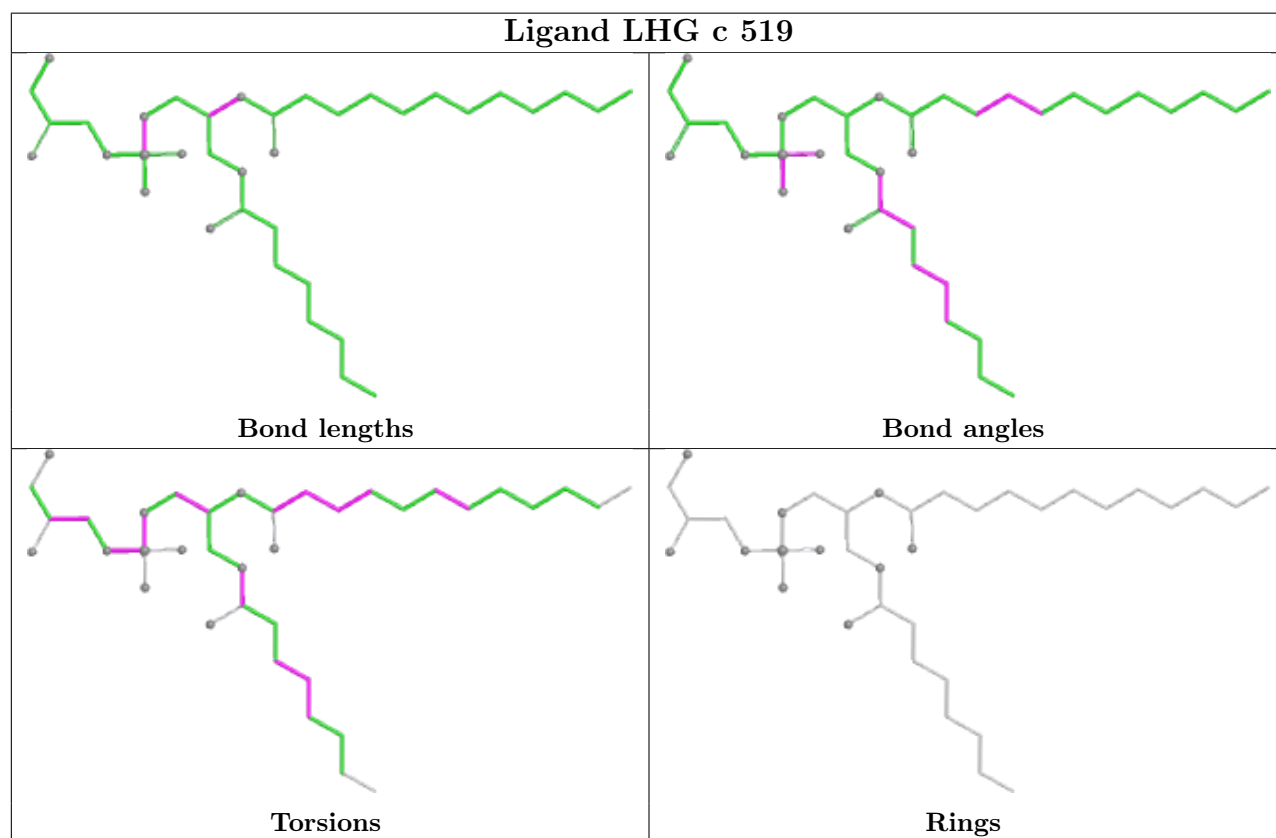
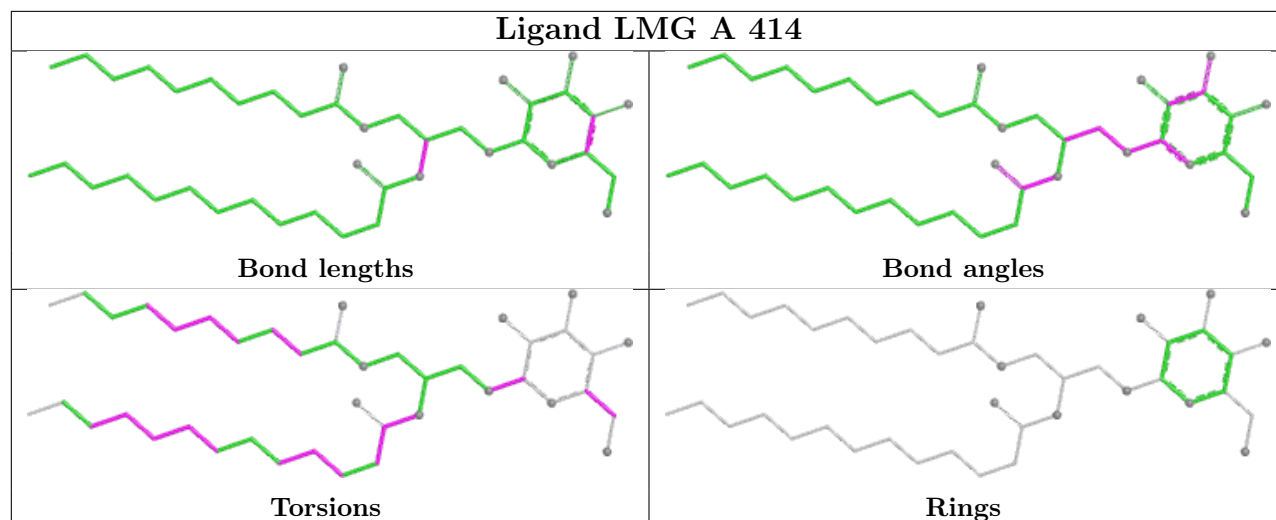
Ligand SQD b 602

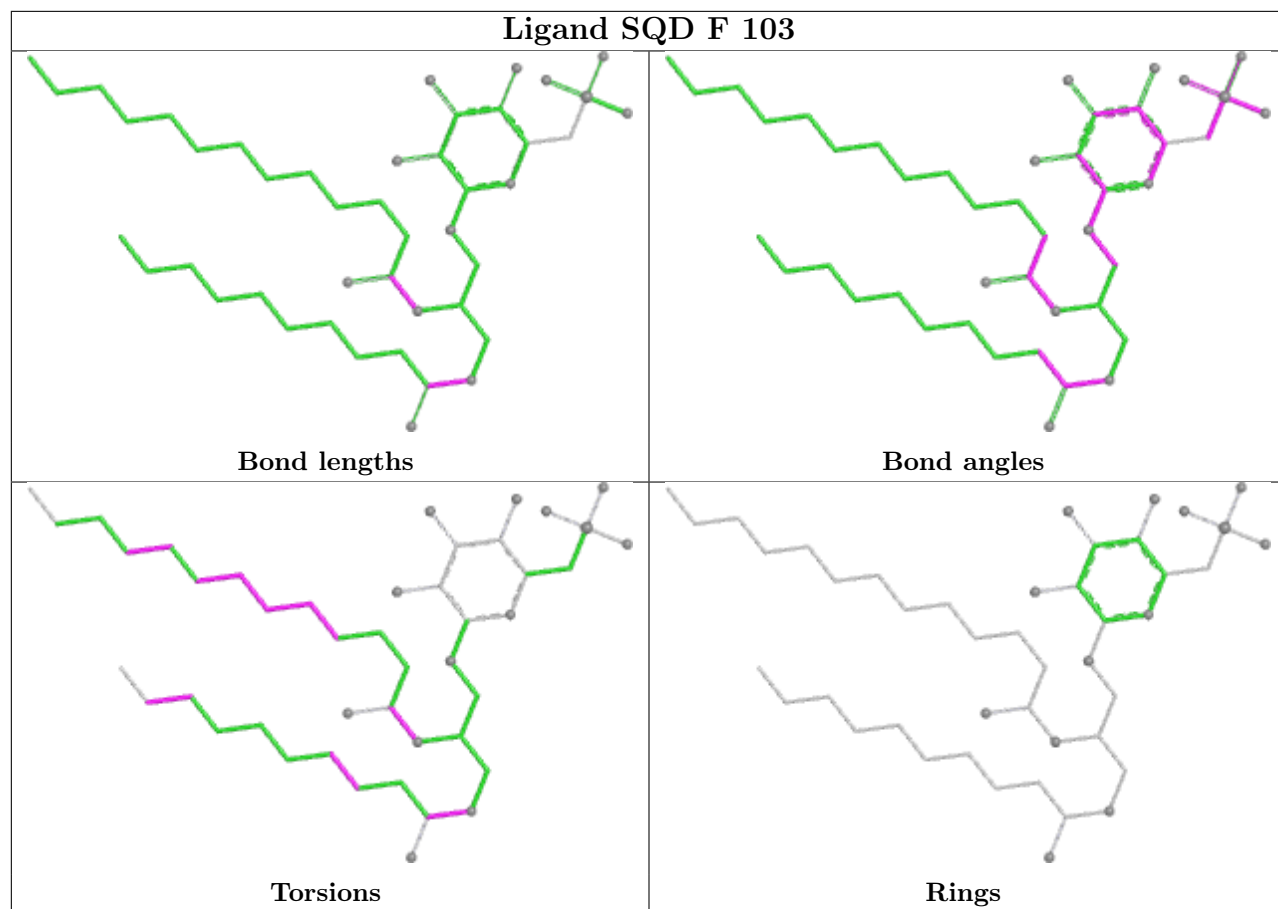












5.7 Other polymers [i](#)

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%)	0.14	8 (2%) 59 48	178, 179, 180, 181	0
1	a	335/344 (97%)	0.00	8 (2%) 59 48	178, 179, 180, 181	0
2	B	490/510 (96%)	0.03	7 (1%) 73 58	178, 179, 180, 181	0
2	b	490/510 (96%)	0.08	12 (2%) 59 48	178, 179, 180, 181	0
3	C	447/461 (96%)	0.05	5 (1%) 78 62	178, 179, 180, 181	0
3	c	447/461 (96%)	-0.05	6 (1%) 75 60	178, 180, 180, 181	0
4	D	340/352 (96%)	0.14	7 (2%) 63 50	177, 179, 180, 181	0
4	d	340/352 (96%)	-0.02	5 (1%) 72 57	177, 179, 180, 181	0
5	E	82/84 (97%)	-0.07	0 100 100	178, 180, 180, 181	0
5	e	82/84 (97%)	-0.04	2 (2%) 59 48	178, 180, 181, 181	0
6	F	35/45 (77%)	0.19	3 (8%) 16 20	179, 179, 180, 180	0
6	f	35/45 (77%)	-0.12	0 100 100	179, 180, 181, 181	0
7	H	65/66 (98%)	0.26	2 (3%) 51 41	179, 180, 180, 181	0
7	h	65/66 (98%)	0.11	2 (3%) 51 41	179, 180, 181, 181	0
8	I	35/38 (92%)	-0.21	0 100 100	178, 179, 180, 181	0
8	i	35/38 (92%)	-0.08	0 100 100	179, 179, 181, 181	0
9	J	34/40 (85%)	-0.13	0 100 100	178, 179, 180, 180	0
9	j	34/40 (85%)	0.06	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	0.03	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.04	0 100 100	179, 180, 181, 181	0
11	L	37/37 (100%)	0.12	1 (2%) 56 44	178, 179, 180, 181	0
11	l	37/37 (100%)	-0.07	0 100 100	178, 179, 180, 181	0
12	M	34/36 (94%)	0.27	0 100 100	178, 179, 180, 181	0
12	m	34/36 (94%)	0.09	0 100 100	178, 179, 180, 181	0

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Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.13	3 (1%) 76 61	177, 179, 180, 181	0
13	o	243/272 (89%)	0.05	2 (0%) 82 68	177, 179, 181, 181	0
14	T	32/32 (100%)	0.08	0 100 100	178, 179, 181, 181	0
14	t	32/32 (100%)	0.18	1 (3%) 51 41	178, 179, 180, 181	0
15	U	97/134 (72%)	0.29	3 (3%) 51 41	178, 179, 180, 181	0
15	u	97/134 (72%)	0.29	2 (2%) 63 50	178, 179, 180, 181	0
16	V	137/163 (84%)	0.20	5 (3%) 46 39	178, 179, 180, 181	0
16	v	137/163 (84%)	0.02	2 (1%) 72 57	178, 180, 181, 181	0
17	g	28/46 (60%)	0.54	0 100 100	179, 180, 181, 182	0
17	y	28/46 (60%)	-0.13	0 100 100	178, 180, 181, 181	0
18	X	37/41 (90%)	-0.14	0 100 100	179, 179, 181, 181	0
18	x	37/41 (90%)	0.19	0 100 100	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.03	1 (1%) 70 55	179, 180, 181, 181	0
20	z	62/62 (100%)	-0.04	1 (1%) 70 55	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.06	88 (1%) 69 55	177, 179, 180, 182	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	V	47	LEU	5.1
2	b	211	ILE	5.0
2	B	161	LEU	4.5
13	O	195	ASP	4.4
2	b	63	LEU	4.3

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
30	LMT	I	102	35/35	0.49	0.17	178,180,182,183	0
30	LMT	d	411	31/35	0.52	0.18	178,181,182,183	0
35	CA	K	101	1/1	0.58	0.18	184,184,184,184	0
30	LMT	i	102	35/35	0.60	0.17	178,181,183,183	0
30	LMT	b	627	35/35	0.60	0.16	178,180,182,182	0
22	CLA	b	605	65/65	0.62	0.22	179,180,182,183	0
30	LMT	D	411	31/35	0.63	0.13	179,180,182,182	0
22	CLA	B	601	65/65	0.63	0.19	177,180,181,182	0
30	LMT	b	626	35/35	0.64	0.14	178,180,182,183	0
30	LMT	b	603	35/35	0.65	0.15	178,179,181,182	0
30	LMT	B	627	35/35	0.65	0.15	178,180,182,182	0
30	LMT	B	628	35/35	0.65	0.21	177,180,182,183	0
30	LMT	B	623	35/35	0.66	0.14	177,181,182,183	0
25	DGD	D	410	63/66	0.70	0.21	178,181,182,183	0
25	DGD	d	410	63/66	0.71	0.23	178,180,183,183	0
23	PL9	J	101	35/55	0.71	0.31	177,180,181,181	0
22	CLA	b	619	65/65	0.72	0.18	177,179,180,181	0
27	LMG	C	518	45/55	0.73	0.17	178,179,180,181	0
24	BCR	J	102	40/40	0.74	0.27	178,180,181,181	0
24	BCR	j	102	40/40	0.75	0.27	179,180,182,183	0
25	DGD	B	625	52/66	0.75	0.19	177,180,182,182	0
29	SQD	B	626	47/54	0.75	0.17	175,179,181,183	0
29	SQD	d	403	43/54	0.75	0.18	178,180,182,186	0
22	CLA	c	512	65/65	0.75	0.16	178,180,181,182	0
26	LHG	C	519	37/49	0.76	0.19	176,180,184,188	0
27	LMG	M	101	42/55	0.77	0.21	178,180,181,182	0
30	LMT	B	624	35/35	0.77	0.15	178,180,182,183	0
25	DGD	b	601	52/66	0.78	0.18	178,180,181,182	0
26	LHG	c	519	37/49	0.78	0.18	178,180,183,187	0
22	CLA	C	506	65/65	0.80	0.18	177,179,180,180	0
27	LMG	A	414	42/55	0.80	0.22	177,179,182,182	0
30	LMT	b	604	35/35	0.81	0.20	177,179,181,182	0
27	LMG	a	402	42/55	0.81	0.23	177,180,181,182	0
27	LMG	I	101	43/55	0.81	0.20	178,180,181,182	0
30	LMT	M	102	35/35	0.82	0.18	178,179,181,182	0
22	CLA	A	405	65/65	0.82	0.17	177,179,180,181	0
23	PL9	A	406	45/55	0.82	0.27	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	DGD	C	516	62/66	0.82	0.15	177,179,180,181	0
29	SQD	b	602	47/54	0.83	0.16	176,179,182,185	0
27	LMG	c	518	45/55	0.83	0.15	178,180,181,181	0
27	LMG	m	101	42/55	0.83	0.20	175,179,181,181	0
25	DGD	c	516	62/66	0.83	0.19	178,179,180,181	0
25	DGD	a	410	56/66	0.84	0.20	178,180,181,182	0
29	SQD	a	415	51/54	0.84	0.18	178,179,181,182	0
24	BCR	b	621	40/40	0.84	0.20	178,178,179,179	0
27	LMG	E	101	44/55	0.84	0.20	176,179,181,182	0
24	BCR	b	623	40/40	0.84	0.18	177,178,180,180	0
29	SQD	A	412	51/54	0.84	0.18	178,179,180,181	0
24	BCR	H	102	40/40	0.85	0.19	178,180,181,182	0
27	LMG	b	625	49/55	0.85	0.20	178,179,180,180	0
25	DGD	A	408	56/66	0.85	0.17	178,179,181,182	0
27	LMG	i	101	43/55	0.85	0.16	177,180,182,184	0
24	BCR	b	622	40/40	0.85	0.27	176,178,179,179	0
23	PL9	j	101	35/55	0.85	0.24	179,180,181,181	0
25	DGD	b	624	58/66	0.86	0.21	177,178,180,180	0
25	DGD	c	515	53/66	0.86	0.20	176,179,181,182	0
24	BCR	a	409	40/40	0.86	0.21	177,178,180,180	0
29	SQD	F	103	45/54	0.86	0.19	178,180,182,182	0
22	CLA	C	512	65/65	0.86	0.13	177,180,181,182	0
27	LMG	e	101	44/55	0.86	0.18	177,179,181,181	0
33	BCT	d	404	4/4	0.86	0.10	178,180,180,180	0
25	DGD	C	517	66/66	0.86	0.18	177,179,180,181	0
35	CA	O	301	1/1	0.86	0.08	182,182,182,182	0
35	CA	k	101	1/1	0.86	0.09	180,180,180,180	0
22	CLA	C	505	65/65	0.87	0.17	177,179,180,181	0
32	CL	D	403	1/1	0.87	0.33	180,180,180,180	0
24	BCR	K	102	40/40	0.87	0.20	178,180,181,182	0
25	DGD	c	517	66/66	0.87	0.17	177,179,181,181	0
24	BCR	c	514	40/40	0.87	0.22	177,179,180,180	0
29	SQD	a	401	54/54	0.87	0.15	178,180,181,183	0
35	CA	o	301	1/1	0.87	0.12	184,184,184,184	0
24	BCR	c	521	40/40	0.88	0.17	178,179,181,181	0
24	BCR	B	619	40/40	0.88	0.16	178,179,180,180	0
22	CLA	c	506	65/65	0.88	0.15	178,179,180,181	0
22	CLA	a	406	65/65	0.88	0.17	177,179,180,181	0
27	LMG	c	522	48/55	0.88	0.21	178,180,180,181	0
22	CLA	C	510	65/65	0.88	0.15	177,179,180,181	0
22	CLA	b	618	65/65	0.88	0.15	177,179,180,180	0
23	PL9	a	408	45/55	0.88	0.19	176,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PL9	d	407	55/55	0.88	0.17	177,179,180,181	0
22	CLA	C	508	65/65	0.88	0.13	177,179,180,180	0
24	BCR	B	617	40/40	0.88	0.19	177,179,180,180	0
30	LMT	M	103	35/35	0.88	0.17	177,179,180,180	0
26	LHG	A	409	39/49	0.89	0.18	178,179,181,181	0
22	CLA	c	510	65/65	0.89	0.12	178,179,181,181	0
24	BCR	g	101	40/40	0.89	0.16	178,179,180,180	0
24	BCR	x	101	40/40	0.89	0.17	178,179,180,181	0
24	BCR	B	616	40/40	0.89	0.17	176,178,180,180	0
27	LMG	D	409	48/55	0.89	0.16	175,178,180,181	0
22	CLA	b	609	65/65	0.89	0.13	178,179,180,181	0
25	DGD	C	515	53/66	0.89	0.17	177,178,179,180	0
22	CLA	C	520	65/65	0.89	0.15	178,179,180,181	0
24	BCR	b	620	40/40	0.89	0.21	177,179,179,180	0
27	LMG	a	412	51/55	0.89	0.20	177,179,180,180	0
22	CLA	c	502	65/65	0.90	0.18	178,179,180,181	0
22	CLA	c	505	65/65	0.90	0.15	177,179,180,181	0
22	CLA	B	615	65/65	0.90	0.13	176,179,180,181	0
22	CLA	A	404	65/65	0.90	0.19	176,178,180,181	0
22	CLA	B	603	65/65	0.90	0.12	176,179,180,180	0
27	LMG	A	410	51/55	0.90	0.17	177,178,180,181	0
22	CLA	h	101	65/65	0.90	0.15	176,179,180,181	0
27	LMG	B	621	49/55	0.90	0.15	177,179,180,180	0
22	CLA	B	605	65/65	0.90	0.12	178,179,180,180	0
27	LMG	C	521	48/55	0.90	0.16	177,179,180,181	0
27	LMG	D	408	49/55	0.90	0.20	177,178,180,180	0
24	BCR	C	514	40/40	0.90	0.17	178,179,180,181	0
29	SQD	A	413	54/54	0.90	0.14	178,180,182,184	0
22	CLA	b	606	65/65	0.91	0.13	177,179,180,181	0
25	DGD	B	620	58/66	0.91	0.18	176,179,181,182	0
22	CLA	c	503	65/65	0.91	0.13	177,179,180,181	0
29	SQD	f	103	45/54	0.91	0.15	177,179,181,182	0
22	CLA	b	607	65/65	0.91	0.13	177,179,180,181	0
24	BCR	c	513	40/40	0.91	0.15	178,179,180,180	0
31	PHO	D	402	64/64	0.91	0.14	177,179,180,181	0
31	PHO	d	401	64/64	0.91	0.16	178,179,180,180	0
22	CLA	C	509	65/65	0.91	0.15	177,179,180,180	0
22	CLA	a	407	65/65	0.91	0.14	178,179,180,181	0
29	SQD	B	622	43/54	0.91	0.14	177,180,182,185	0
22	CLA	B	613	65/65	0.91	0.13	177,179,180,180	0
24	BCR	A	407	40/40	0.91	0.19	177,179,180,180	0
22	CLA	c	520	65/65	0.91	0.16	177,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	503	65/65	0.92	0.13	177,179,180,180	0
24	BCR	F	102	40/40	0.92	0.18	177,179,180,180	0
27	LMG	D	412	46/55	0.92	0.14	178,179,180,181	0
22	CLA	c	501	65/65	0.92	0.13	177,179,180,181	0
22	CLA	C	507	65/65	0.92	0.17	178,179,180,181	0
22	CLA	C	504	65/65	0.92	0.16	177,179,180,180	0
24	BCR	y	101	40/40	0.92	0.15	177,179,180,180	0
22	CLA	D	405	65/65	0.92	0.13	177,179,180,180	0
31	PHO	D	401	64/64	0.92	0.15	177,179,180,180	0
22	CLA	a	405	65/65	0.92	0.20	174,178,179,180	0
22	CLA	c	508	65/65	0.92	0.11	177,179,180,181	0
22	CLA	c	509	65/65	0.92	0.12	177,179,180,180	0
27	LMG	d	408	49/55	0.92	0.15	178,179,180,180	0
27	LMG	d	409	48/55	0.92	0.14	177,179,180,180	0
22	CLA	b	613	65/65	0.92	0.13	178,179,180,181	0
22	CLA	c	511	65/65	0.92	0.12	178,180,181,182	0
22	CLA	C	501	65/65	0.92	0.12	178,179,180,180	0
22	CLA	B	606	65/65	0.93	0.12	177,179,180,180	0
22	CLA	c	504	65/65	0.93	0.15	177,179,180,180	0
23	PL9	D	407	55/55	0.93	0.18	177,178,179,180	0
22	CLA	B	607	65/65	0.93	0.14	178,179,180,181	0
22	CLA	b	608	65/65	0.93	0.12	178,179,180,181	0
22	CLA	c	507	65/65	0.93	0.14	177,179,180,181	0
22	CLA	H	101	65/65	0.93	0.15	177,179,180,181	0
22	CLA	a	404	65/65	0.93	0.16	177,178,180,180	0
27	LMG	d	412	46/55	0.93	0.13	177,178,180,180	0
22	CLA	B	608	65/65	0.93	0.14	177,179,180,180	0
33	BCT	D	404	4/4	0.93	0.06	178,179,179,179	0
22	CLA	B	604	65/65	0.93	0.10	177,179,180,180	0
22	CLA	C	511	65/65	0.93	0.13	178,179,180,181	0
24	BCR	C	513	40/40	0.93	0.15	177,179,180,180	0
22	CLA	B	602	65/65	0.93	0.13	176,178,180,180	0
22	CLA	d	406	65/65	0.93	0.13	177,179,180,181	0
22	CLA	b	615	65/65	0.94	0.11	177,179,180,180	0
22	CLA	b	617	65/65	0.94	0.17	178,179,180,182	0
26	LHG	a	411	39/49	0.94	0.14	177,179,180,181	0
22	CLA	B	610	65/65	0.94	0.12	177,179,180,180	0
22	CLA	B	612	65/65	0.94	0.14	176,178,180,181	0
31	PHO	d	402	64/64	0.94	0.10	178,179,180,181	0
24	BCR	f	102	40/40	0.94	0.14	177,179,181,181	0
22	CLA	C	502	65/65	0.94	0.14	178,179,180,180	0
22	CLA	D	406	65/65	0.94	0.13	177,179,180,181	0

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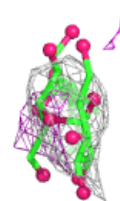
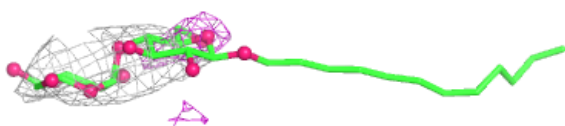
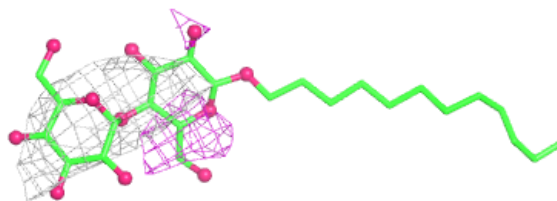
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HEM	f	101	43/43	0.94	0.12	178,180,180,181	0
22	CLA	b	610	65/65	0.94	0.12	177,179,180,180	0
22	CLA	b	611	65/65	0.94	0.13	177,179,180,180	0
22	CLA	b	612	65/65	0.94	0.13	176,179,181,181	0
22	CLA	B	609	65/65	0.94	0.12	178,179,180,181	0
28	OEX	a	414	10/10	0.95	0.10	174,177,179,182	0
22	CLA	d	405	65/65	0.95	0.15	177,178,179,180	0
22	CLA	B	614	65/65	0.95	0.10	177,179,180,181	0
34	HEM	v	201	43/43	0.95	0.12	177,179,180,180	0
22	CLA	A	402	65/65	0.95	0.14	178,179,180,181	0
22	CLA	A	403	65/65	0.95	0.14	177,179,179,180	0
24	BCR	B	618	40/40	0.95	0.18	177,178,179,179	0
32	CL	a	413	1/1	0.95	0.15	177,177,177,177	0
22	CLA	b	614	65/65	0.96	0.13	178,179,180,180	0
22	CLA	B	611	65/65	0.96	0.12	177,179,180,180	0
28	OEX	A	411	10/10	0.96	0.09	172,175,178,178	0
22	CLA	b	616	65/65	0.96	0.13	177,179,180,180	0
34	HEM	F	101	43/43	0.96	0.11	178,180,181,182	0
34	HEM	V	201	43/43	0.96	0.14	176,178,180,180	0
21	FE2	A	401	1/1	0.97	0.07	176,176,176,176	0
21	FE2	a	403	1/1	0.97	0.10	182,182,182,182	0

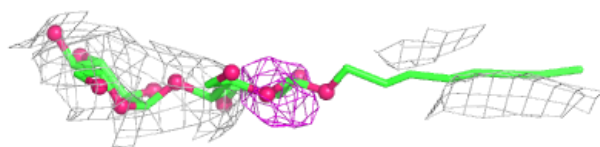
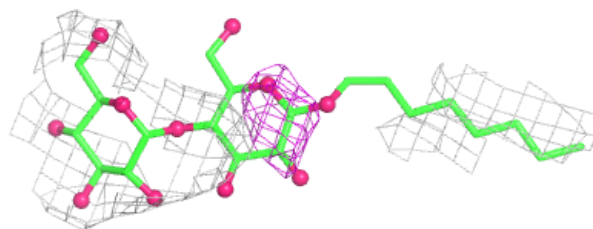
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

