



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:46 AM JST

PDB ID : 5WS6 / pdb_00005ws6
Title : Native XFEL structure of Photosystem II (preflash two-flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-12-05
Resolution : 2.35 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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

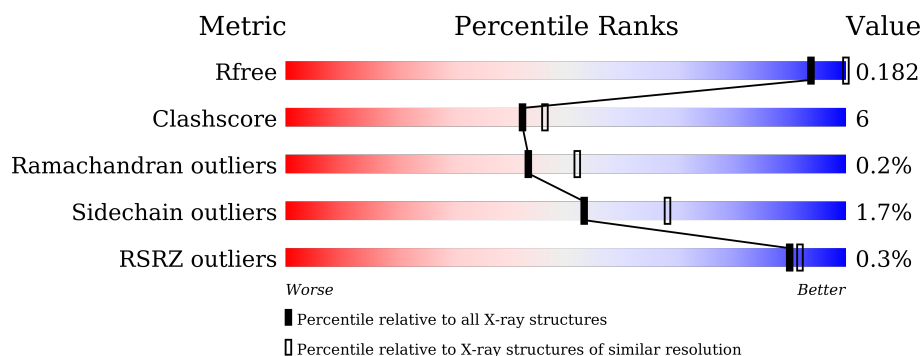
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

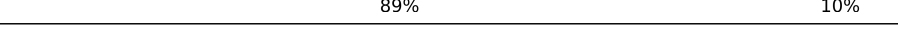
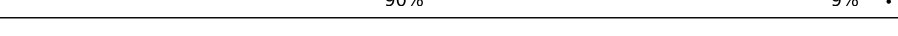
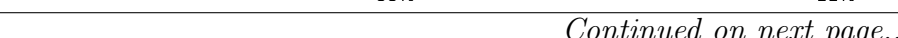
The reported resolution of this entry is 2.35 Å.

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.



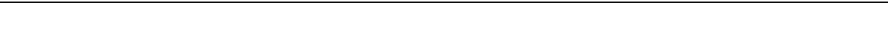
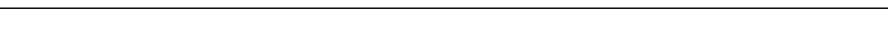
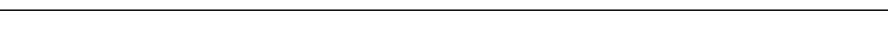
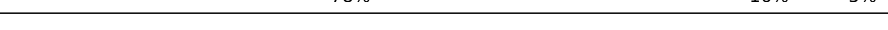
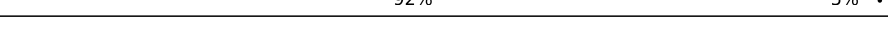
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	
1	a	344	
2	B	505	
2	b	505	
3	C	455	
3	c	455	

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	 90% 9% .
17	X	40	 90% 5% 5%
17	x	40	 88% 8% 5%
18	Y	30	 73% 20% . .
18	y	30	 3% 80% 17% .
19	Z	62	 85% 13% .
19	z	62	 2% 87% 13%
20	R	34	 12% 82% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
41	HEC	V	203	X	-	-	-
41	HEC	v	203	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 53280 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 II D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	29	0
			2850	1865	467	502	16			
1	a	334	Total	C	N	O	S	0	29	0
			2852	1867	466	503	16			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	10	0
			3542	2315	590	624	13			
3	c	455	Total	C	N	O	S	0	10	0
			3577	2340	595	629	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2748	1819	450	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2739	1814	449	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	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	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	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	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
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
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		

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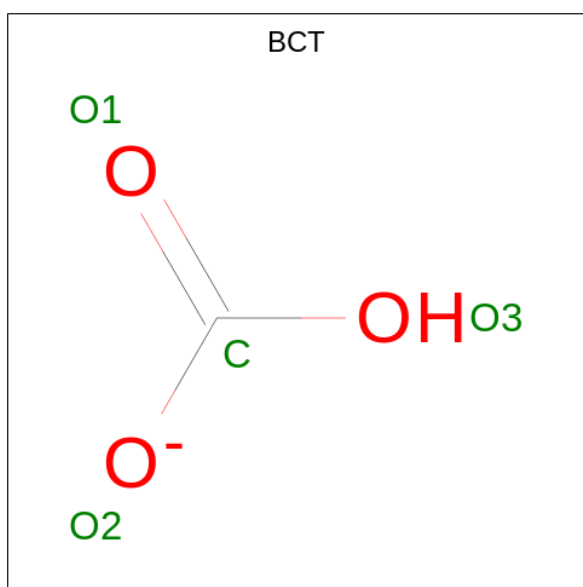
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	1
			2	2		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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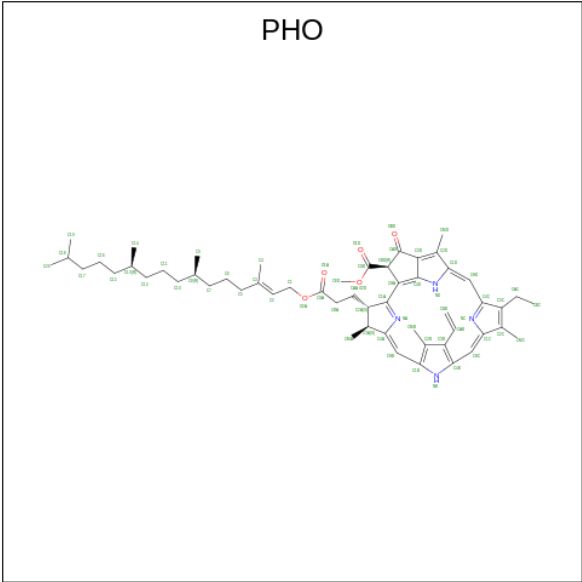
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24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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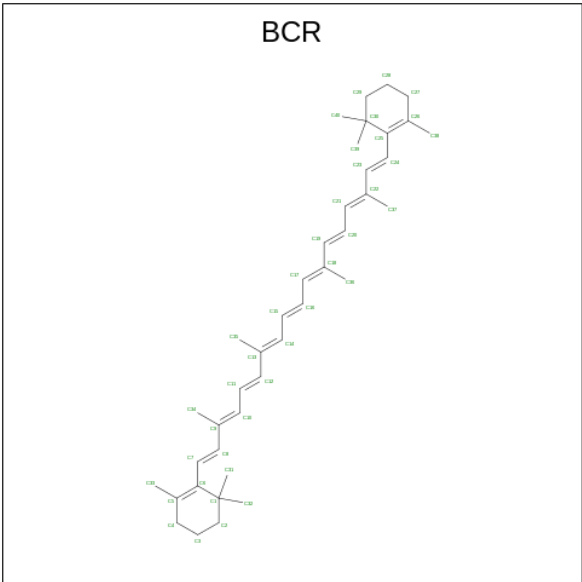
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



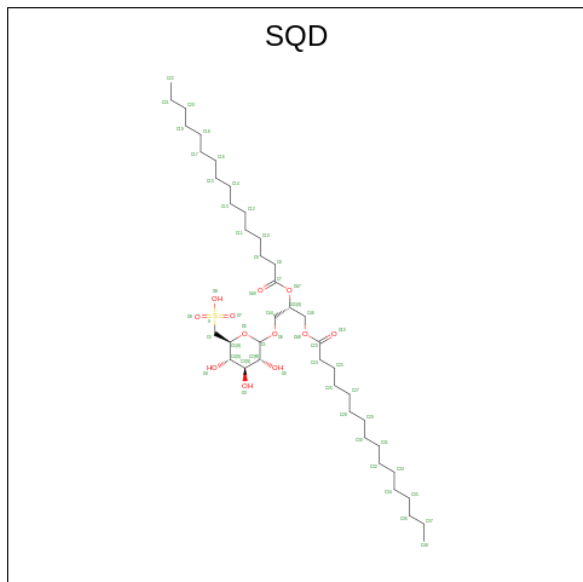
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



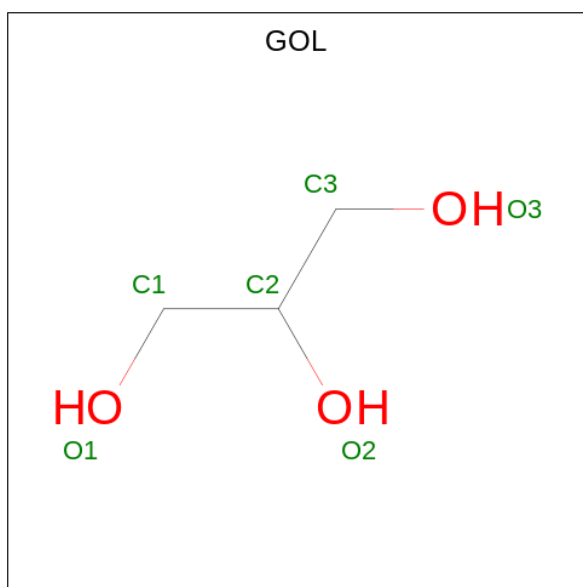
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



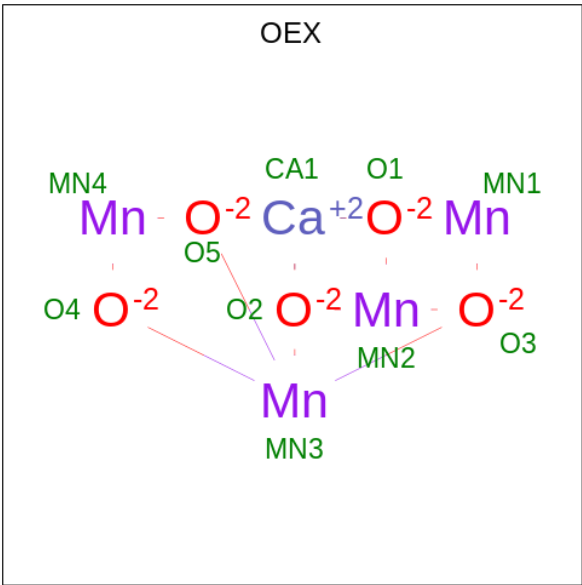
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



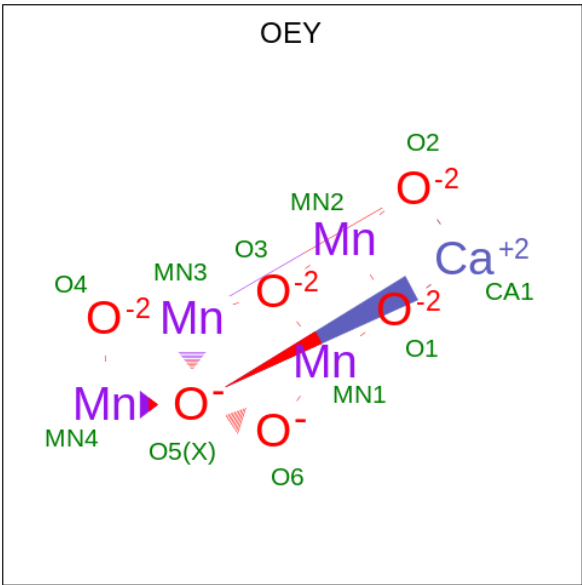
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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



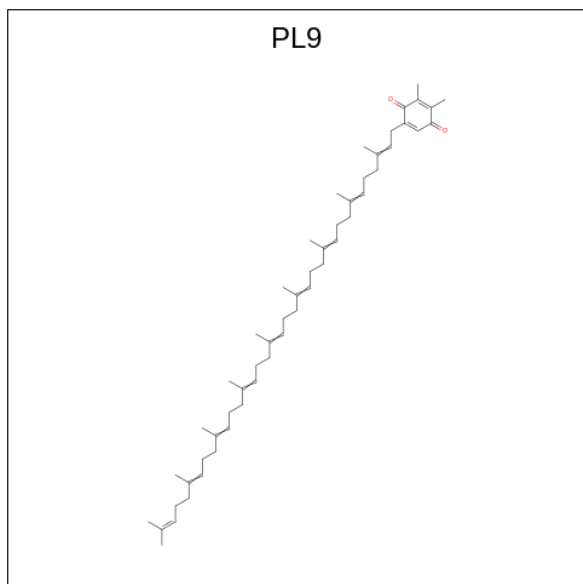
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 31 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: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

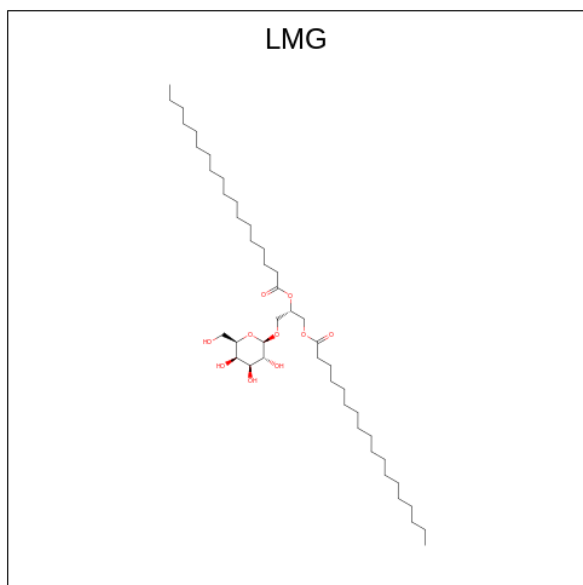
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	K	1	Total	C	O	0	0
			34	29	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	2	Total C O 53 47 6	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0
32	x	1	Total C O 18 16 2	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



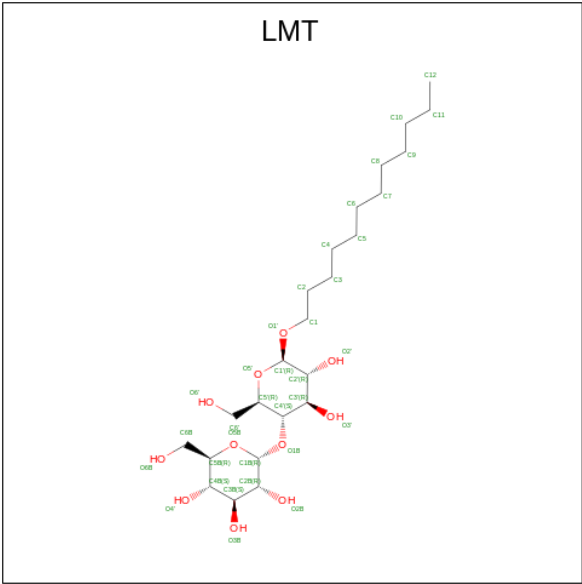
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 51 41 10	0	0

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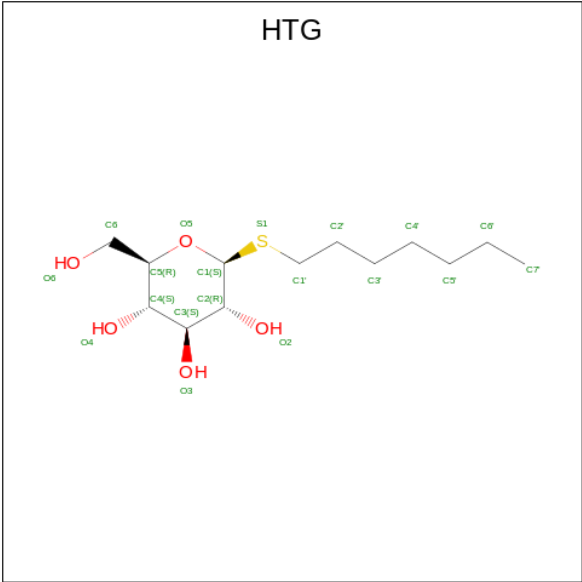
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			25	19	6		
34	E	1	Total	C	O	0	0
			35	24	11		
34	I	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	b	1	Total	C	O	0	0
			25	19	6		
34	e	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



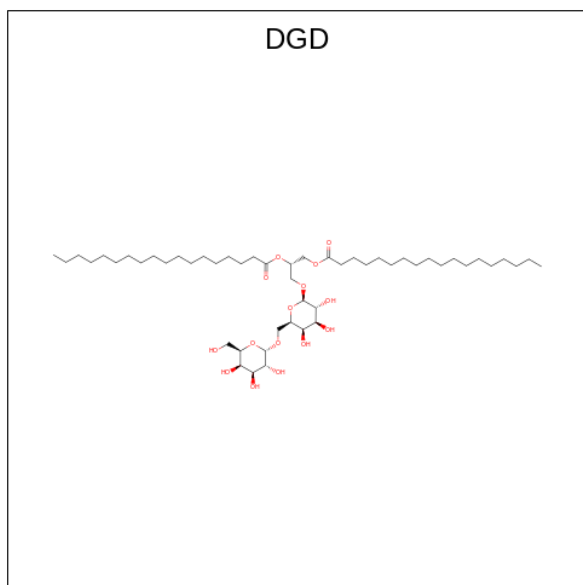
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

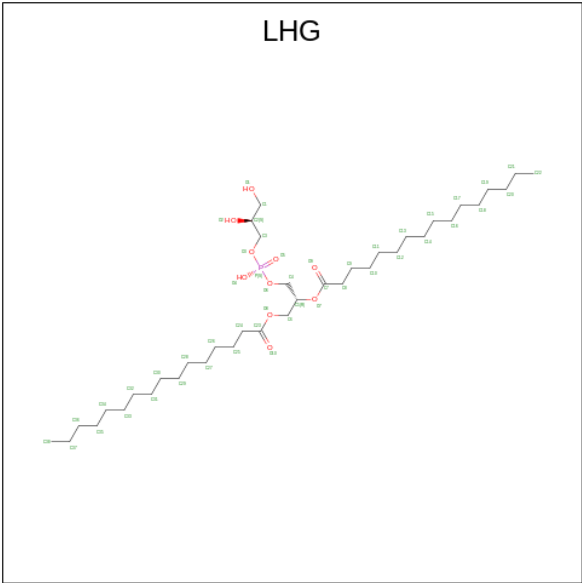


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	h	1	Total	C	O		0	0
			62	47	15			

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	V	1	Total Ca 1 1	0	0
37	b	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0
37	o	1	Total Ca 1 1	0	0
37	v	1	Total Ca 1 1	0	0

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



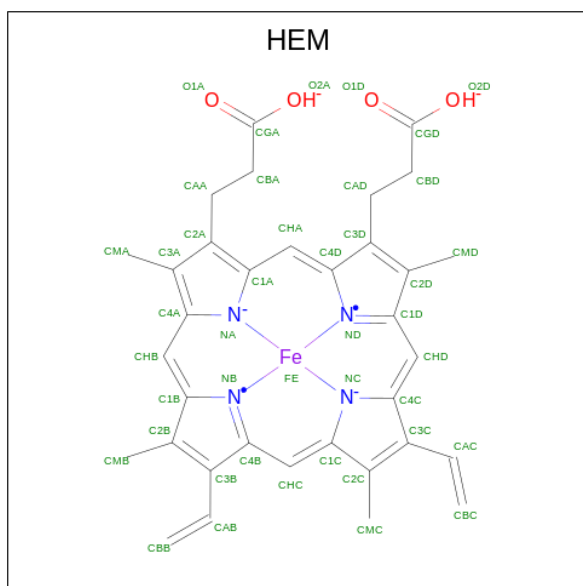
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	E	1	Total C O P 42 31 10 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	a	1	Total	C	O	P	0	0
			42	31	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
39	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
39	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

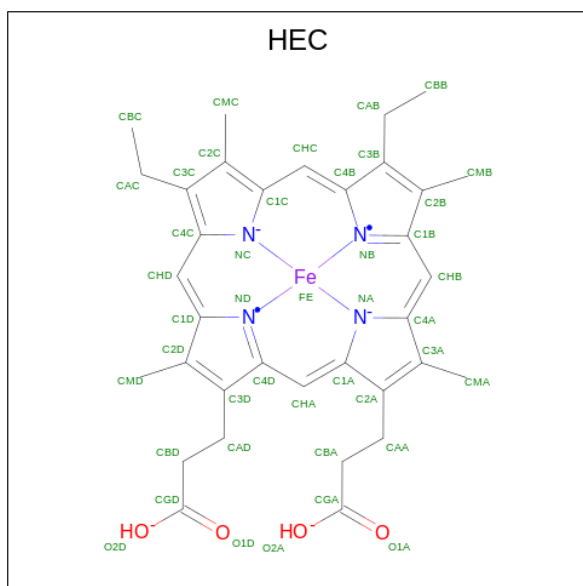
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	j	1	Total	Mg	0	0
			1	1		

- Molecule 41 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	125	Total	O	0	5
			130	130		
42	B	164	Total	O	0	0
			164	164		
42	C	147	Total	O	0	0
			147	147		
42	D	112	Total	O	0	0
			112	112		
42	E	14	Total	O	0	0
			14	14		
42	F	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	H	20	Total 20	O 20	0	0
42	I	6	Total 6	O 6	0	0
42	J	4	Total 4	O 4	0	0
42	K	7	Total 7	O 7	0	0
42	L	4	Total 4	O 4	0	0
42	M	7	Total 7	O 7	0	0
42	O	74	Total 74	O 74	0	0
42	T	8	Total 8	O 8	0	0
42	U	33	Total 33	O 33	0	0
42	V	65	Total 65	O 65	0	0
42	X	2	Total 2	O 2	0	0
42	Y	1	Total 1	O 1	0	0
42	a	128	Total 133	O 133	0	5
42	b	185	Total 185	O 185	0	0
42	c	122	Total 122	O 122	0	0
42	d	109	Total 109	O 109	0	0
42	e	7	Total 7	O 7	0	0
42	f	3	Total 3	O 3	0	0
42	h	14	Total 14	O 14	0	0
42	i	3	Total 3	O 3	0	0
42	j	2	Total 2	O 2	0	0

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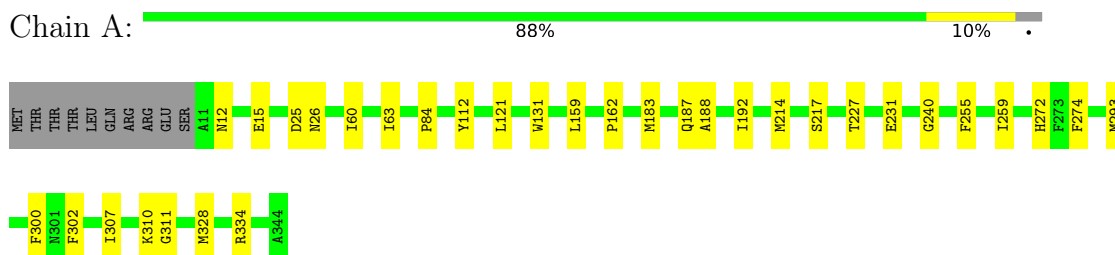
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	k	3	Total 3	O 3	0	0
42	l	6	Total 6	O 6	0	0
42	m	11	Total 11	O 11	0	0
42	o	78	Total 78	O 78	0	0
42	t	5	Total 5	O 5	0	0
42	u	47	Total 47	O 47	0	0
42	v	49	Total 49	O 49	0	0
42	x	4	Total 4	O 4	0	0
42	y	1	Total 1	O 1	0	0

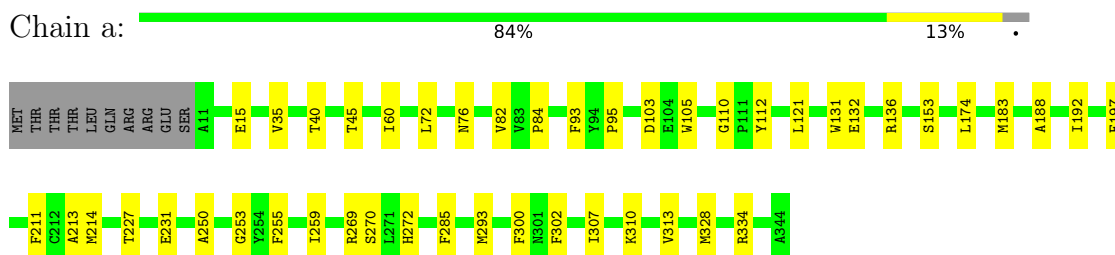
3 Residue-property plots [i](#)

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

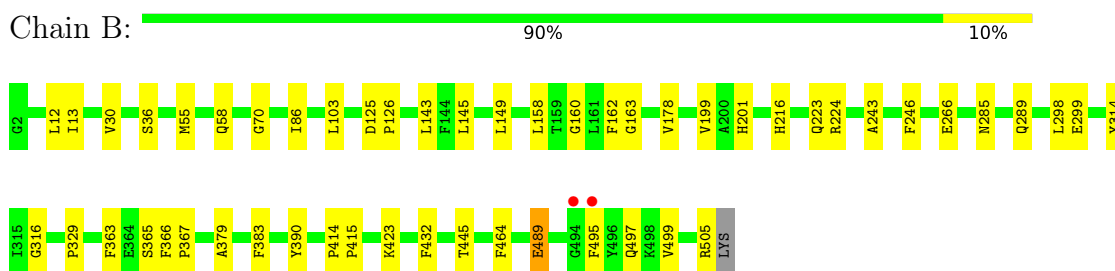
- Molecule 1: Photosystem II D1 protein



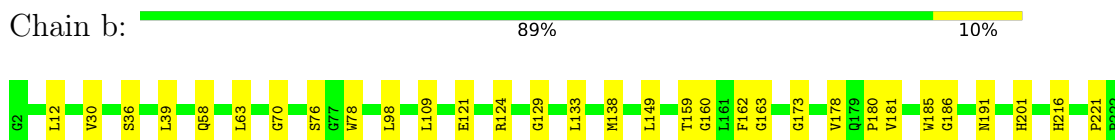
- Molecule 1: Photosystem II D1 protein



- Molecule 2: Photosystem II CP47 reaction center protein

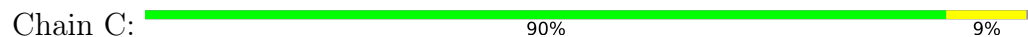


- Molecule 2: Photosystem II CP47 reaction center protein

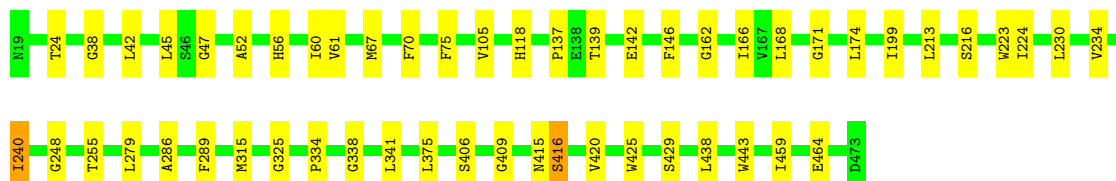
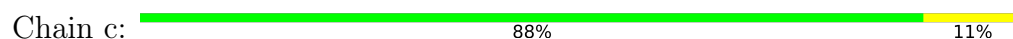




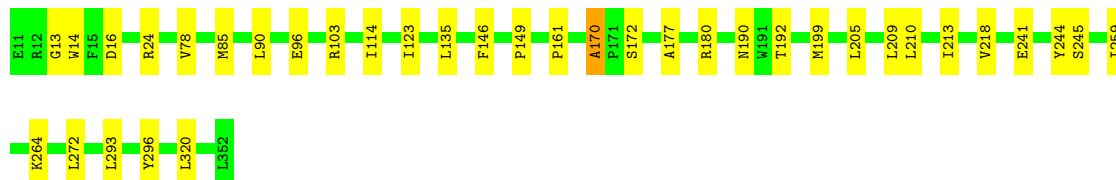
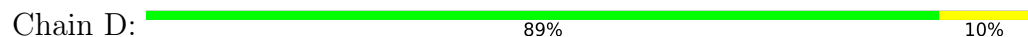
• Molecule 3: Photosystem II CP43 chlorophyll protein



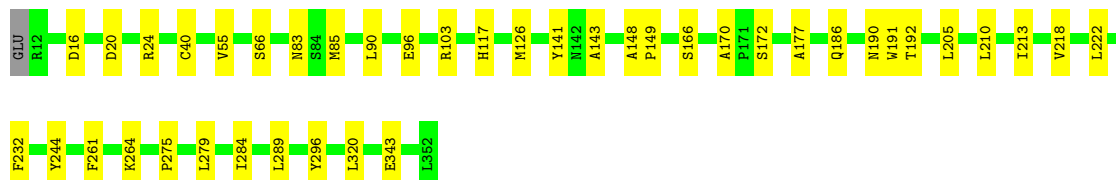
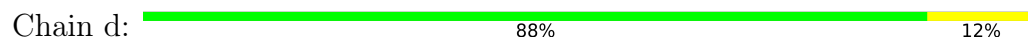
• Molecule 3: Photosystem II CP43 chlorophyll protein



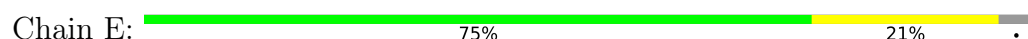
• Molecule 4: Photosystem II D2 protein

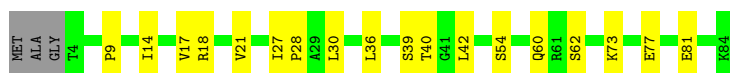


• Molecule 4: Photosystem II D2 protein

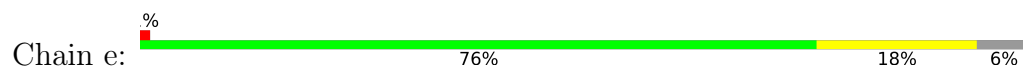


• Molecule 5: Cytochrome b559 subunit alpha





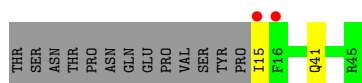
- Molecule 5: Cytochrome b559 subunit alpha



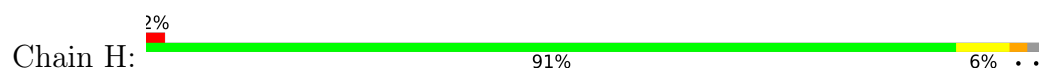
- Molecule 6: Cytochrome b559 subunit beta



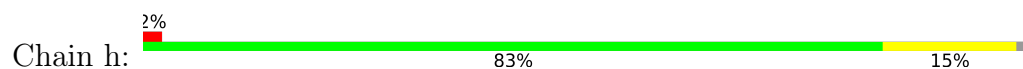
- Molecule 6: Cytochrome b559 subunit beta



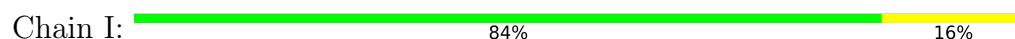
- Molecule 7: Photosystem II reaction center protein H



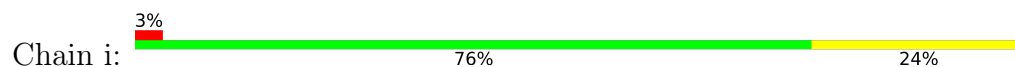
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



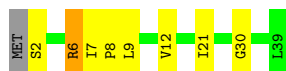
- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 77% 18% . .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 90% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 76% 19% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 92% 5% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 78% 14% 8%



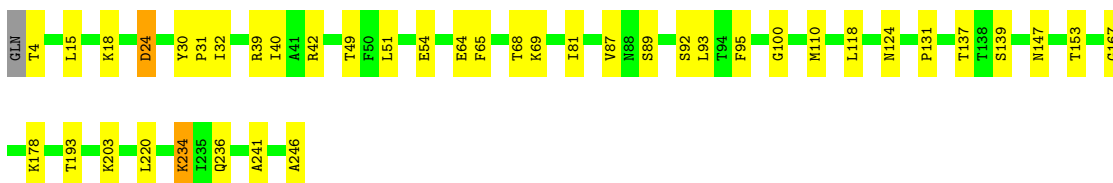
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% 6%



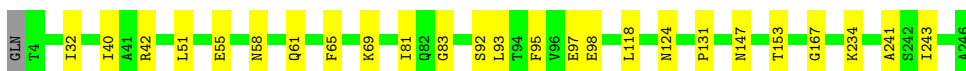
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 83% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 84% 6% 6%



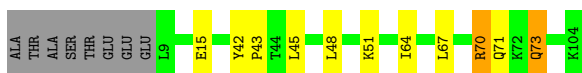
- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 81% 6% 6% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 82% 9% 8%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 5% • 7%



- Molecule 16: Cytochrome c-550

Chain V:  93% 7%



- Molecule 16: Cytochrome c-550

Chain v:  90% 9% •



- Molecule 17: Photosystem II reaction center protein X

Chain X:  90% 5% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  73% 20% • •



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  3% 80% 17% •



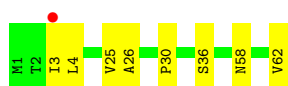
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  85% 13% .



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  2% 87% 13%



- Molecule 20: Photosystem II protein Y

Chain R:  12% 82% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 99.8 (20.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.129 , 0.175 0.140 , 0.182	Depositor DCC
R_{free} test set	17126 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 91.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: BCR, PHO, HTG, LMG, OEY, PL9, FME, CLA, SQD, HEM, CA, BCT, HEC, CL, UNL, GOL, OEX, MG, DGD, LHG, FE2, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/2952	0.84	0/4019
1	a	0.52	0/2957	0.79	0/4027
2	B	0.53	0/4171	0.80	0/5683
2	b	0.51	0/4138	0.80	0/5640
3	C	0.52	0/3667	0.81	2/4992 (0.0%)
3	c	0.46	0/3703	0.79	0/5041
4	D	0.57	0/2847	0.82	2/3878 (0.1%)
4	d	0.52	0/2838	0.79	2/3866 (0.1%)
5	E	0.47	0/687	0.78	0/936
5	e	0.44	0/667	0.77	0/908
6	F	0.59	0/284	0.74	0/387
6	f	0.48	0/257	0.81	0/349
7	H	0.46	0/530	0.90	0/723
7	h	0.43	0/519	0.80	0/708
8	I	0.47	0/311	0.69	0/419
8	i	0.45	0/311	0.80	0/419
9	J	0.41	0/278	0.74	0/376
9	j	0.41	0/283	0.74	0/383
10	K	0.48	0/303	0.79	0/416
10	k	0.51	0/303	0.86	0/416
11	L	0.49	0/311	0.68	0/423
11	l	0.51	0/311	0.75	0/423
12	M	0.59	0/261	0.97	0/357
12	m	0.53	0/262	0.94	0/357
13	O	0.49	0/1935	0.80	0/2623
13	o	0.49	0/1910	0.81	2/2589 (0.1%)
14	T	0.59	0/257	0.74	0/349
14	t	0.54	0/257	0.78	0/349
15	U	0.48	0/776	0.77	0/1052
15	u	0.47	0/785	0.72	0/1064
16	V	0.49	0/1085	0.75	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.45	0/1085	0.77	0/1473
17	X	0.44	0/284	0.73	0/384
17	x	0.42	0/284	0.75	0/384
18	Y	0.41	0/216	0.77	0/289
18	y	0.41	0/216	0.81	0/289
19	Z	0.43	0/490	0.84	0/669
19	z	0.39	0/490	0.80	0/669
20	R	0.41	0/279	0.73	0/383
All	All	0.51	0/43500	0.80	8/59185 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	170	ALA	CA-C-N	-6.56	113.22	119.85
4	d	170	ALA	C-N-CA	-6.56	113.22	119.85
13	o	55	GLU	CA-C-N	6.29	126.05	119.76
13	o	55	GLU	C-N-CA	6.29	126.05	119.76
4	D	170	ALA	CA-C-N	-5.94	113.82	119.76

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	2850	0	2705	26	0
1	a	2852	0	2708	40	0
2	B	4007	0	3879	41	0
2	b	3986	0	3855	44	0
3	C	3542	0	3462	30	0
3	c	3577	0	3498	38	0
4	D	2748	0	2650	30	0
4	d	2739	0	2644	30	0
5	E	665	0	653	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	648	0	634	16	0
6	F	275	0	282	7	0
6	f	250	0	261	1	0
7	H	514	0	542	4	0
7	h	506	0	529	10	0
8	I	314	0	328	4	0
8	i	314	0	328	4	0
9	J	272	0	279	6	0
9	j	277	0	284	3	0
10	K	293	0	305	7	0
10	k	293	0	305	5	0
11	L	301	0	315	2	0
11	l	301	0	315	3	0
12	M	265	0	286	3	0
12	m	269	0	288	7	0
13	O	1889	0	1871	23	0
13	o	1873	0	1852	14	0
14	T	258	0	261	4	0
14	t	258	0	261	3	0
15	U	765	0	767	6	0
15	u	774	0	773	4	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	10	0
17	X	281	0	312	2	0
17	x	281	0	312	4	0
18	Y	215	0	246	6	0
18	y	215	0	246	4	0
19	Z	479	0	516	4	0
19	z	479	0	516	3	0
20	R	273	0	305	6	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	14	0
24	B	1040	0	1152	37	0
24	C	845	0	936	40	0
24	D	130	0	144	6	0
24	a	260	0	288	14	0
24	b	1040	0	1152	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	c	845	0	936	50	0
24	d	130	0	144	7	0
25	A	128	0	148	6	0
25	a	128	0	148	5	0
26	A	40	0	56	2	0
26	B	120	0	168	7	0
26	C	80	0	112	6	0
26	D	40	0	56	3	0
26	H	40	0	56	3	0
26	K	40	0	56	1	0
26	T	40	0	56	6	0
26	Y	40	0	56	3	0
26	a	40	0	56	2	0
26	b	120	0	168	10	0
26	c	80	0	112	7	0
26	d	40	0	56	3	0
26	h	40	0	56	5	0
26	k	40	0	56	1	0
26	t	40	0	56	5	0
26	y	40	0	56	4	0
27	A	108	0	156	8	0
27	B	54	0	78	1	0
27	F	43	0	53	1	0
27	a	108	0	156	5	0
27	b	54	0	78	2	0
27	f	43	0	53	3	0
28	A	6	0	8	0	0
28	B	12	0	16	2	0
28	C	6	0	8	0	0
28	V	6	0	8	0	0
28	a	12	0	16	2	0
28	b	6	0	8	0	0
28	c	6	0	8	0	0
28	v	6	0	8	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	11	0	0	0	0
30	a	11	0	0	1	0
31	A	110	0	160	9	0
31	D	55	0	80	5	0
31	a	110	0	160	14	0
31	d	55	0	80	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	1	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	53	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
32	x	18	0	0	0	0
33	A	51	0	72	1	0
33	B	51	0	72	1	0
33	C	102	0	144	3	0
33	J	51	0	72	2	0
33	Z	37	0	44	5	0
33	a	51	0	72	3	0
33	b	51	0	72	1	0
33	c	102	0	144	2	0
33	j	51	0	72	4	0
33	z	39	0	48	2	0
34	A	35	0	46	2	0
34	B	60	0	81	3	0
34	E	35	0	46	1	0
34	I	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	4	0
34	b	50	0	70	0	0
34	e	35	0	46	1	0
34	m	35	0	46	1	0
34	t	26	0	35	1	0
35	B	76	0	104	5	0
35	C	38	0	52	2	0
35	D	16	0	17	2	0
35	V	11	0	10	0	0
35	b	76	0	104	7	0
35	c	38	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	h	16	0	17	0	0
36	C	186	0	246	4	0
36	H	62	0	82	2	0
36	c	186	0	246	6	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	b	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
37	v	1	0	0	0	0
38	D	147	0	222	10	0
38	E	42	0	57	6	0
38	L	49	0	74	2	0
38	a	42	0	57	3	0
38	d	147	0	222	12	0
38	l	49	0	74	2	0
39	E	43	0	30	2	0
39	e	43	0	30	4	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	130	0	0	1	0
42	B	164	0	0	2	0
42	C	147	0	0	1	0
42	D	112	0	0	1	0
42	E	14	0	0	1	0
42	F	4	0	0	0	0
42	H	20	0	0	0	0
42	I	6	0	0	1	0
42	J	4	0	0	0	0
42	K	7	0	0	0	0
42	L	4	0	0	0	0
42	M	7	0	0	0	0
42	O	74	0	0	1	0
42	T	8	0	0	0	0
42	U	33	0	0	0	0
42	V	65	0	0	0	0
42	X	2	0	0	0	0
42	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	a	133	0	0	1	0
42	b	185	0	0	2	0
42	c	122	0	0	3	0
42	d	109	0	0	0	0
42	e	7	0	0	0	0
42	f	3	0	0	0	0
42	h	14	0	0	0	0
42	i	3	0	0	0	0
42	j	2	0	0	0	0
42	k	3	0	0	0	0
42	l	6	0	0	0	0
42	m	11	0	0	1	0
42	o	78	0	0	1	0
42	t	5	0	0	0	0
42	u	47	0	0	1	0
42	v	49	0	0	1	0
42	x	4	0	0	0	0
42	y	1	0	0	0	0
All	All	53280	0	52671	660	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 6.

The worst 5 of 660 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)
24:C:514:CLA:HBB1	26:C:515:BCR:H24C	1.35	1.05
24:B:604:CLA:H42	24:B:605:CLA:H2	1.47	0.95
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.19	0.89
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.54	0.88
5:e:67:THR:H	5:e:75:GLN:HE22	1.27	0.83

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	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	36	43
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	36	43
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	30	34
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	30	34
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100	100
4	d	342/342 (100%)	336 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	6
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	2
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	6
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	6
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	43	52

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER

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	295/279 (106%)	295 (100%)	0	100	100
1	a	296/279 (106%)	295 (100%)	1 (0%)	86	92
2	B	410/403 (102%)	406 (99%)	4 (1%)	68	81
2	b	406/403 (101%)	398 (98%)	8 (2%)	48	63
3	C	360/356 (101%)	355 (99%)	5 (1%)	59	73
3	c	364/356 (102%)	358 (98%)	6 (2%)	55	70
4	D	280/277 (101%)	279 (100%)	1 (0%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	279/277 (101%)	279 (100%)	0	100	100
5	E	73/73 (100%)	72 (99%)	1 (1%)	59	73
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	28	37
7	H	55/54 (102%)	51 (93%)	4 (7%)	13	14
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	49
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	13
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	39
10	K	30/30 (100%)	25 (83%)	5 (17%)	2	2
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	3
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	49
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	44
13	O	211/207 (102%)	204 (97%)	7 (3%)	33	44
13	o	208/207 (100%)	207 (100%)	1 (0%)	81	89
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	39
14	t	26/28 (93%)	25 (96%)	1 (4%)	29	39
15	U	83/89 (93%)	80 (96%)	3 (4%)	31	41
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	57
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	82
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	43
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	9
18	y	22/23 (96%)	21 (96%)	1 (4%)	24	32
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	22
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4416/4403 (100%)	4341 (98%)	75 (2%)	53	68

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	17	ILE
18	y	45	ASN
10	k	24	VAL
15	u	16	LYS
13	O	24	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	81	HIS
15	u	78	ASN
2	b	53	ASN
19	z	58	ASN
5	e	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.06	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.65	0	7,9,11	1.22	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.37	0
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.30	0
14	FME	t	1	14	8,9,10	0.66	0	7,9,11	1.57	2 (28%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.21	1 (14%)

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
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.72	117.64	124.78
14	t	1	FME	C-CA-N	2.26	113.81	109.73
12	M	1	FME	O-C-CA	-2.09	119.30	124.78
8	I	1	FME	O-C-CA	-2.05	119.39	124.78
8	i	1	FME	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	O-C-CA-CB
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 227 ligands modelled in this entry, 18 are monoatomic and 18 are unknown - leaving 191 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
24	CLA	b	611	2	69,73,73	2.01	19 (27%)	83,113,113	2.86	28 (33%)
24	CLA	c	514	3	69,73,73	2.04	19 (27%)	83,113,113	2.92	34 (40%)
38	LHG	l	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.10	3 (5%)
24	CLA	b	616	2	69,73,73	2.02	19 (27%)	83,113,113	2.86	32 (38%)
24	CLA	b	609	2	69,73,73	2.01	21 (30%)	83,113,113	2.78	30 (36%)
24	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.69	28 (33%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.16	5 (6%)
36	DGD	h	103	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	3 (3%)
28	GOL	a	416	-	5,5,5	0.35	0	5,5,5	0.65	0
24	CLA	C	514	3	69,73,73	2.05	20 (28%)	83,113,113	2.83	29 (34%)
24	CLA	C	503	3	69,73,73	2.00	19 (27%)	83,113,113	2.79	28 (33%)
34	LMT	a	359	-	36,36,36	0.50	1 (2%)	47,47,47	0.90	2 (4%)
31	PL9	A	416[A]	-	55,55,55	0.63	1 (1%)	68,69,69	2.01	23 (33%)
27	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.40	8 (12%)
29	OEX	a	412[A]	3,42,1	0,14,14	-	-	-	-	-
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.09	5 (9%)
24	CLA	B	604	2	69,73,73	1.96	19 (27%)	83,113,113	2.75	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	c	517	-	41,41,41	1.04	1 (2%)	56,56,56	1.64	13 (23%)
38	LHG	D	407	-	48,48,48	0.90	2 (4%)	51,54,54	0.99	3 (5%)
34	LMT	I	101	-	36,36,36	0.48	1 (2%)	47,47,47	1.07	3 (6%)
35	HTG	b	625	-	19,19,19	1.09	2 (10%)	23,24,24	1.75	3 (13%)
28	GOL	b	627	-	5,5,5	0.34	0	5,5,5	0.37	0
24	CLA	B	613	2	69,73,73	1.96	19 (27%)	83,113,113	2.85	32 (38%)
25	PHO	A	408	-	58,69,69	2.73	14 (24%)	56,99,99	3.06	18 (32%)
35	HTG	C	523	-	19,19,19	1.06	2 (10%)	23,24,24	1.82	5 (21%)
31	PL9	A	416[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.87	20 (29%)
24	CLA	C	513	3	69,73,73	2.05	20 (28%)	83,113,113	2.85	30 (36%)
36	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.94	4 (5%)
24	CLA	b	607	42	69,73,73	1.97	19 (27%)	83,113,113	2.86	30 (36%)
33	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.18	6 (10%)
24	CLA	c	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.85	30 (36%)
24	CLA	B	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.85	33 (39%)
24	CLA	B	605	2	69,73,73	2.01	19 (27%)	83,113,113	2.93	31 (37%)
24	CLA	b	613	2	69,73,73	2.04	18 (26%)	83,113,113	2.80	28 (33%)
28	GOL	B	627	-	5,5,5	0.47	0	5,5,5	0.38	0
27	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.47	9 (14%)
36	DGD	c	518	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	4 (5%)
24	CLA	c	505	3	69,73,73	2.02	19 (27%)	83,113,113	2.79	26 (31%)
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.08	3 (6%)
25	PHO	a	406	-	58,69,69	2.76	14 (24%)	56,99,99	2.90	17 (30%)
24	CLA	c	507	3	69,73,73	1.98	20 (28%)	83,113,113	2.71	27 (32%)
24	CLA	c	512	3	69,73,73	2.02	20 (28%)	83,113,113	2.80	32 (38%)
24	CLA	b	604	2	69,73,73	1.98	17 (24%)	83,113,113	2.76	29 (34%)
34	LMT	E	102	-	36,36,36	0.47	0	47,47,47	0.82	0
39	HEM	e	102	5,6	50,50,50	1.52	8 (16%)	66,82,82	1.72	13 (19%)
26	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.75	14 (25%)
24	CLA	C	504	3	69,73,73	2.01	18 (26%)	83,113,113	2.88	26 (31%)
24	CLA	b	614	2	69,73,73	1.96	20 (28%)	83,113,113	2.89	30 (36%)
33	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.21	5 (8%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	3 (5%)
24	CLA	A	406	42	69,73,73	2.06	19 (27%)	83,113,113	2.88	33 (39%)
38	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	0.90	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	601	42	69,73,73	2.08	20 (28%)	83,113,113	2.80	28 (33%)
24	CLA	D	403	4	69,73,73	2.02	18 (26%)	83,113,113	2.89	33 (39%)
28	GOL	B	626	-	5,5,5	0.37	0	5,5,5	0.47	0
34	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.87	1 (2%)
36	DGD	c	520	-	63,63,67	0.82	2 (3%)	77,77,81	1.09	3 (3%)
24	CLA	c	506	42	69,73,73	2.02	21 (30%)	83,113,113	2.85	32 (38%)
30	OEY	a	413[B]	3,42,1	0,16,16	-	-	-	-	-
24	CLA	B	615	2	69,73,73	1.99	17 (24%)	83,113,113	2.91	31 (37%)
24	CLA	C	512	3	69,73,73	2.03	21 (30%)	83,113,113	2.76	29 (34%)
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.95	2 (4%)
24	CLA	B	608	2	69,73,73	1.98	19 (27%)	83,113,113	2.84	29 (34%)
24	CLA	a	407	1	69,73,73	2.01	20 (28%)	83,113,113	2.79	32 (38%)
27	SQD	A	413	-	53,54,54	1.01	3 (5%)	62,65,65	1.10	6 (9%)
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.66	8 (15%)
24	CLA	C	511	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	31 (37%)
24	CLA	c	510	3	69,73,73	2.02	20 (28%)	83,113,113	2.83	27 (32%)
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.73	1 (3%)
26	BCR	a	408	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	11 (19%)
28	GOL	a	410	-	5,5,5	0.36	0	5,5,5	0.35	0
34	LMT	B	622	-	36,36,36	0.41	0	47,47,47	1.07	2 (4%)
41	HEC	V	203	16	50,50,50	1.70	10 (20%)	68,82,82	1.91	17 (25%)
24	CLA	a	350	42	69,73,73	2.02	18 (26%)	83,113,113	2.90	29 (34%)
24	CLA	C	507	3	69,73,73	2.03	21 (30%)	83,113,113	2.81	33 (39%)
24	CLA	d	402	4	69,73,73	1.96	20 (28%)	83,113,113	2.74	32 (38%)
24	CLA	C	510	3	69,73,73	2.05	21 (30%)	83,113,113	2.82	29 (34%)
38	LHG	E	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.11	5 (11%)
24	CLA	c	511	3	69,73,73	2.09	20 (28%)	83,113,113	2.81	31 (37%)
39	HEM	E	103	5,6	50,50,50	1.54	7 (14%)	66,82,82	1.84	16 (24%)
38	LHG	D	406	-	48,48,48	0.89	3 (6%)	51,54,54	0.99	3 (5%)
27	SQD	a	411	-	53,54,54	1.05	3 (5%)	62,65,65	1.25	7 (11%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.14	2 (6%)
24	CLA	C	505	42	69,73,73	1.98	20 (28%)	83,113,113	2.86	35 (42%)
24	CLA	b	602	2	69,73,73	2.05	20 (28%)	83,113,113	2.91	32 (38%)
24	CLA	B	610	42	69,73,73	2.05	19 (27%)	83,113,113	2.82	31 (37%)
29	OEX	A	414[A]	3,42,1	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	509	42	69,73,73	2.03	19 (27%)	83,113,113	2.84	29 (34%)
24	CLA	C	506	3	69,73,73	2.00	20 (28%)	83,113,113	2.76	30 (36%)
25	PHO	a	405	-	58,69,69	2.71	16 (27%)	56,99,99	3.01	15 (26%)
34	LMT	b	630	-	25,25,36	0.52	1 (4%)	30,30,47	0.85	0
24	CLA	C	509	3	69,73,73	2.04	21 (30%)	83,113,113	2.74	29 (34%)
31	PL9	a	414[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.89	21 (30%)
34	LMT	b	622	-	25,25,36	0.46	0	30,30,47	0.70	0
24	CLA	a	403	1	69,73,73	2.00	20 (28%)	83,113,113	2.84	34 (40%)
28	GOL	A	412	-	5,5,5	0.40	0	5,5,5	0.35	0
30	OEY	A	415[B]	3,42,1	0,16,16	-	-	-		
26	BCR	b	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.63	12 (21%)
36	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	0.93	4 (5%)
26	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.75	14 (25%)
35	HTG	b	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.51	3 (13%)
24	CLA	B	603	2	69,73,73	1.98	20 (28%)	83,113,113	2.96	32 (38%)
28	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.12	0
26	BCR	D	404	-	41,41,41	1.04	1 (2%)	56,56,56	1.84	18 (32%)
24	CLA	b	608	2	69,73,73	2.03	20 (28%)	83,113,113	2.83	33 (39%)
24	CLA	A	404	1	69,73,73	2.01	20 (28%)	83,113,113	2.89	29 (34%)
38	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
24	CLA	A	409	1	69,73,73	2.00	21 (30%)	83,113,113	2.94	32 (38%)
26	BCR	h	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	11 (19%)
27	SQD	a	409	-	53,54,54	0.96	3 (5%)	62,65,65	1.78	13 (20%)
31	PL9	D	405	-	55,55,55	0.67	2 (3%)	68,69,69	1.74	20 (29%)
35	HTG	B	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.39	5 (21%)
34	LMT	e	101	-	36,36,36	0.47	0	47,47,47	0.80	1 (2%)
35	HTG	h	101	-	16,16,19	1.15	2 (12%)	20,21,24	1.62	2 (10%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.71	15 (26%)
26	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	12 (21%)
33	LMG	b	621	-	51,51,55	0.86	2 (3%)	59,59,63	1.27	5 (8%)
35	HTG	b	624	-	19,19,19	1.02	1 (5%)	23,24,24	1.37	1 (4%)
34	LMT	A	359	-	36,36,36	0.55	1 (2%)	47,47,47	0.86	0
38	LHG	D	357	-	48,48,48	0.89	2 (4%)	51,54,54	1.20	5 (9%)
24	CLA	c	504	3	69,73,73	1.97	21 (30%)	83,113,113	2.83	30 (36%)
24	CLA	a	404	42	69,73,73	2.02	20 (28%)	83,113,113	2.88	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	508	3	69,73,73	2.07	19 (27%)	83,113,113	2.70	31 (37%)
25	PHO	A	407	-	58,69,69	2.63	13 (22%)	56,99,99	3.00	15 (26%)
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	6 (7%)
23	BCT	a	420[A]	21	2,3,3	0.67	0	2,3,3	0.97	0
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
23	BCT	A	403[B]	21	2,3,3	0.69	0	2,3,3	0.83	0
33	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.10	4 (8%)
35	HTG	V	204	-	11,11,19	0.23	0	15,15,24	1.05	1 (6%)
24	CLA	c	515	3	69,73,73	2.09	21 (30%)	83,113,113	2.88	31 (37%)
31	PL9	a	414[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.98	22 (32%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
33	LMG	J	101	40	51,51,55	0.88	2 (3%)	59,59,63	0.90	3 (5%)
33	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.13	6 (10%)
33	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.48	7 (15%)
24	CLA	d	403	4	69,73,73	2.07	19 (27%)	83,113,113	2.92	33 (39%)
23	BCT	a	420[B]	21	2,3,3	0.66	0	2,3,3	0.86	0
24	CLA	B	601	42	69,73,73	2.06	19 (27%)	83,113,113	2.83	29 (34%)
27	SQD	A	411	-	53,54,54	0.94	3 (5%)	62,65,65	1.81	13 (20%)
26	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.68	11 (19%)
26	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	8 (14%)
24	CLA	B	616	2	69,73,73	2.01	20 (28%)	83,113,113	2.87	31 (37%)
24	CLA	B	609	2	69,73,73	1.99	17 (24%)	83,113,113	2.86	28 (33%)
24	CLA	C	502	3	69,73,73	2.01	21 (30%)	83,113,113	2.89	31 (37%)
24	CLA	A	405	42	69,73,73	2.01	19 (27%)	83,113,113	2.96	30 (36%)
24	CLA	b	603	2	69,73,73	2.02	20 (28%)	83,113,113	2.89	29 (34%)
24	CLA	b	606	2	69,73,73	1.98	20 (28%)	83,113,113	2.91	32 (38%)
38	LHG	a	419	-	41,41,48	1.03	2 (4%)	44,47,54	0.90	2 (4%)
36	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	0.94	4 (5%)
35	HTG	D	410	-	16,16,19	1.08	2 (12%)	20,21,24	1.36	1 (5%)
35	HTG	B	628	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	3 (13%)
24	CLA	C	508	42	69,73,73	1.99	20 (28%)	83,113,113	2.72	31 (37%)
28	GOL	c	502	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	B	606	2	69,73,73	1.94	19 (27%)	83,113,113	3.02	29 (34%)
24	CLA	B	611	2	69,73,73	1.96	20 (28%)	83,113,113	2.93	31 (37%)
24	CLA	b	610	42	69,73,73	2.07	19 (27%)	83,113,113	2.86	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.62	12 (21%)
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.77	12 (21%)
26	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	16 (28%)
23	BCT	A	403[A]	21	2,3,3	0.67	0	2,3,3	0.79	0
26	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.49	14 (25%)
41	HEC	v	203	16	50,50,50	1.74	10 (20%)	68,82,82	1.81	18 (26%)
26	BCR	b	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.56	10 (17%)
24	CLA	B	607	42	69,73,73	1.98	18 (26%)	83,113,113	2.89	29 (34%)
24	CLA	c	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	b	605	2	69,73,73	1.96	21 (30%)	83,113,113	2.98	28 (33%)
24	CLA	b	615	2	69,73,73	2.02	19 (27%)	83,113,113	2.85	30 (36%)
35	HTG	B	624	-	19,19,19	0.90	1 (5%)	23,24,24	1.39	1 (4%)
26	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	11 (19%)
28	GOL	v	202	-	5,5,5	0.37	0	5,5,5	0.29	0
38	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	4 (7%)
24	CLA	D	402	4	69,73,73	1.93	21 (30%)	83,113,113	2.93	31 (37%)
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.41	2 (8%)
24	CLA	B	612	2	69,73,73	1.93	21 (30%)	83,113,113	2.84	30 (36%)
26	BCR	d	404	-	41,41,41	1.14	1 (2%)	56,56,56	1.83	14 (25%)
33	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.07	5 (8%)
35	HTG	c	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.35	1 (4%)
31	PL9	d	405	-	55,55,55	0.61	1 (1%)	68,69,69	1.73	19 (27%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.57	14 (25%)
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.83	0
35	HTG	B	625	-	19,19,19	0.99	1 (5%)	23,24,24	1.60	3 (13%)
35	HTG	b	628	-	19,19,19	0.91	2 (10%)	23,24,24	1.29	3 (13%)
24	CLA	B	614	2	69,73,73	1.94	20 (28%)	83,113,113	3.07	30 (36%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.19	4 (6%)
33	LMG	j	101	40	51,51,55	0.88	2 (3%)	59,59,63	1.13	5 (8%)
26	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	12 (21%)
28	GOL	V	202	-	5,5,5	0.37	0	5,5,5	0.35	0
27	SQD	f	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.43	9 (17%)
26	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.54	10 (17%)
35	HTG	c	526	-	19,19,19	1.03	2 (10%)	23,24,24	1.49	3 (13%)

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
24	CLA	b	611	2	-	3/39/115/115	-
24	CLA	c	514	3	-	9/39/115/115	-
38	LHG	l	101	-	-	16/53/53/53	-
24	CLA	b	616	2	-	12/39/115/115	-
24	CLA	b	609	2	-	6/39/115/115	-
24	CLA	b	612	2	-	6/39/115/115	-
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
36	DGD	h	103	-	-	11/51/91/95	0/2/2/2
28	GOL	a	416	-	-	3/4/4/4	-
24	CLA	C	514	3	-	11/39/115/115	-
24	CLA	C	503	3	-	11/39/115/115	-
34	LMT	a	359	-	-	7/21/61/61	0/2/2/2
31	PL9	A	416[A]	-	-	15/53/73/73	0/1/1/1
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
38	LHG	d	406	-	-	8/53/53/53	-
24	CLA	B	604	2	-	11/39/115/115	-
26	BCR	c	517	-	-	4/29/63/63	0/2/2/2
38	LHG	D	407	-	-	10/53/53/53	-
34	LMT	I	101	-	-	9/21/61/61	0/2/2/2
35	HTG	b	625	-	-	2/10/30/30	0/1/1/1
28	GOL	b	627	-	-	2/4/4/4	-
24	CLA	B	613	2	-	6/39/115/115	-
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
31	PL9	A	416[B]	-	-	18/53/73/73	0/1/1/1
24	CLA	C	513	3	-	11/39/115/115	-
36	DGD	c	519	-	-	11/51/91/95	0/2/2/2
24	CLA	b	607	42	-	4/39/115/115	-
33	LMG	a	417	-	-	13/46/66/70	0/1/1/1
24	CLA	c	513	3	-	5/39/115/115	-
24	CLA	B	602	2	-	7/39/115/115	-
24	CLA	B	605	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	613	2	-	8/39/115/115	-
28	GOL	B	627	-	-	3/4/4/4	-
27	SQD	b	620	-	-	20/49/69/69	0/1/1/1
36	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	c	505	3	-	1/39/115/115	-
34	LMT	M	101	-	-	3/21/61/61	0/2/2/2
25	PHO	a	406	-	-	2/37/103/103	0/5/6/6
24	CLA	c	507	3	-	5/39/115/115	-
24	CLA	c	512	3	-	8/39/115/115	-
24	CLA	b	604	2	-	9/39/115/115	-
34	LMT	E	102	-	-	9/21/61/61	0/2/2/2
39	HEM	e	102	5,6	-	9/14/54/54	-
26	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
24	CLA	C	504	3	-	3/39/115/115	-
24	CLA	b	614	2	-	13/39/115/115	-
33	LMG	A	418	-	-	10/46/66/70	0/1/1/1
33	LMG	B	621	-	-	12/46/66/70	0/1/1/1
24	CLA	A	406	42	-	4/39/115/115	-
38	LHG	d	407	-	-	15/53/53/53	-
24	CLA	b	601	42	-	16/39/115/115	-
24	CLA	D	403	4	-	10/39/115/115	-
28	GOL	B	626	-	-	4/4/4/4	-
34	LMT	m	102	-	-	5/21/61/61	0/2/2/2
36	DGD	c	520	-	-	11/51/91/95	0/2/2/2
24	CLA	c	506	42	-	7/39/115/115	-
24	CLA	B	615	2	-	10/39/115/115	-
24	CLA	C	512	3	-	5/39/115/115	-
34	LMT	M	103	-	-	7/21/61/61	0/2/2/2
24	CLA	B	608	2	-	4/39/115/115	-
24	CLA	a	407	1	-	9/39/115/115	-
27	SQD	A	413	-	-	7/49/69/69	0/1/1/1
27	SQD	F	101	-	-	10/38/58/69	0/1/1/1
24	CLA	C	511	3	-	10/39/115/115	-
24	CLA	c	510	3	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	B	630	-	-	11/17/37/61	0/1/1/2
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
28	GOL	a	410	-	-	4/4/4/4	-
34	LMT	B	622	-	-	8/21/61/61	0/2/2/2
41	HEC	V	203	16	1/1/3/7	6/14/54/54	-
24	CLA	a	350	42	-	7/39/115/115	-
24	CLA	C	507	3	-	11/39/115/115	-
24	CLA	d	402	4	-	6/39/115/115	-
24	CLA	C	510	3	-	4/39/115/115	-
38	LHG	E	101	-	-	16/46/46/53	-
24	CLA	c	511	3	-	10/39/115/115	-
39	HEM	E	103	5,6	-	7/14/54/54	-
38	LHG	D	406	-	-	16/53/53/53	-
27	SQD	a	411	-	-	15/49/69/69	0/1/1/1
34	LMT	t	101	-	-	5/17/38/61	0/1/1/2
24	CLA	C	505	42	-	8/39/115/115	-
24	CLA	b	602	2	-	6/39/115/115	-
24	CLA	B	610	42	-	8/39/115/115	-
24	CLA	c	509	42	-	11/39/115/115	-
24	CLA	C	506	3	-	9/39/115/115	-
25	PHO	a	405	-	-	2/37/103/103	0/5/6/6
34	LMT	b	630	-	-	9/17/37/61	0/1/1/2
24	CLA	C	509	3	-	4/39/115/115	-
31	PL9	a	414[B]	-	-	21/53/73/73	0/1/1/1
34	LMT	b	622	-	-	5/17/37/61	0/1/1/2
24	CLA	a	403	1	-	1/39/115/115	-
28	GOL	A	412	-	-	2/4/4/4	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
36	DGD	H	102	-	-	15/51/91/95	0/2/2/2
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
35	HTG	b	623	-	-	6/10/30/30	0/1/1/1
24	CLA	B	603	2	-	6/39/115/115	-
28	GOL	C	525	-	-	2/4/4/4	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CLA	b	608	2	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	404	1	-	1/39/115/115	-
38	LHG	L	101	-	-	13/53/53/53	-
24	CLA	A	409	1	-	10/39/115/115	-
26	BCR	h	102	-	-	2/29/63/63	0/2/2/2
27	SQD	a	409	-	-	12/49/69/69	0/1/1/1
31	PL9	D	405	-	-	15/53/73/73	0/1/1/1
35	HTG	B	623	-	-	2/10/30/30	0/1/1/1
34	LMT	e	101	-	-	6/21/61/61	0/2/2/2
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
33	LMG	b	621	-	-	10/46/66/70	0/1/1/1
35	HTG	b	624	-	-	3/10/30/30	0/1/1/1
34	LMT	A	359	-	-	4/21/61/61	0/2/2/2
38	LHG	D	357	-	-	14/53/53/53	-
24	CLA	c	504	3	-	9/39/115/115	-
24	CLA	a	404	42	-	5/39/115/115	-
24	CLA	c	508	3	-	13/39/115/115	-
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
36	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
24	CLA	c	515	3	-	8/39/115/115	-
31	PL9	a	414[A]	-	-	16/53/73/73	0/1/1/1
33	LMG	C	520	-	-	14/46/66/70	0/1/1/1
33	LMG	J	101	40	-	11/46/66/70	0/1/1/1
33	LMG	c	522	-	-	10/46/66/70	0/1/1/1
33	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	CLA	d	403	4	-	6/39/115/115	-
24	CLA	B	601	42	-	12/39/115/115	-
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
26	BCR	y	101	-	-	6/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	CLA	B	616	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	609	2	-	6/39/115/115	-
24	CLA	C	502	3	-	6/39/115/115	-
24	CLA	A	405	42	-	6/39/115/115	-
24	CLA	b	603	2	-	7/39/115/115	-
24	CLA	b	606	2	-	10/39/115/115	-
38	LHG	a	419	-	-	9/46/46/53	-
36	DGD	C	519	-	-	11/51/91/95	0/2/2/2
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
24	CLA	C	508	42	-	8/39/115/115	-
28	GOL	c	502	-	-	0/4/4/4	-
24	CLA	B	606	2	-	9/39/115/115	-
24	CLA	B	611	2	-	3/39/115/115	-
24	CLA	b	610	42	-	7/39/115/115	-
26	BCR	C	516	-	-	1/29/63/63	0/2/2/2
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
41	HEC	v	203	16	1/1/3/7	6/14/54/54	-
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
24	CLA	B	607	42	-	6/39/115/115	-
24	CLA	c	503	3	-	4/39/115/115	-
24	CLA	b	605	2	-	5/39/115/115	-
24	CLA	b	615	2	-	4/39/115/115	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
28	GOL	v	202	-	-	2/4/4/4	-
38	LHG	d	408	-	-	12/53/53/53	-
24	CLA	D	402	4	-	2/39/115/115	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	CLA	B	612	2	-	5/39/115/115	-
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1
35	HTG	c	523	-	-	4/10/30/30	0/1/1/1
31	PL9	d	405	-	-	9/53/73/73	0/1/1/1
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
35	HTG	B	625	-	-	4/10/30/30	0/1/1/1
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	B	614	2	-	13/39/115/115	-
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
33	LMG	j	101	40	-	9/46/66/70	0/1/1/1
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
27	SQD	f	101	-	-	13/38/58/69	0/1/1/1
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
35	HTG	c	526	-	-	1/10/30/30	0/1/1/1

The worst 5 of 1617 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	PHO	C1D-C2D	8.83	1.49	1.39
25	a	405	PHO	C1B-C2B	8.74	1.49	1.39
25	a	405	PHO	C1D-C2D	8.58	1.49	1.39
25	a	406	PHO	C1B-C2B	8.49	1.49	1.39
25	A	408	PHO	C1B-C2B	8.24	1.48	1.39

The worst 5 of 2906 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	PHO	C2D-C1D-ND	12.40	118.09	109.53
25	A	407	PHO	C2D-C1D-ND	12.30	118.02	109.53
25	A	408	PHO	C2D-C1D-ND	12.22	117.96	109.53
25	a	406	PHO	C2D-C1D-ND	10.82	117.00	109.53
24	a	404	CLA	C1D-ND-C4D	-10.11	99.15	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
41	V	203	HEC	NA
41	v	203	HEC	NA

5 of 1292 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	C2B-C3B-CAB-CBB
24	B	603	CLA	C4B-C3B-CAB-CBB
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6

There are no ring outliers.

154 monomers are involved in 383 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	611	CLA	1	0
24	c	514	CLA	7	0
38	l	101	LHG	2	0
24	b	616	CLA	1	0
24	b	609	CLA	4	0
24	b	612	CLA	4	0
36	C	517	DGD	2	0
28	a	416	GOL	1	0
24	C	514	CLA	5	0
24	C	503	CLA	3	0
34	a	359	LMT	3	0
31	A	416[A]	PL9	4	0
27	B	620	SQD	1	0
38	d	406	LHG	2	0
24	B	604	CLA	3	0
26	c	517	BCR	2	0
38	D	407	LHG	5	0
34	I	101	LMT	1	0
35	b	625	HTG	1	0
24	B	613	CLA	3	0
25	A	408	PHO	4	0
31	A	416[B]	PL9	5	0
24	C	513	CLA	2	0
36	c	519	DGD	5	0
24	b	607	CLA	1	0
33	a	417	LMG	3	0
24	c	513	CLA	4	0
24	B	602	CLA	5	0
24	B	605	CLA	4	0
24	b	613	CLA	4	0
28	B	627	GOL	2	0
27	b	620	SQD	2	0
36	c	518	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	505	CLA	5	0
34	M	101	LMT	1	0
25	a	406	PHO	3	0
24	c	507	CLA	8	0
24	c	512	CLA	6	0
24	b	604	CLA	1	0
34	E	102	LMT	1	0
39	e	102	HEM	4	0
26	Y	101	BCR	3	0
24	C	504	CLA	5	0
24	b	614	CLA	6	0
33	A	418	LMG	1	0
33	B	621	LMG	1	0
24	A	406	CLA	4	0
38	d	407	LHG	3	0
24	b	601	CLA	2	0
24	D	403	CLA	1	0
34	m	102	LMT	1	0
24	c	506	CLA	4	0
30	a	413[B]	OEY	1	0
24	B	615	CLA	2	0
24	C	512	CLA	2	0
34	M	103	LMT	2	0
24	a	407	CLA	3	0
27	A	413	SQD	2	0
27	F	101	SQD	1	0
24	C	511	CLA	2	0
24	c	510	CLA	5	0
26	a	408	BCR	2	0
28	a	410	GOL	1	0
34	B	622	LMT	3	0
24	a	350	CLA	4	0
24	C	507	CLA	8	0
24	d	402	CLA	3	0
24	C	510	CLA	3	0
38	E	101	LHG	6	0
24	c	511	CLA	3	0
39	E	103	HEM	2	0
38	D	406	LHG	3	0
34	t	101	LMT	1	0
24	C	505	CLA	1	0
24	b	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	610	CLA	2	0
24	c	509	CLA	4	0
24	C	506	CLA	4	0
25	a	405	PHO	2	0
24	C	509	CLA	5	0
31	a	414[B]	PL9	8	0
24	a	403	CLA	5	0
26	b	619	BCR	4	0
36	H	102	DGD	2	0
26	T	101	BCR	6	0
35	b	623	HTG	4	0
26	D	404	BCR	3	0
24	A	404	CLA	6	0
38	L	101	LHG	2	0
24	A	409	CLA	3	0
26	h	102	BCR	5	0
27	a	409	SQD	5	0
31	D	405	PL9	5	0
35	B	623	HTG	3	0
34	e	101	LMT	1	0
26	t	102	BCR	5	0
26	K	102	BCR	1	0
33	b	621	LMG	1	0
35	b	624	HTG	2	0
34	A	359	LMT	2	0
38	D	357	LHG	2	0
24	c	504	CLA	4	0
24	a	404	CLA	3	0
24	c	508	CLA	4	0
25	A	407	PHO	2	0
36	C	518	DGD	1	0
26	A	410	BCR	2	0
33	z	101	LMG	2	0
24	c	515	CLA	5	0
31	a	414[A]	PL9	6	0
33	J	101	LMG	2	0
33	Z	101	LMG	5	0
24	d	403	CLA	4	0
24	B	601	CLA	1	0
27	A	411	SQD	6	0
26	y	101	BCR	4	0
26	C	515	BCR	4	0

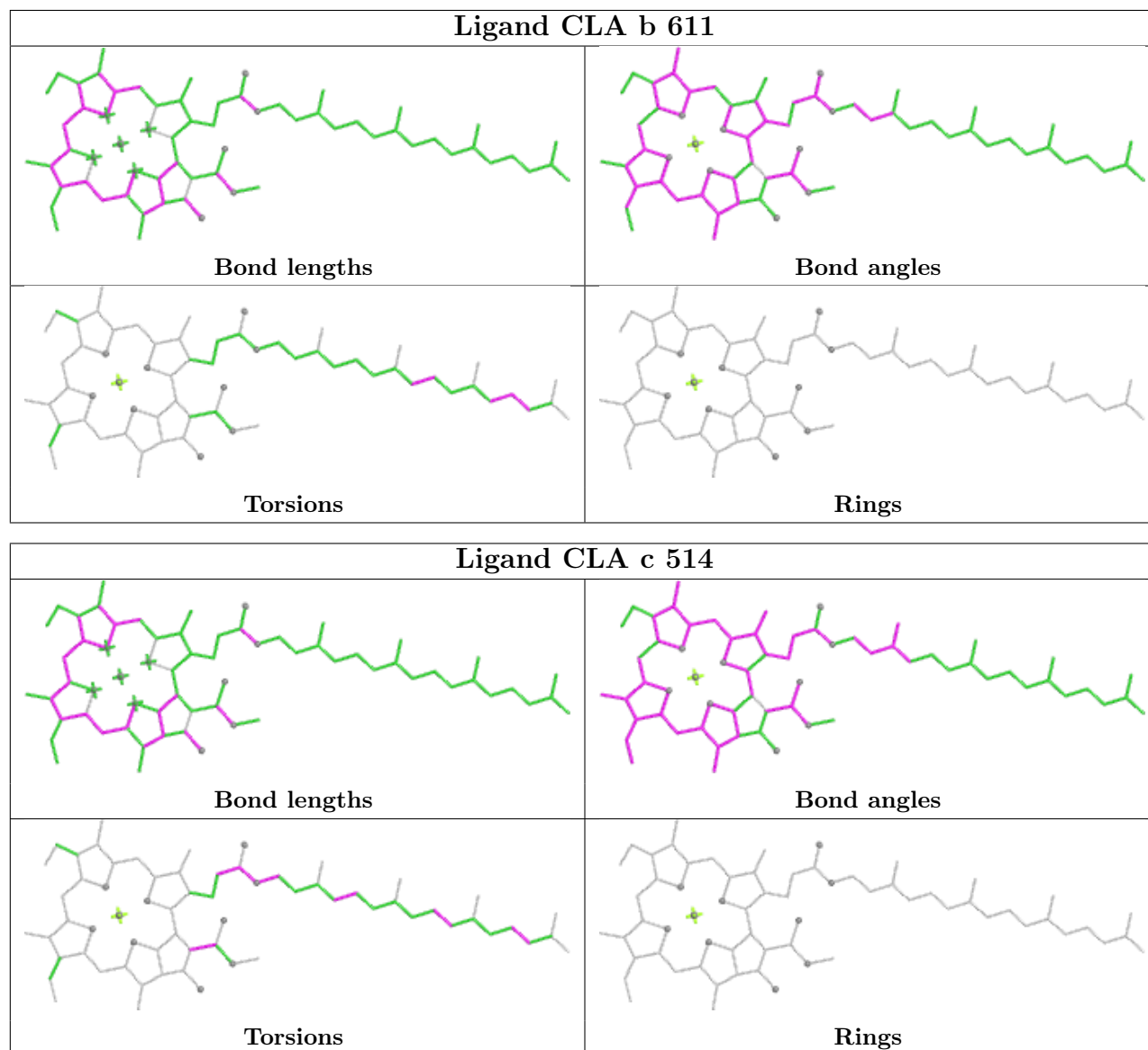
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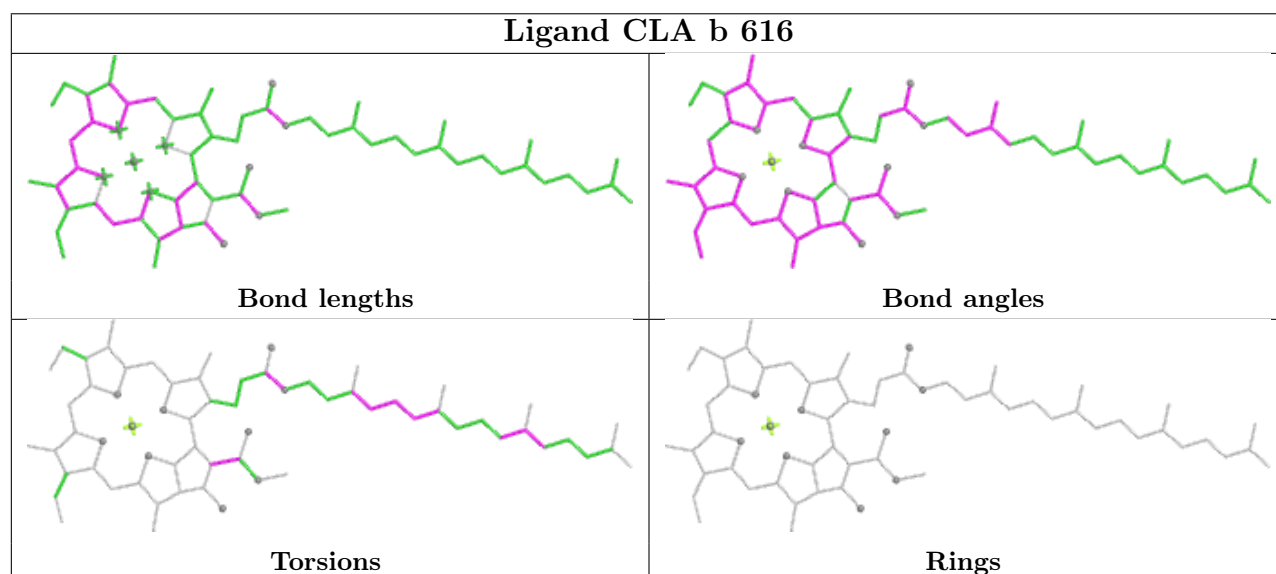
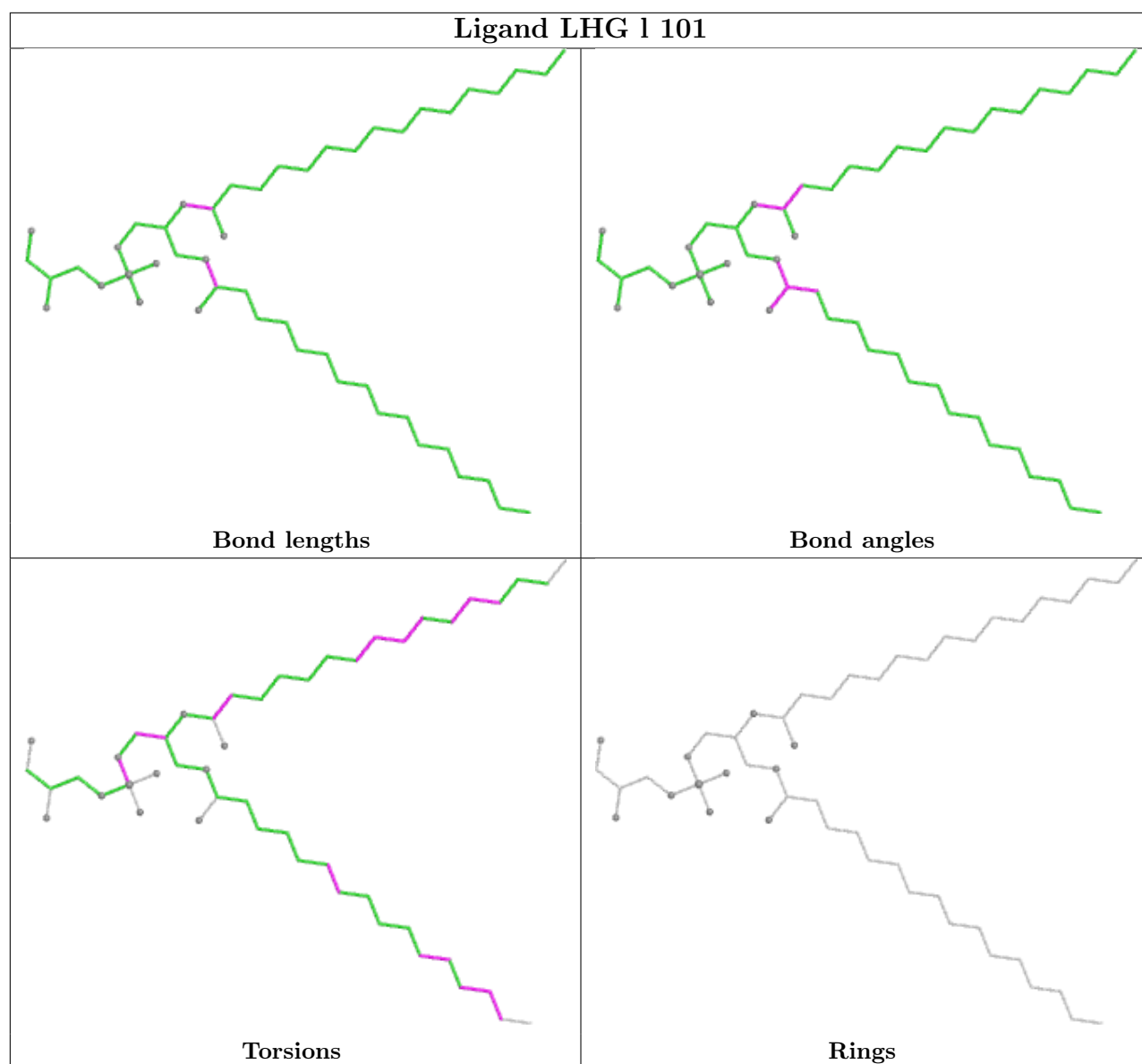
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	616	CLA	5	0
24	B	609	CLA	6	0
24	C	502	CLA	5	0
24	A	405	CLA	3	0
24	b	603	CLA	3	0
24	b	606	CLA	5	0
38	a	419	LHG	3	0
36	C	519	DGD	1	0
35	D	410	HTG	2	0
24	C	508	CLA	2	0
24	B	606	CLA	3	0
24	B	611	CLA	1	0
24	b	610	CLA	1	0
26	C	516	BCR	2	0
26	c	516	BCR	5	0
26	b	618	BCR	3	0
26	B	619	BCR	3	0
26	b	617	BCR	3	0
24	c	503	CLA	2	0
24	b	605	CLA	8	0
24	b	615	CLA	1	0
35	B	624	HTG	2	0
26	H	101	BCR	3	0
38	d	408	LHG	7	0
24	D	402	CLA	5	0
35	C	522	HTG	2	0
24	B	612	CLA	3	0
26	d	404	BCR	3	0
33	c	521	LMG	2	0
31	d	405	PL9	3	0
26	B	618	BCR	4	0
34	a	418	LMT	1	0
24	B	614	CLA	5	0
33	C	521	LMG	3	0
33	j	101	LMG	4	0
26	k	101	BCR	1	0
27	f	101	SQD	3	0

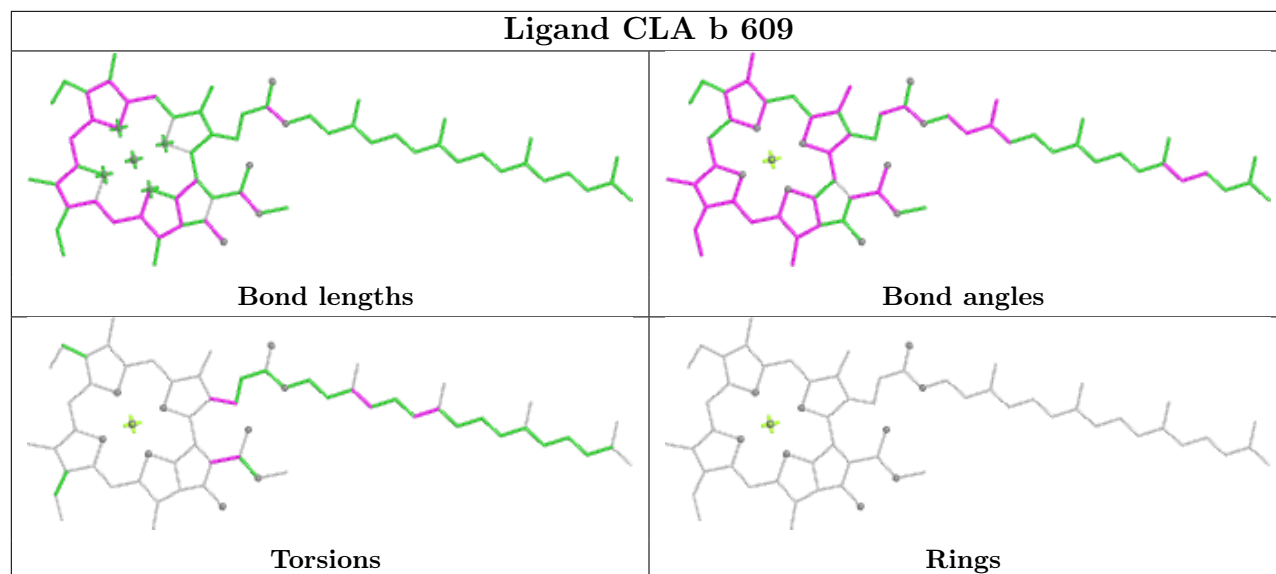
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

