



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 06:18 PM BST

PDB ID : 4UB8
Title : Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors : Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on : 2014-08-12
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

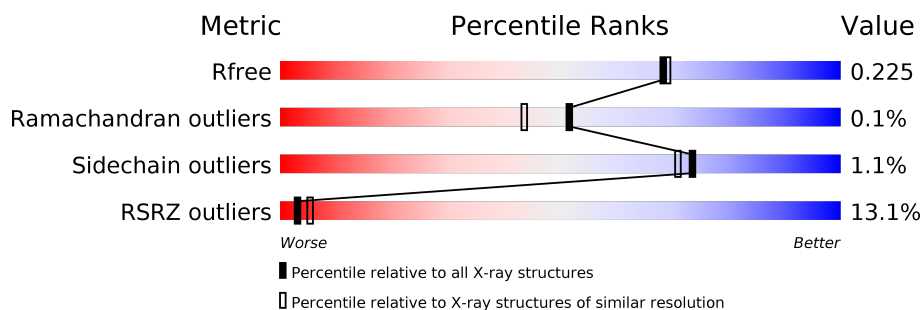
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	<div> <div>13%</div> <div>97%</div> <div>.</div> </div>
1	a	344	<div> <div>17%</div> <div>97%</div> <div>..</div> </div>
2	B	505	<div> <div>8%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>10%</div> <div>99%</div> <div>.</div> </div>
3	C	455	<div> <div>6%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>8%</div> <div>99%</div> <div>.</div> </div>
4	D	342	<div> <div>18%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
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	31	
14	t	31	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	404	X	-	-	-
28	GOL	B	635	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	k	102	-	-	-	X
30	LMT	a	417	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2631	1725	431	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2634	1727	431	461	15			

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4023	2642	667	701	13			
2	b	504	Total	C	N	O	S	0	11	0
			4028	2645	668	702	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	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	0	0
			2726	1805	445	464	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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	0	0
			662	432	107	123			

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	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
			282	188	43	49	2			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	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	3	0
			1879	1175	315	384	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	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	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 Ycf12.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	1	0
			292	196	46	50				
18	x	39	Total	C	N	O		0	0	0
			287	191	46	50				

- 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 (three-letter code: FE2) (formula: Fe).

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

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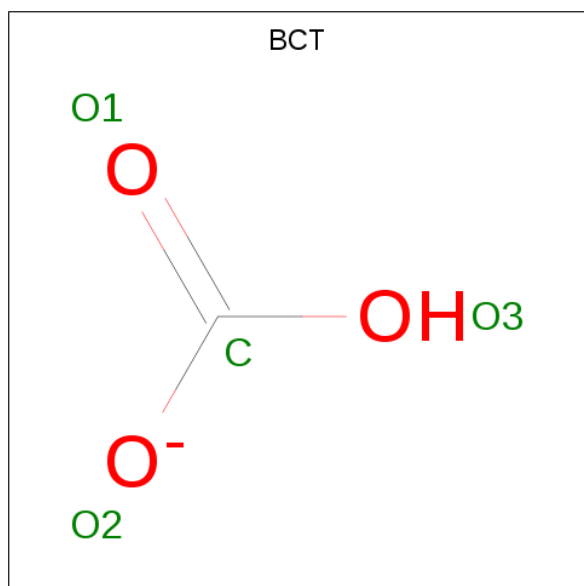
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

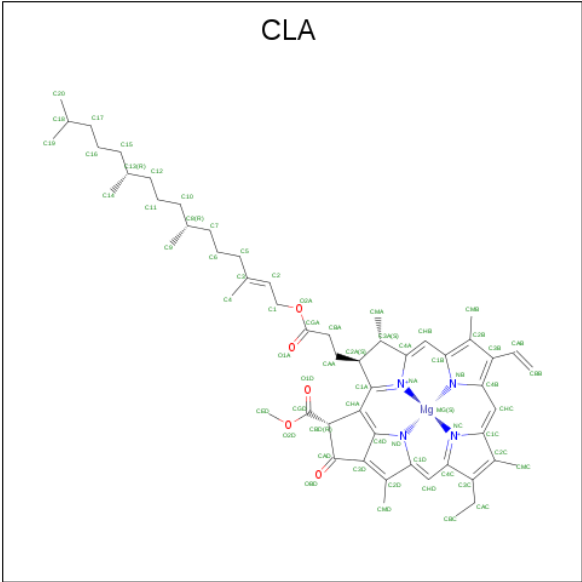
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	u	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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



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

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

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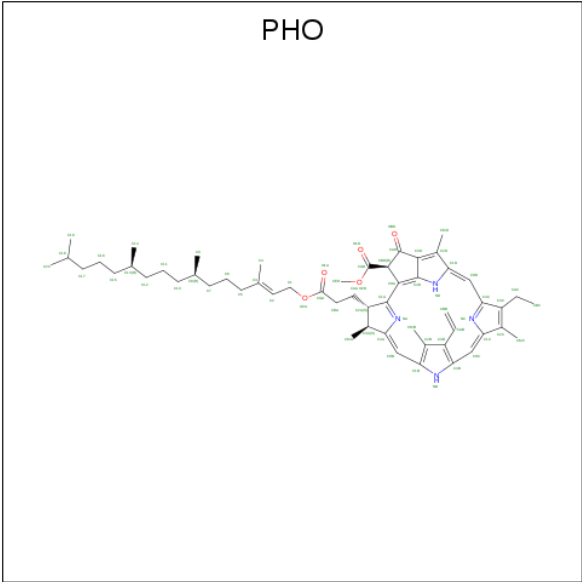
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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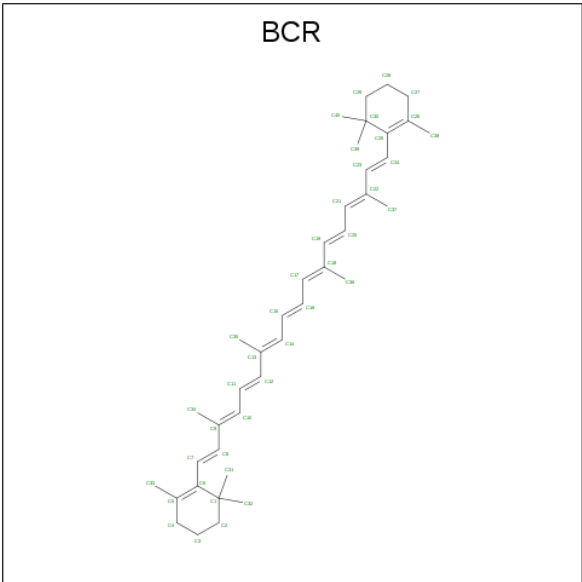
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



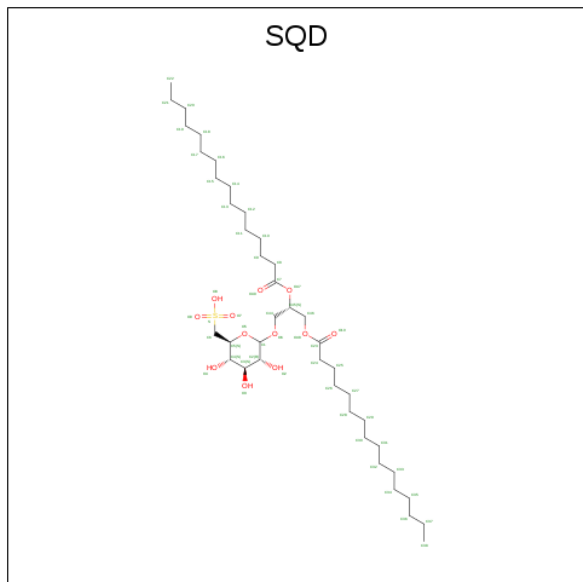
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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



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

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	F	1	Total	C	O	0	0
			6	3	3		
28	O	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	f	1	Total 6	C 3	O 3	0	0
28	t	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

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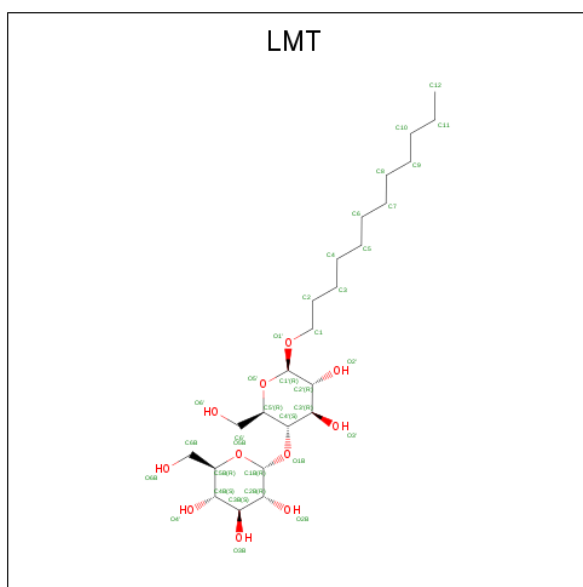
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

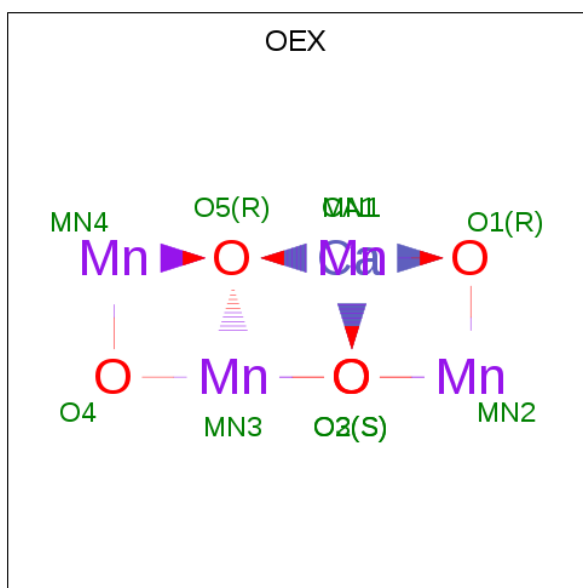
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	J	1	Total	C		0	0
			10	10			
29	i	1	Total	C	O	0	0
			40	35	5		
29	D	2	Total	C	O	0	0
			57	51	6		
29	k	2	Total	C	O	0	0
			42	37	5		
29	B	1	Total	C	O	0	0
			33	28	5		
29	I	1	Total	C	O	0	0
			40	35	5		
29	C	1	Total	C	O	0	0
			34	29	5		
29	a	1	Total	C	O	0	0
			30	25	5		
29	x	1	Total	C		0	0
			10	10			
29	A	1	Total	C	O	0	0
			28	23	5		
29	j	1	Total	C		0	0
			10	10			
29	X	1	Total	C		0	0
			10	10			
29	d	2	Total	C	O	0	0
			53	47	6		
29	m	1	Total	C		0	0
			10	10			
29	b	1	Total	C	O	0	0
			33	28	5		
29	M	1	Total	C		0	0
			10	10			

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



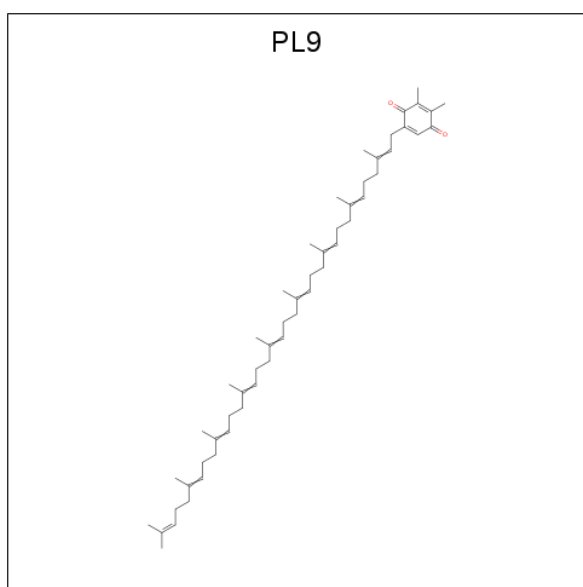
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total 33	C 22	O 11	0	0
30	B	1	Total 25	C 19	O 6	0	0
30	D	1	Total 35	C 24	O 11	0	0
30	E	1	Total 35	C 24	O 11	0	0
30	I	1	Total 35	C 24	O 11	0	0
30	M	1	Total 35	C 24	O 11	0	0
30	M	1	Total 35	C 24	O 11	0	0
30	a	1	Total 35	C 24	O 11	0	0
30	a	1	Total 35	C 24	O 11	0	0
30	b	1	Total 25	C 19	O 6	0	0
30	b	1	Total 25	C 19	O 6	0	0
30	f	1	Total 35	C 24	O 11	0	0
30	m	1	Total 35	C 24	O 11	0	0
30	m	1	Total 35	C 24	O 11	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 32 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 (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).

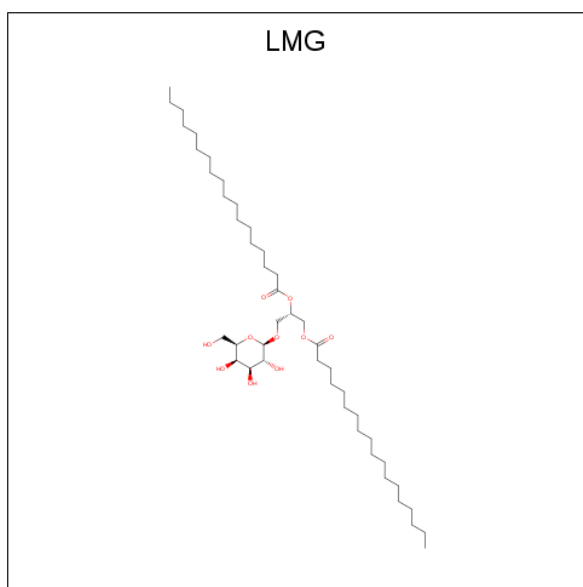


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			55	53	2		
32	D	1	Total	C	O	0	0
			55	53	2		
32	a	1	Total	C	O	0	0
			55	53	2		
32	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

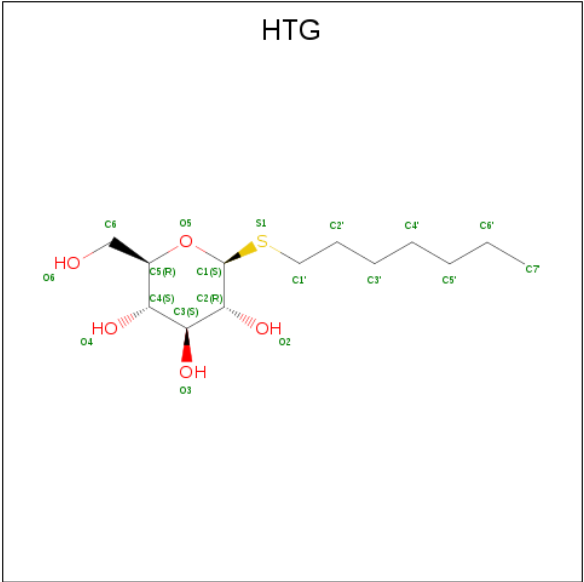
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		
33	F	1	Total	Ca	0	0
			1	1		
33	o	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	f	1	Total	Ca	0	0
			1	1		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



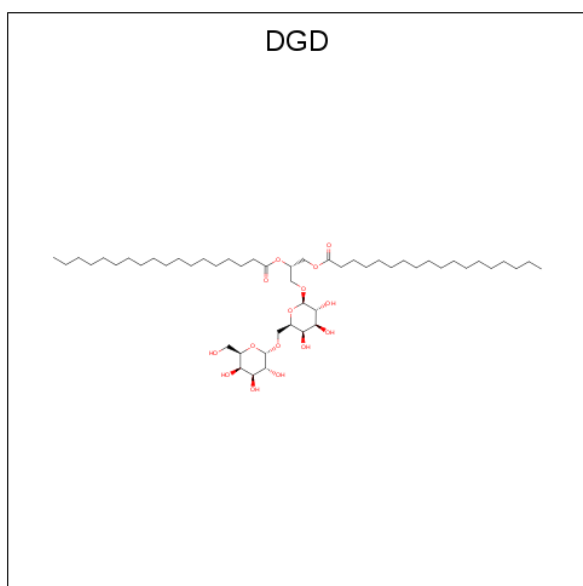
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			16	10	5	1		

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



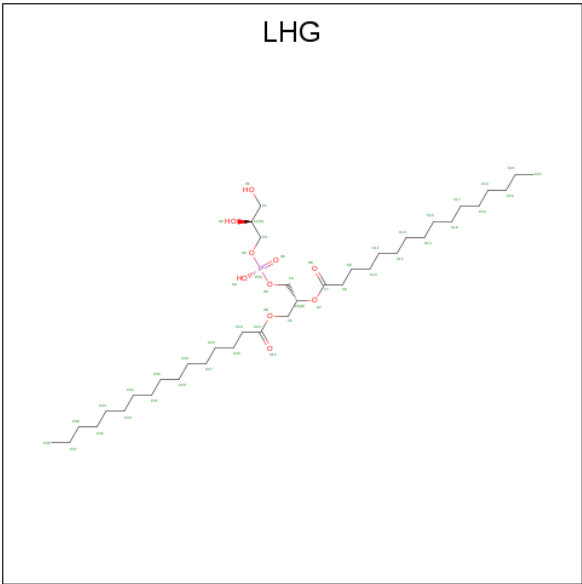
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