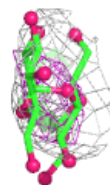
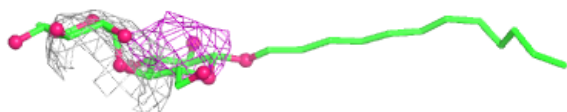
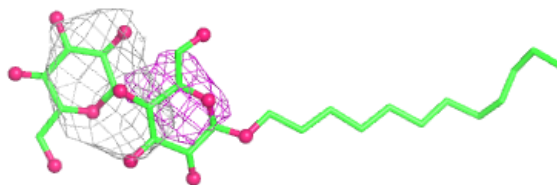
**Electron density around LMT d 411:**

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

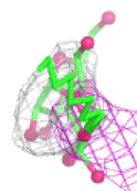
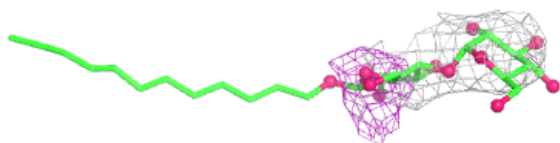
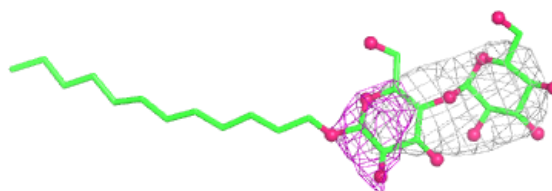


Electron density around LMT i 102:

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

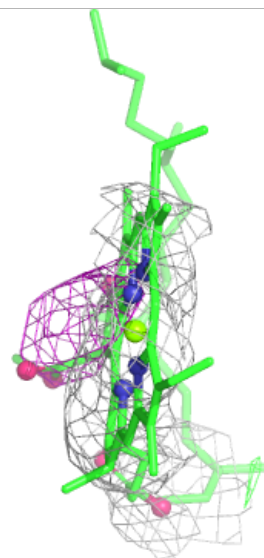
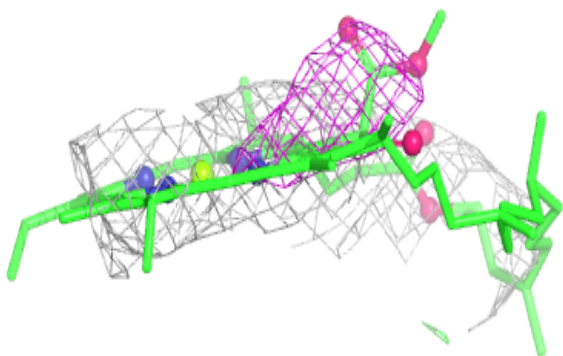
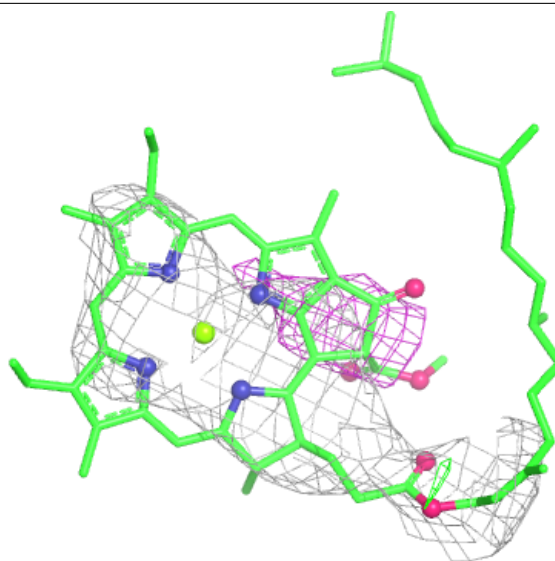
**Electron density around LMT b 627:**

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



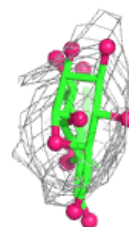
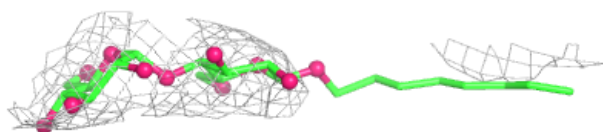
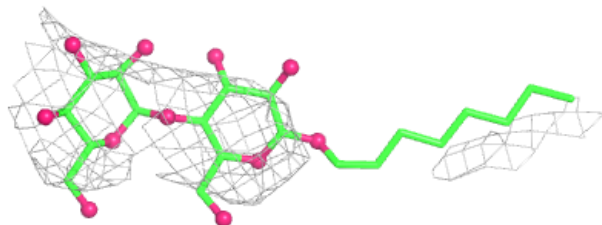
Electron density around CLA b 605:

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



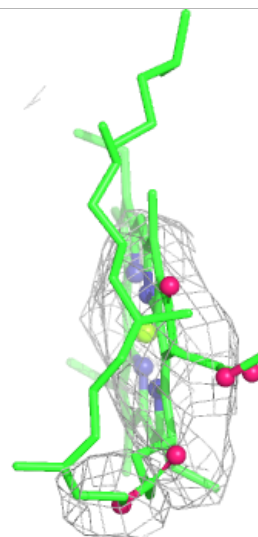
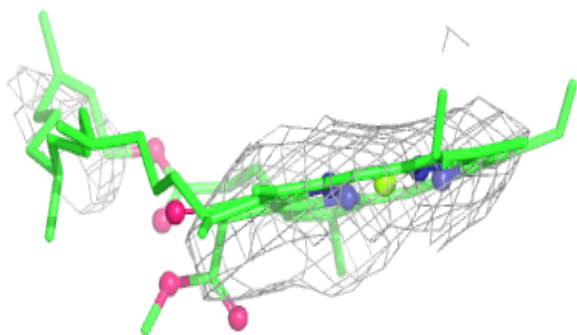
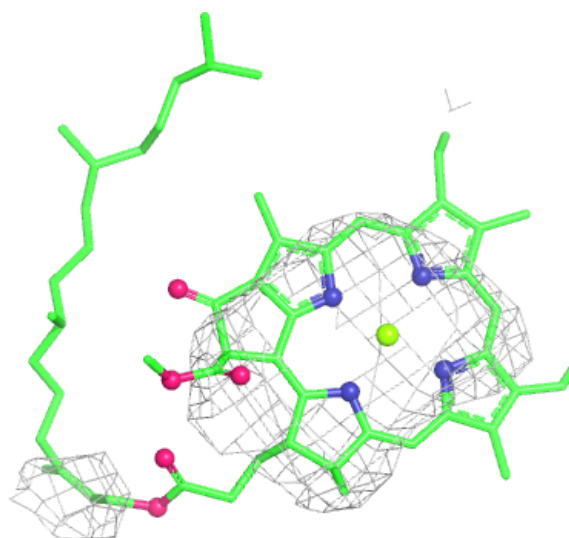
Electron density around LMT D 411:

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



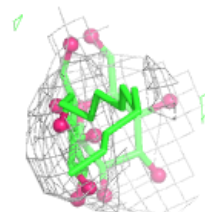
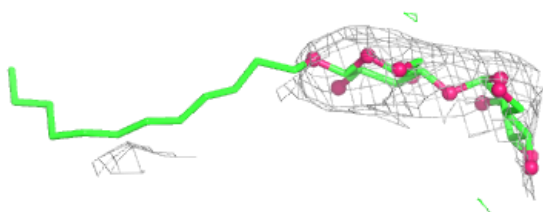
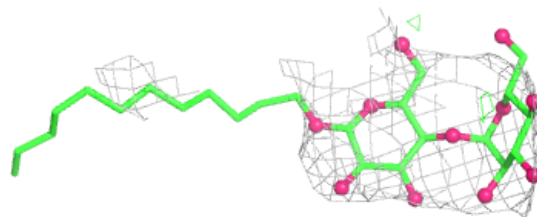
Electron density around CLA B 601:

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

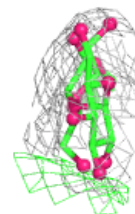
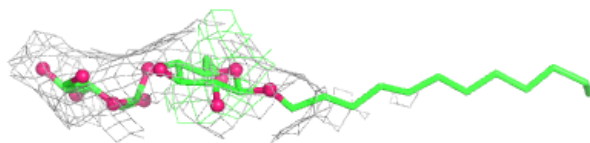
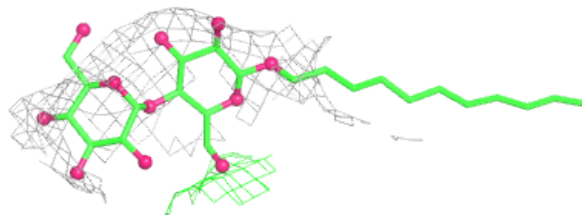


Electron density around LMT b 626:

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

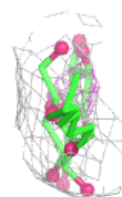
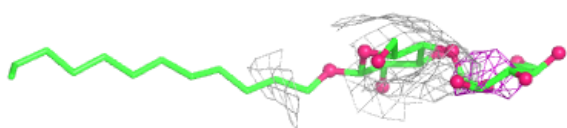
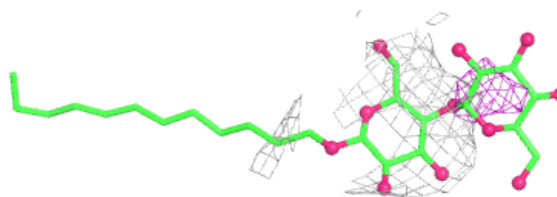
**Electron density around LMT b 603:**

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

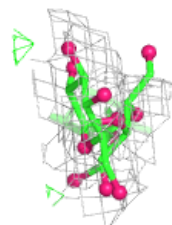
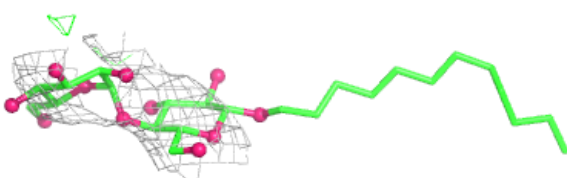
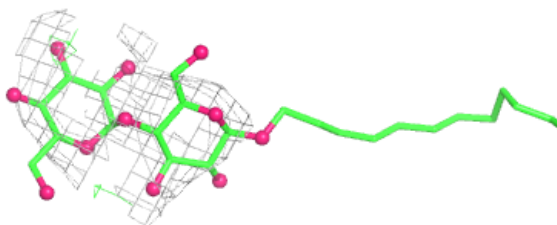


Electron density around LMT B 627:

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

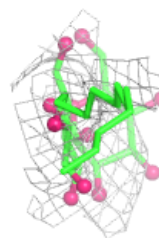
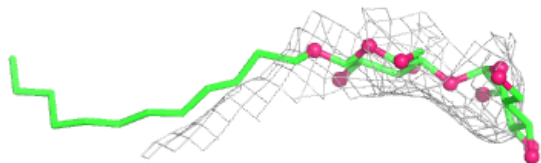
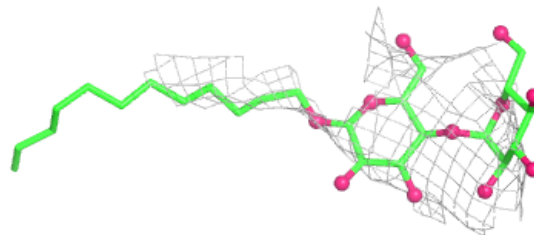
**Electron density around LMT B 628:**

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

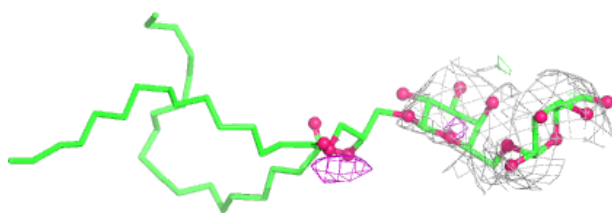
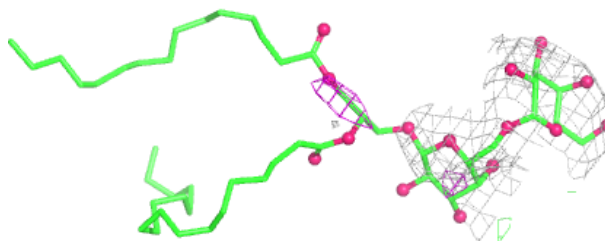


Electron density around LMT B 623:

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

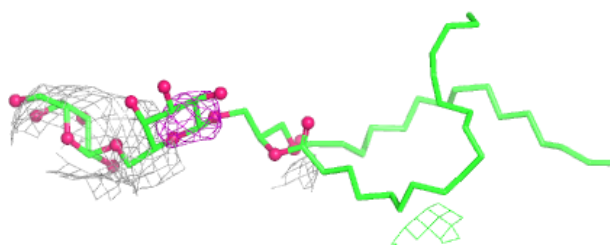
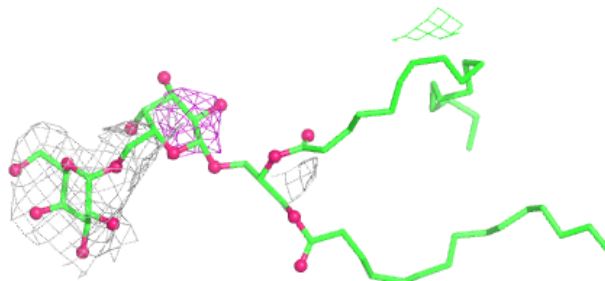
**Electron density around DGD D 410:**

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

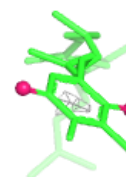
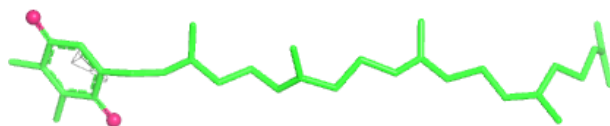
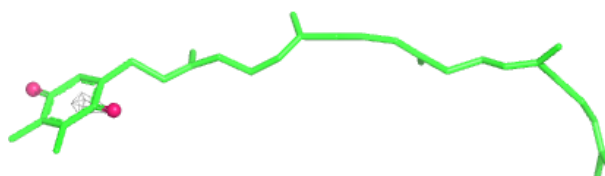


Electron density around DGD d 410:

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

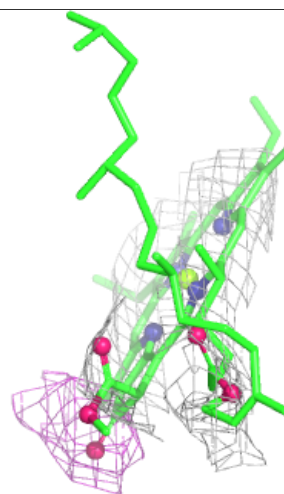
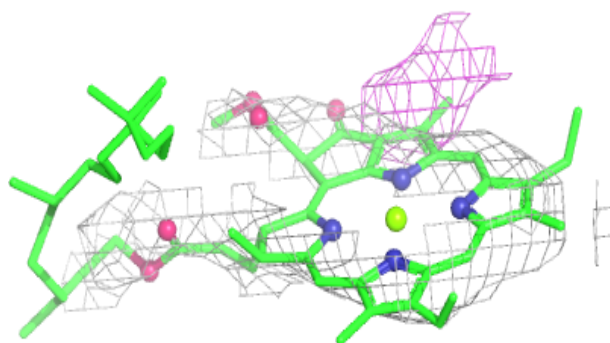
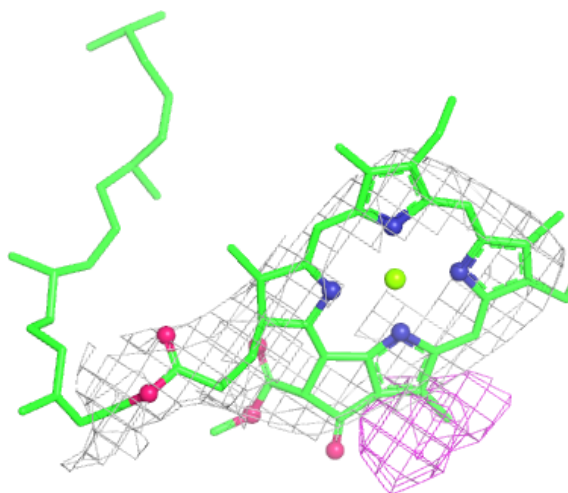
**Electron density around PL9 J 101:**

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



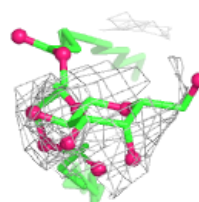
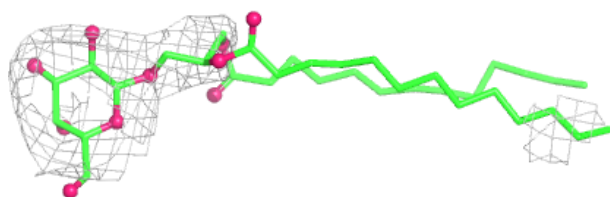
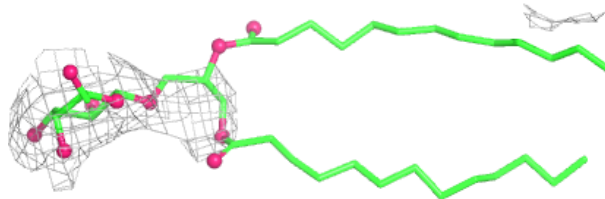
Electron density around CLA b 619:

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

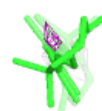
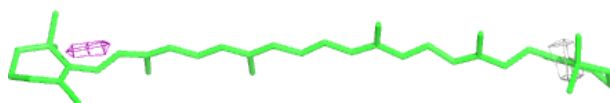
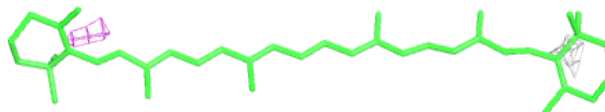


Electron density around LMG C 518:

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

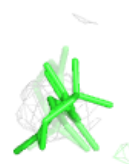
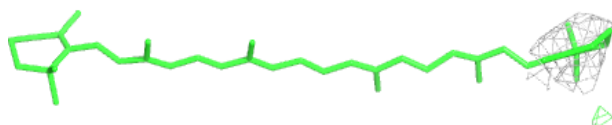
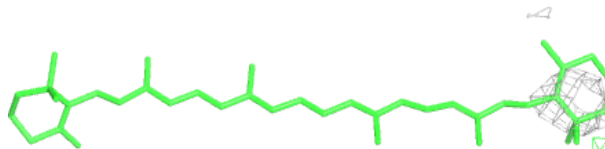
**Electron density around BCR J 102:**

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

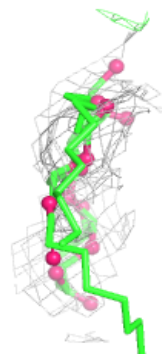
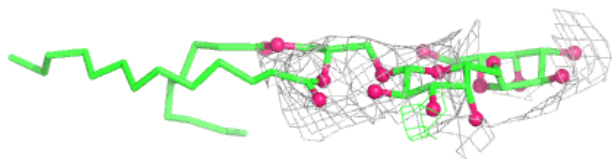
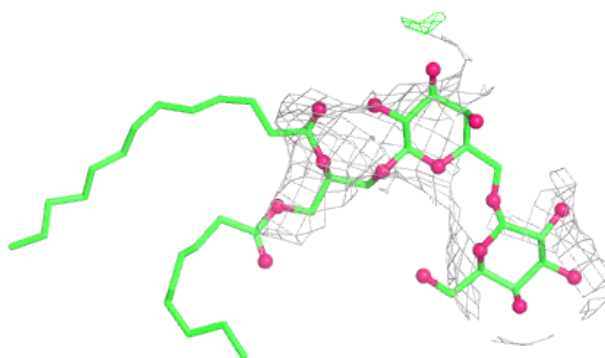


Electron density around BCR j 102:

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

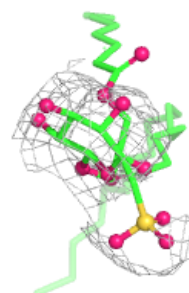
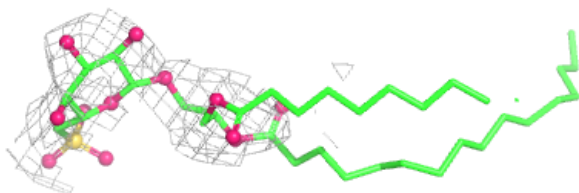
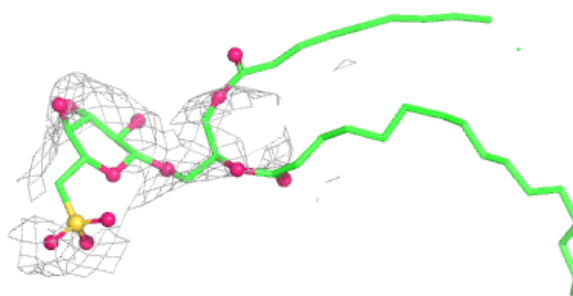
**Electron density around DGD B 625:**

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

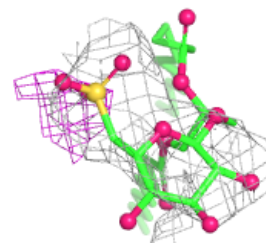
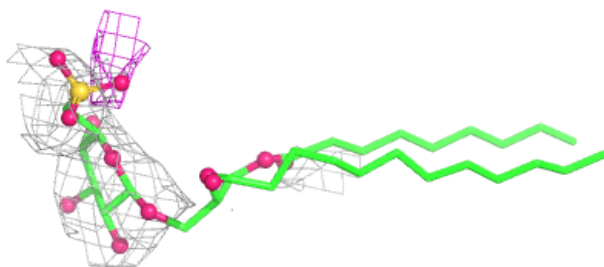
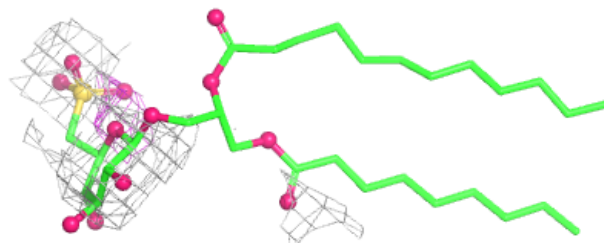


Electron density around SQD B 626:

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

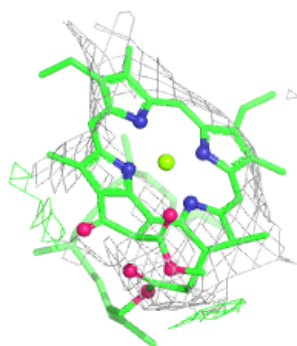
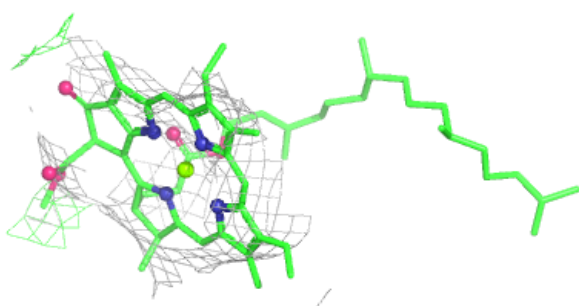
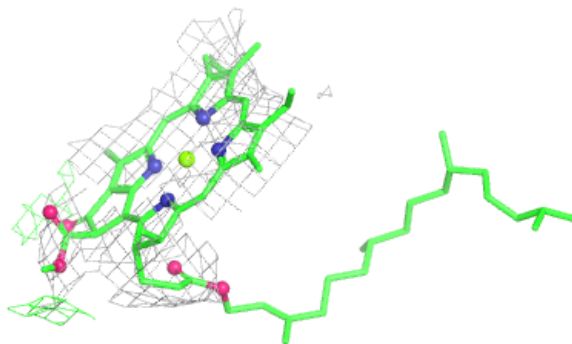
**Electron density around SQD d 403:**

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

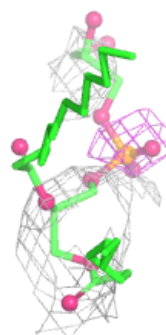
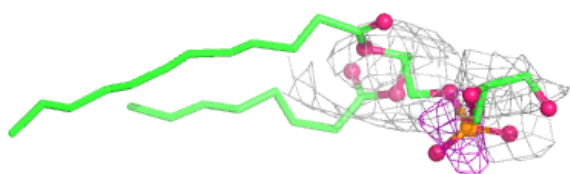
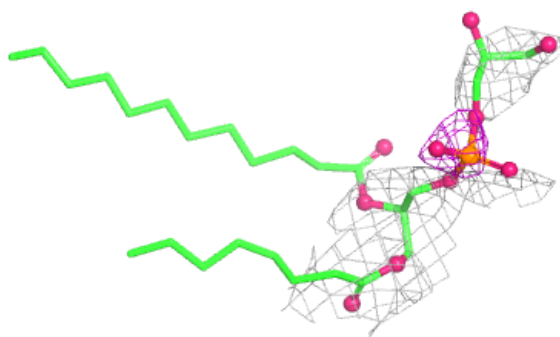


Electron density around CLA c 512:

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

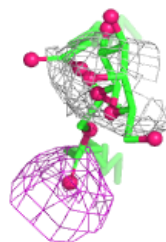
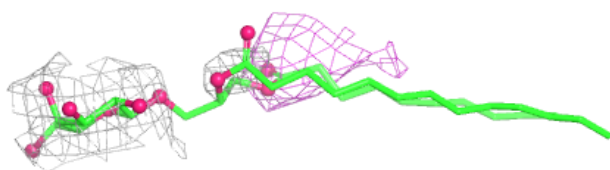
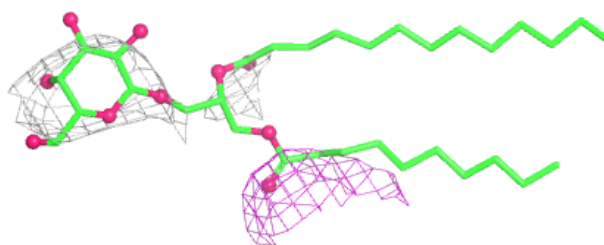
**Electron density around LHG C 519:**

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

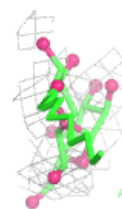
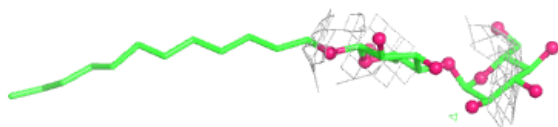
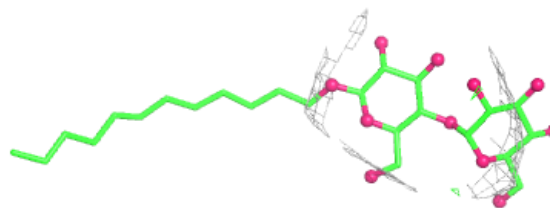


Electron density around LMG M 101:

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

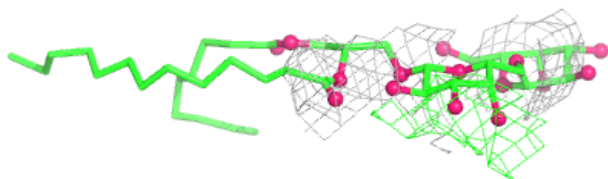
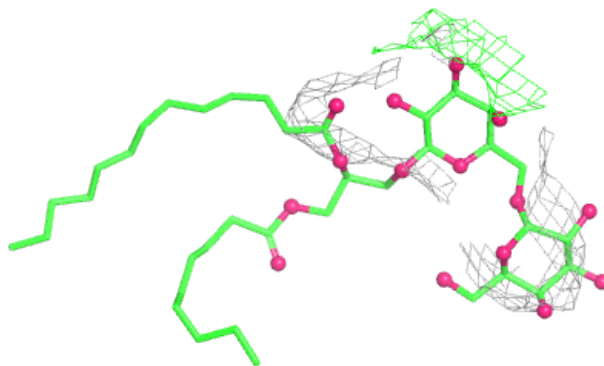
**Electron density around LMT B 624:**