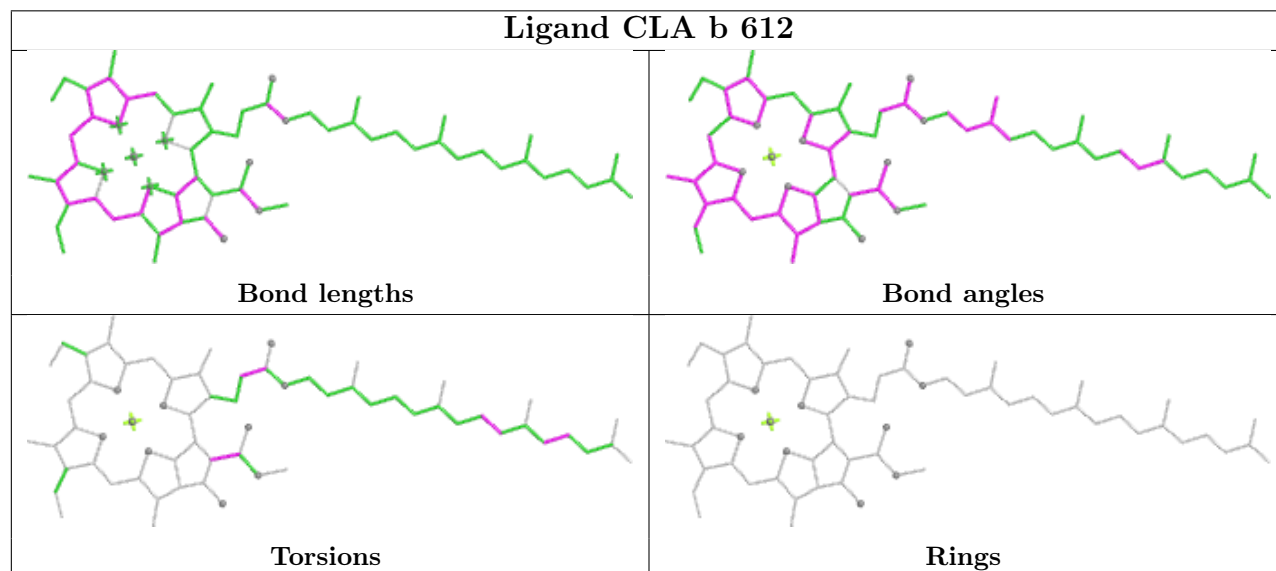




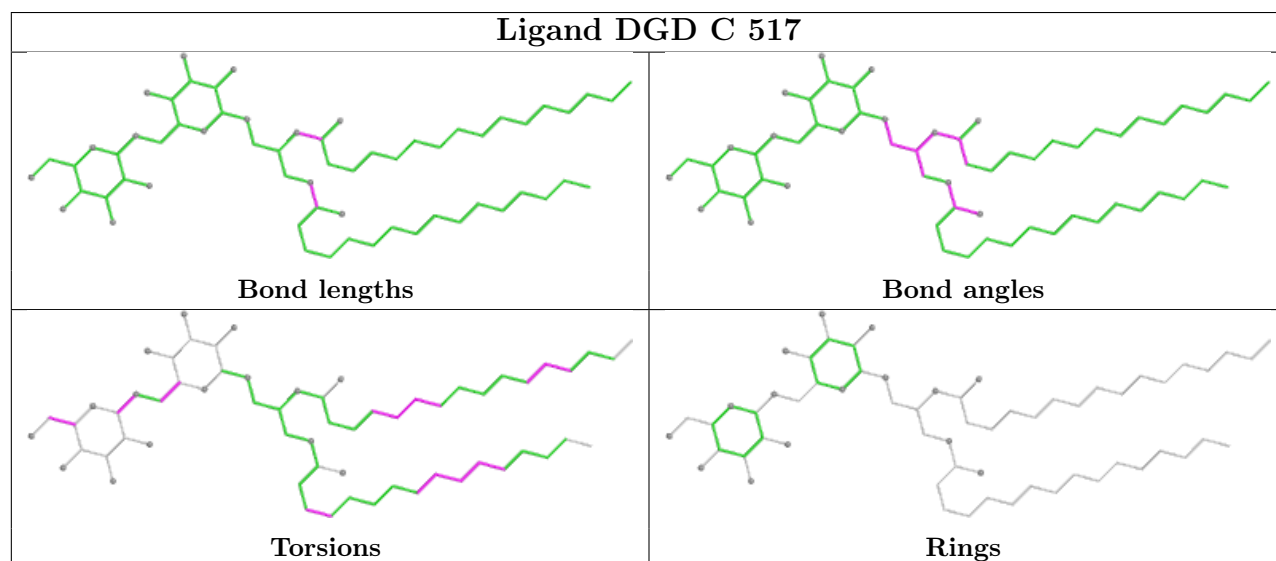
Ligand CLA b 609

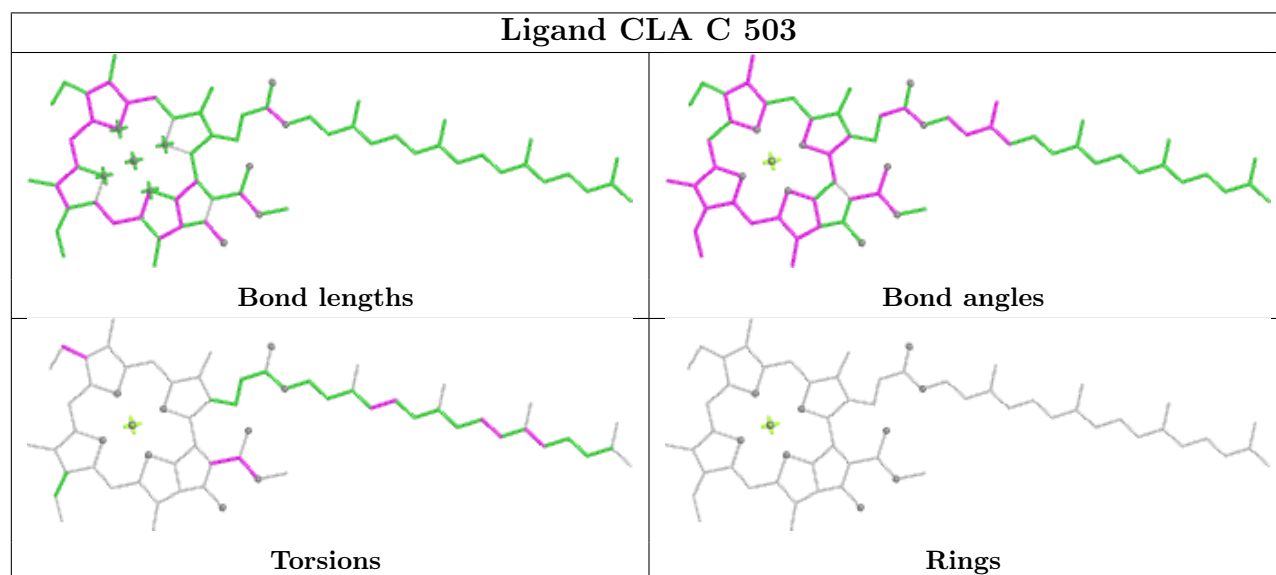
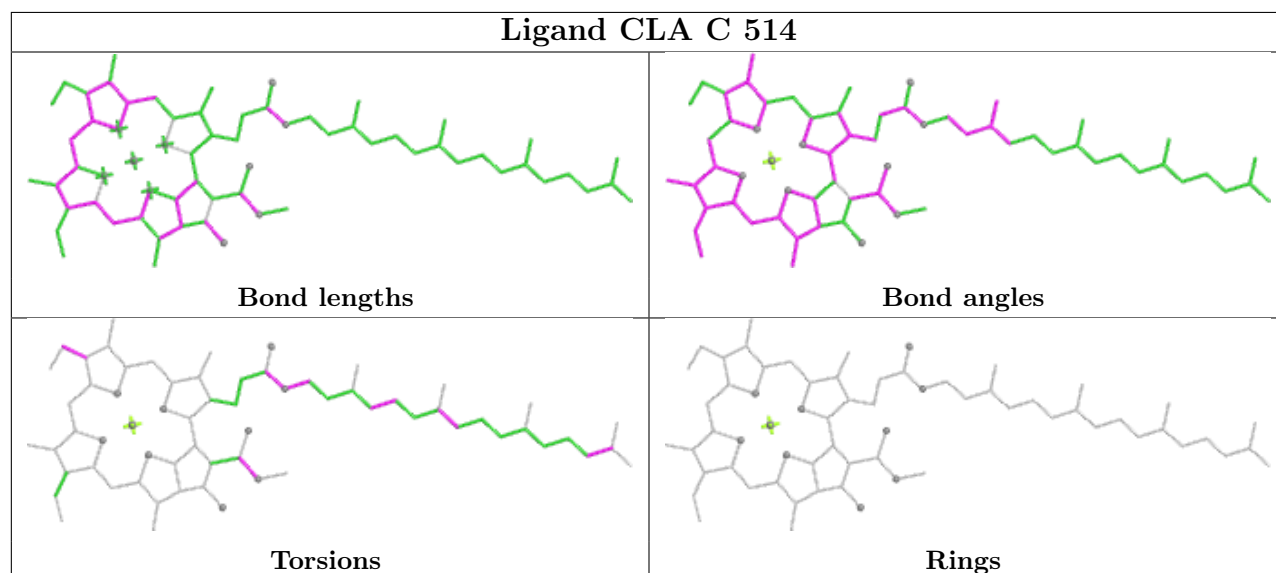
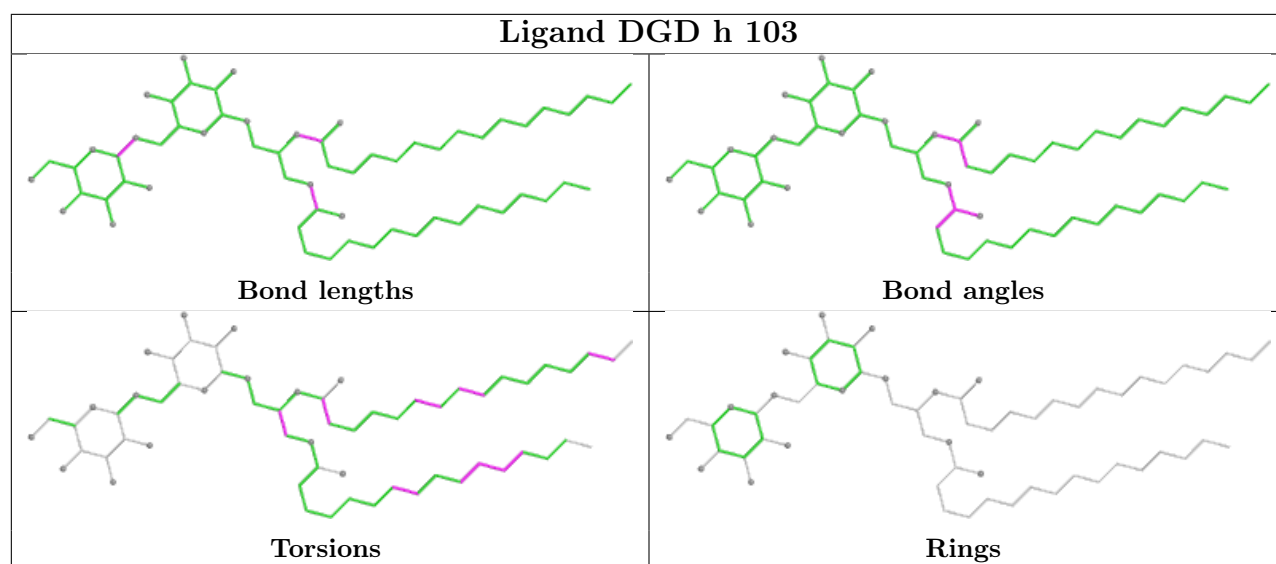


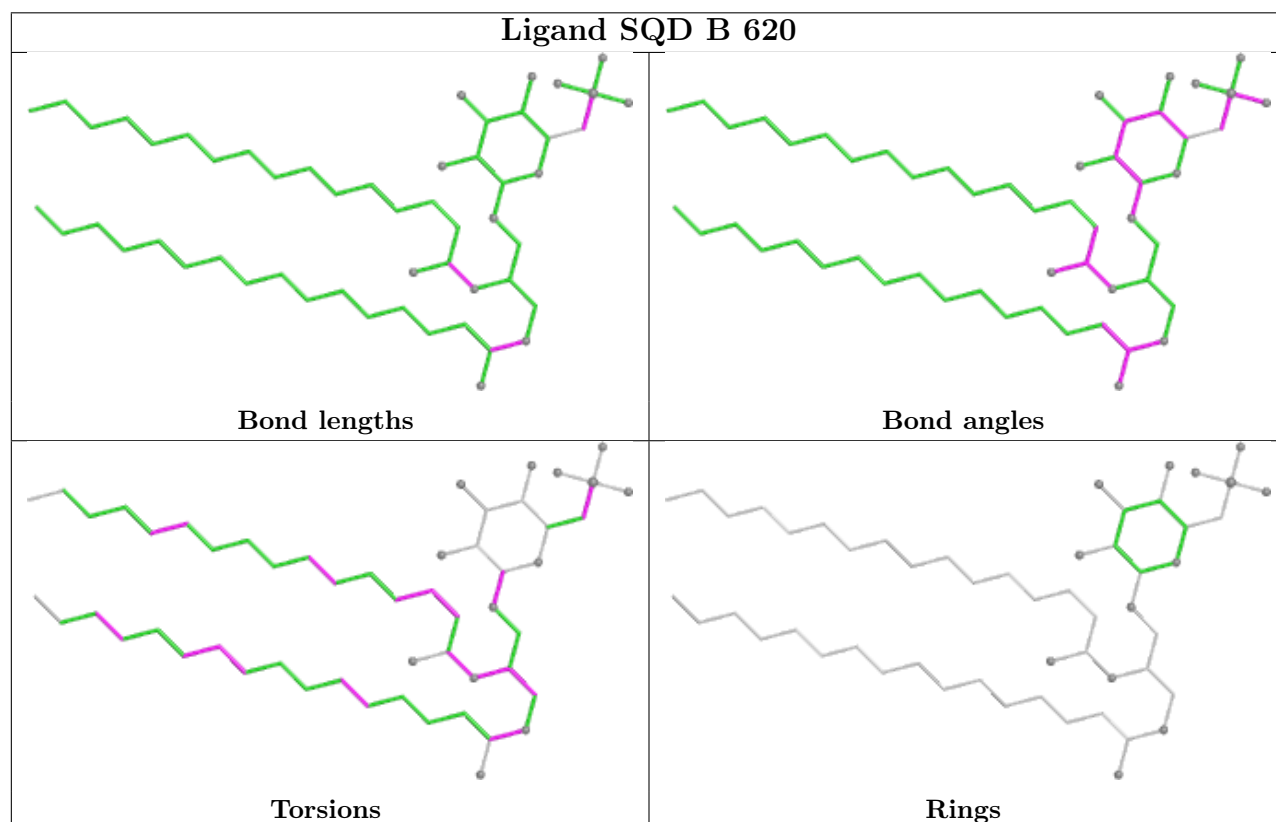
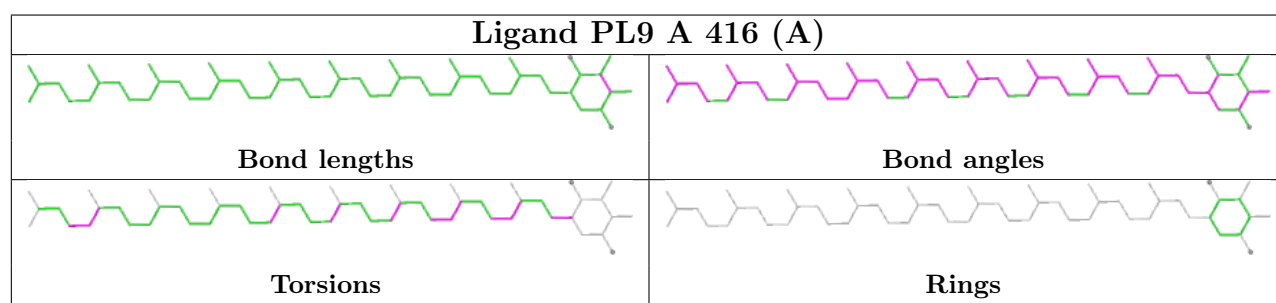
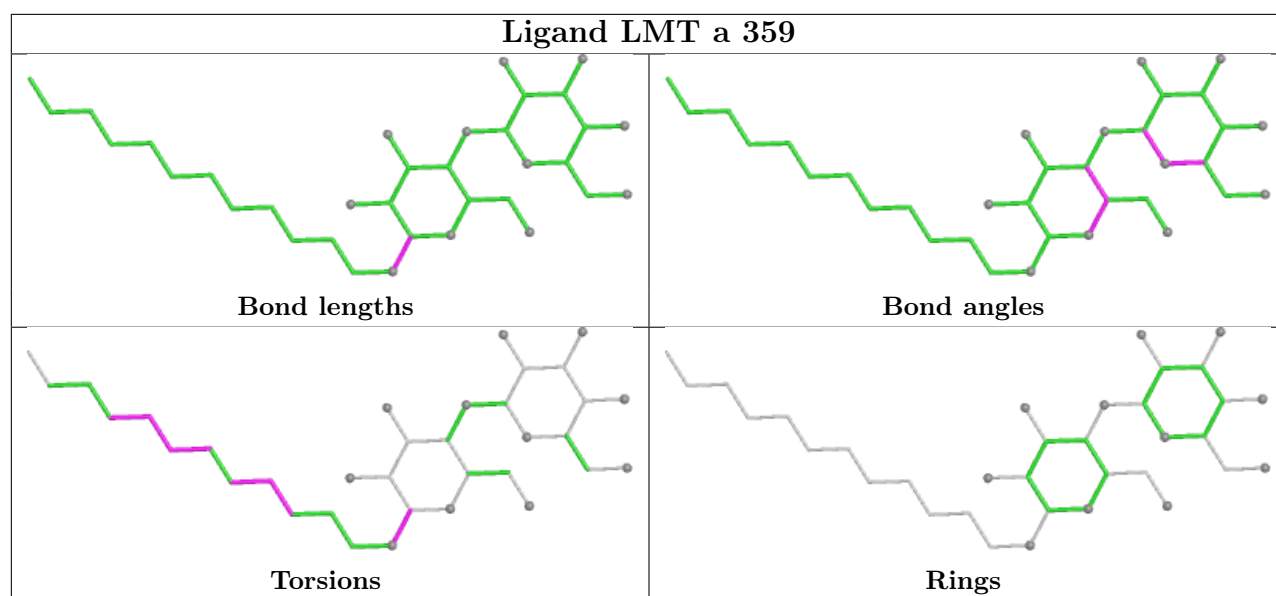
Ligand CLA b 612

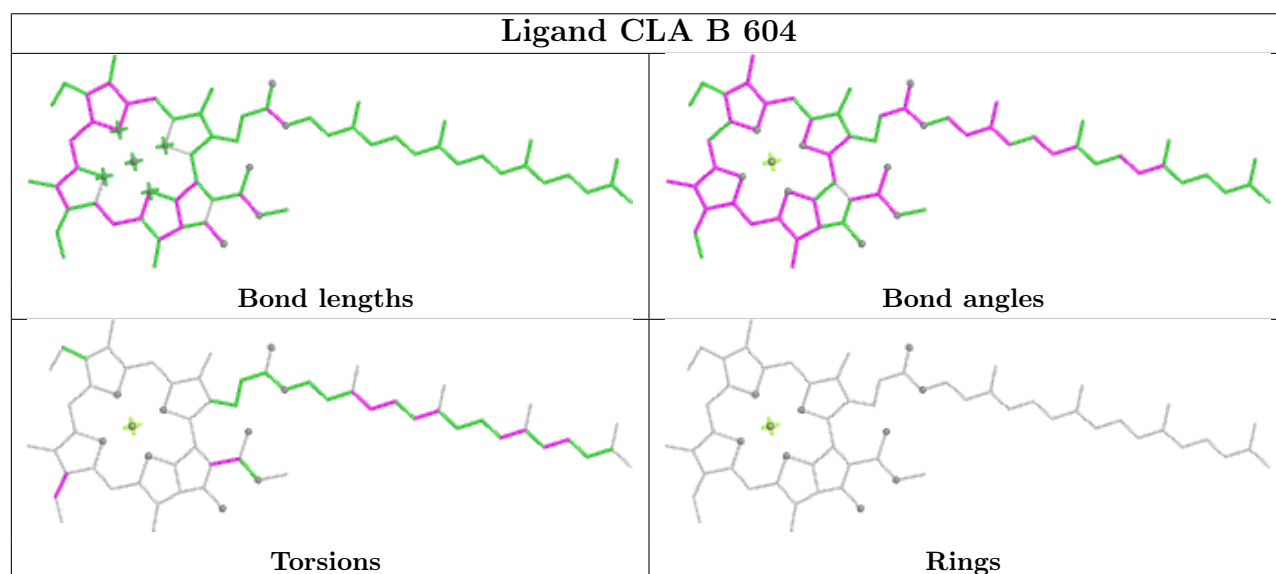
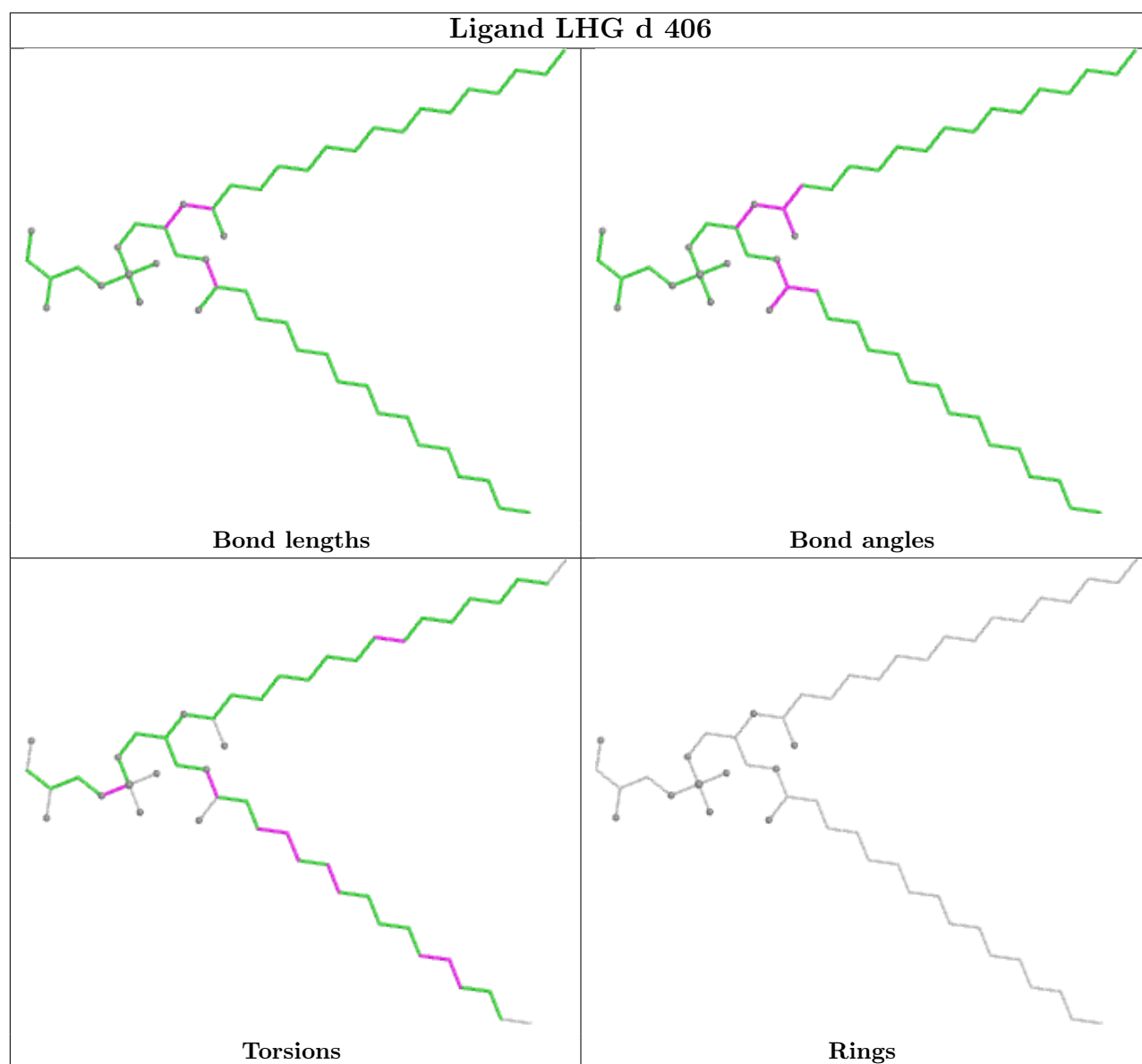


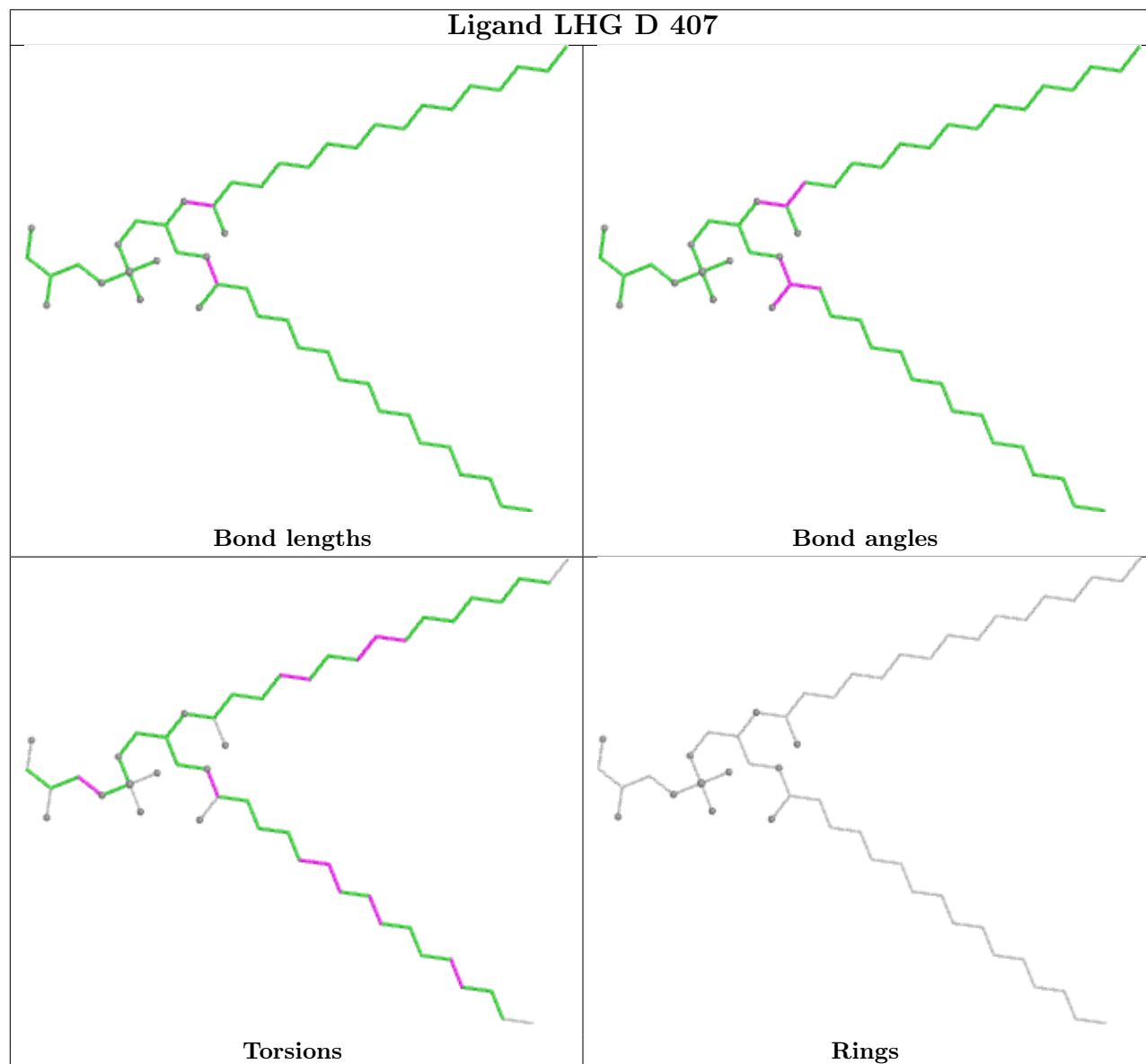
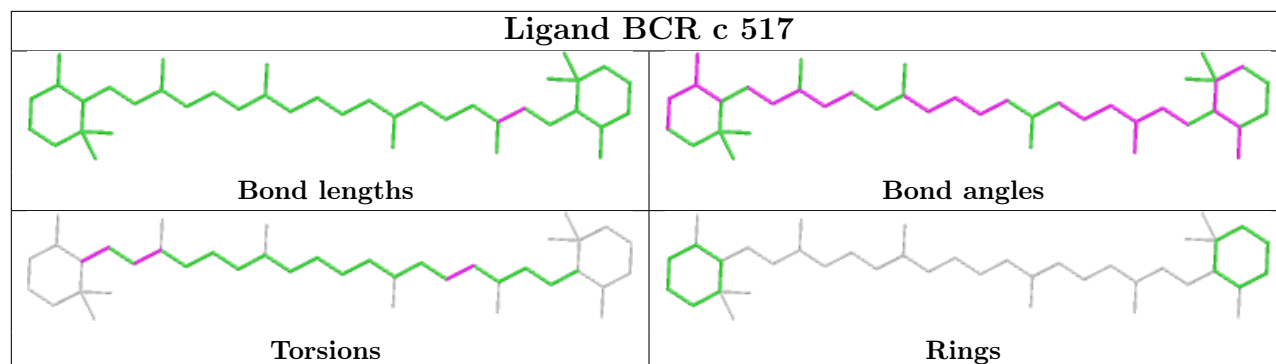
Ligand DGD C 517

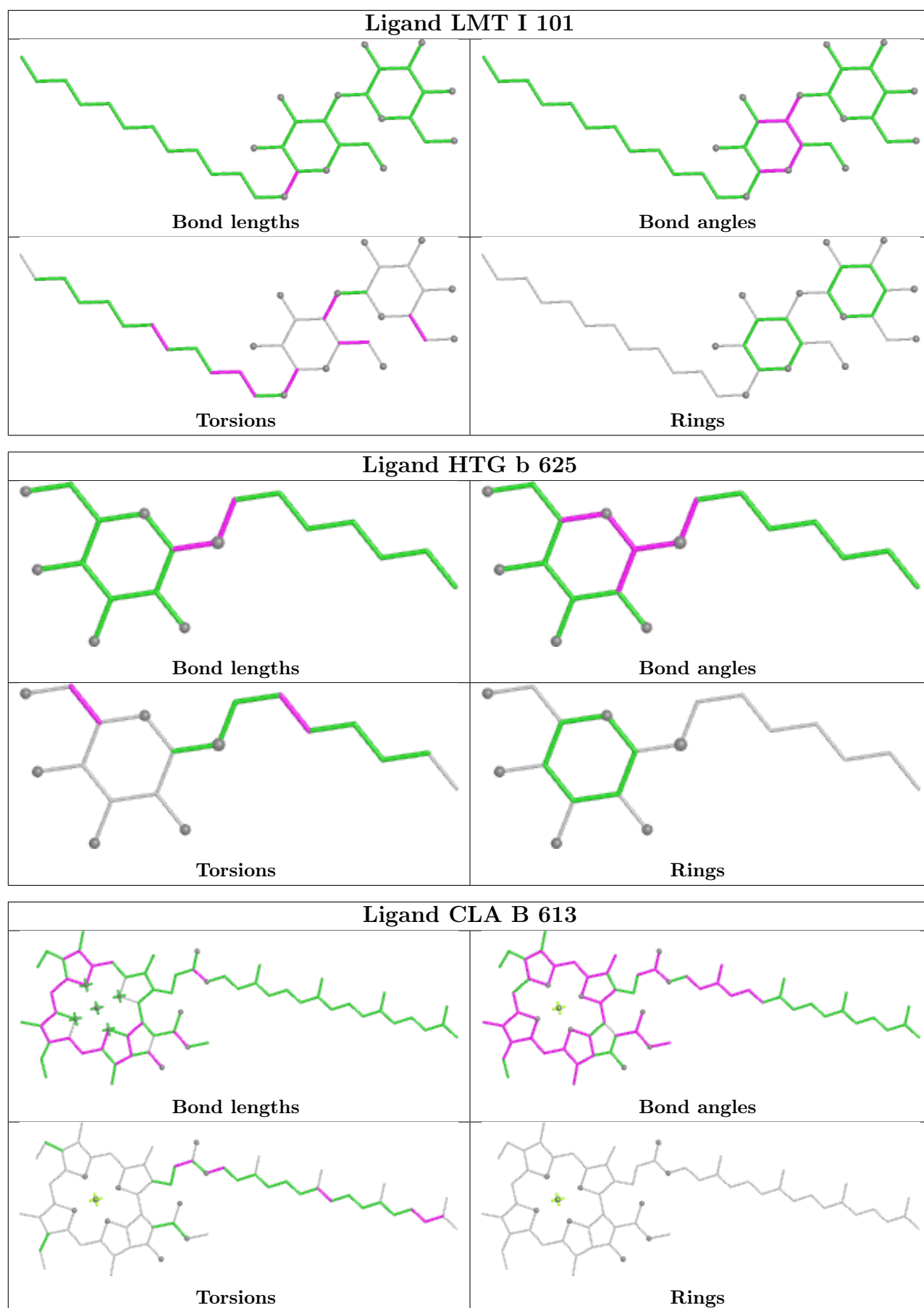


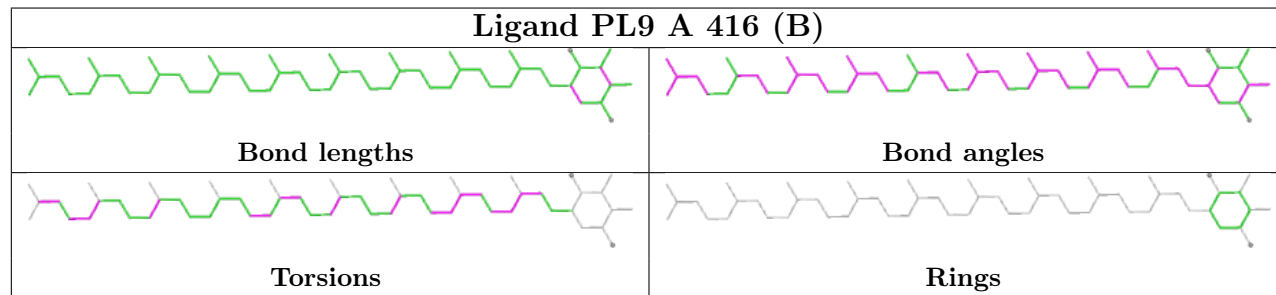
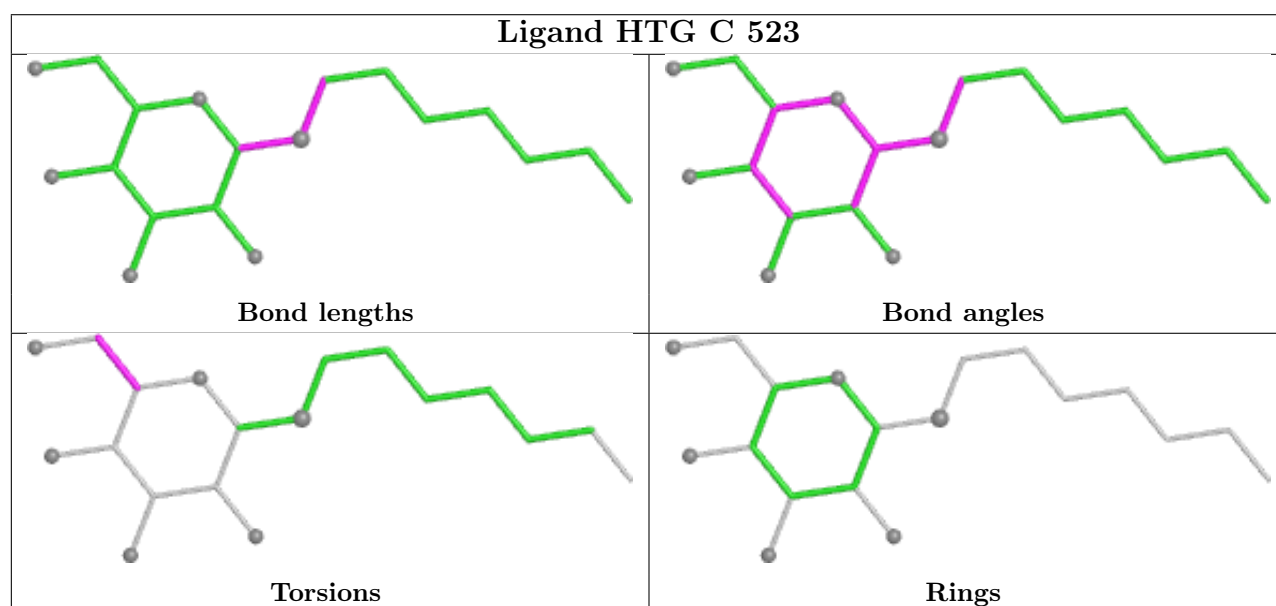
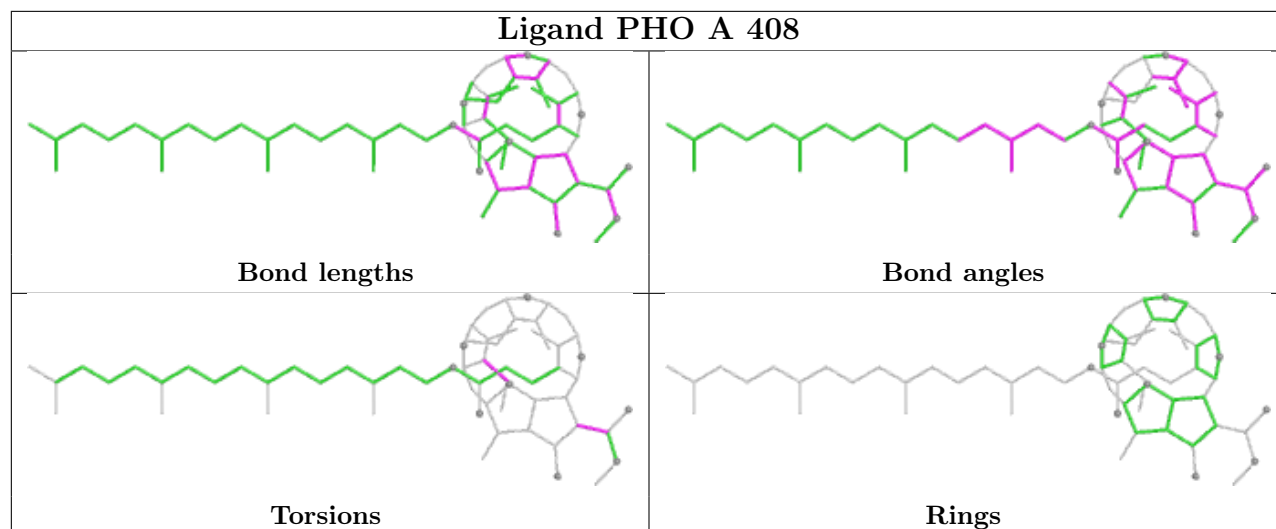


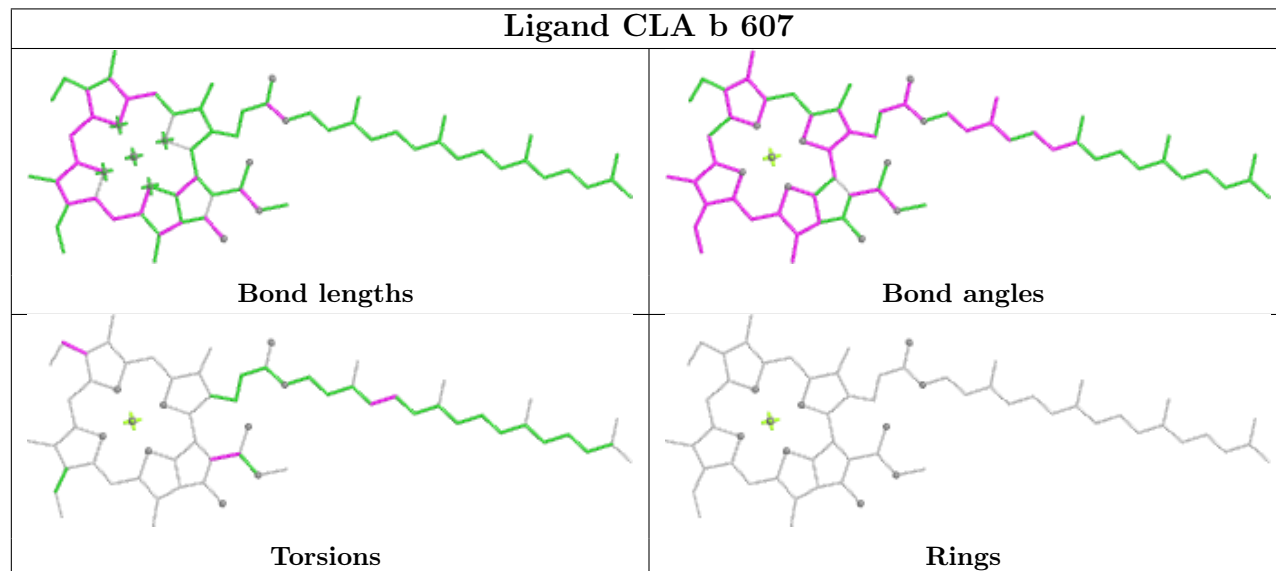
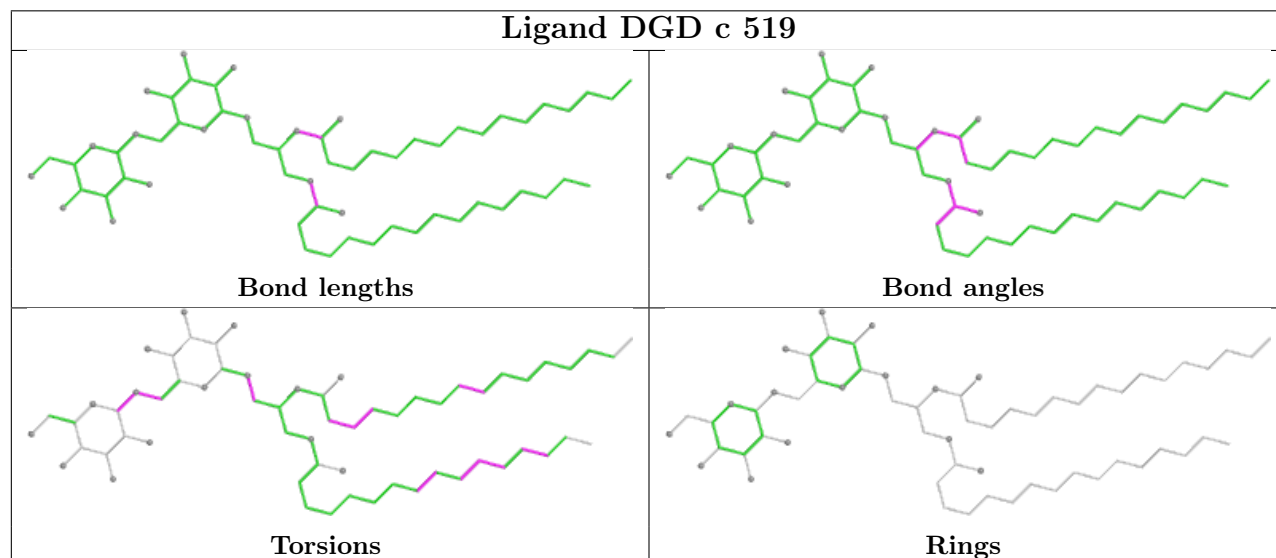
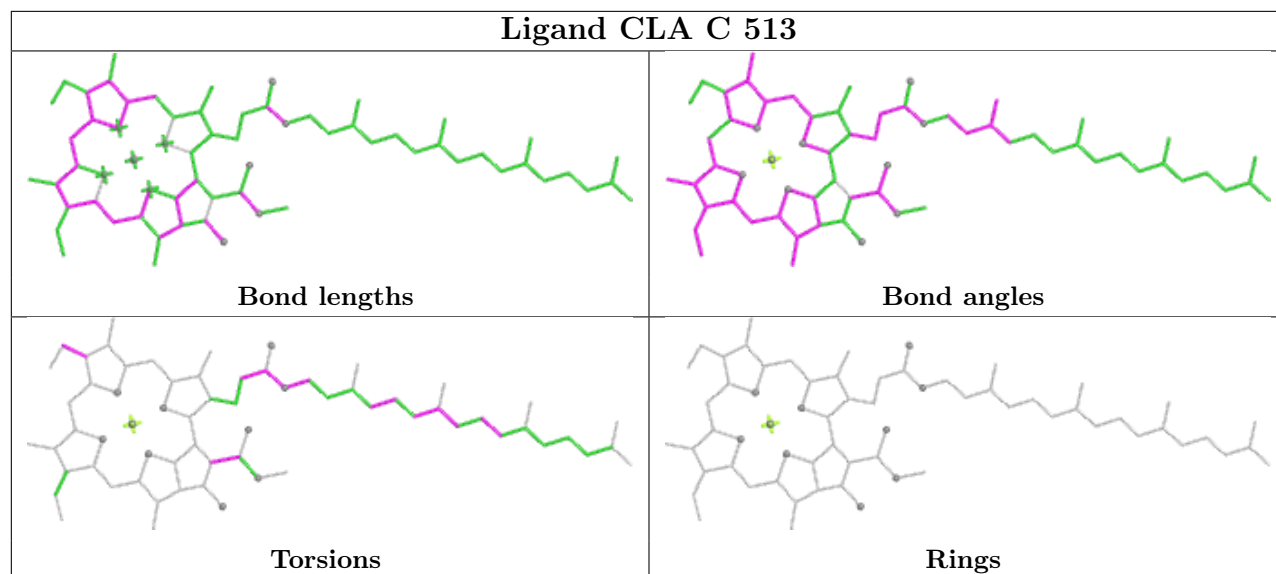


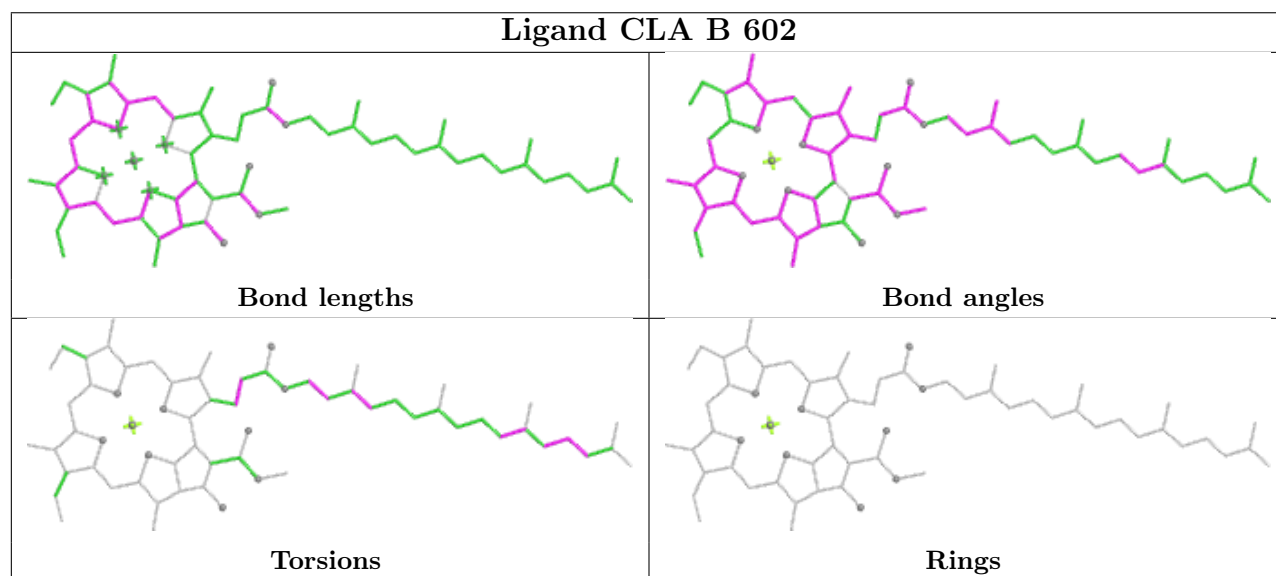
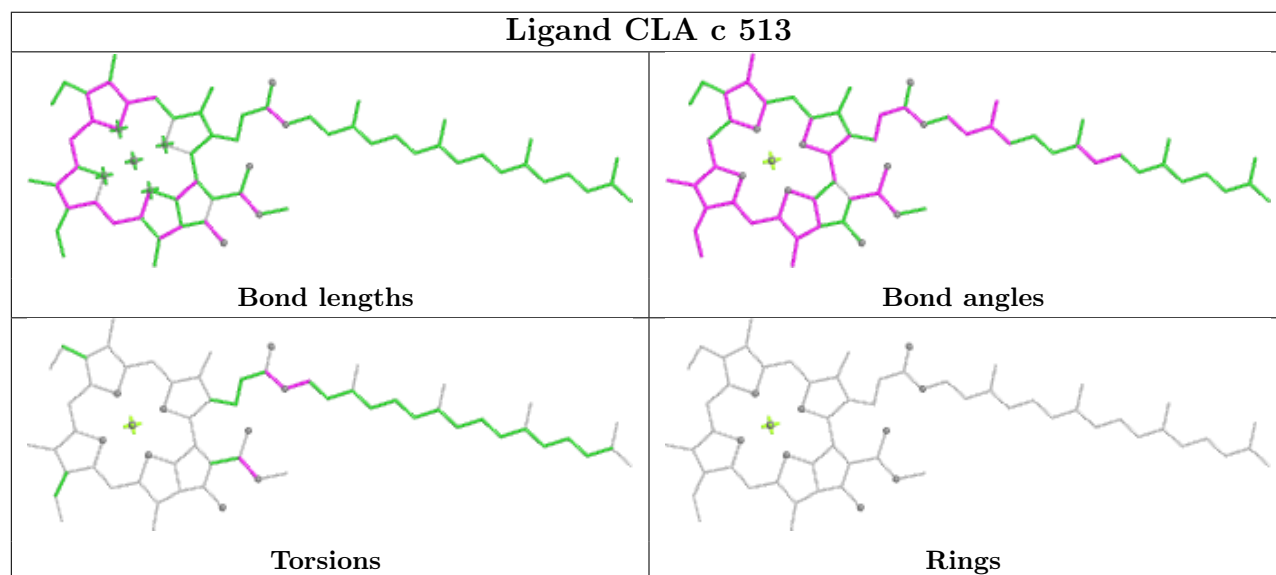
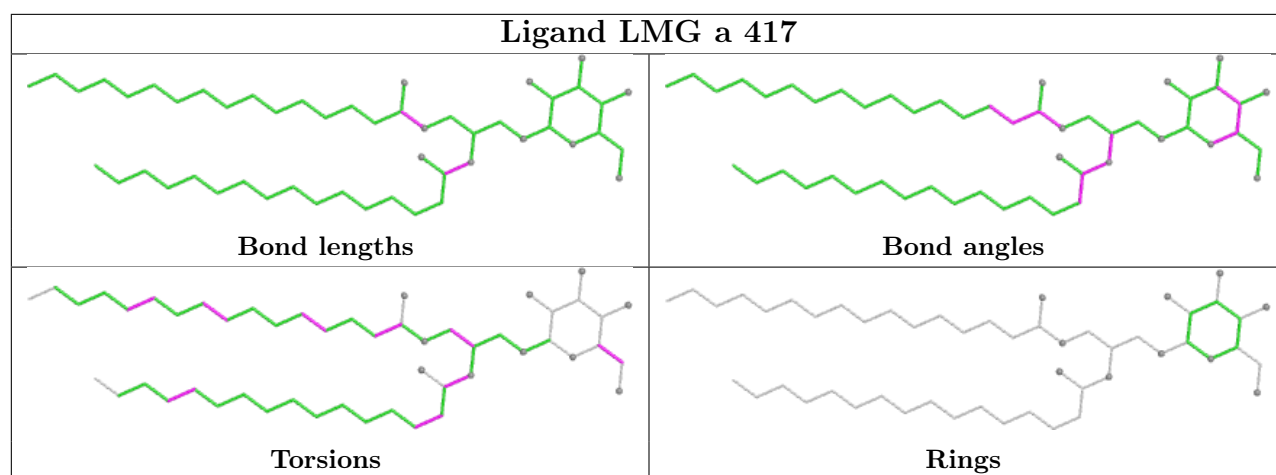


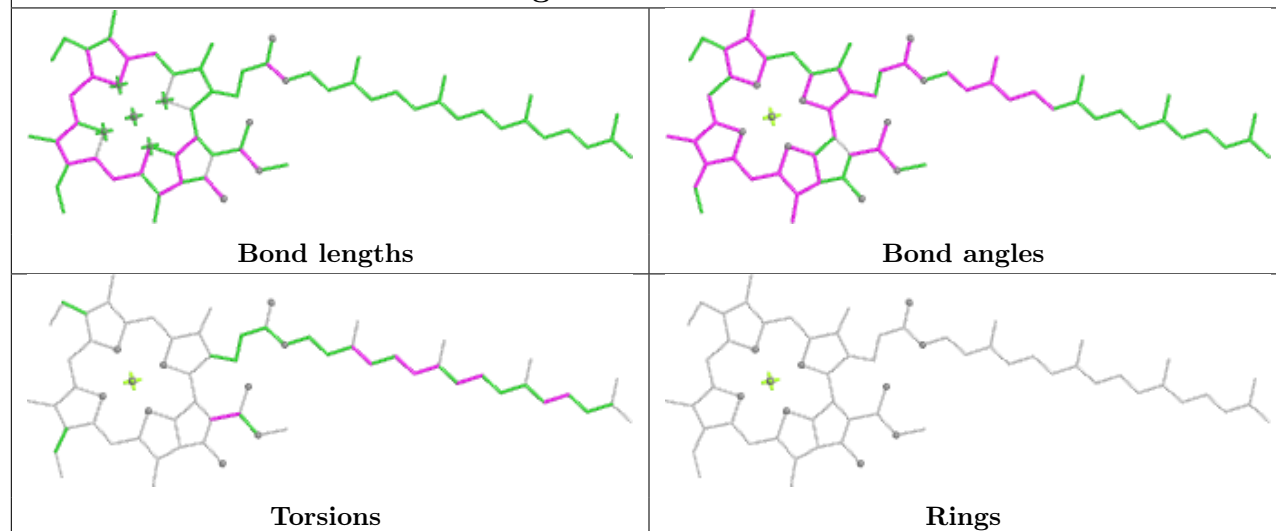
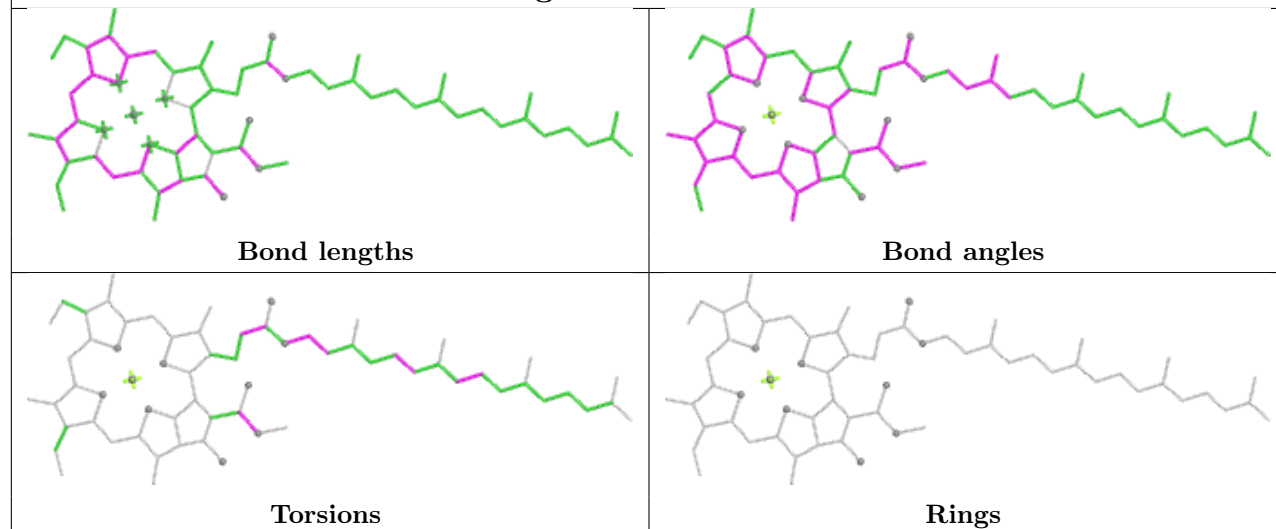


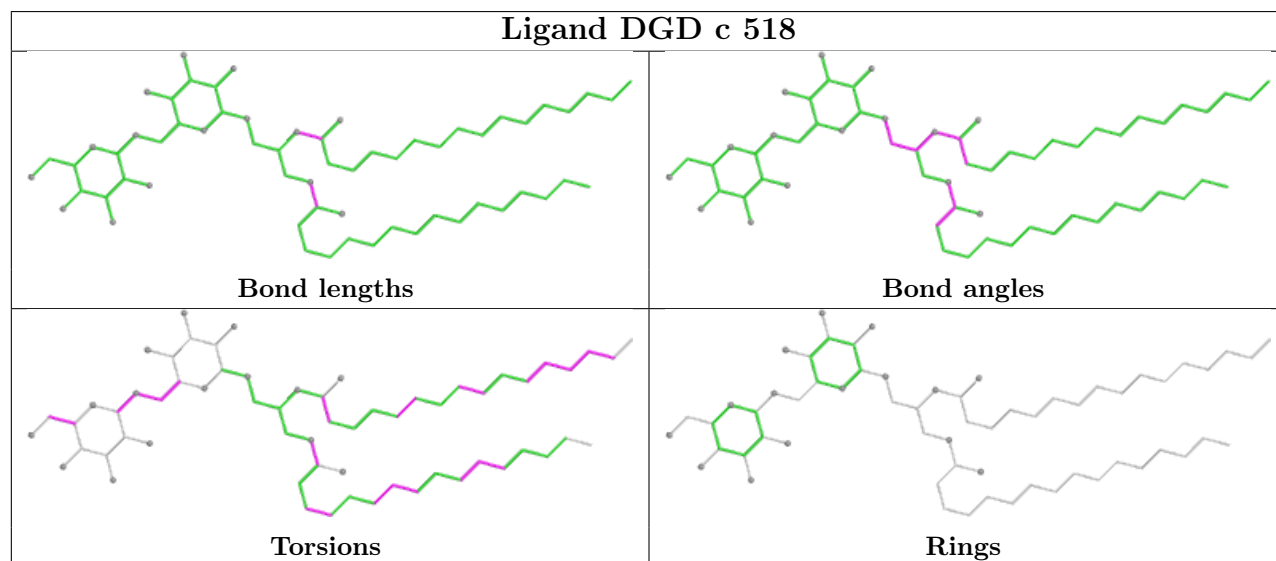
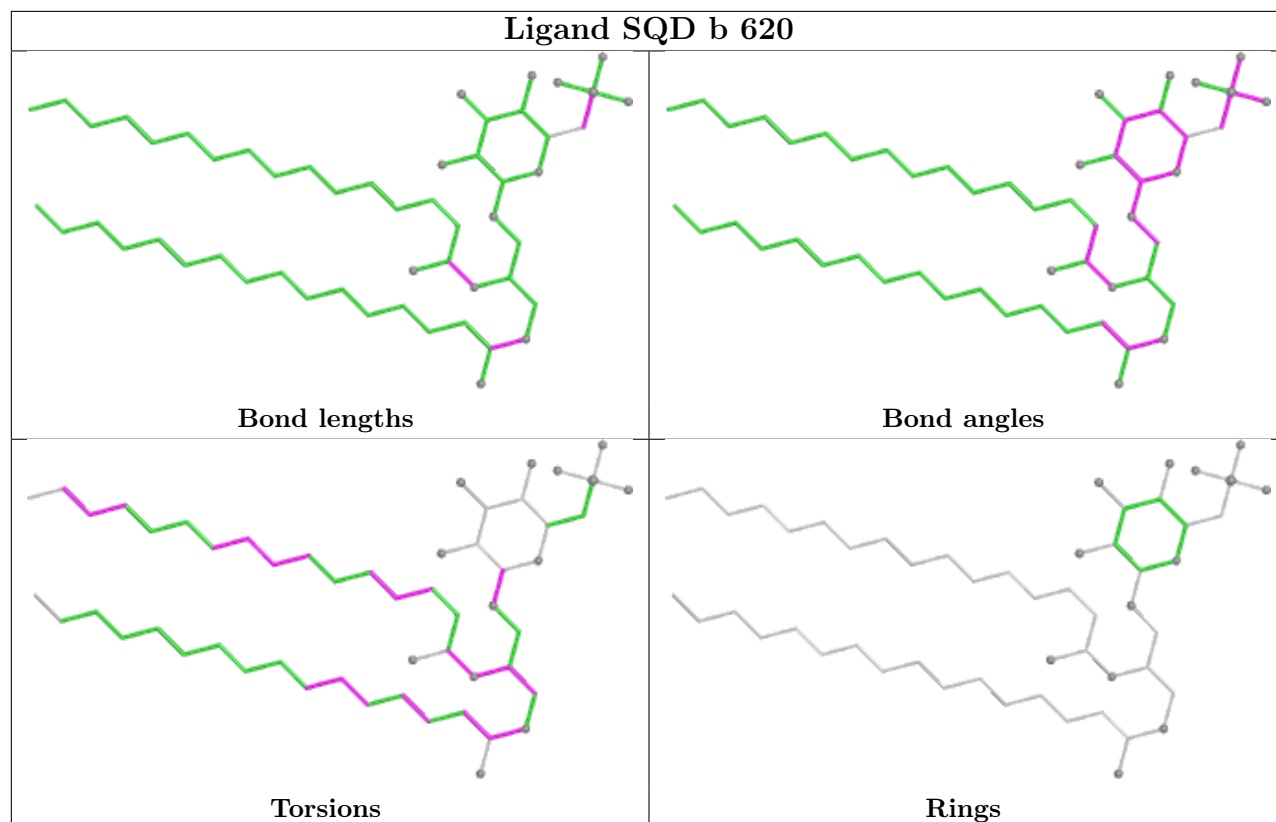




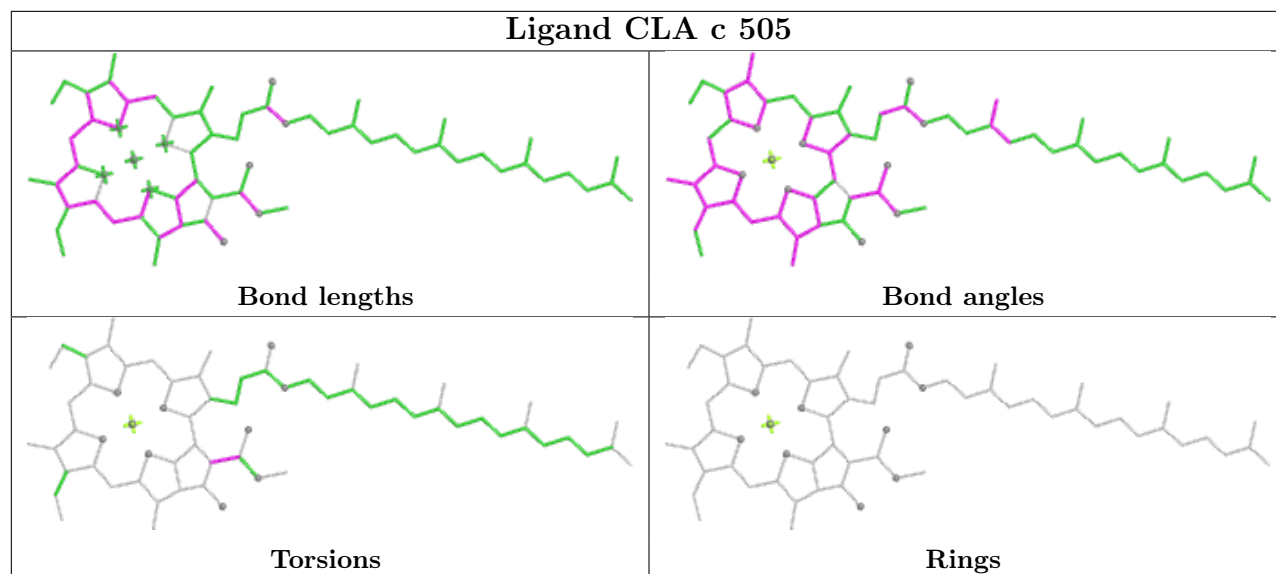




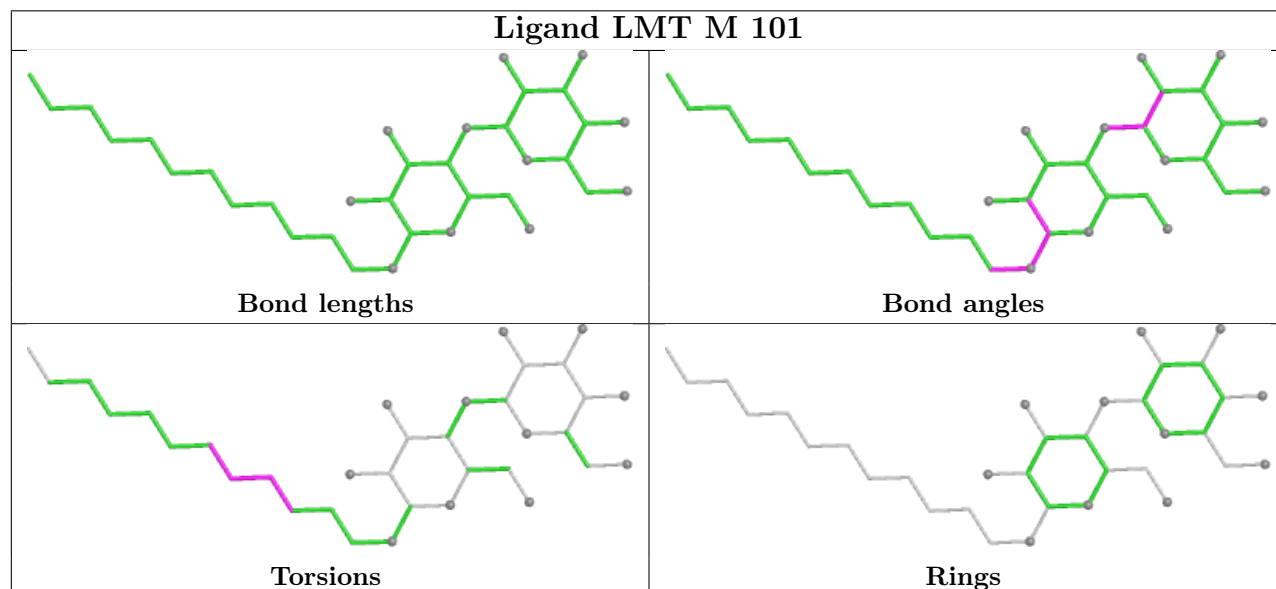
Ligand CLA B 605**Ligand CLA b 613**



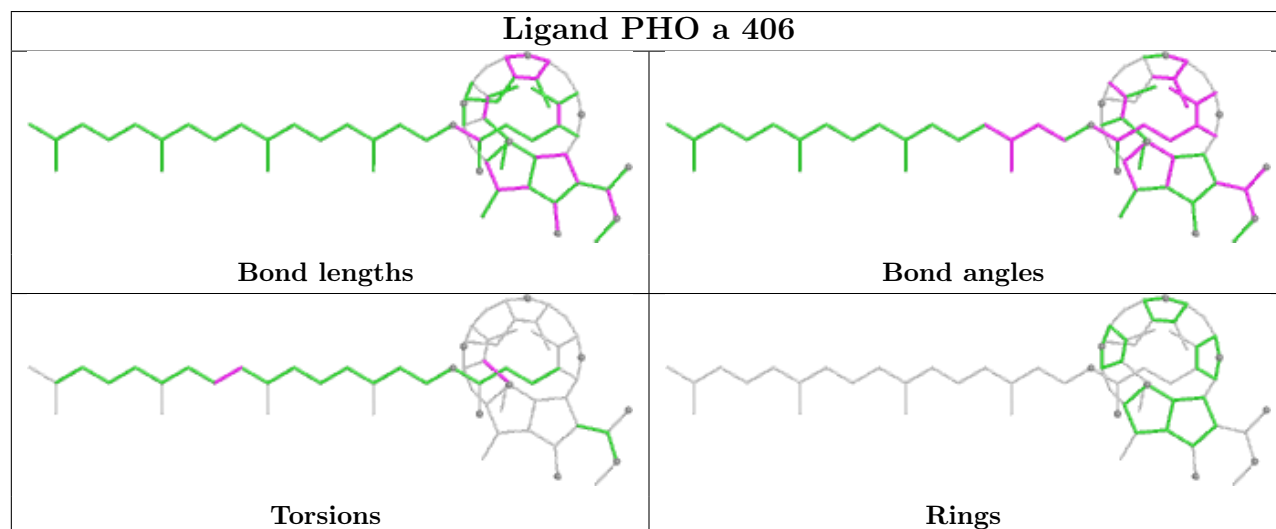
Ligand CLA c 505



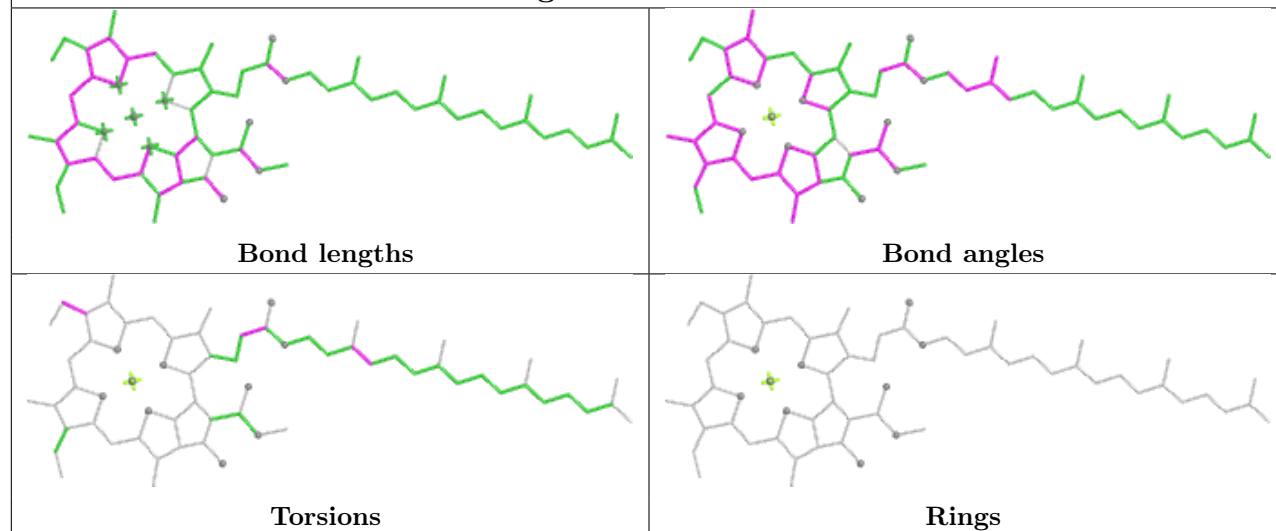
Ligand LMT M 101



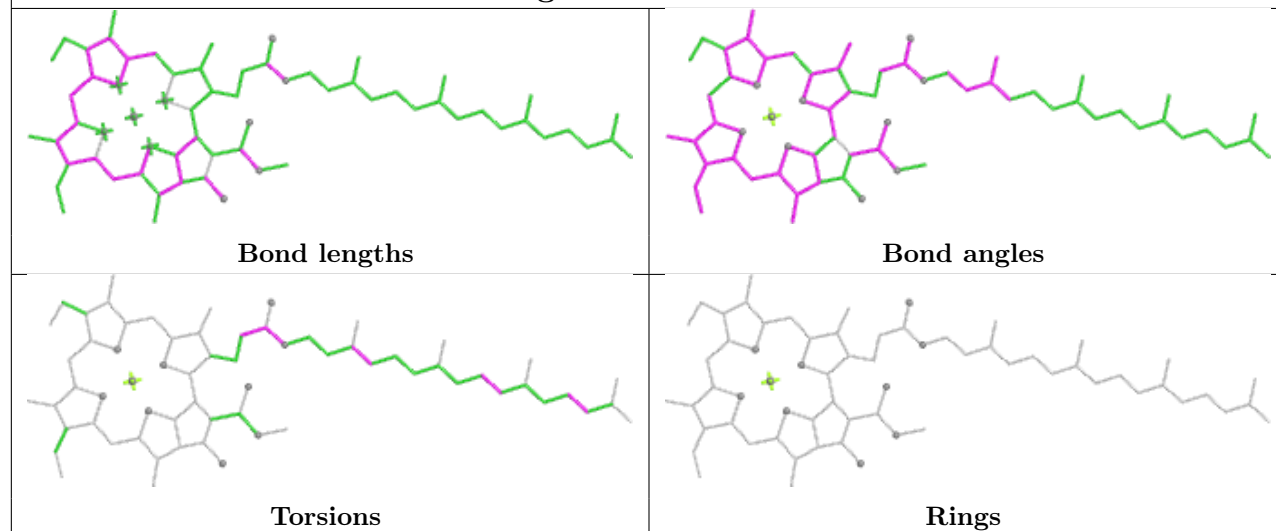
Ligand PHO a 406



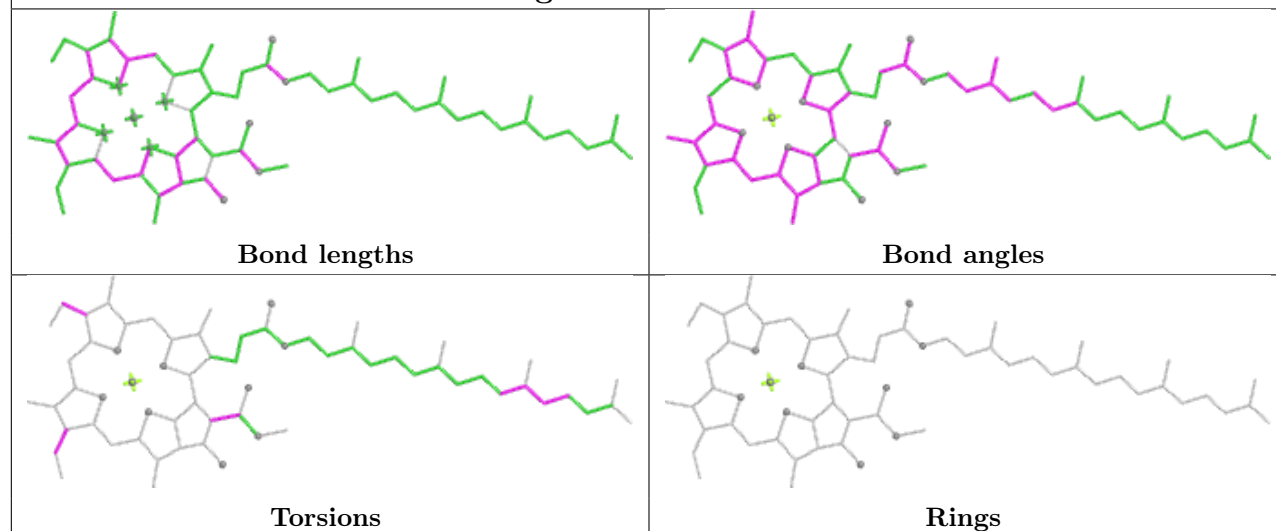
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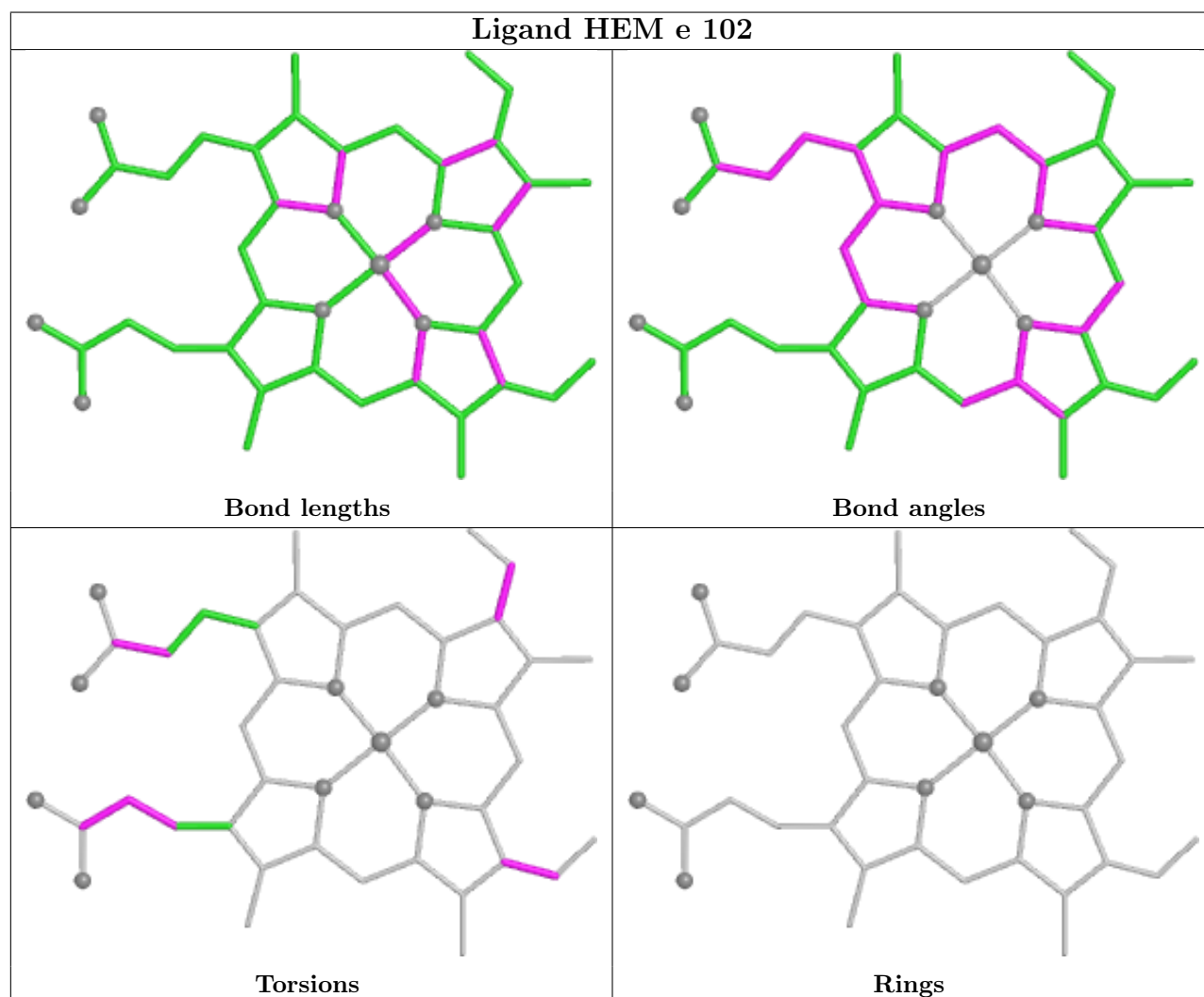
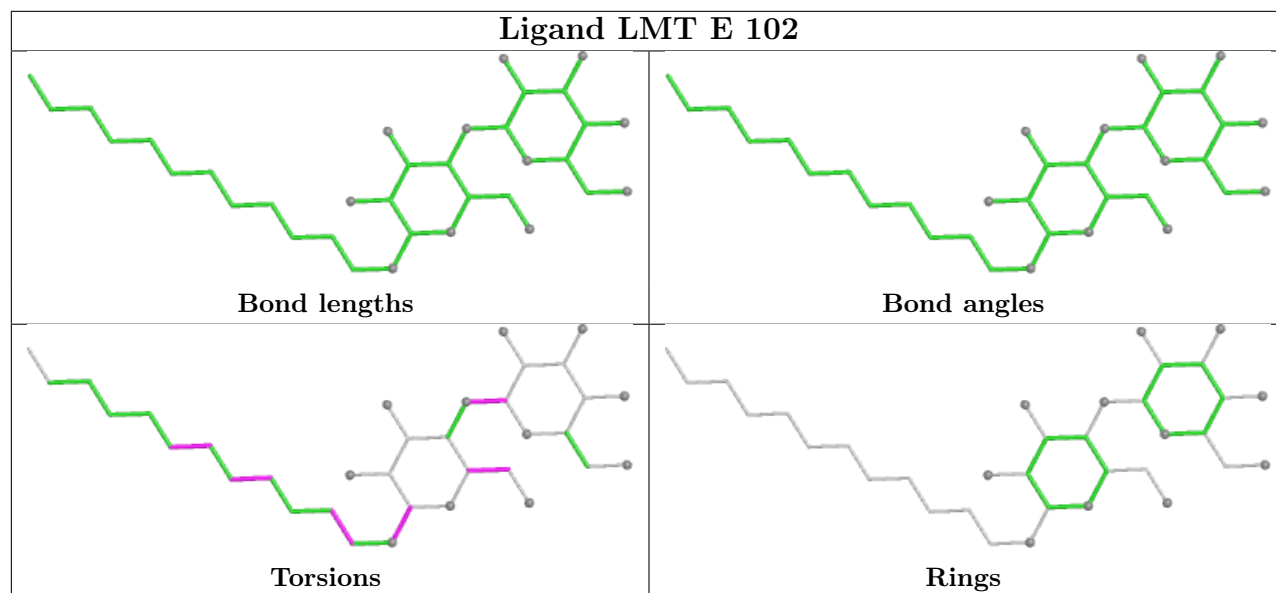


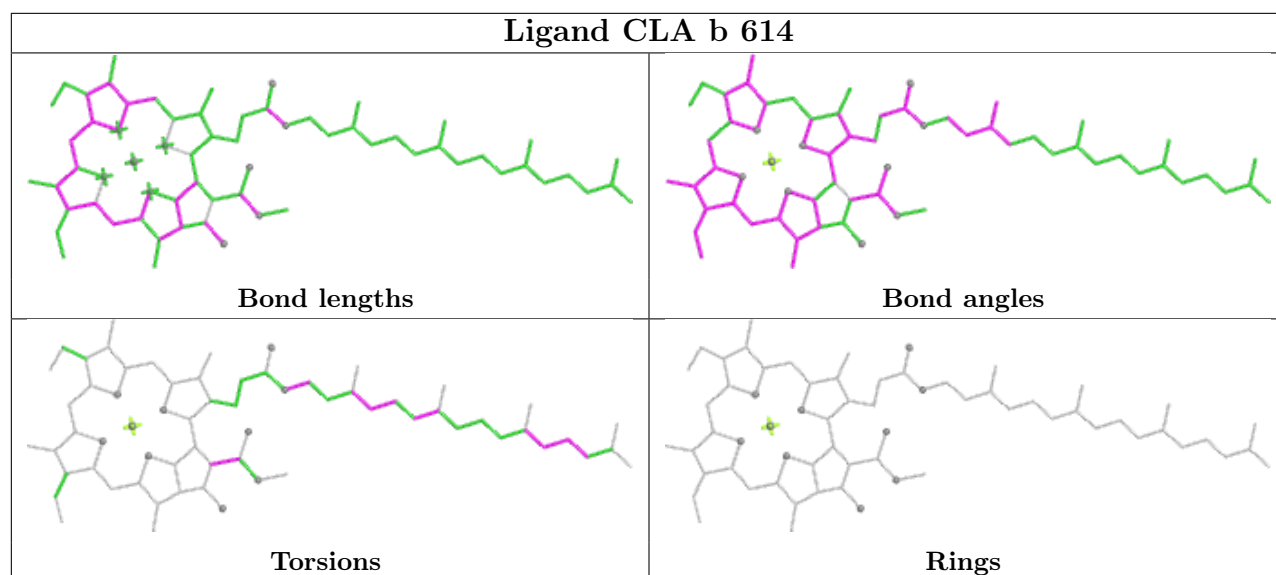
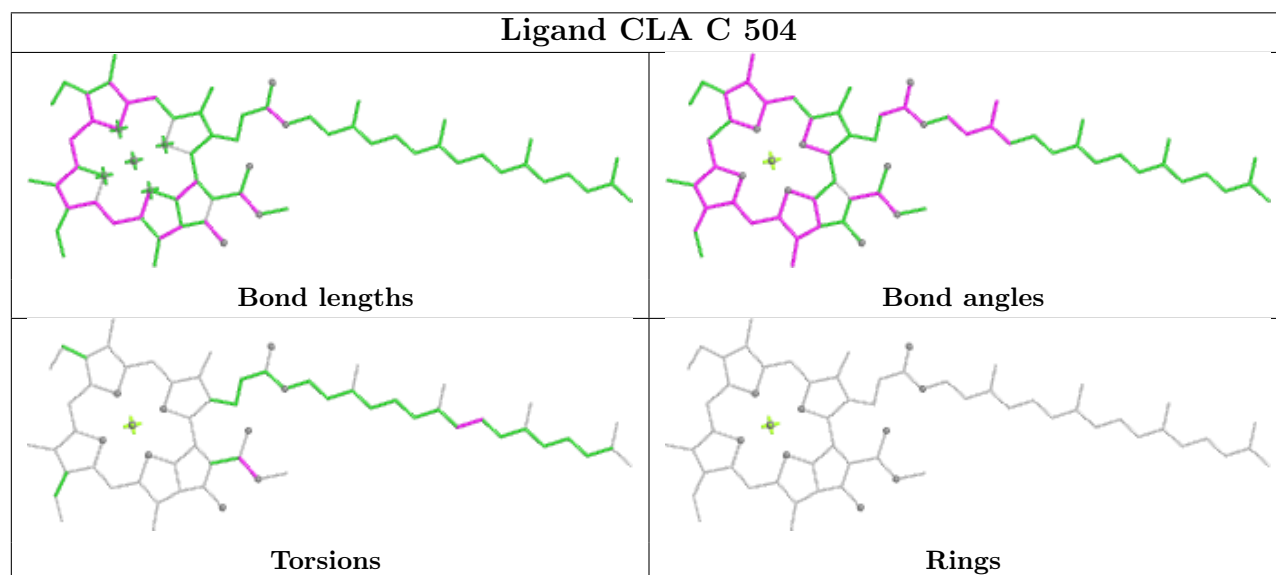
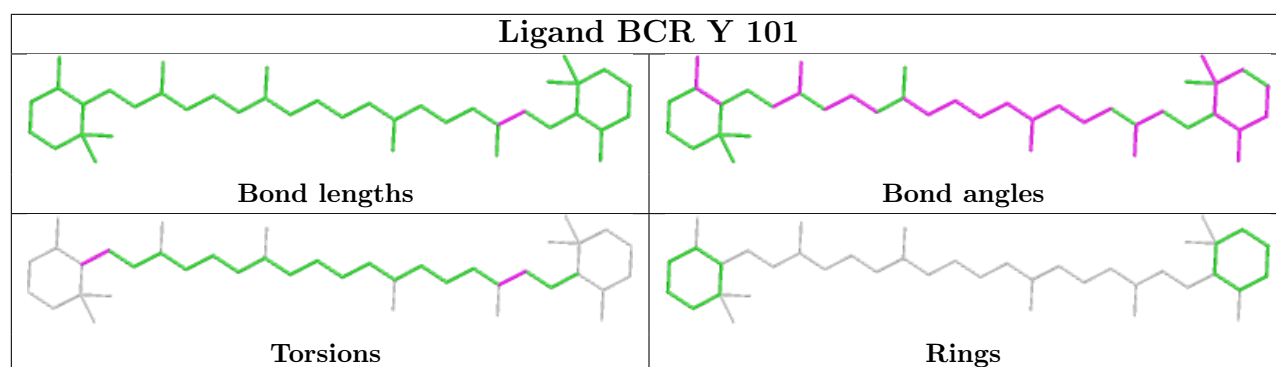
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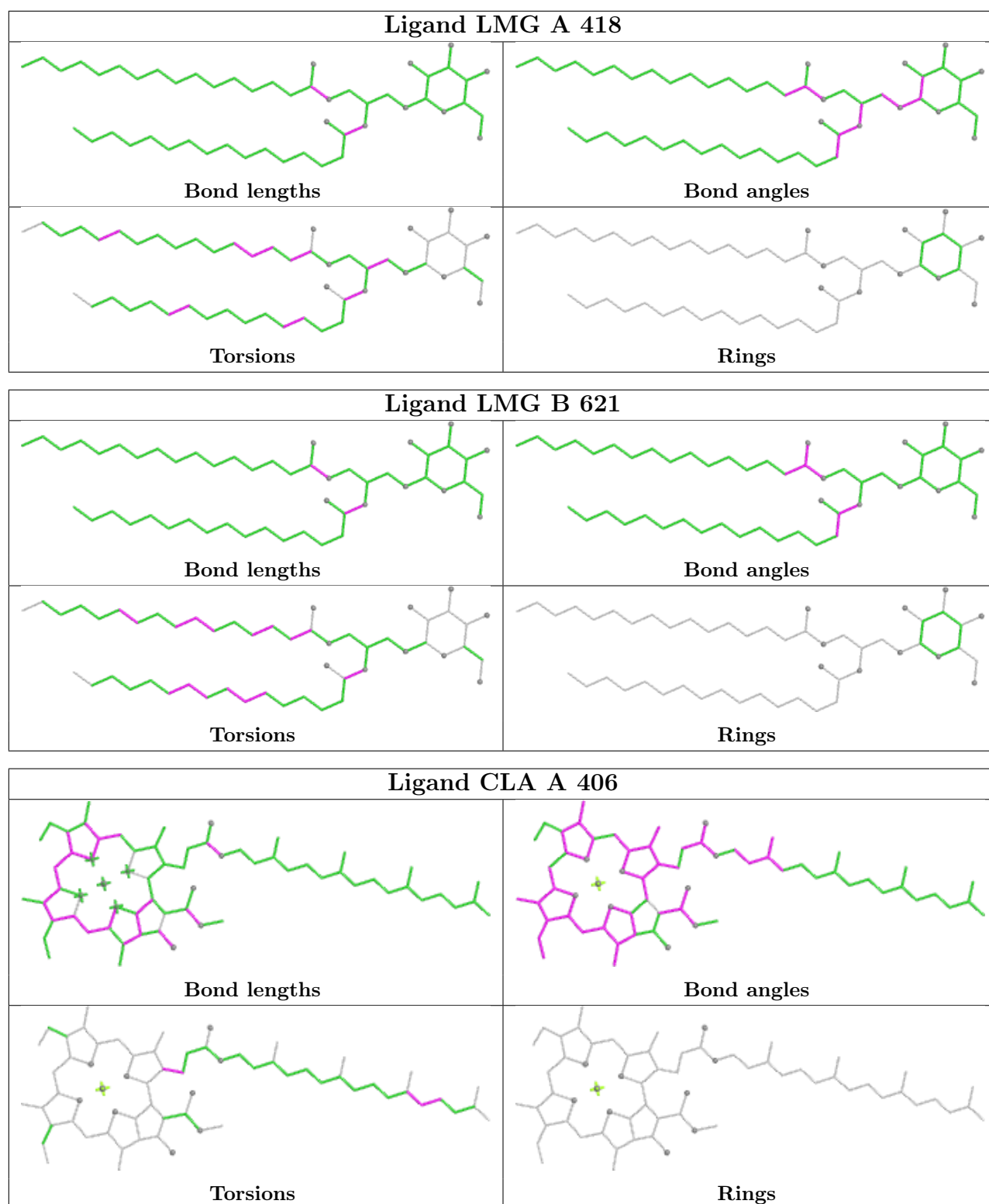