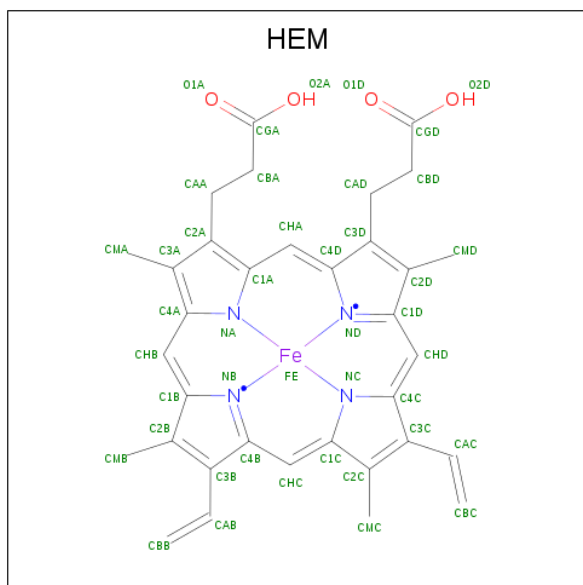
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

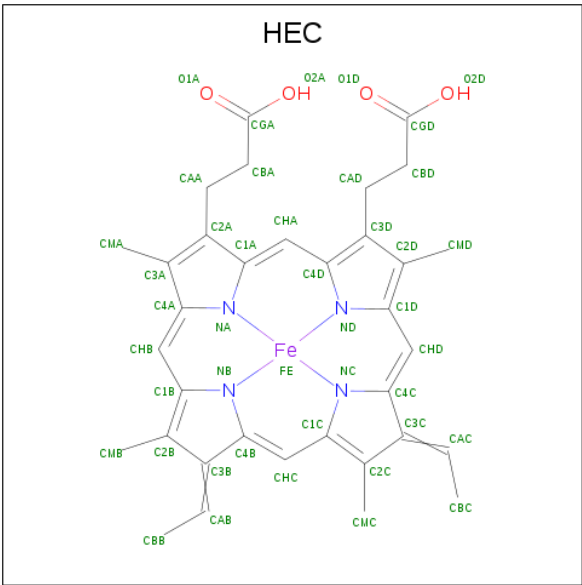


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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	146	Total	O	0	3
			149	149		
41	B	277	Total	O	0	3
			280	280		
41	C	206	Total	O	0	3
			209	209		
41	D	157	Total	O	0	4
			161	161		
41	E	28	Total	O	0	0
			28	28		
41	F	7	Total	O	0	0
			7	7		
41	H	39	Total	O	0	1
			40	40		
41	I	8	Total	O	0	0
			8	8		
41	J	12	Total	O	0	0
			12	12		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	12	Total 12	O 12	0	0
41	M	15	Total 15	O 15	0	0
41	O	164	Total 165	O 165	0	1
41	T	12	Total 13	O 13	0	1
41	U	75	Total 76	O 76	0	1
41	V	111	Total 111	O 111	0	0
41	Y	1	Total 1	O 1	0	0
41	X	8	Total 8	O 8	0	0
41	a	151	Total 151	O 151	0	0
41	b	247	Total 249	O 249	0	2
41	c	187	Total 189	O 189	0	2
41	d	136	Total 139	O 139	0	3
41	e	15	Total 15	O 15	0	0
41	f	7	Total 7	O 7	0	0
41	h	36	Total 36	O 36	0	0
41	i	5	Total 5	O 5	0	0
41	j	7	Total 7	O 7	0	0
41	k	3	Total 3	O 3	0	0
41	l	10	Total 10	O 10	0	0
41	m	12	Total 12	O 12	0	0
41	o	137	Total 137	O 137	0	0

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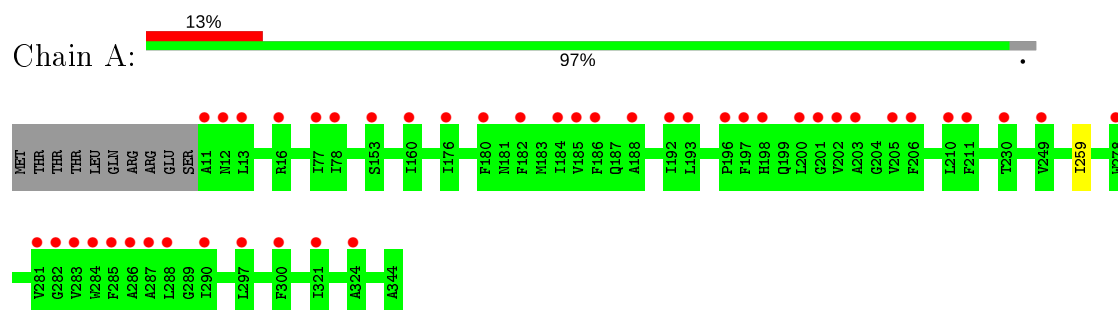
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	t	10	Total 10	O 10	0	0
41	u	89	Total 89	O 89	0	0
41	v	80	Total 80	O 80	0	0
41	y	4	Total 4	O 4	0	0
41	x	5	Total 5	O 5	0	0

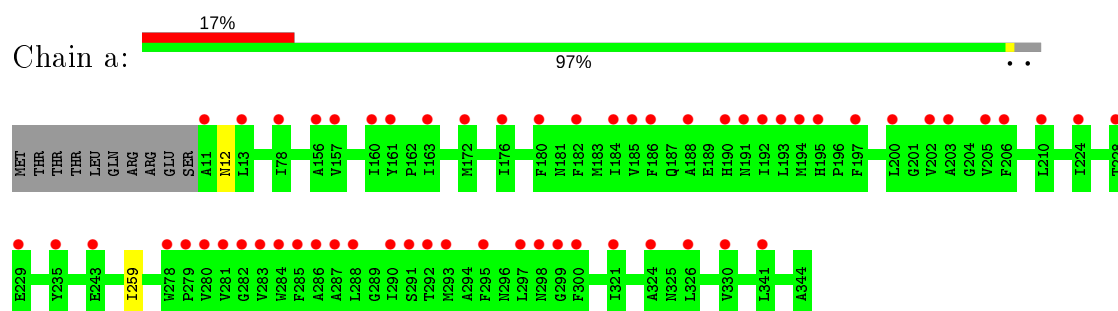
3 Residue-property plots [i](#)

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

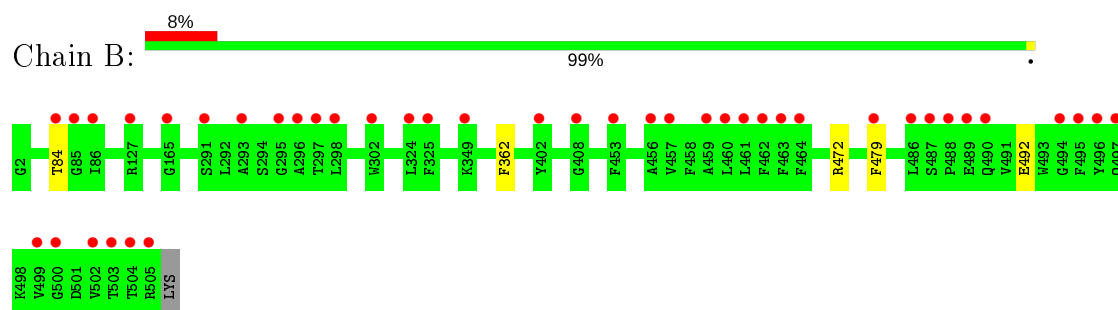
- Molecule 1: Photosystem Q(B) protein



- Molecule 1: Photosystem Q(B) protein

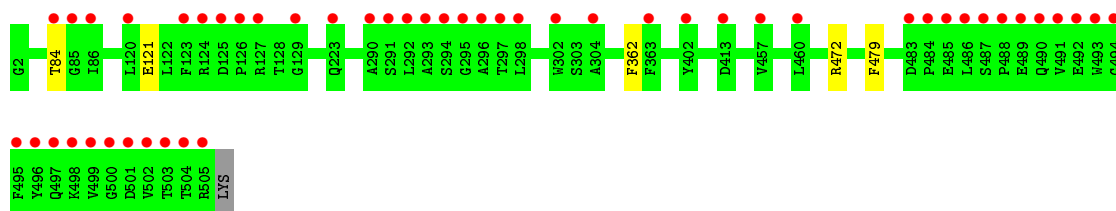


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

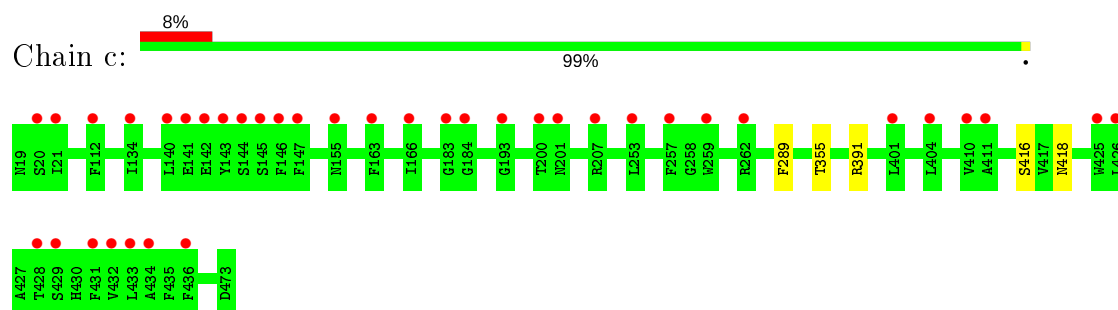




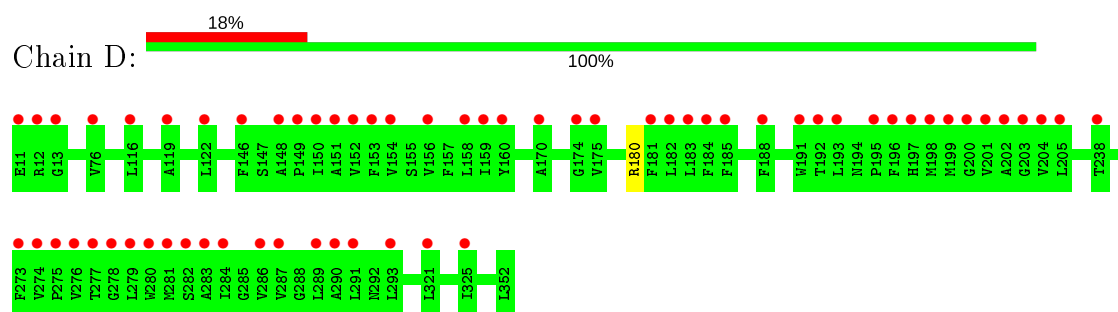
- Molecule 3: Photosystem II 44 kDa reaction center protein



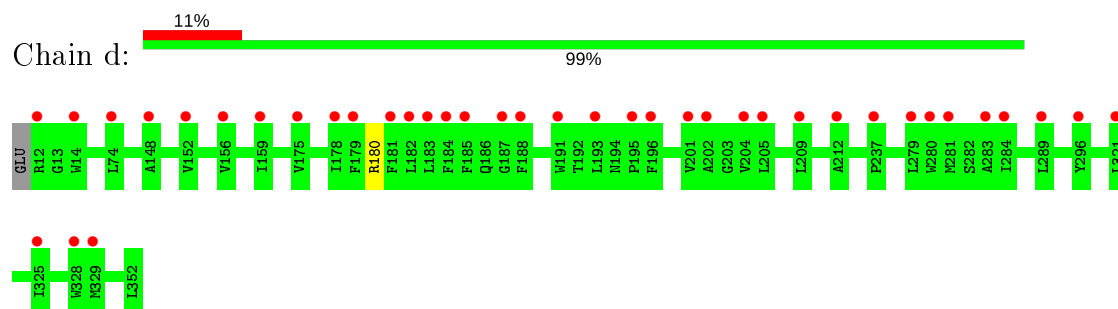
- Molecule 3: Photosystem II 44 kDa reaction center protein



- Molecule 4: Photosystem II D2 protein

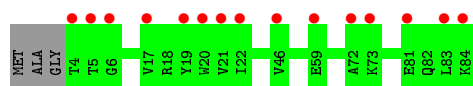


- Molecule 4: Photosystem II D2 protein

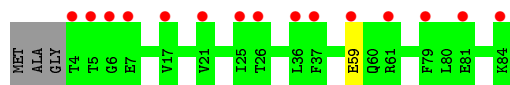


- Molecule 5: Cytochrome b559 subunit alpha

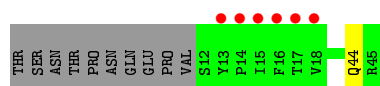
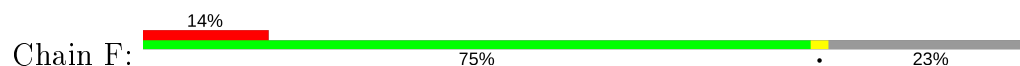




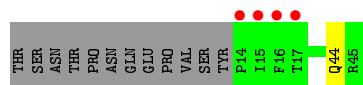
- Molecule 5: Cytochrome b559 subunit alpha



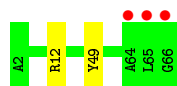
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



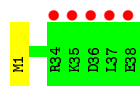
- Molecule 7: Photosystem II reaction center protein H



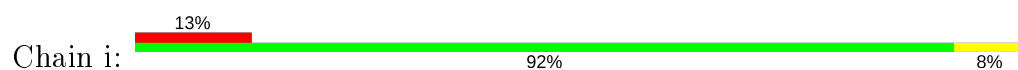
- Molecule 7: Photosystem II reaction center protein H



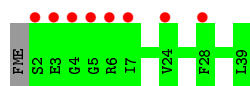
- Molecule 8: Photosystem II reaction center protein I



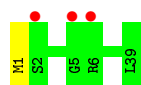
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



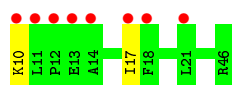
- Molecule 9: Photosystem II reaction center protein J



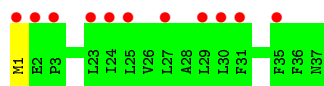
- Molecule 10: Photosystem II reaction center protein K



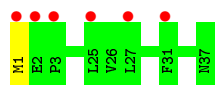
- Molecule 10: Photosystem II reaction center protein K



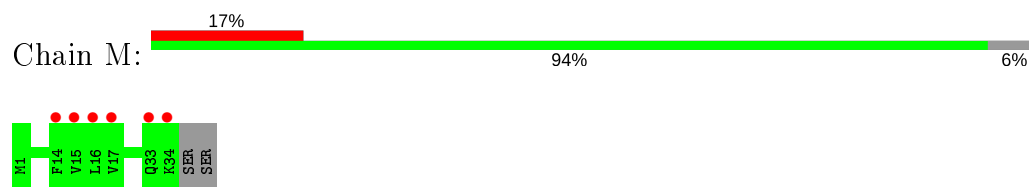
- Molecule 11: Photosystem II reaction center protein L



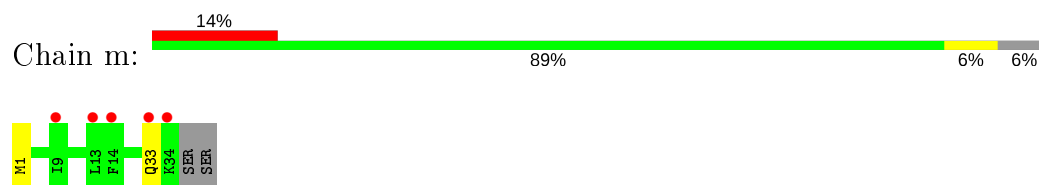
- Molecule 11: Photosystem II reaction center protein L



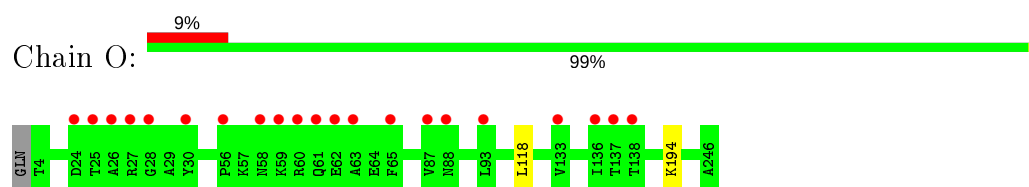
- Molecule 12: Photosystem II reaction center protein M



