



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 05:19 AM UTC

PDB ID : 5WS5 / pdb_00005ws5
Title : Native XFEL structure of photosystem II (preflash dark 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

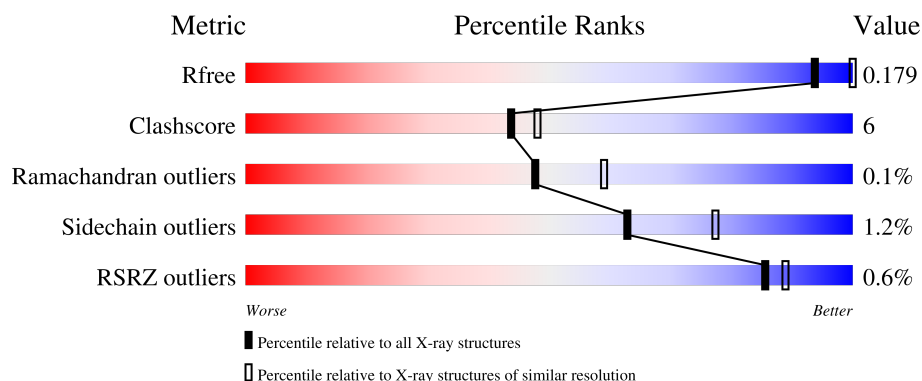
1 Overall quality at a glance

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.



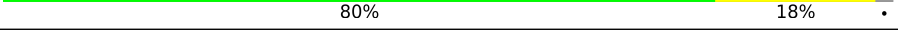
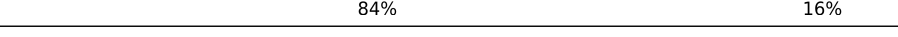
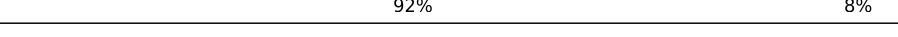
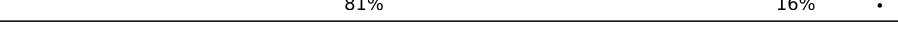
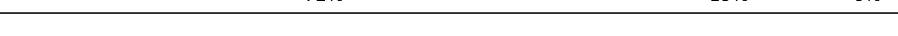
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	87% 10% .
1	a	344	84% 13% .
2	B	505	89% 10% .
2	b	505	% 92% 8%
3	C	455	91% 7% .

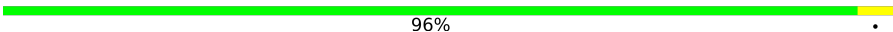
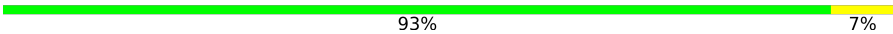
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 93% 7%
17	X	40	 92% . 5%
17	x	40	 88% 8% 5%
18	Y	30	 73% 23% .
18	y	30	 73% 23% .
19	Z	62	 85% 15%
19	z	62	 79% 19% .
20	R	34	 88% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
27	GOL	B	625	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52545 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	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	4	0
			2636	1730	431	460	15			

- 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2316	589	618	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	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	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 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 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	4	0
			1883	1178	315	385	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	0
			1	1		

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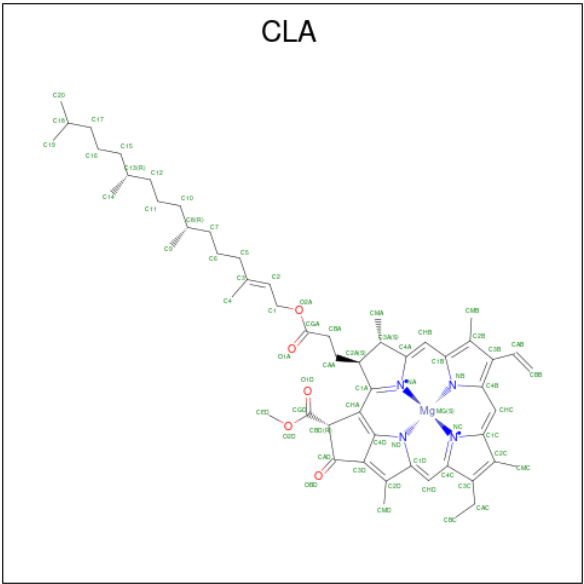
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

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



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

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

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

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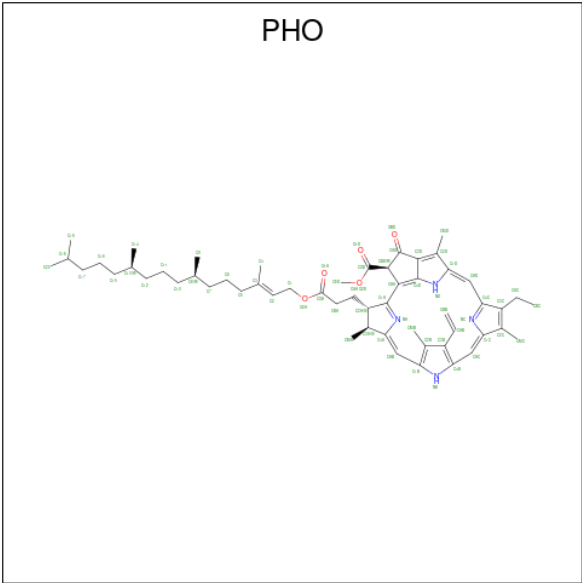
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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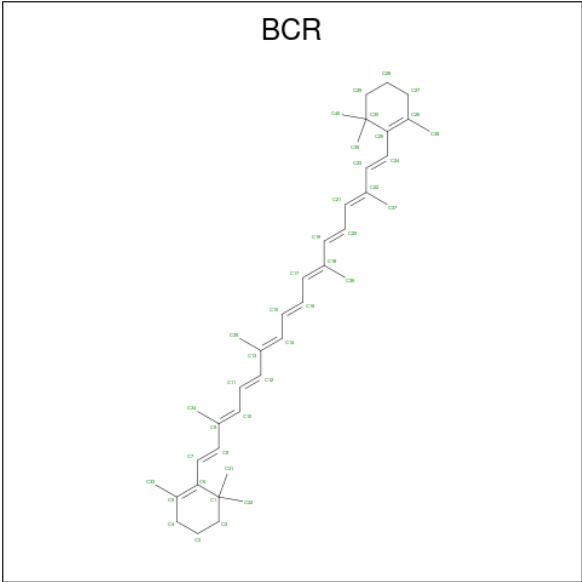
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

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



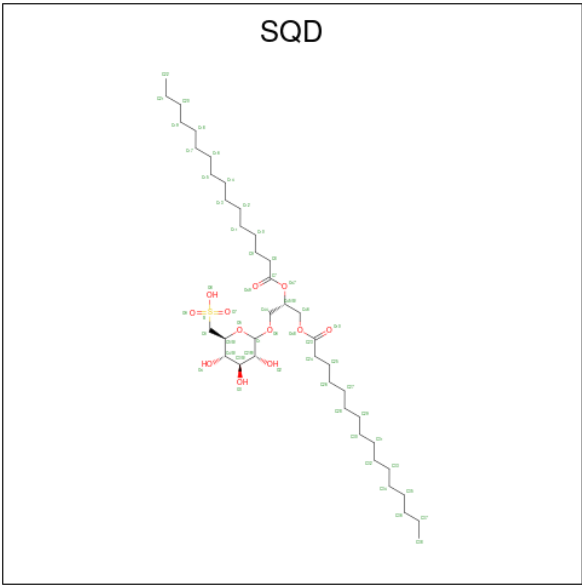
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



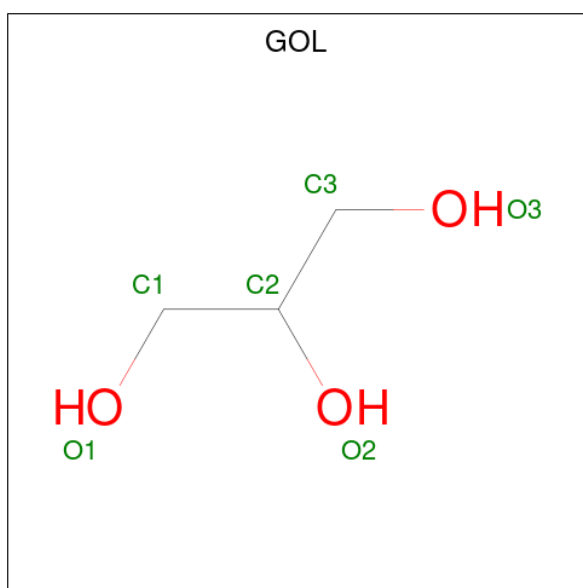
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



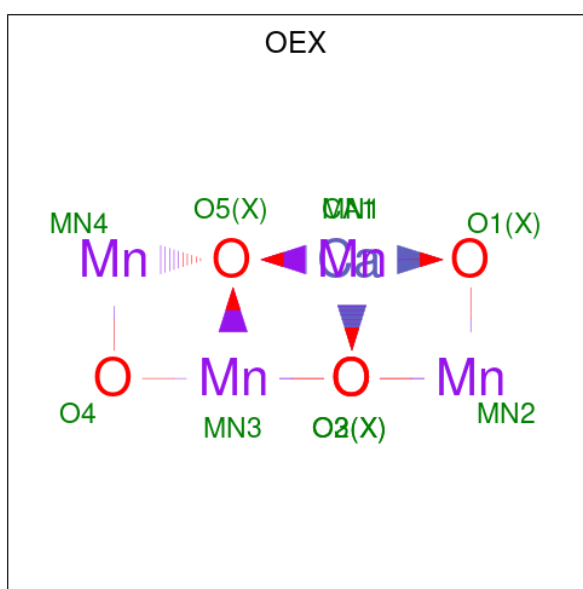
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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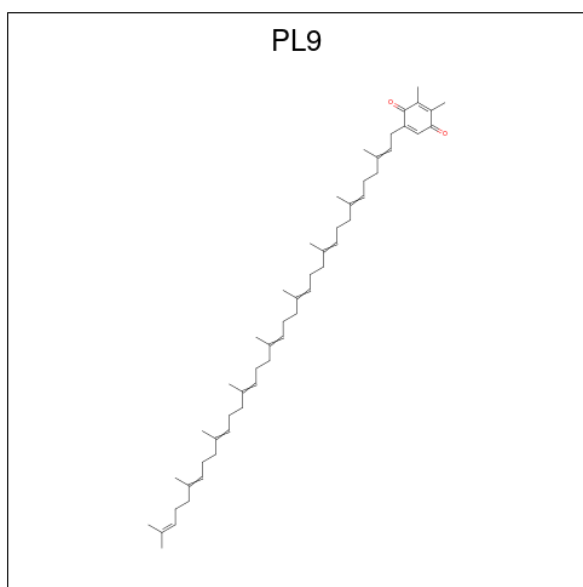
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 29 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

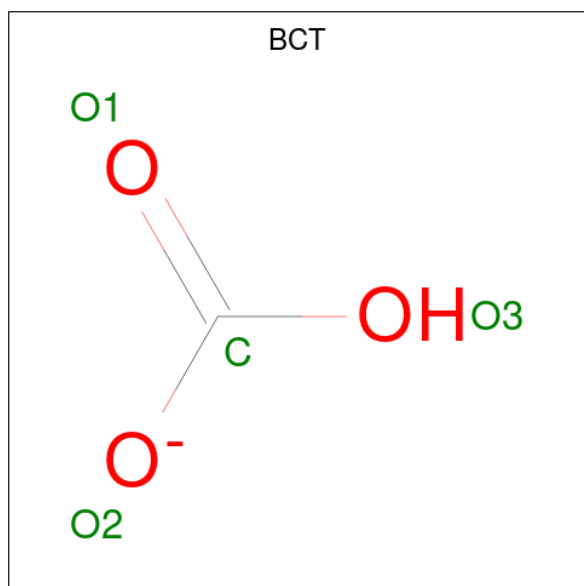
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		

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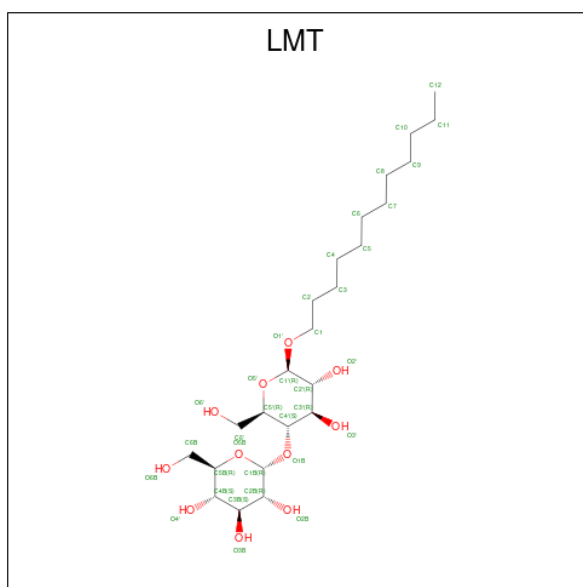
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
		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

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



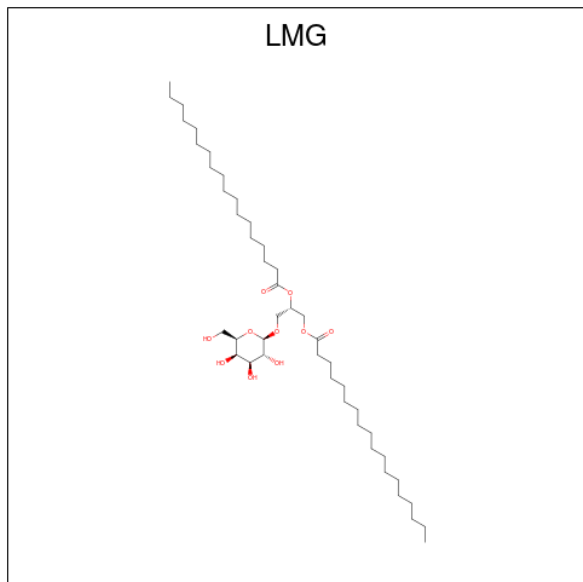
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



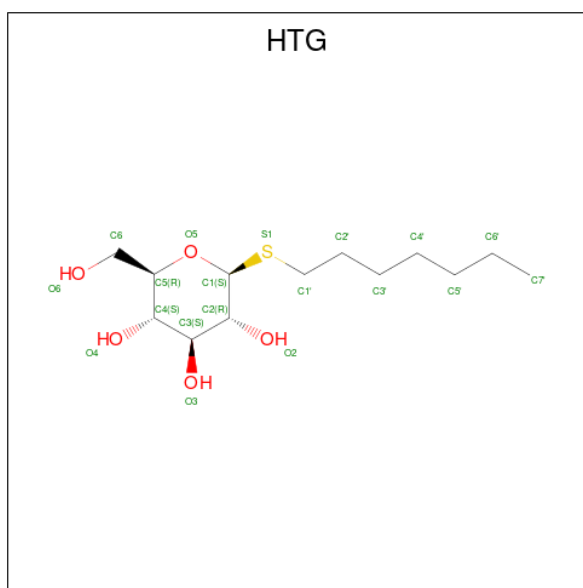
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total 35	C 24	O 11	0	0
32	D	1	Total 35	C 24	O 11	0	0
32	E	1	Total 35	C 24	O 11	0	0
32	I	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	M	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0
32	a	1	Total 35	C 24	O 11	0	0
32	b	1	Total 25	C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

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



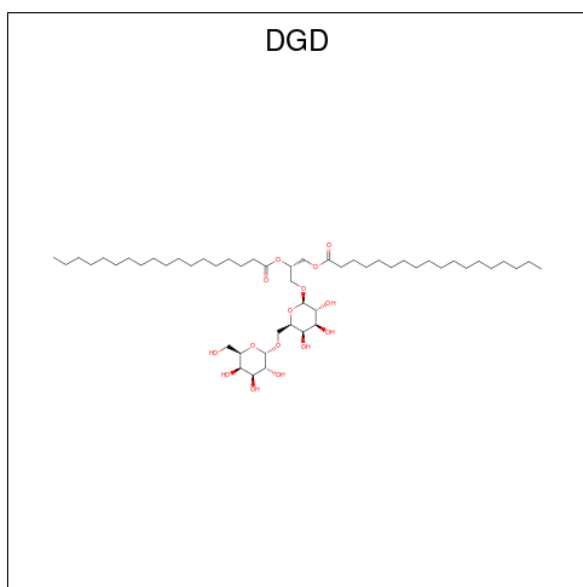
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

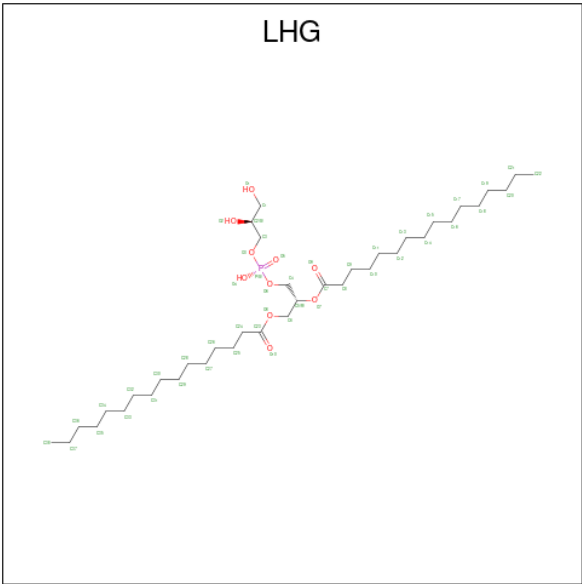
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	f	1	Total	Ca	0	0
			1	1		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



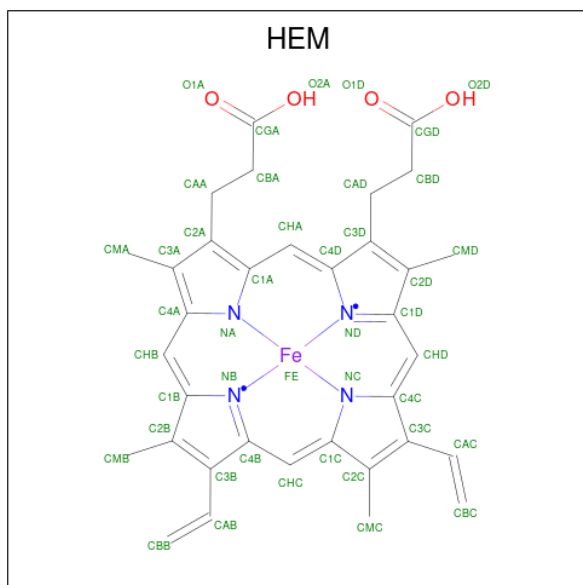
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	1	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

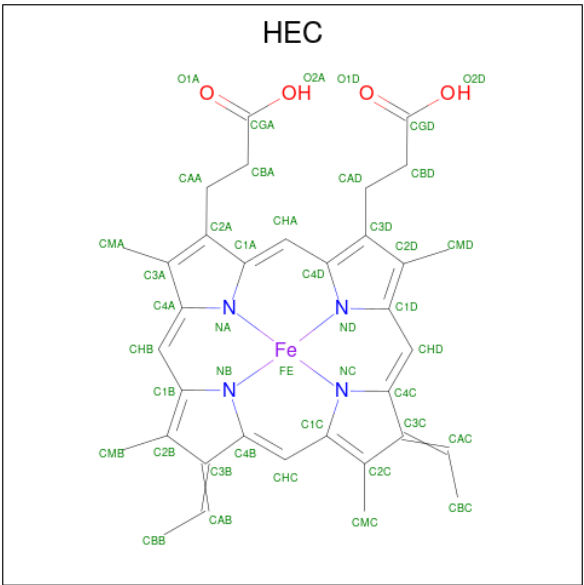


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	e	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	130	Total	O	0	0
			130	130		
41	B	167	Total	O	0	0
			167	167		
41	C	144	Total	O	0	0
			144	144		
41	D	122	Total	O	0	0
			122	122		
41	E	15	Total	O	0	0
			15	15		
41	F	4	Total	O	0	0
			4	4		
41	H	19	Total	O	0	0
			19	19		
41	I	6	Total	O	0	0
			6	6		
41	J	5	Total	O	0	0
			5	5		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	3	Total 3	O 3	0	0
41	M	7	Total 7	O 7	0	0
41	O	71	Total 71	O 71	0	0
41	T	9	Total 9	O 9	0	0
41	U	32	Total 32	O 32	0	0
41	V	67	Total 67	O 67	0	0
41	X	1	Total 1	O 1	0	0
41	Y	1	Total 1	O 1	0	0
41	a	133	Total 133	O 133	0	0
41	b	193	Total 193	O 193	0	0
41	c	142	Total 142	O 142	0	0
41	d	114	Total 114	O 114	0	0
41	e	8	Total 8	O 8	0	0
41	f	4	Total 4	O 4	0	0
41	h	16	Total 16	O 16	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	4	Total 4	O 4	0	0
41	m	15	Total 15	O 15	0	0
41	o	77	Total 77	O 77	0	0

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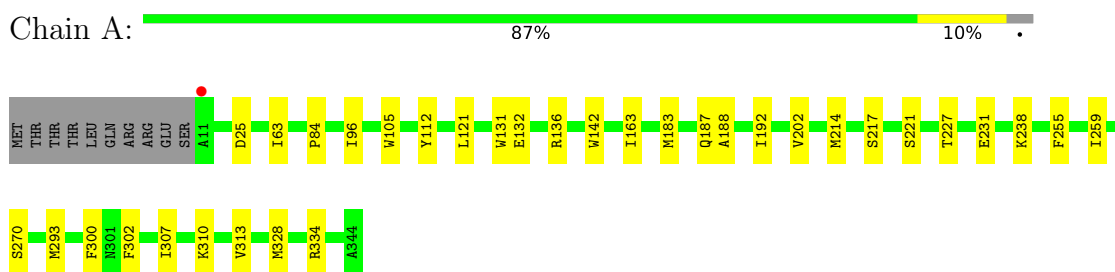
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	t	6	Total 6	O 6	0	0
41	u	47	Total 47	O 47	0	0
41	v	47	Total 47	O 47	0	0
41	x	2	Total 2	O 2	0	0
41	y	1	Total 1	O 1	0	0

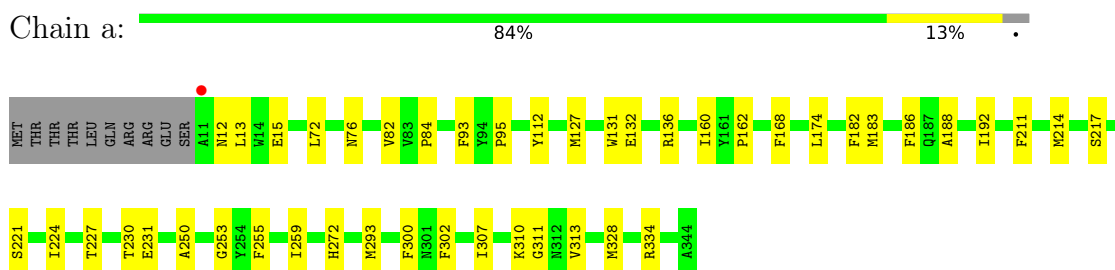
3 Residue-property plots

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

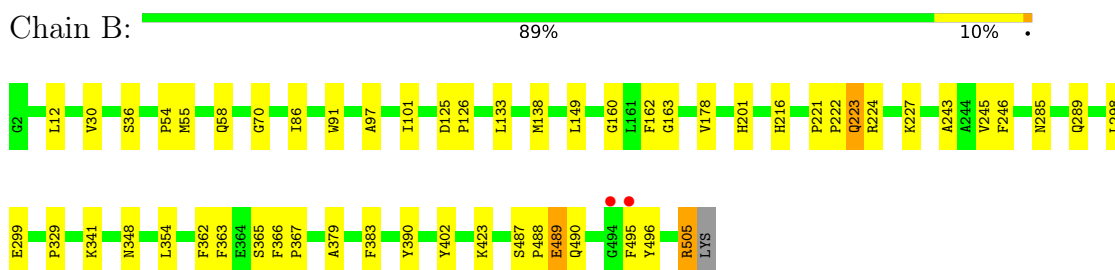
- Molecule 1: Photosystem II D1 protein



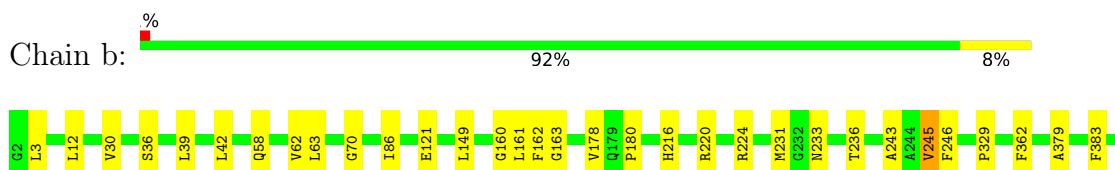
- Molecule 1: Photosystem II D1 protein

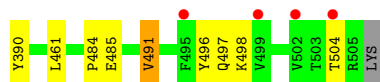


- Molecule 2: Photosystem II CP47 reaction center protein



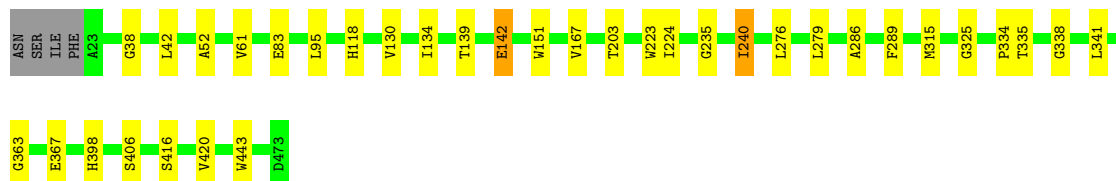
- Molecule 2: Photosystem II CP47 reaction center protein





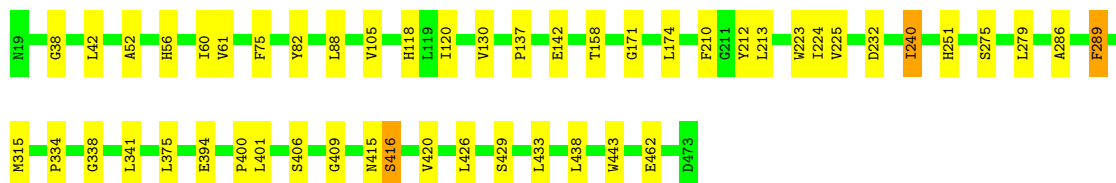
• Molecule 3: Photosystem II CP43 protein

Chain C: 91% 7% .



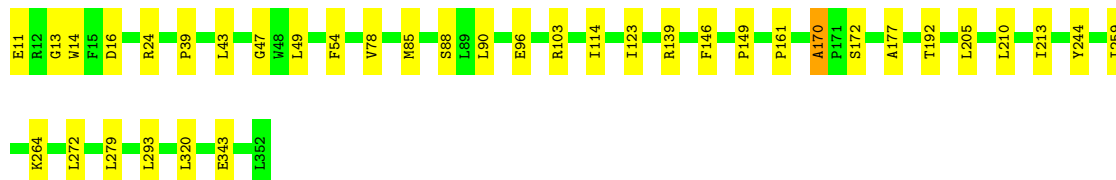
• Molecule 3: Photosystem II CP43 protein

Chain c: 89% 10% .



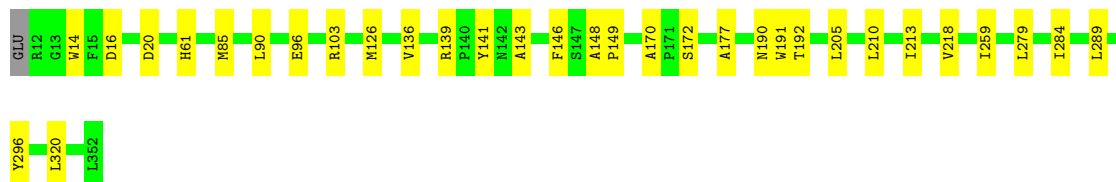
• Molecule 4: Photosystem II D2 protein

Chain D: 89% 11% .



• Molecule 4: Photosystem II D2 protein

Chain d: 90% 9% .



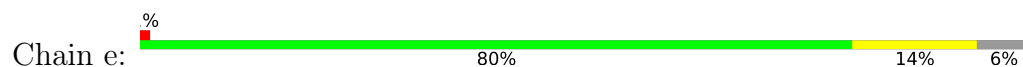
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 80% 17% .





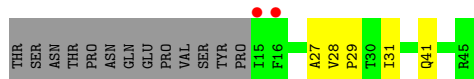
- Molecule 5: Cytochrome b559 subunit alpha



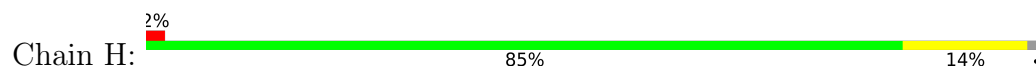
- Molecule 6: Cytochrome b559 subunit beta



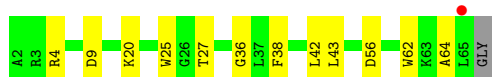
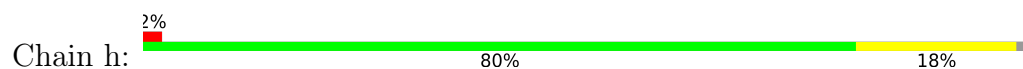
- Molecule 6: Cytochrome b559 subunit beta



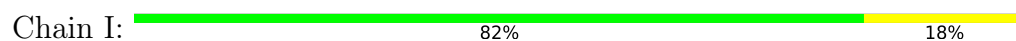
- Molecule 7: Photosystem II reaction center protein H



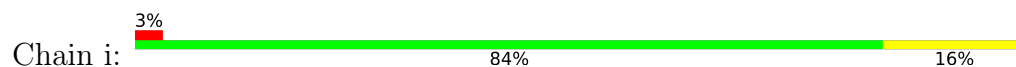
- Molecule 7: Photosystem II reaction center protein H

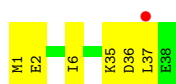


- Molecule 8: Photosystem II reaction center protein I



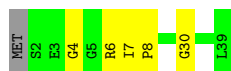
- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 85% 13% .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



- Molecule 10: Photosystem II protein K

Chain K: 81% 16% .



- Molecule 10: Photosystem II protein K

Chain k: 84% 14% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 89% 8% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 89% 8% .



- Molecule 12: Photosystem II protein M

Chain M: 83% 8% 8%



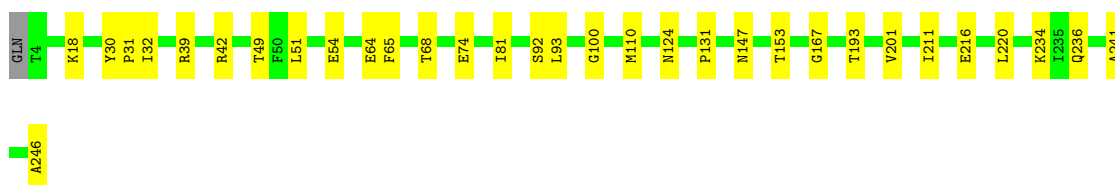
- Molecule 12: Photosystem II protein M

Chain m: 72% 19% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 86% 13%



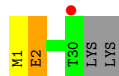
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 91% 9%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 88% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 72% 16% 6% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 84% 9% 8%

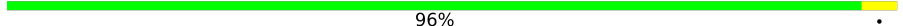


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



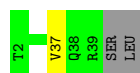
- Molecule 16: Cytochrome c-550

Chain v:  93% 7%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  92% . 5%



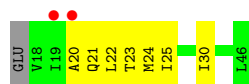
- Molecule 17: Photosystem II reaction center protein X

Chain x:  2% 88% 8% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  7% 73% 23% .

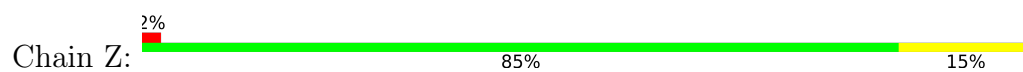


- Molecule 18: Photosystem II reaction center protein Ycf12

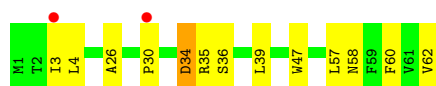
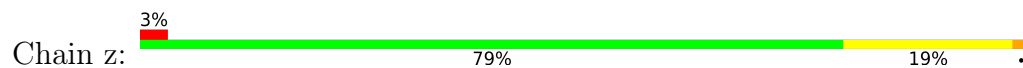
Chain y:  73% 23% .



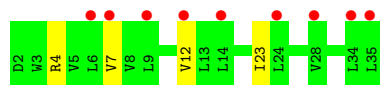
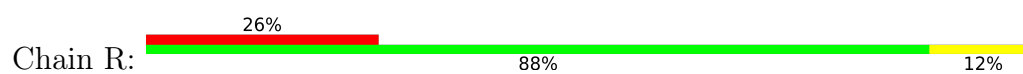
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.70Å 229.89Å 285.50Å 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	1.41 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.133 , 0.171 0.144 , 0.179	Depositor DCC
R_{free} test set	17049 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 89.7	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	52545	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.60	0/2728	0.85	1/3719 (0.0%)
1	a	0.57	0/2733	0.85	0/3727
2	B	0.56	0/4171	0.80	0/5683
2	b	0.55	0/4138	0.80	2/5640 (0.0%)
3	C	0.54	0/3626	0.81	0/4936
3	c	0.51	0/3662	0.81	0/4985
4	D	0.60	0/2827	0.81	2/3852 (0.1%)
4	d	0.56	0/2818	0.81	2/3840 (0.1%)
5	E	0.51	0/687	0.83	0/936
5	e	0.49	0/667	0.81	0/908
6	F	0.59	0/284	0.79	0/387
6	f	0.54	0/257	0.82	0/349
7	H	0.49	0/530	0.80	0/723
7	h	0.45	0/519	0.77	0/708
8	I	0.49	0/311	0.76	0/419
8	i	0.48	0/311	0.77	0/419
9	J	0.46	0/278	0.82	0/376
9	j	0.44	0/283	0.77	0/383
10	K	0.47	0/303	0.79	0/416
10	k	0.49	0/303	0.83	0/416
11	L	0.58	0/311	0.68	0/423
11	l	0.57	0/311	0.71	0/423
12	M	0.62	0/261	1.00	0/357
12	m	0.57	0/262	0.95	0/357
13	O	0.54	0/1926	0.81	0/2611
13	o	0.53	0/1910	0.82	2/2589 (0.1%)
14	T	0.63	0/257	0.79	0/349
14	t	0.56	0/257	0.77	0/349
15	U	0.53	0/776	0.78	0/1052
15	u	0.53	0/785	0.76	0/1064
16	V	0.52	0/1085	0.79	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.48	0/1085	0.78	0/1473
17	X	0.47	0/284	0.79	0/384
17	x	0.45	0/284	0.77	0/384
18	Y	0.44	0/216	0.81	0/289
18	y	0.44	0/216	0.91	0/289
19	Z	0.41	0/490	0.84	0/669
19	z	0.41	0/490	0.84	0/669
20	R	0.44	0/279	0.74	0/383
All	All	0.54	0/42921	0.81	9/58409 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	55	GLU	CA-C-N	6.24	126.19	119.76
13	o	55	GLU	C-N-CA	6.24	126.19	119.76
4	d	170	ALA	CA-C-N	-6.21	113.55	119.76
4	d	170	ALA	C-N-CA	-6.21	113.55	119.76
2	b	163	GLY	CA-C-N	5.79	125.48	119.64

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	2634	0	2546	23	0
1	a	2636	0	2549	33	0
2	B	4007	0	3879	45	0
2	b	3986	0	3855	37	0
3	C	3501	0	3428	24	0
3	c	3536	0	3463	37	0
4	D	2729	0	2632	29	0
4	d	2720	0	2626	23	0
5	E	665	0	653	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	648	0	634	9	0
6	F	275	0	282	7	0
6	f	250	0	261	5	0
7	H	514	0	542	7	0
7	h	506	0	529	14	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	4	0
9	j	277	0	284	2	0
10	K	293	0	305	6	0
10	k	293	0	305	3	0
11	L	301	0	315	2	0
11	l	301	0	315	3	0
12	M	265	0	286	2	0
12	m	269	0	288	10	0
13	O	1883	0	1865	20	0
13	o	1873	0	1852	13	0
14	T	258	0	261	2	0
14	t	258	0	261	6	0
15	U	765	0	767	5	0
15	u	774	0	773	4	0
16	V	1064	0	1073	3	0
16	v	1064	0	1073	6	0
17	X	281	0	312	1	0
17	x	281	0	312	3	0
18	Y	215	0	246	5	0
18	y	215	0	246	3	0
19	Z	479	0	516	4	0
19	z	479	0	516	8	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	14	0
23	B	1040	0	1152	40	0
23	C	845	0	936	43	0
23	D	130	0	144	4	0
23	a	260	0	288	11	0
23	b	1040	0	1152	41	0
23	c	845	0	936	51	0
23	d	130	0	144	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	128	0	148	5	0
24	a	128	0	148	6	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	80	0	112	6	0
25	D	40	0	56	4	0
25	H	40	0	56	3	0
25	K	40	0	56	2	0
25	T	40	0	56	8	0
25	Y	40	0	56	3	0
25	a	40	0	56	2	0
25	b	120	0	168	11	0
25	c	80	0	112	10	0
25	d	40	0	56	1	0
25	h	40	0	56	4	0
25	k	40	0	56	2	0
25	t	40	0	56	6	0
25	y	40	0	56	2	0
26	A	108	0	156	6	0
26	B	54	0	78	3	0
26	F	43	0	53	2	0
26	a	108	0	156	3	0
26	b	54	0	78	4	0
26	f	43	0	53	2	0
27	A	6	0	8	0	0
27	B	12	0	16	4	0
27	C	6	0	8	0	0
27	V	6	0	8	0	0
27	a	12	0	16	2	0
27	b	6	0	8	0	0
27	c	6	0	8	0	0
27	v	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	4	0
29	D	55	0	80	0	0
29	a	55	0	80	7	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	1	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	32	0	0	1	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	A	35	0	46	2	0
32	D	35	0	46	2	0
32	E	35	0	46	1	0
32	I	35	0	46	1	0
32	M	70	0	92	5	0
32	a	70	0	92	4	0
32	b	50	0	70	2	0
32	e	35	0	46	0	0
32	m	35	0	46	2	0
32	t	51	0	70	1	0
33	B	51	0	72	0	0
33	C	153	0	216	7	0
33	D	51	0	72	2	0
33	Z	37	0	44	2	0
33	a	51	0	72	1	0
33	c	102	0	144	3	0
33	d	51	0	71	1	0
33	m	51	0	72	0	0
33	z	39	0	48	1	0
34	B	57	0	78	4	0
34	C	19	0	26	0	0
34	D	16	0	17	2	0
34	V	11	0	10	0	0
34	b	57	0	78	1	0
34	c	19	0	26	0	0
34	d	16	0	17	2	0
35	C	186	0	246	8	0
35	H	62	0	82	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	186	0	246	7	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	147	0	222	4	0
37	E	42	0	57	3	0
37	L	49	0	74	1	0
37	d	147	0	222	12	0
37	e	42	0	57	2	0
37	l	49	0	74	0	0
38	E	43	0	30	4	0
38	e	43	0	30	5	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	130	0	0	1	0
41	B	167	0	0	1	0
41	C	144	0	0	2	0
41	D	122	0	0	2	0
41	E	15	0	0	0	0
41	F	4	0	0	0	0
41	H	19	0	0	0	0
41	I	6	0	0	1	0
41	J	5	0	0	1	0
41	K	6	0	0	0	0
41	L	3	0	0	0	0
41	M	7	0	0	0	0
41	O	71	0	0	0	0
41	T	9	0	0	0	0
41	U	32	0	0	0	0
41	V	67	0	0	0	0
41	X	1	0	0	0	0
41	Y	1	0	0	0	0
41	a	133	0	0	0	0
41	b	193	0	0	0	0
41	c	142	0	0	2	0
41	d	114	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	e	8	0	0	0	0
41	f	4	0	0	0	0
41	h	16	0	0	0	0
41	i	3	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	4	0	0	0	0
41	m	15	0	0	1	0
41	o	77	0	0	0	0
41	t	6	0	0	0	0
41	u	47	0	0	0	0
41	v	47	0	0	2	0
41	x	2	0	0	0	0
41	y	1	0	0	0	0
All	All	52545	0	51977	630	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 630 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)
23:b:604:CLA:H42	23:b:605:CLA:H2	1.43	0.99
23:C:514:CLA:HBB1	25:C:515:BCR:H24C	1.48	0.93
23:B:604:CLA:H42	23:B:605:CLA:H2	1.50	0.91
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.51	0.90
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.58	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36	43
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	36	43
2	B	510/505 (101%)	505 (99%)	5 (1%)	0	100	100
2	b	506/505 (100%)	500 (99%)	6 (1%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	30	34
3	c	457/455 (100%)	446 (98%)	9 (2%)	2 (0%)	30	34
4	D	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (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%)	58 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
9	J	36/39 (92%)	36 (100%)	0	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%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	238 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	237 (98%)	6 (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%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	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%)	59 (98%)	0	1 (2%)	7	6
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	6
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5251/5384 (98%)	5147 (98%)	95 (2%)	9 (0%)	48	52

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
1	a	259	ILE
3	c	416[A]	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	272/279 (98%)	270 (99%)	2 (1%)	76	86
1	a	273/279 (98%)	271 (99%)	2 (1%)	76	86
2	B	410/403 (102%)	405 (99%)	5 (1%)	63	77
2	b	406/403 (101%)	401 (99%)	5 (1%)	63	77
3	C	356/356 (100%)	352 (99%)	4 (1%)	65	79
3	c	360/356 (101%)	354 (98%)	6 (2%)	53	68
4	D	278/277 (100%)	277 (100%)	1 (0%)	84	91
4	d	277/277 (100%)	276 (100%)	1 (0%)	84	91
5	E	73/73 (100%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	25 (100%)	0	100	100
7	H	55/54 (102%)	52 (94%)	3 (6%)	19	24
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%)	34 (100%)	0	100	100
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	39
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	7
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	44
13	O	210/207 (101%)	210 (100%)	0	100	100
13	o	208/207 (100%)	206 (99%)	2 (1%)	68	81
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%)	82 (99%)	1 (1%)	63	77
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	82
16	v	117/117 (100%)	116 (99%)	1 (1%)	70	82
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%)	21 (96%)	1 (4%)	24	32
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	9
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	22
19	z	52/52 (100%)	48 (92%)	4 (8%)	12	13
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	43
All	All	4357/4403 (99%)	4302 (99%)	55 (1%)	63	76

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	63	LEU
3	c	289	PHE
19	z	62	VAL
18	y	30	ILE
2	b	245	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	53	ASN
3	c	44	ASN
15	u	78	ASN
2	b	374	ASN
3	c	201	ASN

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	8,9,11	1.10	1 (12%)
12	FME	M	1	12	8,9,10	0.62	0	8,9,11	1.40	2 (25%)
14	FME	T	1	14	8,9,10	0.60	0	8,9,11	1.88	3 (37%)
8	FME	i	1	8	8,9,10	0.61	0	8,9,11	1.31	1 (12%)
14	FME	t	1	14	8,9,10	0.65	0	8,9,11	1.56	2 (25%)
12	FME	m	1	12	8,9,10	0.60	0	8,9,11	1.42	2 (25%)

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-3.57	104.02	110.52
14	t	1	FME	O-C-CA	-2.71	117.79	124.77
14	t	1	FME	CA-N-CN	-2.55	118.89	122.82
12	m	1	FME	CA-N-CN	-2.50	118.98	122.82
12	M	1	FME	O-C-CA	-2.37	118.67	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
12	M	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	CB-CA-N-CN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 214 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 181 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
23	CLA	D	406	4	69,73,73	2.01	18 (26%)	82,113,113	2.71	32 (39%)
25	BCR	B	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	10 (17%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.20	6 (10%)
33	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.06	3 (5%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.76	14 (25%)
35	DGD	c	518	-	63,63,67	0.90	3 (4%)	77,77,81	0.98	4 (5%)
24	PHO	A	353	-	58,69,69	2.70	13 (22%)	55,99,99	3.19	18 (32%)
25	BCR	b	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	13 (23%)
23	CLA	c	507	3	69,73,73	2.00	18 (26%)	82,113,113	2.59	31 (37%)
32	LMT	a	414	-	36,36,36	0.56	1 (2%)	47,47,47	1.11	4 (8%)
23	CLA	A	408	1	69,73,73	2.00	20 (28%)	82,113,113	2.82	33 (40%)
32	LMT	m	103	-	36,36,36	0.47	0	47,47,47	0.93	1 (2%)
27	GOL	V	201	-	5,5,5	0.43	0	5,5,5	0.51	0
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.54	11 (19%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.26	4 (6%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.79	13 (23%)
24	PHO	a	408	-	58,69,69	2.72	12 (20%)	55,99,99	3.10	17 (30%)
31	BCT	A	348	21	3,3,3	0.53	0	2,3,3	1.11	0
26	SQD	b	620	-	52,54,54	0.98	2 (3%)	62,65,65	1.54	9 (14%)
23	CLA	B	603	2	69,73,73	1.92	20 (28%)	82,113,113	2.80	34 (41%)
27	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.50	0
34	HTG	B	622	-	19,19,19	0.95	1 (5%)	23,24,24	1.48	5 (21%)
29	PL9	a	416	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	23 (33%)
32	LMT	A	359	-	36,36,36	0.59	1 (2%)	47,47,47	0.89	1 (2%)
26	SQD	B	620	-	52,54,54	0.97	3 (5%)	62,65,65	1.43	8 (12%)
23	CLA	C	509	3	69,73,73	2.00	21 (30%)	82,113,113	2.62	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	609	2	69,73,73	1.98	20 (28%)	82,113,113	2.72	31 (37%)
33	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.17	4 (6%)
26	SQD	a	411	-	52,54,54	0.88	2 (3%)	62,65,65	1.68	13 (20%)
23	CLA	c	510	3	69,73,73	2.05	20 (28%)	82,113,113	2.76	33 (40%)
23	CLA	B	606	2	69,73,73	1.90	19 (27%)	82,113,113	2.84	32 (39%)
32	LMT	e	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.93	2 (4%)
34	HTG	C	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.27	2 (8%)
29	PL9	A	414	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	b	603	2	69,73,73	1.98	20 (28%)	82,113,113	2.76	34 (41%)
23	CLA	c	513	3	69,73,73	1.99	19 (27%)	82,113,113	2.76	33 (40%)
23	CLA	C	508	41	69,73,73	1.99	18 (26%)	82,113,113	2.65	29 (35%)
35	DGD	c	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.05	6 (7%)
23	CLA	C	507	3	69,73,73	1.99	20 (28%)	82,113,113	2.65	34 (41%)
34	HTG	b	625	-	19,19,19	0.86	2 (10%)	23,24,24	1.31	3 (13%)
35	DGD	c	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.14	8 (10%)
29	PL9	D	408	-	55,55,55	0.67	1 (1%)	68,69,69	1.76	19 (27%)
32	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.12	3 (6%)
33	LMG	a	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.13	6 (10%)
23	CLA	b	612	2	69,73,73	1.96	20 (28%)	82,113,113	2.67	29 (35%)
23	CLA	C	503	3	69,73,73	1.99	20 (28%)	82,113,113	2.66	29 (35%)
23	CLA	C	512	3	69,73,73	1.99	20 (28%)	82,113,113	2.58	31 (37%)
23	CLA	b	606	2	69,73,73	1.96	19 (27%)	82,113,113	2.75	33 (40%)
23	CLA	C	510	3	69,73,73	2.02	21 (30%)	82,113,113	2.67	32 (39%)
25	BCR	c	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.83	16 (28%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.59	9 (16%)
23	CLA	B	616	2	69,73,73	1.99	19 (27%)	82,113,113	2.67	28 (34%)
23	CLA	C	513	3	69,73,73	2.01	20 (28%)	82,113,113	2.67	31 (37%)
23	CLA	a	406	41	69,73,73	2.01	18 (26%)	82,113,113	2.77	30 (36%)
23	CLA	B	609	2	69,73,73	1.99	17 (24%)	82,113,113	2.67	27 (32%)
27	GOL	c	501	-	5,5,5	0.32	0	5,5,5	0.45	0
34	HTG	b	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.55	1 (4%)
38	HEM	E	103	5,6	50,50,50	1.51	7 (14%)	67,82,82	1.74	15 (22%)
23	CLA	c	506	3	69,73,73	1.97	19 (27%)	82,113,113	2.58	30 (36%)
23	CLA	C	506	3	69,73,73	1.97	19 (27%)	82,113,113	2.68	33 (40%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.89	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	502	3	69,73,73	1.93	20 (28%)	82,113,113	2.76	31 (37%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.25	0
23	CLA	B	604	2	69,73,73	1.94	19 (27%)	82,113,113	2.67	33 (40%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.54	6 (10%)
23	CLA	A	405	41	69,73,73	2.02	18 (26%)	82,113,113	2.76	33 (40%)
23	CLA	c	502	3	69,73,73	2.02	20 (28%)	82,113,113	2.68	32 (39%)
34	HTG	d	411	-	16,16,19	1.06	2 (12%)	20,21,24	1.49	2 (10%)
23	CLA	D	405	4	69,73,73	1.85	19 (27%)	82,113,113	2.71	32 (39%)
35	DGD	C	519	-	63,63,67	0.83	3 (4%)	77,77,81	1.05	6 (7%)
23	CLA	a	409	1	69,73,73	1.96	19 (27%)	82,113,113	2.65	34 (41%)
23	CLA	a	405	1	69,73,73	2.00	20 (28%)	82,113,113	2.64	36 (43%)
32	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.93	2 (4%)
23	CLA	c	503	3	69,73,73	1.92	20 (28%)	82,113,113	2.66	30 (36%)
33	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
26	SQD	A	412	-	52,54,54	0.95	2 (3%)	62,65,65	1.18	9 (14%)
31	BCT	a	404	21	3,3,3	0.51	0	2,3,3	1.13	0
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	c	514	3	69,73,73	2.05	21 (30%)	82,113,113	2.69	32 (39%)
33	LMG	D	415	39	51,51,55	0.88	3 (5%)	59,59,63	0.89	3 (5%)
25	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.70	13 (23%)
23	CLA	b	604	2	69,73,73	1.92	18 (26%)	82,113,113	2.72	31 (37%)
23	CLA	A	406	41	69,73,73	1.96	19 (27%)	82,113,113	2.70	32 (39%)
23	CLA	b	611	2	69,73,73	1.93	18 (26%)	82,113,113	2.81	30 (36%)
25	BCR	a	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	13 (23%)
32	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.10	4 (8%)
33	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.10	4 (8%)
32	LMT	a	420	-	36,36,36	0.49	1 (2%)	47,47,47	0.93	1 (2%)
33	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.48	7 (15%)
23	CLA	B	611	2	69,73,73	1.99	19 (27%)	82,113,113	2.68	31 (37%)
29	PL9	d	405	-	55,55,55	0.67	1 (1%)	68,69,69	1.79	19 (27%)
35	DGD	h	102	-	63,63,67	0.85	2 (3%)	77,77,81	0.98	4 (5%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.63	15 (26%)
23	CLA	b	610	41	69,73,73	1.98	20 (28%)	82,113,113	2.76	32 (39%)
23	CLA	b	615	2	69,73,73	1.97	18 (26%)	82,113,113	2.67	30 (36%)
27	GOL	B	625	-	5,5,5	0.62	0	5,5,5	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	D	410	-	48,48,48	0.87	3 (6%)	51,54,54	1.00	3 (5%)
23	CLA	C	511	3	69,73,73	2.01	20 (28%)	82,113,113	2.79	32 (39%)
27	GOL	b	624	-	5,5,5	0.30	0	5,5,5	0.57	0
37	LHG	D	411	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	3 (5%)
34	HTG	V	203	-	11,11,19	0.24	0	15,15,24	1.06	1 (6%)
23	CLA	b	605	2	69,73,73	1.94	19 (27%)	82,113,113	2.88	30 (36%)
23	CLA	c	504	3	69,73,73	2.01	19 (27%)	82,113,113	2.69	29 (35%)
23	CLA	C	504	3	69,73,73	1.97	20 (28%)	82,113,113	2.70	32 (39%)
32	LMT	b	621	-	25,25,36	0.48	0	30,30,47	0.72	0
26	SQD	A	410	-	52,54,54	0.87	2 (3%)	62,65,65	1.91	12 (19%)
37	LHG	L	101	-	48,48,48	0.94	3 (6%)	51,54,54	1.09	2 (3%)
32	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.89	0
37	LHG	D	409	-	48,48,48	0.91	3 (6%)	51,54,54	1.18	6 (11%)
25	BCR	D	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.95	15 (26%)
23	CLA	C	505	41	69,73,73	1.98	20 (28%)	82,113,113	2.70	31 (37%)
37	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.12	5 (9%)
23	CLA	B	608	2	69,73,73	1.94	21 (30%)	82,113,113	2.65	31 (37%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
34	HTG	b	622	-	19,19,19	0.97	1 (5%)	23,24,24	1.67	4 (17%)
23	CLA	b	614	2	69,73,73	1.91	20 (28%)	82,113,113	2.76	31 (37%)
24	PHO	A	407	-	58,69,69	2.59	14 (24%)	55,99,99	3.06	19 (34%)
23	CLA	c	505	41	69,73,73	1.97	20 (28%)	82,113,113	2.78	34 (41%)
23	CLA	d	403	4	69,73,73	2.02	20 (28%)	82,113,113	2.78	36 (43%)
32	LMT	t	101	-	25,25,36	0.53	1 (4%)	30,30,47	1.04	1 (3%)
23	CLA	a	407	41	69,73,73	1.96	19 (27%)	82,113,113	2.74	32 (39%)
23	CLA	b	607	41	69,73,73	1.92	18 (26%)	82,113,113	2.71	31 (37%)
34	HTG	D	414	-	16,16,19	0.95	2 (12%)	20,21,24	1.39	1 (5%)
37	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	4 (7%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
28	OEX	a	415	41,1,3	0,15,15	-	-	-	-	-
24	PHO	a	353	-	58,69,69	2.75	13 (22%)	55,99,99	3.07	17 (30%)
32	LMT	b	627	-	25,25,36	0.53	1 (4%)	30,30,47	0.76	0
33	LMG	c	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.06	4 (6%)
38	HEM	e	87	5,6	50,50,50	1.54	8 (16%)	67,82,82	1.63	13 (19%)
23	CLA	B	610	41	69,73,73	2.00	21 (30%)	82,113,113	2.67	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	F	101	-	41,43,54	1.11	3 (7%)	51,54,65	1.75	11 (21%)
32	LMT	t	102	-	26,26,36	0.57	1 (3%)	31,31,47	0.97	2 (6%)
25	BCR	t	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.77	15 (26%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.52	12 (21%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.32	6 (10%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.17	5 (11%)
25	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	14 (25%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.00	4 (5%)
23	CLA	d	402	4	69,73,73	1.93	19 (27%)	82,113,113	2.65	32 (39%)
40	HEC	v	202	16	46,50,50	1.78	9 (19%)	58,82,82	1.73	13 (22%)
23	CLA	b	608	2	69,73,73	2.02	20 (28%)	82,113,113	2.70	35 (42%)
26	SQD	a	413	-	52,54,54	1.00	2 (3%)	62,65,65	1.18	7 (11%)
27	GOL	B	624	-	5,5,5	0.37	0	5,5,5	0.59	0
23	CLA	B	601	41	69,73,73	2.06	21 (30%)	82,113,113	2.72	31 (37%)
23	CLA	B	612	2	69,73,73	1.89	19 (27%)	82,113,113	2.74	34 (41%)
23	CLA	b	613	2	69,73,73	1.98	19 (27%)	82,113,113	2.68	30 (36%)
25	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	12 (21%)
23	CLA	B	605	2	69,73,73	1.97	19 (27%)	82,113,113	2.83	32 (39%)
28	OEX	A	413	41,1,3	0,15,15	-	-	-	-	-
23	CLA	B	607	41	69,73,73	1.97	19 (27%)	82,113,113	2.76	33 (40%)
27	GOL	a	418	-	5,5,5	0.38	0	5,5,5	0.71	0
25	BCR	c	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.63	12 (21%)
25	BCR	C	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.65	14 (25%)
32	LMT	M	101	-	36,36,36	0.48	0	47,47,47	1.07	3 (6%)
23	CLA	b	601	41	69,73,73	2.08	22 (31%)	82,113,113	2.63	28 (34%)
27	GOL	v	201	-	5,5,5	0.42	0	5,5,5	0.38	0
34	HTG	B	623	-	19,19,19	0.84	1 (5%)	23,24,24	1.34	3 (13%)
40	HEC	V	202	16	46,50,50	1.71	8 (17%)	58,82,82	1.70	13 (22%)
34	HTG	B	626	-	19,19,19	0.92	2 (10%)	23,24,24	1.43	4 (17%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	13 (23%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	11 (19%)
23	CLA	c	511	3	69,73,73	1.98	20 (28%)	82,113,113	2.72	34 (41%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	82,113,113	2.71	32 (39%)
23	CLA	c	509	3	69,73,73	2.00	19 (27%)	82,113,113	2.72	30 (36%)
37	LHG	d	407	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	508	41	69,73,73	1.97	18 (26%)	82,113,113	2.71	30 (36%)
33	LMG	c	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.17	5 (8%)
23	CLA	B	614	2	69,73,73	1.94	19 (27%)	82,113,113	2.98	32 (39%)
34	HTG	c	522	-	19,19,19	0.90	1 (5%)	23,24,24	1.39	1 (4%)
35	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.23	8 (10%)
23	CLA	A	404	1	69,73,73	1.97	19 (27%)	82,113,113	2.77	32 (39%)
23	CLA	b	602	2	69,73,73	2.01	19 (27%)	82,113,113	2.79	35 (42%)
23	CLA	b	616	2	69,73,73	1.99	18 (26%)	82,113,113	2.71	33 (40%)
26	SQD	f	102	-	41,43,54	1.10	2 (4%)	51,54,65	1.44	9 (17%)
27	GOL	C	523	-	5,5,5	0.48	0	5,5,5	0.14	0
23	CLA	B	615	2	69,73,73	1.94	18 (26%)	82,113,113	2.68	33 (40%)
23	CLA	c	512	3	69,73,73	1.98	18 (26%)	82,113,113	2.72	29 (35%)
23	CLA	B	613	2	69,73,73	1.99	19 (27%)	82,113,113	2.69	31 (37%)
25	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	7 (12%)
23	CLA	B	602	2	69,73,73	2.05	19 (27%)	82,113,113	2.77	33 (40%)

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
23	CLA	D	406	4	1/1/15/20	7/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	LMG	m	101	-	-	14/46/66/70	0/1/1/1
33	LMG	d	412	39	-	7/46/66/70	0/1/1/1
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
35	DGD	c	518	-	-	11/51/91/95	0/2/2/2
24	PHO	A	353	-	-	1/37/103/103	0/5/6/6
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	c	507	3	1/1/15/20	11/39/115/115	-
32	LMT	a	414	-	-	7/21/61/61	0/2/2/2
23	CLA	A	408	1	1/1/15/20	13/39/115/115	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
27	GOL	V	201	-	-	2/4/4/4	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	521	-	-	9/46/66/70	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
24	PHO	a	408	-	-	5/37/103/103	0/5/6/6
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
23	CLA	B	603	2	1/1/15/20	4/39/115/115	-
27	GOL	a	412	-	-	4/4/4/4	-
34	HTG	B	622	-	-	5/10/30/30	0/1/1/1
29	PL9	a	416	-	-	16/53/73/73	0/1/1/1
32	LMT	A	359	-	-	3/21/61/61	0/2/2/2
26	SQD	B	620	-	-	18/49/69/69	0/1/1/1
23	CLA	C	509	3	1/1/15/20	2/39/115/115	-
23	CLA	b	609	2	1/1/15/20	8/39/115/115	-
33	LMG	B	621	-	-	15/46/66/70	0/1/1/1
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
23	CLA	c	510	3	1/1/15/20	13/39/115/115	-
23	CLA	B	606	2	1/1/15/20	8/39/115/115	-
32	LMT	e	102	-	-	7/21/61/61	0/2/2/2
34	HTG	C	522	-	-	1/10/30/30	0/1/1/1
29	PL9	A	414	-	-	16/53/73/73	0/1/1/1
23	CLA	b	603	2	1/1/15/20	5/39/115/115	-
23	CLA	c	513	3	1/1/15/20	12/39/115/115	-
23	CLA	C	508	41	1/1/15/20	8/39/115/115	-
35	DGD	c	519	-	-	7/51/91/95	0/2/2/2
23	CLA	C	507	3	1/1/15/20	11/39/115/115	-
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1
35	DGD	c	517	-	-	21/51/91/95	0/2/2/2
29	PL9	D	408	-	-	7/53/73/73	0/1/1/1
32	LMT	I	101	-	-	9/21/61/61	0/2/2/2
33	LMG	a	419	-	-	12/46/66/70	0/1/1/1
23	CLA	b	612	2	1/1/15/20	2/39/115/115	-
23	CLA	C	503	3	1/1/15/20	8/39/115/115	-
23	CLA	C	512	3	1/1/15/20	4/39/115/115	-
23	CLA	b	606	2	1/1/15/20	5/39/115/115	-
23	CLA	C	510	3	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	B	616	2	1/1/15/20	7/39/115/115	-
23	CLA	C	513	3	1/1/15/20	10/39/115/115	-
23	CLA	a	406	41	-	3/39/115/115	-
23	CLA	B	609	2	1/1/15/20	3/39/115/115	-
27	GOL	c	501	-	-	0/4/4/4	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
38	HEM	E	103	5,6	-	8/14/54/54	-
23	CLA	c	506	3	1/1/15/20	3/39/115/115	-
23	CLA	C	506	3	1/1/15/20	7/39/115/115	-
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
23	CLA	C	502	3	1/1/15/20	4/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	604	2	1/1/15/20	7/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	A	405	41	1/1/15/20	2/39/115/115	-
23	CLA	c	502	3	1/1/15/20	3/39/115/115	-
34	HTG	d	411	-	-	0/7/27/30	0/1/1/1
23	CLA	D	405	4	1/1/15/20	5/39/115/115	-
35	DGD	C	519	-	-	14/51/91/95	0/2/2/2
23	CLA	a	409	1	1/1/15/20	13/39/115/115	-
23	CLA	a	405	1	1/1/15/20	2/39/115/115	-
32	LMT	M	103	-	-	10/21/61/61	0/2/2/2
23	CLA	c	503	3	1/1/15/20	7/39/115/115	-
33	LMG	C	520	-	-	12/46/66/70	0/1/1/1
26	SQD	A	412	-	-	11/49/69/69	0/1/1/1
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	c	514	3	1/1/15/20	8/39/115/115	-
33	LMG	D	415	39	-	10/46/66/70	0/1/1/1
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	604	2	1/1/15/20	5/39/115/115	-
23	CLA	b	611	2	1/1/15/20	4/39/115/115	-
23	CLA	A	406	41	-	6/39/115/115	-
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	D	404	-	-	7/21/61/61	0/2/2/2
33	LMG	z	101	-	-	8/34/54/70	0/1/1/1
32	LMT	a	420	-	-	5/21/61/61	0/2/2/2
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
23	CLA	B	611	2	1/1/15/20	2/39/115/115	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
35	DGD	h	102	-	-	10/51/91/95	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	41	1/1/15/20	9/39/115/115	-
23	CLA	b	615	2	1/1/15/20	5/39/115/115	-
27	GOL	B	625	-	-	3/4/4/4	-
37	LHG	D	410	-	-	15/53/53/53	-
23	CLA	C	511	3	1/1/15/20	12/39/115/115	-
27	GOL	b	624	-	-	0/4/4/4	-
37	LHG	D	411	-	-	14/53/53/53	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	b	605	2	1/1/15/20	4/39/115/115	-
23	CLA	c	504	3	1/1/15/20	1/39/115/115	-
23	CLA	C	504	3	1/1/15/20	3/39/115/115	-
32	LMT	b	621	-	-	7/17/37/61	0/1/1/2
26	SQD	A	410	-	-	15/49/69/69	0/1/1/1
37	LHG	L	101	-	-	18/53/53/53	-
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
37	LHG	D	409	-	-	10/53/53/53	-
25	BCR	D	407	-	-	6/29/63/63	0/2/2/2
23	CLA	C	505	41	1/1/15/20	6/39/115/115	-
37	LHG	l	101	-	-	18/53/53/53	-
23	CLA	B	608	2	-	3/39/115/115	-
37	LHG	e	101	-	-	11/46/46/53	-
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	614	2	1/1/15/20	11/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	c	505	41	1/1/15/20	4/39/115/115	-
23	CLA	d	403	4	1/1/15/20	7/39/115/115	-
32	LMT	t	101	-	-	6/17/37/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	607	41	1/1/15/20	4/39/115/115	-
23	CLA	a	407	41	-	6/39/115/115	-
34	HTG	D	414	-	-	0/7/27/30	0/1/1/1
37	LHG	d	406	-	-	5/53/53/53	-
37	LHG	d	408	-	-	13/53/53/53	-
24	PHO	a	353	-	-	2/37/103/103	0/5/6/6
32	LMT	b	627	-	-	8/17/37/61	0/1/1/2
33	LMG	c	520	-	-	15/46/66/70	0/1/1/1
38	HEM	e	87	5,6	-	9/14/54/54	-
23	CLA	B	610	41	1/1/15/20	4/39/115/115	-
26	SQD	F	101	-	-	14/38/58/69	0/1/1/1
32	LMT	t	102	-	-	5/17/38/61	0/1/1/2
25	BCR	t	103	-	-	5/29/63/63	0/2/2/2
25	BCR	H	101	-	-	5/29/63/63	0/2/2/2
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
37	LHG	E	101	-	-	18/46/46/53	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	d	402	4	1/1/15/20	4/39/115/115	-
40	HEC	v	202	16	-	6/14/54/54	-
23	CLA	b	608	2	-	4/39/115/115	-
26	SQD	a	413	-	-	16/49/69/69	0/1/1/1
27	GOL	B	624	-	-	4/4/4/4	-
23	CLA	B	601	41	1/1/15/20	12/39/115/115	-
23	CLA	B	612	2	1/1/15/20	3/39/115/115	-
23	CLA	b	613	2	1/1/15/20	7/39/115/115	-
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
23	CLA	B	605	2	1/1/15/20	6/39/115/115	-
23	CLA	B	607	41	1/1/15/20	3/39/115/115	-
27	GOL	a	418	-	-	2/4/4/4	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	b	601	41	1/1/15/20	18/39/115/115	-
27	GOL	v	201	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
40	HEC	V	202	16	-	6/14/54/54	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	c	511	3	1/1/15/20	9/39/115/115	-
23	CLA	C	514	3	1/1/15/20	7/39/115/115	-
23	CLA	c	509	3	1/1/15/20	1/39/115/115	-
37	LHG	d	407	-	-	15/53/53/53	-
23	CLA	c	508	41	1/1/15/20	8/39/115/115	-
33	LMG	c	521	-	-	7/46/66/70	0/1/1/1
23	CLA	B	614	2	1/1/15/20	10/39/115/115	-
34	HTG	c	522	-	-	4/10/30/30	0/1/1/1
35	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	A	404	1	1/1/15/20	3/39/115/115	-
23	CLA	b	602	2	1/1/15/20	3/39/115/115	-
23	CLA	b	616	2	1/1/15/20	10/39/115/115	-
26	SQD	f	102	-	-	13/38/58/69	0/1/1/1
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	B	615	2	1/1/15/20	8/39/115/115	-
23	CLA	c	512	3	1/1/15/20	7/39/115/115	-
23	CLA	B	613	2	1/1/15/20	6/39/115/115	-
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
23	CLA	B	602	2	1/1/15/20	6/39/115/115	-

The worst 5 of 1581 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	353	PHO	C1D-C2D	9.50	1.49	1.39
24	a	408	PHO	C1B-C2B	9.41	1.49	1.39
24	A	353	PHO	C1D-C2D	8.75	1.49	1.39
24	A	407	PHO	C1D-C2D	8.59	1.48	1.39
24	a	408	PHO	C1D-C2D	8.58	1.48	1.39

The worst 5 of 2970 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	353	PHO	C2D-C1D-ND	12.09	118.17	109.43
24	A	407	PHO	C2D-C1D-ND	11.39	117.66	109.43
24	a	408	PHO	C2D-C1D-ND	10.78	117.22	109.43
24	a	353	PHO	C2D-C1D-ND	10.55	117.06	109.43
23	A	408	CLA	C1D-ND-C4D	-10.52	98.93	106.31

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

5 of 1203 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

146 monomers are involved in 367 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	406	CLA	1	0
33	d	412	LMG	1	0
25	Y	101	BCR	3	0
35	c	518	DGD	4	0
24	A	353	PHO	4	0
25	b	619	BCR	3	0
23	c	507	CLA	2	0
32	a	414	LMT	3	0
23	A	408	CLA	4	0
32	m	103	LMT	2	0
25	B	619	BCR	2	0
33	C	521	LMG	1	0
25	y	101	BCR	2	0
24	a	408	PHO	2	0
26	b	620	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	603	CLA	5	0
27	a	412	GOL	1	0
34	B	622	HTG	3	0
29	a	416	PL9	7	0
32	A	359	LMT	2	0
26	B	620	SQD	3	0
23	C	509	CLA	4	0
23	b	609	CLA	4	0
26	a	411	SQD	3	0
23	c	510	CLA	6	0
23	B	606	CLA	3	0
29	A	414	PL9	4	0
23	b	603	CLA	2	0
23	c	513	CLA	6	0
23	C	508	CLA	4	0
35	c	519	DGD	1	0
23	C	507	CLA	4	0
35	c	517	DGD	2	0
32	I	101	LMT	1	0
33	a	419	LMG	1	0
23	b	612	CLA	3	0
23	C	503	CLA	2	0
23	C	512	CLA	3	0
23	b	606	CLA	6	0
23	C	510	CLA	3	0
25	c	515	BCR	5	0
25	C	515	BCR	5	0
23	B	616	CLA	4	0
23	C	513	CLA	2	0
23	a	406	CLA	6	0
23	B	609	CLA	4	0
38	E	103	HEM	4	0
23	c	506	CLA	9	0
23	C	506	CLA	12	0
25	d	404	BCR	1	0
23	C	502	CLA	3	0
23	B	604	CLA	4	0
25	b	617	BCR	2	0
23	A	405	CLA	4	0
23	c	502	CLA	2	0
34	d	411	HTG	2	0
23	D	405	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	519	DGD	1	0
23	a	409	CLA	1	0
23	a	405	CLA	5	0
32	M	103	LMT	3	0
23	c	503	CLA	3	0
26	A	412	SQD	2	0
35	C	518	DGD	2	0
23	c	514	CLA	5	0
33	D	415	LMG	2	0
25	T	101	BCR	8	0
23	b	604	CLA	2	0
23	A	406	CLA	3	0
25	a	410	BCR	2	0
32	D	404	LMT	2	0
33	z	101	LMG	1	0
32	a	420	LMT	1	0
33	Z	101	LMG	2	0
29	d	405	PL9	1	0
25	B	618	BCR	6	0
23	b	610	CLA	1	0
23	b	615	CLA	3	0
27	B	625	GOL	4	0
23	C	511	CLA	4	0
37	D	411	LHG	3	0
23	b	605	CLA	5	0
23	c	504	CLA	4	0
23	C	504	CLA	4	0
32	b	621	LMT	2	0
26	A	410	SQD	4	0
37	L	101	LHG	1	0
32	E	102	LMT	1	0
37	D	409	LHG	1	0
25	D	407	BCR	4	0
23	C	505	CLA	1	0
37	e	101	LHG	2	0
34	b	622	HTG	1	0
23	b	614	CLA	6	0
24	A	407	PHO	1	0
23	c	505	CLA	3	0
23	d	403	CLA	4	0
32	t	101	LMT	1	0
23	a	407	CLA	1	0

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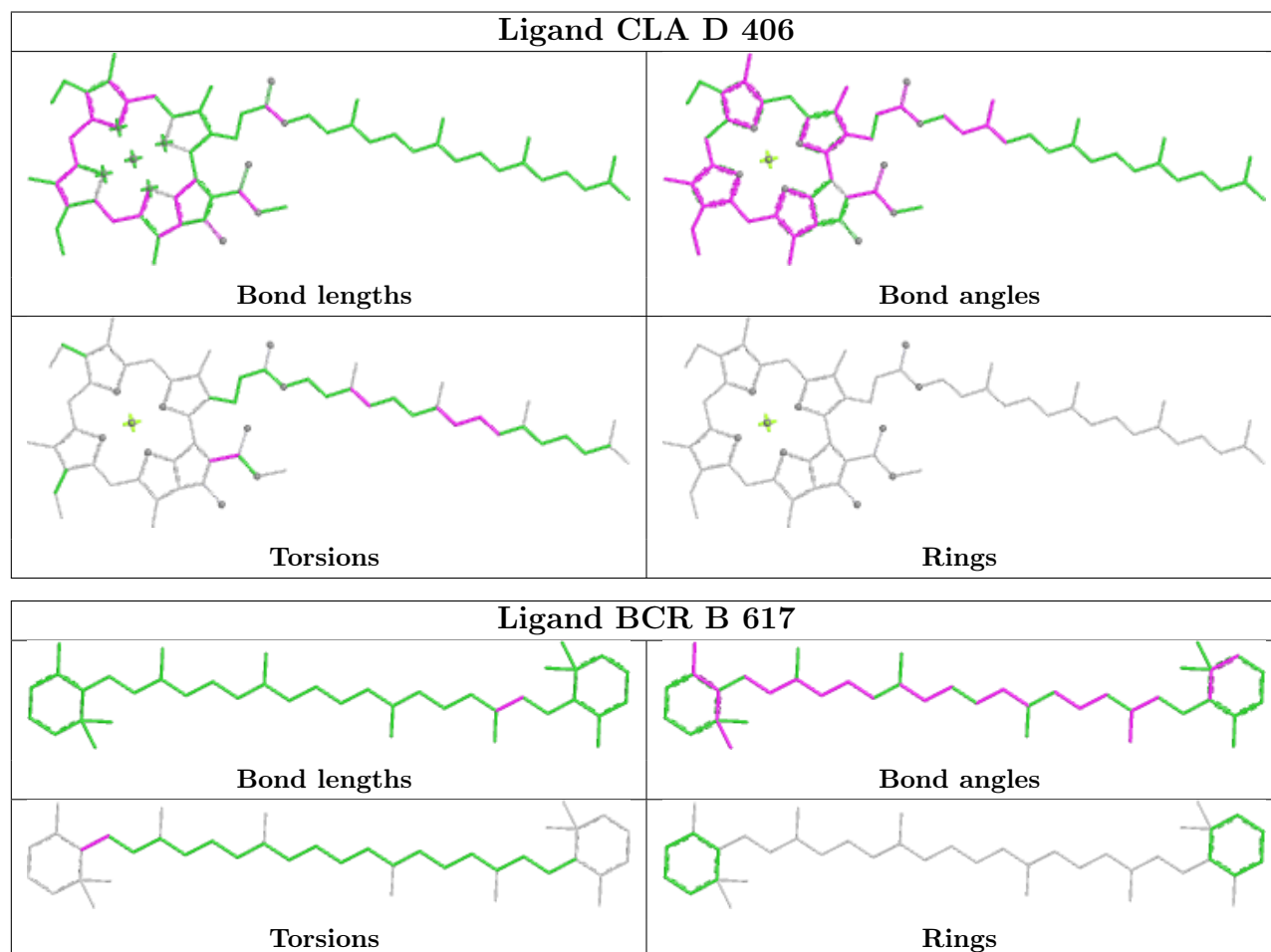
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34	D	414	HTG	2	0
37	d	406	LHG	2	0
37	d	408	LHG	7	0
24	a	353	PHO	4	0
33	c	520	LMG	1	0
38	e	87	HEM	5	0
23	B	610	CLA	1	0
26	F	101	SQD	2	0
25	t	103	BCR	6	0
25	H	101	BCR	3	0
33	C	501	LMG	6	0
37	E	101	LHG	3	0
25	A	409	BCR	1	0
35	H	102	DGD	2	0
23	d	402	CLA	2	0
23	b	608	CLA	1	0
23	B	601	CLA	1	0
23	B	612	CLA	3	0
23	b	613	CLA	4	0
25	K	102	BCR	2	0
23	B	605	CLA	8	0
27	a	418	GOL	1	0
25	c	516	BCR	5	0
25	C	516	BCR	1	0
32	M	101	LMT	2	0
23	b	601	CLA	1	0
34	B	623	HTG	1	0
25	k	101	BCR	2	0
25	b	618	BCR	6	0
23	c	511	CLA	5	0
23	C	514	CLA	4	0
23	c	509	CLA	8	0
37	d	407	LHG	3	0
23	c	508	CLA	5	0
33	c	521	LMG	2	0
23	B	614	CLA	4	0
35	C	517	DGD	5	0
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23	b	602	CLA	2	0
23	b	616	CLA	2	0
26	f	102	SQD	2	0

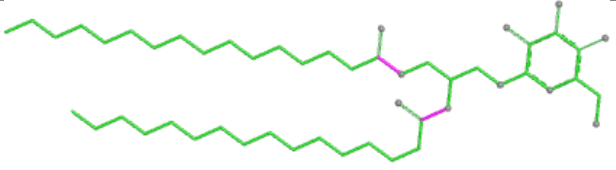
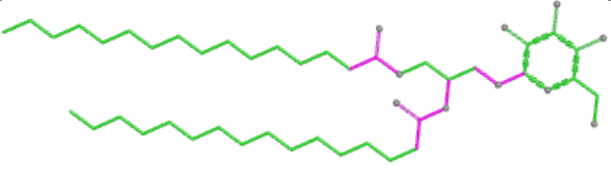
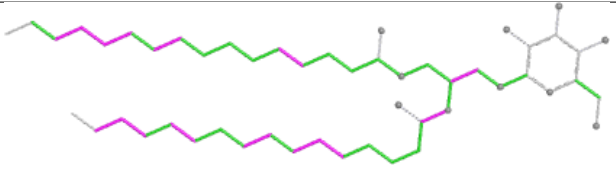
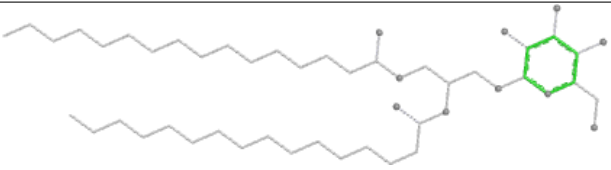
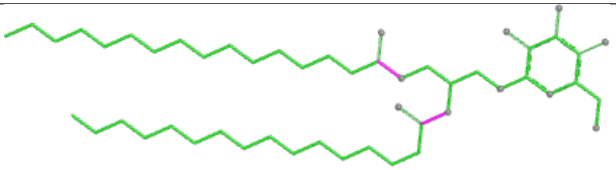
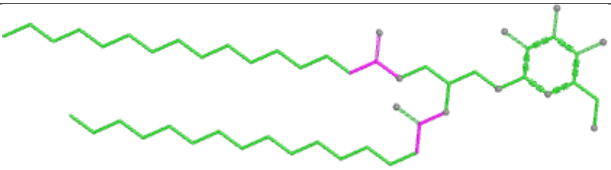
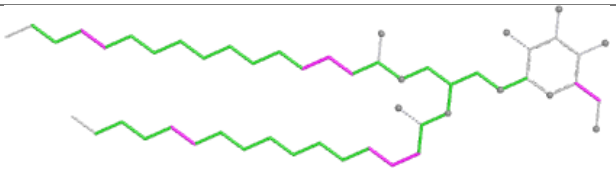
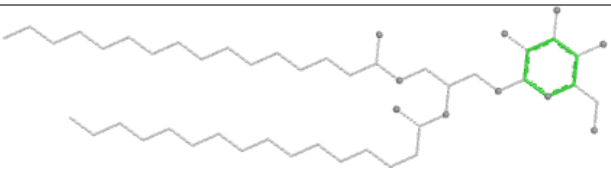
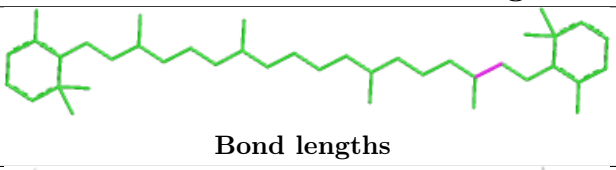
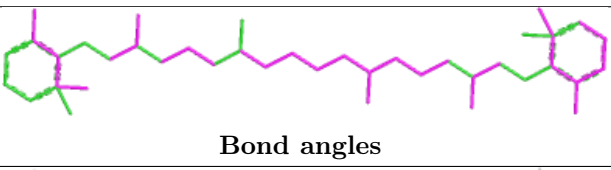
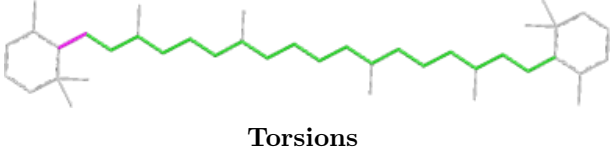
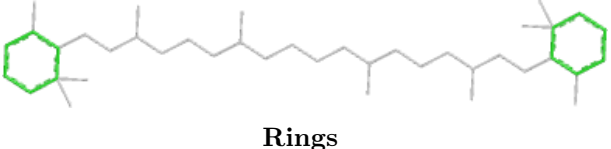
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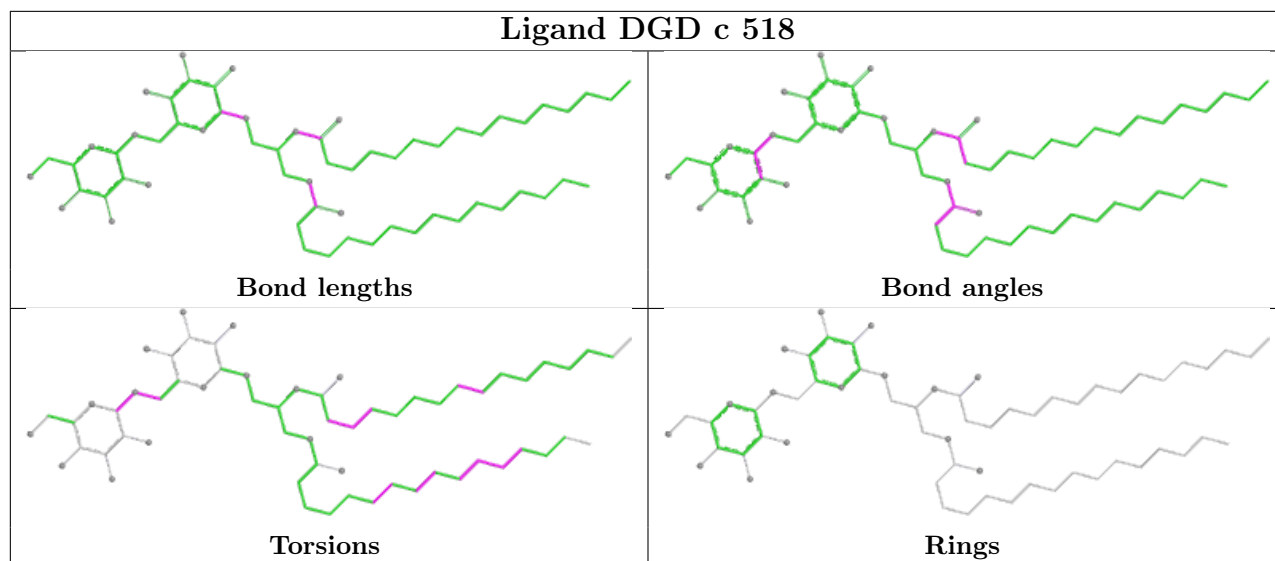
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	615	CLA	3	0
23	c	512	CLA	6	0
23	B	613	CLA	4	0
25	h	101	BCR	4	0
23	B	602	CLA	5	0

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

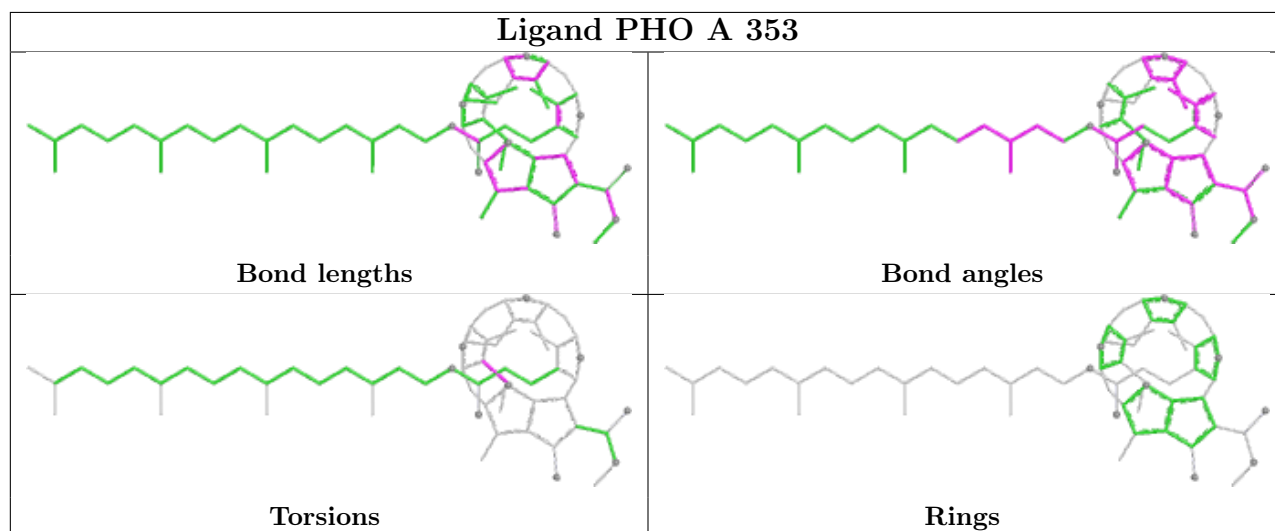


Ligand LMG m 101			
 Bond lengths	 Bond angles		
 Torsions	 Rings		
Ligand LMG d 412			
 Bond lengths	 Bond angles		
 Torsions	 Rings		
Ligand BCR Y 101			
 Bond lengths	 Bond angles		
 Torsions	 Rings		