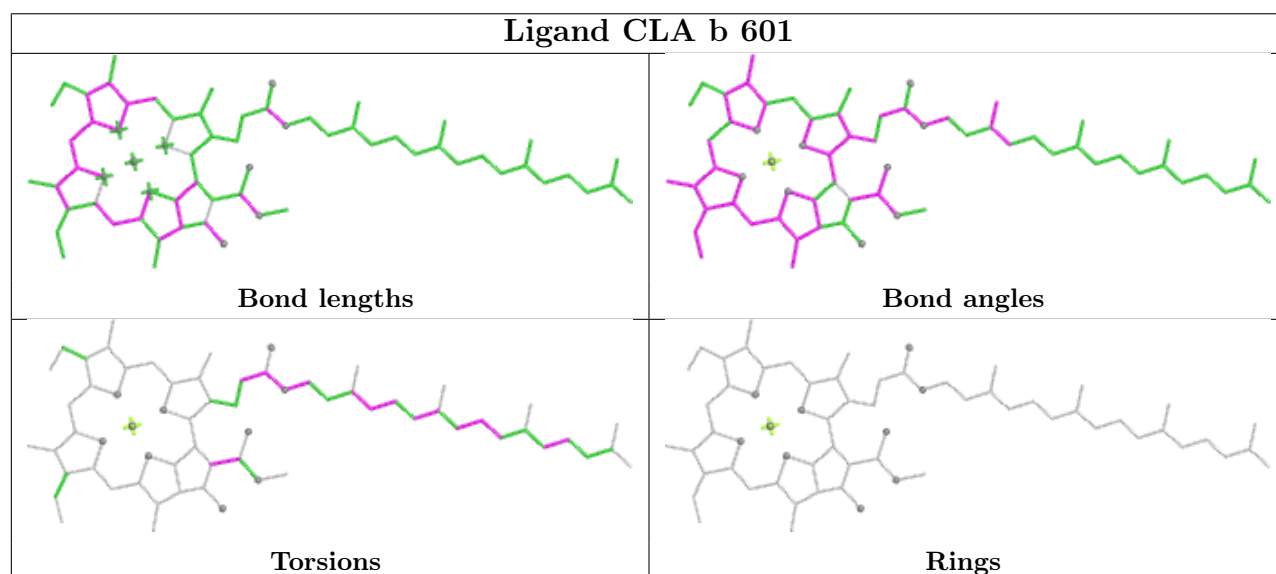
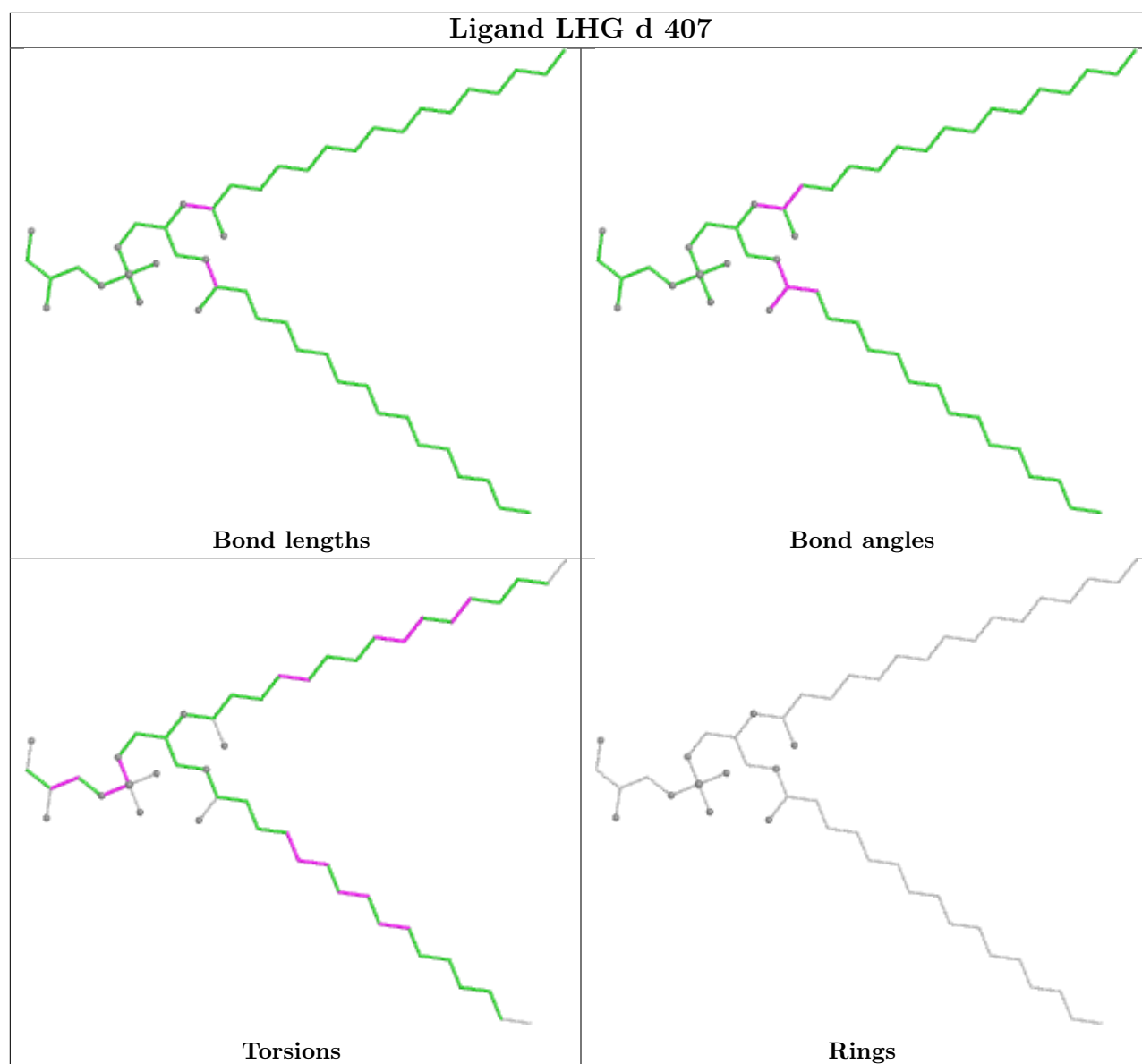
Ligand CLA b 604

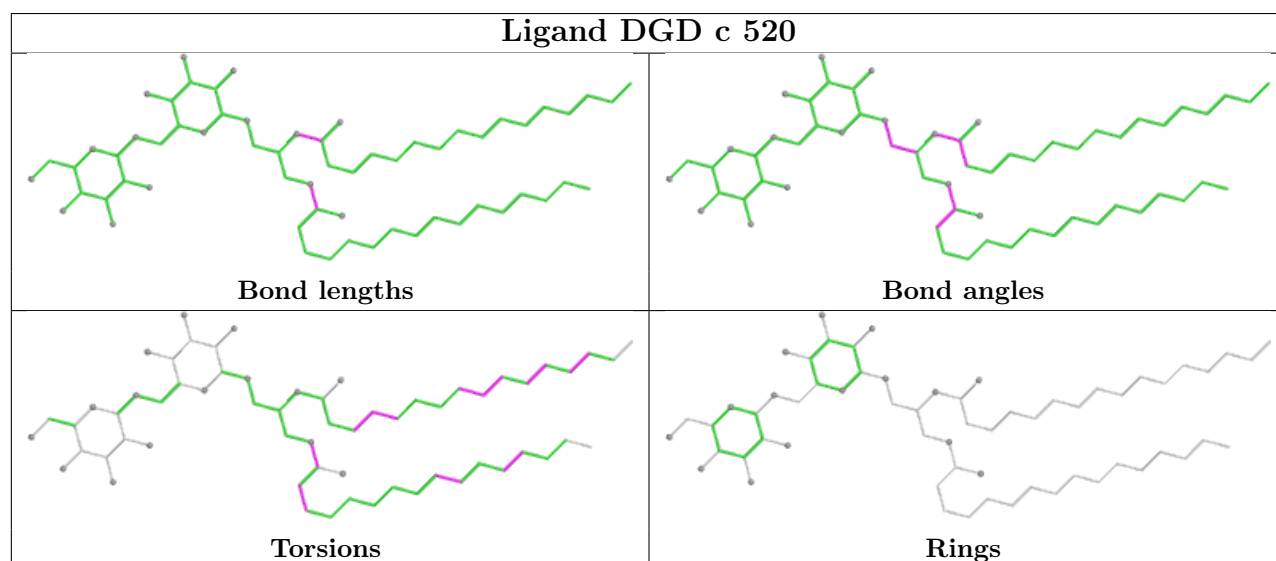
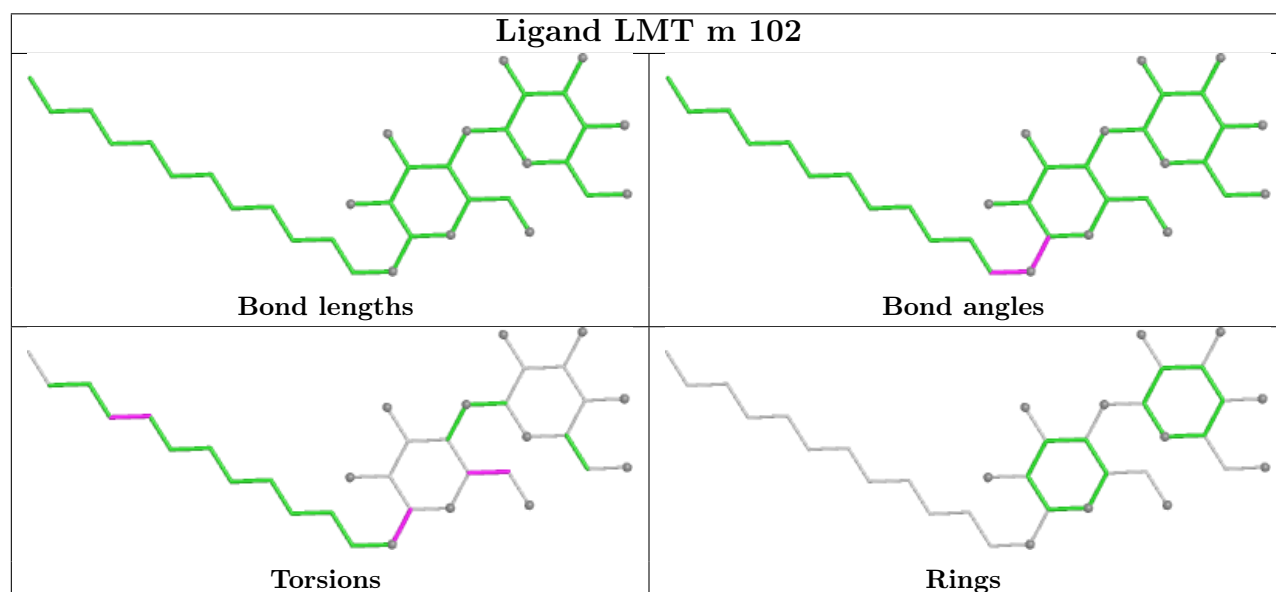
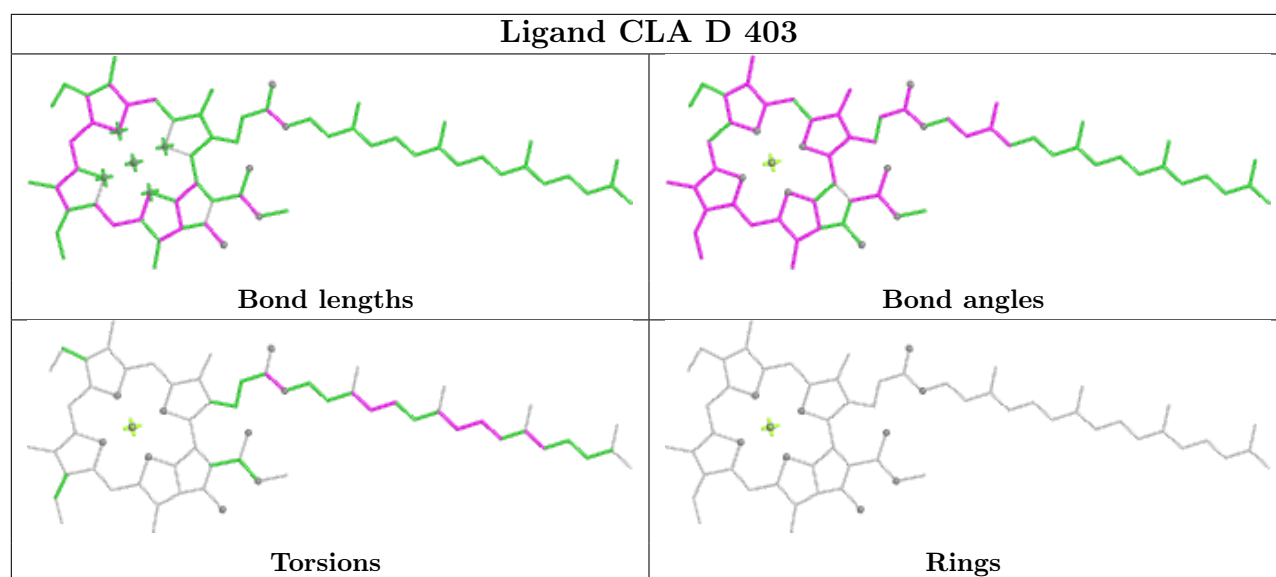


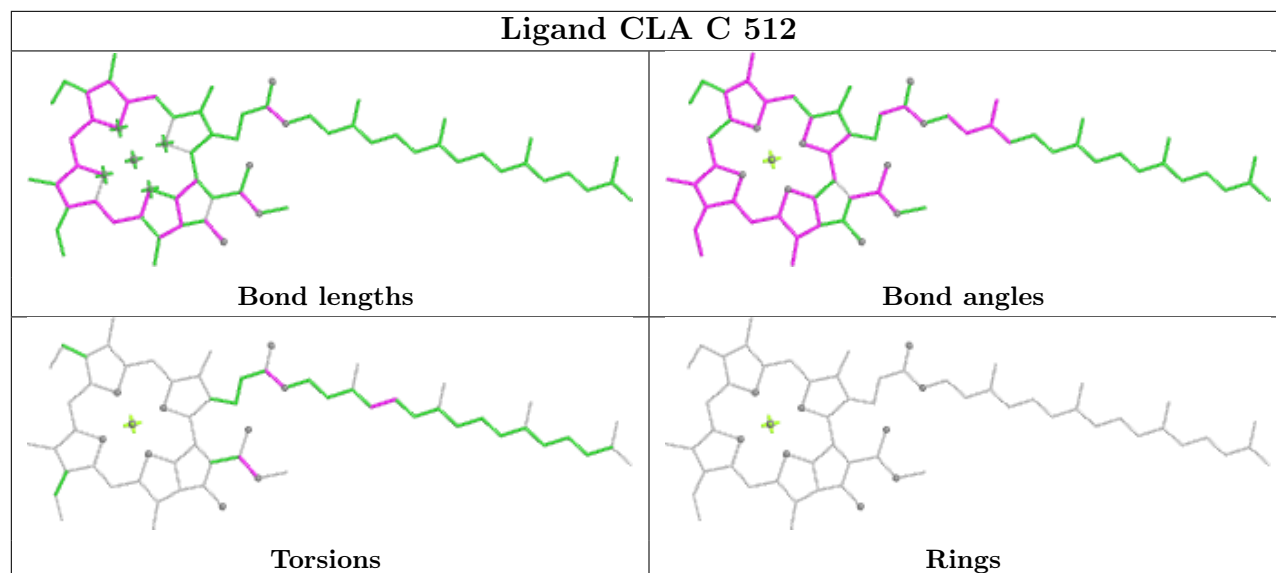
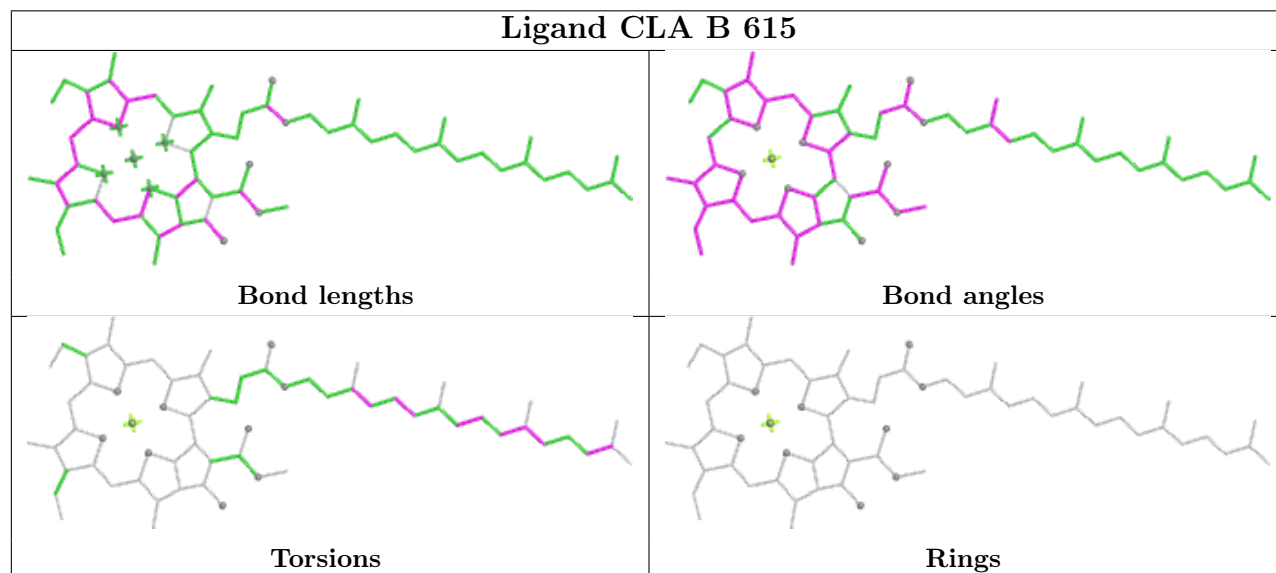
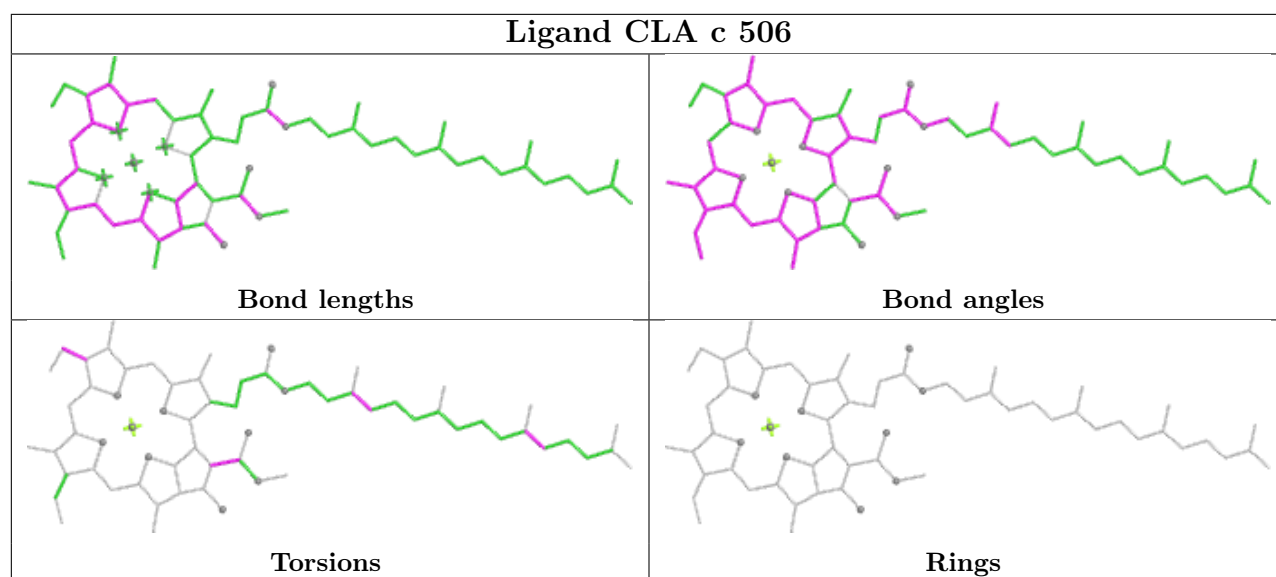


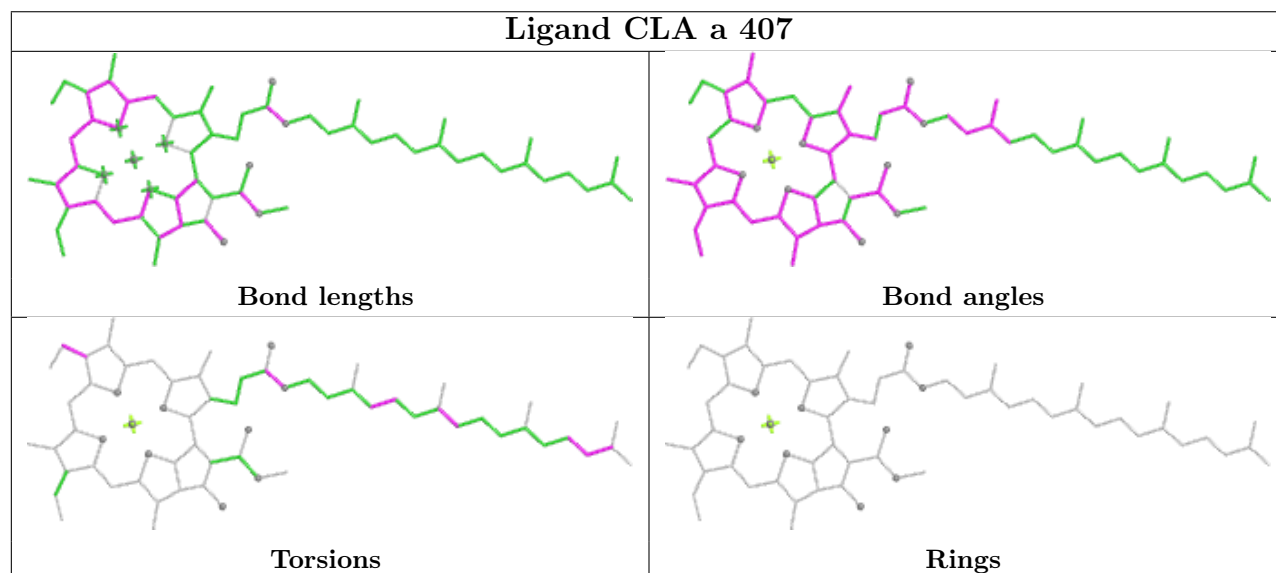
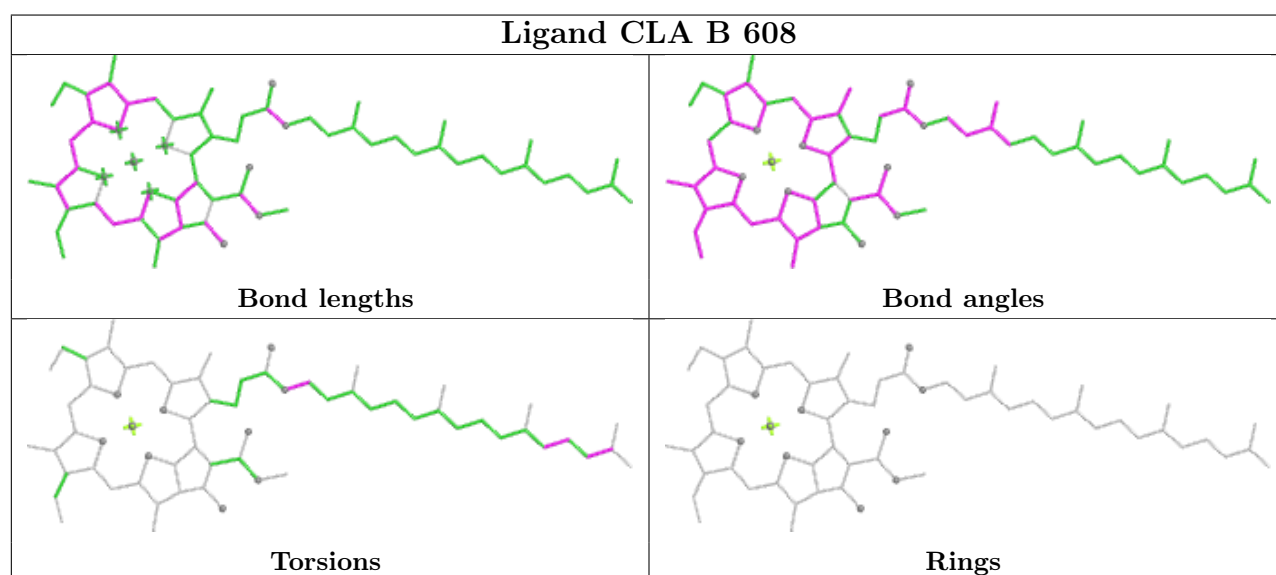
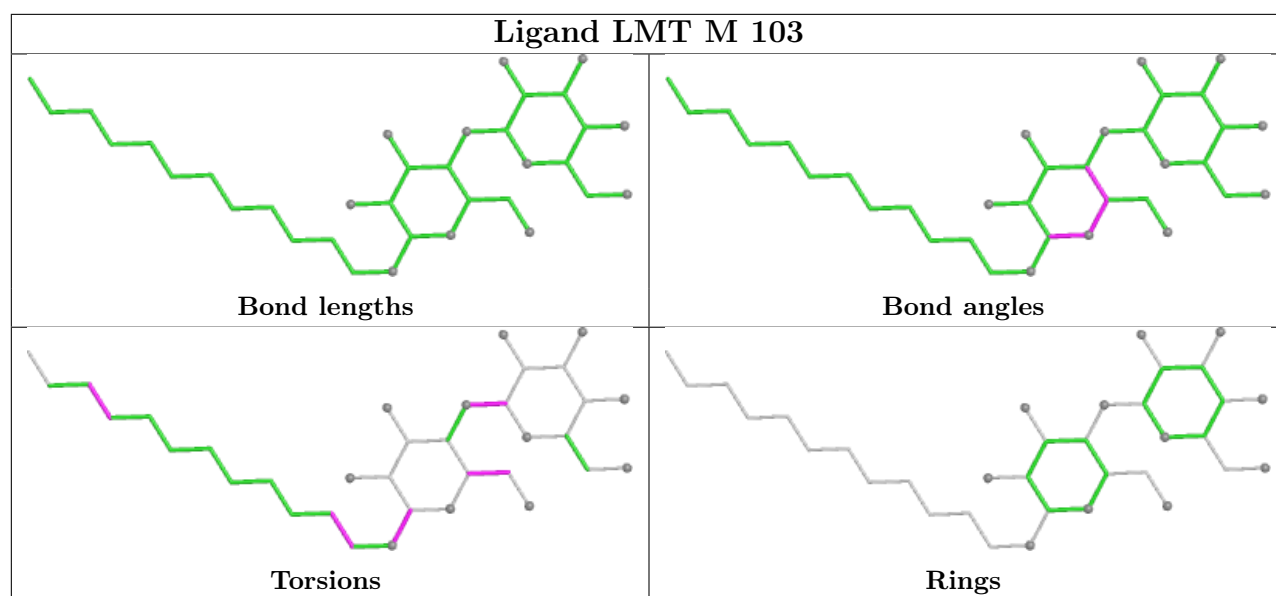


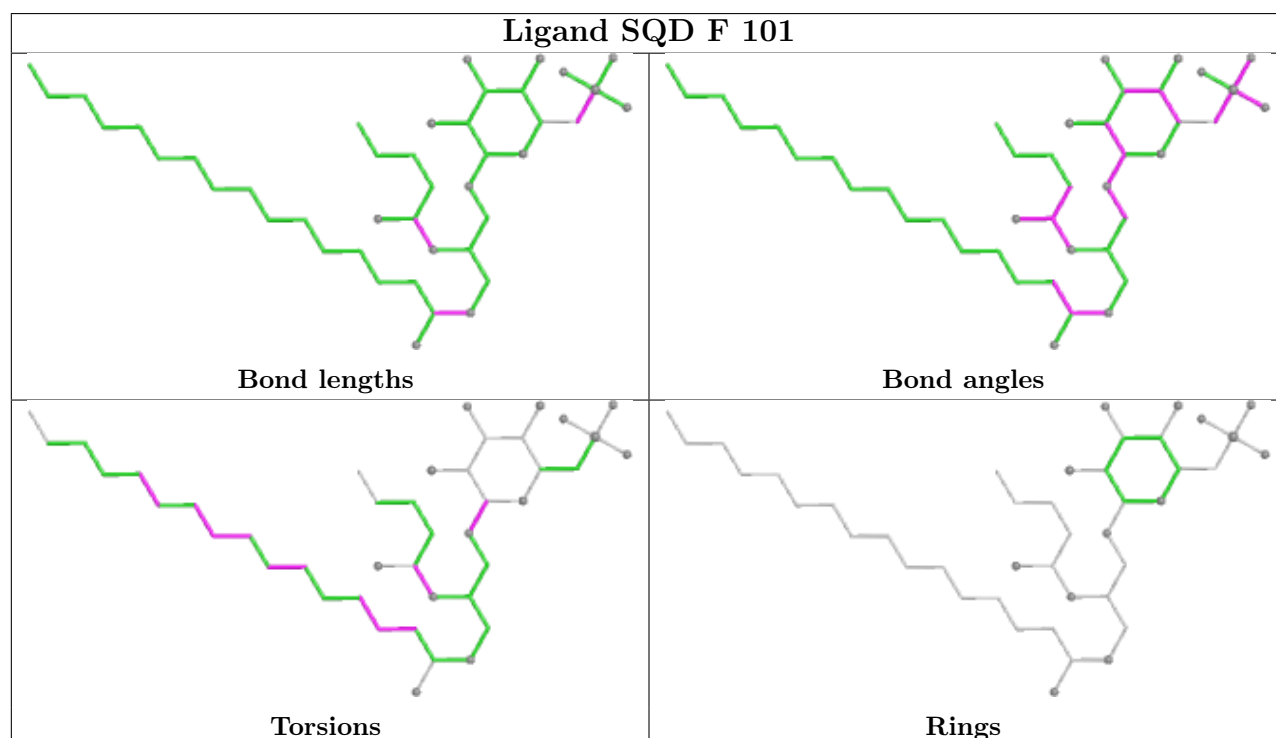
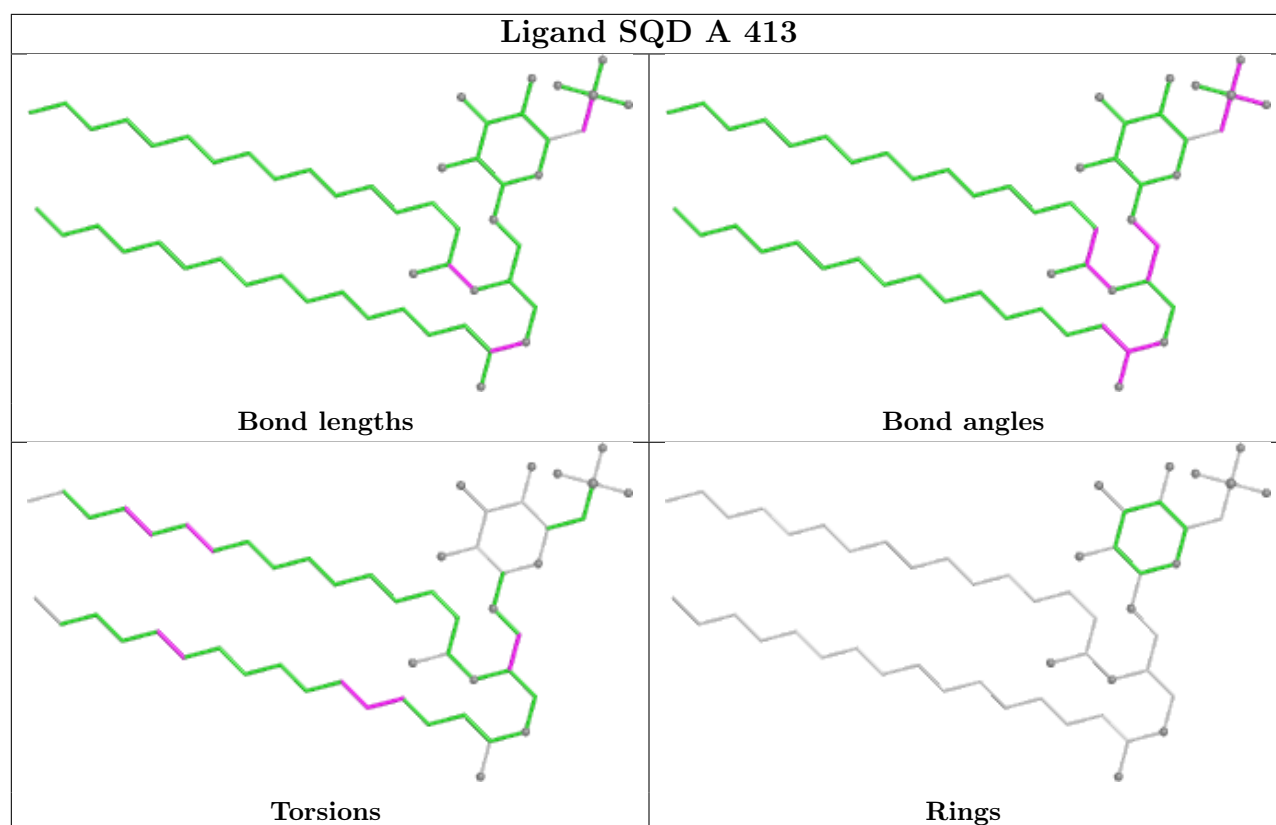


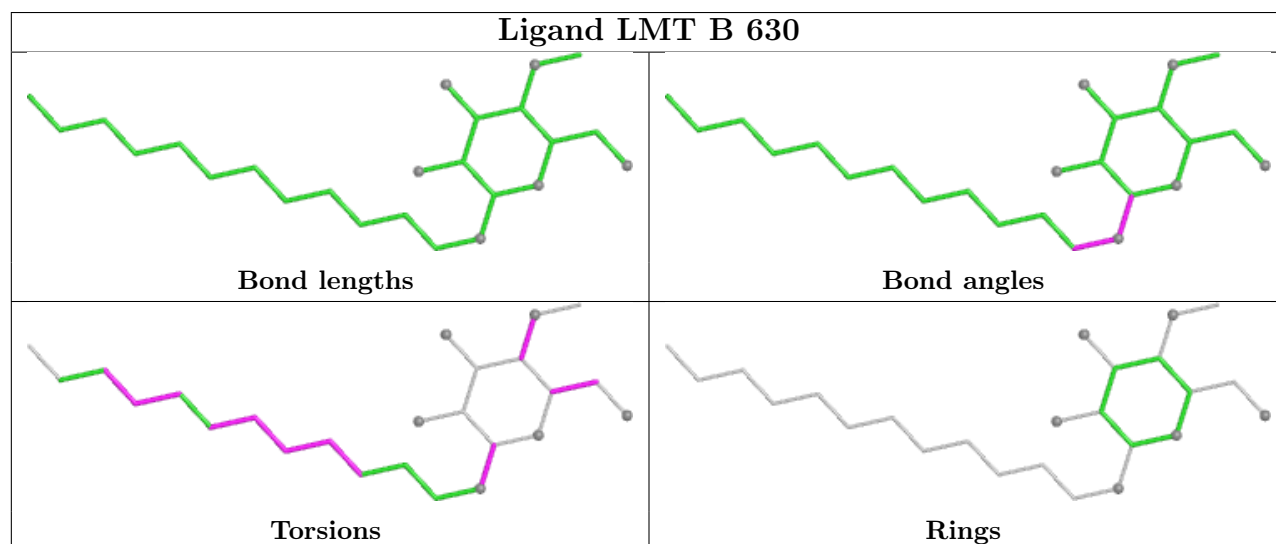
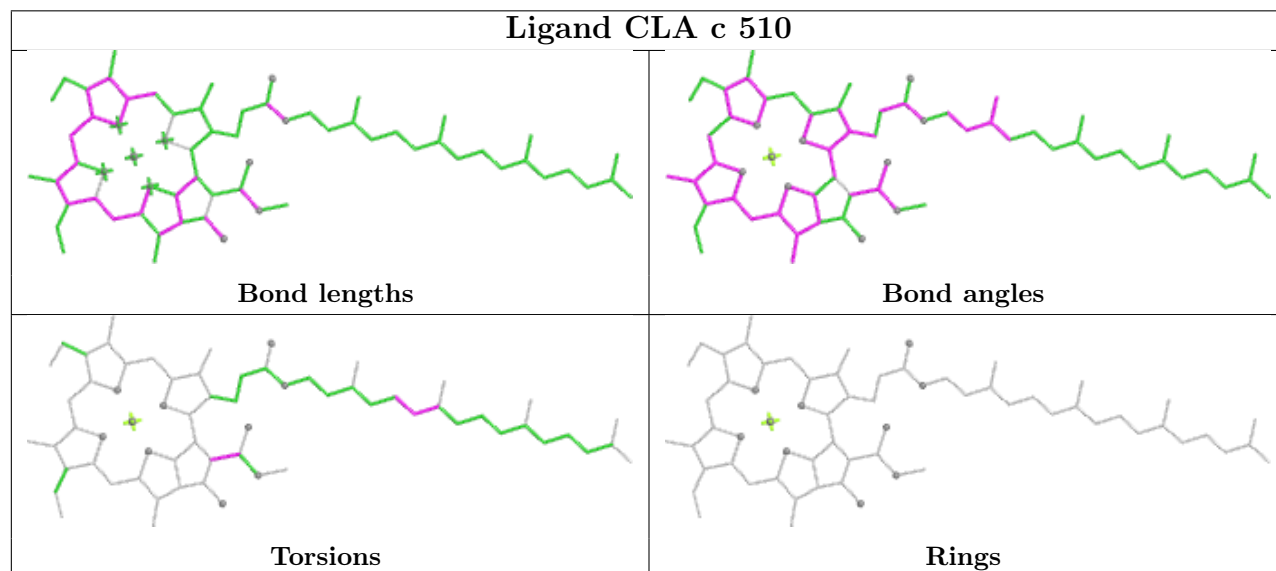
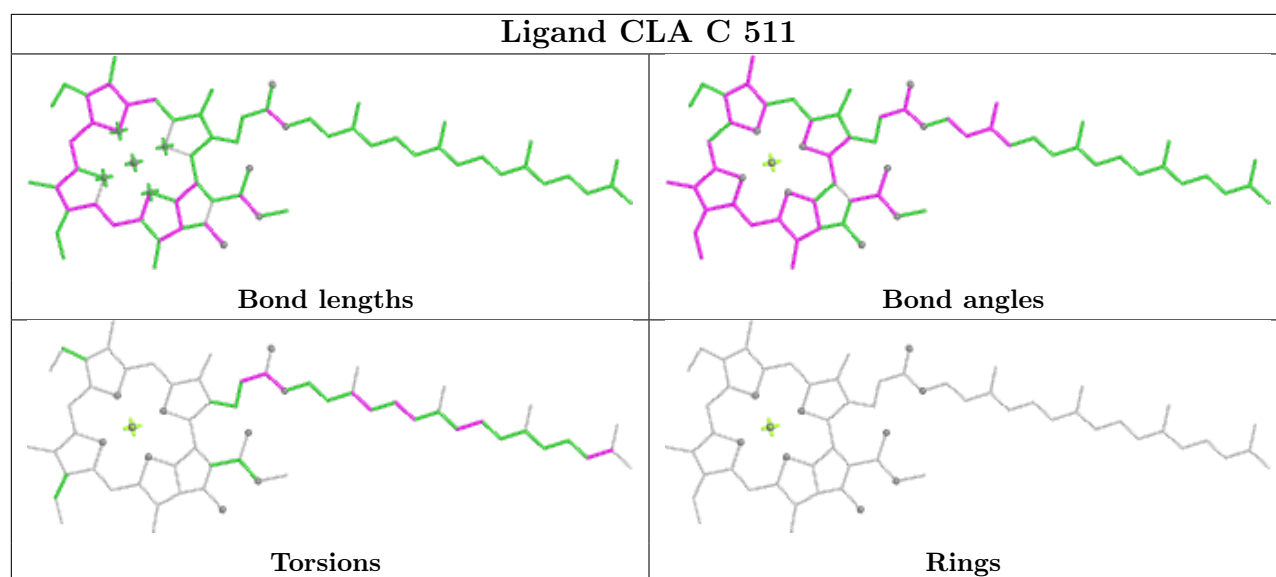


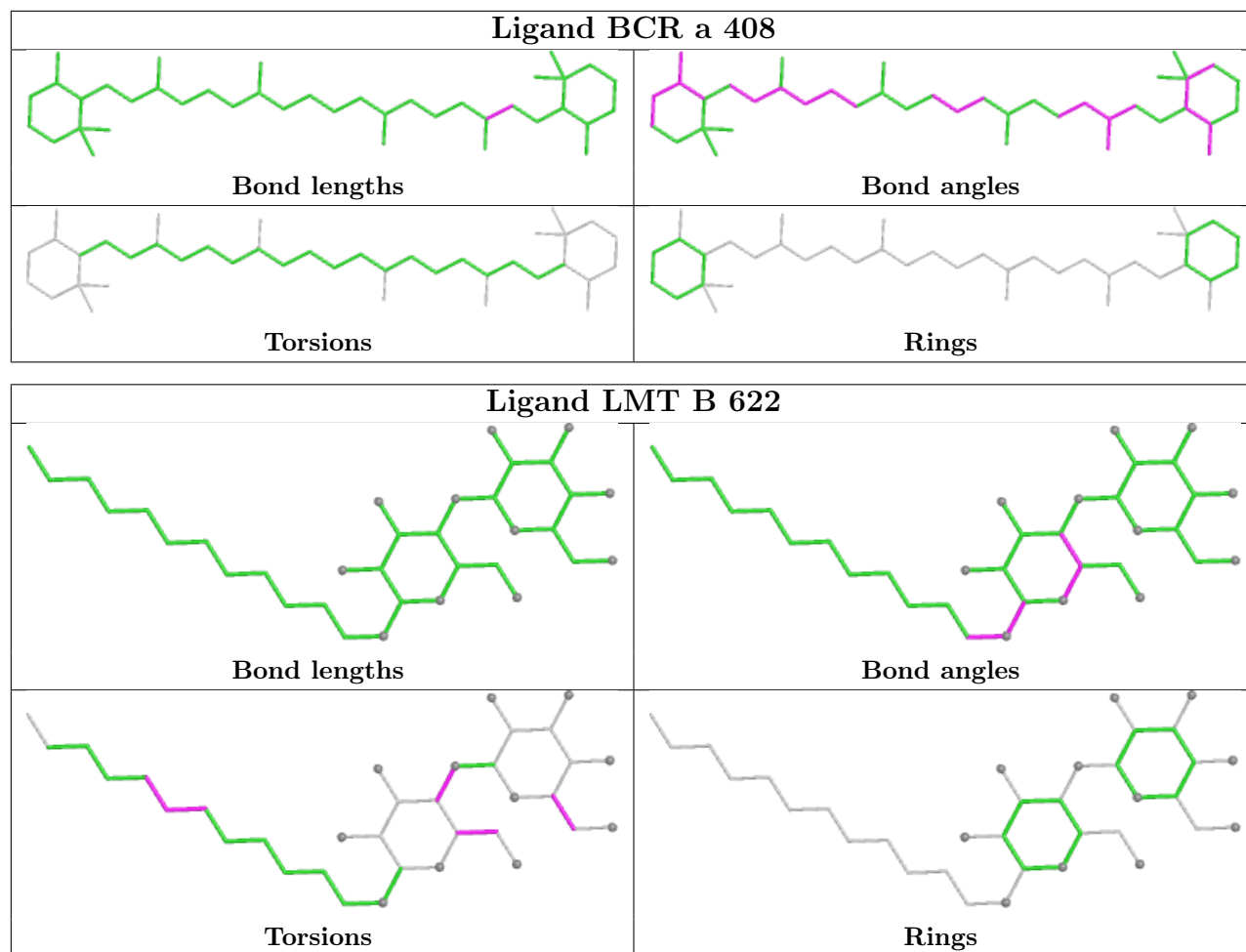




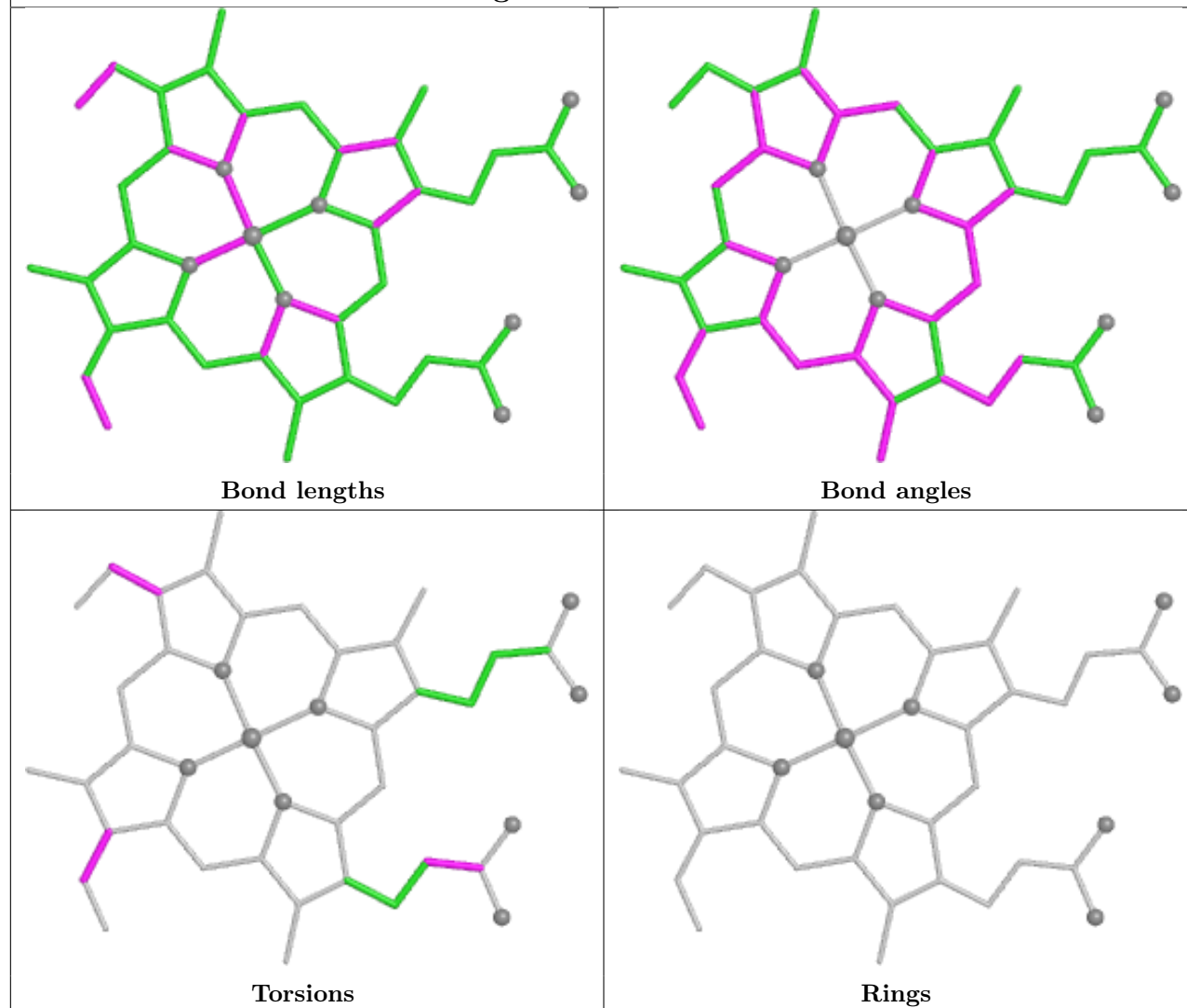




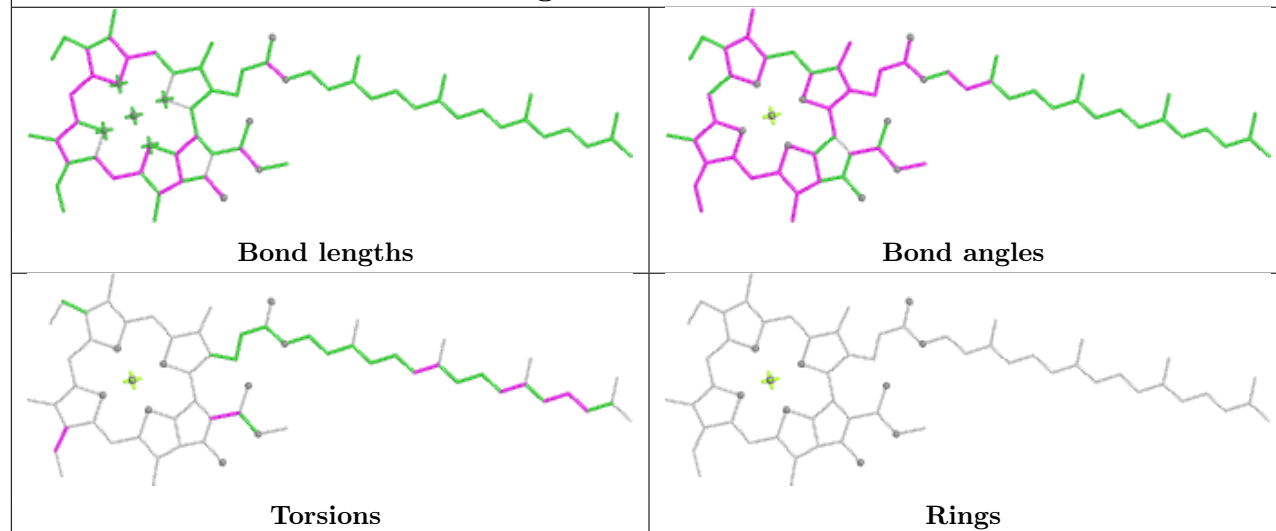


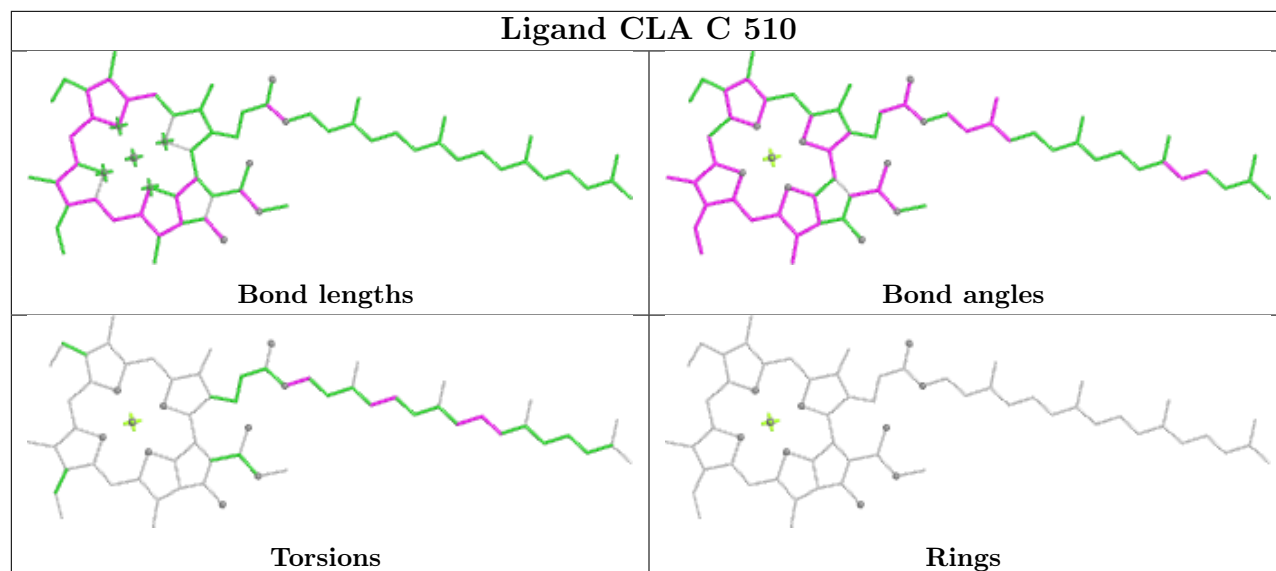
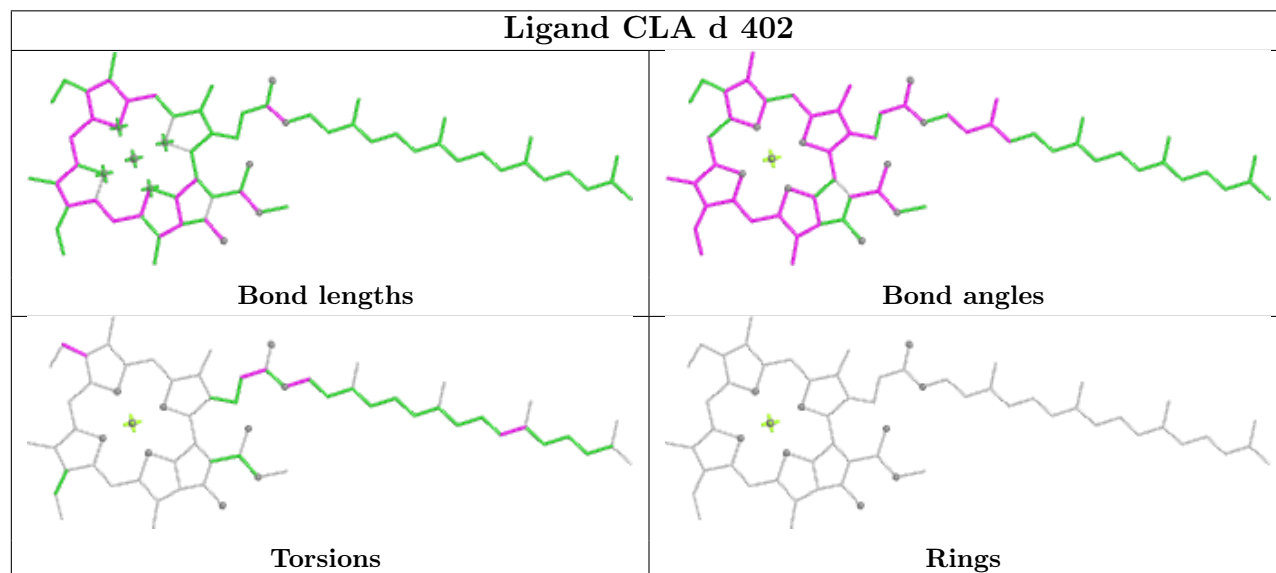
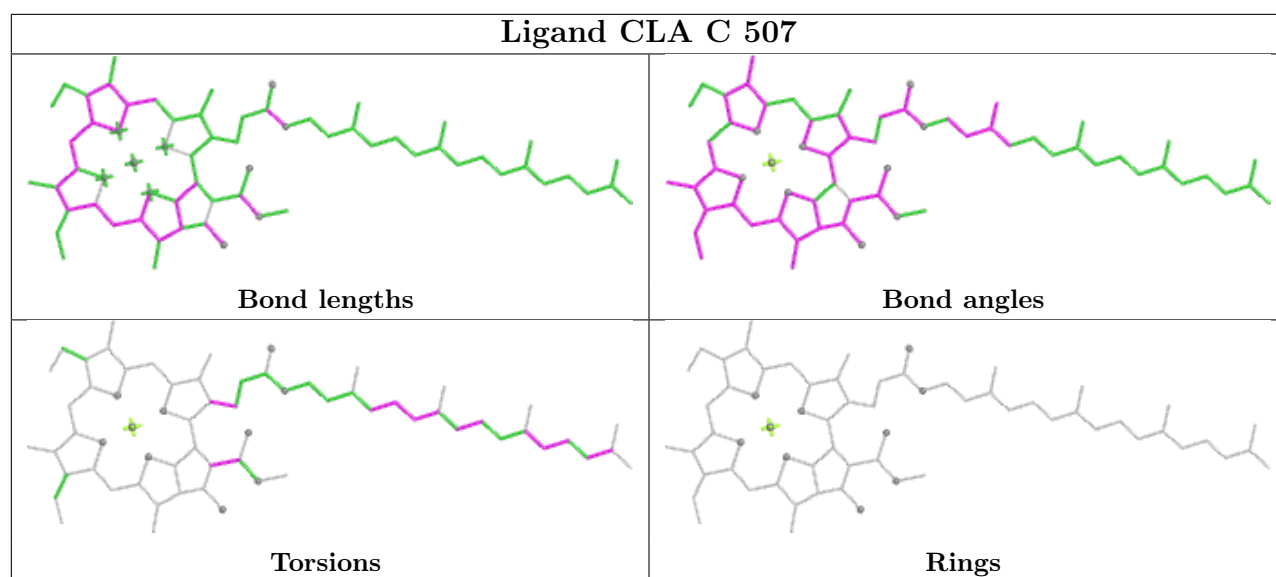


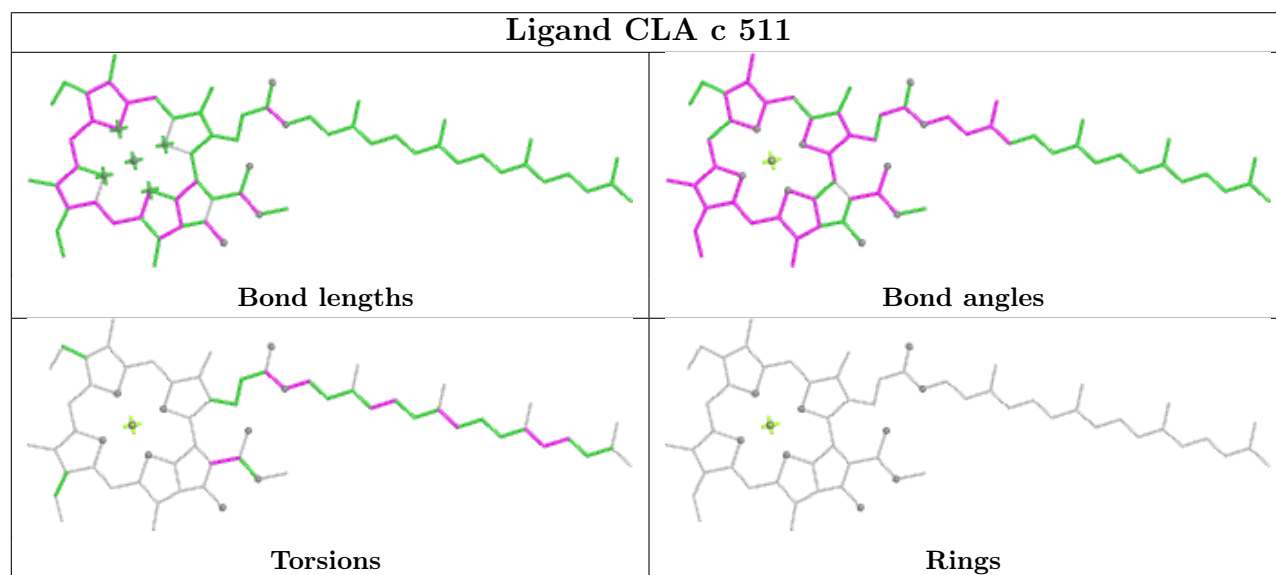
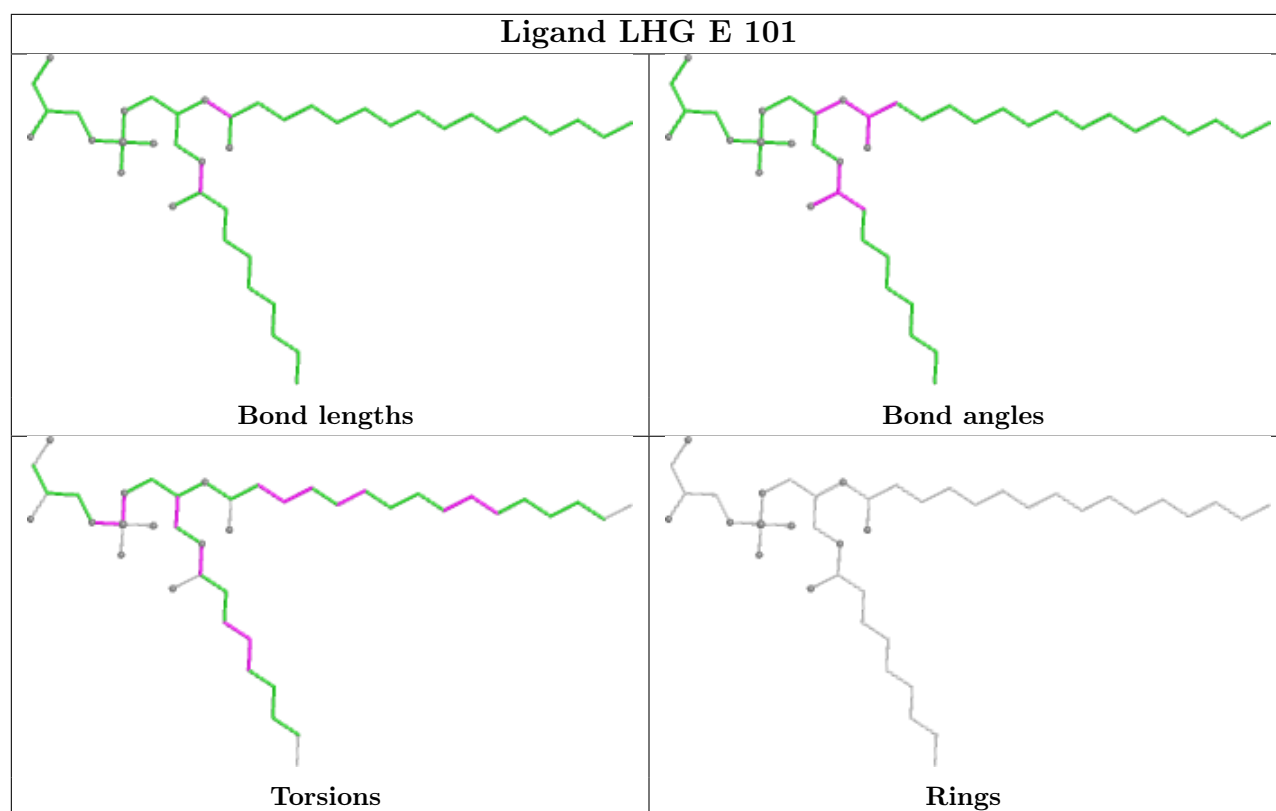
Ligand HEC V 203

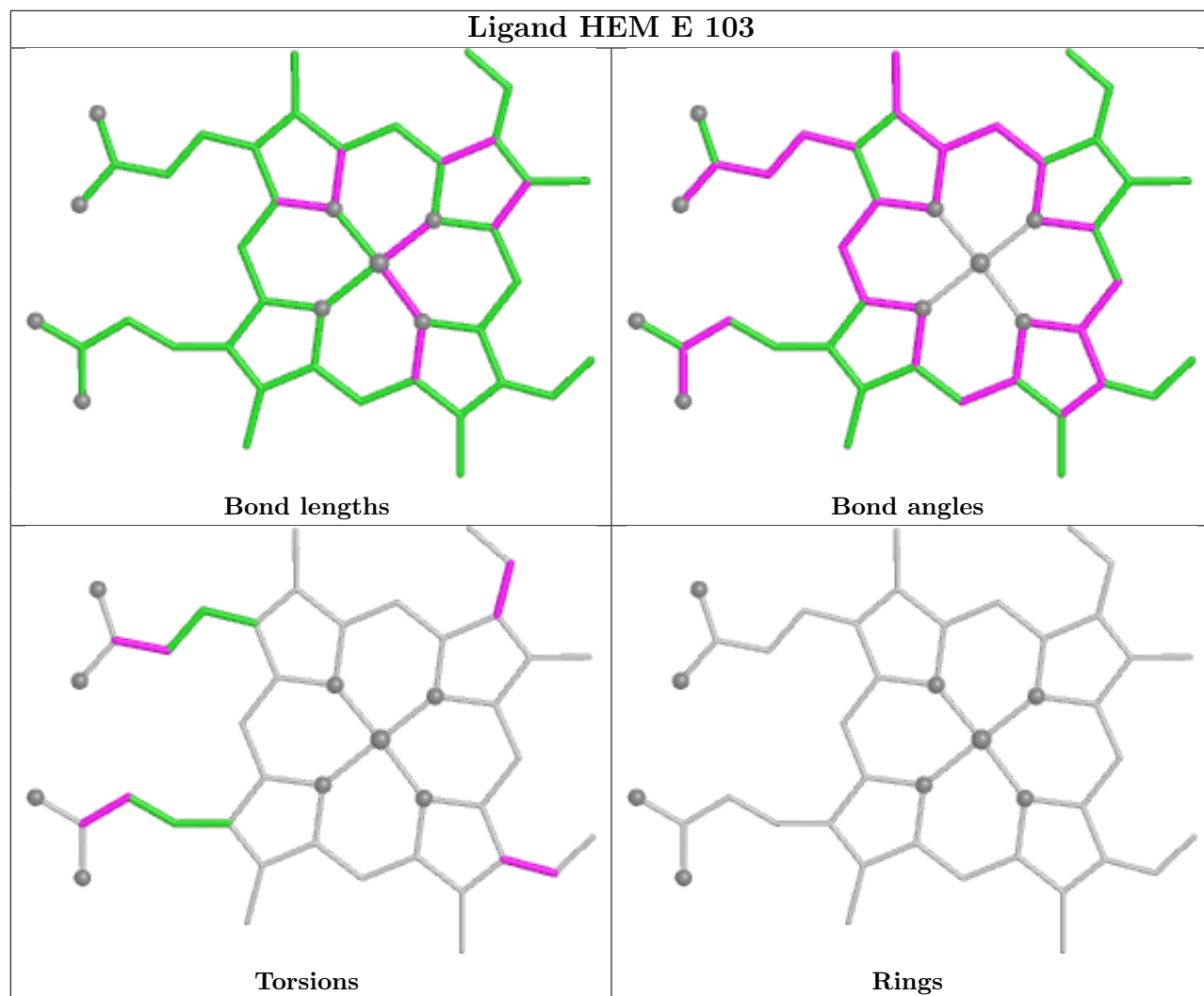


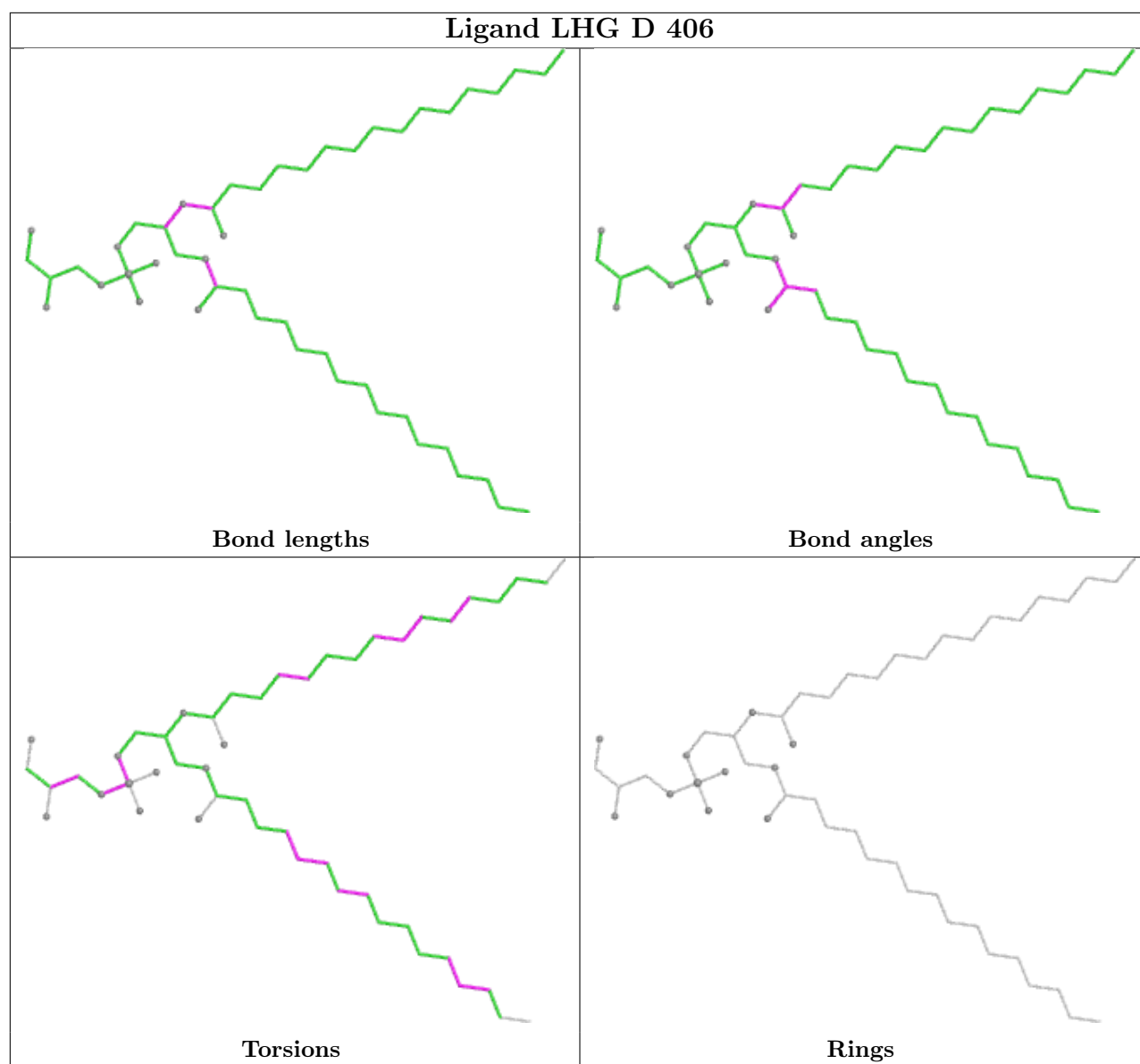
Ligand CLA a 350

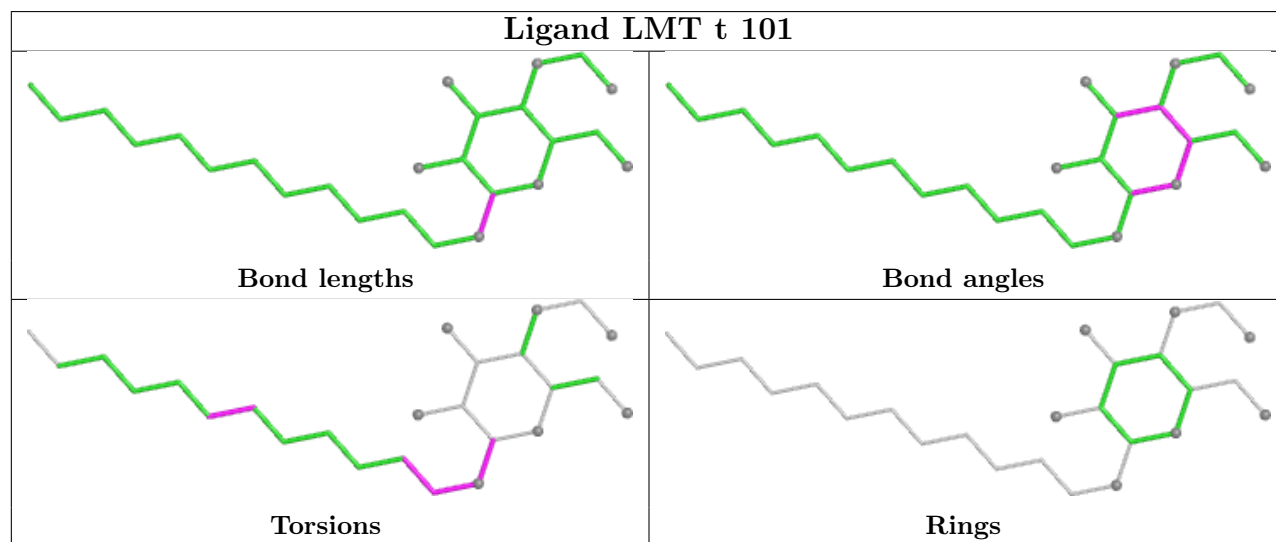
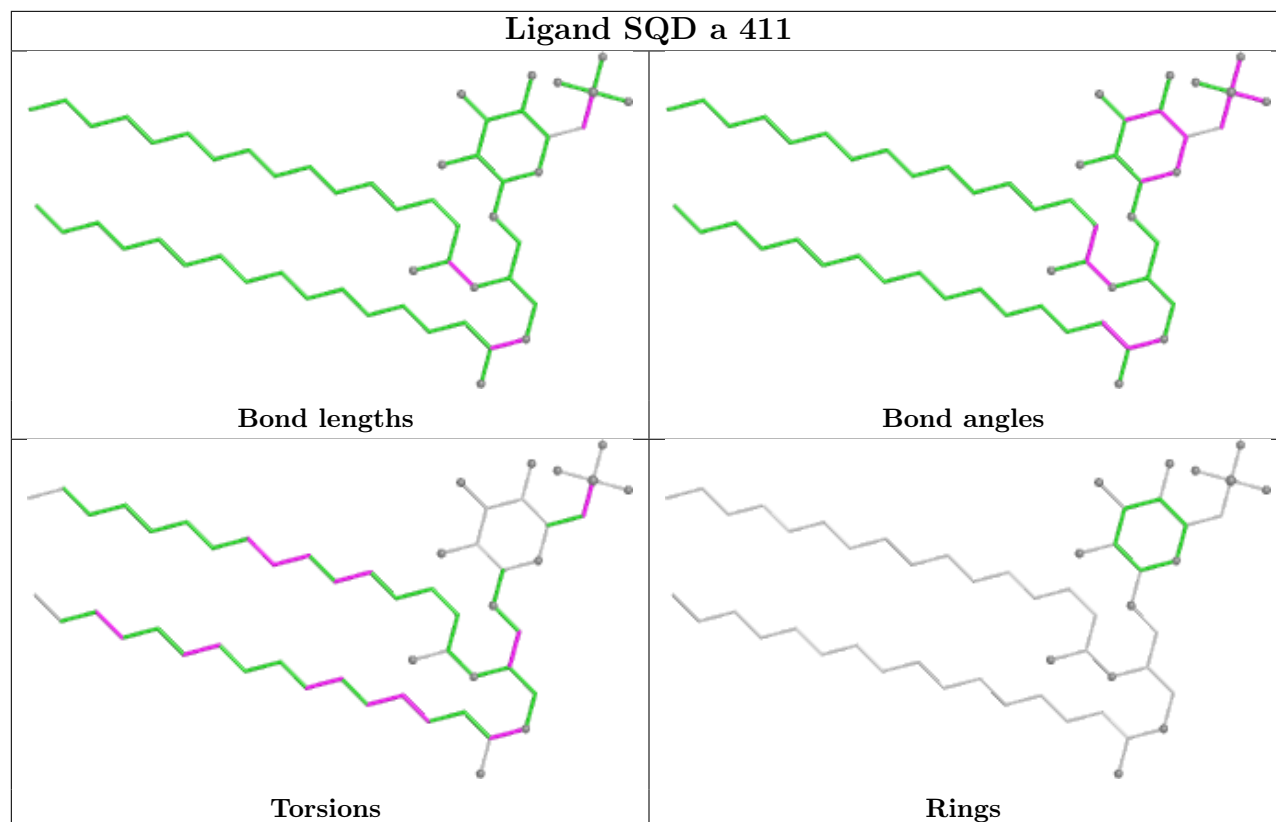


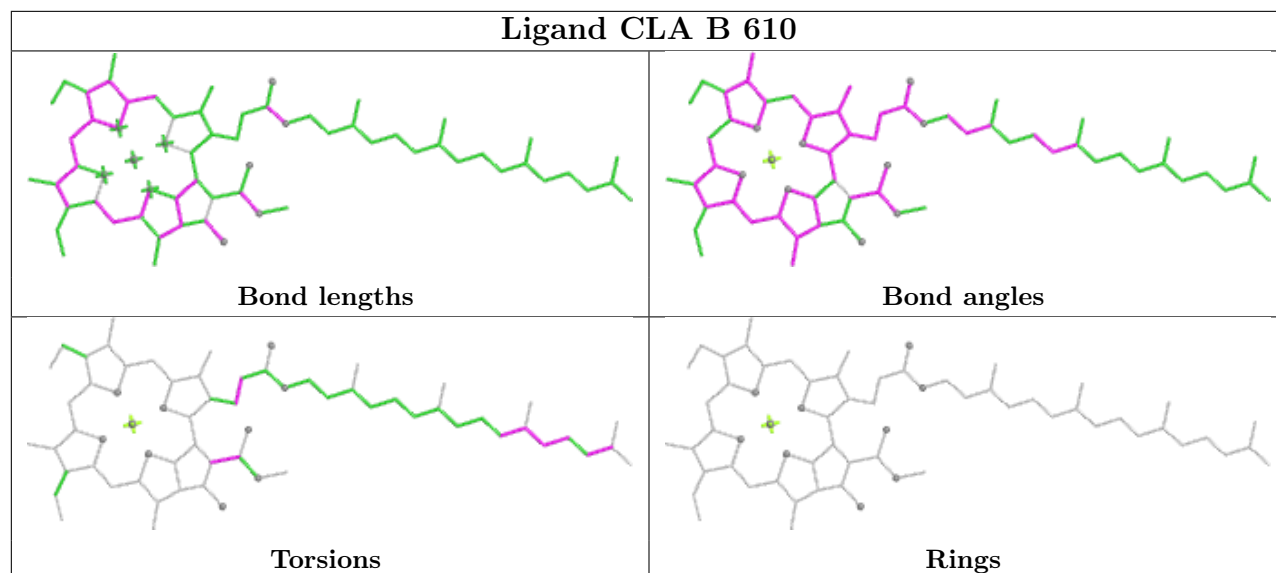
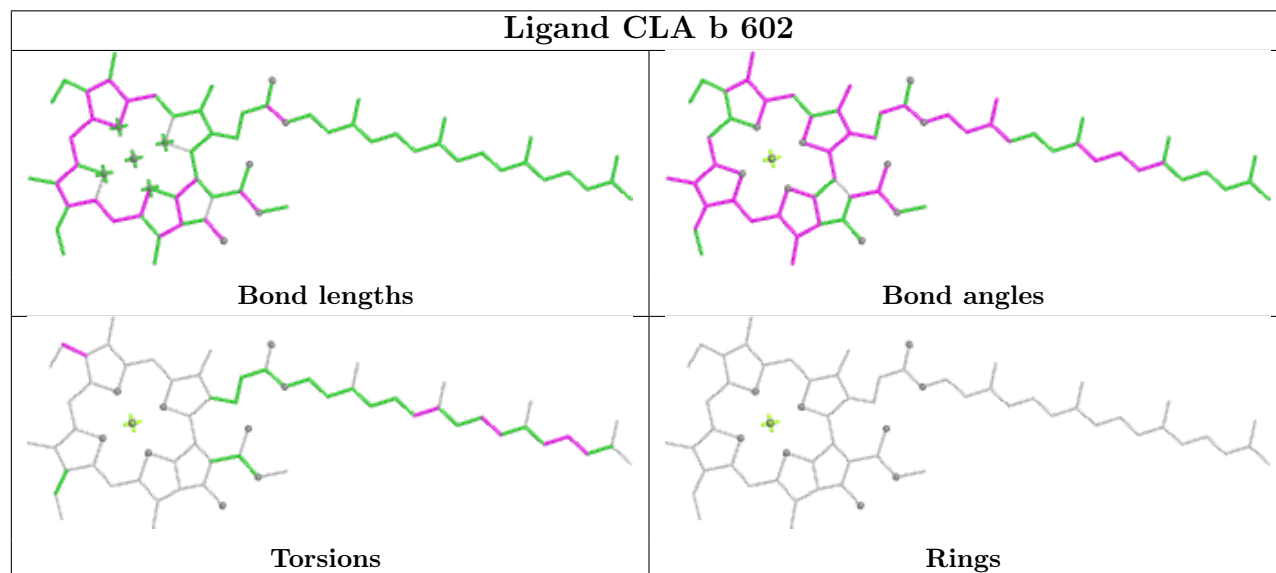
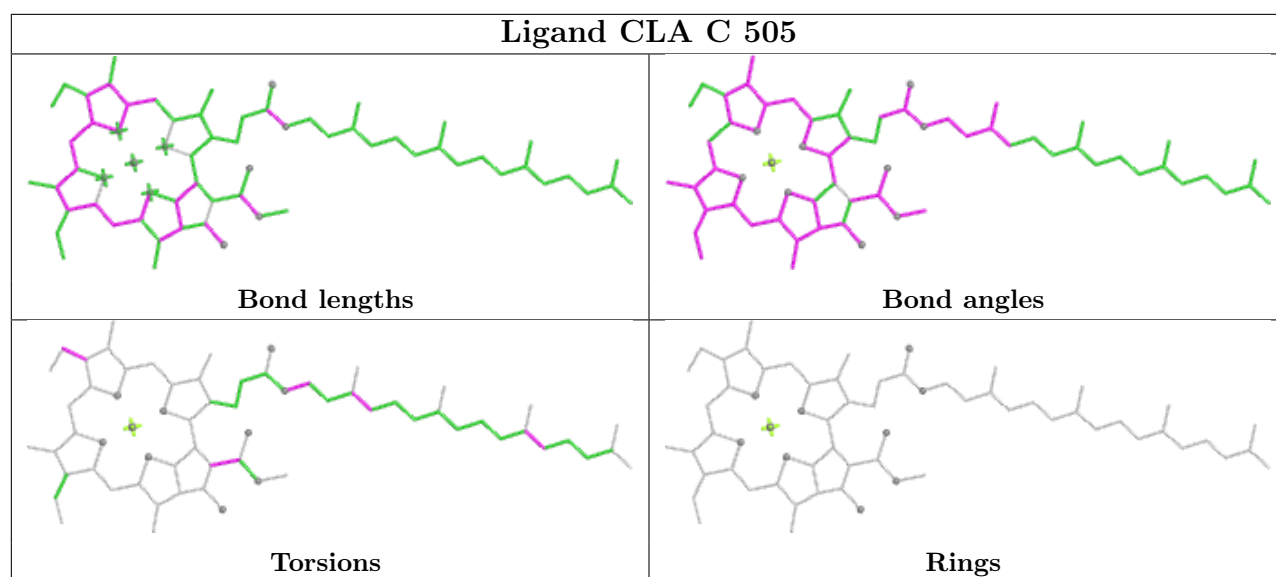




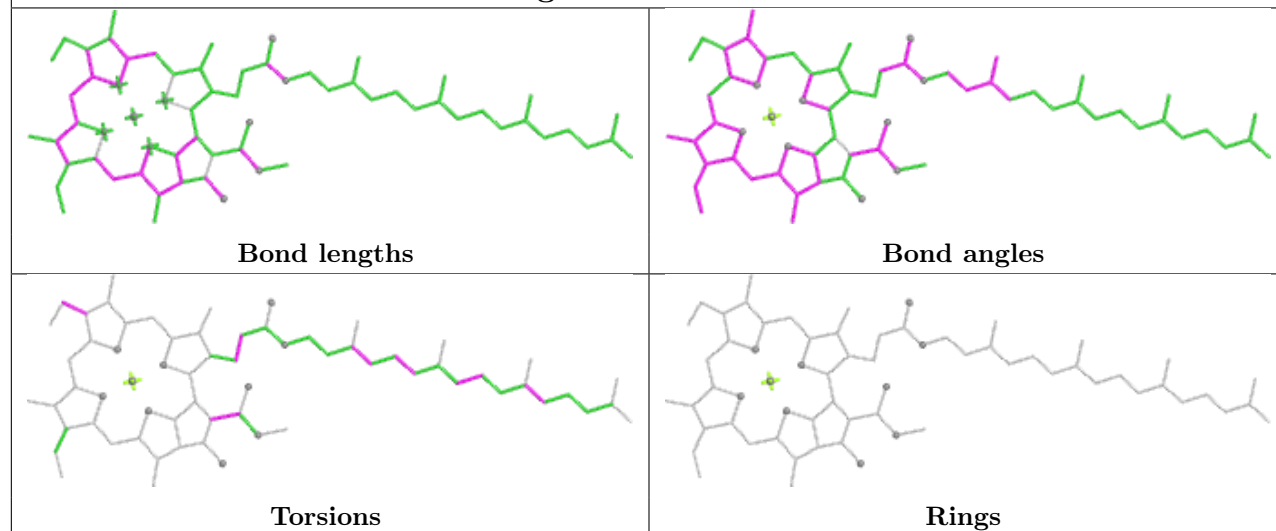




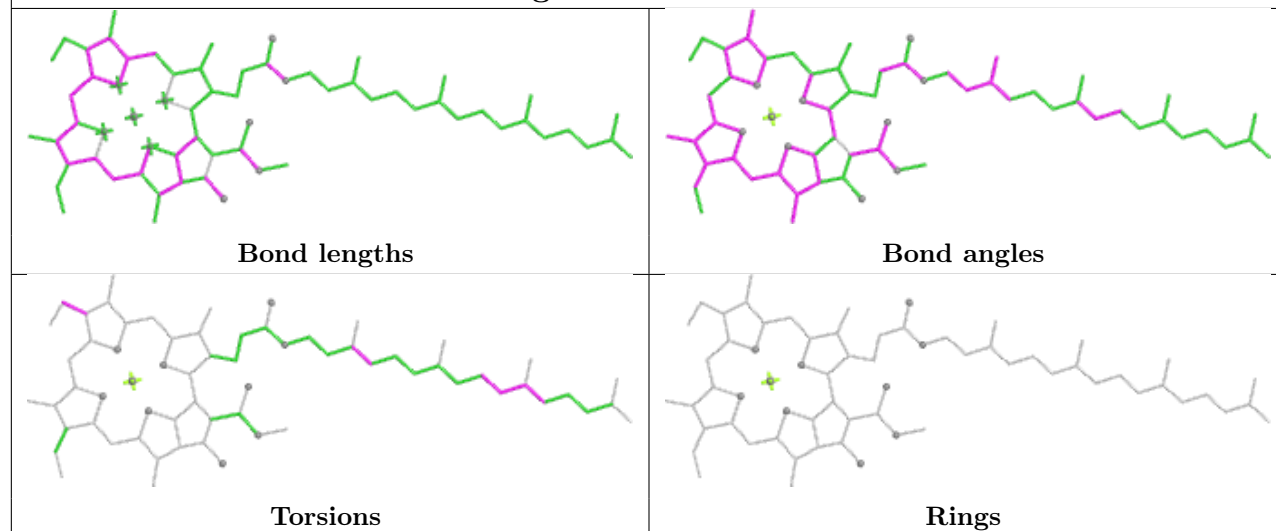




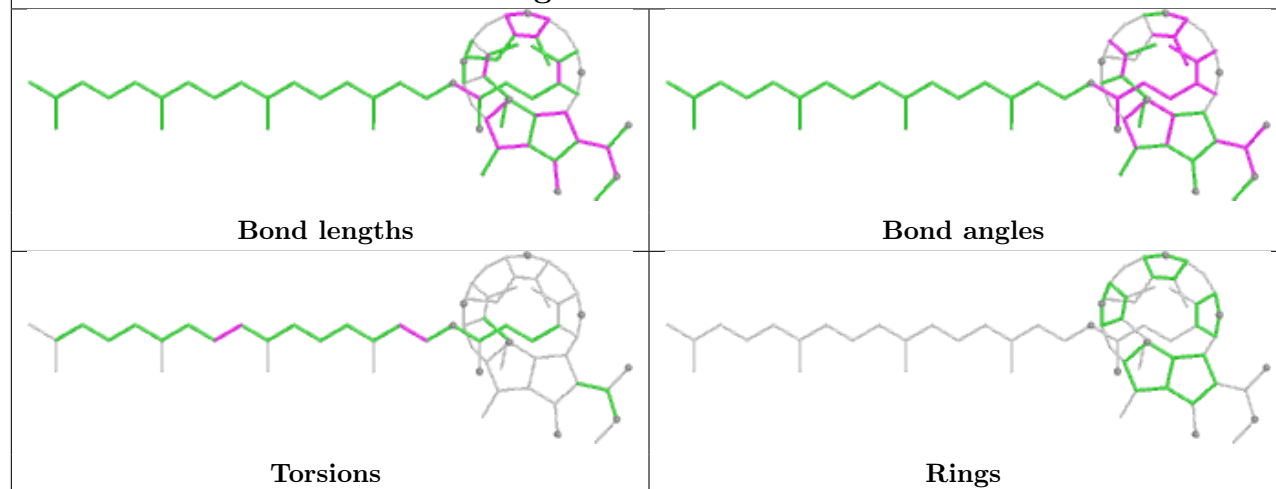
Ligand CLA c 509

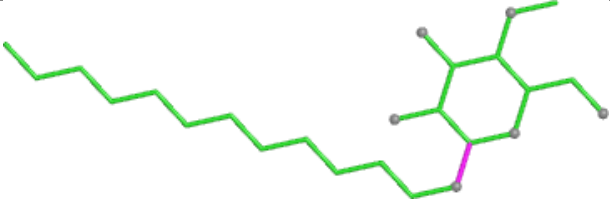
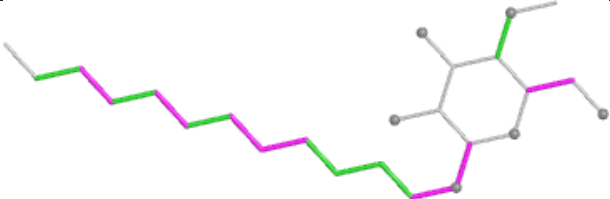
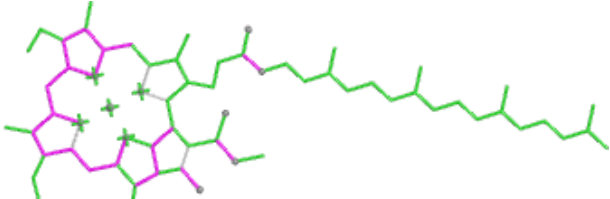
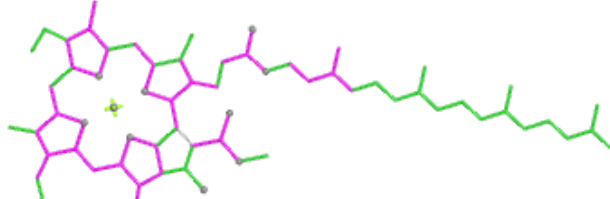
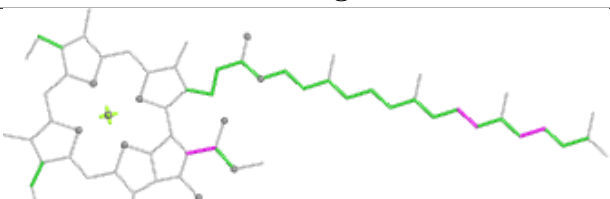
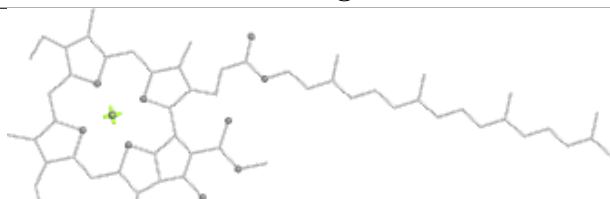
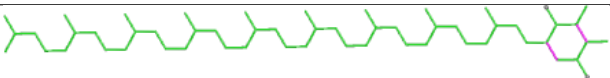
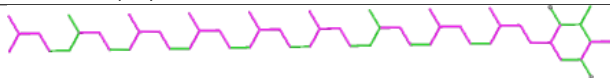
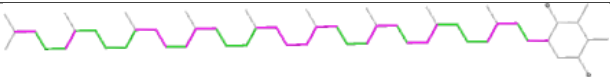
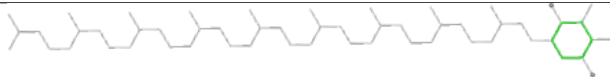