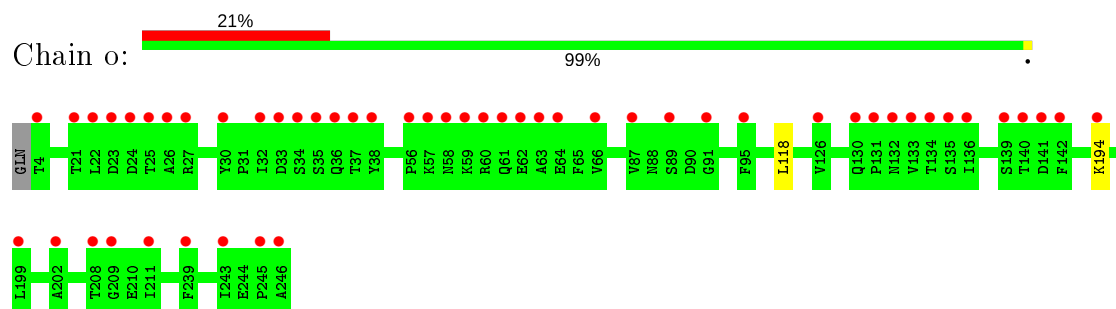
- Molecule 12: Photosystem II reaction center protein M



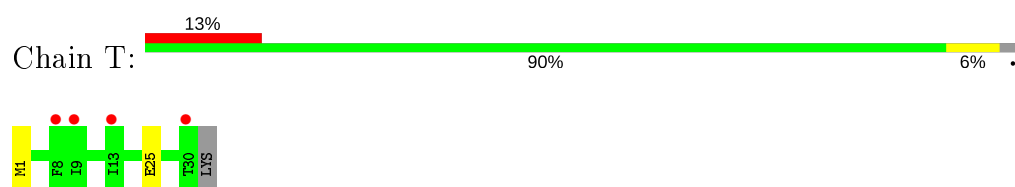
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



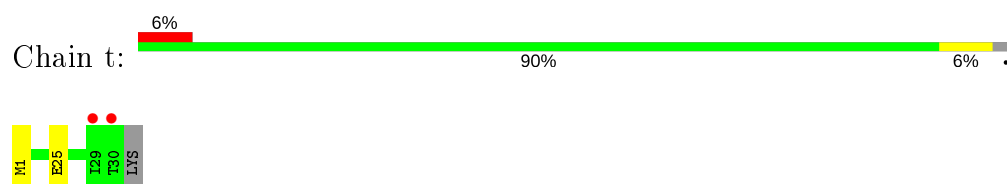
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



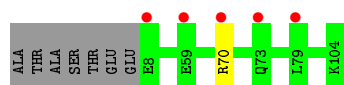
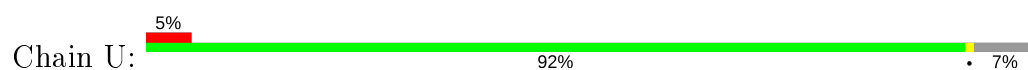
- Molecule 14: Photosystem II reaction center protein T



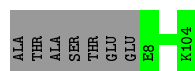
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



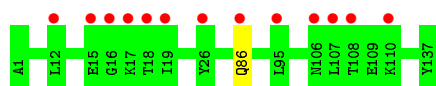
- Molecule 15: Photosystem II 12 kDa extrinsic protein



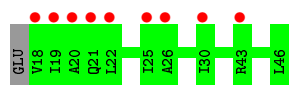
- Molecule 16: Cytochrome c-550



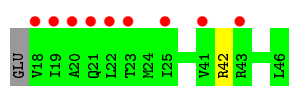
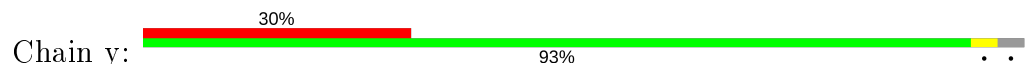
- Molecule 16: Cytochrome c-550



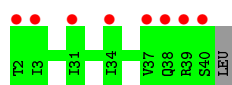
- Molecule 17: Photosystem II reaction center protein Ycf12



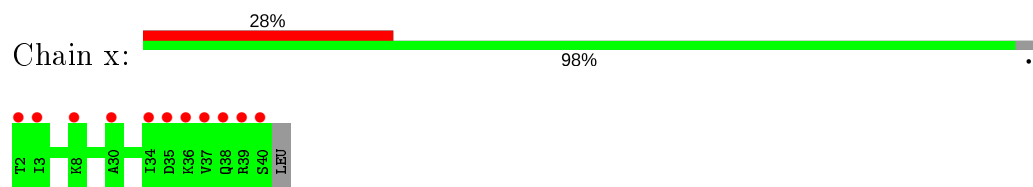
- Molecule 17: Photosystem II reaction center protein Ycf12



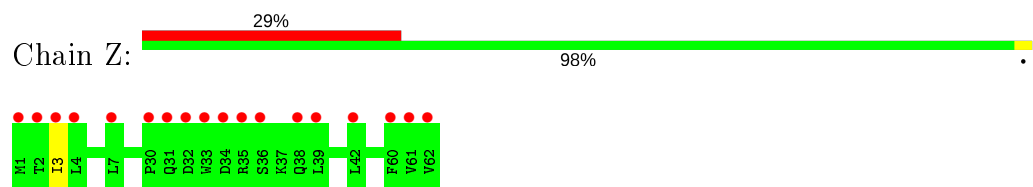
- Molecule 18: Photosystem II reaction center protein X



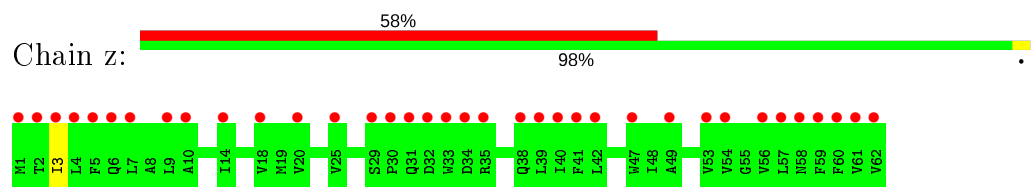
- Molecule 18: Photosystem II reaction center protein X



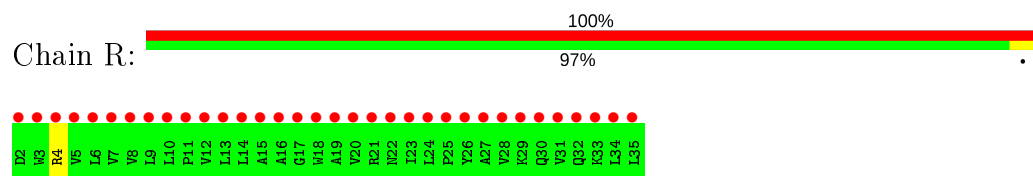
- Molecule 19: Photosystem II reaction center protein Z



- 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	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 85.6 (61.90-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.08 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.187 , 0.225	Depositor DCC
R_{free} test set	29342 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/2725	0.59	0/3716
1	a	0.55	0/2731	0.58	0/3724
2	B	0.49	0/4193	0.56	0/5712
2	b	0.47	0/4201	0.55	0/5723
3	C	0.46	0/3634	0.54	0/4947
3	c	0.46	0/3676	0.54	0/5004
4	D	0.53	0/2821	0.56	0/3844
4	d	0.52	0/2818	0.55	0/3840
5	E	0.36	0/693	0.52	0/944
5	e	0.33	0/681	0.52	0/928
6	F	0.39	0/284	0.48	0/387
6	f	0.37	0/265	0.51	0/360
7	H	0.40	0/535	0.53	0/728
7	h	0.35	0/524	0.50	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.37	0/278	0.46	0/376
9	j	0.38	0/278	0.48	0/376
10	K	0.36	0/303	0.48	0/416
10	k	0.36	0/303	0.51	0/416
11	L	0.48	0/319	0.49	0/433
11	l	0.49	0/319	0.50	0/433
12	M	0.43	0/270	0.58	0/368
12	m	0.47	0/262	0.58	0/357
13	O	0.41	0/1926	0.56	0/2611
13	o	0.40	0/1919	0.57	0/2601
14	T	0.54	0/266	0.56	0/362
14	t	0.54	0/266	0.56	0/362
15	U	0.44	0/785	0.55	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.45	0/1096	0.54	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.41	0/1085	0.53	0/1473
17	Y	0.29	0/216	0.46	0/289
17	y	0.28	0/216	0.46	0/289
18	X	0.34	0/298	0.44	0/403
18	x	0.34	0/290	0.48	0/392
19	Z	0.31	0/490	0.43	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.24	0/279	0.38	0/383
All	All	0.46	0/43142	0.55	0/58701

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	330 (98%)	4 (1%)	1 (0%)	41	30
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	41	30
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	34	22
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	242 (99%)	3 (1%)	0	100	100
13	o	244/244 (100%)	238 (98%)	6 (2%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	29/31 (94%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	51	43

5 of 7 Ramachandran outliers are listed below:

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

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%)	272 (100%)	0	100	100
1	a	273/279 (98%)	272 (100%)	1 (0%)	91	90
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	68
2	b	413/403 (102%)	408 (99%)	5 (1%)	71	68
3	C	357/356 (100%)	352 (99%)	5 (1%)	67	62
3	c	362/356 (102%)	358 (99%)	4 (1%)	73	71
4	D	277/277 (100%)	276 (100%)	1 (0%)	91	90
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	90
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	72/73 (99%)	71 (99%)	1 (1%)	67	62
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	23
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	21
7	H	55/54 (102%)	52 (94%)	3 (6%)	21	9
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	31
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	5
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	5
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	33
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	33
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	26
13	O	210/207 (101%)	208 (99%)	2 (1%)	76	74
13	o	209/207 (101%)	207 (99%)	2 (1%)	76	74
14	T	27/27 (100%)	25 (93%)	2 (7%)	13	4
14	t	27/27 (100%)	25 (93%)	2 (7%)	13	4
15	U	84/89 (94%)	83 (99%)	1 (1%)	71	68
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	80
16	v	117/117 (100%)	116 (99%)	1 (1%)	78	77
17	Y	22/23 (96%)	22 (100%)	0	100	100
17	y	22/23 (96%)	21 (96%)	1 (4%)	27	15
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	50
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	50
20	R	29/29 (100%)	28 (97%)	1 (3%)	37	25
All	All	4383/4399 (100%)	4331 (99%)	52 (1%)	73	68

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	86	GLN
2	b	362	PHE
14	t	25[B]	GLU

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Mol	Chain	Res	Type
19	Z	3	ILE
1	a	12	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	497	GLN
19	z	6	GLN
13	o	109	GLN
4	D	142	ASN
15	u	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.32	0
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.73	3 (42%)
12	FME	m	1	12	8,9,10	0.69	0	7,9,11	1.05	1 (14%)
9	FME	j	1	9	8,9,10	0.63	0	7,9,11	1.32	1 (14%)
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.28	4 (57%)
8	FME	i	1	8	8,9,10	0.62	0	7,9,11	1.17	1 (14%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.32	2 (28%)