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

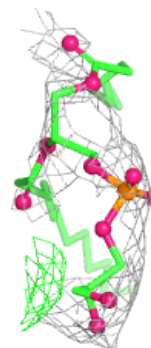
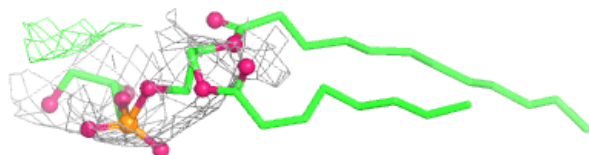
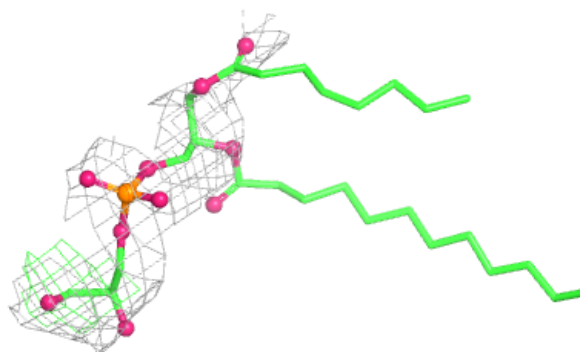


Electron density around DGD b 601:

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

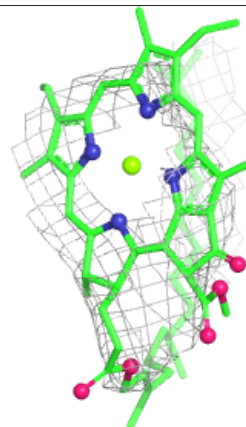
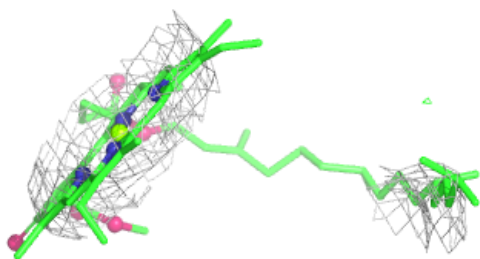
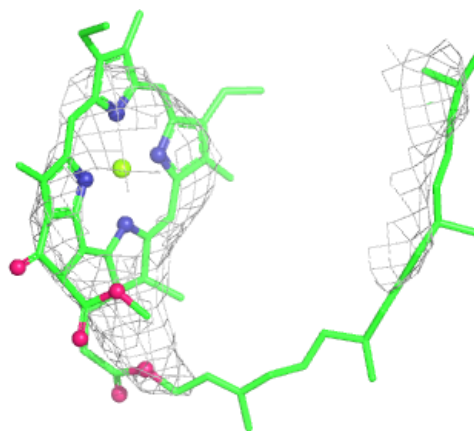
**Electron density around LHG c 519:**

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

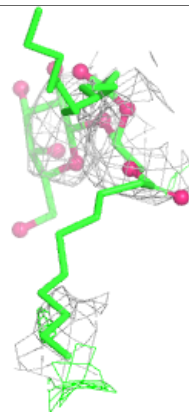
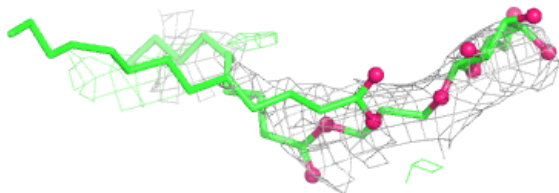


Electron density around CLA C 506:

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

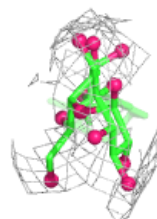
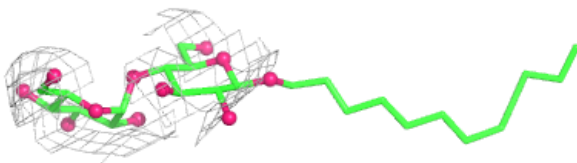
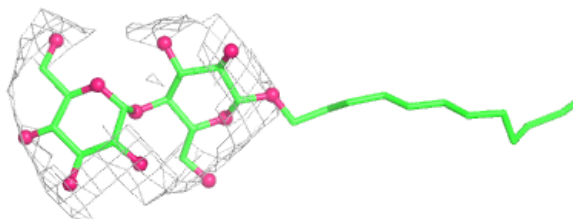
**Electron density around LMG A 414:**

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

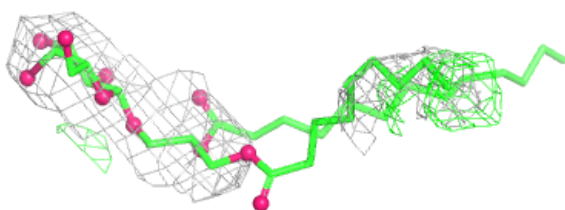
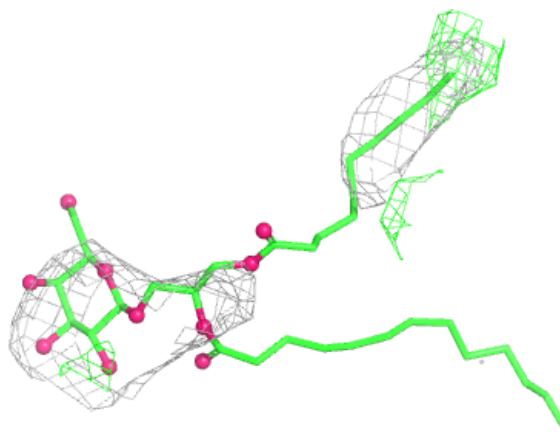


Electron density around LMT b 604:

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

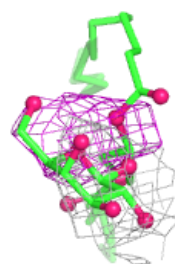
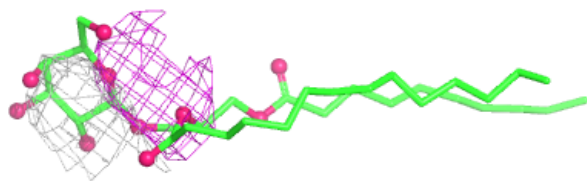
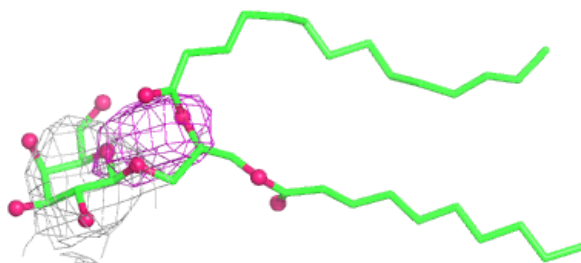
**Electron density around LMG a 402:**

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

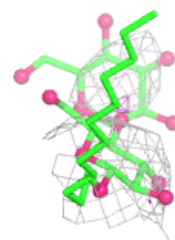
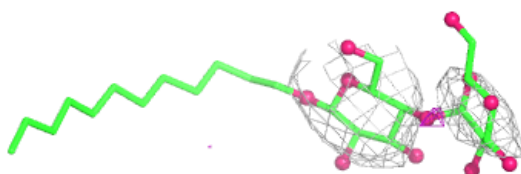
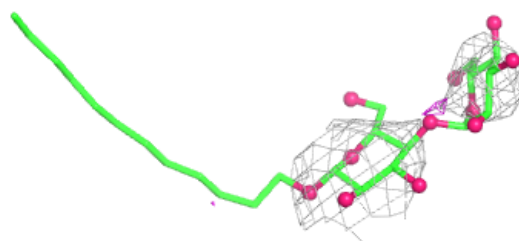


Electron density around LMG I 101:

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

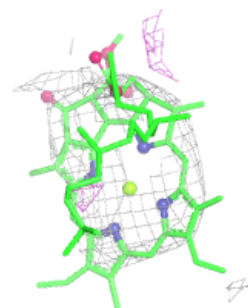
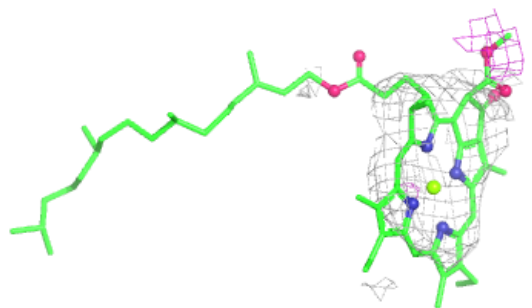
**Electron density around LMT M 102:**

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

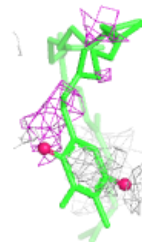
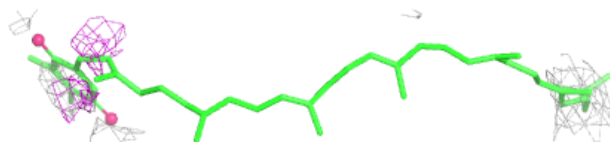
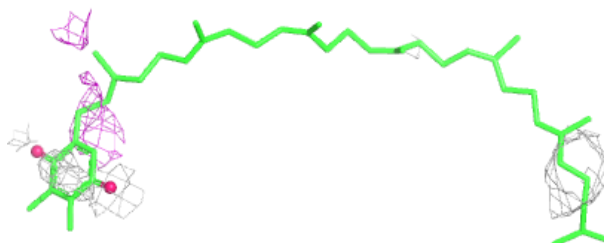


Electron density around CLA A 405:

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

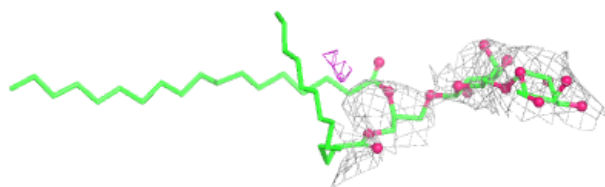
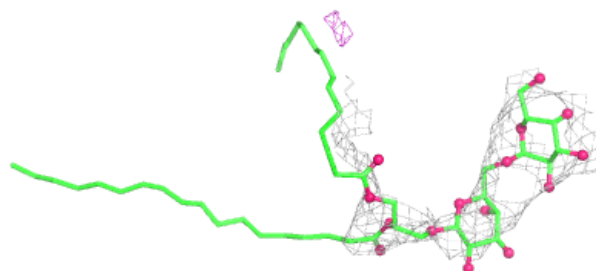
**Electron density around PL9 A 406:**

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

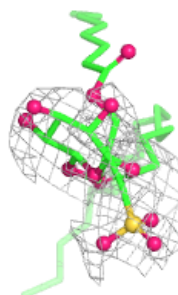
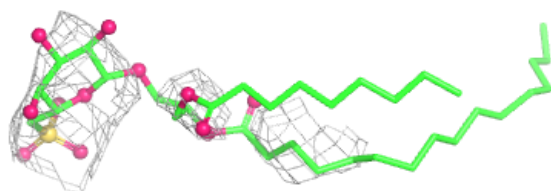
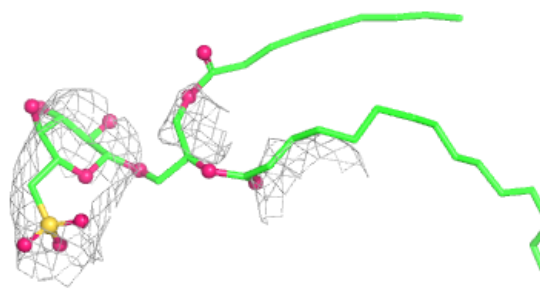


Electron density around DGD C 516:

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

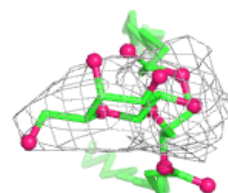
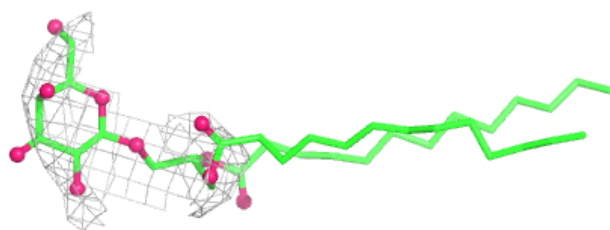
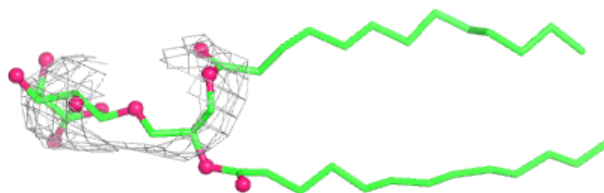
**Electron density around SQD b 602:**

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

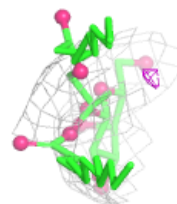
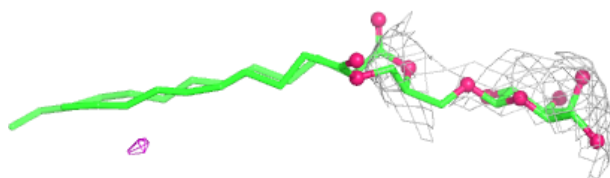
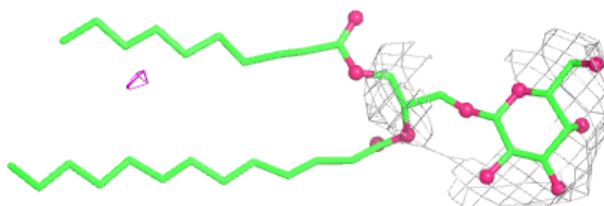


Electron density around LMG c 518:

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

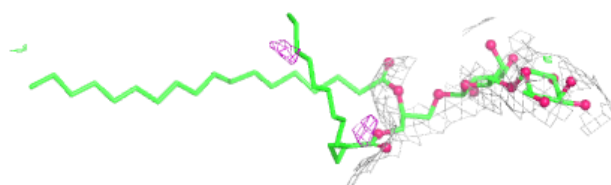
**Electron density around LMG m 101:**

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

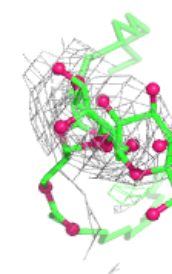
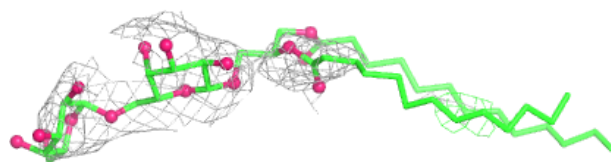


Electron density around DGD c 516:

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

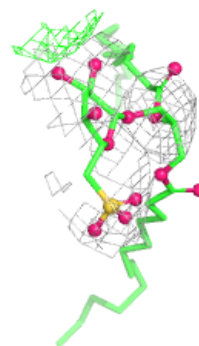
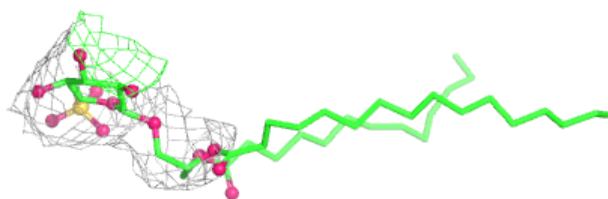
**Electron density around DGD a 410:**

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

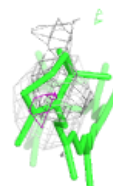
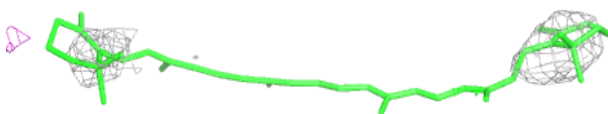
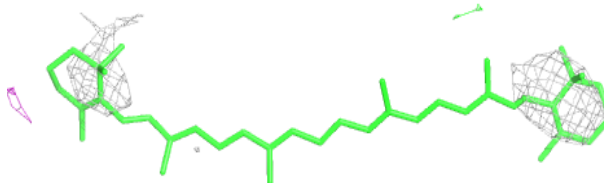


Electron density around SQD a 415:

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

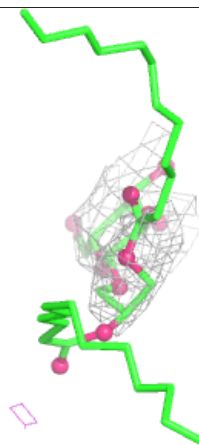
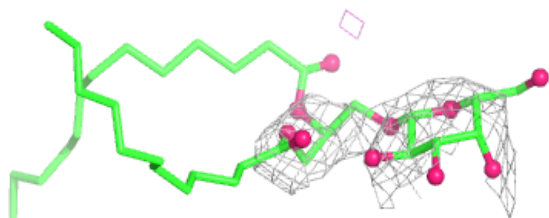
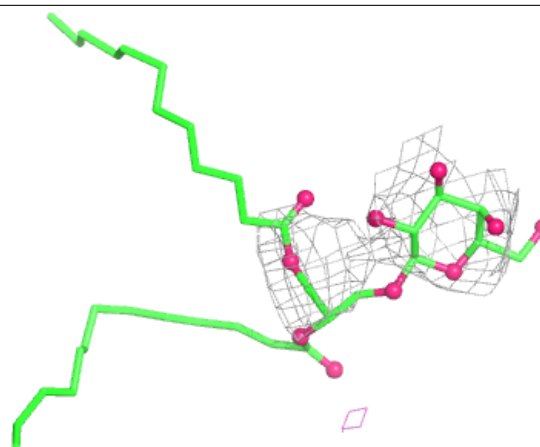
**Electron density around BCR b 621:**

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

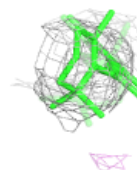
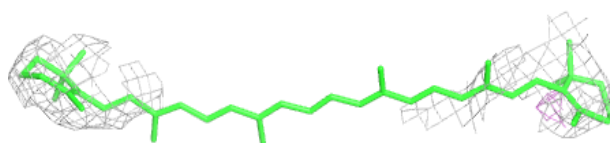
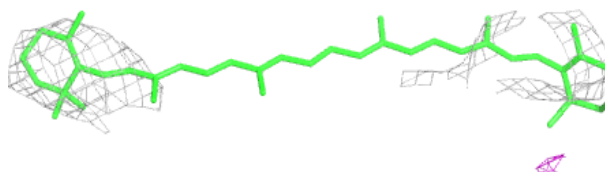


Electron density around LMG E 101:

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

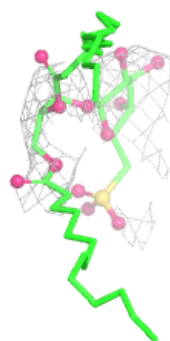
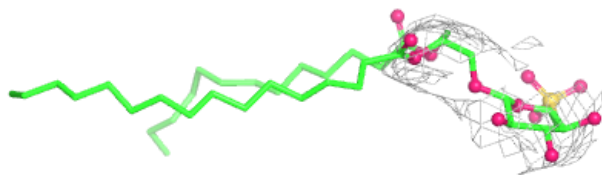
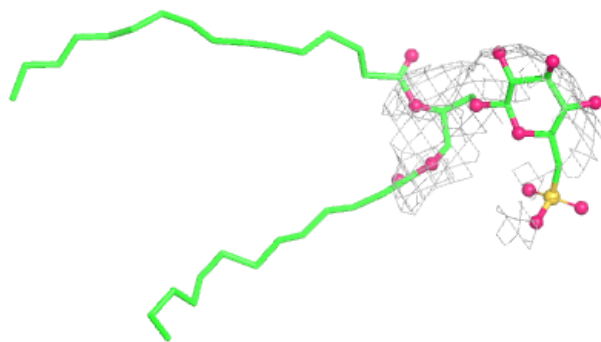
**Electron density around BCR b 623:**

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

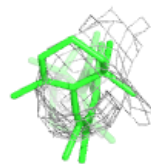
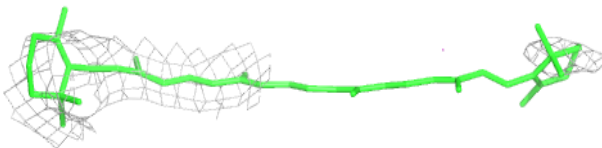
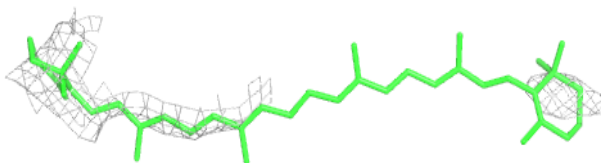


Electron density around SQD A 412:

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

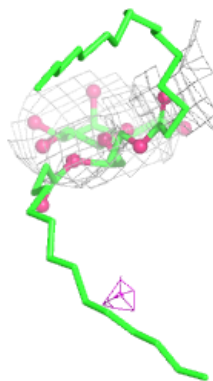
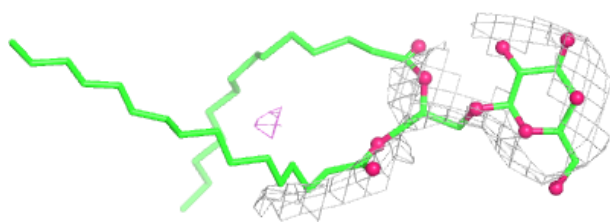
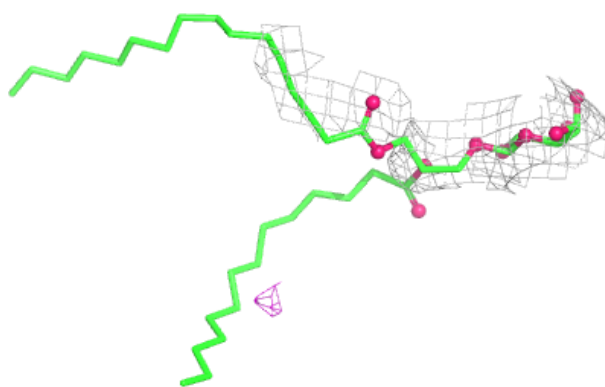
**Electron density around BCR H 102:**

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

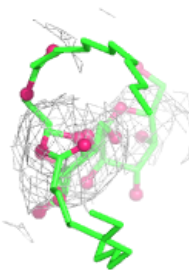
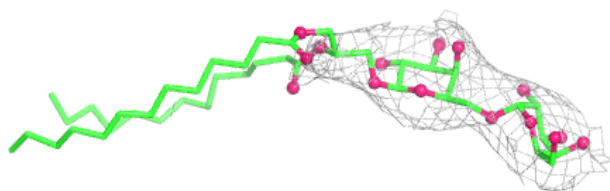
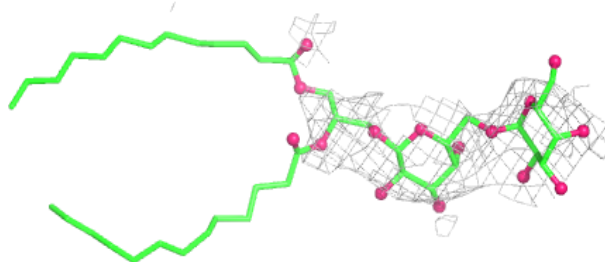


Electron density around LMG b 625:

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

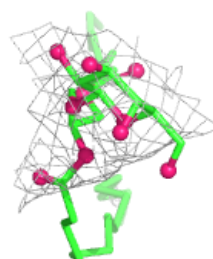
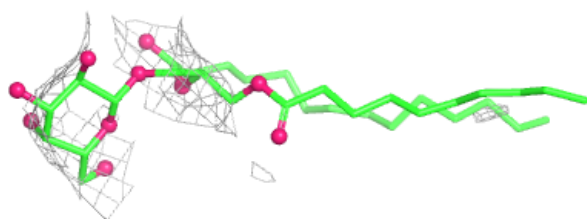
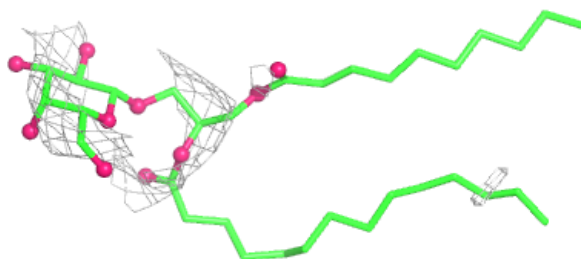
**Electron density around DGD A 408:**

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

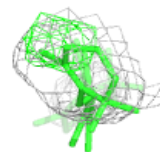
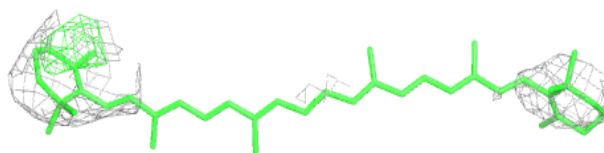


Electron density around LMG i 101:

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

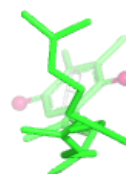
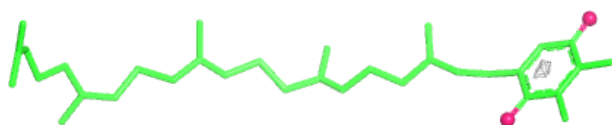
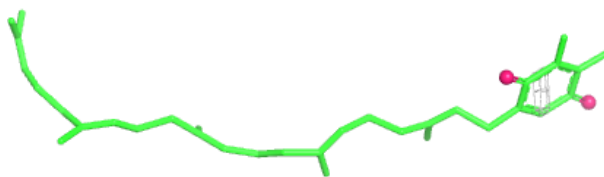
**Electron density around BCR b 622:**

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

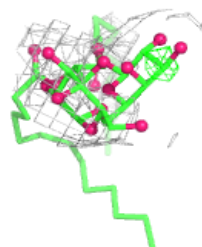
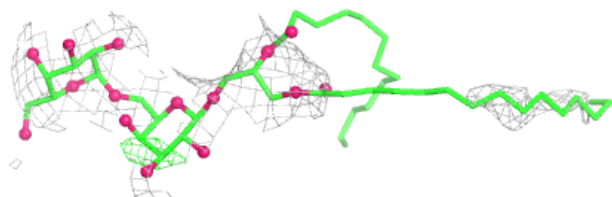


Electron density around PL9 j 101:

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

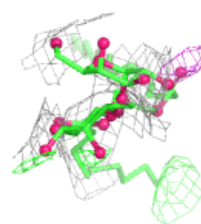
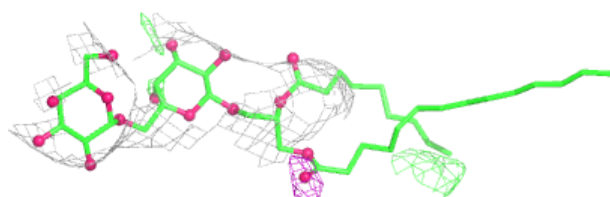
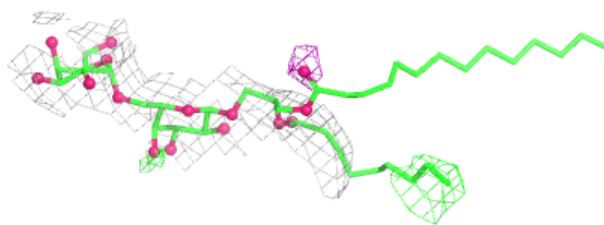
**Electron density around DGD b 624:**

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

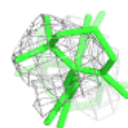
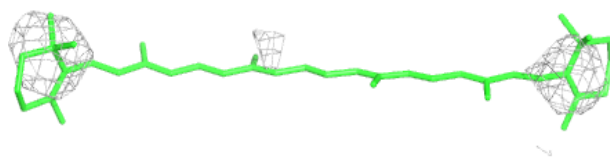
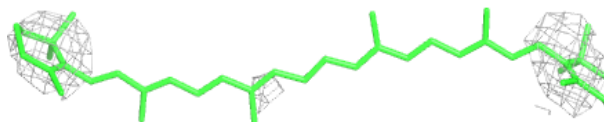


Electron density around DGD c 515:

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

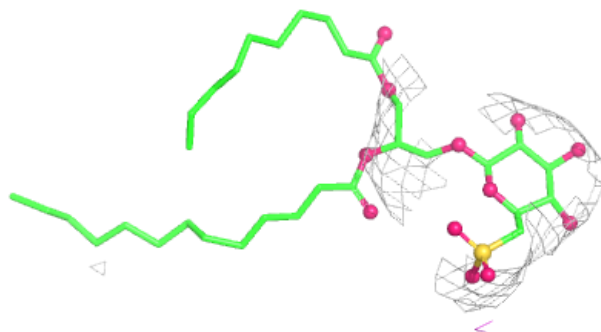
**Electron density around BCR a 409:**

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

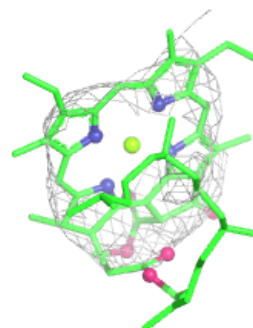
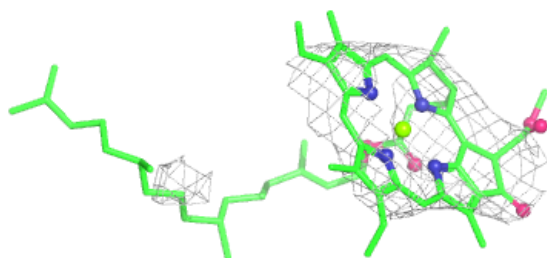
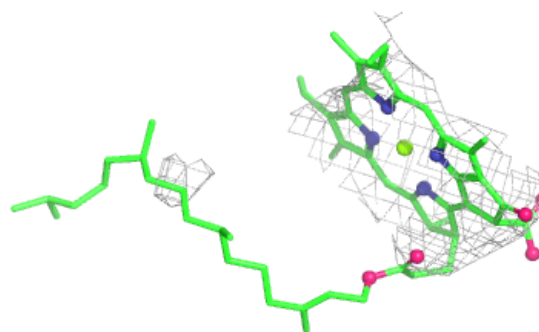


Electron density around SQD F 103:

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

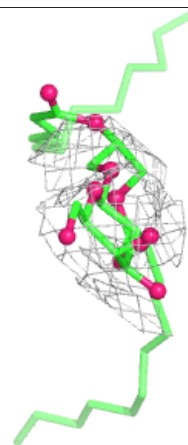
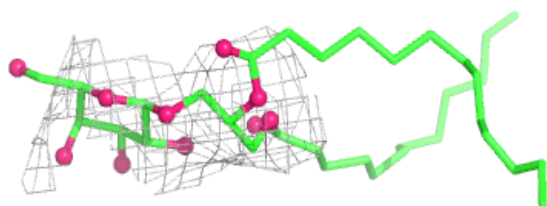
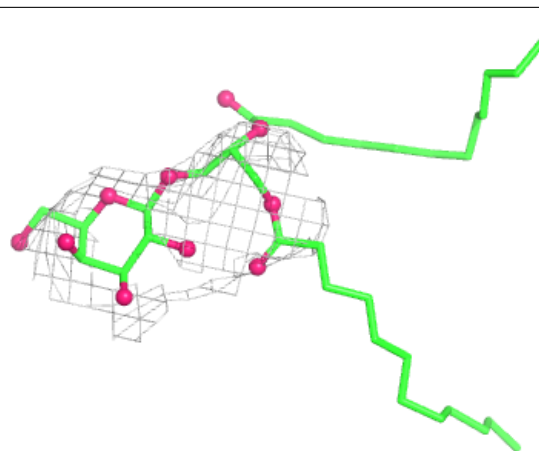
**Electron density around CLA C 512:**

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

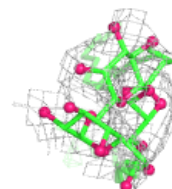
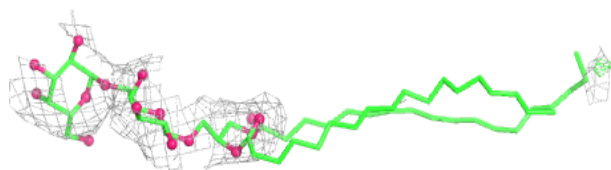


Electron density around LMG e 101:

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

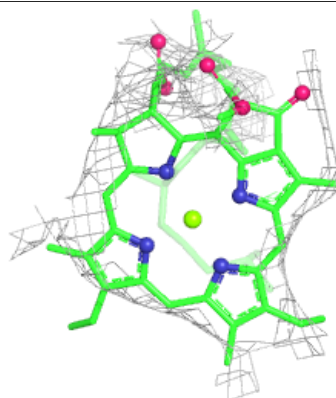
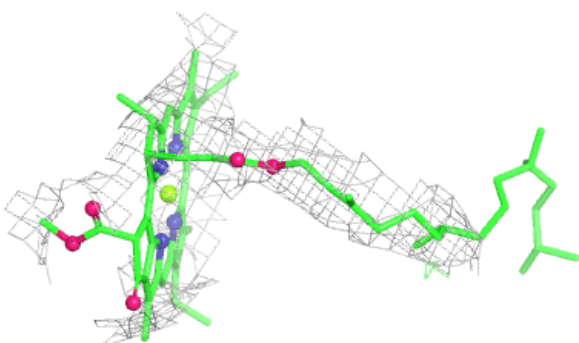
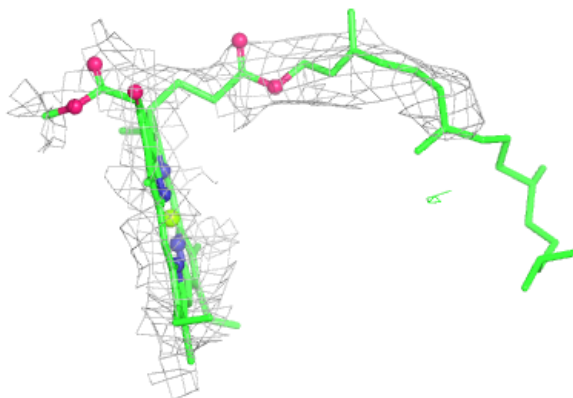
**Electron density around DGD C 517:**

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

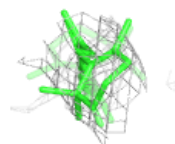
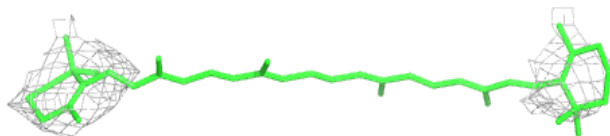
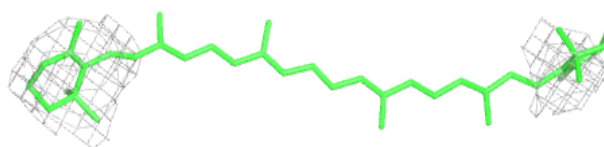


Electron density around CLA C 505:

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

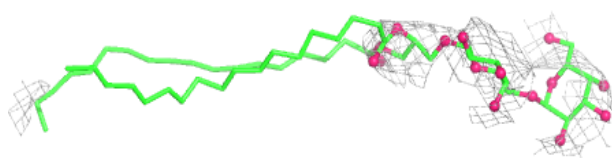
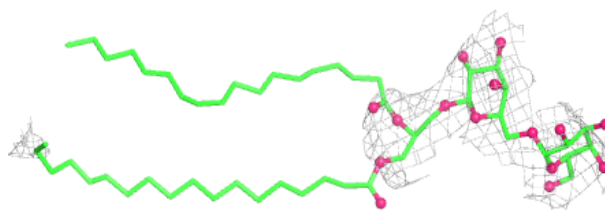
**Electron density around BCR K 102:**

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

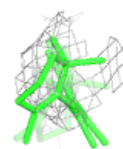
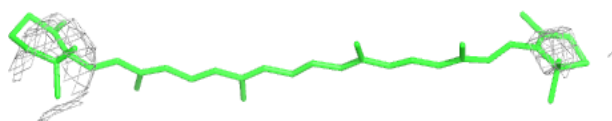
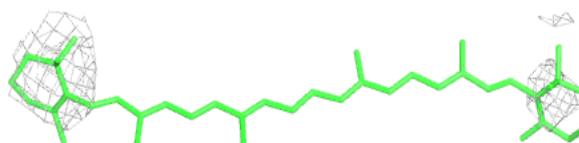


Electron density around DGD c 517:

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

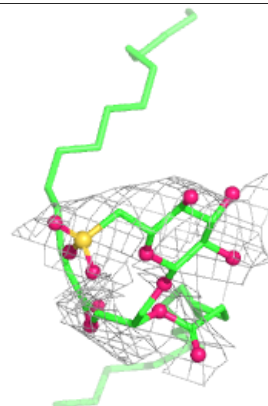
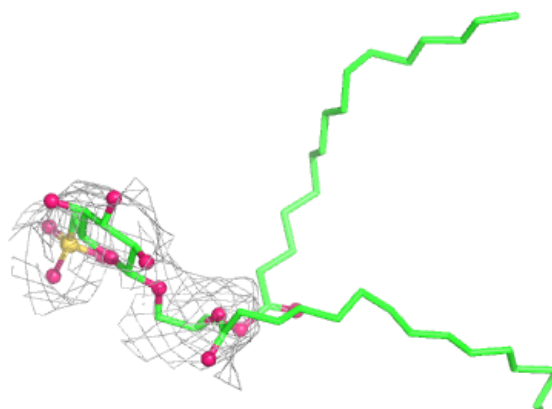
**Electron density around BCR c 514:**

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

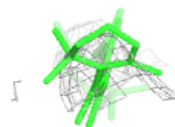
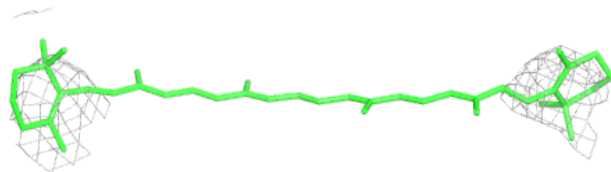
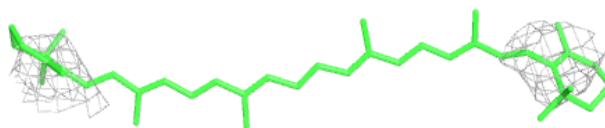


Electron density around SQD a 401:

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

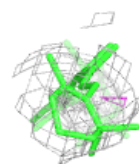
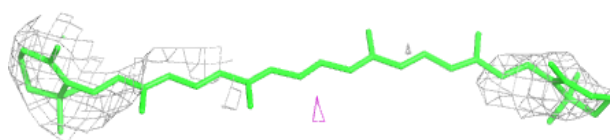
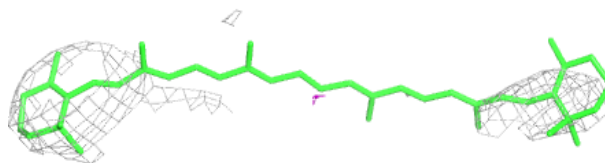
**Electron density around BCR c 521:**

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

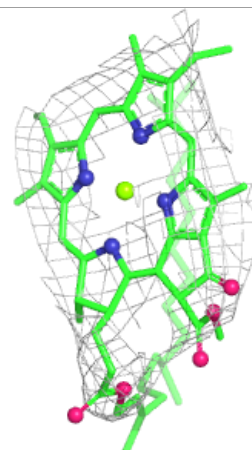
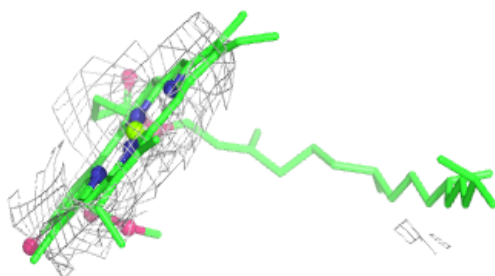
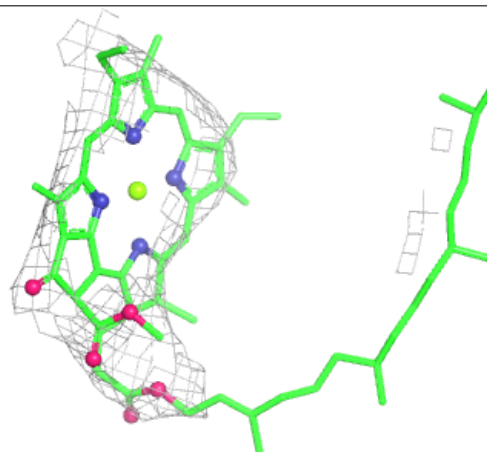


Electron density around BCR B 619:

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

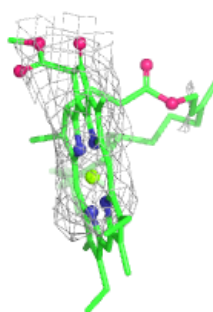
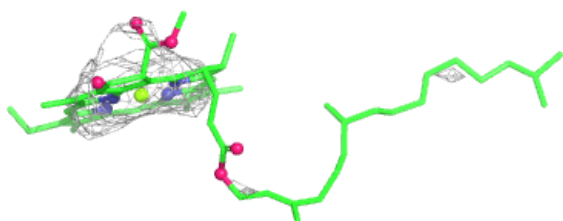
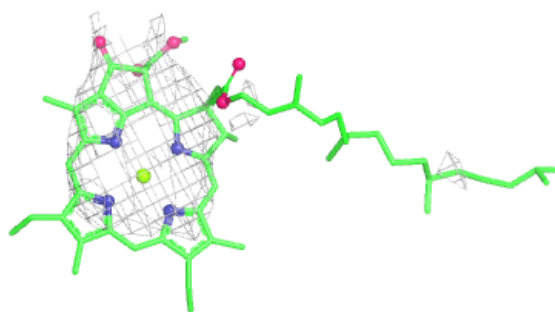
**Electron density around CLA c 506:**

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

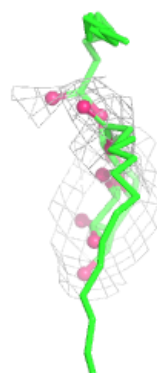
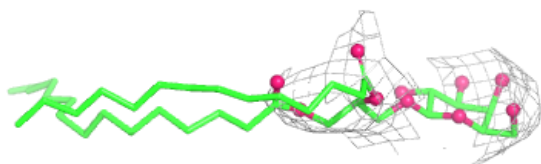


Electron density around CLA a 406:

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

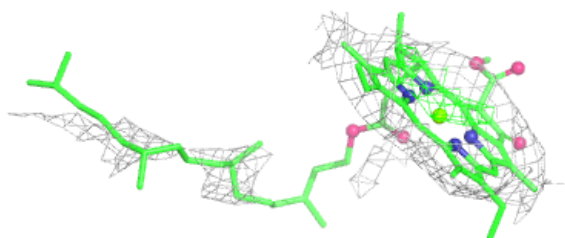
**Electron density around LMG c 522:**

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



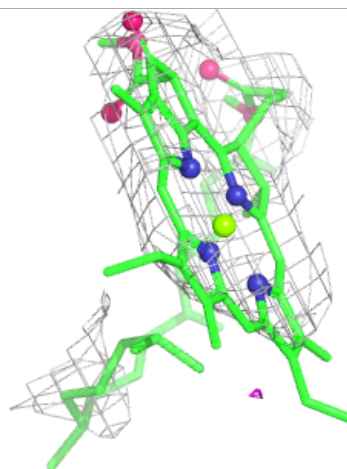
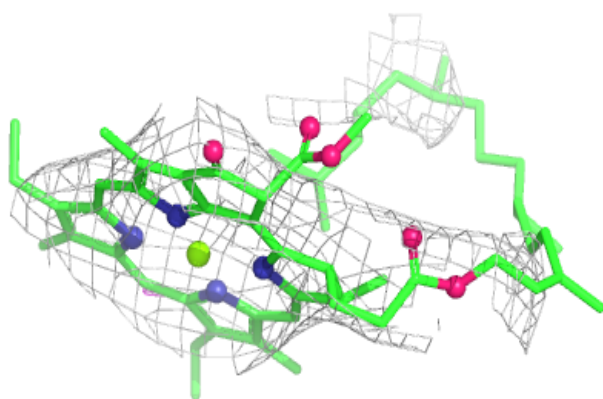
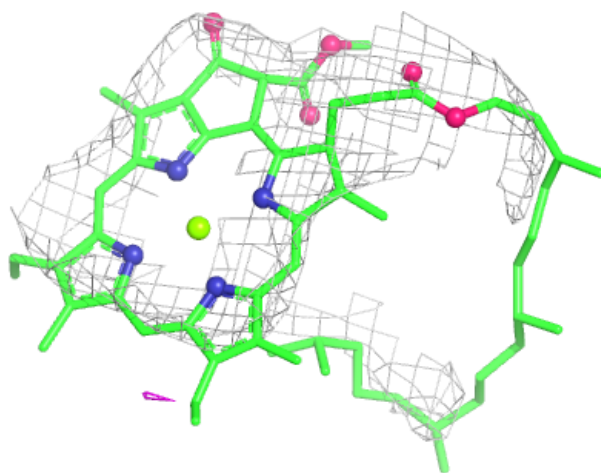
Electron density around CLA C 510:

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



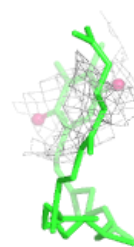
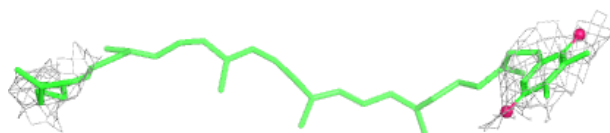
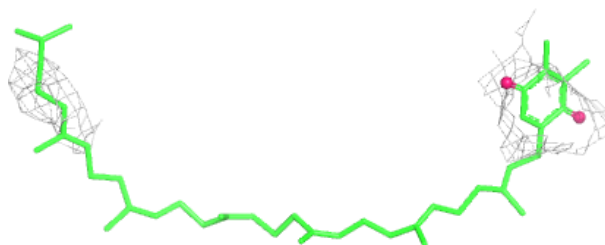
Electron density around CLA b 618:

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

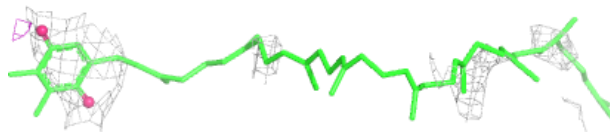
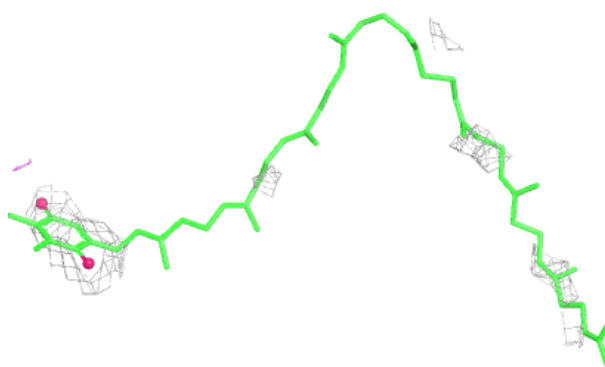


Electron density around PL9 a 408:

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

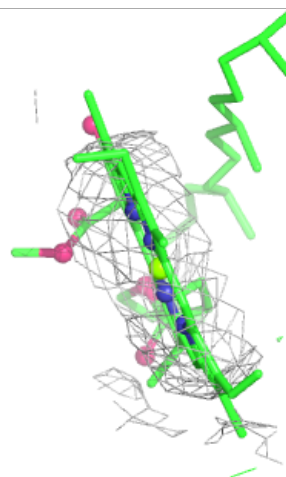
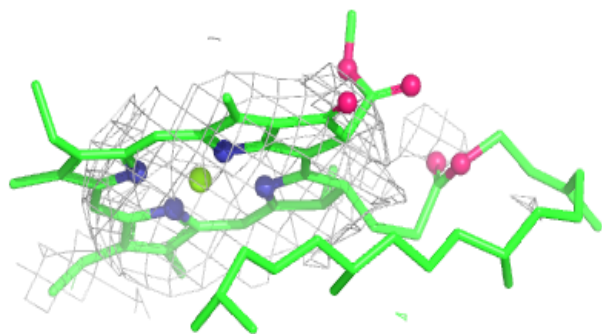
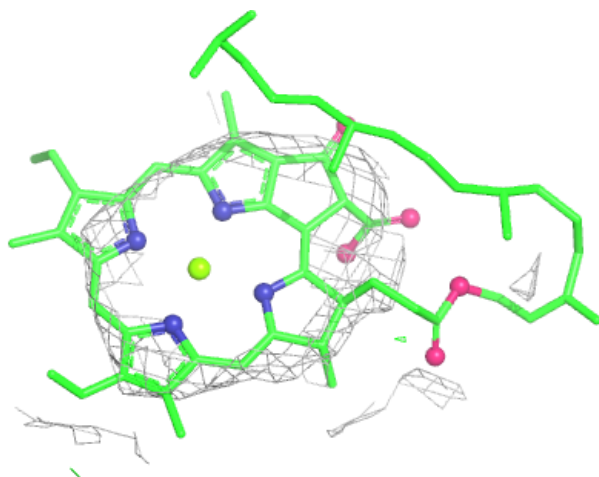
**Electron density around PL9 d 407:**

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



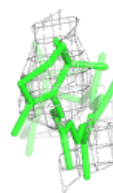
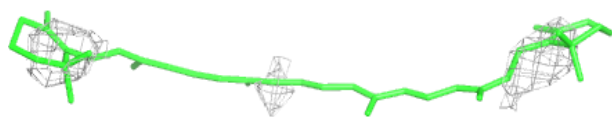
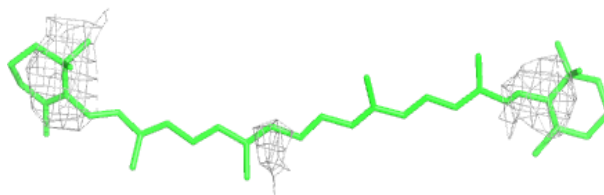
Electron density around CLA C 508:

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

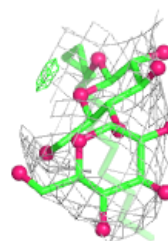
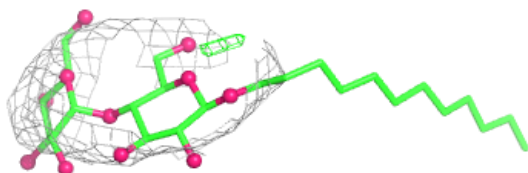
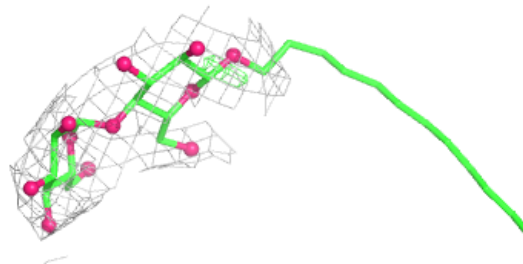


Electron density around BCR B 617:

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

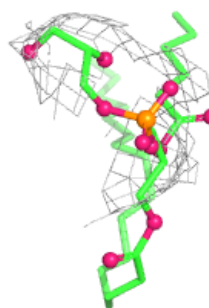
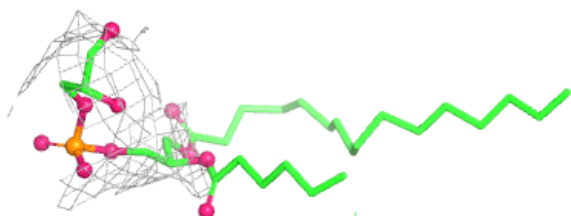
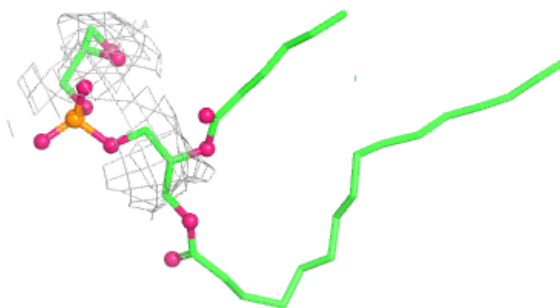
**Electron density around LMT M 103:**

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

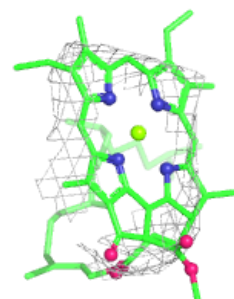
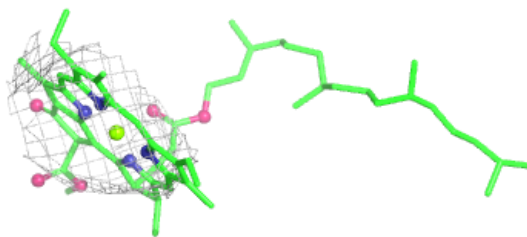
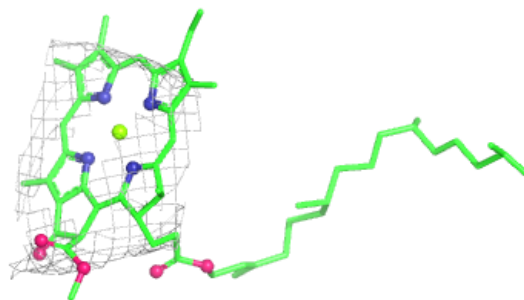


Electron density around LHG A 409:

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

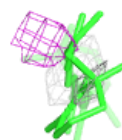
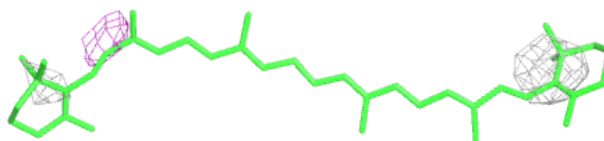
**Electron density around CLA c 510:**

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

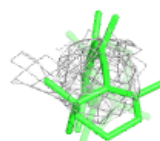
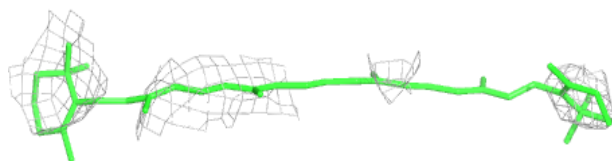
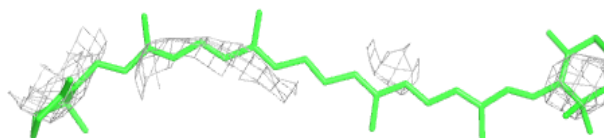


Electron density around BCR g 101:

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

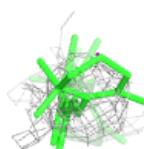
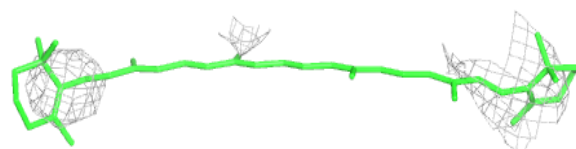
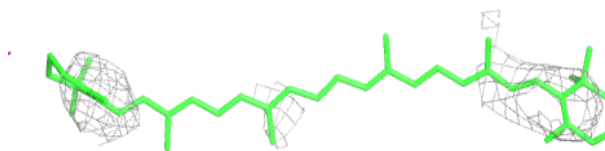
**Electron density around BCR x 101:**

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

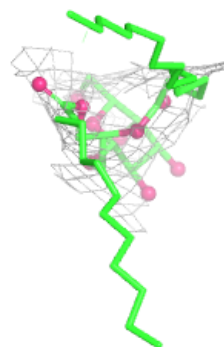
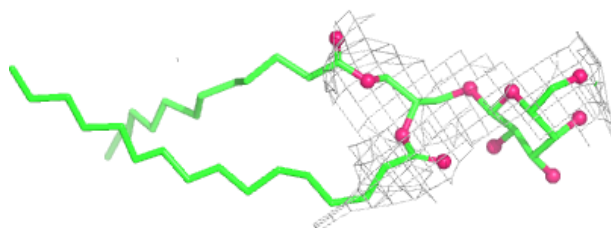
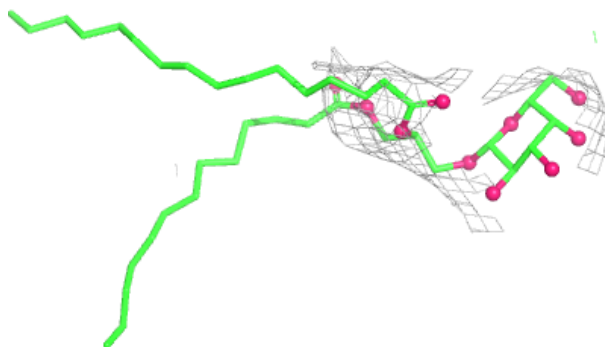