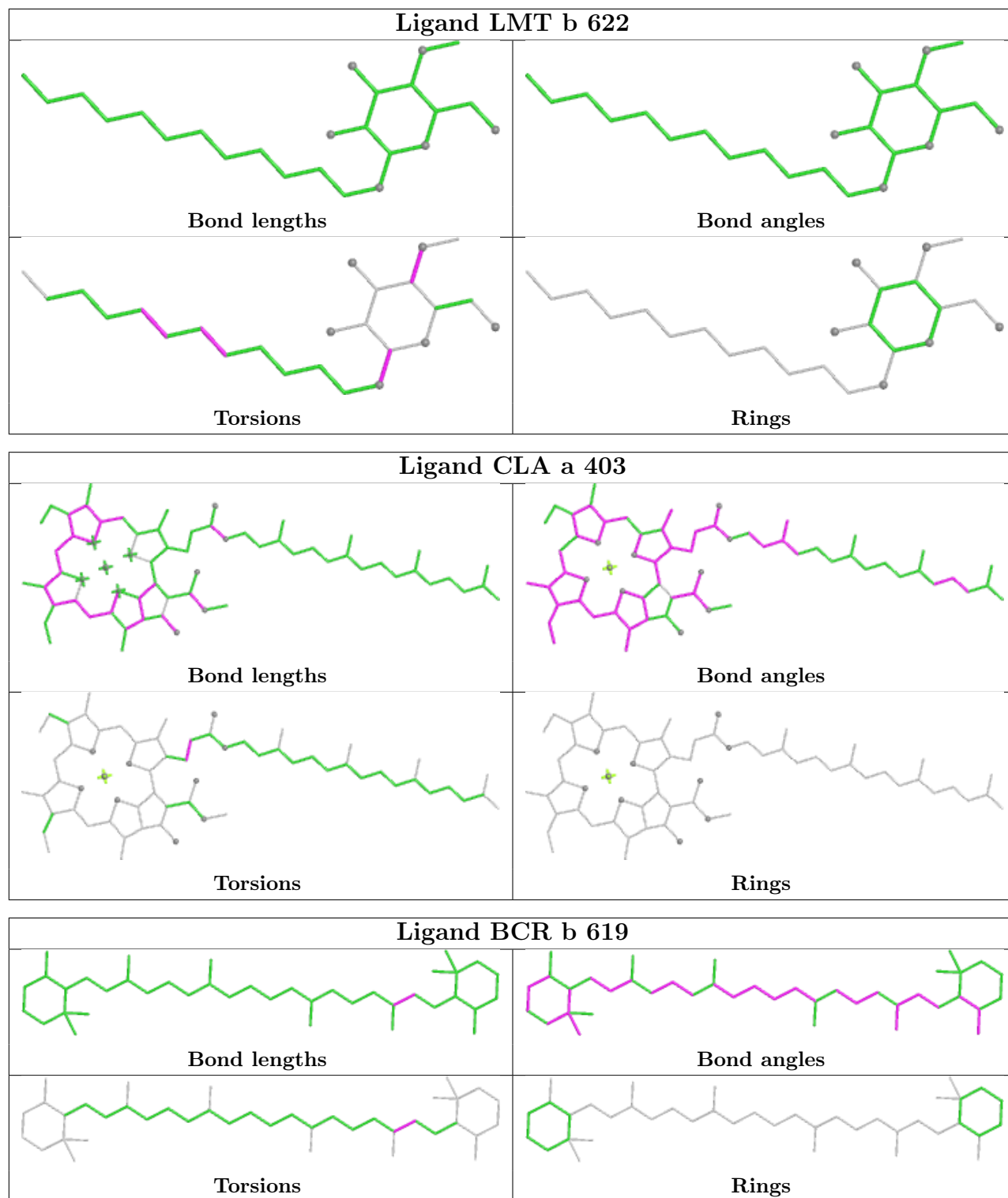
Ligand CLA C 506

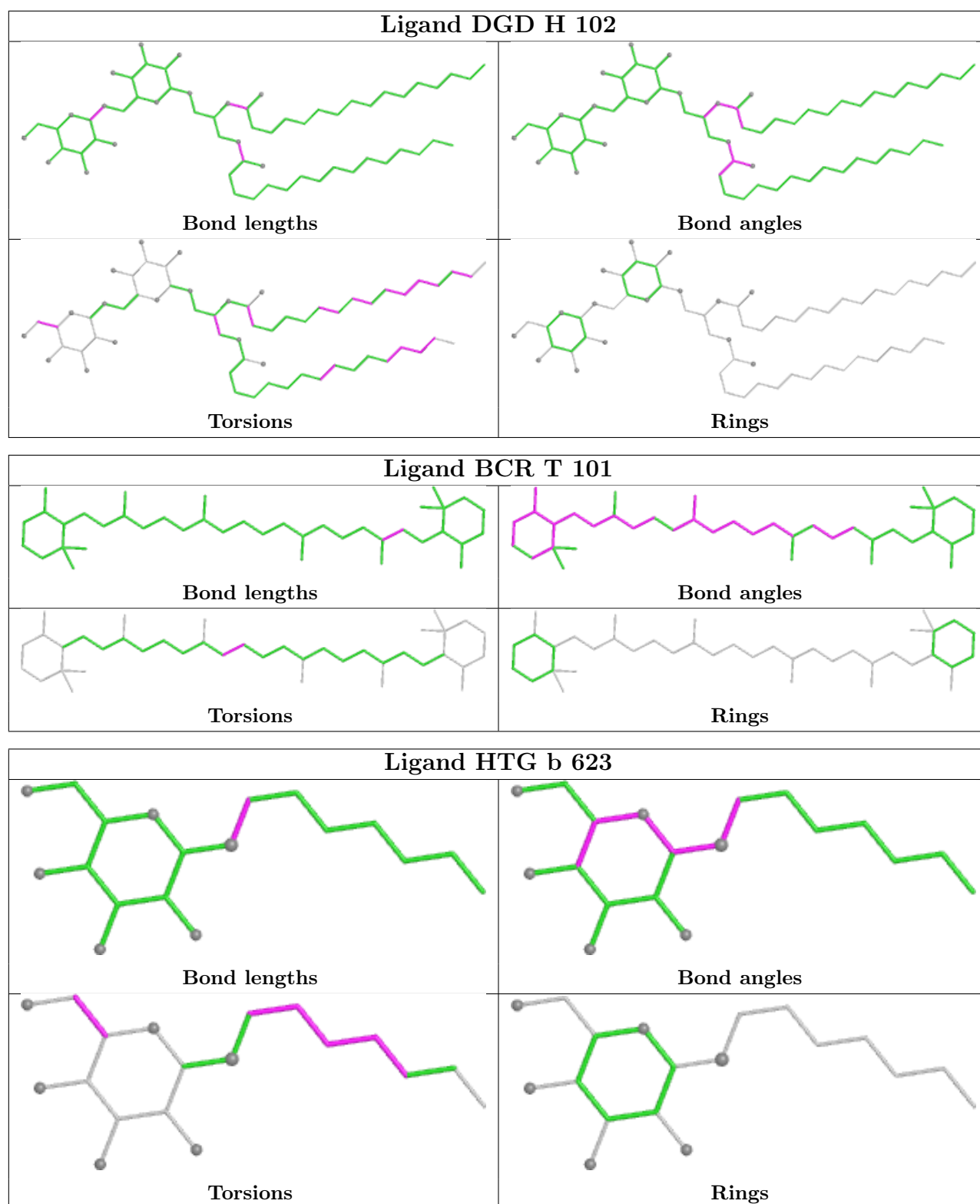


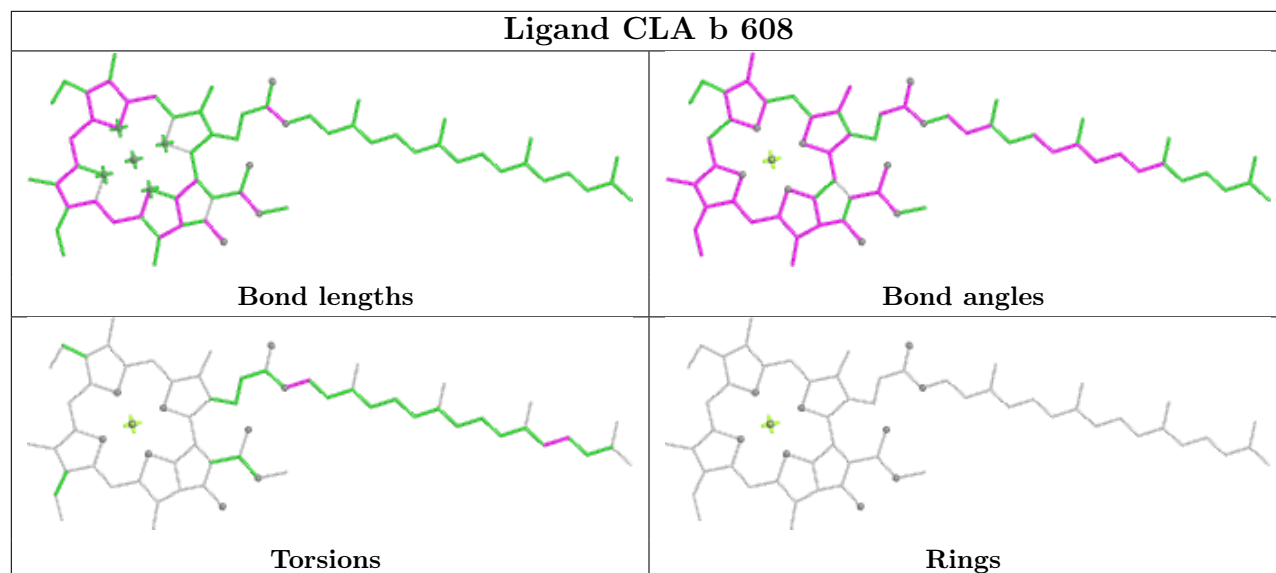
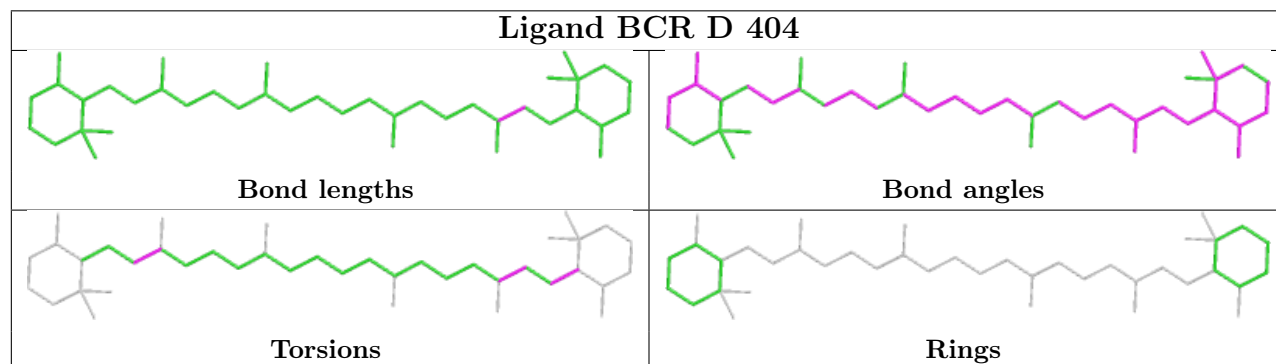
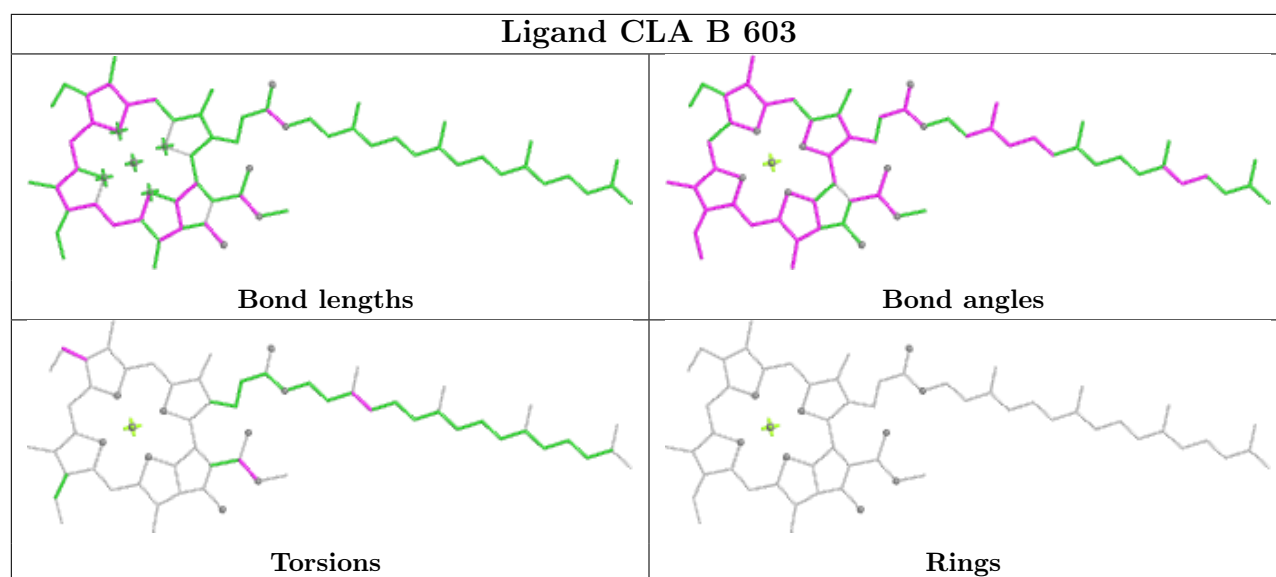
Ligand PHO a 405

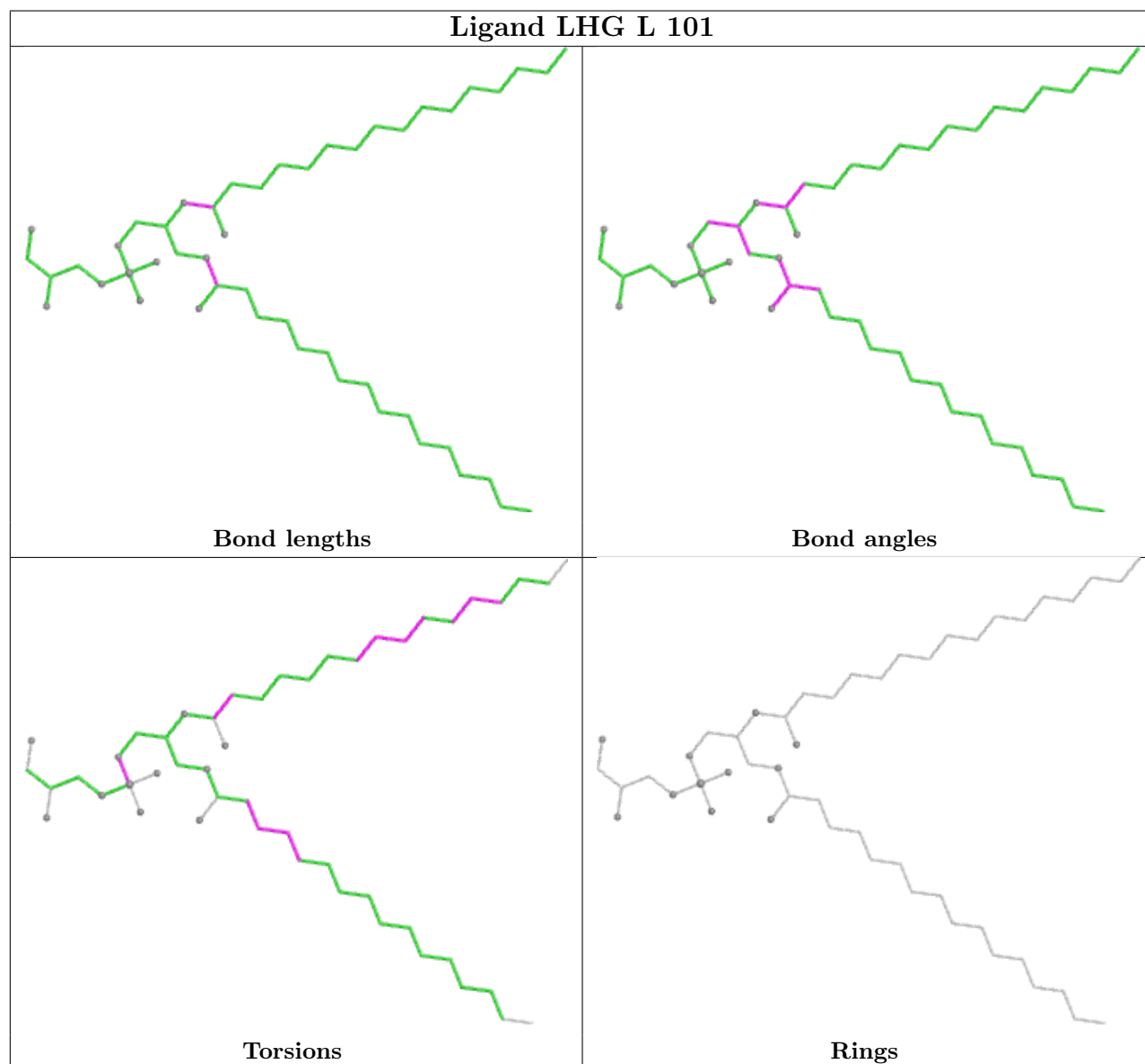
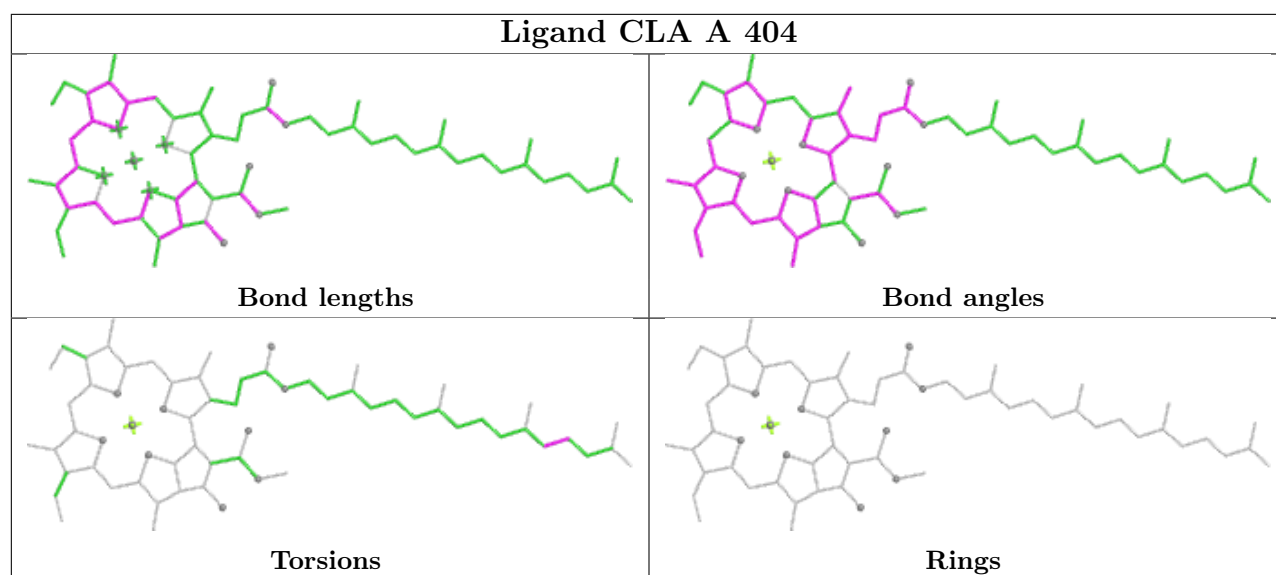


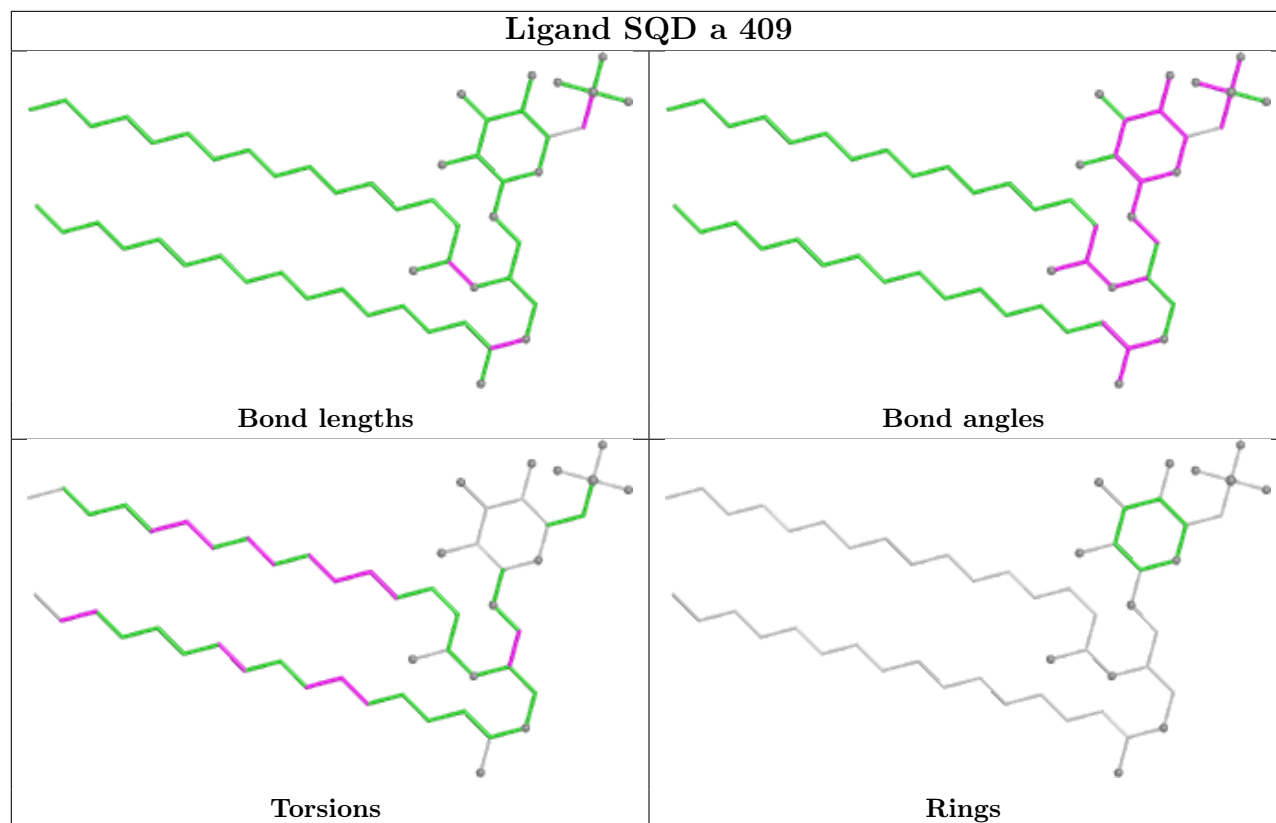
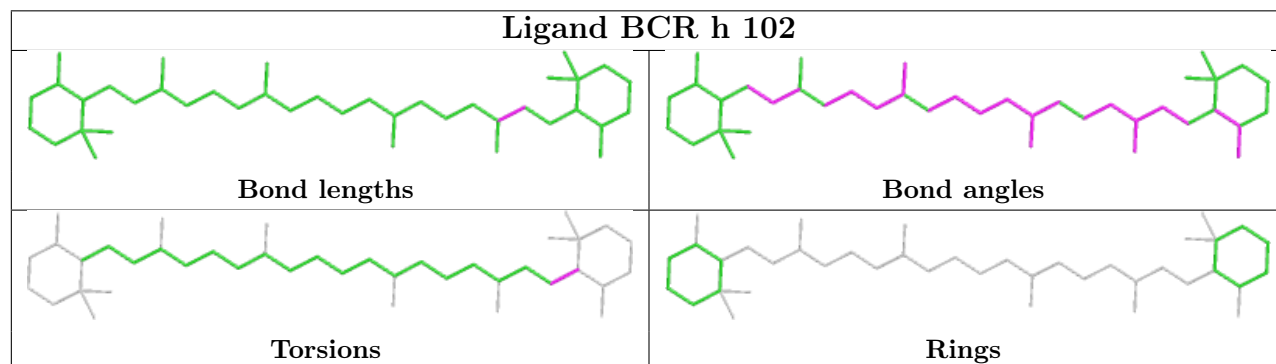
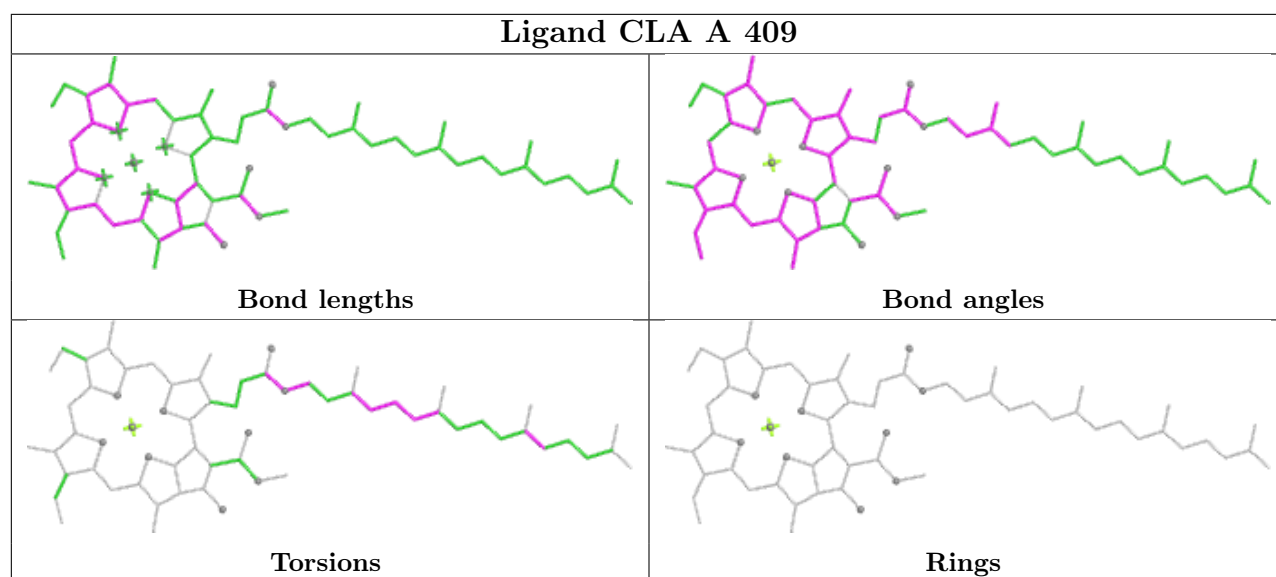
Ligand LMT b 630	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 414 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

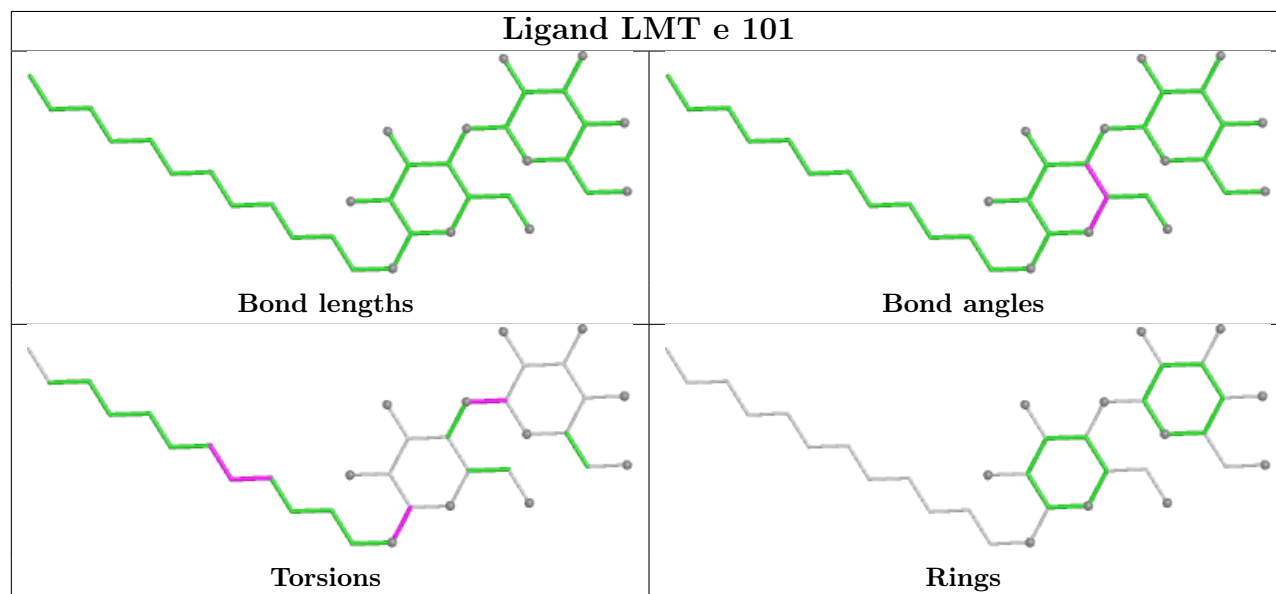
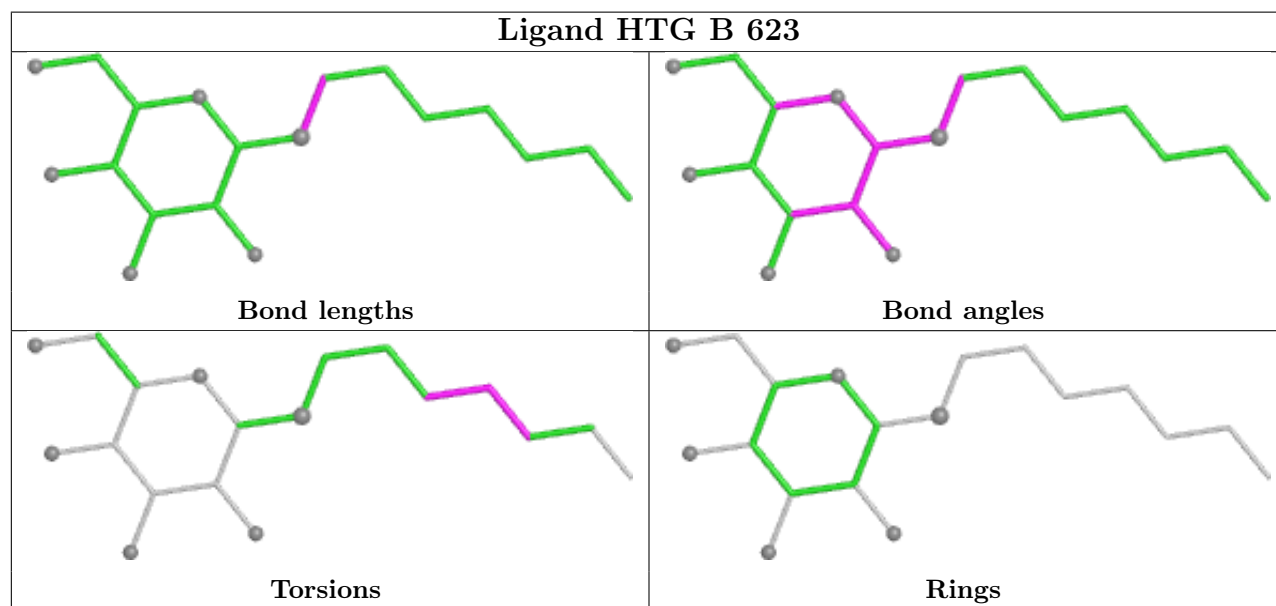
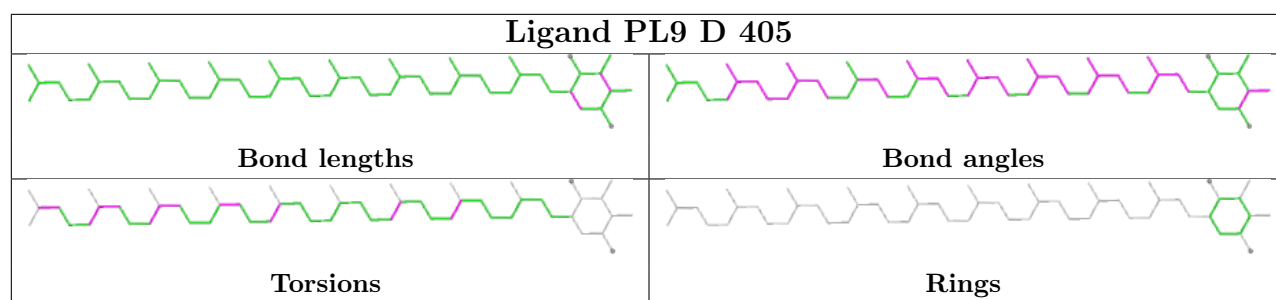


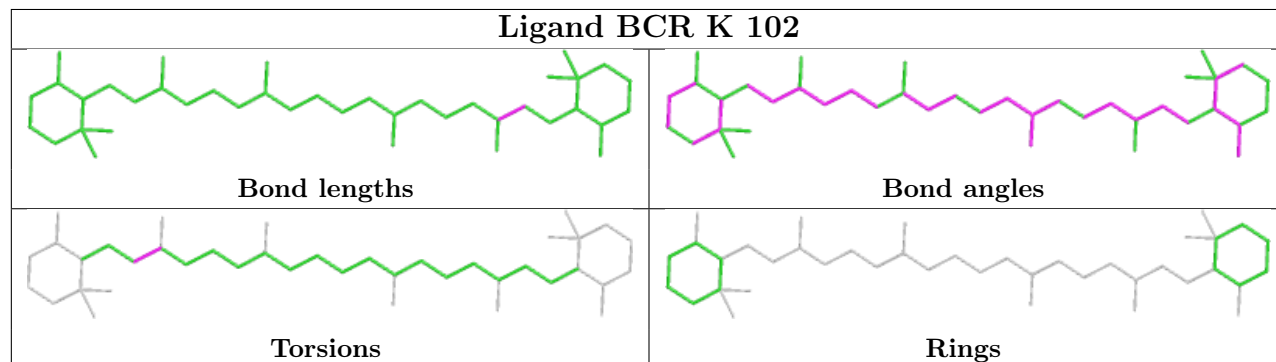
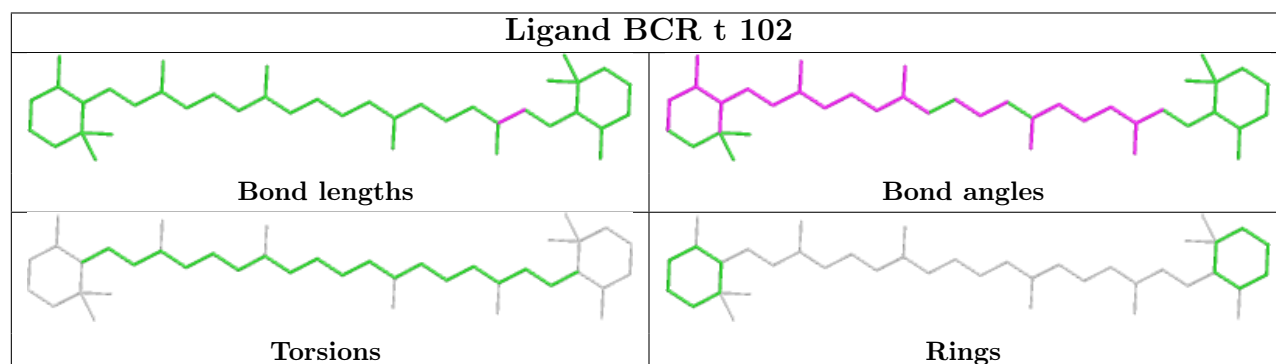
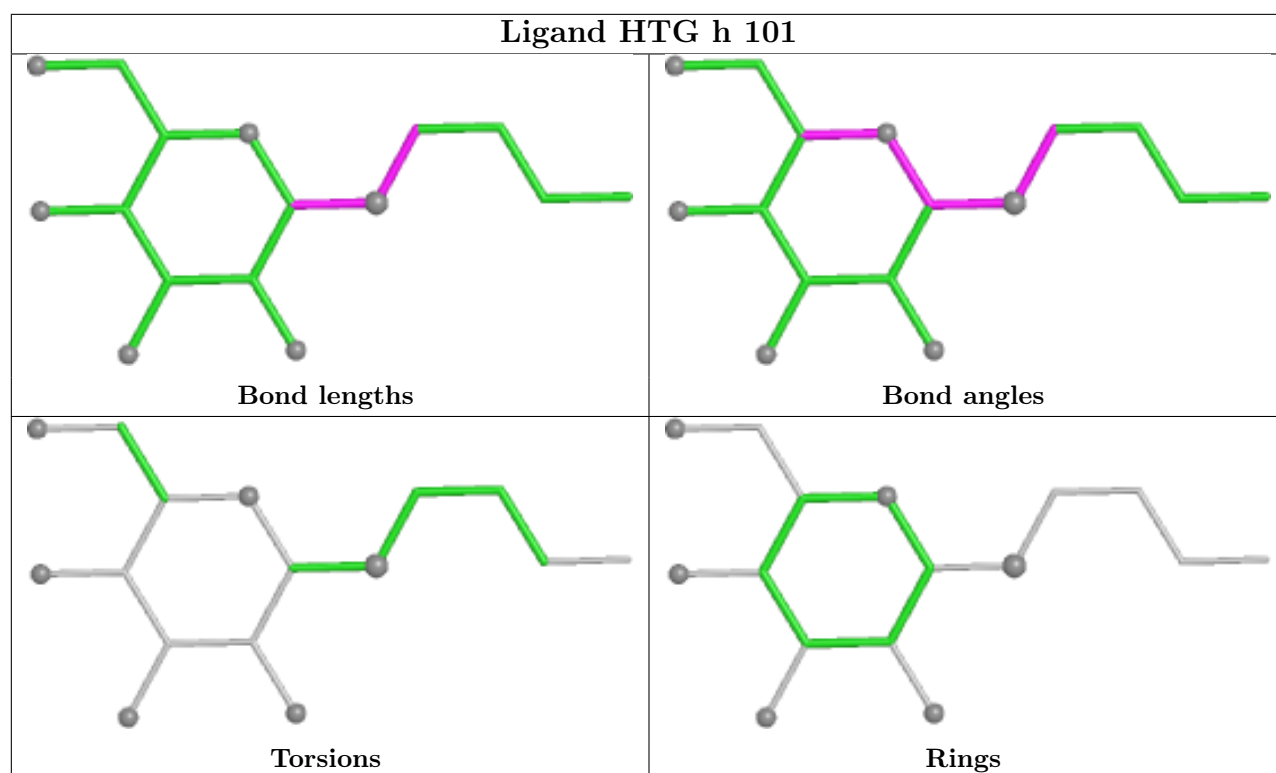


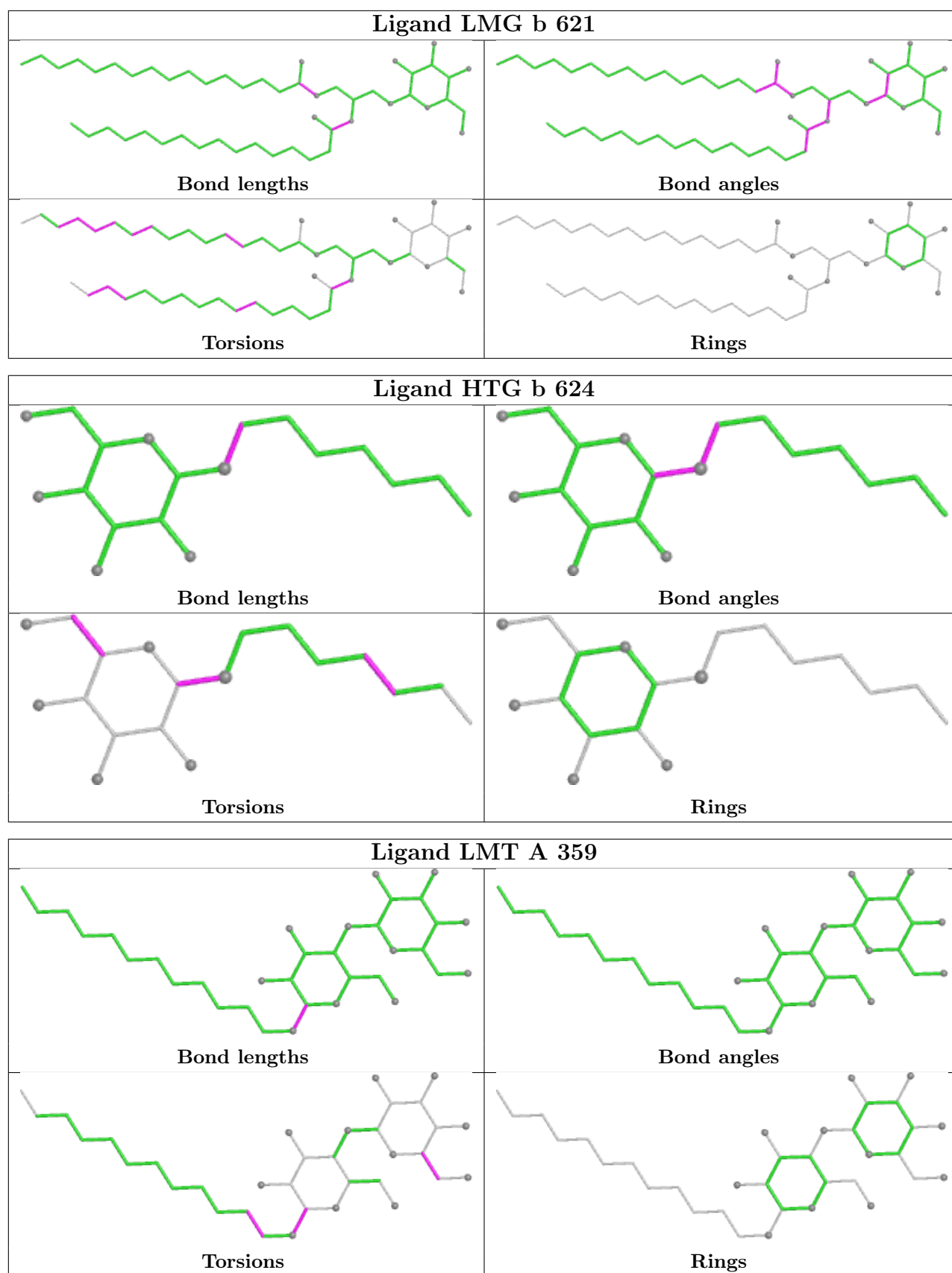


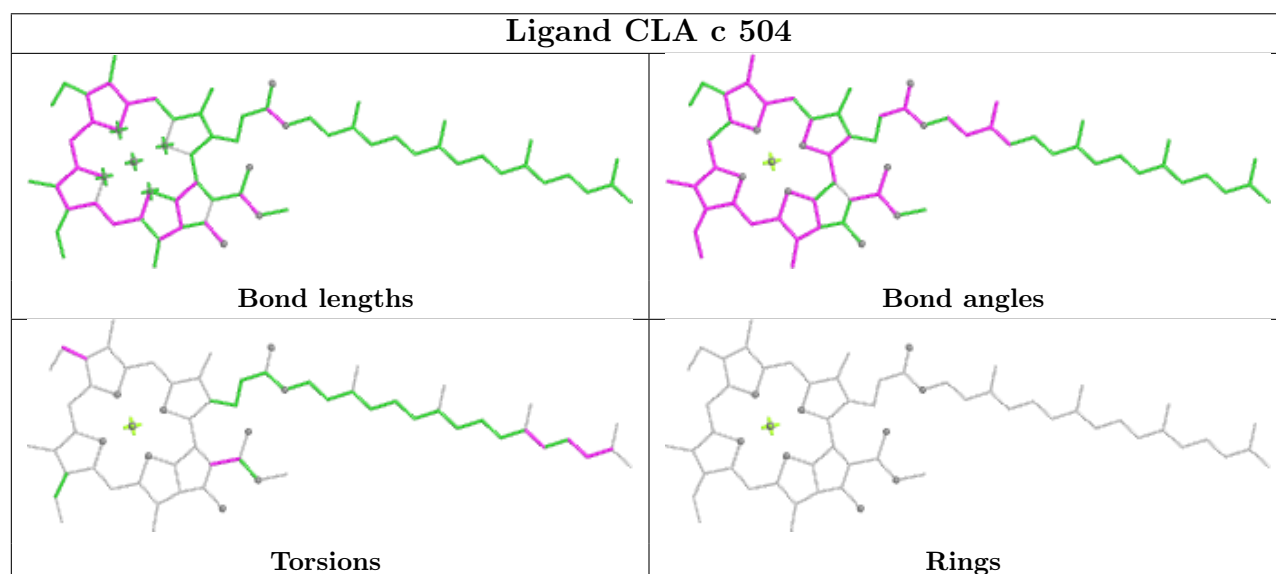
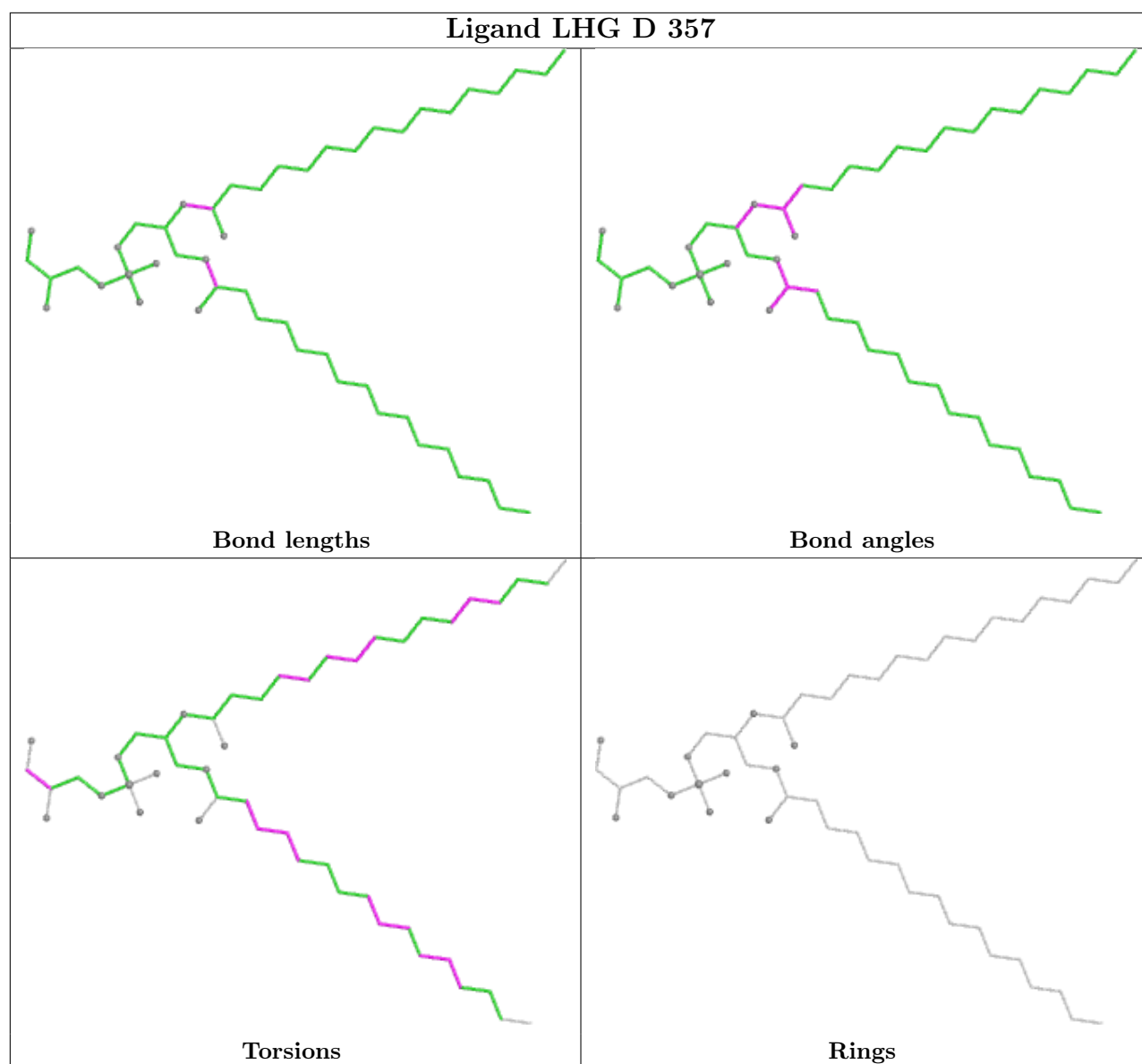


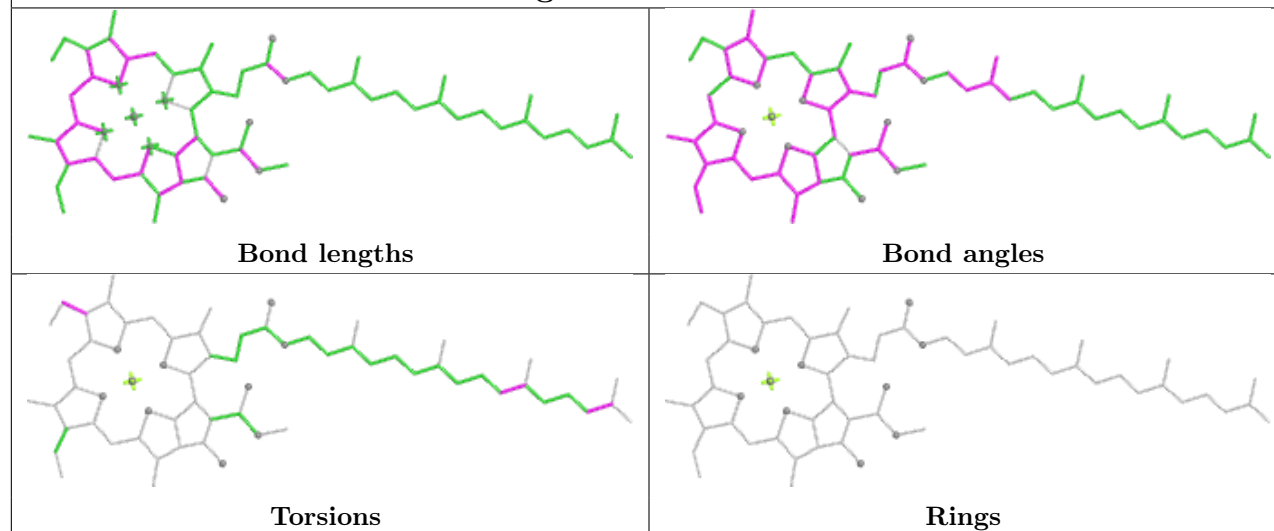
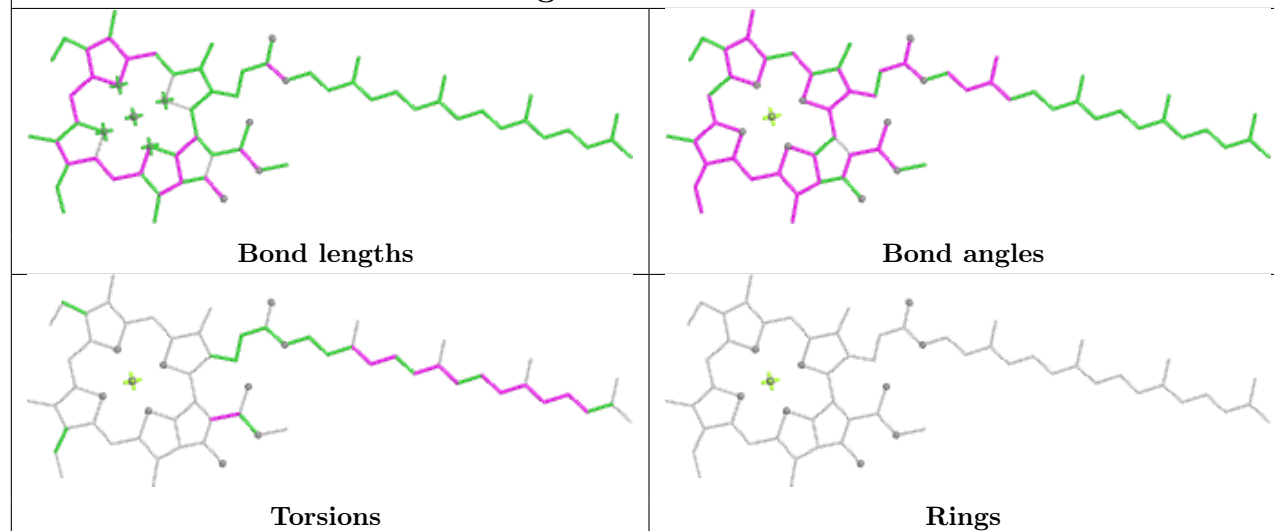
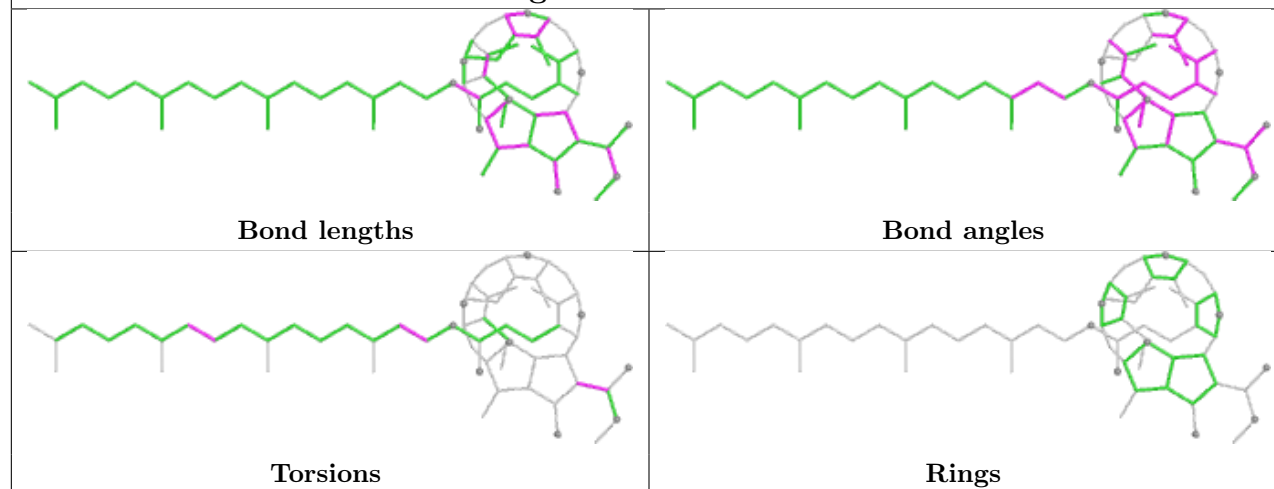


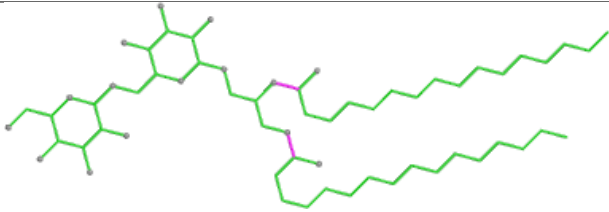
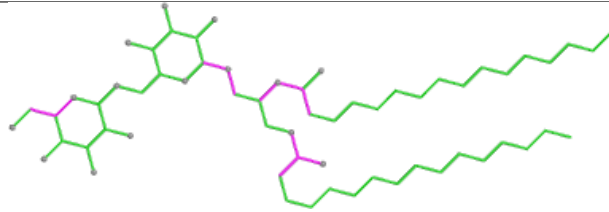
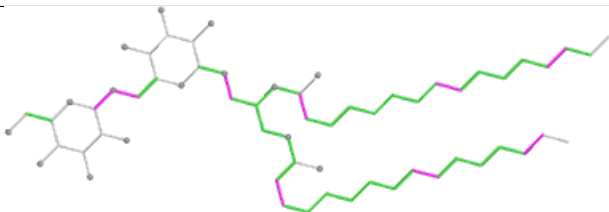
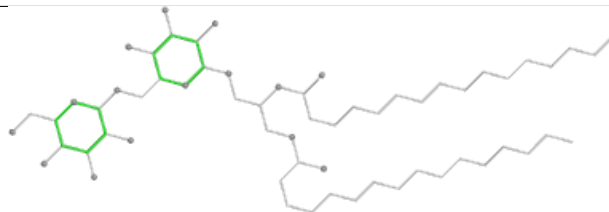


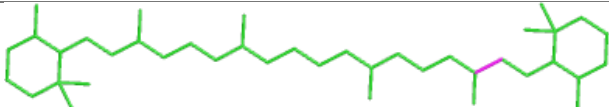
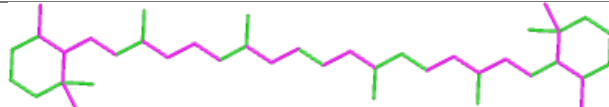
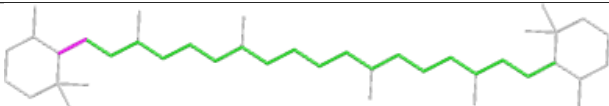
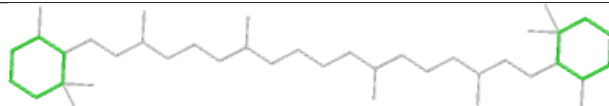


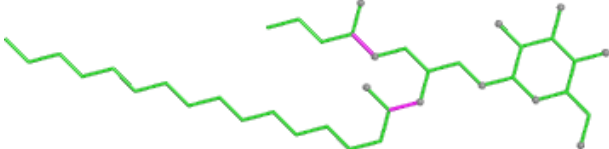
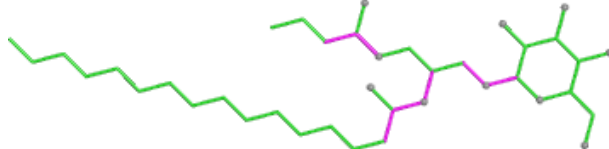
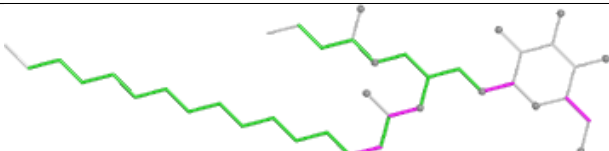


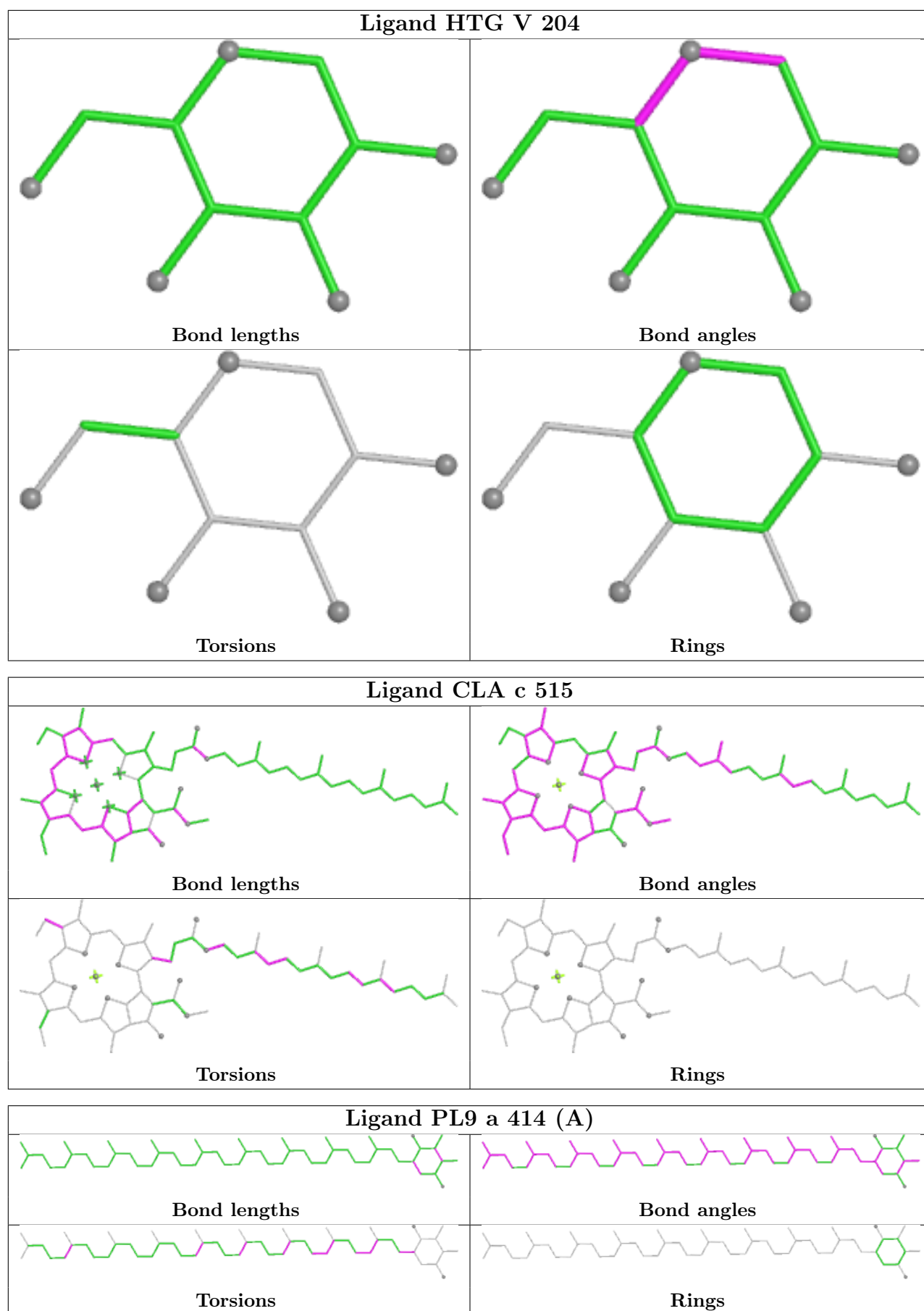


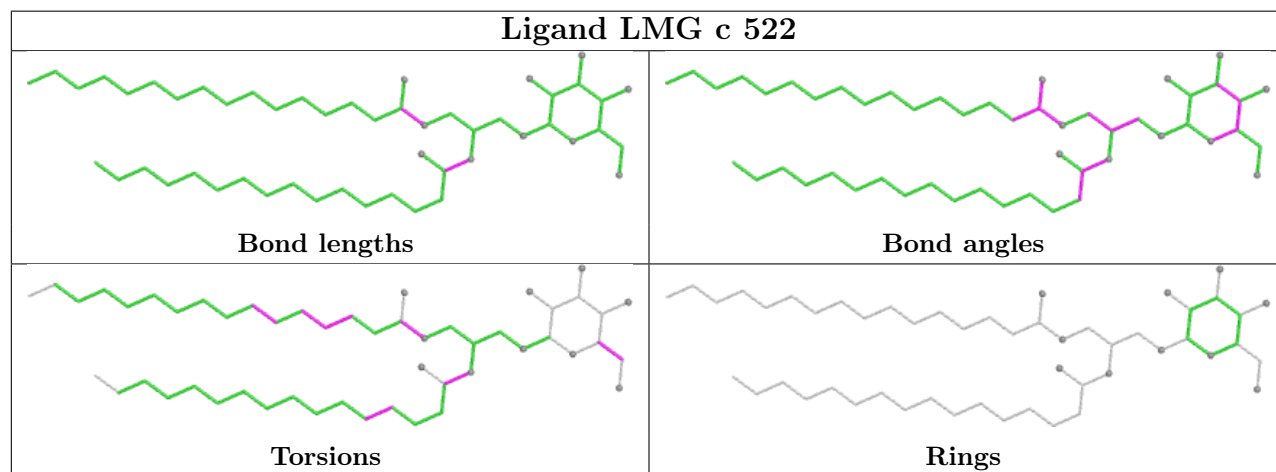
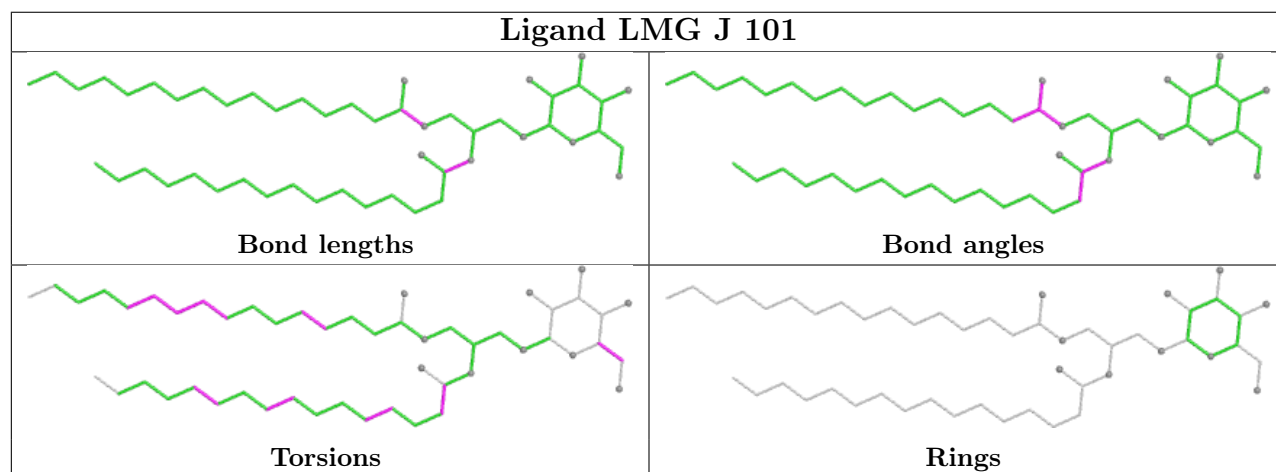
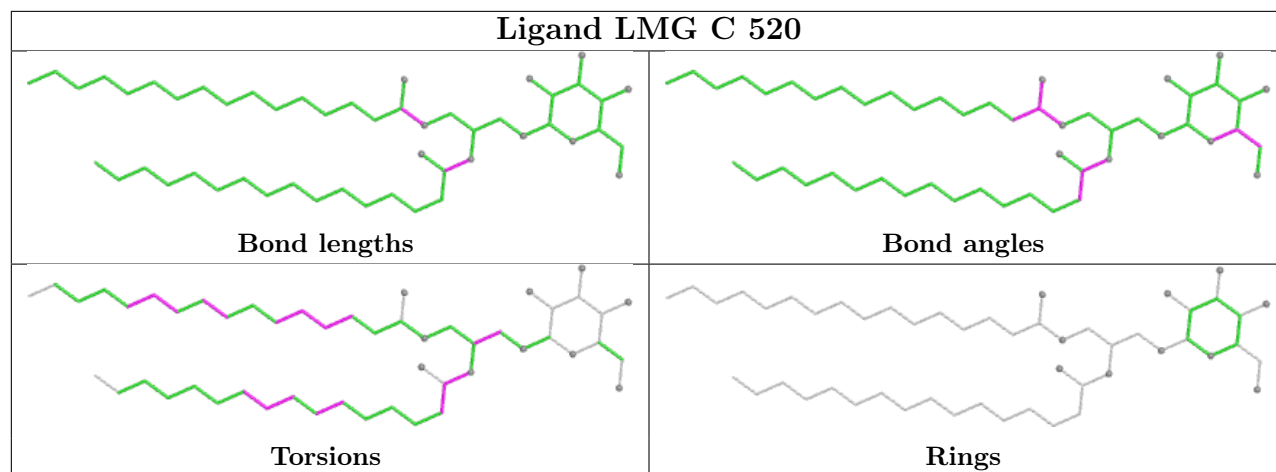
Ligand CLA a 404**Ligand CLA c 508****Ligand PHO A 407**

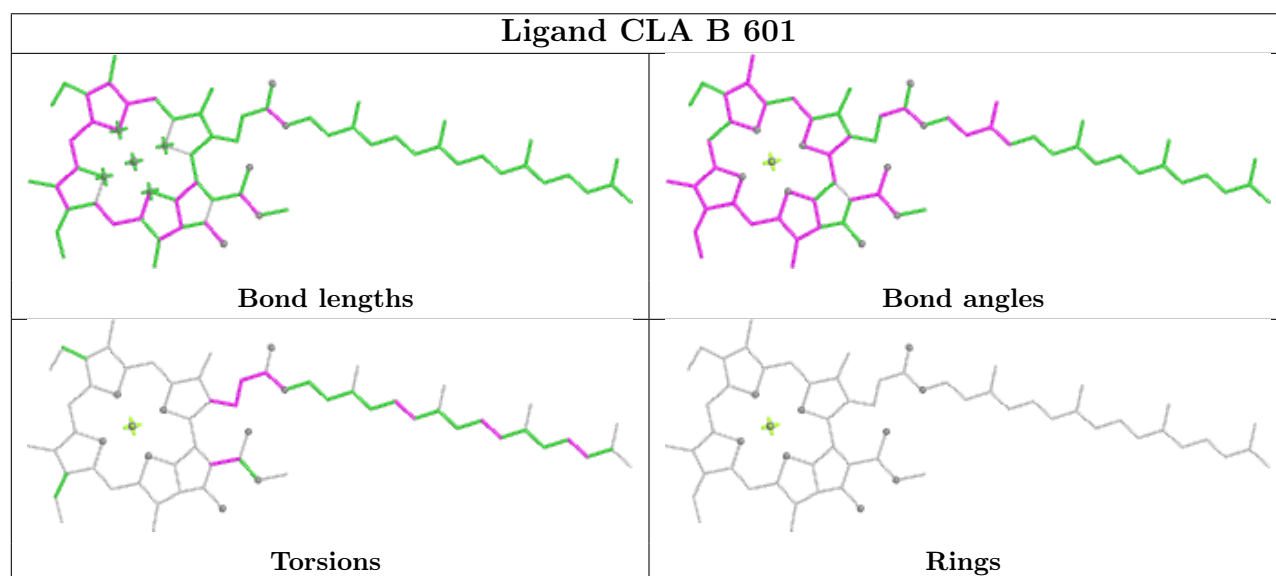
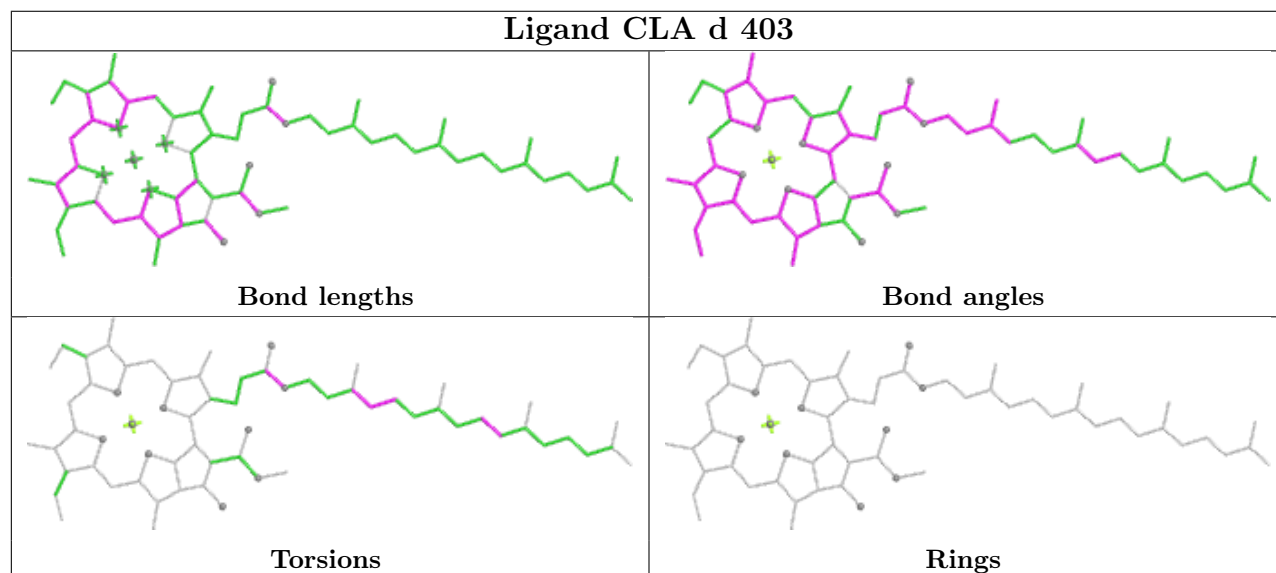
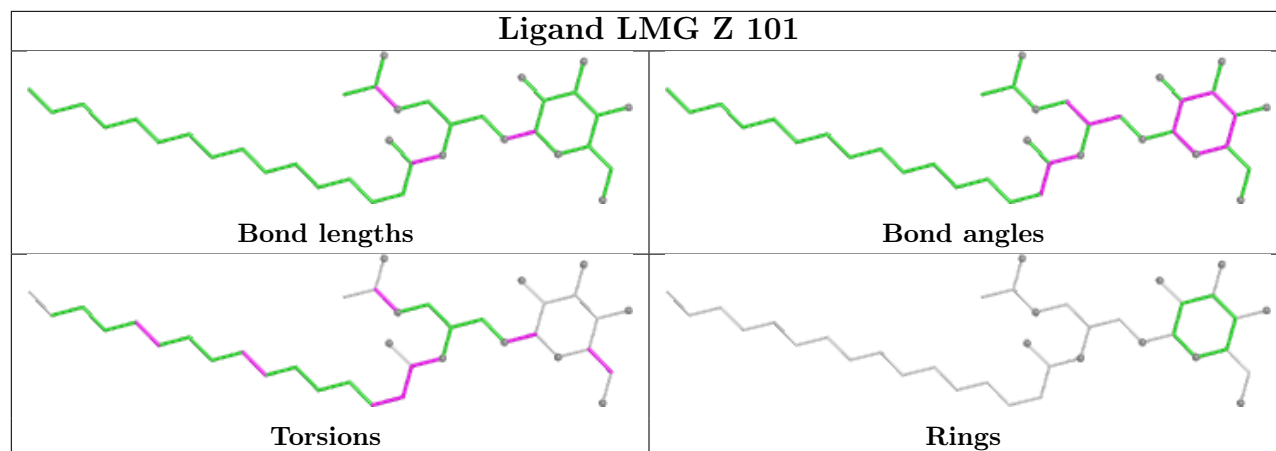
Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

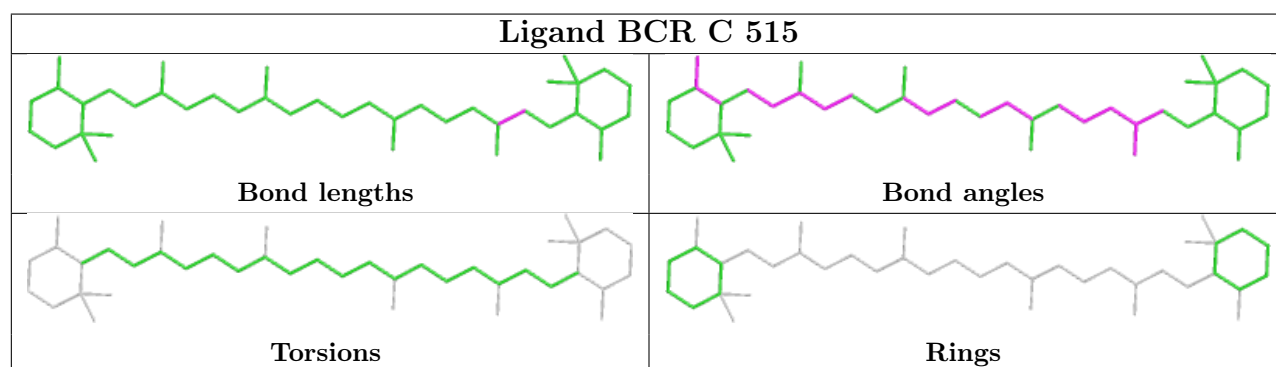
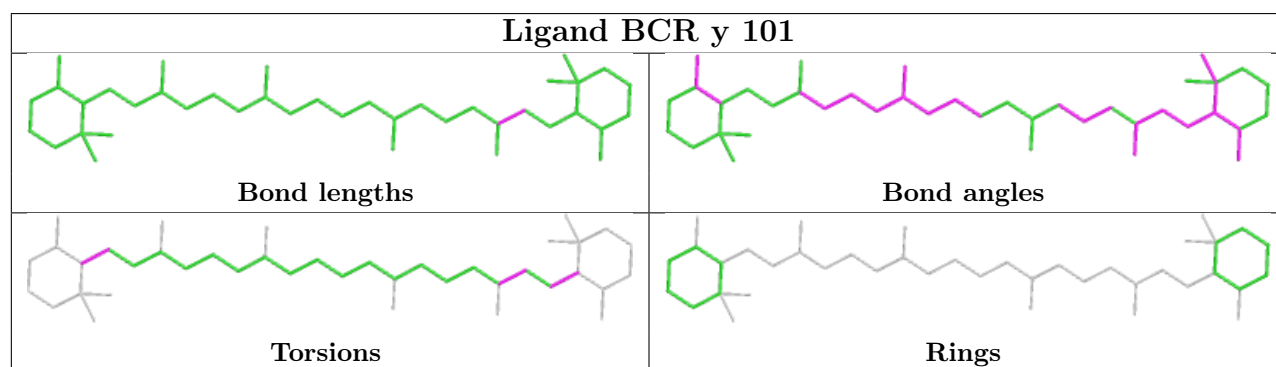
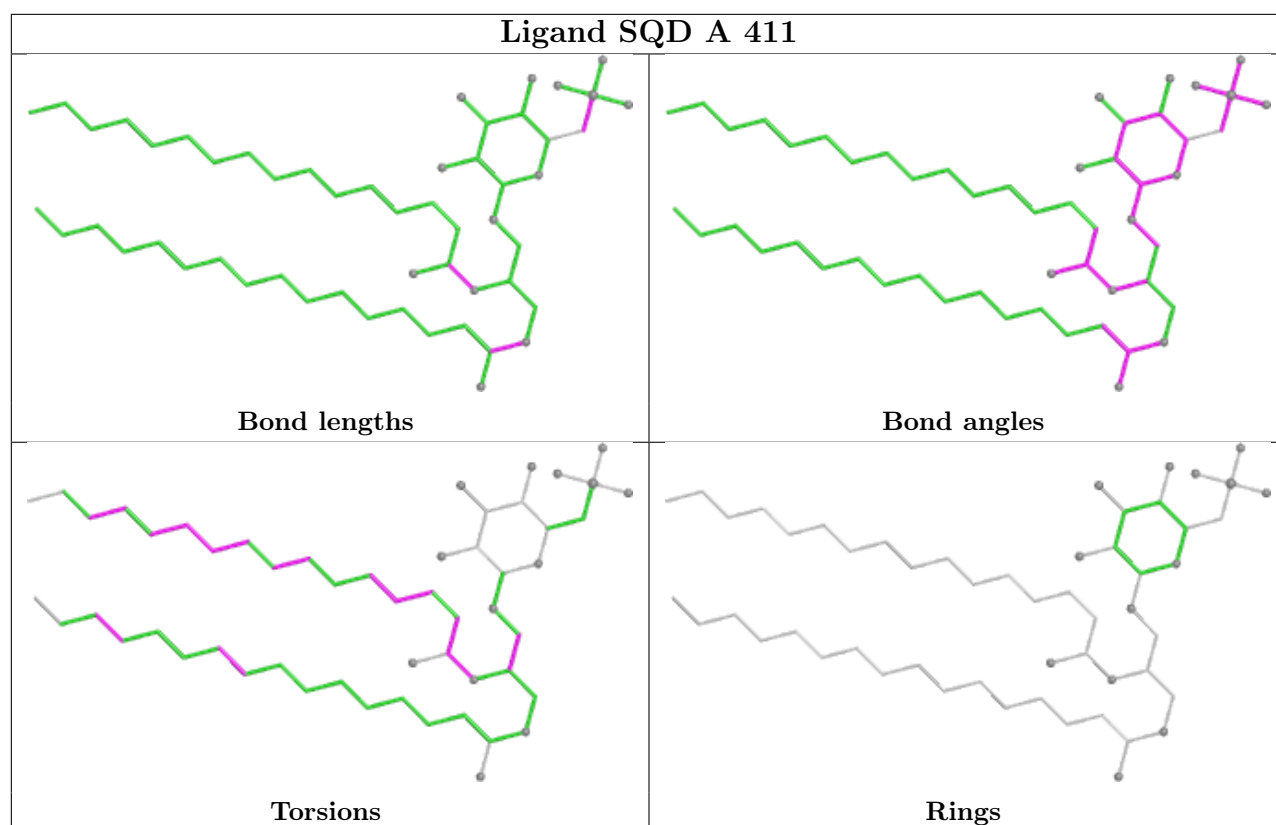
Ligand BCR A 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

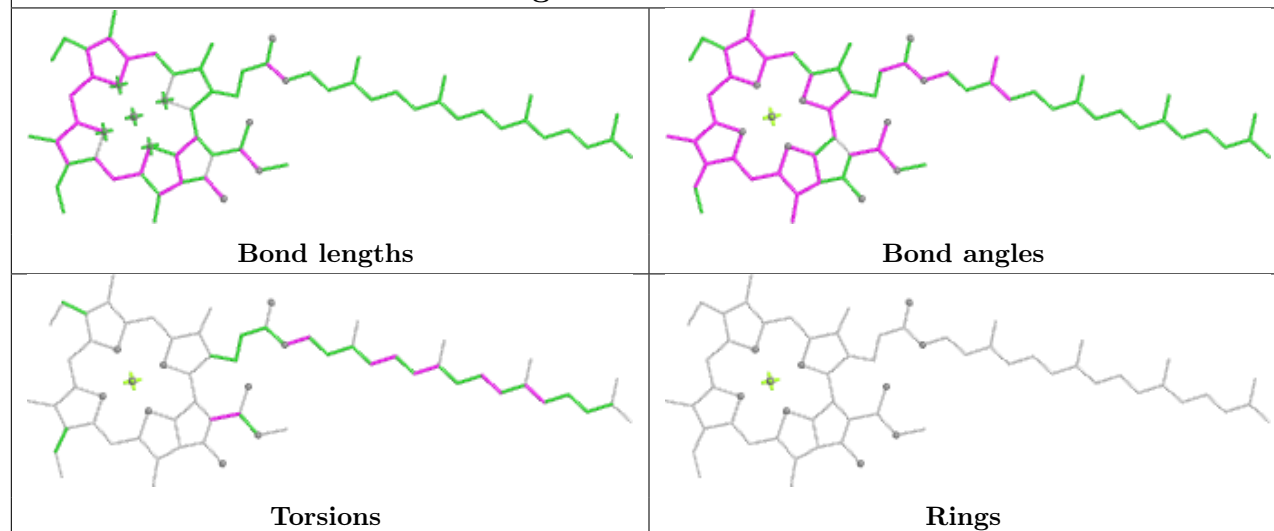
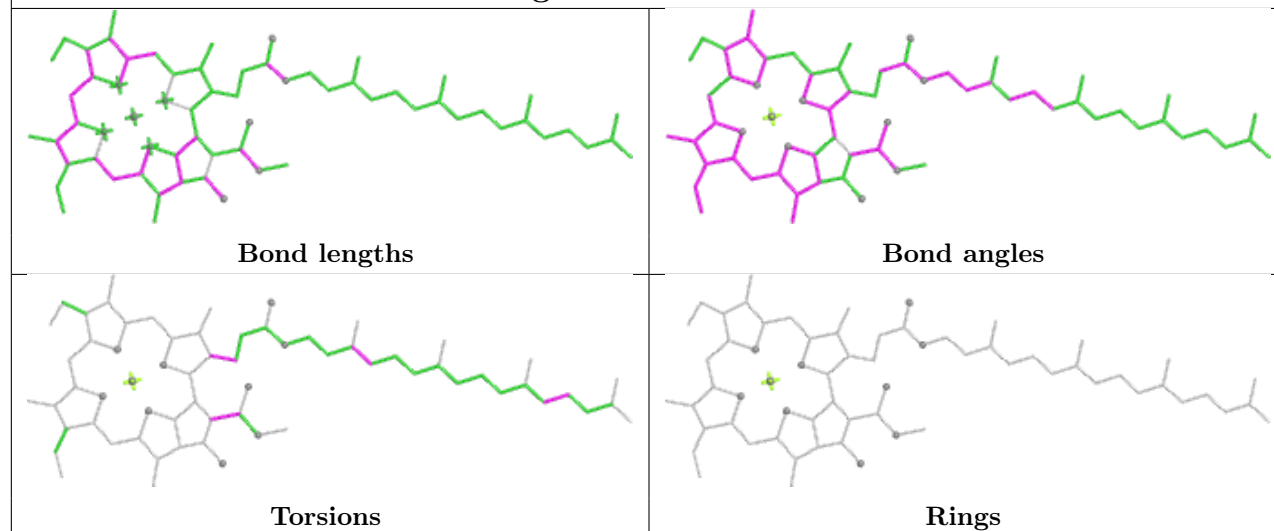
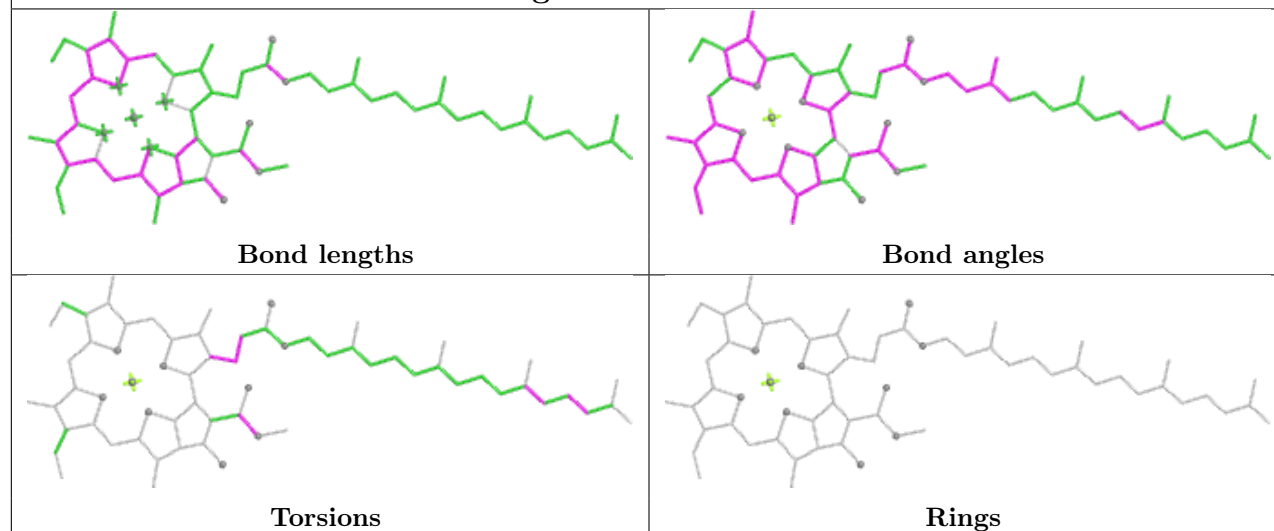
Ligand LMG z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