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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.68	116.36	109.73
14	t	1	FME	O-C-CA	-3.00	116.92	124.78
14	T	1	FME	O-C-CA	-2.78	117.48	124.78
14	T	1	FME	C-CA-N	2.35	113.97	109.73
14	T	1	FME	CA-N-CN	-2.29	119.31	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 252 ligands modelled in this entry, 19 are unknown and 17 are monoatomic - leaving 216 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$
28	GOL	B	628	-	5,5,5	0.40	0	5,5,5	0.29	0
24	CLA	c	513	3	59,73,73	1.98	12 (20%)	67,113,113	2.09	20 (29%)
24	CLA	B	612	-	59,73,73	2.03	13 (22%)	67,113,113	2.27	21 (31%)
24	CLA	D	403	-	59,73,73	2.00	14 (23%)	67,113,113	2.28	20 (29%)
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.06	3 (6%)
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	8 (14%)
30	LMT	D	402	-	36,36,36	0.48	0	47,47,47	1.01	3 (6%)
26	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	V	201	-	5,5,5	0.38	0	5,5,5	0.43	0
24	CLA	B	607	-	59,73,73	2.00	14 (23%)	67,113,113	2.39	24 (35%)
24	CLA	c	514	-	59,73,73	2.00	13 (22%)	67,113,113	2.18	24 (35%)
24	CLA	B	613	-	59,73,73	2.02	14 (23%)	67,113,113	2.18	19 (28%)
35	HTG	b	627	-	19,19,19	0.86	1 (5%)	23,24,24	1.35	4 (17%)
24	CLA	c	510	-	59,73,73	2.08	13 (22%)	67,113,113	2.27	25 (37%)
34	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.44	7 (15%)
24	CLA	B	603	-	59,73,73	2.03	15 (25%)	67,113,113	2.30	23 (34%)
24	CLA	C	504	-	59,73,73	2.04	13 (22%)	67,113,113	2.15	20 (29%)
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	18 (26%)
28	GOL	v	203	-	5,5,5	0.27	0	5,5,5	0.49	0
28	GOL	B	633	-	5,5,5	0.30	0	5,5,5	0.66	0
26	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	13 (23%)
24	CLA	b	608	-	59,73,73	2.01	13 (22%)	67,113,113	2.40	25 (37%)
28	GOL	V	206	-	5,5,5	0.37	0	5,5,5	0.46	0
28	GOL	A	412	-	5,5,5	0.26	0	5,5,5	0.68	0
35	HTG	C	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.77	5 (21%)
25	PHO	a	408	-	67,69,69	2.15	16 (23%)	85,99,99	1.85	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.29	0
24	CLA	d	404	-	59,73,73	2.00	14 (23%)	67,113,113	2.16	22 (32%)
31	OEX	a	415	1,3,41	0,15,15	0.00	-	-	-	-
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	5 (9%)
34	LMG	c	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
26	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
28	GOL	c	525	-	5,5,5	0.36	0	5,5,5	0.58	0
24	CLA	b	620	-	59,73,73	2.03	13 (22%)	67,113,113	2.23	20 (29%)
24	CLA	C	513	-	59,73,73	2.01	13 (22%)	67,113,113	2.25	27 (40%)
34	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	5 (8%)
27	SQD	F	101	-	42,43,54	1.12	3 (7%)	51,54,65	1.55	9 (17%)
31	OEX	A	418	1,3,41	0,15,15	0.00	-	-	-	-
24	CLA	c	506	41	59,73,73	2.04	13 (22%)	67,113,113	2.16	22 (32%)
28	GOL	c	524	-	5,5,5	0.32	0	5,5,5	0.37	0
27	SQD	a	402	-	53,54,54	1.03	3 (5%)	62,65,65	1.19	6 (9%)
30	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.77	0
24	CLA	C	506	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	17 (25%)
35	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.89	4 (17%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	7 (12%)
25	PHO	A	407	-	67,69,69	2.15	17 (25%)	85,99,99	1.85	19 (22%)
24	CLA	a	409	-	59,73,73	1.99	14 (23%)	67,113,113	2.22	24 (35%)
24	CLA	b	616	-	59,73,73	1.99	13 (22%)	67,113,113	2.24	21 (31%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.39	0
24	CLA	b	614	-	59,73,73	2.02	13 (22%)	67,113,113	2.22	22 (32%)
30	LMT	a	417	-	36,36,36	0.44	0	47,47,47	0.84	2 (4%)
28	GOL	A	413	-	5,5,5	0.43	0	5,5,5	0.62	0
26	BCR	d	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	13 (23%)
27	SQD	l	101	-	53,54,54	1.00	3 (5%)	62,65,65	1.40	9 (14%)
24	CLA	B	604	-	59,73,73	2.05	13 (22%)	67,113,113	2.29	26 (38%)
30	LMT	M	101	-	36,36,36	0.57	1 (2%)	47,47,47	0.84	0
24	CLA	B	606	-	59,73,73	1.94	13 (22%)	67,113,113	2.32	23 (34%)
27	SQD	A	411	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	11 (17%)
24	CLA	B	609	-	59,73,73	2.05	13 (22%)	67,113,113	2.23	23 (34%)
28	GOL	V	208	-	5,5,5	0.37	0	5,5,5	0.27	0
24	CLA	b	621	-	59,73,73	2.04	14 (23%)	67,113,113	2.21	23 (34%)
24	CLA	B	614	-	59,73,73	2.03	13 (22%)	67,113,113	2.17	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	D	404	-	59,73,73	2.00	13 (22%)	67,113,113	2.17	24 (35%)
24	CLA	B	610	-	59,73,73	1.96	12 (20%)	67,113,113	2.20	21 (31%)
28	GOL	A	414	-	5,5,5	0.41	0	5,5,5	0.20	0
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.13	5 (8%)
28	GOL	T	103	-	5,5,5	0.41	0	5,5,5	0.24	0
32	PL9	d	406	-	55,55,55	0.71	1 (1%)	68,69,69	1.55	14 (20%)
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
24	CLA	C	503	-	59,73,73	2.03	13 (22%)	67,113,113	2.24	24 (35%)
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	4 (5%)
28	GOL	b	630	-	5,5,5	0.34	0	5,5,5	0.16	0
28	GOL	T	101	-	5,5,5	0.45	0	5,5,5	0.31	0
24	CLA	c	504	-	59,73,73	1.96	13 (22%)	67,113,113	2.18	20 (29%)
25	PHO	d	403	-	67,69,69	2.15	17 (25%)	85,99,99	1.95	22 (25%)
24	CLA	C	508	41	59,73,73	2.02	13 (22%)	67,113,113	2.18	22 (32%)
26	BCR	k	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.33	5 (8%)
27	SQD	A	416	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	7 (11%)
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.50	2 (8%)
24	CLA	C	502	-	59,73,73	1.99	13 (22%)	67,113,113	2.15	21 (31%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.03	3 (15%)
28	GOL	F	103	33	5,5,5	0.36	0	5,5,5	0.37	0
34	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.11	5 (8%)
24	CLA	b	606	41	59,73,73	2.04	13 (22%)	67,113,113	2.15	19 (28%)
24	CLA	B	605	-	59,73,73	1.85	13 (22%)	67,113,113	2.28	21 (31%)
24	CLA	A	409	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	24 (35%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.43	3 (13%)
28	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.57	0
35	HTG	b	604	-	19,19,19	1.02	2 (10%)	23,24,24	1.10	2 (8%)
24	CLA	b	618	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	20 (29%)
25	PHO	A	408	-	67,69,69	2.08	16 (23%)	85,99,99	1.96	22 (25%)
26	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.00	3 (5%)
35	HTG	V	204	-	19,19,19	1.00	2 (10%)	23,24,24	1.33	3 (13%)
34	LMG	J	101	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	4 (6%)
30	LMT	I	102	-	36,36,36	0.45	0	47,47,47	1.18	4 (8%)
24	CLA	b	617	-	59,73,73	1.99	13 (22%)	67,113,113	2.16	20 (29%)
24	CLA	C	514	-	59,73,73	1.99	13 (22%)	67,113,113	2.14	22 (32%)
24	CLA	a	406	-	59,73,73	1.99	13 (22%)	67,113,113	2.23	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	1.85	19 (27%)
26	BCR	b	622	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	4 (7%)
26	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.24	5 (8%)
24	CLA	b	609	-	59,73,73	2.01	14 (23%)	67,113,113	2.24	20 (29%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)
34	LMG	c	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	6 (10%)
28	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.37	0
24	CLA	c	512	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	24 (35%)
34	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
24	CLA	b	611	-	59,73,73	1.98	13 (22%)	67,113,113	2.22	23 (34%)
23	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
40	HEC	V	203	16	26,50,50	1.45	4 (15%)	18,82,82	1.61	4 (22%)
26	BCR	t	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	8 (14%)
34	LMG	j	101	39	51,51,55	0.93	3 (5%)	59,59,63	0.98	3 (5%)
27	SQD	b	601	-	53,54,54	1.02	3 (5%)	62,65,65	1.63	10 (16%)
28	GOL	f	104	33	5,5,5	0.35	0	5,5,5	0.24	0
24	CLA	D	401	41	59,73,73	2.07	13 (22%)	67,113,113	2.18	25 (37%)
36	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
38	HEM	e	102	5,6	27,50,50	0.83	1 (3%)	17,82,82	2.37	3 (17%)
34	LMG	b	625	-	51,51,55	0.90	2 (3%)	59,59,63	1.03	4 (6%)
24	CLA	C	505	41	59,73,73	2.02	13 (22%)	67,113,113	2.17	22 (32%)
24	CLA	B	615	-	59,73,73	1.96	14 (23%)	67,113,113	2.25	23 (34%)
35	HTG	b	628	-	19,19,19	1.10	2 (10%)	23,24,24	1.83	3 (13%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.04	3 (6%)
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	0.89	3 (3%)
24	CLA	c	507	-	59,73,73	1.94	13 (22%)	67,113,113	2.17	15 (22%)
37	LHG	D	409	-	48,48,48	0.85	2 (4%)	51,54,54	1.08	5 (9%)
30	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
36	DGD	D	407	-	63,63,67	0.96	4 (6%)	77,77,81	1.30	9 (11%)
28	GOL	B	625	-	5,5,5	0.31	0	5,5,5	0.56	0
35	HTG	B	623	-	19,19,19	0.88	1 (5%)	23,24,24	1.25	3 (13%)
30	LMT	E	102	-	36,36,36	0.46	0	47,47,47	0.75	0
24	CLA	A	406	41	59,73,73	2.04	12 (20%)	67,113,113	2.17	25 (37%)
24	CLA	d	401	41	59,73,73	2.04	11 (18%)	67,113,113	2.16	23 (34%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.25	5 (8%)
37	LHG	d	408	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	0.97	3 (3%)
36	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.90	3 (3%)
28	GOL	b	632	-	5,5,5	0.44	0	5,5,5	0.52	0
40	HEC	v	202	16	26,50,50	1.55	4 (15%)	18,82,82	1.26	2 (11%)
28	GOL	O	302	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	B	626	-	5,5,5	0.29	0	5,5,5	0.48	0
24	CLA	B	616	-	59,73,73	1.99	14 (23%)	67,113,113	2.21	23 (34%)
24	CLA	C	512	3	59,73,73	1.97	13 (22%)	67,113,113	2.07	18 (26%)
24	CLA	c	508	-	59,73,73	1.97	14 (23%)	67,113,113	2.18	27 (40%)
26	BCR	b	624	-	41,41,41	0.99	1 (2%)	56,56,56	1.25	8 (14%)
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.28	2 (8%)
26	BCR	D	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.70	12 (21%)
37	LHG	D	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	3 (5%)
28	GOL	b	631	-	5,5,5	0.34	0	5,5,5	0.45	0
24	CLA	b	613	-	59,73,73	2.04	13 (22%)	67,113,113	2.21	25 (37%)
28	GOL	t	102	-	5,5,5	0.34	0	5,5,5	0.30	0
24	CLA	B	602	41	59,73,73	2.04	13 (22%)	67,113,113	2.21	24 (35%)
28	GOL	V	207	-	5,5,5	0.37	0	5,5,5	0.46	0
24	CLA	b	615	41	59,73,73	2.04	13 (22%)	67,113,113	2.15	22 (32%)
37	LHG	D	408	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
24	CLA	b	610	-	59,73,73	1.92	13 (22%)	67,113,113	2.25	23 (34%)
28	GOL	B	635	-	5,5,5	0.40	0	5,5,5	0.25	0
27	SQD	a	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.60	11 (17%)
24	CLA	B	617	-	59,73,73	2.02	13 (22%)	67,113,113	2.21	21 (31%)
30	LMT	b	626	-	25,25,36	0.50	0	30,30,47	0.64	0
30	LMT	a	401	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
35	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.44	2 (8%)
28	GOL	c	527	-	5,5,5	0.41	0	5,5,5	0.31	0
35	HTG	O	303	-	19,19,19	1.07	1 (5%)	23,24,24	0.93	1 (4%)
30	LMT	m	103	-	36,36,36	0.56	1 (2%)	47,47,47	1.05	4 (8%)
36	DGD	d	407	-	63,63,67	0.94	3 (4%)	77,77,81	1.04	6 (7%)
34	LMG	C	501	-	51,51,55	0.97	2 (3%)	59,59,63	1.10	3 (5%)
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
30	LMT	b	602	-	25,25,36	0.46	0	30,30,47	1.26	3 (10%)
24	CLA	B	611	41	59,73,73	2.01	13 (22%)	67,113,113	2.24	24 (35%)
28	GOL	a	413	-	5,5,5	0.43	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	515	-	59,73,73	2.03	13 (22%)	67,113,113	2.10	23 (34%)
28	GOL	B	629	-	5,5,5	0.32	0	5,5,5	0.39	0
32	PL9	D	406	-	55,55,55	0.77	2 (3%)	68,69,69	1.50	16 (23%)
35	HTG	d	411	-	16,16,19	1.21	2 (12%)	20,21,24	1.55	1 (5%)
24	CLA	C	511	-	59,73,73	2.04	13 (22%)	67,113,113	2.20	23 (34%)
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
38	HEM	E	103	5,6	27,50,50	0.78	1 (3%)	17,82,82	2.42	4 (23%)
26	BCR	c	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.41	9 (16%)
24	CLA	C	507	-	59,73,73	2.01	13 (22%)	67,113,113	2.21	25 (37%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.39	0
24	CLA	b	607	-	59,73,73	2.07	13 (22%)	67,113,113	2.37	27 (40%)
34	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.17	4 (8%)
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.71	0
24	CLA	c	505	-	59,73,73	1.96	13 (22%)	67,113,113	2.23	21 (31%)
24	CLA	A	405	-	59,73,73	2.06	14 (23%)	67,113,113	2.35	24 (35%)
24	CLA	C	509	-	59,73,73	2.05	13 (22%)	67,113,113	2.30	22 (32%)
37	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)
35	HTG	b	603	-	19,19,19	1.07	2 (10%)	23,24,24	1.28	1 (4%)
30	LMT	B	634	-	25,25,36	0.49	0	30,30,47	0.71	0
30	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
24	CLA	c	511	-	59,73,73	2.09	13 (22%)	67,113,113	2.24	21 (31%)
28	GOL	C	524	-	5,5,5	0.34	0	5,5,5	0.89	0
24	CLA	B	608	41	59,73,73	2.01	13 (22%)	67,113,113	2.20	24 (35%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	7 (9%)
24	CLA	c	503	-	59,73,73	2.01	13 (22%)	67,113,113	2.21	22 (32%)
26	BCR	a	410	-	41,41,41	1.14	1 (2%)	56,56,56	1.35	8 (14%)
24	CLA	d	402	-	59,73,73	2.01	14 (23%)	67,113,113	2.39	22 (32%)
36	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	3 (3%)
37	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	5 (9%)
24	CLA	b	619	-	59,73,73	1.98	13 (22%)	67,113,113	2.30	25 (37%)
24	CLA	b	612	41	59,73,73	1.96	11 (18%)	67,113,113	2.23	23 (34%)
28	GOL	v	205	-	5,5,5	0.35	0	5,5,5	0.46	0
24	CLA	a	407	41	59,73,73	1.98	13 (22%)	67,113,113	2.21	23 (34%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
24	CLA	c	509	41	59,73,73	1.99	13 (22%)	67,113,113	2.19	21 (31%)
37	LHG	l	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.33	8 (14%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.30	0
26	BCR	c	526	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)
37	LHG	d	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
27	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.44	7 (13%)
35	HTG	B	630	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	1 (4%)
28	GOL	C	525	-	5,5,5	0.33	0	5,5,5	0.72	0
24	CLA	C	510	-	59,73,73	2.08	13 (22%)	67,113,113	2.19	22 (32%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.14	5 (8%)

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
28	GOL	B	628	-	-	2/4/4/4	-
24	CLA	c	513	3	3/3/20/25	5/37/135/135	-
24	CLA	B	612	-	1/1/20/25	3/37/135/135	-
24	CLA	D	403	-	1/1/20/25	2/37/135/135	-
30	LMT	A	417	-	-	3/19/59/61	0/2/2/2
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
30	LMT	D	402	-	-	9/21/61/61	0/2/2/2
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	V	201	-	-	0/4/4/4	-
24	CLA	B	607	-	3/3/20/25	4/37/135/135	-
24	CLA	c	514	-	3/3/20/25	12/37/135/135	-
24	CLA	B	613	-	3/3/20/25	2/37/135/135	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
24	CLA	c	510	-	3/3/20/25	2/37/135/135	-
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	CLA	B	603	-	2/2/20/25	7/37/135/135	-
24	CLA	C	504	-	2/2/20/25	4/37/135/135	-
32	PL9	a	416	-	-	17/53/73/73	0/1/1/1
28	GOL	v	203	-	-	4/4/4/4	-
28	GOL	B	633	-	-	0/4/4/4	-
26	BCR	B	620	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	608	-	2/2/20/25	7/37/135/135	-
28	GOL	V	206	-	-	2/4/4/4	-
28	GOL	A	412	-	-	2/4/4/4	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
25	PHO	a	408	-	-	2/53/103/103	0/5/6/6
28	GOL	b	629	-	-	2/4/4/4	-
24	CLA	d	404	-	3/3/20/25	6/37/135/135	-
37	LHG	d	409	-	-	11/53/53/53	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
28	GOL	c	525	-	-	1/4/4/4	-
24	CLA	b	620	-	3/3/20/25	4/37/135/135	-
24	CLA	C	513	-	3/3/20/25	10/37/135/135	-
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
27	SQD	F	101	-	-	12/38/58/69	0/1/1/1
37	LHG	d	410	-	-	13/53/53/53	-
28	GOL	c	524	-	-	0/4/4/4	-
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
30	LMT	f	102	-	-	7/21/61/61	0/2/2/2
24	CLA	C	506	-	1/1/20/25	5/37/135/135	-
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
25	PHO	A	407	-	-	3/53/103/103	0/5/6/6
24	CLA	a	409	-	3/3/20/25	11/37/135/135	-
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	b	614	-	2/2/20/25	3/37/135/135	-
30	LMT	a	417	-	-	2/21/61/61	0/2/2/2
28	GOL	A	413	-	-	2/4/4/4	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1
27	SQD	l	101	-	-	20/49/69/69	0/1/1/1
24	CLA	B	604	-	2/2/20/25	3/37/135/135	-
30	LMT	M	101	-	-	8/21/61/61	0/2/2/2
24	CLA	c	504	-	3/3/20/25	3/37/135/135	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	V	208	-	-	2/4/4/4	-
24	CLA	b	621	-	3/3/20/25	10/37/135/135	-
24	CLA	B	614	-	3/3/20/25	9/37/135/135	-
24	CLA	D	404	-	3/3/20/25	5/37/135/135	-
24	CLA	B	610	-	2/2/20/25	3/37/135/135	-
28	GOL	A	414	-	-	2/4/4/4	-
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
28	GOL	T	103	-	-	3/4/4/4	-
36	DGD	d	407	-	-	20/51/91/95	0/2/2/2
32	PL9	d	406	-	-	3/53/73/73	0/1/1/1
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	CLA	C	503	-	2/2/20/25	8/37/135/135	-
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
28	GOL	b	630	-	-	0/4/4/4	-
28	GOL	T	101	-	-	2/4/4/4	-
24	CLA	B	606	-	2/2/20/25	3/37/135/135	-
25	PHO	d	403	-	-	4/53/103/103	0/5/6/6
24	CLA	C	508	41	3/3/20/25	11/37/135/135	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
27	SQD	A	416	-	-	17/49/69/69	0/1/1/1
28	GOL	F	103	33	-	2/4/4/4	-
24	CLA	C	502	-	3/3/20/25	9/37/135/135	-
35	HTG	c	522	-	-	1/10/30/30	0/1/1/1
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
24	CLA	b	606	41	3/3/20/25	14/37/135/135	-
24	CLA	c	507	-	1/1/20/25	3/37/135/135	-
24	CLA	A	409	-	2/2/20/25	11/37/135/135	-
24	CLA	A	406	41	2/2/20/25	5/37/135/135	-
28	GOL	a	412	-	-	2/4/4/4	-
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
24	CLA	b	618	-	3/3/20/25	6/37/135/135	-
25	PHO	A	408	-	-	2/53/103/103	0/5/6/6
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	HTG	V	204	-	-	3/10/30/30	0/1/1/1
34	LMG	J	101	39	-	9/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	I	102	-	-	10/21/61/61	0/2/2/2
24	CLA	b	617	-	3/3/20/25	3/37/135/135	-
24	CLA	C	514	-	2/2/20/25	3/37/135/135	-
28	GOL	t	102	-	-	0/4/4/4	-
24	CLA	a	407	41	2/2/20/25	3/37/135/135	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	b	609	-	3/3/20/25	3/37/135/135	-
36	DGD	C	518	-	-	19/51/91/95	0/2/2/2
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
28	GOL	v	204	-	-	2/4/4/4	-
24	CLA	c	512	-	3/3/20/25	7/37/135/135	-
34	LMG	B	621	-	-	7/46/66/70	0/1/1/1
24	CLA	b	611	-	2/2/20/25	8/37/135/135	-
40	HEC	V	203	16	-	0/6/54/54	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
34	LMG	j	101	39	-	12/46/66/70	0/1/1/1
27	SQD	b	601	-	-	20/49/69/69	0/1/1/1
28	GOL	f	104	33	-	3/4/4/4	-
24	CLA	D	401	41	3/3/20/25	5/37/135/135	-
36	DGD	c	517	-	-	12/51/91/95	0/2/2/2
38	HEM	e	102	5,6	-	0/6/54/54	-
34	LMG	b	625	-	-	18/46/66/70	0/1/1/1
24	CLA	b	607	-	2/2/20/25	3/37/135/135	-
24	CLA	B	615	-	2/2/20/25	14/37/135/135	-
35	HTG	b	628	-	-	2/10/30/30	0/1/1/1
37	LHG	e	101	-	-	18/46/46/53	-
36	DGD	C	519	-	-	5/51/91/95	0/2/2/2
24	CLA	B	605	-	3/3/20/25	4/37/135/135	-
37	LHG	D	409	-	-	9/53/53/53	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
36	DGD	D	407	-	-	17/51/91/95	0/2/2/2
28	GOL	B	625	-	-	2/4/4/4	-
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
30	LMT	E	102	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
24	CLA	d	401	41	3/3/20/25	7/37/135/135	-
26	BCR	H	101	-	-	1/29/63/63	0/2/2/2
37	LHG	d	408	-	-	9/53/53/53	-
36	DGD	c	519	-	-	12/51/91/95	0/2/2/2
36	DGD	H	102	-	-	11/51/91/95	0/2/2/2
28	GOL	b	632	-	-	2/4/4/4	-
40	HEC	v	202	16	-	0/6/54/54	-
28	GOL	O	302	-	-	2/4/4/4	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	B	616	-	3/3/20/25	8/37/135/135	-
24	CLA	C	512	3	3/3/20/25	1/37/135/135	-
24	CLA	c	508	-	3/3/20/25	8/37/135/135	-
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
24	CLA	c	506	41	3/3/20/25	6/37/135/135	-
26	BCR	D	405	-	-	6/29/63/63	0/2/2/2
24	CLA	C	505	41	3/3/20/25	4/37/135/135	-
37	LHG	D	410	-	-	14/53/53/53	-
28	GOL	b	631	-	-	2/4/4/4	-
24	CLA	b	613	-	2/2/20/25	2/37/135/135	-
24	CLA	a	406	-	3/3/20/25	3/37/135/135	-
24	CLA	B	602	41	3/3/20/25	15/37/135/135	-
28	GOL	V	207	-	-	0/4/4/4	-
24	CLA	b	615	41	3/3/20/25	6/37/135/135	-
37	LHG	D	408	-	-	9/53/53/53	-
24	CLA	b	610	-	3/3/20/25	5/37/135/135	-
28	GOL	B	635	-	-	2/4/4/4	-
27	SQD	a	411	-	-	9/49/69/69	0/1/1/1
24	CLA	B	617	-	3/3/20/25	9/37/135/135	-
30	LMT	b	626	-	-	6/17/37/61	0/1/1/2
30	LMT	a	401	-	-	9/21/61/61	0/2/2/2
26	BCR	C	516	-	-	3/29/63/63	0/2/2/2
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
28	GOL	c	527	-	-	2/4/4/4	-
35	HTG	O	303	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	m	103	-	-	6/21/61/61	0/2/2/2
24	CLA	d	402	-	1/1/20/25	1/37/135/135	-
34	LMG	C	501	-	-	16/46/66/70	0/1/1/1
35	HTG	c	523	-	-	1/10/30/30	0/1/1/1
30	LMT	b	602	-	-	7/17/37/61	0/1/1/2
24	CLA	B	611	41	3/3/20/25	3/37/135/135	-
28	GOL	a	413	-	-	4/4/4/4	-
24	CLA	c	515	-	2/2/20/25	4/37/135/135	-
28	GOL	B	629	-	-	0/4/4/4	-
32	PL9	D	406	-	-	1/53/73/73	0/1/1/1
35	HTG	d	411	-	-	2/7/27/30	0/1/1/1
24	CLA	C	511	-	3/3/20/25	8/37/135/135	-
34	LMG	c	520	-	-	5/46/66/70	0/1/1/1
38	HEM	E	103	5,6	-	0/6/54/54	-
26	BCR	c	516	-	-	4/29/63/63	0/2/2/2
24	CLA	C	507	-	3/3/20/25	8/37/135/135	-
28	GOL	v	201	-	-	0/4/4/4	-
24	CLA	b	616	-	3/3/20/25	2/37/135/135	-
34	LMG	z	101	-	-	13/34/54/70	0/1/1/1
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	c	505	-	3/3/20/25	4/37/135/135	-
24	CLA	A	405	-	3/3/20/25	1/37/135/135	-
24	CLA	C	509	-	2/2/20/25	3/37/135/135	-
37	LHG	E	101	-	-	20/46/46/53	-
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
30	LMT	B	634	-	-	5/17/37/61	0/1/1/2
30	LMT	m	102	-	-	3/21/61/61	0/2/2/2
24	CLA	c	511	-	3/3/20/25	9/37/135/135	-
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	B	608	41	3/3/20/25	5/37/135/135	-
36	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	c	503	-	3/3/20/25	3/37/135/135	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
36	DGD	c	518	-	-	15/51/91/95	0/2/2/2
37	LHG	L	101	-	-	12/53/53/53	-
24	CLA	b	619	-	3/3/20/25	14/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	612	41	2/2/20/25	3/37/135/135	-
28	GOL	v	205	-	-	2/4/4/4	-
32	PL9	A	419	-	-	8/53/73/73	0/1/1/1
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	509	41	3/3/20/25	3/37/135/135	-
37	LHG	l	102	-	-	18/53/53/53	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	205	-	-	4/4/4/4	-
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
27	SQD	f	101	-	-	16/38/58/69	0/1/1/1
35	HTG	B	630	-	-	1/10/30/30	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
24	CLA	C	510	-	3/3/20/25	4/37/135/135	-
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1