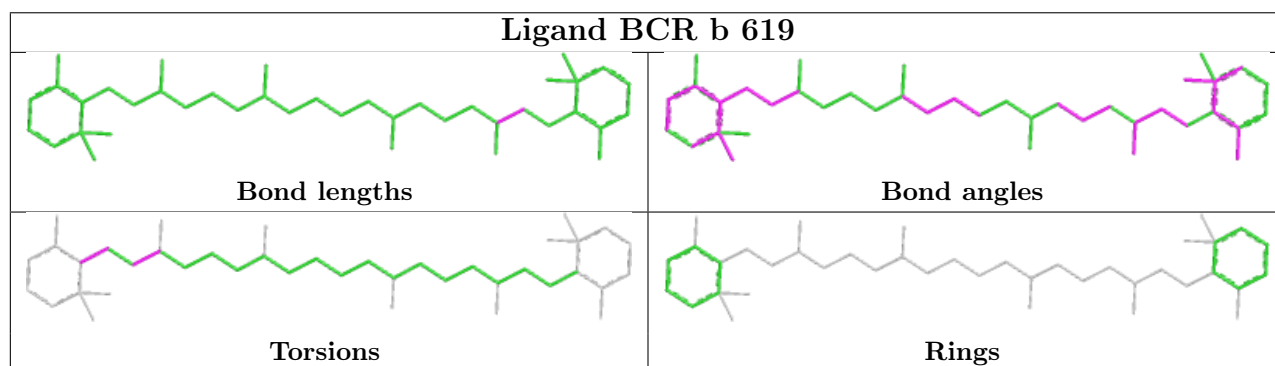
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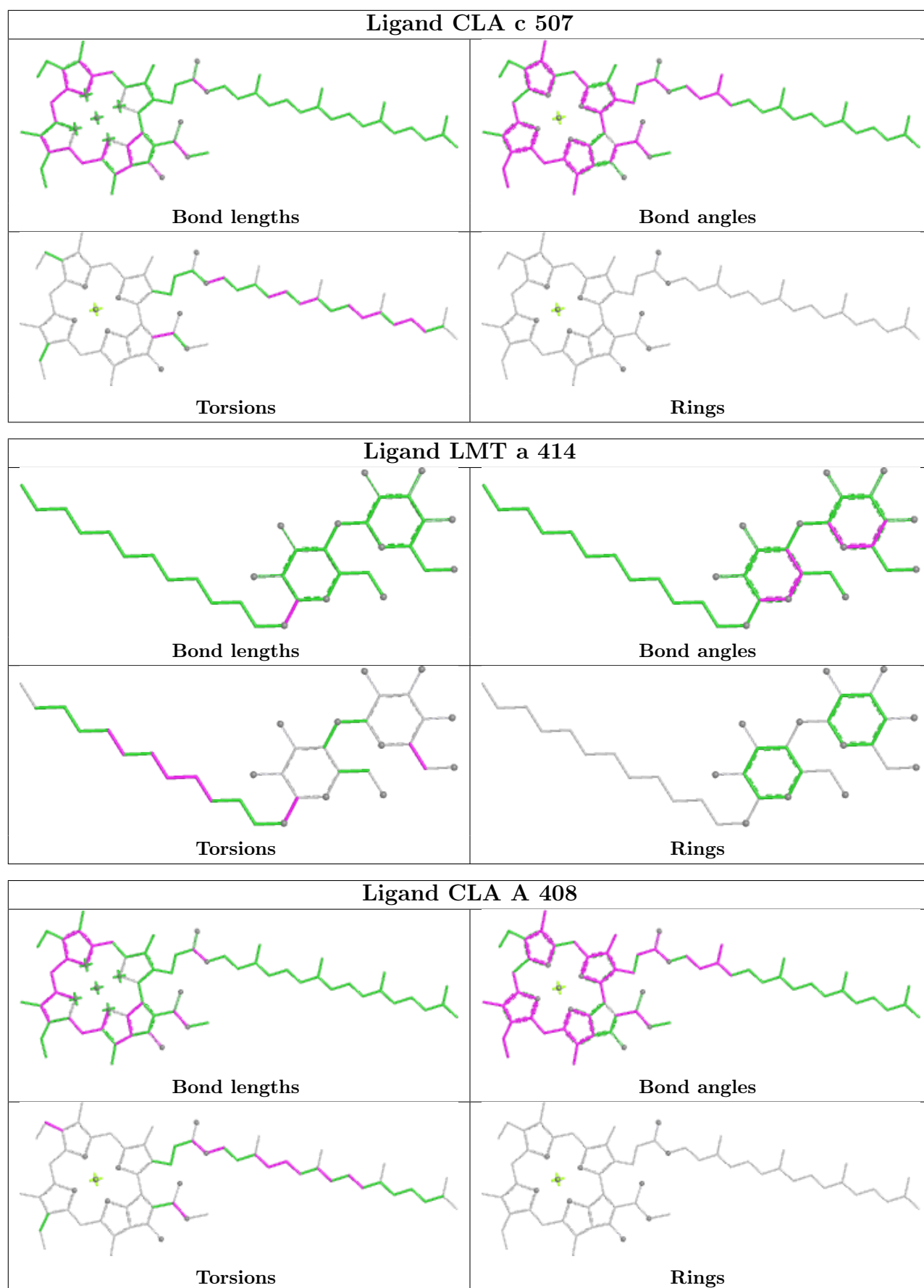


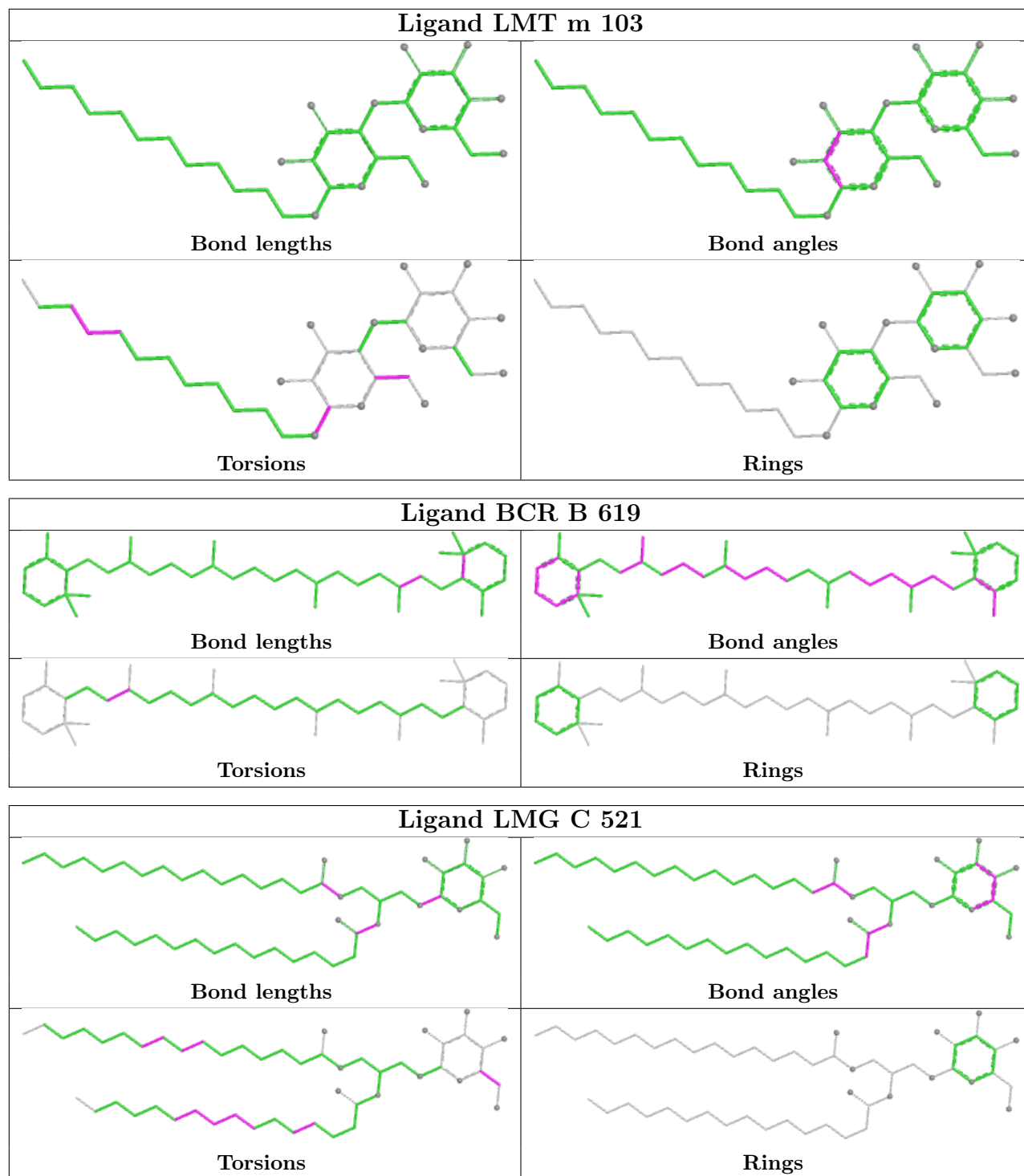
Ligand PHO A 353

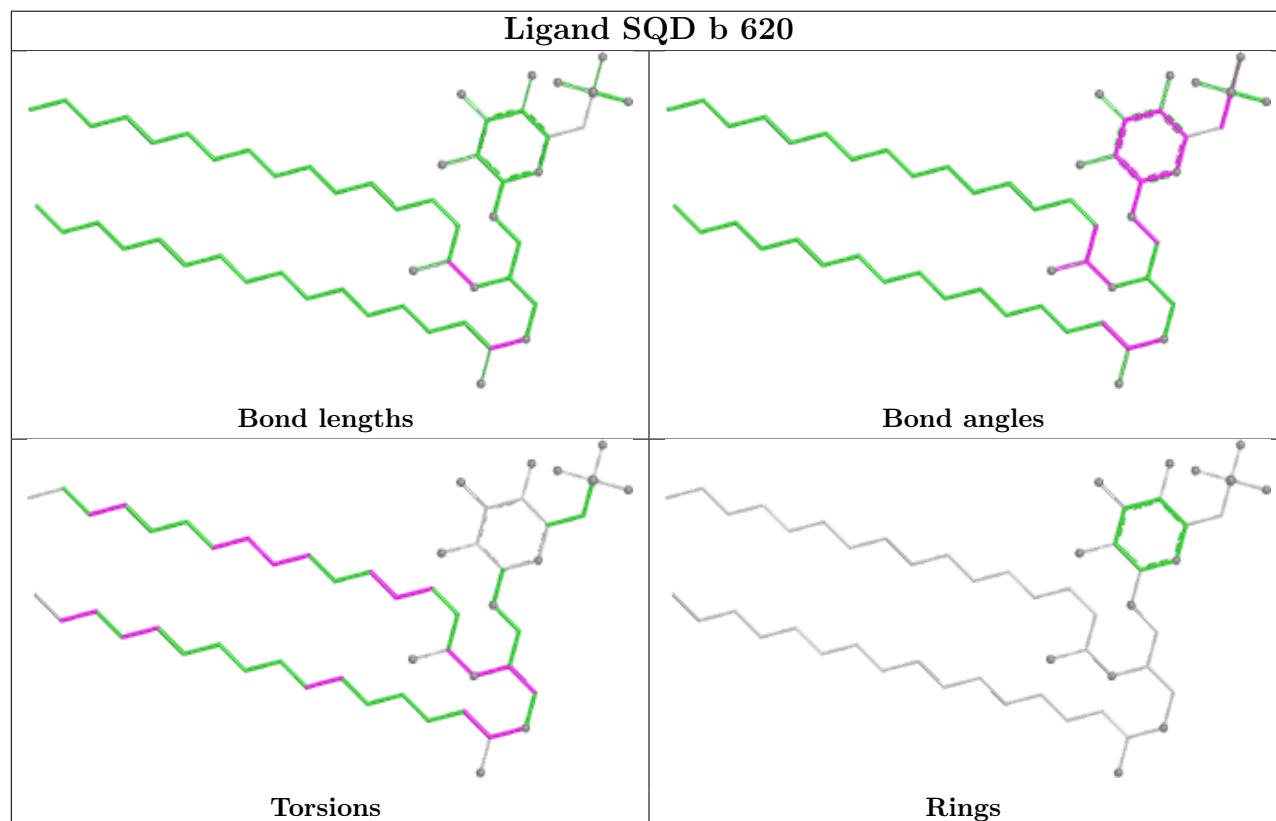
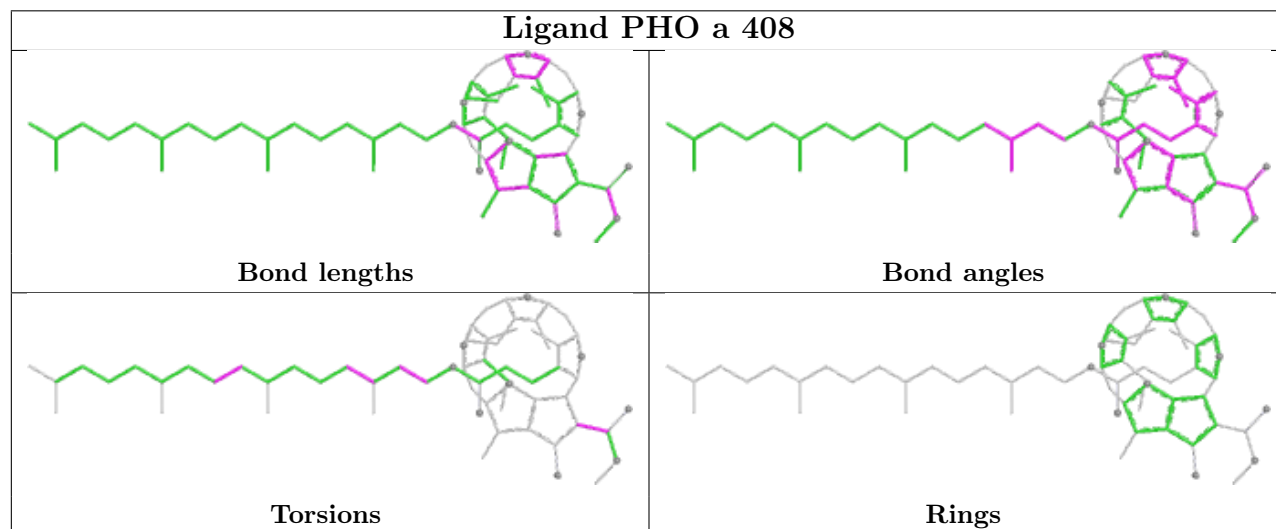
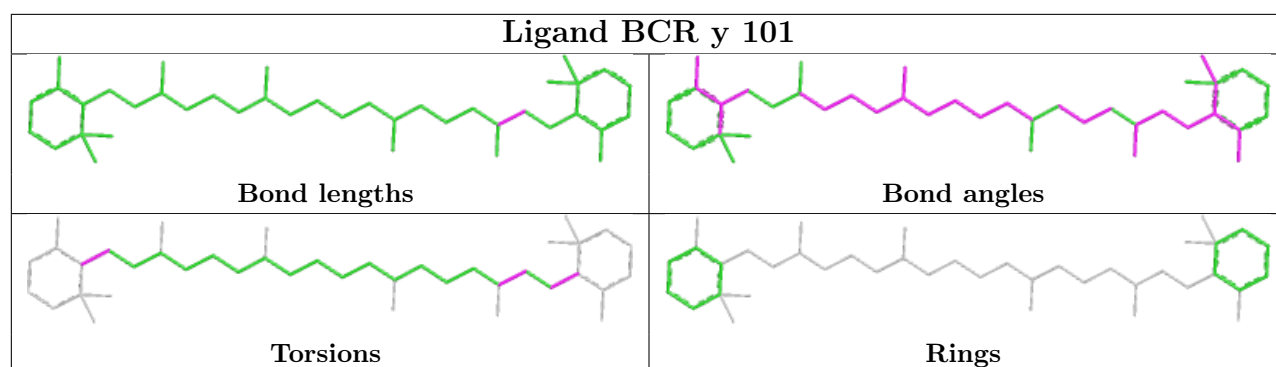


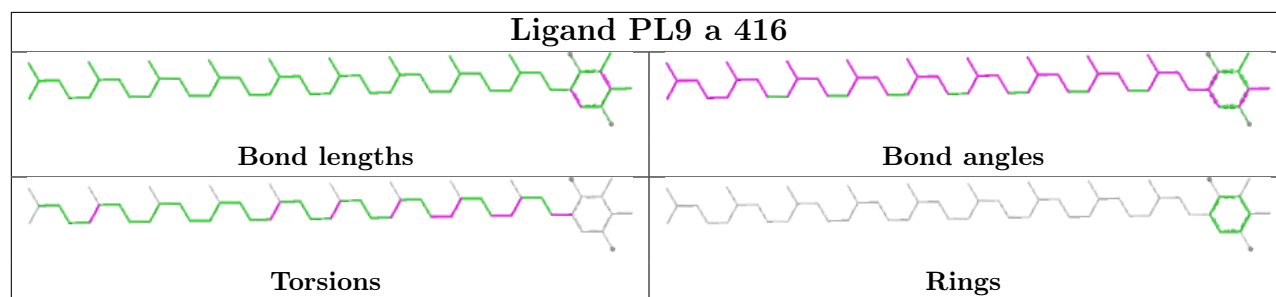
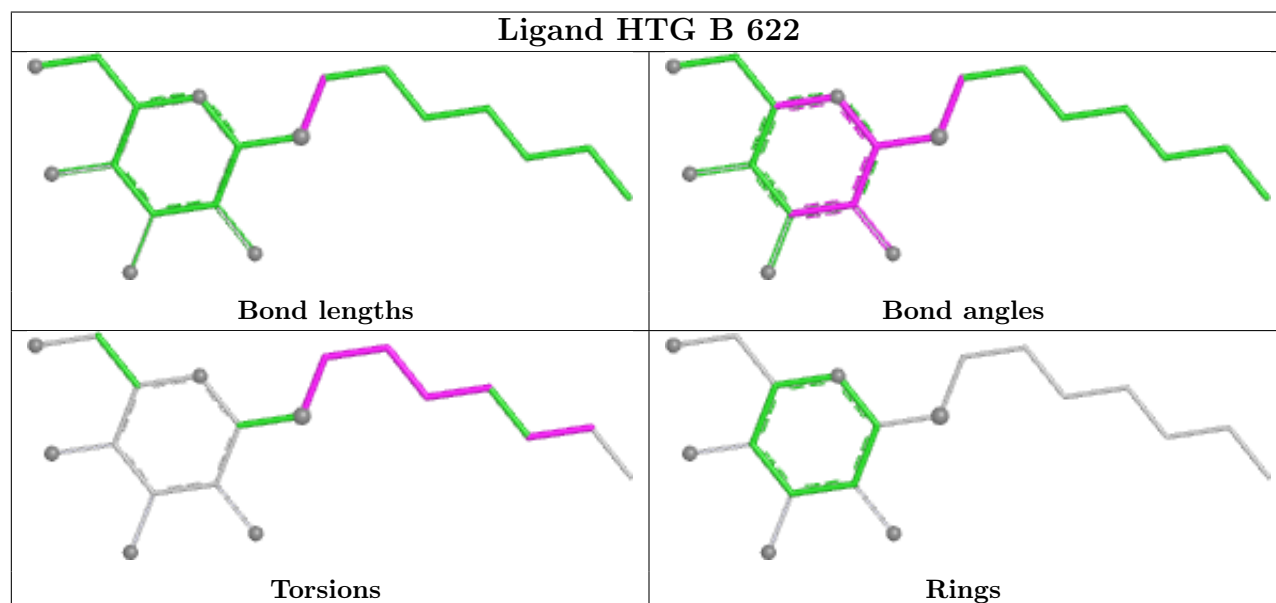
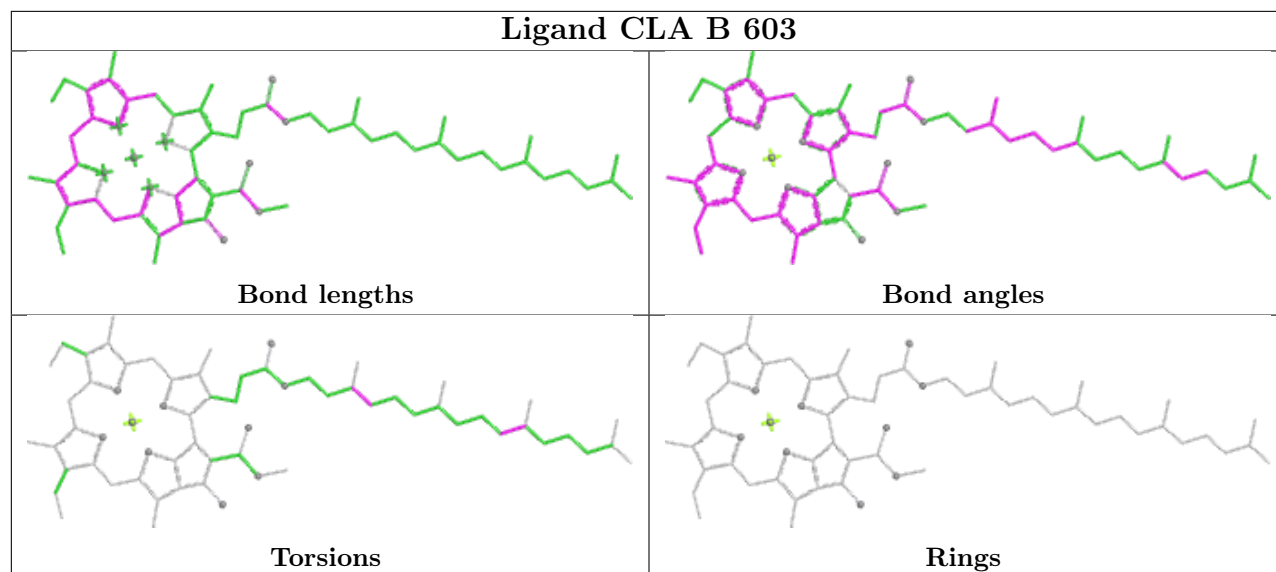
Ligand BCR b 619

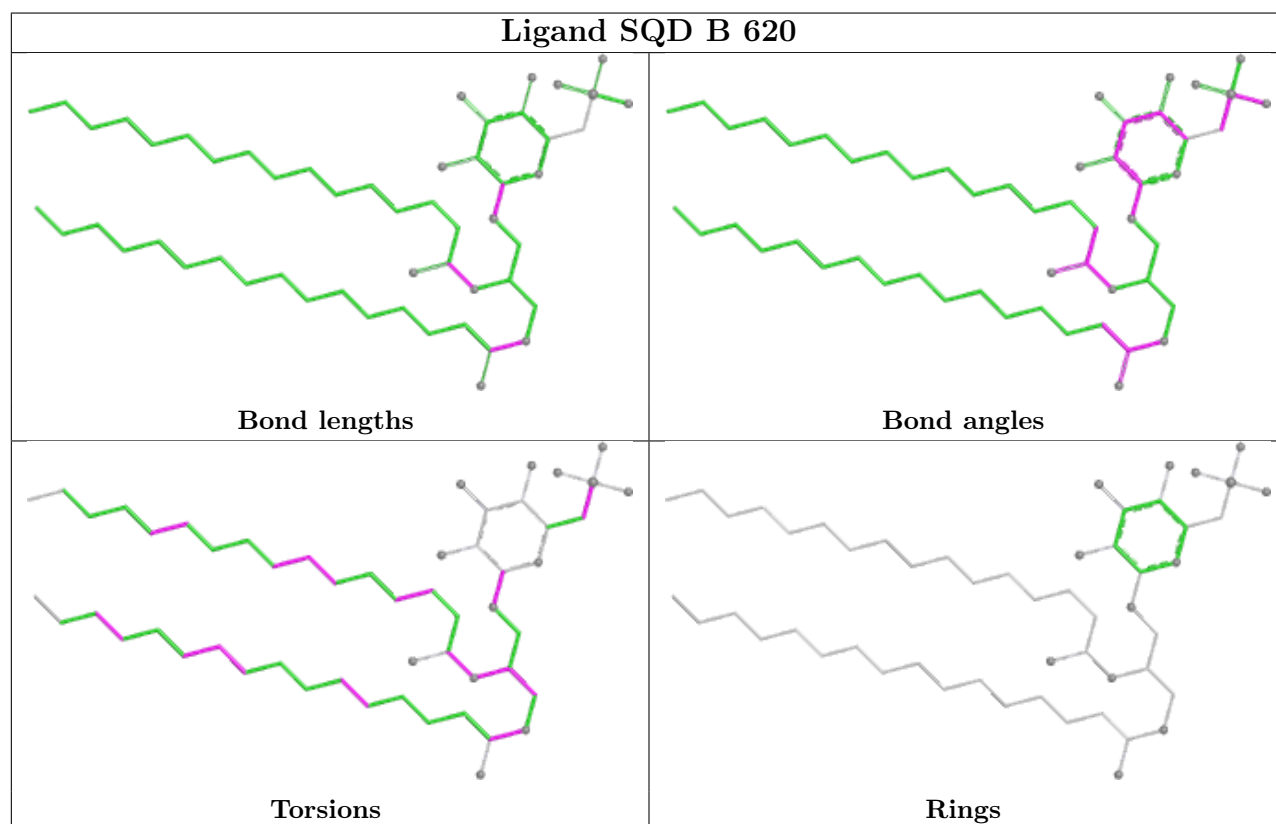
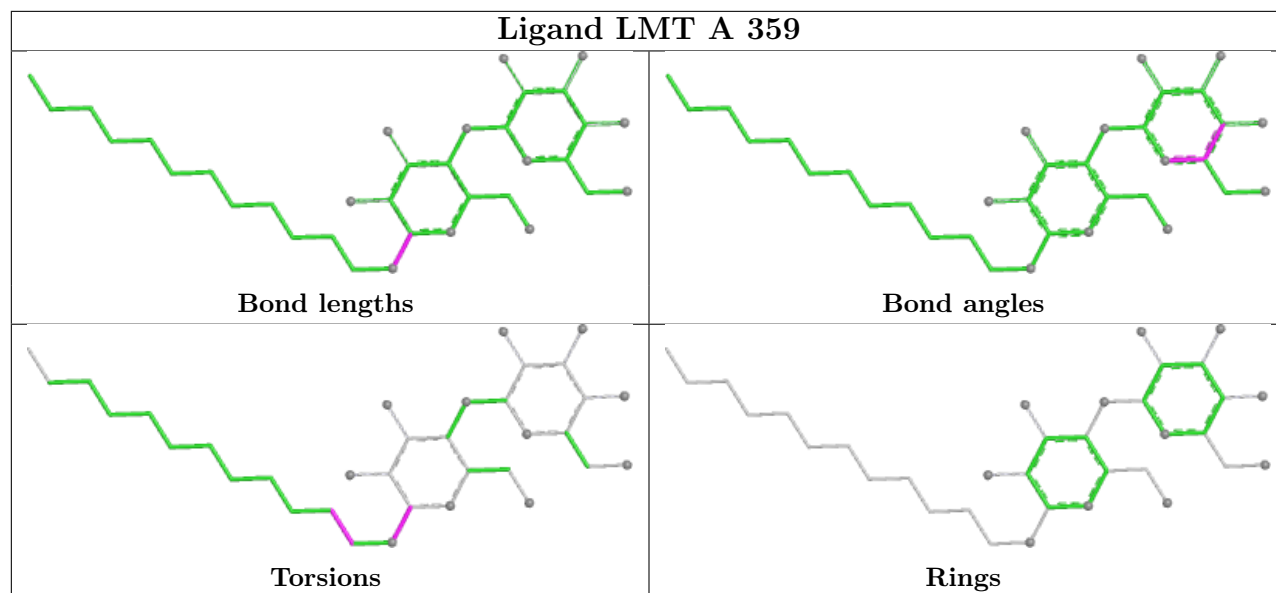


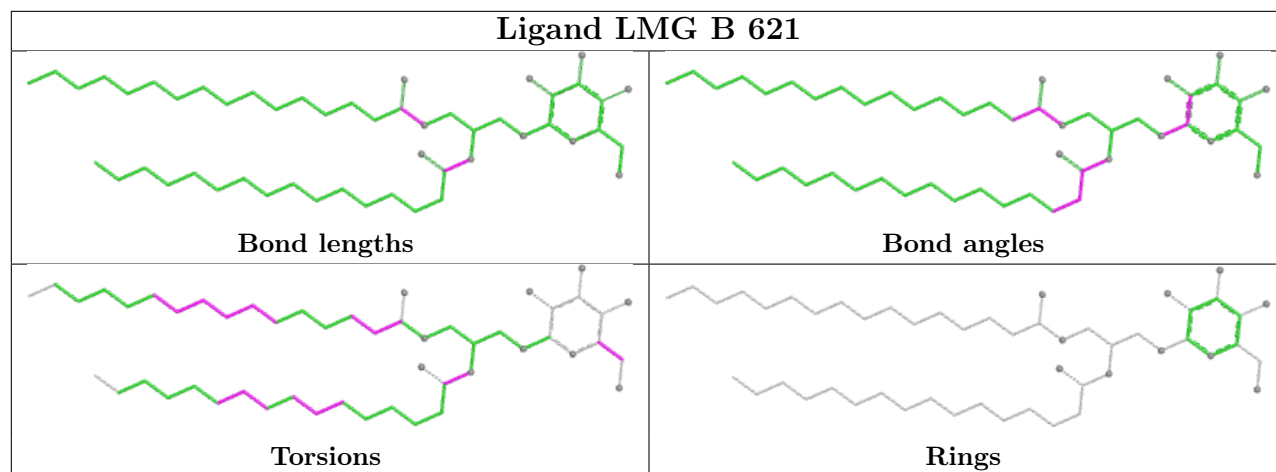
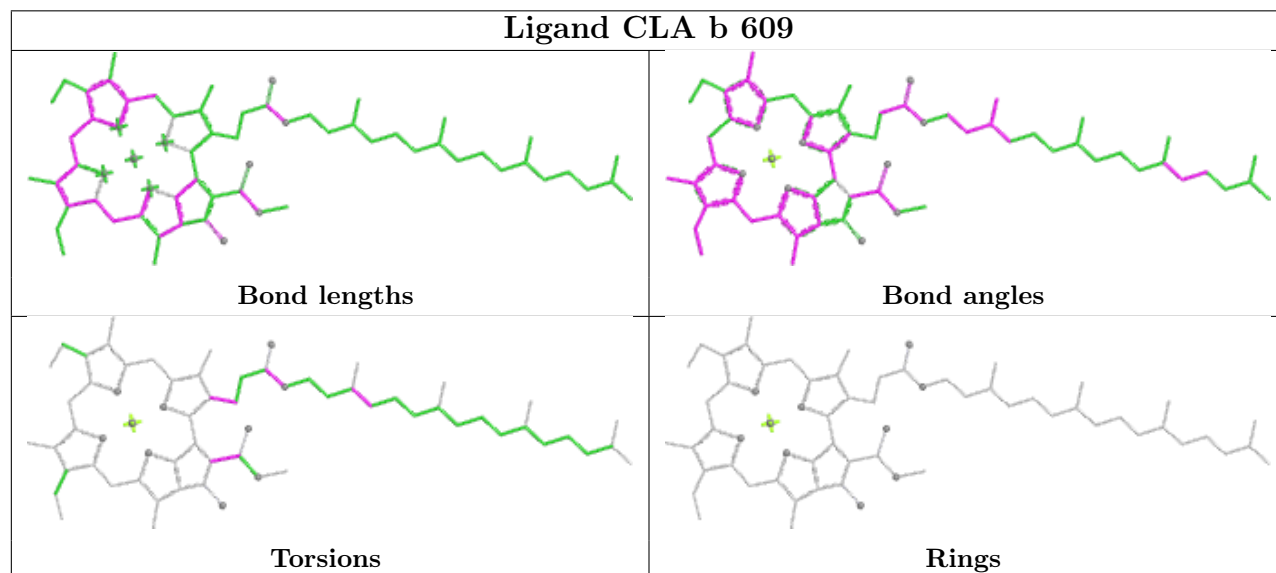
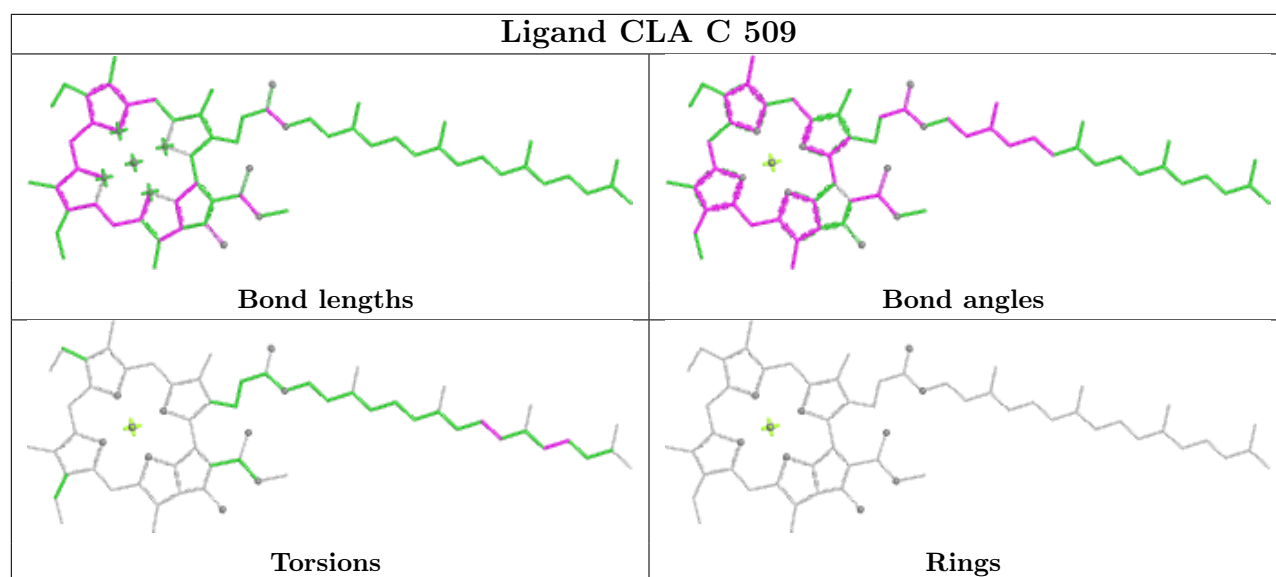


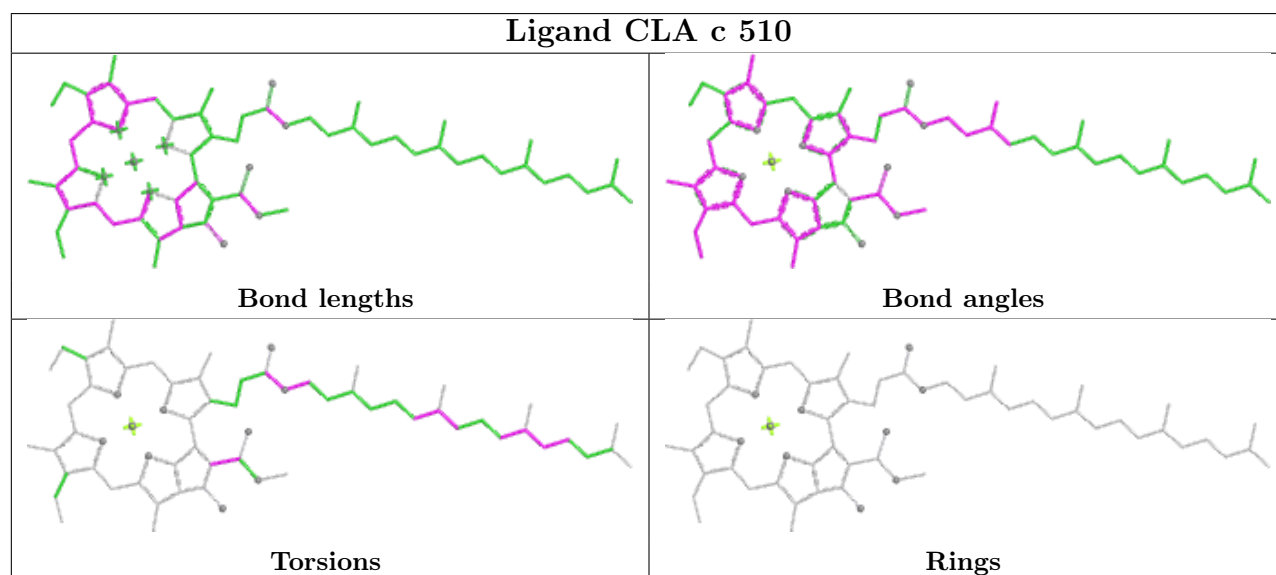
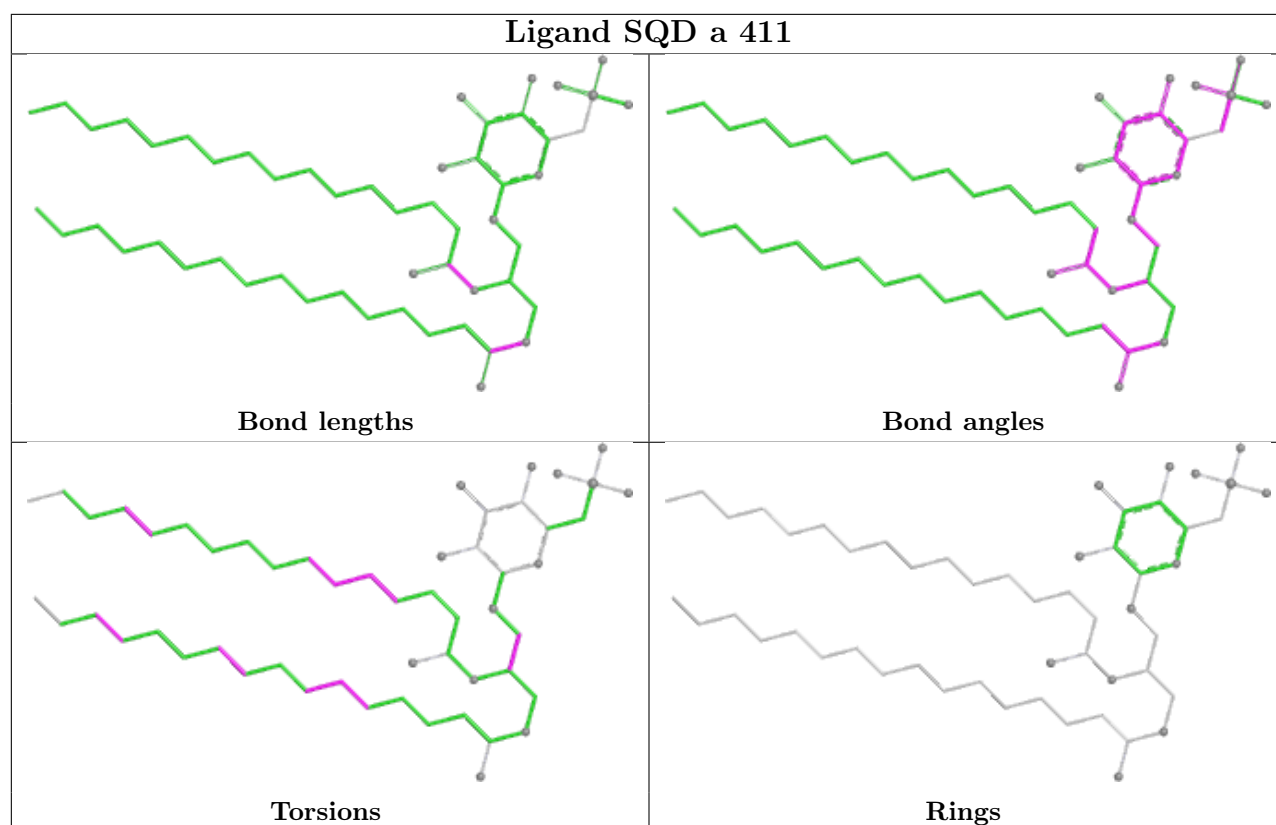


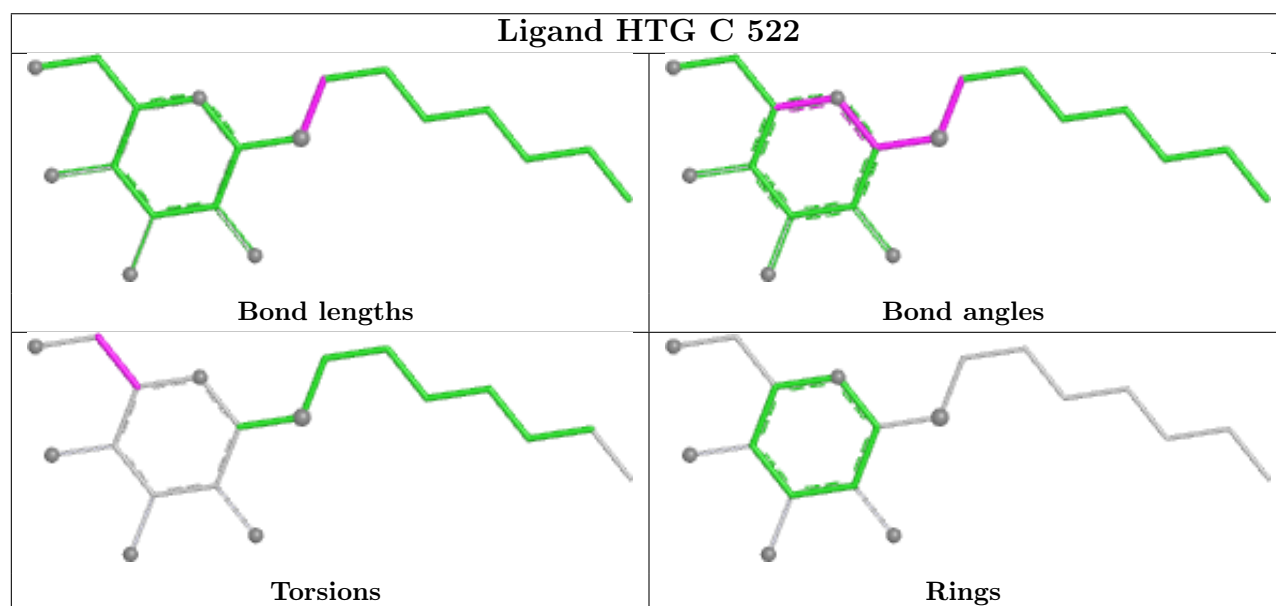
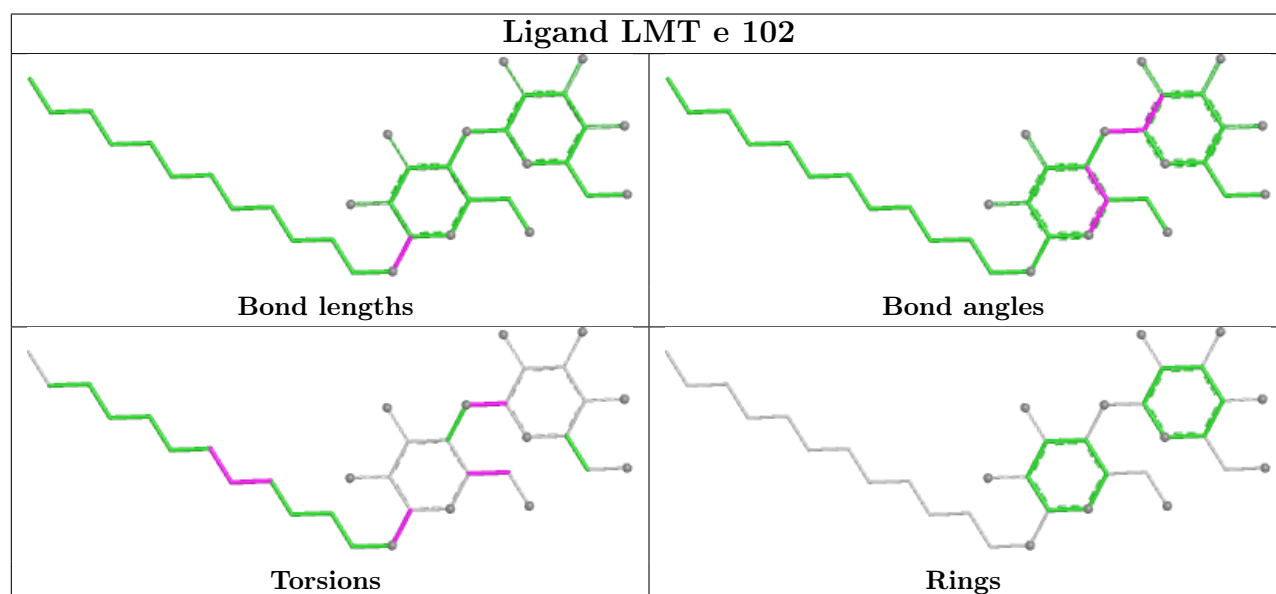
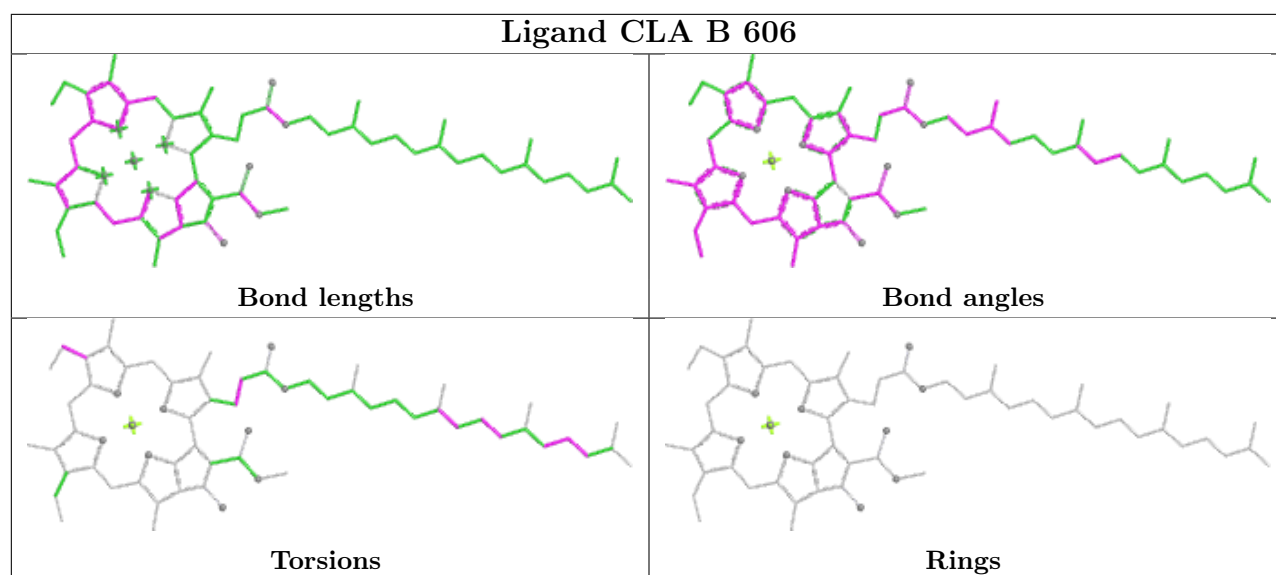


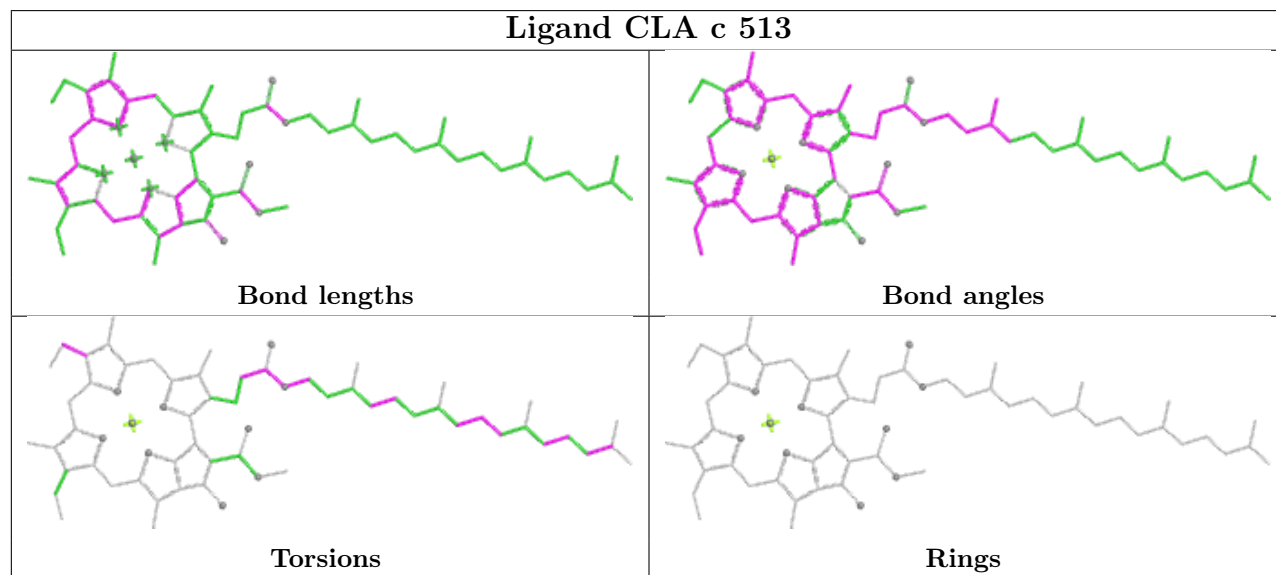
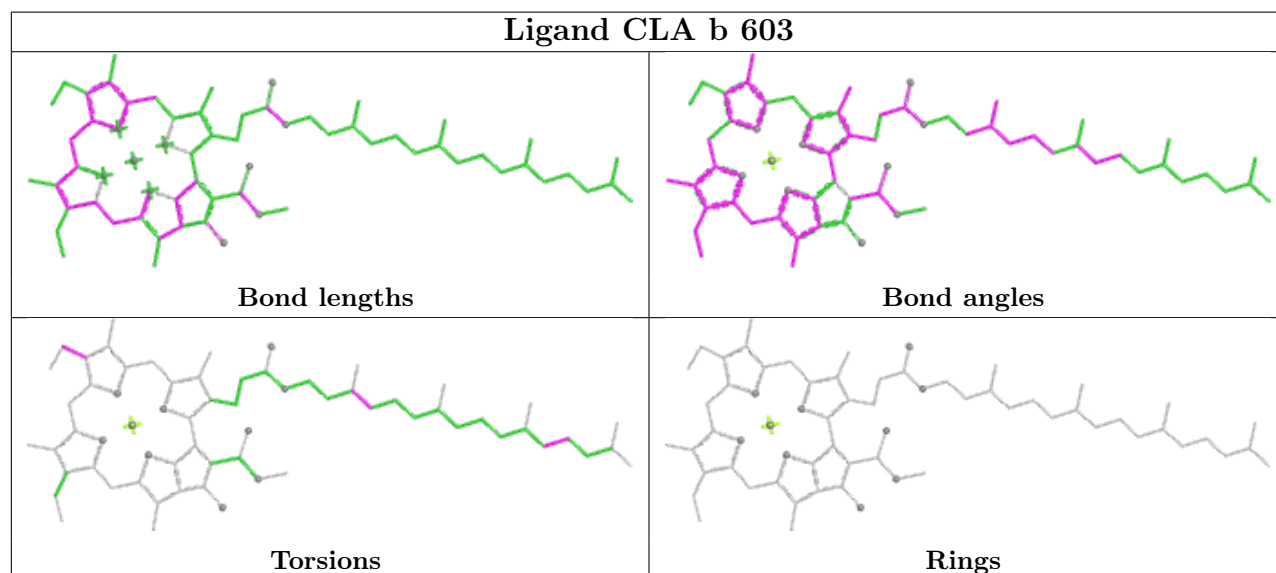
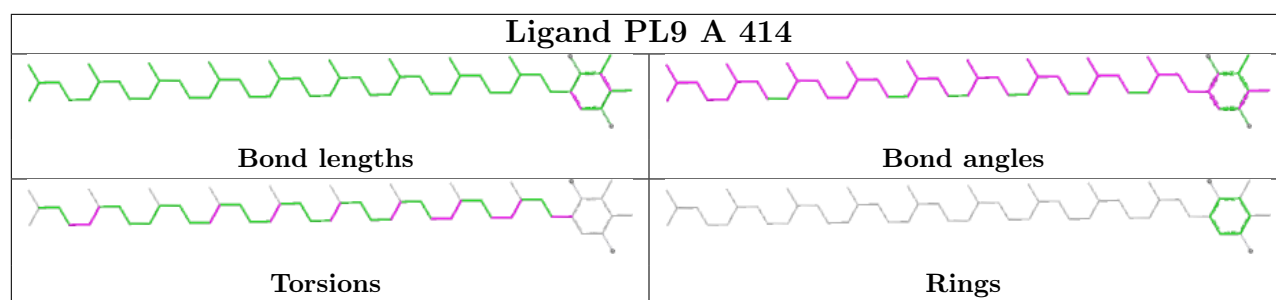


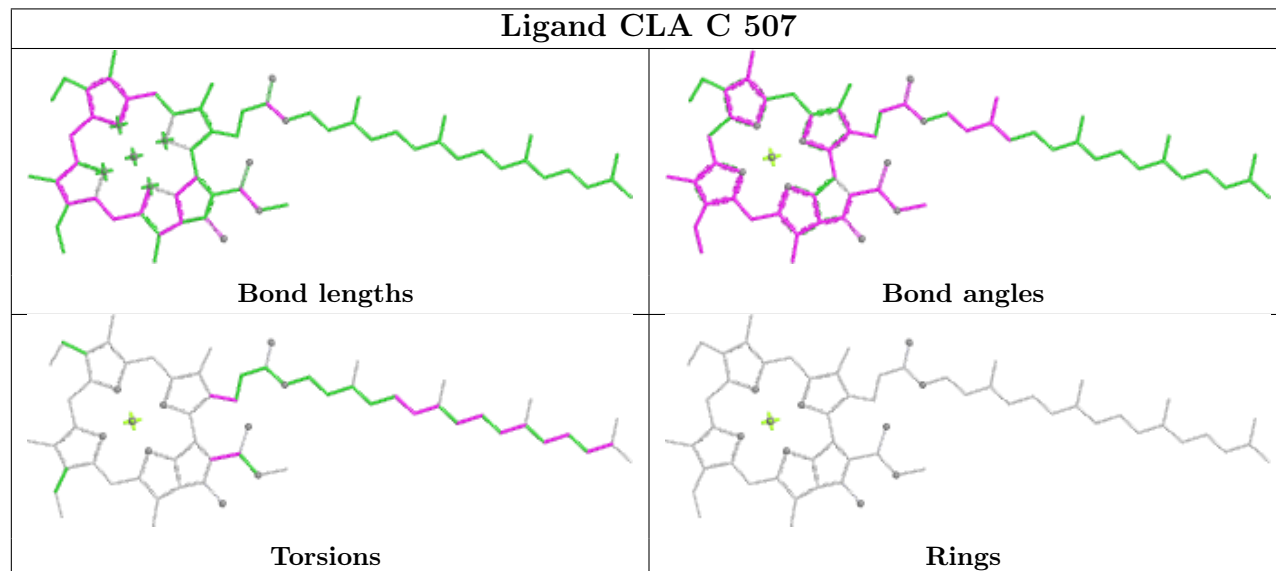
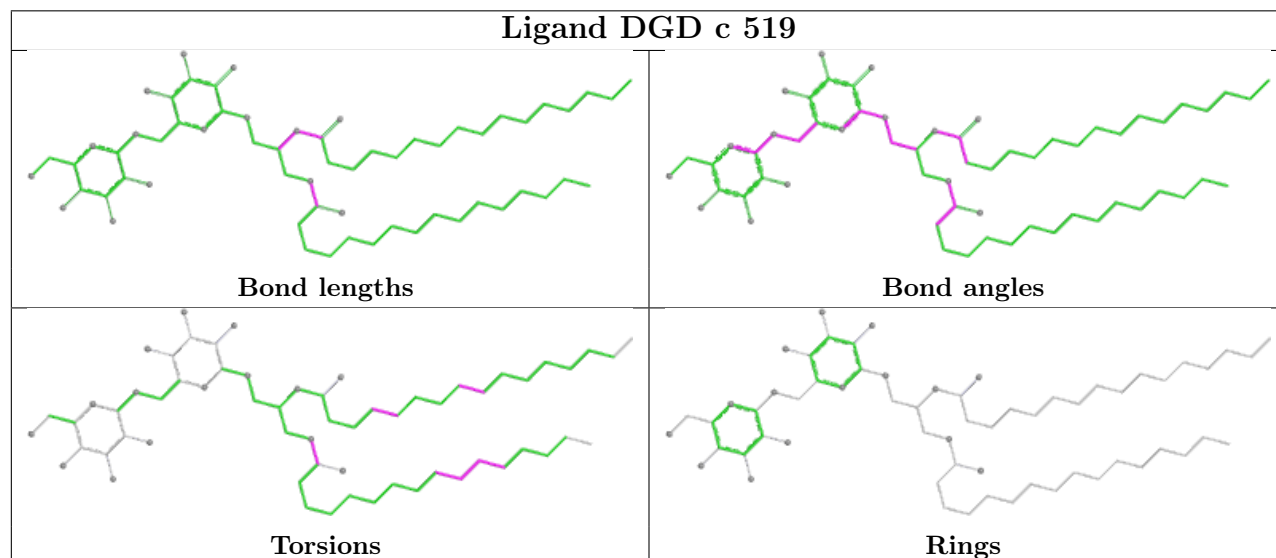
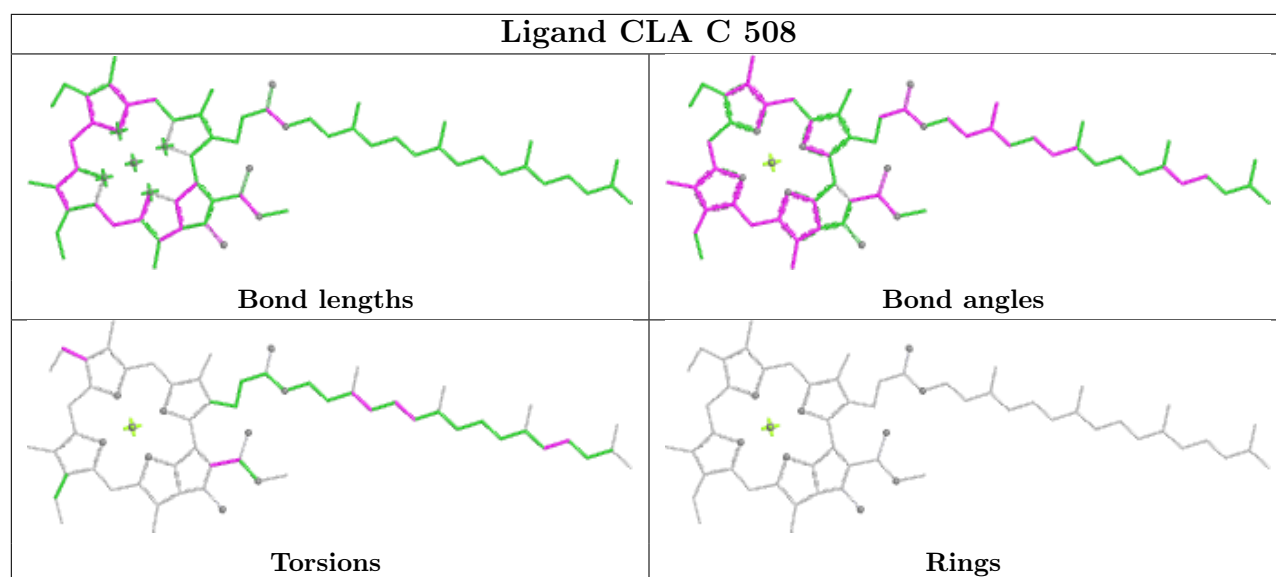


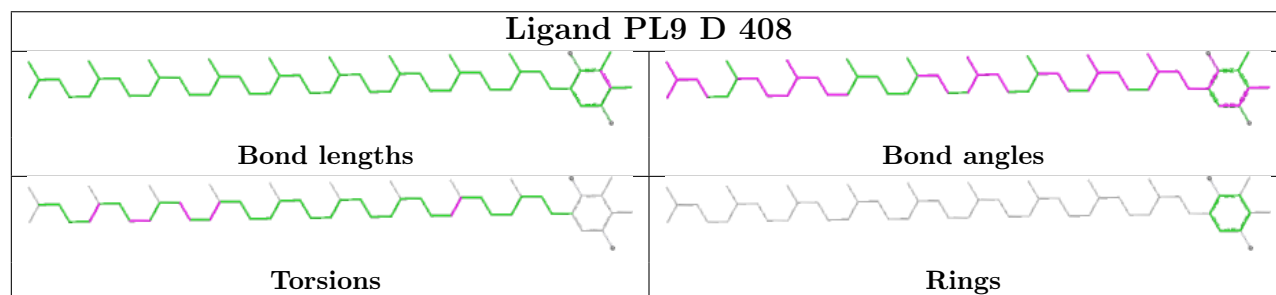
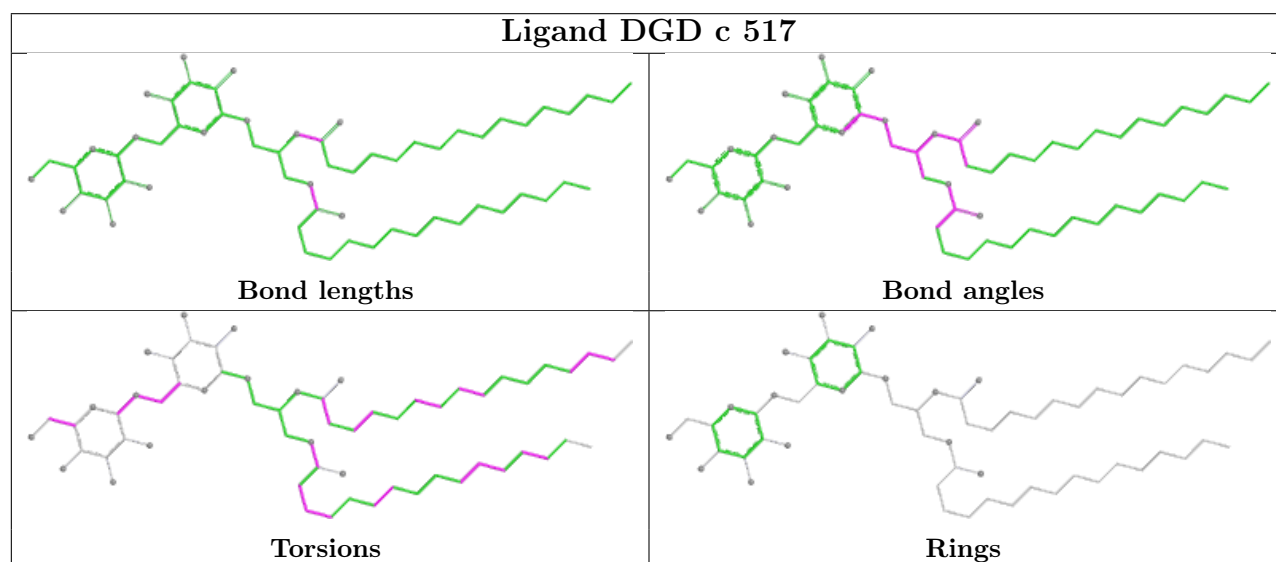
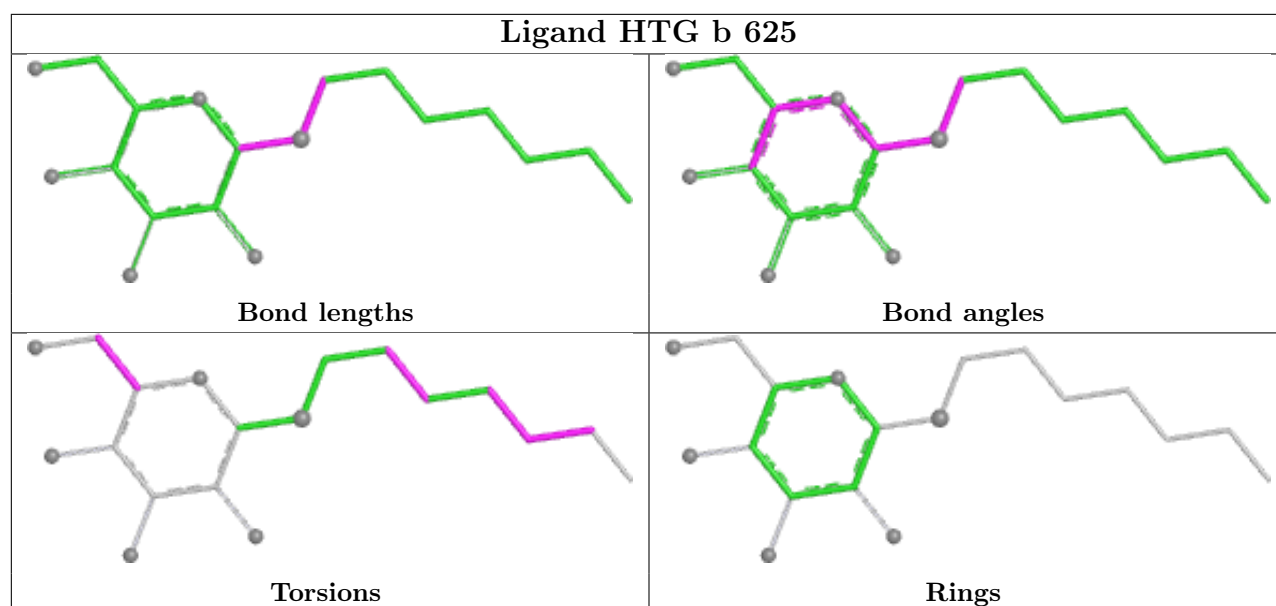


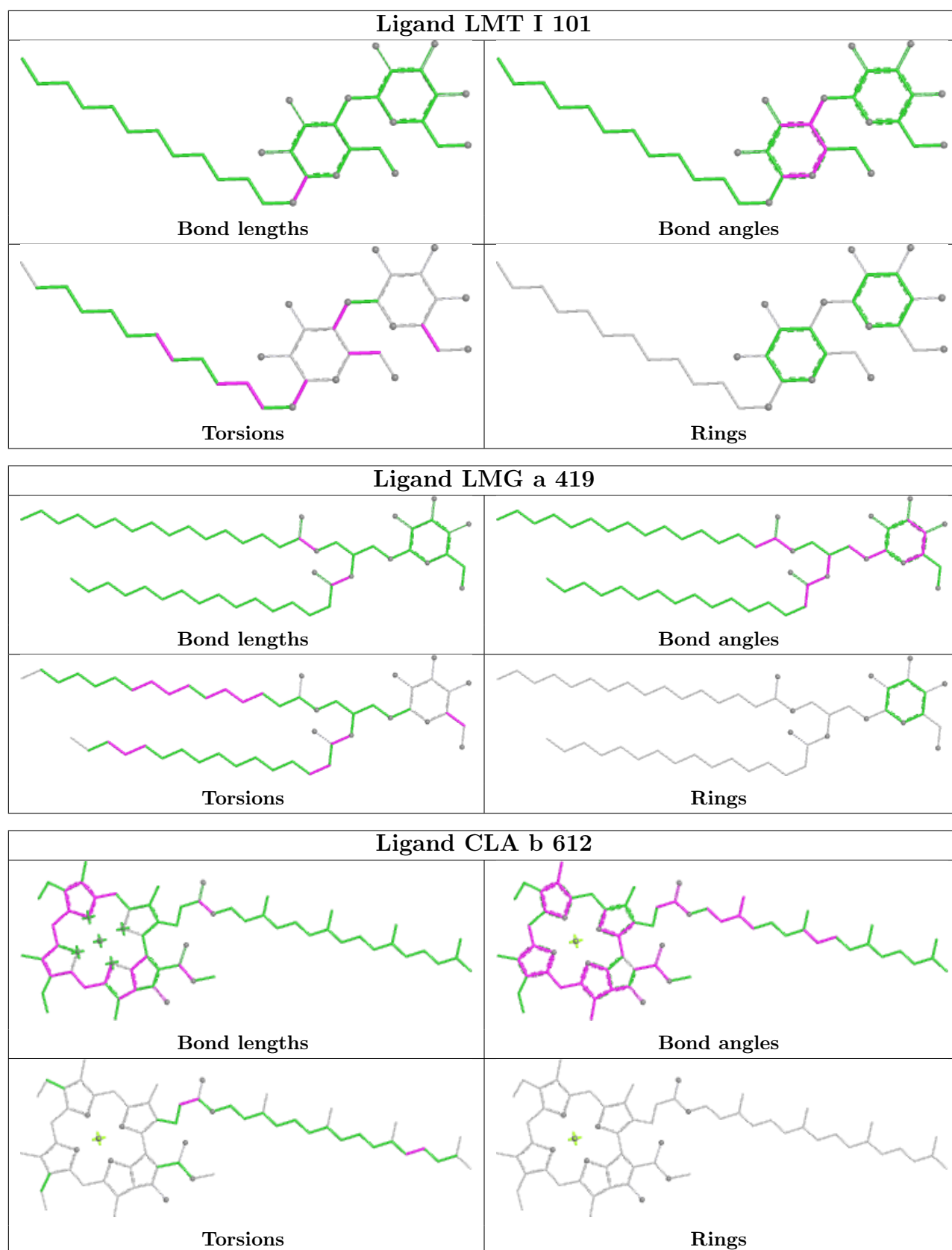


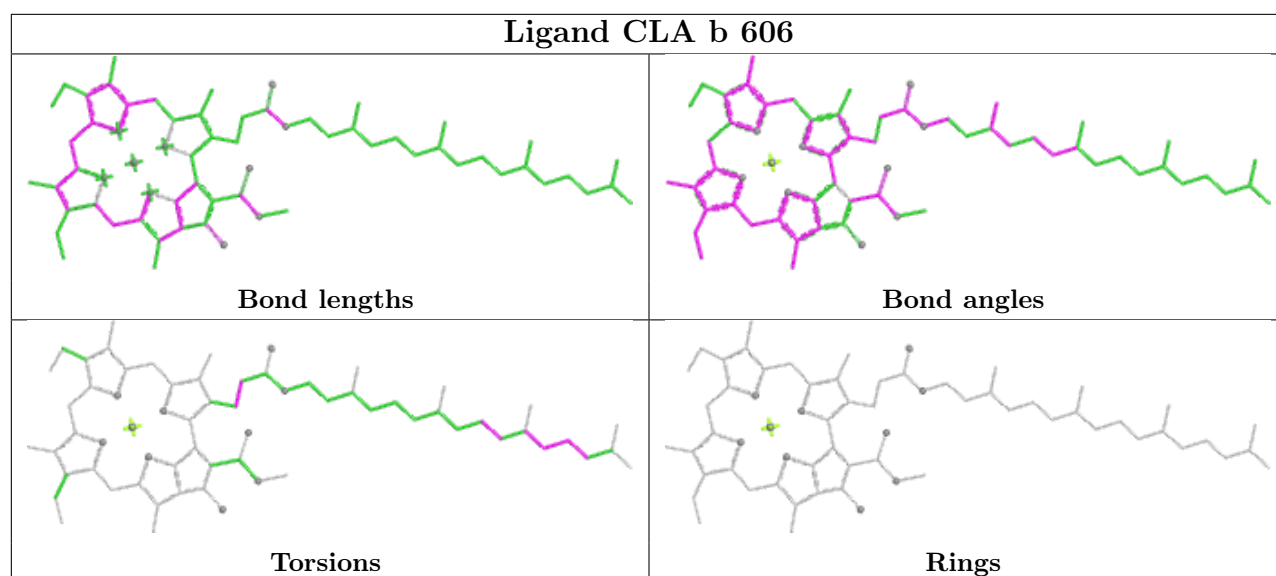
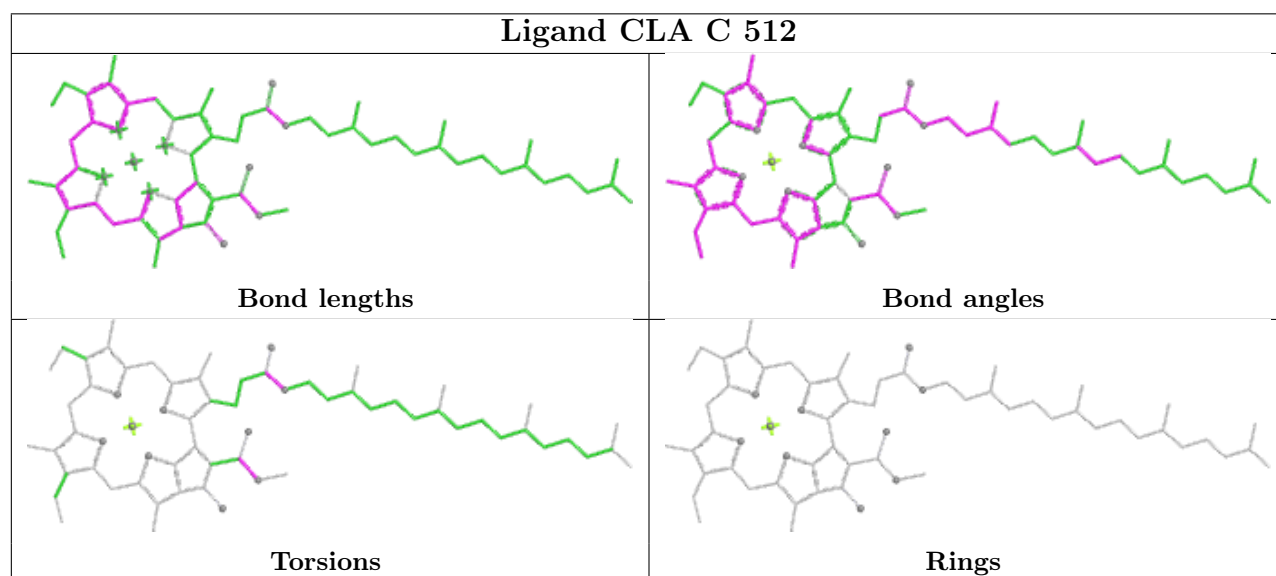
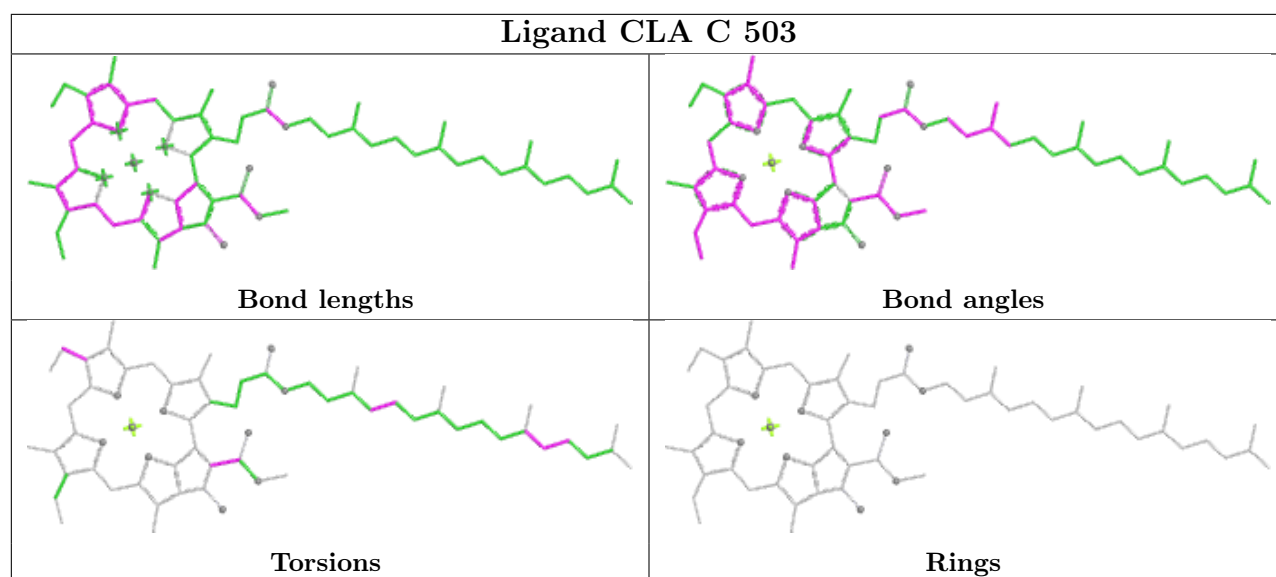


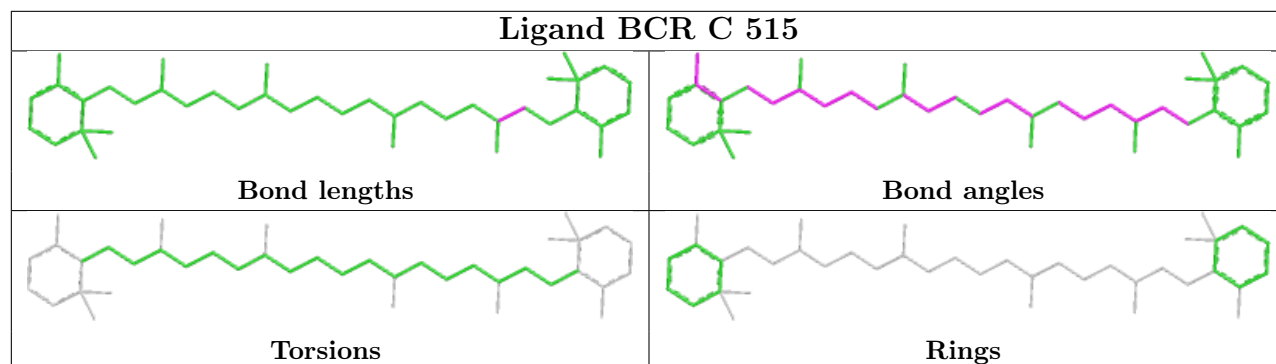
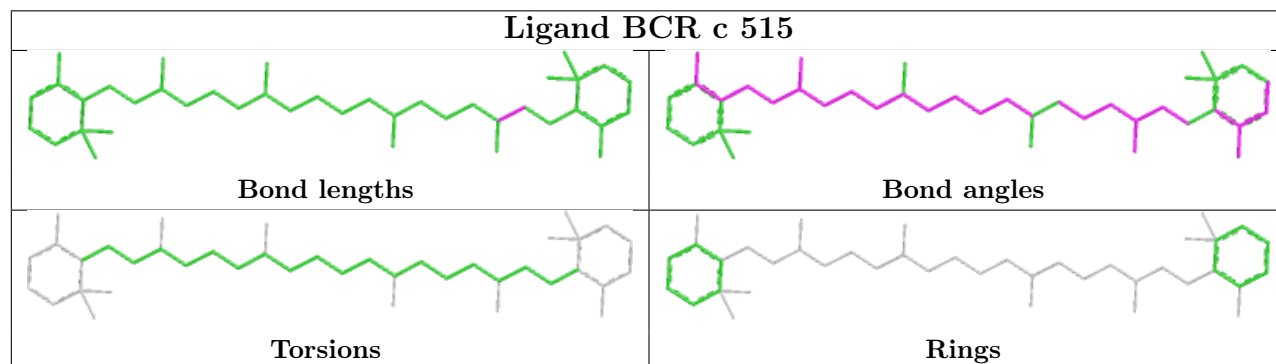
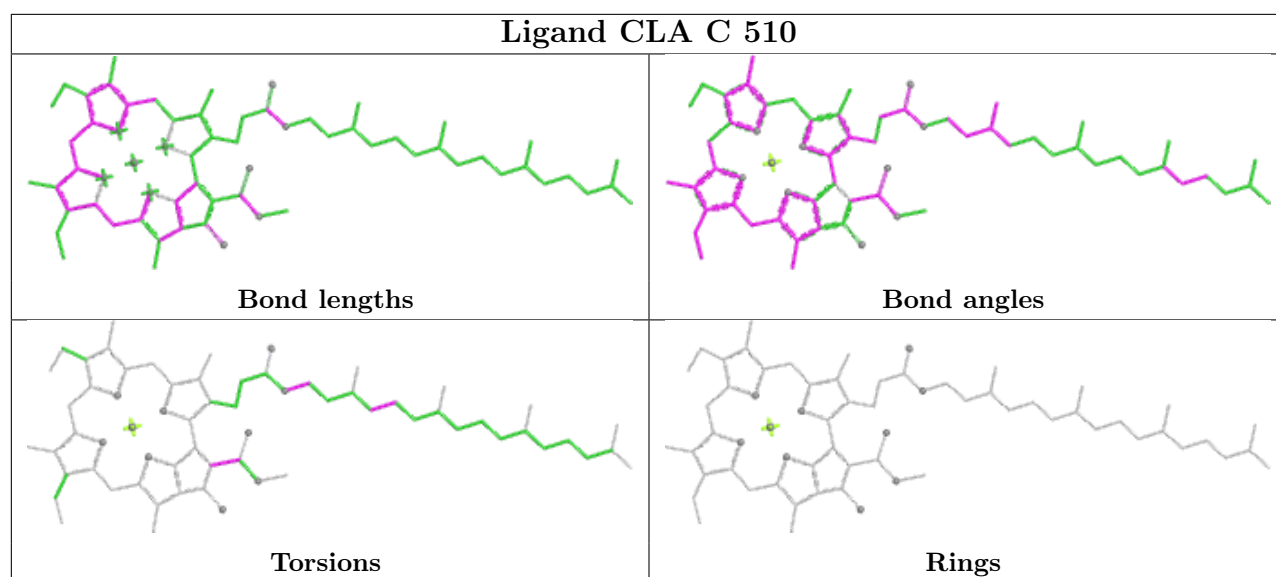


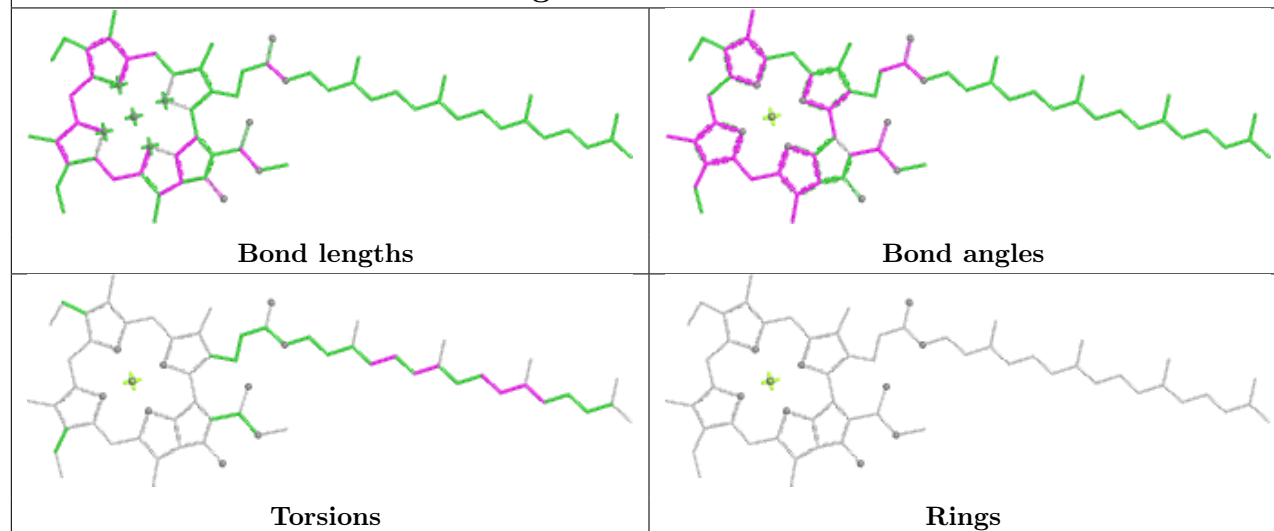
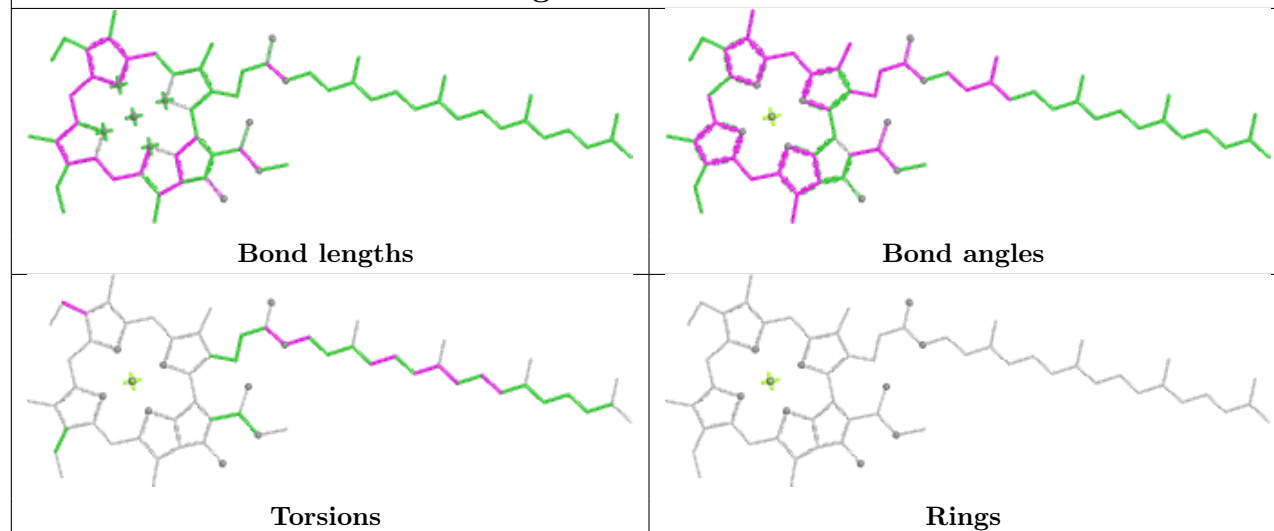
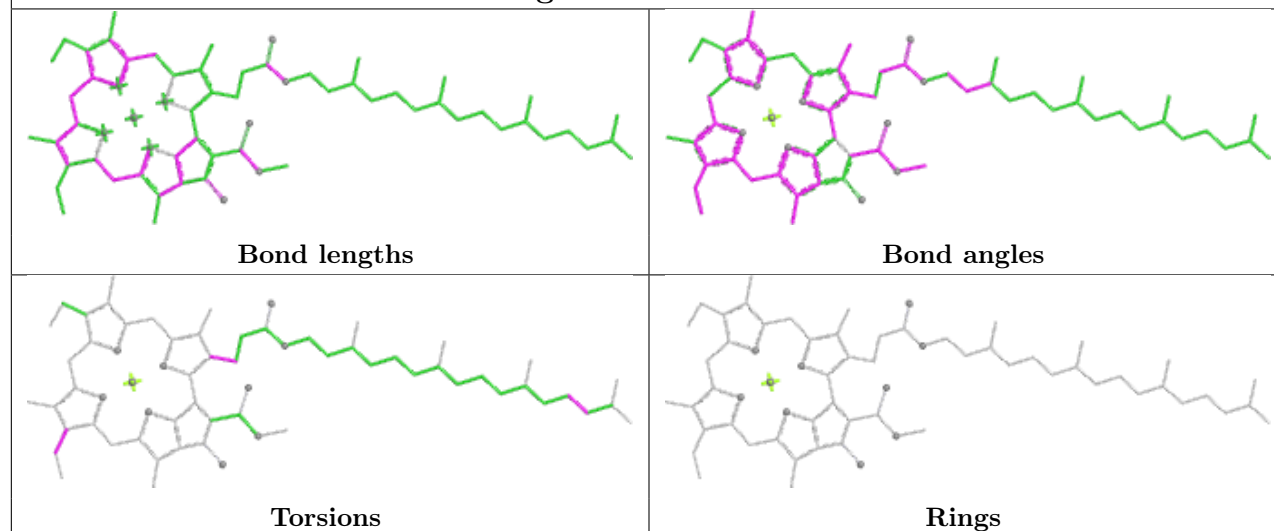