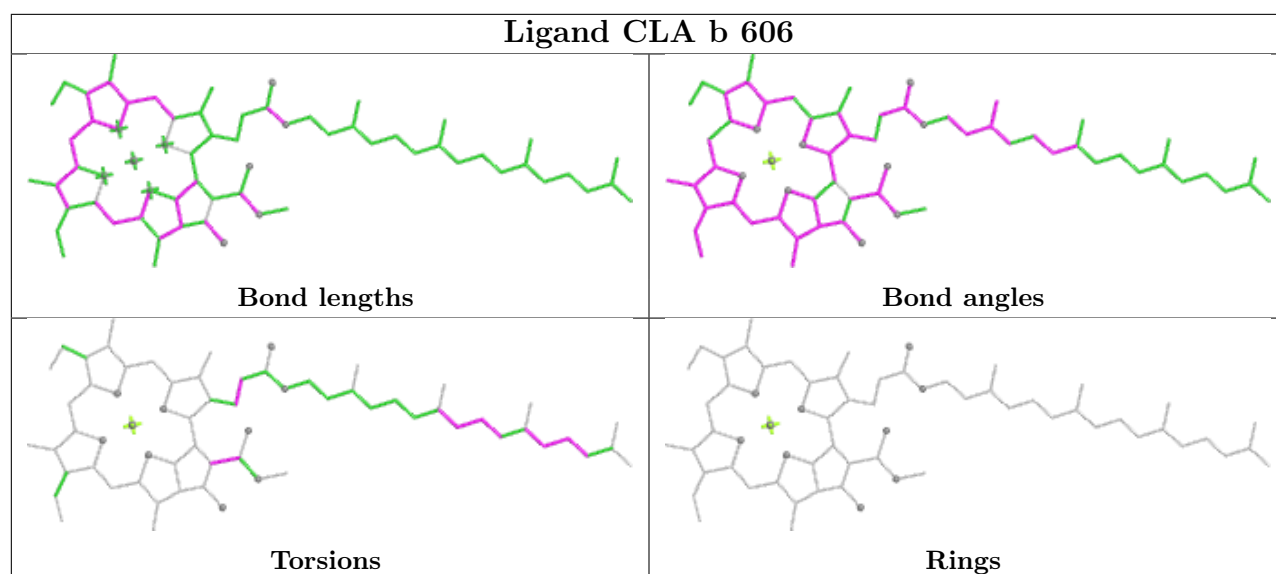
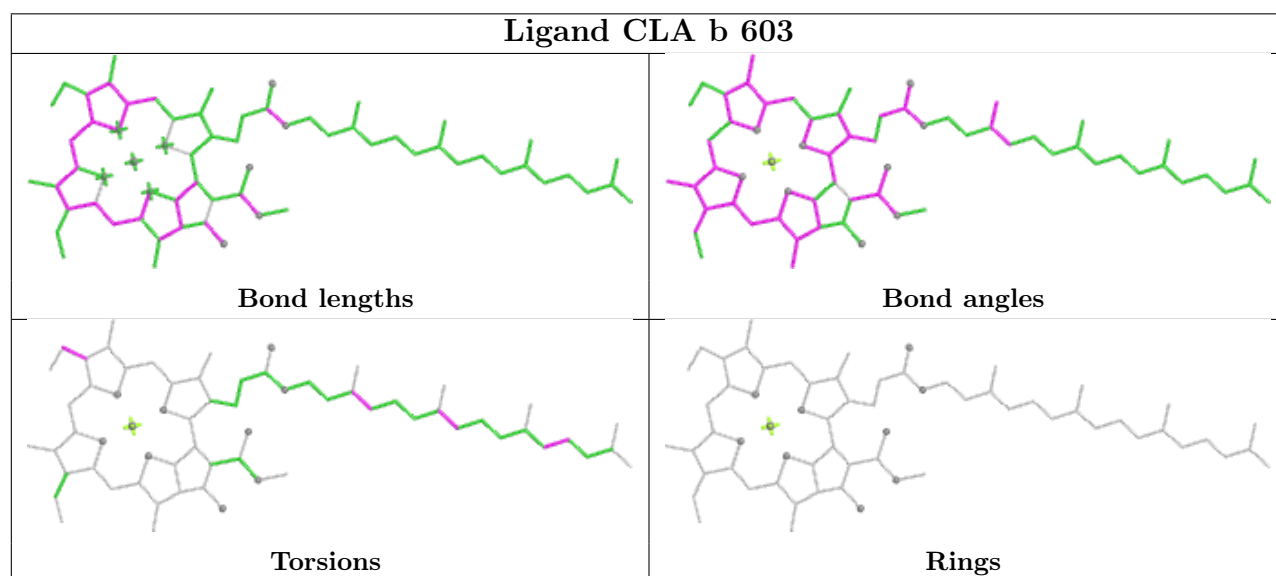
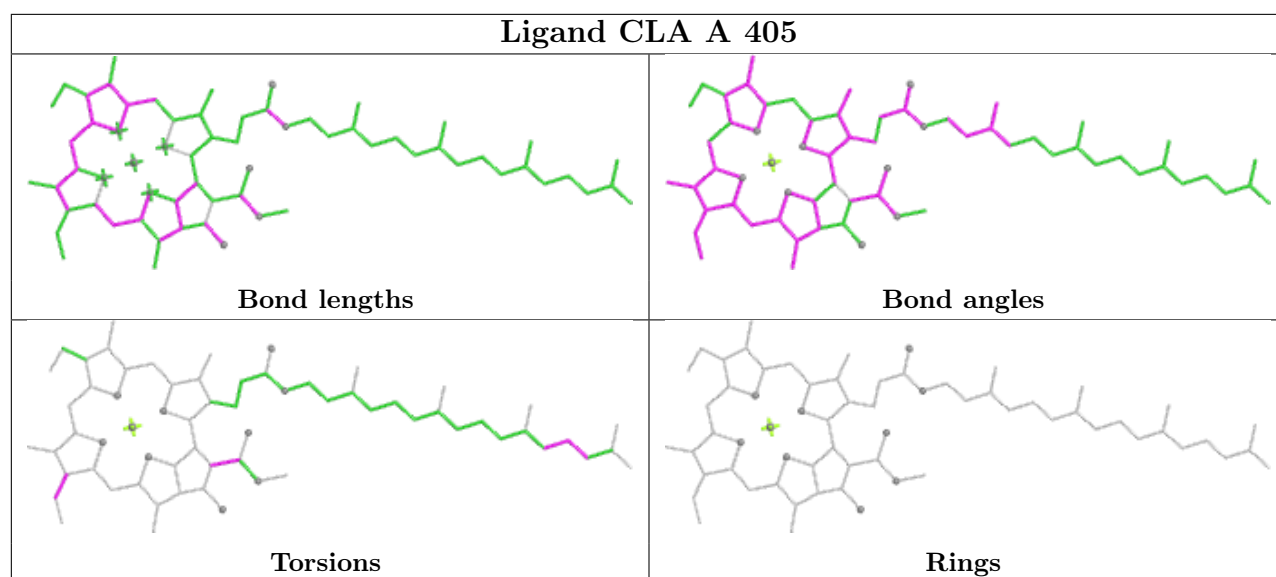




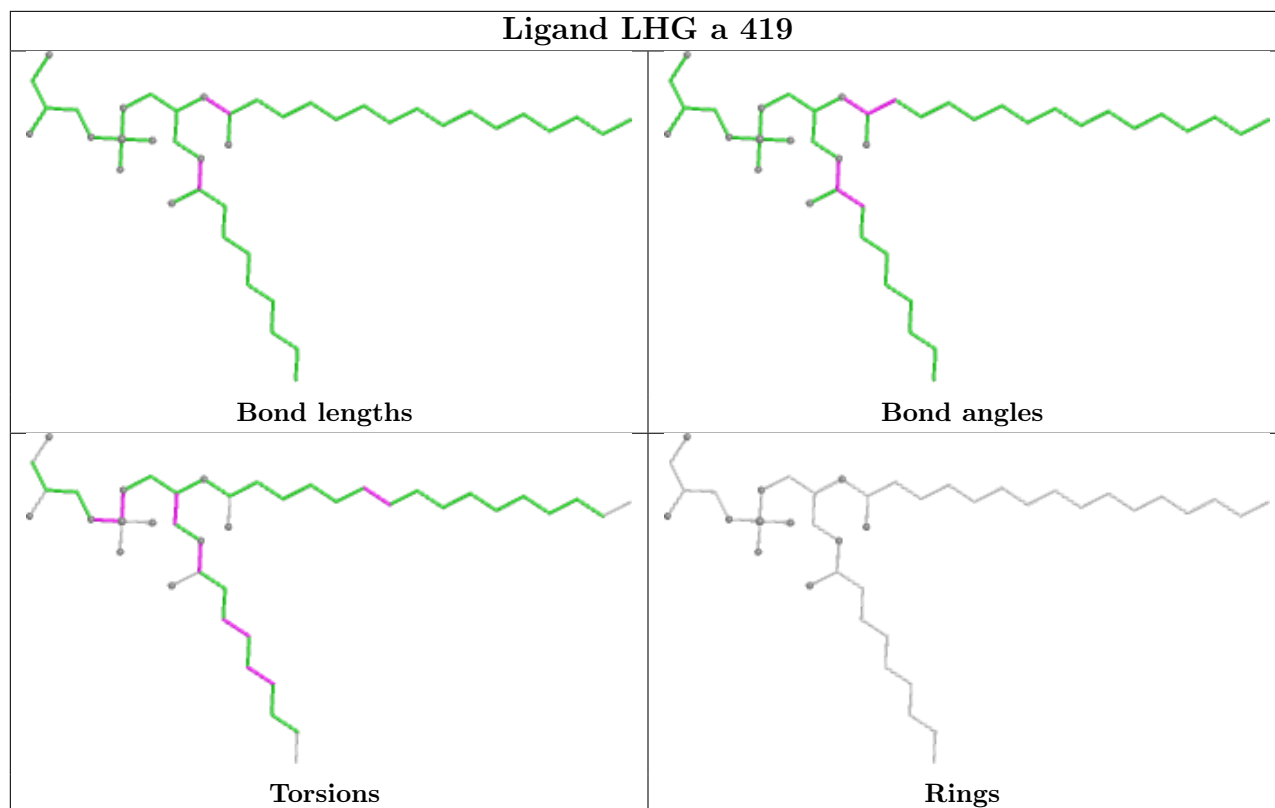




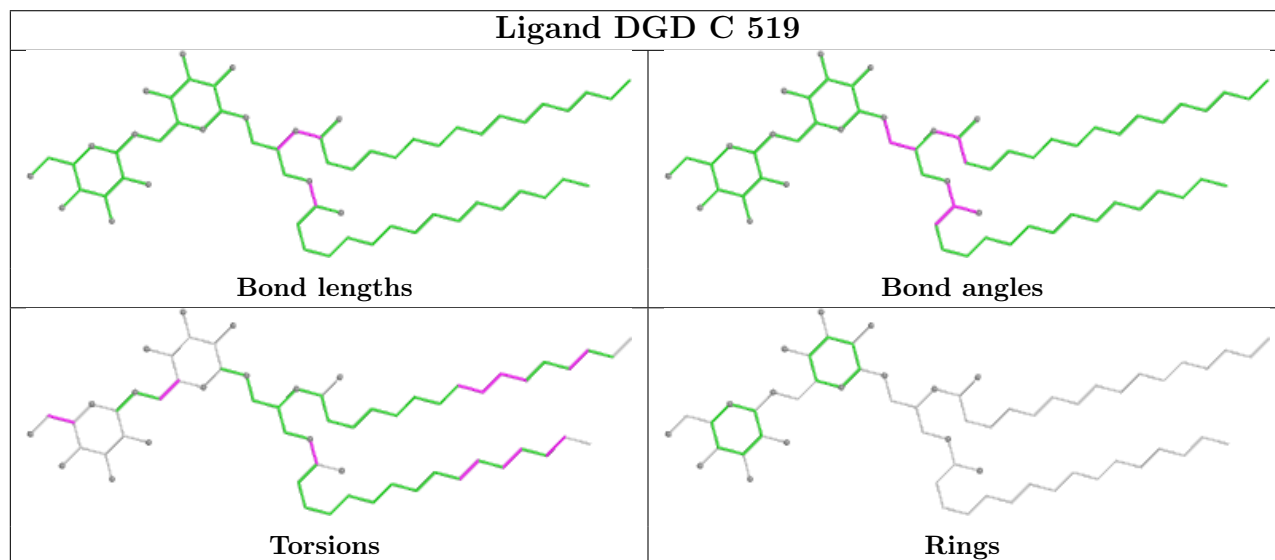
Ligand CLA B 616**Ligand CLA B 609****Ligand CLA C 502**

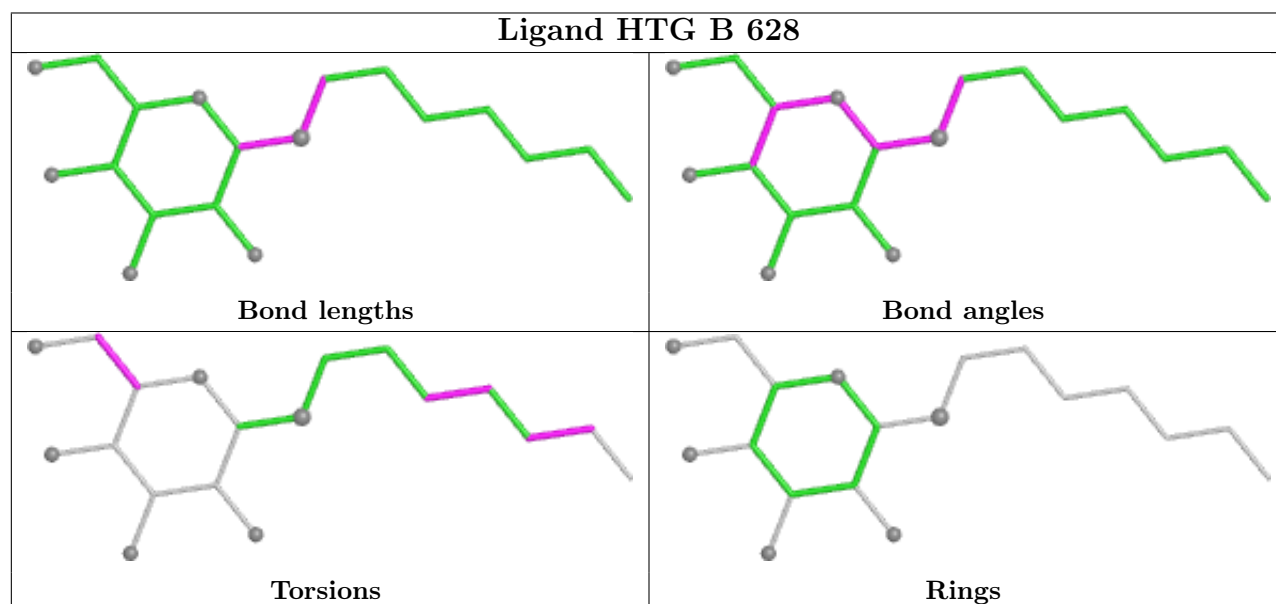
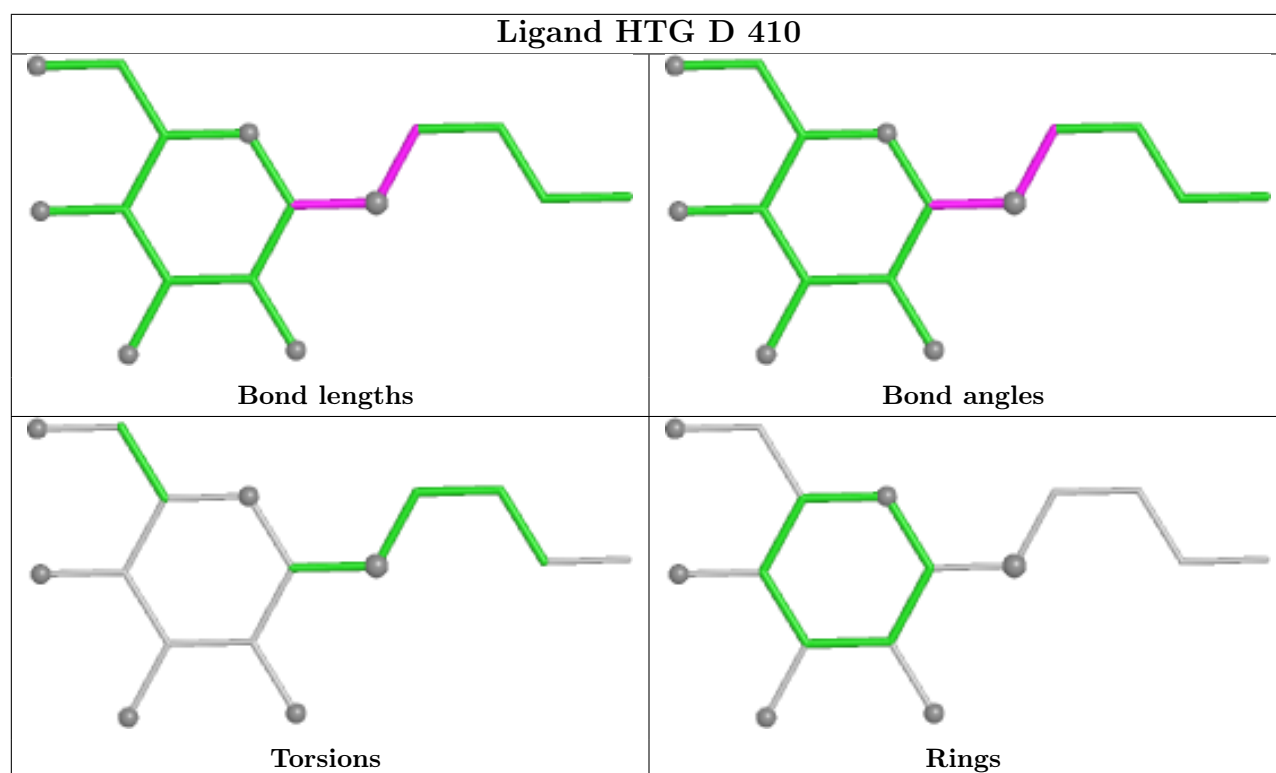


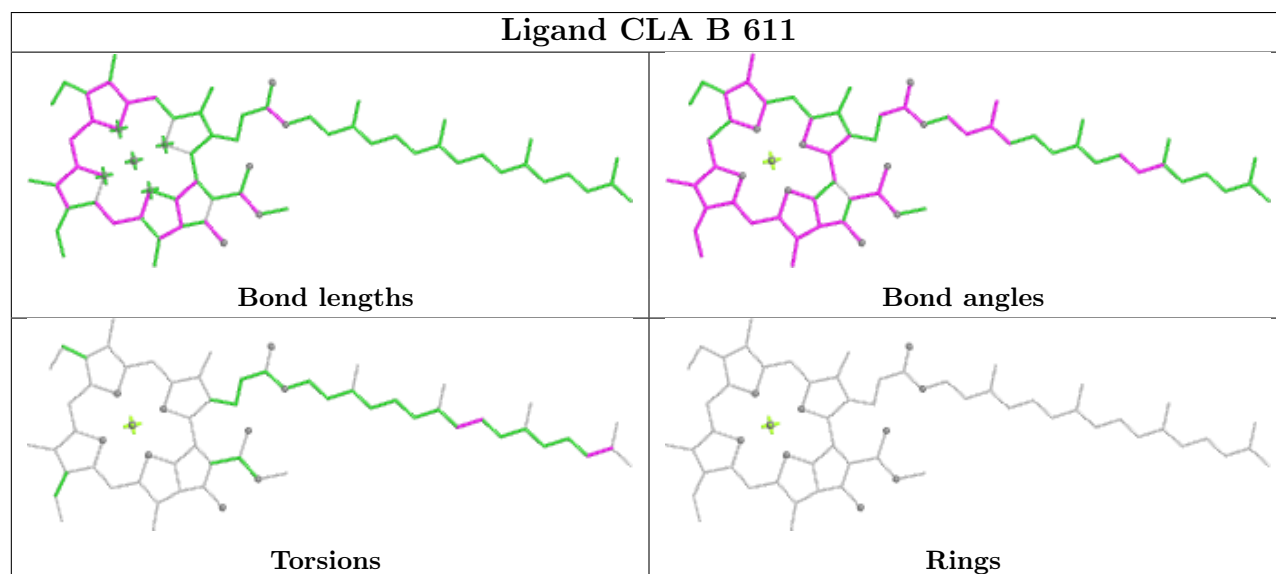
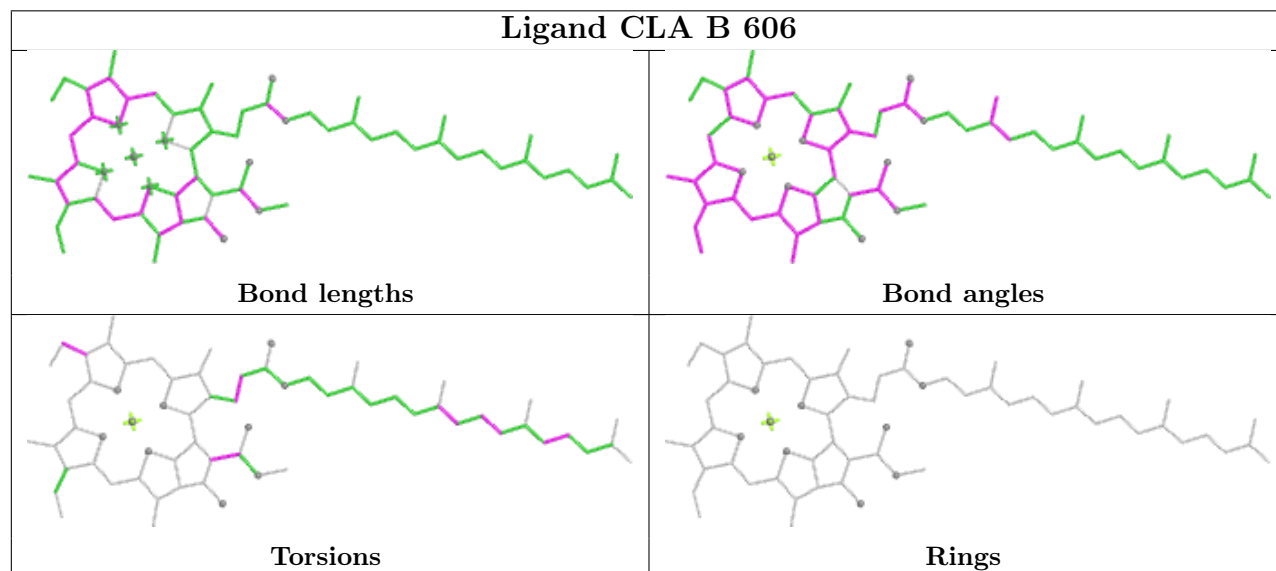
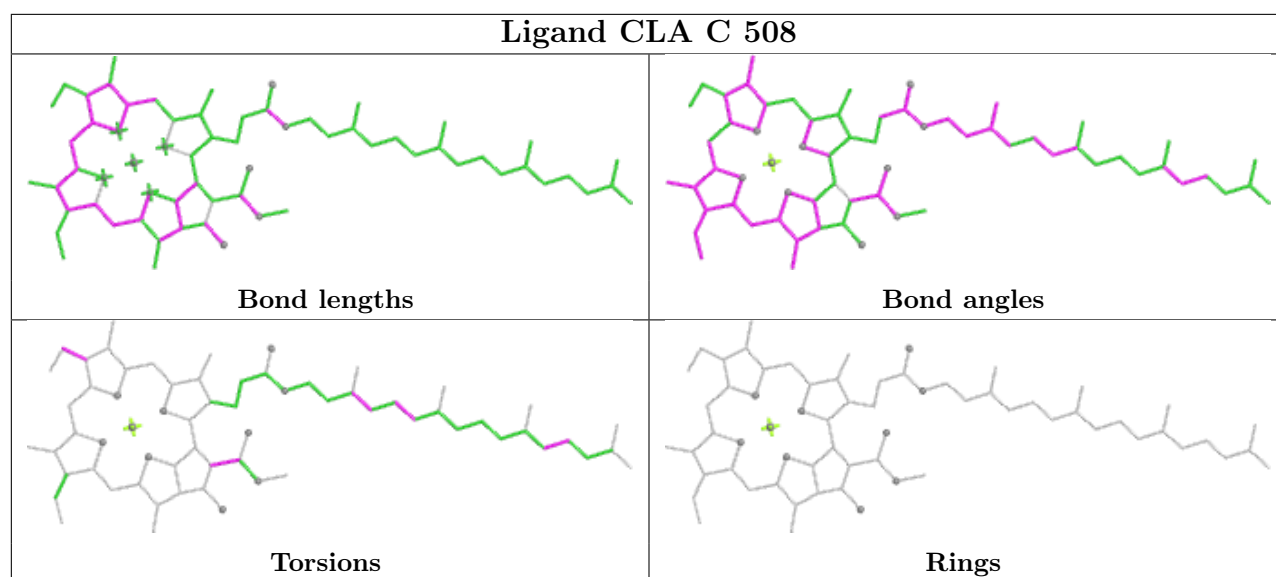
Ligand LHG a 419

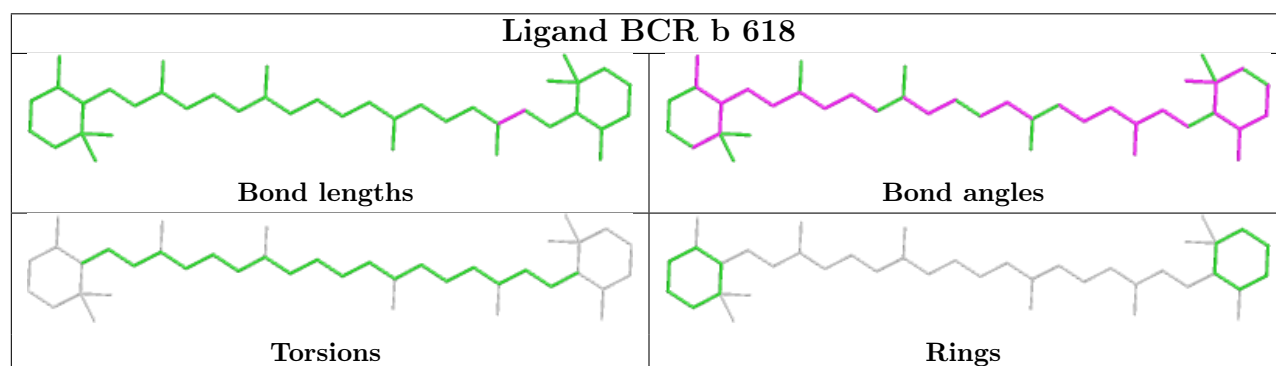
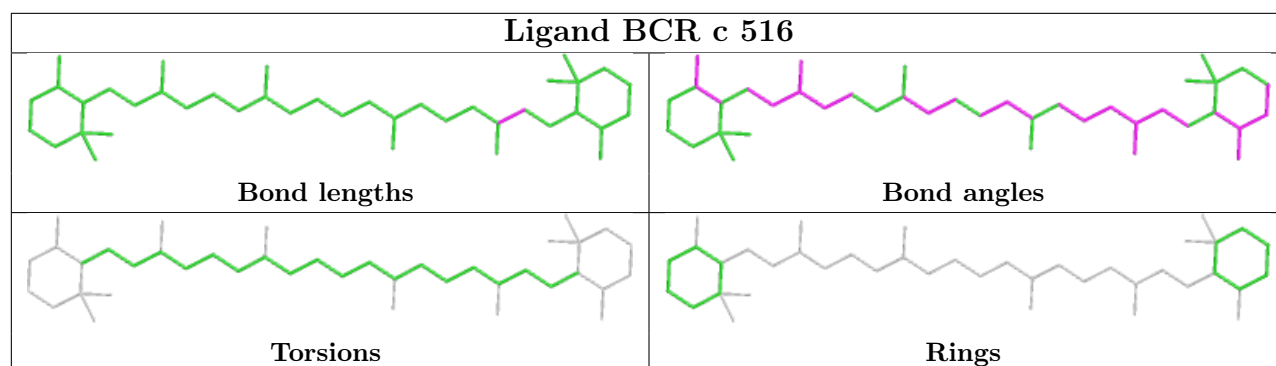
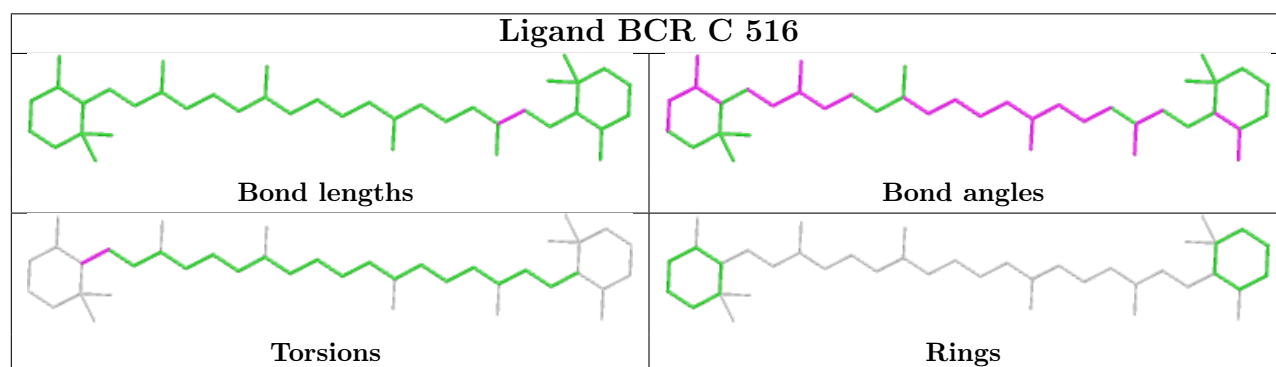
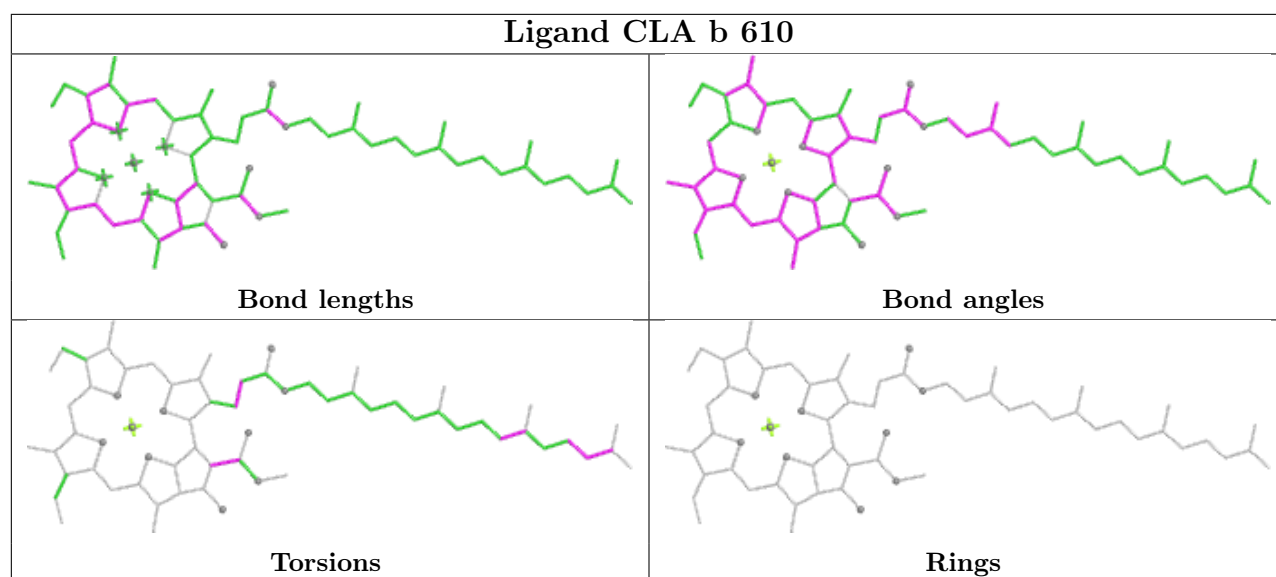


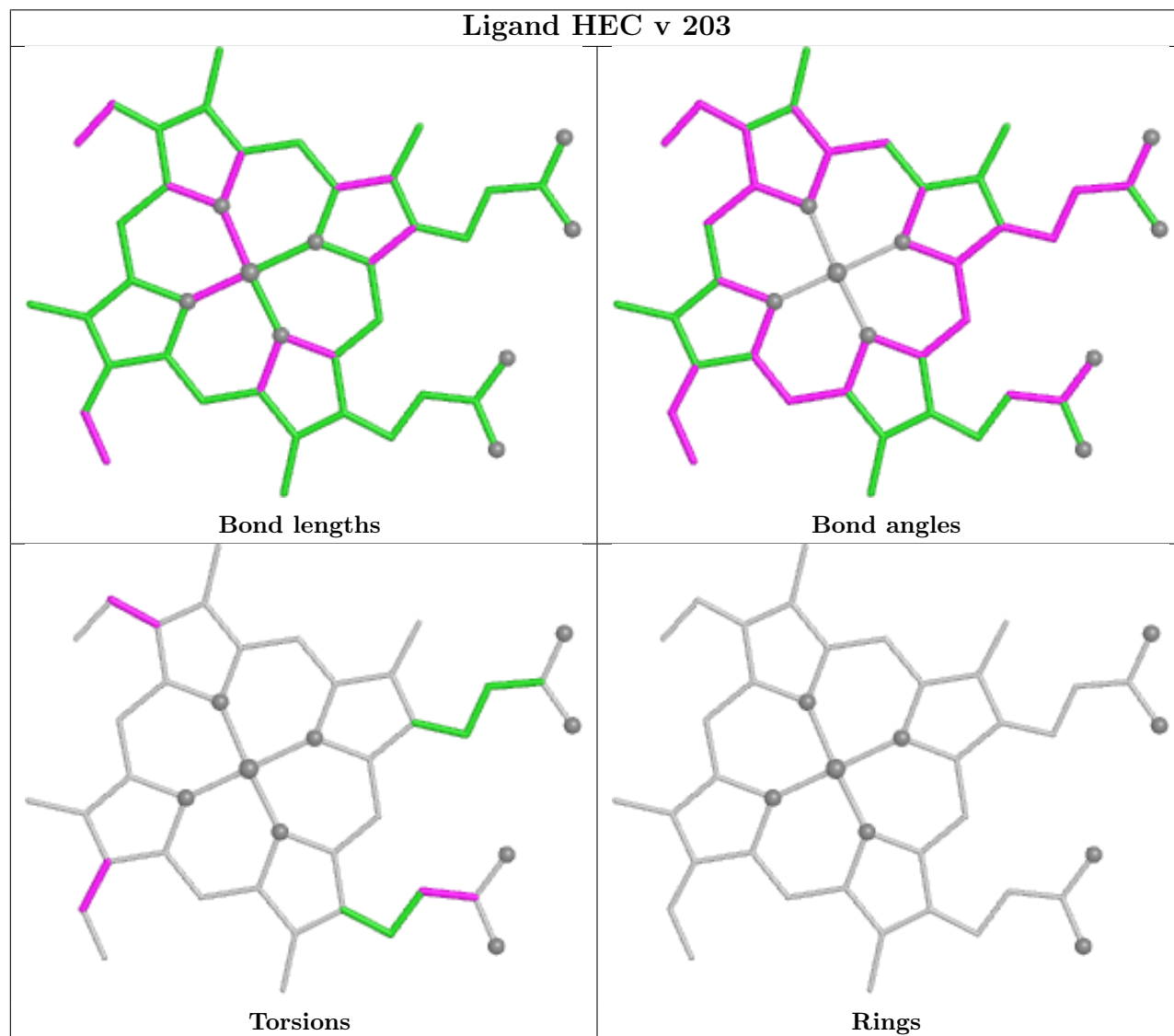
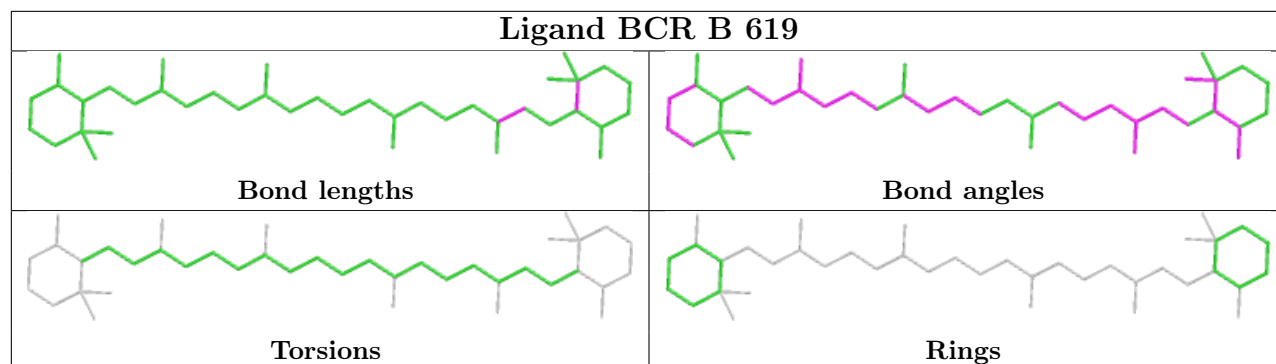
Ligand DGD C 519

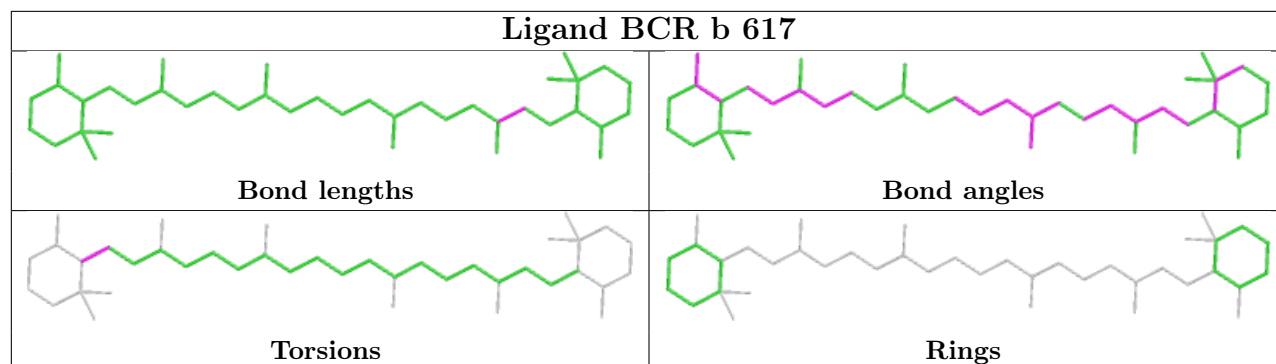
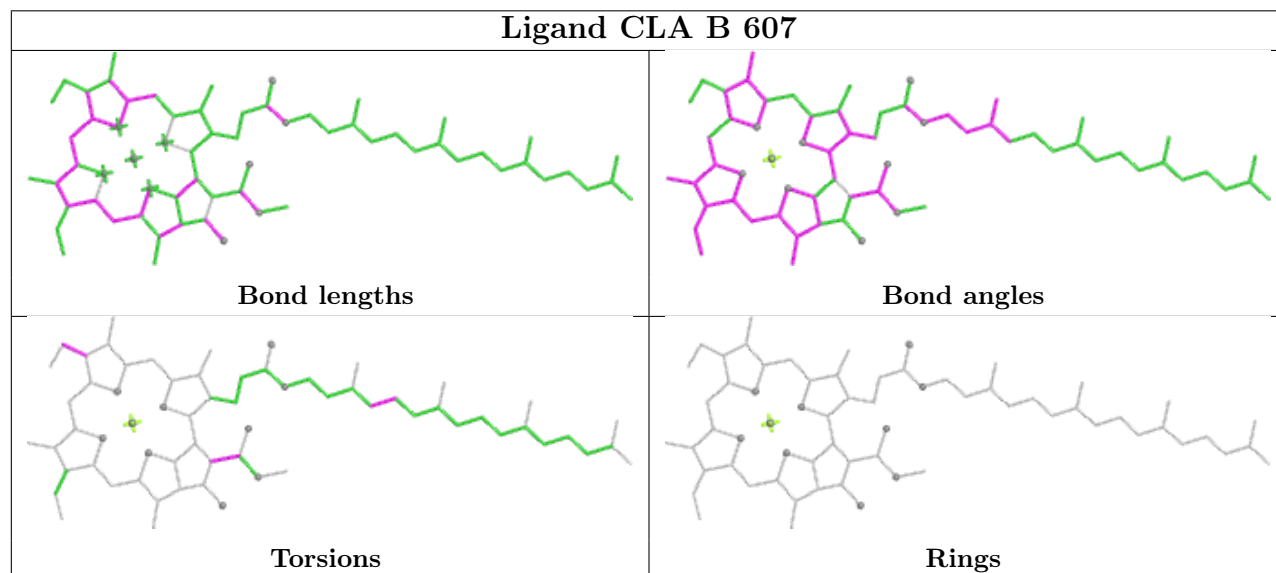
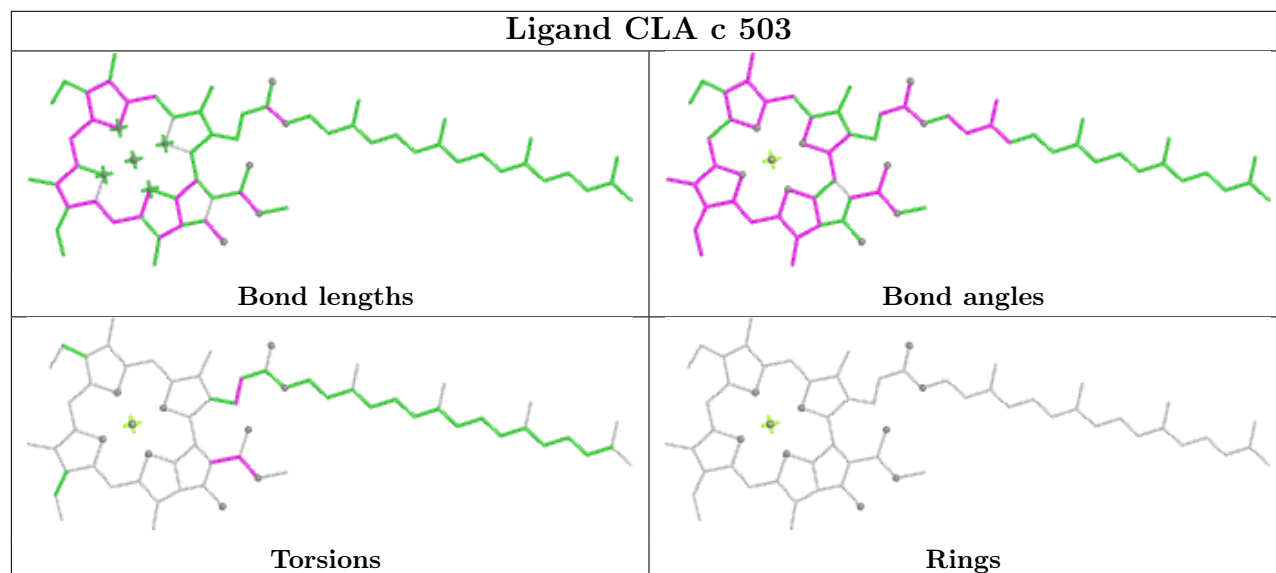


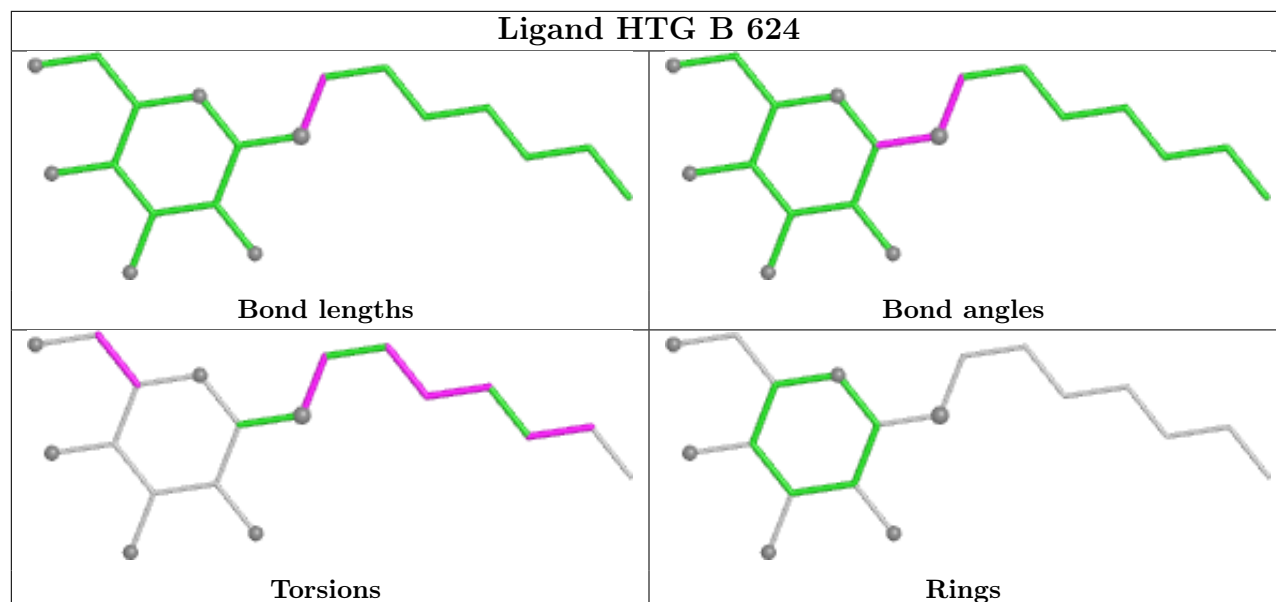
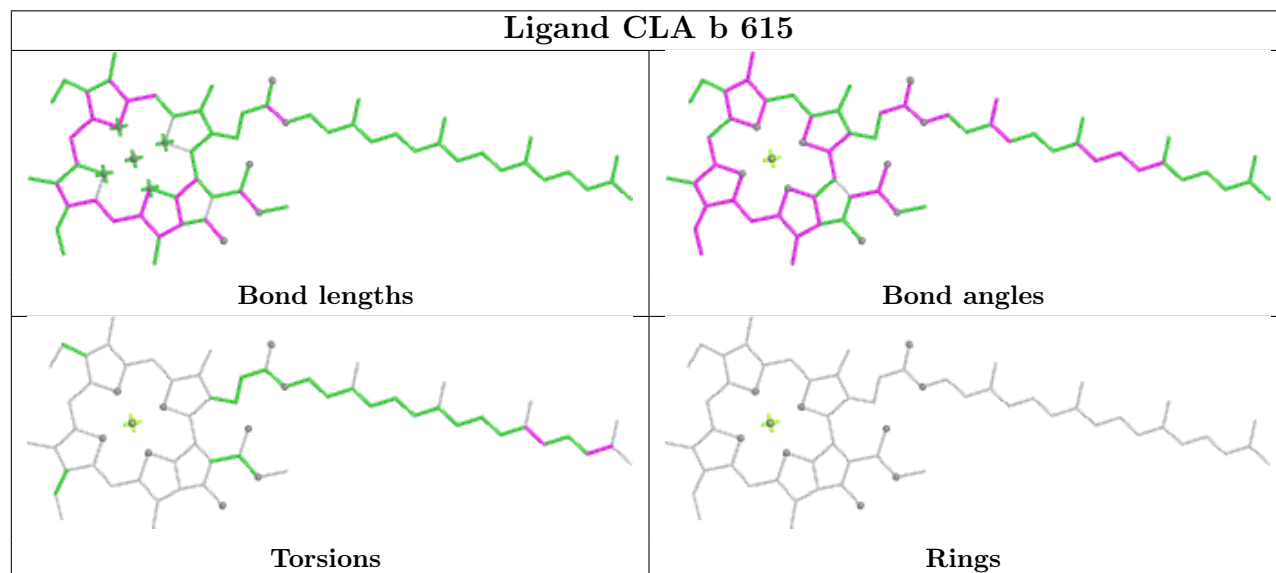
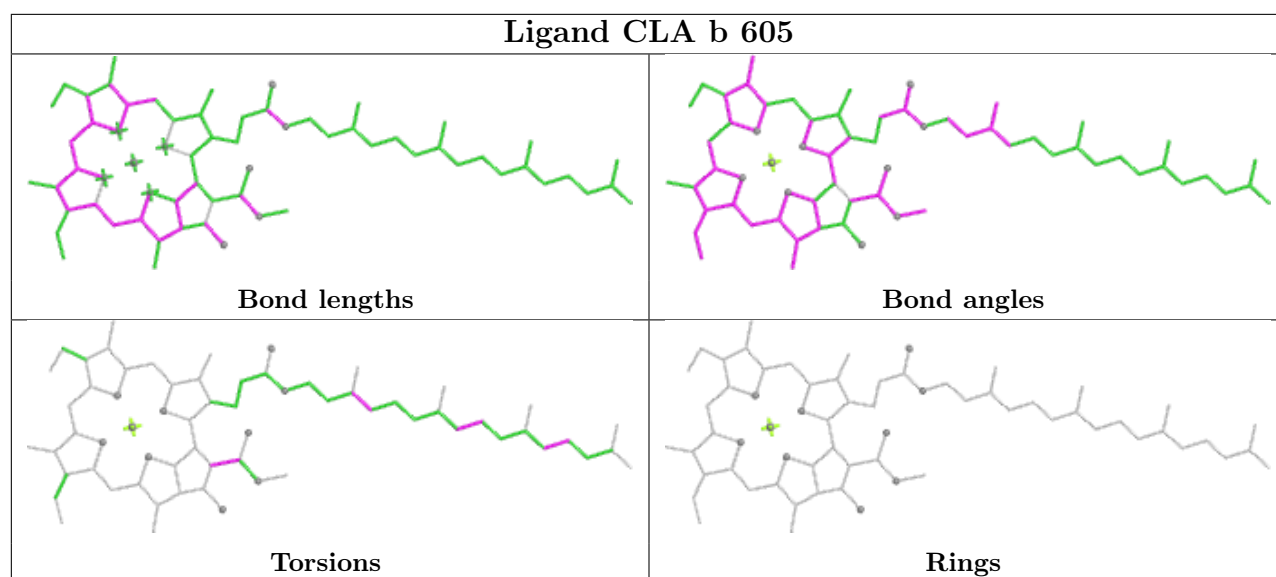


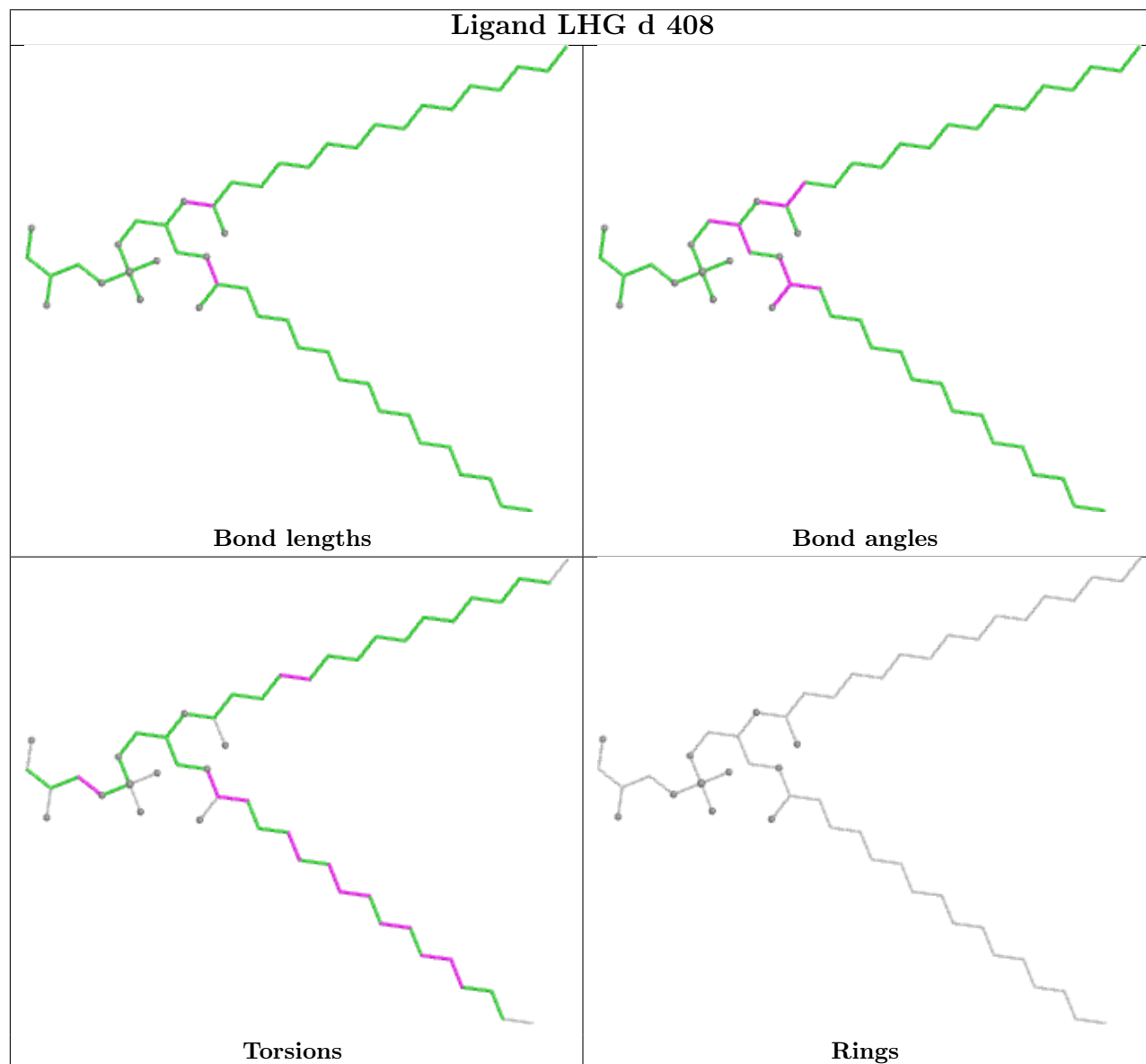
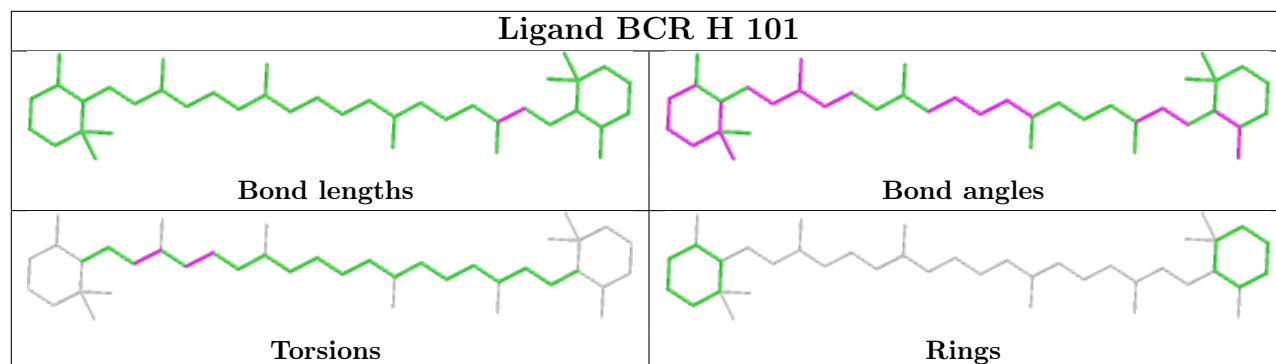




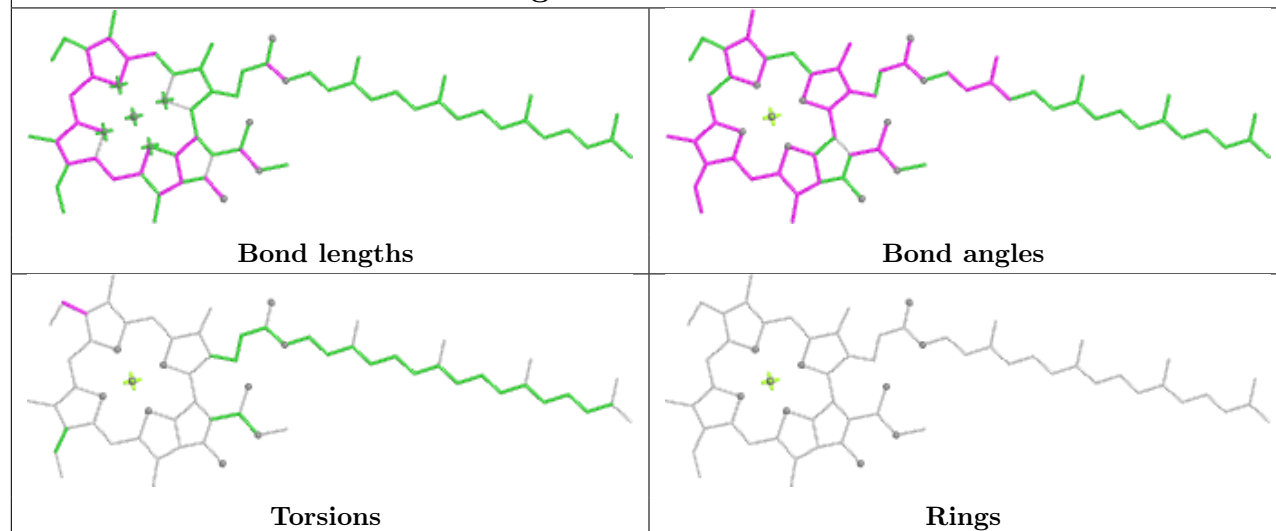


Ligand BCR b 617**Ligand CLA B 607****Ligand CLA c 503**

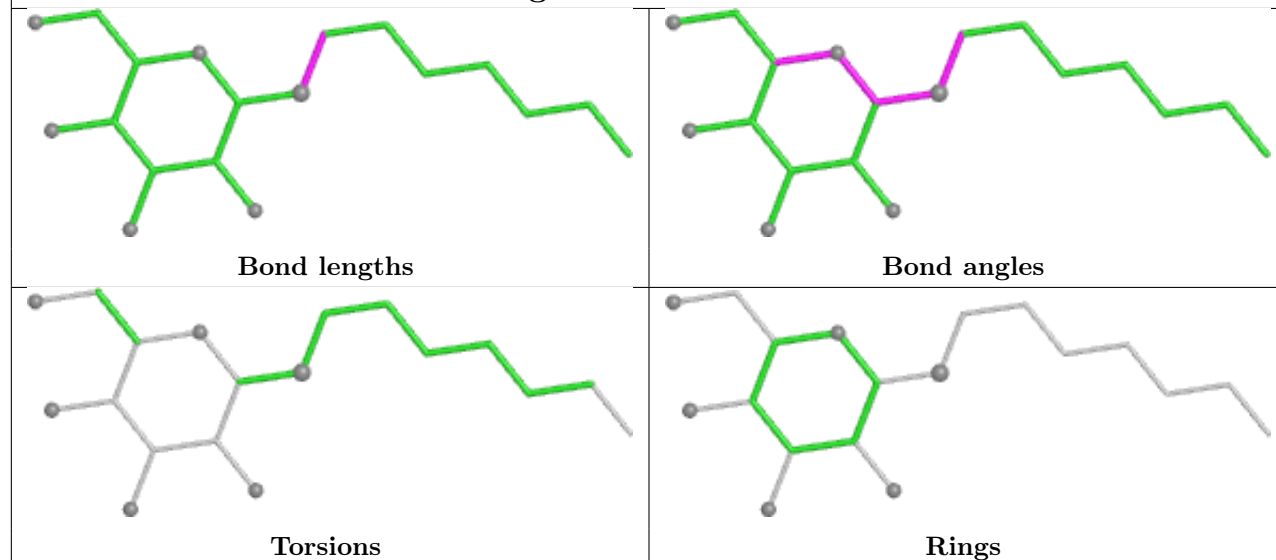




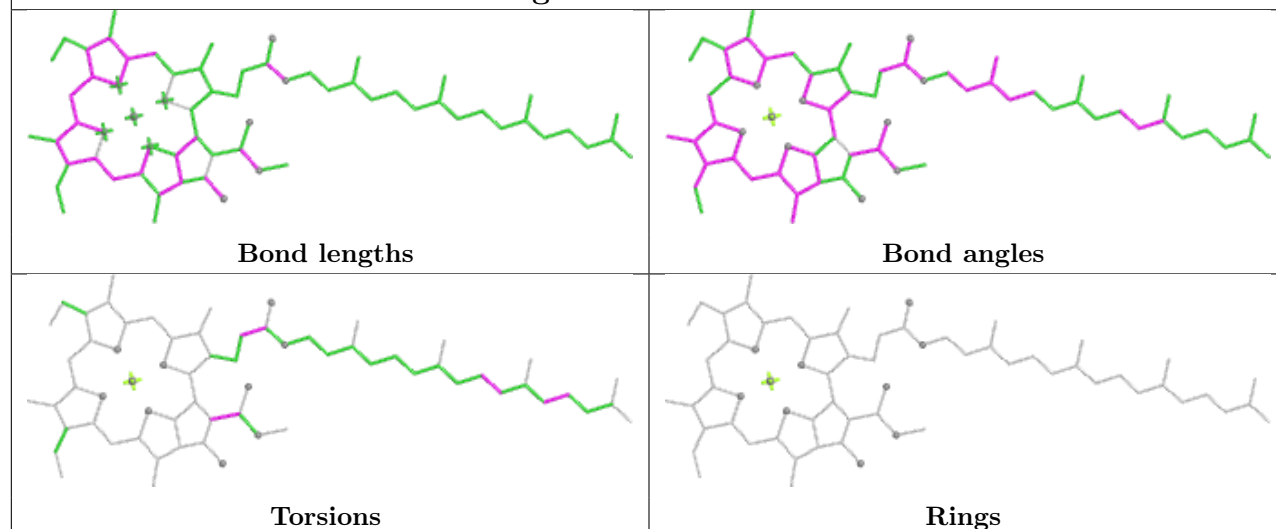
Ligand CLA D 402

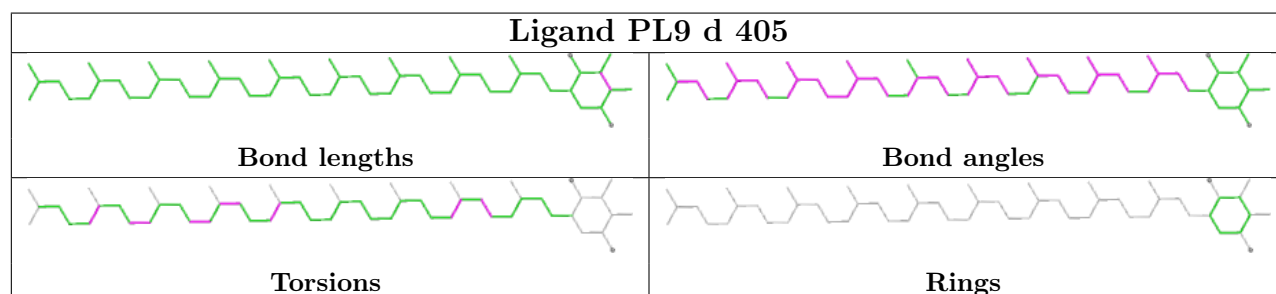
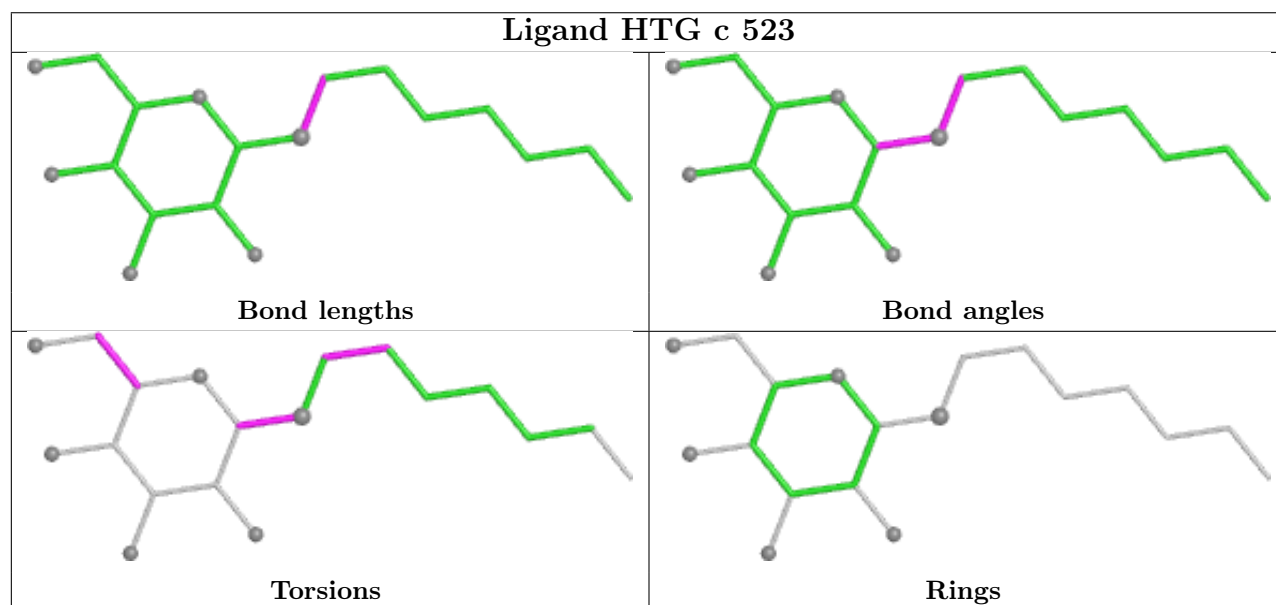
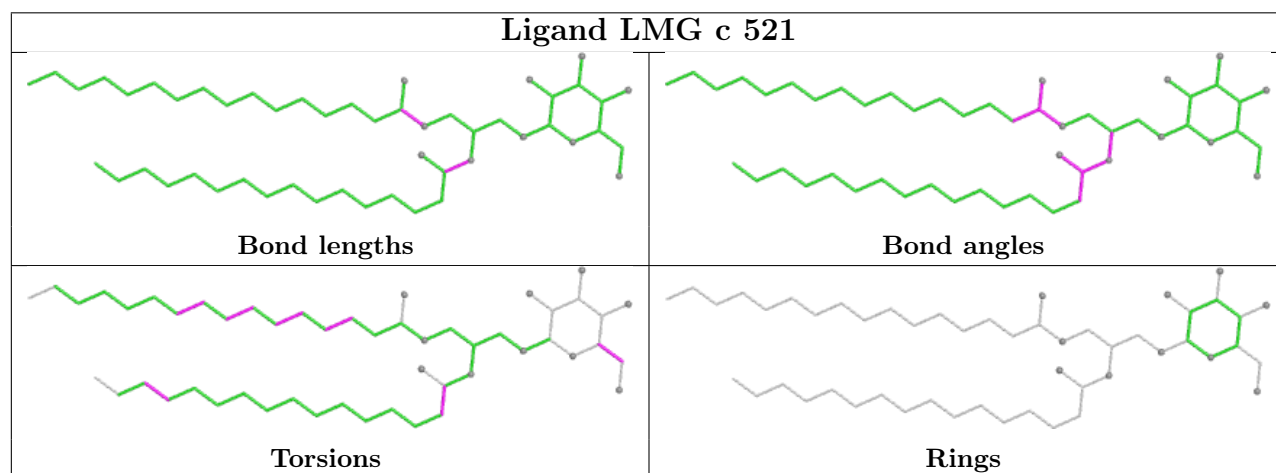
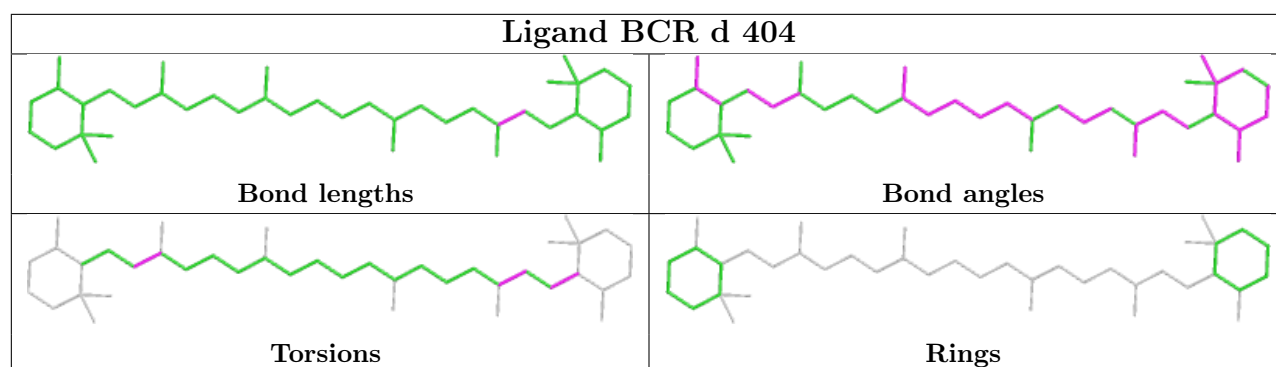


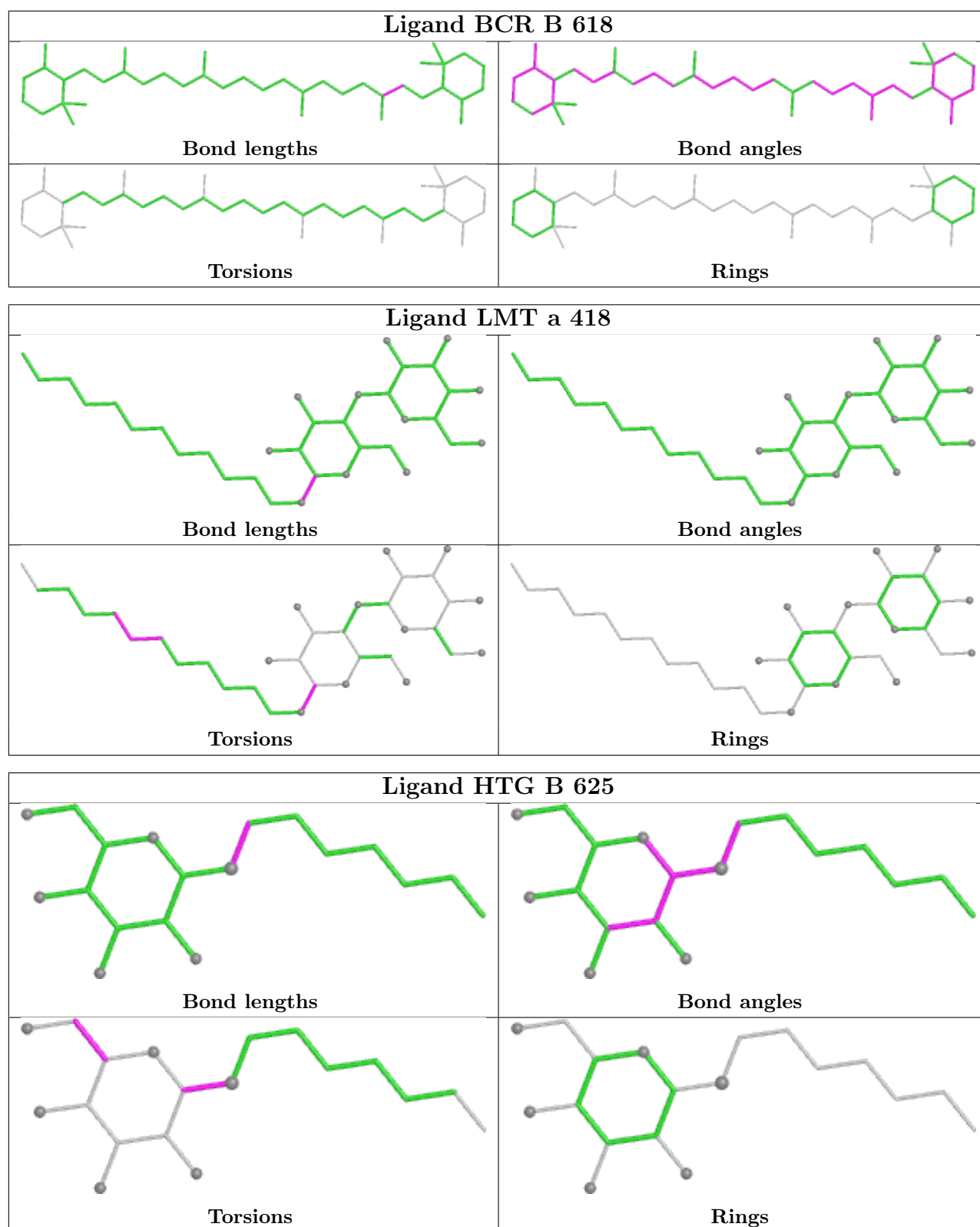
Ligand HTG C 522

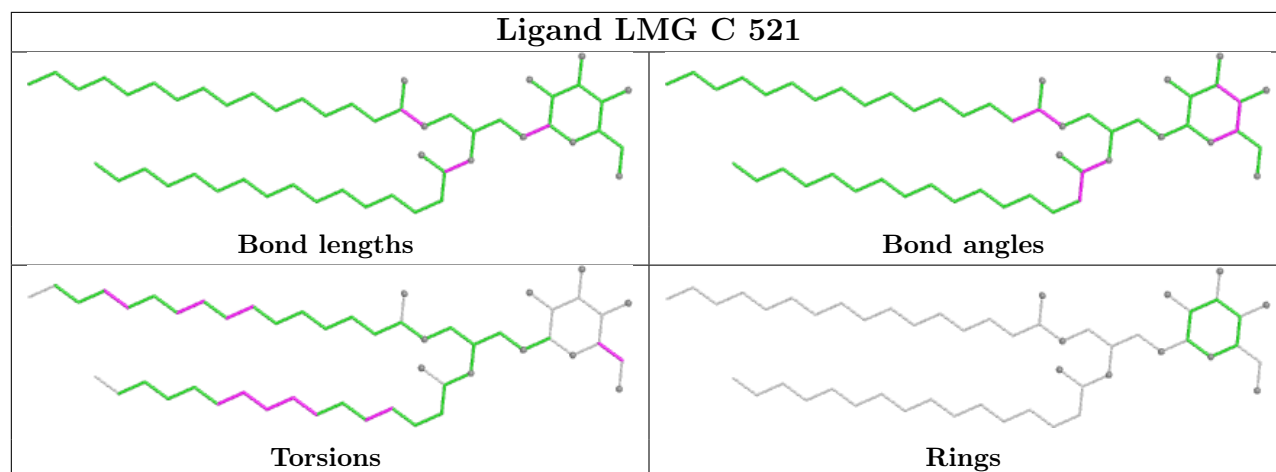
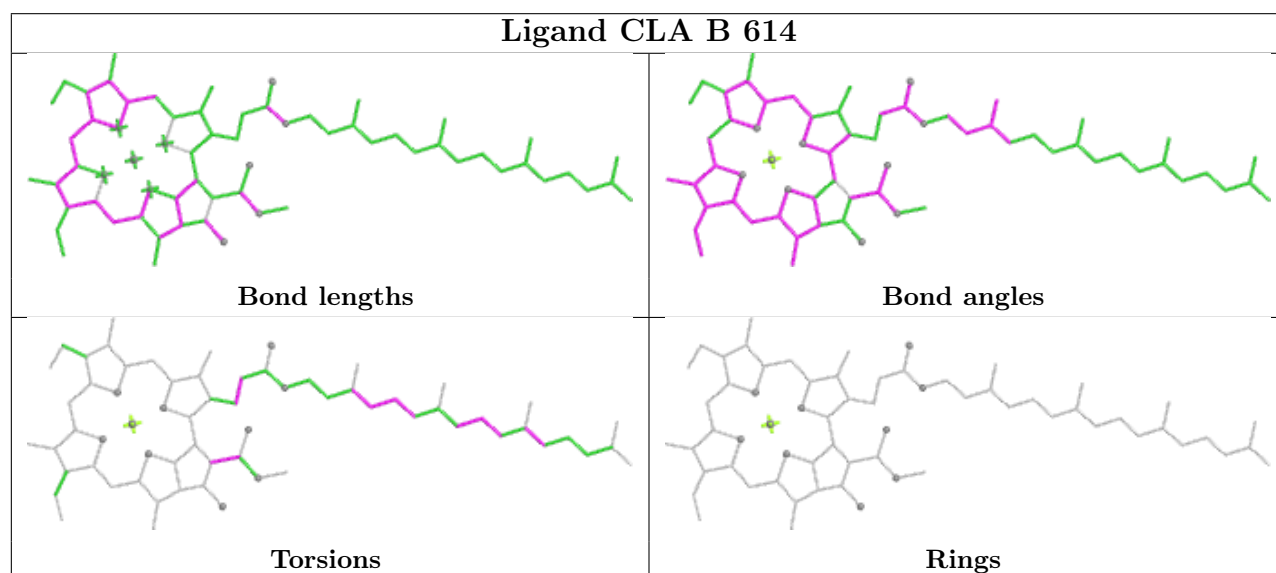
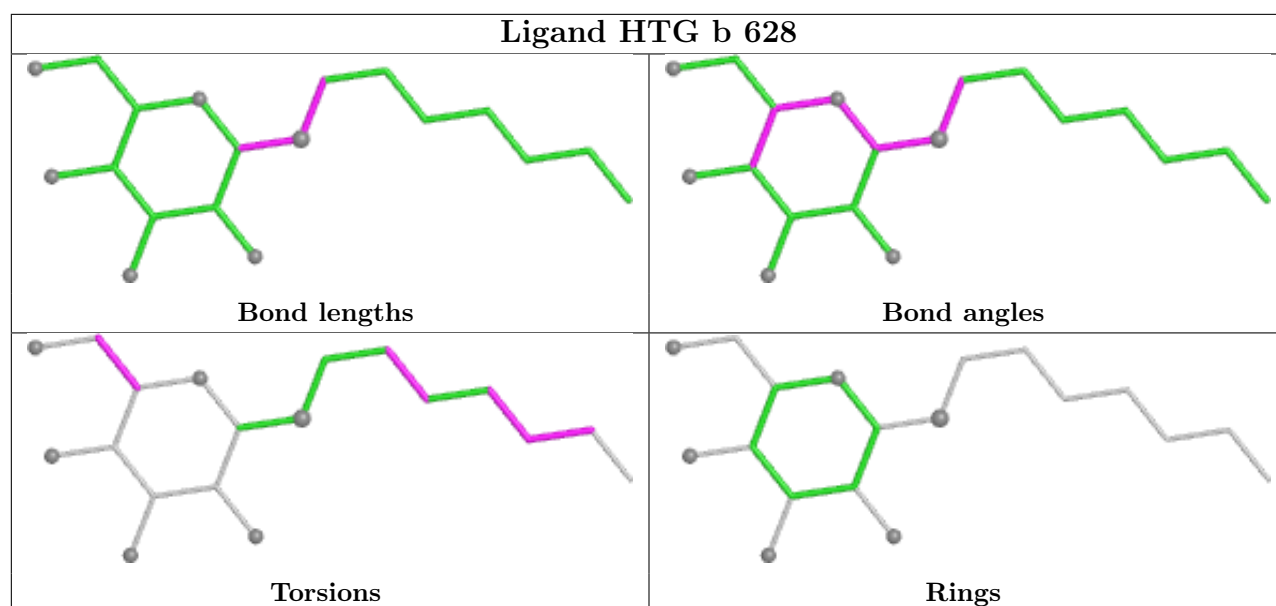


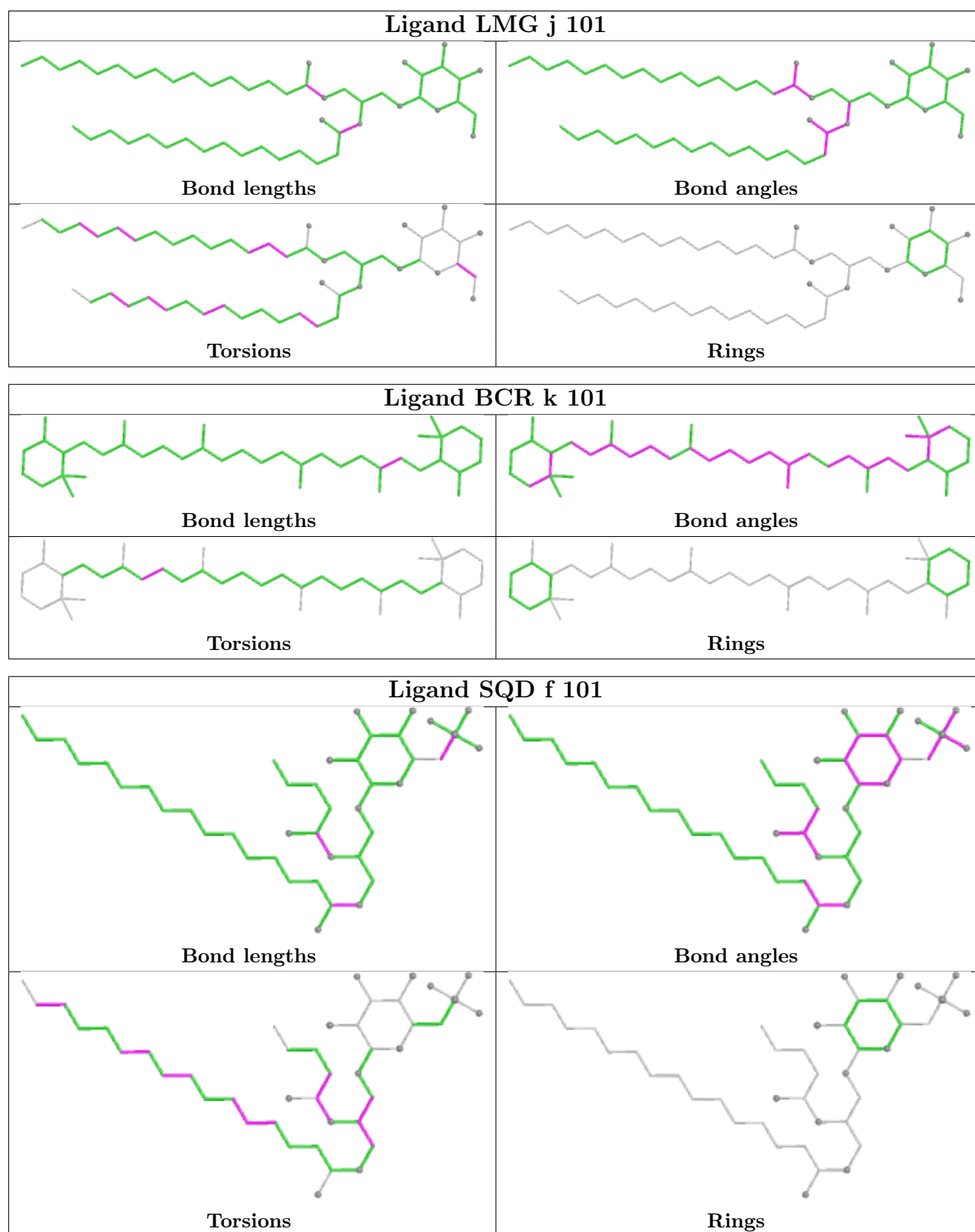
Ligand CLA B 612

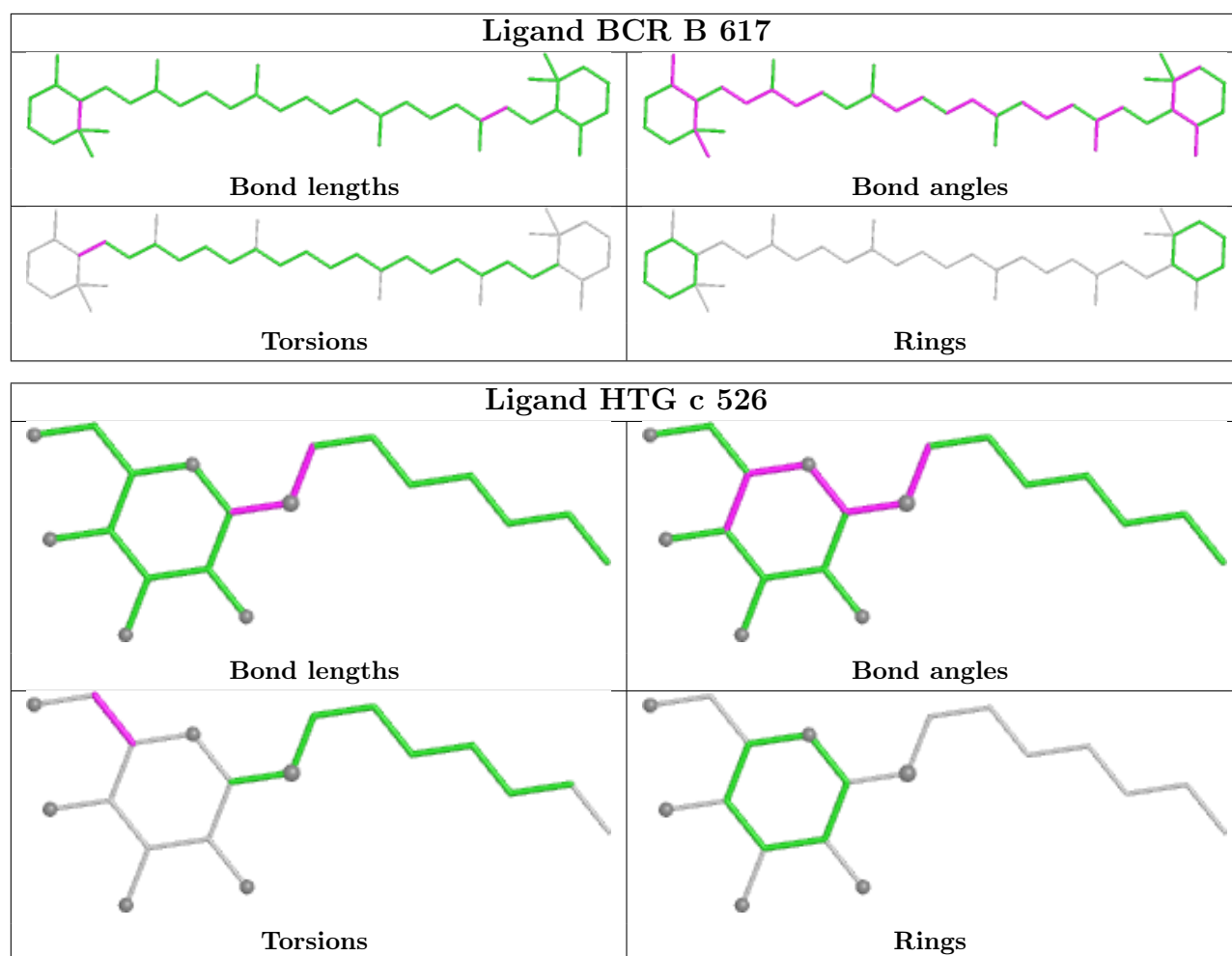












5.7 Other polymers [i](#)

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	334/344 (97%)	-0.68	0 100 100	22, 47, 68, 120	29 (8%)
1	a	334/344 (97%)	-0.62	0 100 100	23, 51, 82, 120	29 (8%)
2	B	504/505 (99%)	-0.60	2 (0%) 88 91	30, 53, 83, 128	8 (1%)
2	b	504/505 (99%)	-0.53	2 (0%) 88 91	35, 57, 97, 149	4 (0%)
3	C	451/455 (99%)	-0.59	0 100 100	23, 59, 80, 142	10 (2%)
3	c	455/455 (100%)	-0.48	0 100 100	26, 67, 89, 129	10 (2%)
4	D	342/342 (100%)	-0.73	0 100 100	23, 49, 68, 139	3 (0%)
4	d	341/342 (99%)	-0.67	0 100 100	24, 55, 78, 147	3 (0%)
5	E	81/84 (96%)	-0.23	0 100 100	53, 70, 100, 151	1 (1%)
5	e	79/84 (94%)	-0.12	1 (1%) 75 79	62, 78, 122, 140	0
6	F	34/44 (77%)	-0.46	0 100 100	52, 63, 90, 117	0
6	f	31/44 (70%)	-0.22	2 (6%) 25 28	62, 68, 100, 140	0
7	H	64/65 (98%)	-0.44	1 (1%) 70 76	33, 62, 81, 129	1 (1%)
7	h	64/65 (98%)	-0.37	1 (1%) 70 76	58, 69, 95, 147	0
8	I	37/38 (97%)	-0.30	0 100 100	55, 62, 127, 147	0
8	i	37/38 (97%)	-0.24	1 (2%) 56 63	57, 66, 123, 138	0
9	J	38/39 (97%)	-0.20	0 100 100	51, 71, 129, 175	0
9	j	39/39 (100%)	0.00	0 100 100	56, 80, 149, 175	0
10	K	37/37 (100%)	-0.43	0 100 100	60, 67, 89, 101	0
10	k	37/37 (100%)	-0.34	0 100 100	70, 77, 101, 117	0
11	L	36/37 (97%)	-0.60	0 100 100	27, 47, 109, 162	1 (2%)
11	l	36/37 (97%)	-0.64	0 100 100	28, 48, 103, 152	1 (2%)
12	M	32/36 (88%)	-0.55	0 100 100	28, 49, 74, 134	1 (3%)
12	m	33/36 (91%)	-0.58	0 100 100	43, 50, 86, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	36, 63, 115, 176	5 (2%)
13	o	243/244 (99%)	-0.44	0 100 100	34, 65, 121, 161	2 (0%)
14	T	29/32 (90%)	-0.65	1 (3%) 48 55	42, 49, 81, 115	0
14	t	29/32 (90%)	-0.64	1 (3%) 48 55	43, 50, 81, 130	0
15	U	96/104 (92%)	-0.62	0 100 100	47, 60, 90, 101	0
15	u	97/104 (93%)	-0.62	0 100 100	51, 62, 84, 121	0
16	V	137/137 (100%)	-0.66	0 100 100	46, 57, 82, 112	0
16	v	137/137 (100%)	-0.48	0 100 100	52, 71, 104, 137	0
17	X	38/40 (95%)	-0.23	0 100 100	59, 71, 96, 126	0
17	x	38/40 (95%)	0.00	0 100 100	65, 78, 117, 154	0
18	Y	29/30 (96%)	0.27	0 100 100	73, 87, 140, 155	0
18	y	29/30 (96%)	0.18	1 (3%) 48 55	79, 97, 126, 136	0
19	Z	62/62 (100%)	-0.11	0 100 100	67, 84, 131, 173	0
19	z	62/62 (100%)	0.31	1 (1%) 70 76	83, 99, 148, 185	0
20	R	34/34 (100%)	1.17	4 (11%) 9 10	97, 125, 149, 154	0
All	All	5283/5384 (98%)	-0.51	18 (0%) 90 92	22, 59, 104, 185	108 (2%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.1
7	h	65	LEU	4.4
2	b	502	VAL	3.2
14	t	30	THR	2.7
2	B	494	GLY	2.7