The worst 5 of 1148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	C3B-C2B	6.62	1.49	1.40
24	B	617	CLA	C3B-C2B	6.61	1.49	1.40
24	C	511	CLA	C3B-C2B	6.55	1.49	1.40
24	A	405	CLA	C3B-C2B	6.45	1.49	1.40
24	B	609	CLA	C3B-C2B	6.41	1.49	1.40

The worst 5 of 2185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	C4A-NA-C1A	-8.26	102.99	106.71
24	A	405	CLA	C4A-NA-C1A	-8.07	103.08	106.71
38	E	103	HEM	CAD-CBD-CGD	7.50	125.25	112.67
24	B	612	CLA	C4A-NA-C1A	-7.20	103.47	106.71
24	B	616	CLA	C4A-NA-C1A	-7.19	103.47	106.71

5 of 180 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA

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Mol	Chain	Res	Type	Atom
24	B	612	CLA	NC
24	D	403	CLA	ND

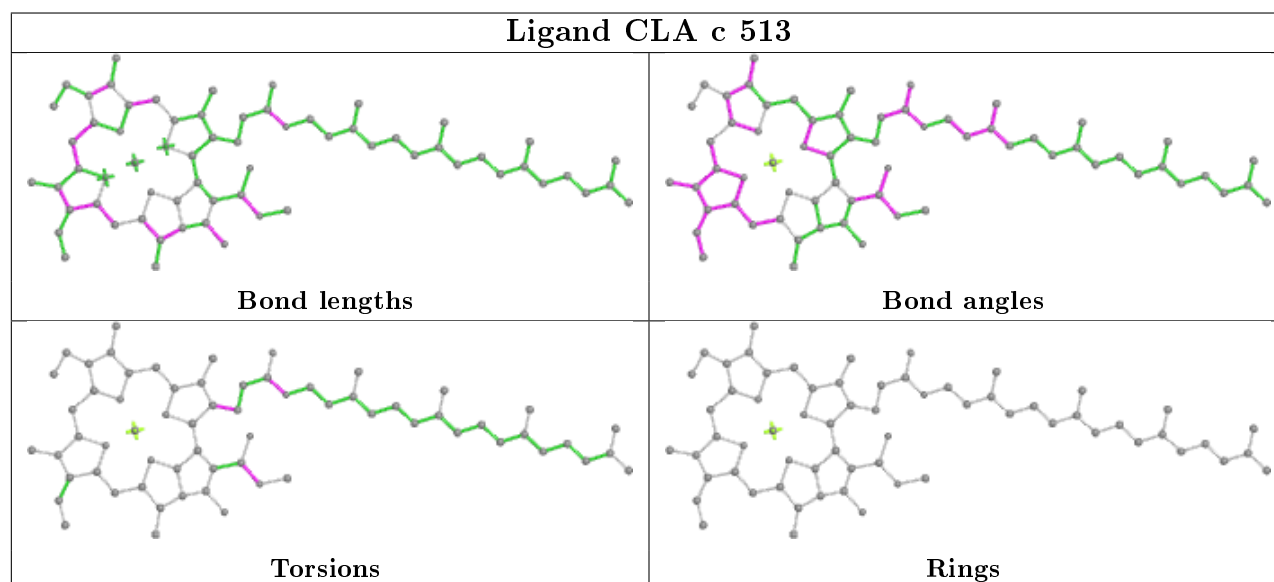
5 of 1180 torsion outliers are listed below:

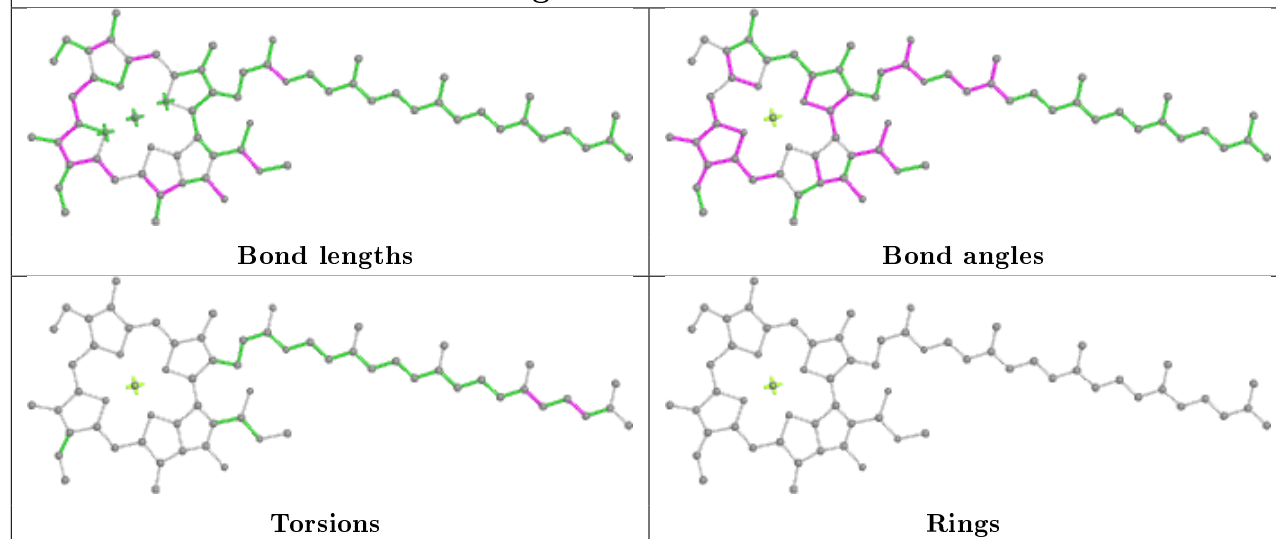
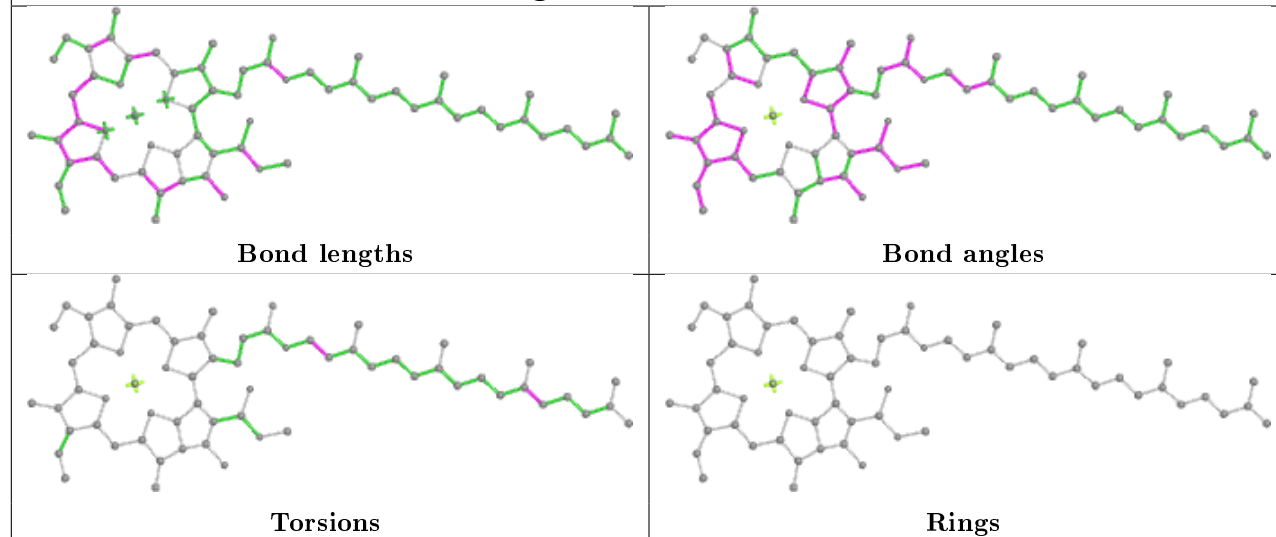
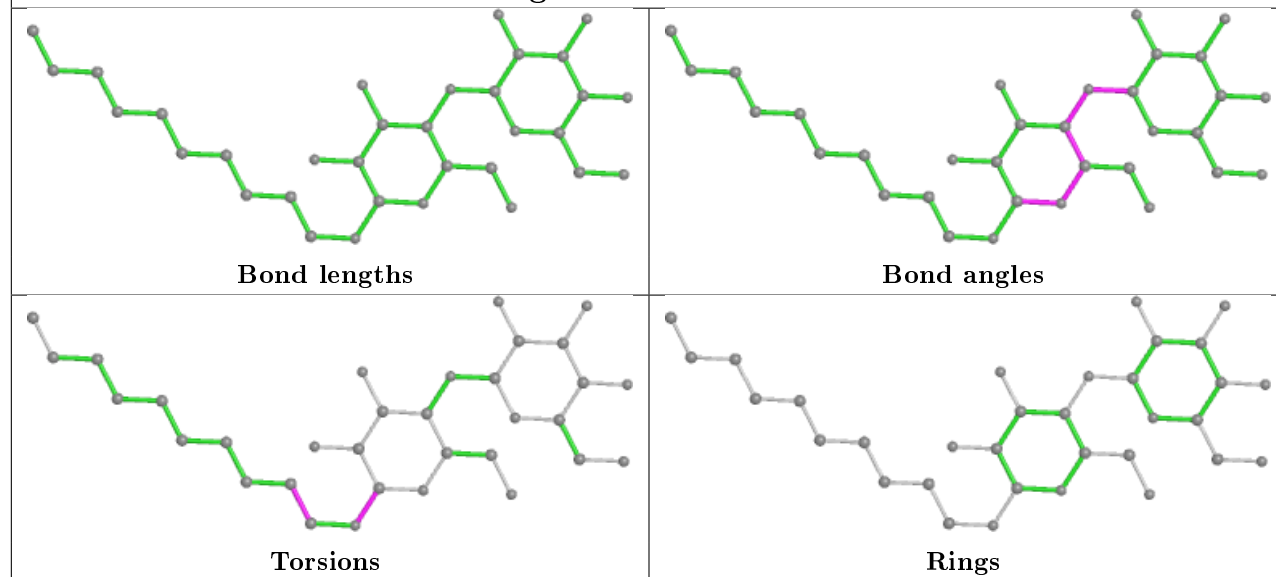
Mol	Chain	Res	Type	Atoms
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D

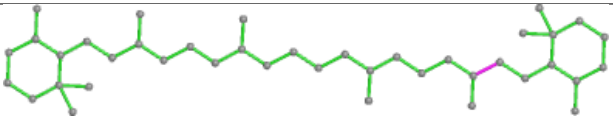
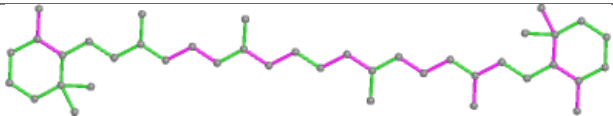
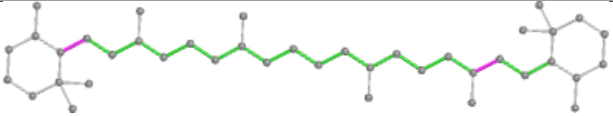
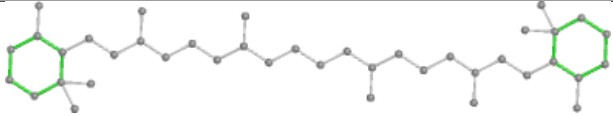
There are no ring outliers.

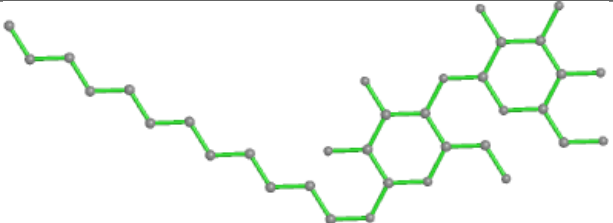
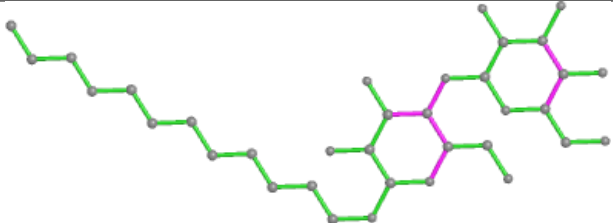
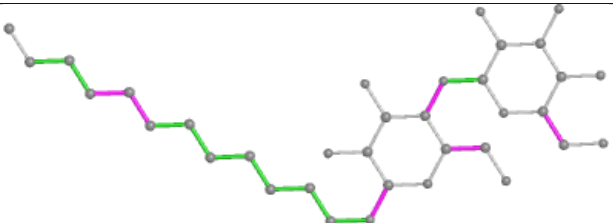
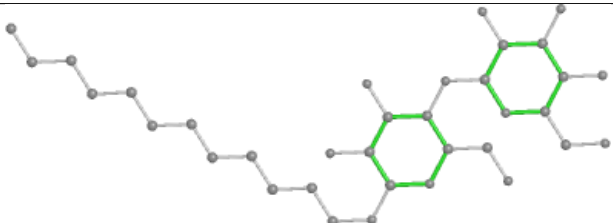
No monomer is involved in short contacts.