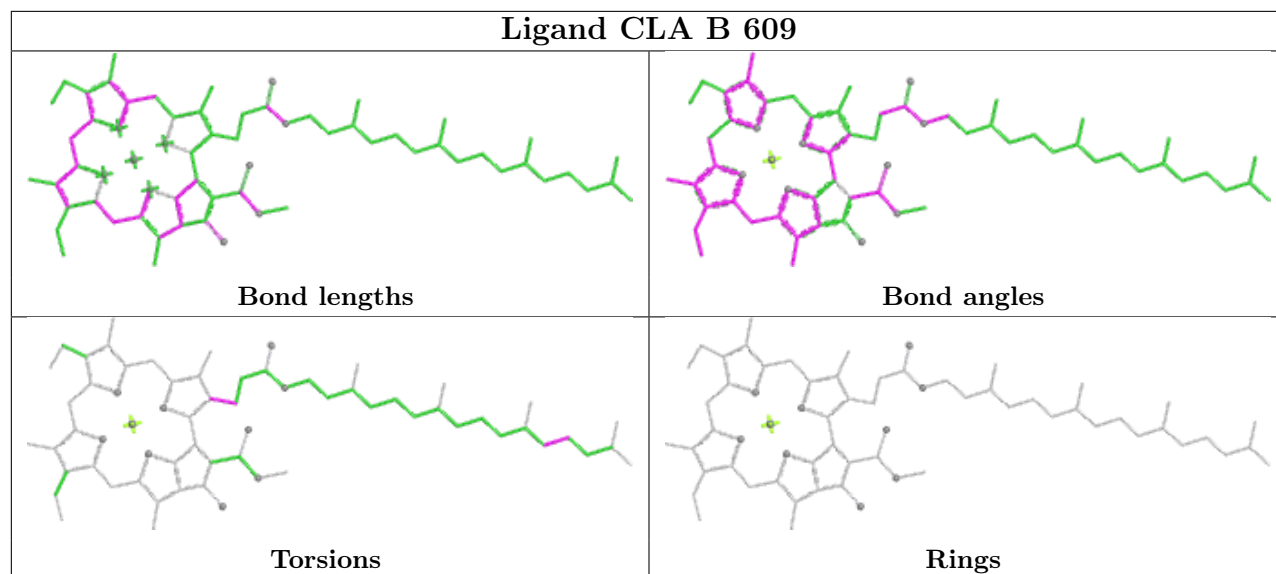




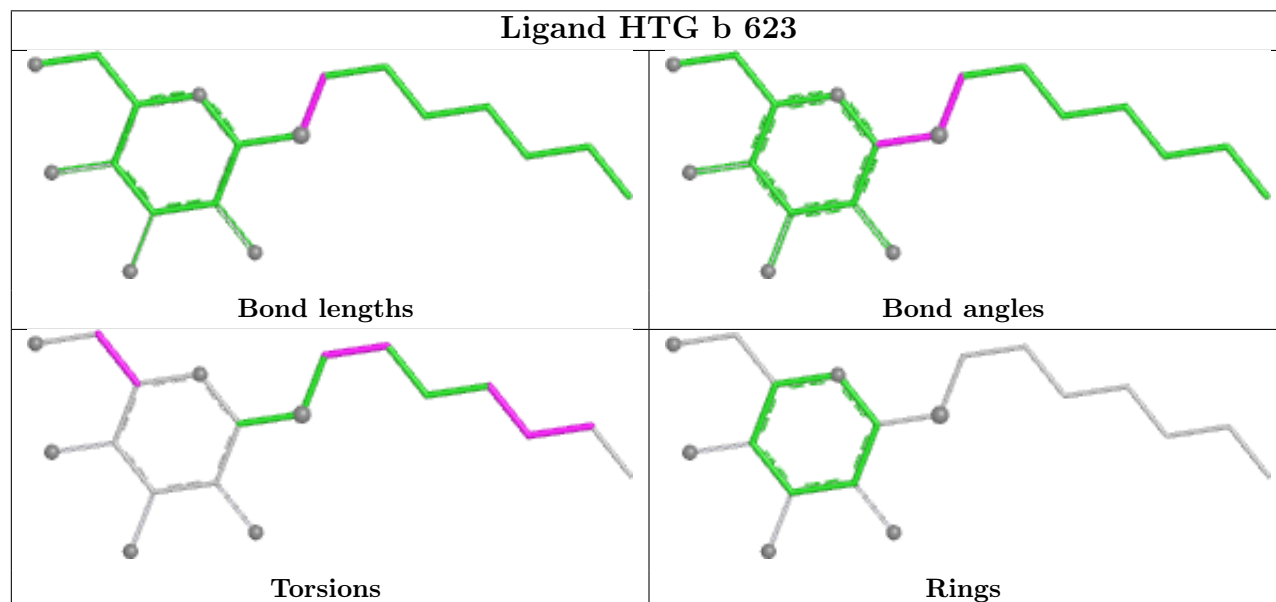


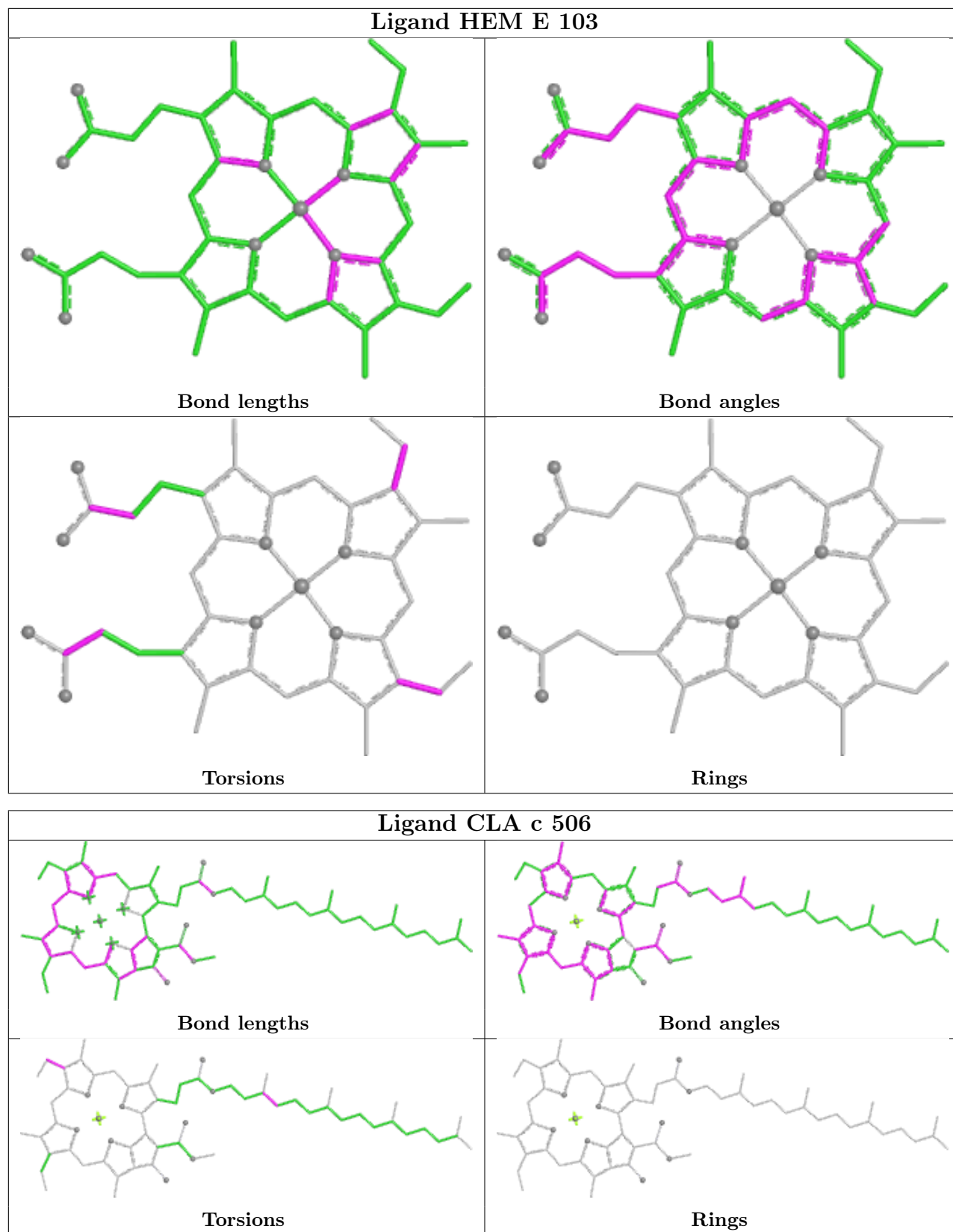
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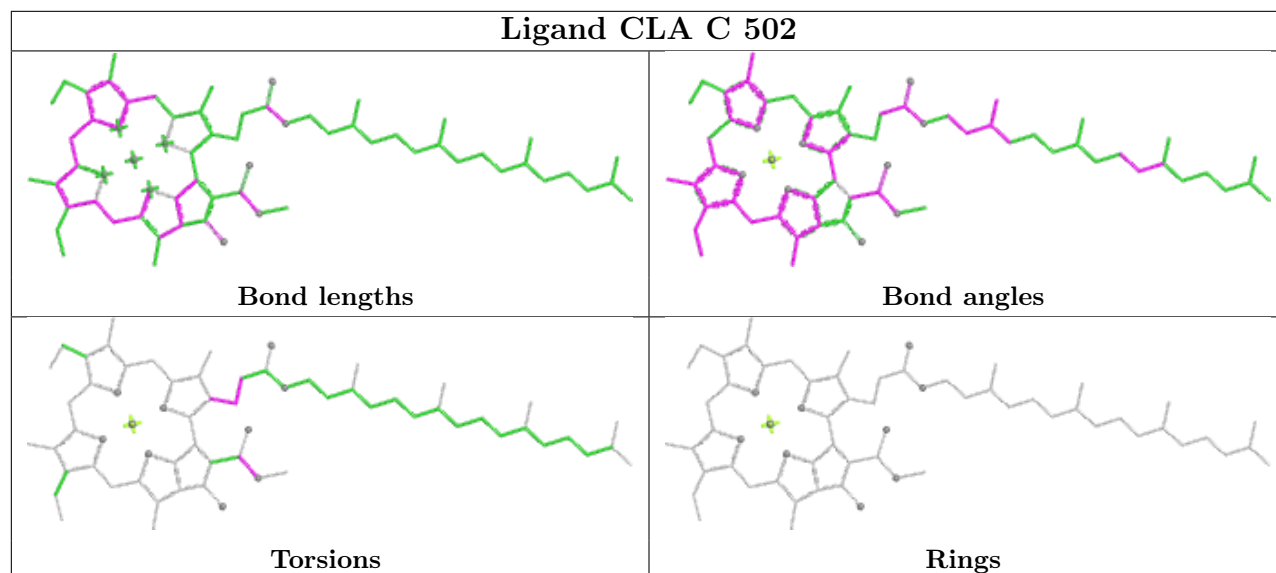
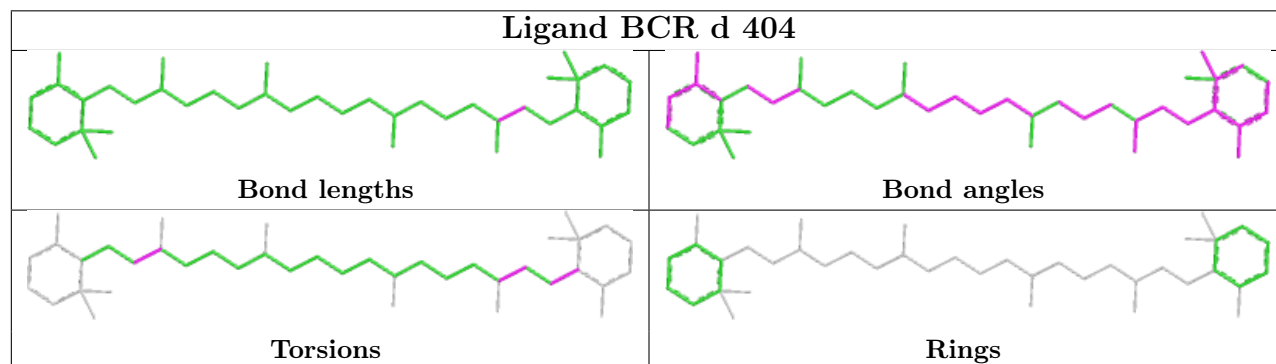
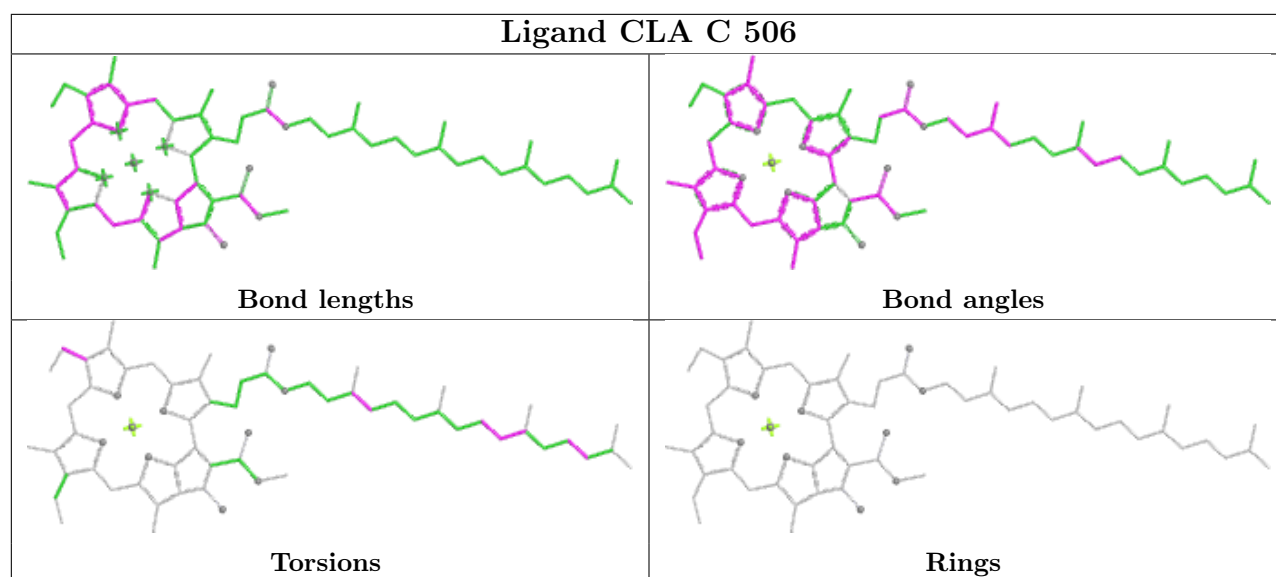
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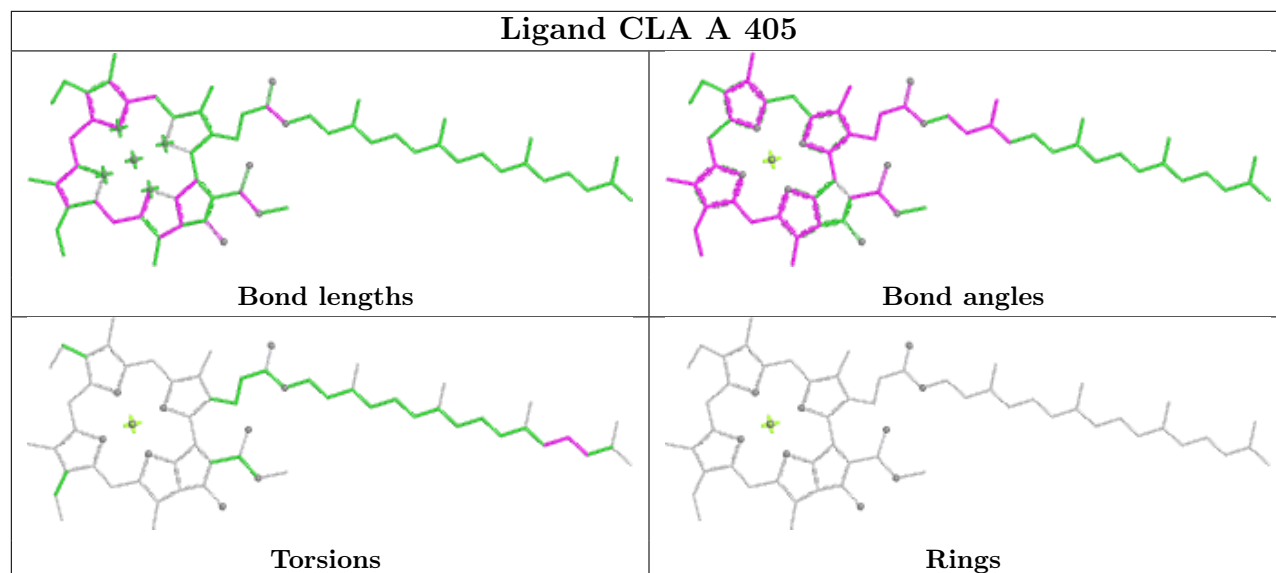
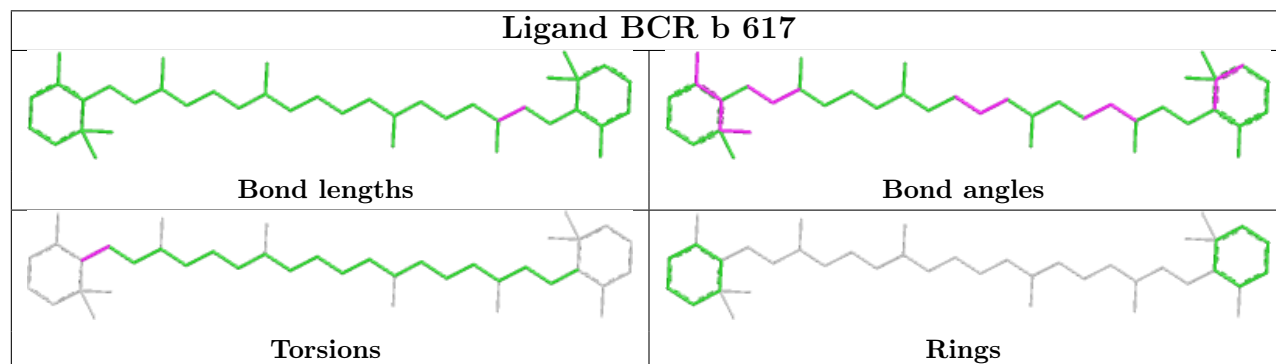
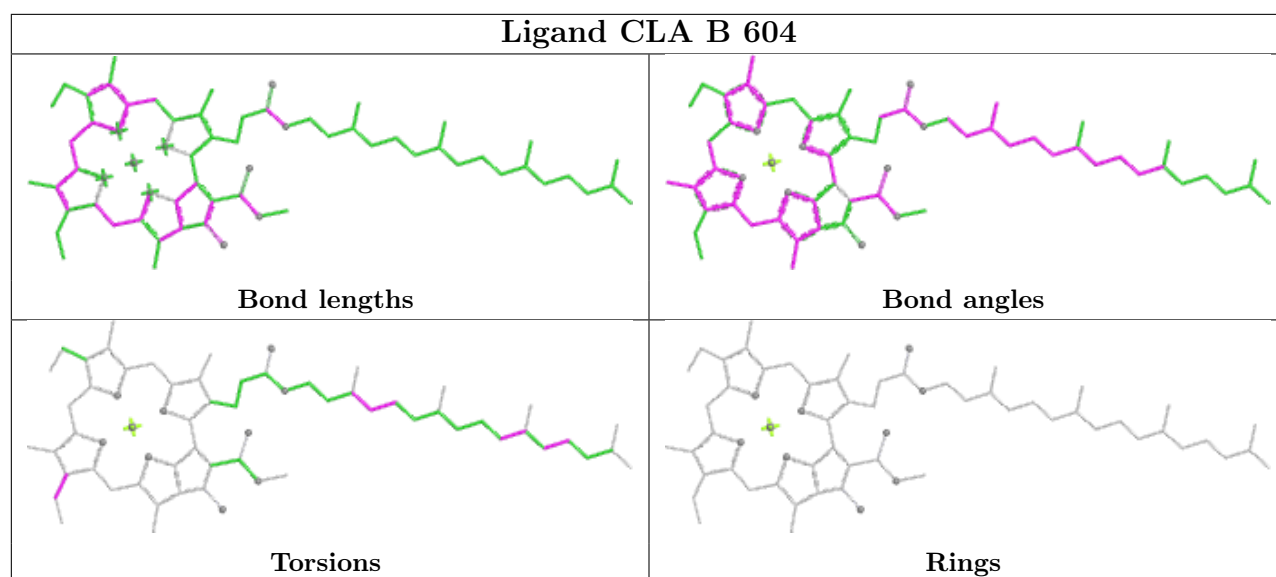


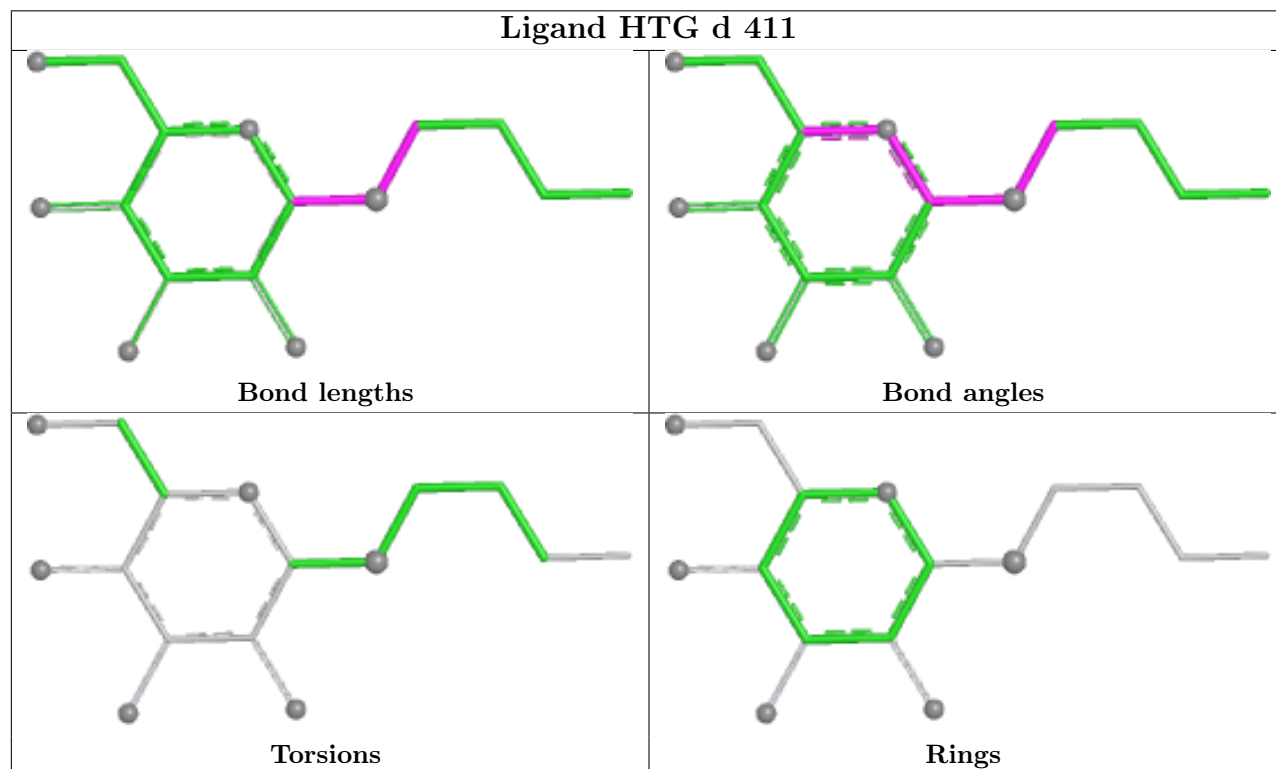
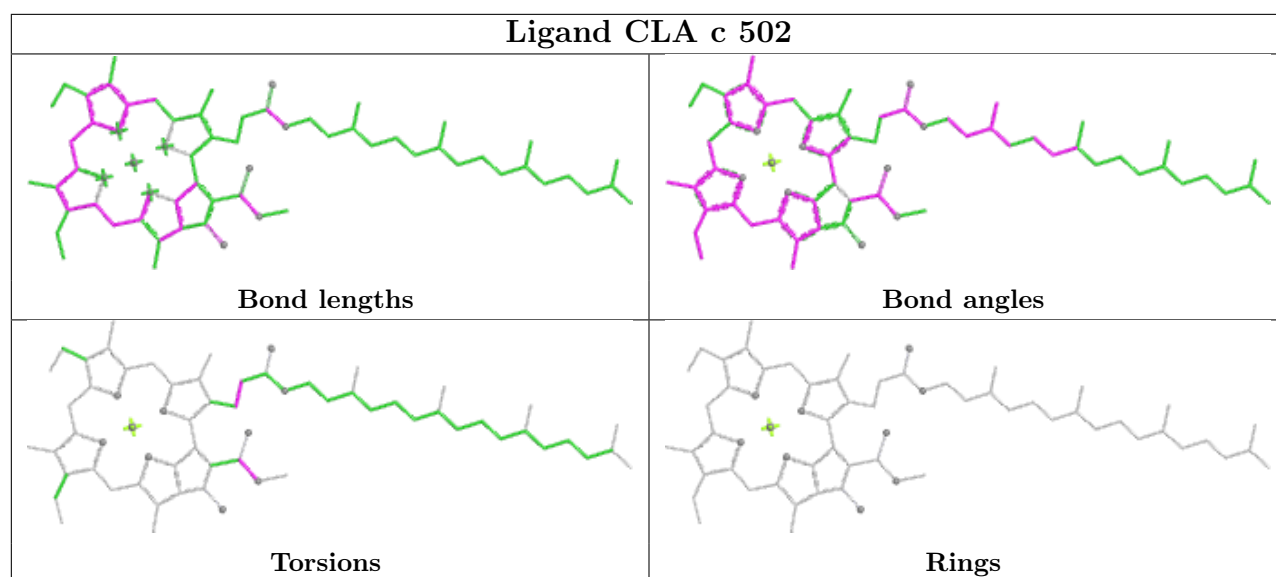
Ligand HTG b 623

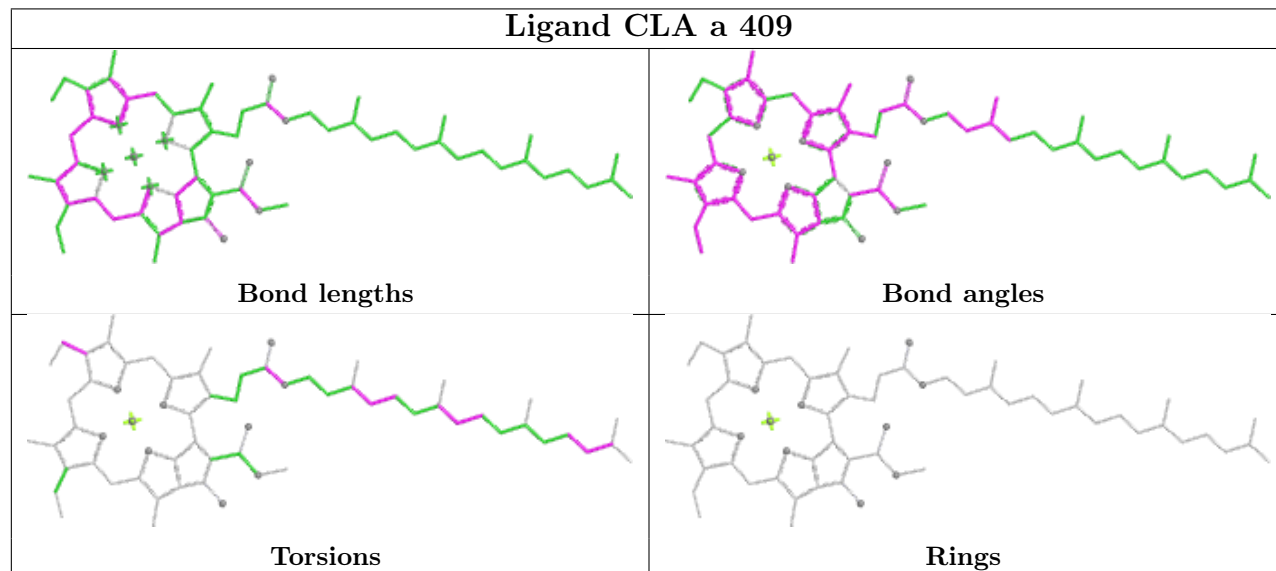
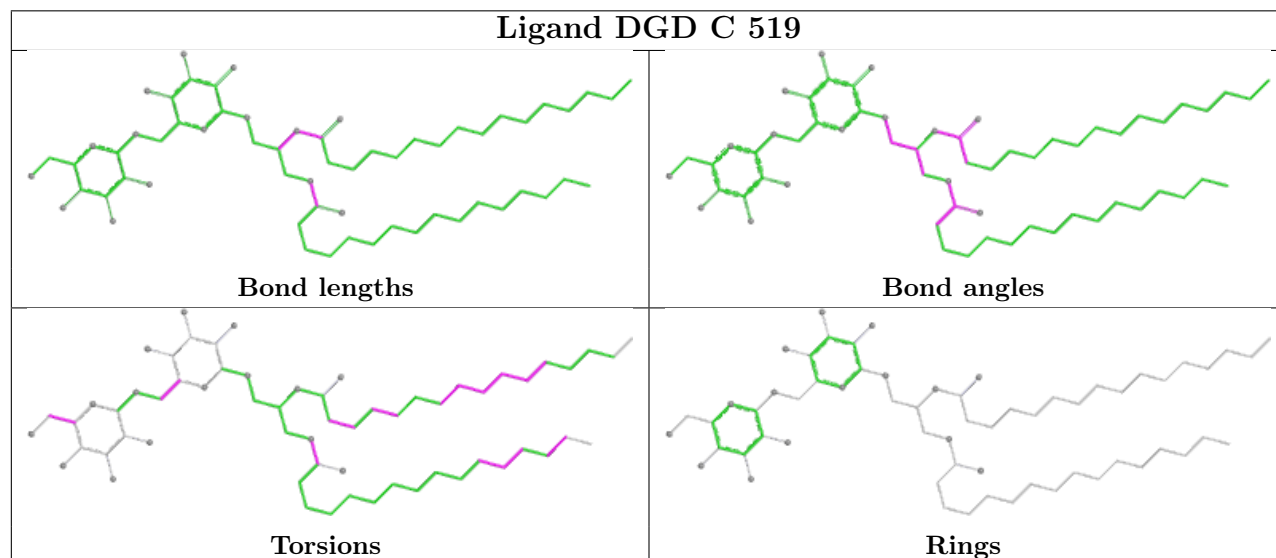
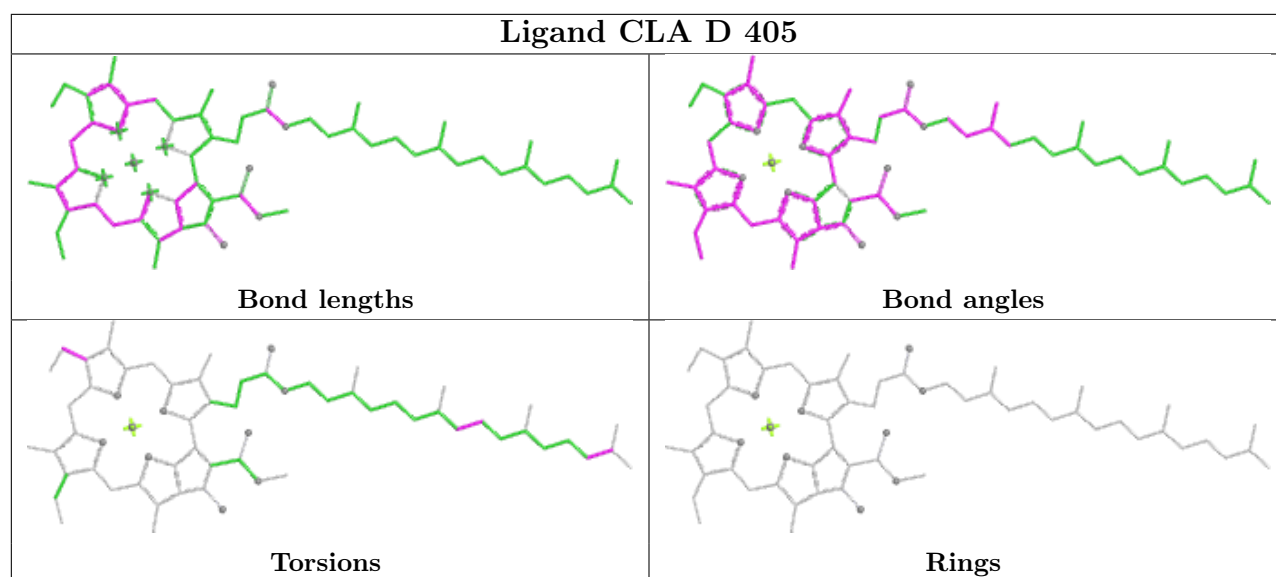




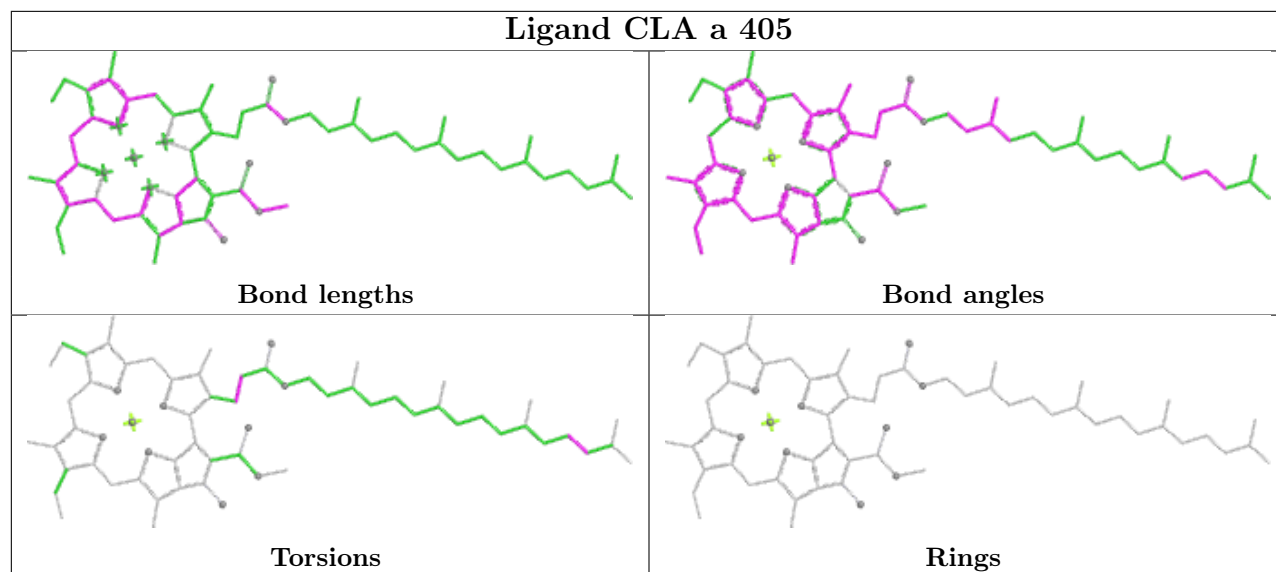




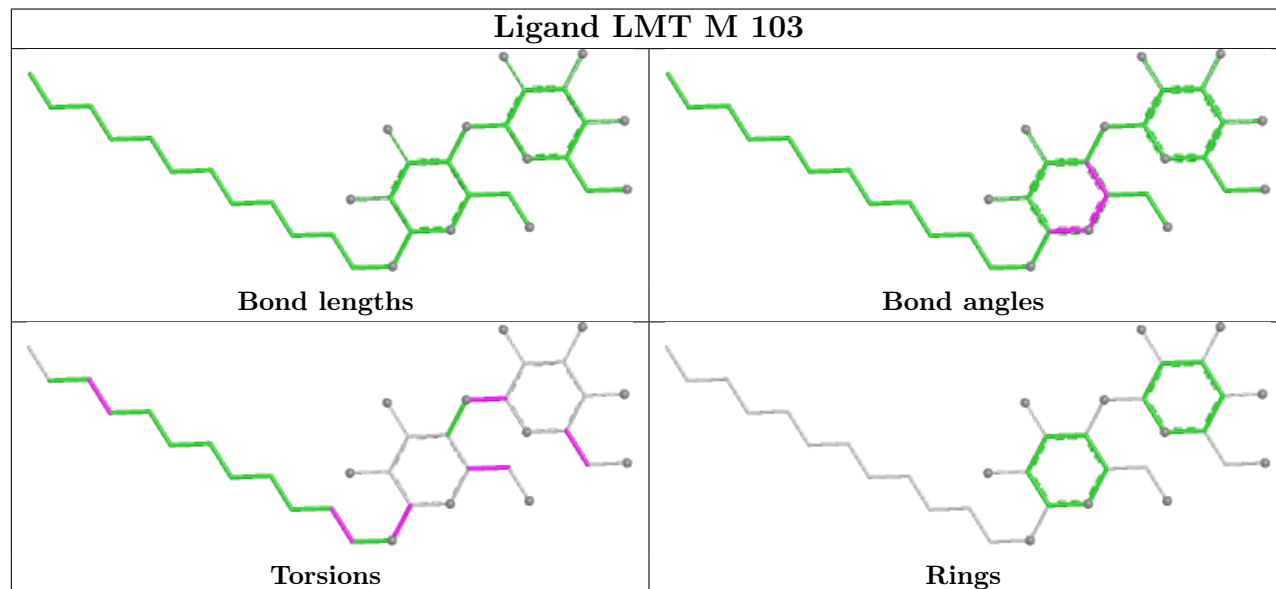




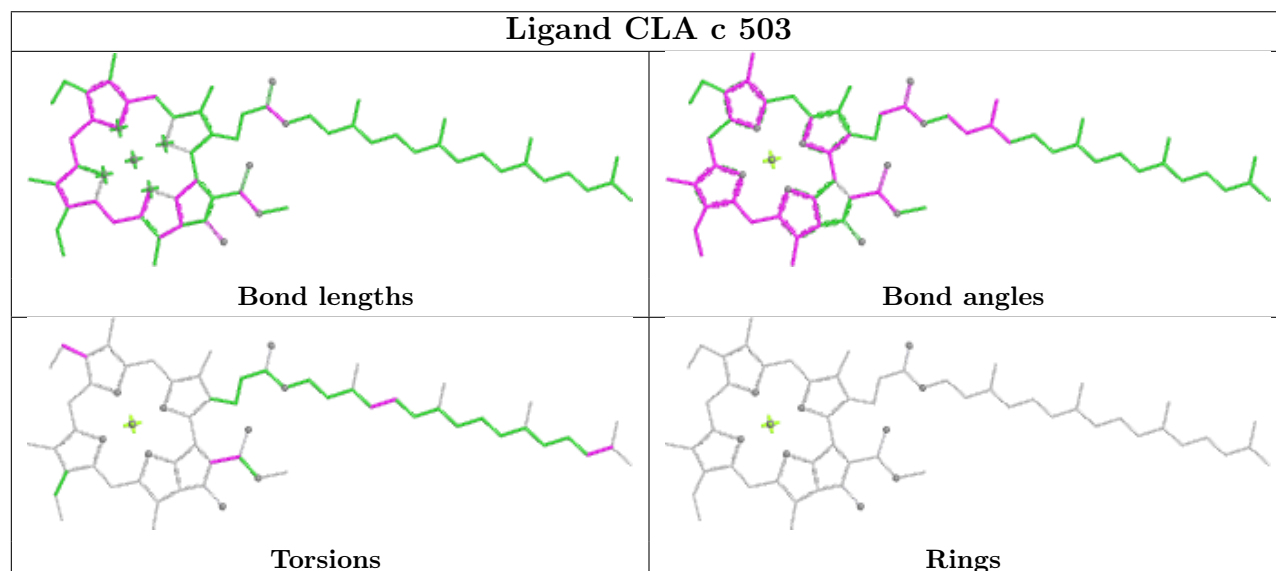
Ligand CLA a 405

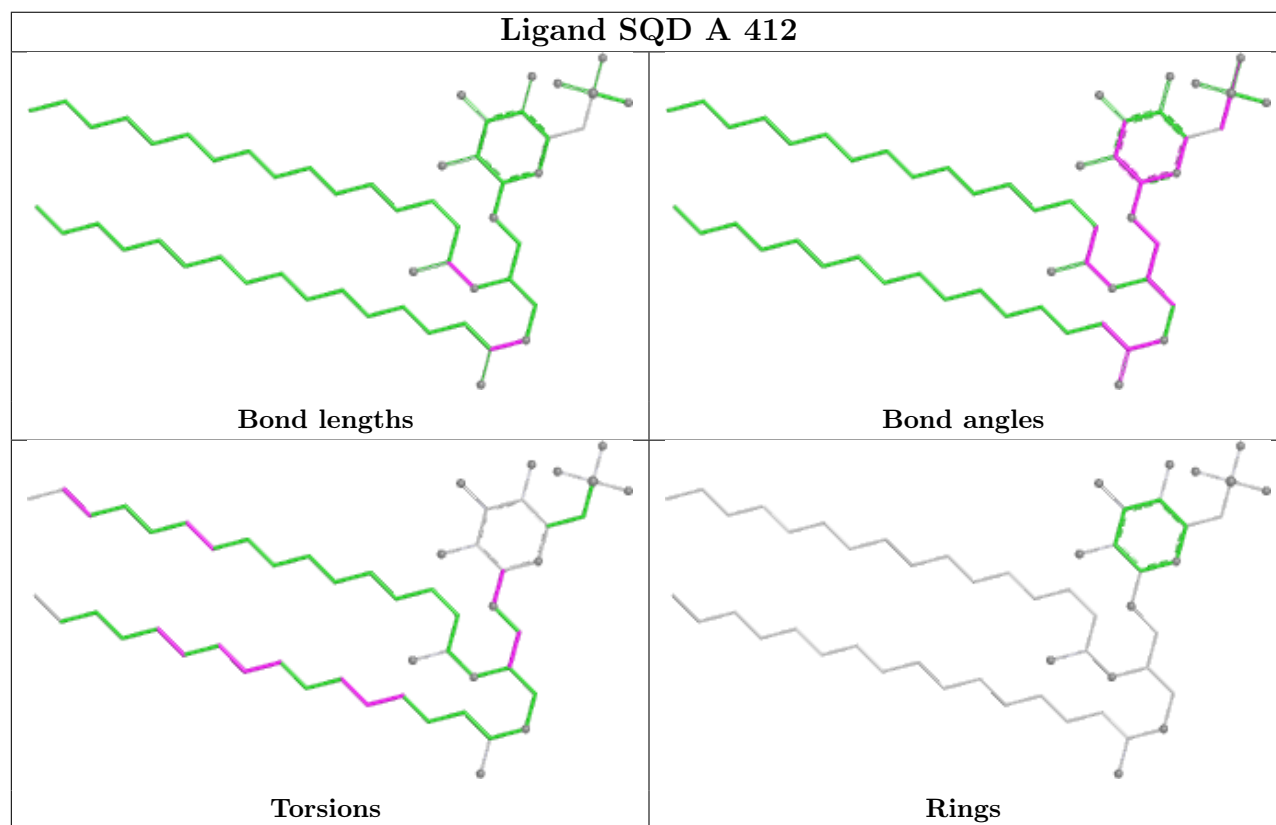
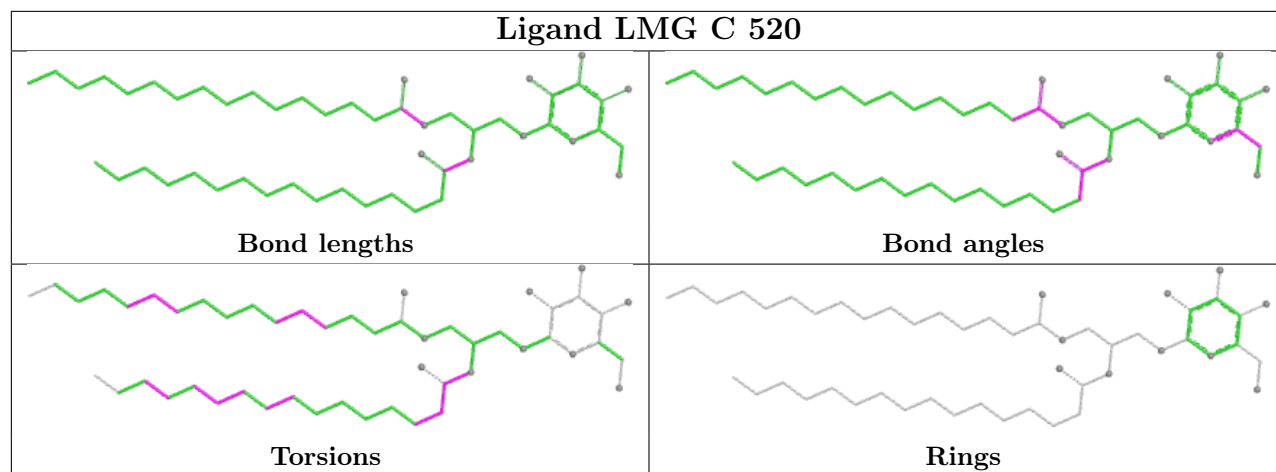


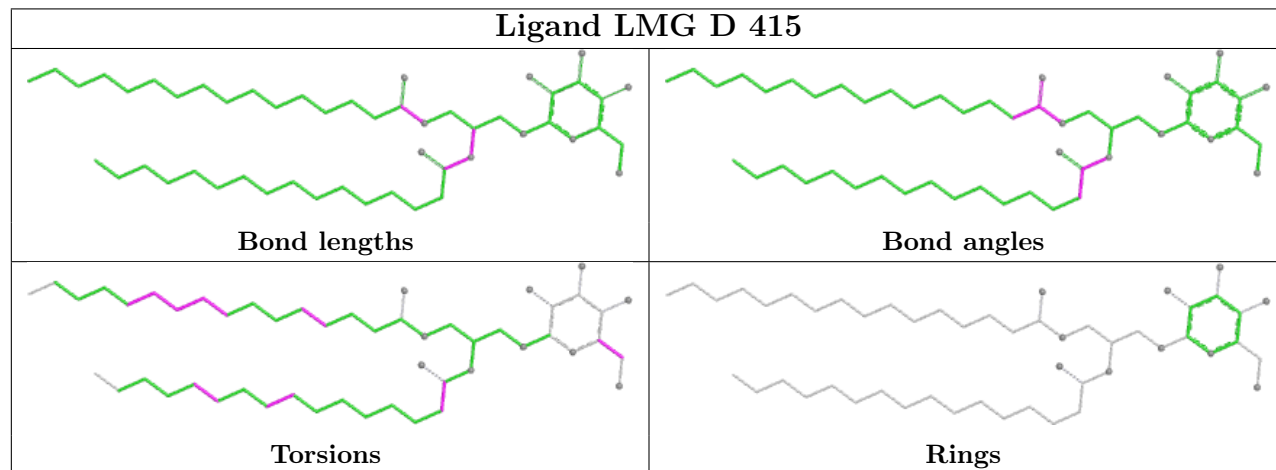
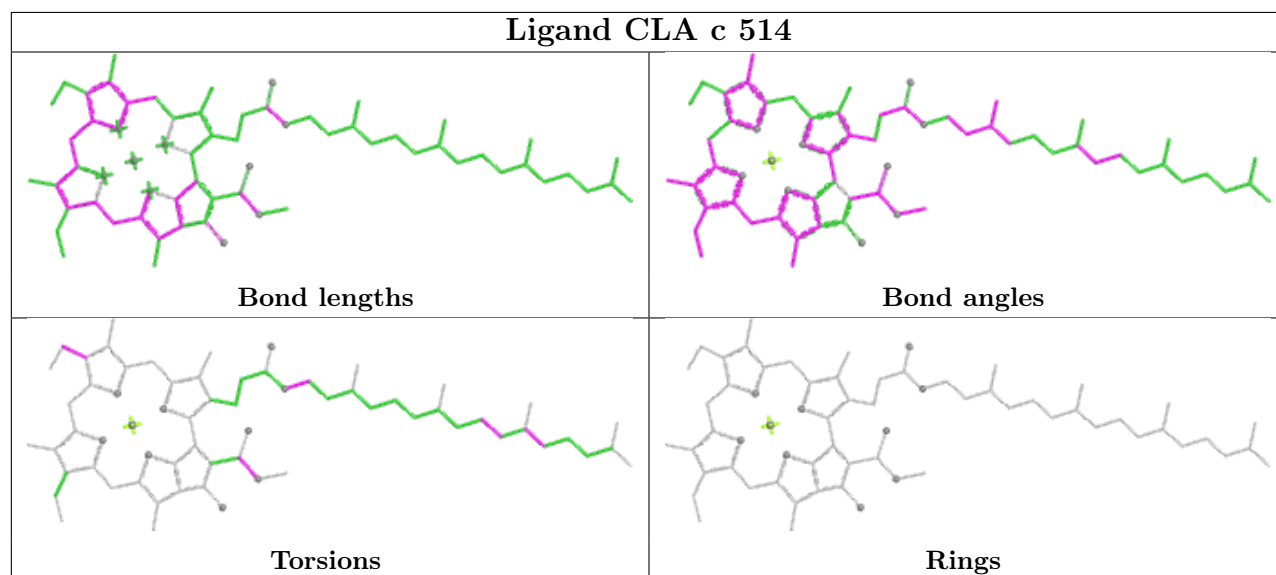
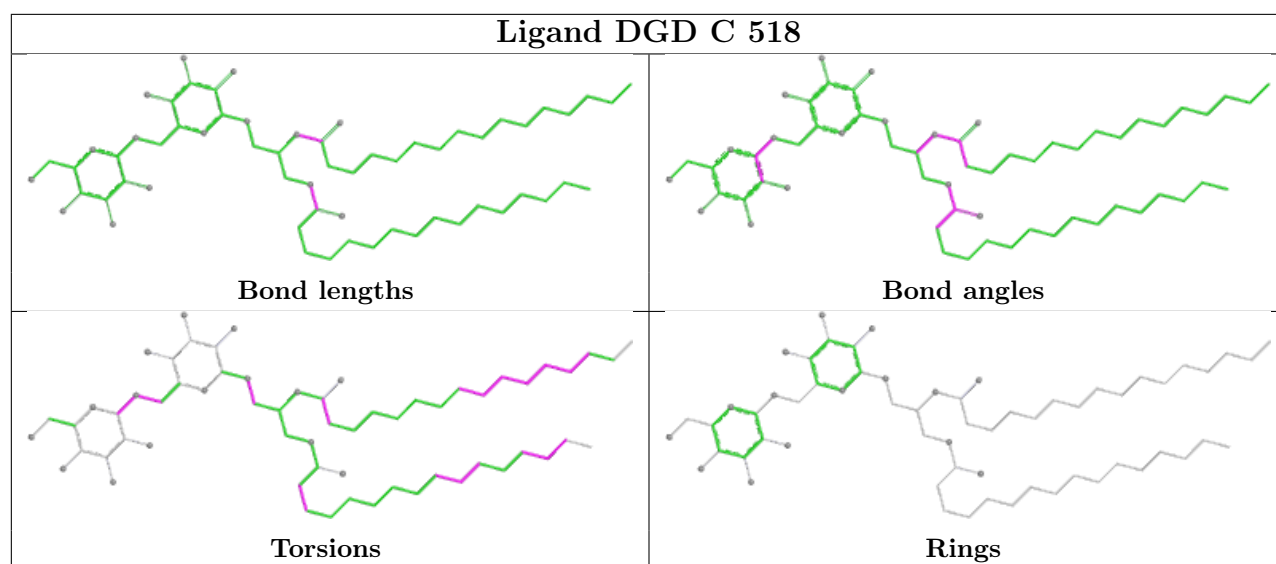
Ligand LMT M 103

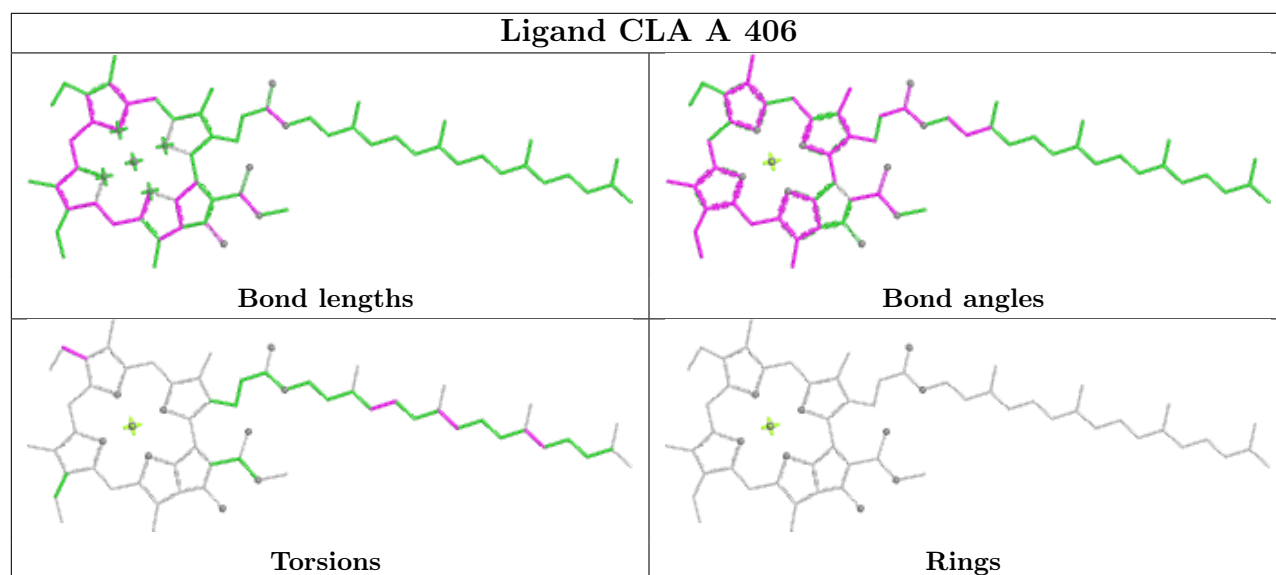
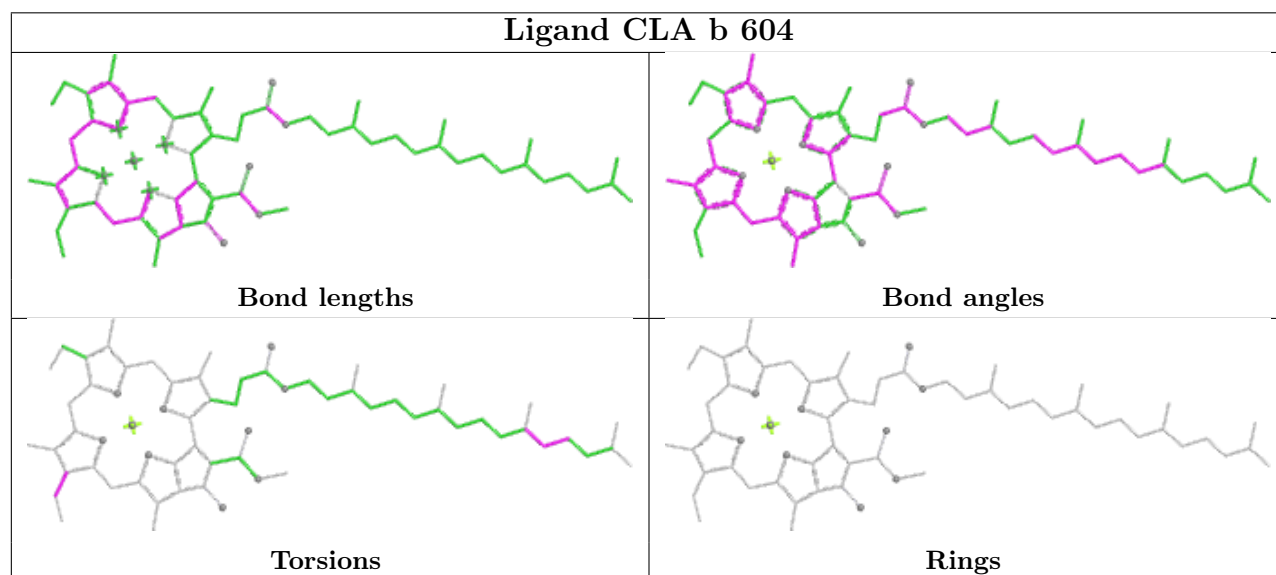
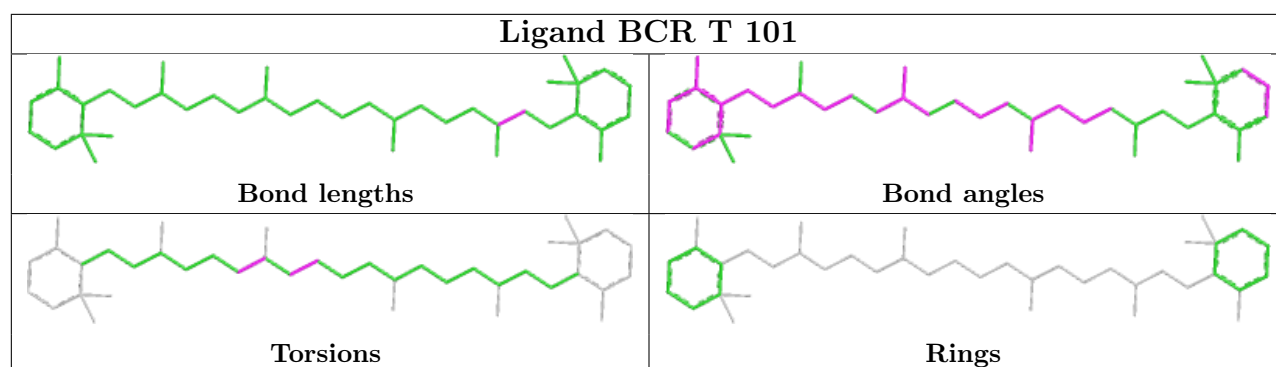


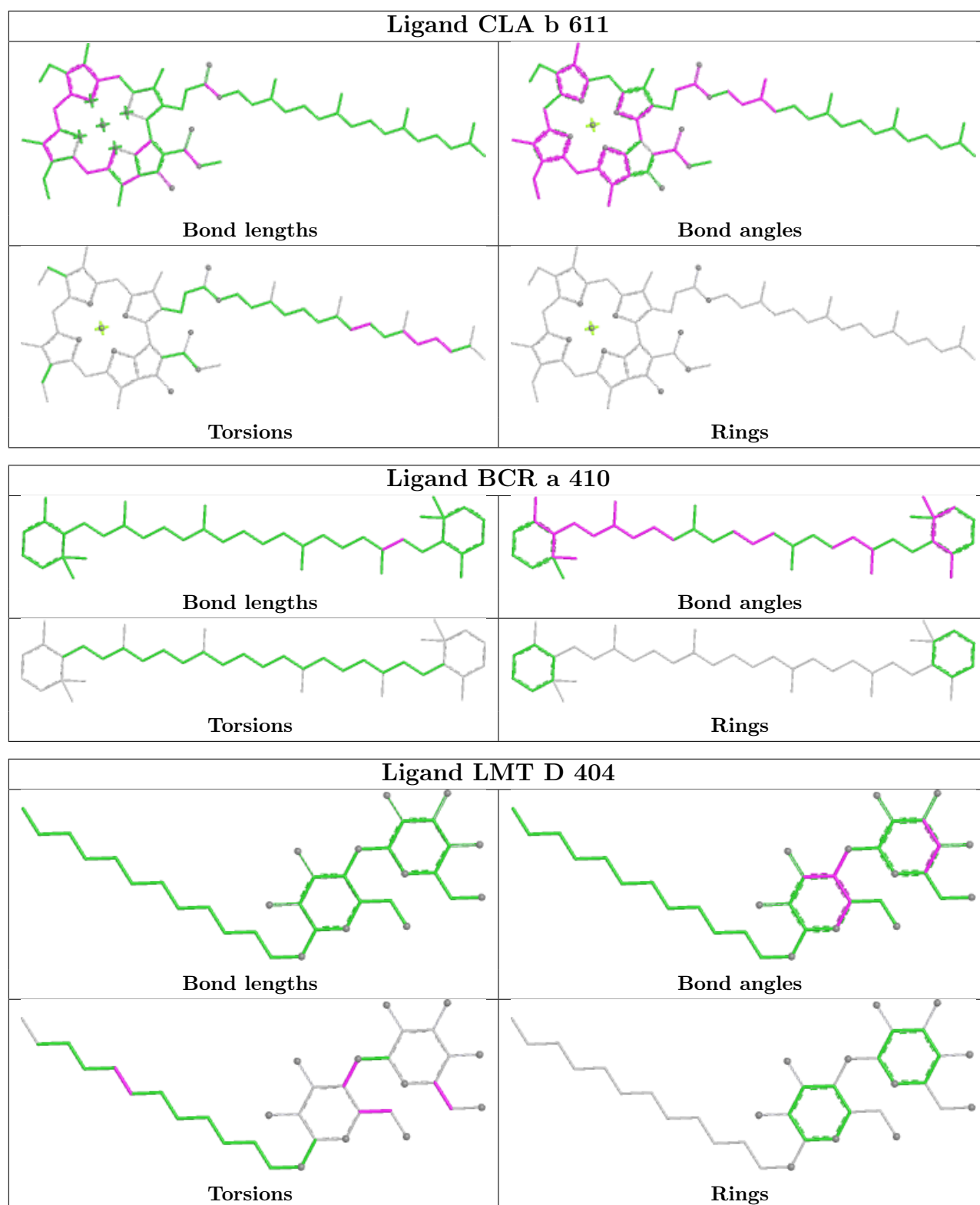
Ligand CLA c 503

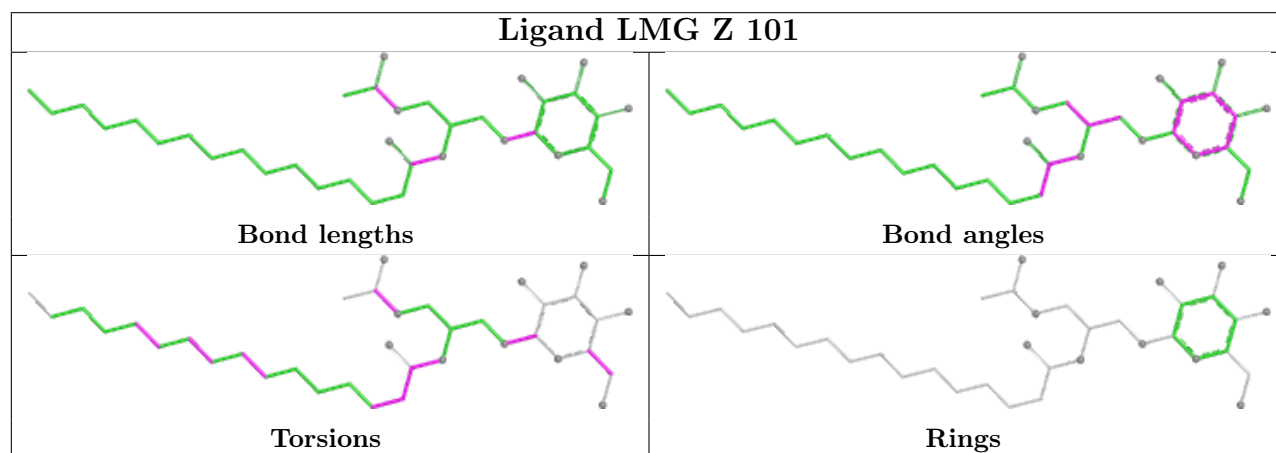
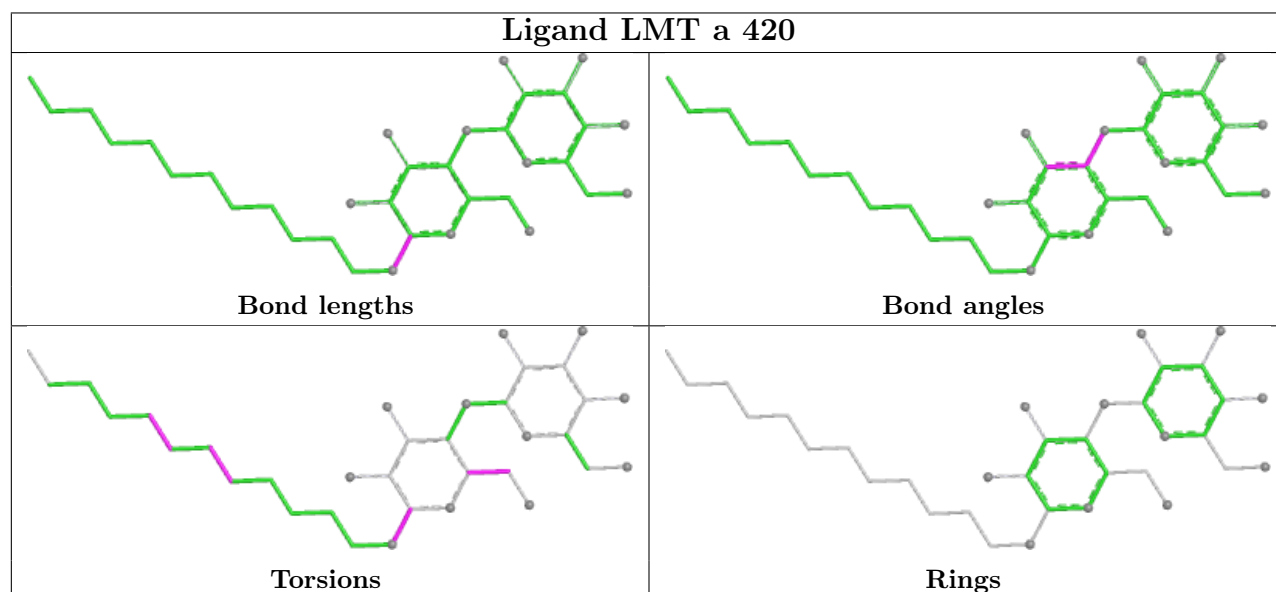
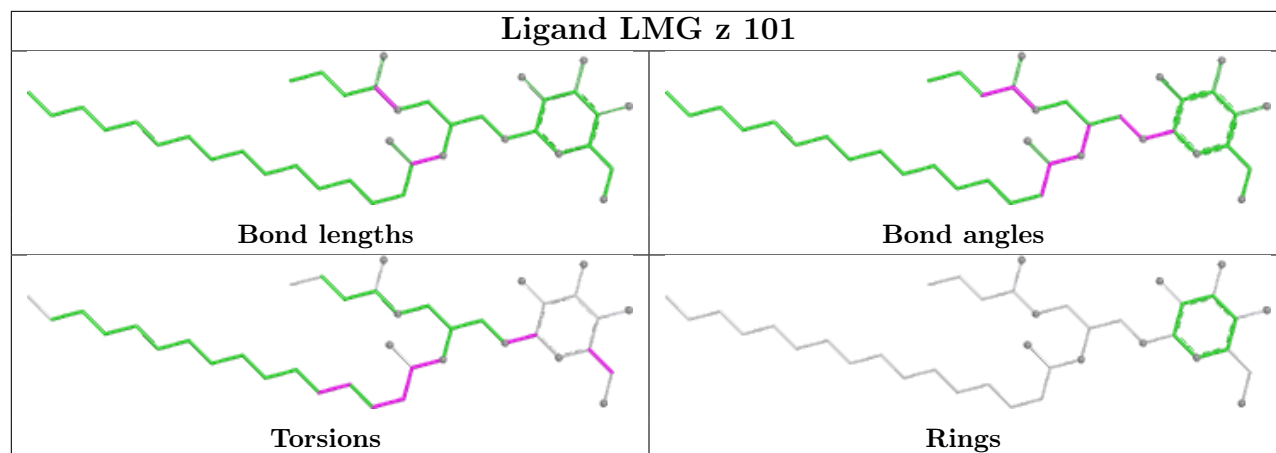


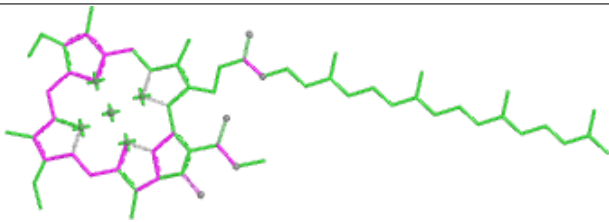
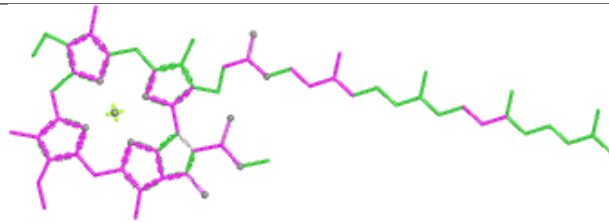
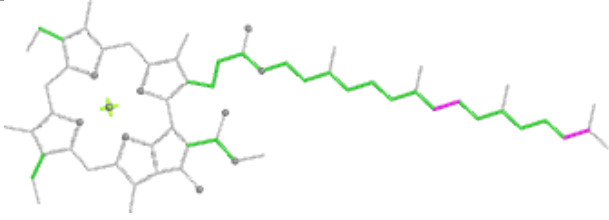
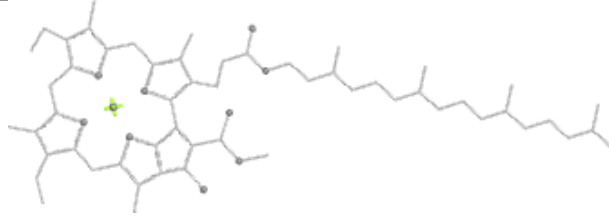


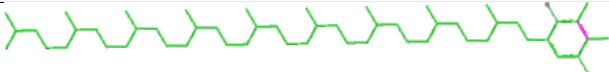
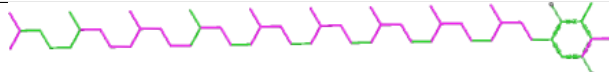


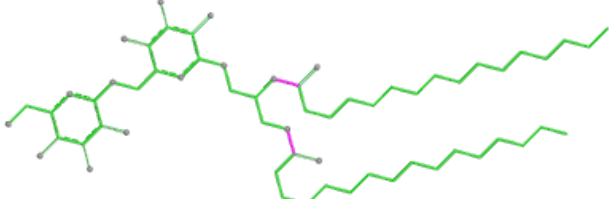
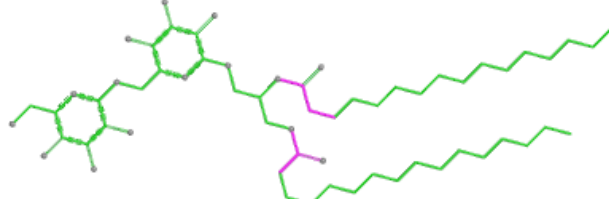
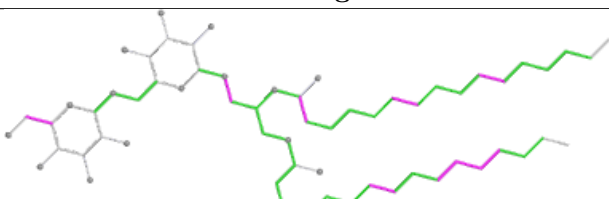
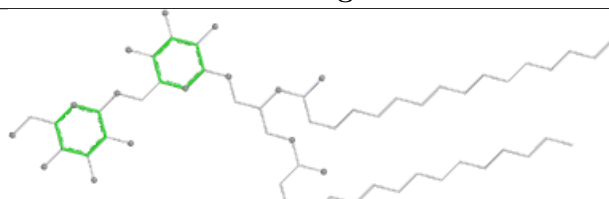


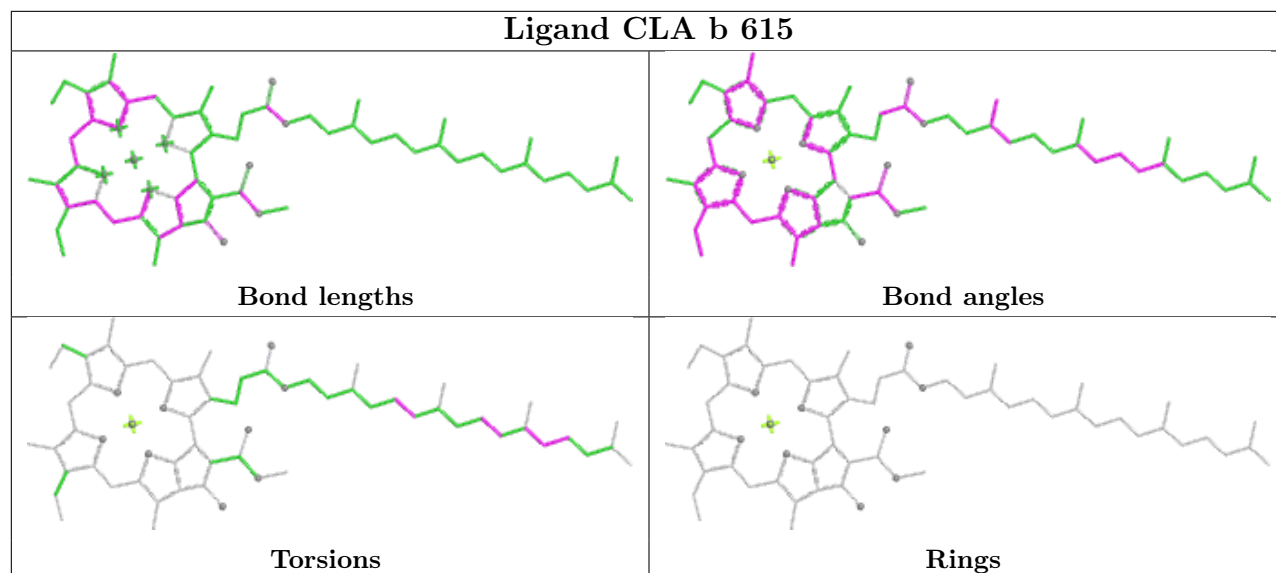
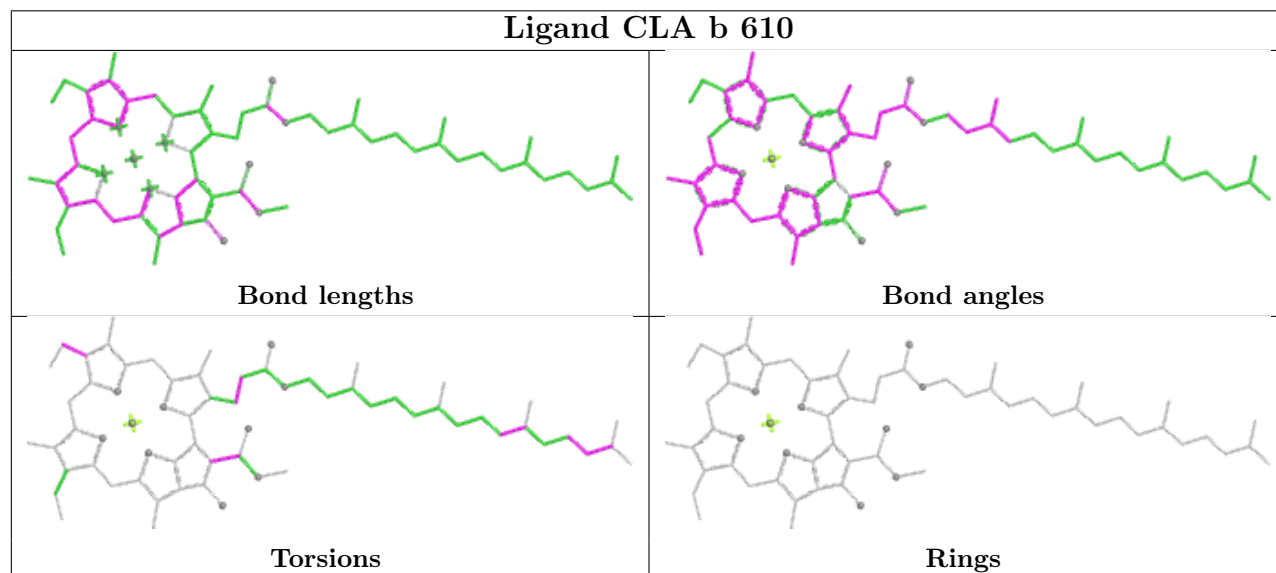
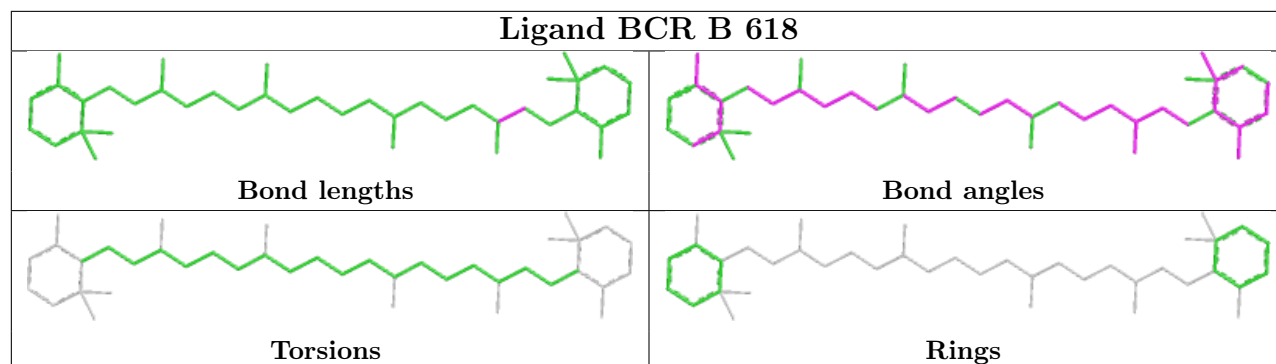


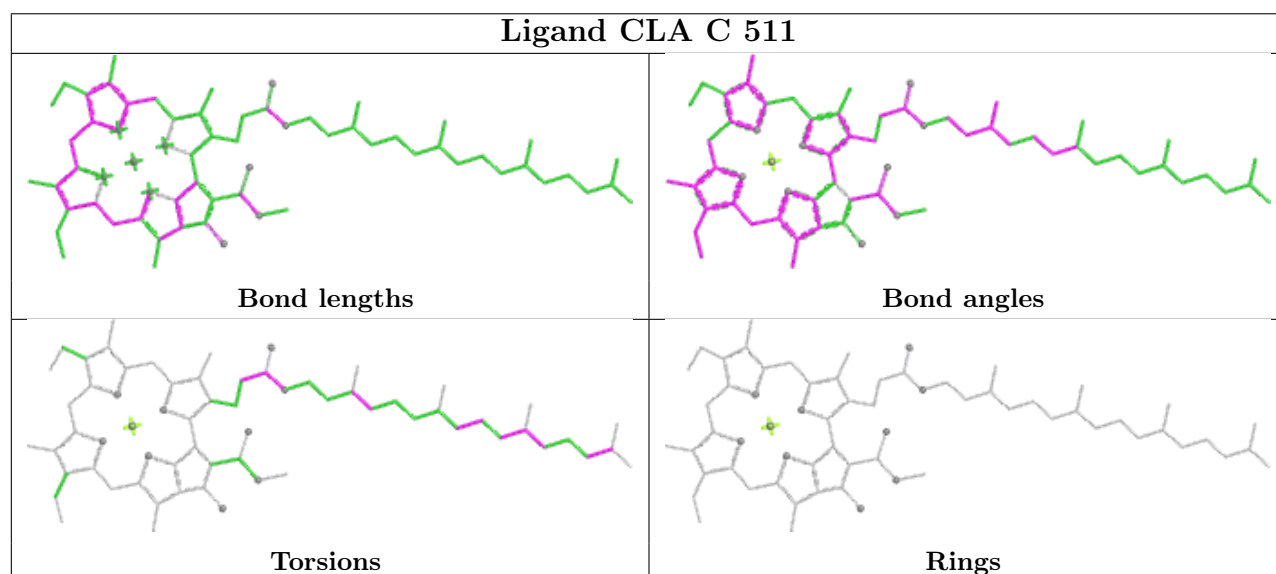
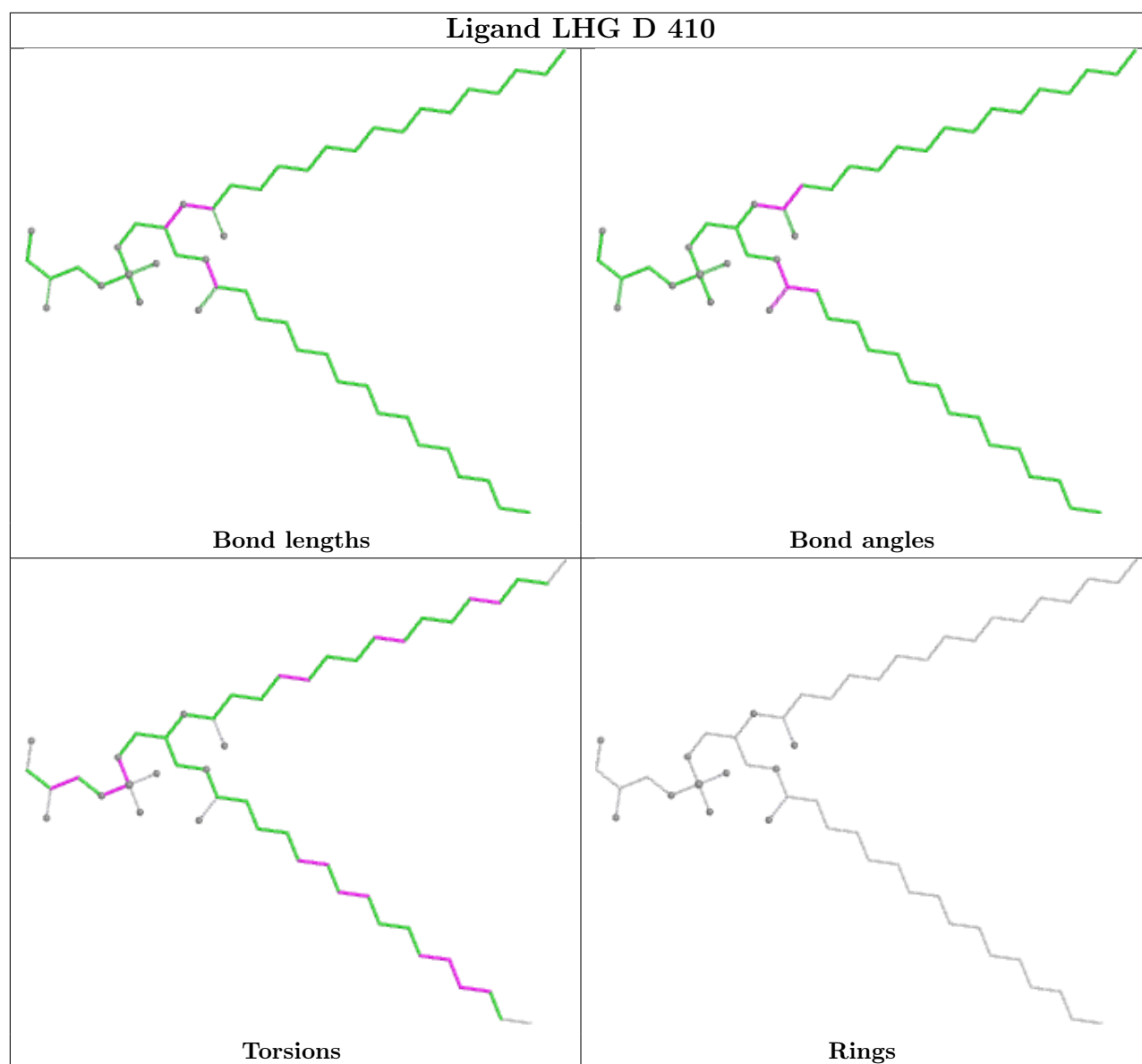


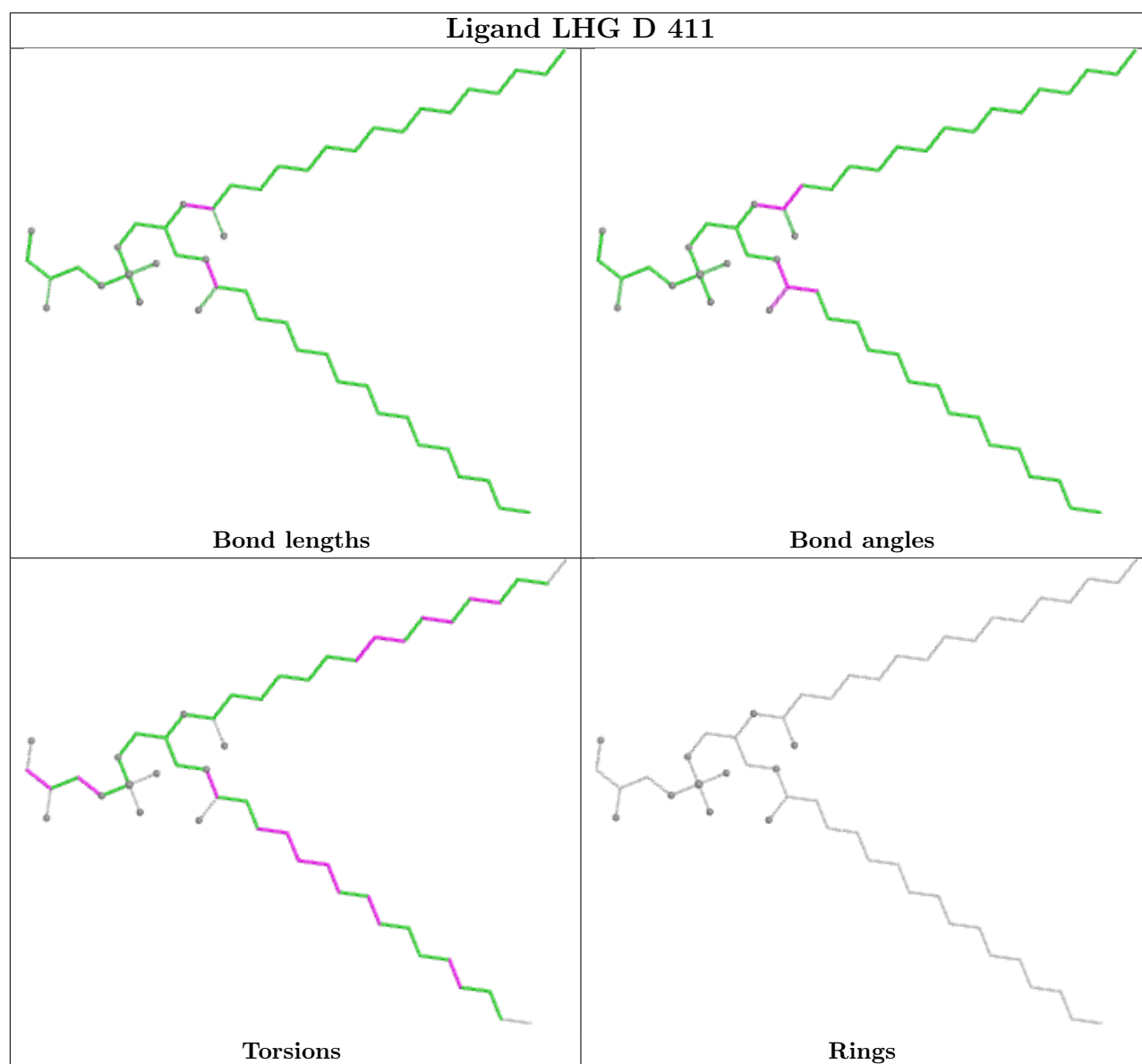
Ligand CLA B 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

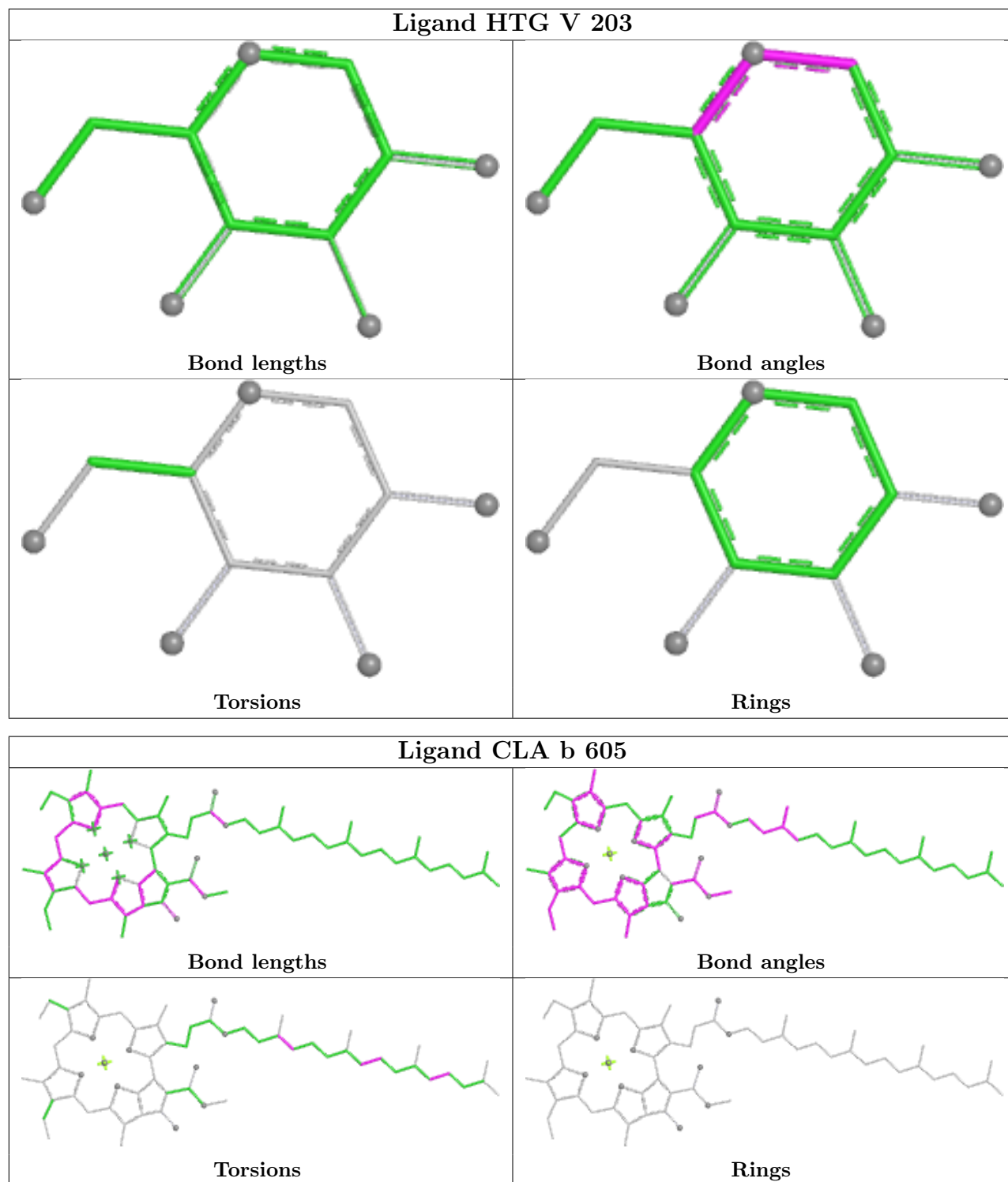
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Bond lengths	Bond angles
	