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

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
14	FME	T	1	10/11	0.96	0.08	44,50,74,88	0
12	FME	m	1	10/11	0.96	0.08	47,60,91,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.97	0.09	34,56,91,100	0
14	FME	t	1	10/11	0.97	0.07	43,51,75,84	0
8	FME	i	1	10/11	0.98	0.06	59,64,77,78	0
8	FME	I	1	10/11	0.98	0.06	46,65,76,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
35	HTG	c	523	19/19	0.74	0.14	118,144,148,169	0
34	LMT	e	101	35/35	0.75	0.15	121,166,181,186	0
34	LMT	a	418	35/35	0.78	0.15	113,136,151,151	0
32	UNL	i	101	40/-	0.78	0.15	77,109,164,165	0
35	HTG	C	522	19/19	0.78	0.14	112,123,133,150	0
34	LMT	A	359	35/35	0.78	0.15	73,134,144,148	0
35	HTG	c	526	19/19	0.78	0.13	114,161,170,200	0
34	LMT	E	102	35/35	0.79	0.15	119,145,171,173	0
32	UNL	a	415	30/-	0.79	0.16	98,115,136,146	0
32	UNL	K	101	34/-	0.80	0.14	83,119,134,150	0
27	SQD	f	101	43/54	0.80	0.14	118,136,170,175	0
32	UNL	A	417	28/-	0.80	0.16	98,110,128,144	0
32	UNL	j	102	10/-	0.80	0.15	87,106,117,118	0
32	UNL	m	101	10/-	0.80	0.12	69,78,80,84	0
32	UNL	J	102	10/-	0.80	0.16	77,81,99,104	0
32	UNL	c	527	32/-	0.81	0.15	93,125,140,143	0
35	HTG	b	624	19/19	0.81	0.18	114,128,145,170	0
34	LMT	a	359	35/35	0.81	0.15	65,144,151,154	0
34	LMT	I	101	35/35	0.81	0.14	110,145,160,162	0
37	CA	b	626	1/1	0.81	0.08	151,151,151,151	0
32	UNL	I	102	40/-	0.82	0.15	66,113,156,158	0
38	LHG	a	419	42/49	0.82	0.11	78,141,167,179	0
33	LMG	C	521	51/55	0.83	0.13	68,121,155,157	0
35	HTG	B	624	19/19	0.83	0.16	71,103,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMT	b	622	25/35	0.84	0.12	88,117,159,160	0
35	HTG	B	625	19/19	0.84	0.13	82,167,178,238	0
32	UNL	b	629	33/-	0.84	0.14	72,108,162,162	0
35	HTG	h	101	16/19	0.84	0.14	98,133,140,163	0
35	HTG	C	523	19/19	0.84	0.12	84,153,166,186	0
35	HTG	D	410	16/19	0.84	0.12	82,121,136,138	0
35	HTG	b	625	19/19	0.85	0.13	91,138,154,196	0
32	UNL	D	409	40/-	0.85	0.12	67,93,136,140	0
31	PL9	A	416[A]	55/55	0.86	0.14	66,93,107,111	55
34	LMT	M	103	35/35	0.86	0.11	68,146,169,171	0
33	LMG	c	522	51/55	0.86	0.11	80,127,154,158	0
31	PL9	A	416[B]	55/55	0.86	0.14	66,93,108,113	55
34	LMT	B	622	35/35	0.86	0.13	78,125,142,144	0
32	UNL	d	410	36/-	0.86	0.12	73,100,136,140	0
33	LMG	Z	101	37/55	0.87	0.13	77,129,150,151	0
33	LMG	z	101	39/55	0.88	0.12	84,133,148,153	0
28	GOL	a	410	6/6	0.88	0.12	79,81,90,95	0
34	LMT	t	101	26/35	0.88	0.11	71,110,152,153	0
27	SQD	a	411	54/54	0.88	0.10	72,95,139,149	0
38	LHG	E	101	42/49	0.88	0.11	72,118,132,132	0
27	SQD	F	101	43/54	0.88	0.12	81,114,134,137	0
35	HTG	V	204	11/19	0.89	0.12	104,117,122,125	0
28	GOL	c	502	6/6	0.89	0.19	68,70,71,75	0
32	UNL	B	629	33/-	0.89	0.12	57,103,166,173	0
35	HTG	B	623	19/19	0.89	0.12	70,88,128,128	0
28	GOL	v	202	6/6	0.89	0.11	75,86,94,96	0
33	LMG	A	418	51/55	0.89	0.11	61,97,118,121	0
32	UNL	M	102	10/-	0.89	0.09	62,72,86,92	0
34	LMT	B	630	25/35	0.89	0.12	54,89,147,148	0
34	LMT	b	630	25/35	0.89	0.12	57,81,151,153	0
28	GOL	B	627	6/6	0.90	0.14	58,77,85,87	0
27	SQD	B	620	54/54	0.90	0.10	65,93,132,134	0
28	GOL	a	416	6/6	0.90	0.21	55,82,84,86	0
28	GOL	b	627	6/6	0.90	0.12	97,106,113,116	0
27	SQD	b	620	54/54	0.90	0.10	68,93,144,152	0
27	SQD	A	413	54/54	0.90	0.10	63,91,128,137	0
28	GOL	A	412	6/6	0.91	0.12	80,82,86,98	0
24	CLA	B	601	65/65	0.91	0.10	53,77,112,132	0
33	LMG	a	417	51/55	0.91	0.10	76,100,122,129	0
24	CLA	c	515	65/65	0.91	0.10	70,91,134,138	0
37	CA	V	201	1/1	0.91	0.14	141,141,141,141	0
34	LMT	m	102	35/35	0.91	0.11	63,95,117,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	CA	v	201	1/1	0.91	0.13	123,123,123,123	0
31	PL9	a	414[A]	55/55	0.91	0.16	97,107,120,124	55
31	PL9	a	414[B]	55/55	0.91	0.16	97,107,120,124	55
34	LMT	M	101	35/35	0.92	0.10	61,99,123,126	0
24	CLA	b	601	65/65	0.92	0.10	58,85,115,130	0
33	LMG	c	521	51/55	0.92	0.09	68,101,145,156	0
33	LMG	C	520	51/55	0.92	0.09	56,90,127,140	0
35	HTG	b	623	19/19	0.92	0.11	68,88,130,131	0
28	GOL	V	202	6/6	0.93	0.11	64,74,85,92	0
24	CLA	c	514	65/65	0.93	0.09	59,80,123,128	0
35	HTG	B	628	19/19	0.93	0.08	65,80,89,95	0
24	CLA	C	514	65/65	0.93	0.09	60,81,122,127	0
28	GOL	C	525	6/6	0.93	0.12	66,73,76,78	0
32	UNL	D	408	17/-	0.93	0.09	66,85,107,110	0
26	BCR	d	404	40/40	0.94	0.08	53,67,96,98	0
24	CLA	C	507	65/65	0.94	0.09	53,69,137,141	0
37	CA	O	301	1/1	0.94	0.07	119,119,119,119	0
24	CLA	C	513	65/65	0.94	0.08	60,73,118,123	0
26	BCR	C	515	40/40	0.94	0.08	63,75,82,85	0
27	SQD	a	409	54/54	0.94	0.09	63,85,127,131	0
33	LMG	b	621	51/55	0.94	0.09	53,74,105,124	0
26	BCR	D	404	40/40	0.94	0.08	46,61,94,95	0
24	CLA	c	506	65/65	0.95	0.07	51,66,116,125	0
24	CLA	c	508	65/65	0.95	0.08	60,72,120,133	0
33	LMG	J	101	51/55	0.95	0.08	48,73,119,126	0
24	CLA	c	509	65/65	0.95	0.08	56,70,86,92	0
24	CLA	C	509	65/65	0.95	0.07	44,57,115,131	0
24	CLA	B	614	65/65	0.95	0.08	38,49,103,113	0
24	CLA	d	403	65/65	0.95	0.08	46,64,132,137	0
24	CLA	C	505	65/65	0.95	0.07	42,56,103,113	0
33	LMG	j	101	51/55	0.95	0.08	60,70,121,138	0
24	CLA	B	606	65/65	0.95	0.08	41,52,104,114	0
26	BCR	K	102	40/40	0.95	0.07	56,67,74,81	0
32	UNL	X	101	18/-	0.95	0.09	57,76,100,100	0
26	BCR	Y	101	40/40	0.95	0.07	57,68,74,81	0
35	HTG	b	628	19/19	0.95	0.08	61,82,106,112	0
24	CLA	b	606	65/65	0.95	0.08	45,58,114,129	0
26	BCR	h	102	40/40	0.95	0.07	56,70,80,81	0
26	BCR	t	102	40/40	0.95	0.07	45,60,76,80	0
36	DGD	C	518	62/66	0.95	0.08	48,67,127,131	0
36	DGD	c	519	62/66	0.95	0.08	56,73,136,145	0
26	BCR	y	101	40/40	0.95	0.08	58,74,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	SQD	A	411	54/54	0.95	0.08	55,86,123,126	0
24	CLA	b	614	65/65	0.95	0.07	41,49,116,120	0
37	CA	o	301	1/1	0.95	0.06	108,108,108,108	0
32	UNL	x	101	18/-	0.95	0.09	70,85,105,106	0
38	LHG	D	407	49/49	0.95	0.09	53,61,120,125	0
24	CLA	b	616	65/65	0.95	0.09	50,60,124,127	0
33	LMG	B	621	51/55	0.95	0.08	53,72,94,108	0
38	LHG	d	406	49/49	0.95	0.08	50,66,90,106	0
38	LHG	d	408	49/49	0.95	0.09	53,68,121,125	0
28	GOL	B	626	6/6	0.96	0.10	85,88,90,95	0
26	BCR	A	410	40/40	0.96	0.06	42,51,61,62	0
26	BCR	B	618	40/40	0.96	0.06	44,57,70,77	0
26	BCR	B	619	40/40	0.96	0.06	45,57,80,87	0
24	CLA	C	504	65/65	0.96	0.07	47,58,76,85	0
24	CLA	b	607	65/65	0.96	0.07	35,49,77,87	0
26	BCR	H	101	40/40	0.96	0.06	50,65,77,82	0
24	CLA	b	609	65/65	0.96	0.07	50,61,83,99	0
26	BCR	T	101	40/40	0.96	0.06	46,57,68,72	0
24	CLA	B	602	65/65	0.96	0.07	45,55,80,84	0
26	BCR	b	617	40/40	0.96	0.06	45,52,63,63	0
26	BCR	b	618	40/40	0.96	0.06	44,60,73,75	0
26	BCR	c	516	40/40	0.96	0.07	77,86,93,96	0
24	CLA	b	615	65/65	0.96	0.07	46,59,81,86	0
24	CLA	B	616	65/65	0.96	0.10	45,58,147,153	0
26	BCR	k	101	40/40	0.96	0.07	58,73,84,90	0
36	DGD	C	517	62/66	0.96	0.07	43,63,104,106	0
24	CLA	c	505	65/65	0.96	0.06	58,67,77,83	0
36	DGD	C	519	62/66	0.96	0.07	43,60,94,116	0
36	DGD	c	518	62/66	0.96	0.07	49,67,95,103	0
24	CLA	D	403	65/65	0.96	0.08	44,58,139,144	0
36	DGD	c	520	62/66	0.96	0.07	55,64,100,116	0
24	CLA	c	507	65/65	0.96	0.07	49,61,91,95	0
24	CLA	a	404	65/65	0.96	0.07	42,53,126,133	0
24	CLA	a	407	65/65	0.96	0.09	44,57,134,140	0
24	CLA	c	510	65/65	0.96	0.07	53,63,141,145	0
24	CLA	c	511	65/65	0.96	0.08	51,69,82,89	0
24	CLA	c	513	65/65	0.96	0.07	57,71,91,97	0
38	LHG	D	357	49/49	0.96	0.07	49,64,86,102	0
24	CLA	C	508	65/65	0.96	0.07	49,60,80,82	0
32	UNL	d	409	17/-	0.96	0.07	68,83,111,114	0
24	CLA	b	602	65/65	0.96	0.07	51,62,79,88	0
24	CLA	b	604	65/65	0.96	0.07	37,50,122,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	LHG	l	101	49/49	0.96	0.07	50,60,74,91	0
39	HEM	e	102	43/43	0.96	0.09	67,93,128,137	0
24	CLA	a	403	65/65	0.97	0.06	36,48,69,86	0
26	BCR	B	617	40/40	0.97	0.05	44,52,59,65	0
31	PL9	D	405	55/55	0.97	0.06	37,49,62,78	0
24	CLA	B	609	65/65	0.97	0.06	47,57,73,80	0
24	CLA	B	610	65/65	0.97	0.07	43,53,64,80	0
31	PL9	d	405	55/55	0.97	0.06	41,50,66,85	0
24	CLA	a	350	65/65	0.97	0.05	36,46,63,77	0
26	BCR	C	516	40/40	0.97	0.06	53,62,72,81	0
24	CLA	B	611	65/65	0.97	0.06	37,47,63,73	0
24	CLA	B	612	65/65	0.97	0.05	35,47,57,74	0
24	CLA	b	603	65/65	0.97	0.06	46,56,85,92	0
24	CLA	B	613	65/65	0.97	0.06	37,47,94,103	0
24	CLA	b	605	65/65	0.97	0.06	43,52,70,74	0
26	BCR	a	408	40/40	0.97	0.05	42,52,65,68	0
24	CLA	A	406	65/65	0.97	0.06	36,47,110,116	0
24	CLA	B	615	65/65	0.97	0.06	37,52,74,83	0
26	BCR	b	619	40/40	0.97	0.06	51,62,81,84	0
24	CLA	b	608	65/65	0.97	0.05	46,58,81,84	0
26	BCR	c	517	40/40	0.97	0.06	56,67,80,81	0
24	CLA	A	409	65/65	0.97	0.08	42,53,136,144	0
24	CLA	b	610	65/65	0.97	0.07	47,58,73,75	0
24	CLA	b	611	65/65	0.97	0.06	41,52,73,82	0
24	CLA	b	612	65/65	0.97	0.06	43,54,64,75	0
24	CLA	C	502	65/65	0.97	0.06	48,59,73,83	0
24	CLA	C	503	65/65	0.97	0.06	47,55,78,95	0
23	BCT	A	403[A]	4/4	0.97	0.06	58,60,60,69	4
36	DGD	H	102	62/66	0.97	0.07	46,63,76,78	0
24	CLA	c	503	65/65	0.97	0.07	56,66,79,86	0
24	CLA	c	504	65/65	0.97	0.06	45,65,86,89	0
23	BCT	A	403[B]	4/4	0.97	0.06	55,61,62,78	4
36	DGD	h	103	62/66	0.97	0.07	52,66,78,86	0
24	CLA	C	506	65/65	0.97	0.06	49,57,92,100	0
24	CLA	B	603	65/65	0.97	0.06	42,52,69,76	0
24	CLA	B	604	65/65	0.97	0.07	34,46,123,127	0
24	CLA	B	605	65/65	0.97	0.06	39,48,65,68	0
24	CLA	C	510	65/65	0.97	0.07	49,60,81,91	0
38	LHG	D	406	49/49	0.97	0.07	47,57,76,93	0
24	CLA	C	511	65/65	0.97	0.06	49,61,74,88	0
24	CLA	c	512	65/65	0.97	0.07	50,65,81,92	0
24	CLA	C	512	65/65	0.97	0.06	52,63,79,86	0

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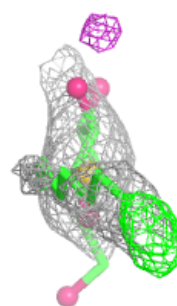
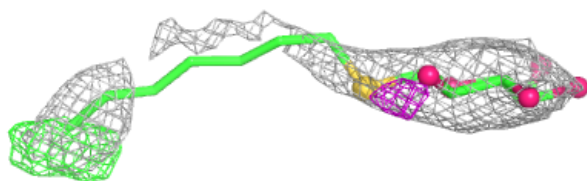
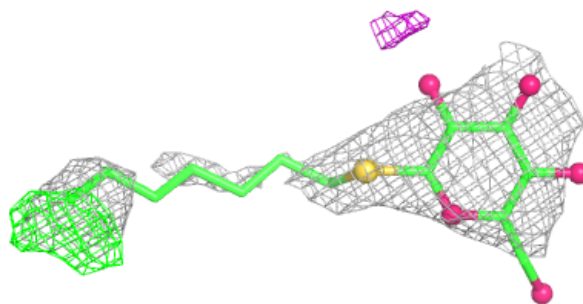
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	LHG	L	101	49/49	0.97	0.06	45,55,67,96	0
24	CLA	A	404	65/65	0.97	0.06	36,43,66,80	0
24	CLA	B	607	65/65	0.97	0.06	32,45,71,78	0
38	LHG	d	407	49/49	0.97	0.06	48,59,73,85	0
24	CLA	B	608	65/65	0.97	0.05	41,54,68,71	0
25	PHO	A	408	64/64	0.97	0.06	37,49,57,60	0
39	HEM	E	103	43/43	0.97	0.07	60,70,80,93	0
25	PHO	a	406	64/64	0.97	0.06	41,55,63,65	0
24	CLA	b	613	65/65	0.98	0.05	42,49,101,106	0
24	CLA	A	405	65/65	0.98	0.05	34,45,54,63	0
24	CLA	d	402	65/65	0.98	0.05	39,48,74,86	0
22	CL	a	347	1/1	0.98	0.09	53,53,53,53	0
37	CA	c	524	1/1	0.98	0.09	78,78,78,78	0
37	CA	c	525	1/1	0.98	0.04	92,92,92,92	0
25	PHO	A	407	64/64	0.98	0.05	35,45,54,58	0
24	CLA	D	402	65/65	0.98	0.05	31,45,68,82	0
25	PHO	a	405	64/64	0.98	0.05	41,49,56,64	0
22	CL	A	347	1/1	0.98	0.06	49,49,49,49	0
40	MG	j	103	1/1	0.98	0.04	64,64,64,64	0
41	HEC	V	203	43/43	0.98	0.05	39,52,58,60	0
41	HEC	v	203	43/43	0.98	0.06	51,64,72,78	0
21	FE2	A	401[A]	1/1	0.99	0.04	62,62,62,62	1
23	BCT	a	420[A]	4/4	0.99	0.05	58,63,63,68	4
23	BCT	a	420[B]	4/4	0.99	0.05	54,63,64,72	4
29	OEX	A	414[A]	10/10	0.99	0.05	44,48,55,59	10
29	OEX	a	412[A]	10/10	0.99	0.05	50,55,61,74	10
30	OXY	A	415[B]	11/11	0.99	0.05	43,49,55,56	11
30	OXY	a	413[B]	11/11	0.99	0.05	50,54,58,74	11
22	CL	a	402	1/1	0.99	0.02	51,51,51,51	0
40	MG	J	103	1/1	0.99	0.06	61,61,61,61	0
21	FE2	A	401[B]	1/1	0.99	0.04	60,60,60,60	1
22	CL	A	402	1/1	0.99	0.04	44,44,44,44	0
37	CA	C	524	1/1	0.99	0.10	72,72,72,72	0
21	FE2	a	401[B]	1/1	1.00	0.05	60,60,60,60	1
21	FE2	a	401[A]	1/1	1.00	0.05	60,60,60,60	1

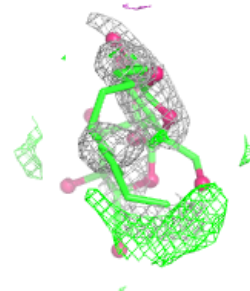
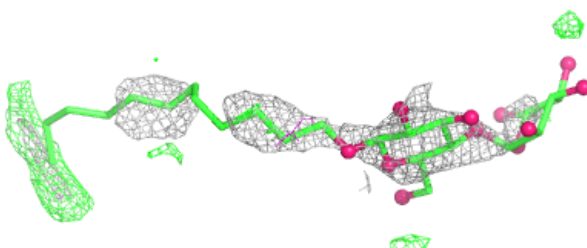
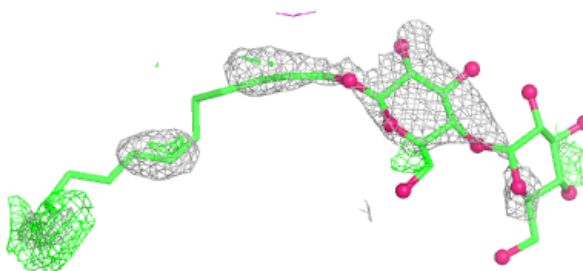
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG c 523:

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

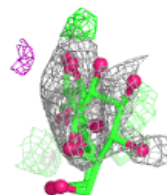
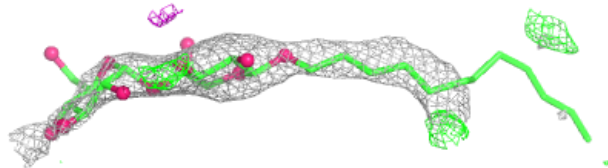
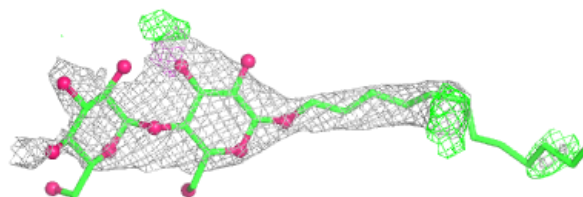
**Electron density around LMT e 101:**

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

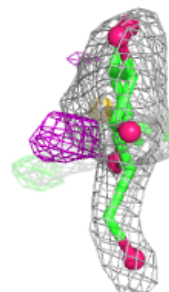
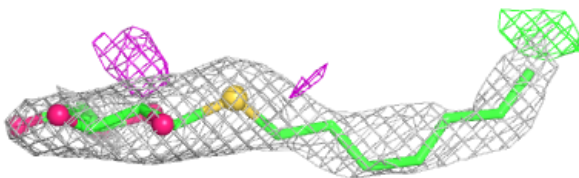
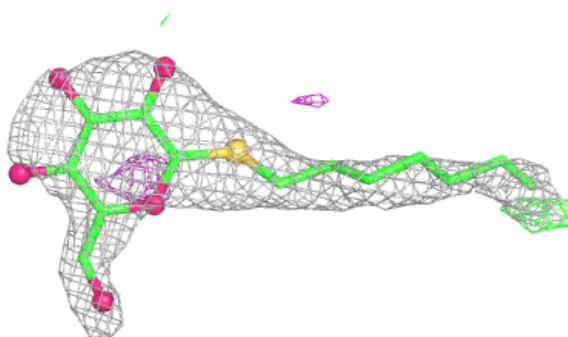


Electron density around LMT a 418:

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

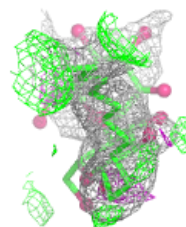
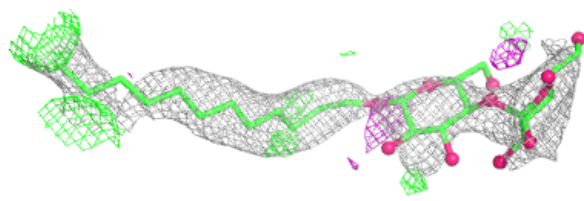
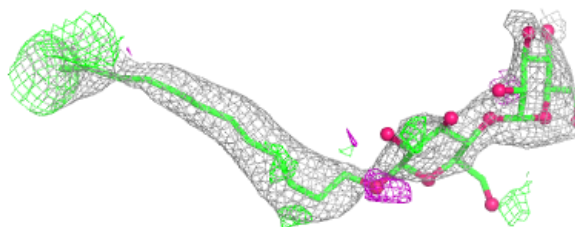
**Electron density around HTG C 522:**

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

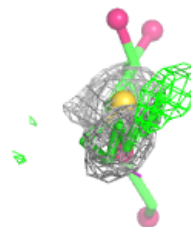
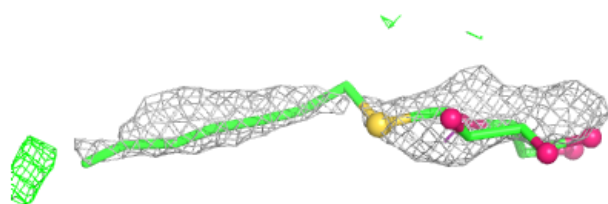
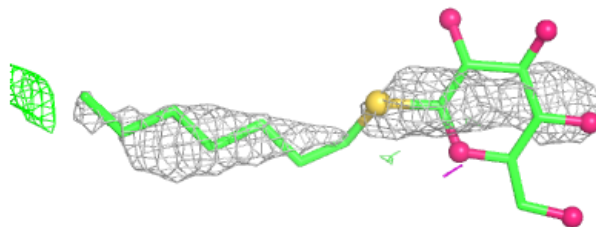


Electron density around LMT A 359:

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

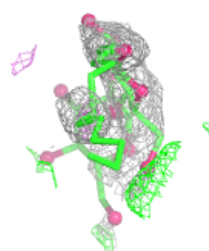
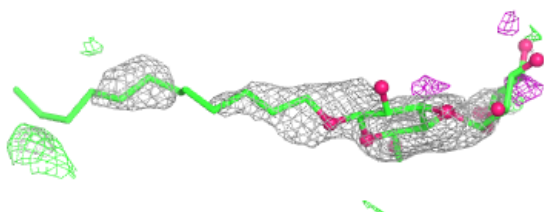
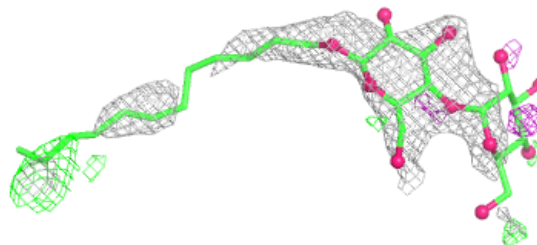
**Electron density around HTG c 526:**

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

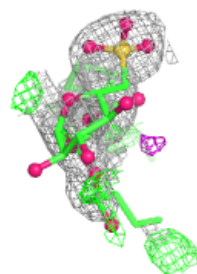
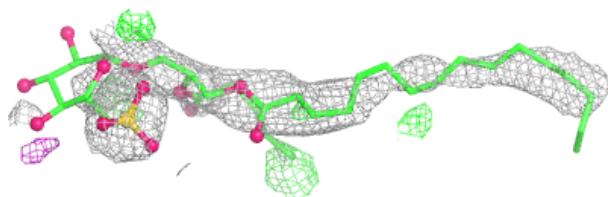
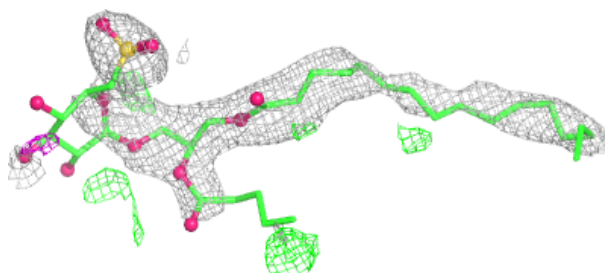


Electron density around LMT E 102:

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

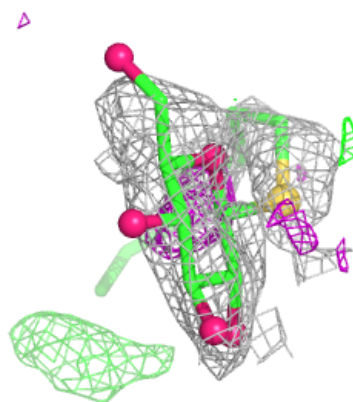
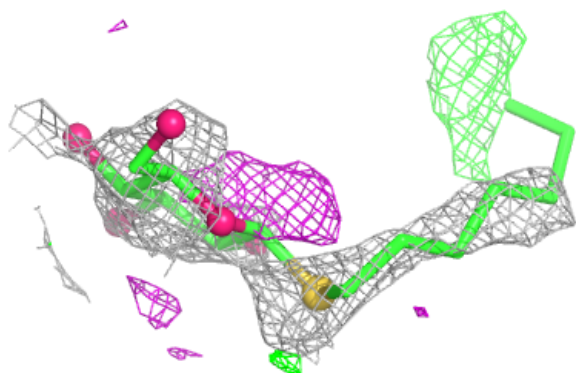
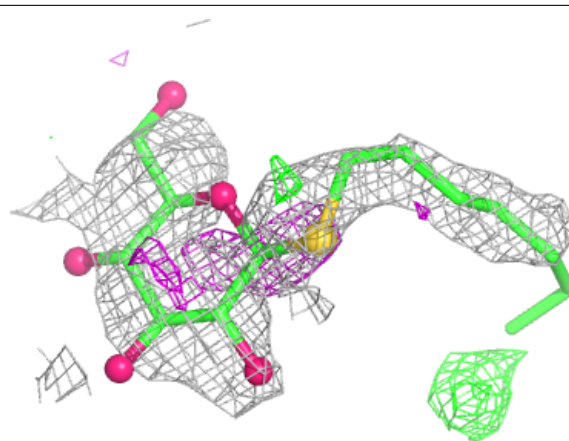
**Electron density around SQD f 101:**

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

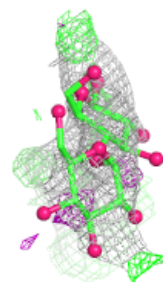
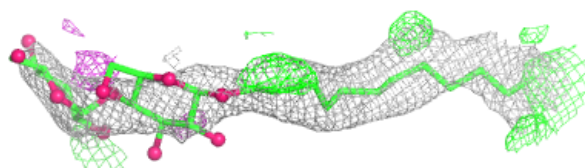
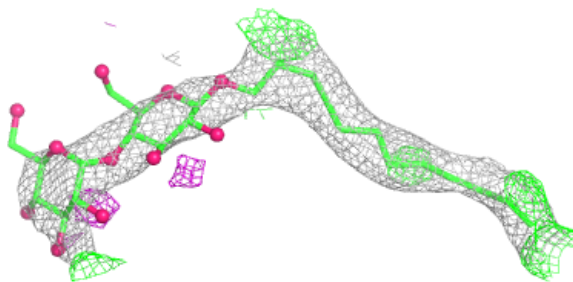


Electron density around HTG b 624:

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

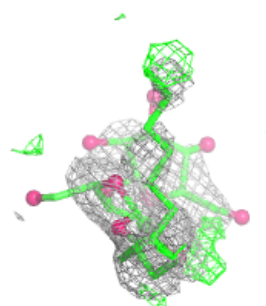
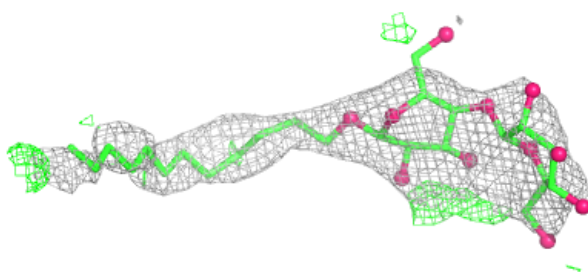
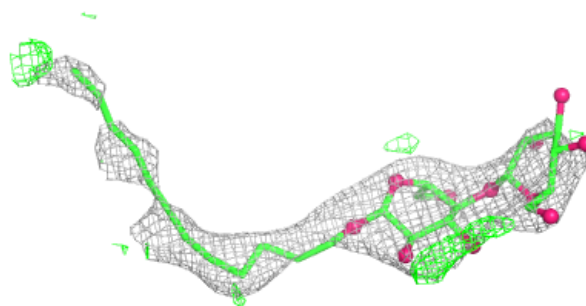
**Electron density around LMT a 359:**

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

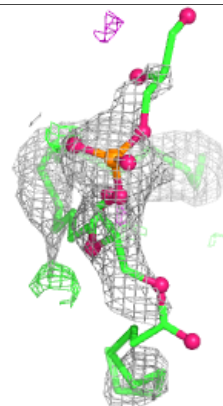
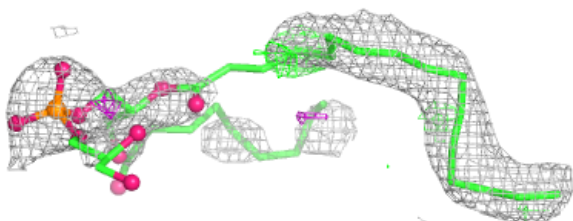
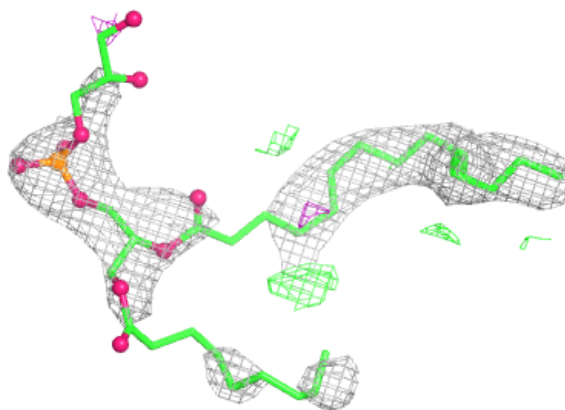


Electron density around LMT I 101:

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

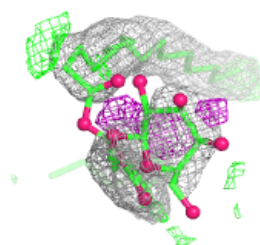
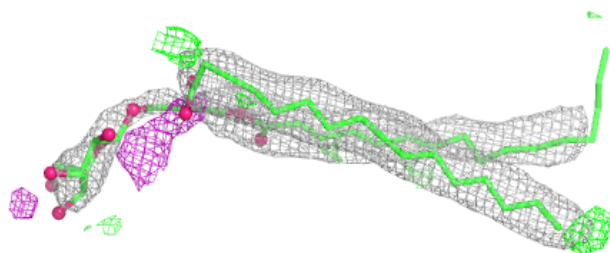
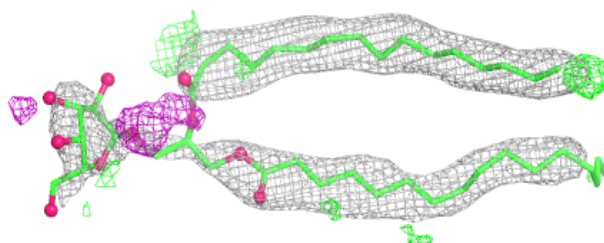
**Electron density around LHG a 419:**

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

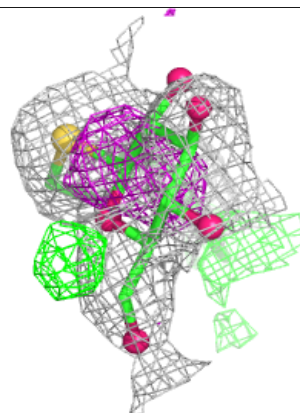
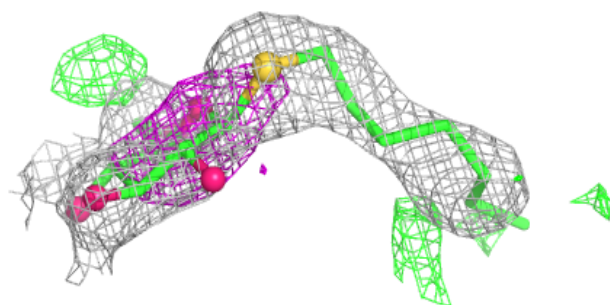
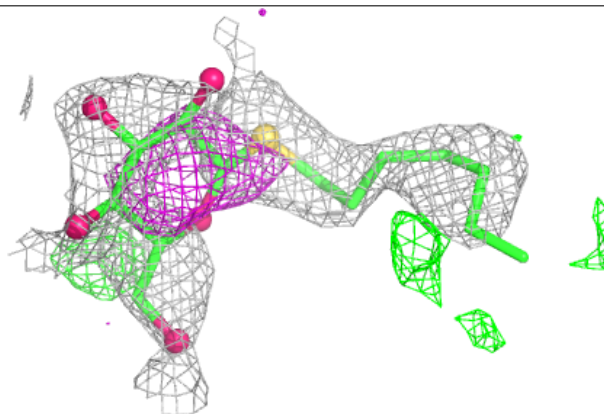


Electron density around LMG C 521:

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

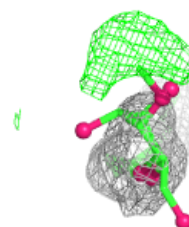
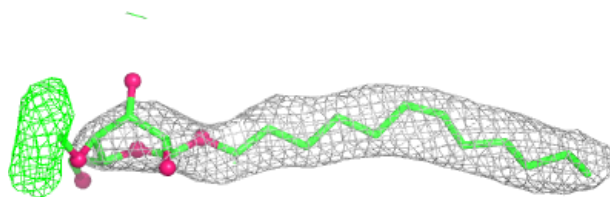
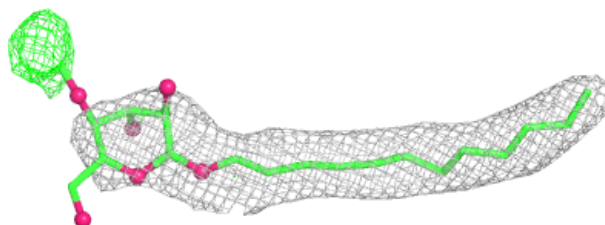
**Electron density around HTG B 624:**

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

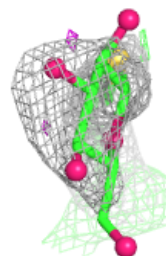
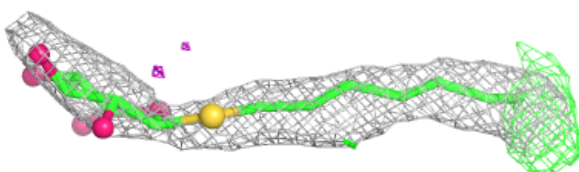
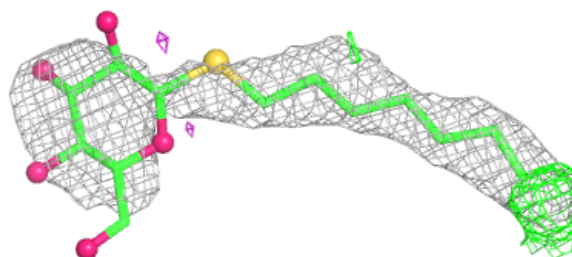


Electron density around LMT b 622:

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

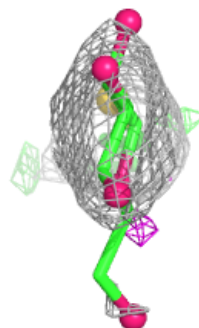
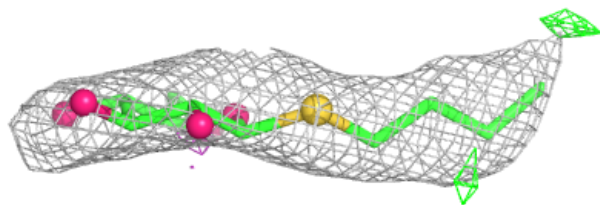
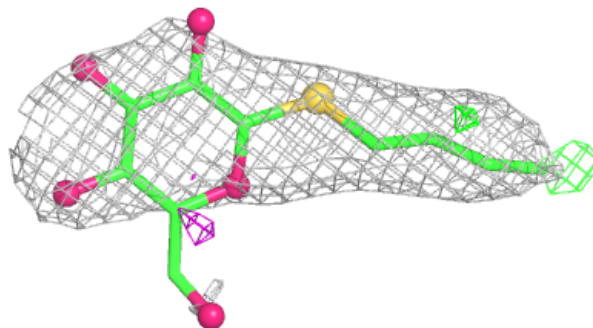
**Electron density around HTG B 625:**

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

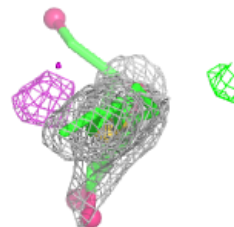
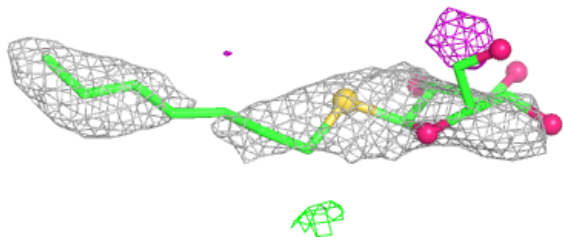
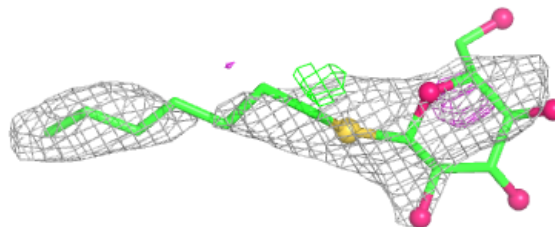


Electron density around HTG h 101:

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

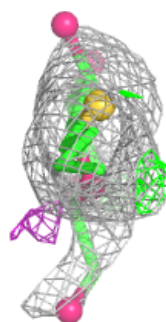
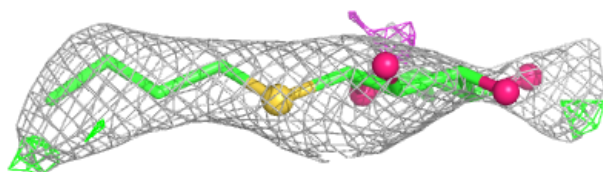
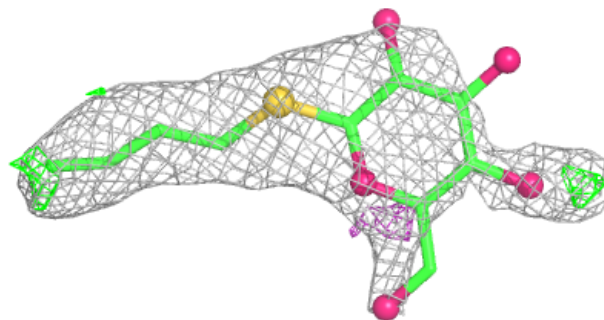
**Electron density around HTG C 523:**

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

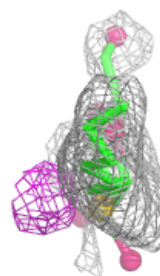
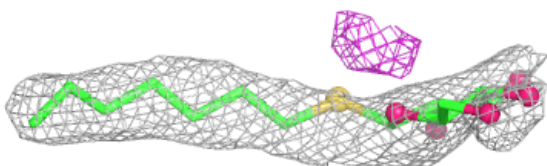
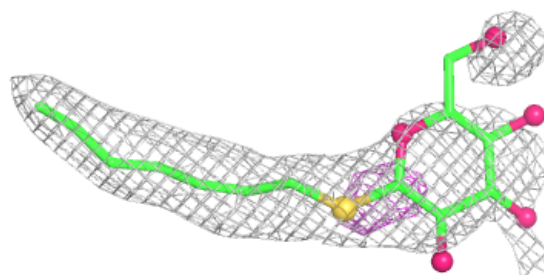


Electron density around HTG D 410:

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

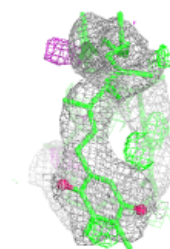
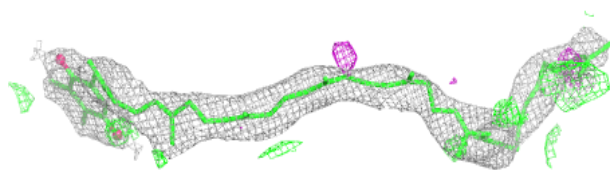
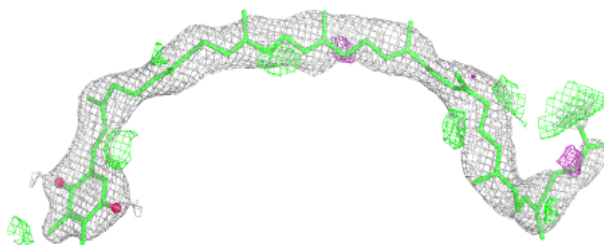
**Electron density around HTG b 625:**

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and green (positive)

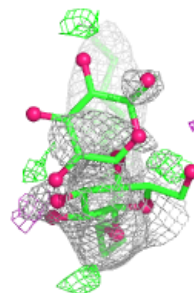
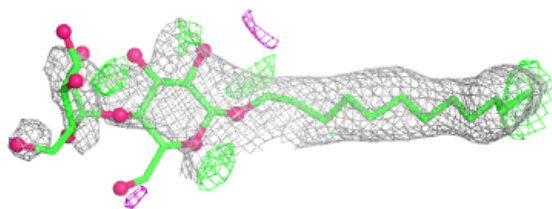
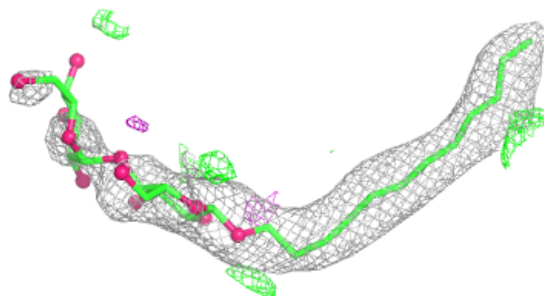


Electron density around PL9 A 416 (A):

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

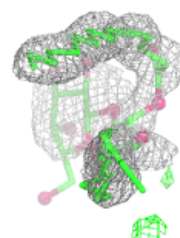
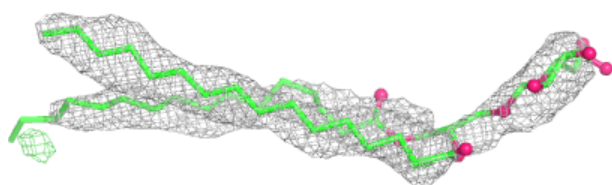
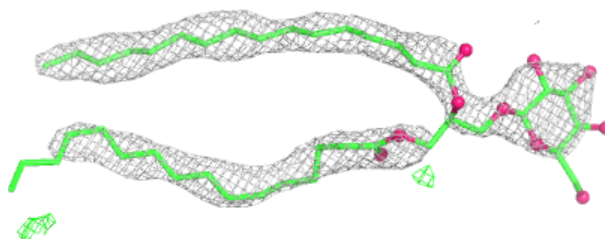
**Electron density around LMT M 103:**

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

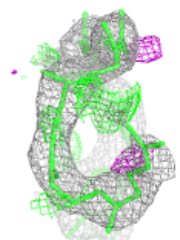
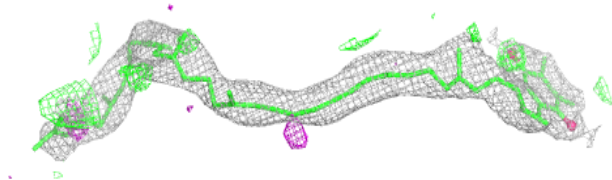
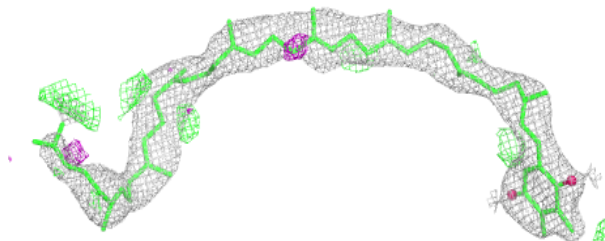


Electron density around LMG c 522:

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

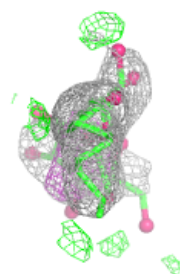
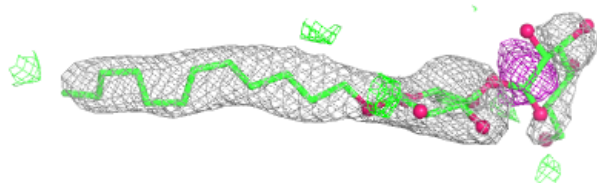
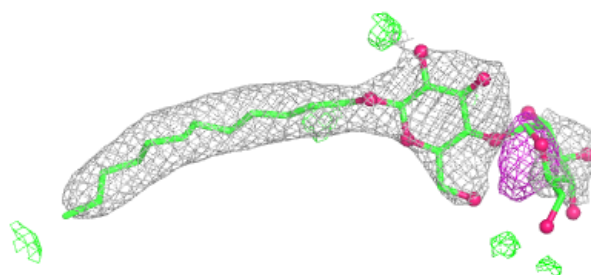
**Electron density around PL9 A 416 (B):**

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

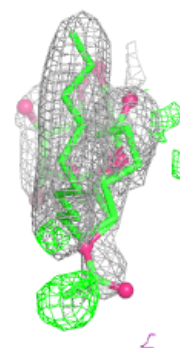
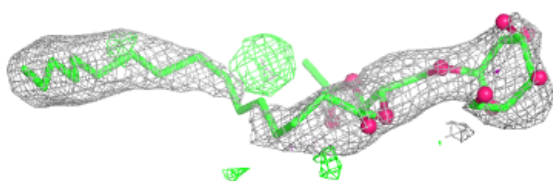
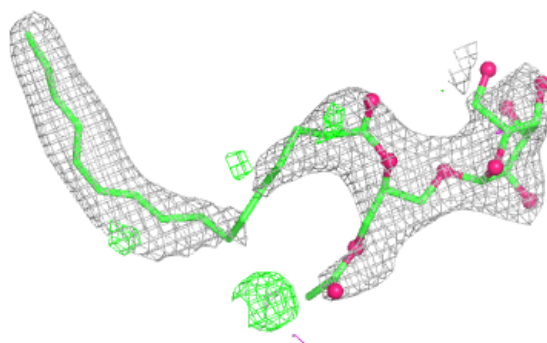


Electron density around LMT B 622:

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

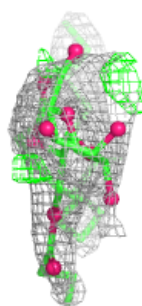
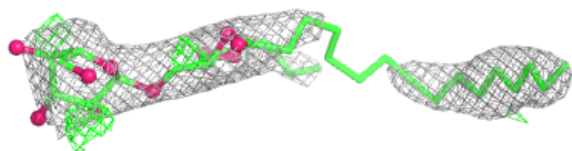
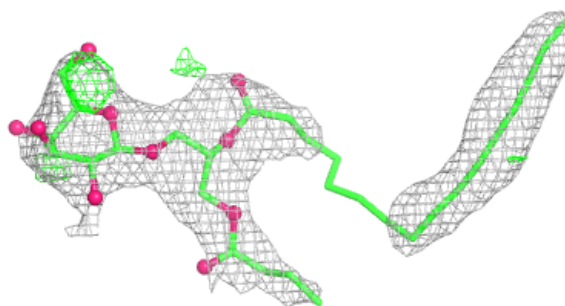
**Electron density around LMG Z 101:**

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

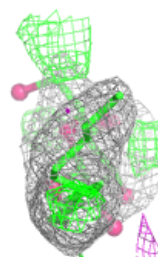
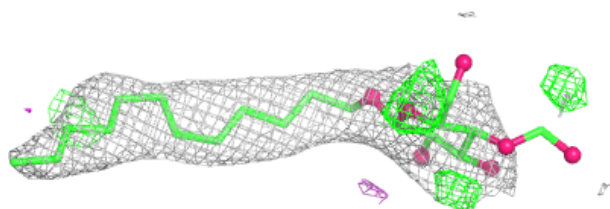
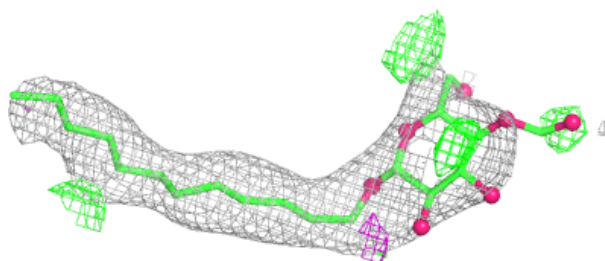


Electron density around LMG z 101:

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

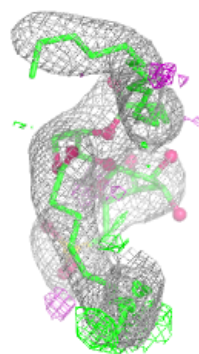
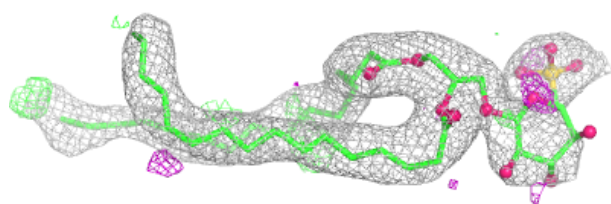
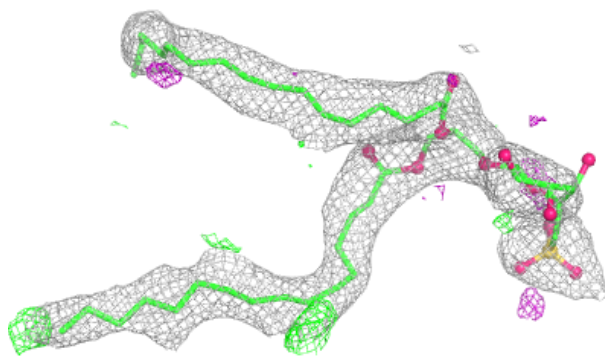
**Electron density around LMT t 101:**

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

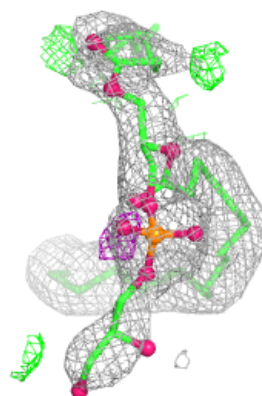
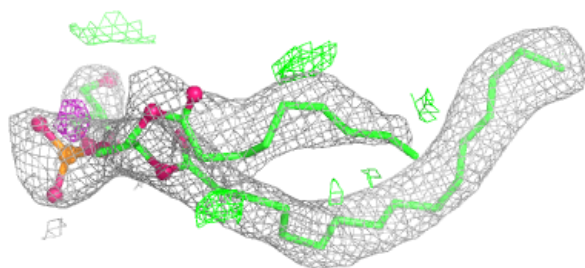
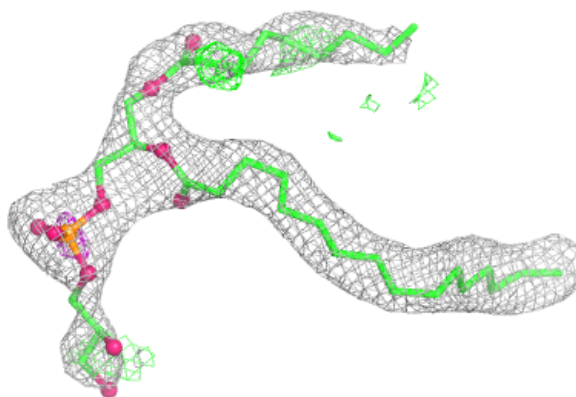


Electron density around SQD a 411:

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

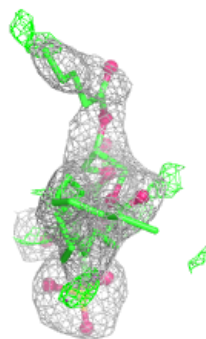
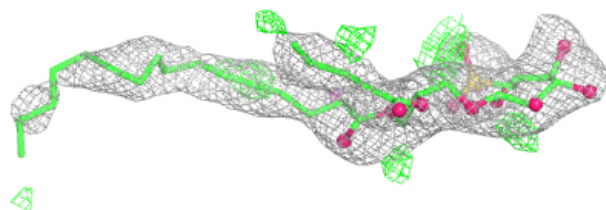
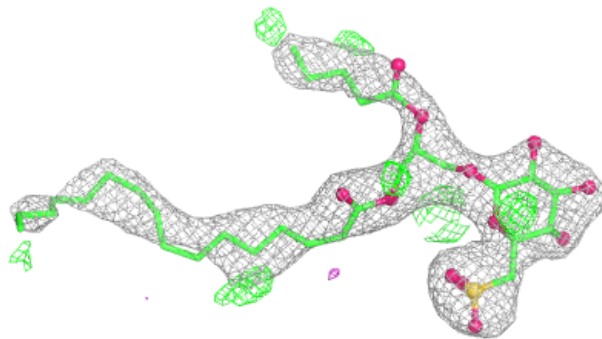
**Electron density around LHG E 101:**

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



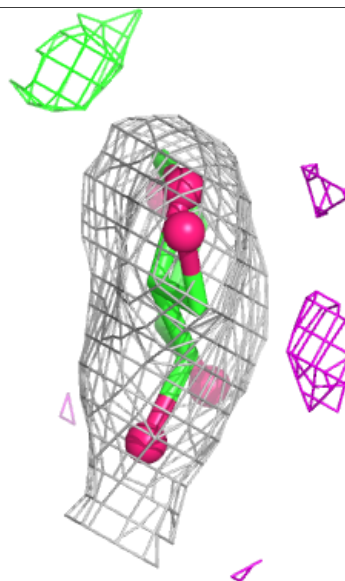
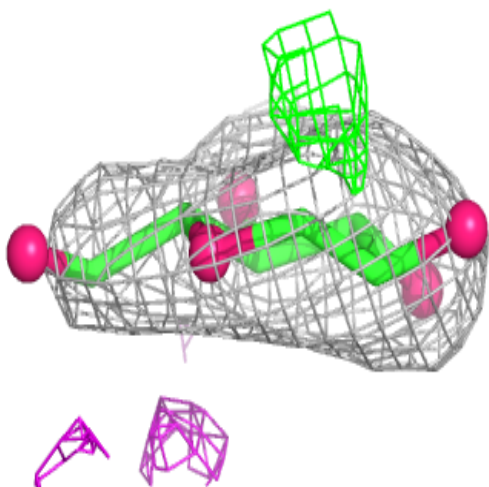
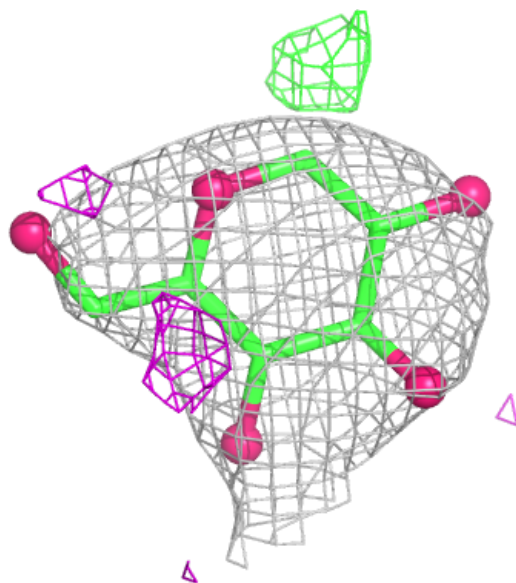
Electron density around SQD F 101:

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



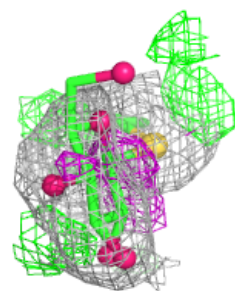
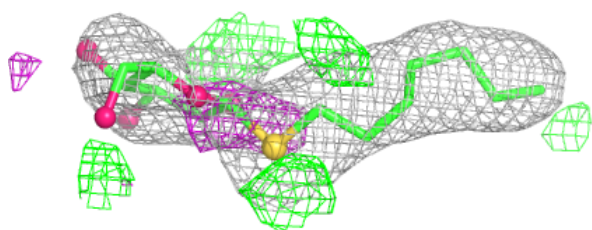
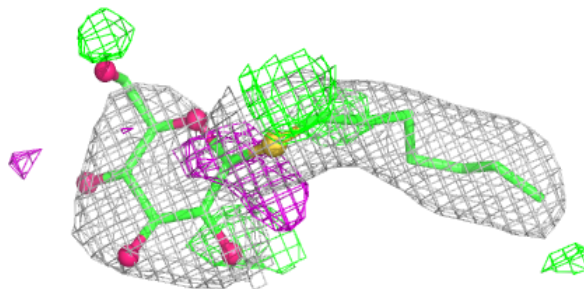
Electron density around HTG V 204:

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

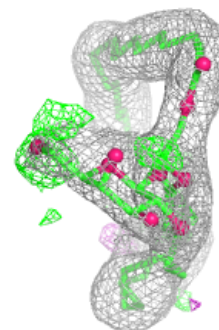
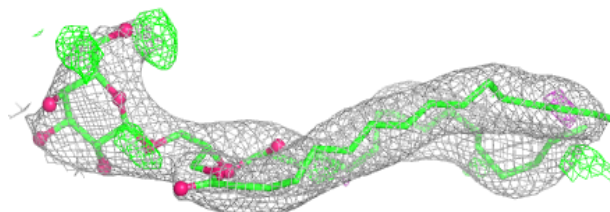
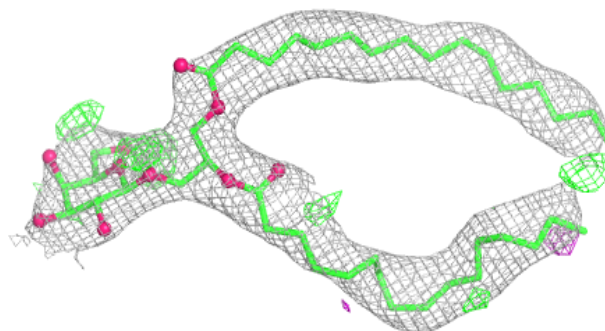


Electron density around HTG B 623:

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

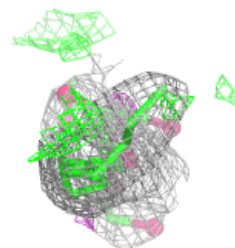
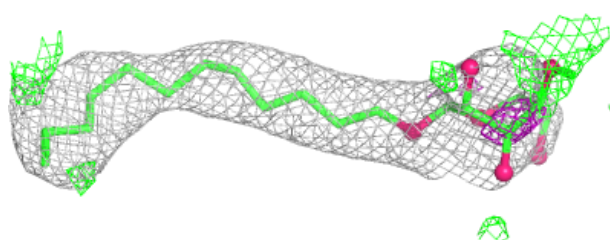
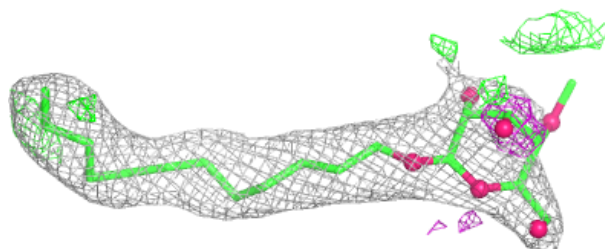
**Electron density around LMG A 418:**

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

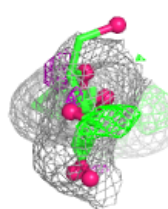
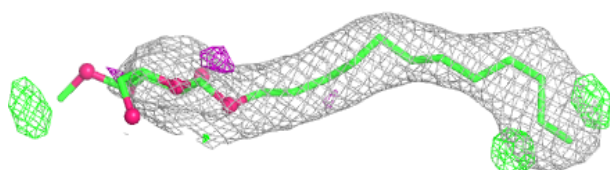
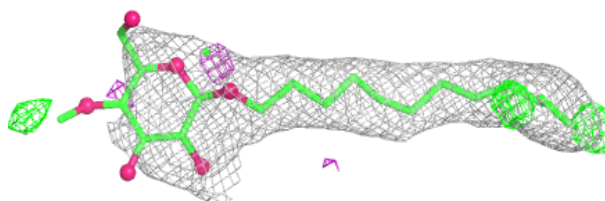


Electron density around LMT B 630:

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

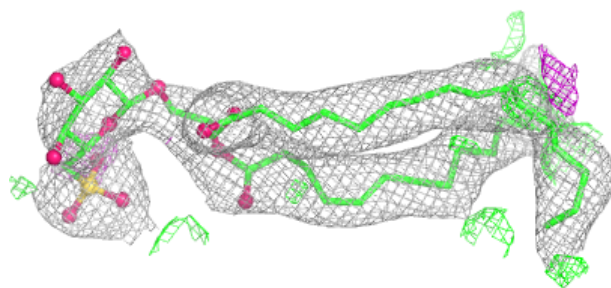
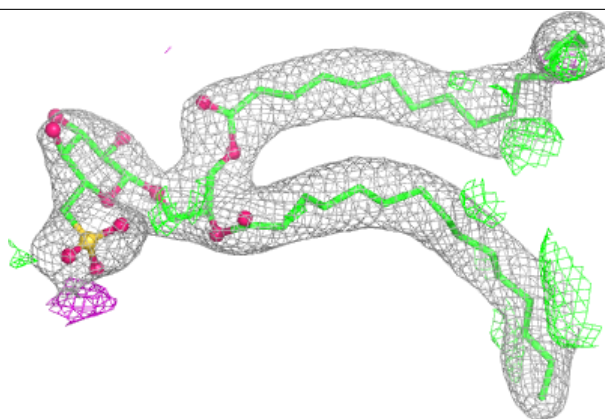
**Electron density around LMT b 630:**

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

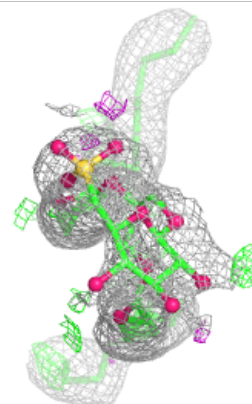
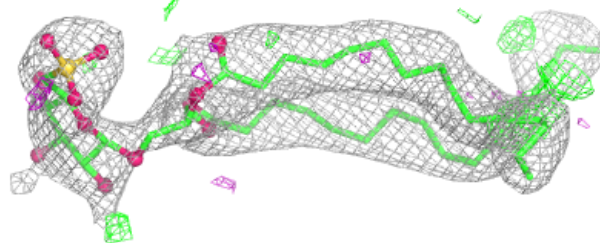
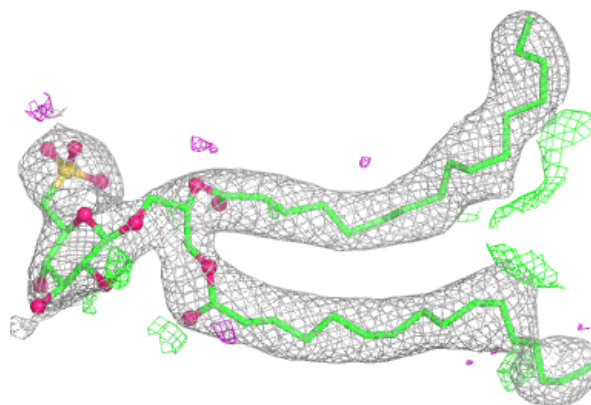


Electron density around SQD B 620:

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

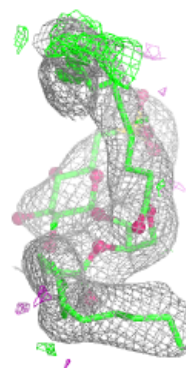
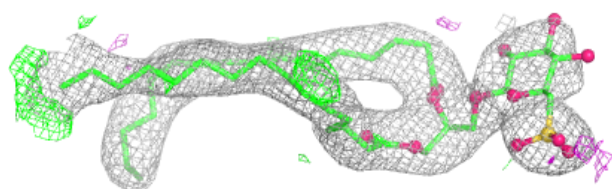
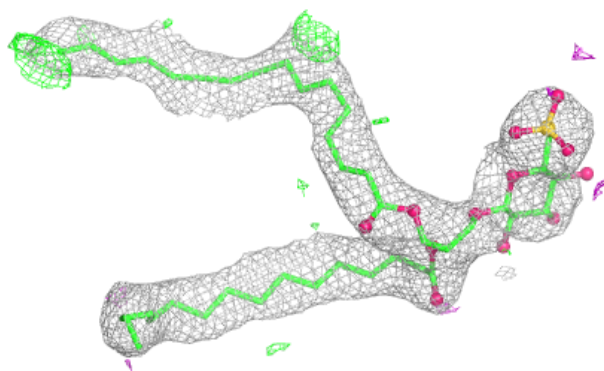
**Electron density around SQD b 620:**

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

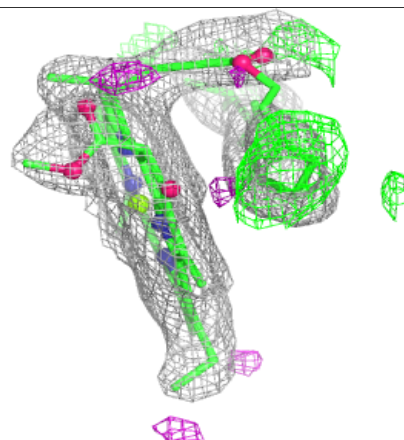
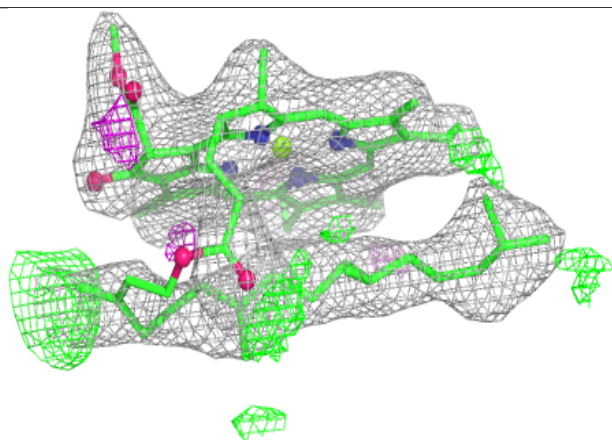
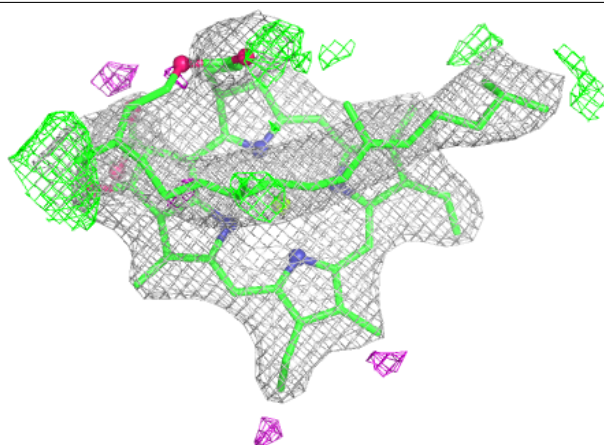


Electron density around SQD A 413:

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

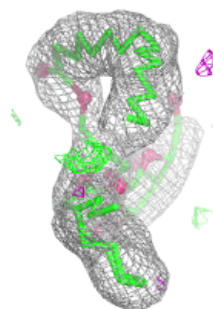
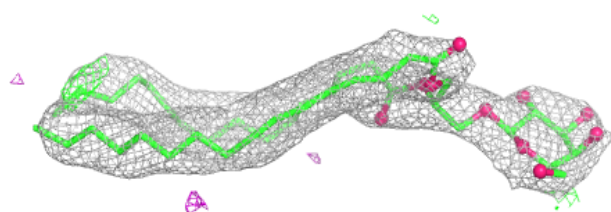
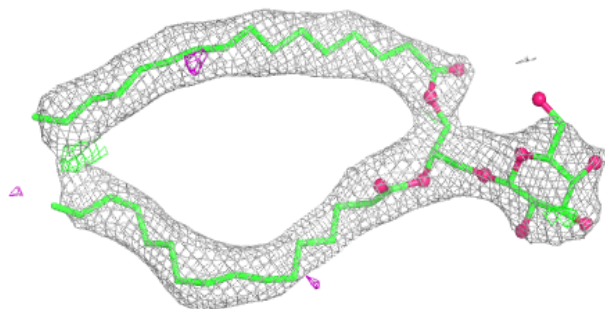
**Electron density around CLA B 601:**

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

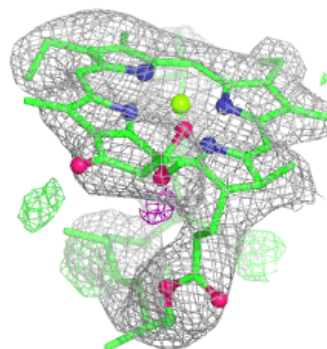
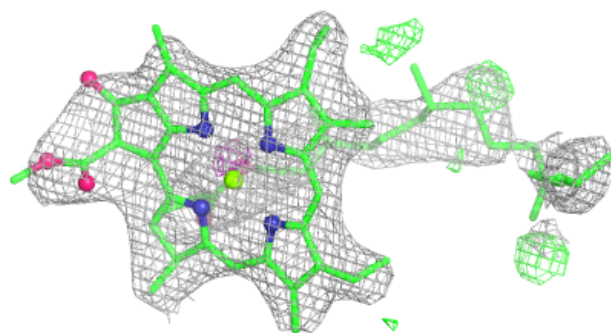
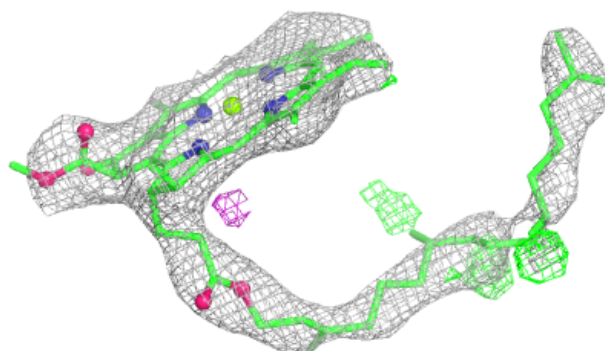


Electron density around LMG a 417:

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

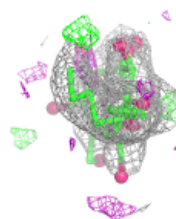
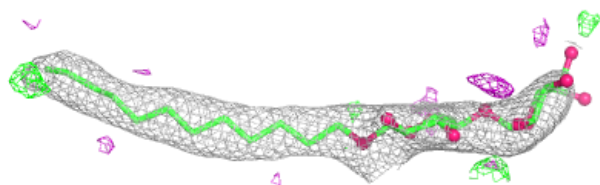
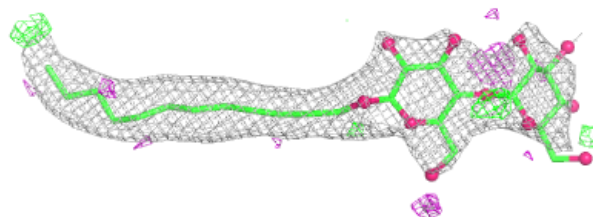
**Electron density around CLA c 515:**

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

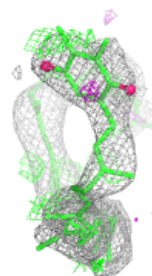
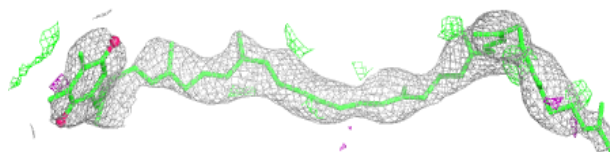
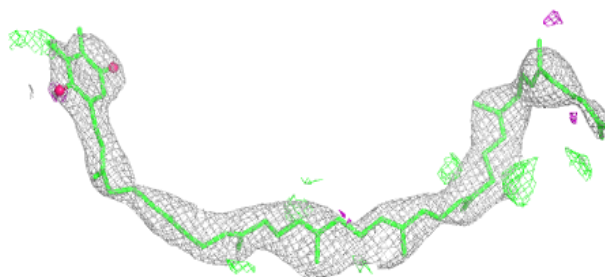


Electron density around LMT m 102:

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

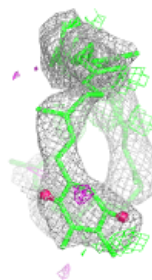
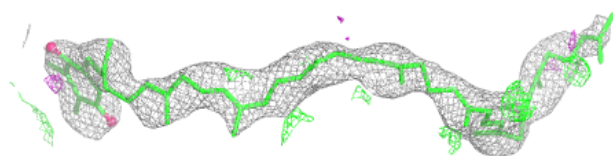
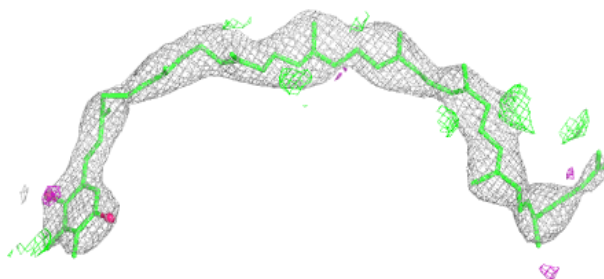
**Electron density around PL9 a 414 (A):**

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

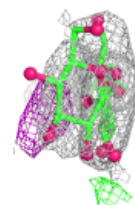
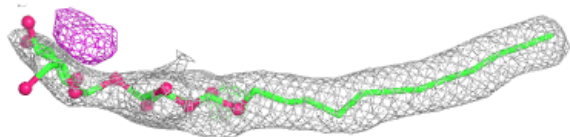
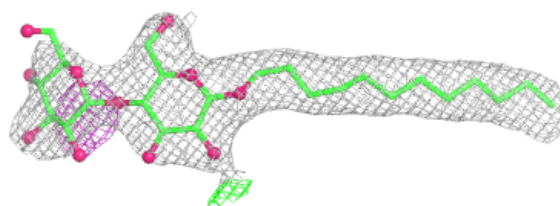


Electron density around PL9 a 414 (B):

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

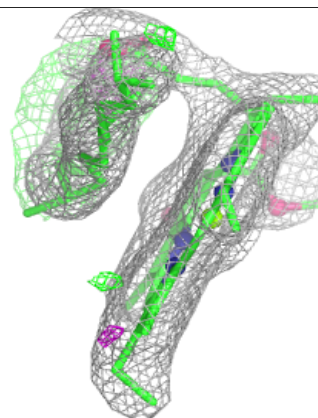
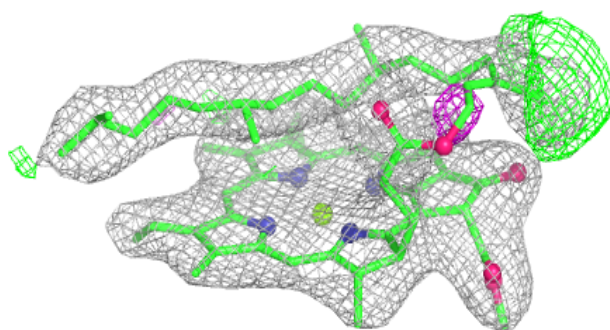
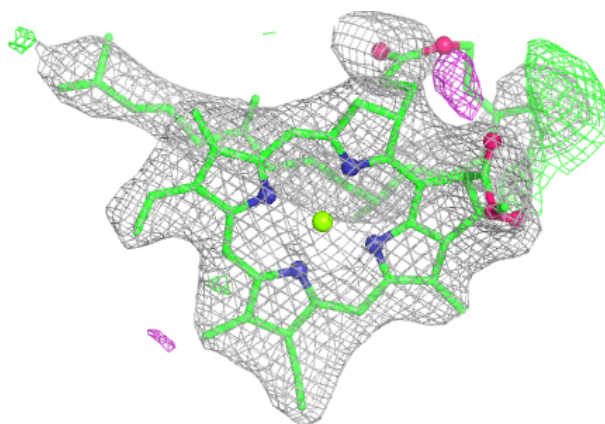
**Electron density around LMT M 101:**

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



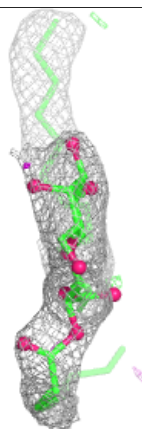
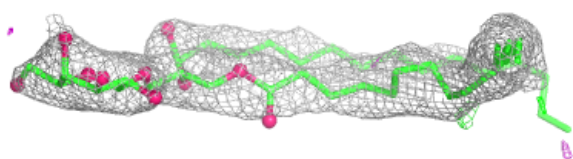
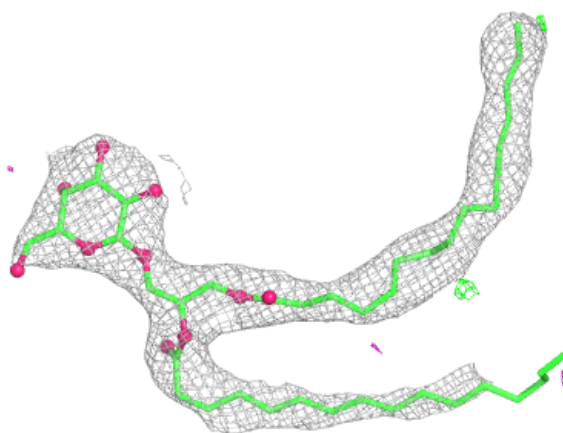
Electron density around CLA b 601:

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



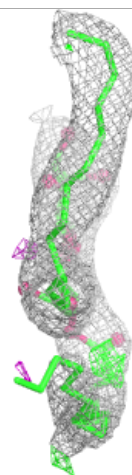
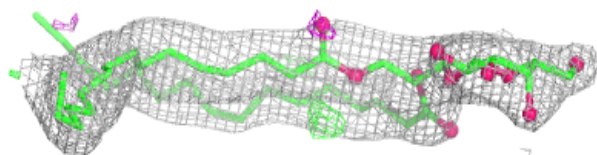
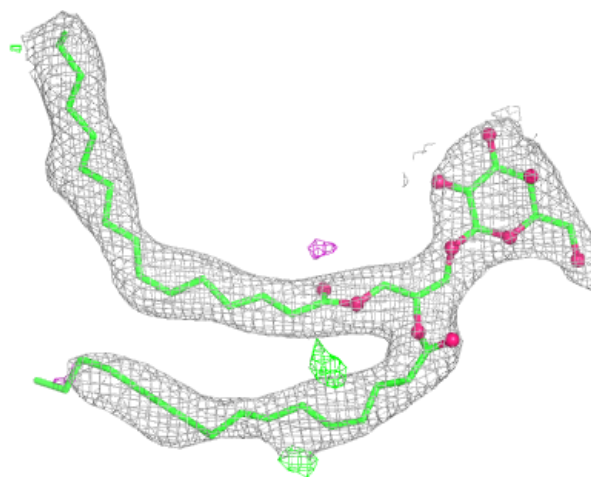
Electron density around LMG c 521:

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



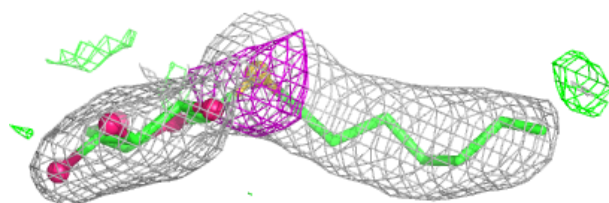
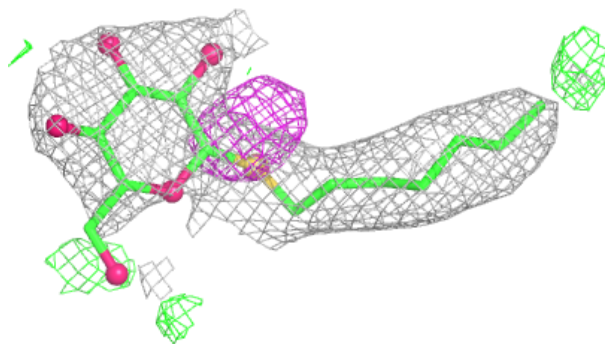
Electron density around LMG C 520:

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



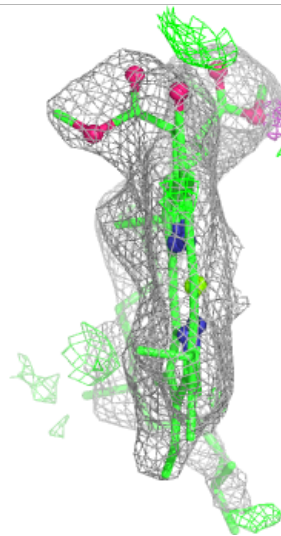
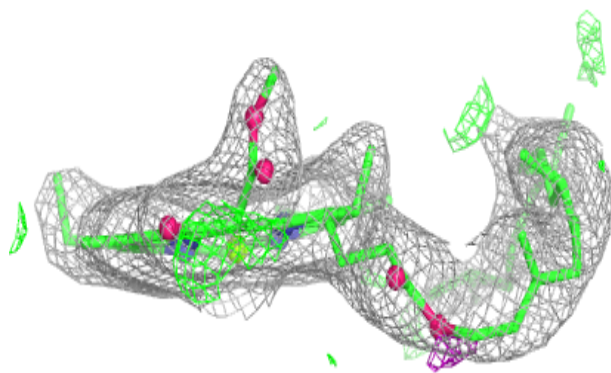
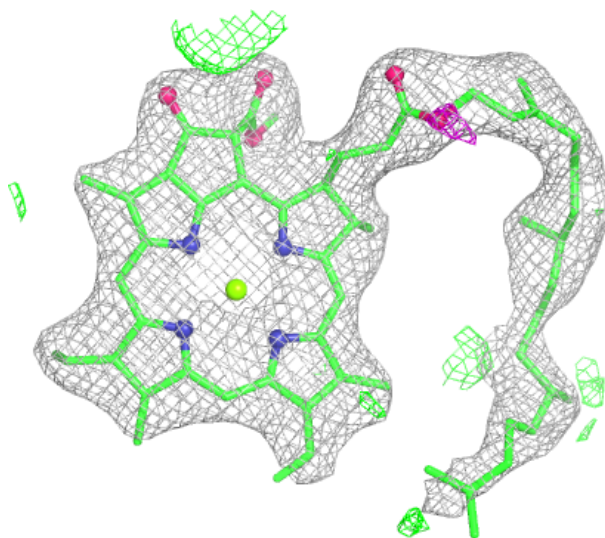
Electron density around HTG b 623:

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



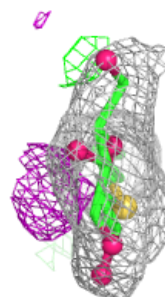
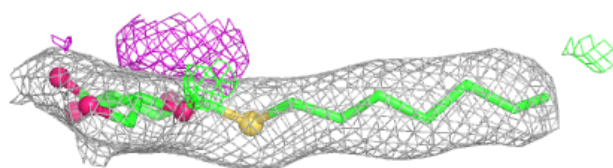
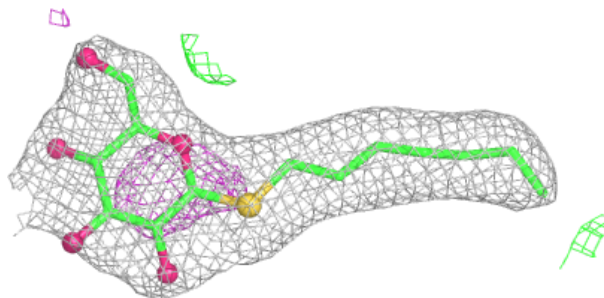
Electron density around CLA c 514:

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

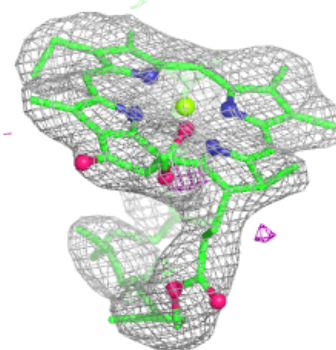
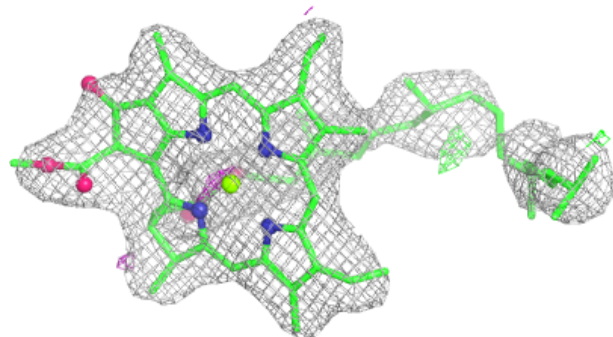
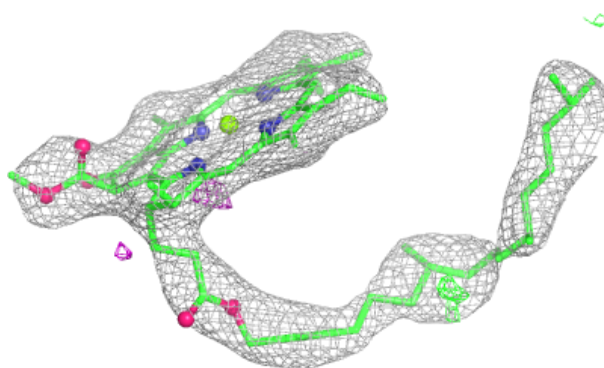


Electron density around HTG B 628:

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

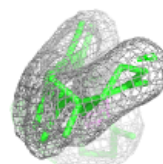
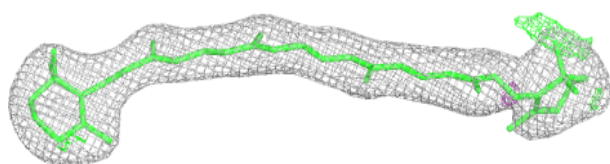
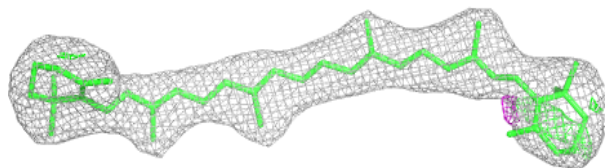
**Electron density around CLA C 514:**