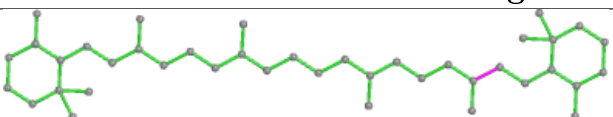
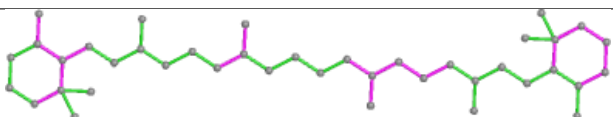
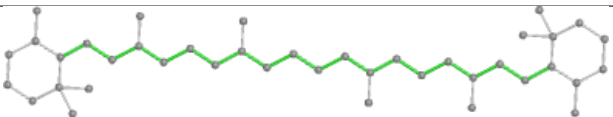
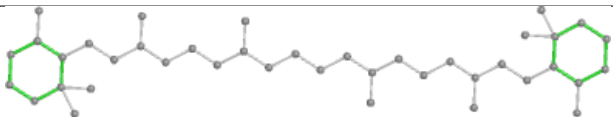
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

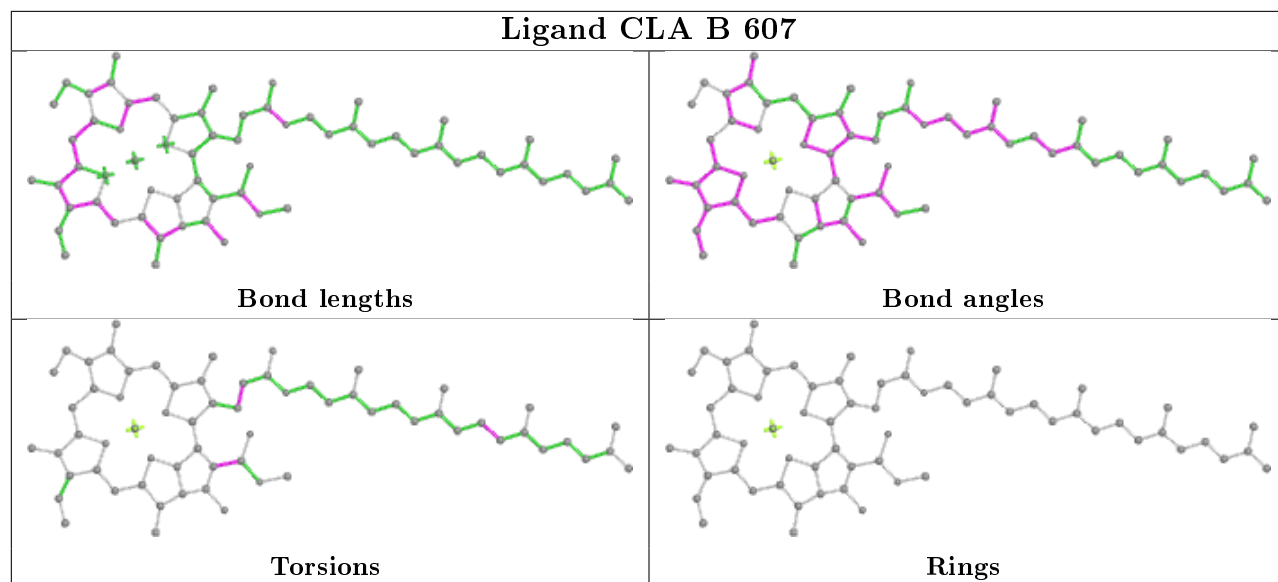
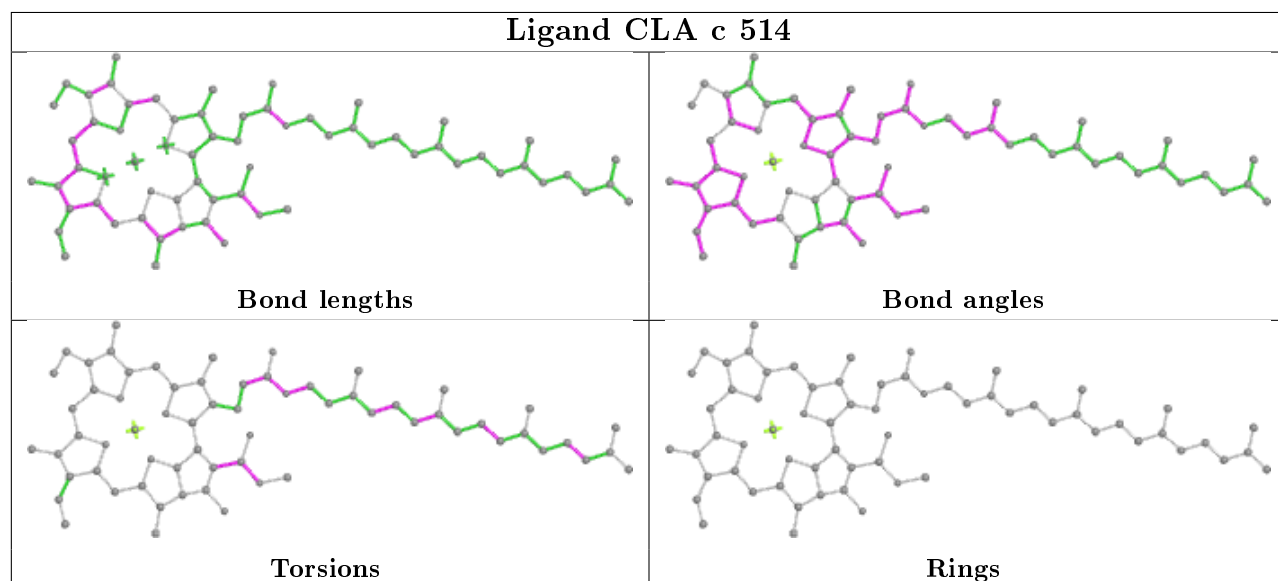
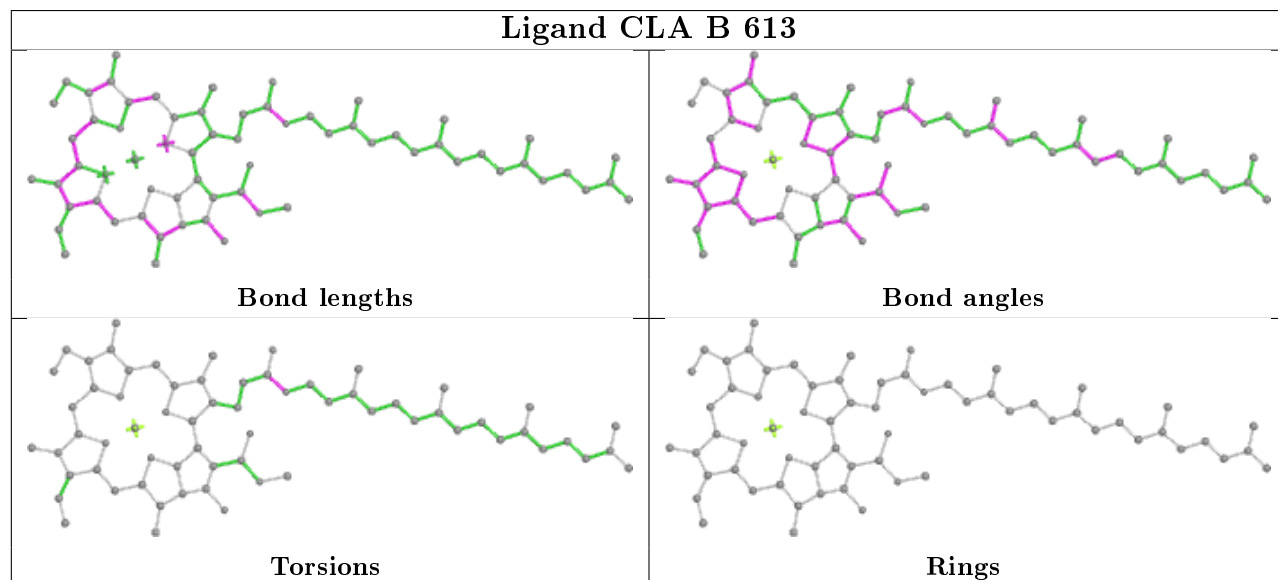


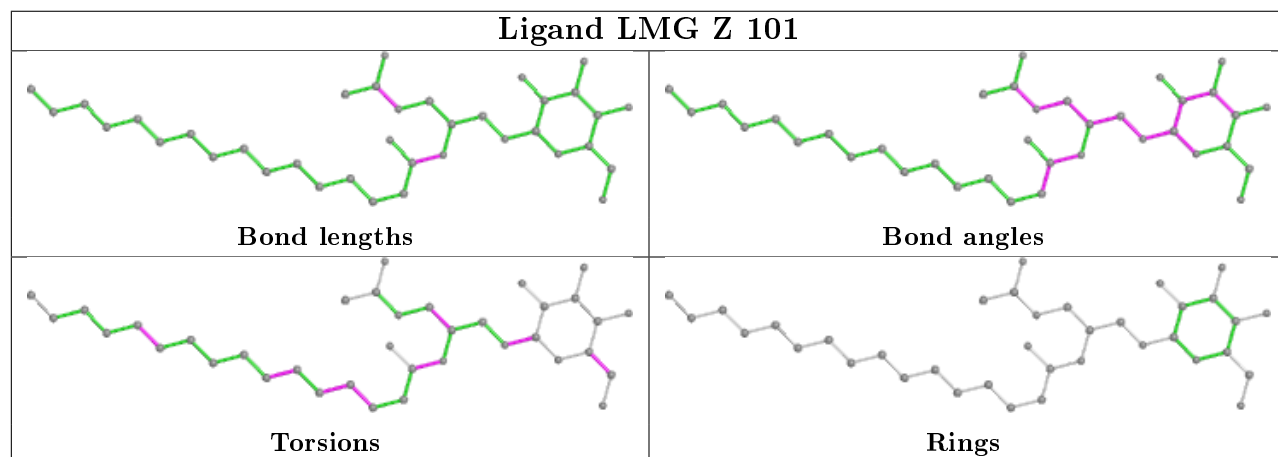
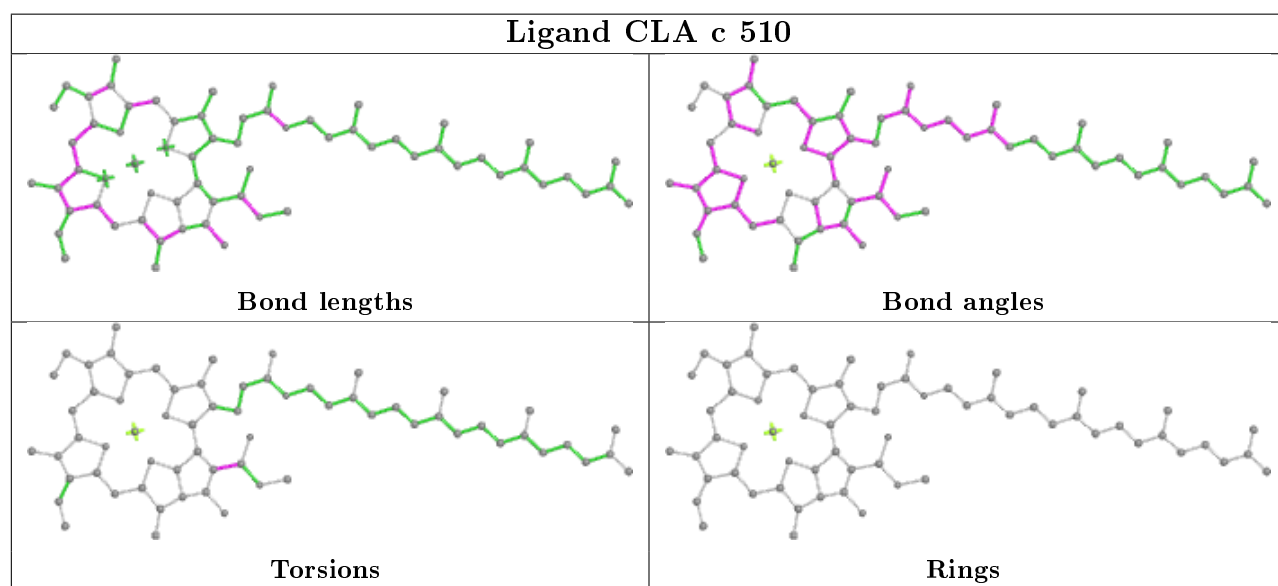
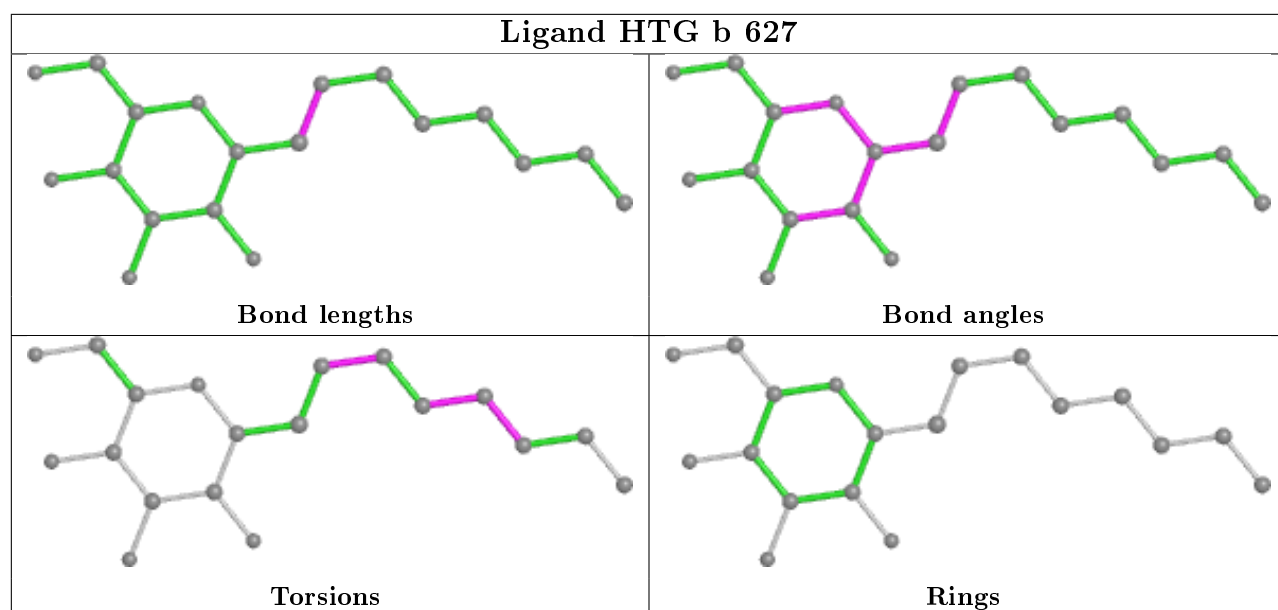
Ligand CLA B 612**Ligand CLA D 403****Ligand LMT A 417**