Torsions	Rings

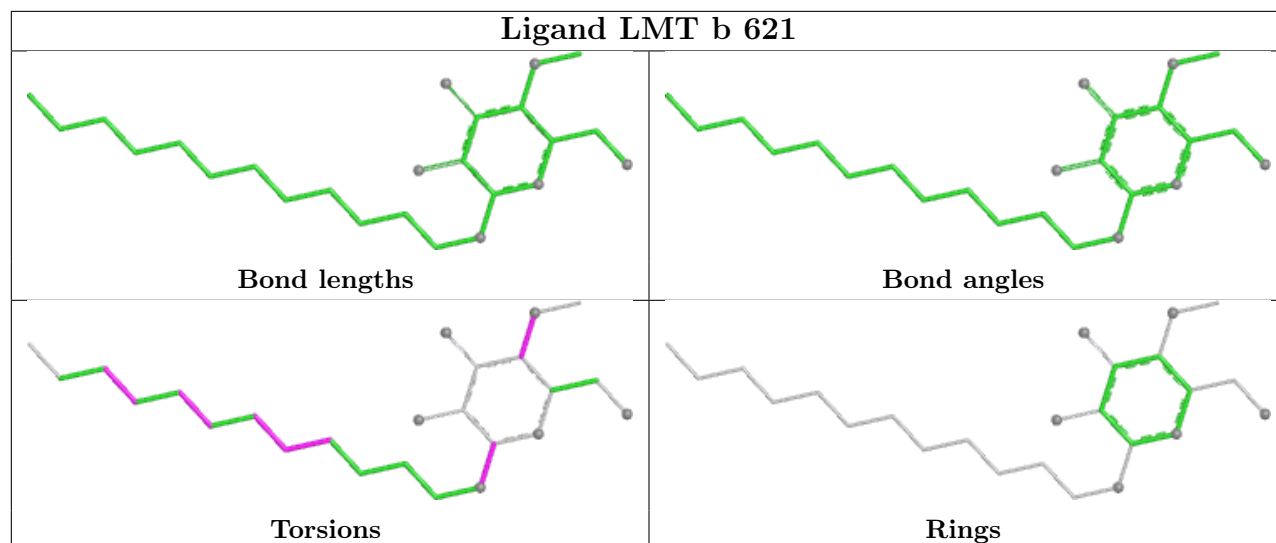
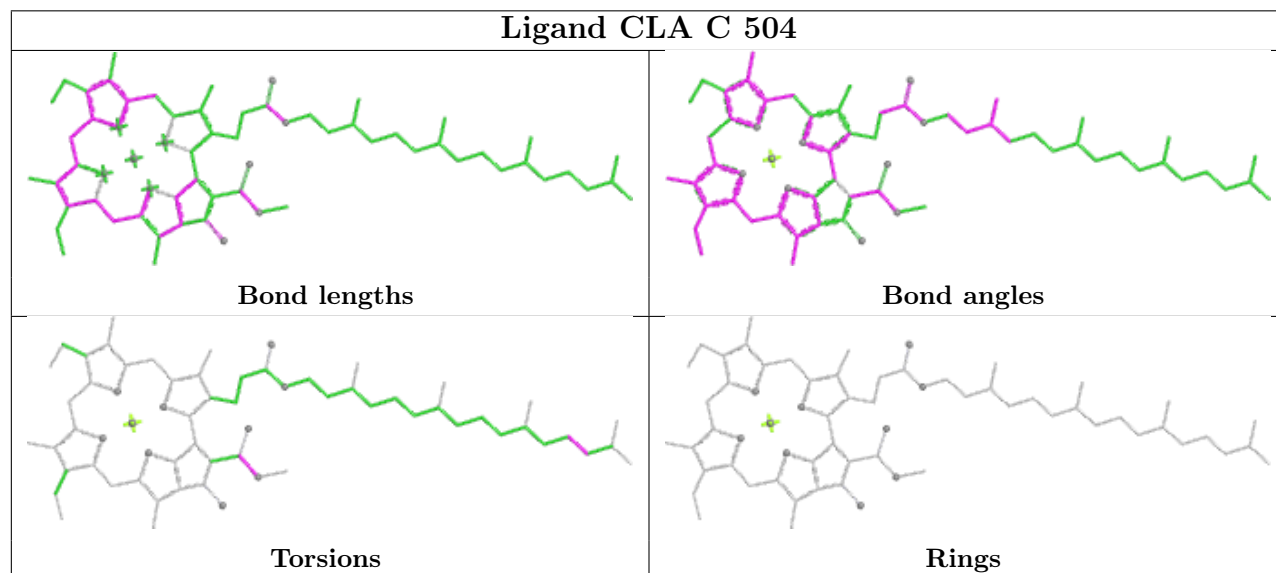
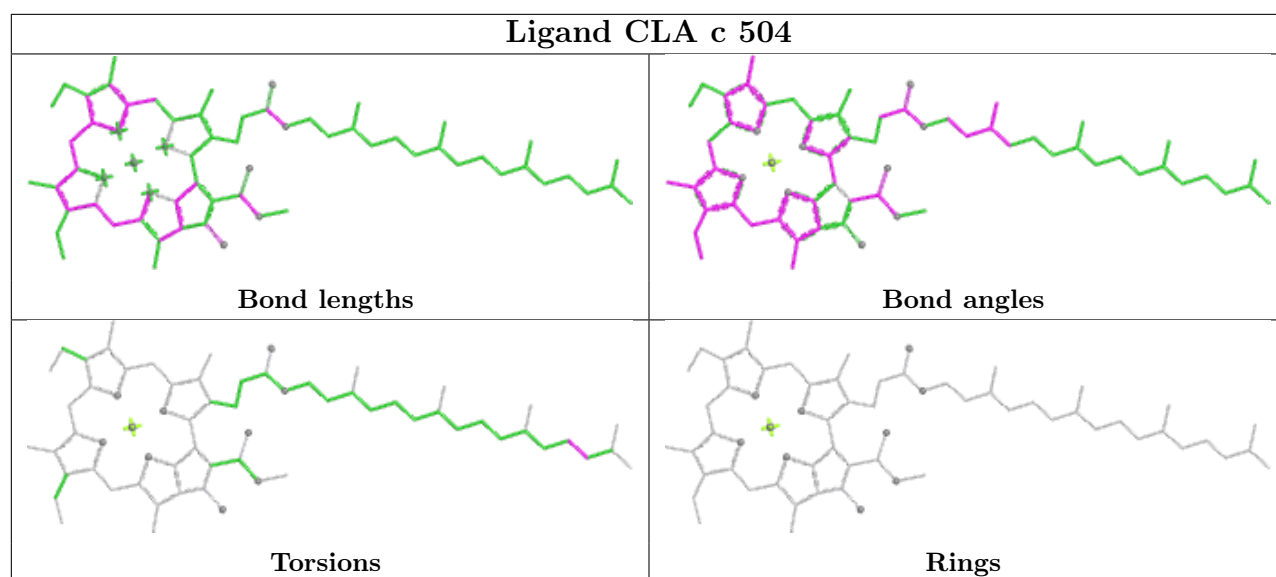
Ligand DGD h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

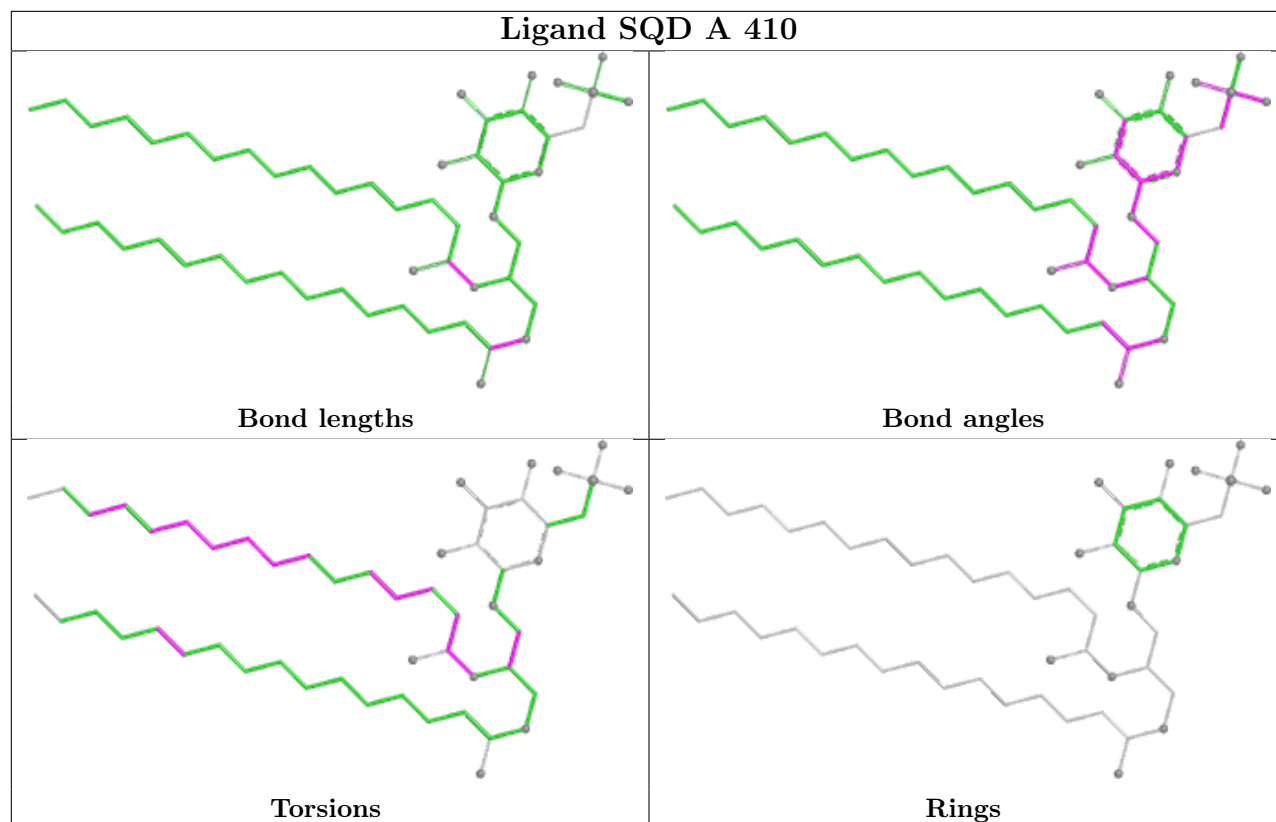


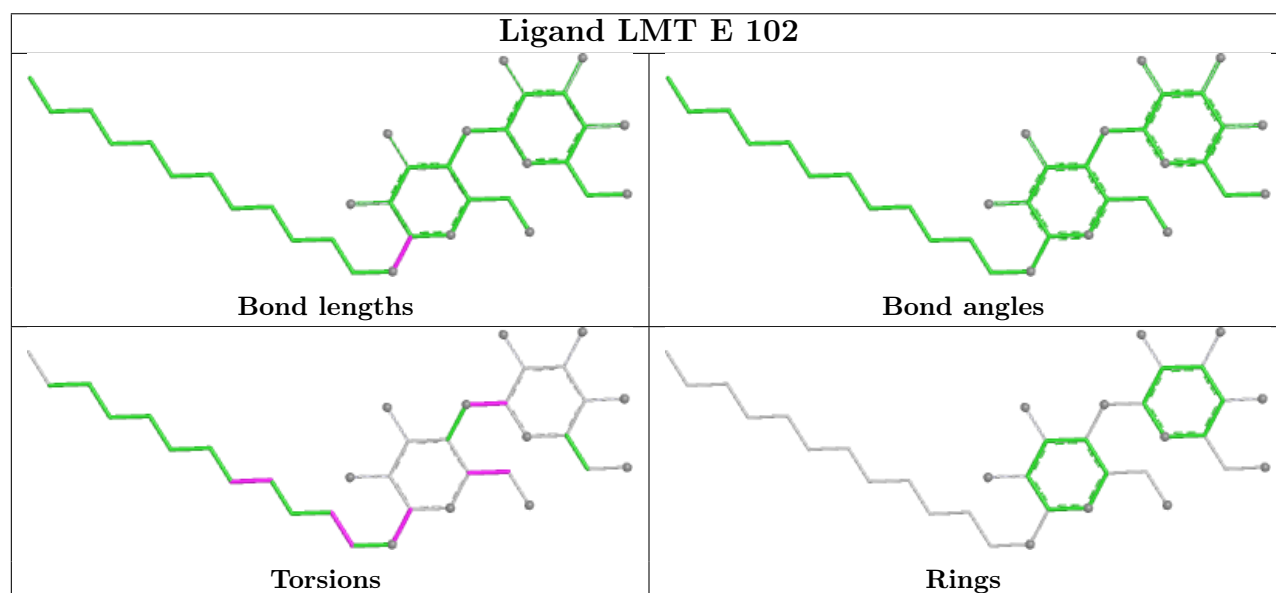
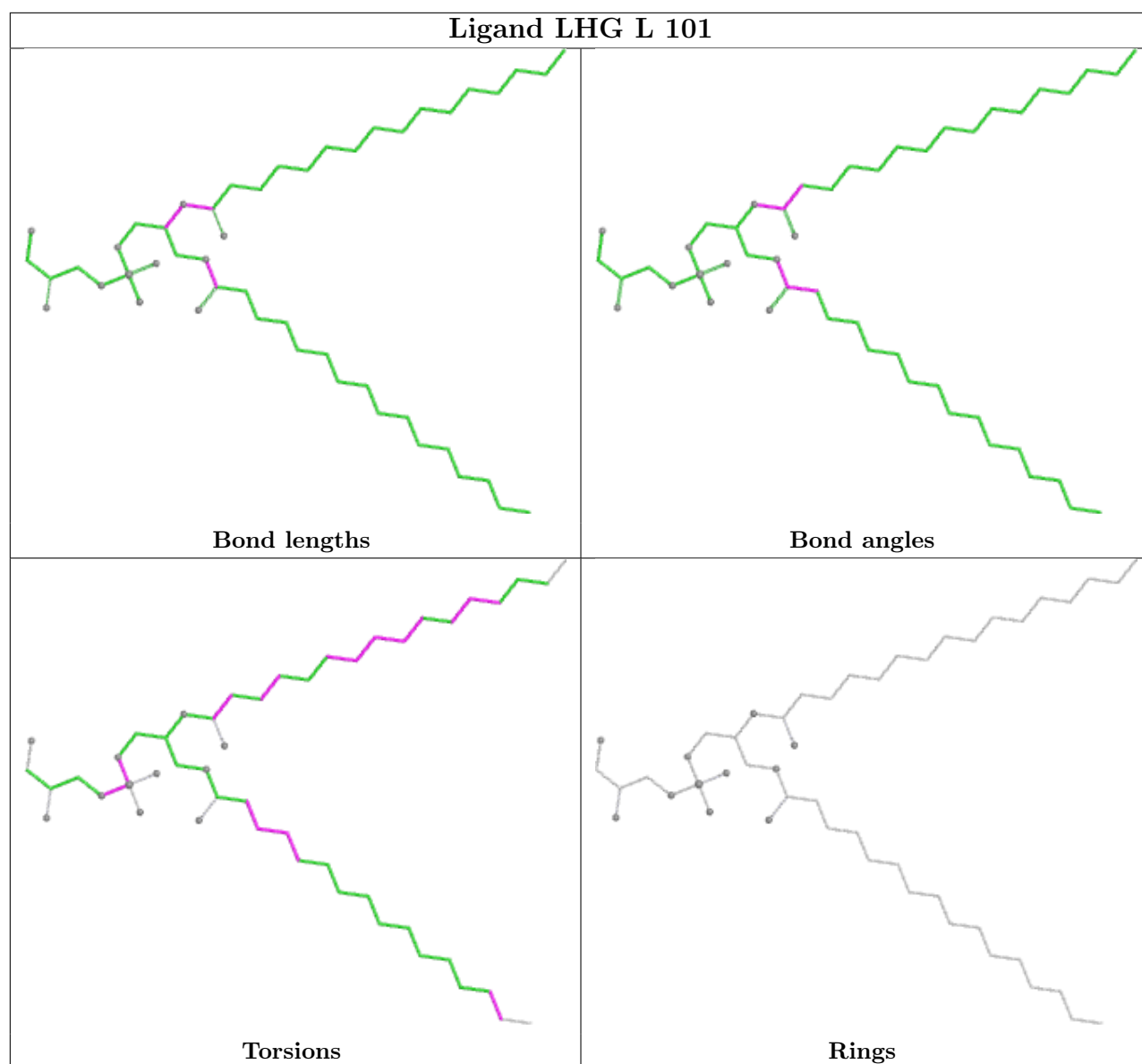


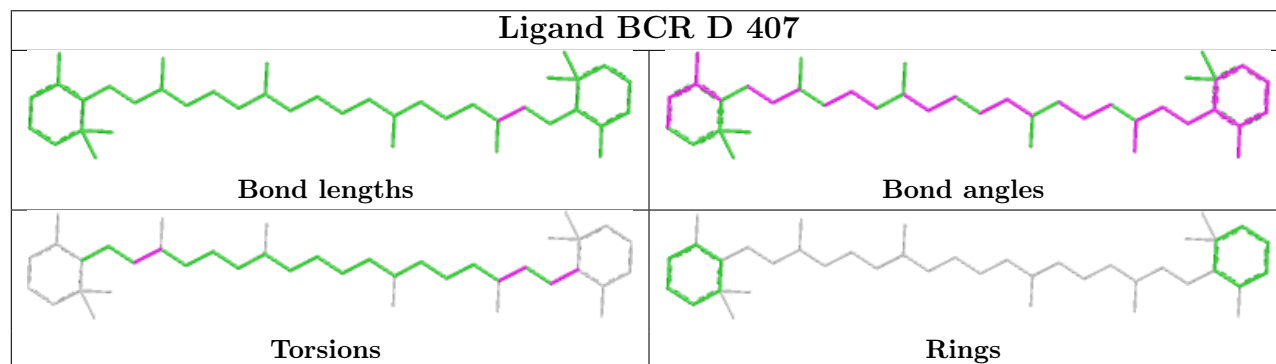
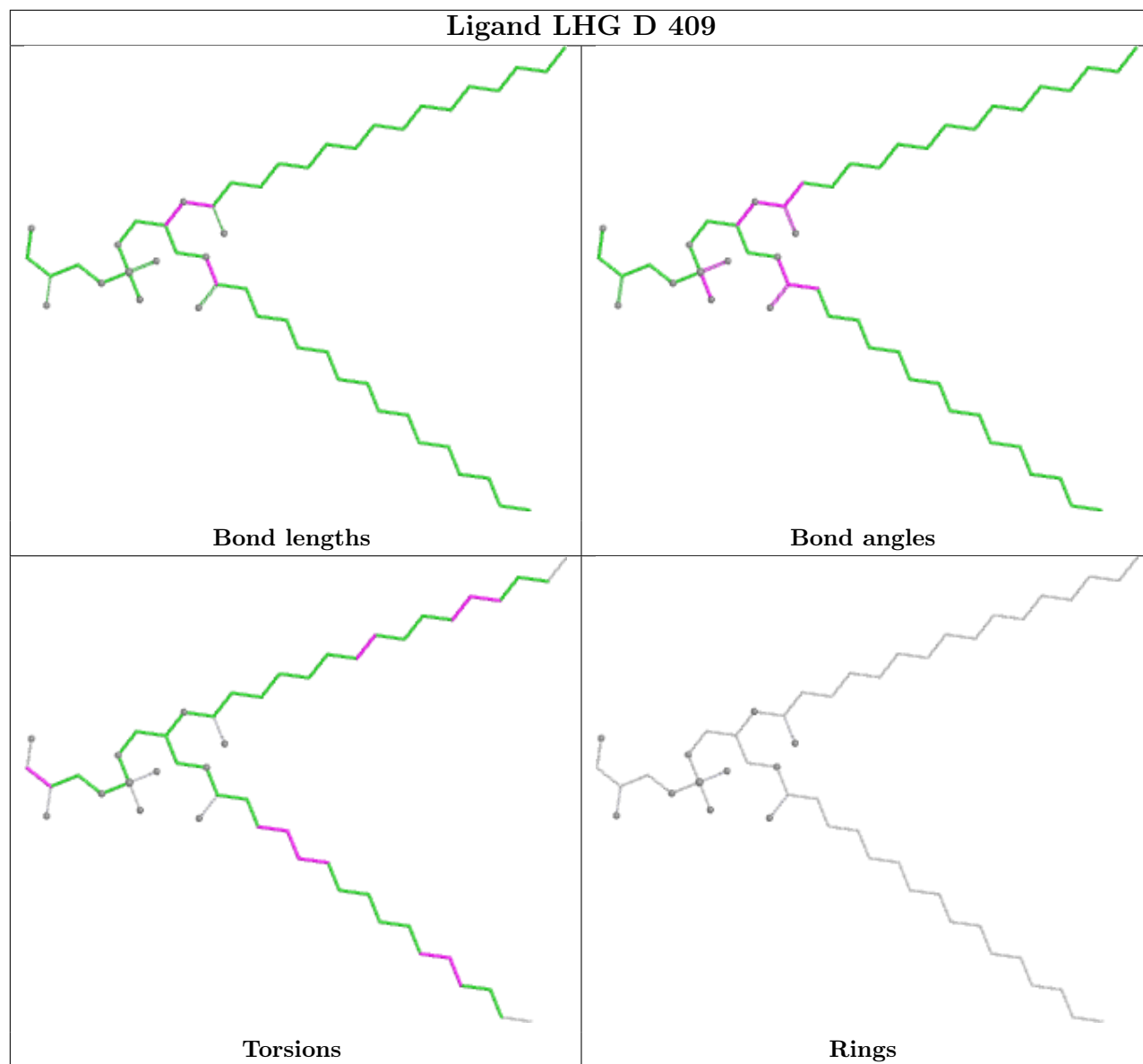


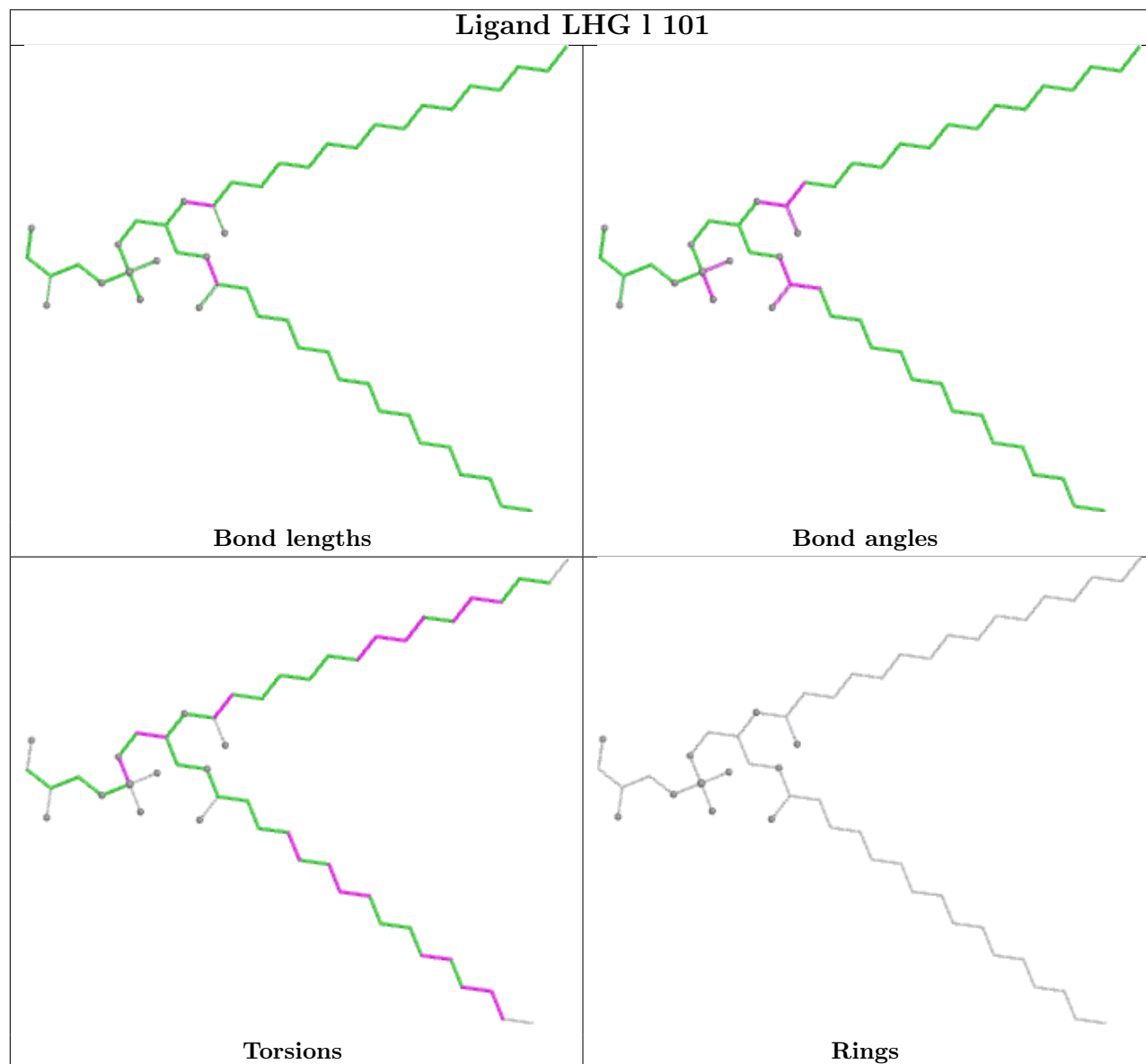
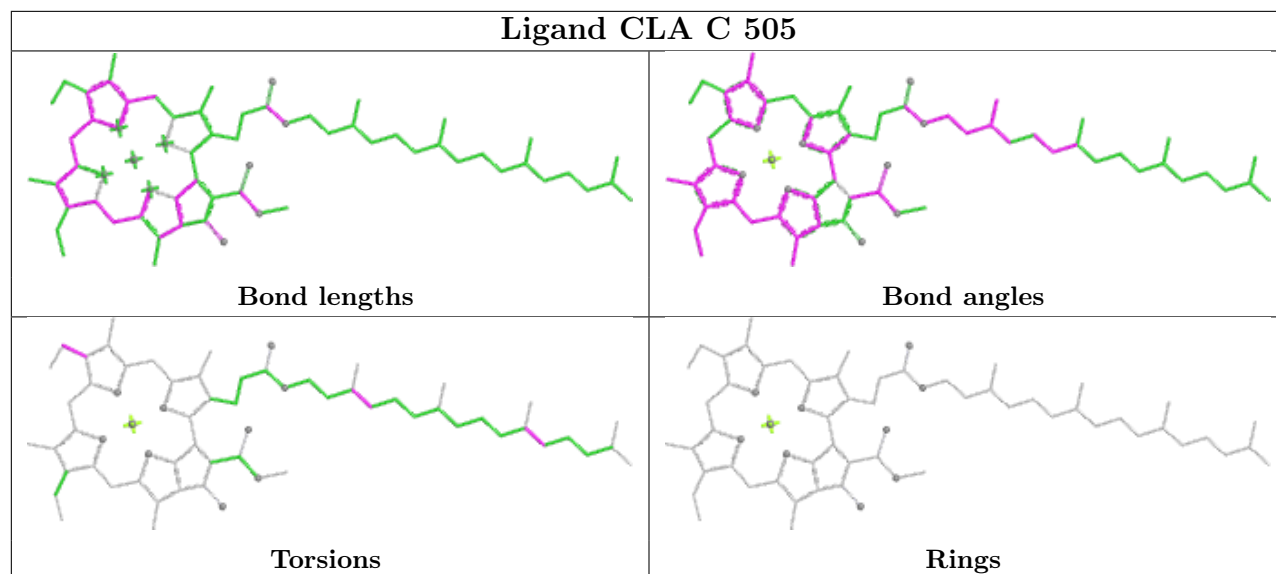


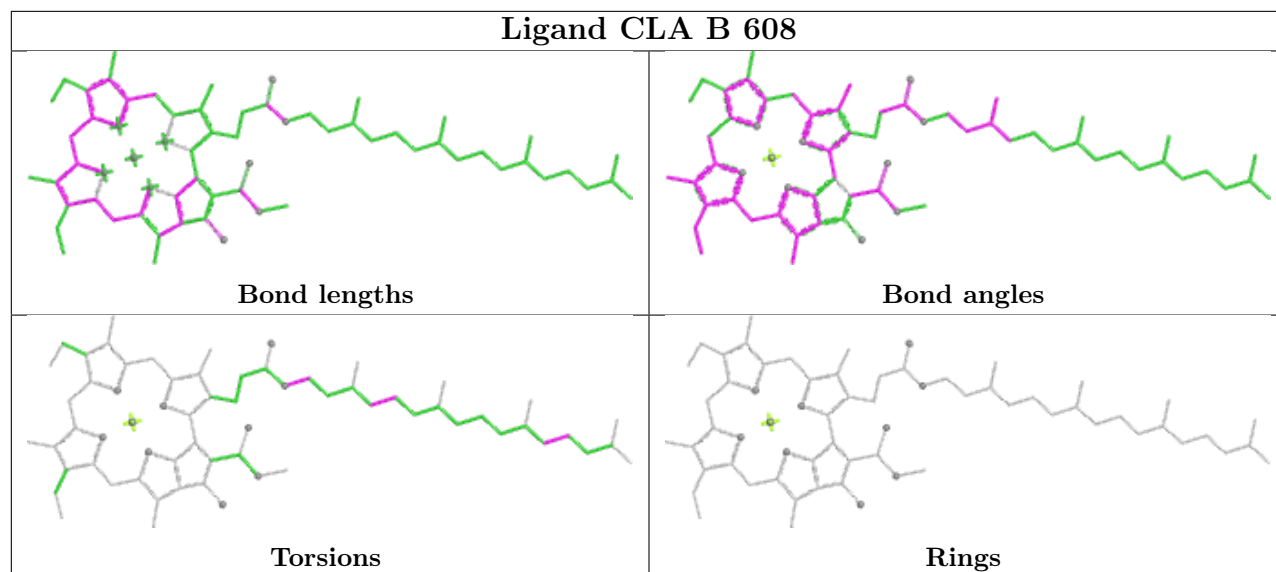
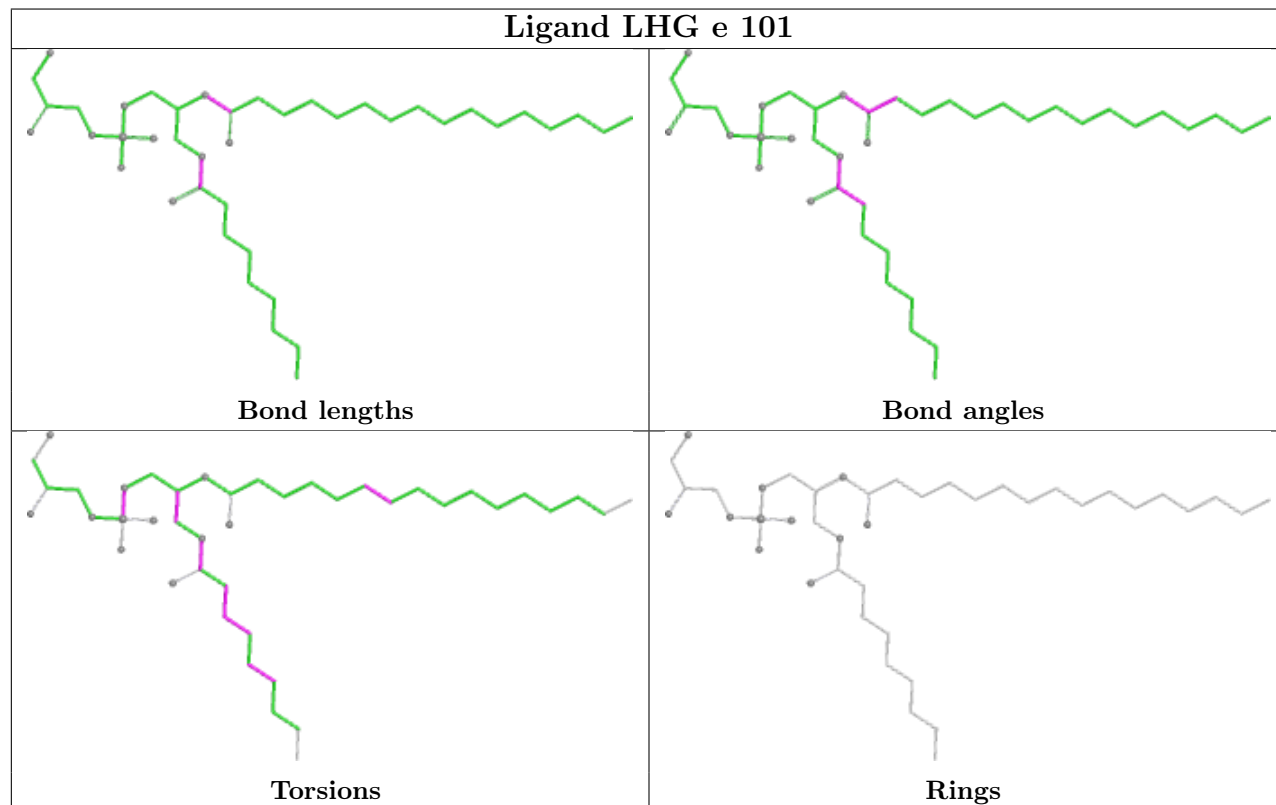


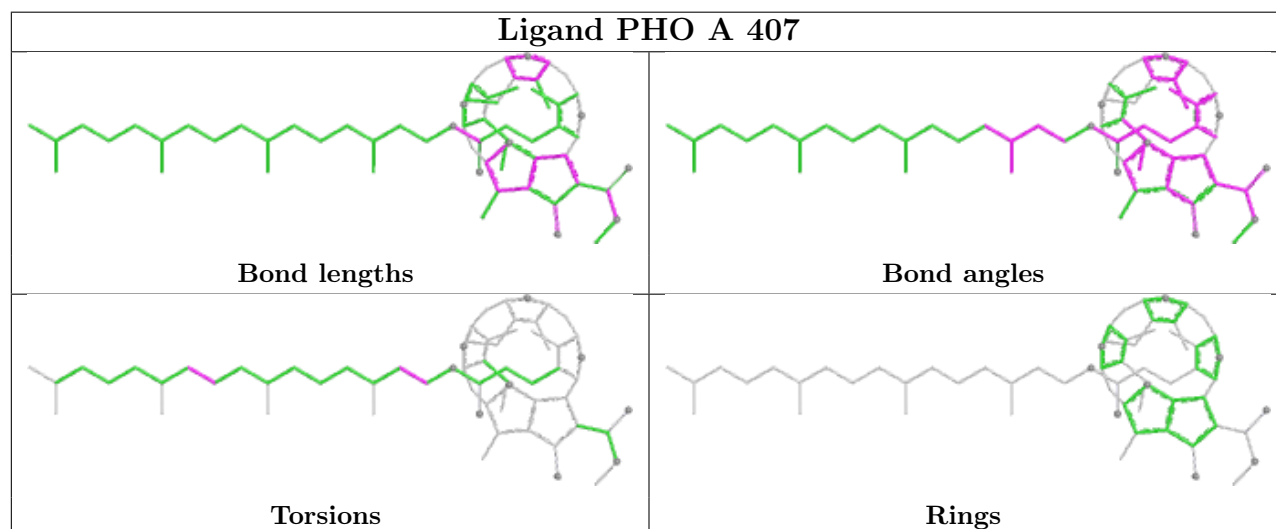
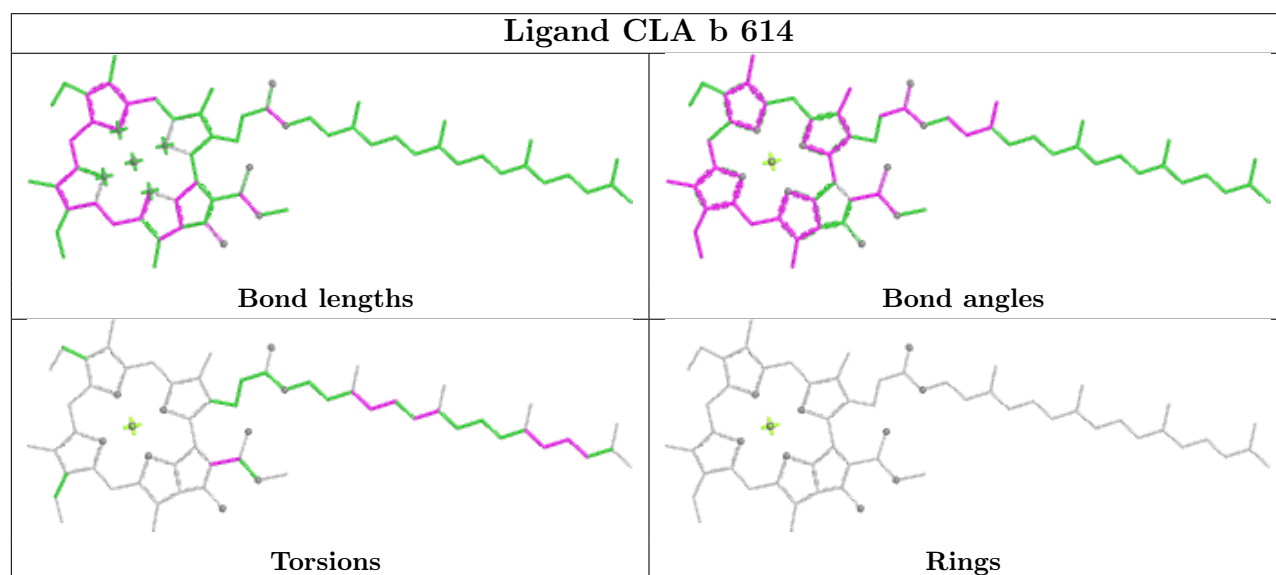
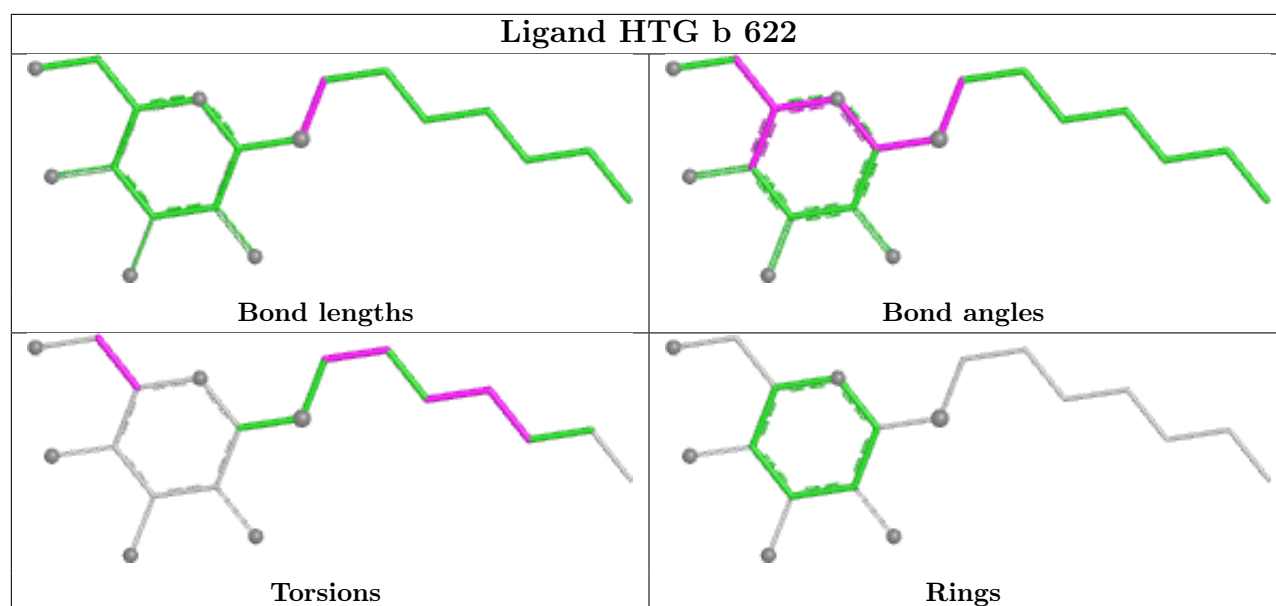


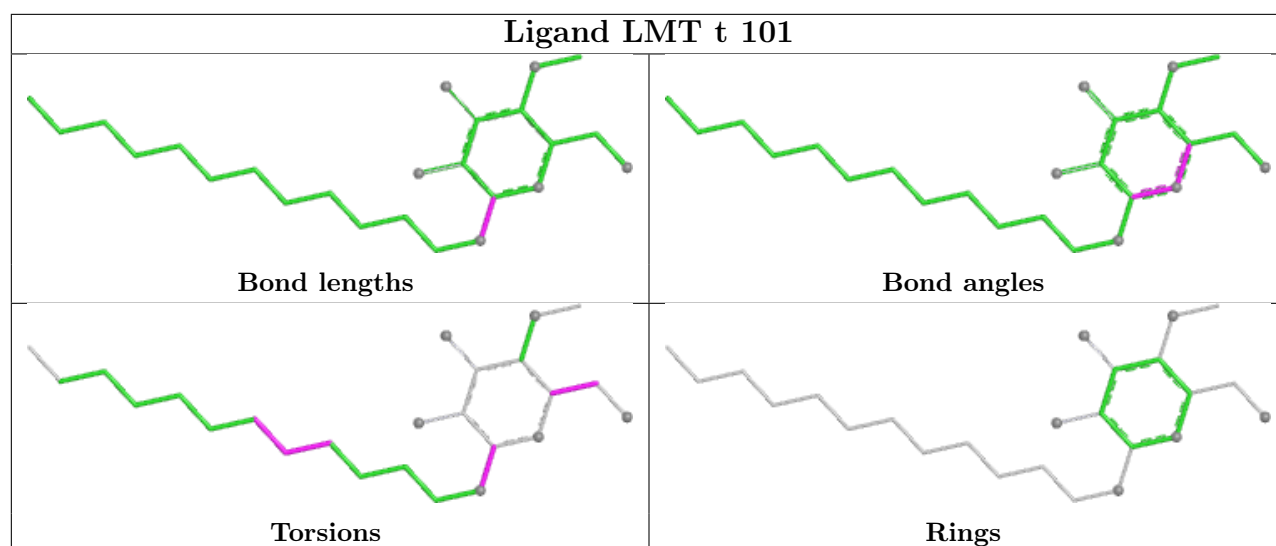
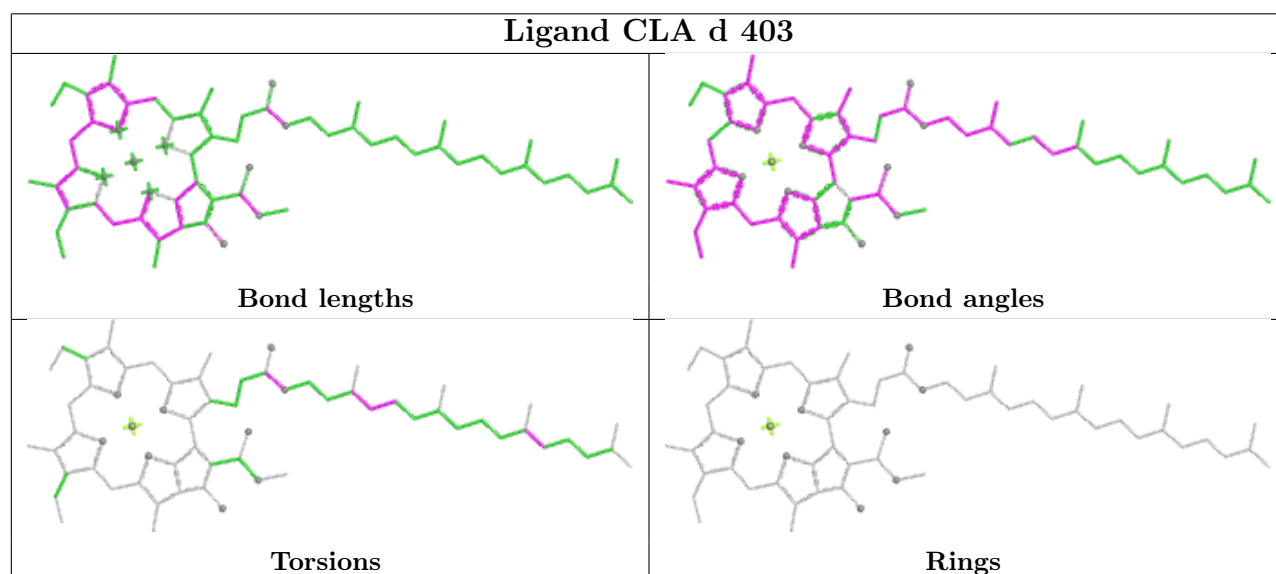
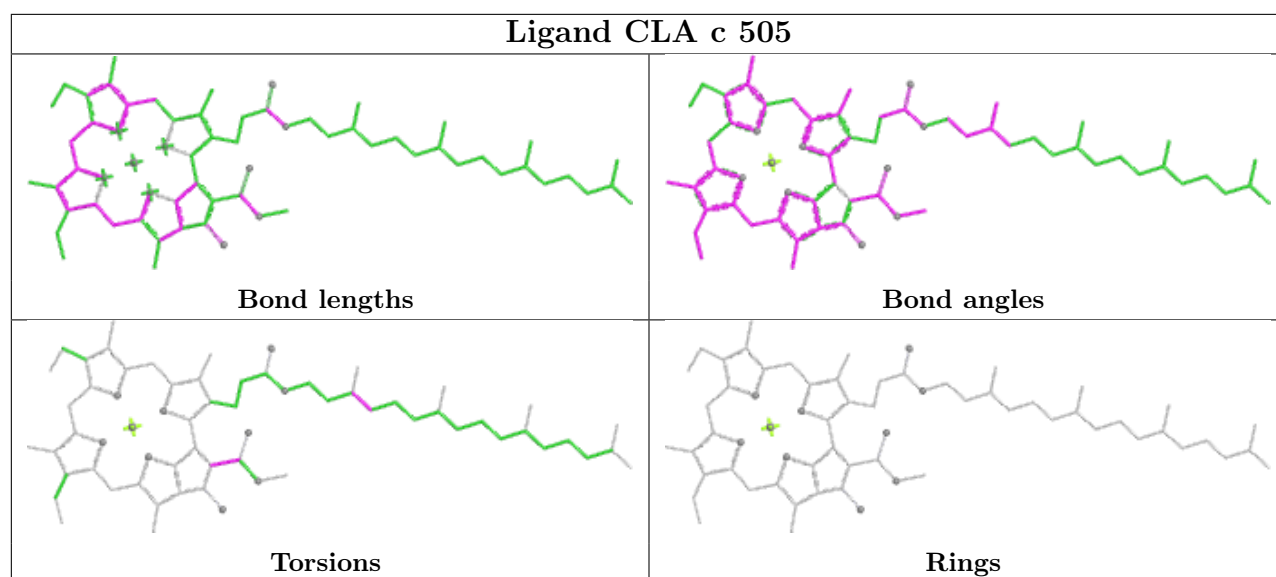


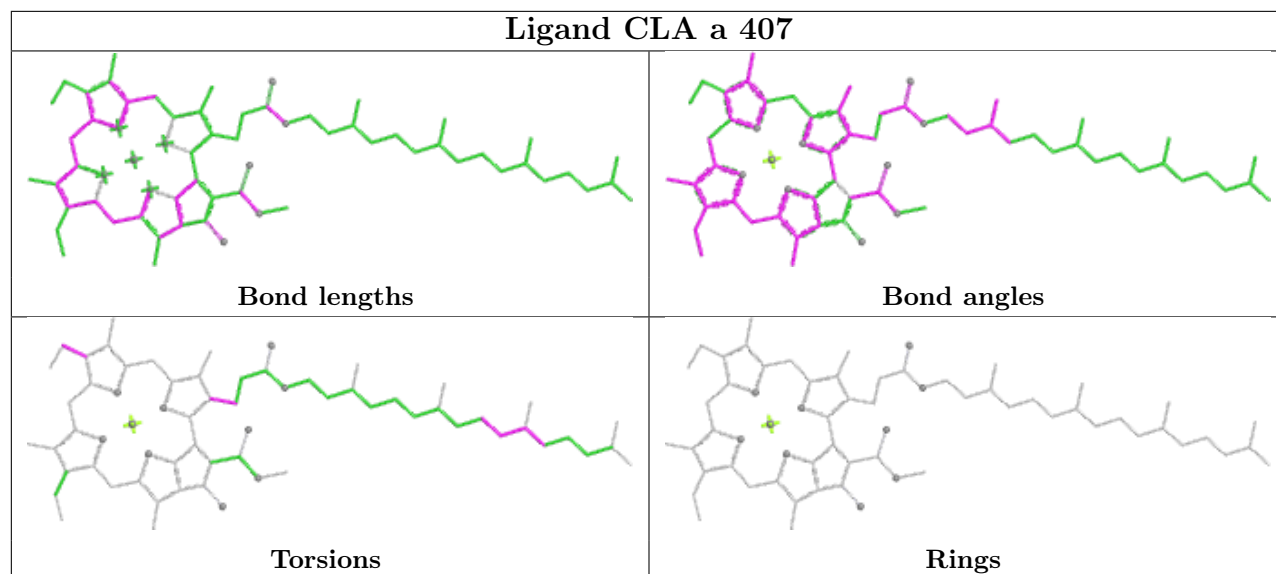
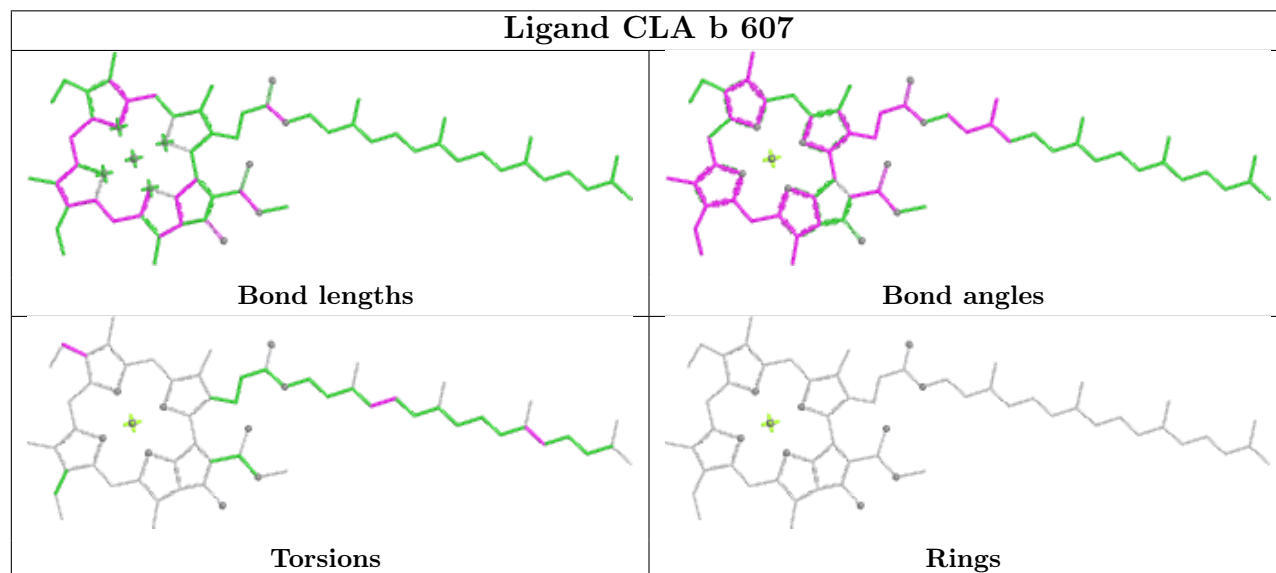


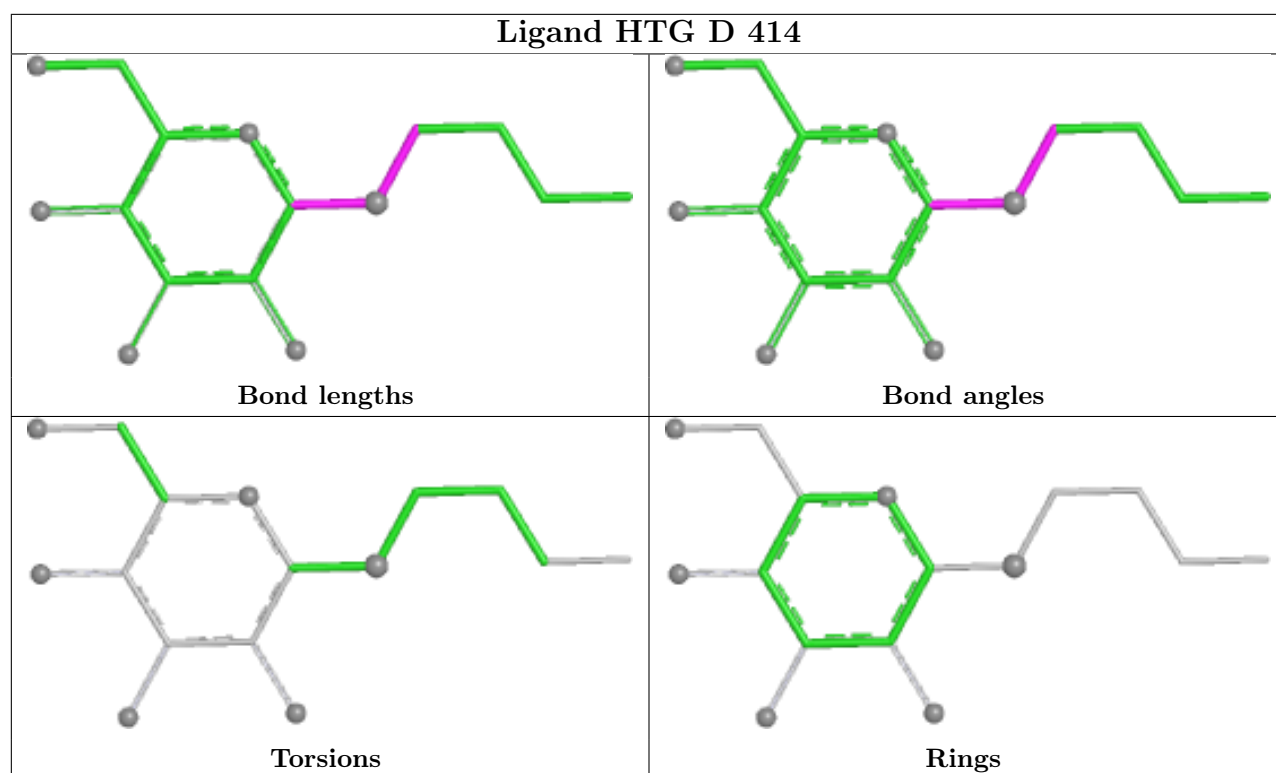


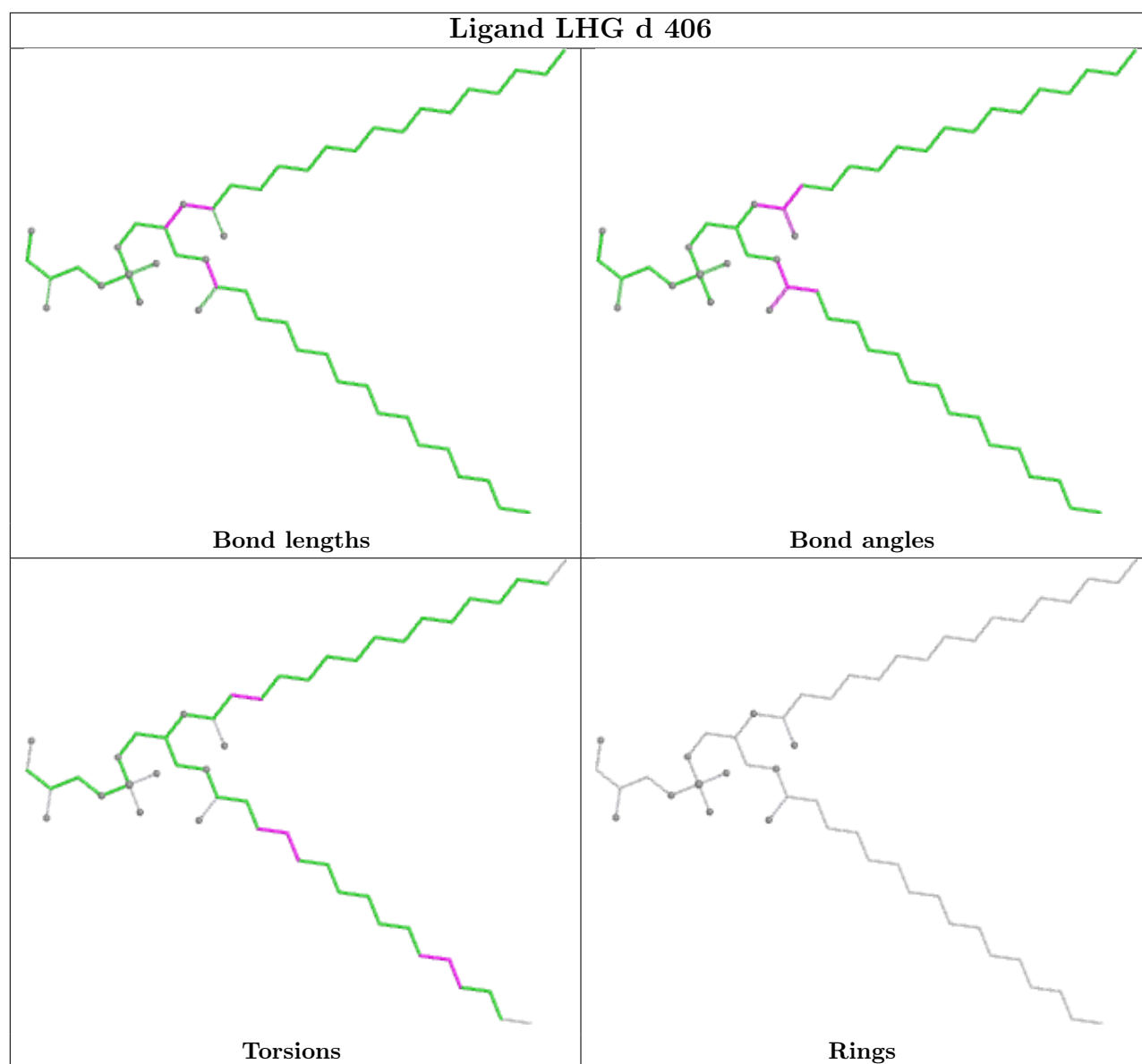
Ligand CLA B 608**Ligand LHG e 101**

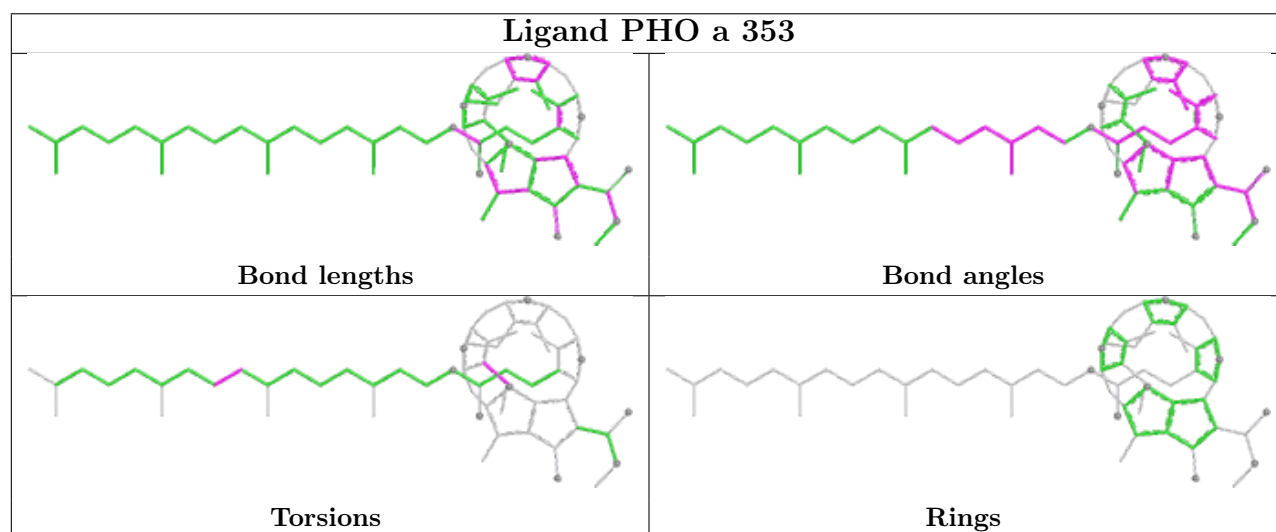
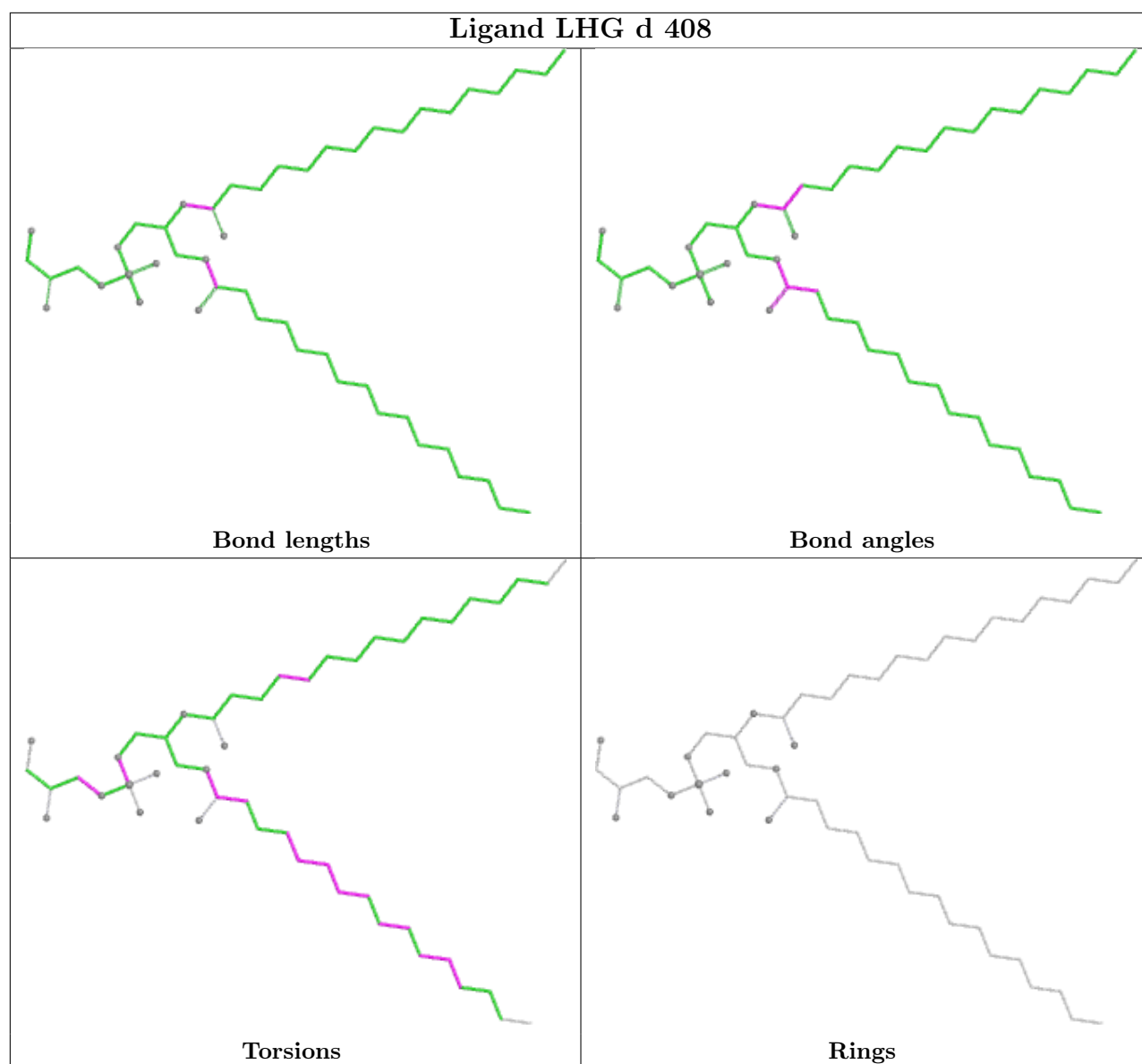


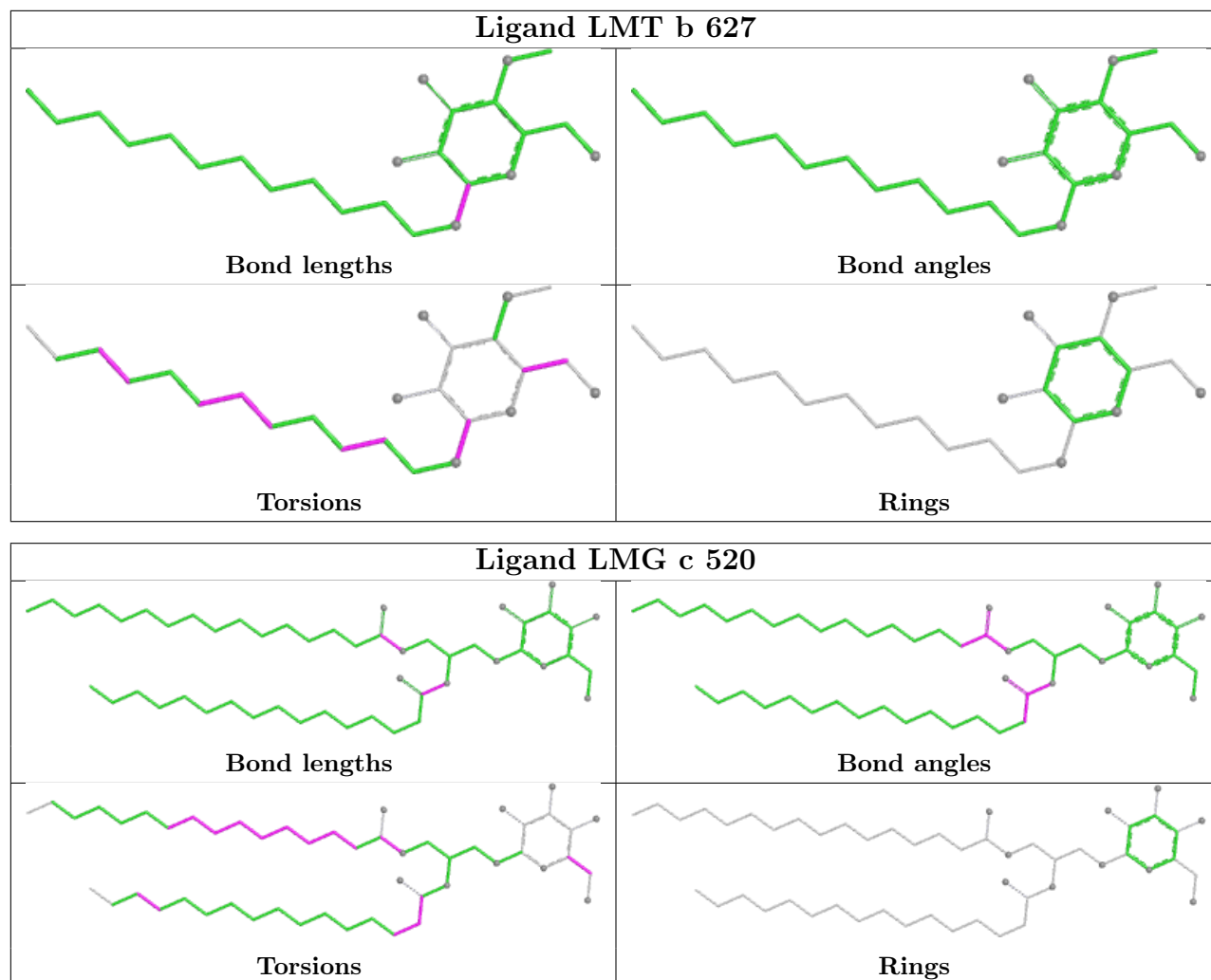


Ligand CLA a 407**Ligand CLA b 607**

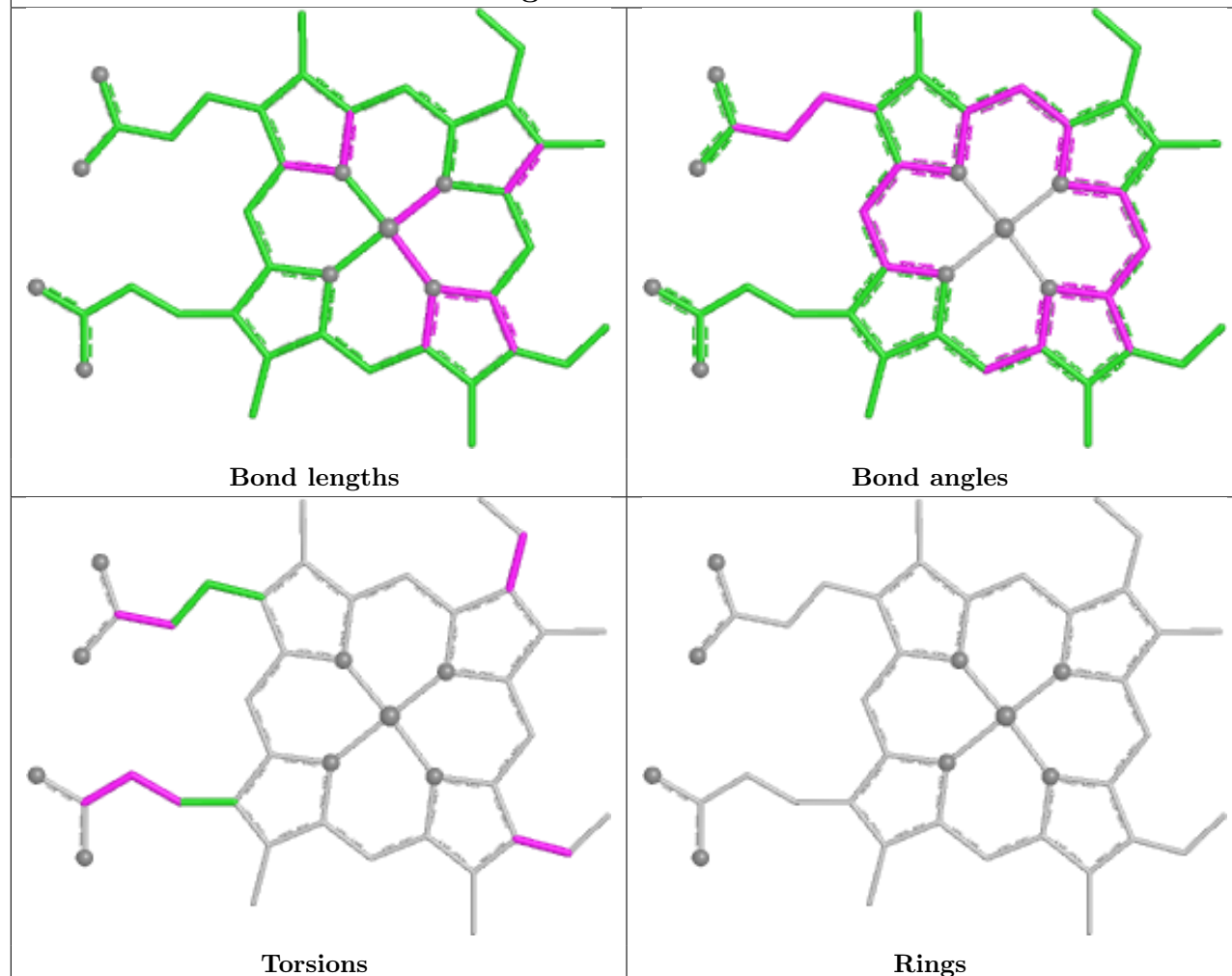




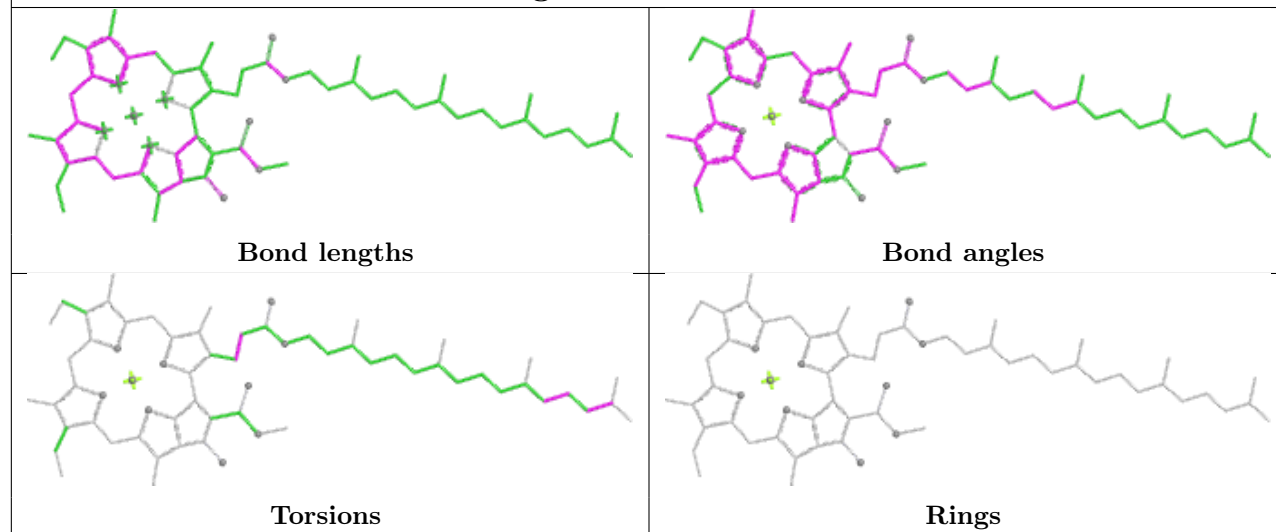


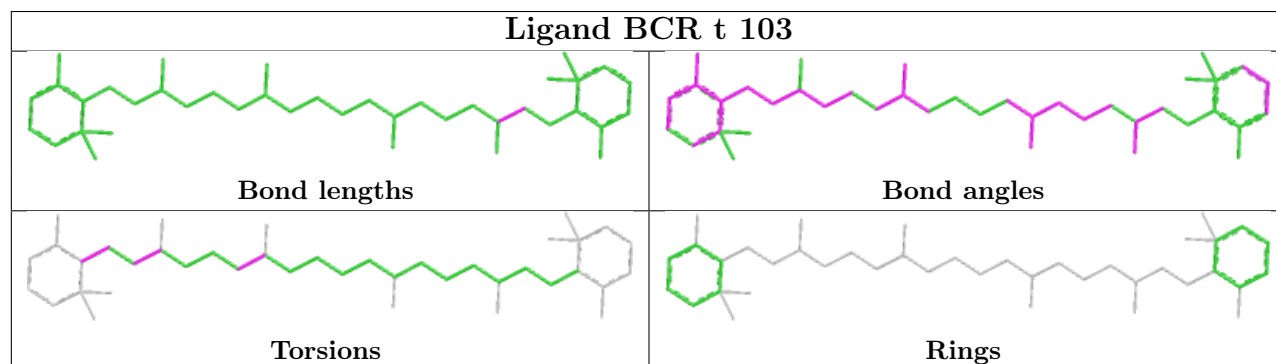
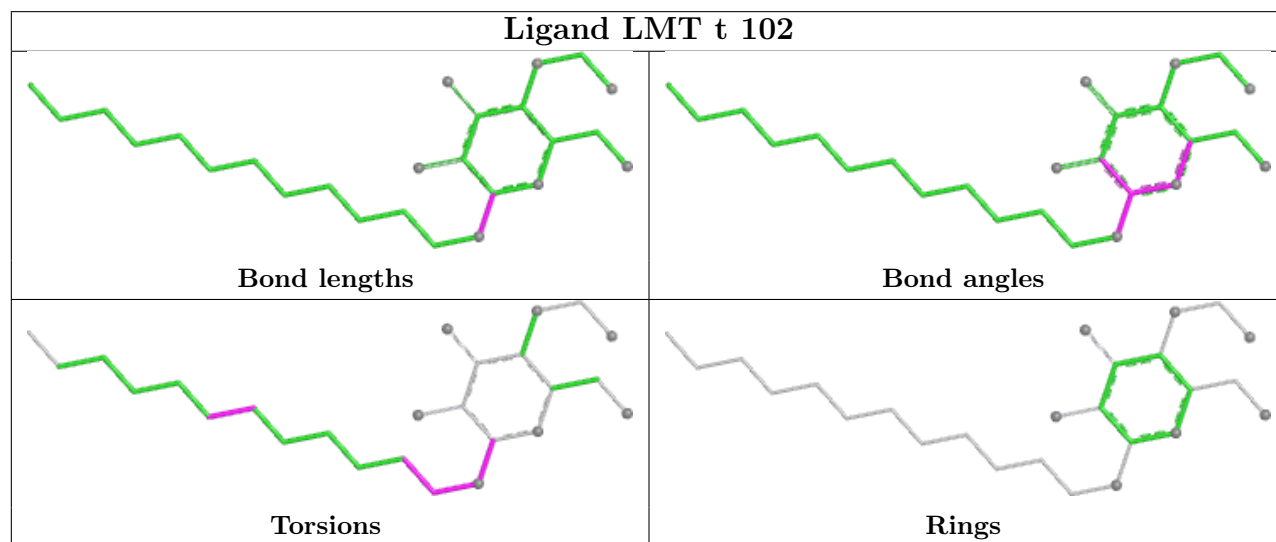
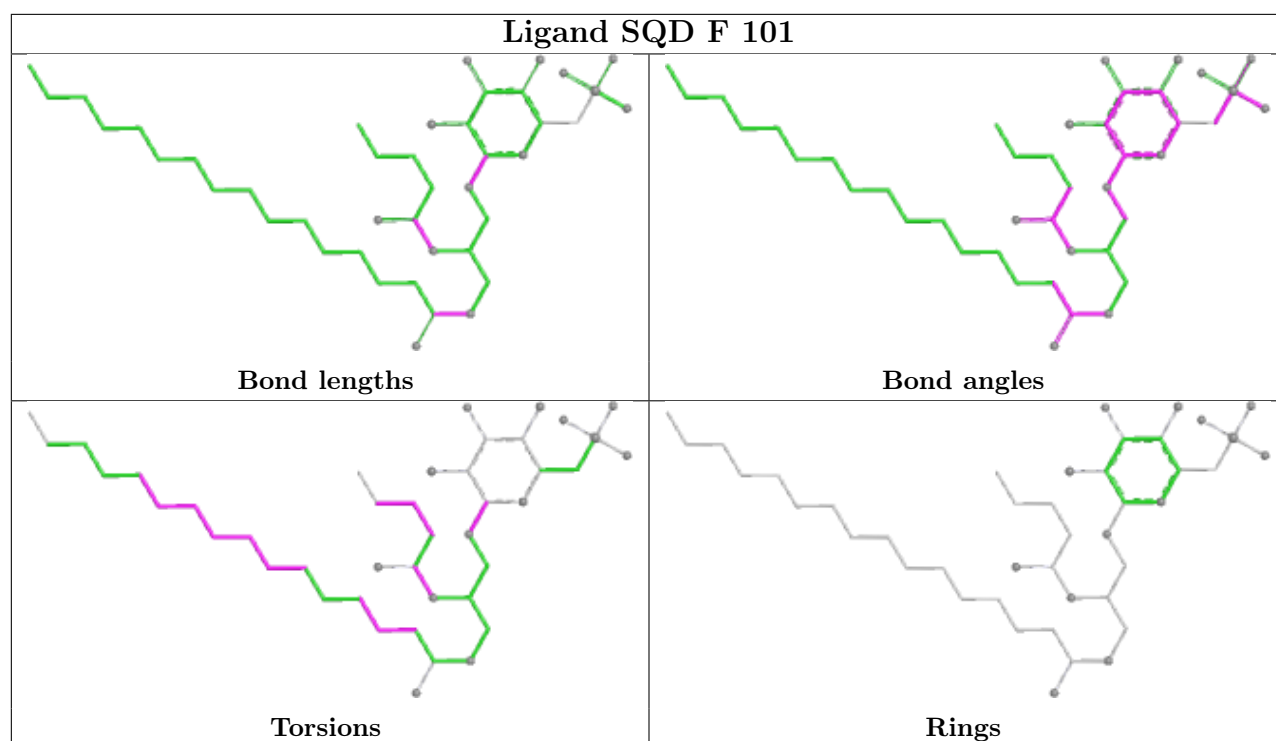


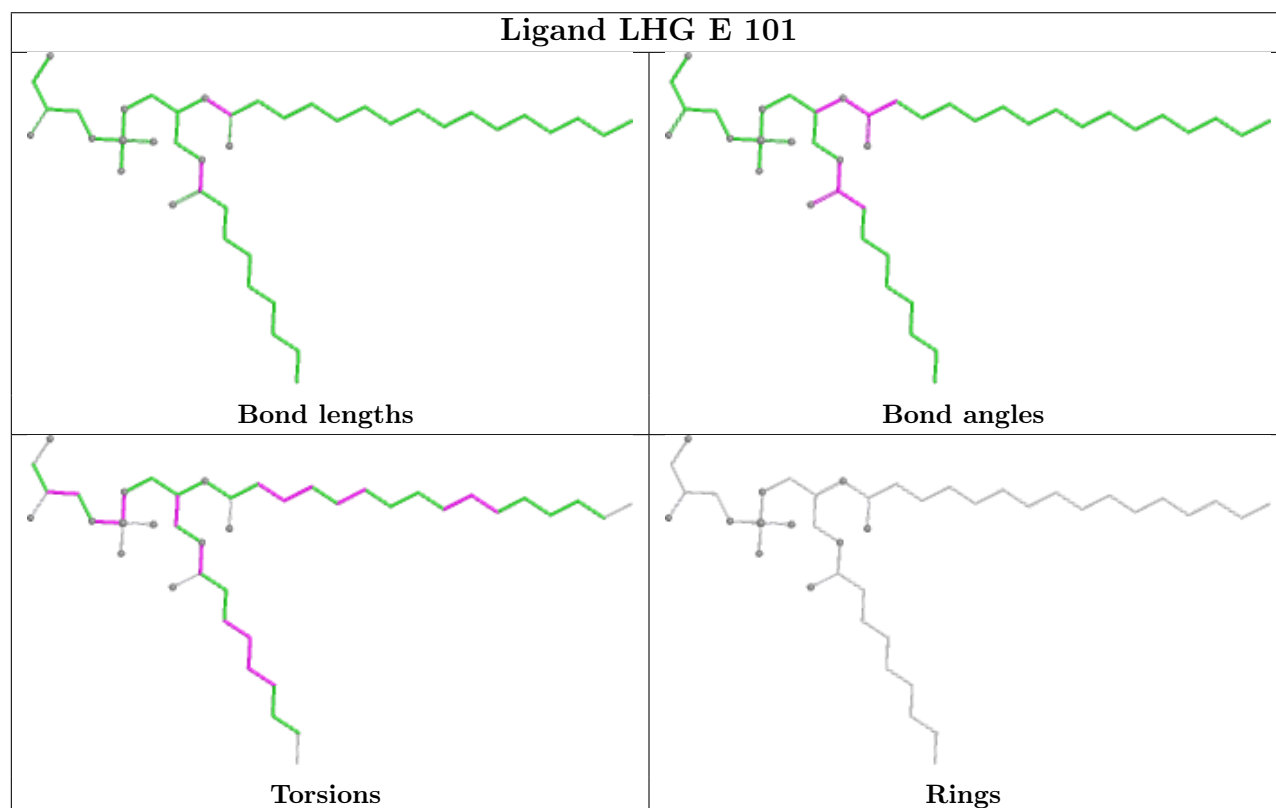
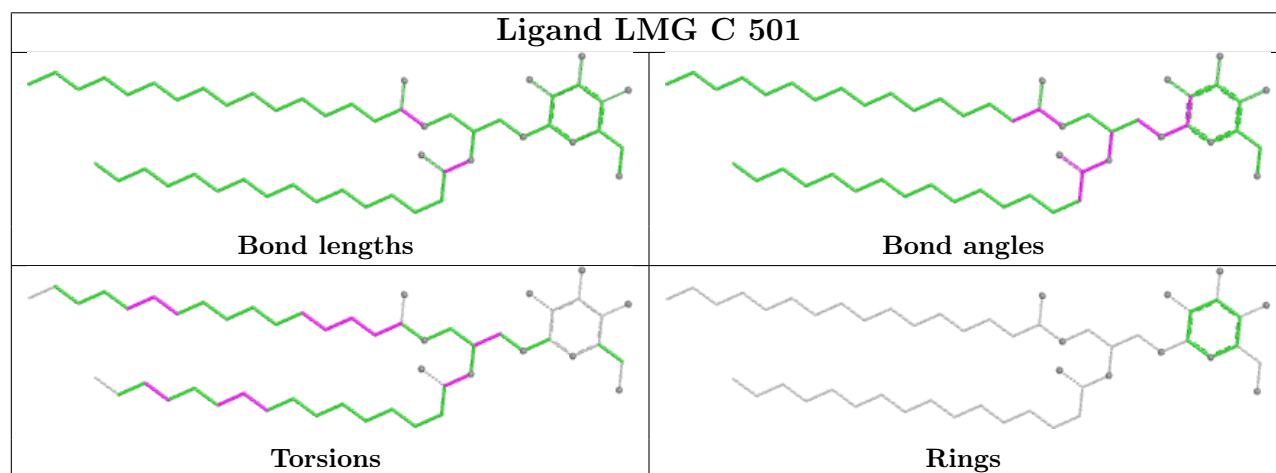
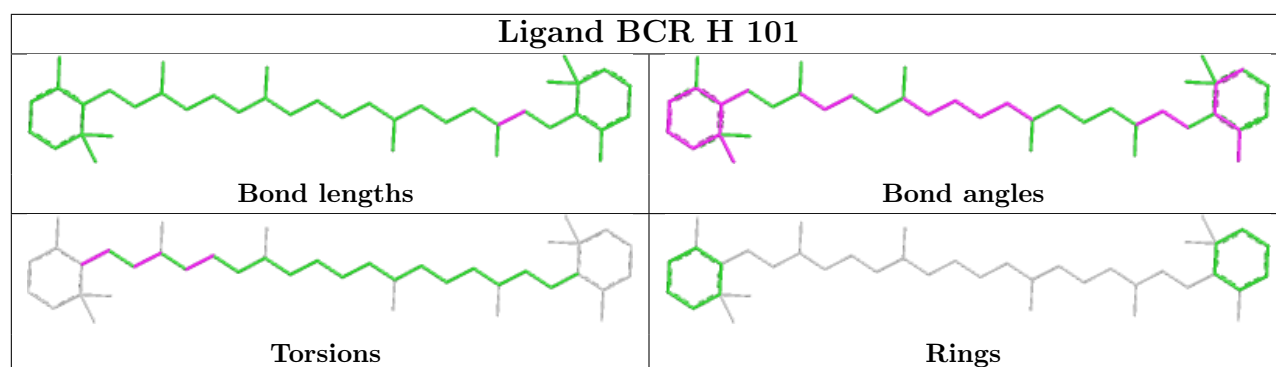
Ligand HEM e 87