Electron density around BCR B 616:

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

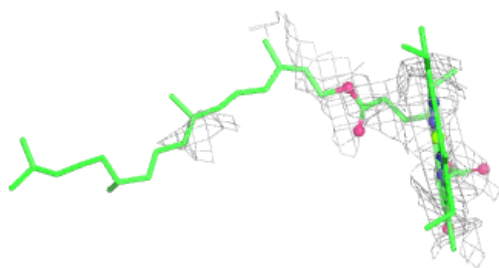
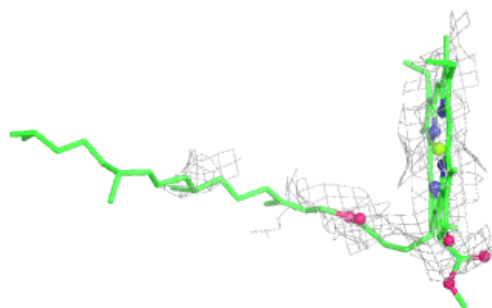
**Electron density around LMG D 409:**

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

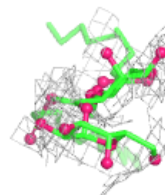
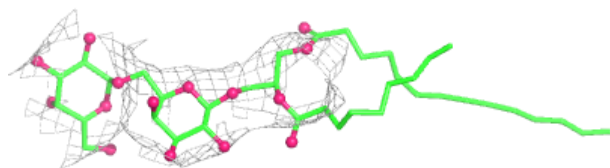


Electron density around CLA b 609:

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

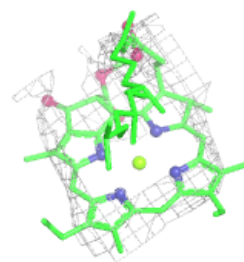
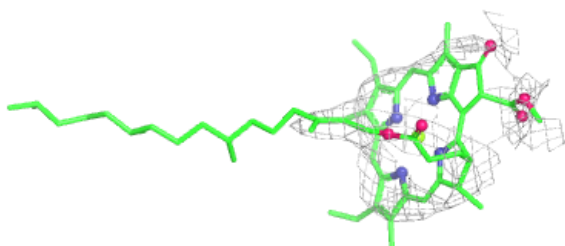
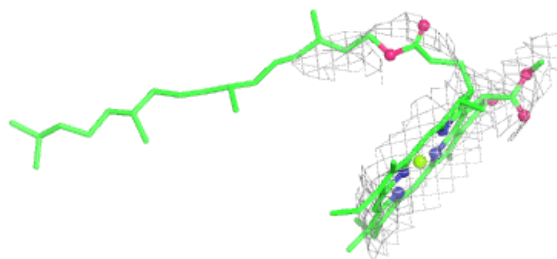
**Electron density around DGD C 515:**

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

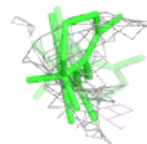
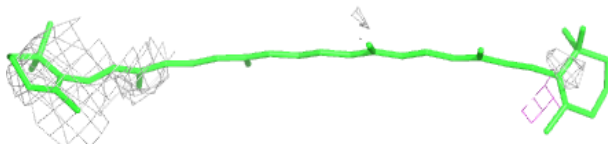
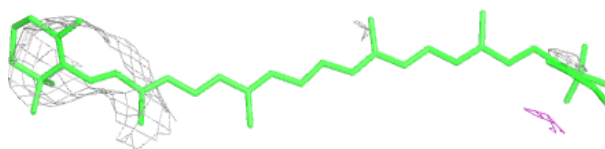


Electron density around CLA C 520:

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

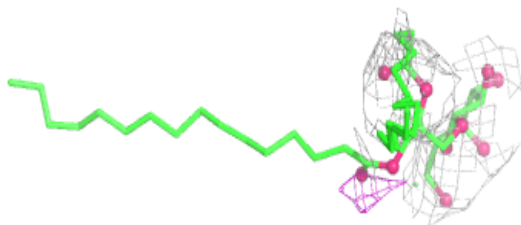
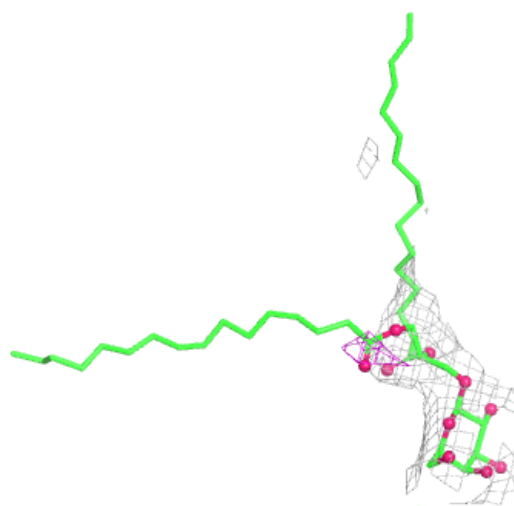
**Electron density around BCR b 620:**

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



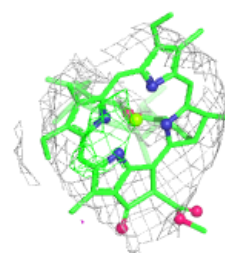
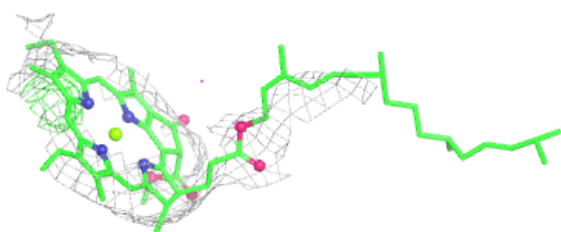
Electron density around LMG a 412:

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

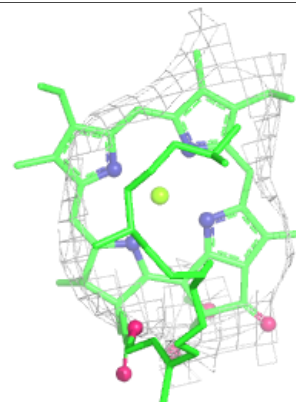
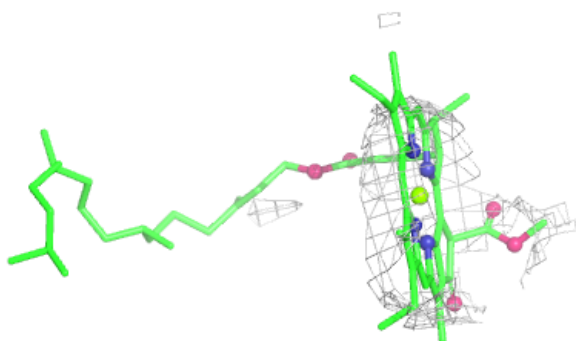
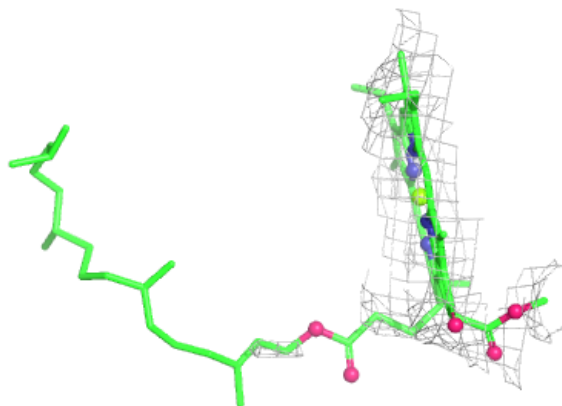


Electron density around CLA c 502:

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

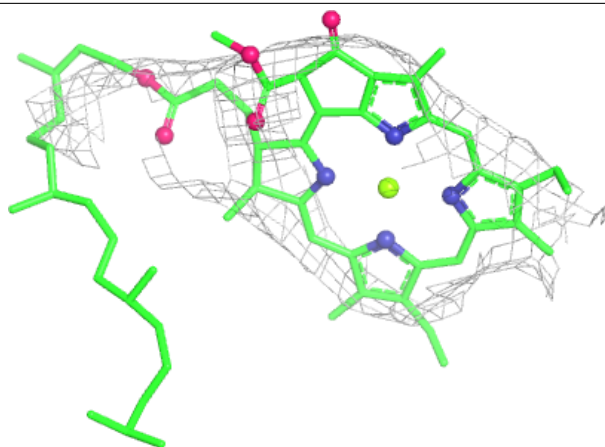
**Electron density around CLA c 505:**

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



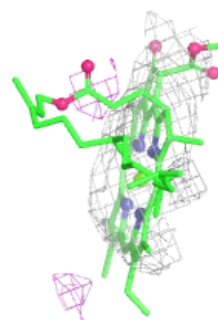
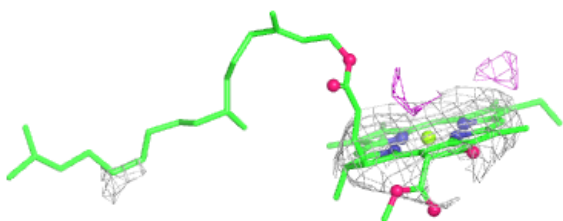
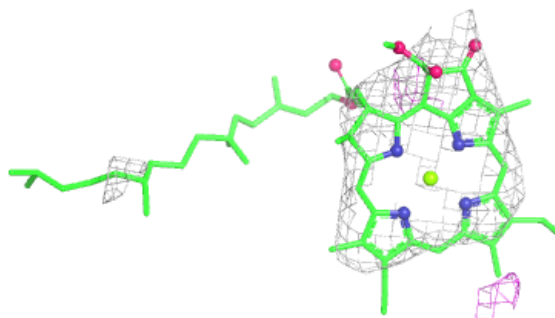
Electron density around CLA B 615:

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

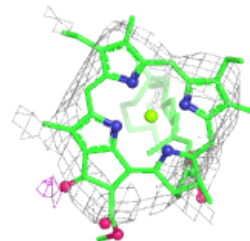
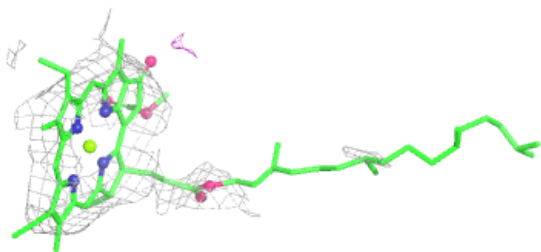
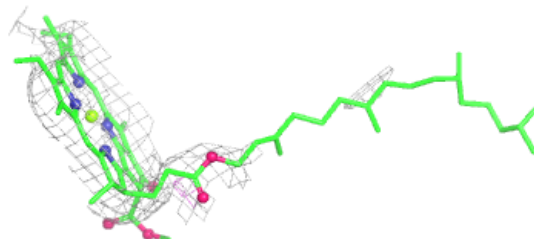


Electron density around CLA A 404:

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

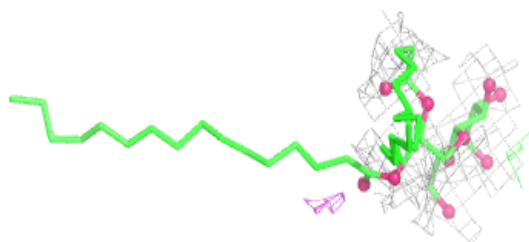
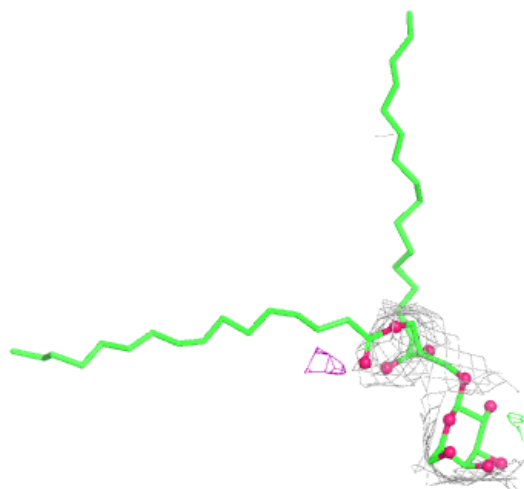
**Electron density around CLA B 603:**

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



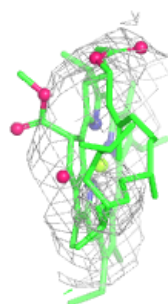
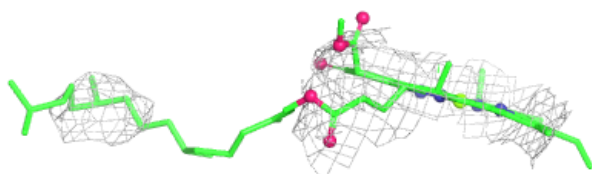
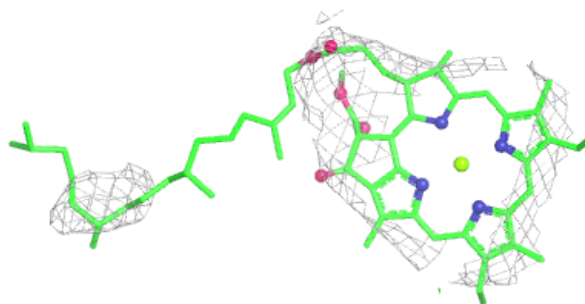
Electron density around LMG A 410:

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

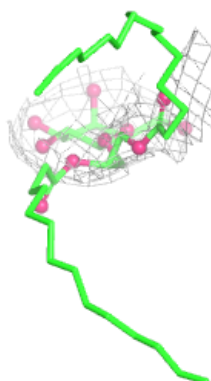


Electron density around CLA h 101:

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

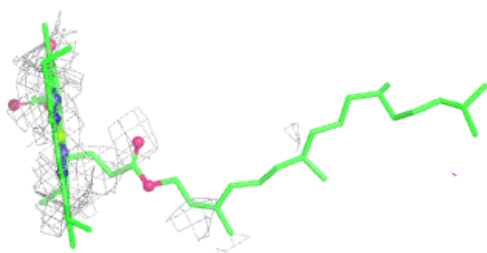
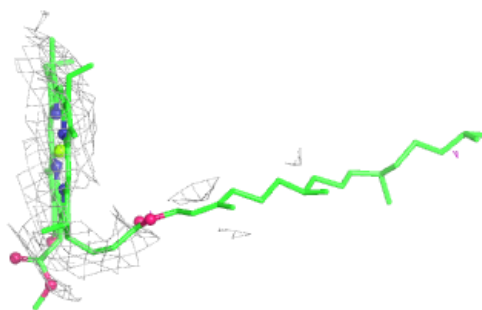
**Electron density around LMG B 621:**

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

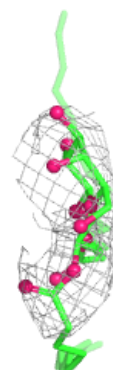
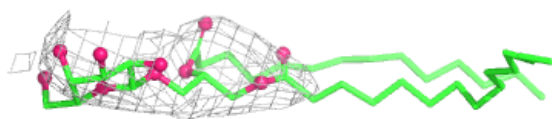
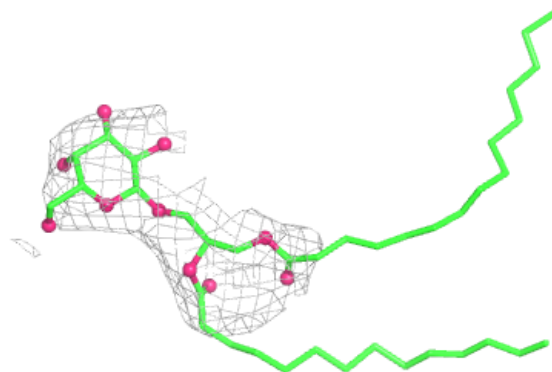


Electron density around CLA B 605:

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

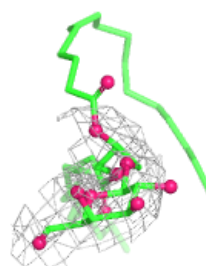
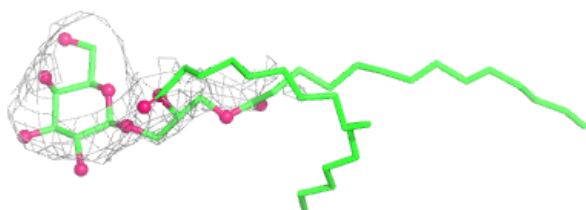
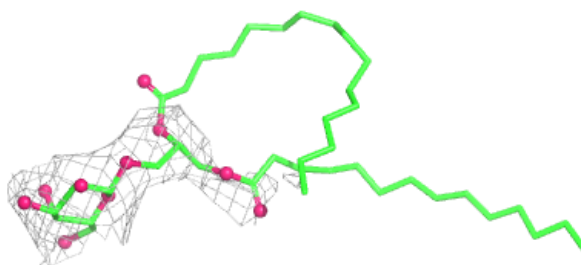
**Electron density around LMG C 521:**

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

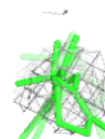
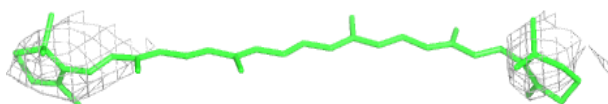
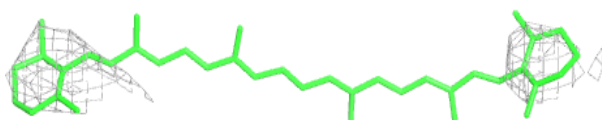


Electron density around LMG D 408:

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

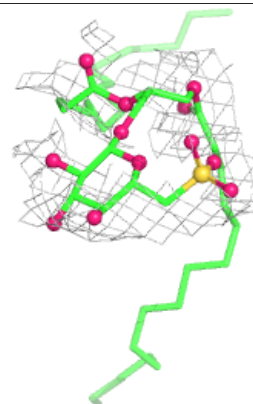
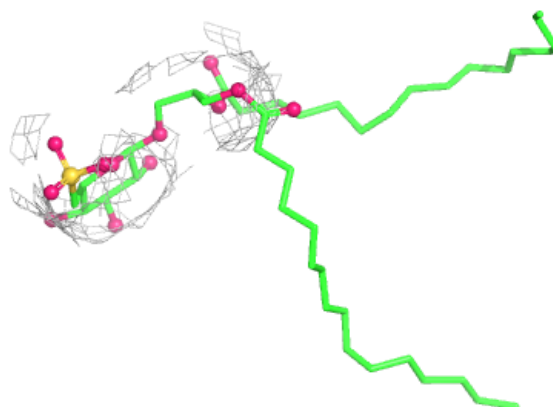
**Electron density around BCR C 514:**

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

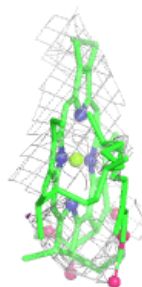
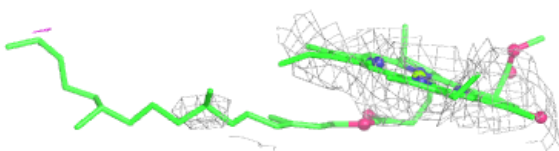
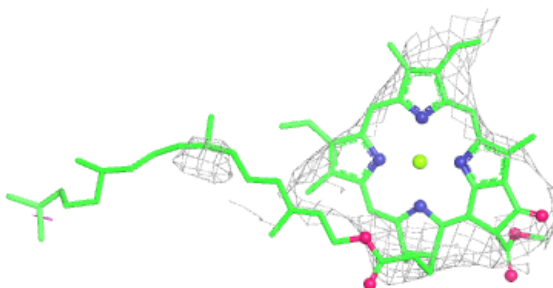


Electron density around SQD A 413:

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

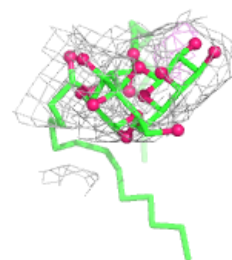
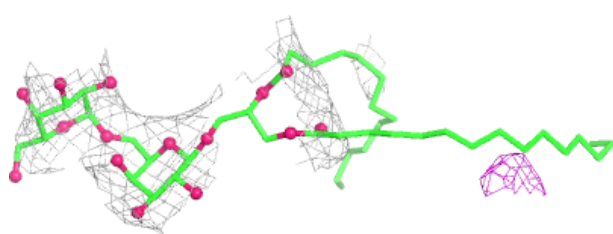
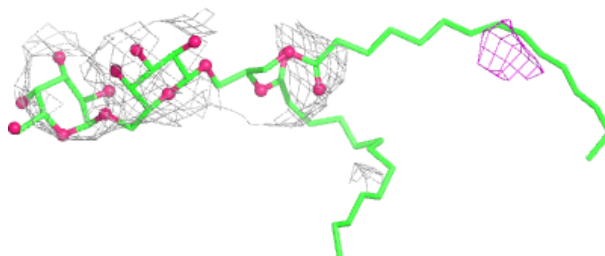
**Electron density around CLA b 606:**

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

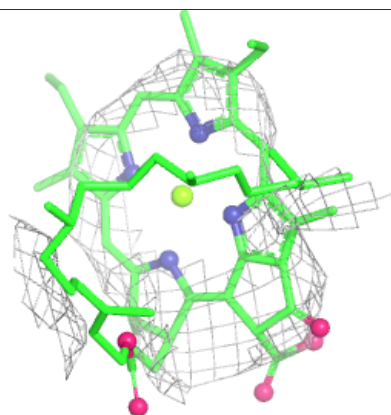
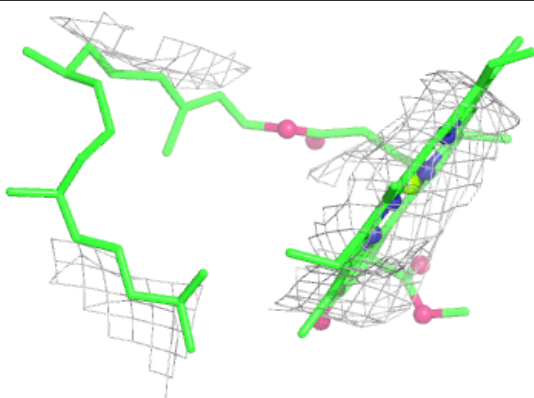
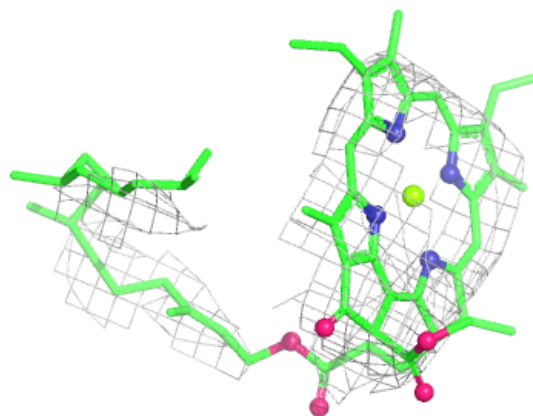


Electron density around DGD B 620:

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

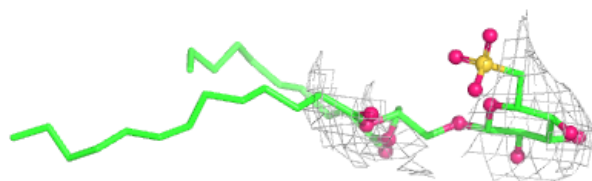
**Electron density around CLA c 503:**

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

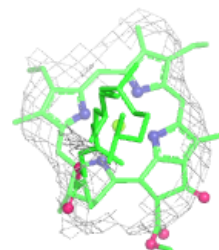


Electron density around SQD f 103:

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

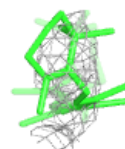
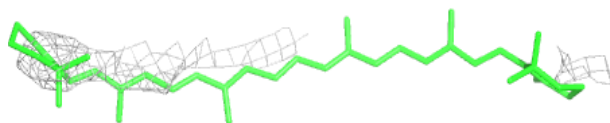
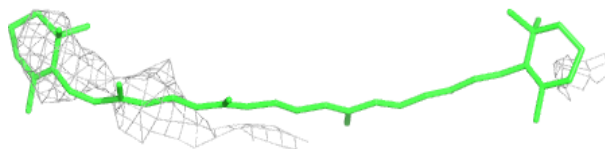
**Electron density around CLA b 607:**

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

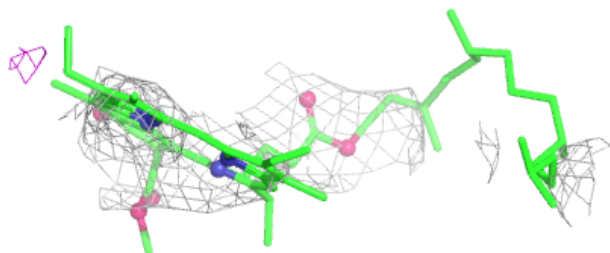
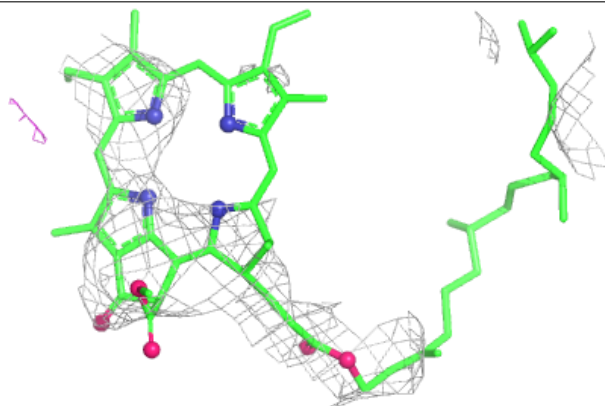


Electron density around BCR c 513:

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

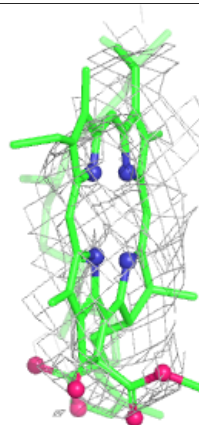
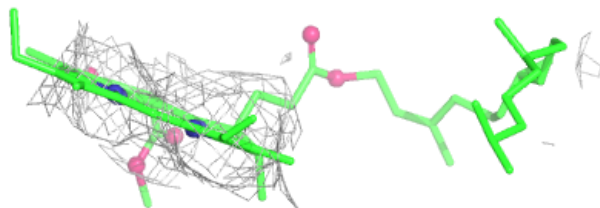
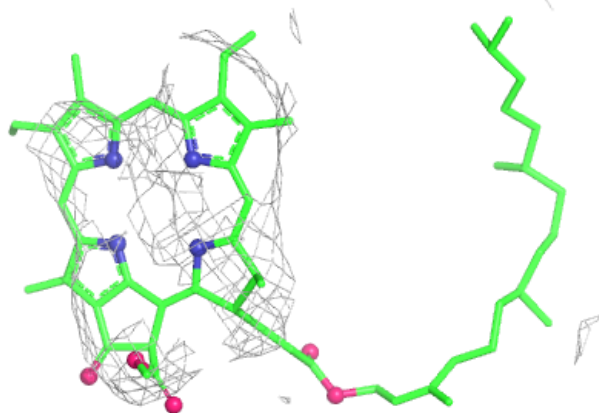
**Electron density around PHO D 402:**