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

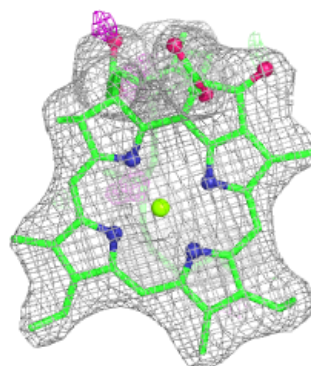
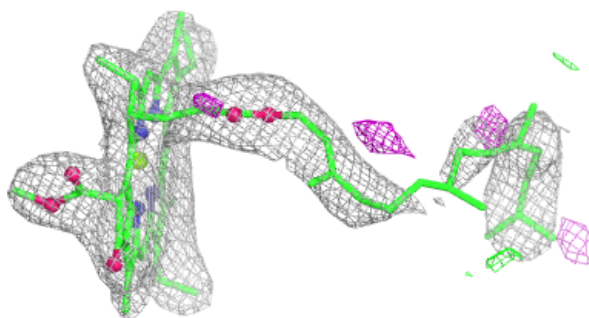
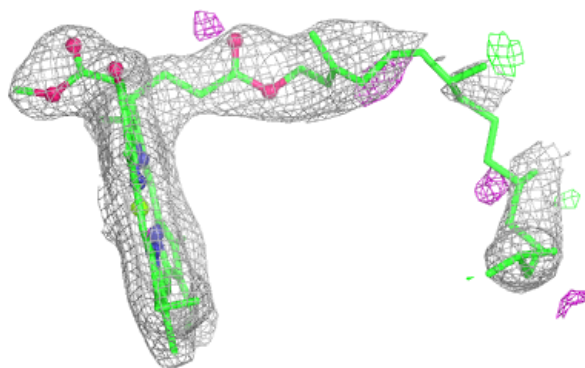


Electron density around BCR d 404:

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

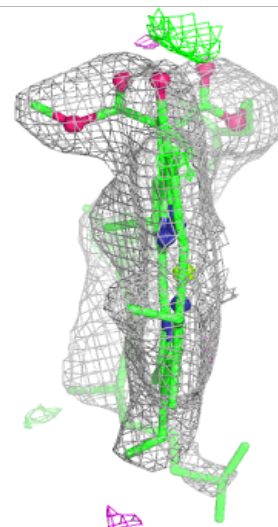
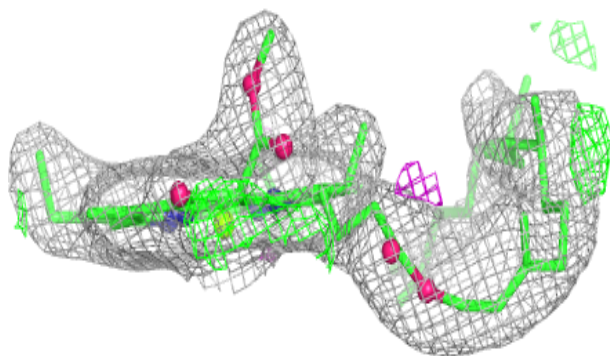
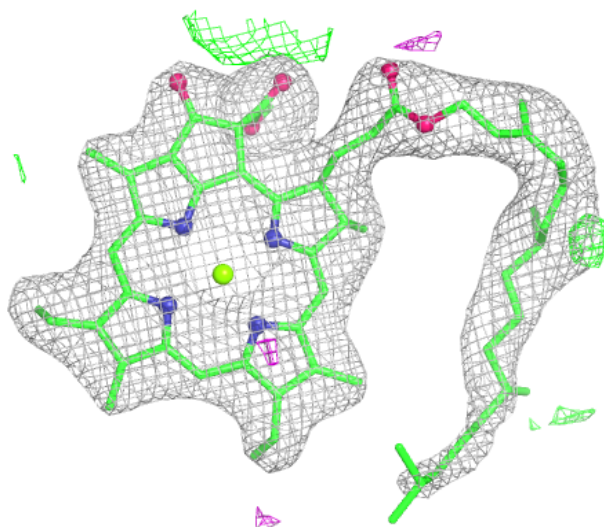
**Electron density around CLA C 507:**

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



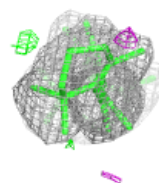
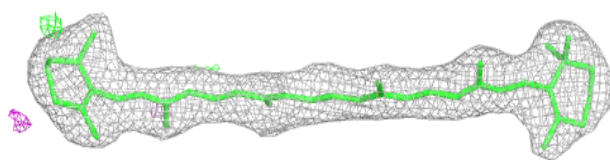
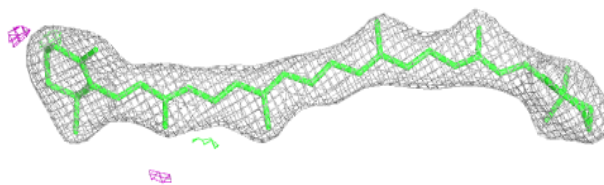
Electron density around CLA C 513:

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



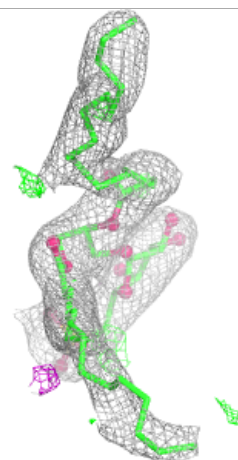
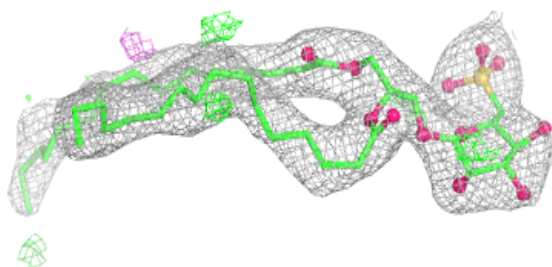
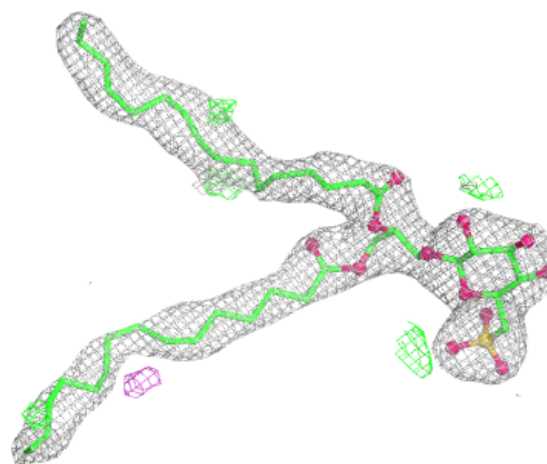
Electron density around BCR C 515:

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



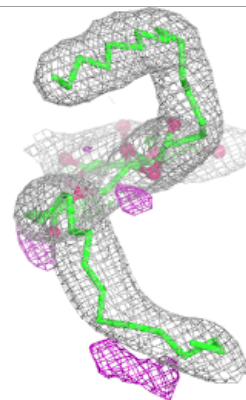
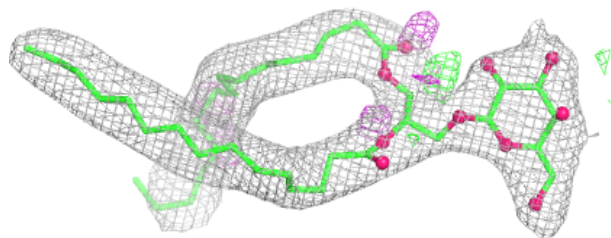
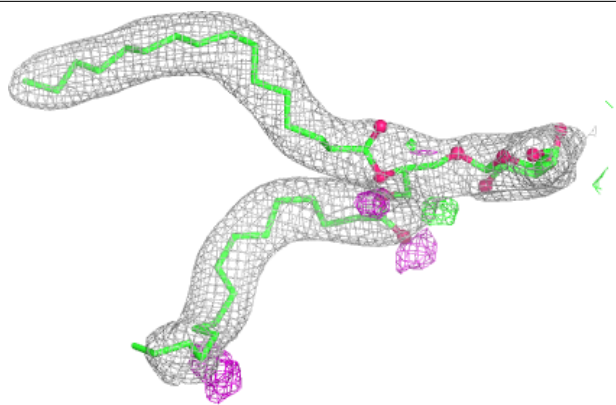
Electron density around SQD a 409:

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

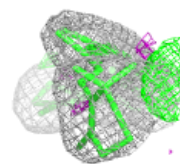
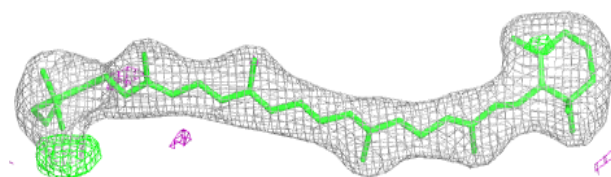
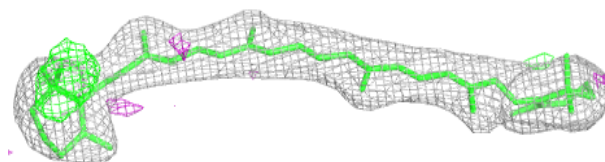


Electron density around LMG b 621:

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

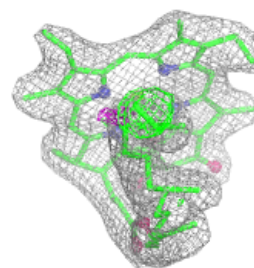
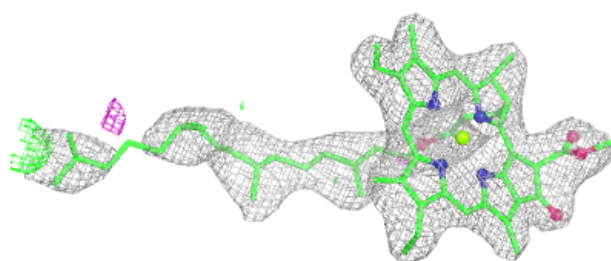
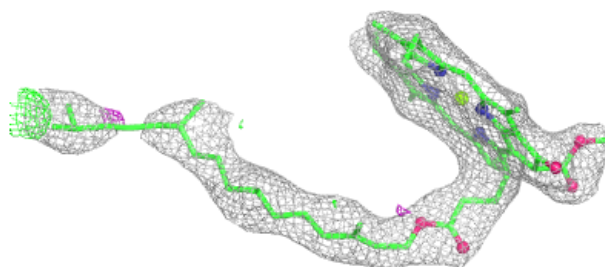
**Electron density around BCR D 404:**

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

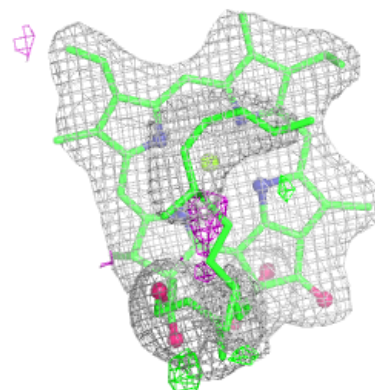
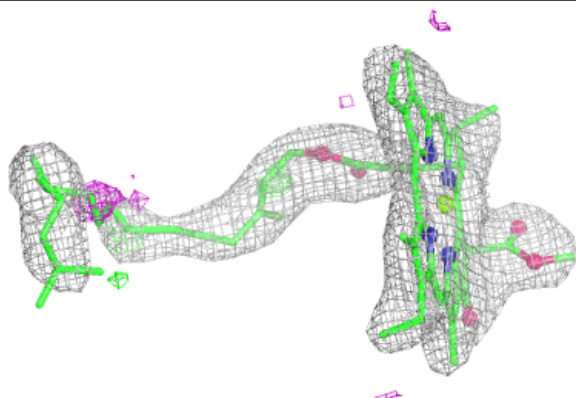
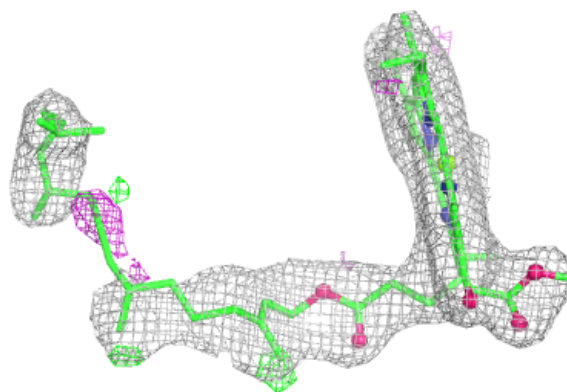


Electron density around CLA c 506:

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

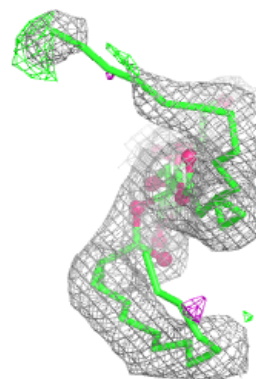
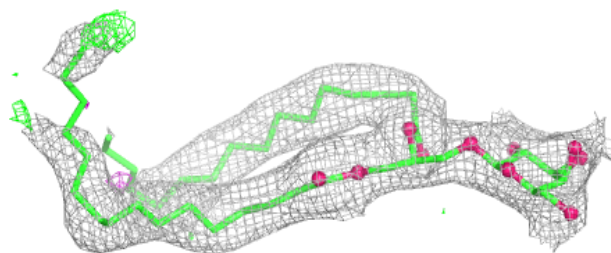
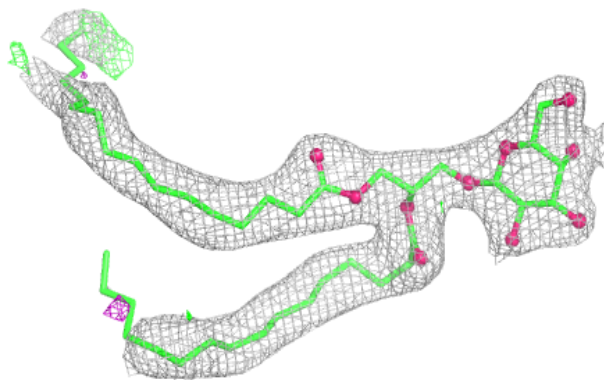
**Electron density around CLA c 508:**

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



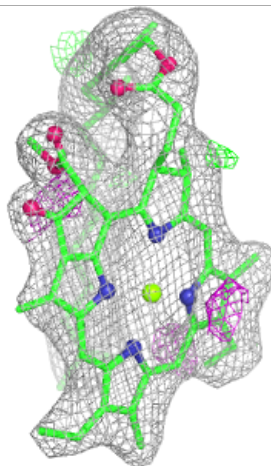
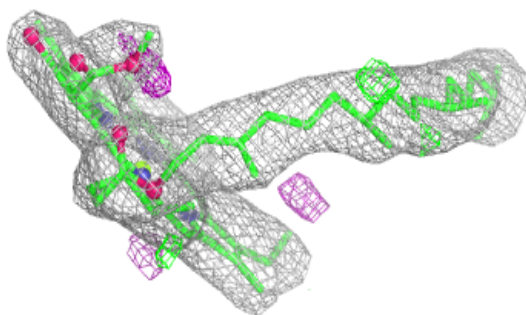
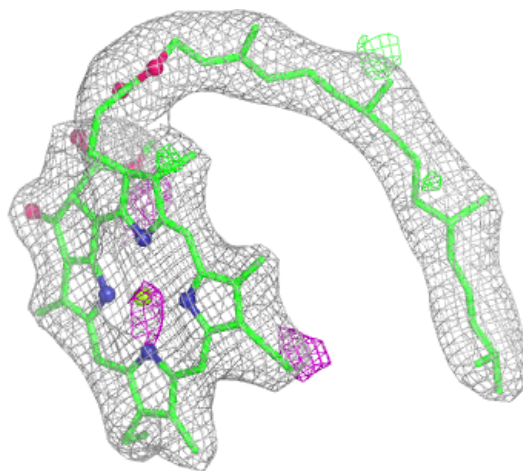
Electron density around LMG J 101:

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



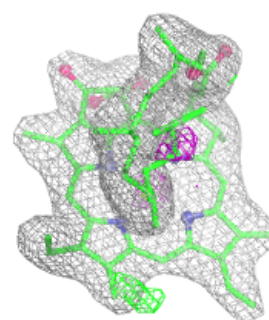
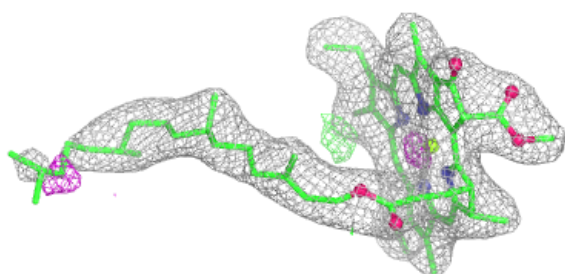
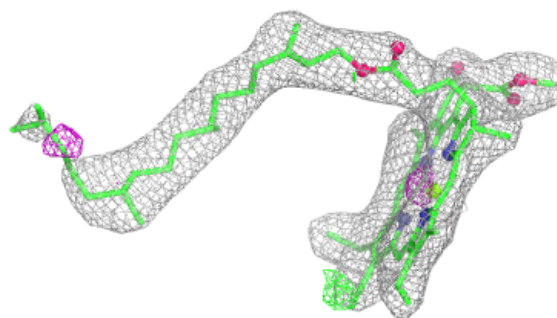
Electron density around CLA c 509:

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

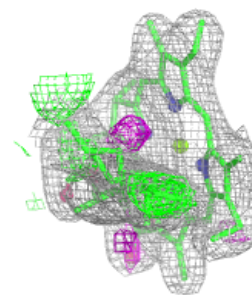
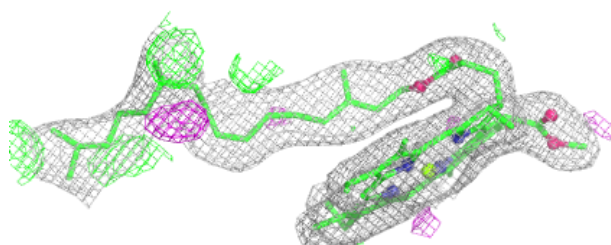
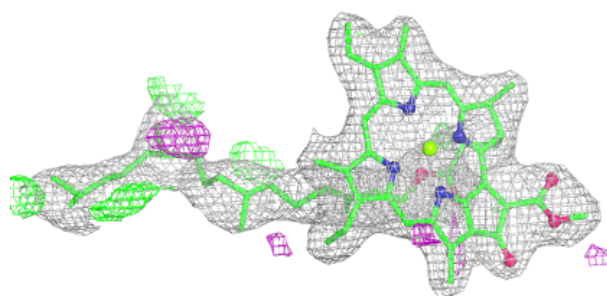


Electron density around CLA C 509:

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

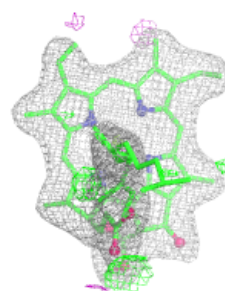
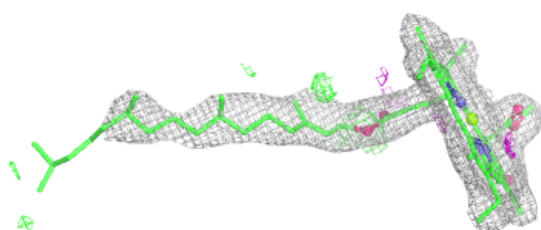
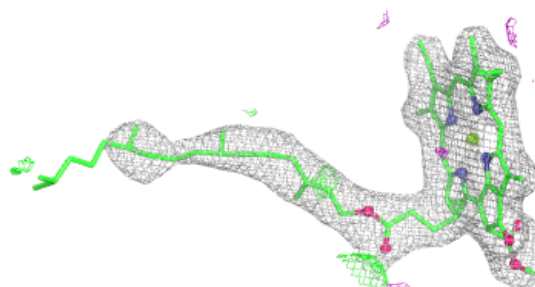
**Electron density around CLA B 614:**

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

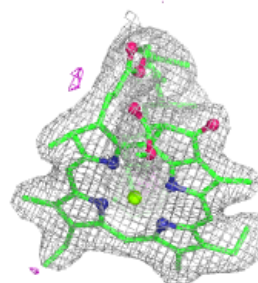
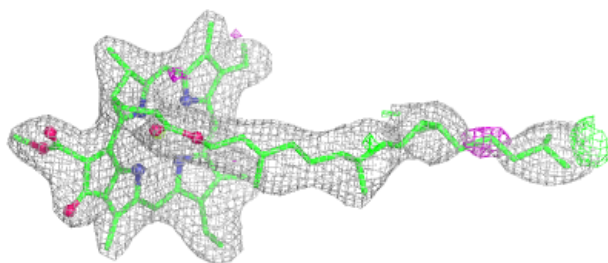
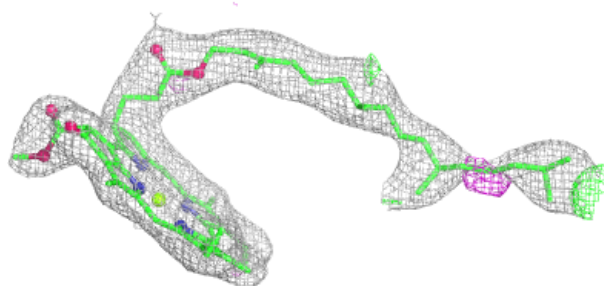


Electron density around CLA d 403:

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

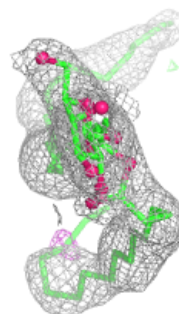
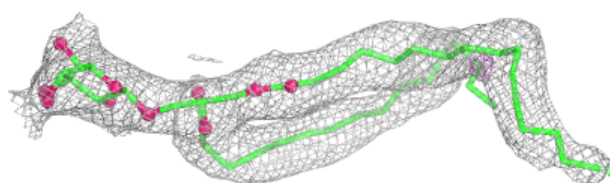
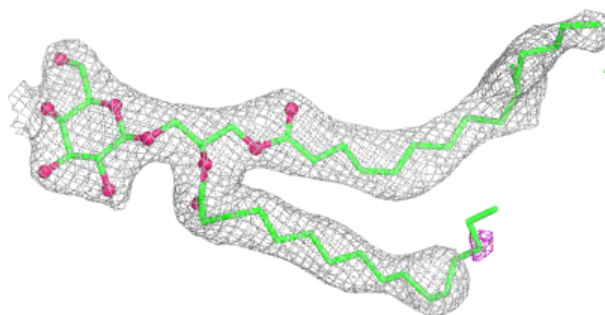
**Electron density around CLA C 505:**

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

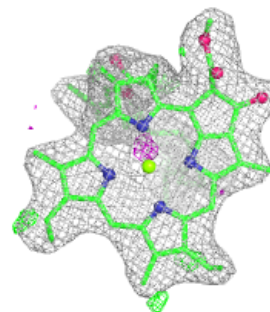
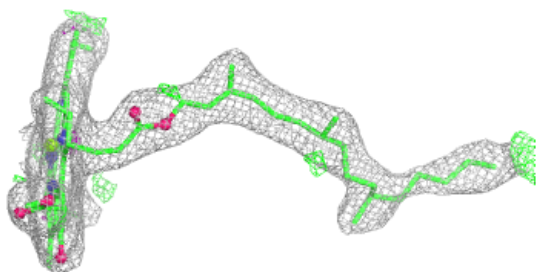
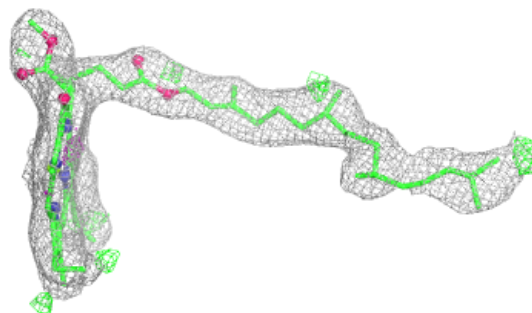


Electron density around LMG j 101:

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

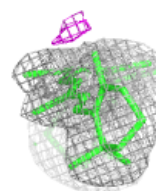
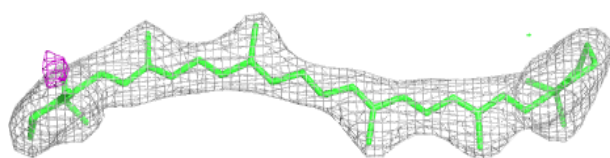
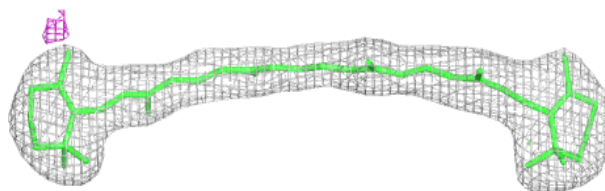
**Electron density around CLA B 606:**

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

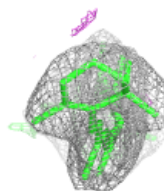
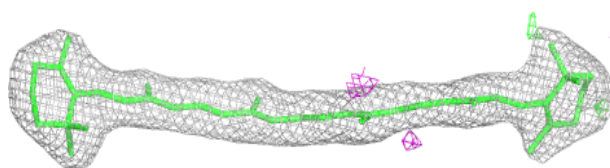
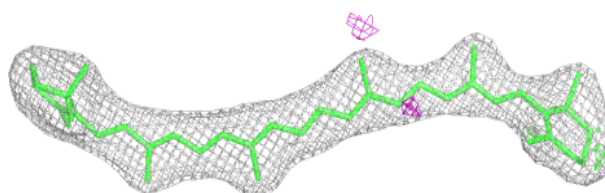


Electron density around BCR K 102:

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

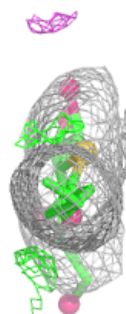
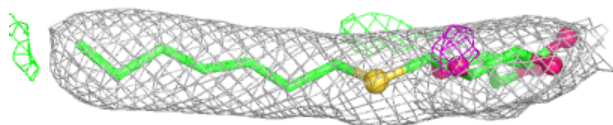
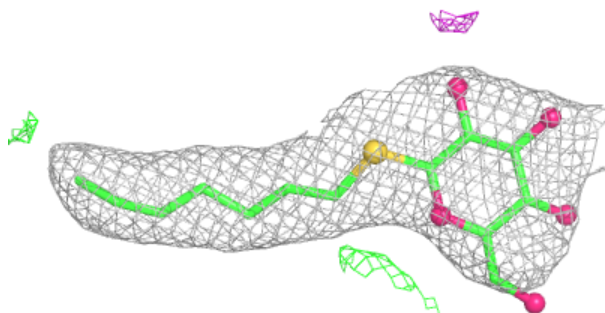
**Electron density around BCR Y 101:**

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

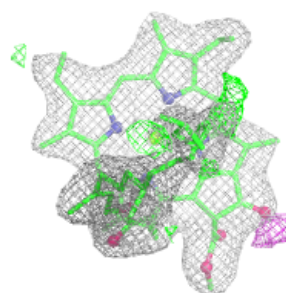
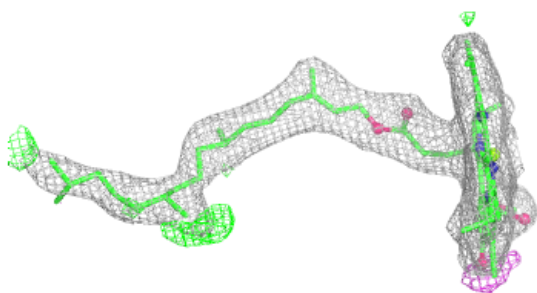
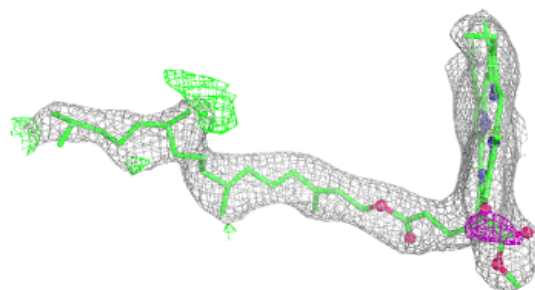


Electron density around HTG b 628:

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

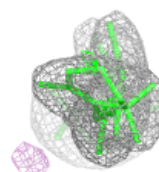
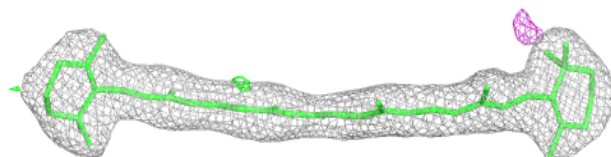
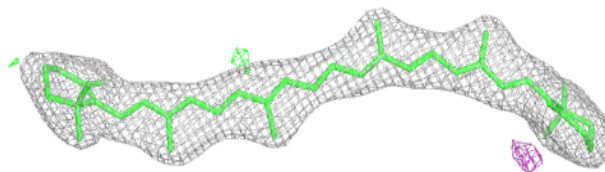
**Electron density around CLA b 606:**

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

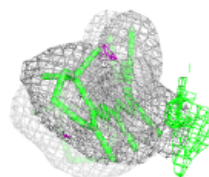
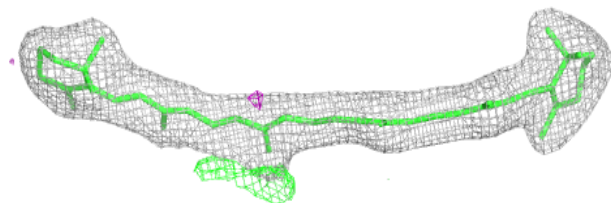
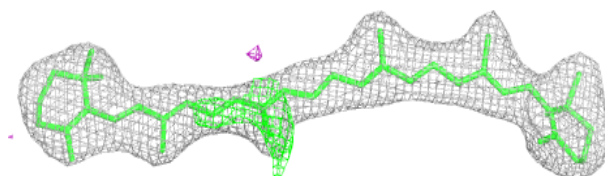


Electron density around BCR h 102:

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

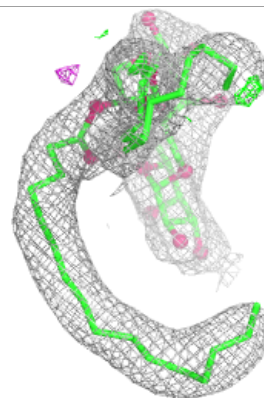
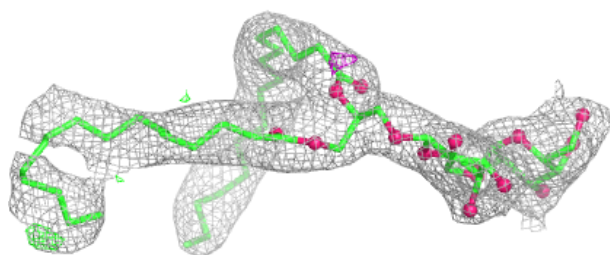
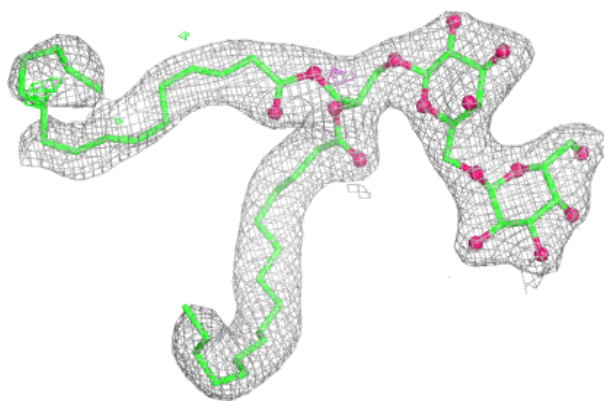
**Electron density around BCR t 102:**

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

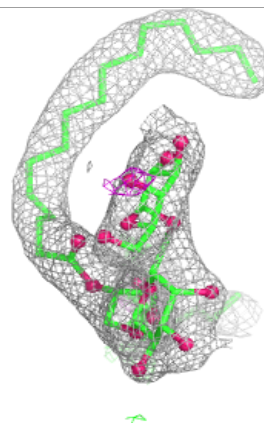
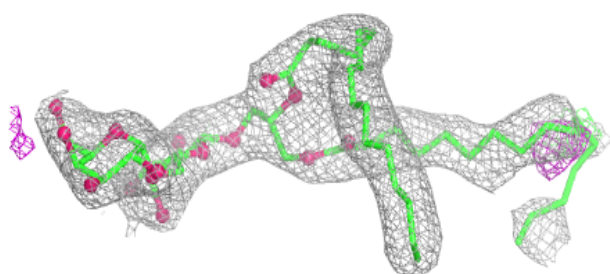
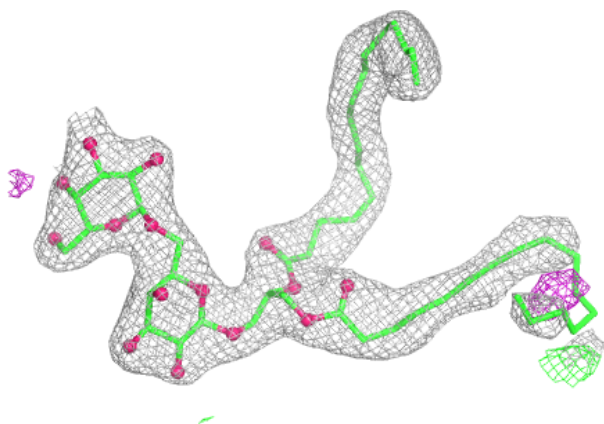


Electron density around DGD C 518:

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

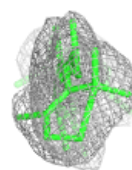
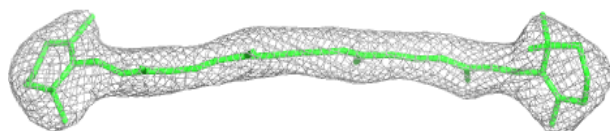
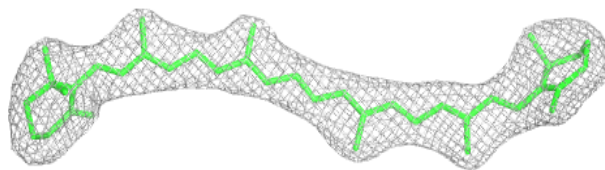
**Electron density around DGD c 519:**

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

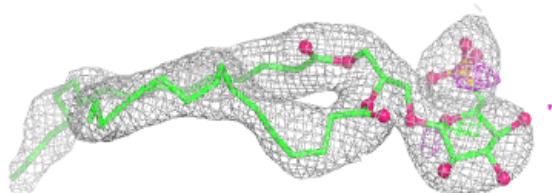
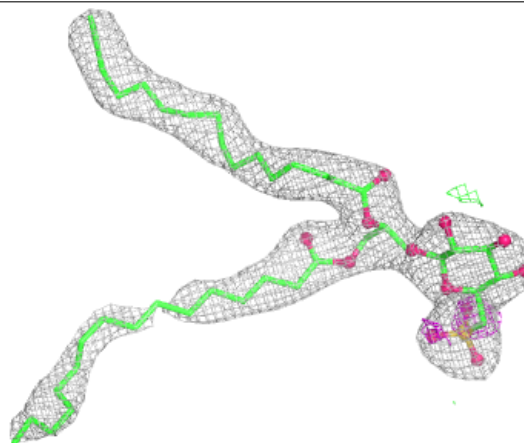


Electron density around BCR y 101:

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

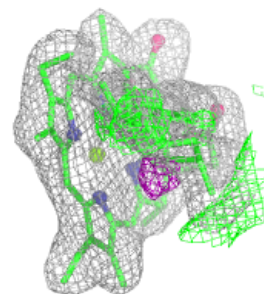
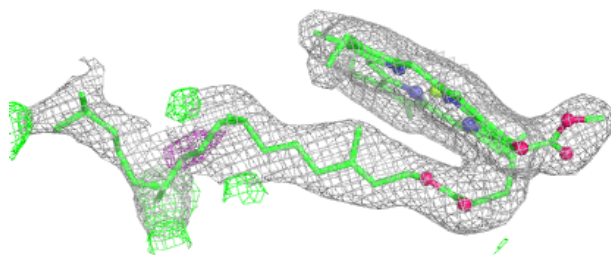
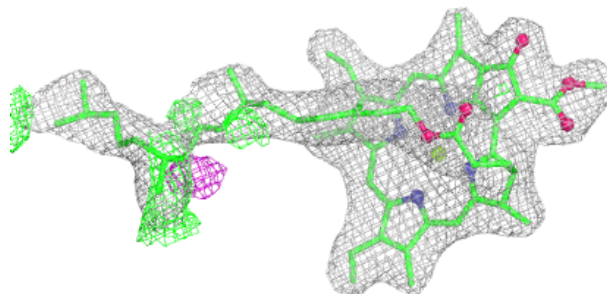
**Electron density around SQD A 411:**

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

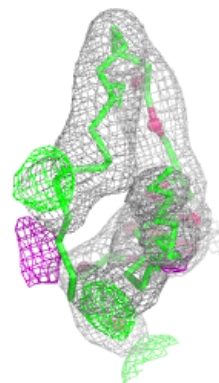
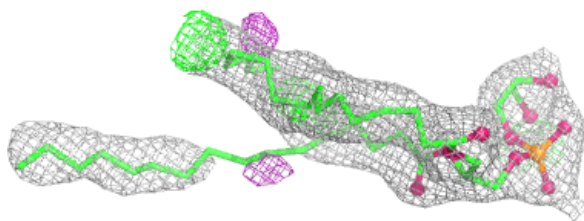
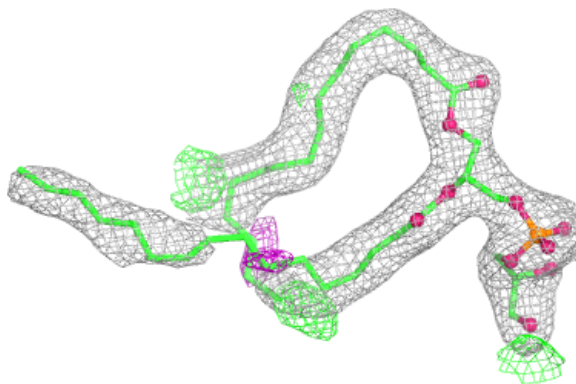


Electron density around CLA b 614:

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

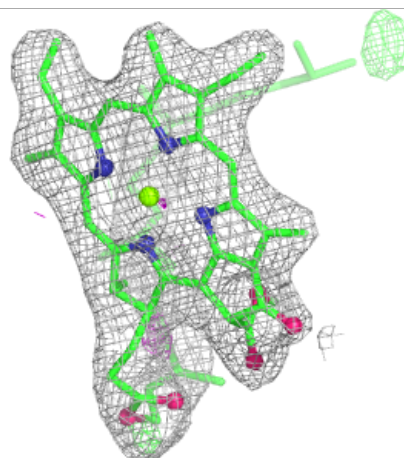
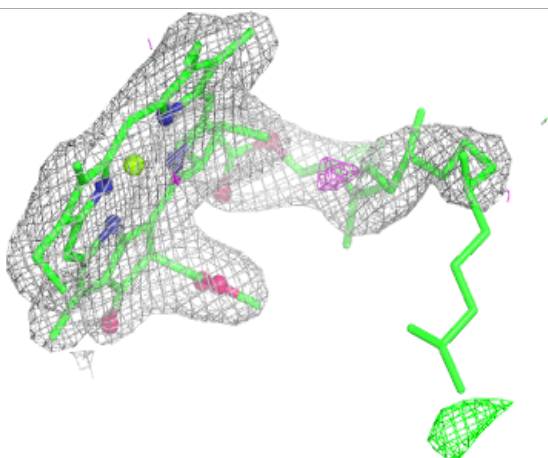
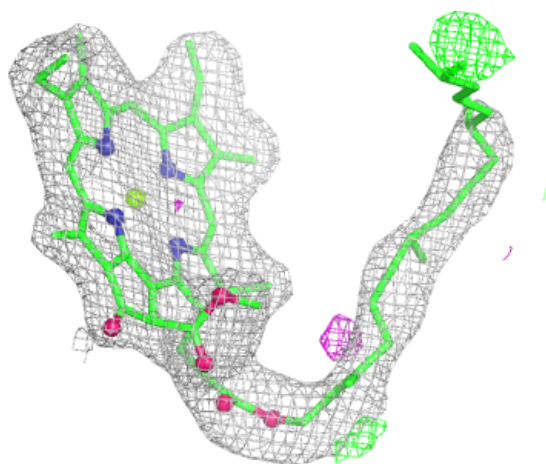
**Electron density around LHG D 407:**

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



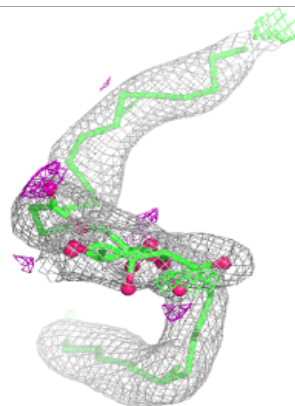
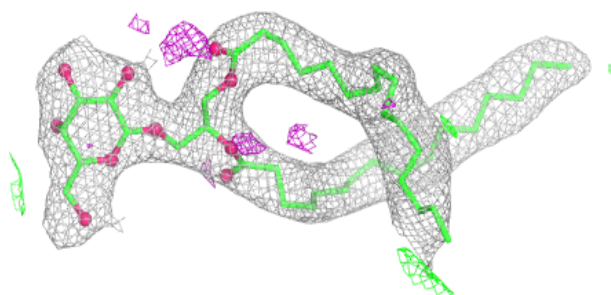
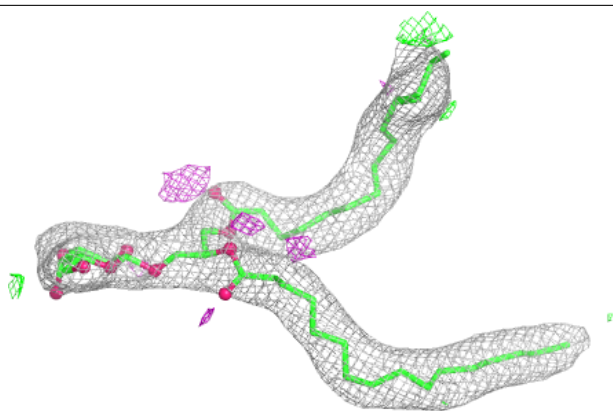
Electron density around CLA b 616:

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

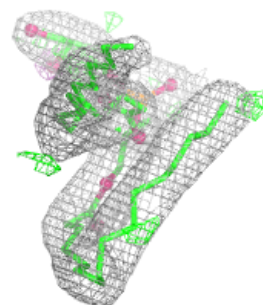
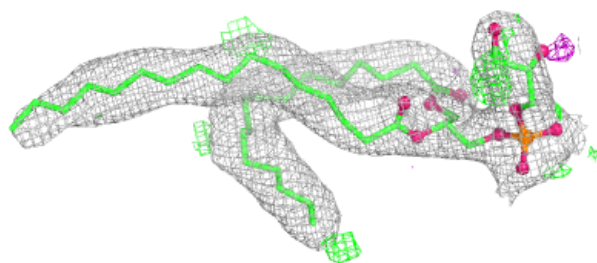
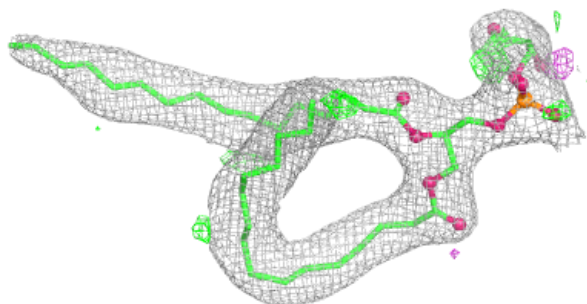


Electron density around LMG B 621:

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

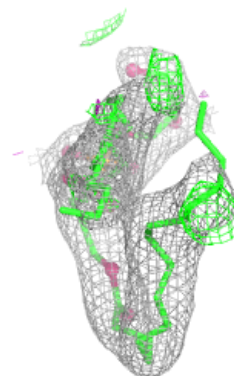
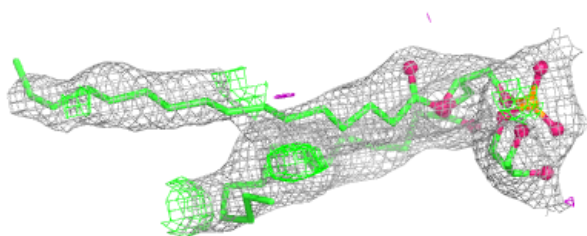
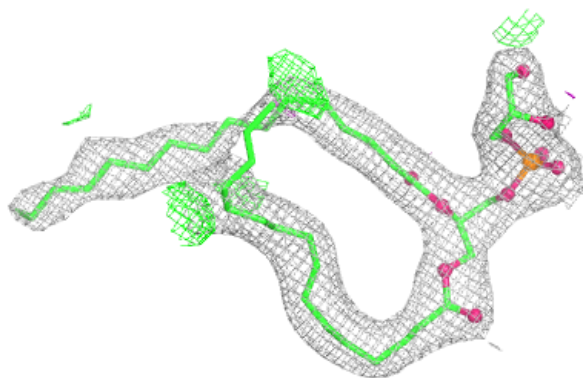
**Electron density around LHG d 406:**

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

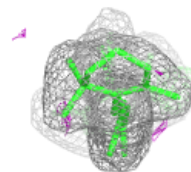
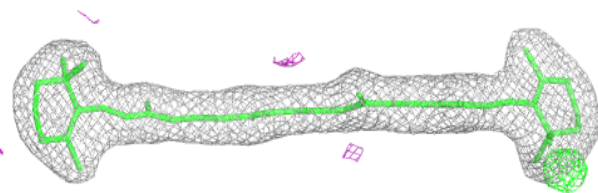
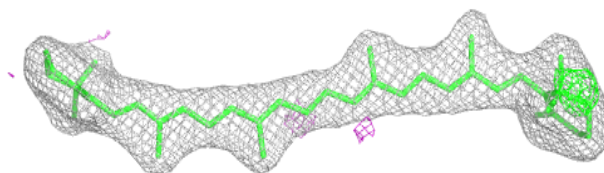


Electron density around LHG d 408:

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

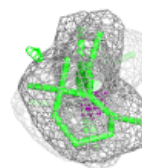
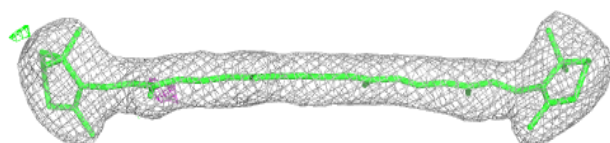
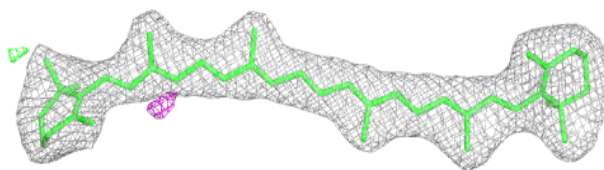
**Electron density around BCR A 410:**

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

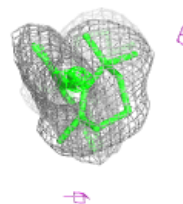
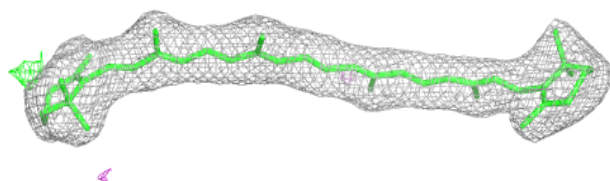
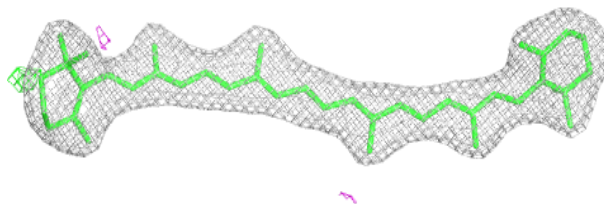


Electron density around BCR B 618:

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

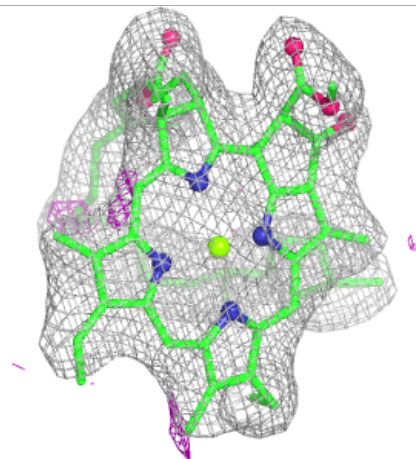
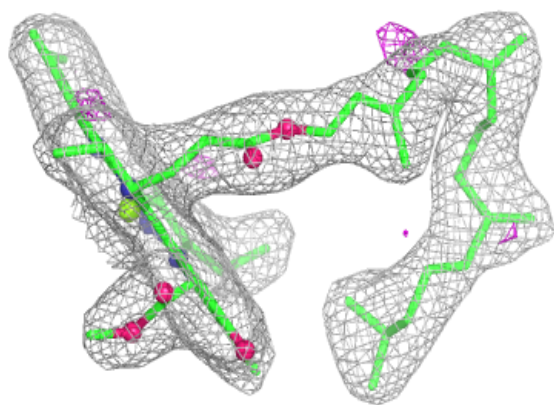
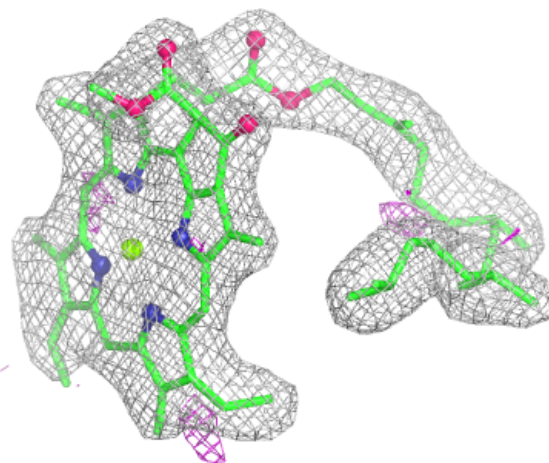
**Electron density around BCR B 619:**

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



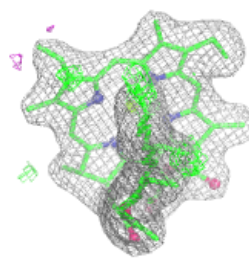
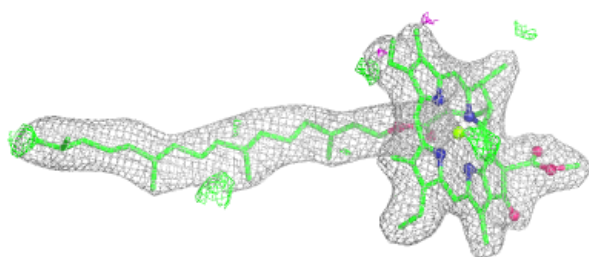
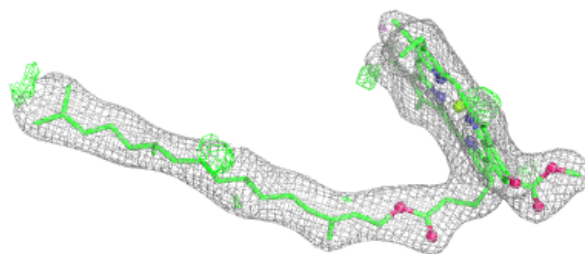
Electron density around CLA C 504:

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

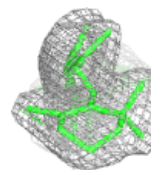
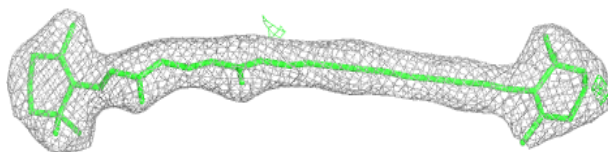
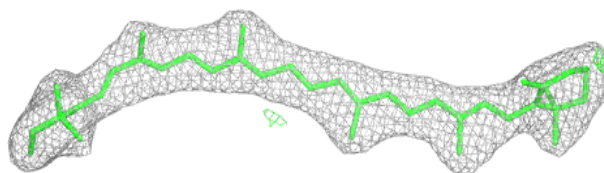


Electron density around CLA b 607:

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

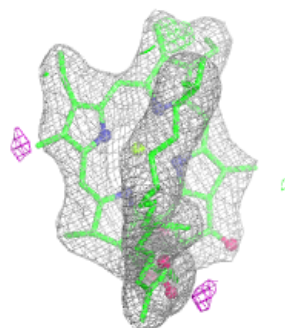
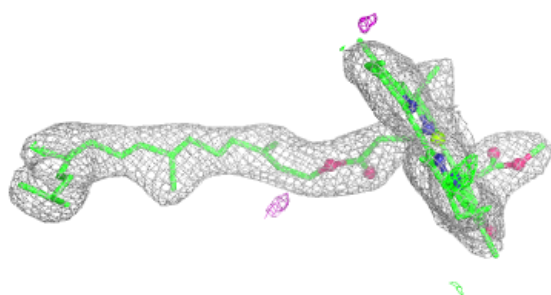
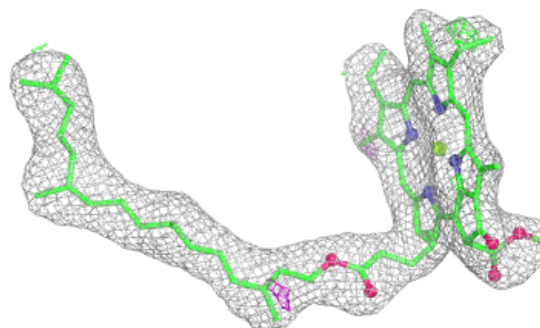
**Electron density around BCR H 101:**

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

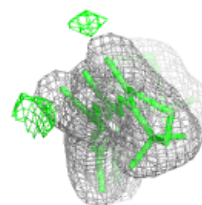
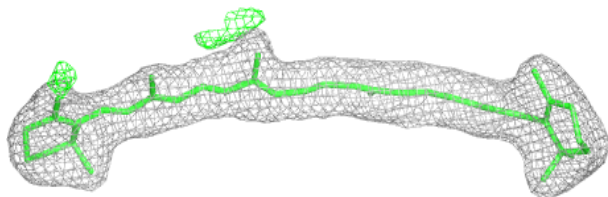
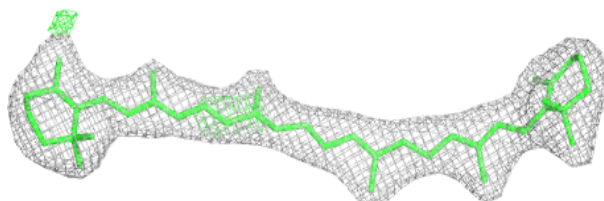


Electron density around CLA b 609:

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

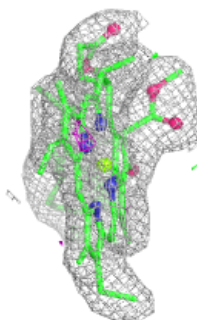
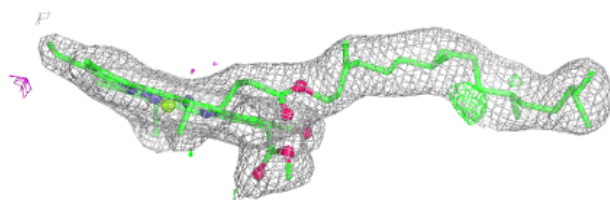
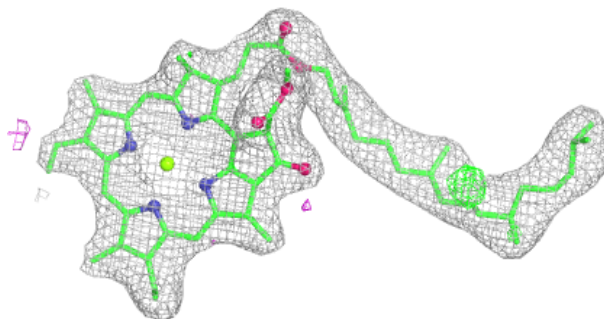
**Electron density around BCR T 101:**

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

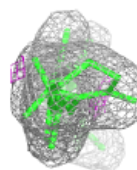
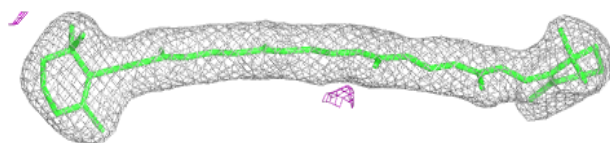
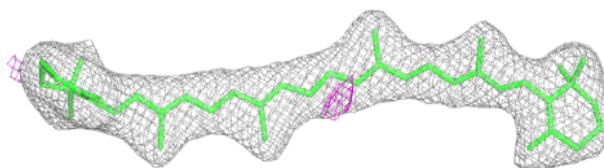


Electron density around CLA B 602:

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

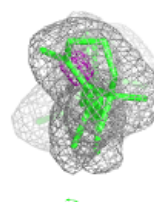
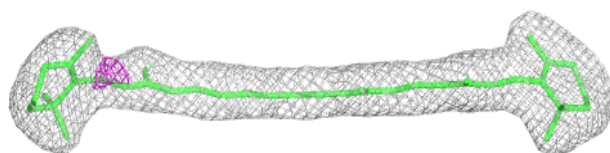
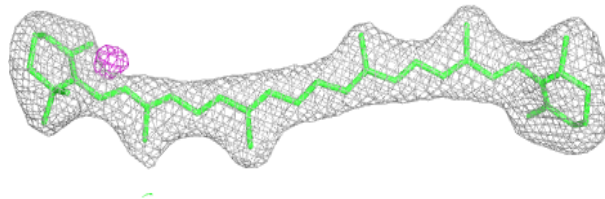
**Electron density around BCR b 617:**

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

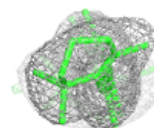
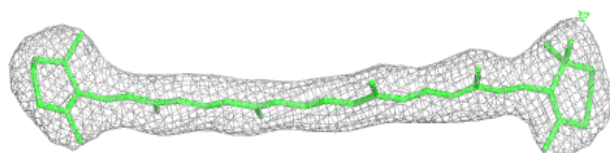
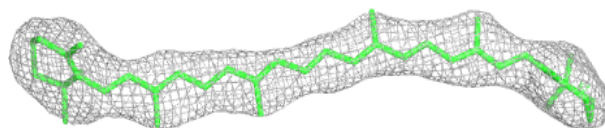


Electron density around BCR b 618:

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

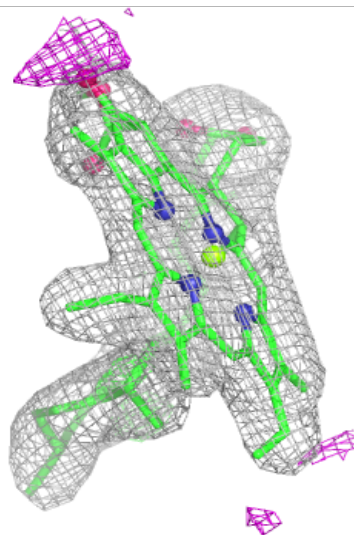
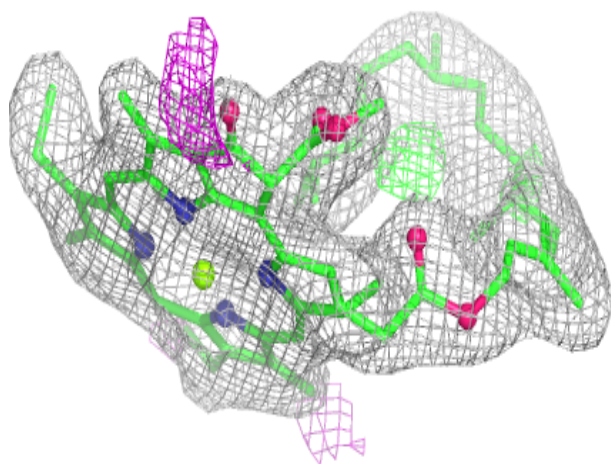
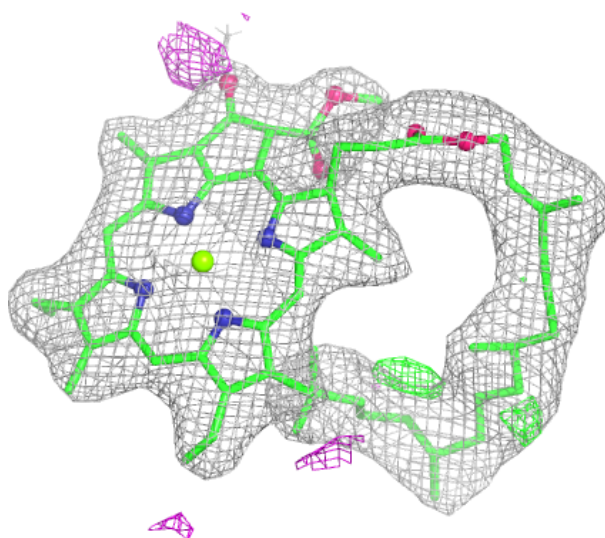
**Electron density around BCR c 516:**

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



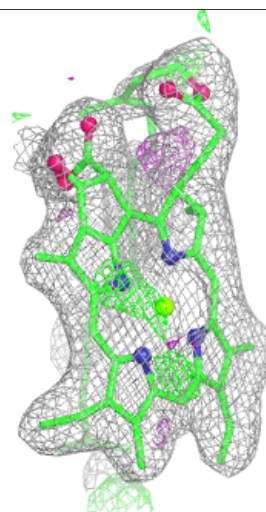
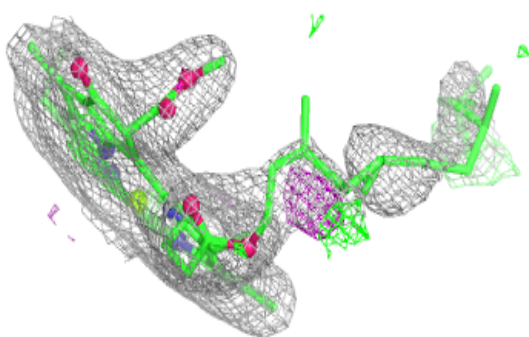
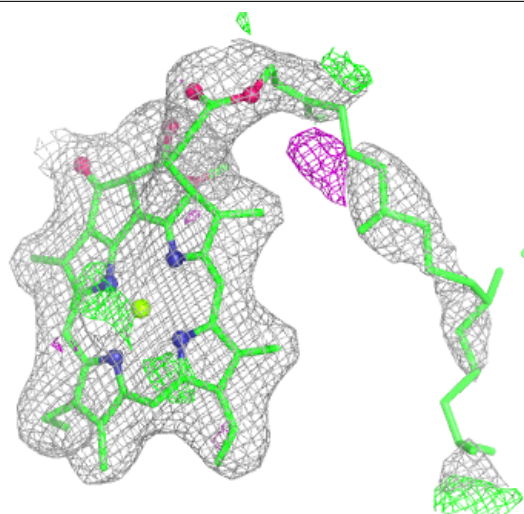
Electron density around CLA b 615:

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



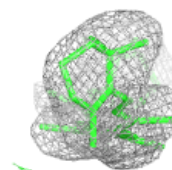
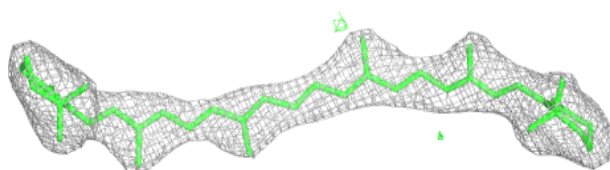
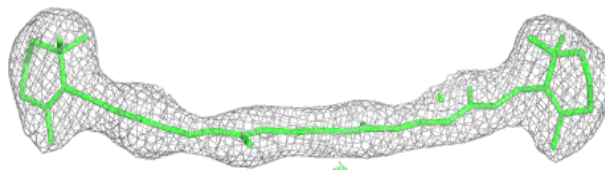
Electron density around CLA B 616:

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

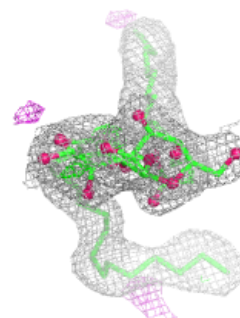
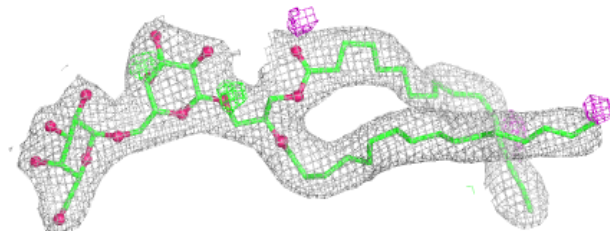
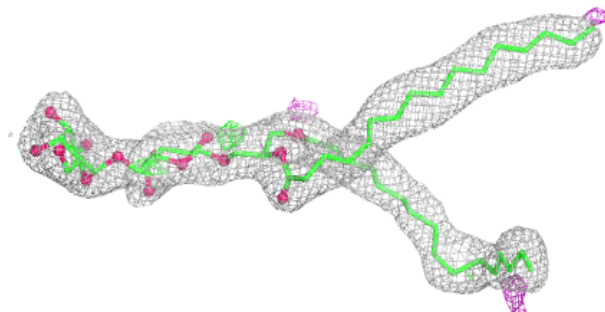


Electron density around BCR k 101:

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

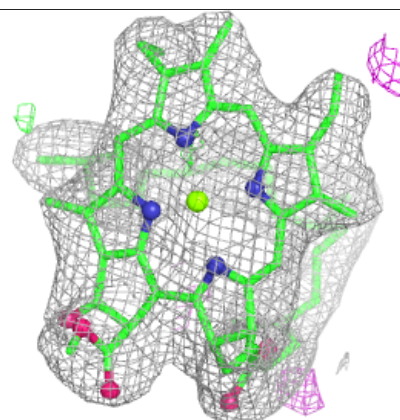
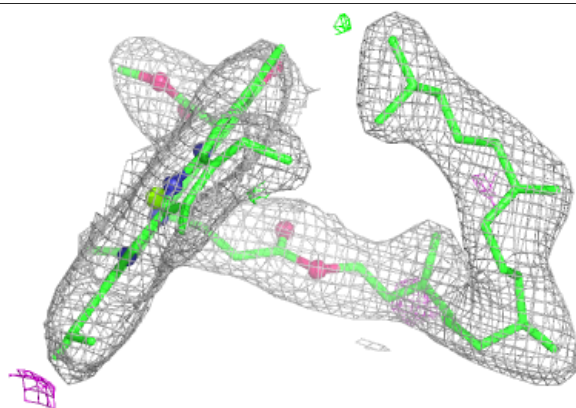
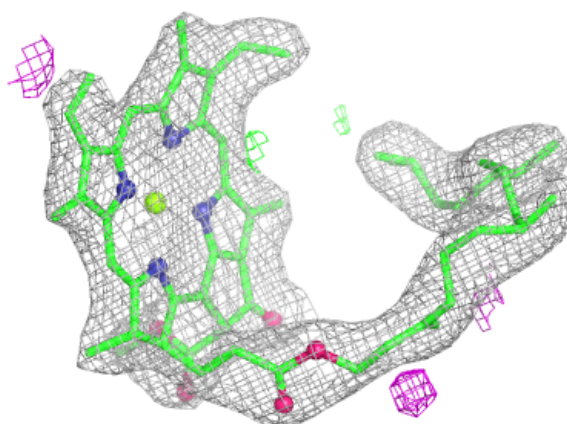
**Electron density around DGD C 517:**

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

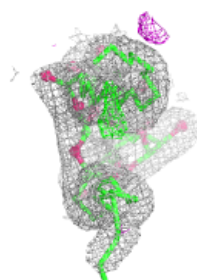
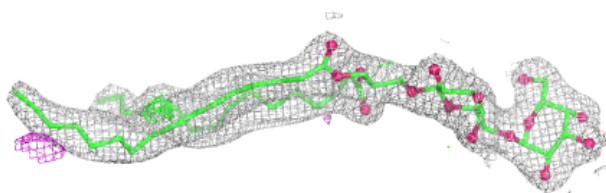
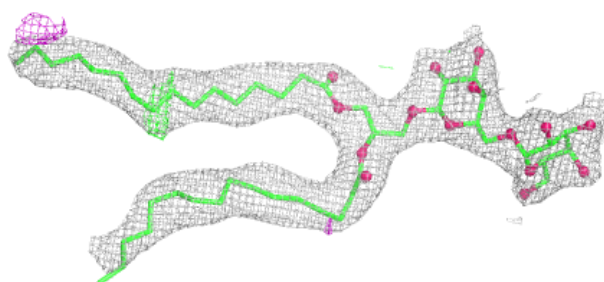


Electron density around CLA c 505:

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

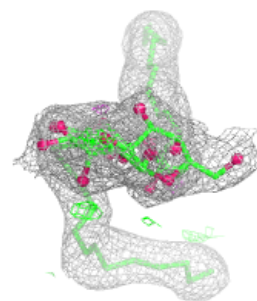
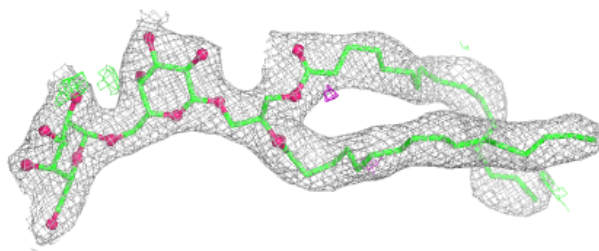
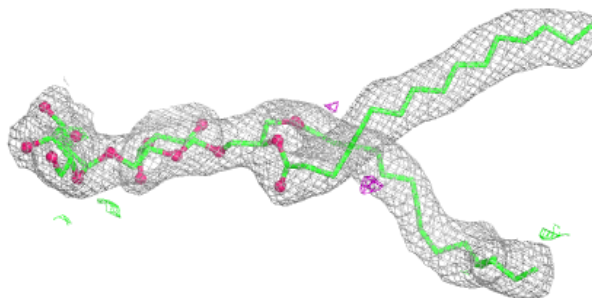
**Electron density around DGD C 519:**

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

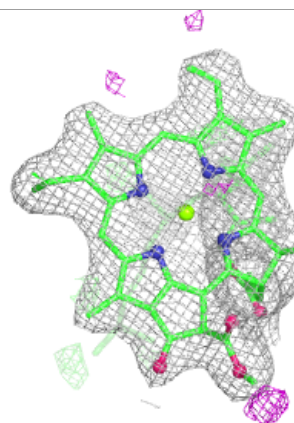
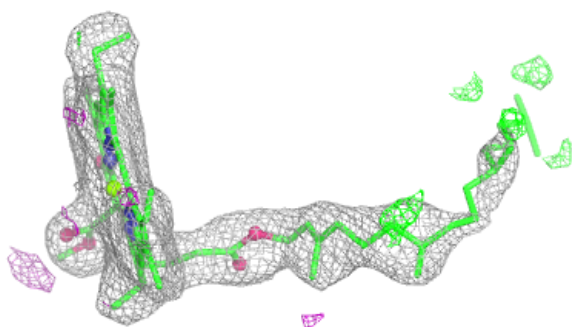
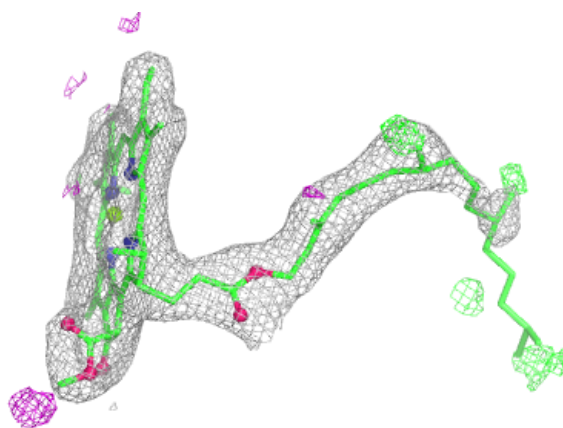


Electron density around DGD c 518:

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

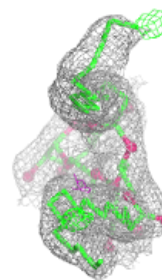
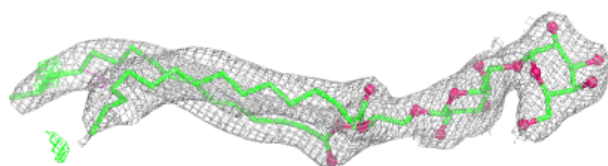
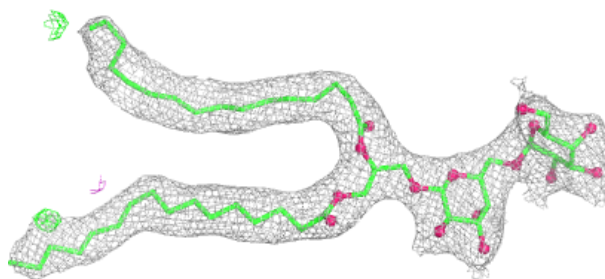
**Electron density around CLA D 403:**

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

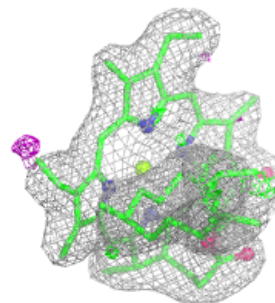
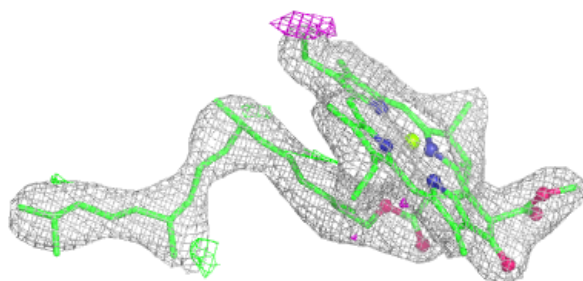
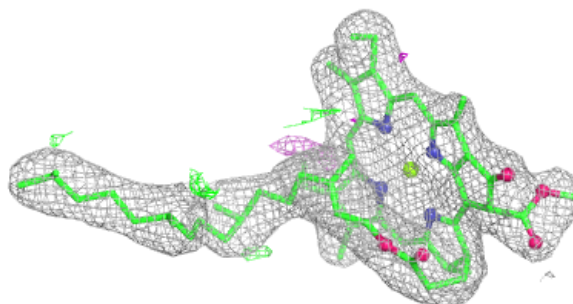


Electron density around DGD c 520:

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

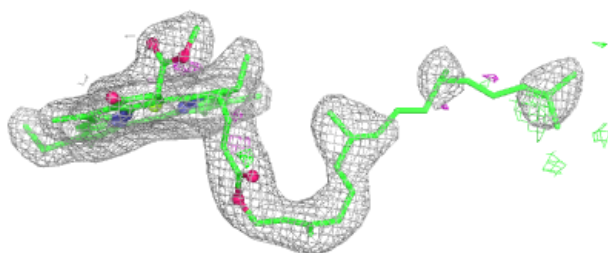
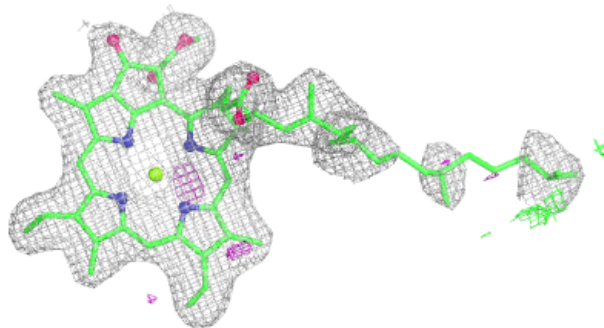
**Electron density around CLA c 507:**

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

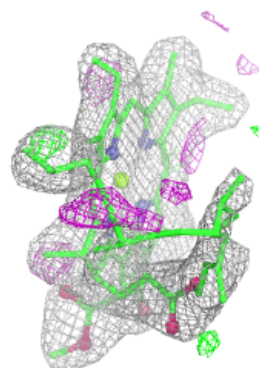
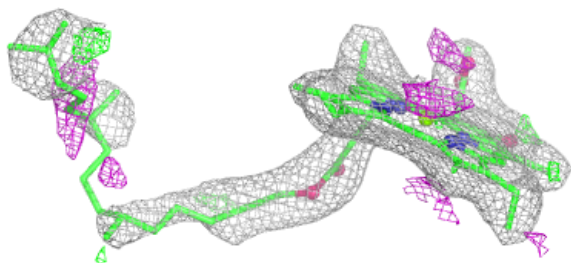
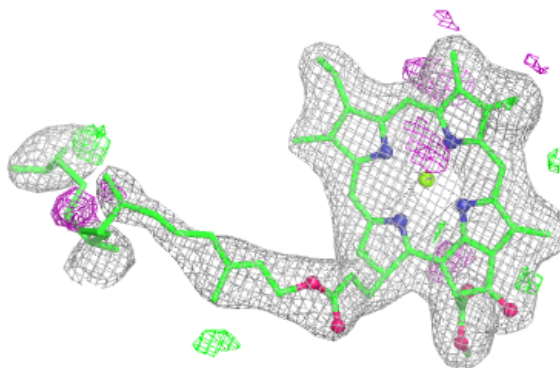


Electron density around CLA a 404:

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

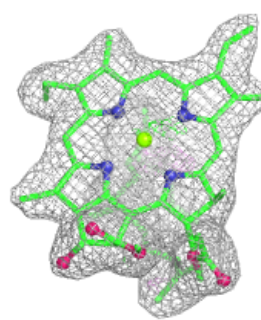
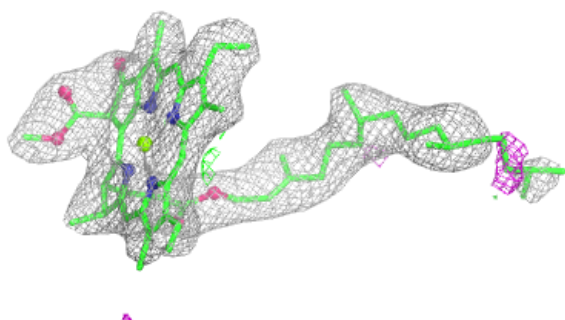
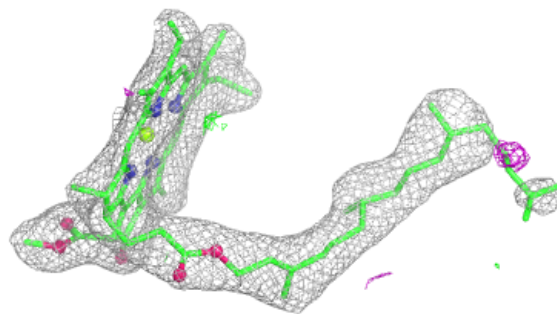
**Electron density around CLA a 407:**

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



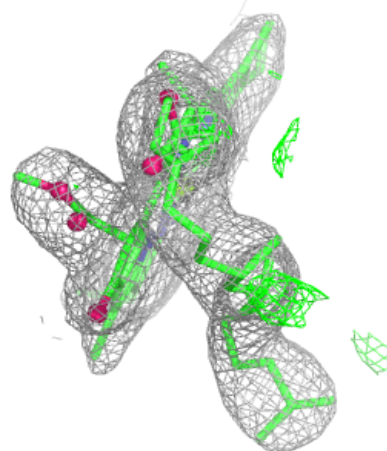
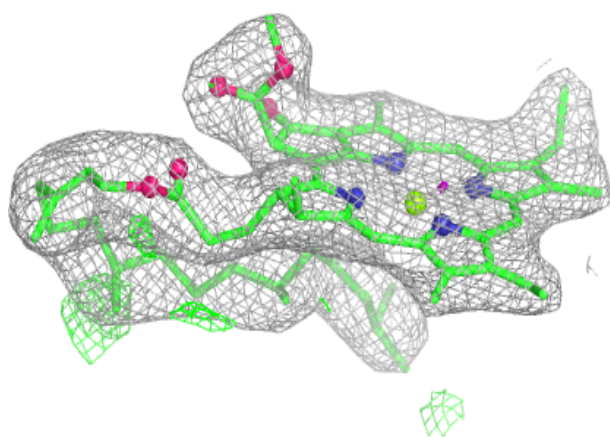
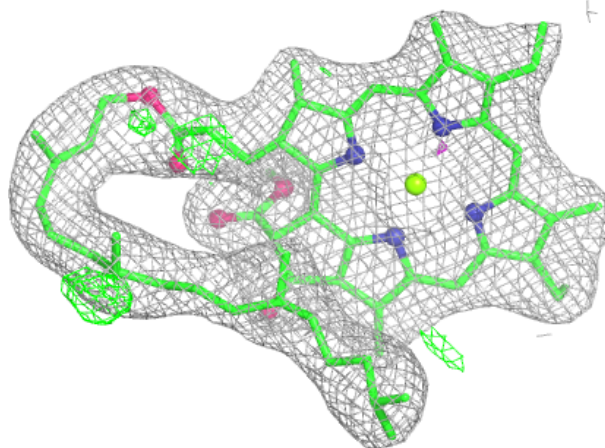
Electron density around CLA c 510:

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



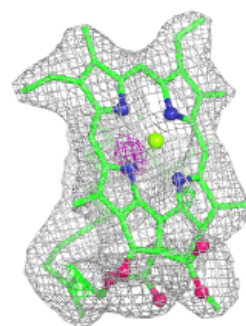
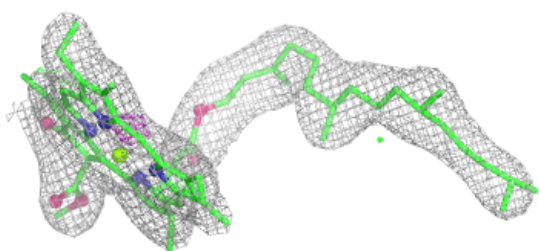
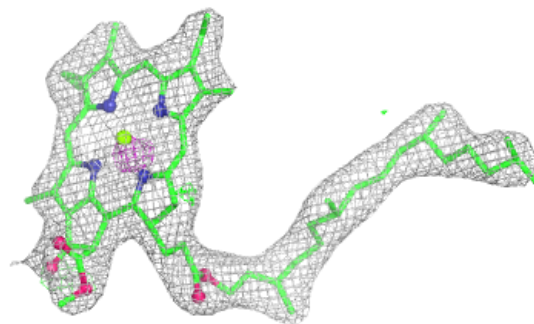
Electron density around CLA c 511:

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

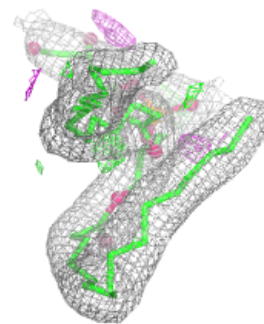
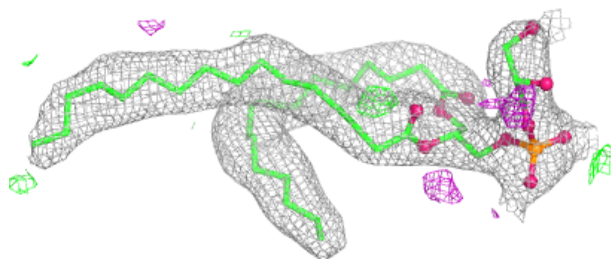
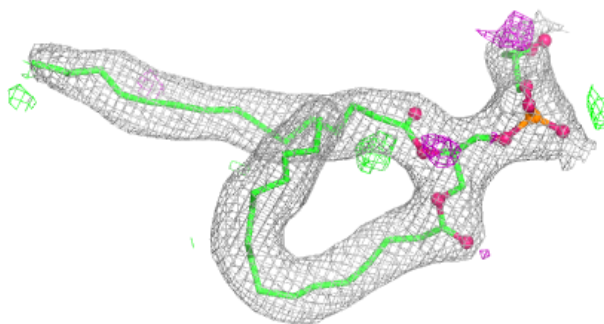


Electron density around CLA c 513:

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

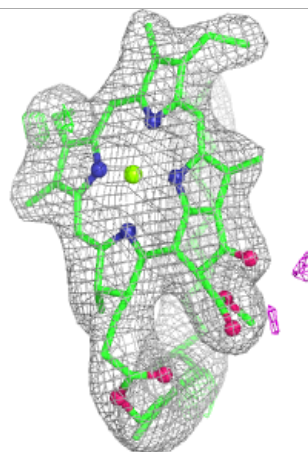
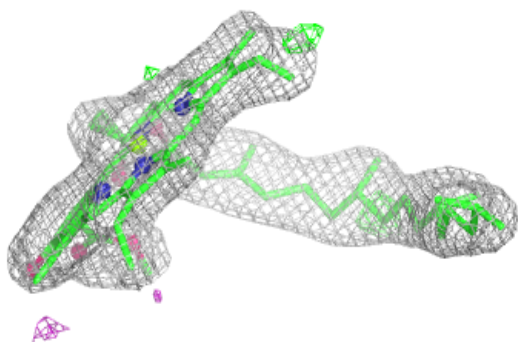
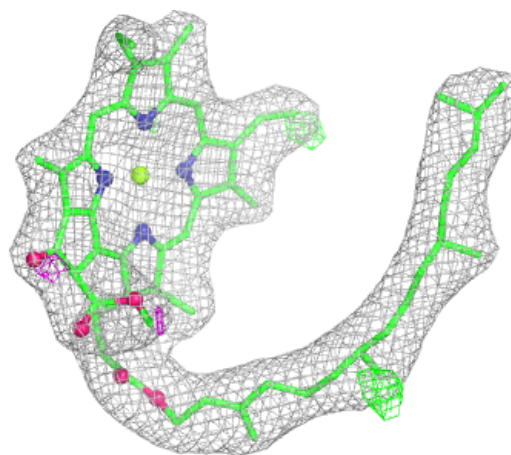
**Electron density around LHG D 357:**

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



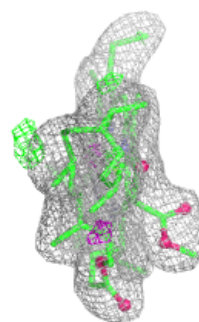
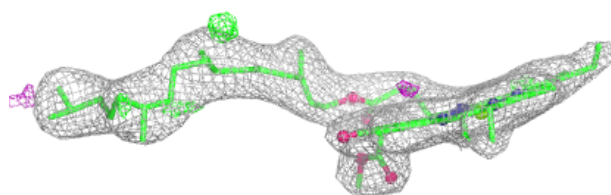
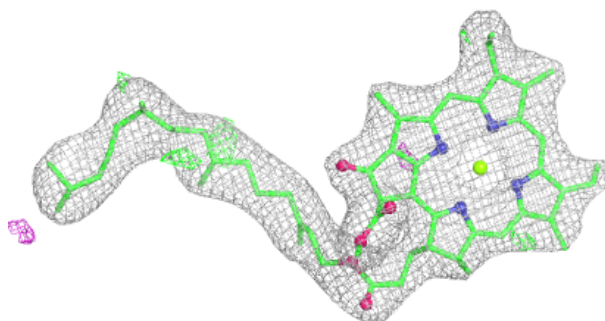
Electron density around CLA C 508:

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

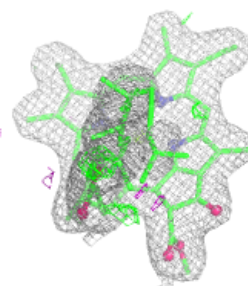
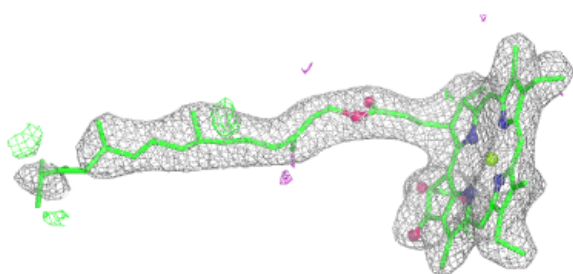
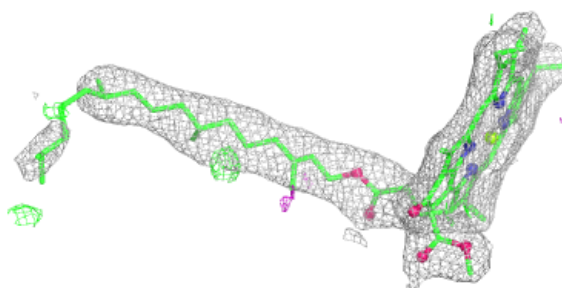


Electron density around CLA b 602:

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

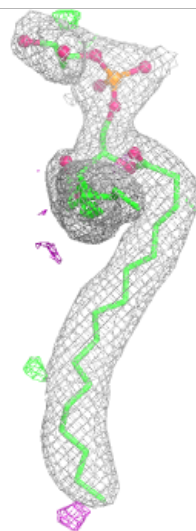
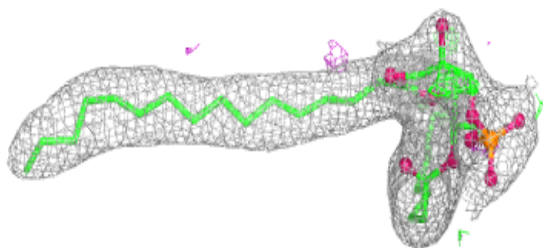
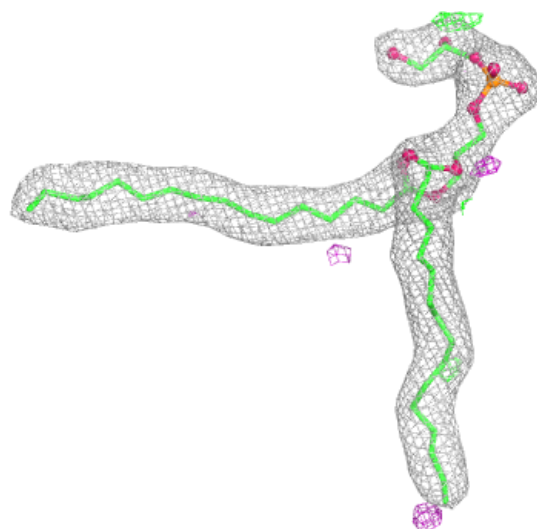
**Electron density around CLA b 604:**