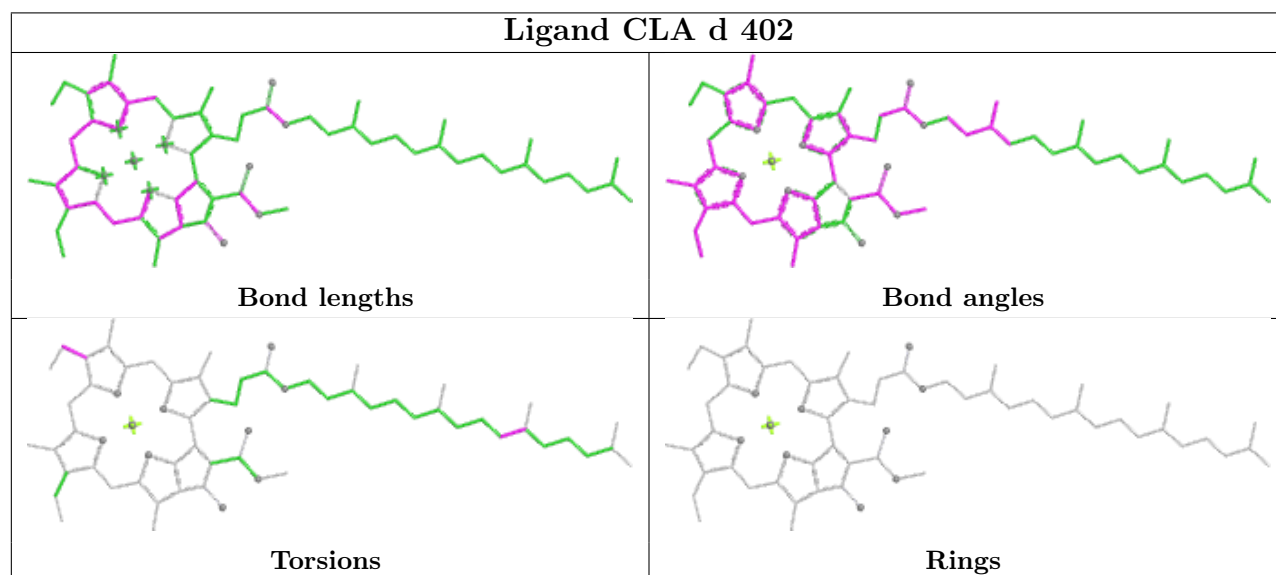
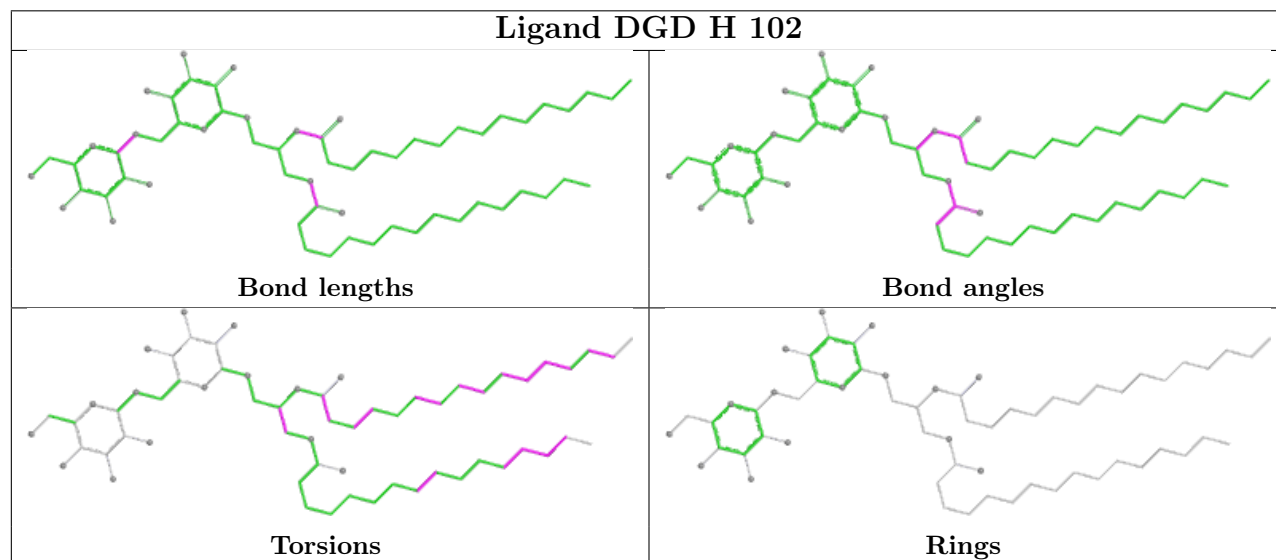
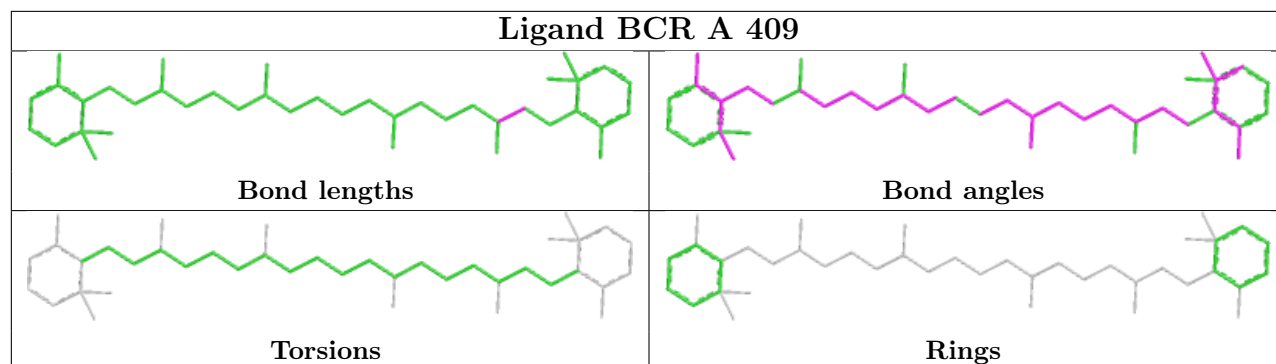


Ligand CLA B 610

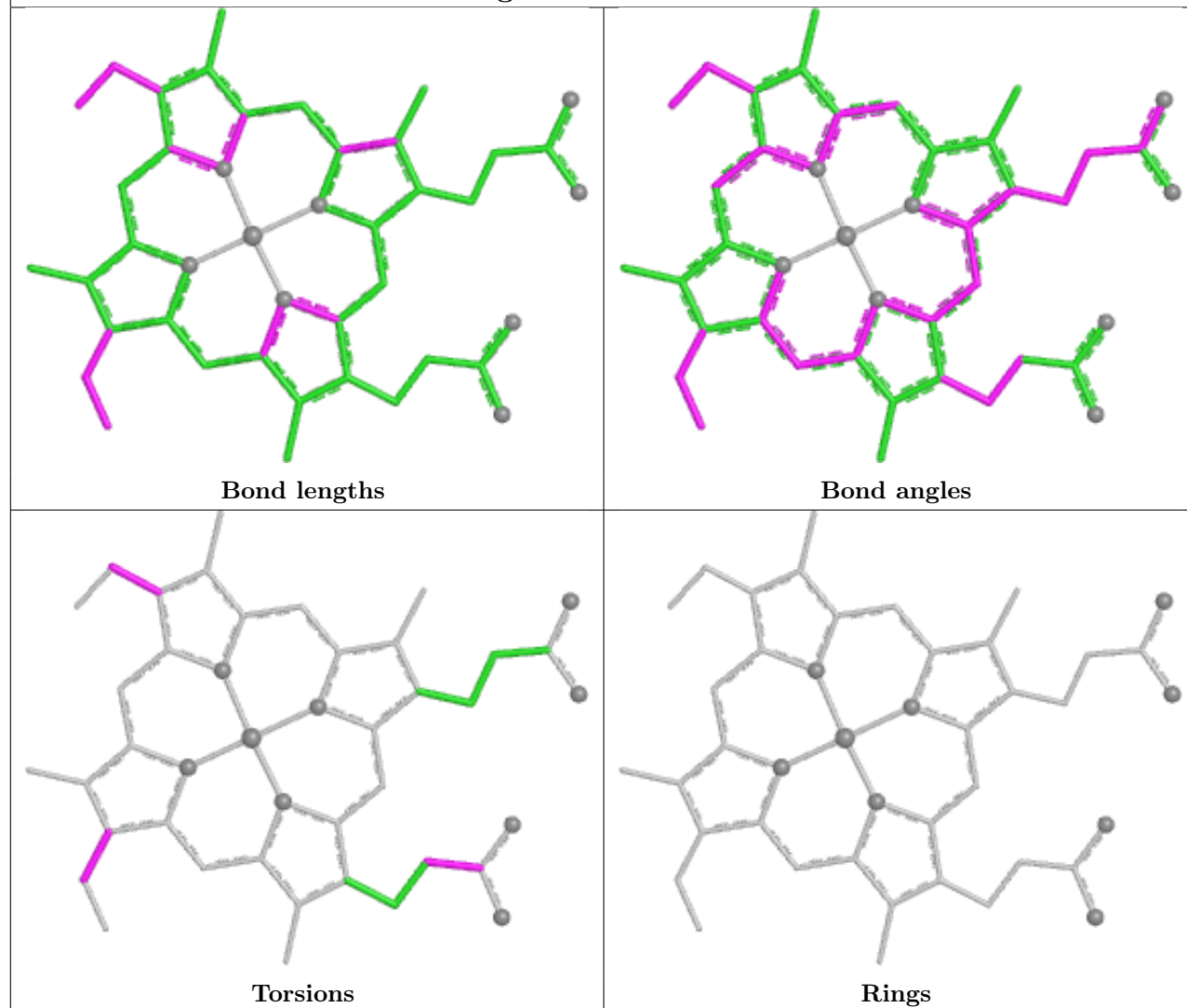




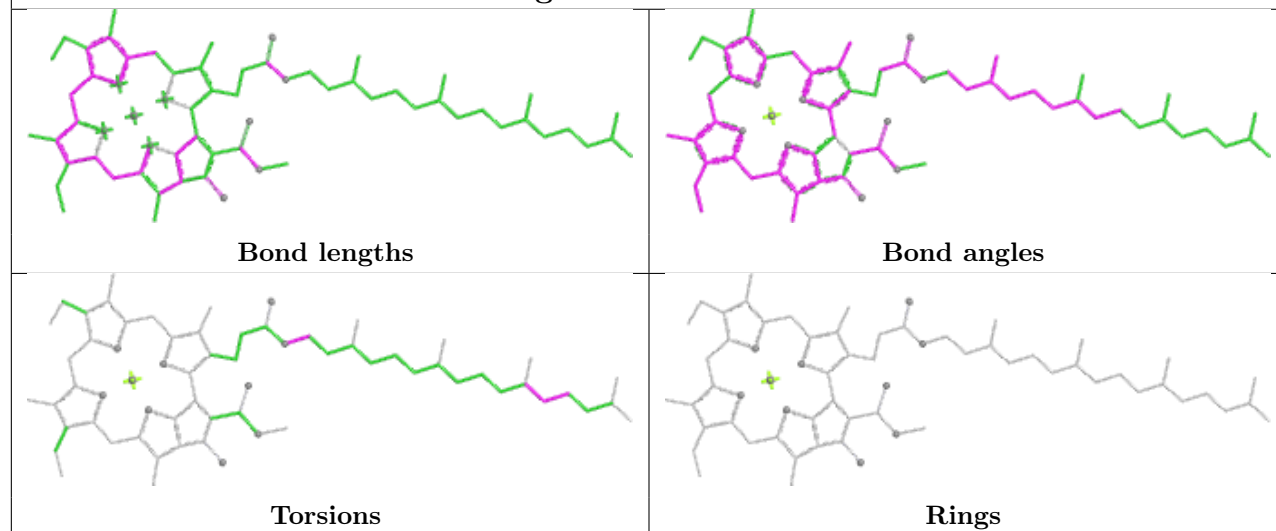


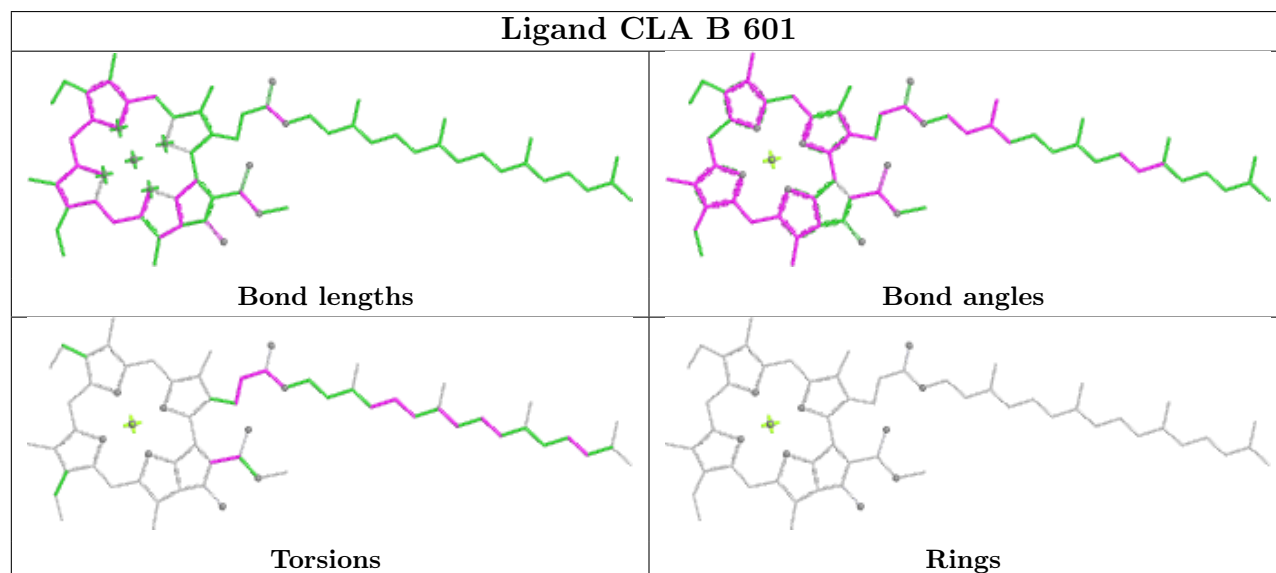
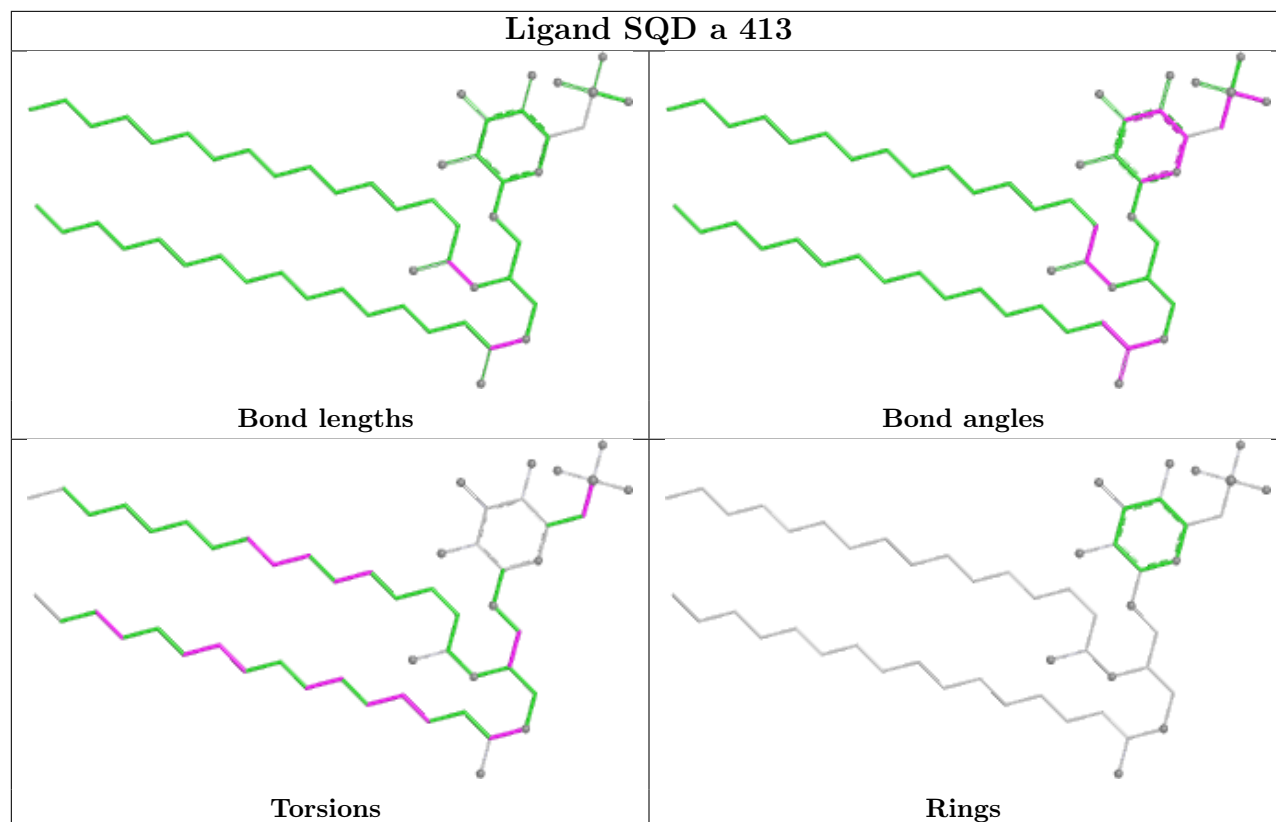


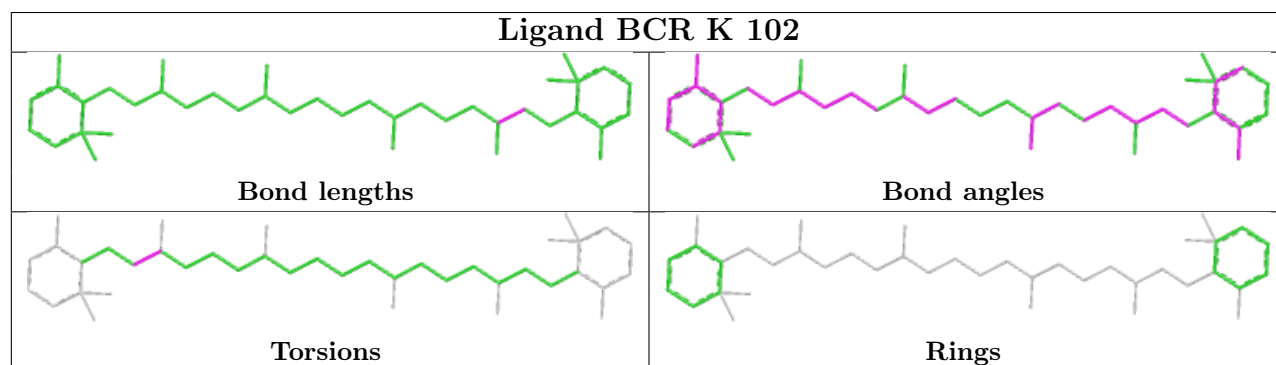
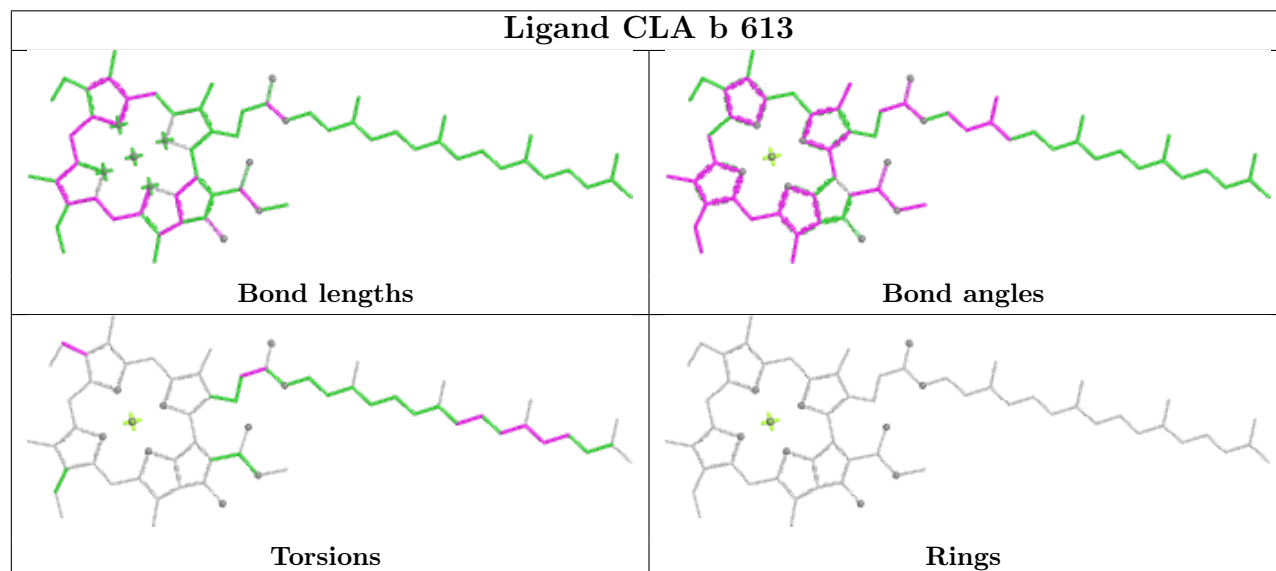
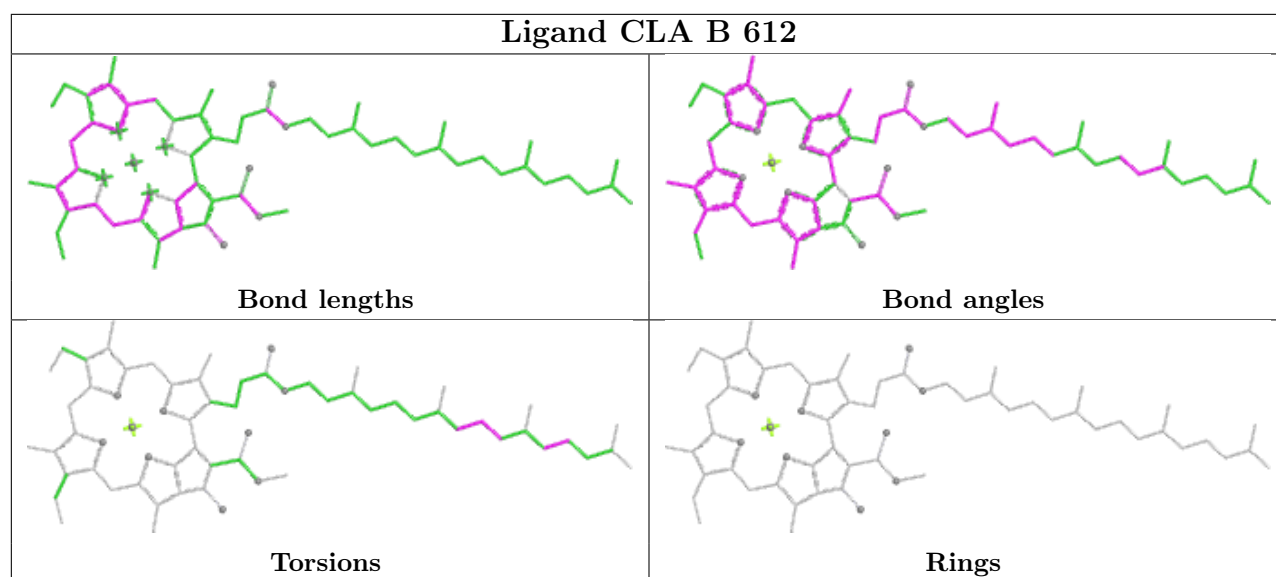
Ligand HEC v 202

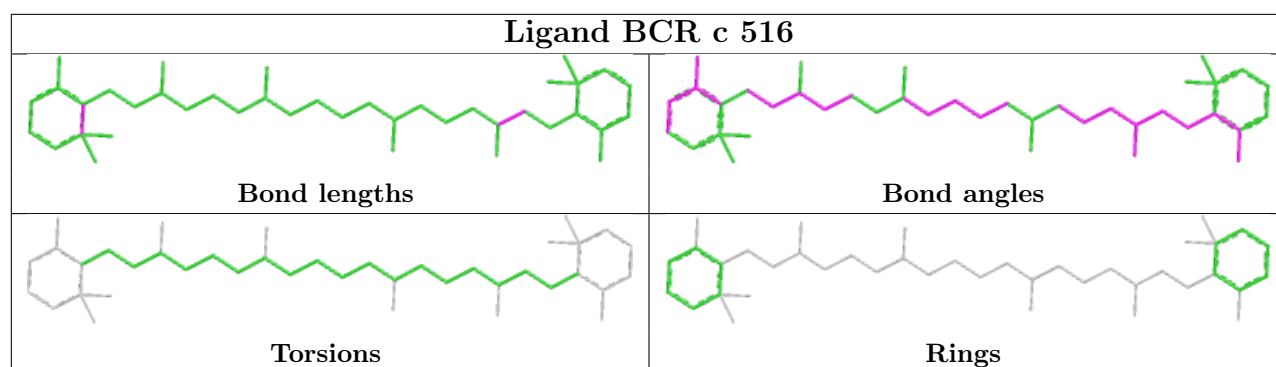
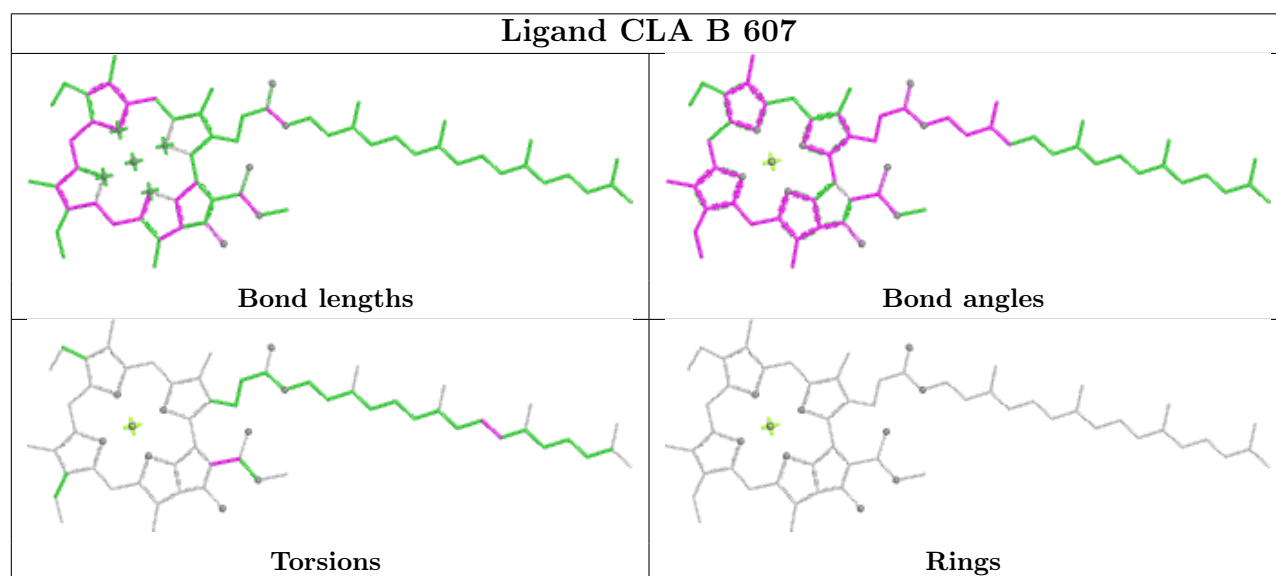
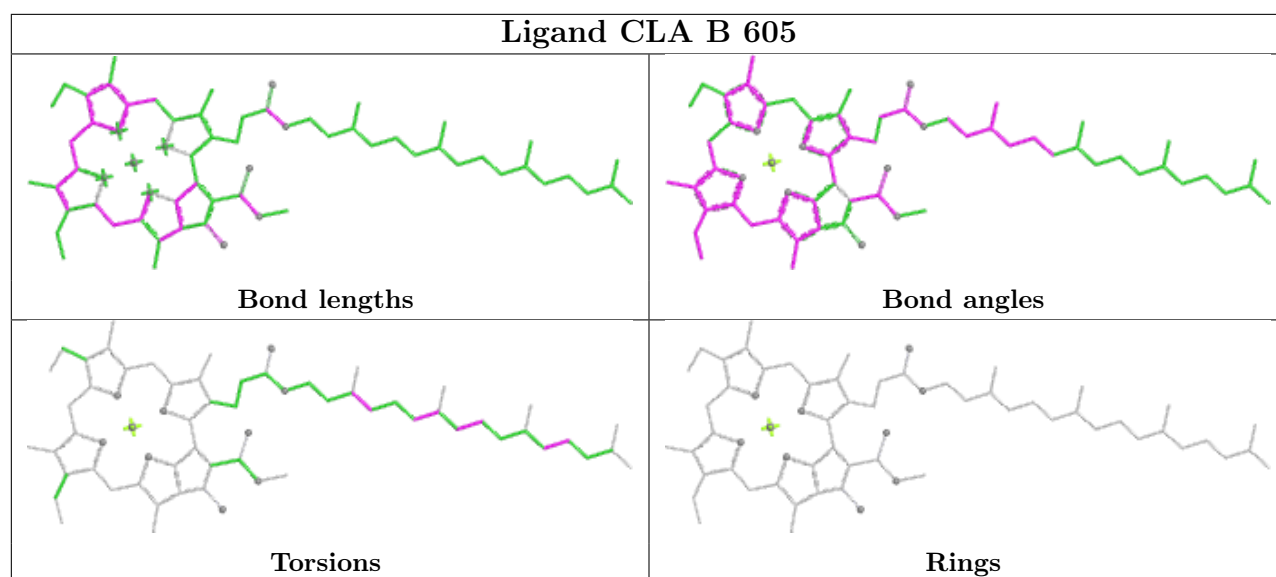


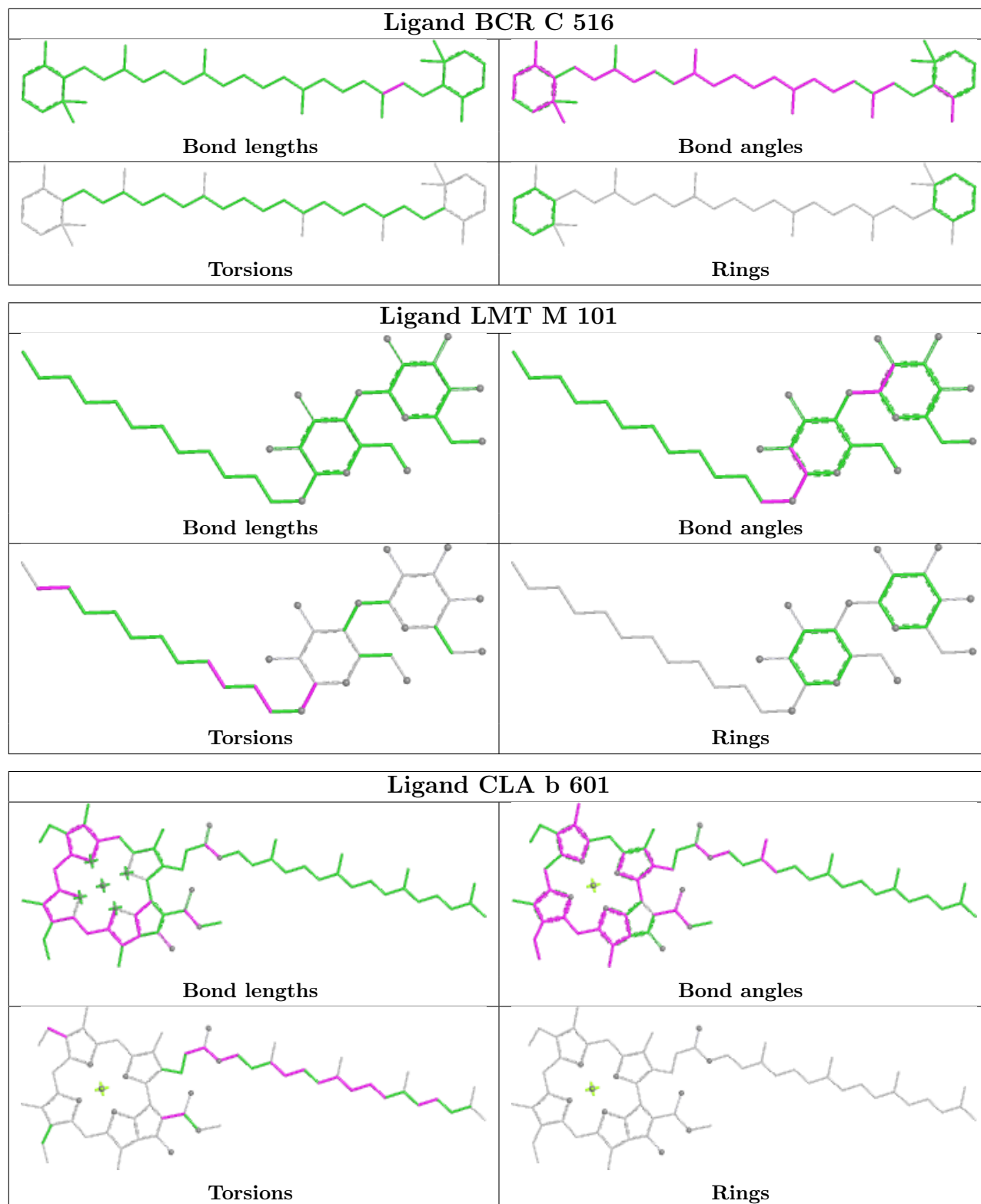
Ligand CLA b 608

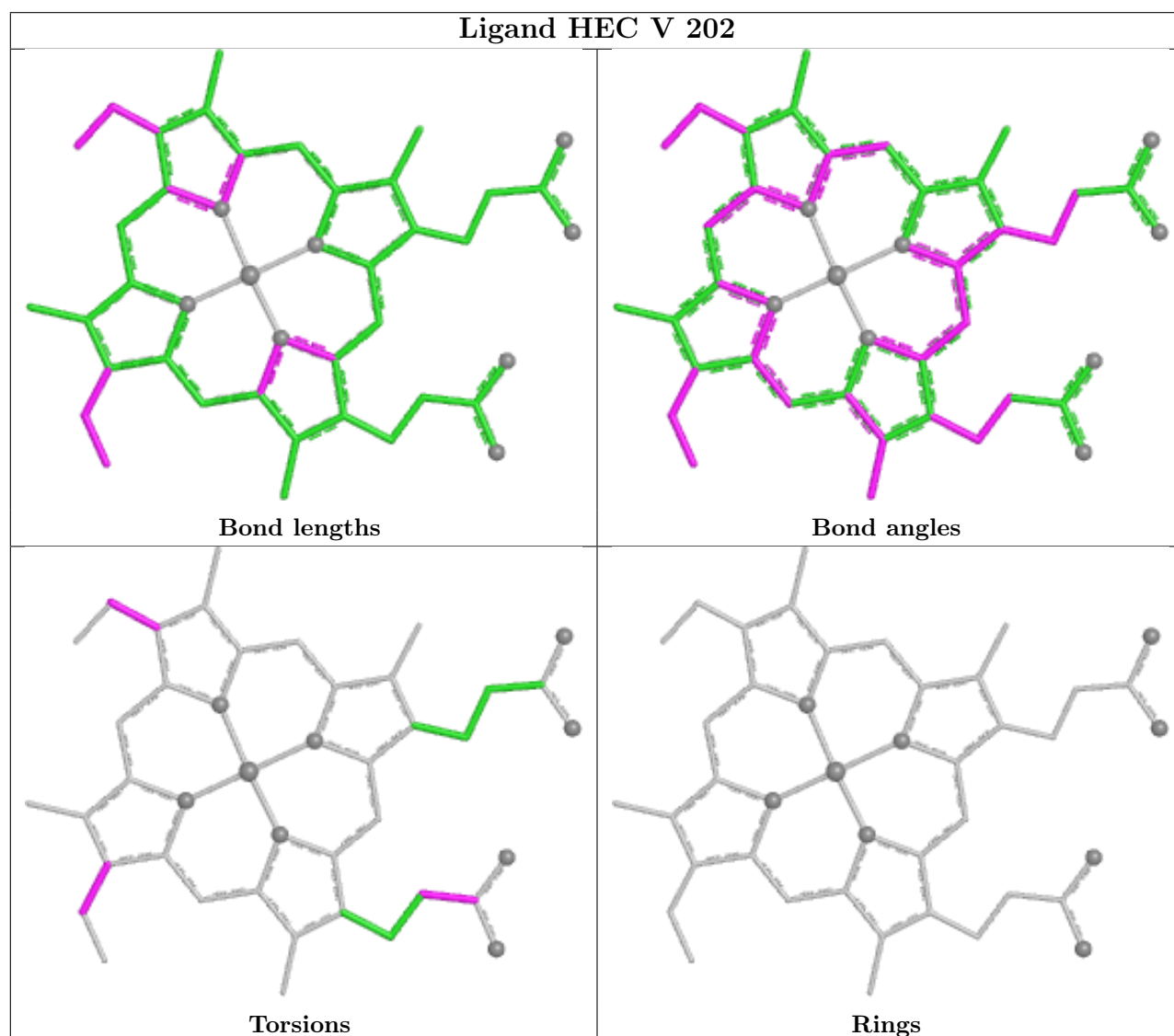
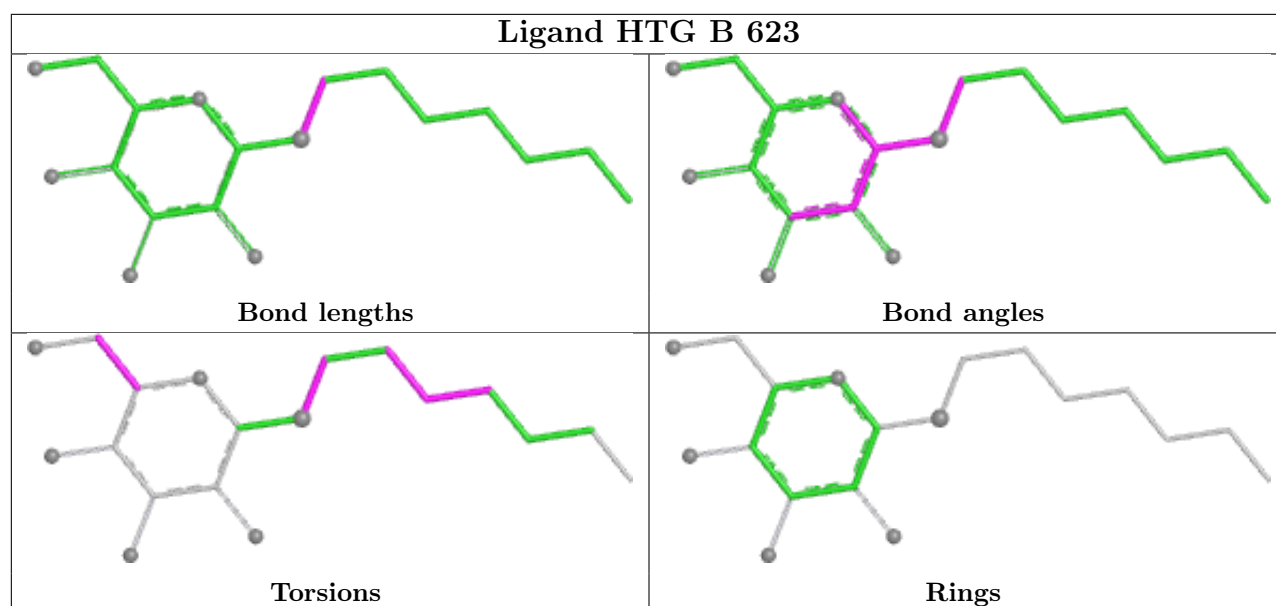


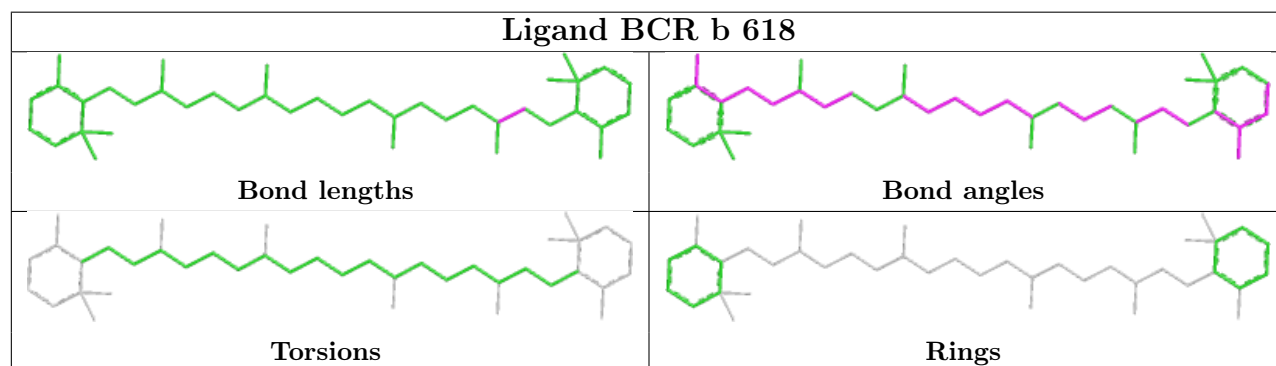
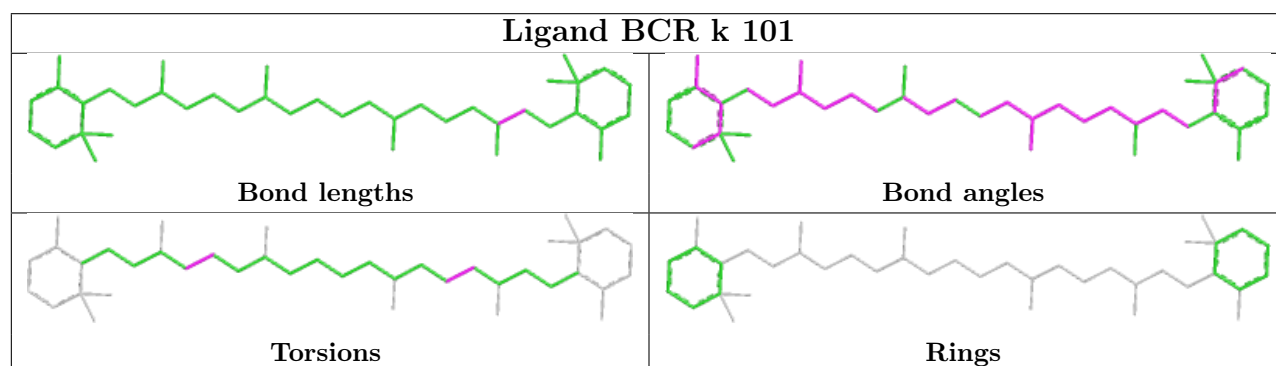
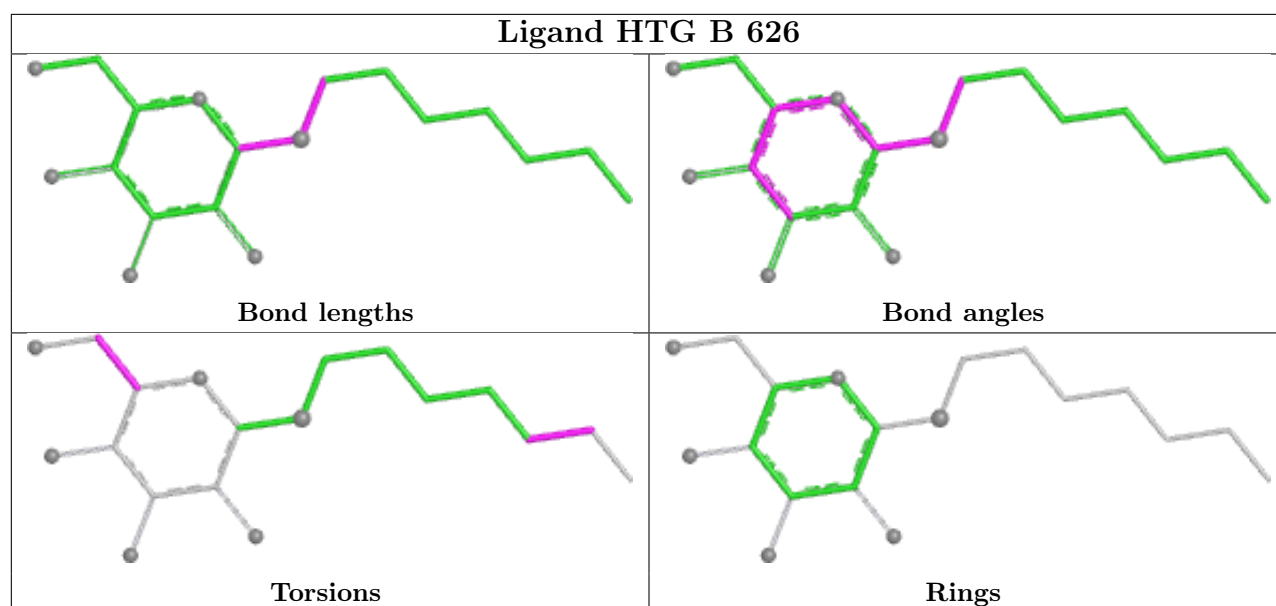




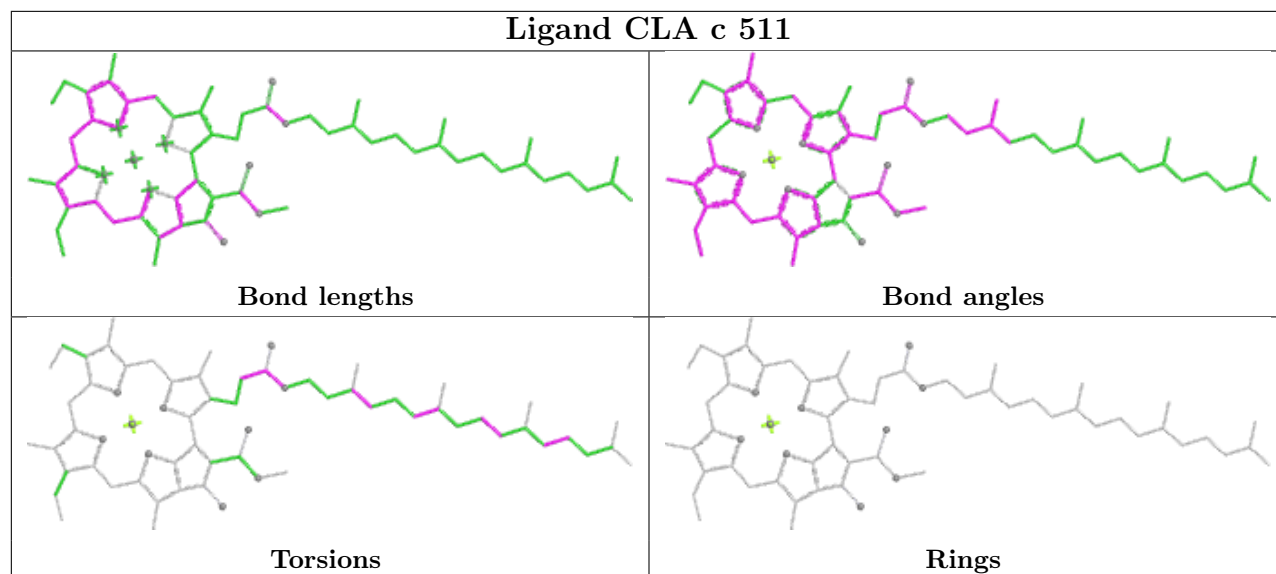




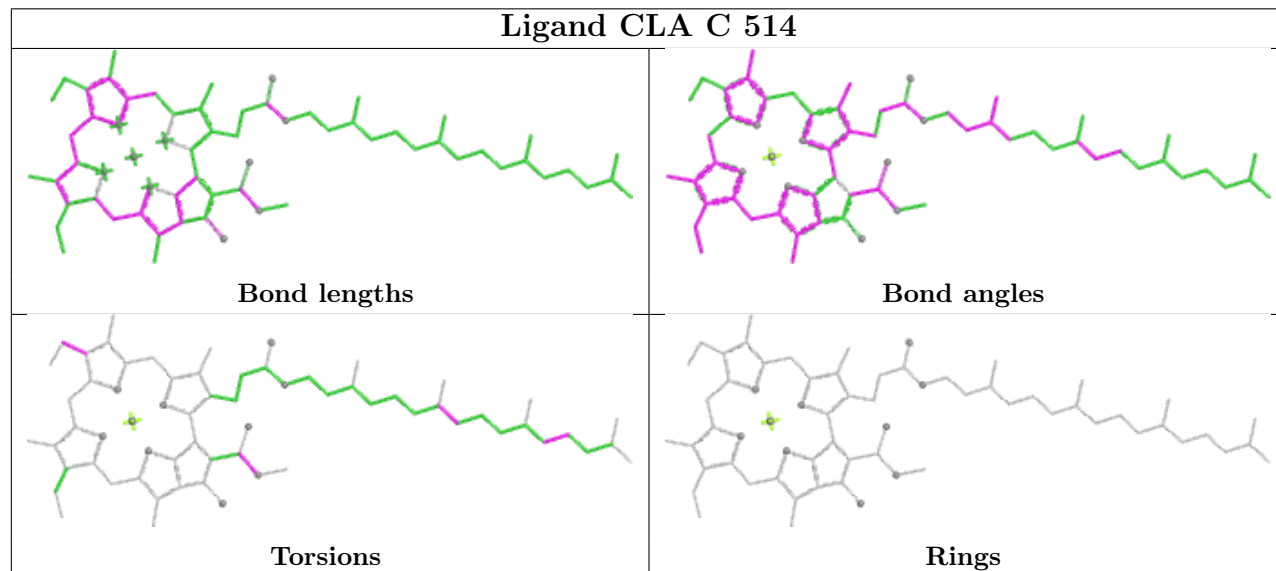




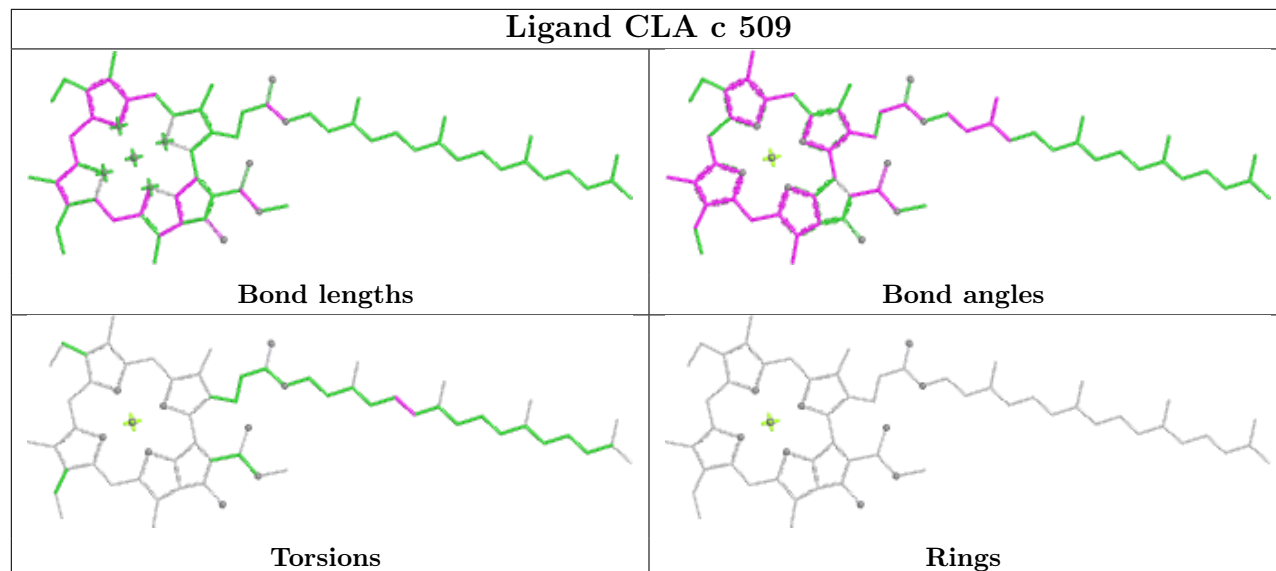
Ligand CLA c 511

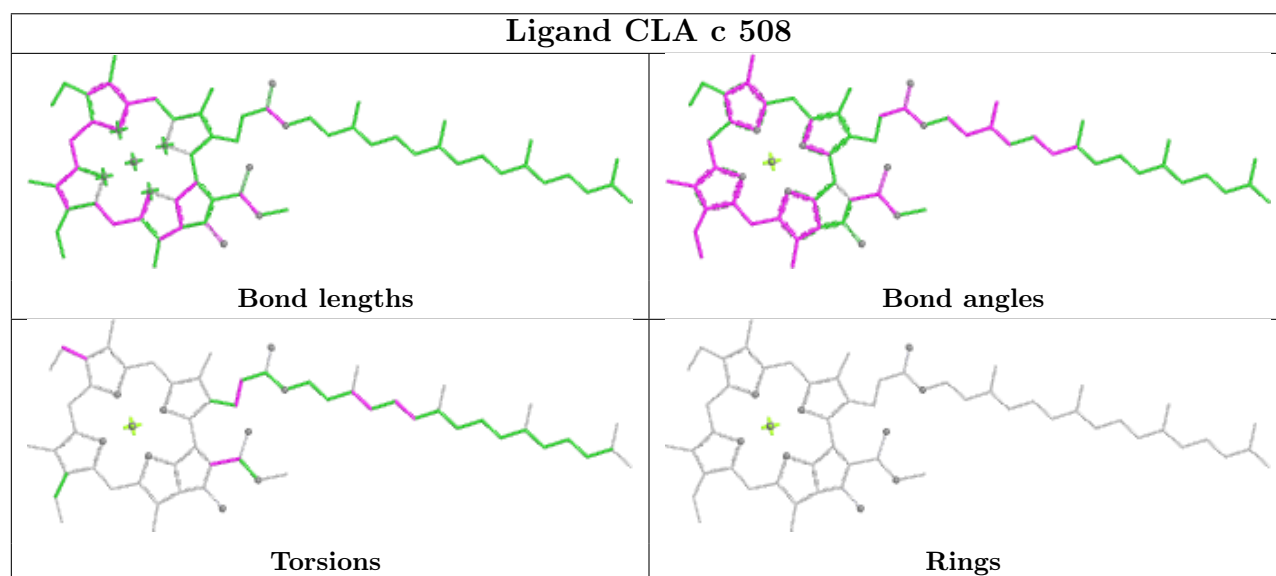
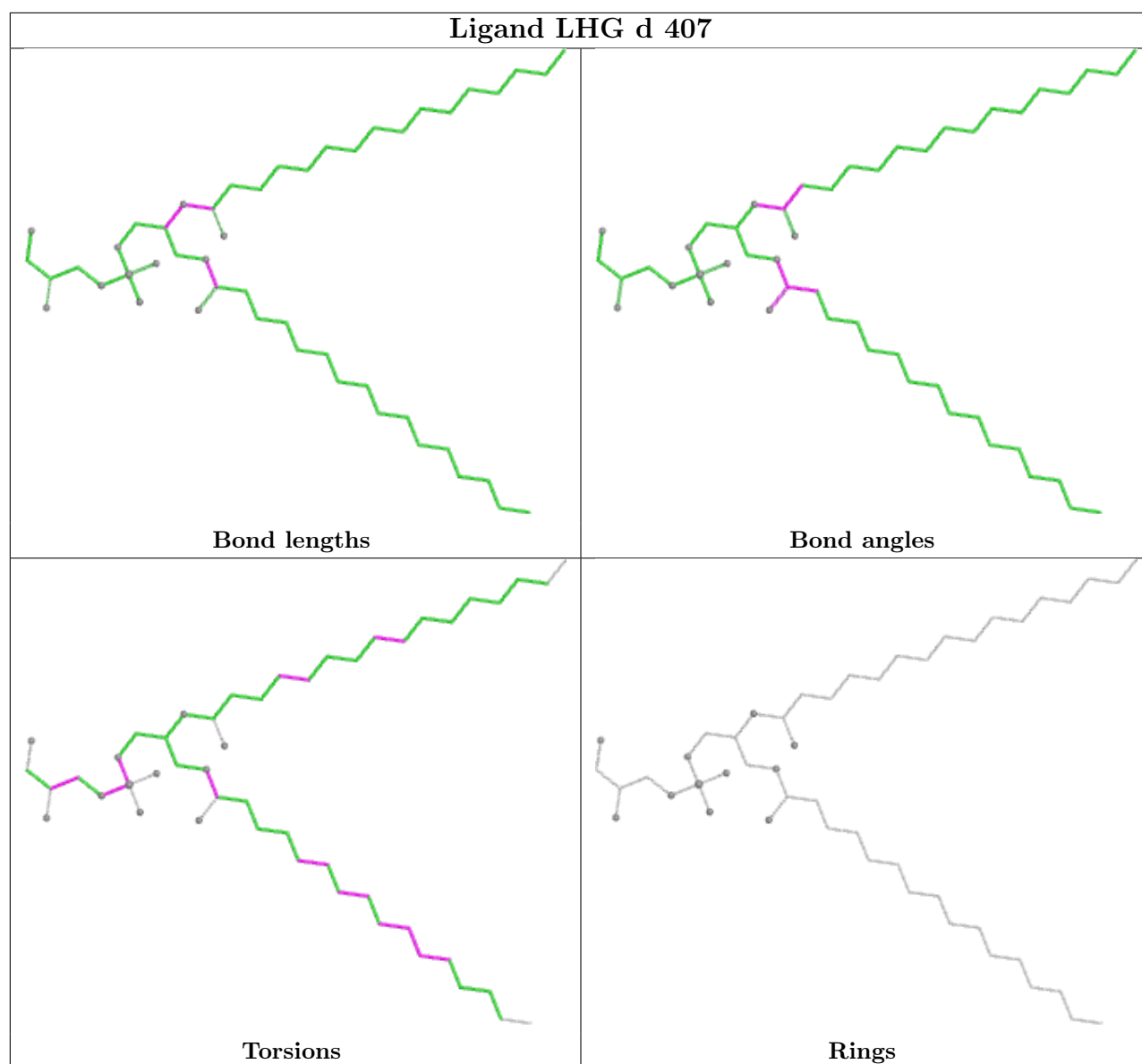


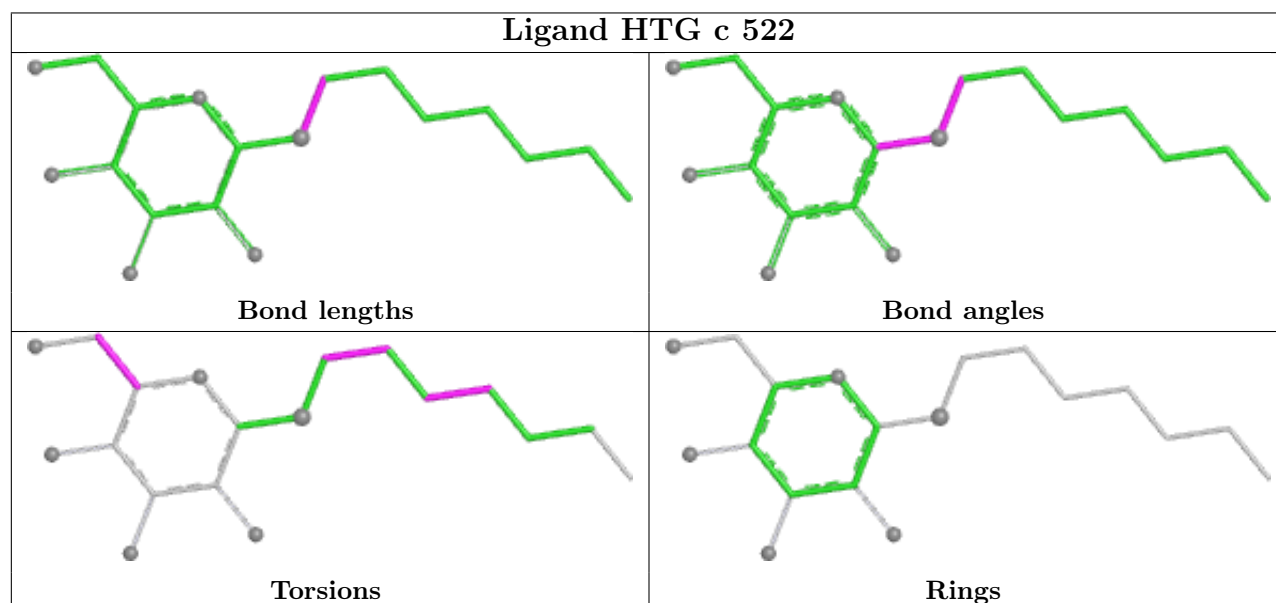
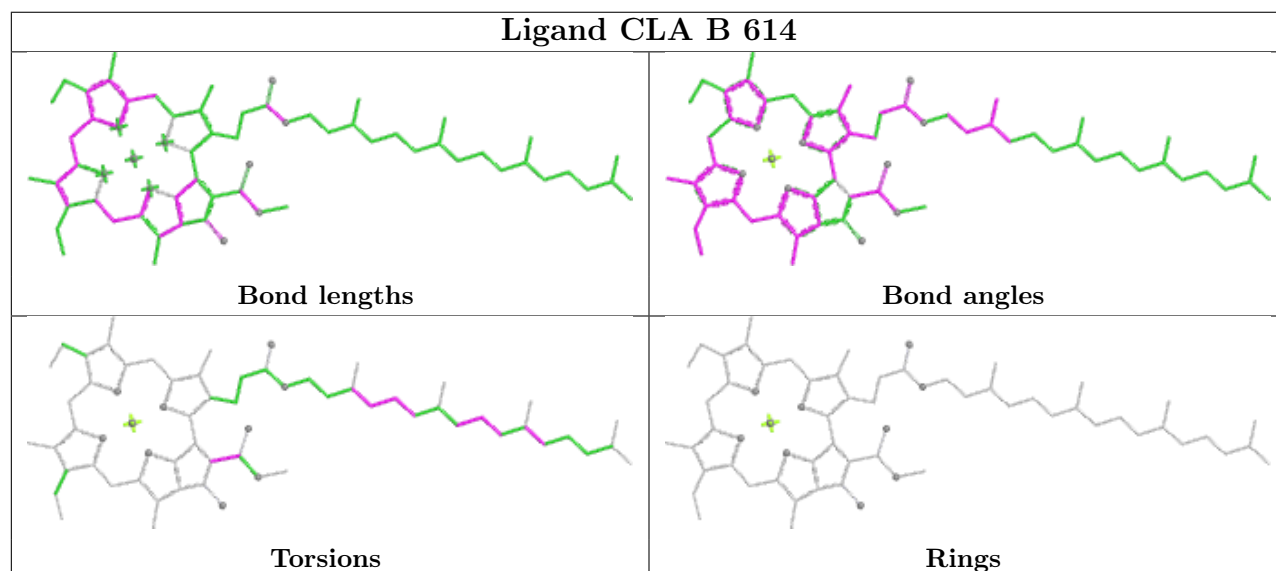
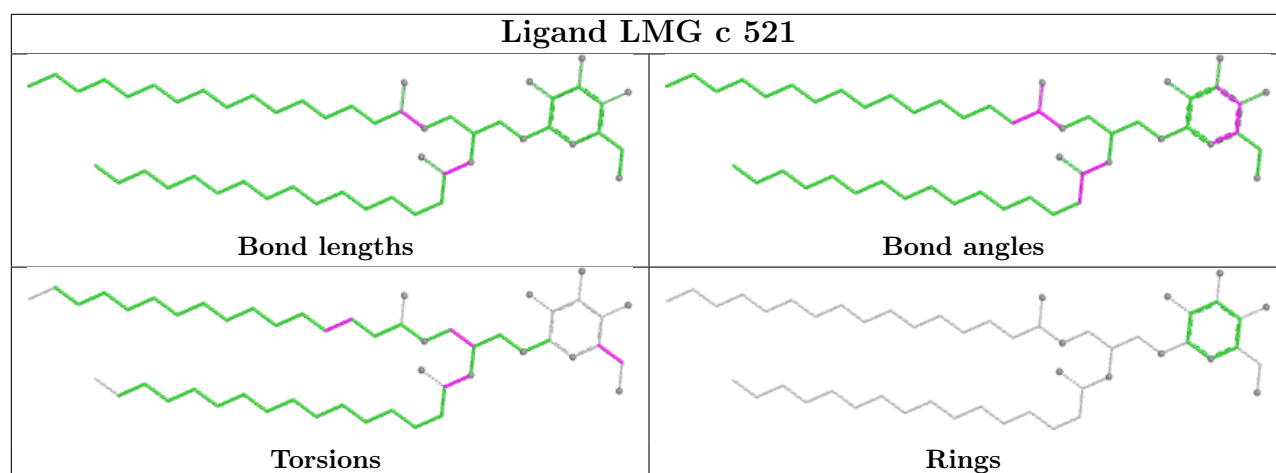
Ligand CLA C 514

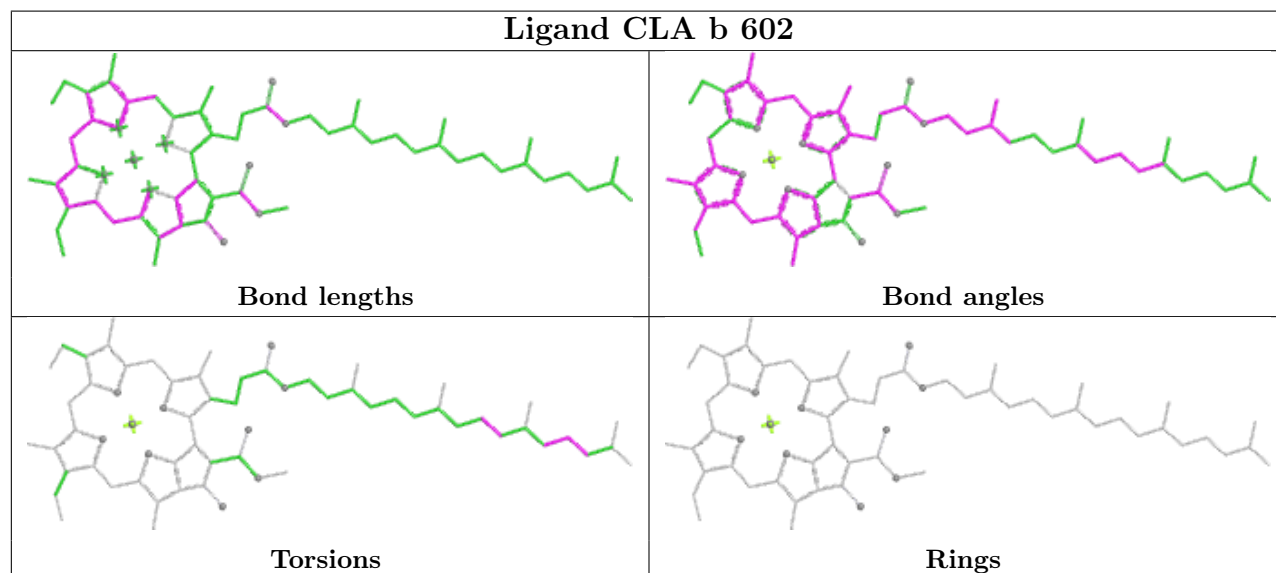
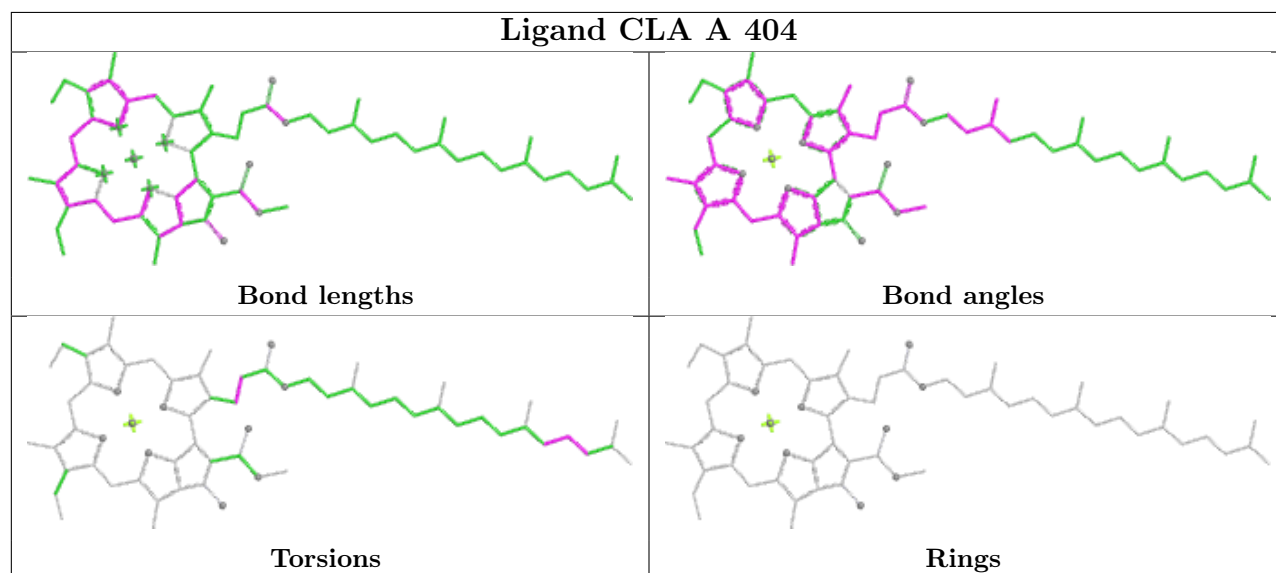
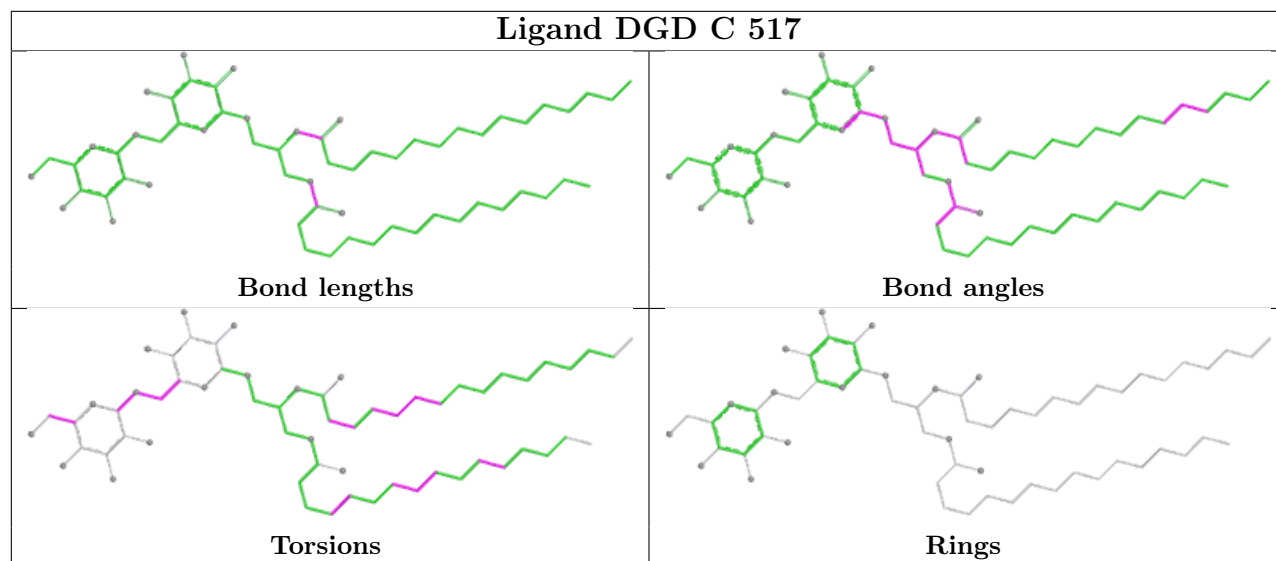


Ligand CLA c 509

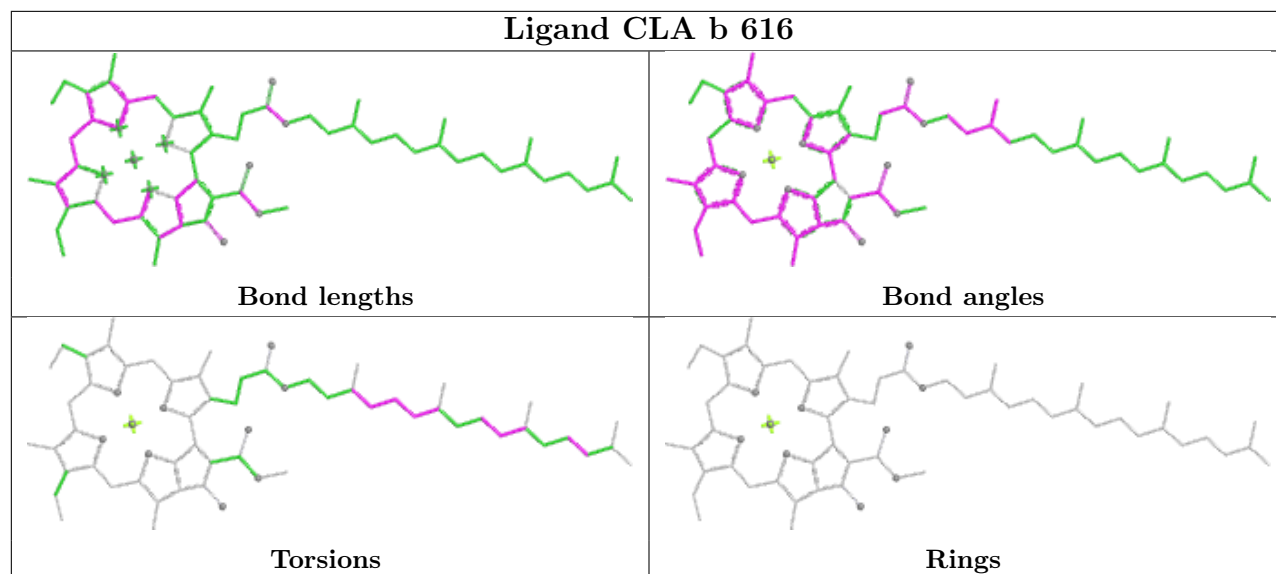




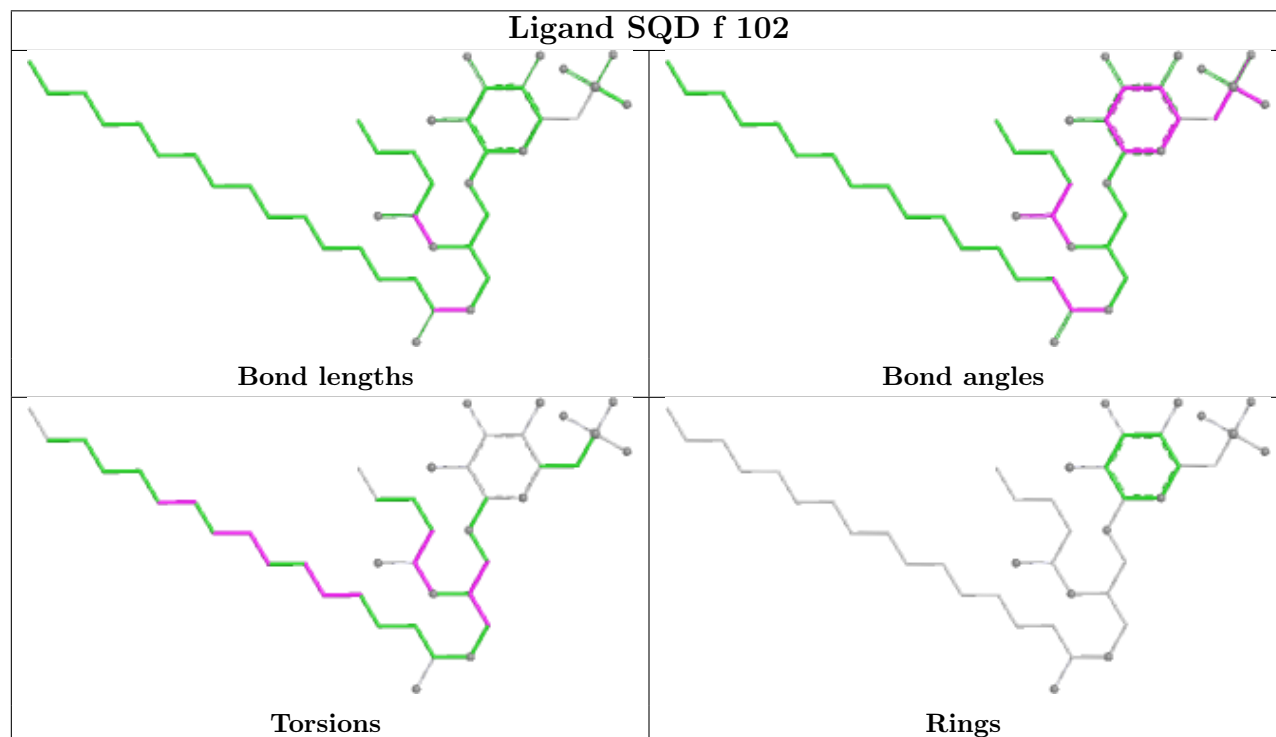


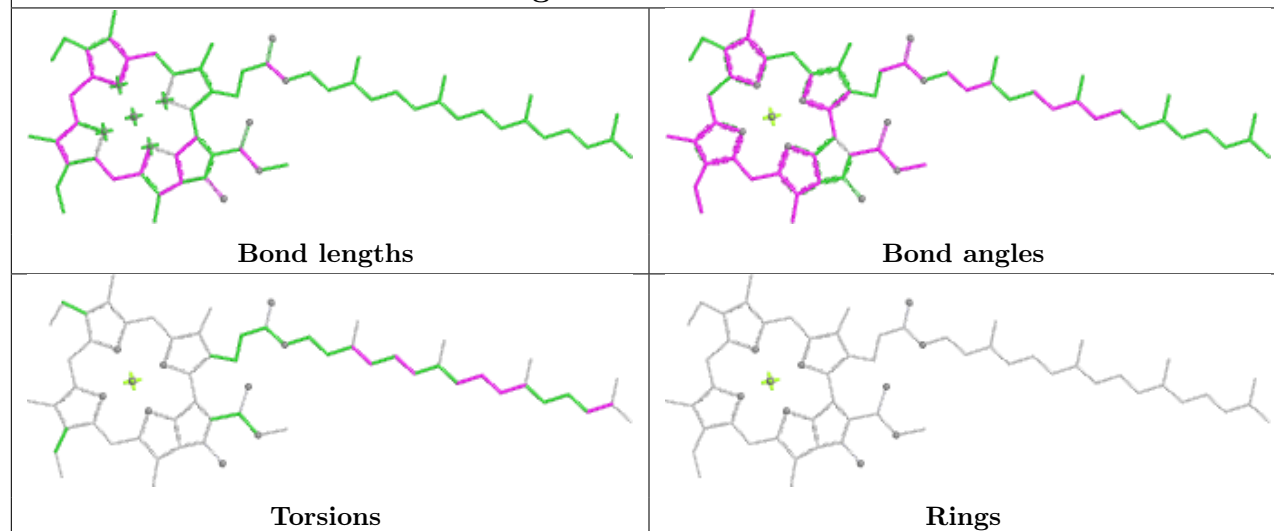
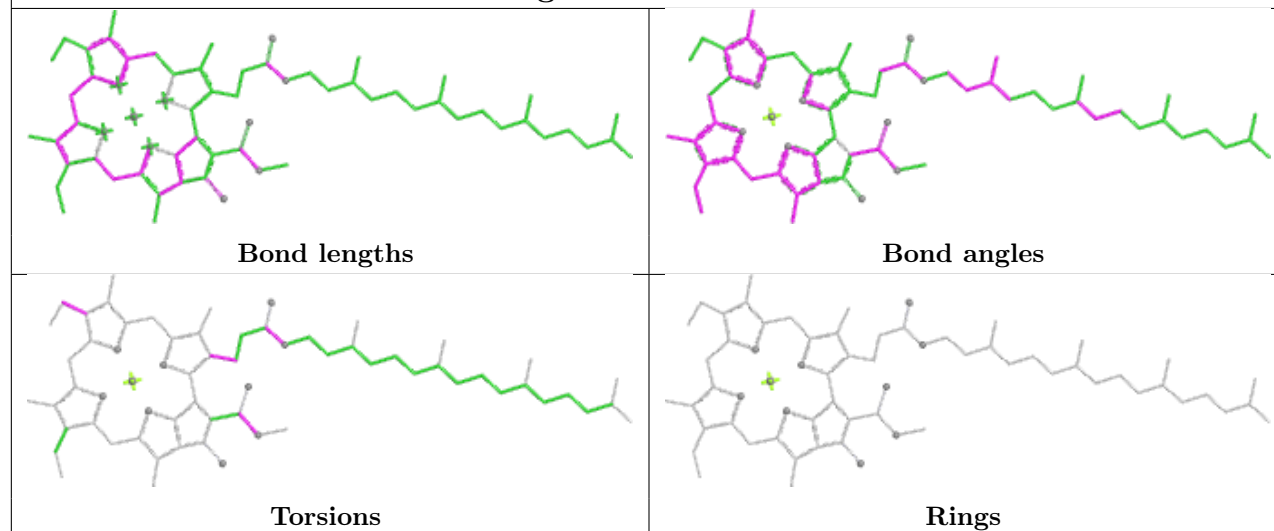
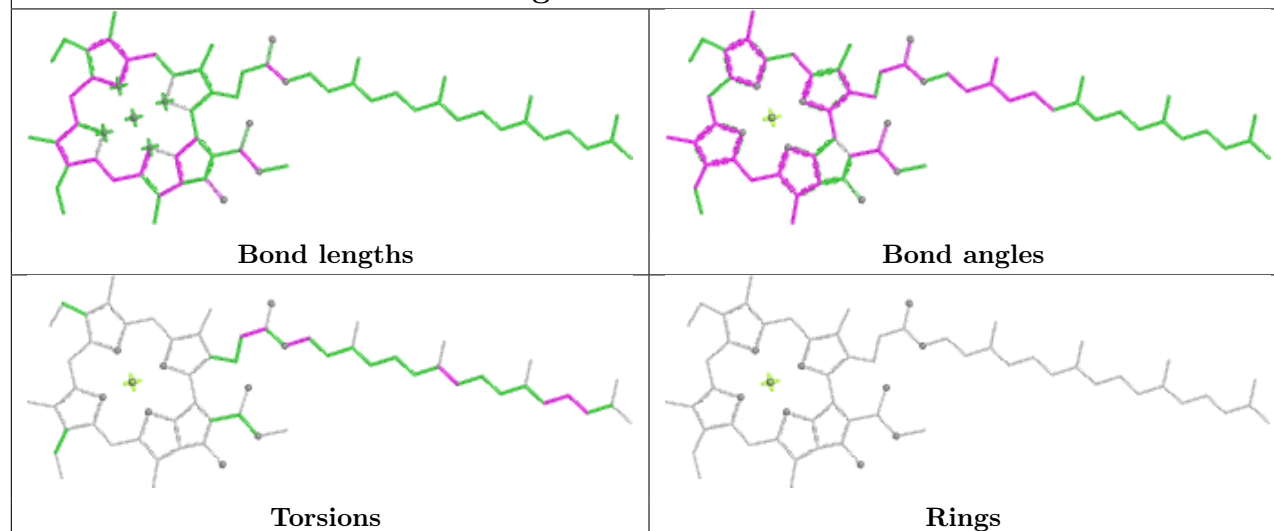


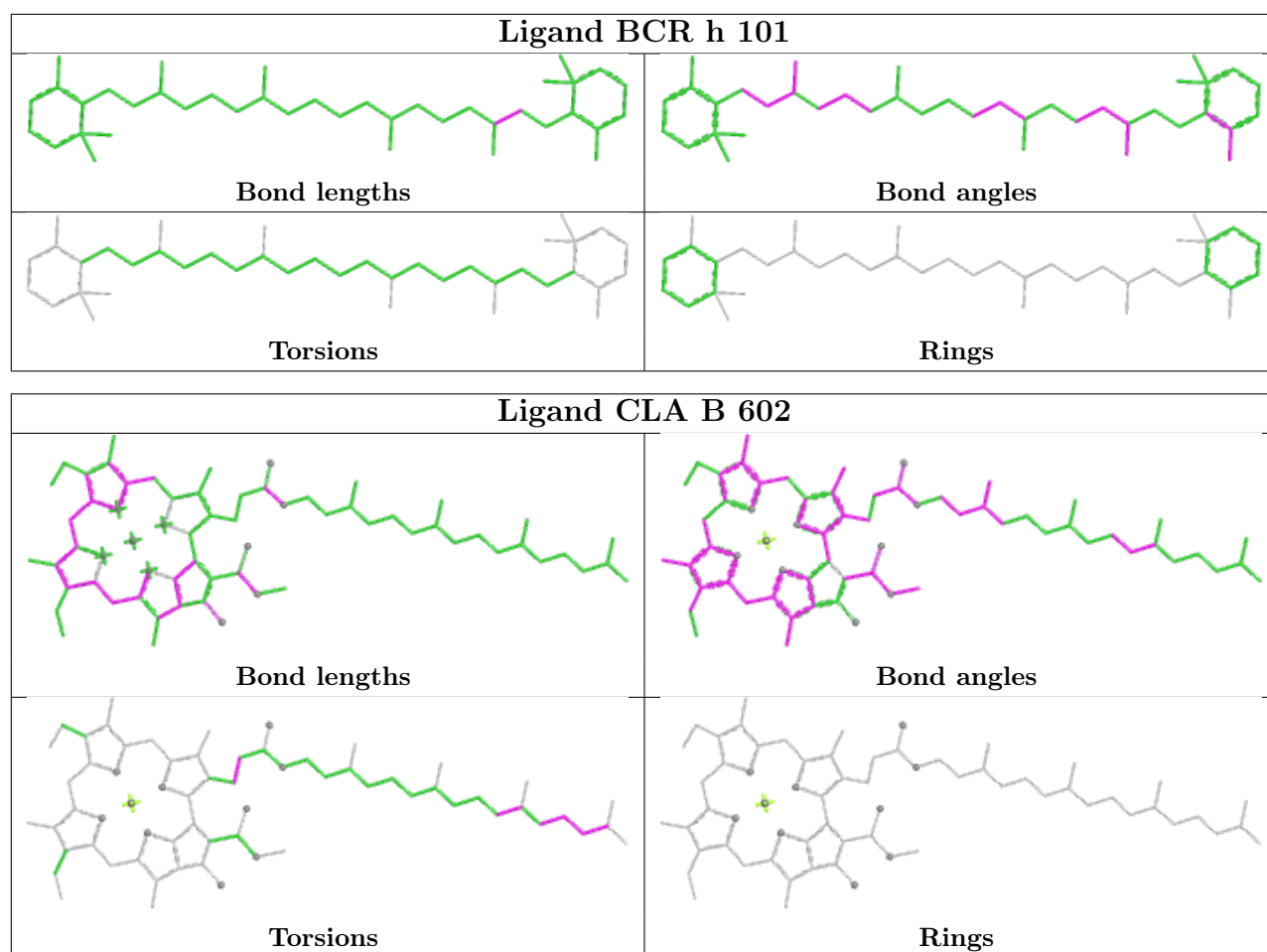
Ligand CLA b 616



Ligand SQD f 102



Ligand CLA B 615**Ligand CLA c 512****Ligand CLA B 613**



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%)	-0.61	1 (0%) 90 92	33, 54, 76, 123	3 (0%)
1	a	334/344 (97%)	-0.54	1 (0%) 90 92	34, 58, 88, 134	4 (1%)
2	B	504/505 (99%)	-0.50	2 (0%) 88 91	34, 59, 88, 130	8 (1%)
2	b	504/505 (99%)	-0.42	4 (0%) 82 86	38, 63, 102, 155	4 (0%)
3	C	451/455 (99%)	-0.48	0 100 100	38, 65, 86, 146	4 (0%)
3	c	455/455 (100%)	-0.42	0 100 100	41, 73, 94, 133	4 (0%)
4	D	342/342 (100%)	-0.65	0 100 100	34, 55, 75, 139	1 (0%)
4	d	341/342 (99%)	-0.58	0 100 100	40, 60, 83, 160	1 (0%)
5	E	81/84 (96%)	-0.14	0 100 100	54, 76, 104, 157	1 (1%)
5	e	79/84 (94%)	-0.01	1 (1%) 75 79	68, 85, 123, 148	0
6	F	34/44 (77%)	-0.39	0 100 100	62, 69, 95, 128	0
6	f	31/44 (70%)	-0.16	2 (6%) 25 28	68, 75, 106, 142	0
7	H	64/65 (98%)	-0.33	1 (1%) 70 76	36, 68, 84, 128	1 (1%)
7	h	64/65 (98%)	-0.29	1 (1%) 70 76	61, 75, 93, 140	0
8	I	37/38 (97%)	-0.23	0 100 100	59, 68, 122, 144	0
8	i	37/38 (97%)	-0.18	1 (2%) 56 63	59, 70, 130, 139	0
9	J	38/39 (97%)	-0.18	0 100 100	59, 78, 130, 185	0
9	j	39/39 (100%)	0.07	0 100 100	67, 85, 134, 172	0
10	K	37/37 (100%)	-0.36	0 100 100	68, 75, 93, 103	0
10	k	37/37 (100%)	-0.21	0 100 100	72, 82, 101, 111	0
11	L	36/37 (97%)	-0.50	0 100 100	31, 52, 103, 152	1 (2%)
11	l	36/37 (97%)	-0.53	0 100 100	32, 54, 106, 151	1 (2%)
12	M	32/36 (88%)	-0.45	0 100 100	32, 55, 76, 144	1 (3%)
12	m	33/36 (91%)	-0.45	0 100 100	49, 55, 83, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.38	0 100 100	40, 70, 117, 175	4 (1%)
13	o	243/244 (99%)	-0.31	0 100 100	38, 71, 121, 168	2 (0%)
14	T	29/32 (90%)	-0.59	1 (3%) 48 55	49, 54, 84, 117	0
14	t	29/32 (90%)	-0.58	1 (3%) 48 55	49, 56, 86, 150	0
15	U	96/104 (92%)	-0.48	0 100 100	52, 66, 90, 101	0
15	u	97/104 (93%)	-0.48	0 100 100	58, 68, 86, 131	0
16	V	137/137 (100%)	-0.53	0 100 100	52, 64, 88, 113	0
16	v	137/137 (100%)	-0.39	0 100 100	59, 76, 106, 153	0
17	X	38/40 (95%)	-0.18	0 100 100	65, 79, 102, 123	0
17	x	38/40 (95%)	0.15	1 (2%) 57 63	70, 86, 123, 162	0
18	Y	29/30 (96%)	0.48	2 (6%) 23 26	76, 92, 127, 141	0
18	y	29/30 (96%)	0.27	0 100 100	85, 103, 127, 133	0
19	Z	62/62 (100%)	0.04	1 (1%) 70 76	75, 90, 138, 173	0
19	z	62/62 (100%)	0.41	2 (3%) 50 57	89, 104, 148, 194	0
20	R	34/34 (100%)	1.45	9 (26%) 1 1	103, 130, 154, 159	0
All	All	5283/5384 (98%)	-0.41	31 (0%) 85 89	31, 65, 107, 194	40 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.8
7	h	65	LEU	4.3
14	t	30	THR	3.4
20	R	24	LEU	3.1
2	B	494	GLY	3.1