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



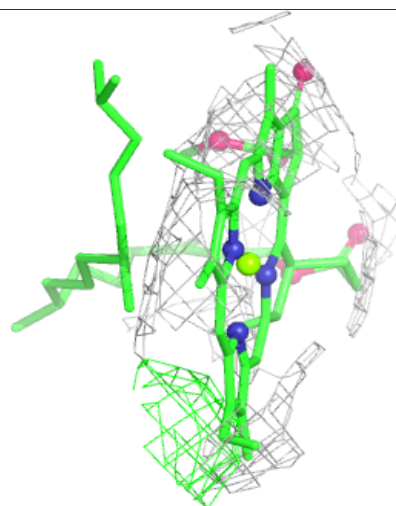
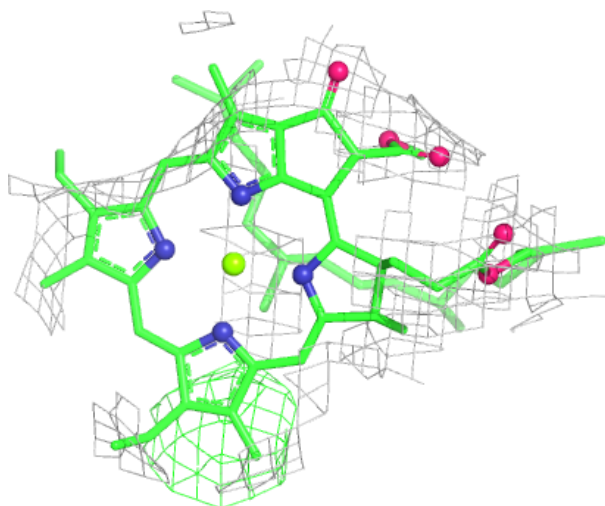
Electron density around PHO d 401:

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



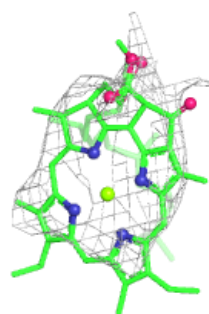
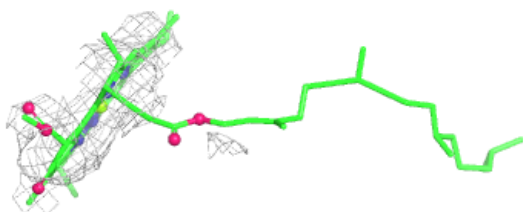
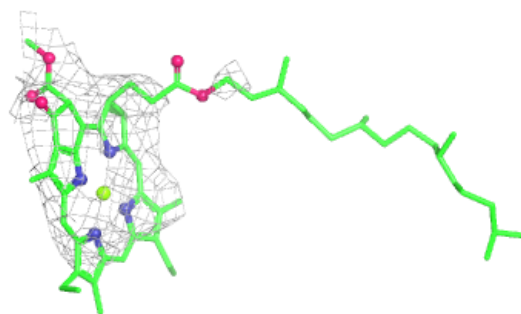
Electron density around CLA C 509:

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

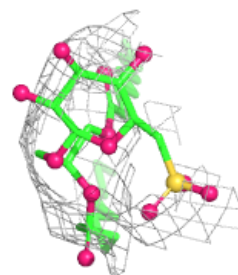
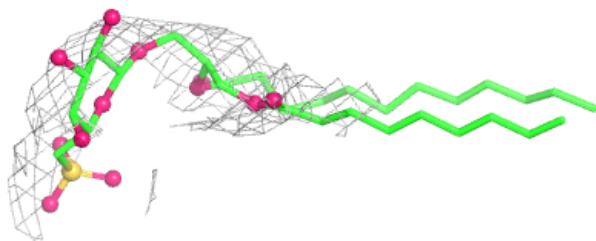


Electron density around CLA a 407:

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

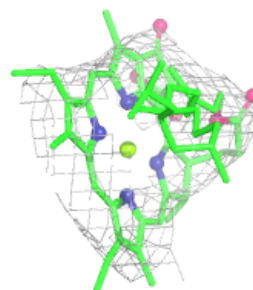
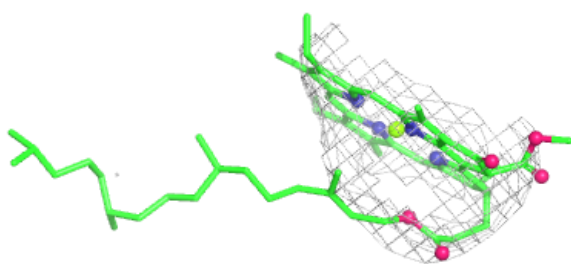
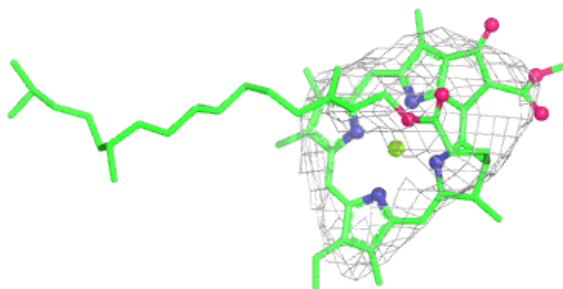
**Electron density around SQD B 622:**

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

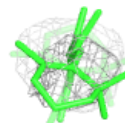
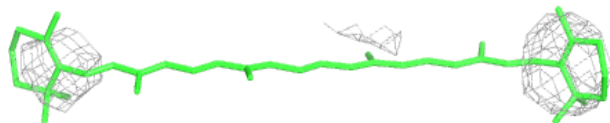
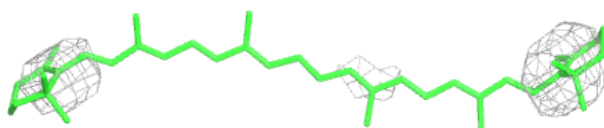


Electron density around CLA B 613:

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

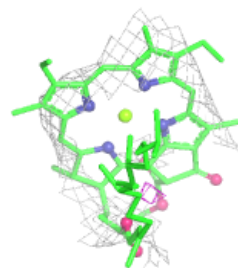
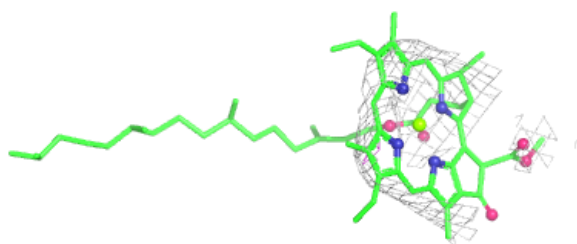
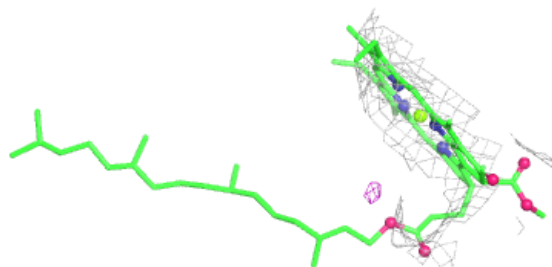
**Electron density around BCR A 407:**

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

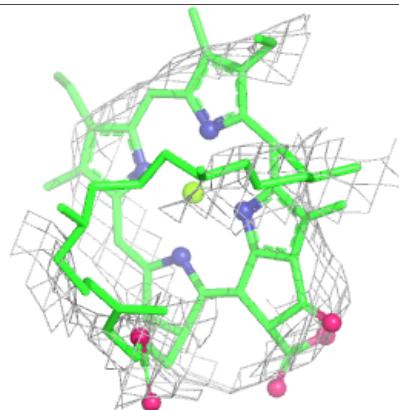
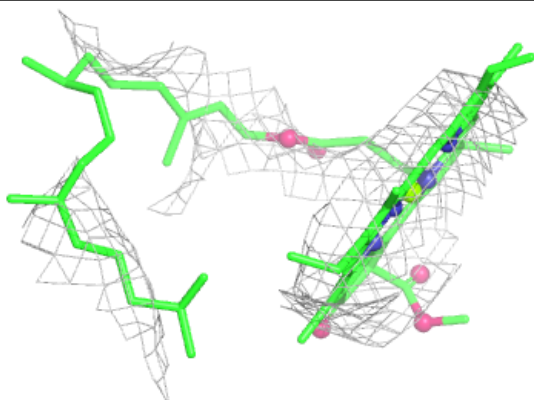
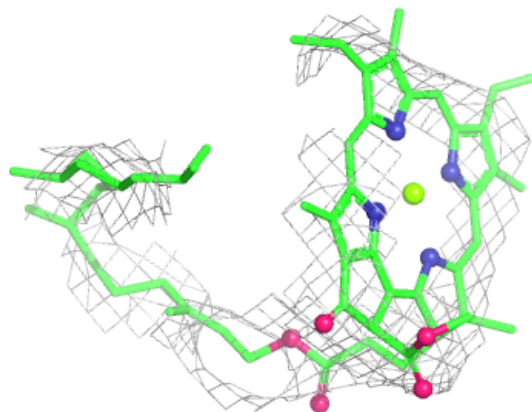


Electron density around CLA c 520:

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

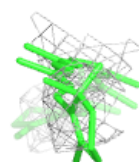
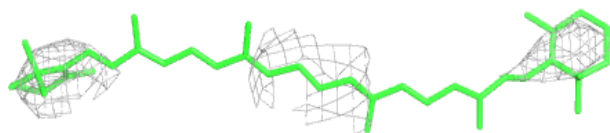
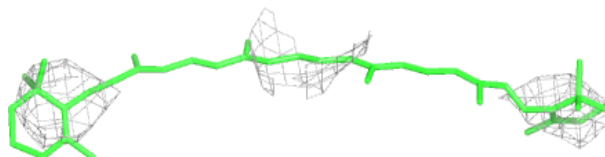
**Electron density around CLA C 503:**

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

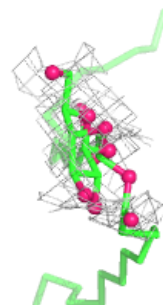
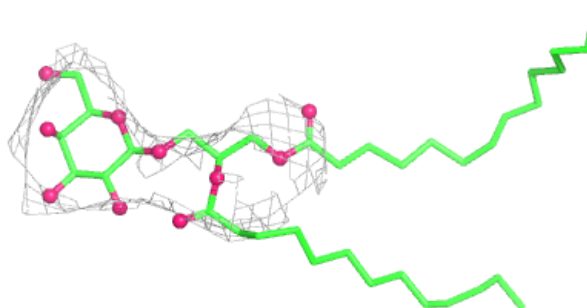


Electron density around BCR F 102:

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

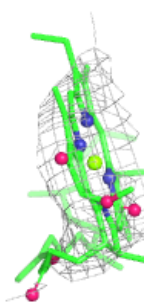
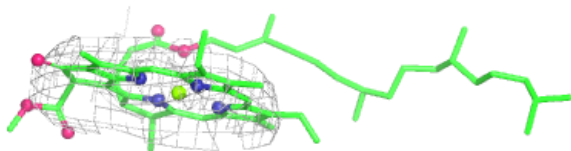
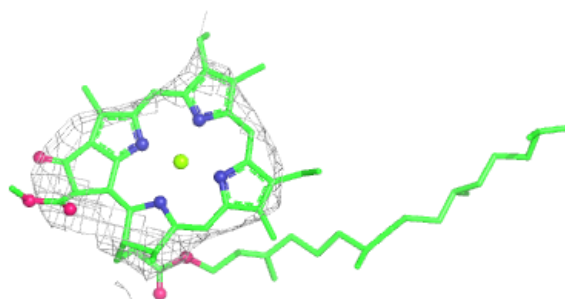
**Electron density around LMG D 412:**

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

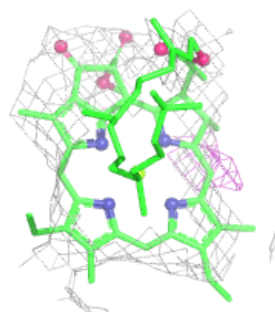
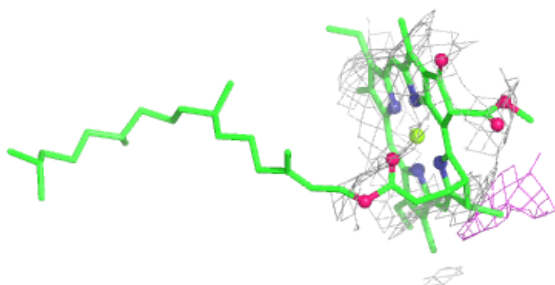
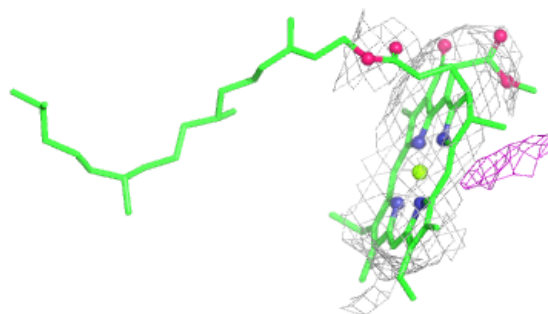


Electron density around CLA c 501:

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

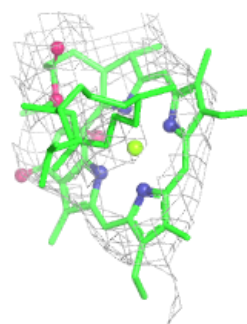
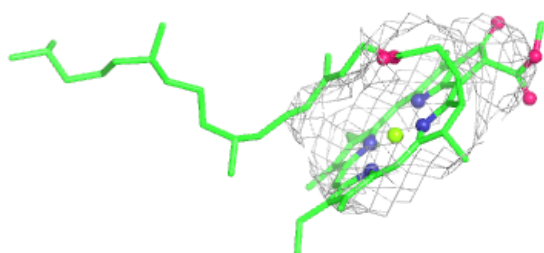
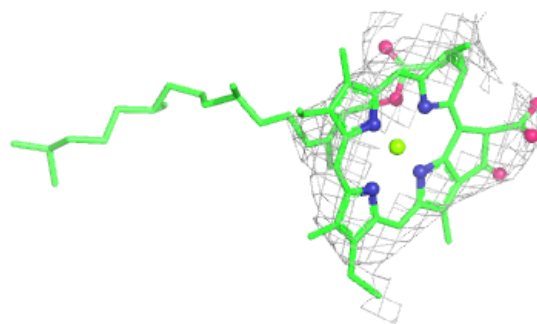
**Electron density around CLA C 507:**

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

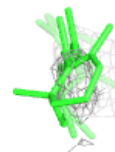
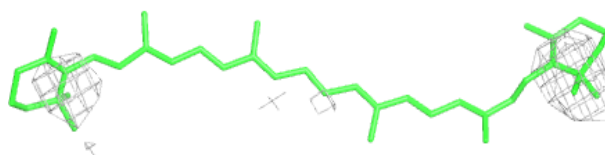


Electron density around CLA C 504:

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

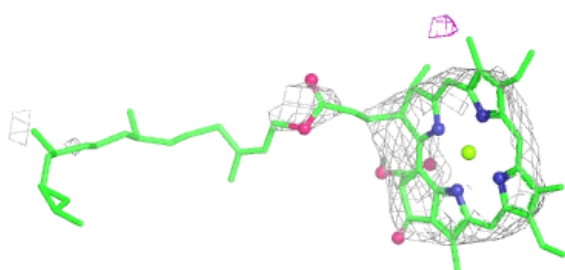
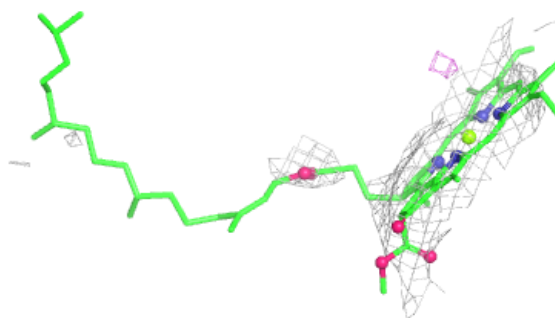
**Electron density around BCR y 101:**

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

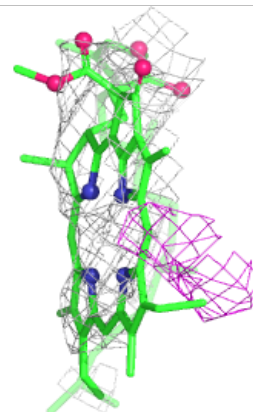
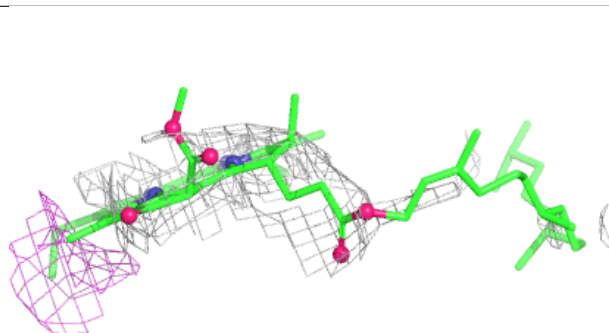
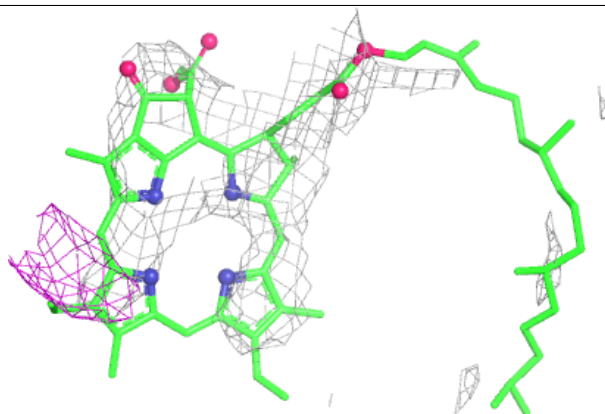


Electron density around CLA D 405:

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

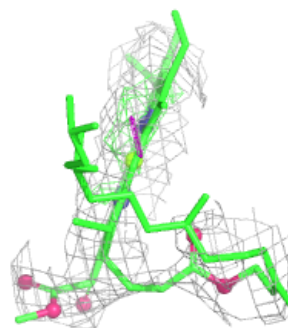
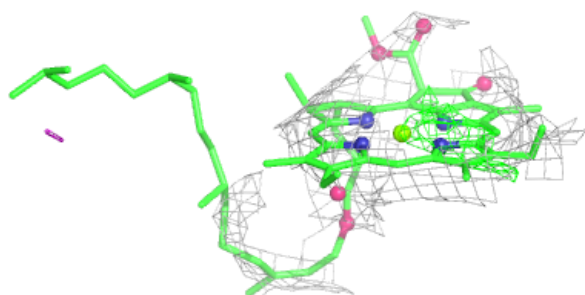
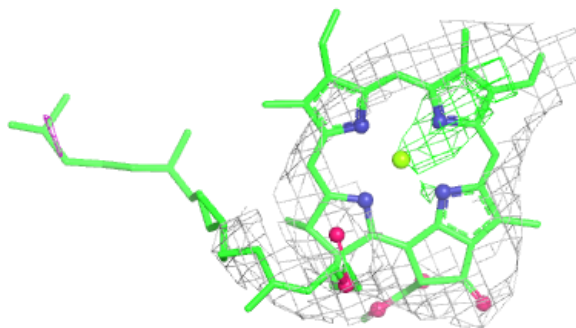
**Electron density around PHO D 401:**

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



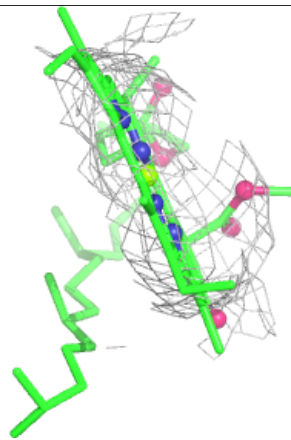
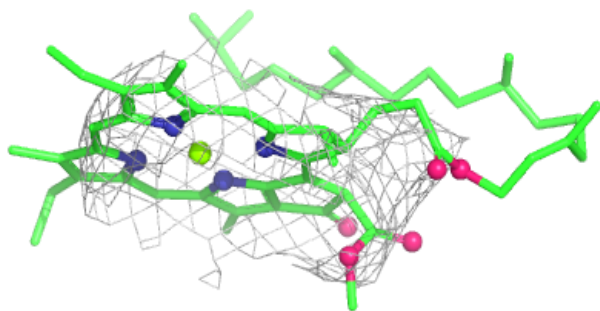
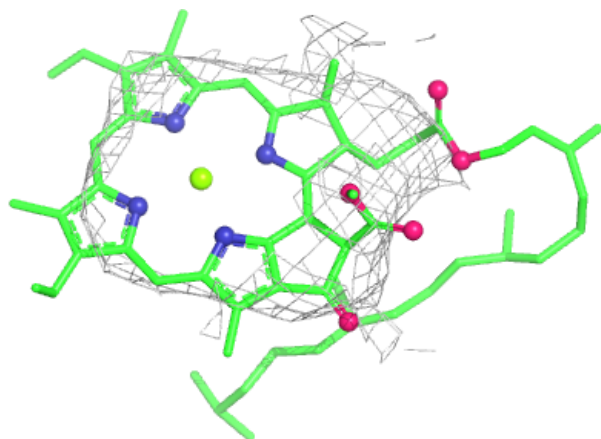
Electron density around CLA a 405:

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



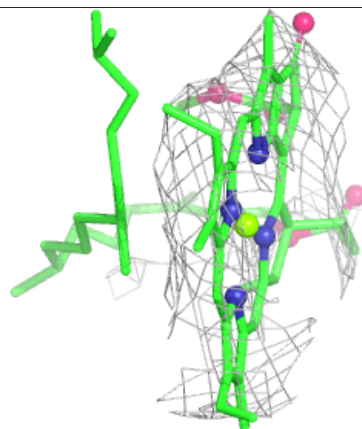
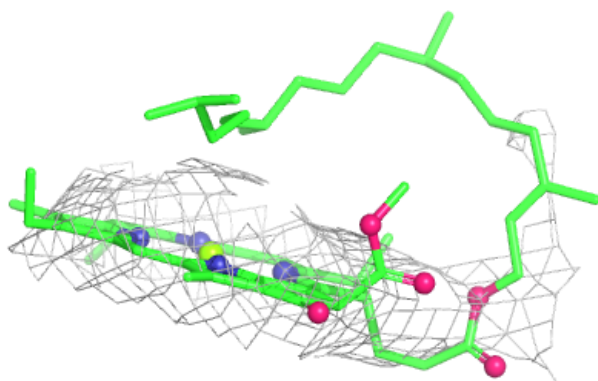
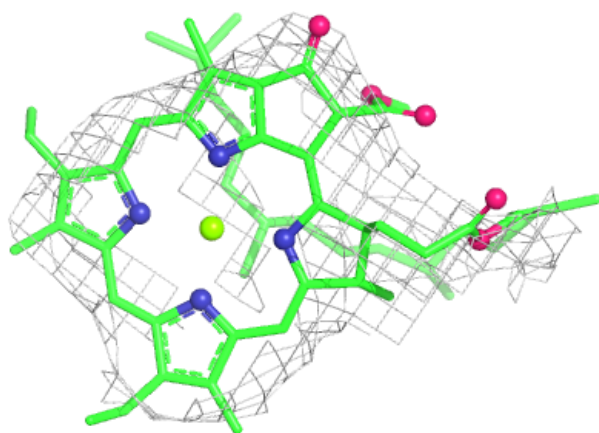
Electron density around CLA c 508:

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

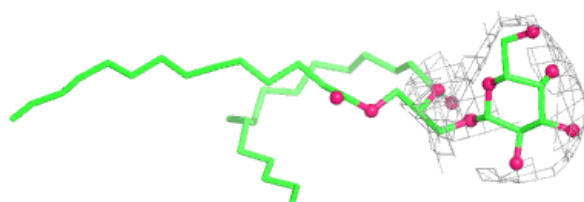
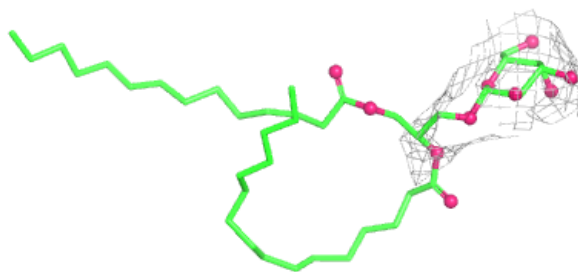


Electron density around CLA c 509:

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

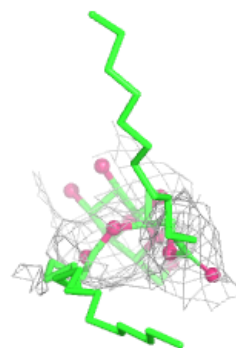
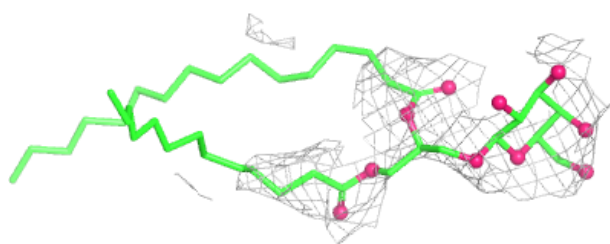
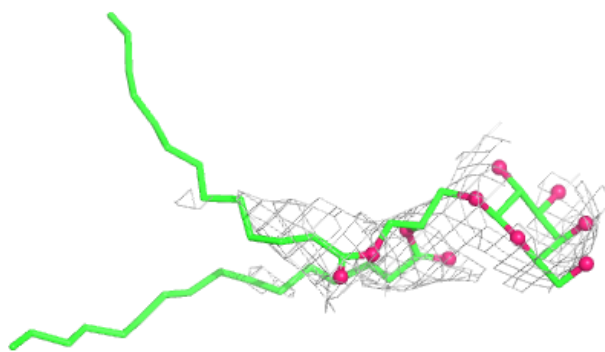
**Electron density around LMG d 408:**

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

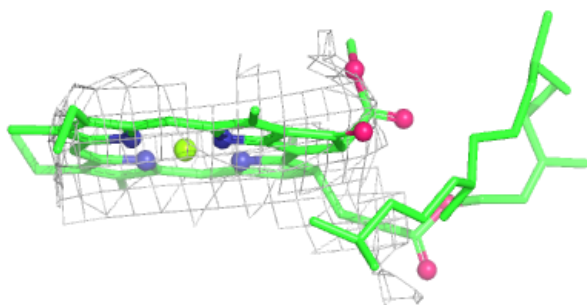
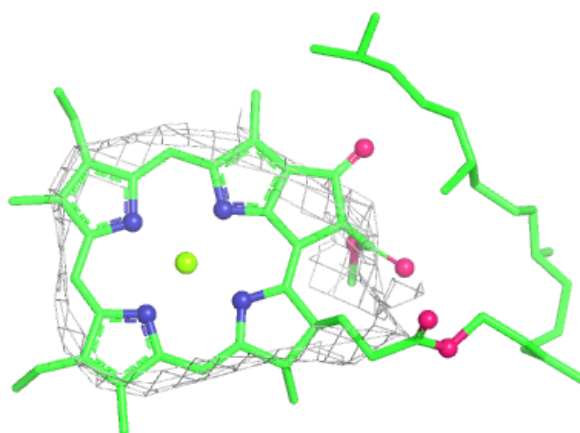


Electron density around LMG d 409:

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

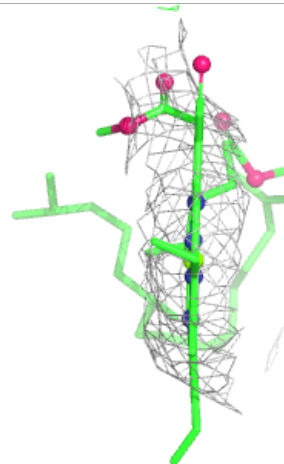
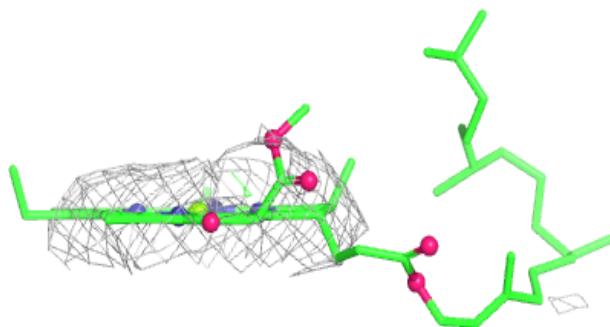
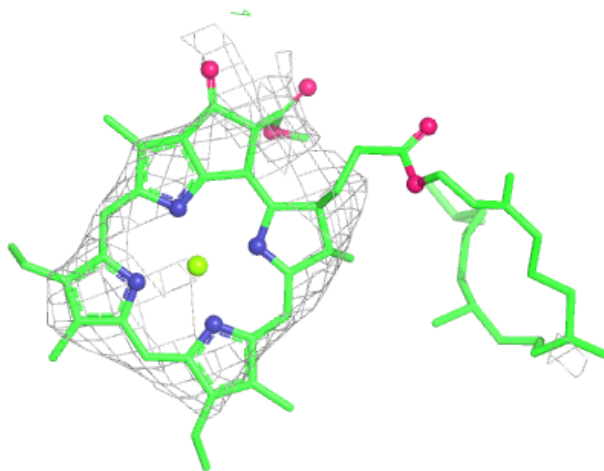
**Electron density around CLA b 613:**