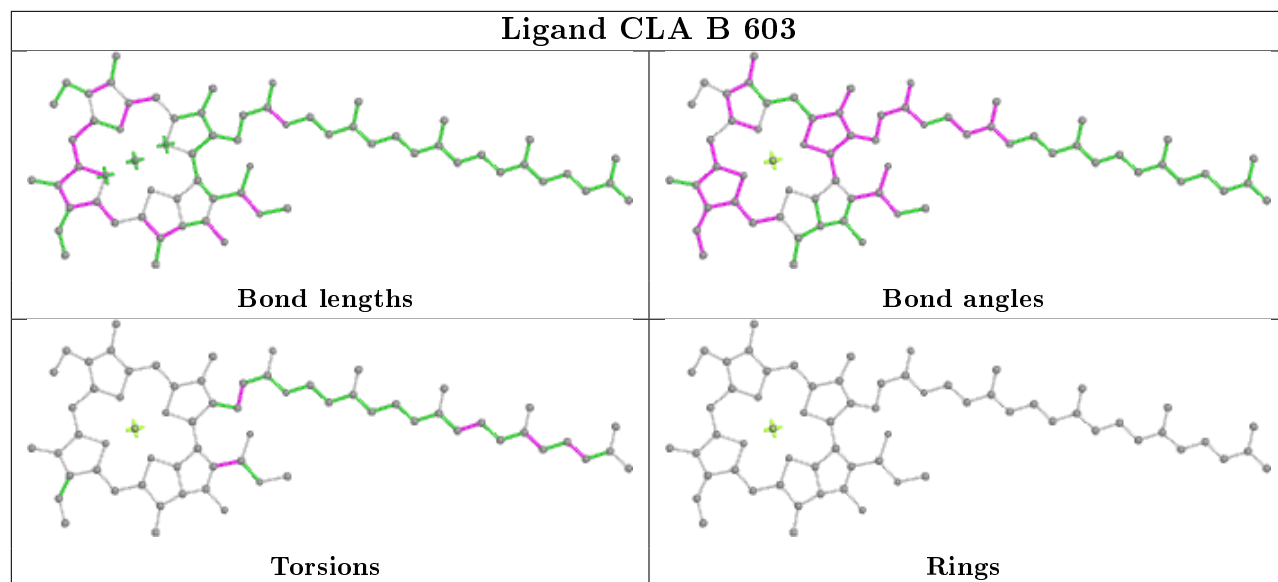
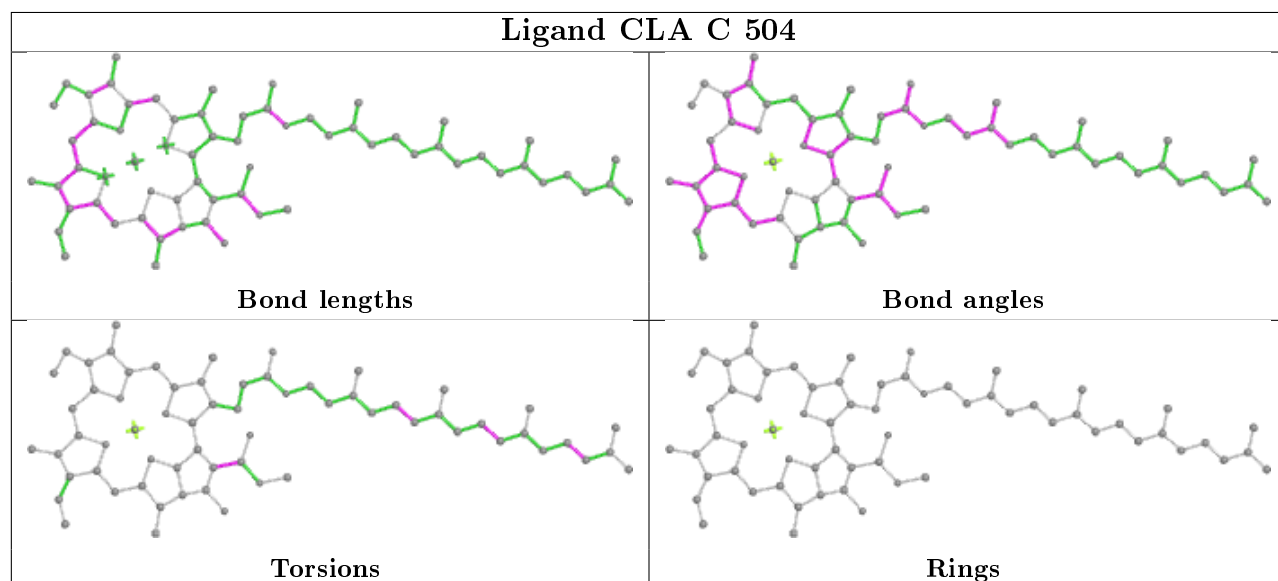
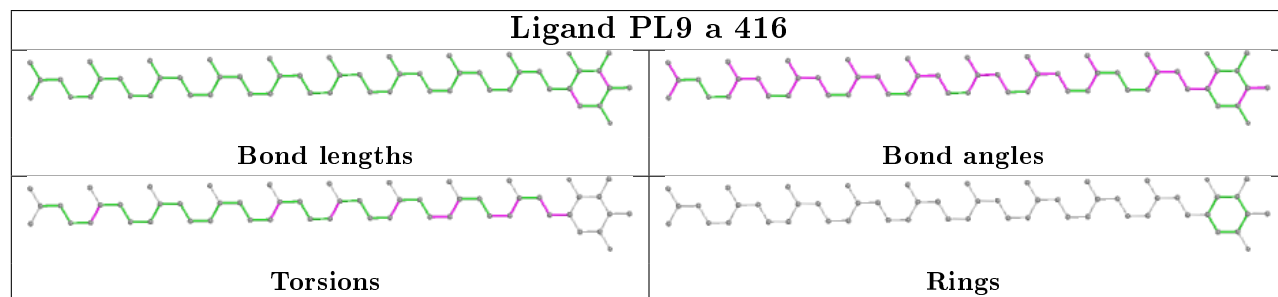
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

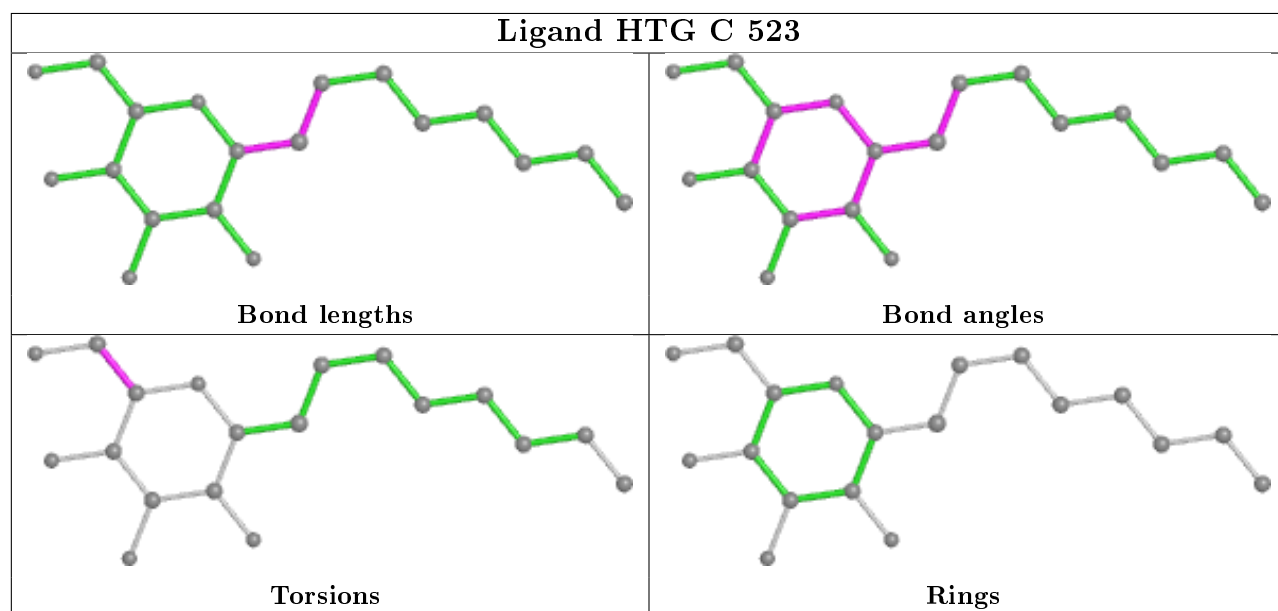
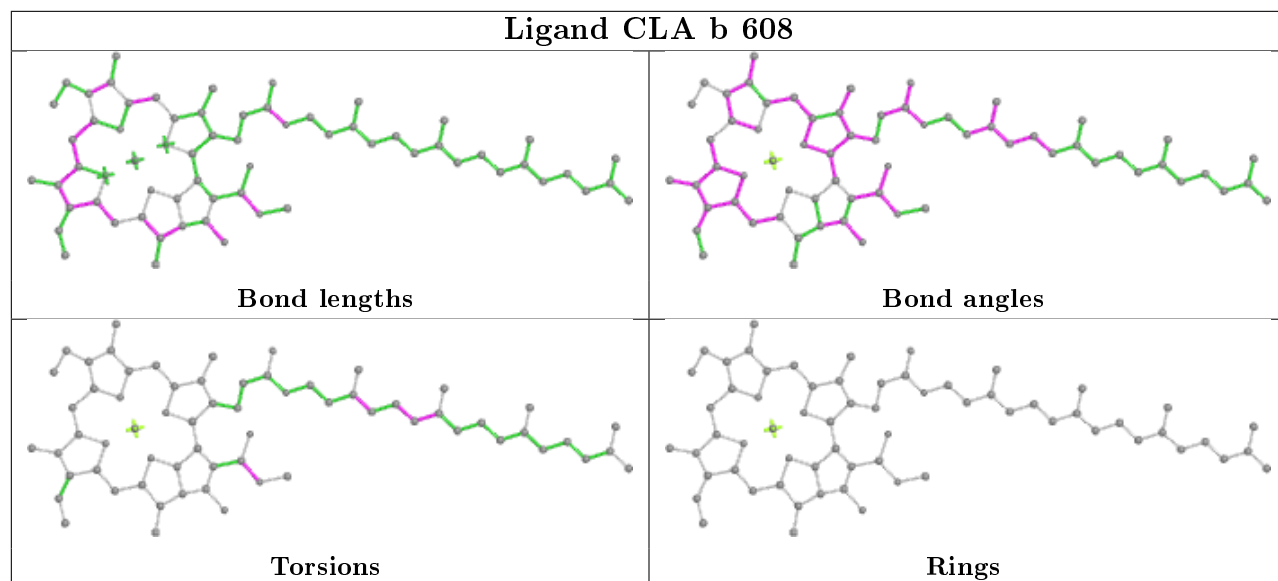
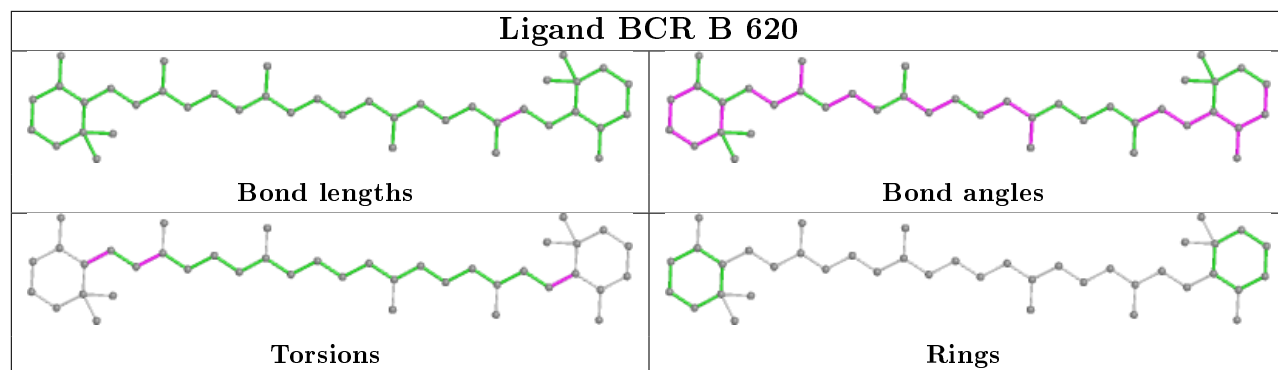
Ligand LMT D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

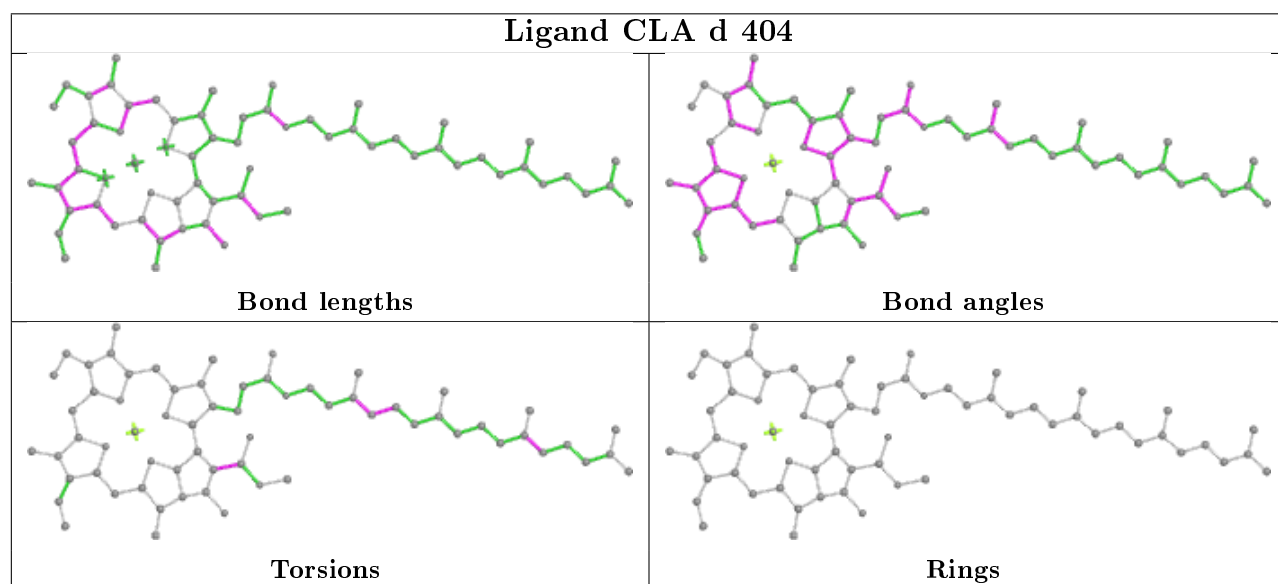
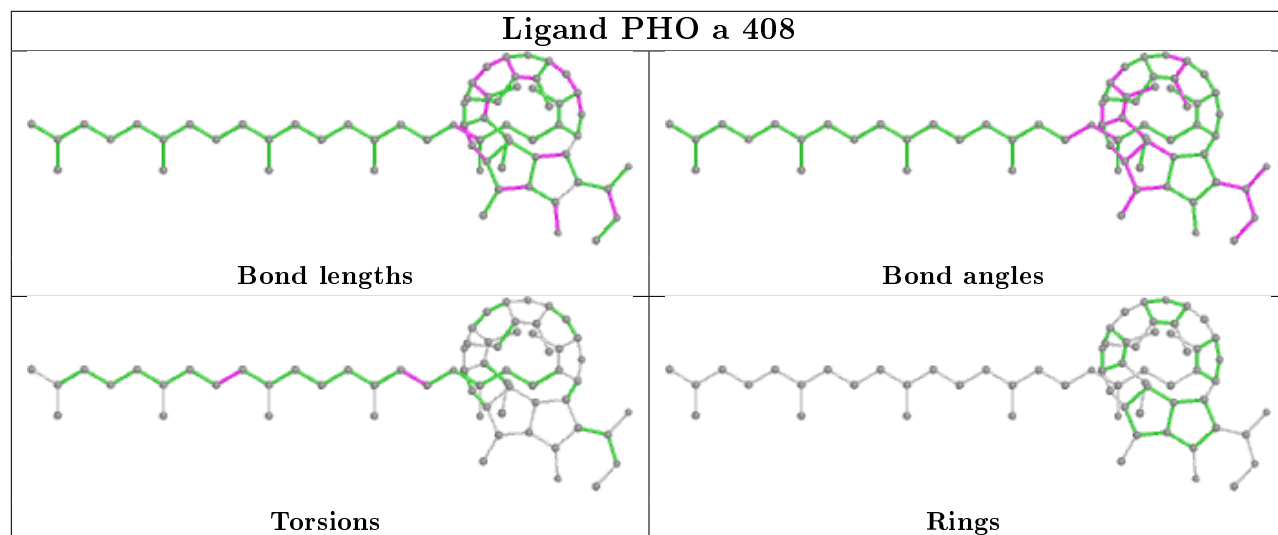
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