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



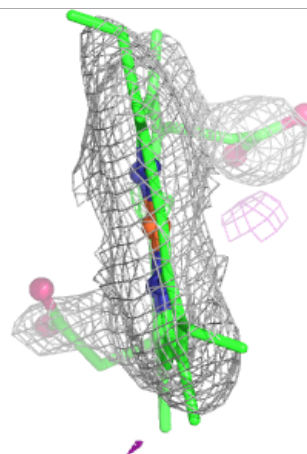
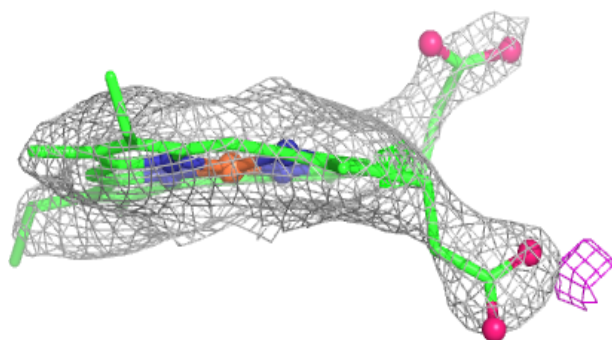
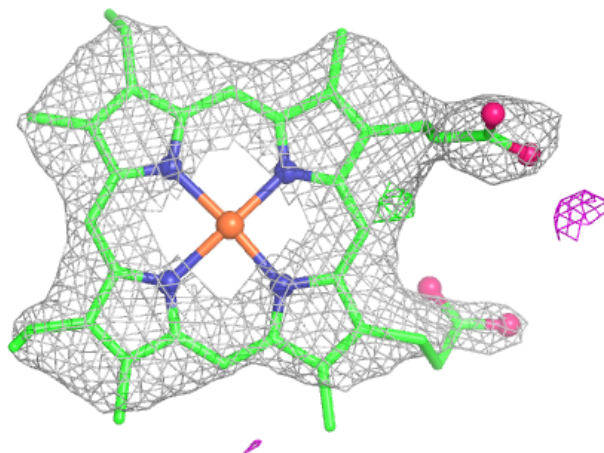
Electron density around LHG 1 101:

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



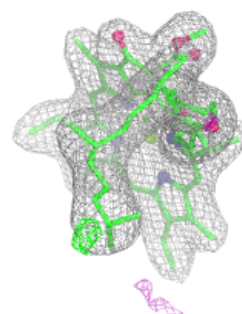
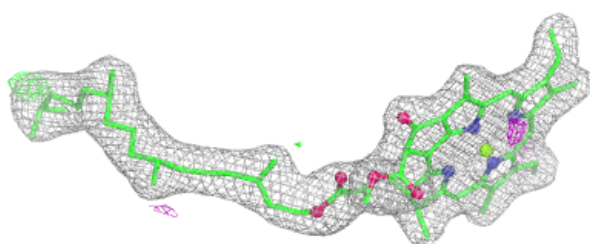
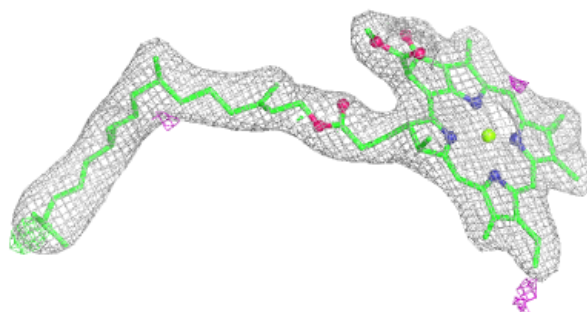
Electron density around HEM e 102:

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

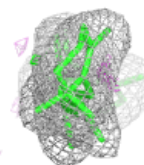
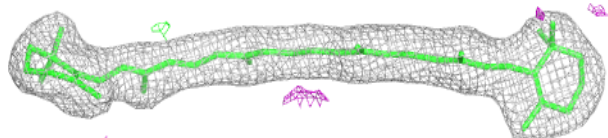
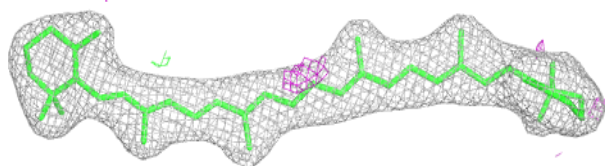


Electron density around CLA a 403:

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

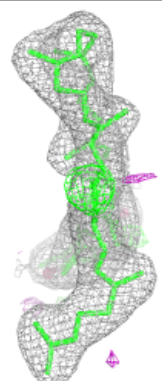
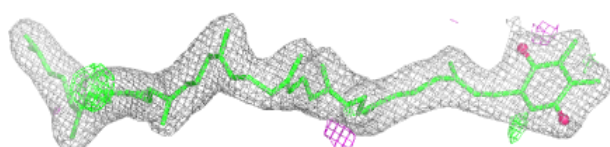
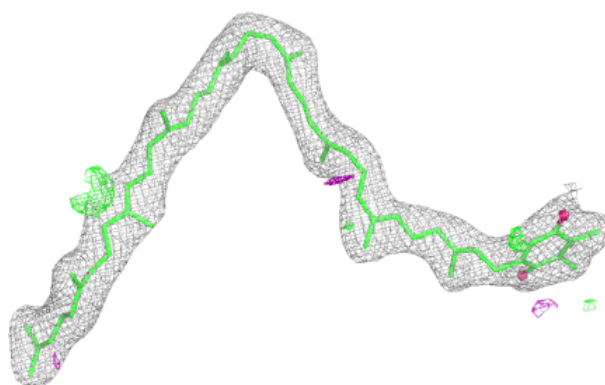
**Electron density around BCR B 617:**

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

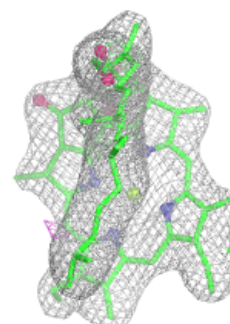
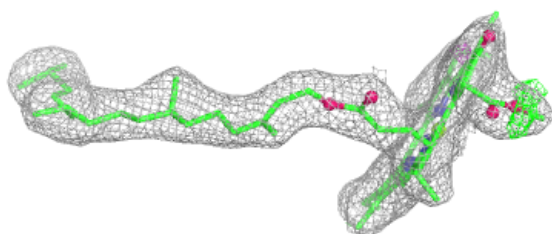
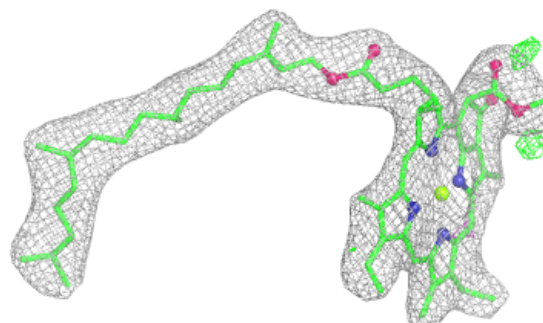


Electron density around PL9 D 405:

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

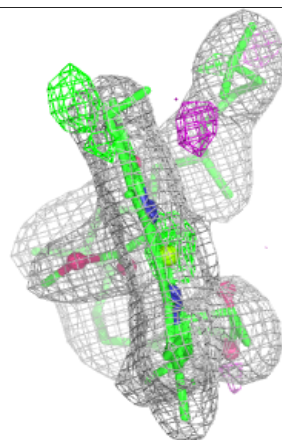
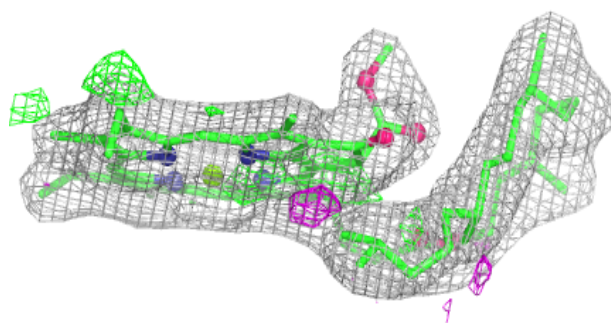
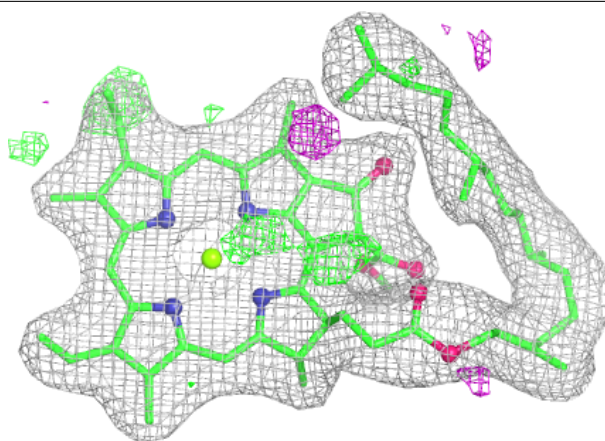
**Electron density around CLA B 609:**

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

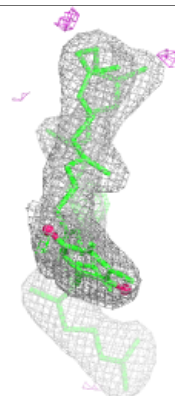
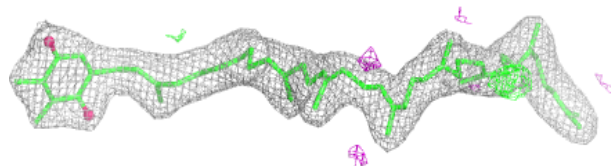
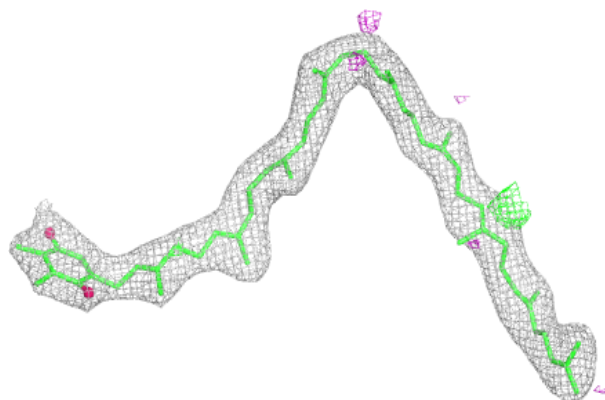


Electron density around CLA B 610:

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

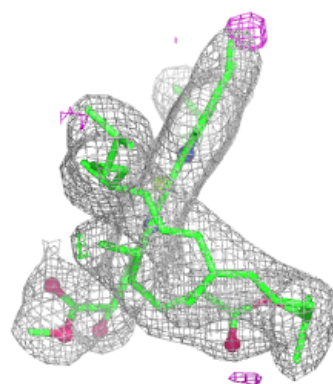
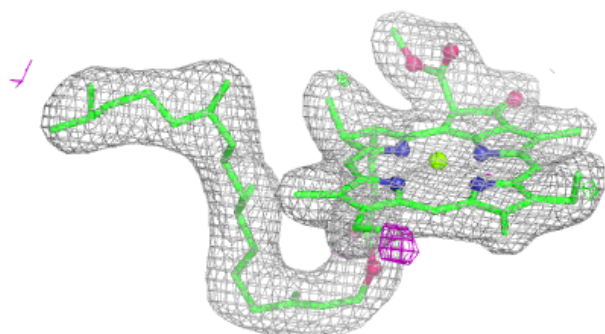
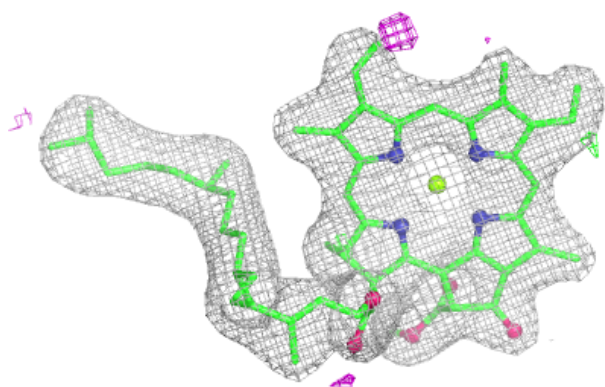
**Electron density around PL9 d 405:**

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

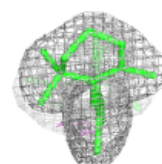
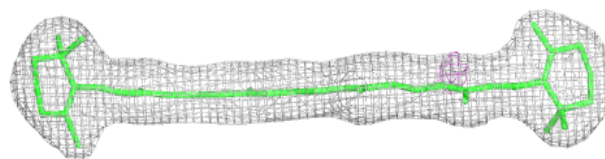
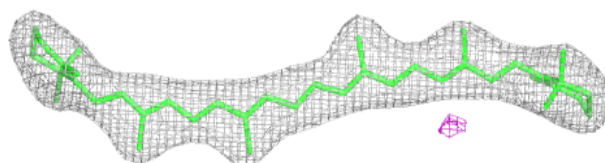


Electron density around CLA a 350:

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

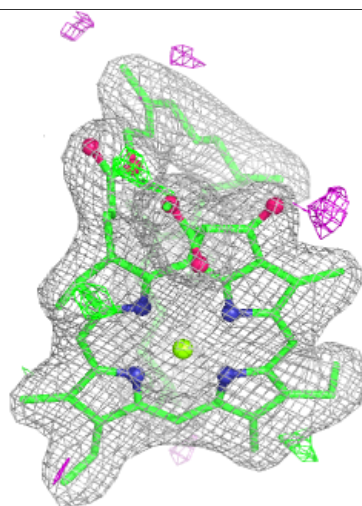
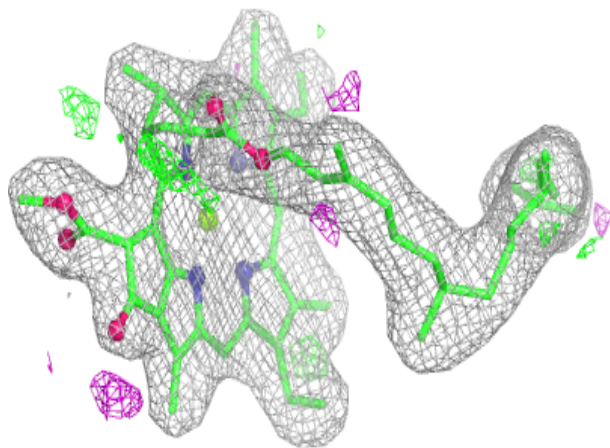
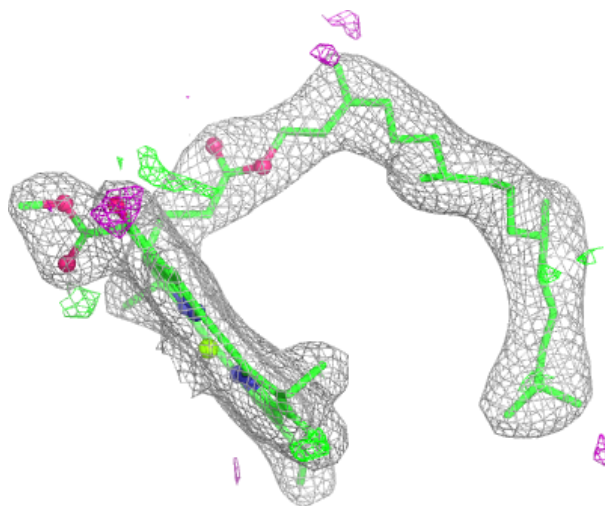
**Electron density around BCR C 516:**

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



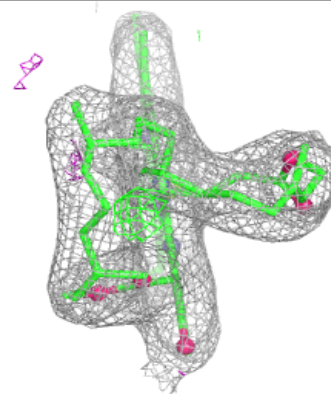
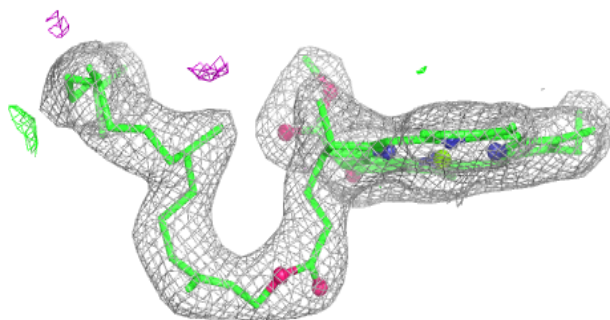
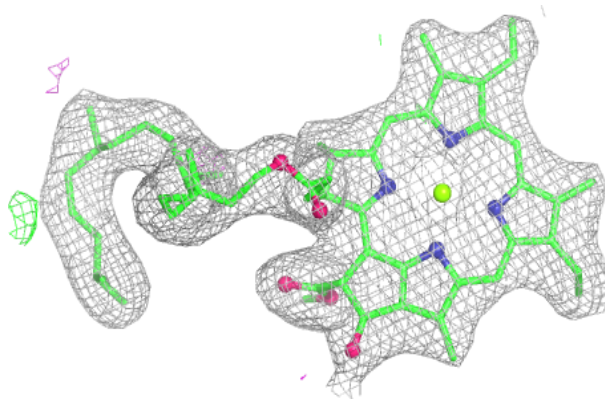
Electron density around CLA B 611:

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

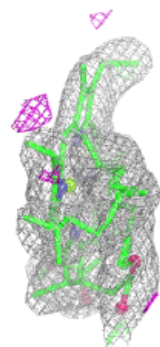
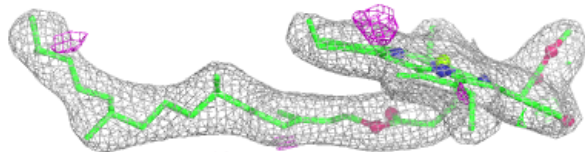
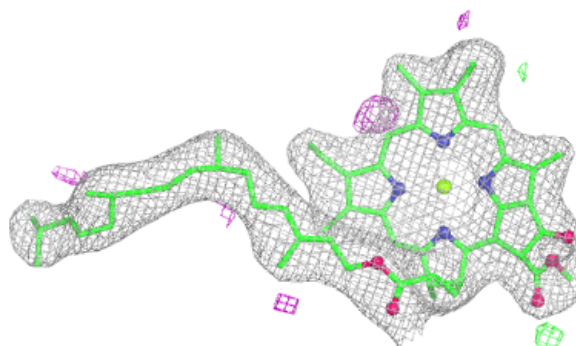


Electron density around CLA B 612:

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

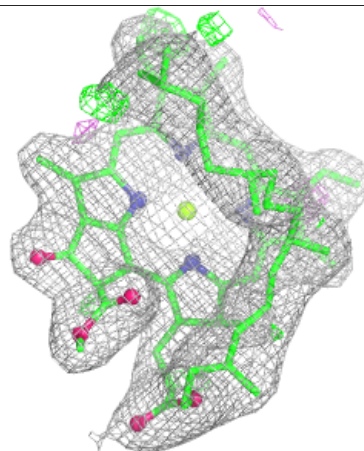
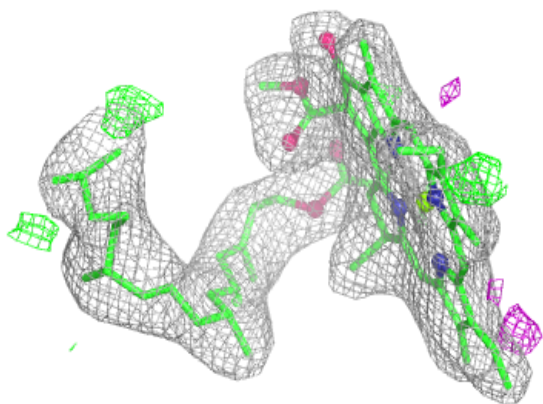
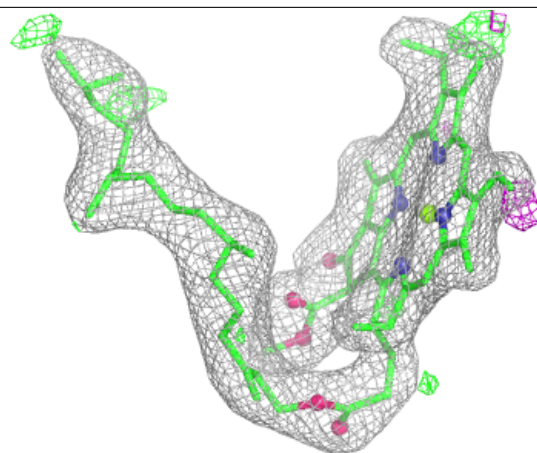
**Electron density around CLA b 603:**

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



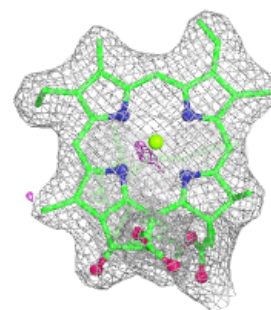
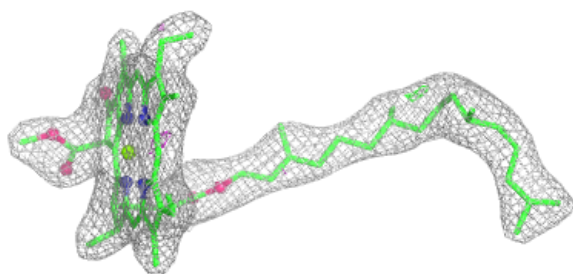
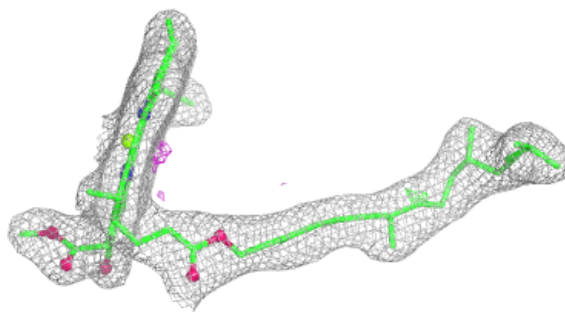
Electron density around CLA B 613:

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

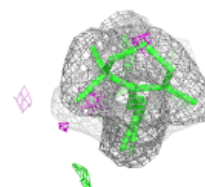
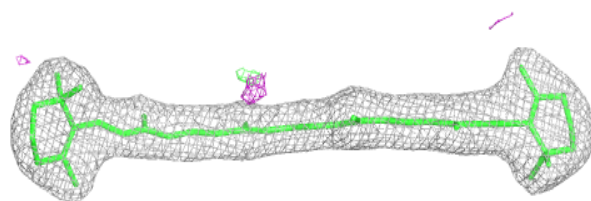
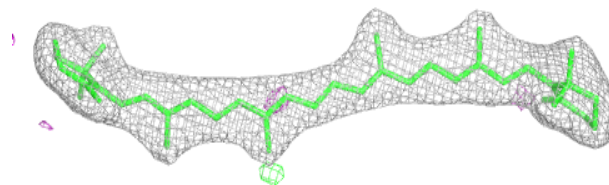


Electron density around CLA b 605:

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

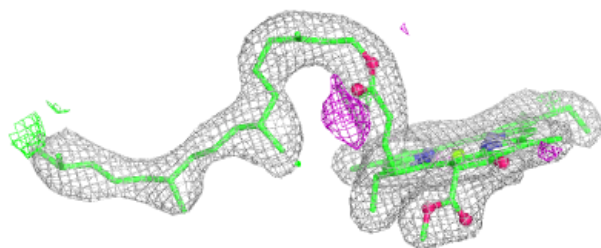
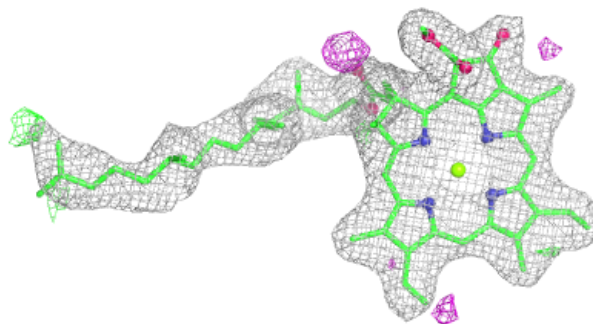
**Electron density around BCR a 408:**

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



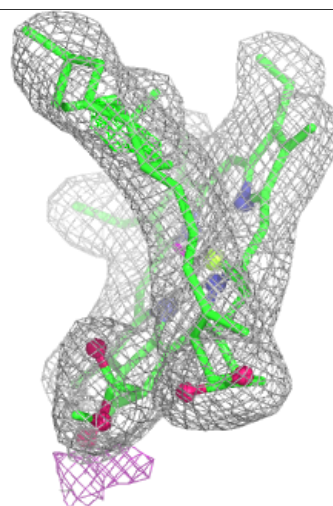
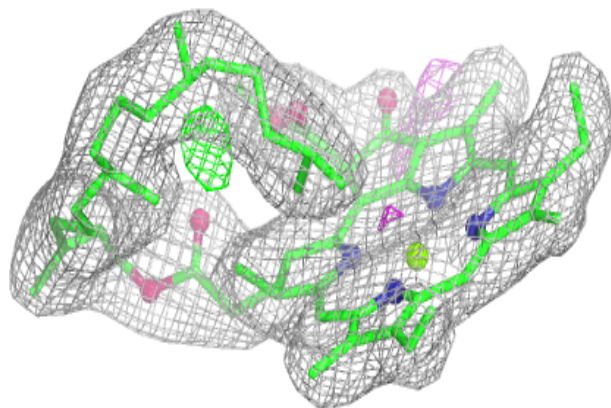
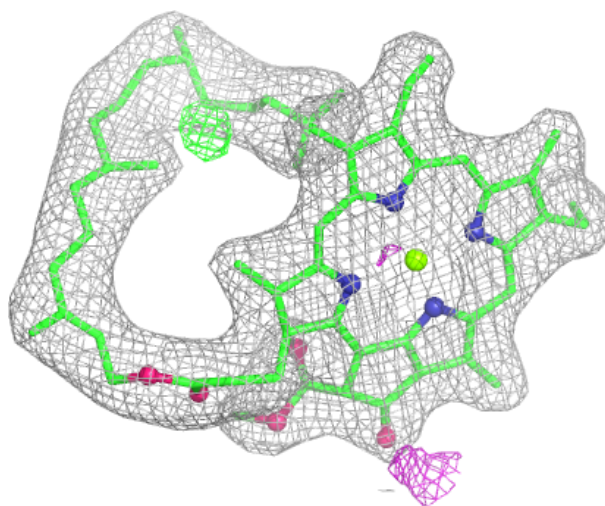
Electron density around CLA A 406:

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



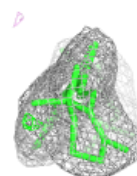
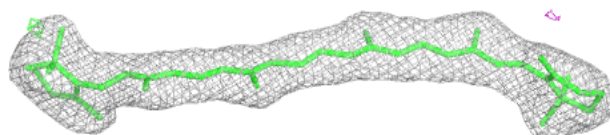
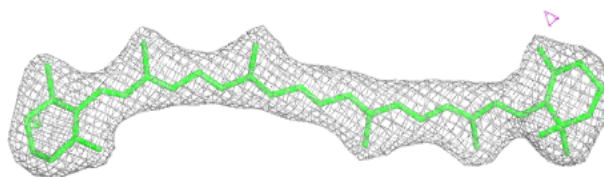
Electron density around CLA B 615:

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

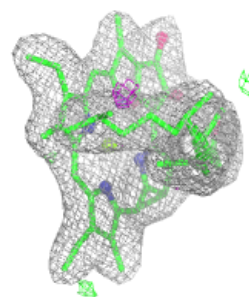
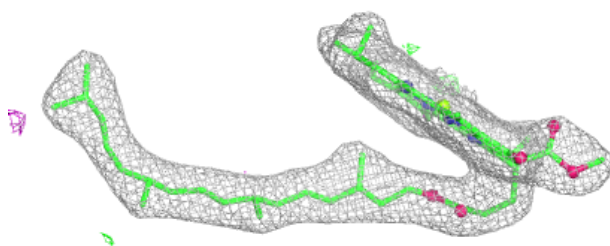
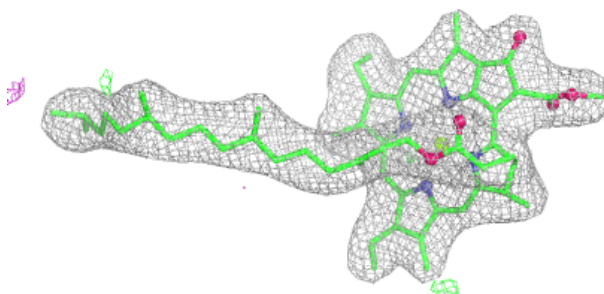


Electron density around BCR b 619:

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

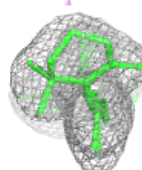
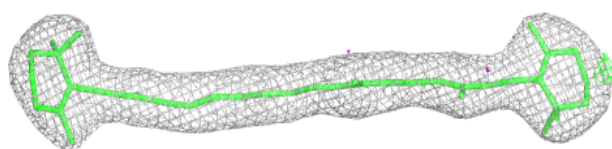
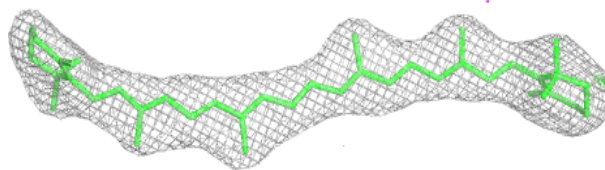
**Electron density around CLA b 608:**

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

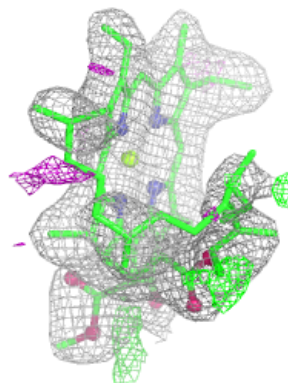
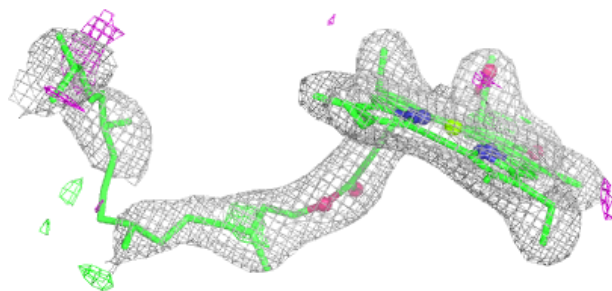
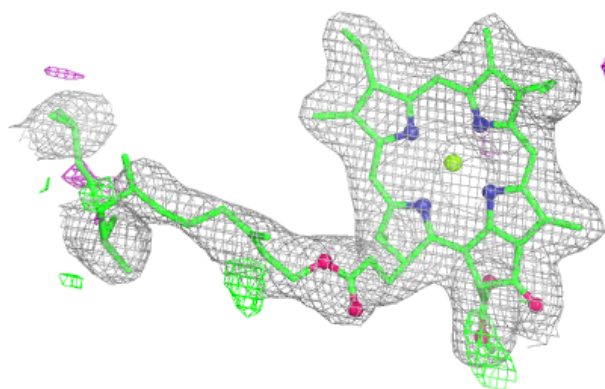


Electron density around BCR c 517:

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

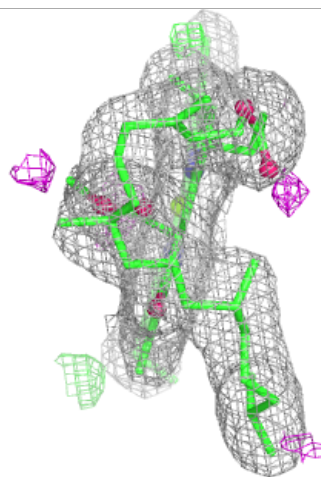
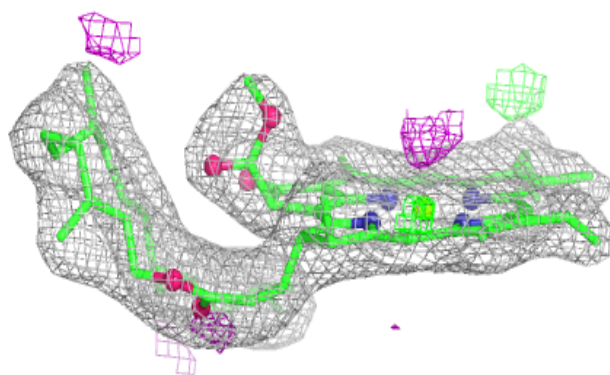
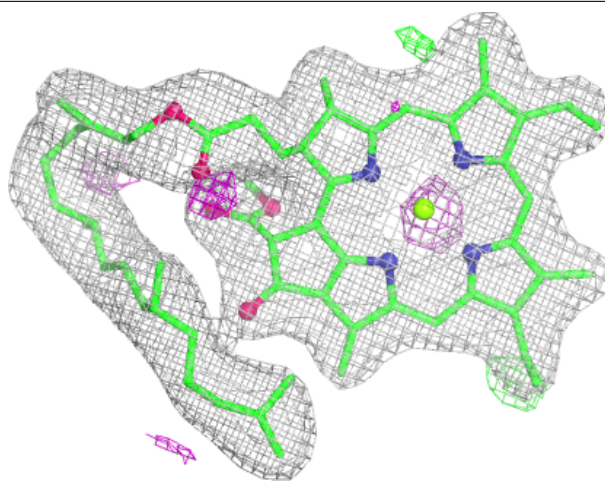
**Electron density around CLA A 409:**

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



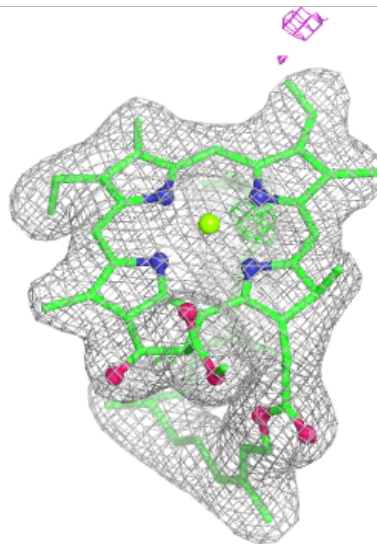
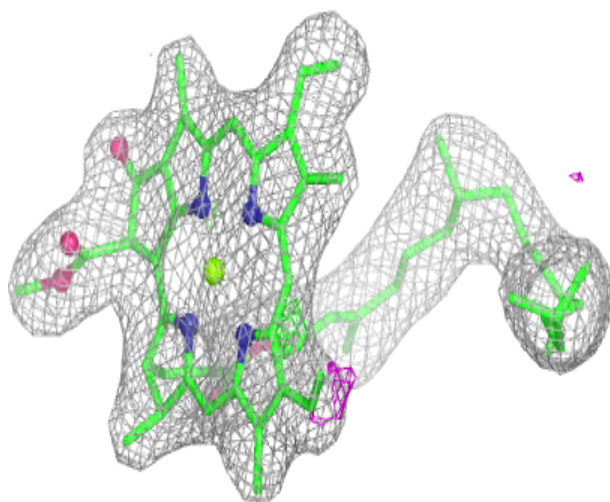
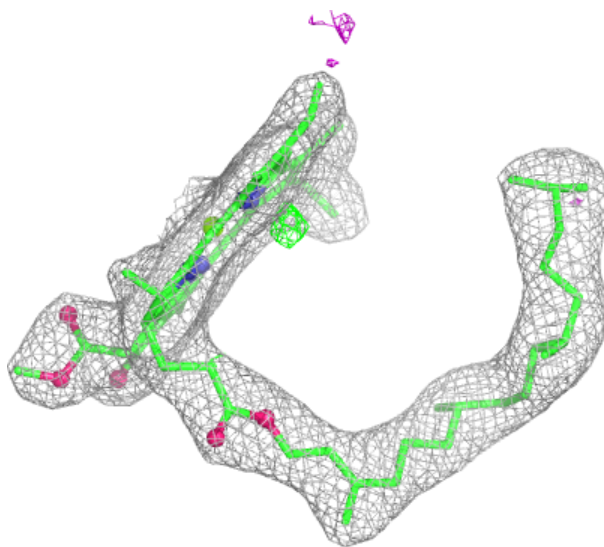
Electron density around CLA b 610:

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



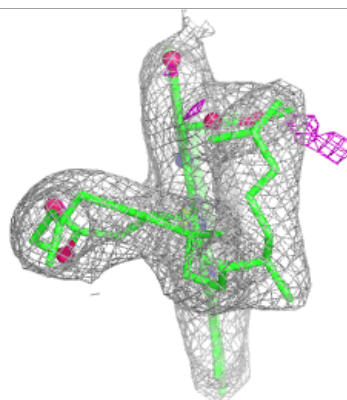
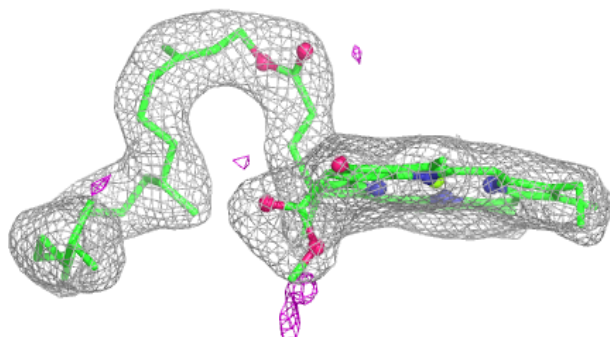
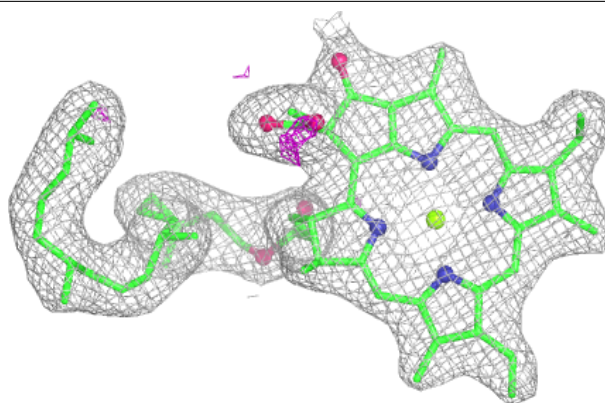
Electron density around CLA b 611:

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

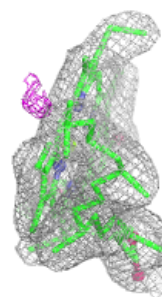
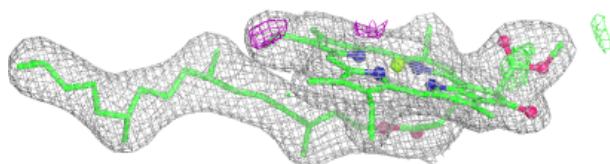
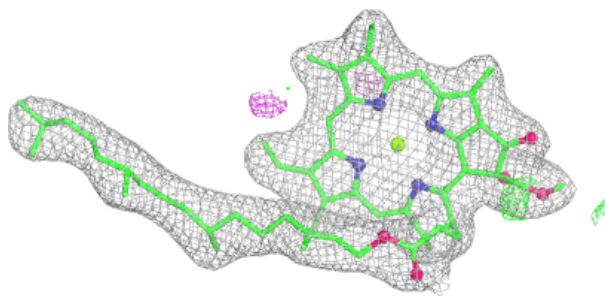


Electron density around CLA b 612:

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

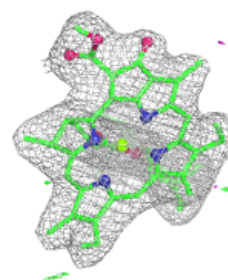
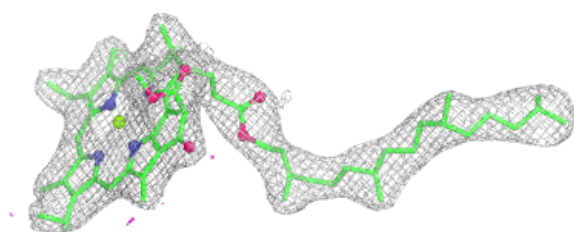
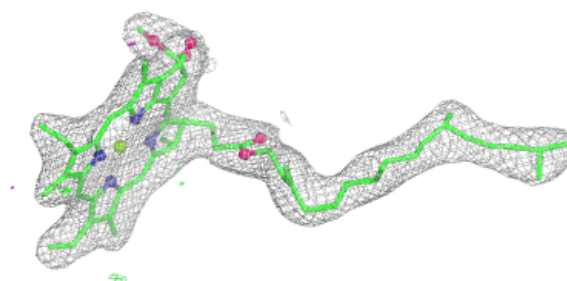
**Electron density around CLA C 502:**

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

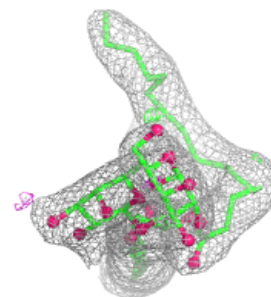
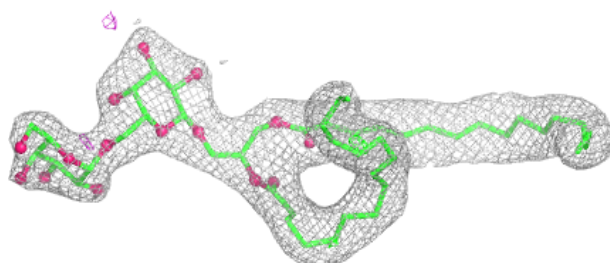
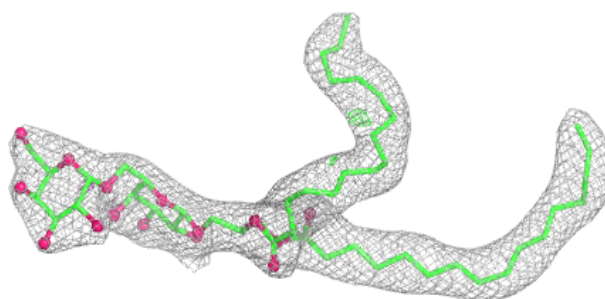


Electron density around CLA C 503:

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

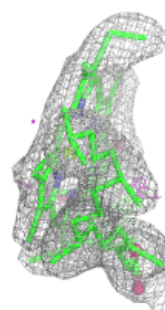
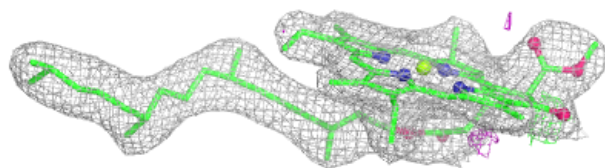
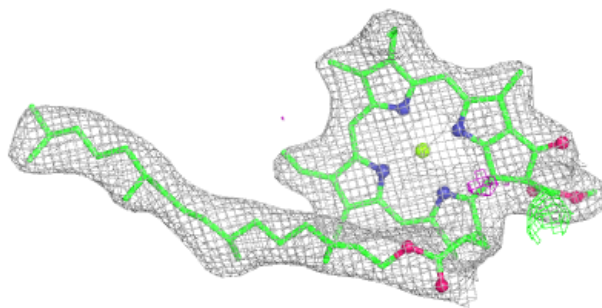
**Electron density around DGD H 102:**

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

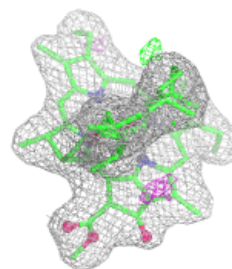
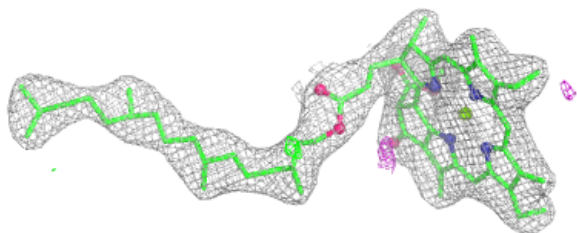
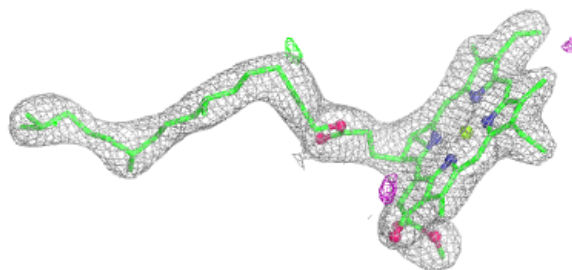


Electron density around CLA c 503:

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

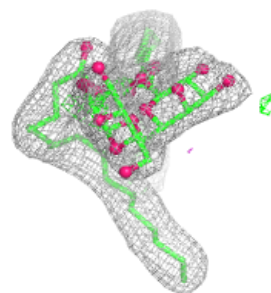
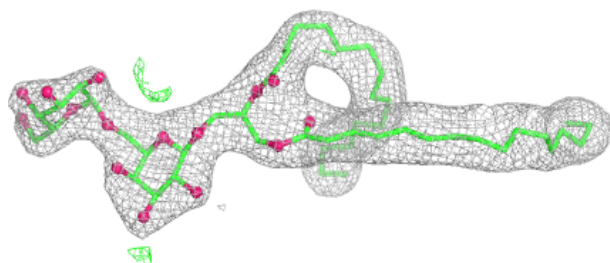
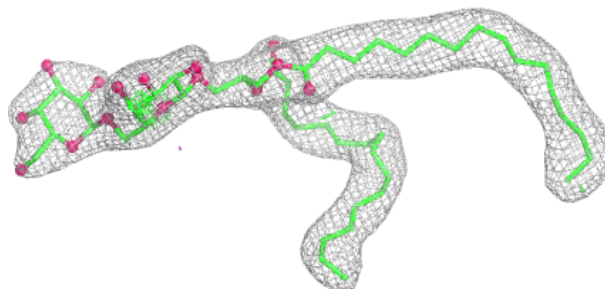
**Electron density around CLA c 504:**

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

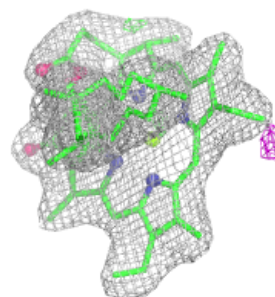
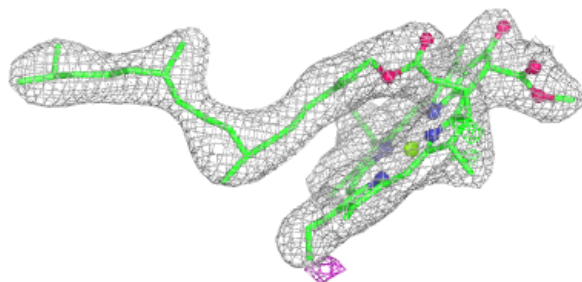
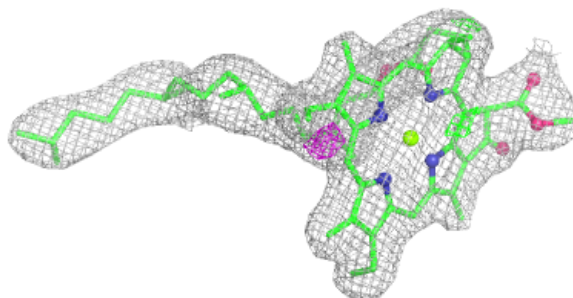


Electron density around DGD h 103:

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

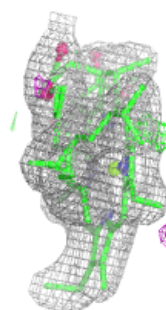
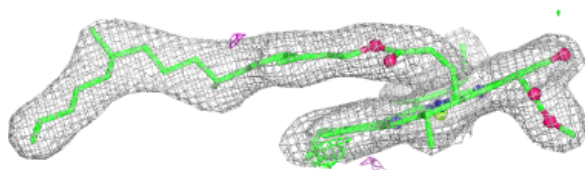
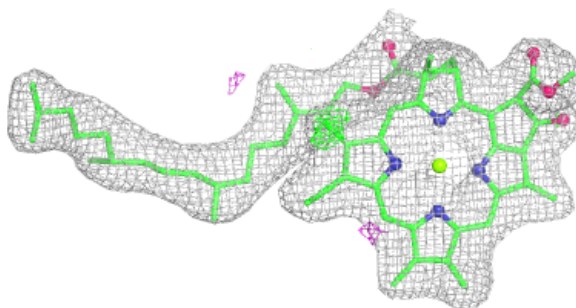
**Electron density around CLA C 506:**

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

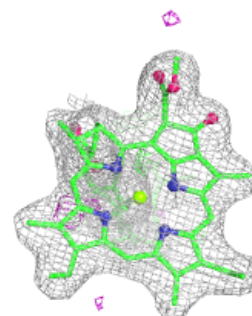
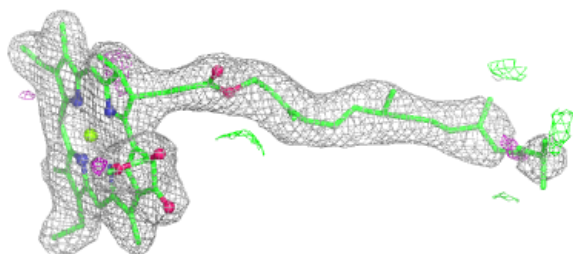
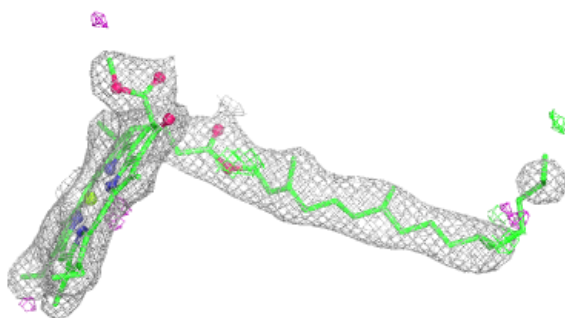


Electron density around CLA B 603:

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

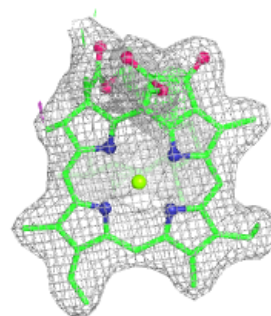
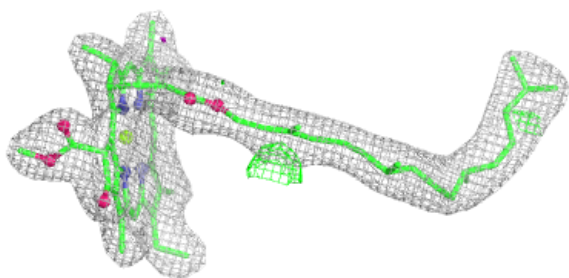
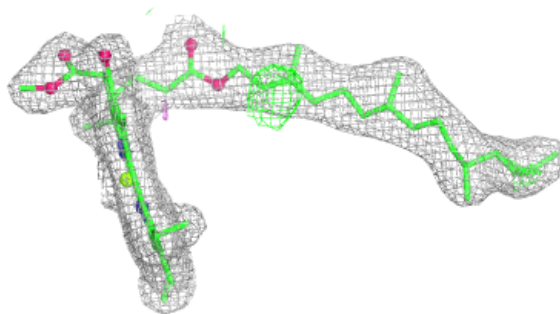
**Electron density around CLA B 604:**

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



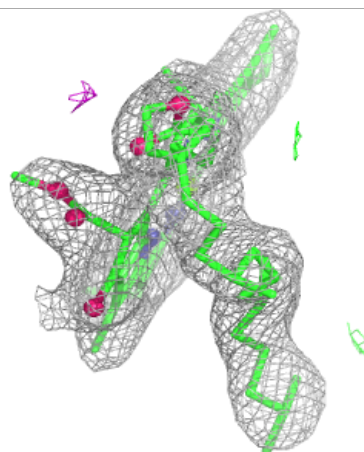
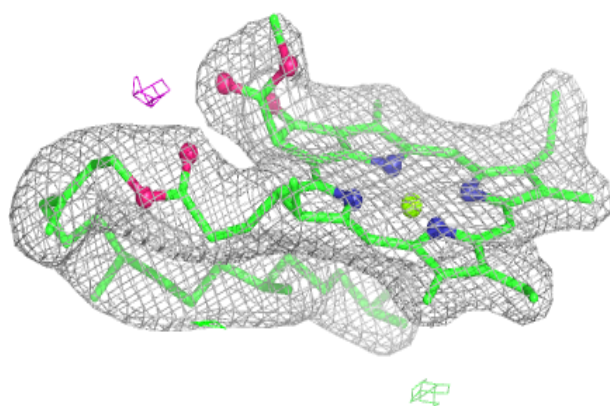
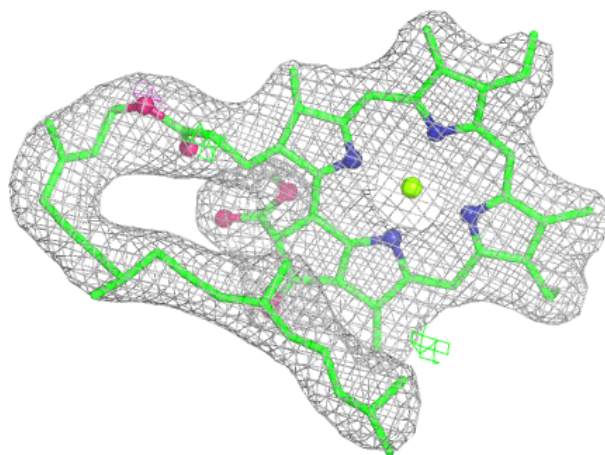
Electron density around CLA B 605:

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



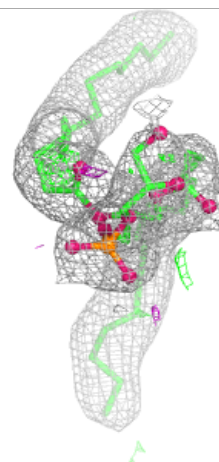
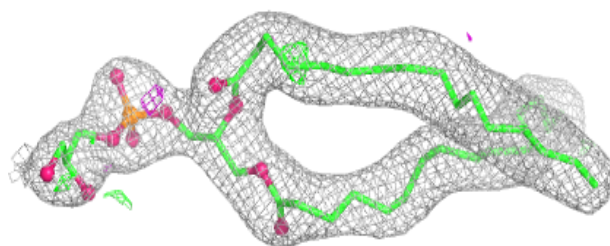
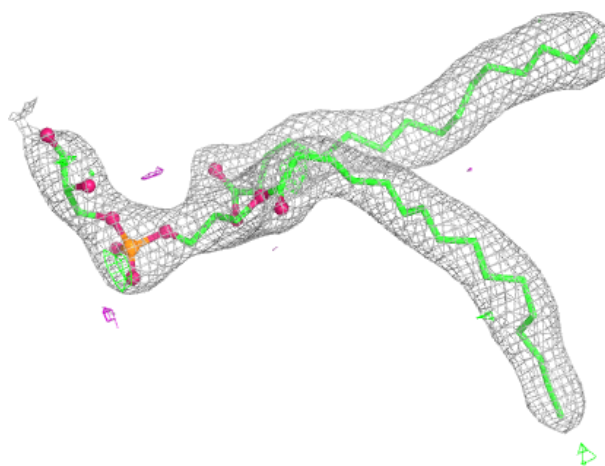
Electron density around CLA C 510:

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



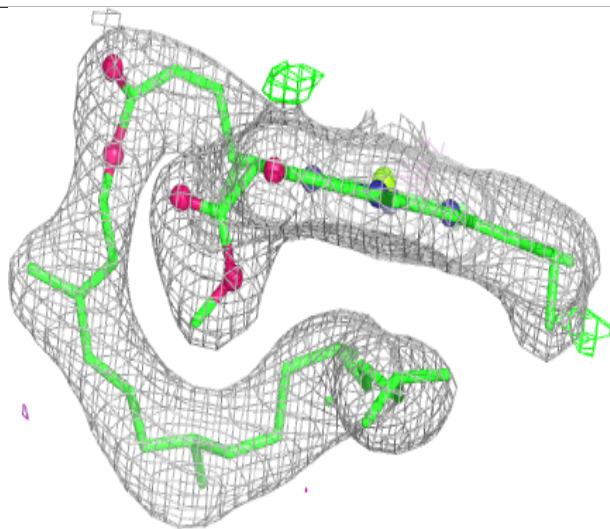
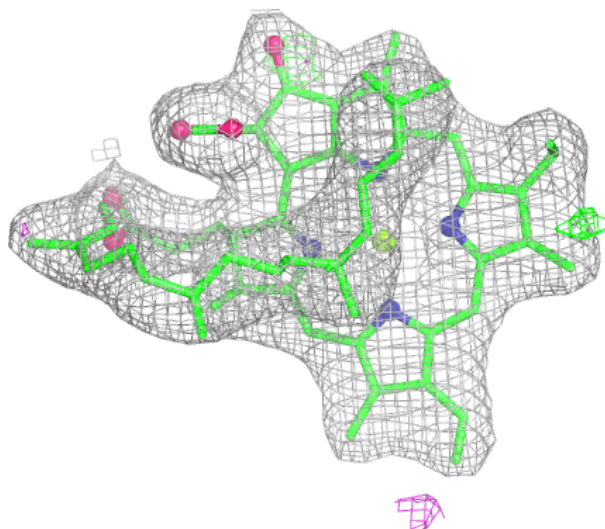
Electron density around LHG D 406:

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



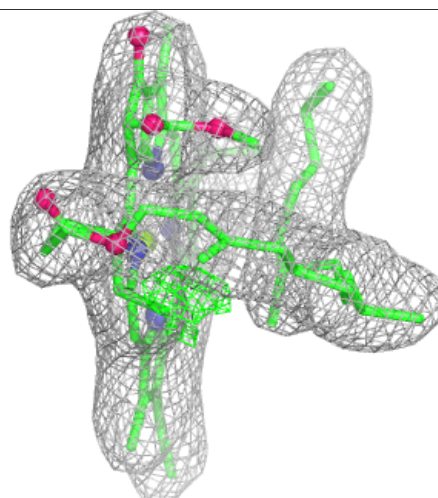
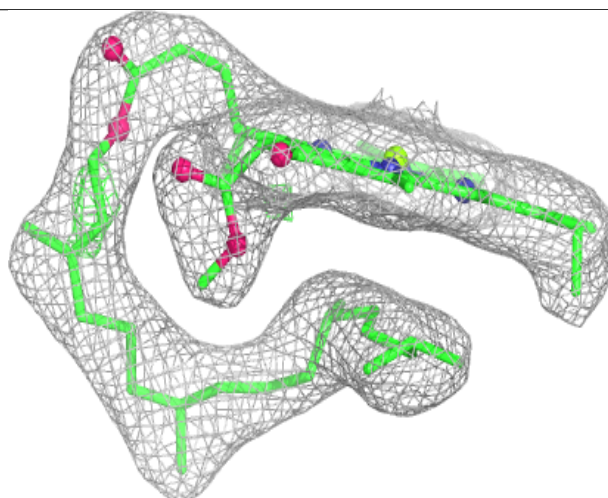
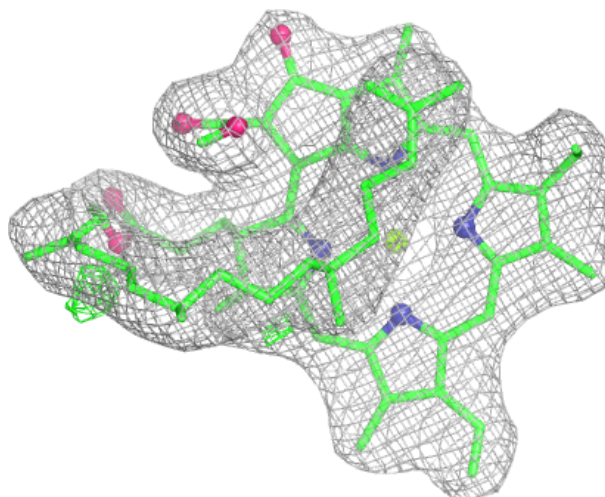
Electron density around CLA C 511:

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



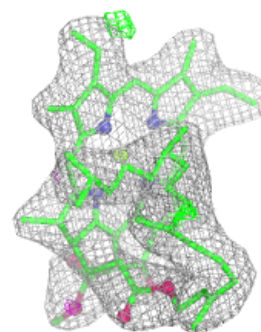
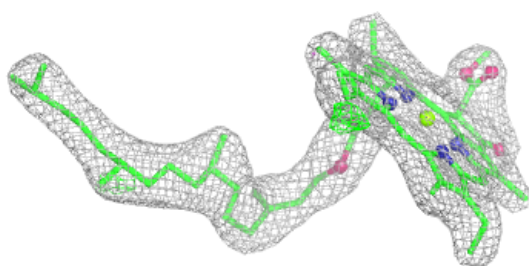
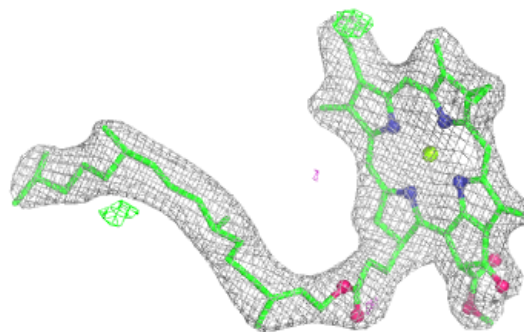
Electron density around CLA c 512:

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



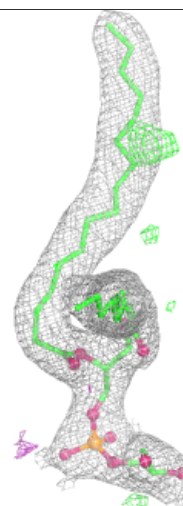
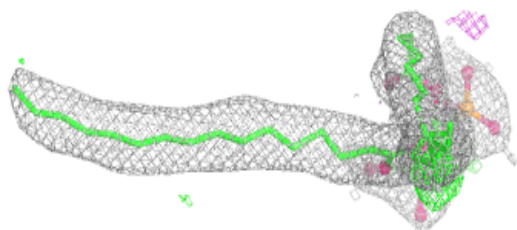
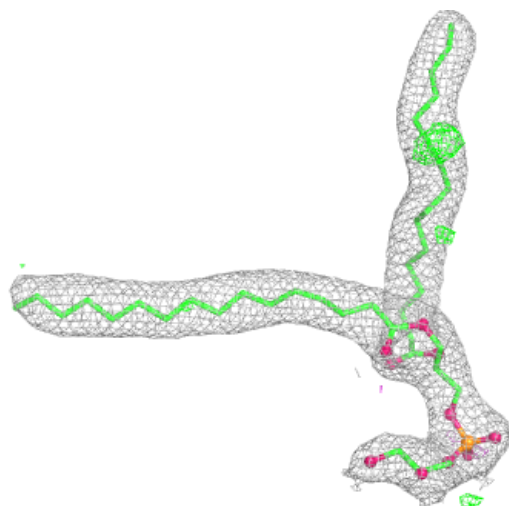
Electron density around CLA C 512:

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



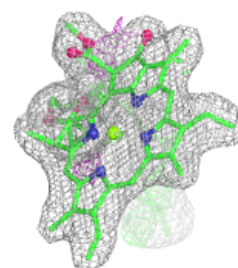
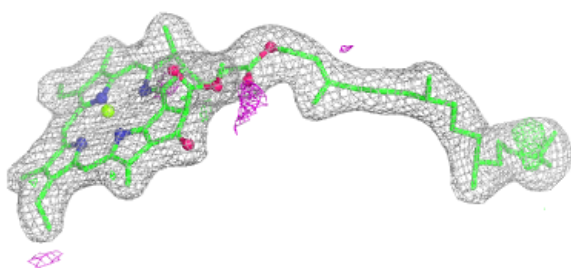
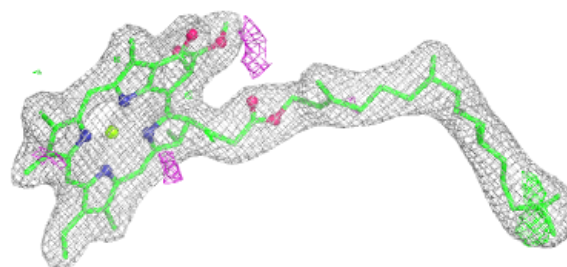
Electron density around LHG L 101:

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

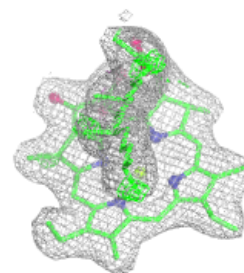
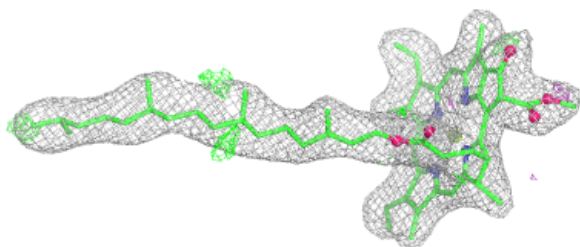
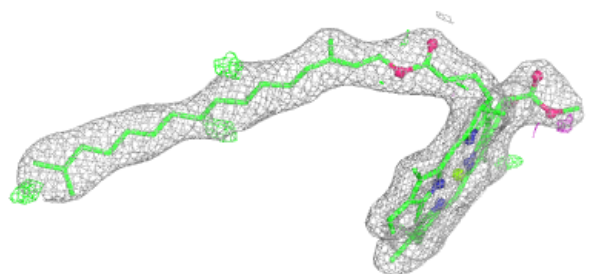


Electron density around CLA A 404:

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

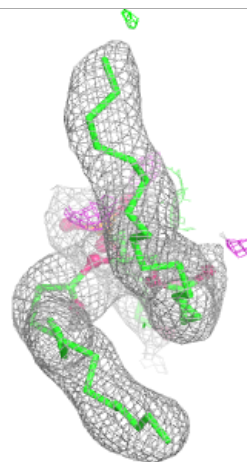
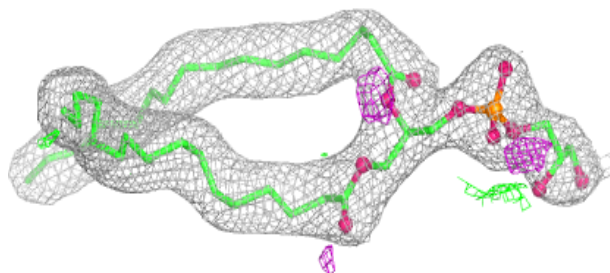
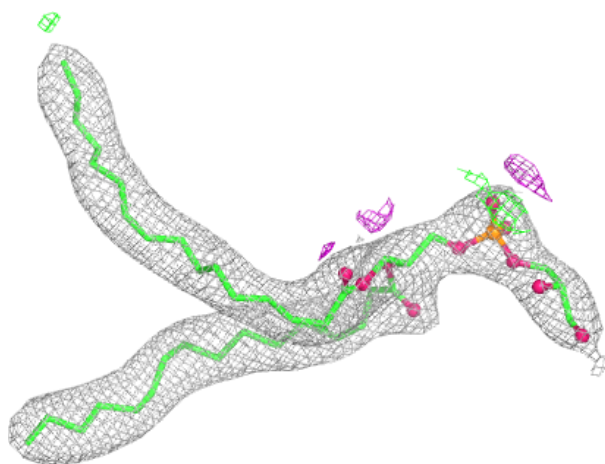
**Electron density around CLA B 607:**

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



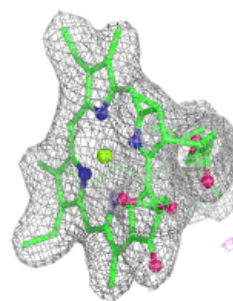
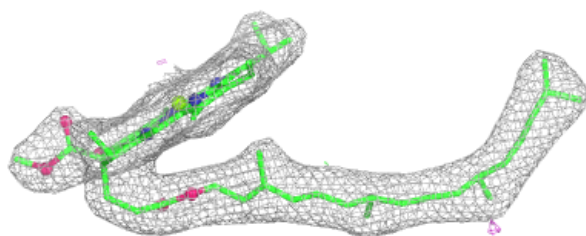
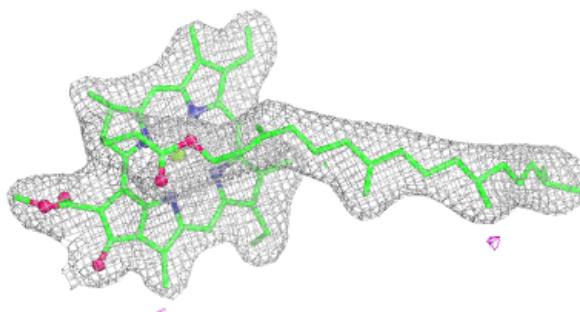
Electron density around LHG d 407:

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

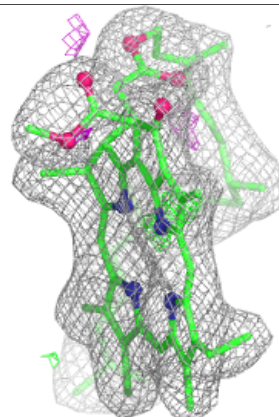
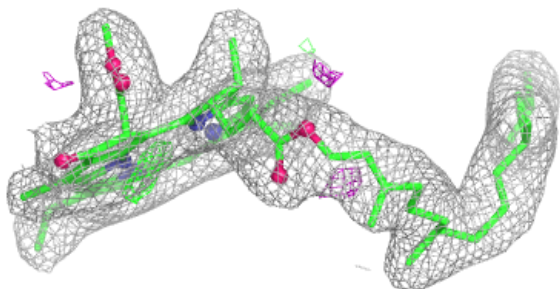
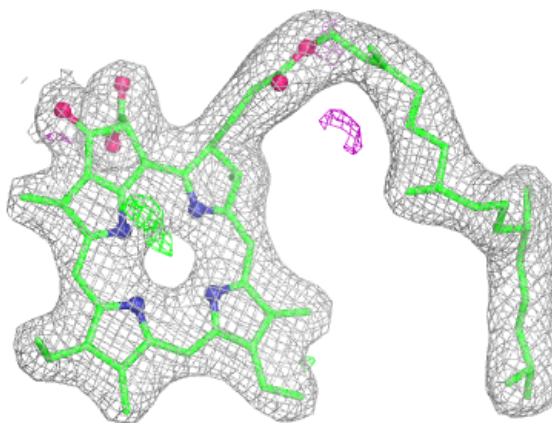


Electron density around CLA B 608:

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

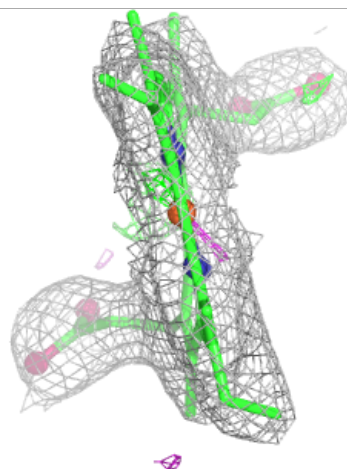
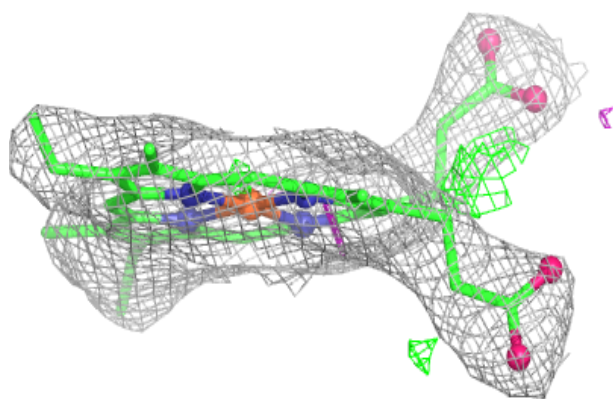
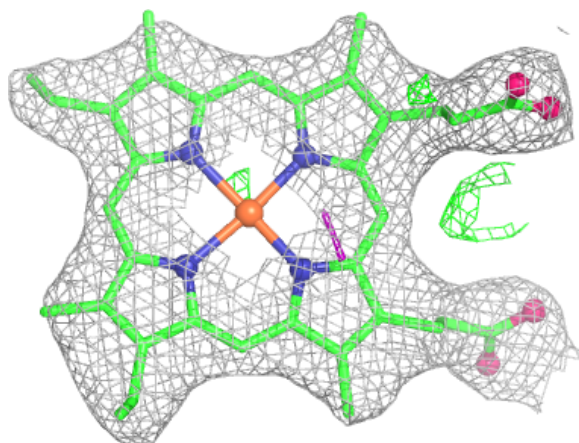
**Electron density around PHO A 408:**

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



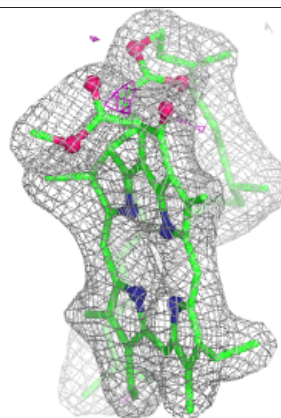
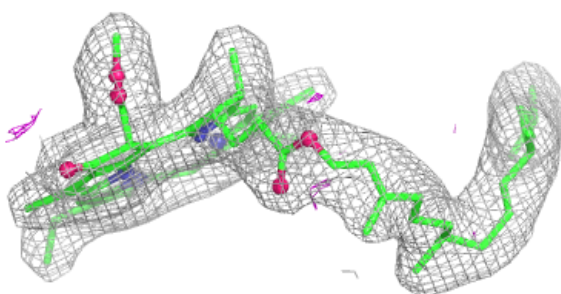
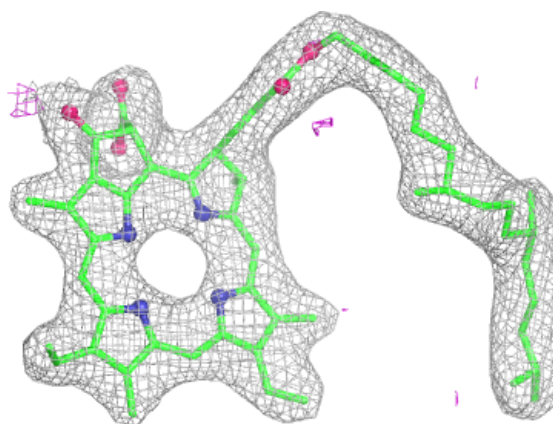
Electron density around HEM E 103:

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



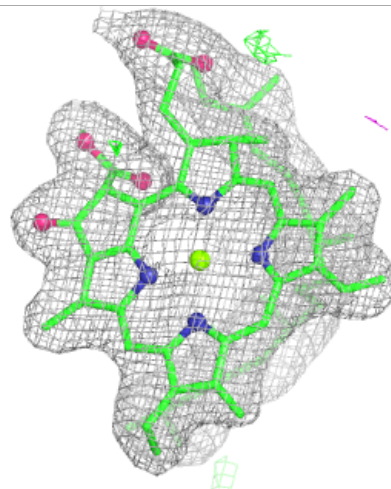
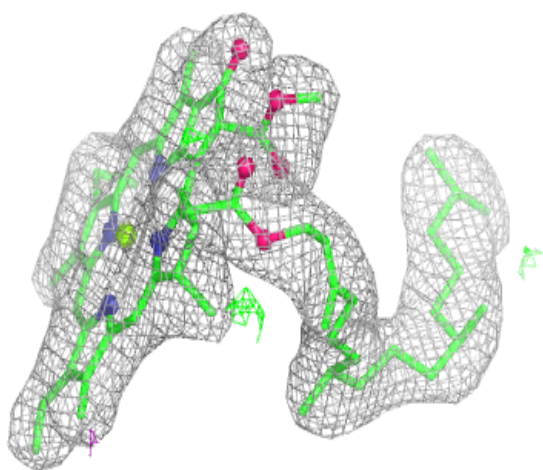
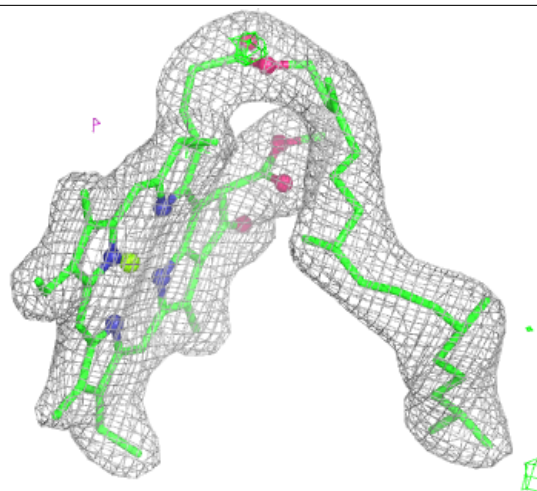
Electron density around PHO a 406:

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



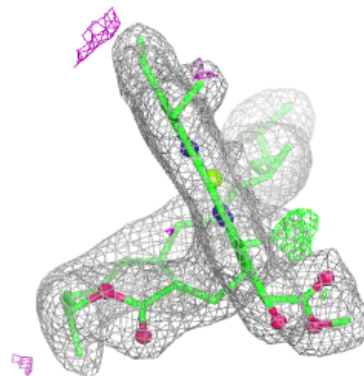
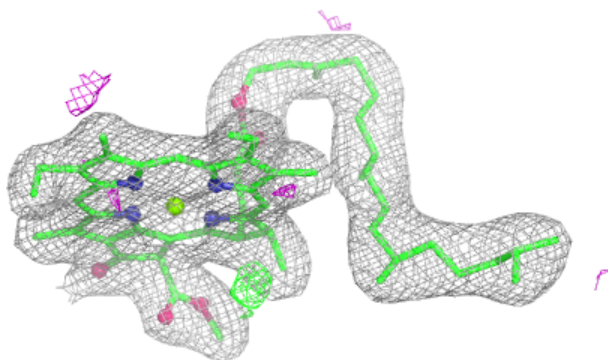
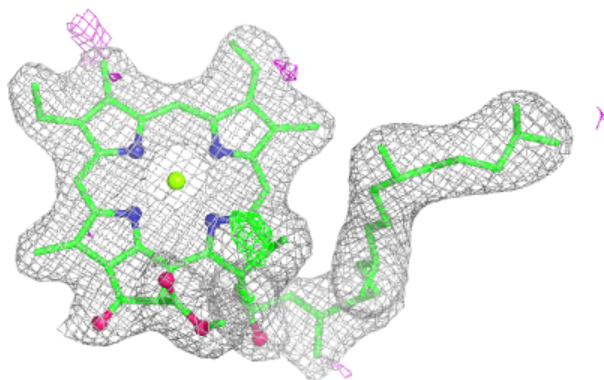
Electron density around CLA b 613:

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

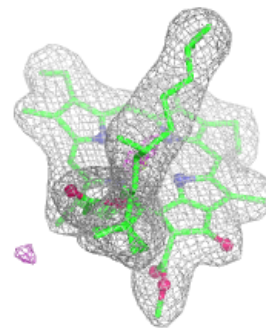
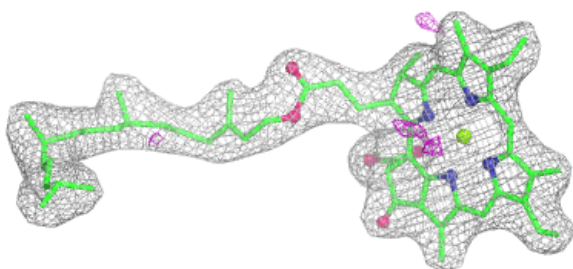
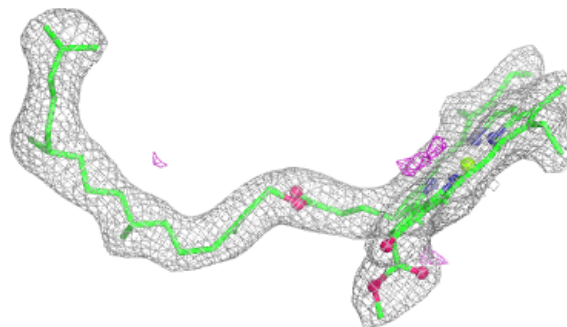


Electron density around CLA A 405:

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

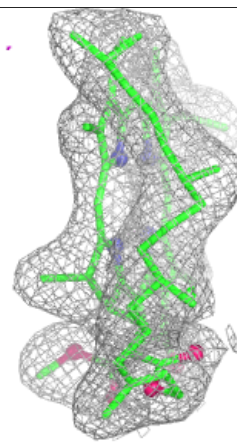
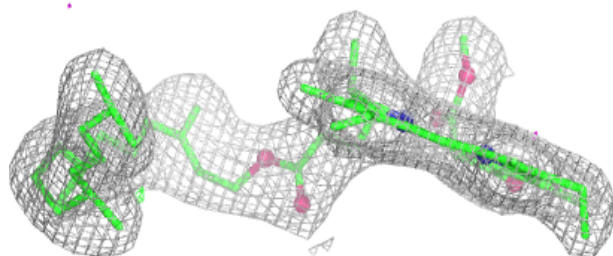
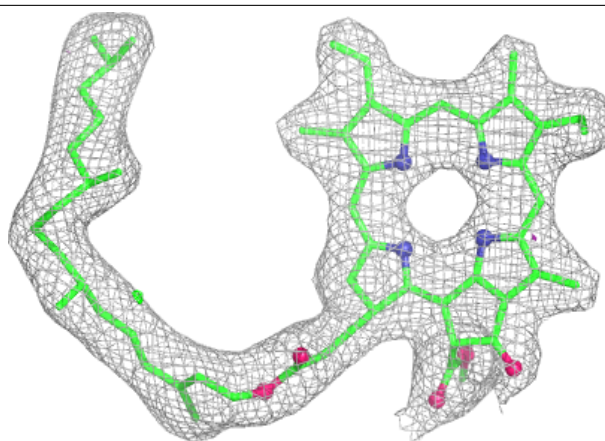
**Electron density around CLA d 402:**

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



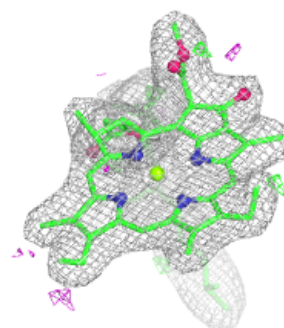
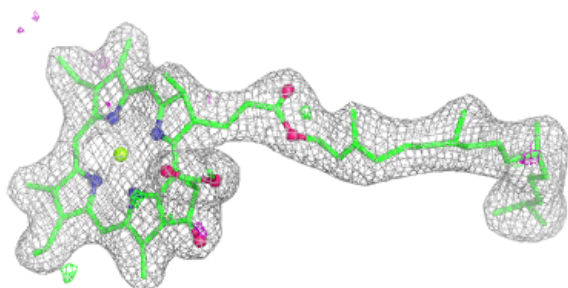
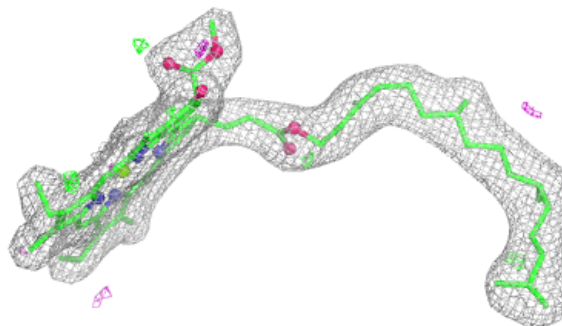
Electron density around PHO A 407:

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



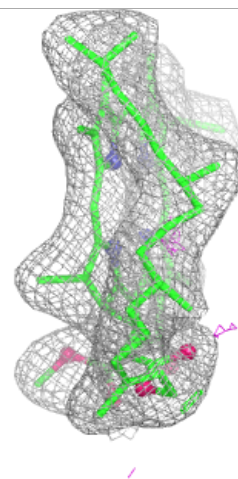
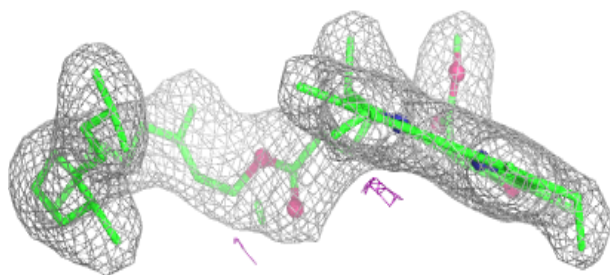
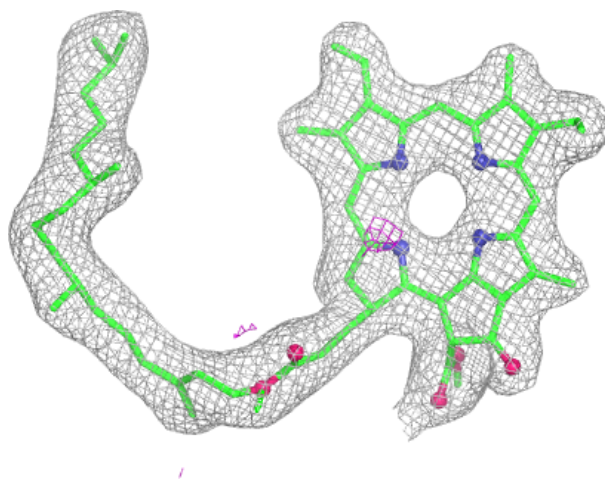
Electron density around CLA D 402:

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



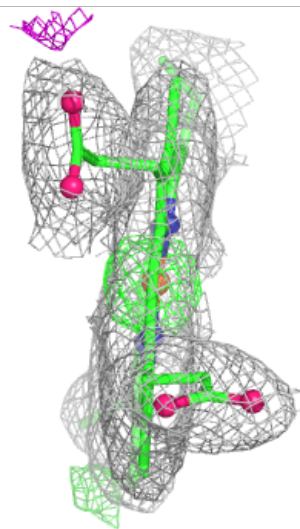
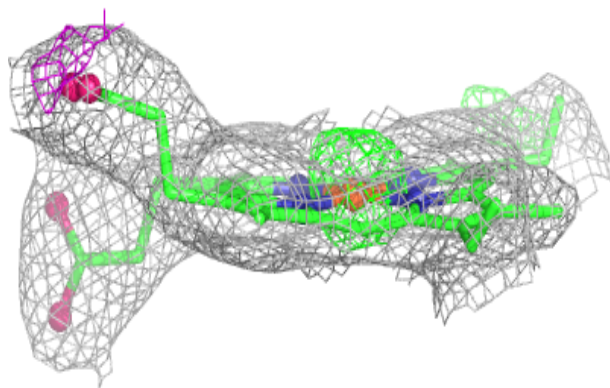
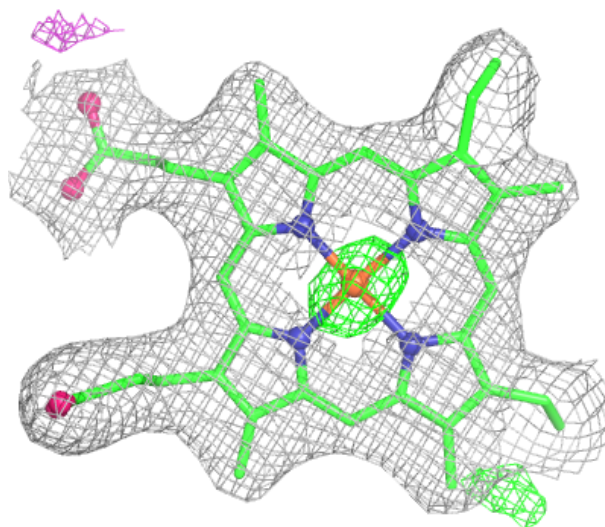
Electron density around PHO a 405:

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



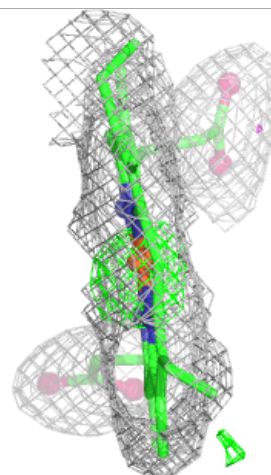
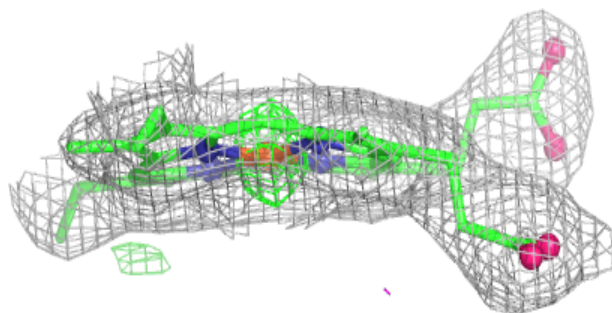
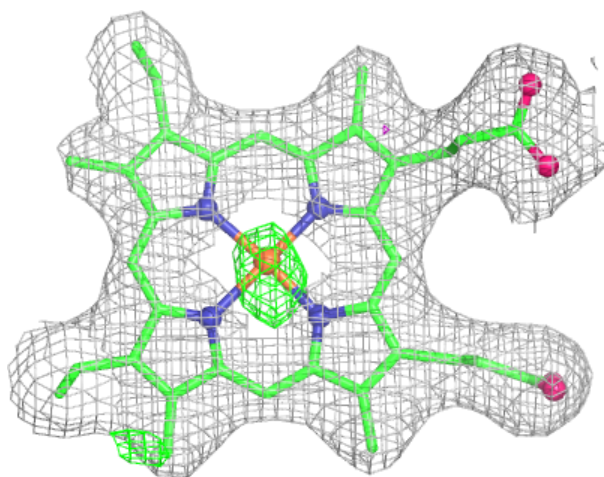
Electron density around HEC V 203:

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



Electron density around HEC v 203:

$2mF_o-DF_c$ (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.