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	49,57,68,72	0
12	FME	m	1	10/11	0.96	0.08	59,67,83,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	I	1	10/11	0.97	0.07	60,72,75,79	0
14	FME	T	1	10/11	0.97	0.07	53,59,69,70	0
12	FME	M	1	10/11	0.98	0.08	54,65,84,92	0
8	FME	i	1	10/11	0.98	0.05	60,70,79,79	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
34	HTG	c	522	19/19	0.74	0.13	122,143,151,152	0
32	LMT	e	102	35/35	0.75	0.16	132,156,166,171	0
30	UNL	J	101	10/-	0.76	0.19	85,93,100,106	0
32	LMT	A	359	35/35	0.76	0.16	85,123,132,134	0
32	LMT	a	414	35/35	0.77	0.15	77,121,131,134	0
34	HTG	C	522	19/19	0.77	0.13	112,128,136,139	0
32	LMT	a	420	35/35	0.77	0.16	124,142,152,152	0
30	UNL	I	102	40/-	0.78	0.17	83,112,137,141	0
26	SQD	f	102	43/54	0.78	0.15	121,146,161,163	0
30	UNL	a	417	30/-	0.78	0.16	105,118,135,144	0
30	UNL	i	101	40/-	0.78	0.15	91,109,147,151	0
30	UNL	A	415	28/-	0.78	0.17	101,116,129,137	0
30	UNL	K	101	34/-	0.79	0.15	98,118,130,146	0
37	LHG	e	101	42/49	0.79	0.13	108,140,159,166	0
30	UNL	j	101	10/-	0.80	0.15	92,102,116,117	0
32	LMT	E	102	35/35	0.80	0.15	118,142,160,165	0
32	LMT	I	101	35/35	0.80	0.15	112,139,150,154	0
30	UNL	c	525	32/-	0.81	0.15	99,116,133,137	0
30	UNL	m	102	10/-	0.81	0.14	70,81,92,93	0
33	LMG	C	521	51/55	0.81	0.14	91,116,139,141	0
32	LMT	b	621	25/35	0.82	0.14	105,119,144,144	0
34	HTG	D	414	16/19	0.82	0.13	93,117,129,133	0
30	UNL	b	626	33/-	0.83	0.14	88,107,143,146	0
33	LMG	c	521	51/55	0.83	0.12	103,127,143,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	d	411	16/19	0.83	0.14	112,133,141,153	0
36	CA	f	103	1/1	0.83	0.14	136,136,136,136	0
32	LMT	M	103	35/35	0.83	0.13	93,135,153,154	0
34	HTG	b	623	19/19	0.84	0.13	103,124,138,158	0
32	LMT	D	404	35/35	0.84	0.13	87,111,134,136	0
34	HTG	B	623	19/19	0.84	0.17	81,103,114,114	0
29	PL9	A	414	55/55	0.84	0.15	90,112,121,124	0
30	UNL	D	413	40/-	0.84	0.13	77,100,127,131	0
33	LMG	Z	101	37/55	0.86	0.14	94,122,137,139	0
27	GOL	v	201	6/6	0.86	0.13	77,89,97,99	0
30	UNL	B	627	33/-	0.86	0.13	76,108,140,145	0
36	CA	F	102	1/1	0.86	0.18	147,147,147,147	0
29	PL9	a	416	55/55	0.86	0.14	104,118,129,130	0
30	UNL	M	102	10/-	0.86	0.10	72,78,87,88	0
33	LMG	z	101	39/55	0.87	0.13	102,127,141,143	0
30	UNL	d	410	36/-	0.87	0.12	84,104,130,135	0
27	GOL	b	624	6/6	0.87	0.12	93,100,106,108	0
26	SQD	a	413	54/54	0.87	0.11	82,98,124,129	0
32	LMT	b	627	25/35	0.87	0.12	68,90,129,132	0
34	HTG	B	622	19/19	0.88	0.13	81,91,122,125	0
26	SQD	F	101	43/54	0.88	0.11	91,107,124,129	0
32	LMT	t	101	25/35	0.89	0.12	80,99,127,128	0
32	LMT	t	102	26/35	0.89	0.11	85,105,128,129	0
26	SQD	b	620	54/54	0.89	0.11	78,97,128,130	0
26	SQD	A	412	54/54	0.89	0.10	72,92,109,117	0
26	SQD	B	620	54/54	0.89	0.11	81,100,120,129	0
37	LHG	E	101	42/49	0.89	0.11	95,119,132,134	0
34	HTG	b	622	19/19	0.89	0.12	71,90,118,119	0
27	GOL	a	412	6/6	0.90	0.10	82,88,94,97	0
27	GOL	A	411	6/6	0.90	0.13	79,87,89,100	0
27	GOL	B	625	6/6	0.90	0.15	65,82,86,93	0
34	HTG	V	203	11/19	0.90	0.11	103,119,123,128	0
23	CLA	B	601	65/65	0.91	0.10	69,81,102,119	0
33	LMG	C	501	51/55	0.91	0.11	79,98,110,117	0
33	LMG	C	520	51/55	0.91	0.09	74,94,110,120	0
32	LMT	M	101	35/35	0.91	0.10	69,95,111,113	0
32	LMT	m	103	35/35	0.91	0.11	73,95,108,111	0
33	LMG	c	520	51/55	0.91	0.09	85,101,121,129	0
27	GOL	c	501	6/6	0.91	0.16	73,74,77,78	0
30	UNL	D	412	17/-	0.92	0.09	70,84,100,106	0
33	LMG	a	419	51/55	0.92	0.09	85,100,111,117	0
27	GOL	a	418	6/6	0.92	0.20	65,79,86,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	514	65/65	0.92	0.09	72,85,107,112	0
23	CLA	b	601	65/65	0.92	0.10	76,88,109,125	0
23	CLA	c	514	65/65	0.92	0.10	83,97,115,122	0
23	CLA	C	507	65/65	0.93	0.09	61,75,112,117	0
23	CLA	c	513	65/65	0.93	0.08	71,87,107,113	0
33	LMG	D	415	51/55	0.93	0.09	62,75,104,108	0
25	BCR	h	101	40/40	0.94	0.08	65,75,84,85	0
23	CLA	b	616	65/65	0.94	0.09	58,67,97,103	0
23	CLA	c	505	65/65	0.94	0.09	63,71,94,111	0
23	CLA	B	616	65/65	0.94	0.11	53,63,108,111	0
33	LMG	B	621	51/55	0.94	0.09	69,78,97,108	0
34	HTG	b	625	19/19	0.94	0.09	79,86,107,111	0
33	LMG	d	412	51/55	0.94	0.09	69,77,107,115	0
33	LMG	m	101	51/55	0.94	0.09	65,77,96,113	0
26	SQD	a	411	54/54	0.94	0.09	79,90,116,119	0
23	CLA	C	513	65/65	0.94	0.08	71,80,101,108	0
25	BCR	D	407	40/40	0.94	0.08	59,68,91,92	0
37	LHG	d	408	49/49	0.94	0.09	64,72,102,105	0
34	HTG	B	626	19/19	0.94	0.08	78,85,96,102	0
38	HEM	E	103	43/43	0.94	0.08	65,73,87,116	0
27	GOL	V	201	6/6	0.95	0.11	64,71,83,87	0
23	CLA	A	408	65/65	0.95	0.08	51,59,101,112	0
30	UNL	x	101	18/-	0.95	0.11	82,91,108,111	0
23	CLA	d	403	65/65	0.95	0.08	58,71,98,106	0
25	BCR	C	515	40/40	0.95	0.08	74,79,87,92	0
23	CLA	D	406	65/65	0.95	0.09	55,65,105,108	0
25	BCR	T	101	40/40	0.95	0.06	52,62,69,72	0
25	BCR	d	404	40/40	0.95	0.08	67,78,91,92	0
23	CLA	a	407	65/65	0.95	0.08	52,59,102,109	0
25	BCR	t	103	40/40	0.95	0.07	54,64,79,80	0
25	BCR	y	101	40/40	0.95	0.08	72,79,88,91	0
26	SQD	A	410	54/54	0.95	0.08	70,87,106,114	0
23	CLA	a	409	65/65	0.95	0.09	53,62,108,115	0
23	CLA	C	505	65/65	0.95	0.07	55,63,88,103	0
23	CLA	b	606	65/65	0.95	0.08	55,65,89,102	0
23	CLA	b	614	65/65	0.95	0.07	49,58,92,99	0
23	CLA	B	606	65/65	0.95	0.08	51,59,90,98	0
35	DGD	C	517	62/66	0.95	0.08	55,65,89,93	0
35	DGD	C	518	62/66	0.95	0.08	60,71,105,112	0
35	DGD	c	517	62/66	0.95	0.07	62,69,85,94	0
35	DGD	c	518	62/66	0.95	0.08	64,76,106,114	0
30	UNL	X	101	18/-	0.95	0.09	72,79,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CA	O	301	1/1	0.95	0.06	121,121,121,121	0
23	CLA	C	509	65/65	0.95	0.08	54,63,97,106	0
37	LHG	D	411	49/49	0.95	0.09	60,67,105,110	0
23	CLA	c	507	65/65	0.95	0.08	71,81,103,112	0
37	LHG	d	406	49/49	0.95	0.08	60,71,88,100	0
23	CLA	c	509	65/65	0.95	0.08	57,69,106,115	0
23	CLA	B	614	65/65	0.95	0.08	48,54,87,95	0
27	GOL	C	523	6/6	0.95	0.10	63,67,73,76	0
23	CLA	A	406	65/65	0.96	0.07	47,54,92,96	0
30	UNL	d	409	17/-	0.96	0.07	78,88,109,111	0
23	CLA	b	607	65/65	0.96	0.07	47,55,76,83	0
25	BCR	A	409	40/40	0.96	0.06	48,55,62,65	0
27	GOL	B	624	6/6	0.96	0.09	85,88,93,95	0
25	BCR	B	618	40/40	0.96	0.06	53,61,74,81	0
25	BCR	B	619	40/40	0.96	0.06	56,64,78,81	0
31	BCT	a	404	4/4	0.96	0.08	59,65,66,76	0
23	CLA	b	609	65/65	0.96	0.07	61,68,82,98	0
23	CLA	C	506	65/65	0.96	0.07	55,63,81,93	0
25	BCR	H	101	40/40	0.96	0.07	58,69,79,80	0
25	BCR	K	102	40/40	0.96	0.07	64,72,81,83	0
23	CLA	b	615	65/65	0.96	0.06	56,64,74,80	0
25	BCR	Y	101	40/40	0.96	0.07	67,75,80,82	0
25	BCR	b	618	40/40	0.96	0.06	53,62,71,76	0
29	PL9	D	408	55/55	0.96	0.06	47,55,61,73	0
25	BCR	c	515	40/40	0.96	0.08	86,93,98,101	0
29	PL9	d	405	55/55	0.96	0.07	51,58,66,90	0
35	DGD	C	519	62/66	0.96	0.08	57,66,90,97	0
35	DGD	H	102	62/66	0.96	0.07	59,68,77,78	0
23	CLA	B	602	65/65	0.96	0.07	55,60,76,82	0
23	CLA	c	504	65/65	0.96	0.07	65,72,82,97	0
35	DGD	c	519	62/66	0.96	0.07	64,74,94,102	0
25	BCR	k	101	40/40	0.96	0.07	71,80,90,95	0
23	CLA	B	604	65/65	0.96	0.07	44,53,90,103	0
36	CA	c	523	1/1	0.96	0.11	84,84,84,84	0
23	CLA	c	506	65/65	0.96	0.07	58,69,85,91	0
36	CA	o	301	1/1	0.96	0.05	107,107,107,107	0
37	LHG	D	409	49/49	0.96	0.07	58,69,84,96	0
23	CLA	C	504	65/65	0.96	0.07	58,65,74,84	0
23	CLA	c	508	65/65	0.96	0.08	64,75,83,90	0
23	CLA	b	602	65/65	0.96	0.07	59,66,79,89	0
23	CLA	c	510	65/65	0.96	0.07	61,73,84,92	0
23	CLA	c	512	65/65	0.96	0.08	67,78,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	LHG	l	101	49/49	0.96	0.07	55,65,77,87	0
23	CLA	b	604	65/65	0.96	0.07	49,56,91,101	0
38	HEM	e	87	43/43	0.96	0.09	80,94,117,126	0
23	CLA	B	605	65/65	0.97	0.06	47,54,63,69	0
23	CLA	A	404	65/65	0.97	0.06	43,50,60,70	0
23	CLA	b	608	65/65	0.97	0.05	57,64,79,88	0
23	CLA	B	607	65/65	0.97	0.06	44,52,69,76	0
25	BCR	a	410	40/40	0.97	0.06	51,59,65,67	0
25	BCR	b	617	40/40	0.97	0.06	51,58,65,67	0
23	CLA	b	610	65/65	0.97	0.07	57,64,73,78	0
25	BCR	b	619	40/40	0.97	0.06	56,67,80,82	0
23	CLA	b	611	65/65	0.97	0.06	52,58,68,75	0
25	BCR	c	516	40/40	0.97	0.07	66,74,81,85	0
23	CLA	b	612	65/65	0.97	0.06	53,60,66,77	0
23	CLA	b	613	65/65	0.97	0.06	48,55,84,89	0
23	CLA	B	609	65/65	0.97	0.07	58,64,70,74	0
23	CLA	C	508	65/65	0.97	0.07	59,66,77,79	0
23	CLA	B	610	65/65	0.97	0.07	52,59,69,75	0
23	CLA	c	502	65/65	0.97	0.06	64,72,80,84	0
23	CLA	c	503	65/65	0.97	0.07	59,69,79,81	0
23	CLA	C	510	65/65	0.97	0.07	57,67,80,86	0
23	CLA	C	511	65/65	0.97	0.07	58,67,77,87	0
23	CLA	C	512	65/65	0.97	0.07	60,73,82,88	0
23	CLA	B	611	65/65	0.97	0.06	46,52,63,68	0
23	CLA	B	612	65/65	0.97	0.06	47,54,61,67	0
23	CLA	D	405	65/65	0.97	0.06	43,50,66,81	0
23	CLA	B	613	65/65	0.97	0.06	47,54,80,87	0
35	DGD	h	102	62/66	0.97	0.07	62,72,79,84	0
23	CLA	c	511	65/65	0.97	0.06	62,71,80,84	0
23	CLA	a	405	65/65	0.97	0.06	48,54,64,81	0
23	CLA	a	406	65/65	0.97	0.05	48,52,63,71	0
23	CLA	B	603	65/65	0.97	0.06	50,58,69,75	0
23	CLA	B	615	65/65	0.97	0.06	48,58,74,77	0
24	PHO	A	353	64/64	0.97	0.06	47,56,61,64	0
37	LHG	D	410	49/49	0.97	0.07	55,61,74,84	0
24	PHO	a	353	64/64	0.97	0.06	53,60,65,67	0
22	CL	a	403	1/1	0.97	0.08	58,58,58,58	0
37	LHG	L	101	49/49	0.97	0.07	55,63,69,84	0
25	BCR	B	617	40/40	0.97	0.05	51,56,63,64	0
37	LHG	d	407	49/49	0.97	0.07	55,62,72,80	0
23	CLA	C	502	65/65	0.97	0.06	56,65,71,76	0
23	CLA	b	603	65/65	0.97	0.06	52,62,78,88	0

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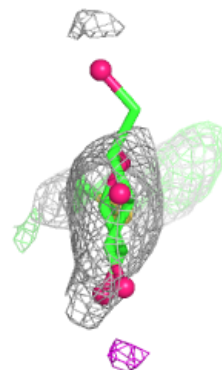
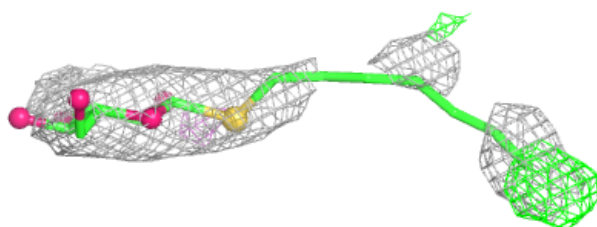
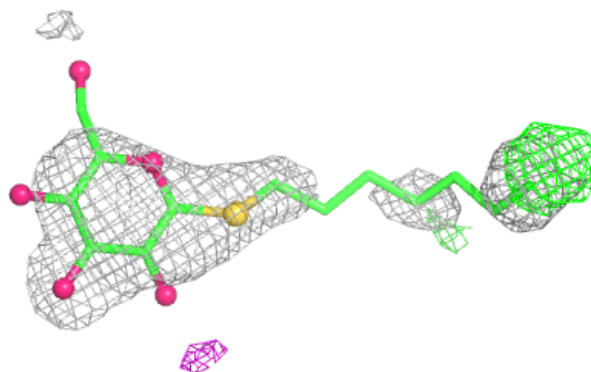
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	503	65/65	0.97	0.07	54,62,73,86	0
25	BCR	C	516	40/40	0.97	0.07	59,69,76,80	0
23	CLA	b	605	65/65	0.97	0.06	51,57,70,72	0
23	CLA	A	405	65/65	0.98	0.05	44,51,59,60	0
24	PHO	A	407	64/64	0.98	0.05	46,51,56,59	0
31	BCT	A	348	4/4	0.98	0.05	60,62,64,69	0
23	CLA	B	608	65/65	0.98	0.05	51,59,69,72	0
24	PHO	a	408	64/64	0.98	0.05	49,55,60,66	0
23	CLA	d	402	65/65	0.98	0.06	48,55,66,78	0
39	MG	J	102	1/1	0.98	0.07	64,64,64,64	0
40	HEC	V	202	43/43	0.98	0.06	50,60,63,64	0
40	HEC	v	202	43/43	0.98	0.06	61,70,75,79	0
36	CA	c	524	1/1	0.99	0.03	93,93,93,93	0
22	CL	A	402	1/1	0.99	0.03	51,51,51,51	0
22	CL	A	403	1/1	0.99	0.05	52,52,52,52	0
22	CL	a	402	1/1	0.99	0.02	56,56,56,56	0
28	OEX	A	413	10/10	0.99	0.05	56,57,57,57	0
36	CA	C	524	1/1	0.99	0.09	81,81,81,81	0
28	OEX	a	415	10/10	0.99	0.04	58,62,66,67	0
39	MG	j	102	1/1	0.99	0.04	70,70,70,70	0
21	FE2	A	401	1/1	0.99	0.03	64,64,64,64	0
21	FE2	a	401	1/1	0.99	0.04	67,67,67,67	0

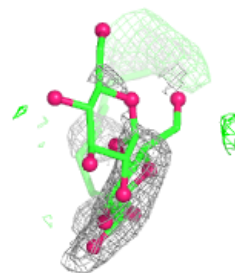
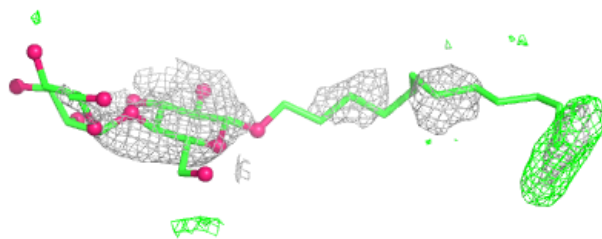
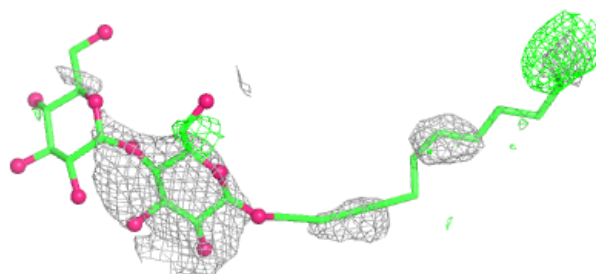
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

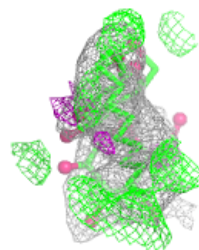
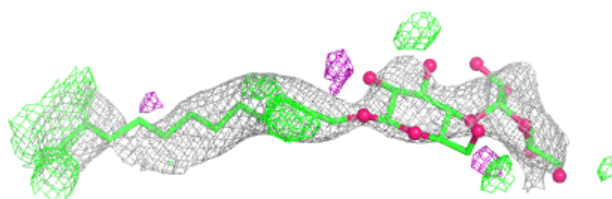
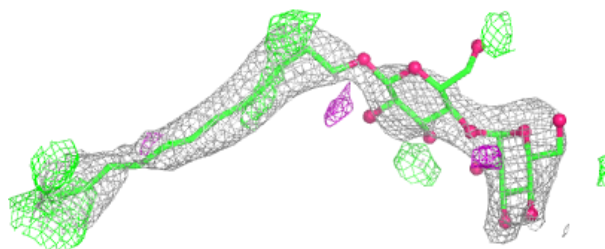
**Electron density around LMT e 102:**

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

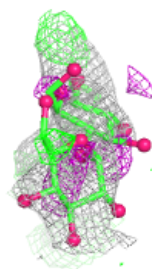
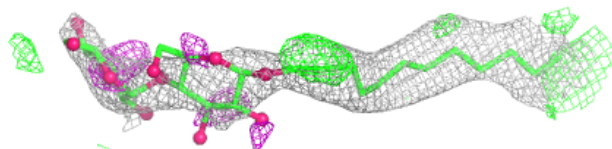
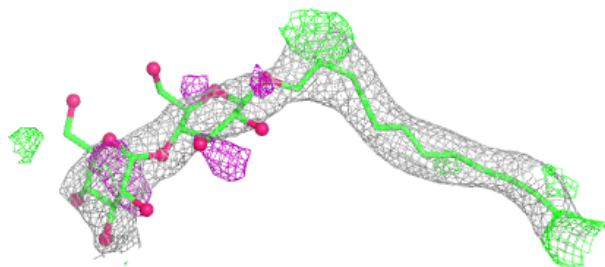


Electron density around LMT A 359:

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

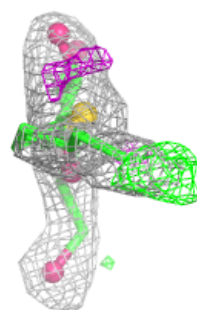
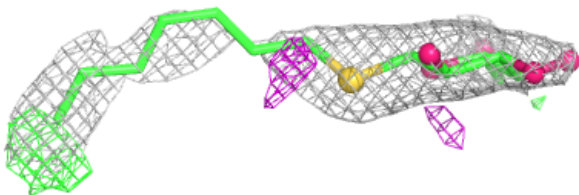
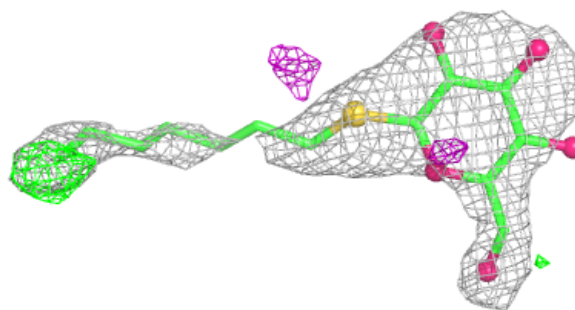
**Electron density around LMT a 414:**

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

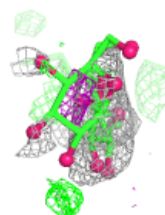
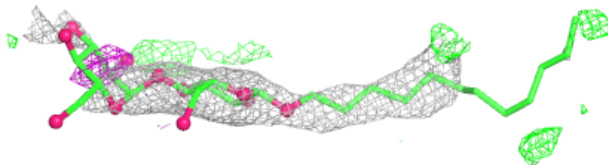
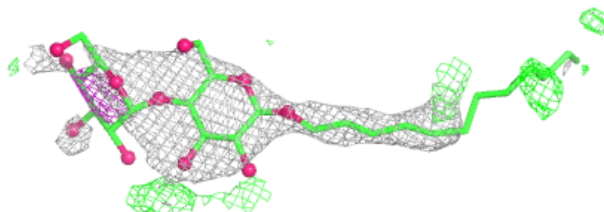


Electron density around HTG C 522:

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

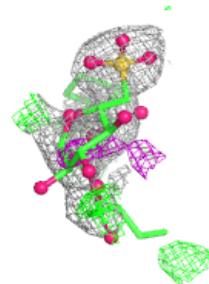
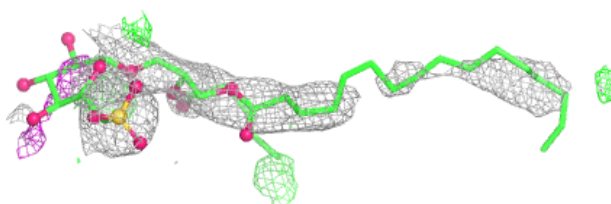
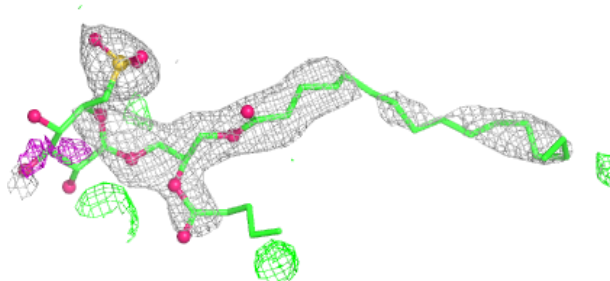
**Electron density around LMT a 420:**

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

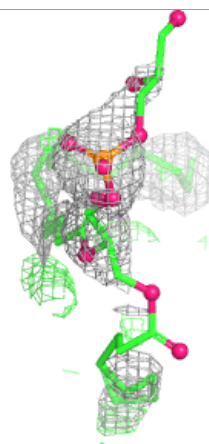
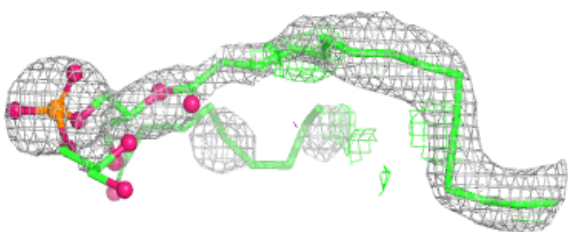
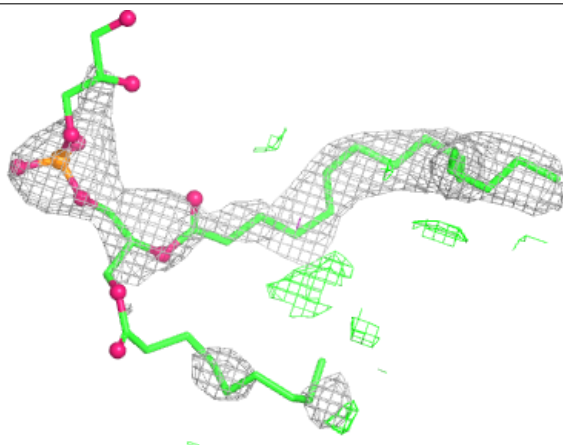


Electron density around SQD f 102:

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

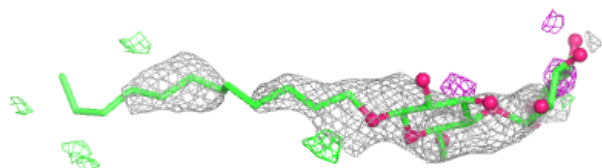
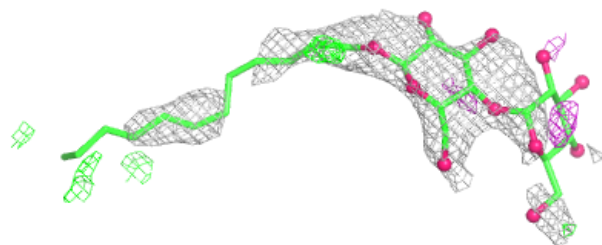
**Electron density around LHG e 101:**

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

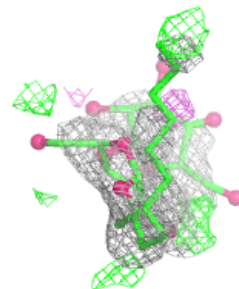
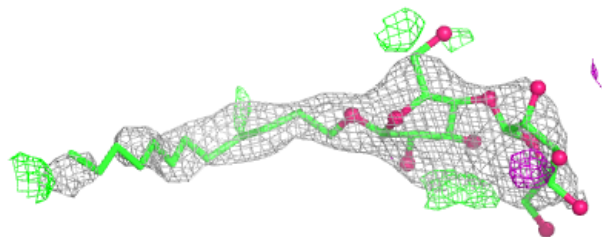
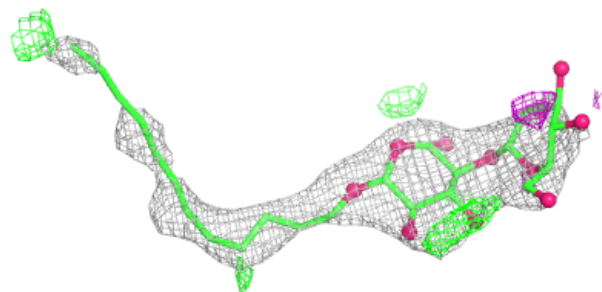


Electron density around LMT E 102:

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

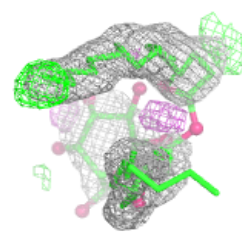
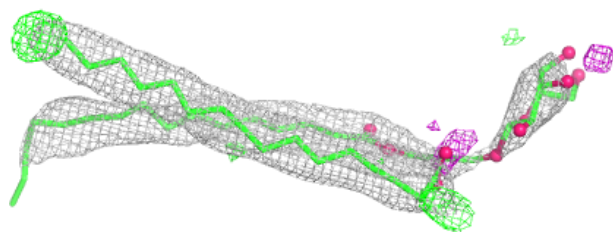
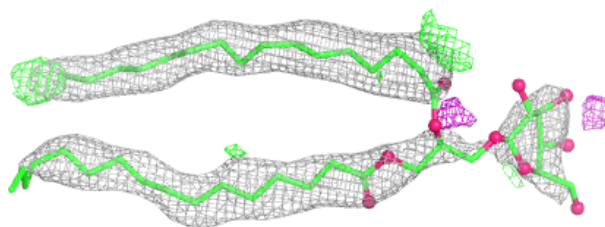
**Electron density around LMT I 101:**

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

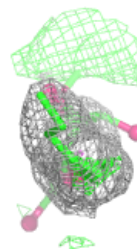
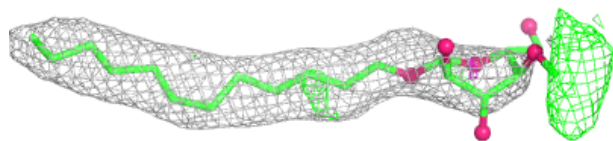
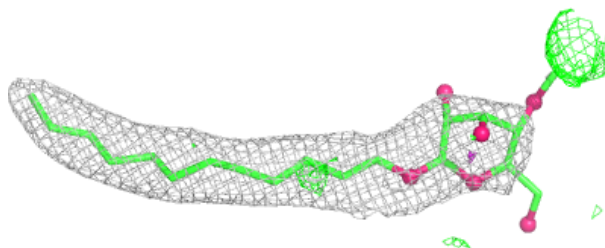


Electron density around LMG C 521:

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

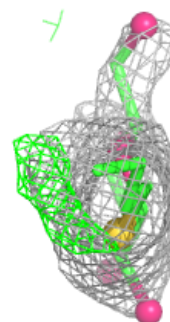
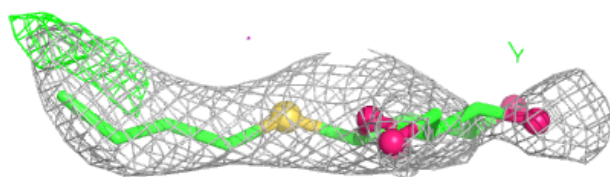
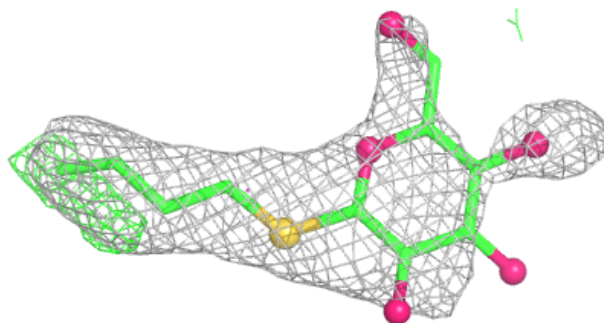
**Electron density around LMT b 621:**

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

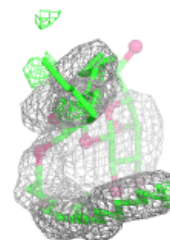
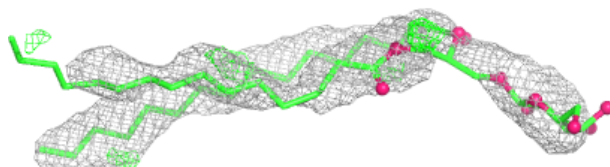
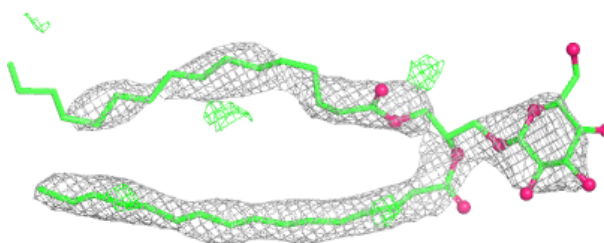


Electron density around HTG D 414:

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

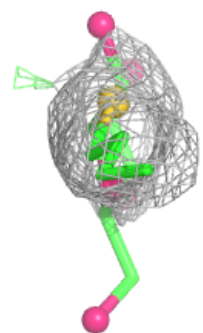
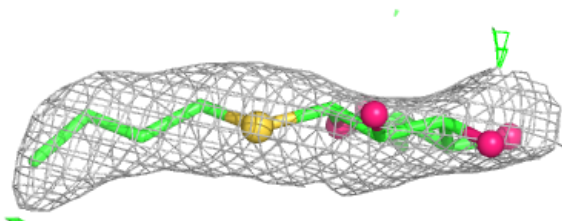
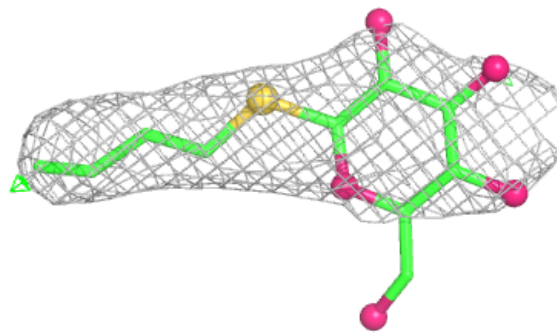
**Electron density around LMG c 521:**

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

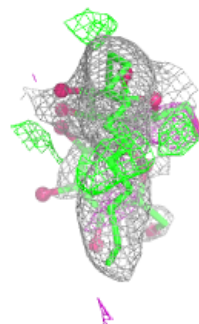
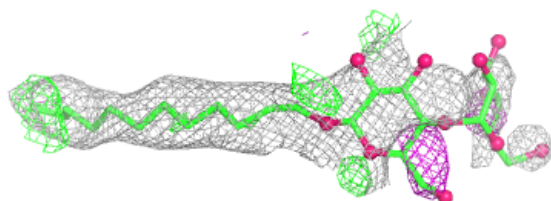
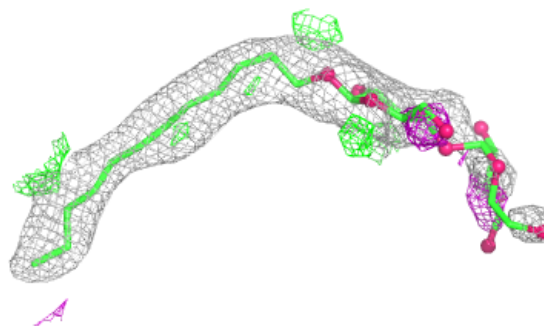


Electron density around HTG d 411:

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

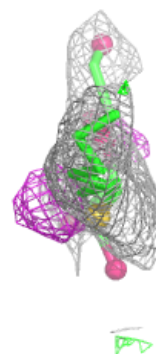
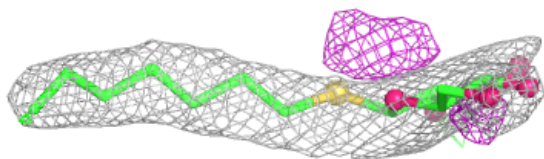
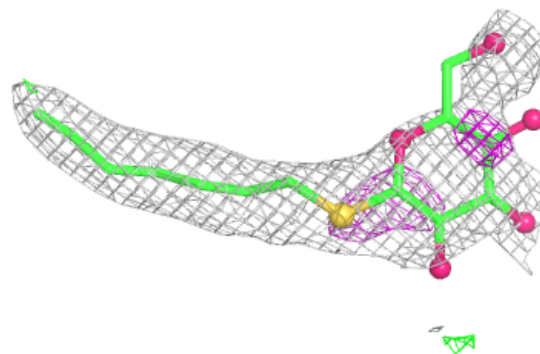
**Electron density around LMT M 103:**

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

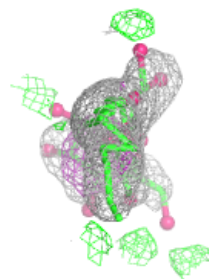
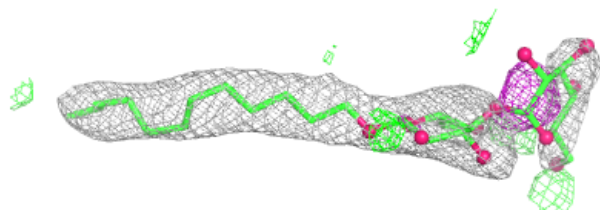
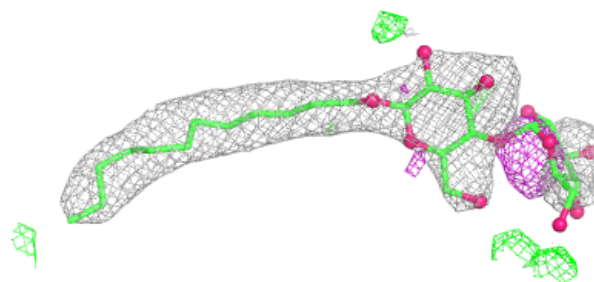


Electron density around HTG b 623:

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

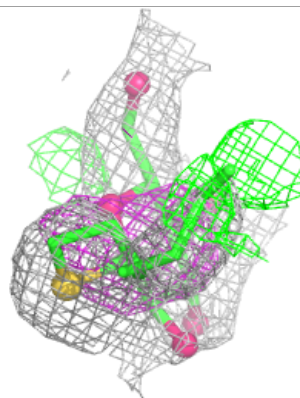
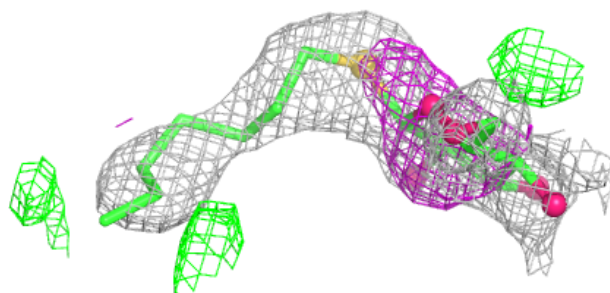
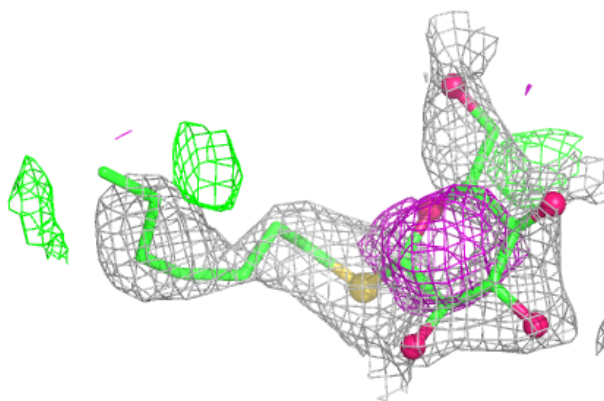
**Electron density around LMT D 404:**

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

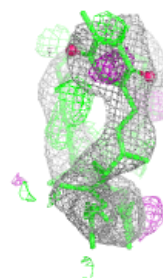
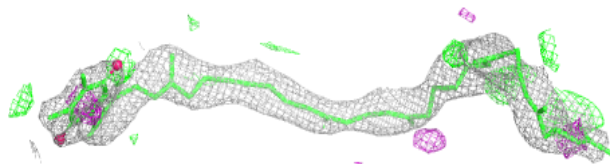
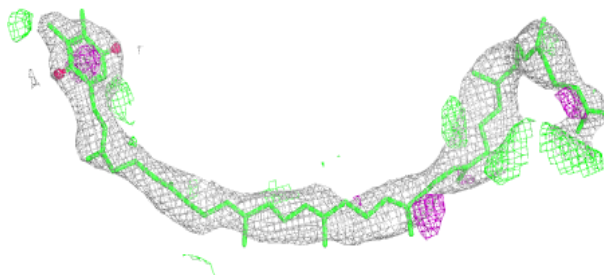


Electron density around HTG B 623:

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

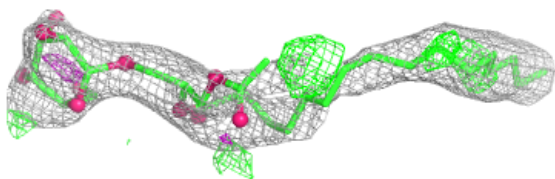
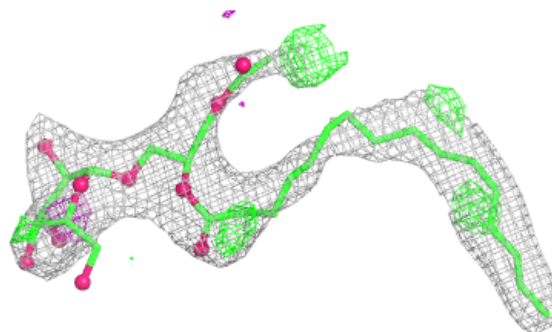
**Electron density around PL9 A 414:**

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

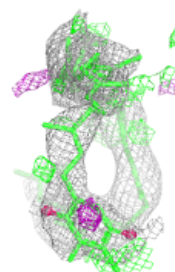
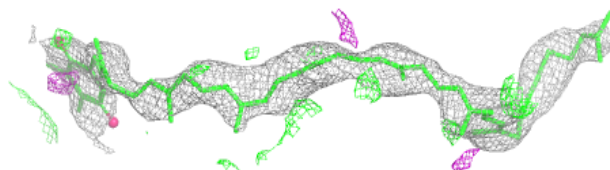
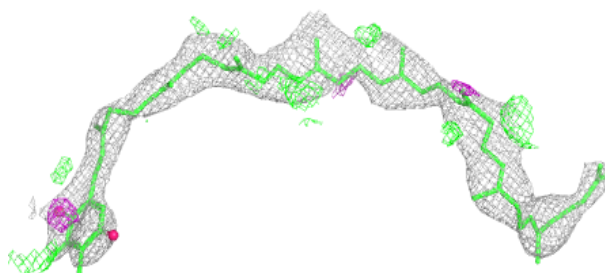


Electron density around LMG Z 101:

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

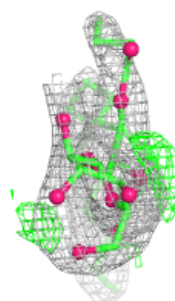
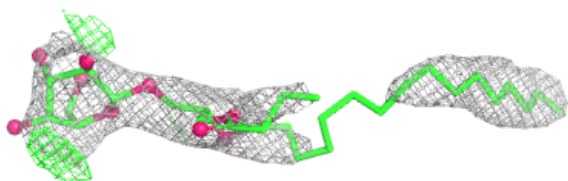
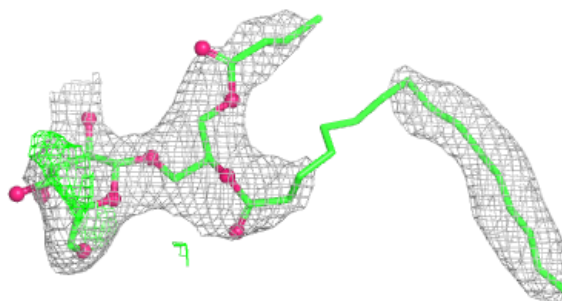
**Electron density around PL9 a 416:**

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

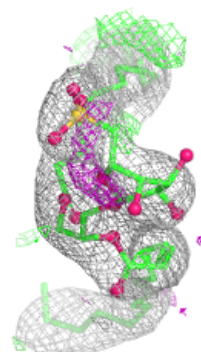
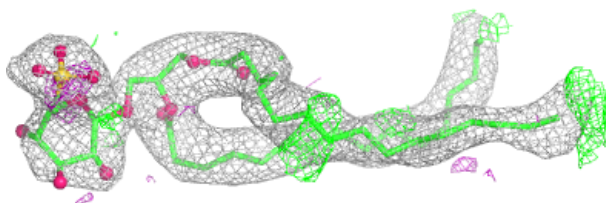
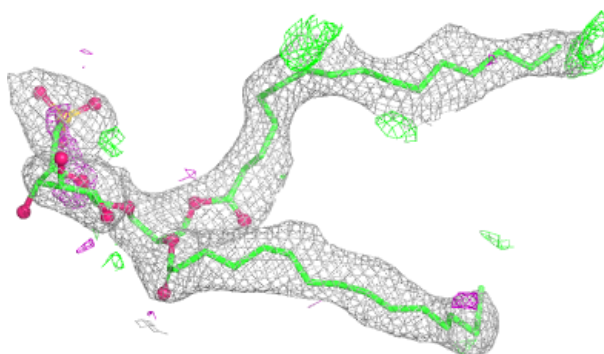


Electron density around LMG z 101:

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

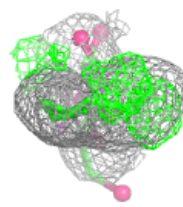
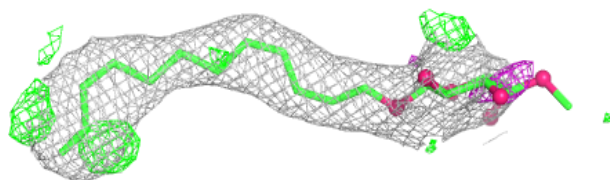
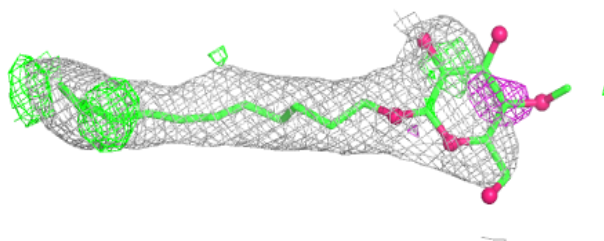
**Electron density around SQD a 413:**

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

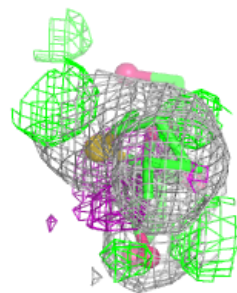
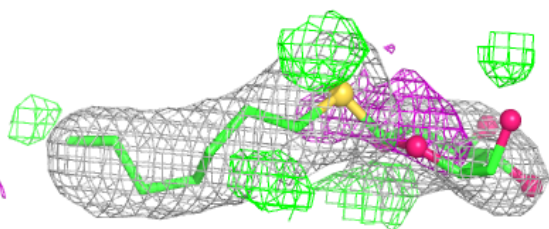
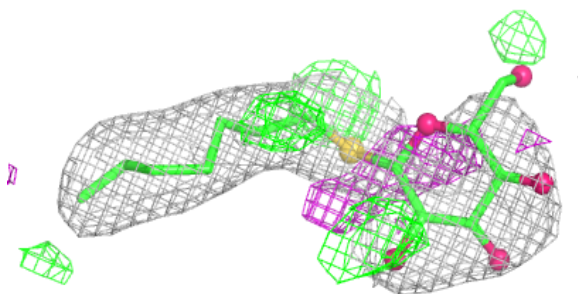


Electron density around LMT b 627:

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

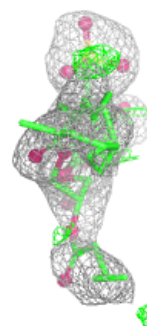
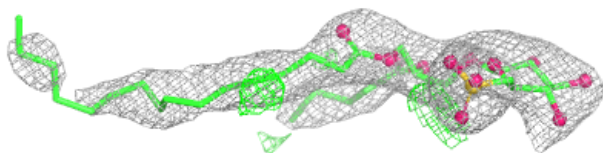
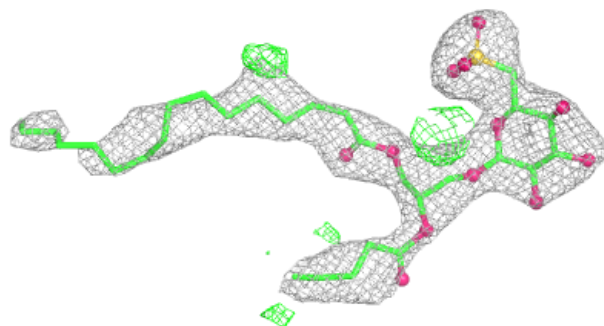
**Electron density around HTG B 622:**

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

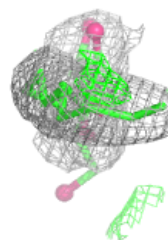
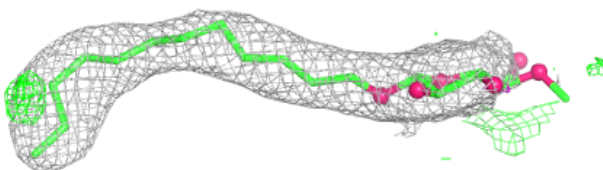
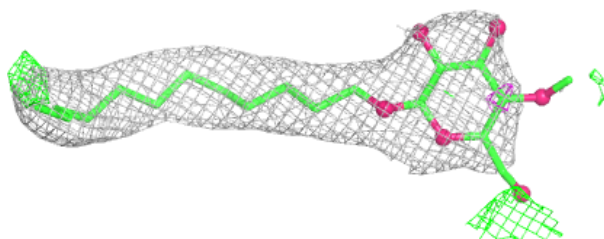


Electron density around SQD F 101:

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

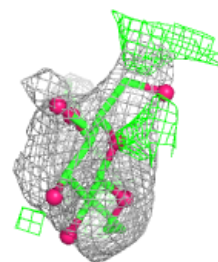
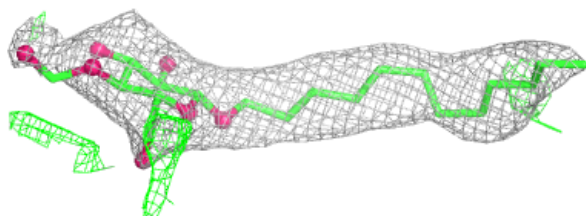
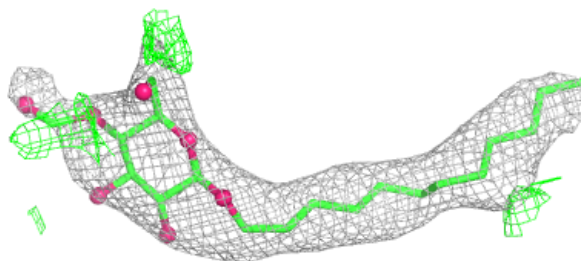
**Electron density around LMT t 101:**

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

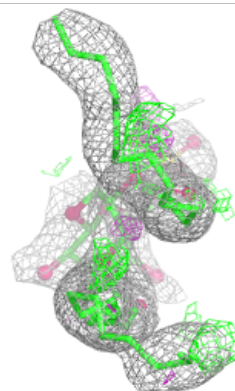
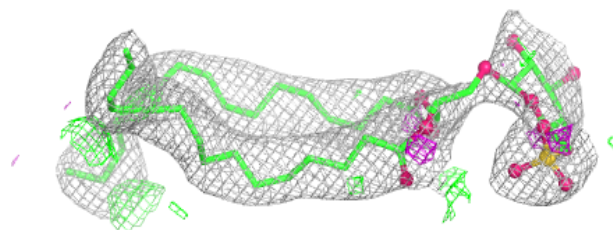
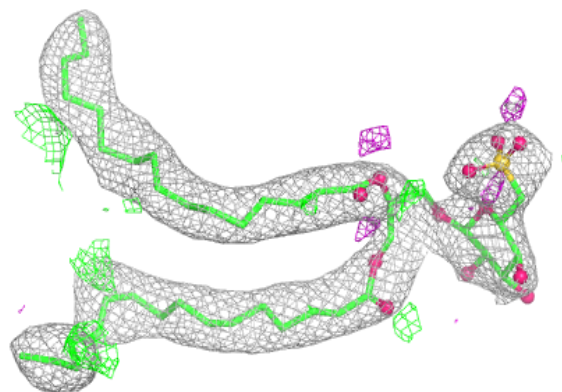


Electron density around LMT t 102:

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

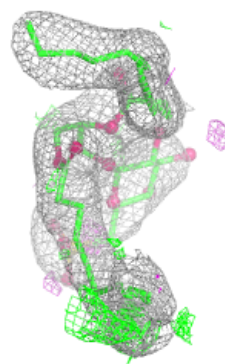
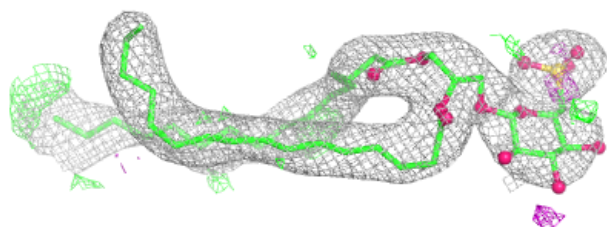
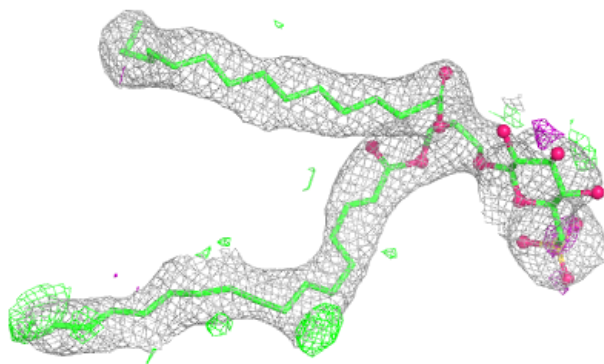
**Electron density around SQD b 620:**

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

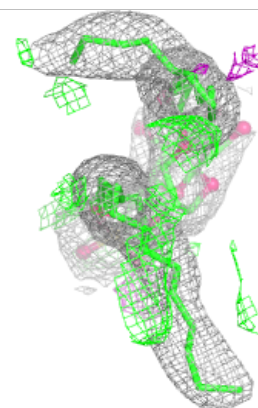
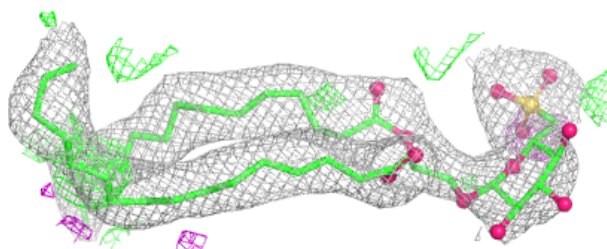
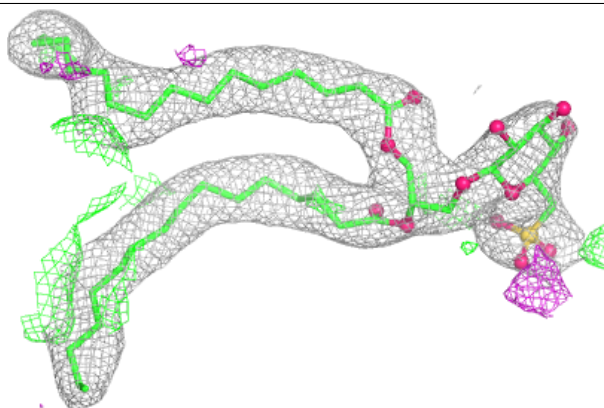


Electron density around SQD A 412:

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

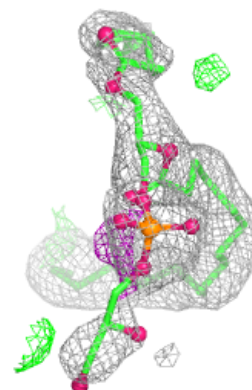
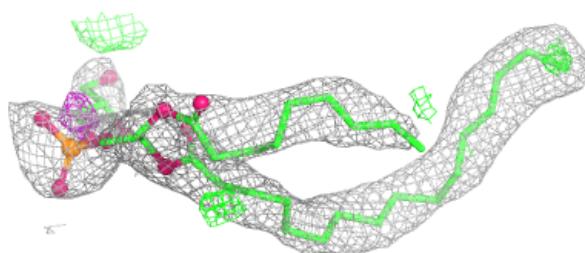
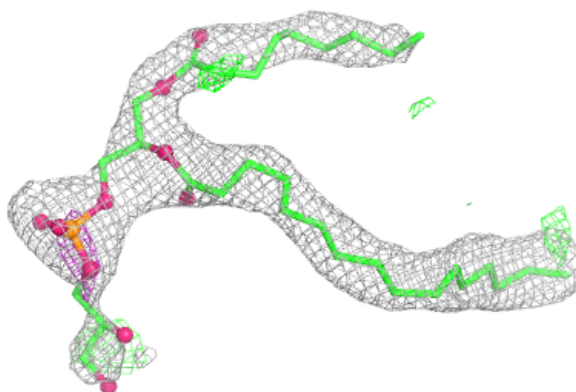
**Electron density around SQD B 620:**

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

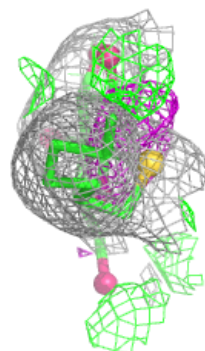
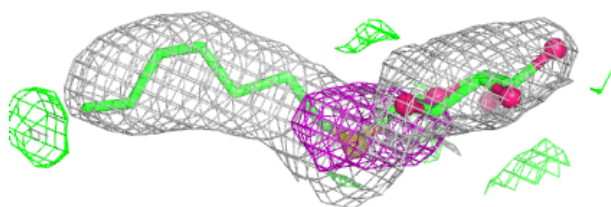
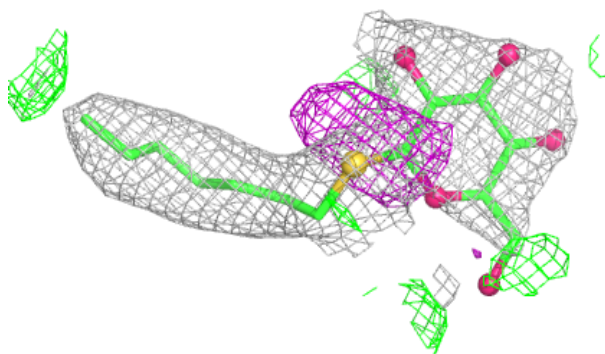


Electron density around LHG E 101:

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

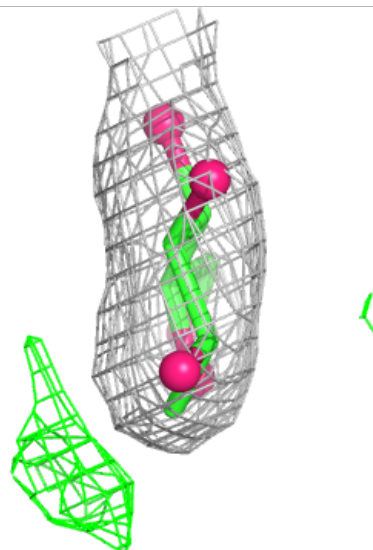
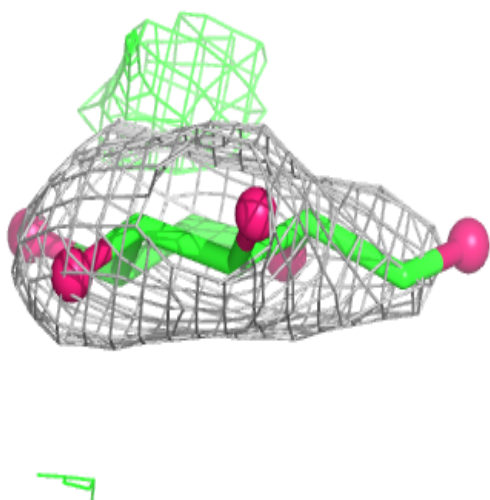
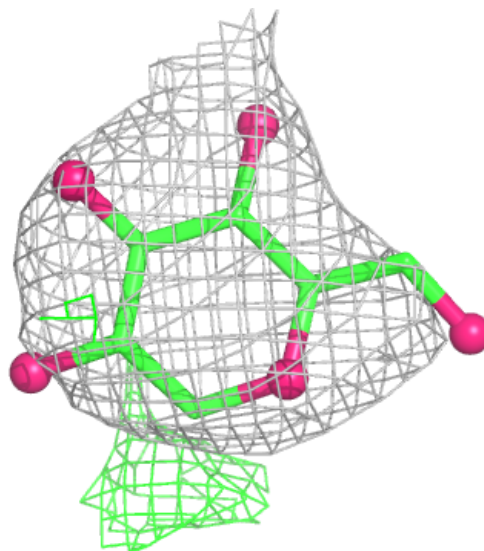
**Electron density around HTG b 622:**

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



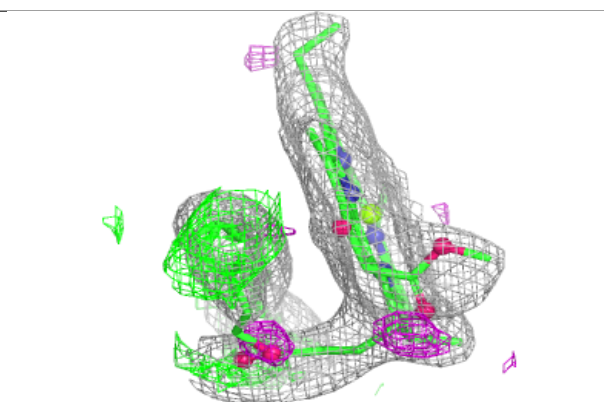
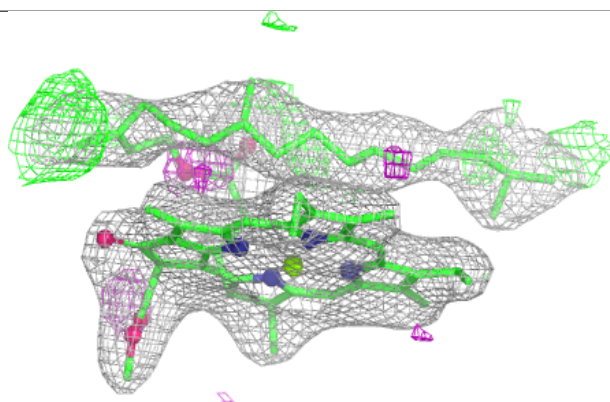
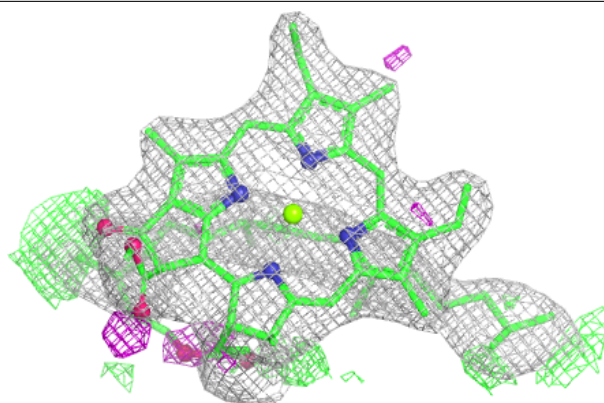
Electron density around HTG V 203:

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

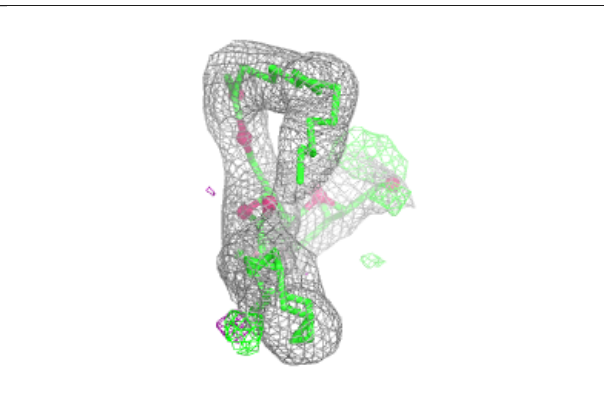
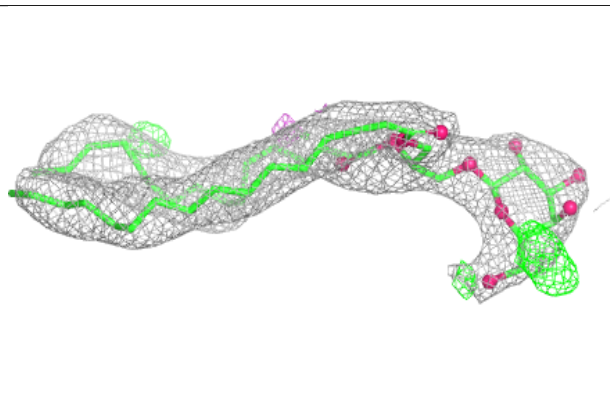
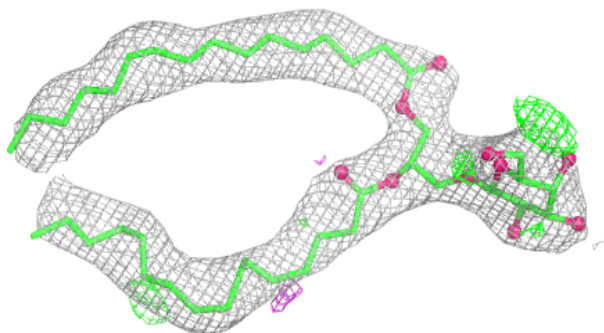


Electron density around CLA B 601:

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

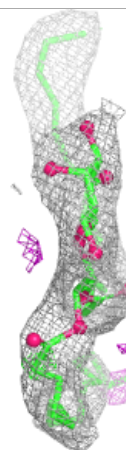
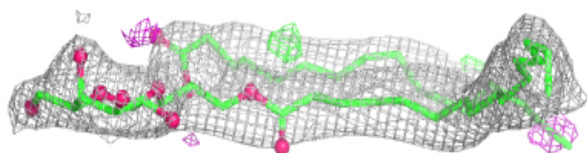
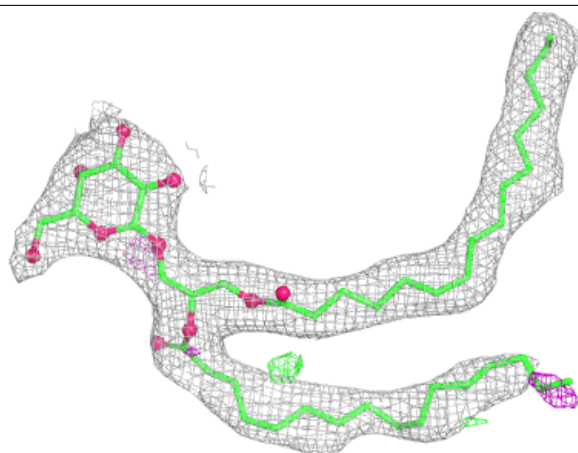
**Electron density around LMG C 501:**

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



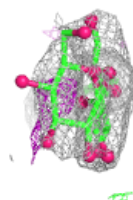
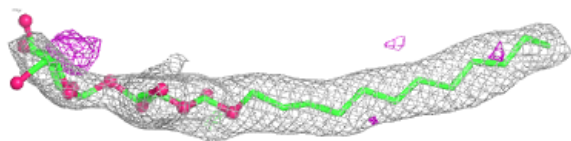
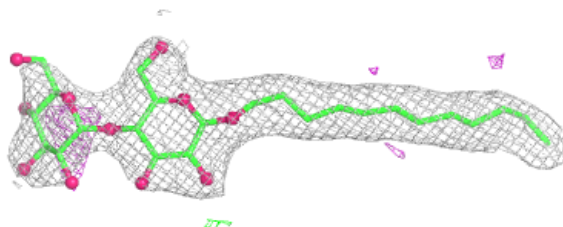
Electron density around LMG C 520:

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

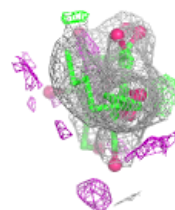
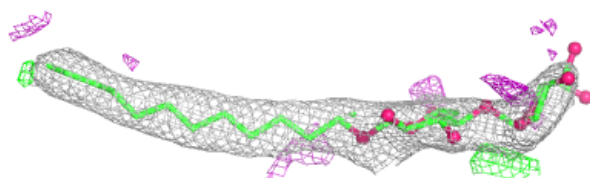
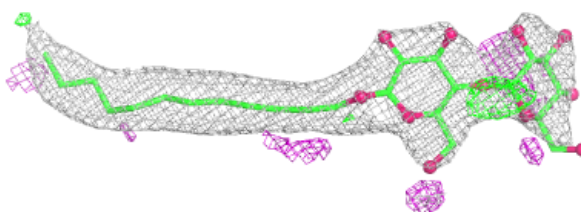


Electron density around LMT M 101:

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

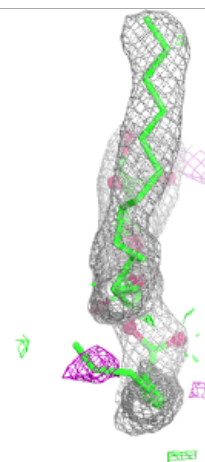
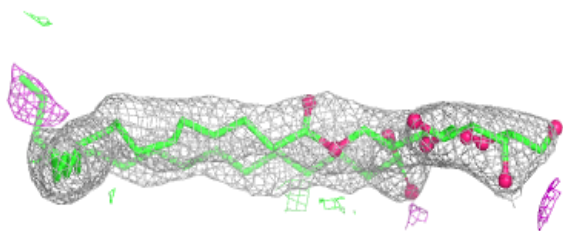
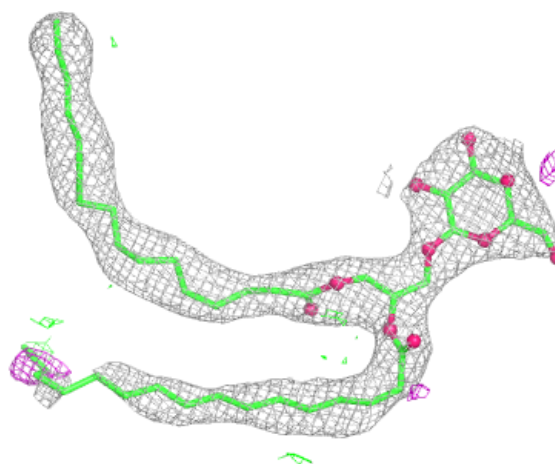
**Electron density around LMT m 103:**

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



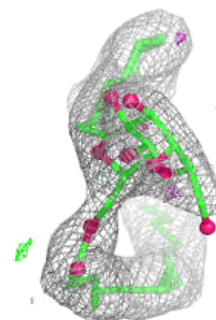
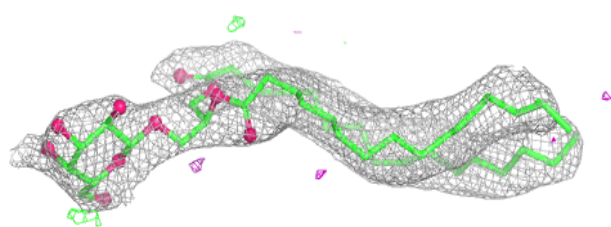
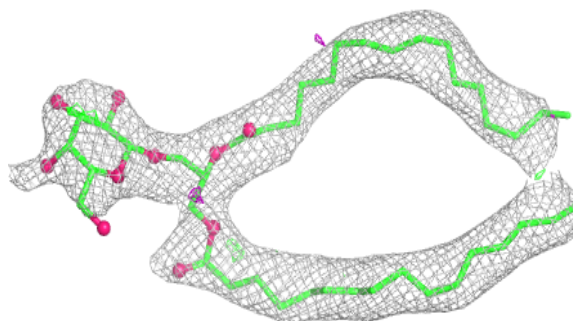
Electron density around LMG c 520:

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

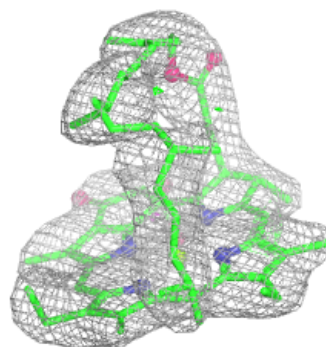
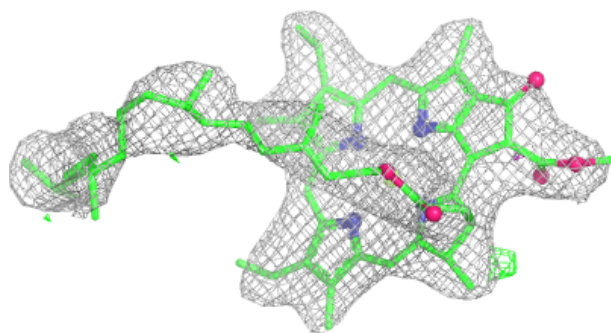
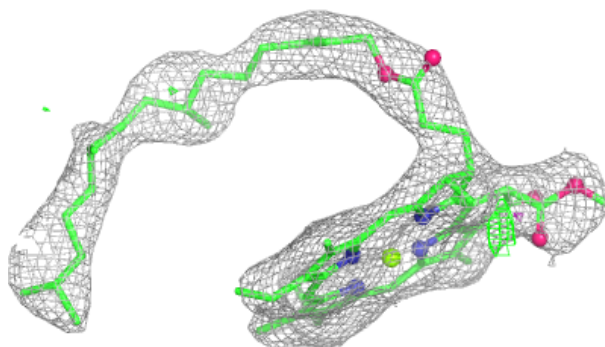


Electron density around LMG a 419:

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

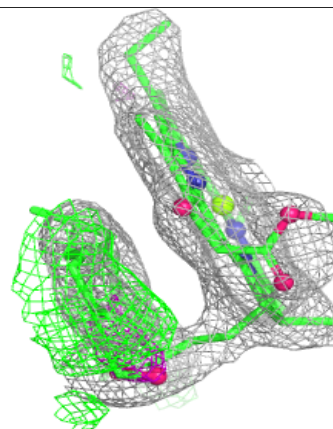
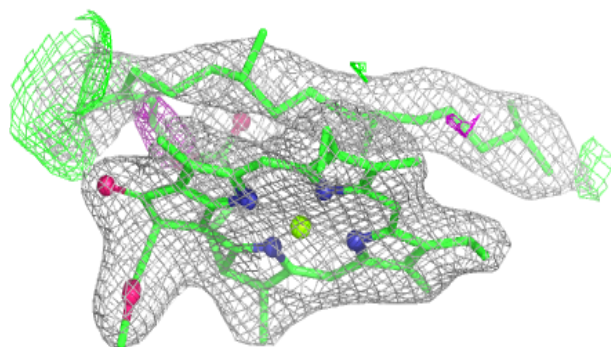
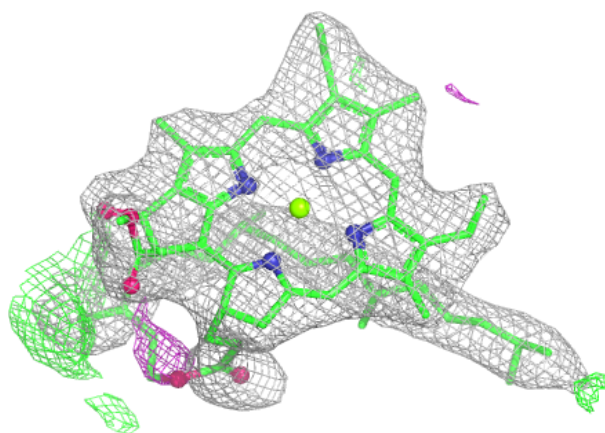
**Electron density around CLA C 514:**

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

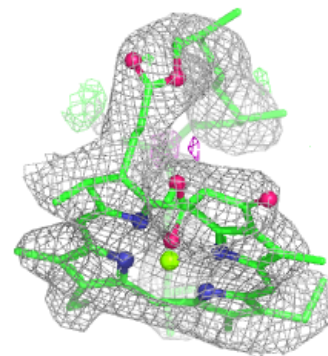
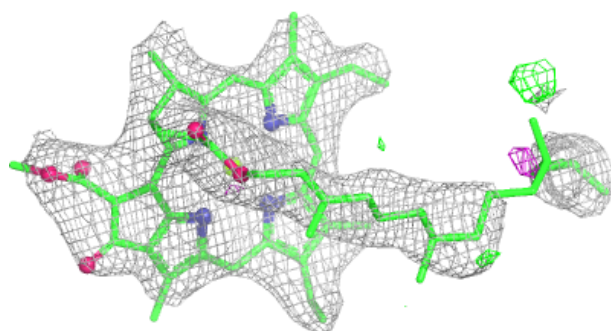
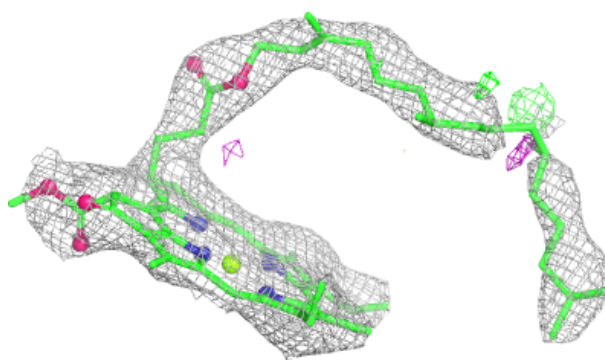


Electron density around CLA b 601:

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

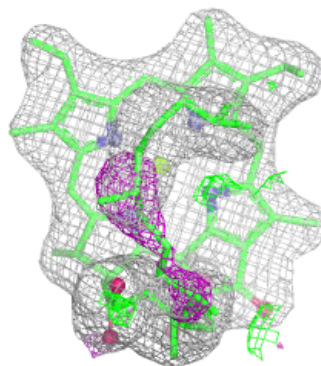
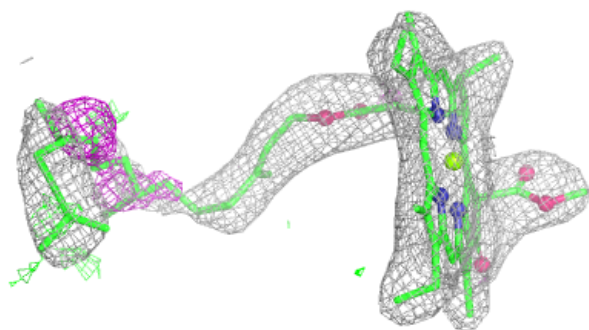
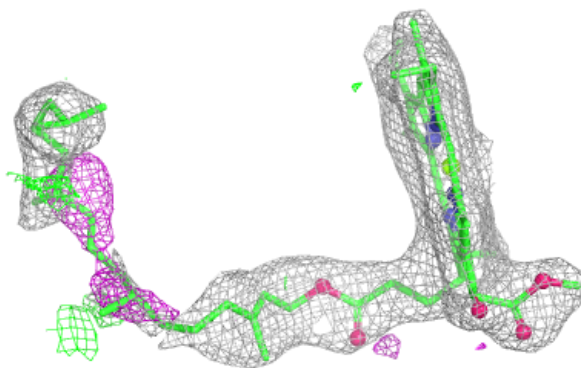
**Electron density around CLA c 514:**

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



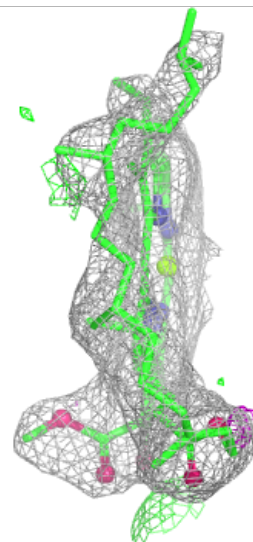
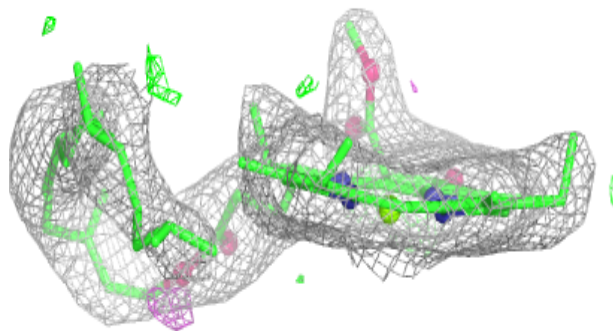
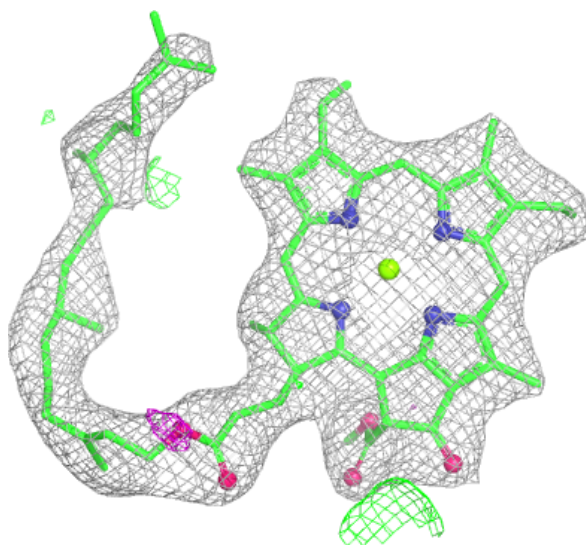
Electron density around CLA C 507:

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



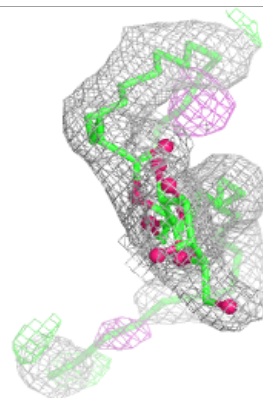
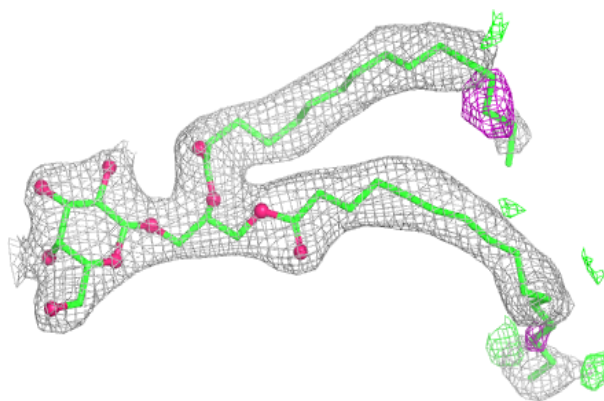
Electron density around CLA c 513:

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

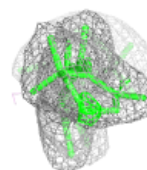
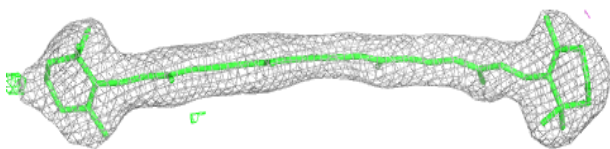
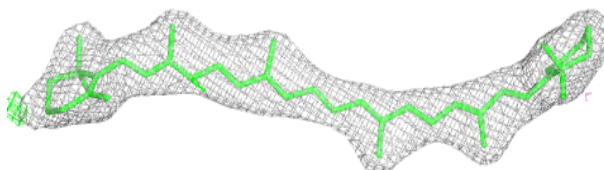


Electron density around LMG D 415:

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

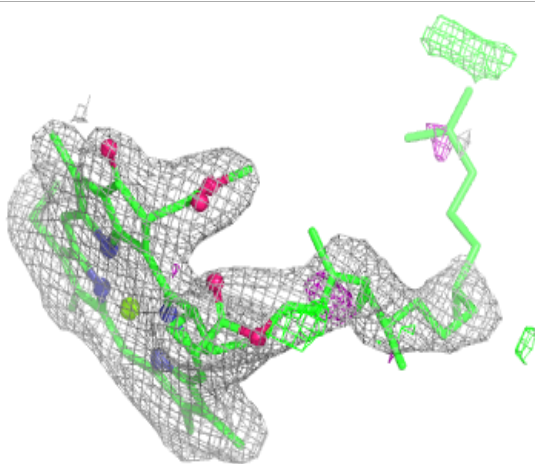
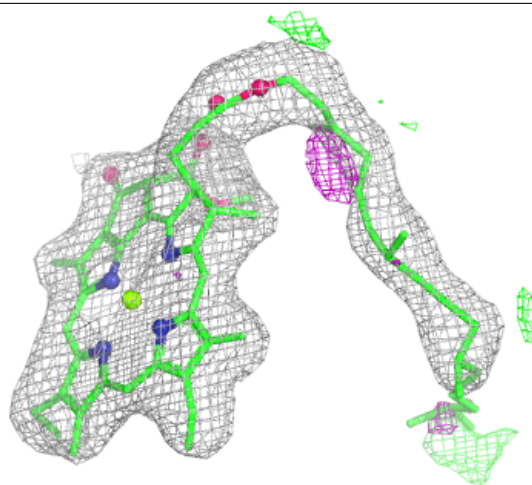
**Electron density around BCR h 101:**

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



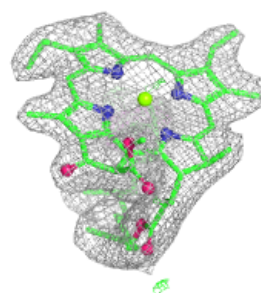
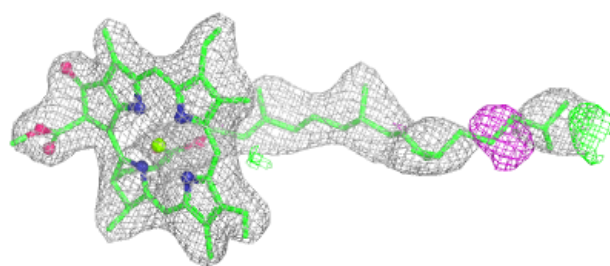
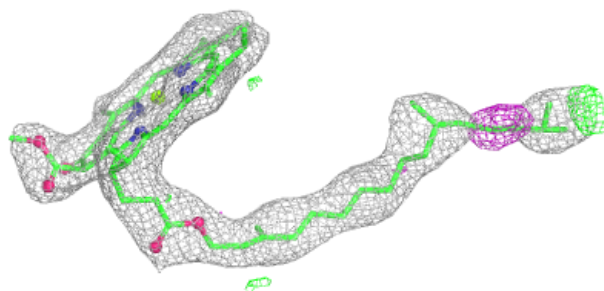
Electron density around CLA b 616:

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



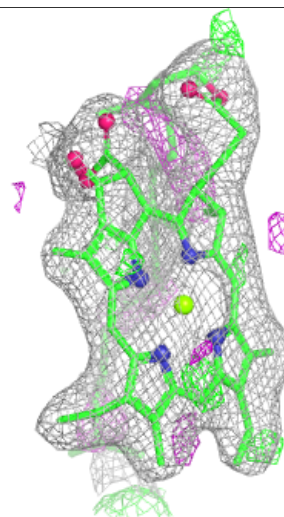
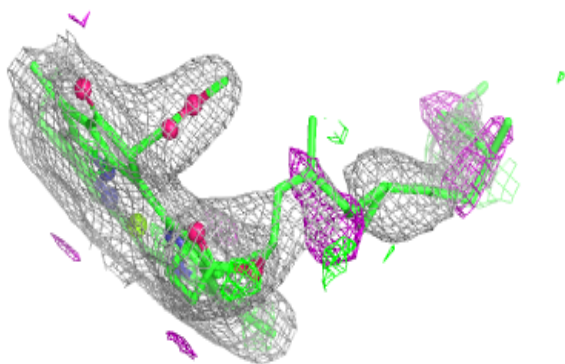
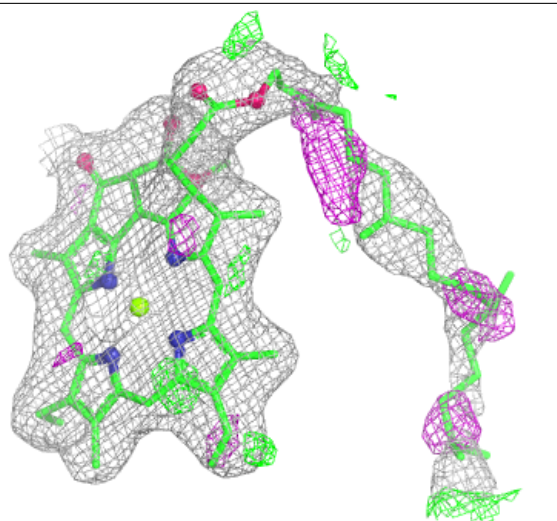
Electron density around CLA c 505:

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



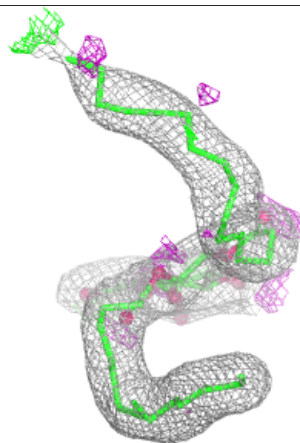
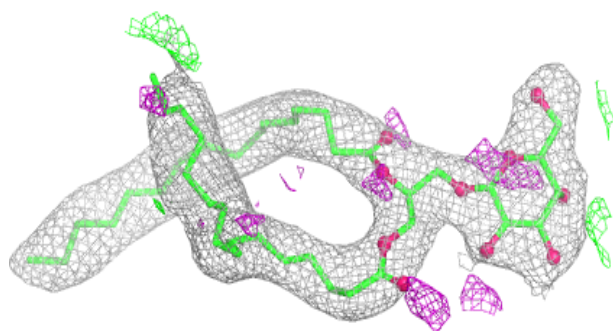
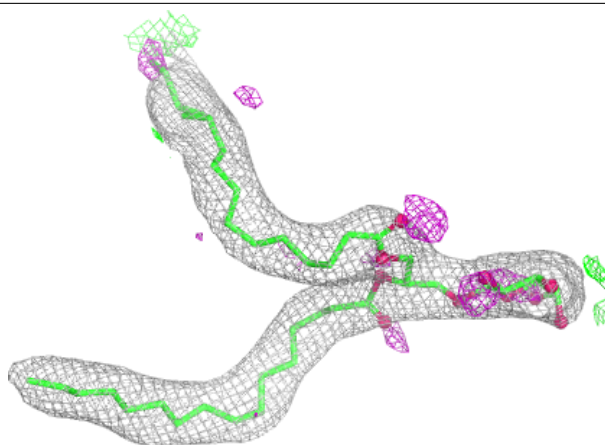
Electron density around CLA B 616:

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

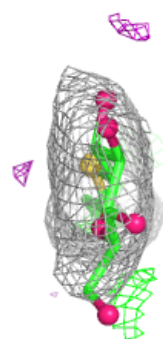
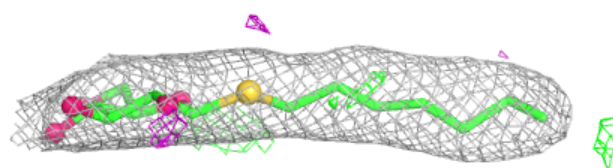
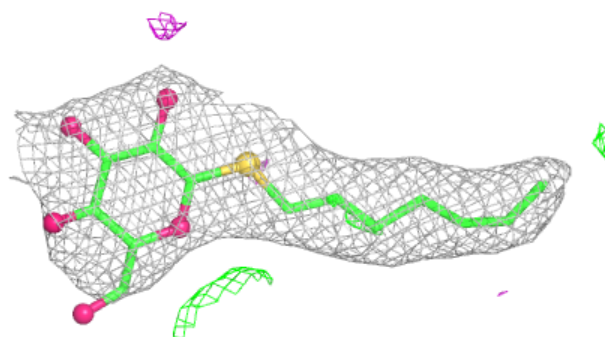


Electron density around LMG B 621:

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

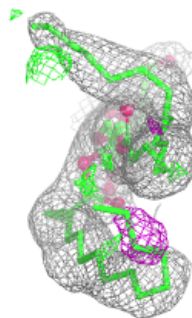
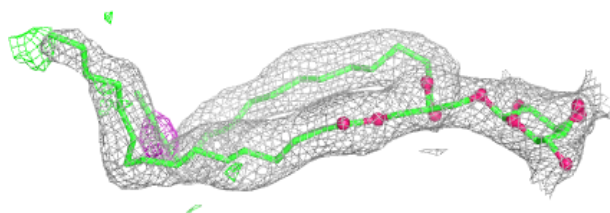
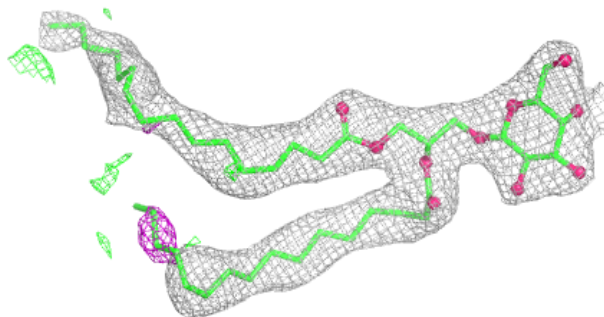
**Electron density around HTG b 625:**

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

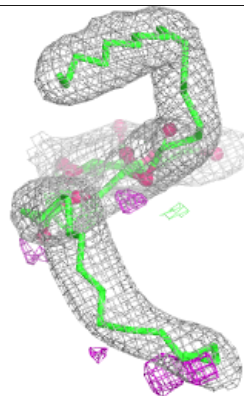
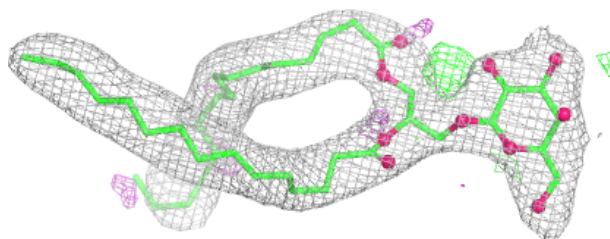
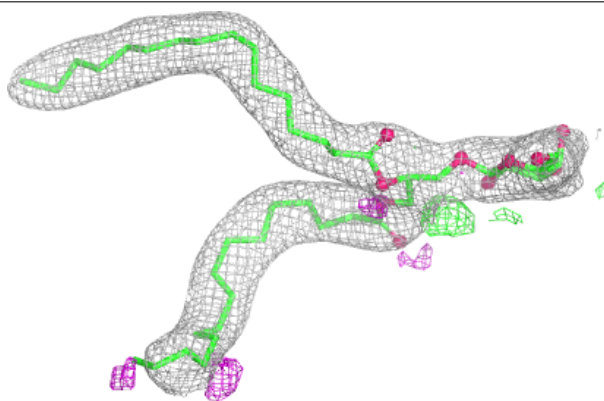


Electron density around LMG d 412:

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

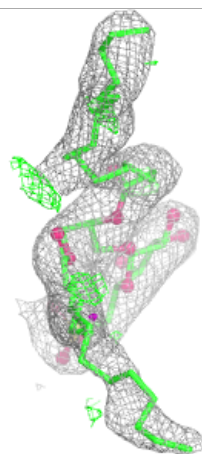
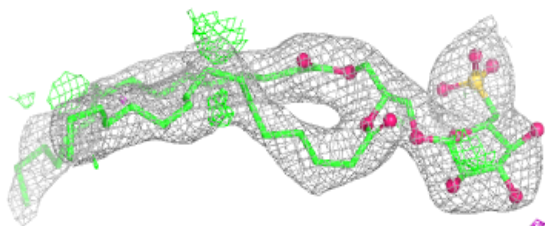
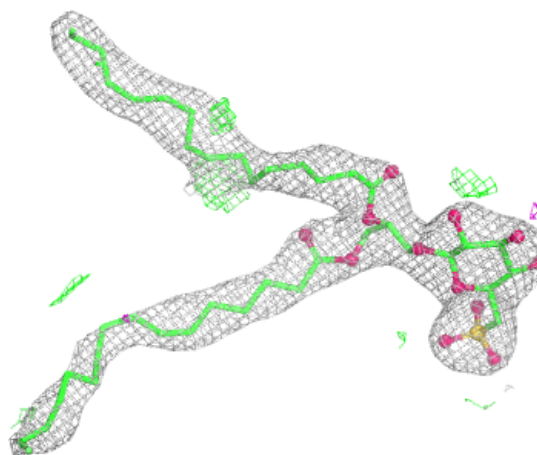
**Electron density around LMG m 101:**

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



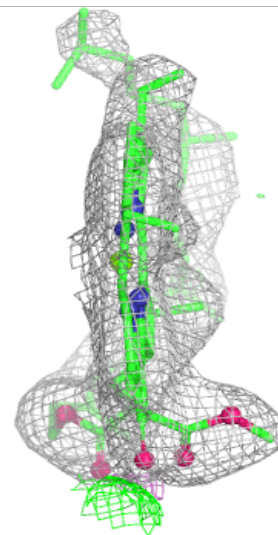
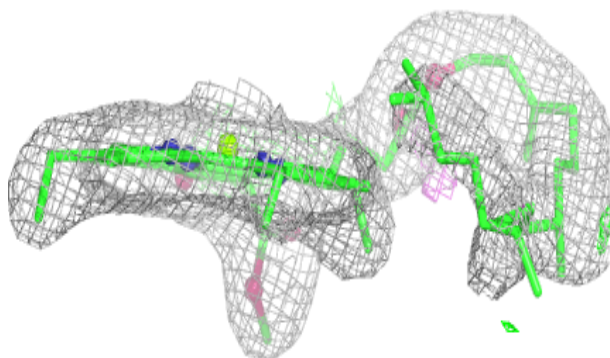
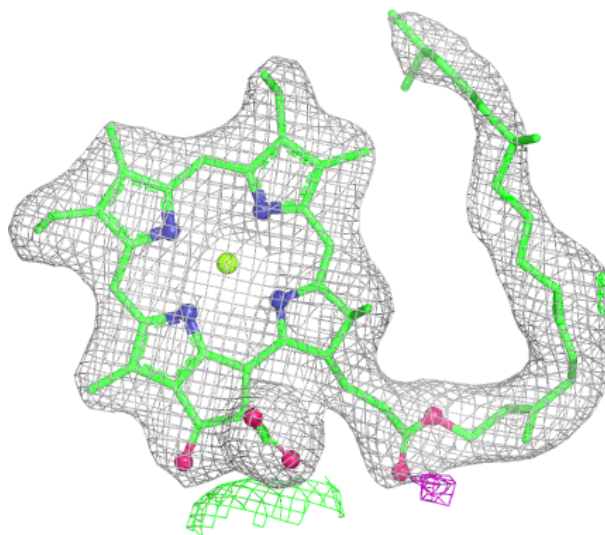
Electron density around SQD a 411:

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



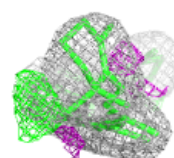
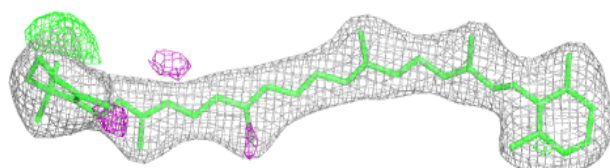
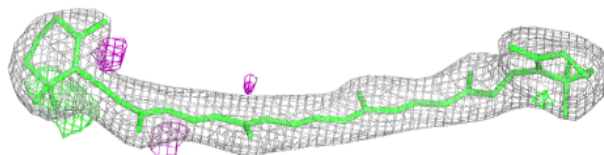
Electron density around CLA C 513:

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

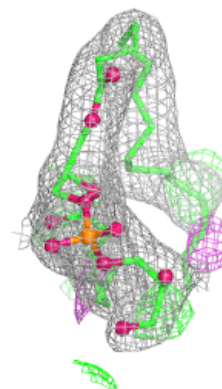
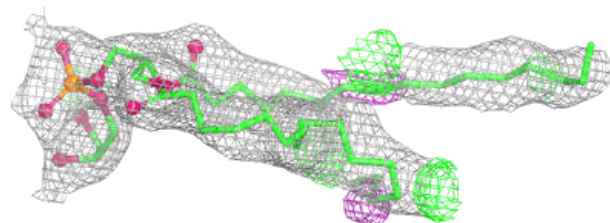
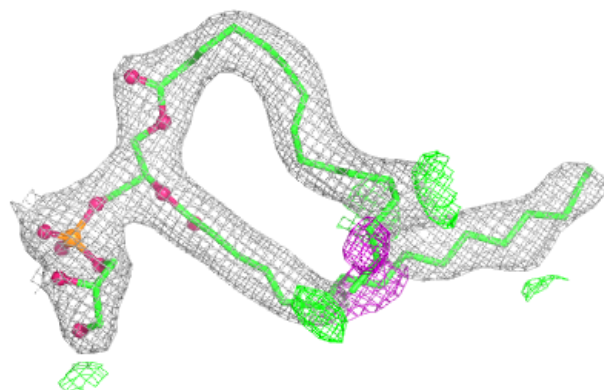


Electron density around BCR D 407:

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

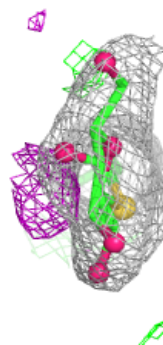
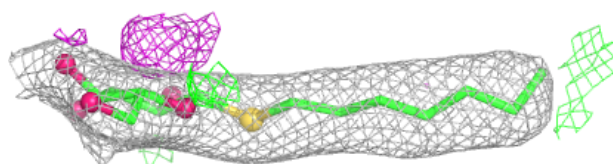
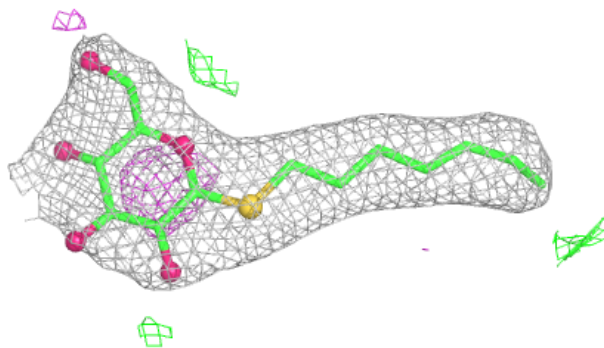
**Electron density around LHG d 408:**

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



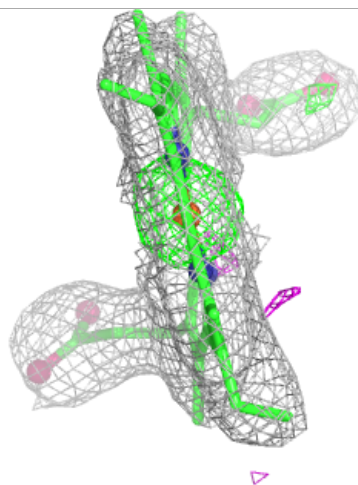
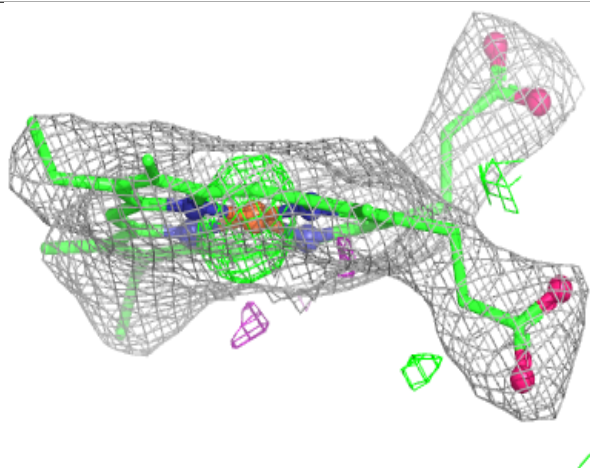
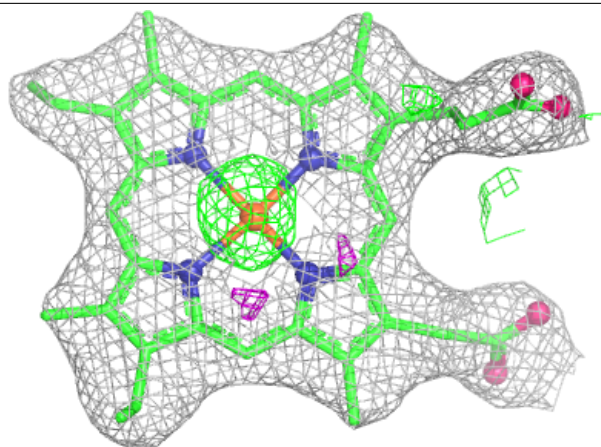
Electron density around HTG B 626:

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



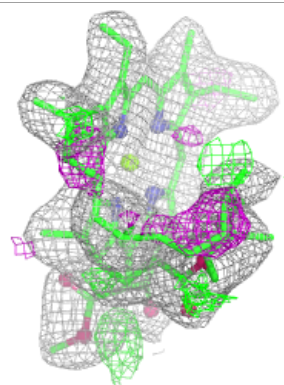
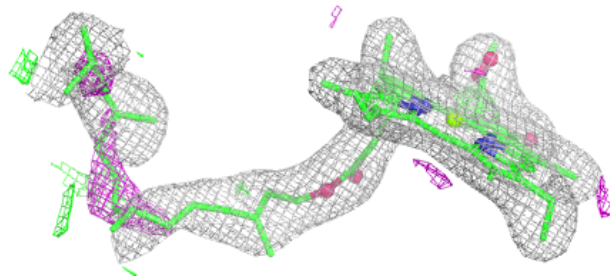
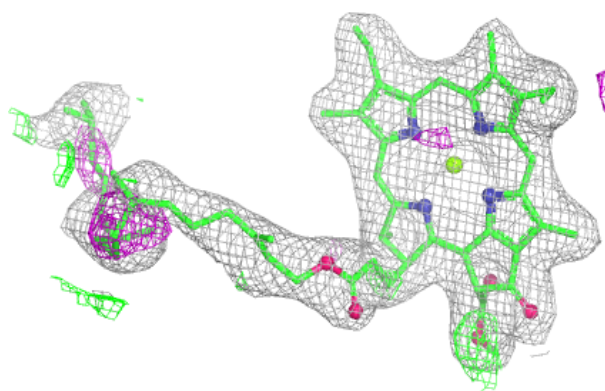
Electron density around HEM E 103:

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

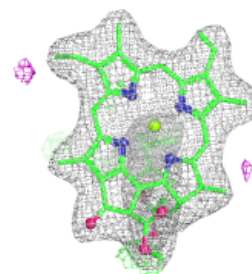
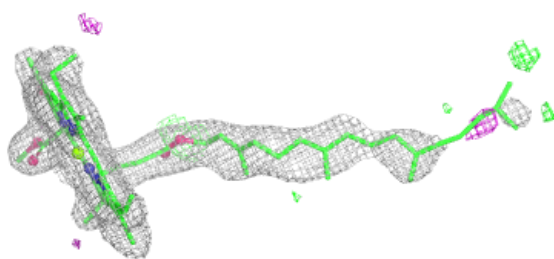
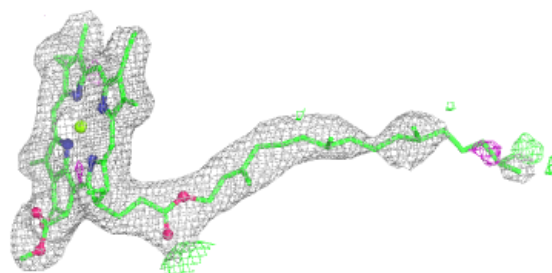


Electron density around CLA A 408:

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

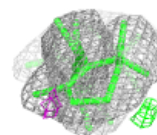
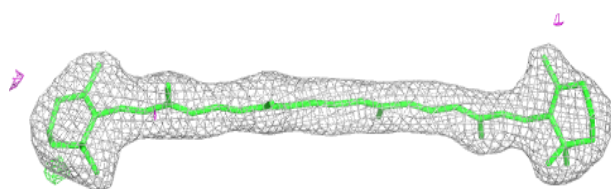
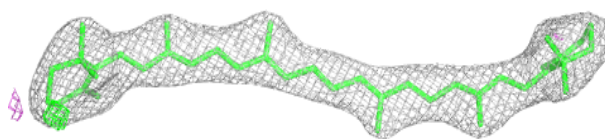
**Electron density around CLA d 403:**

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

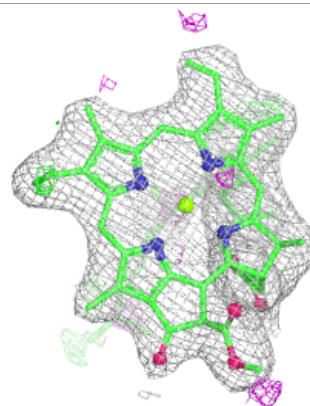
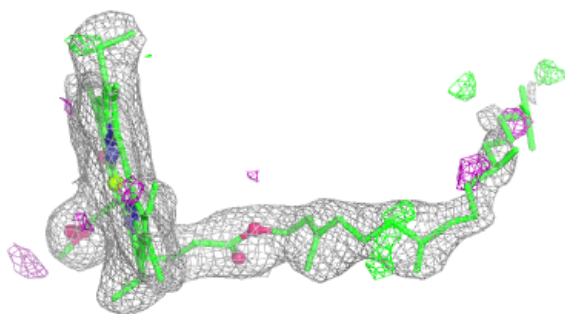
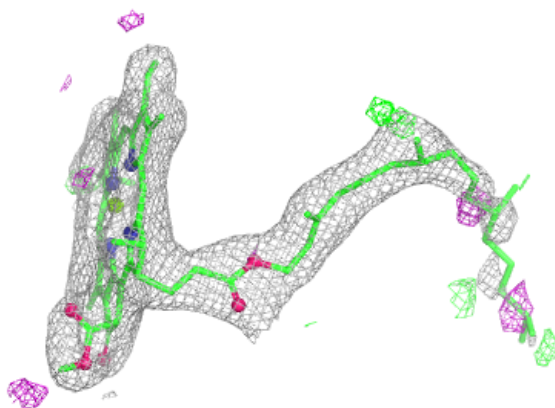


Electron density around BCR C 515:

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

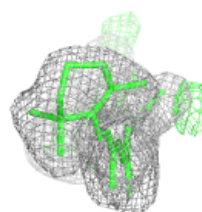
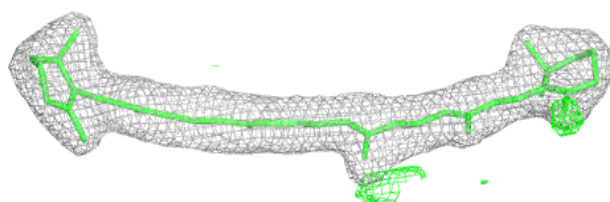
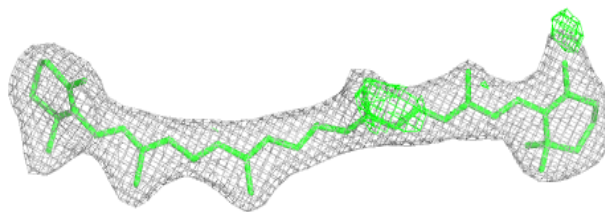
**Electron density around CLA D 406:**

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

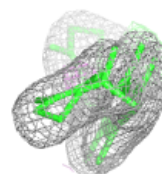
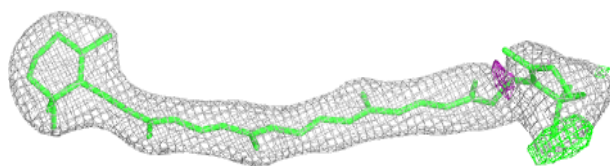
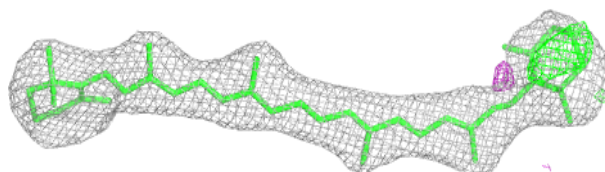


Electron density around BCR T 101:

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

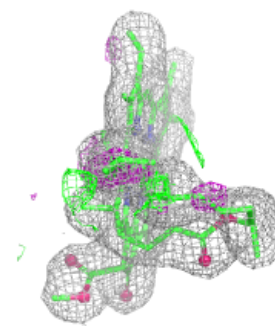
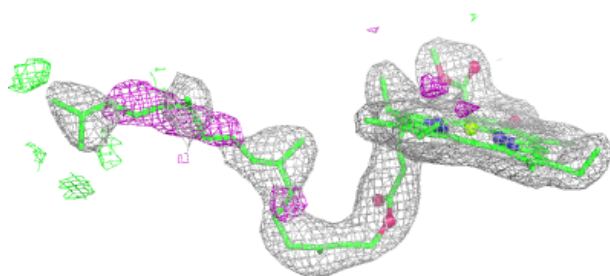
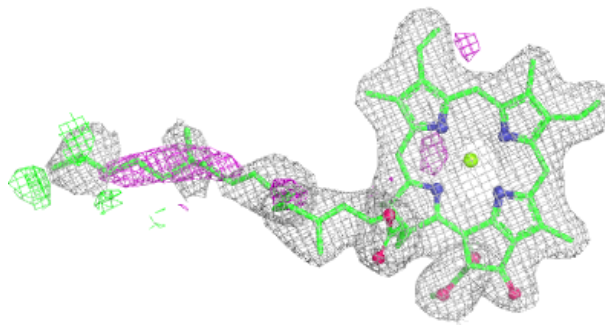
**Electron density around BCR d 404:**

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

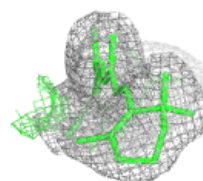
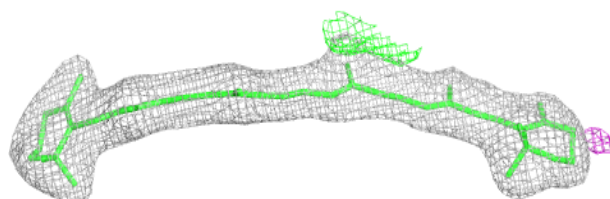
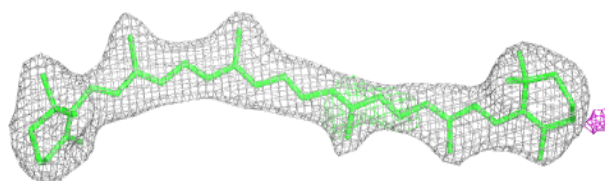


Electron density around CLA a 407:

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

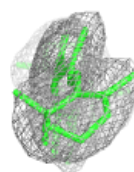
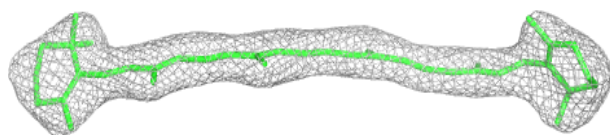
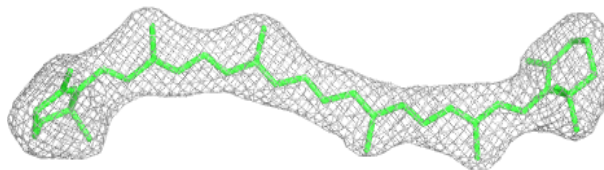
**Electron density around BCR t 103:**

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



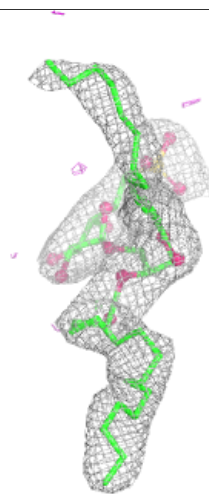
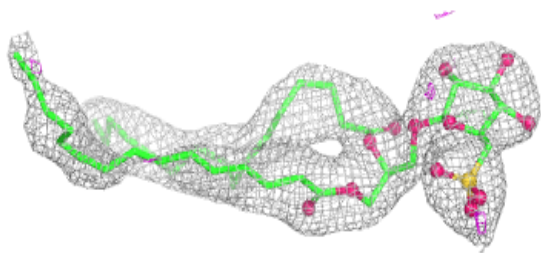
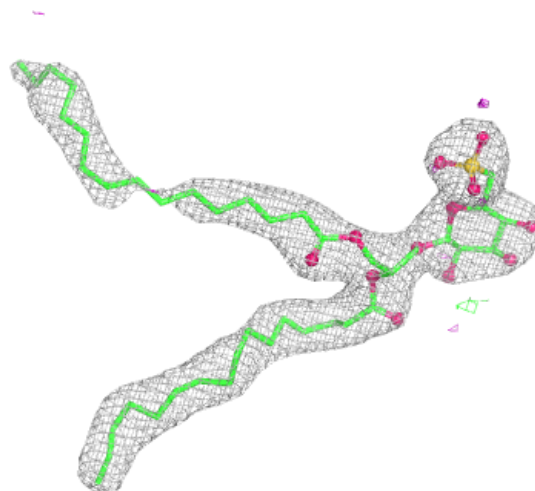
Electron density around BCR y 101:

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



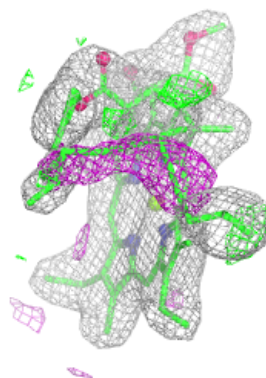
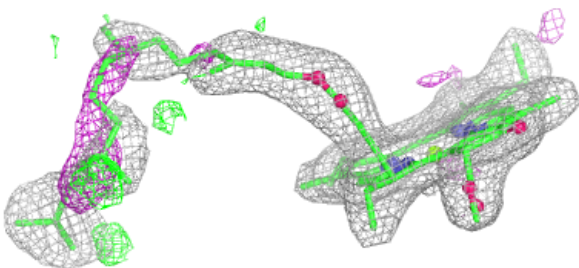
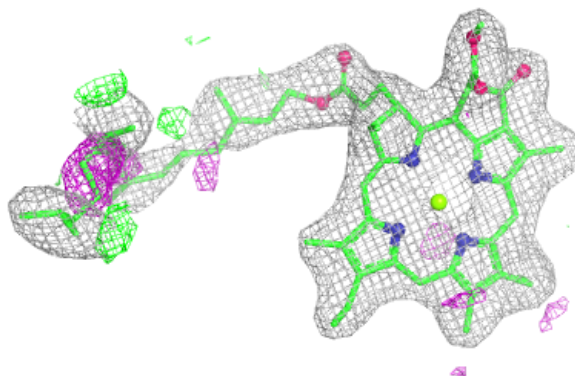
Electron density around SQD A 410:

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

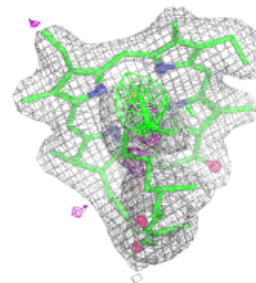
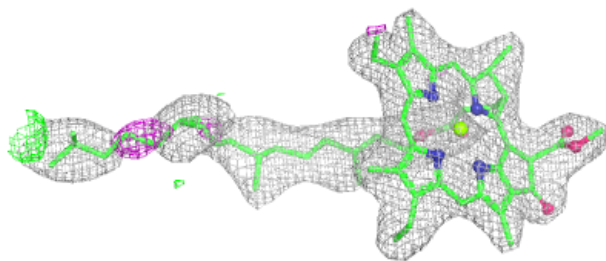
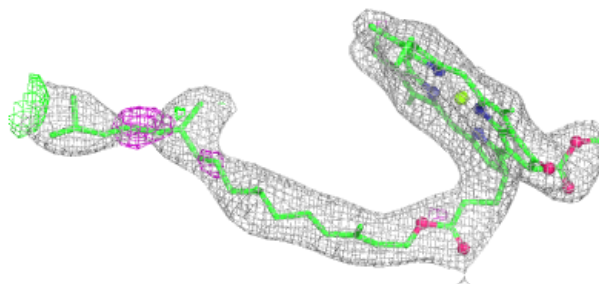


Electron density around CLA a 409:

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

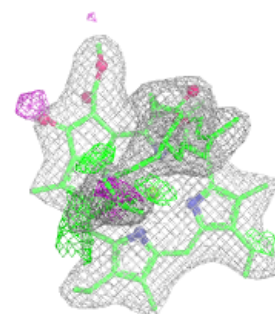
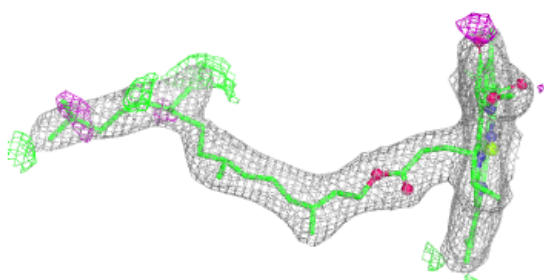
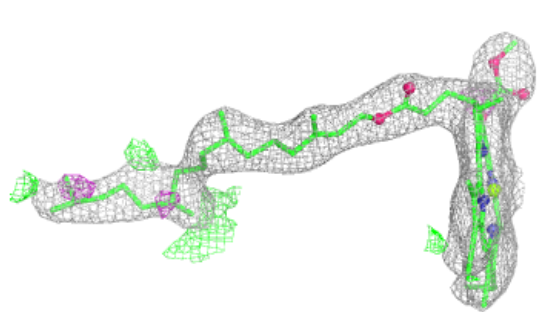
**Electron density around CLA C 505:**

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

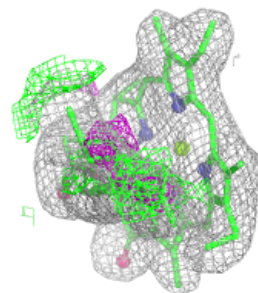
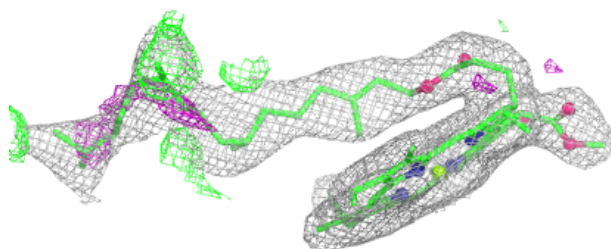
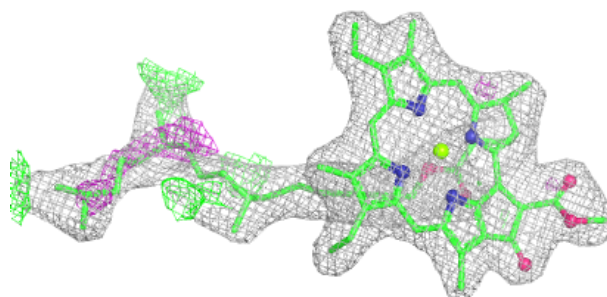


Electron density around CLA b 606:

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

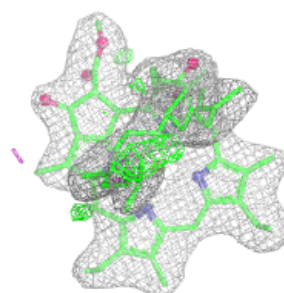
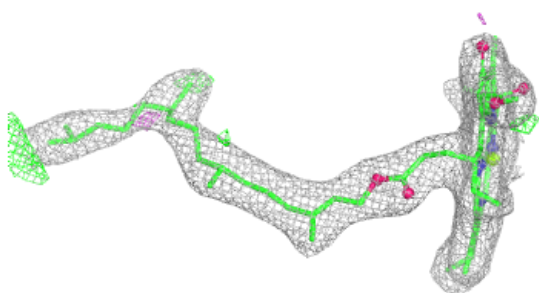
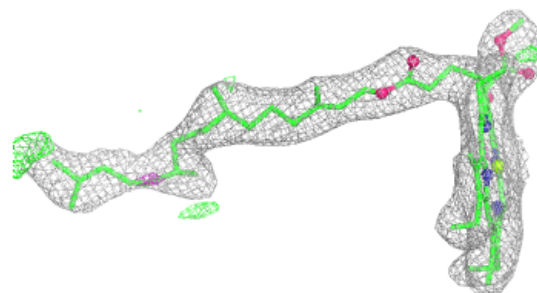
**Electron density around CLA b 614:**

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

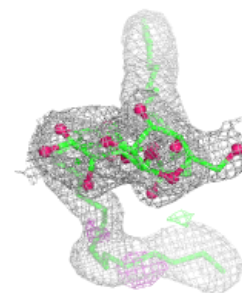
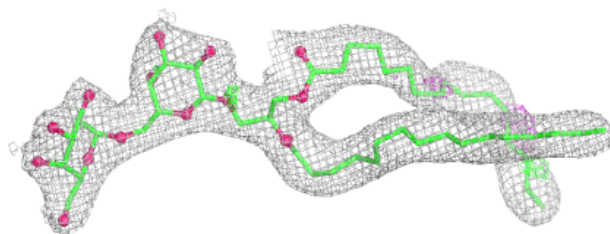
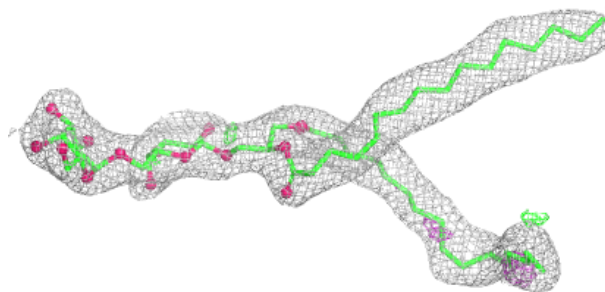


Electron density around CLA B 606:

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

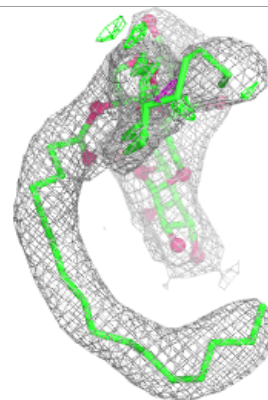
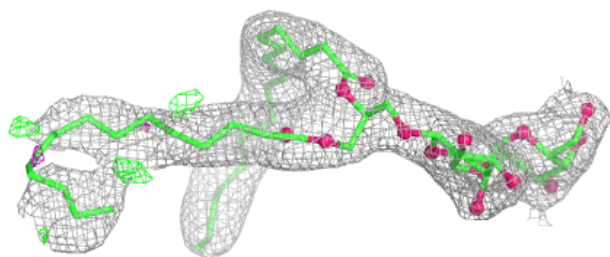
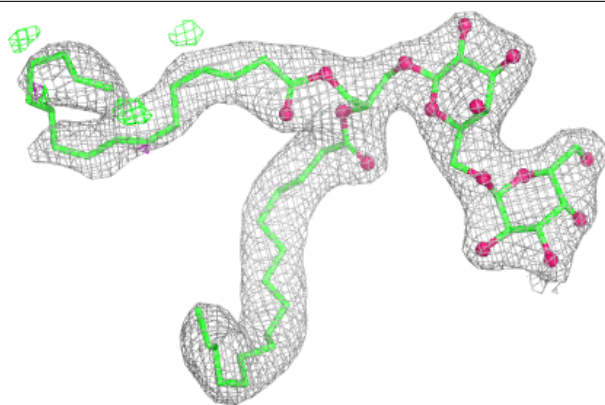
**Electron density around DGD C 517:**

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

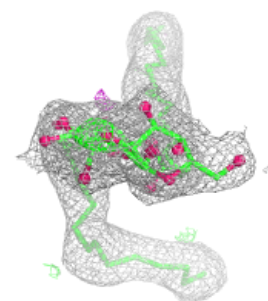
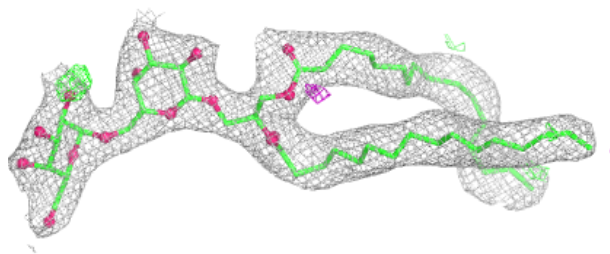
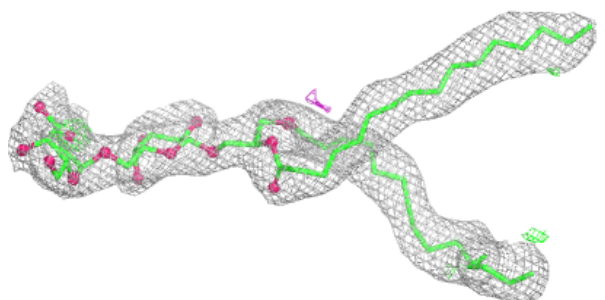


Electron density around DGD C 518:

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

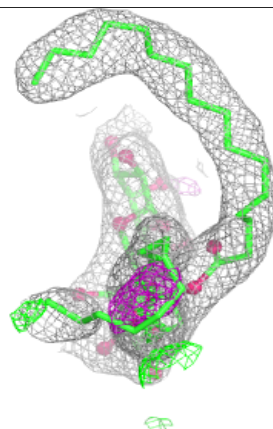
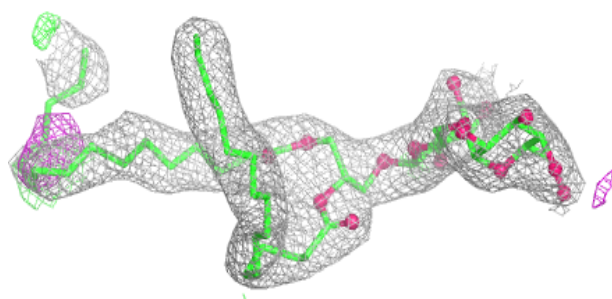
**Electron density around DGD c 517:**

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

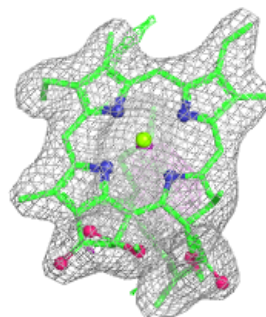
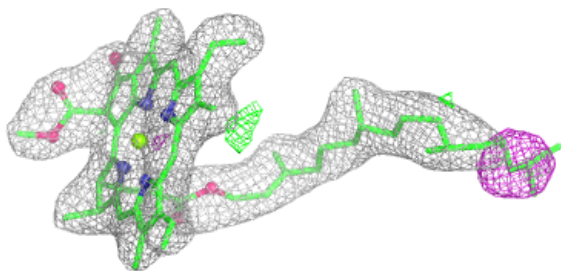
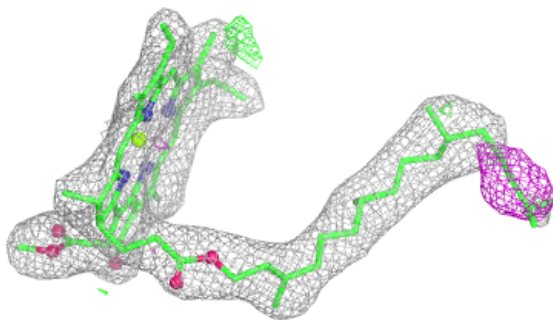


Electron density around DGD c 518:

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

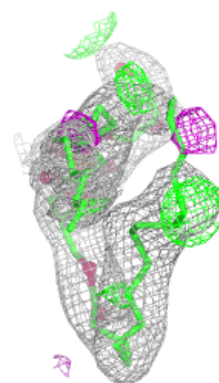
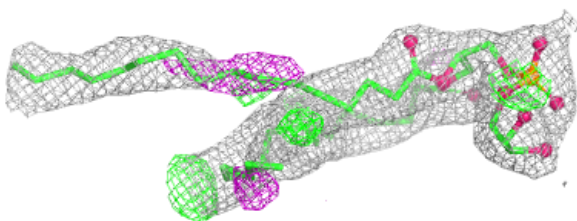
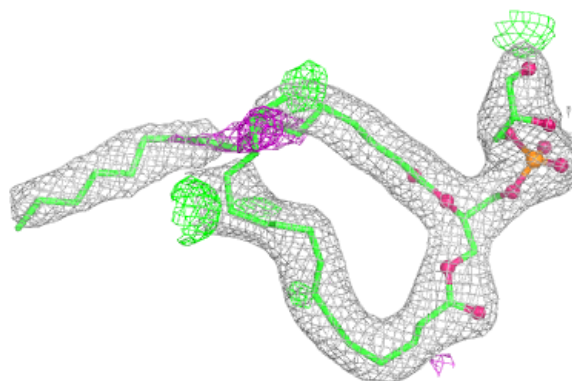
**Electron density around CLA C 509:**

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

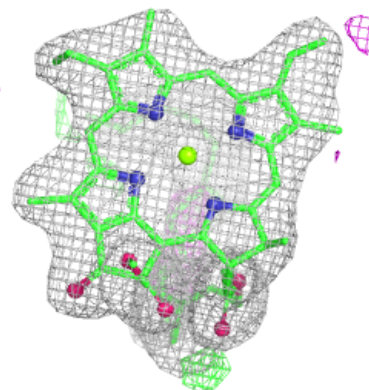
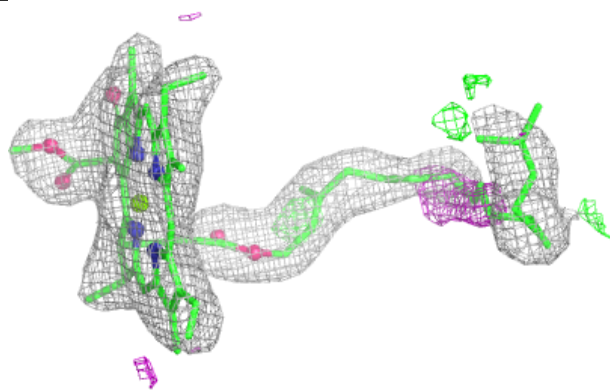
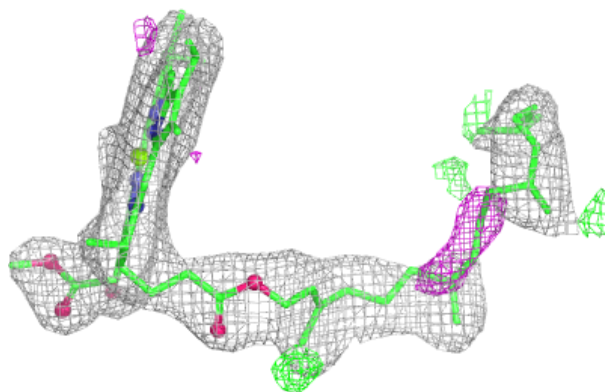


Electron density around LHG D 411:

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

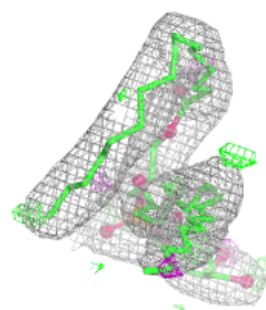
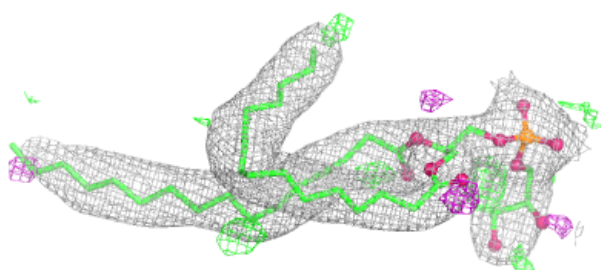
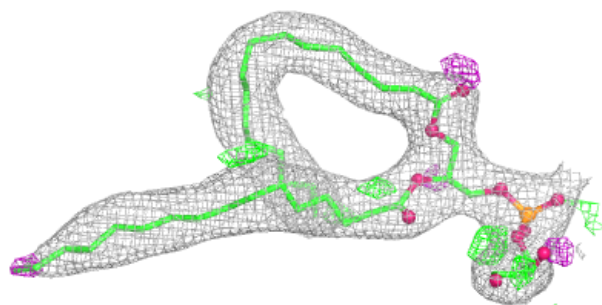
**Electron density around CLA c 507:**

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

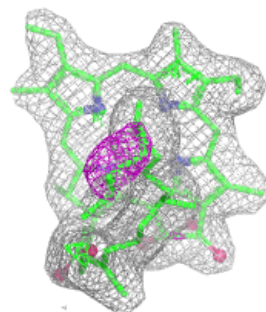
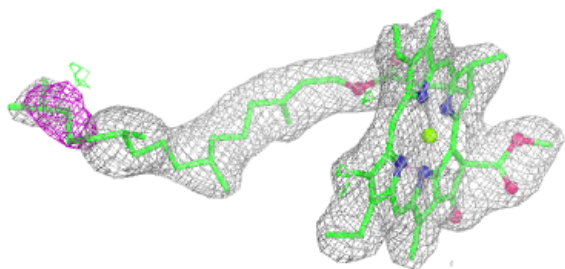
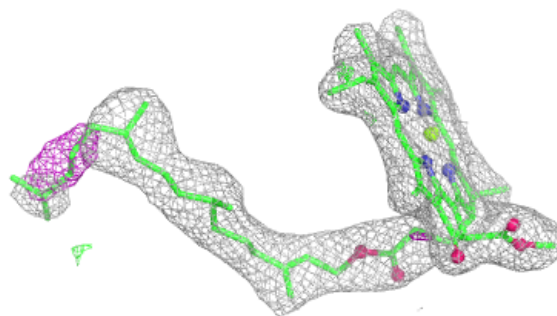


Electron density around LHG d 406:

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

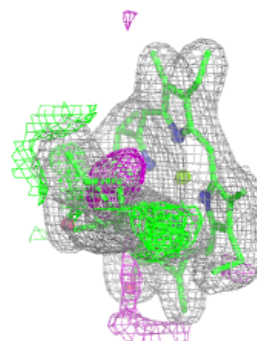
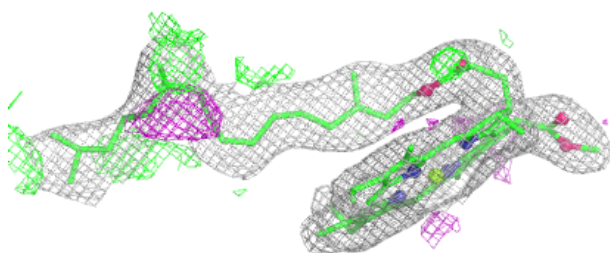
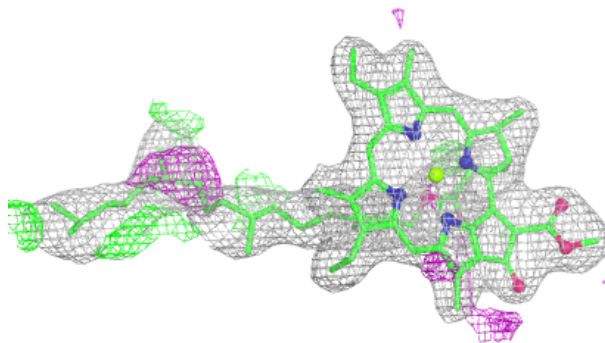
**Electron density around CLA c 509:**

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

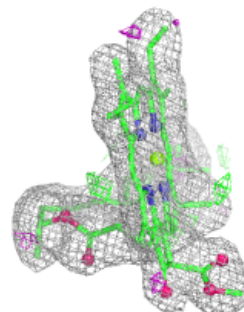
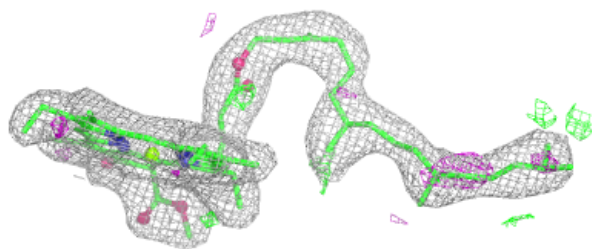
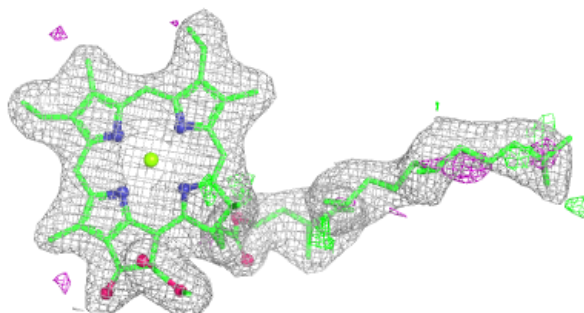


Electron density around CLA B 614:

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

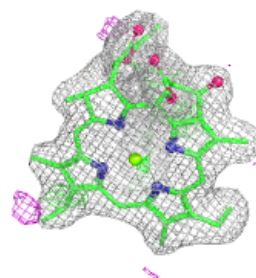
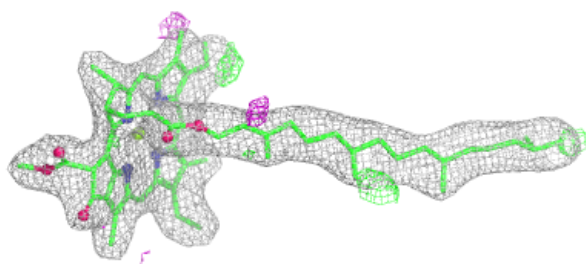
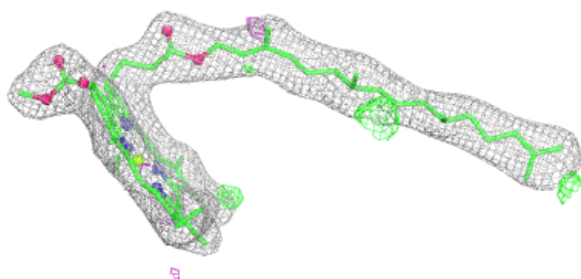
**Electron density around CLA A 406:**

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

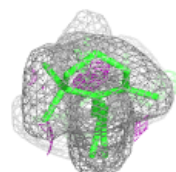
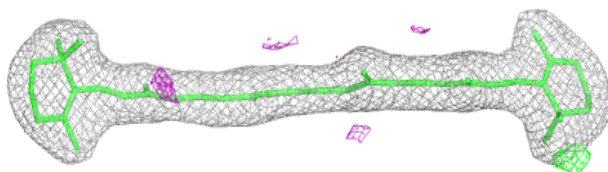
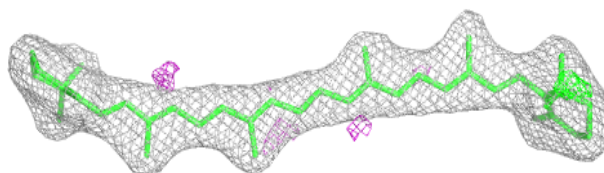


Electron density around CLA b 607:

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

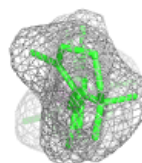
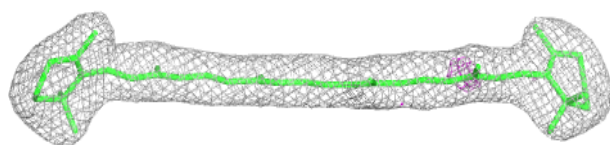
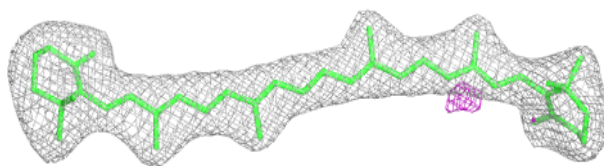
**Electron density around BCR A 409:**

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

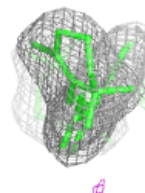
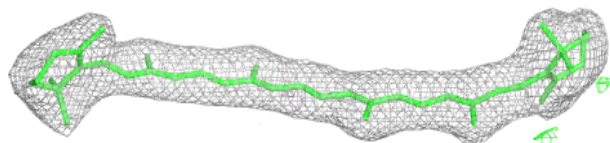
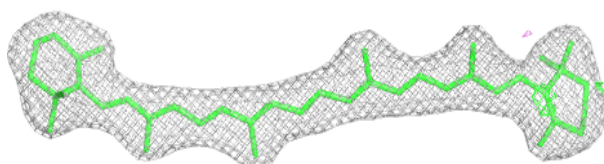


Electron density around BCR B 618:

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

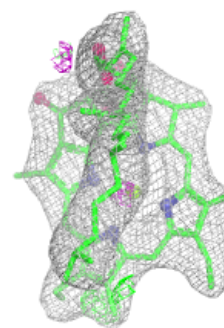
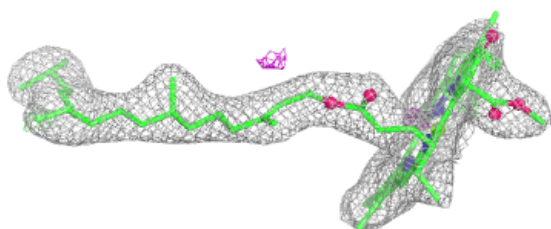
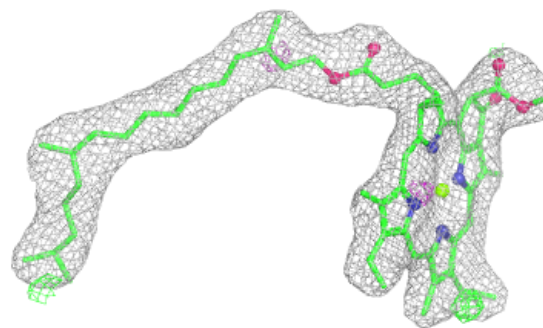
**Electron density around BCR B 619:**

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

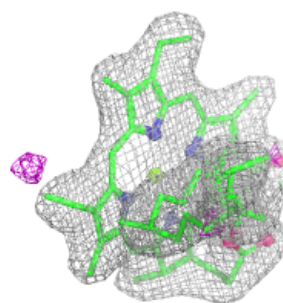
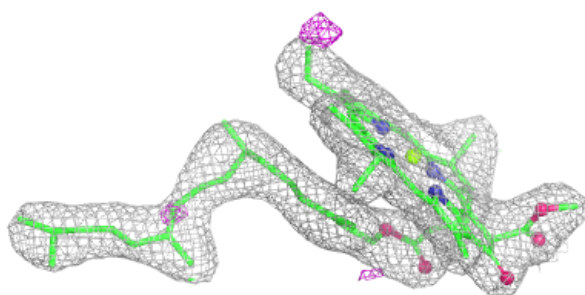
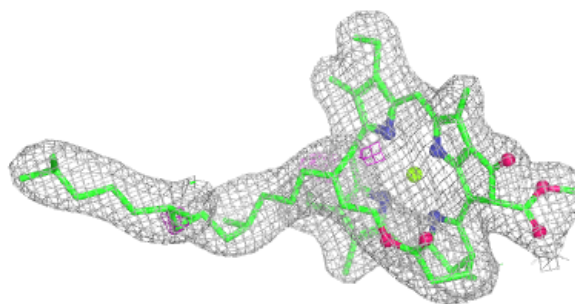


Electron density around CLA b 609:

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

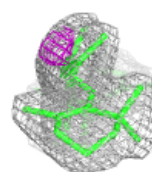
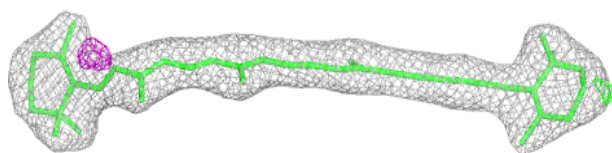
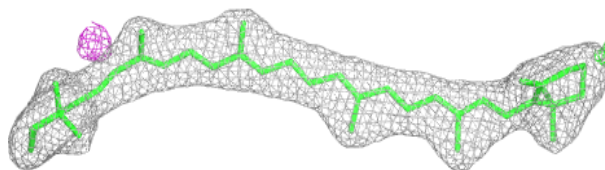
**Electron density around CLA C 506:**

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

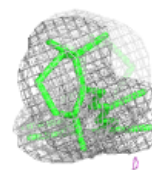
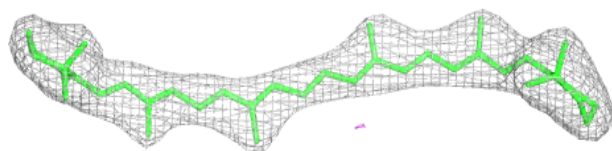
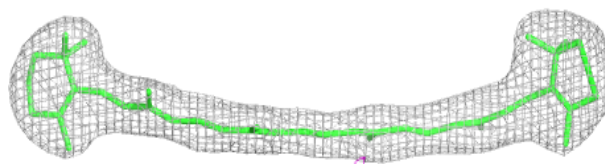


Electron density around BCR H 101:

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

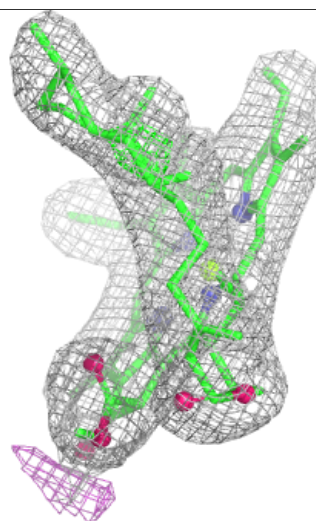
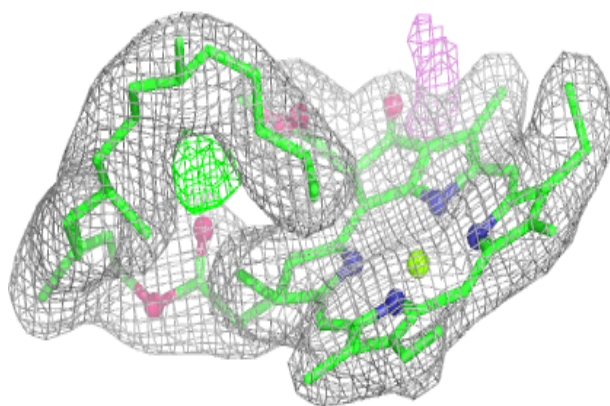
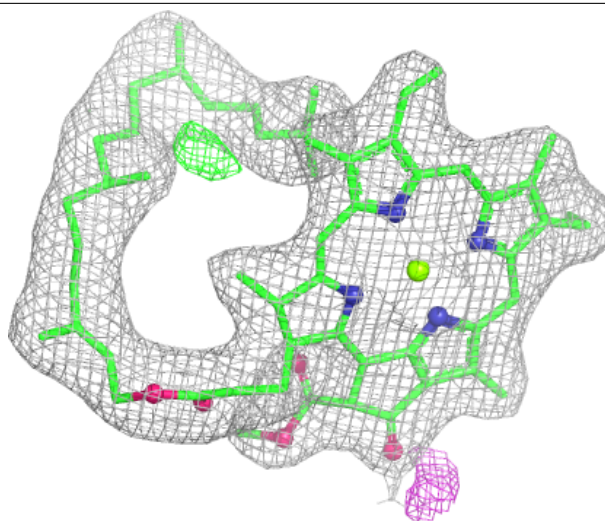
**Electron density around BCR K 102:**

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



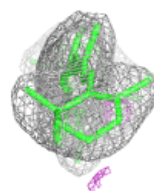
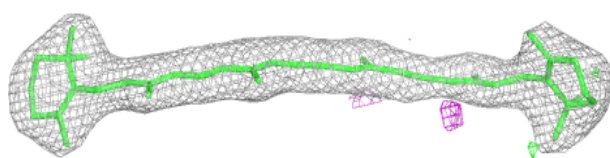
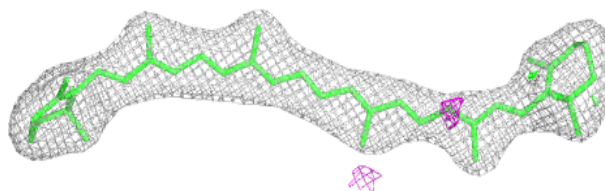
Electron density around CLA b 615:

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

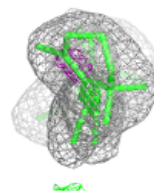
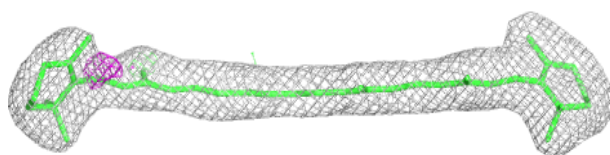
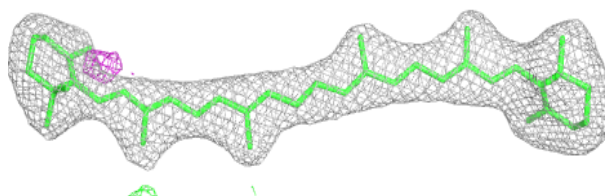


Electron density around BCR Y 101:

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

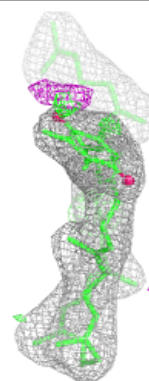
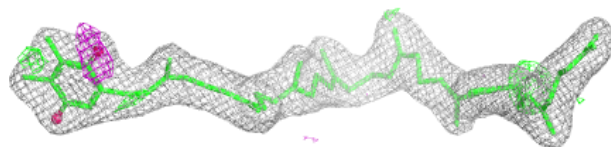
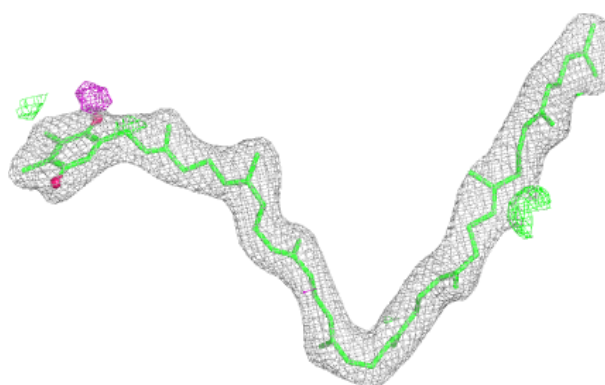
**Electron density around BCR b 618:**

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

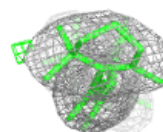
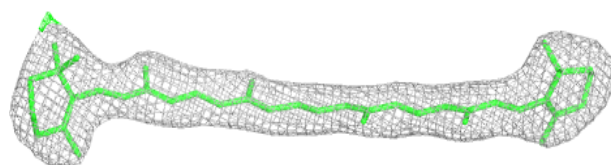


Electron density around PL9 D 408:

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

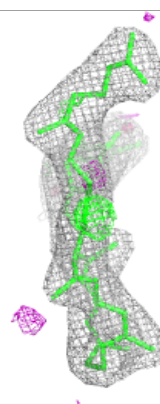
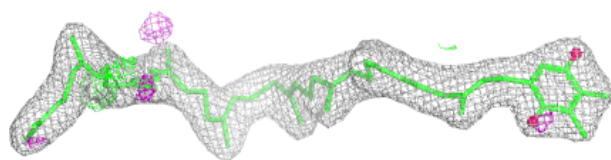
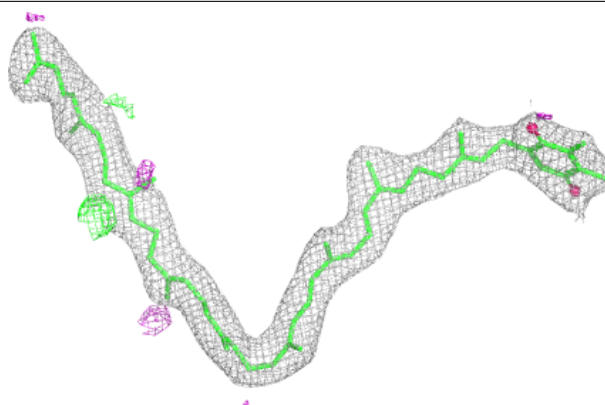
**Electron density around BCR c 515:**

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

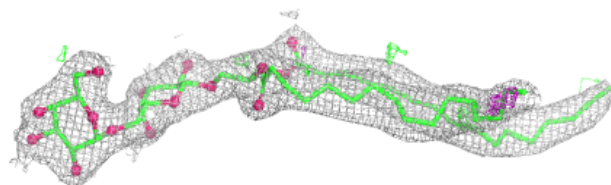
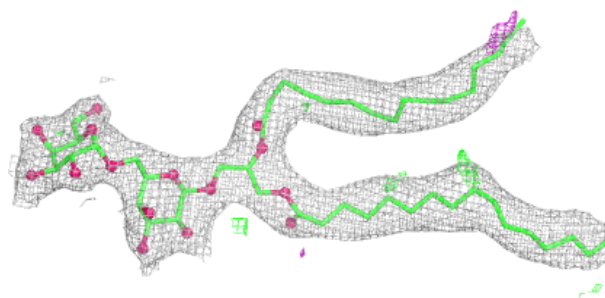


Electron density around PL9 d 405:

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

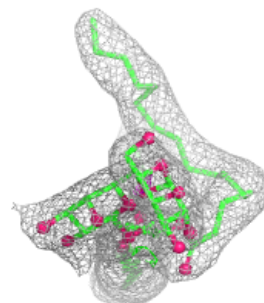
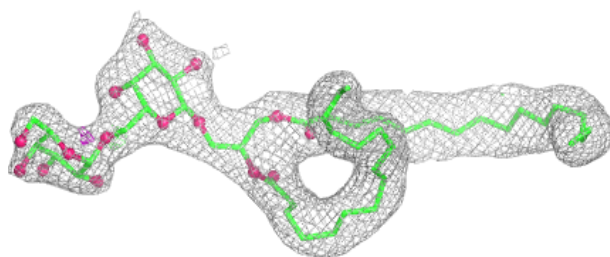
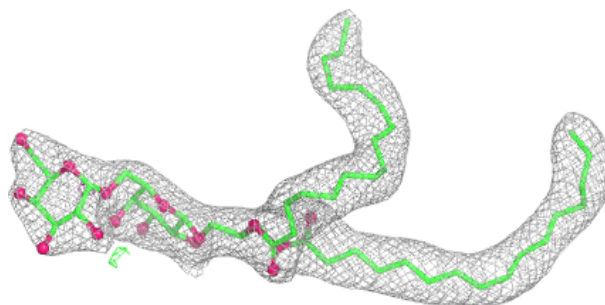
**Electron density around DGD C 519:**

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

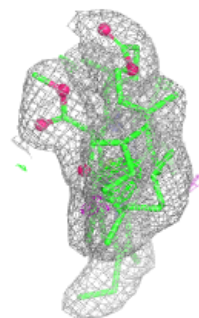
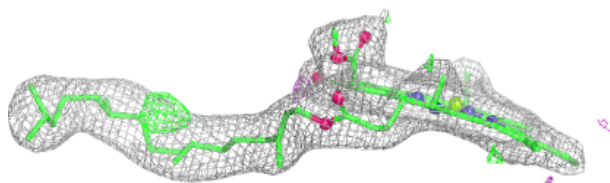
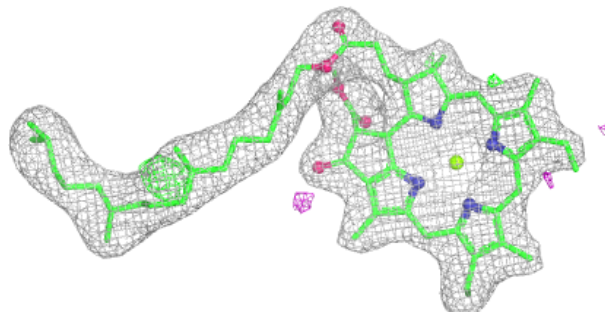


Electron density around DGD H 102:

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

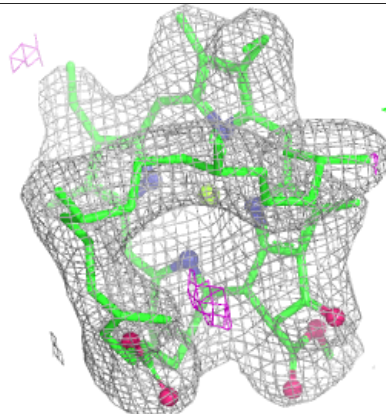
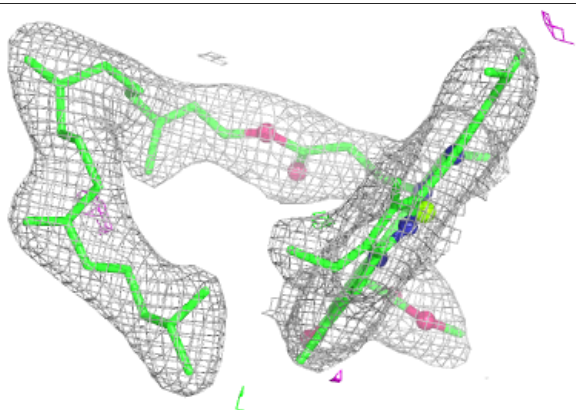
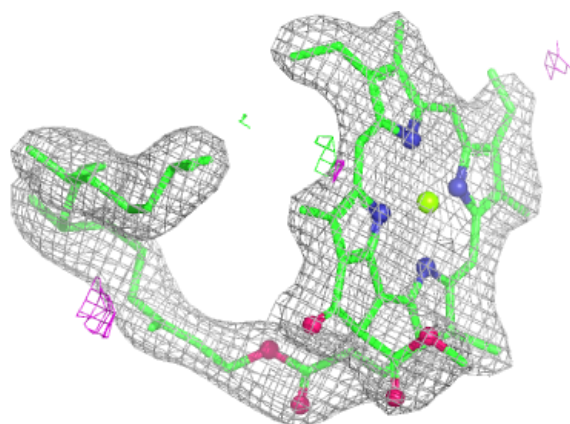
**Electron density around CLA B 602:**

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

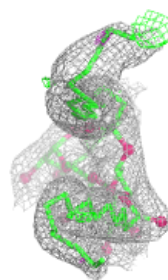
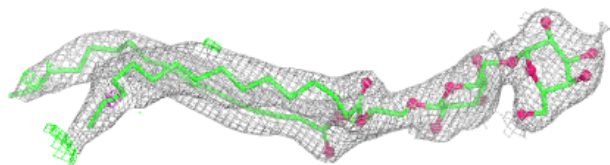
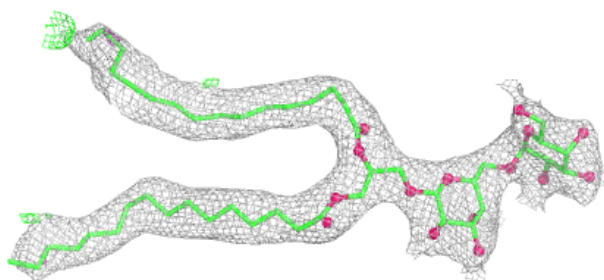


Electron density around CLA c 504:

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

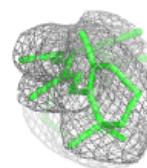
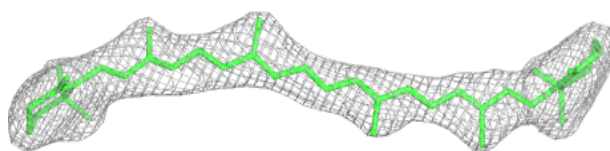
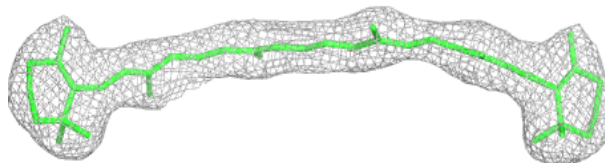
**Electron density around DGD c 519:**

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

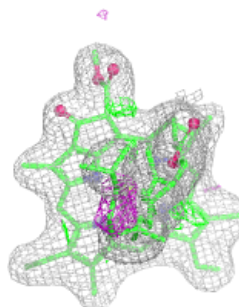
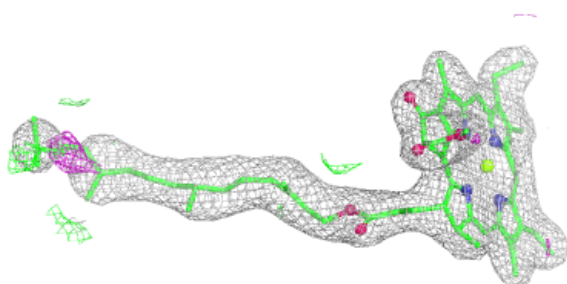
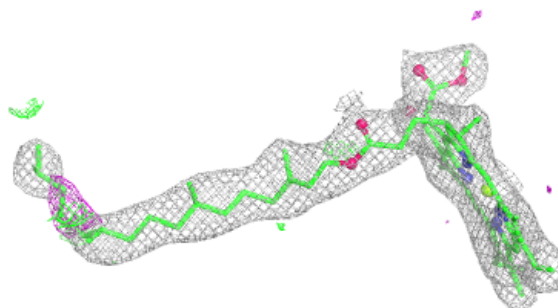


Electron density around BCR k 101:

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

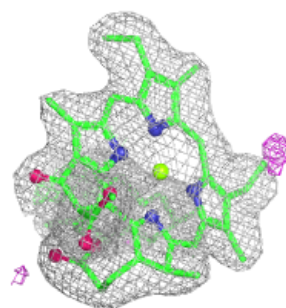
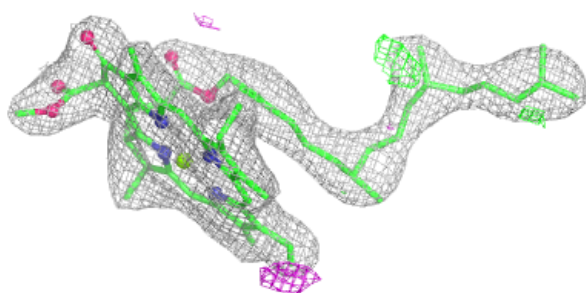
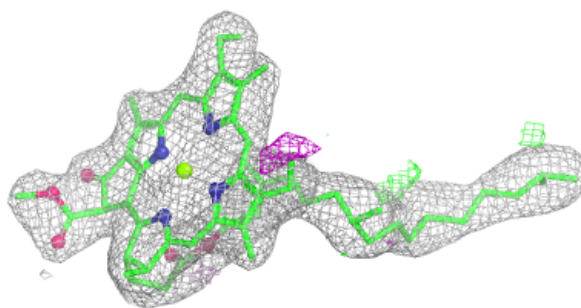
**Electron density around CLA B 604:**

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

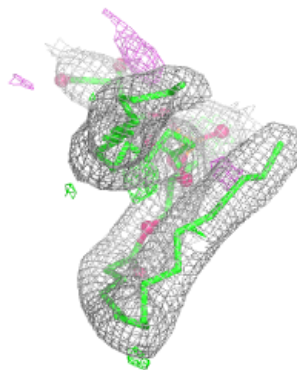
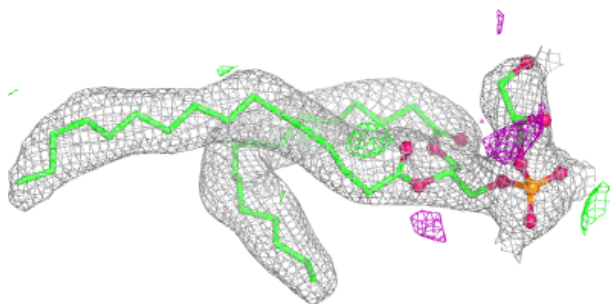
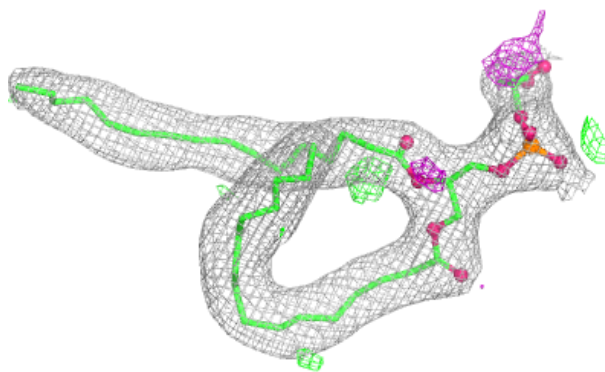


Electron density around CLA c 506:

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

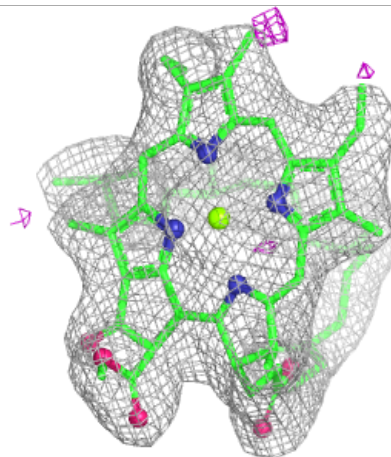
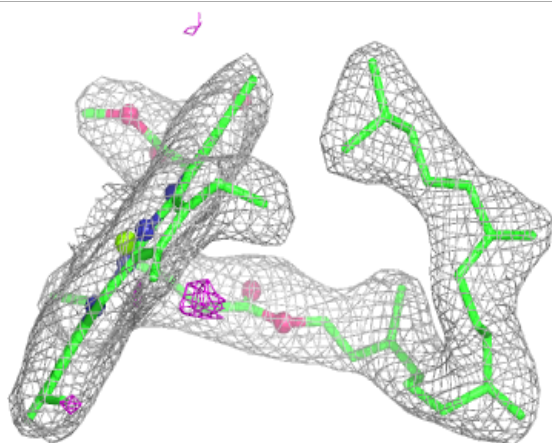
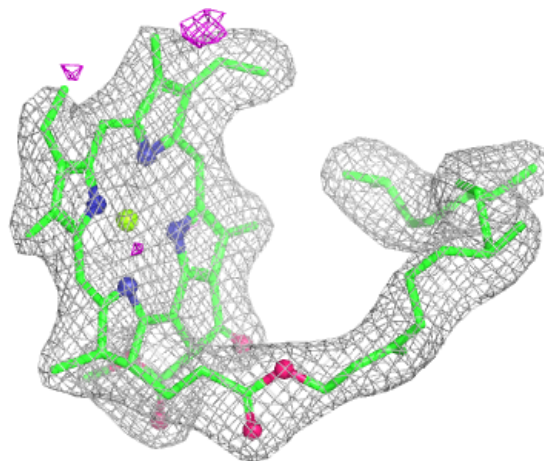
**Electron density around LHG D 409:**

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



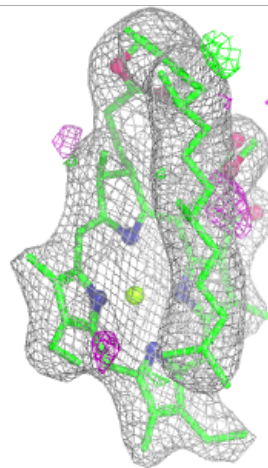
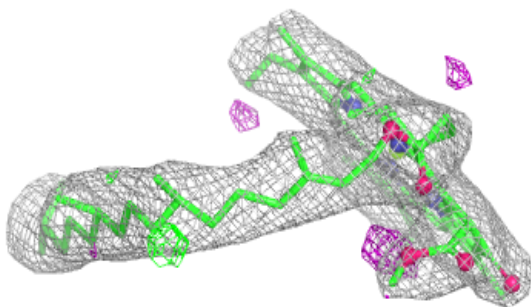
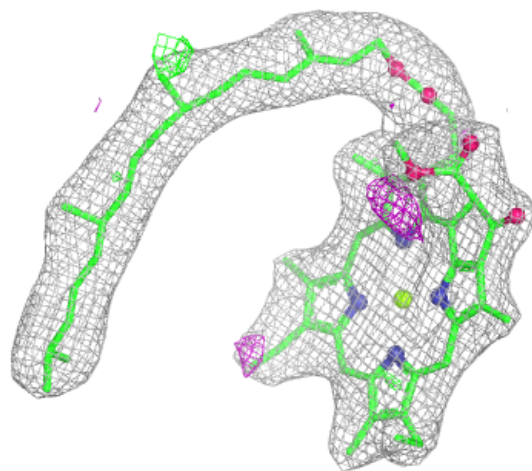
Electron density around CLA C 504:

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



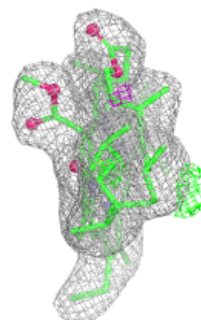
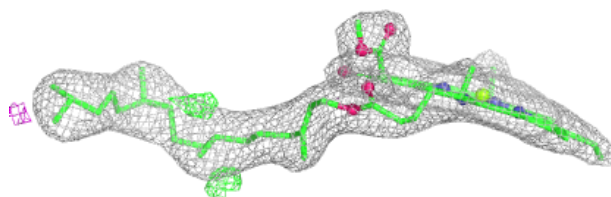
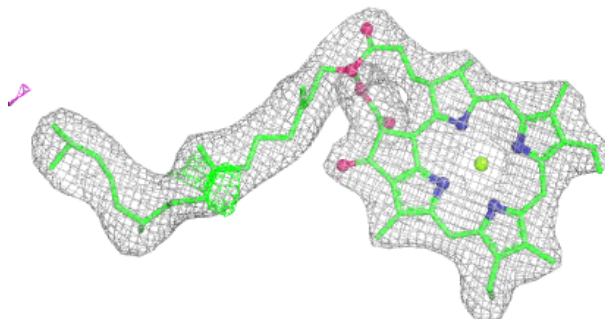
Electron density around CLA c 508:

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



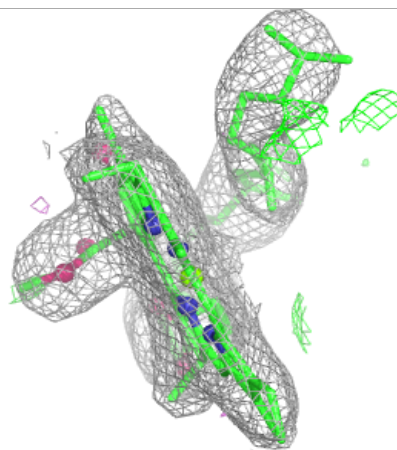
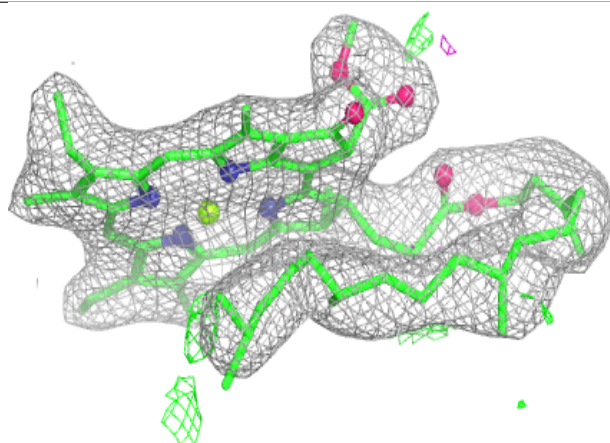
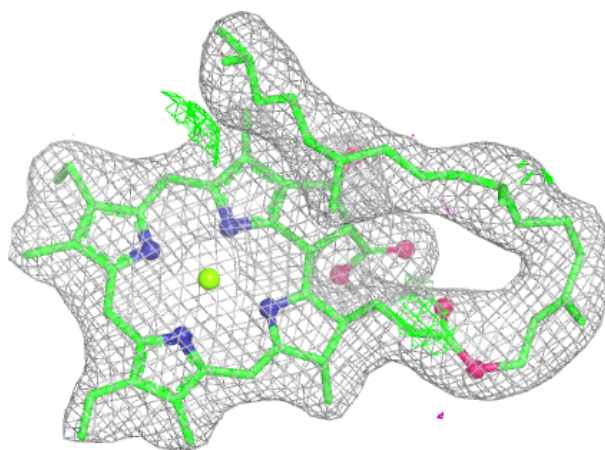
Electron density around CLA b 602:

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



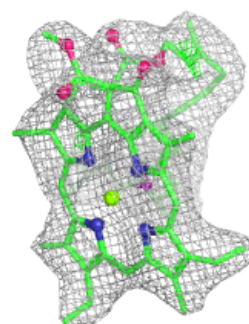
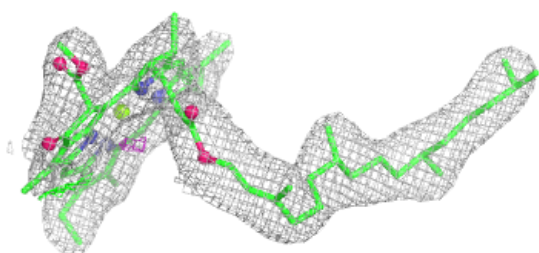
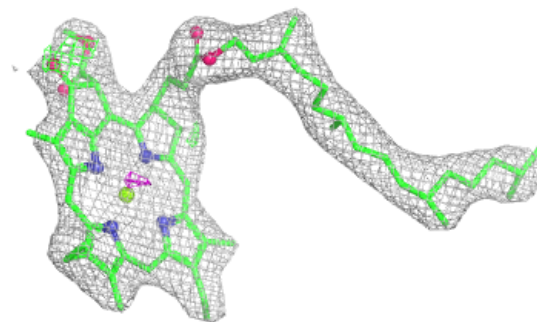
Electron density around CLA c 510:

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



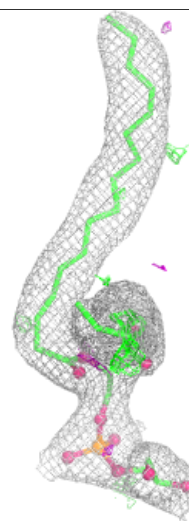
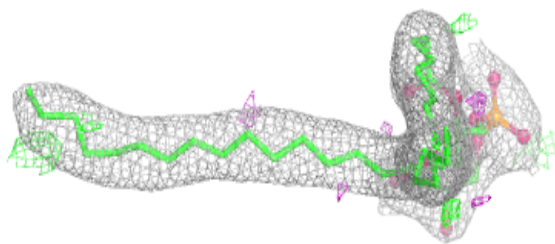
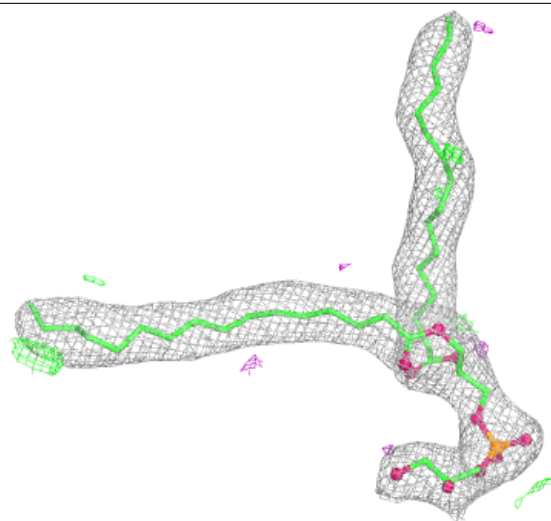
Electron density around CLA c 512:

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



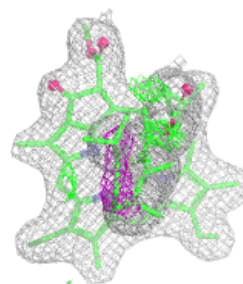
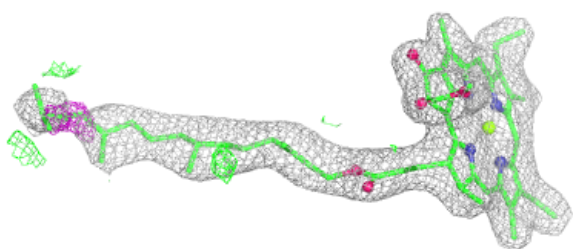
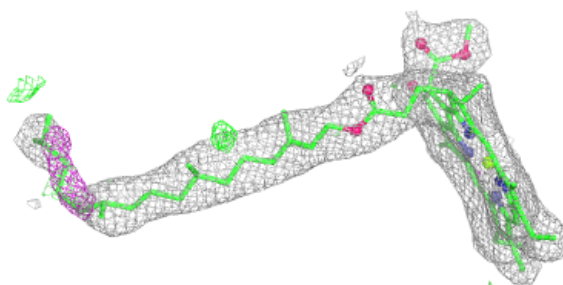
Electron density around LHG 1 101:

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



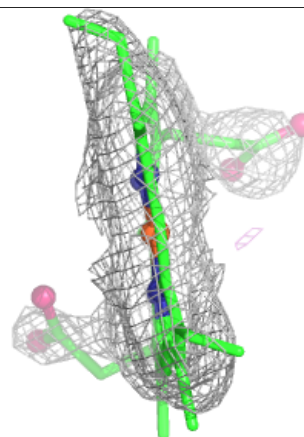
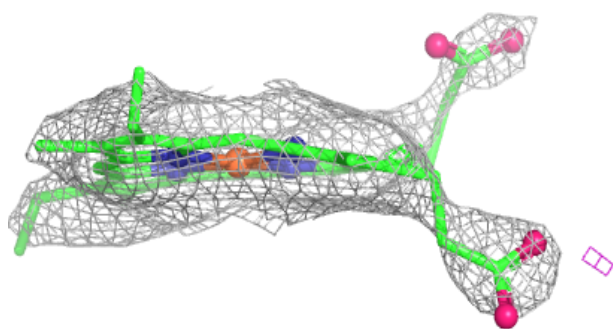
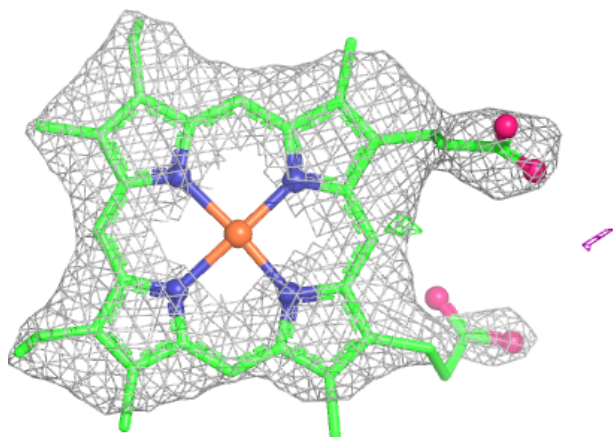
Electron density around CLA b 604:

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



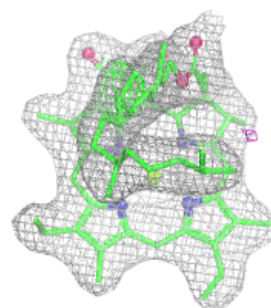
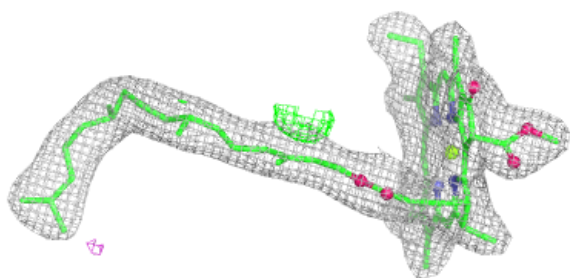
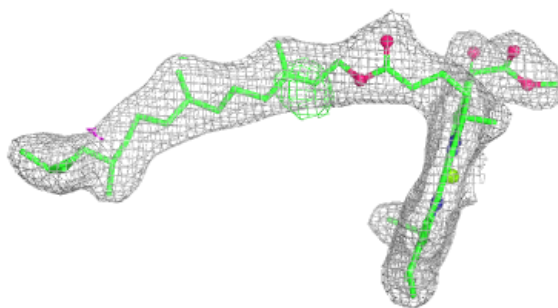
Electron density around HEM e 87:

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

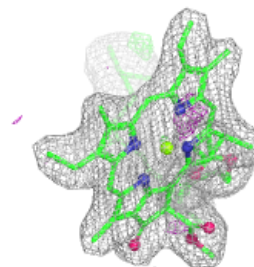
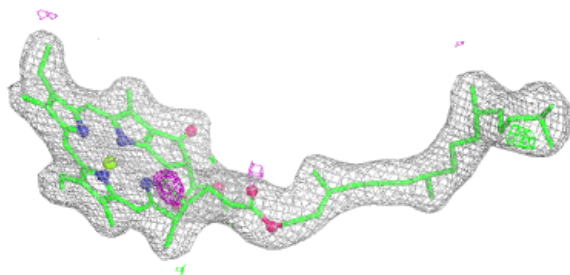
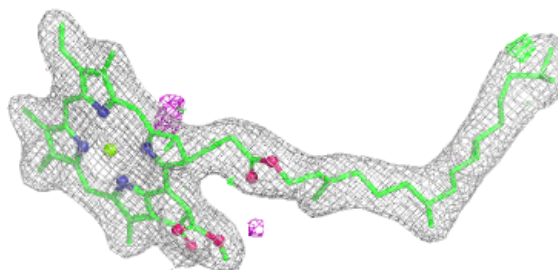


Electron density around CLA B 605:

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

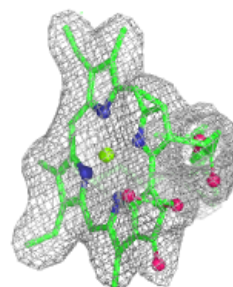
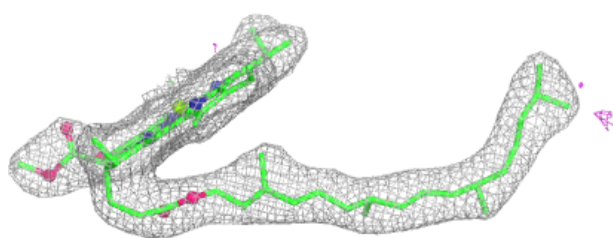
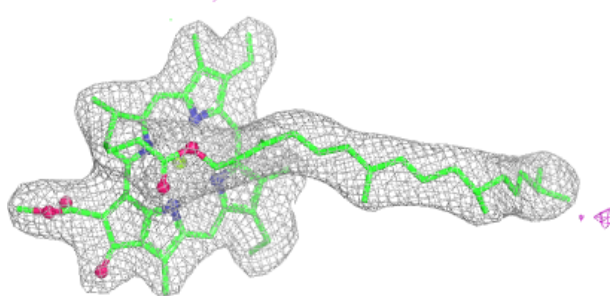
**Electron density around CLA A 404:**

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

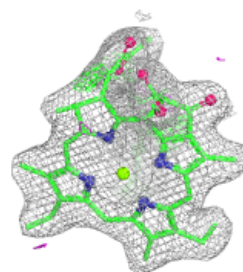
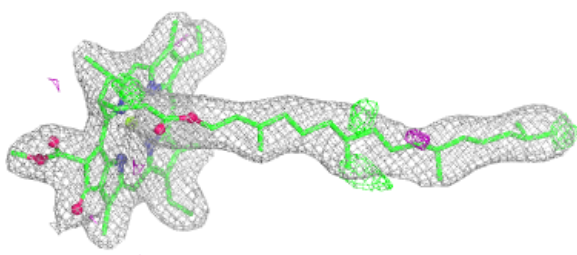
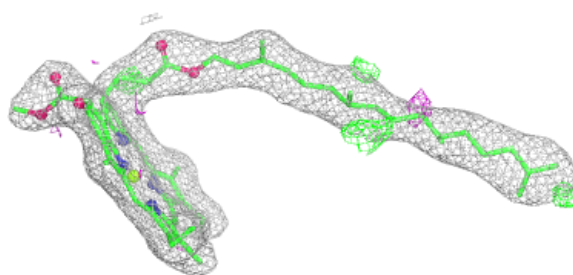


Electron density around CLA b 608:

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

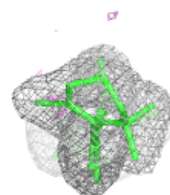
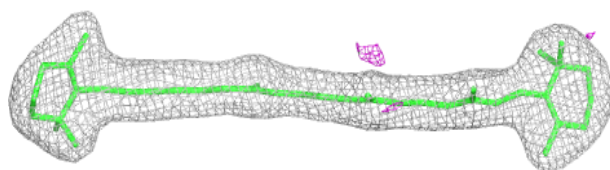
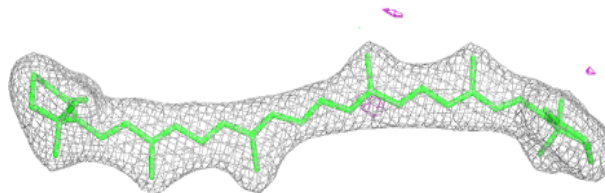
**Electron density around CLA B 607:**

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

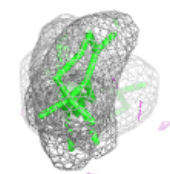
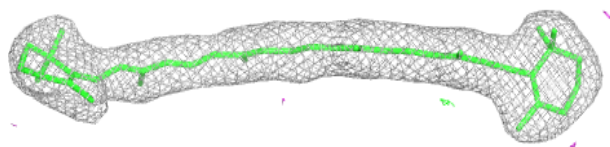
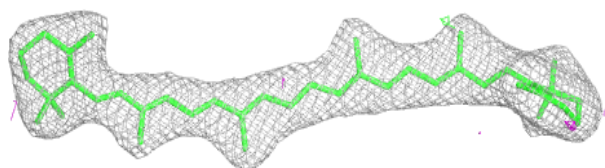


Electron density around BCR a 410:

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

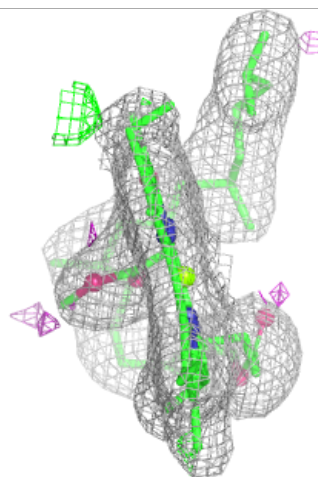
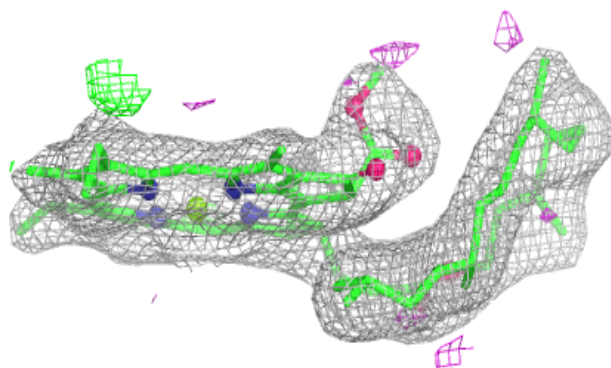
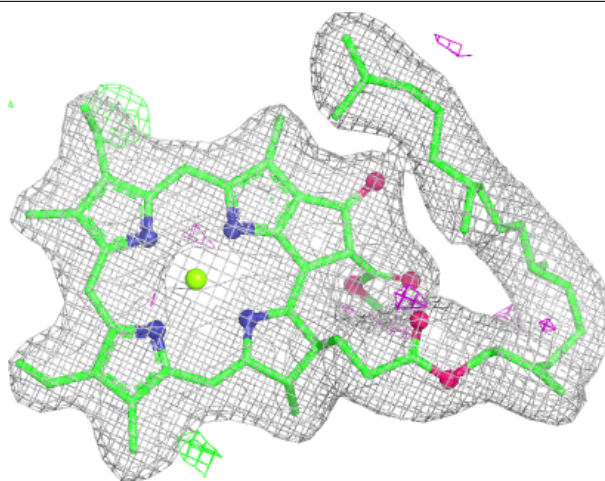
**Electron density around BCR b 617:**

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



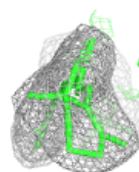
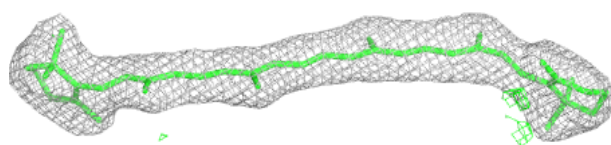
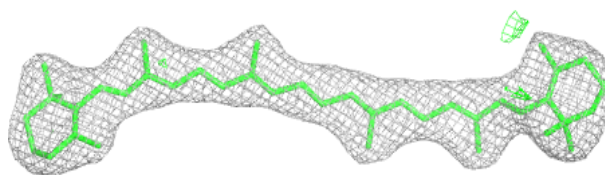
Electron density around CLA b 610:

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



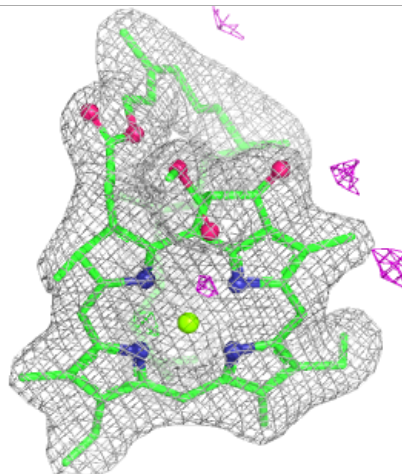
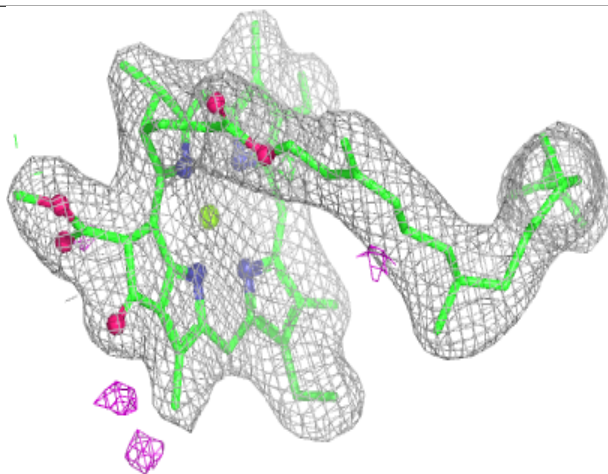
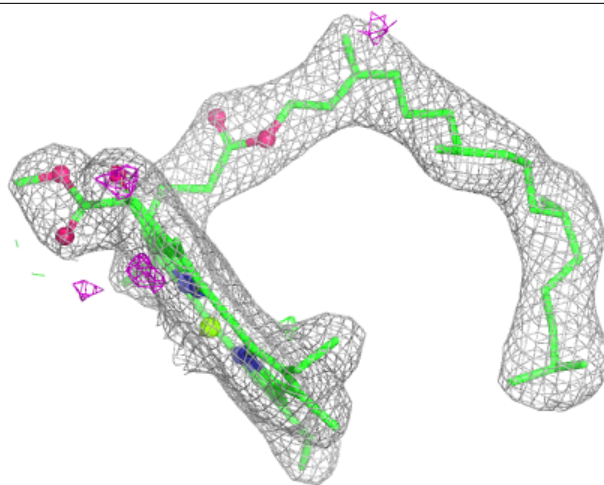
Electron density around BCR b 619:

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



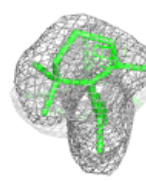
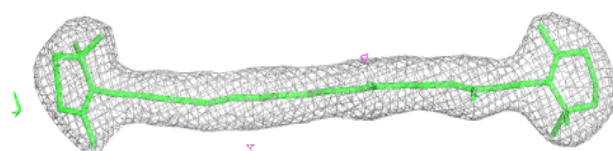
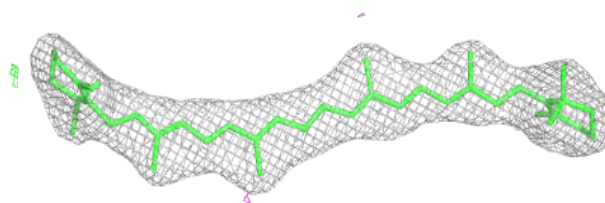
Electron density around CLA b 611:

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

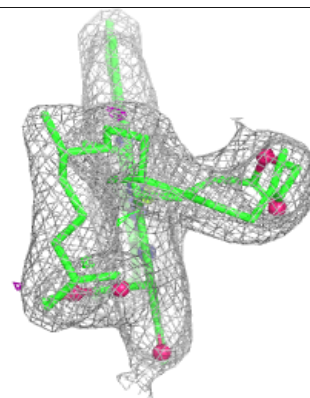
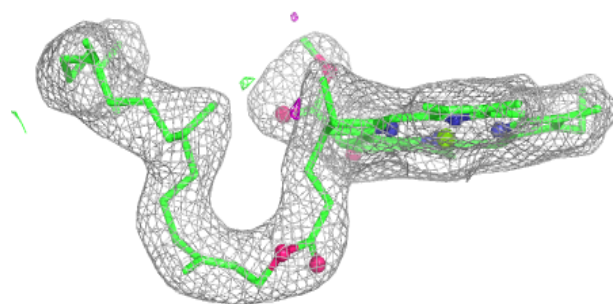
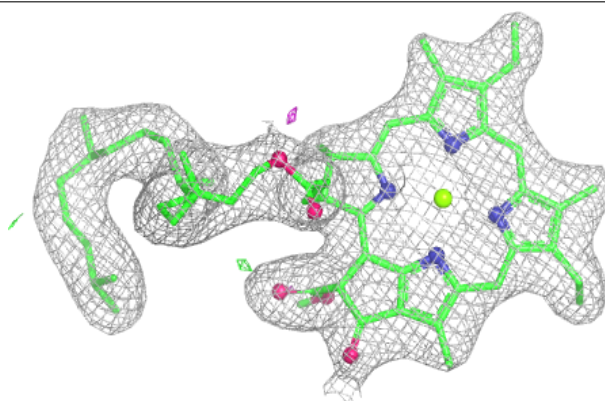


Electron density around BCR c 516:

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

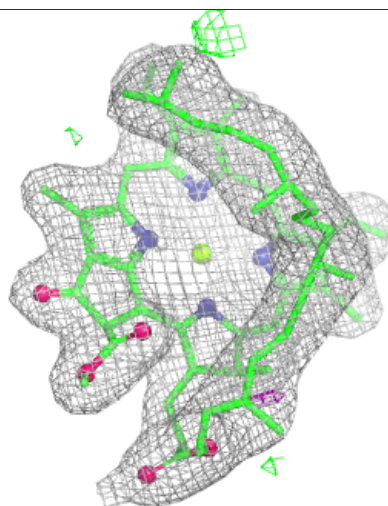
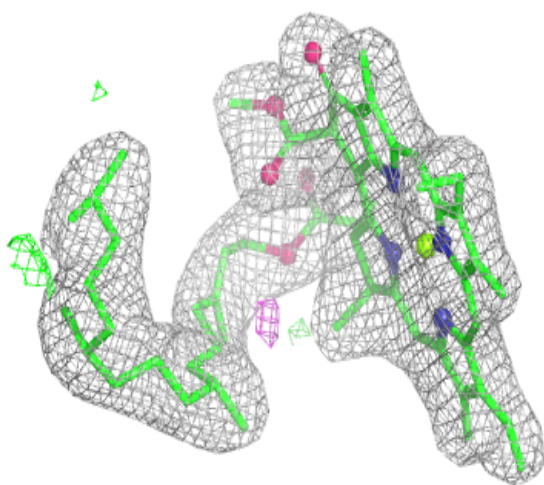
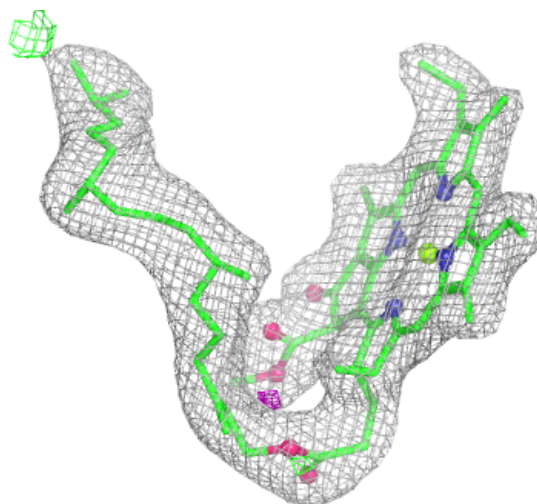
**Electron density around CLA b 612:**

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



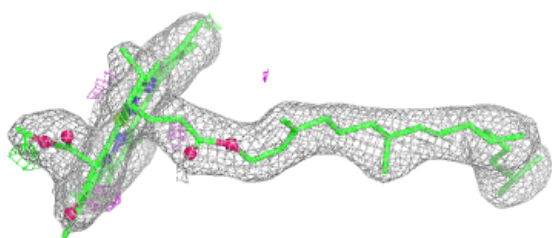
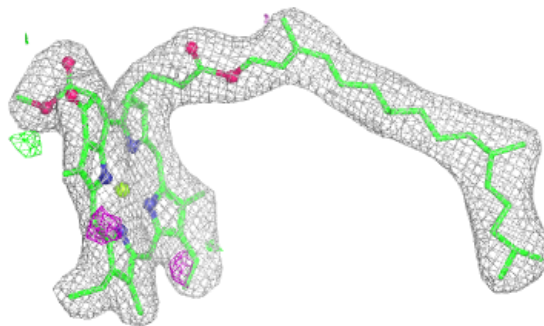
Electron density around CLA b 613:

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



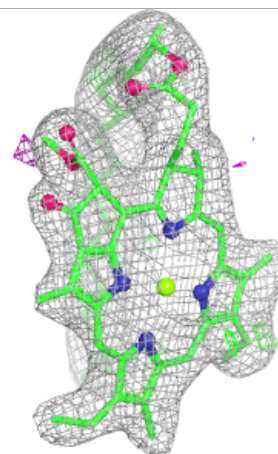
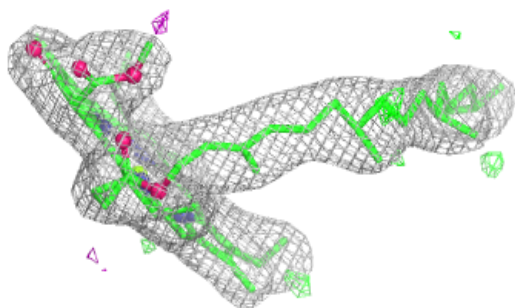
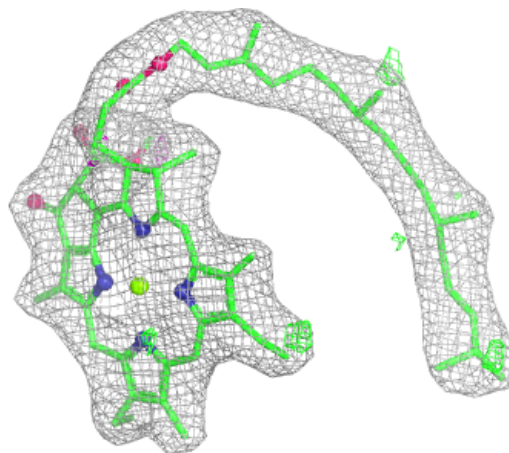
Electron density around CLA B 609:

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



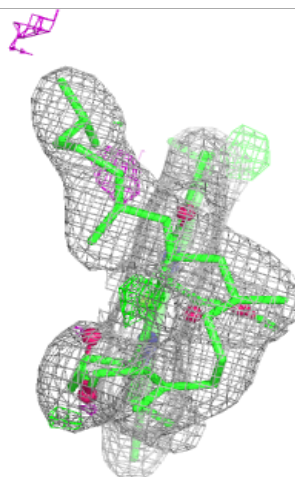
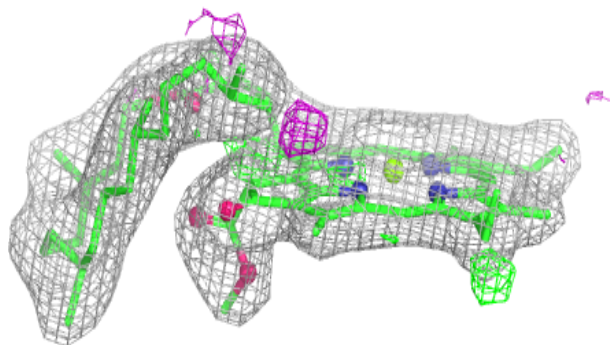
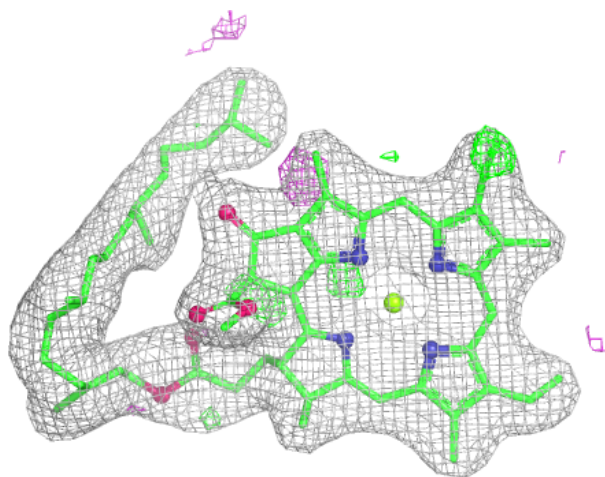
Electron density around CLA C 508:

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



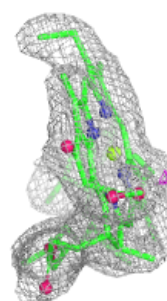
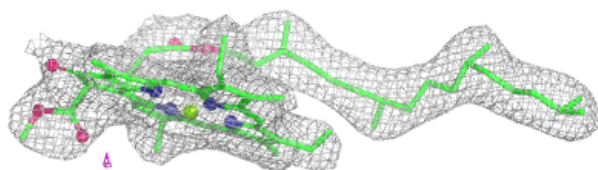
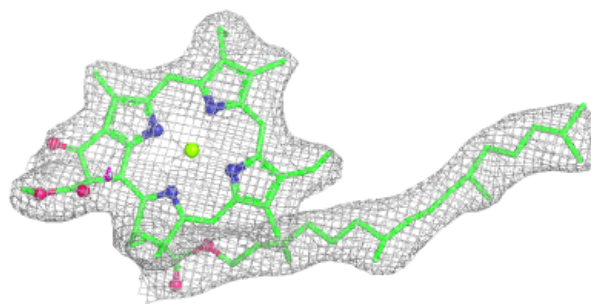
Electron density around CLA B 610:

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

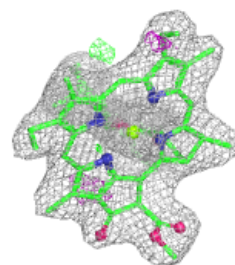
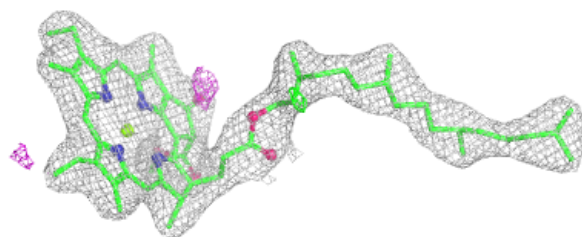
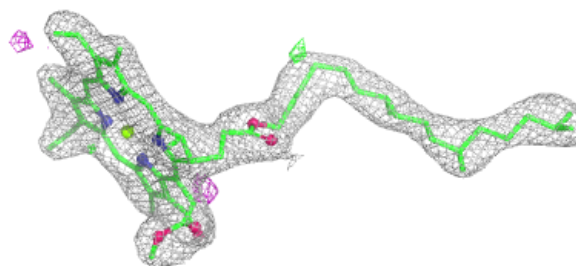


Electron density around CLA c 502:

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

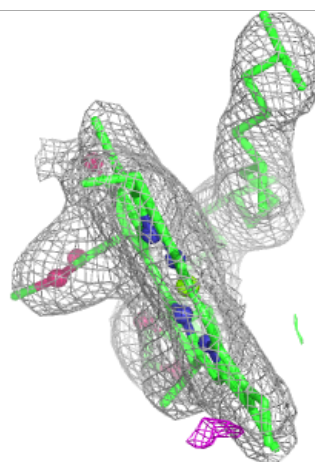
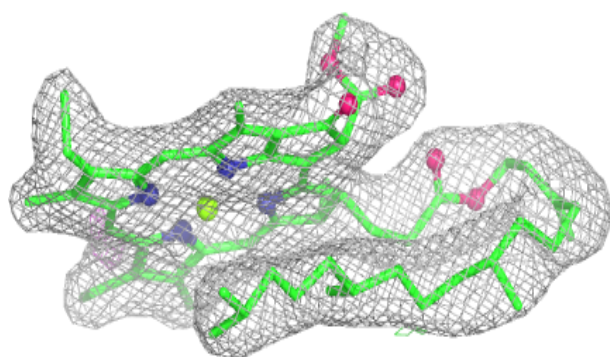
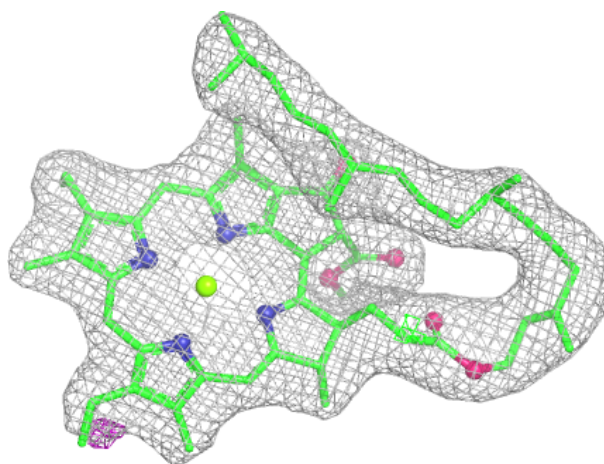
**Electron density around CLA c 503:**

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



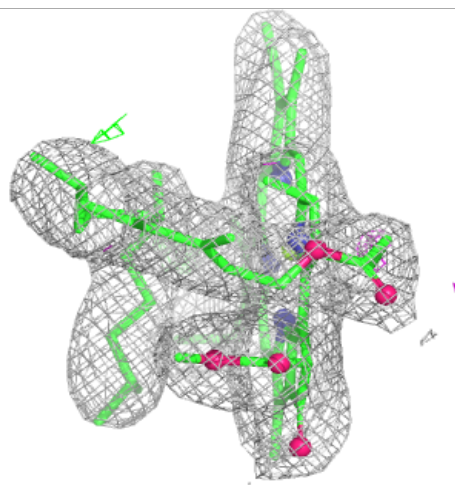
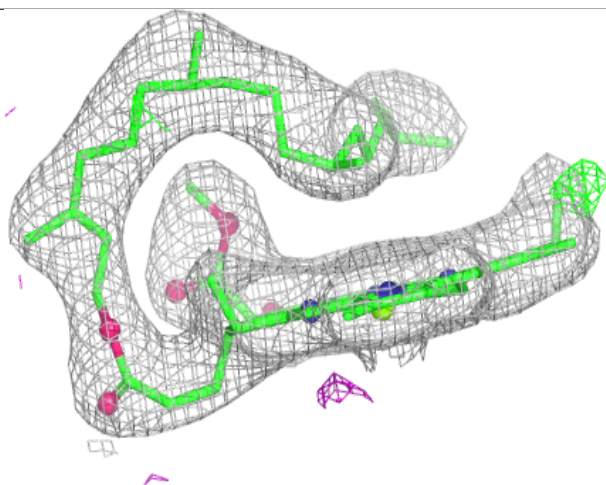
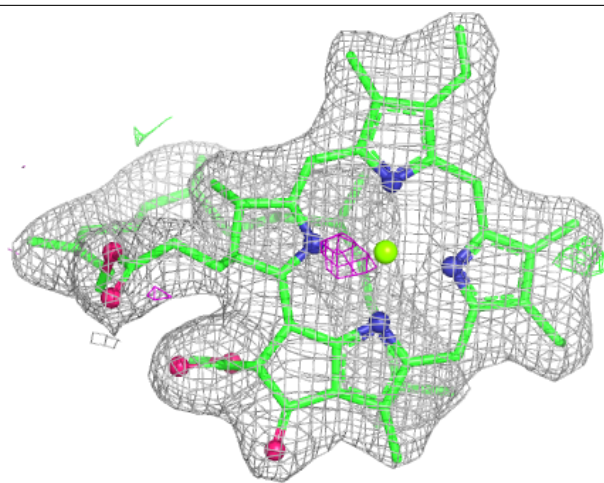
Electron density around CLA C 510:

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



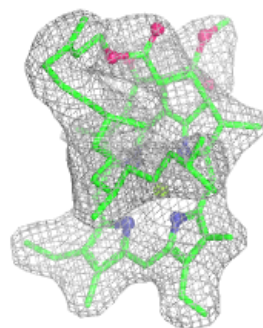
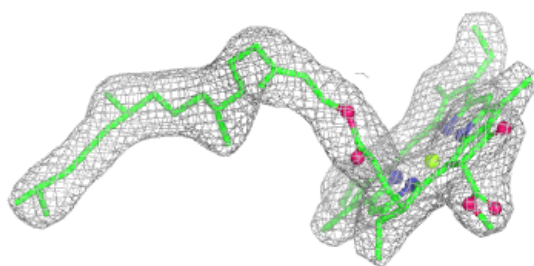
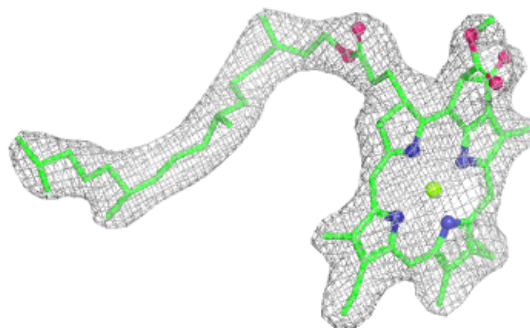
Electron density around CLA C 511:

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



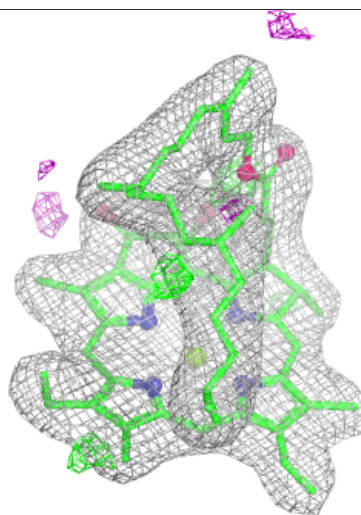
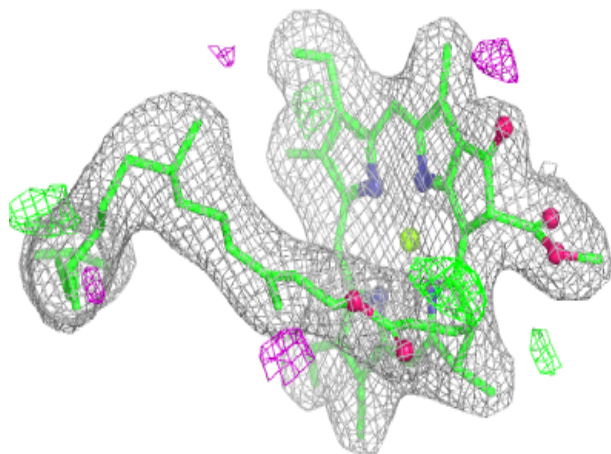
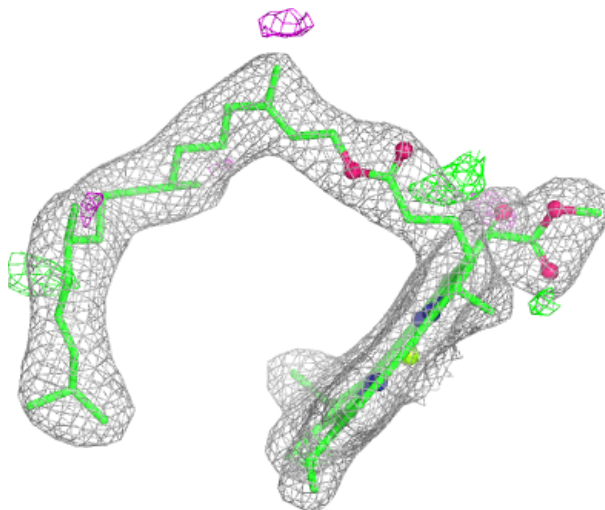
Electron density around CLA C 512:

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



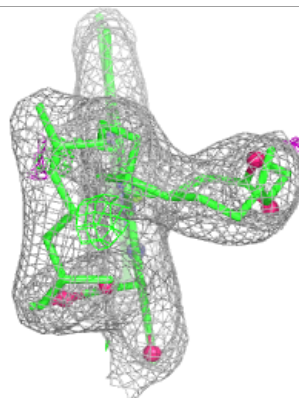
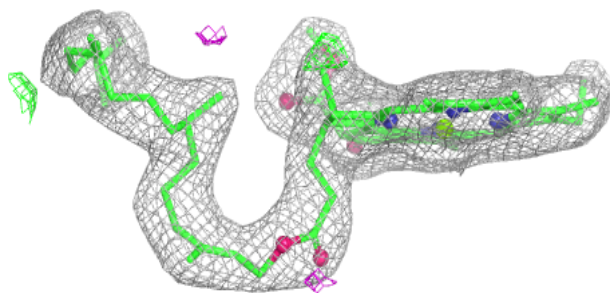
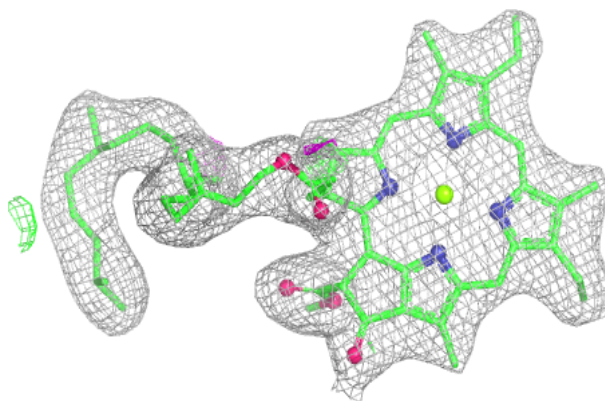
Electron density around CLA B 611:

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

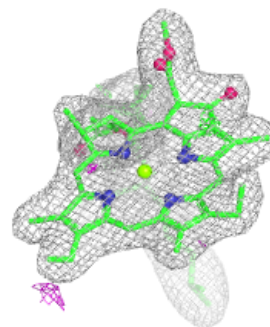
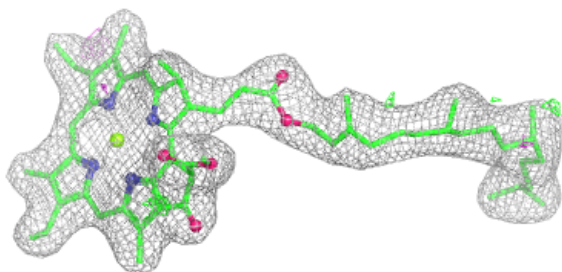
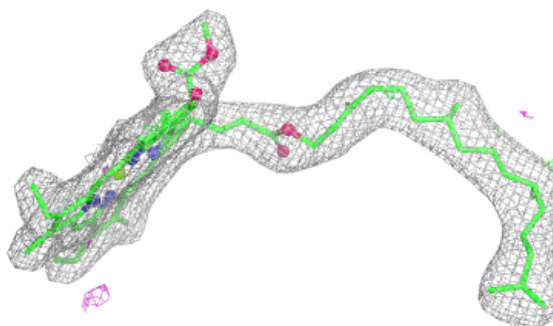


Electron density around CLA B 612:

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

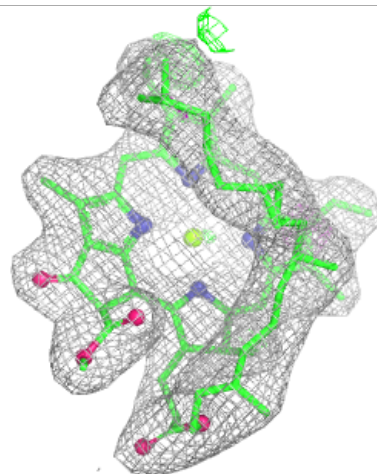
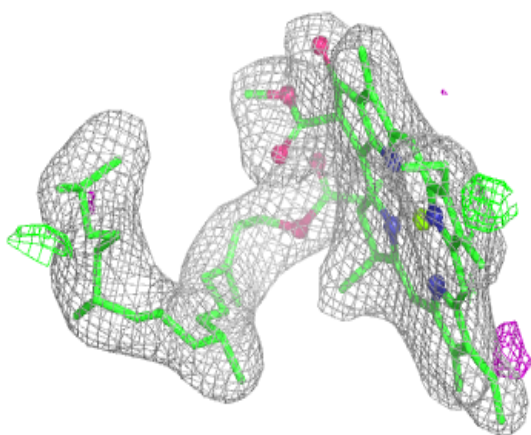
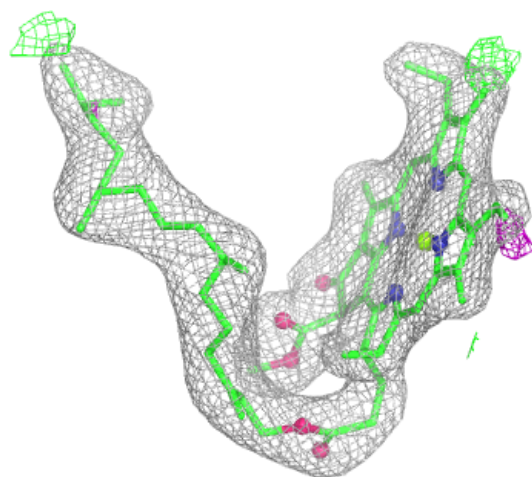
**Electron density around CLA D 405:**

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



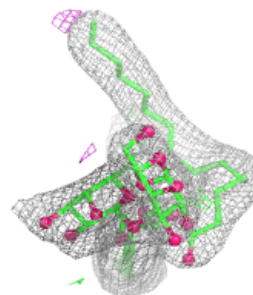
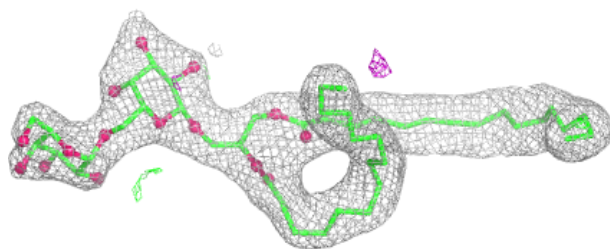
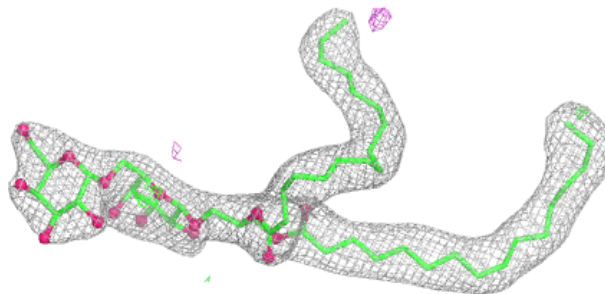
Electron density around CLA B 613:

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



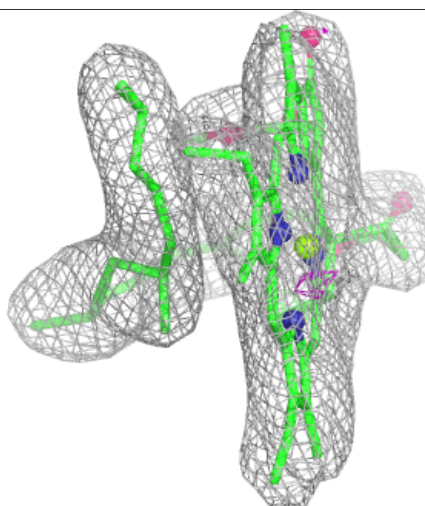
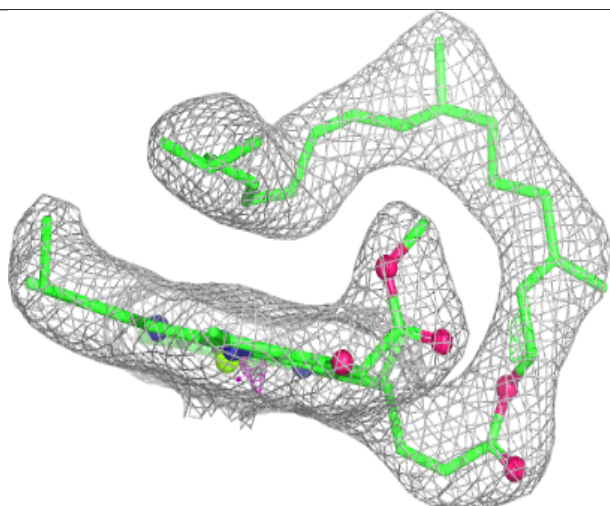
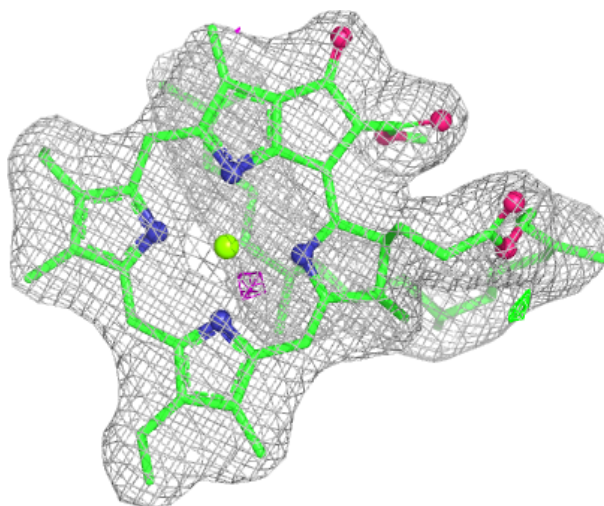
Electron density around DGD h 102:

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



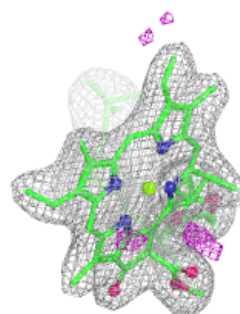
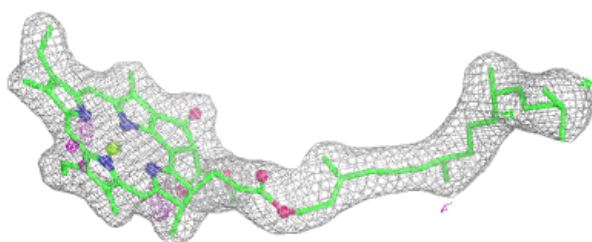
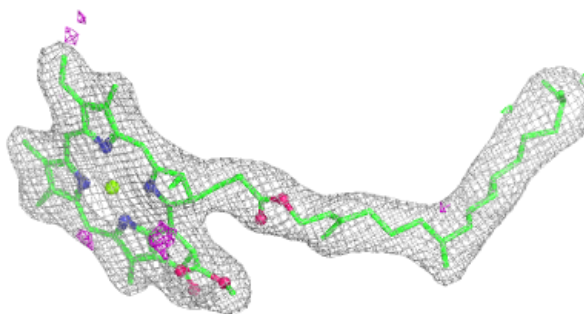
Electron density around CLA c 511:

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

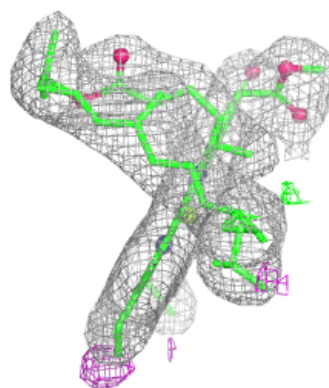
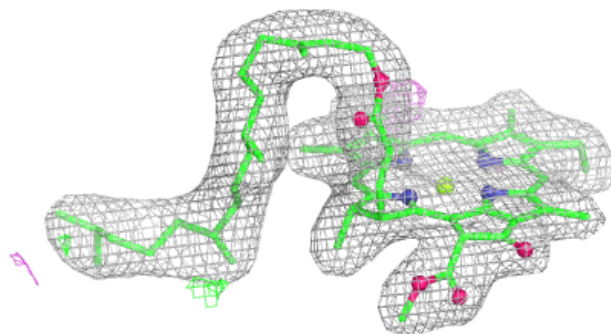
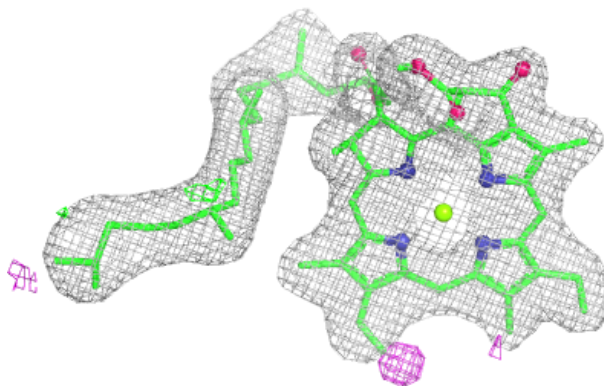


Electron density around CLA a 405:

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

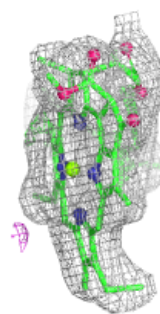
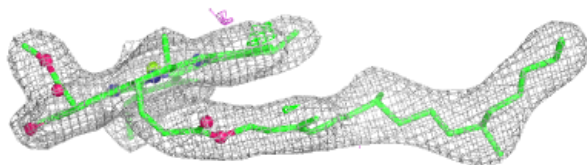
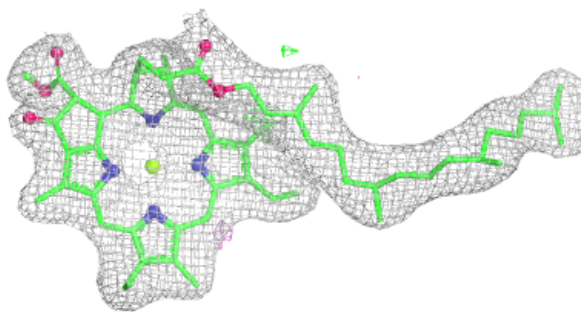
**Electron density around CLA a 406:**

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



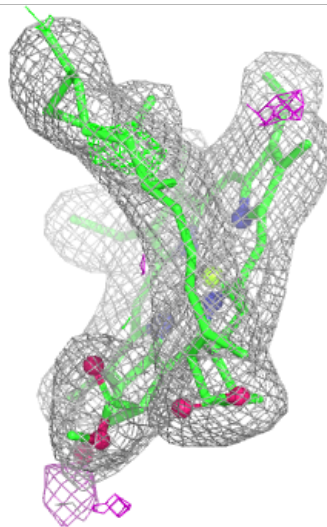
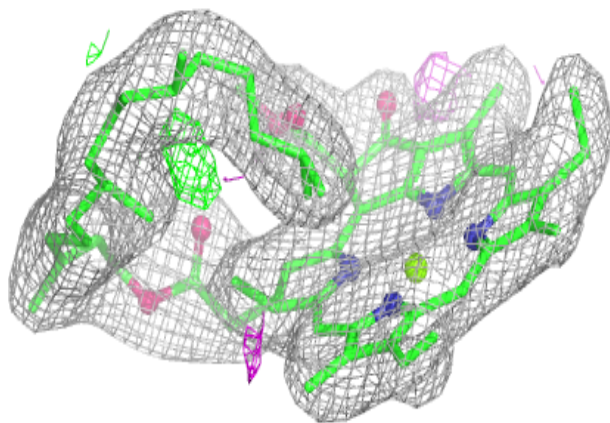
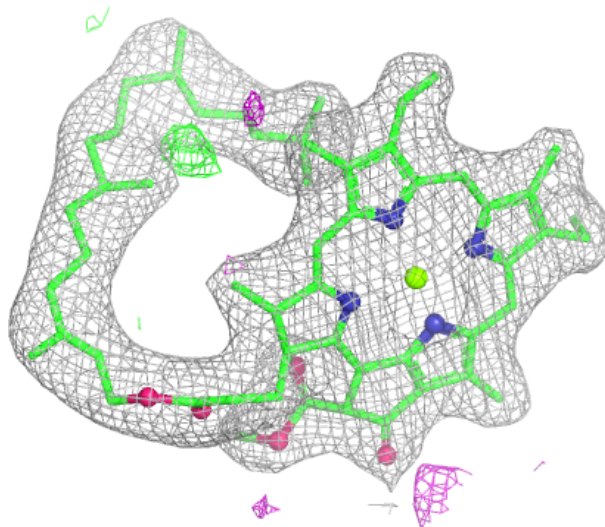
Electron density around CLA B 603:

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



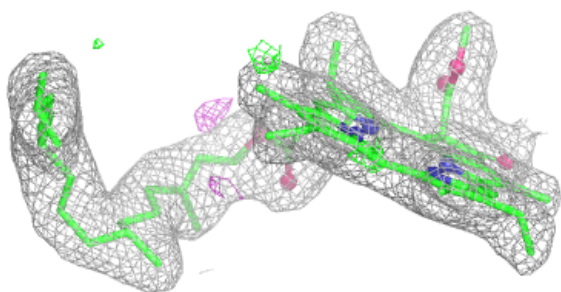
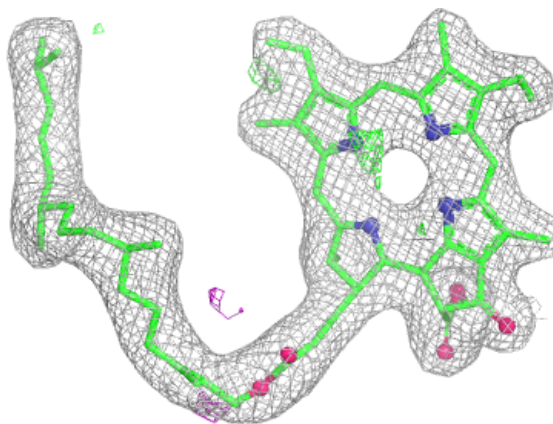
Electron density around CLA B 615:

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



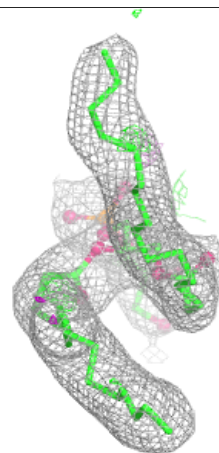
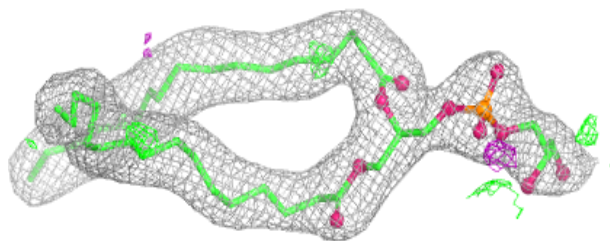
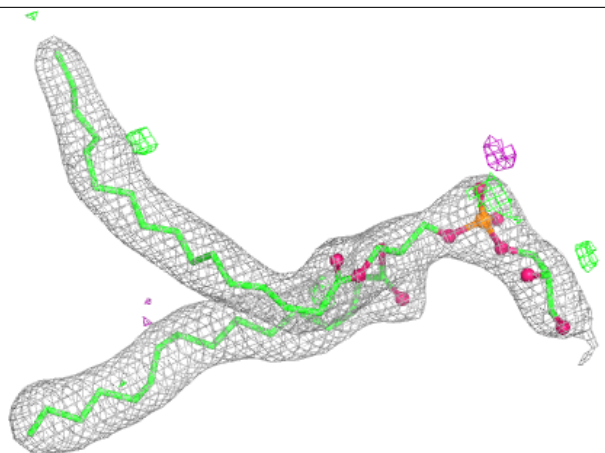
Electron density around PHO A 353:

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



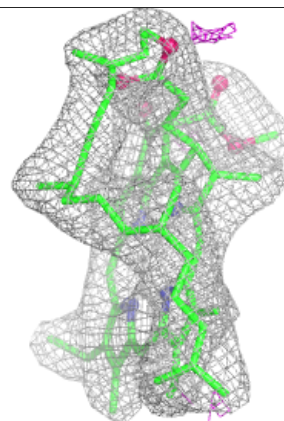
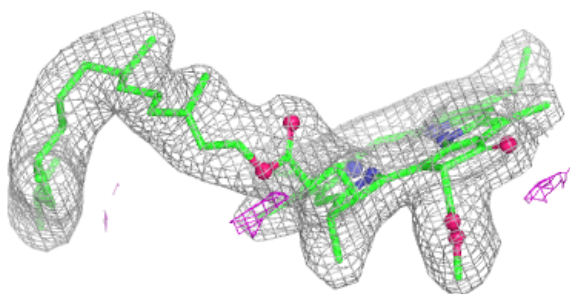
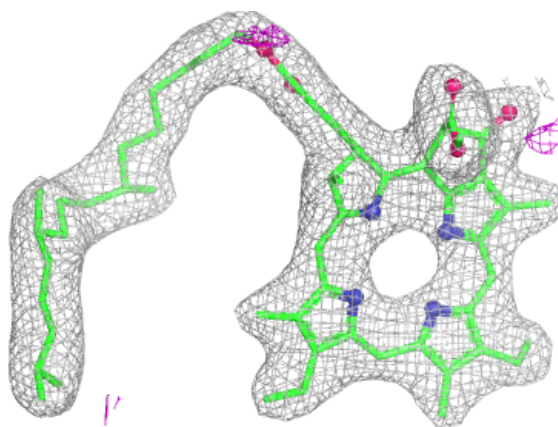
Electron density around LHG D 410:

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



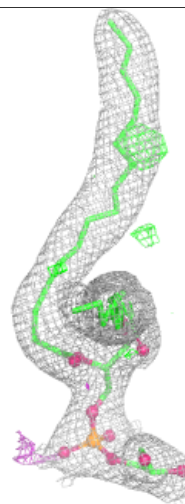
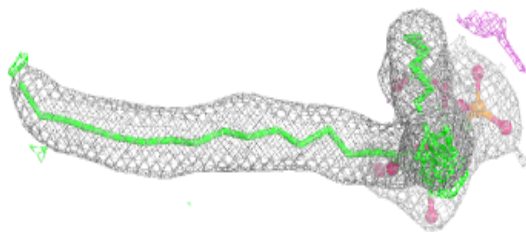
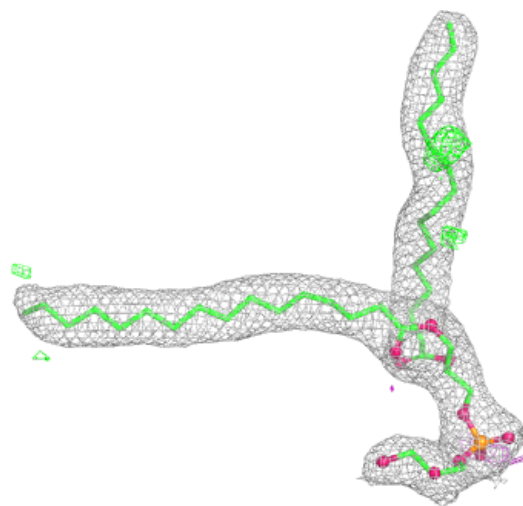
Electron density around PHO a 353:

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



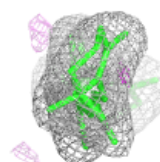
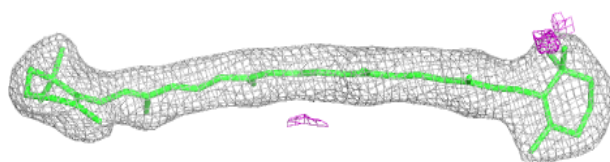
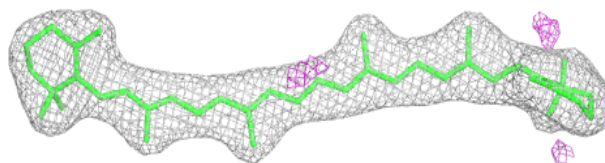
Electron density around LHG L 101:

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



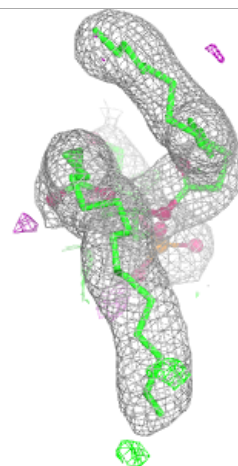
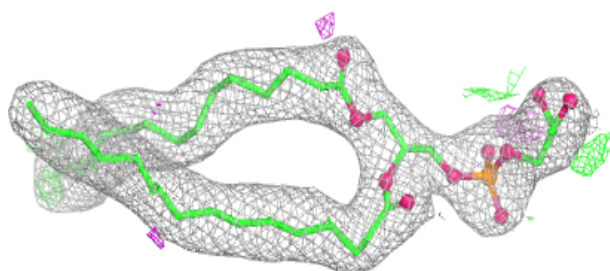
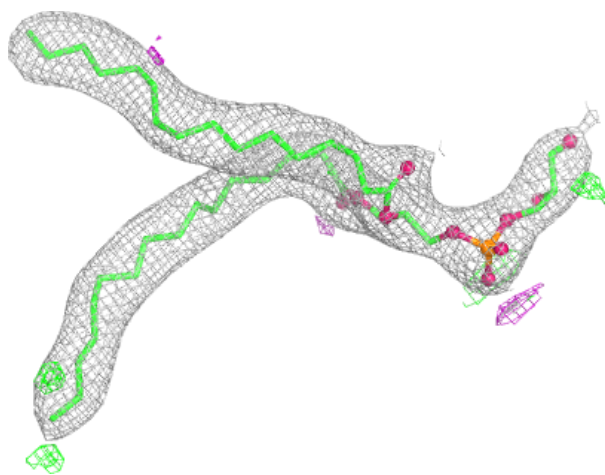
Electron density around BCR B 617:

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



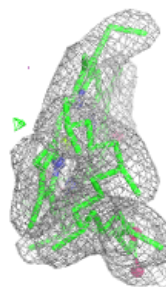
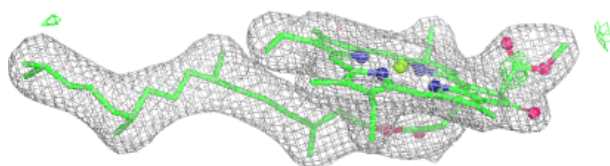
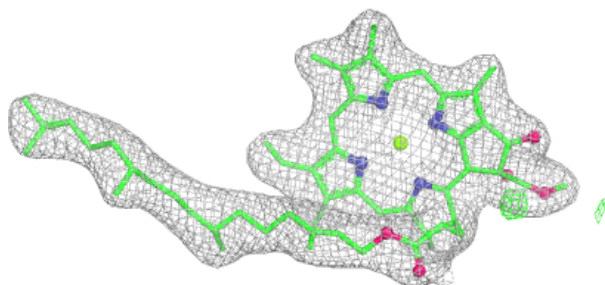
Electron density around LHG d 407:

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

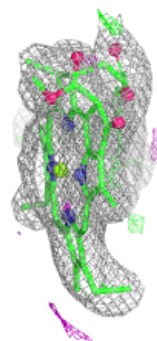
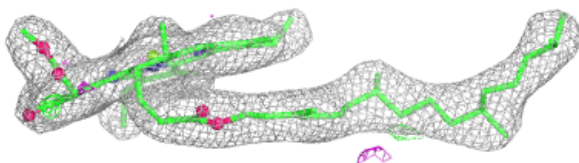
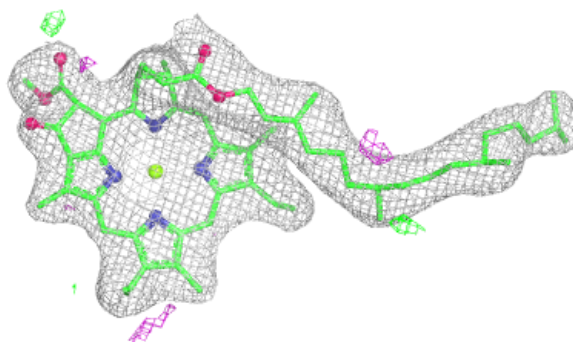


Electron density around CLA C 502:

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

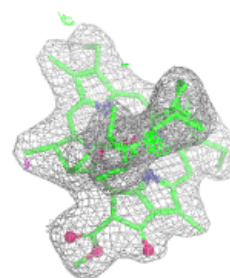
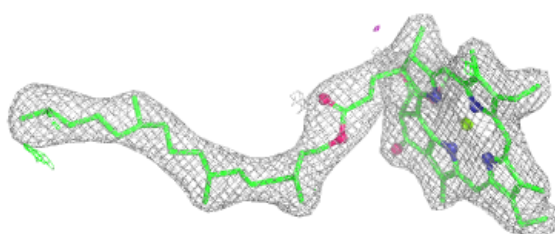
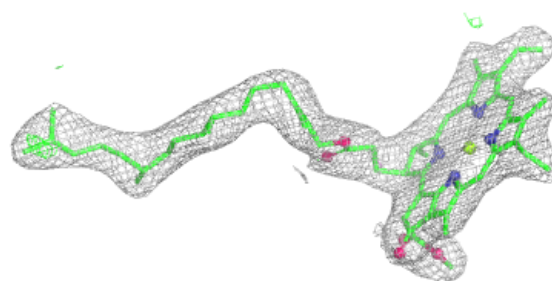
**Electron density around CLA b 603:**

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

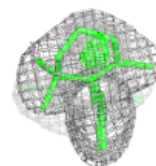
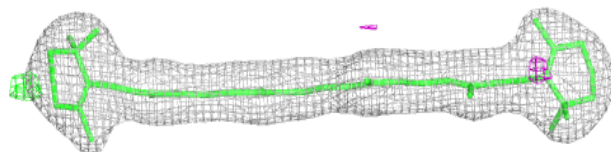
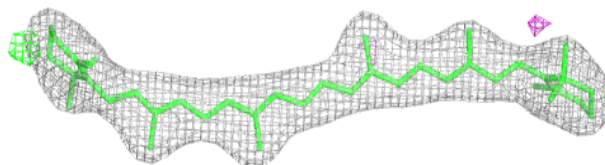


Electron density around CLA C 503:

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

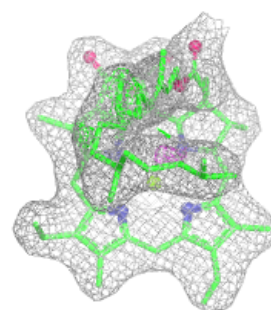
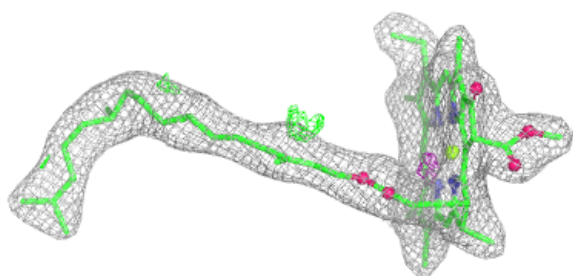
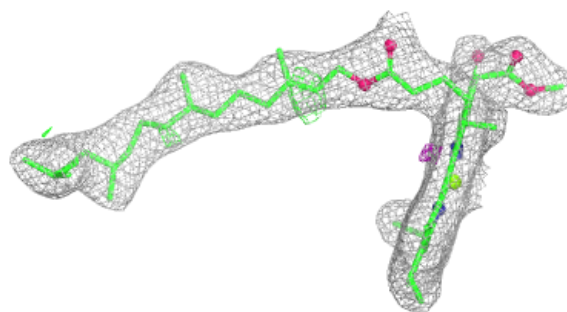
**Electron density around BCR C 516:**

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

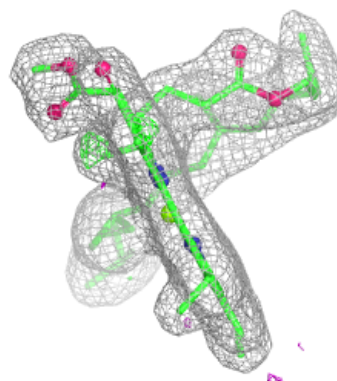
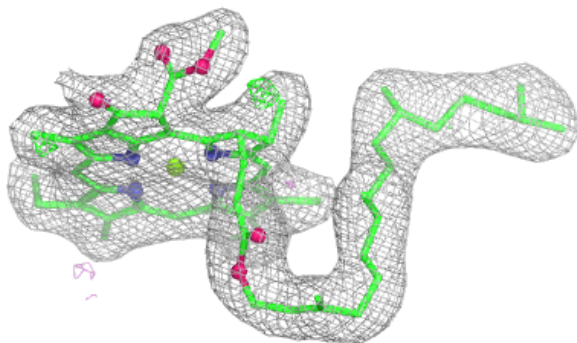
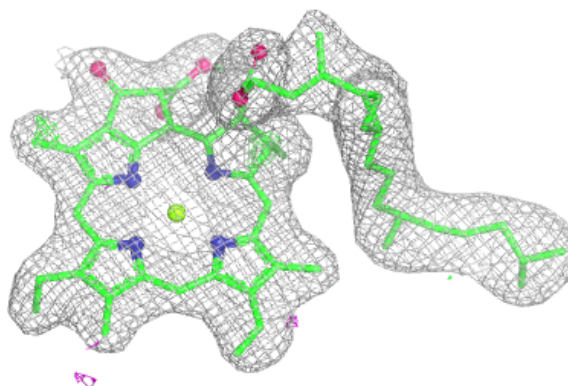


Electron density around CLA b 605:

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

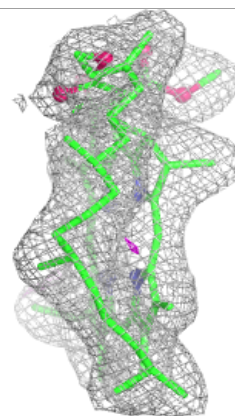
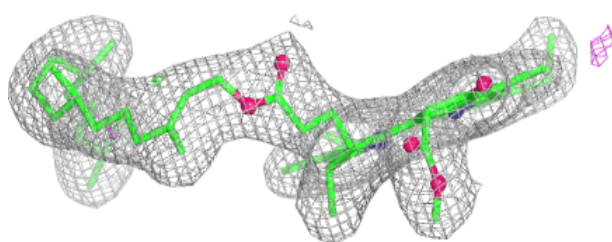
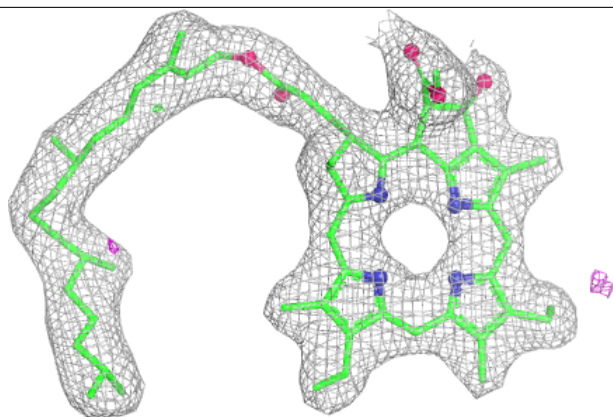
**Electron density around CLA A 405:**

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

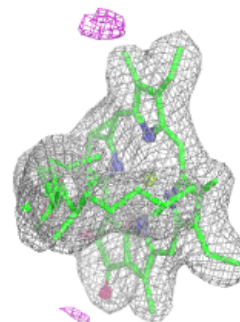
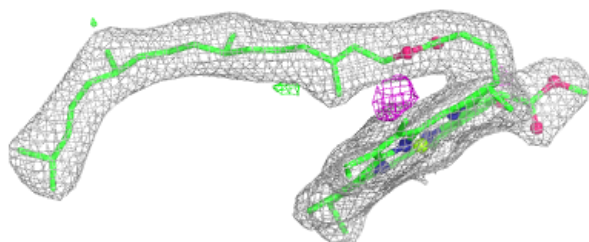
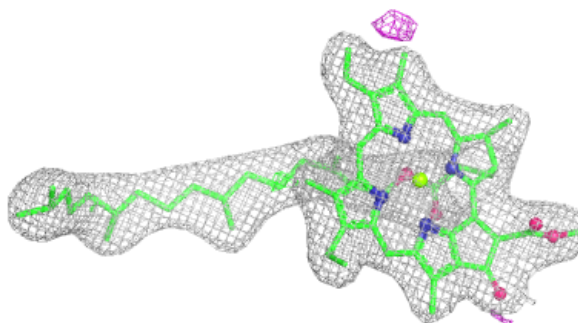


Electron density around PHO A 407:

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

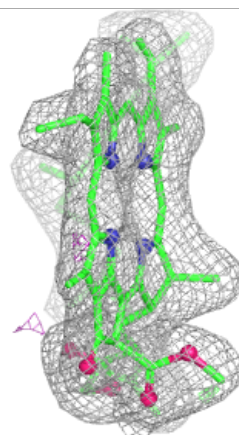
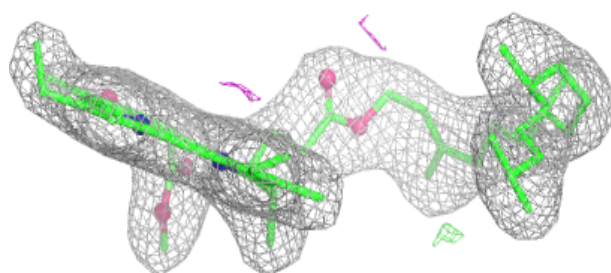
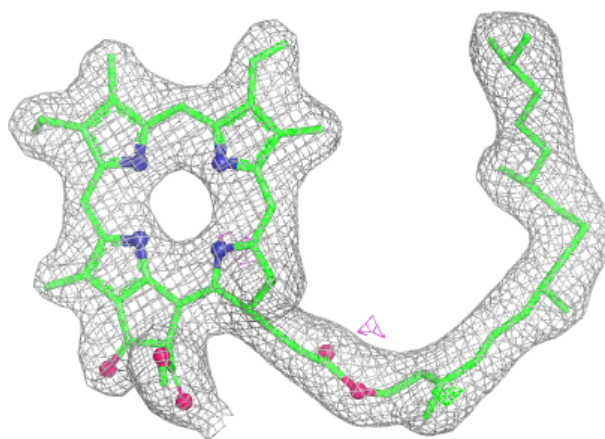
**Electron density around CLA B 608:**

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



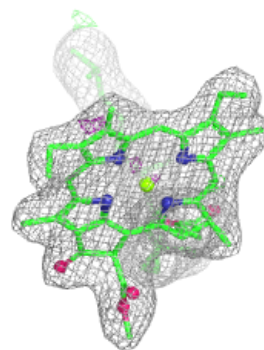
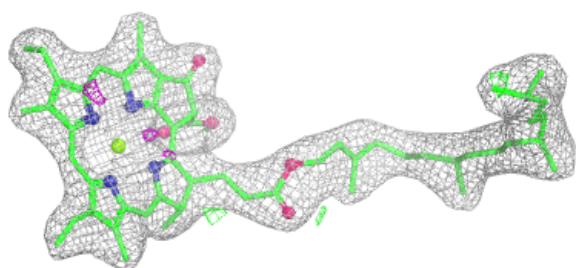
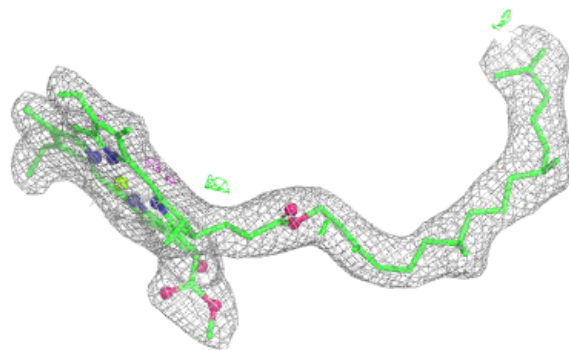
Electron density around PHO a 408:

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



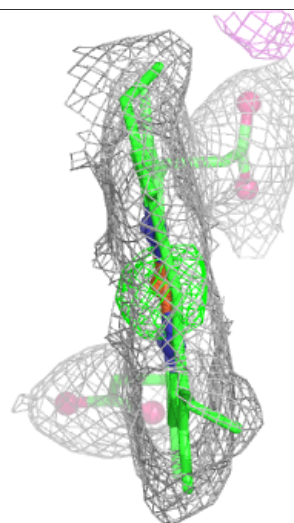
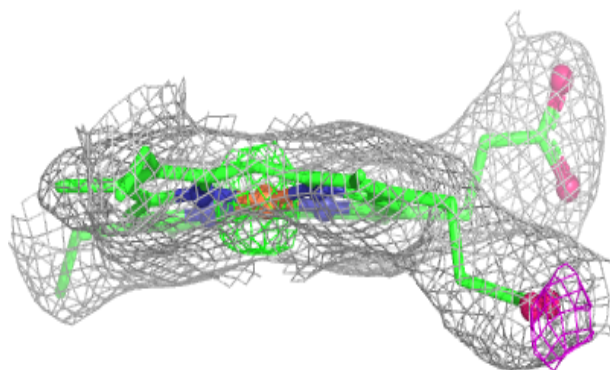
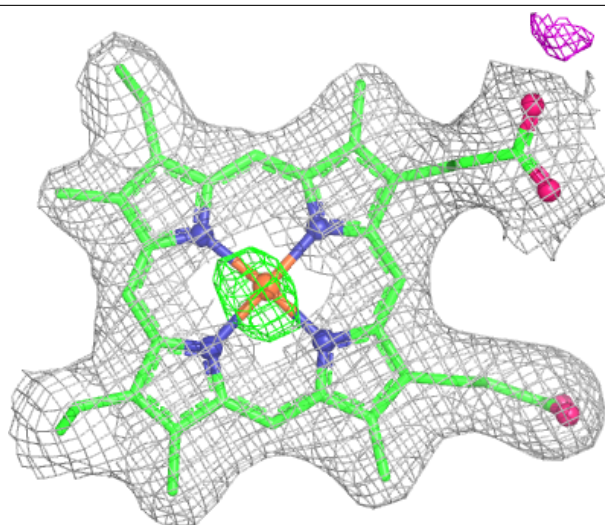
Electron density around CLA d 402:

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



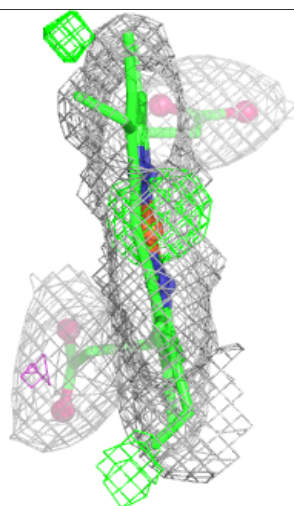
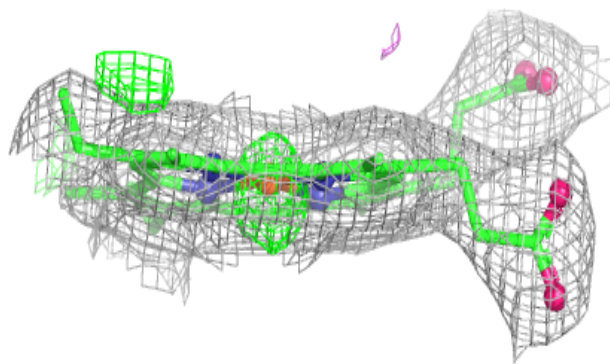
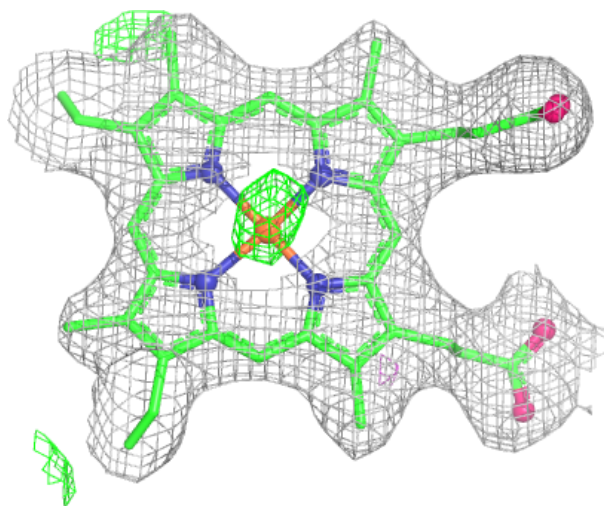
Electron density around HEC V 202:

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



Electron density around HEC v 202:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.