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



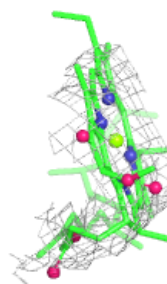
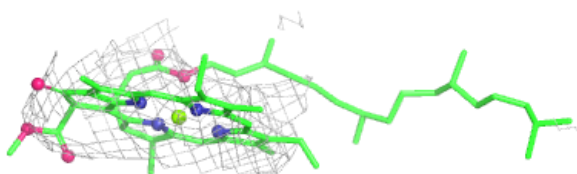
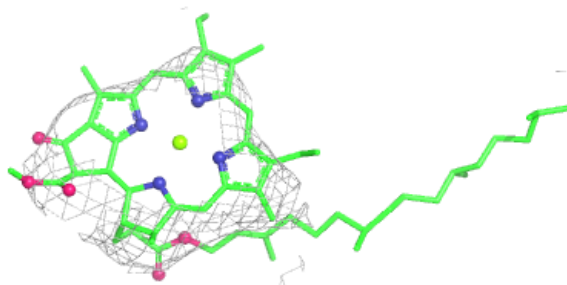
Electron density around CLA c 511:

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

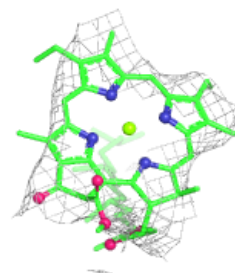
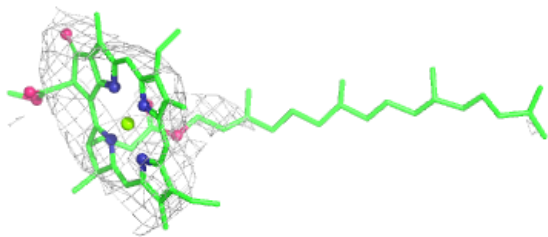
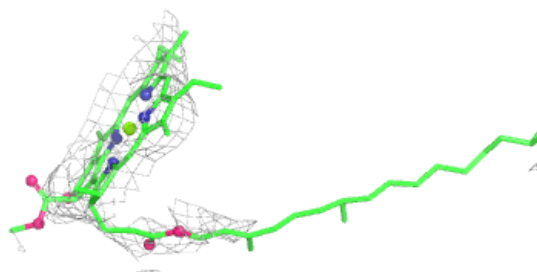


Electron density around CLA C 501:

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

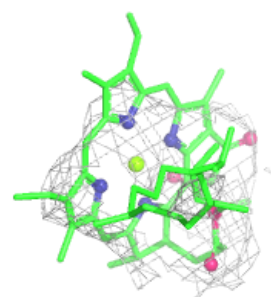
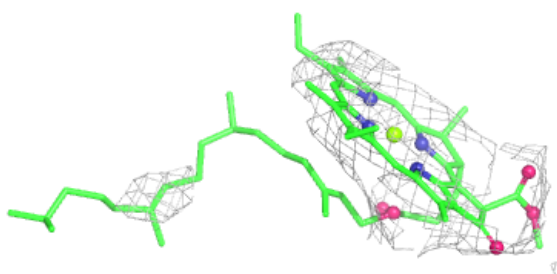
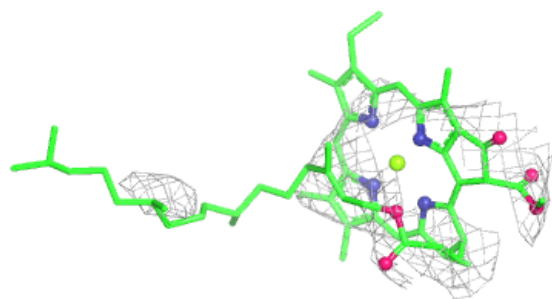
**Electron density around CLA B 606:**

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

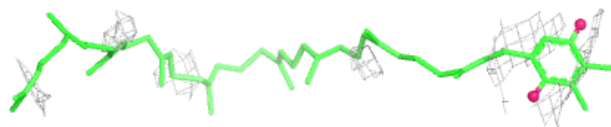
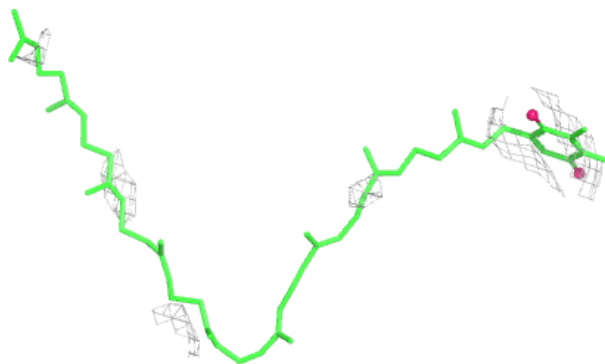


Electron density around CLA c 504:

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

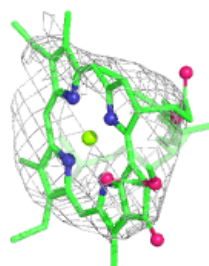
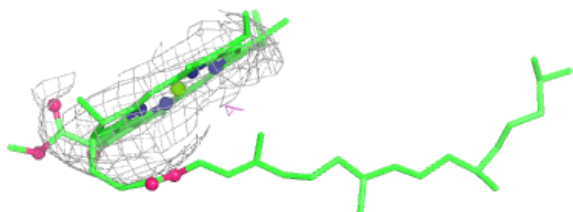
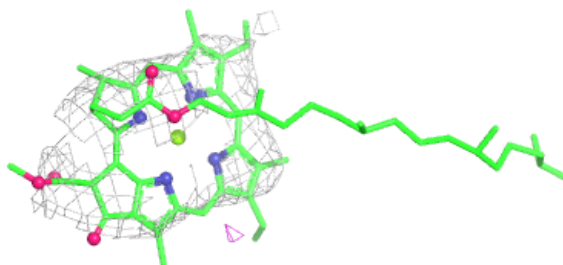
**Electron density around PL9 D 407:**

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

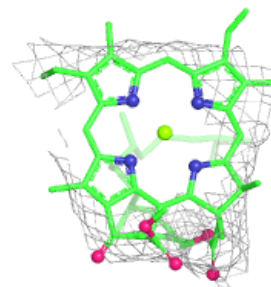
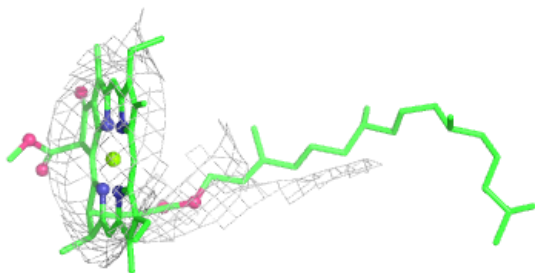
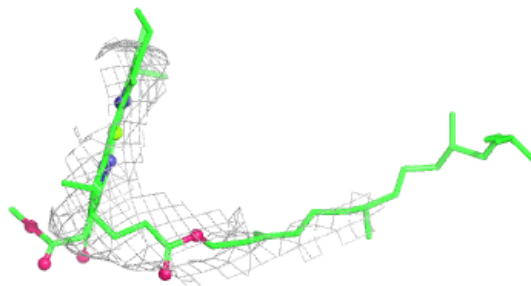


Electron density around CLA B 607:

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

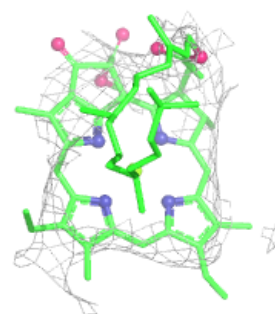
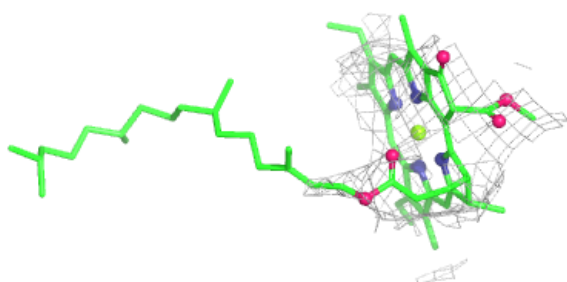
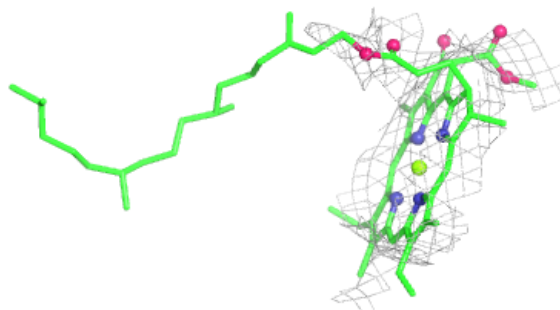
**Electron density around CLA b 608:**

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

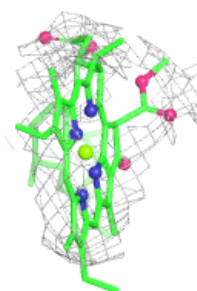
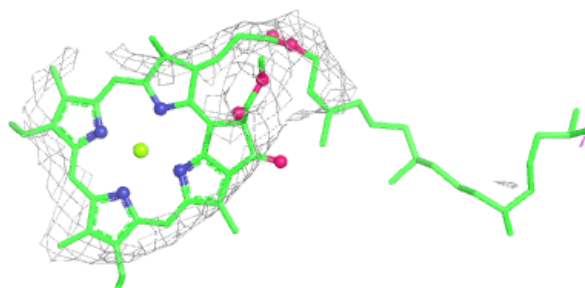


Electron density around CLA c 507:

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

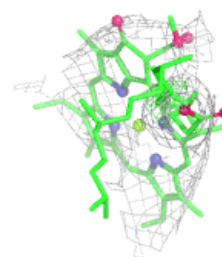
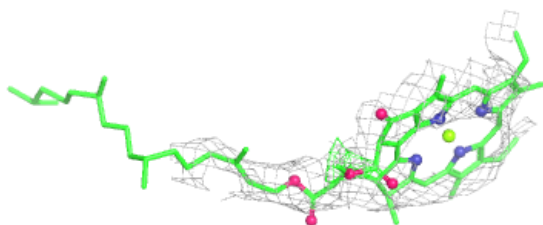
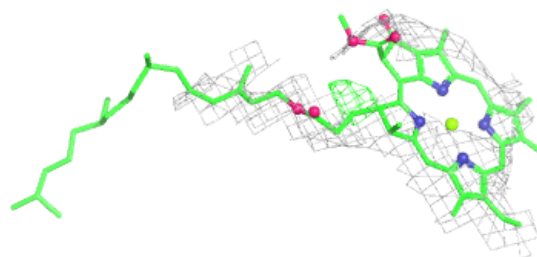
**Electron density around CLA H 101:**

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

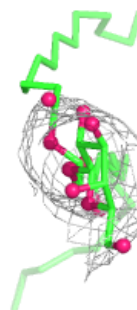
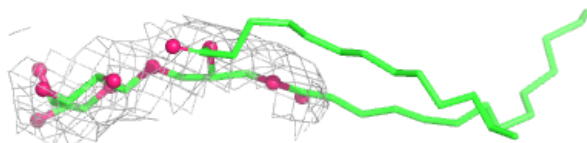
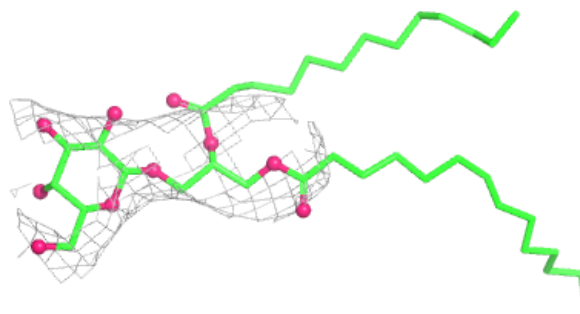


Electron density around CLA a 404:

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

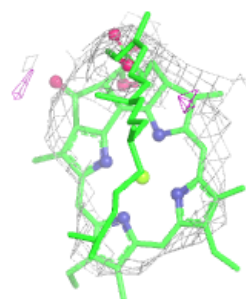
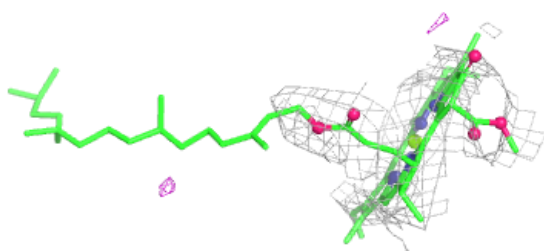
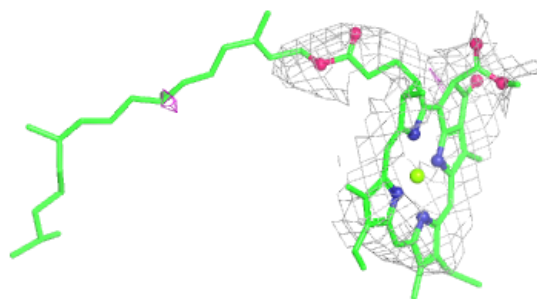
**Electron density around LMG d 412:**

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

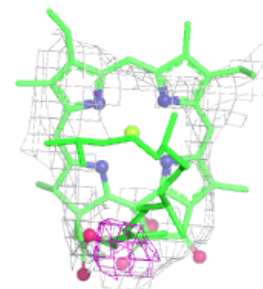
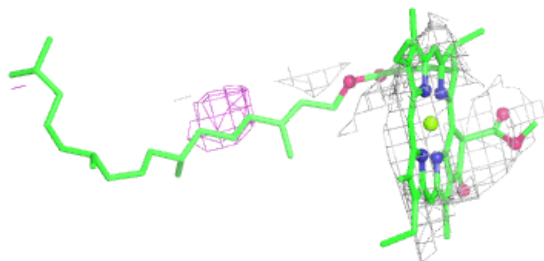
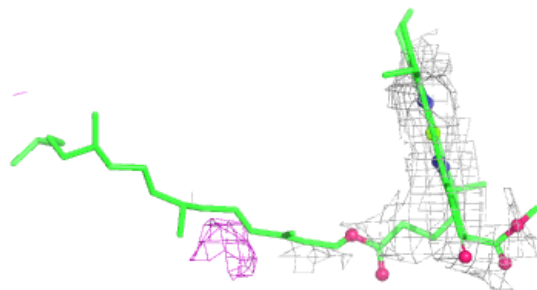


Electron density around CLA B 608:

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

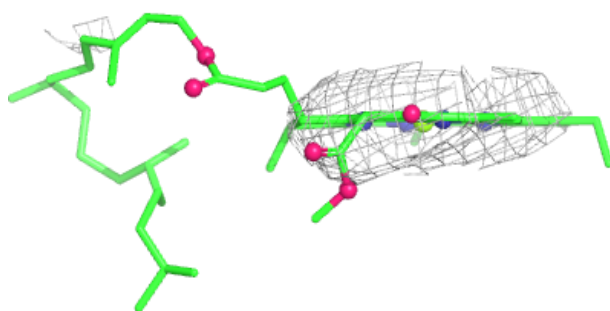
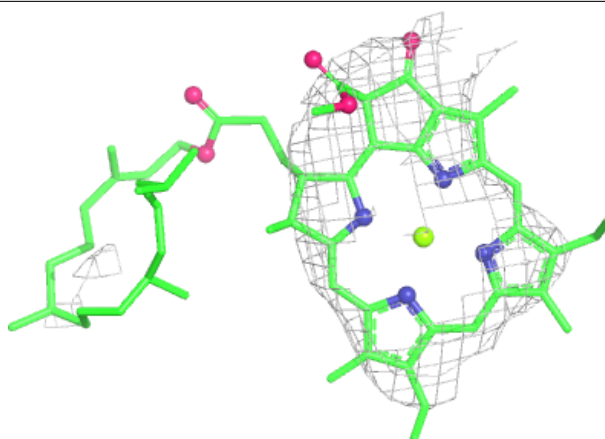
**Electron density around CLA B 604:**

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

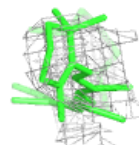
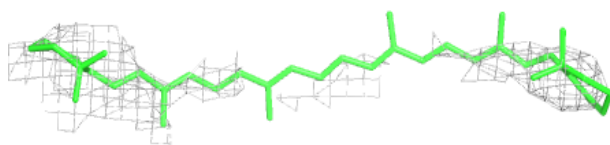
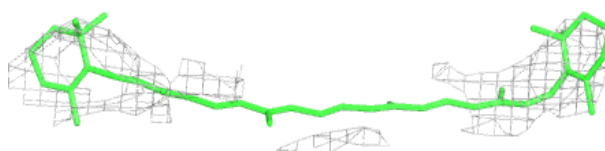


Electron density around CLA C 511:

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

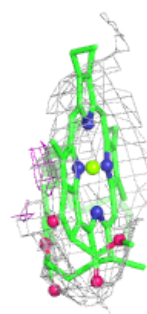
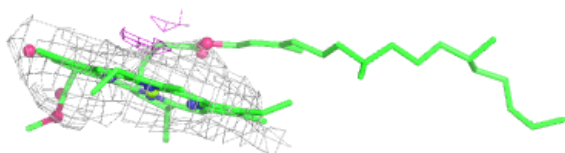
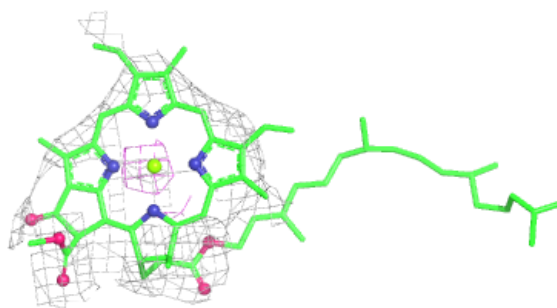
**Electron density around BCR C 513:**

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

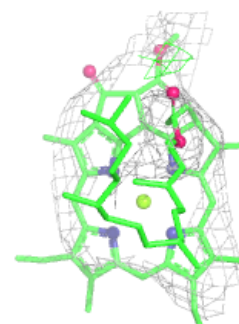
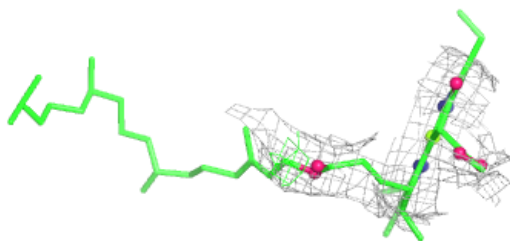
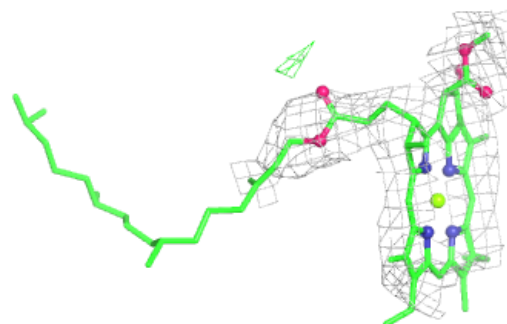


Electron density around CLA B 602:

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

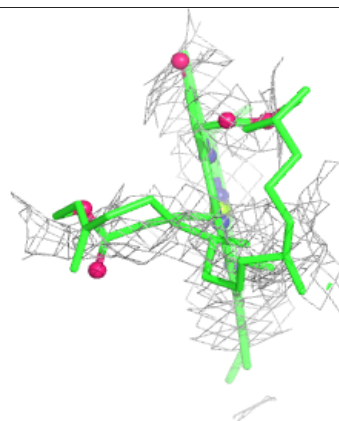
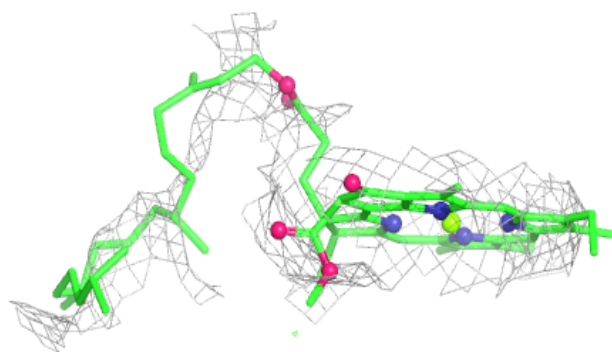
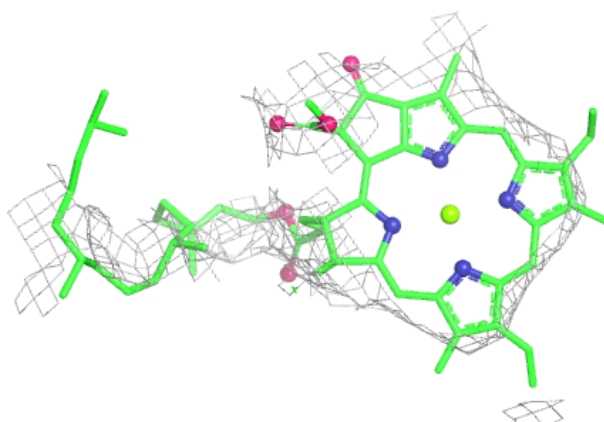
**Electron density around CLA d 406:**

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

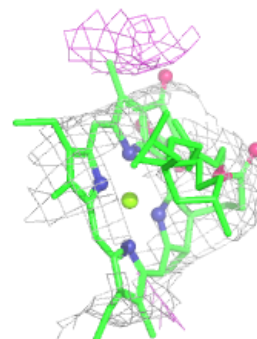
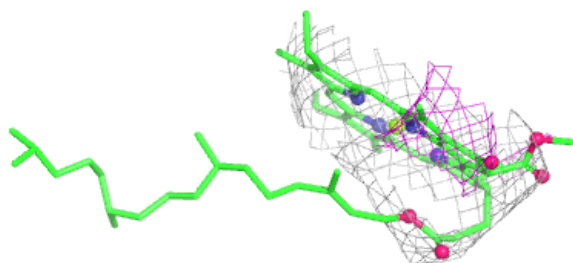
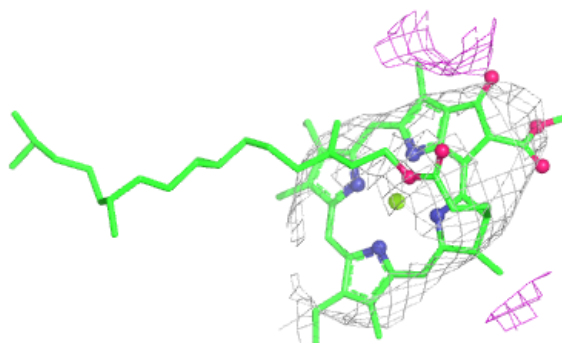


Electron density around CLA b 615:

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

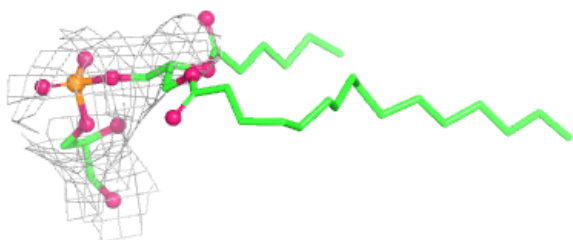
**Electron density around CLA b 617:**

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



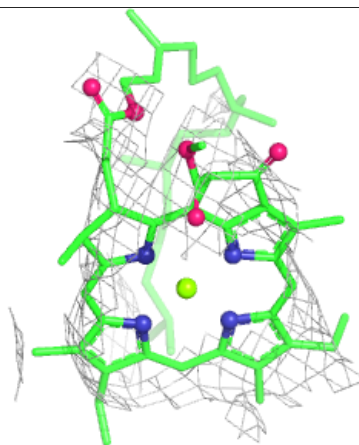
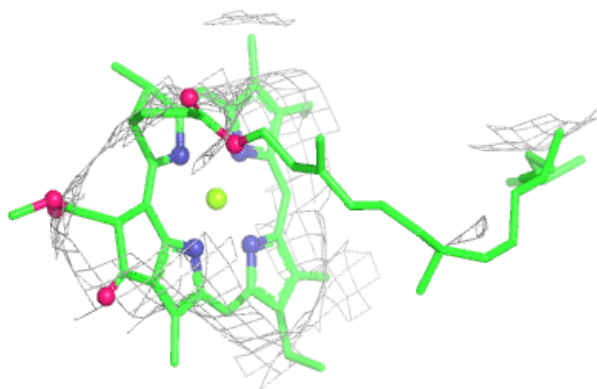
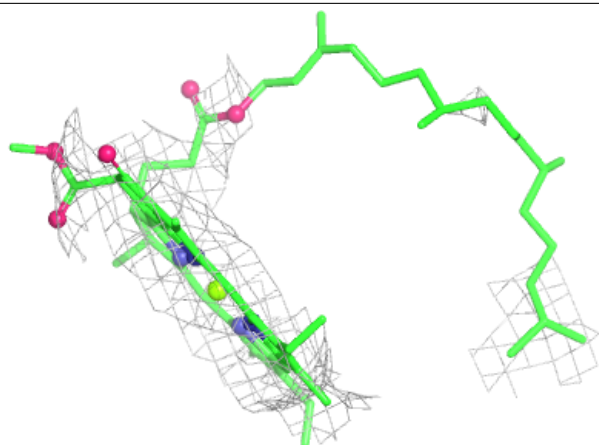
Electron density around LHG a 411:

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



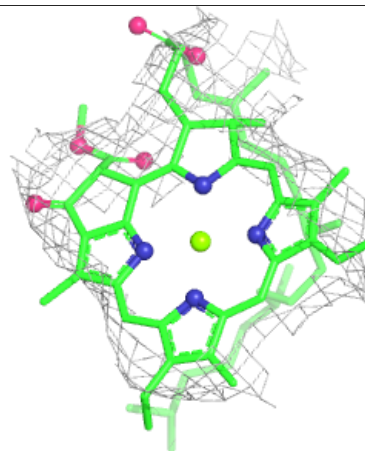
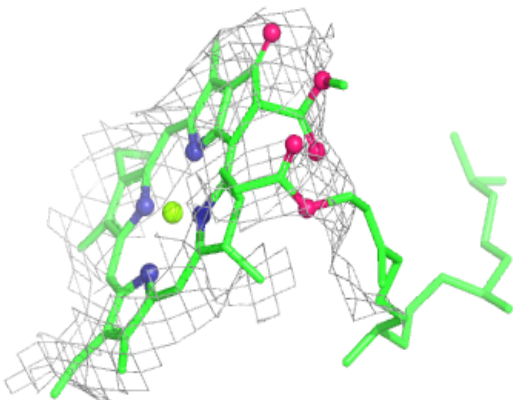
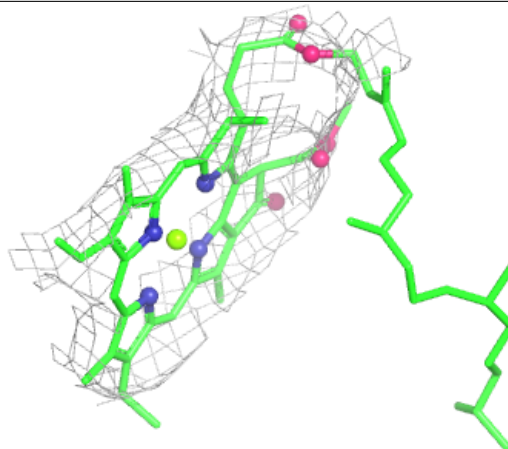
Electron density around CLA B 610:

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



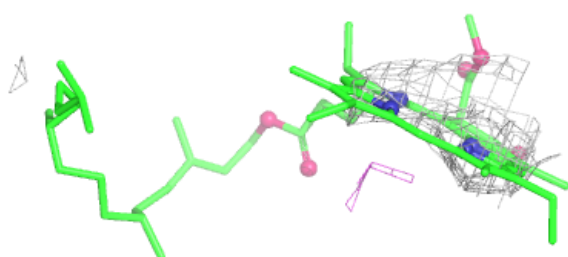
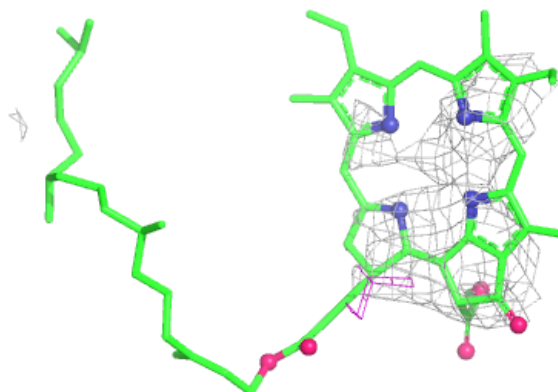
Electron density around CLA B 612:

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

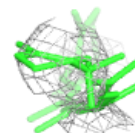
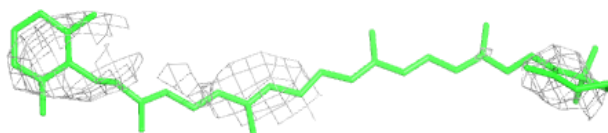
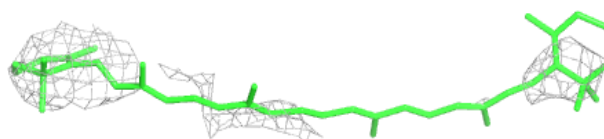


Electron density around PHO d 402:

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

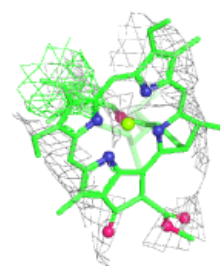
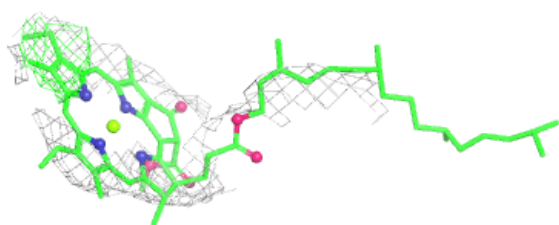
**Electron density around BCR f 102:**

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

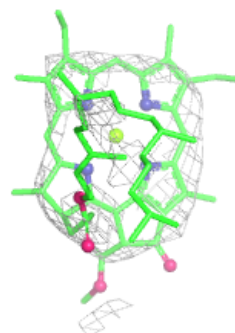
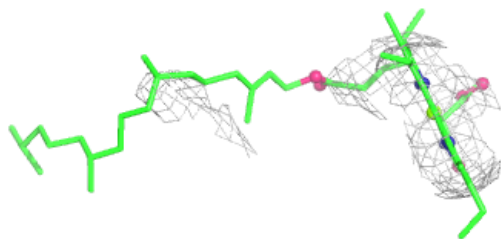
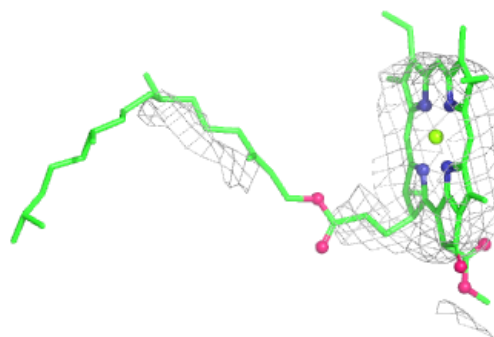


Electron density around CLA C 502:

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

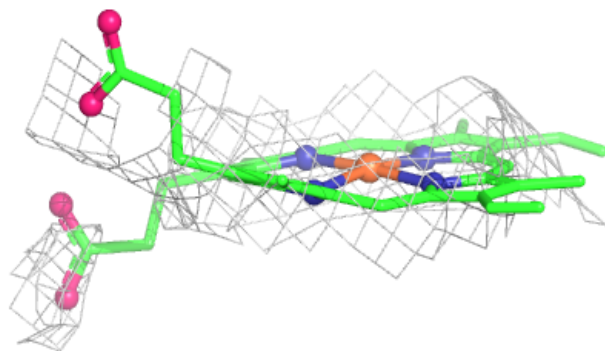
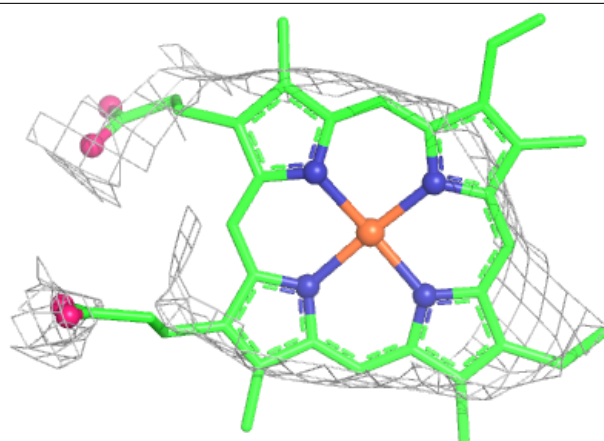
**Electron density around CLA D 406:**

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



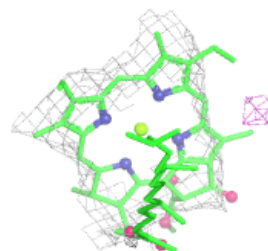
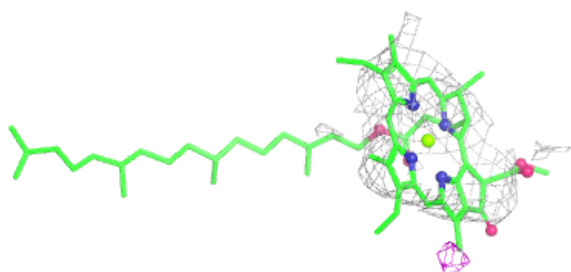
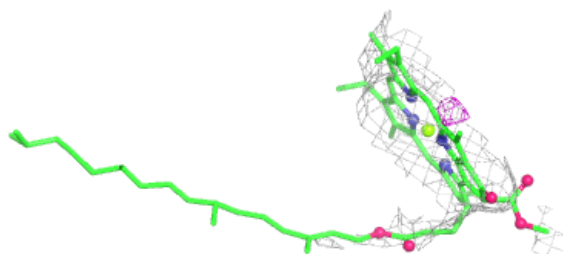
Electron density around HEM f 101:

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

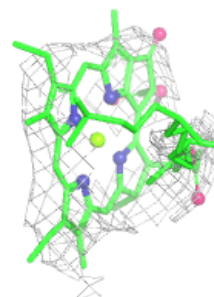
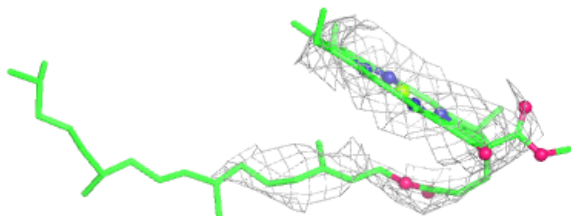
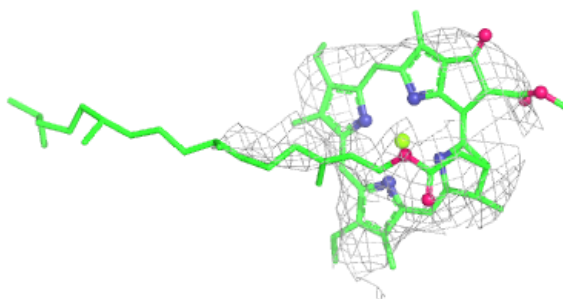


Electron density around CLA b 610:

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

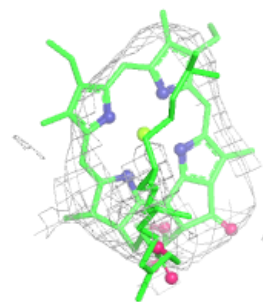
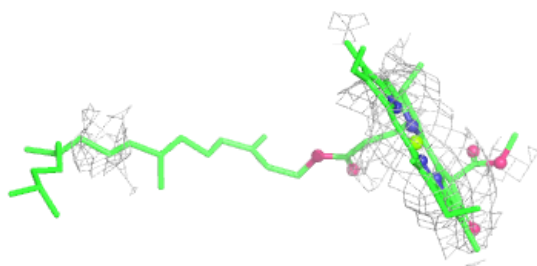
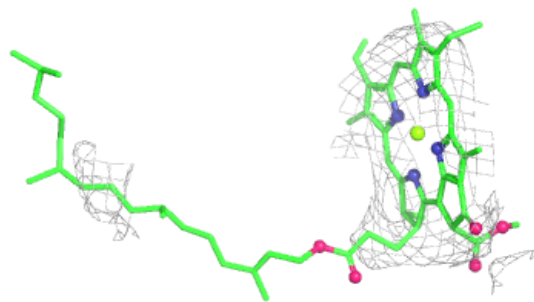
**Electron density around CLA b 611:**

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



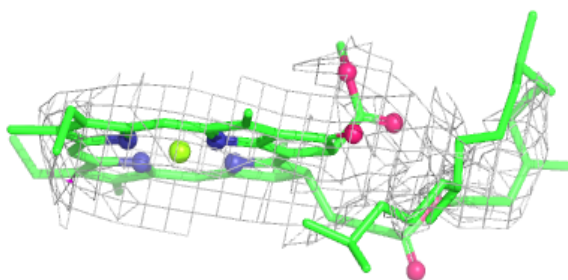
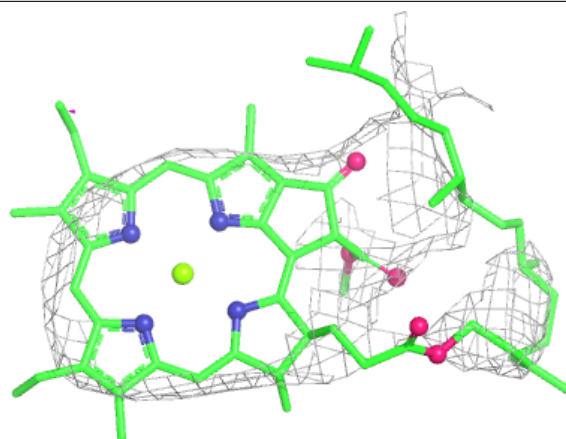
Electron density around CLA b 612:

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



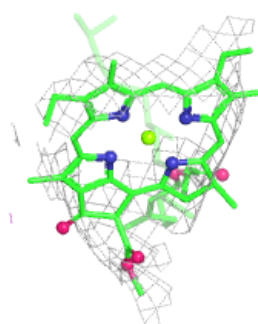
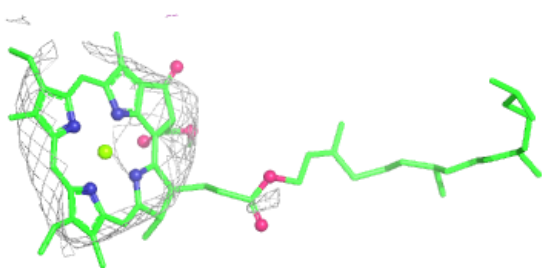
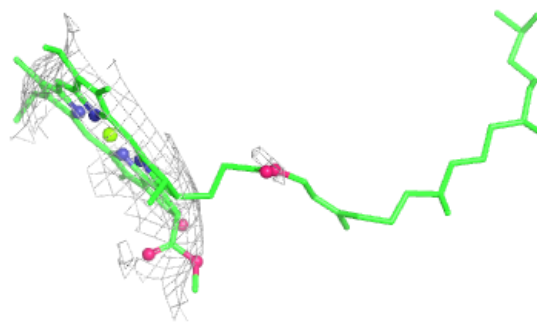
Electron density around CLA B 609:

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



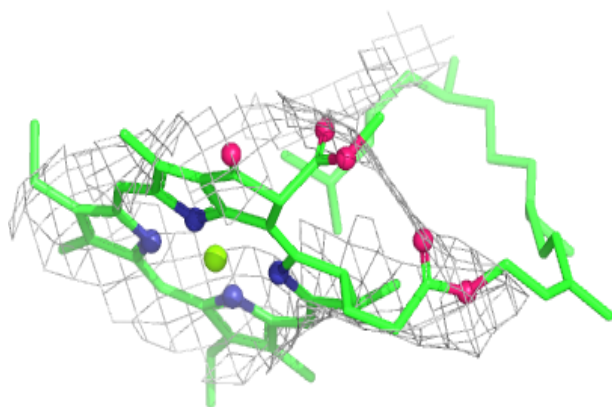
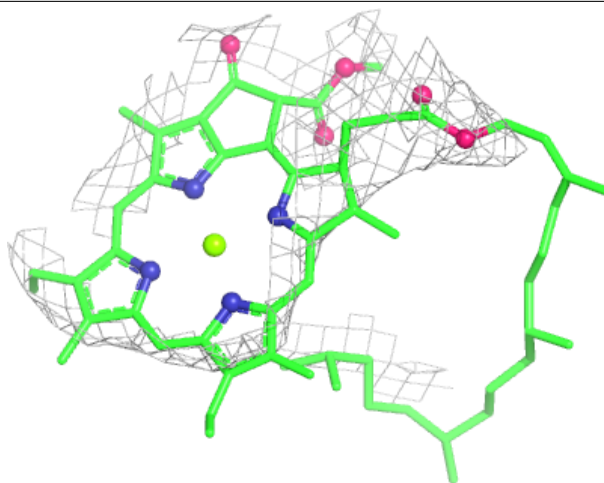
Electron density around CLA d 405:

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



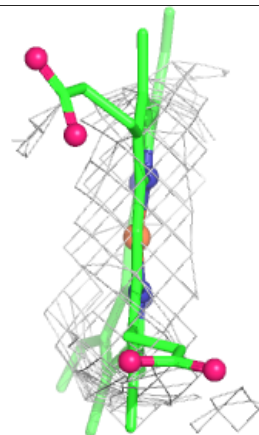
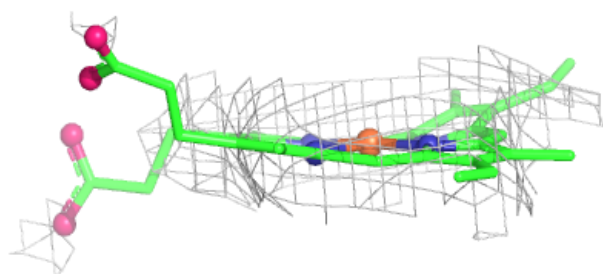
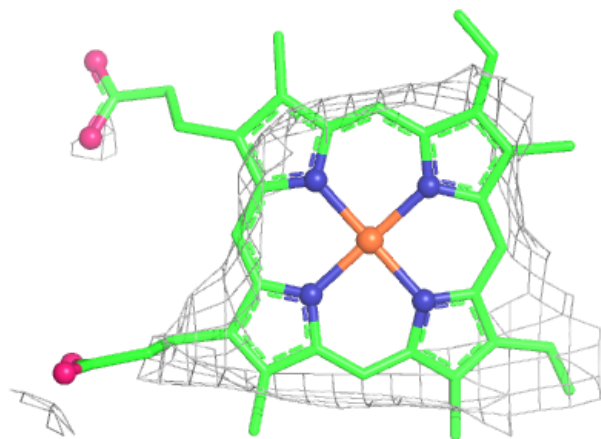
Electron density around CLA B 614:

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



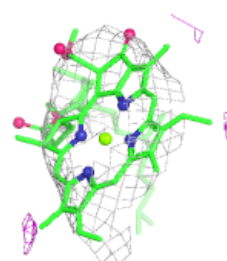
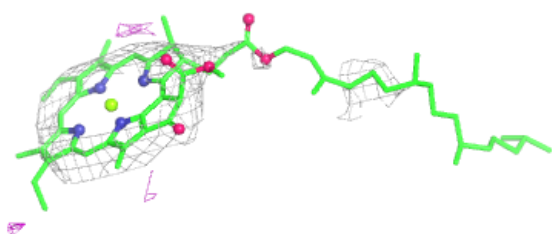
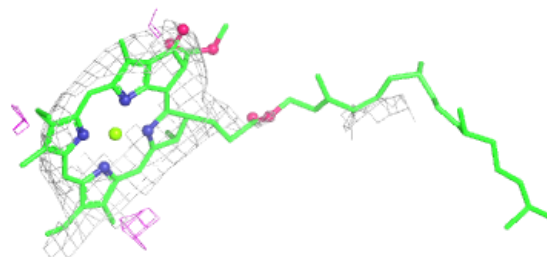
Electron density around HEM v 201:

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

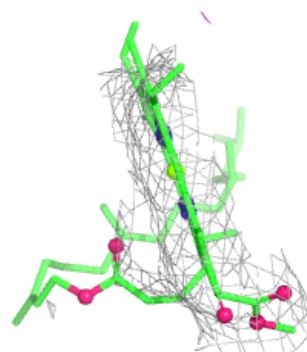
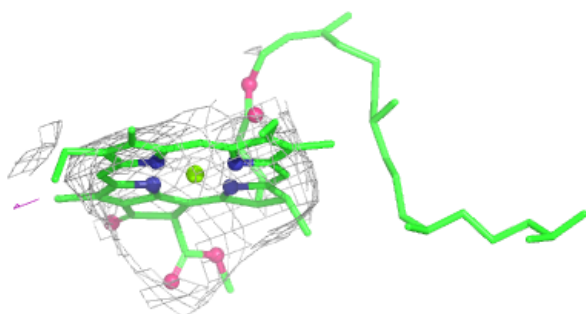
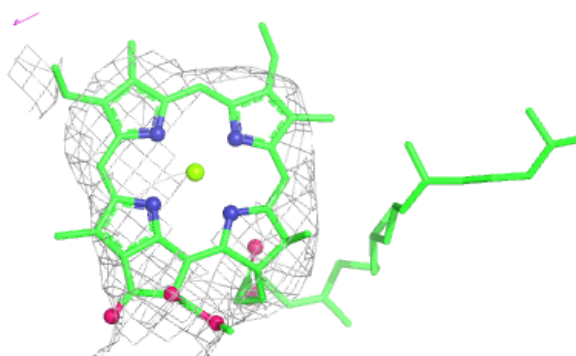


Electron density around CLA A 402:

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

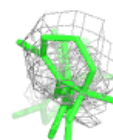
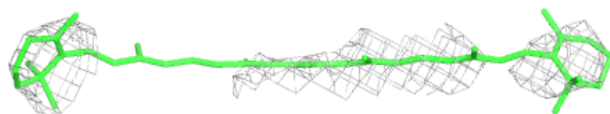
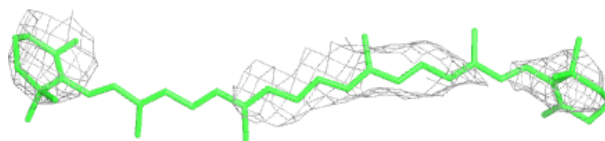
**Electron density around CLA A 403:**

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

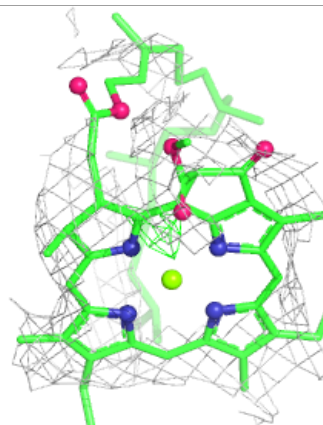
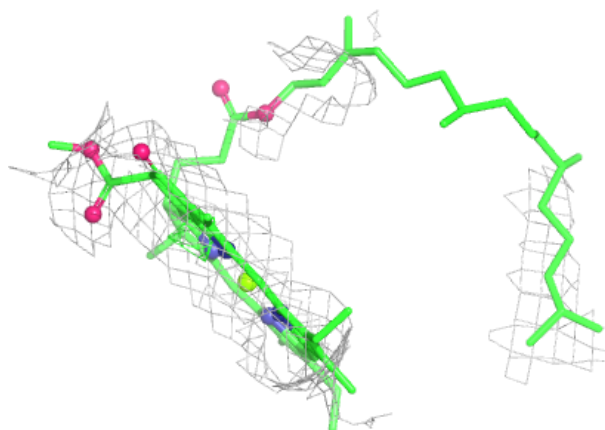


Electron density around BCR B 618:

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

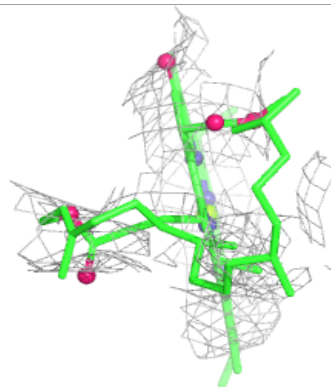
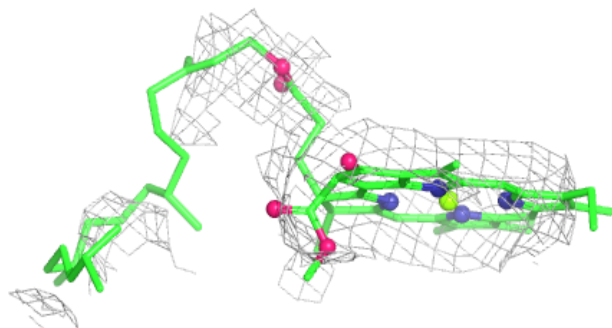
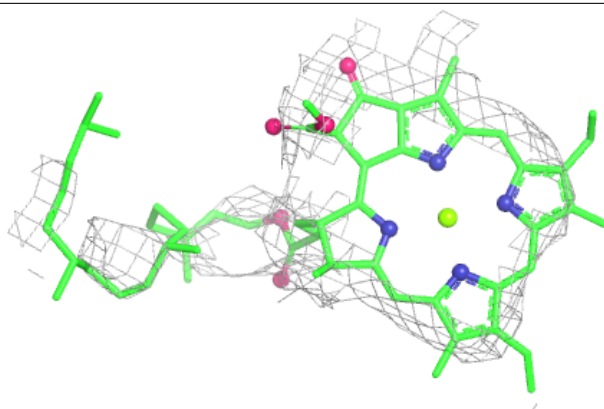
**Electron density around CLA b 614:**

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



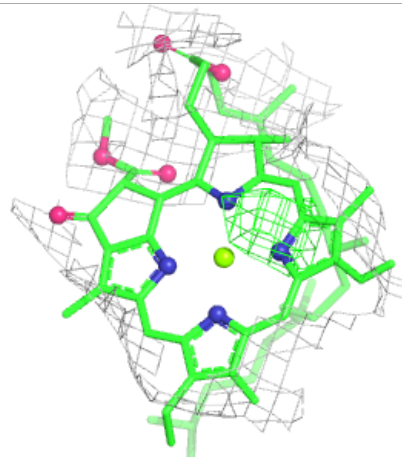
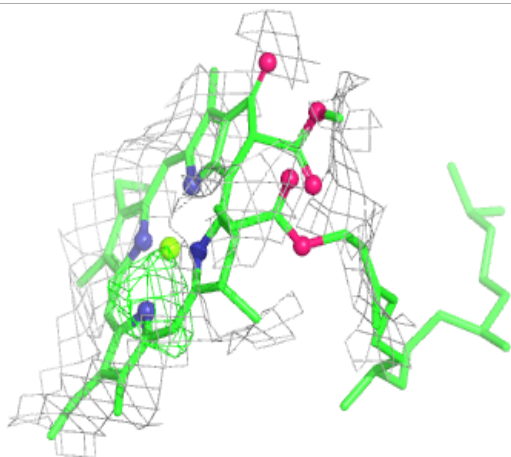
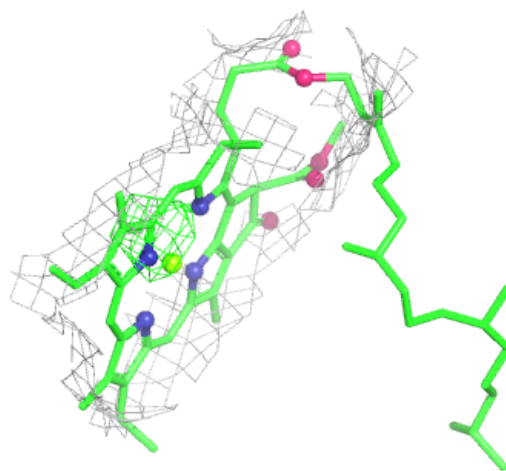
Electron density around CLA B 611:

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



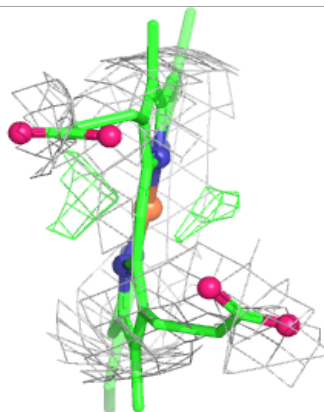
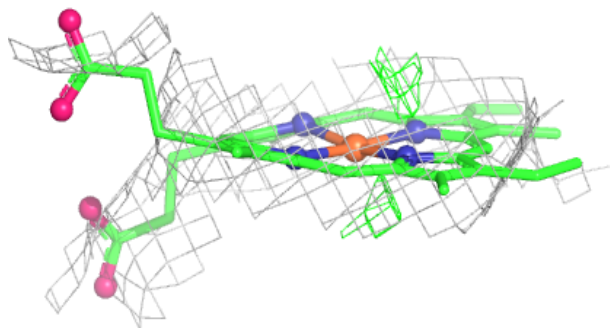
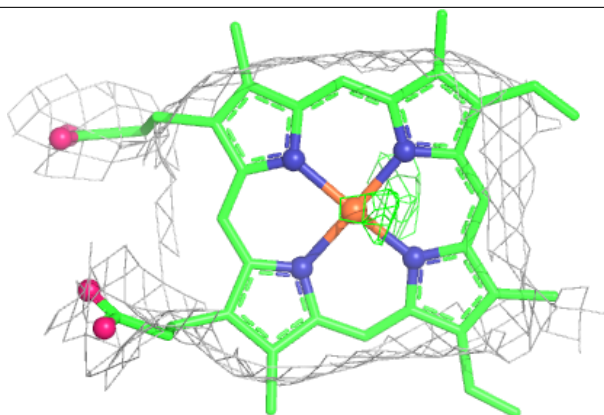
Electron density around CLA b 616:

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

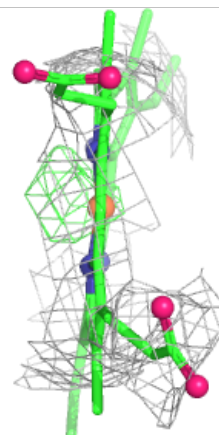
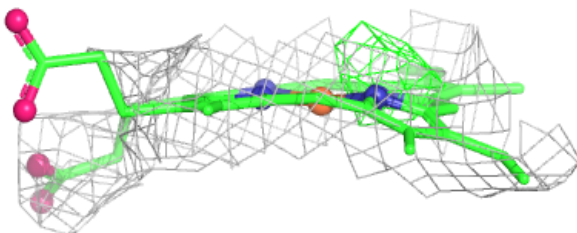
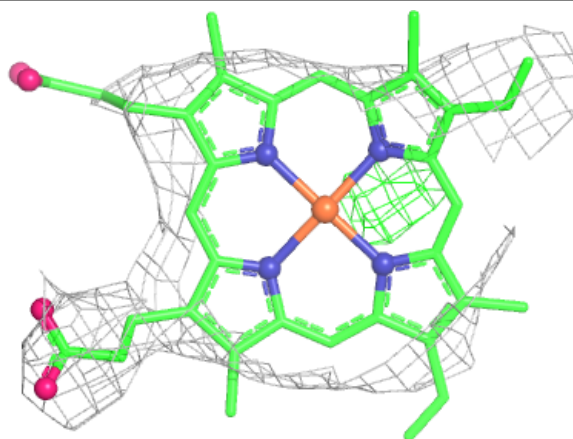


Electron density around HEM F 101:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.