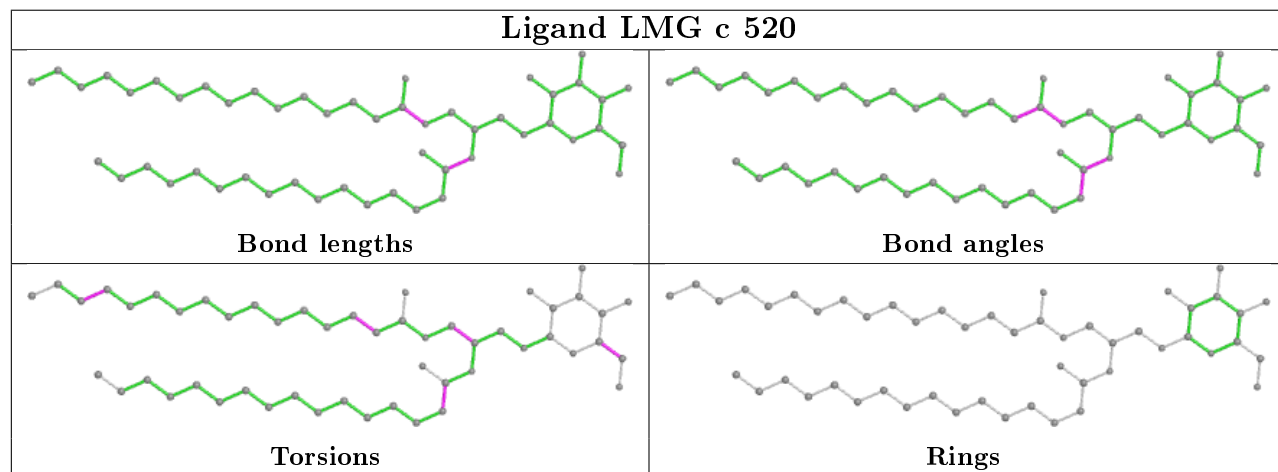
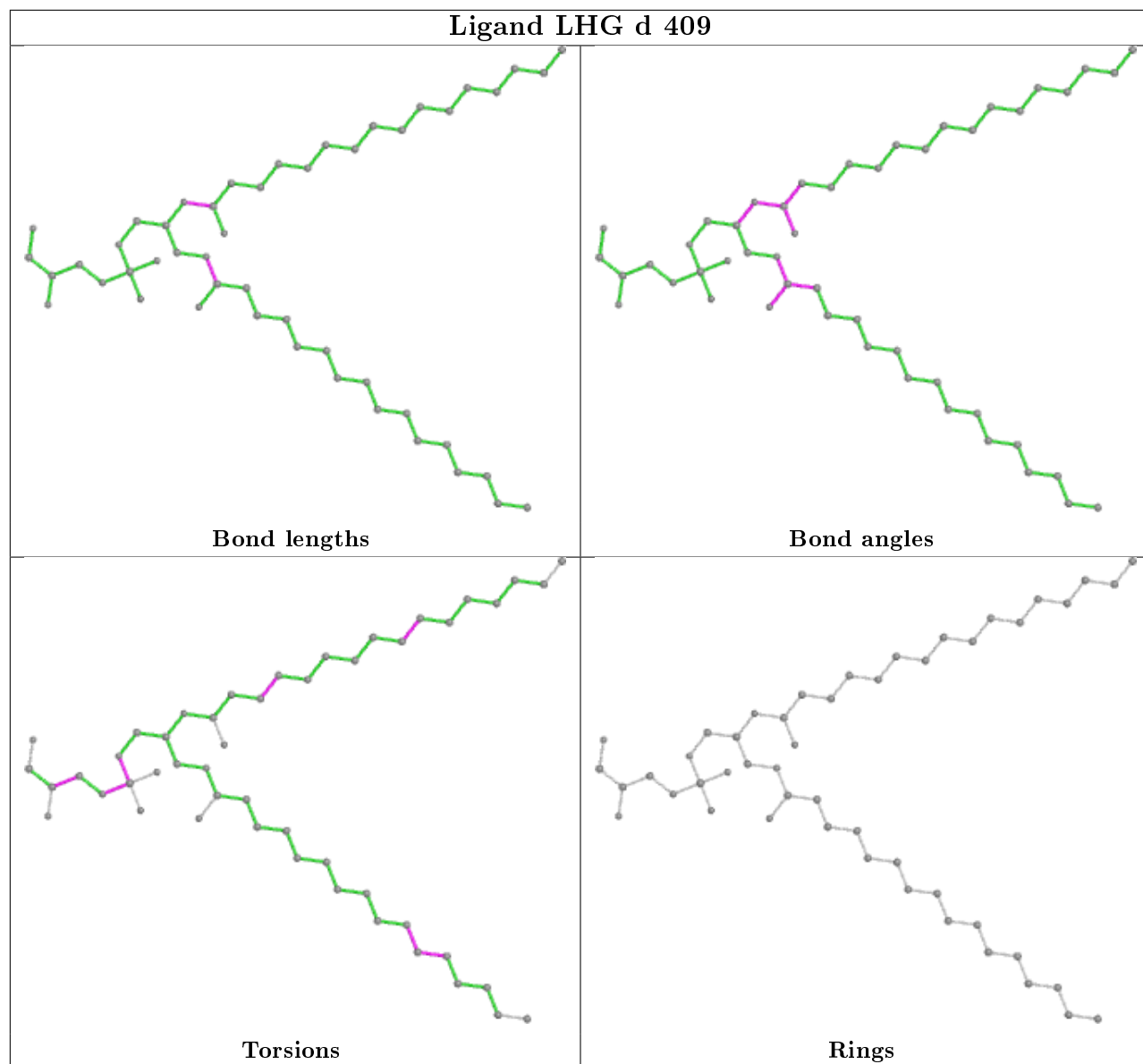
Ligand CLA B 607**Ligand CLA c 514****Ligand CLA B 613**

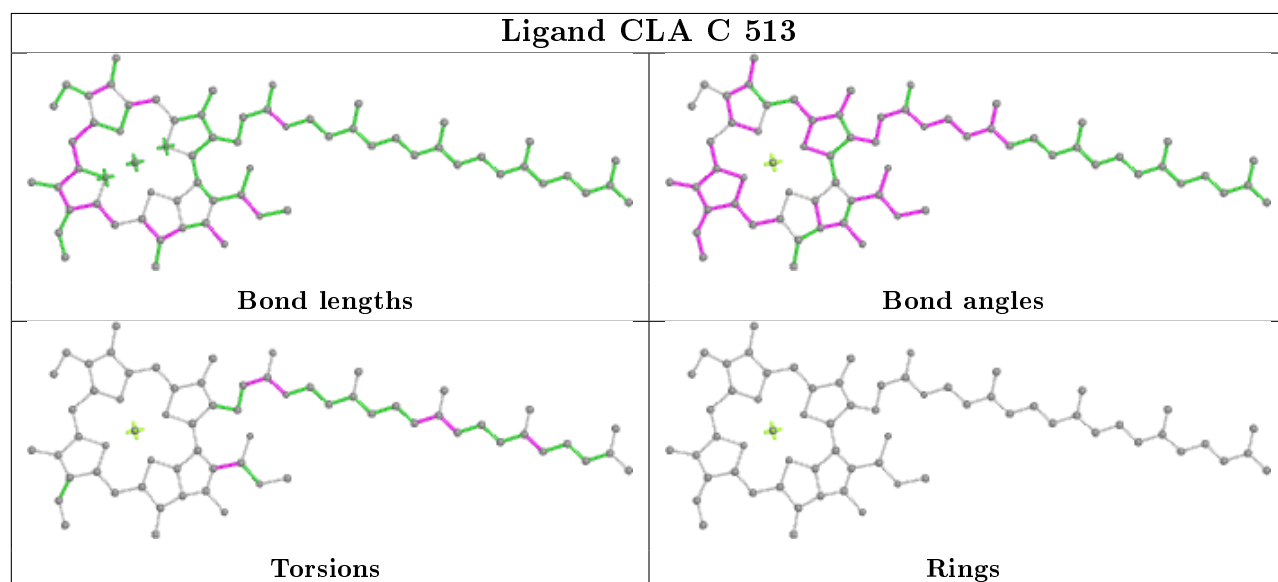
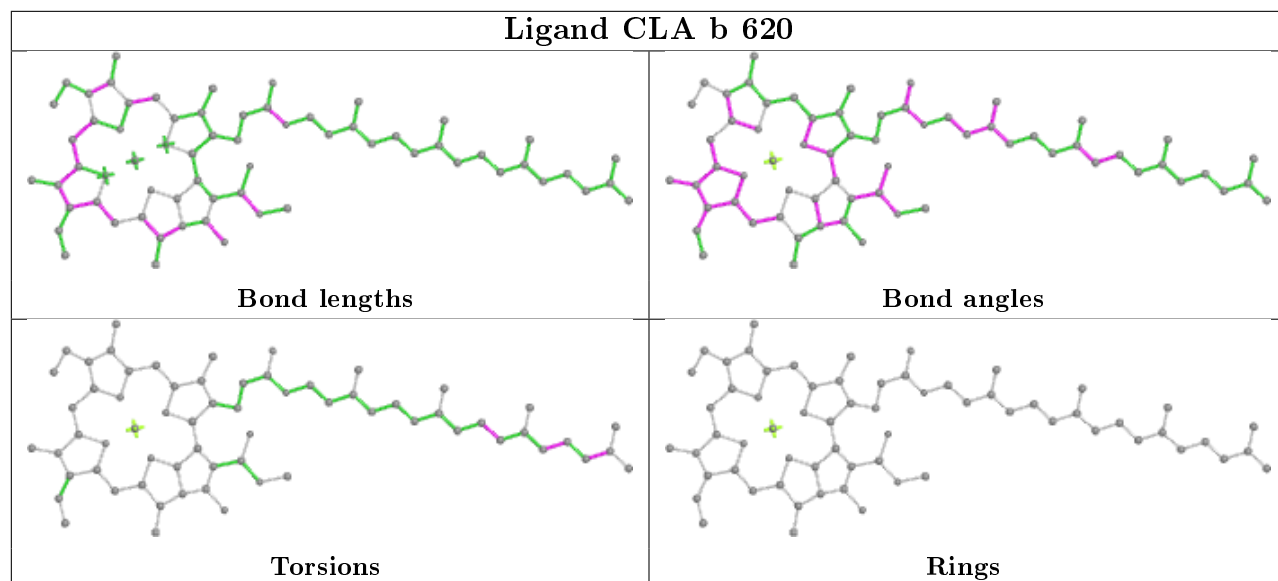
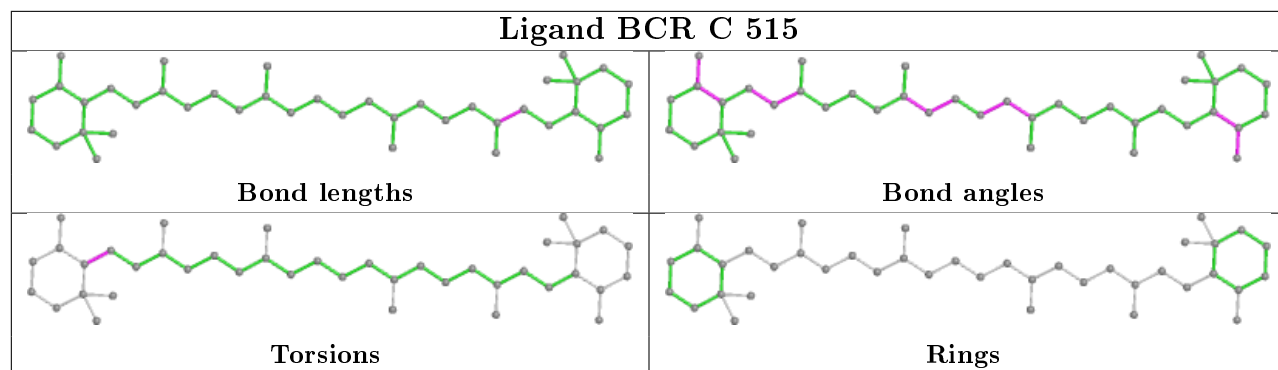


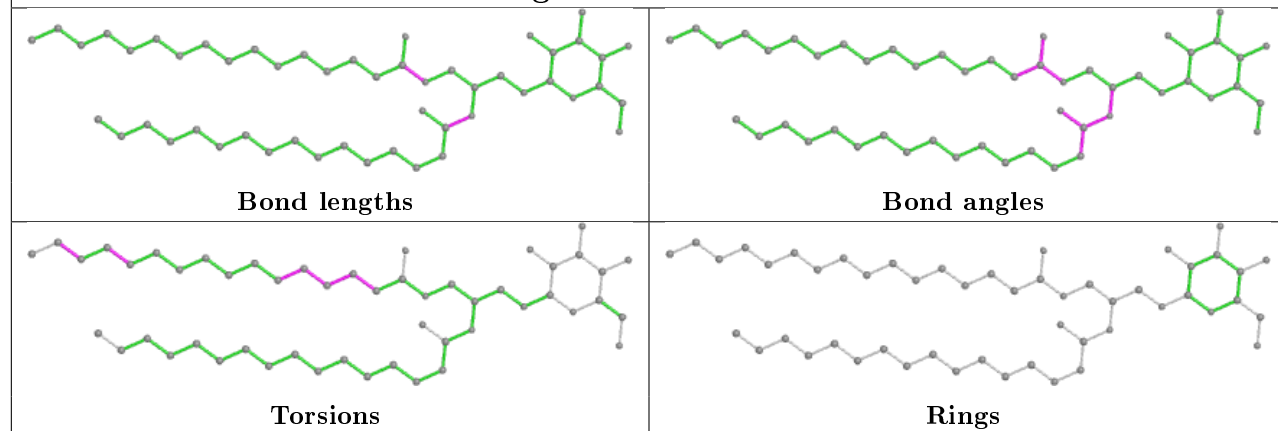
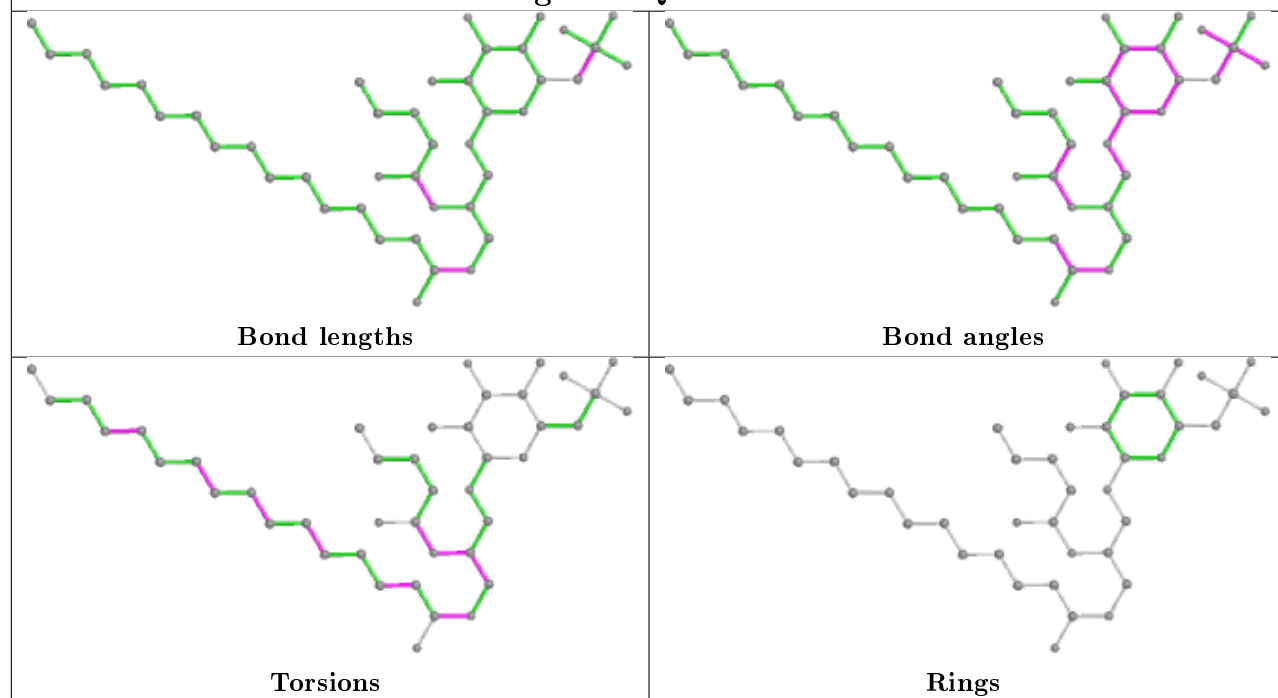
Ligand CLA B 603**Ligand CLA C 504****Ligand PL9 a 416**



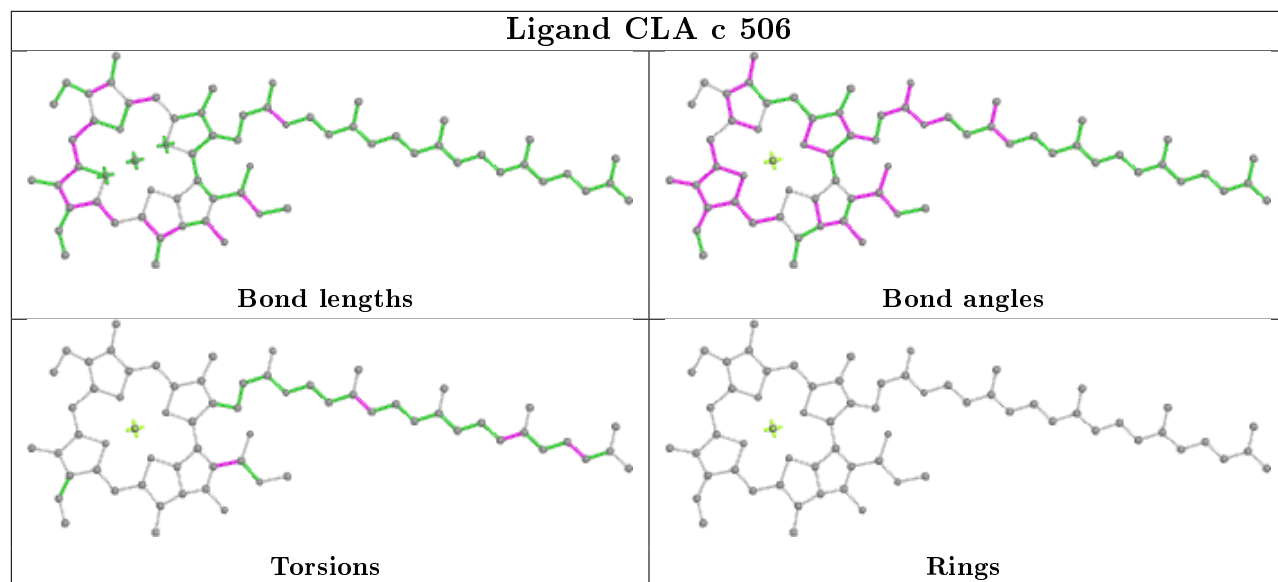




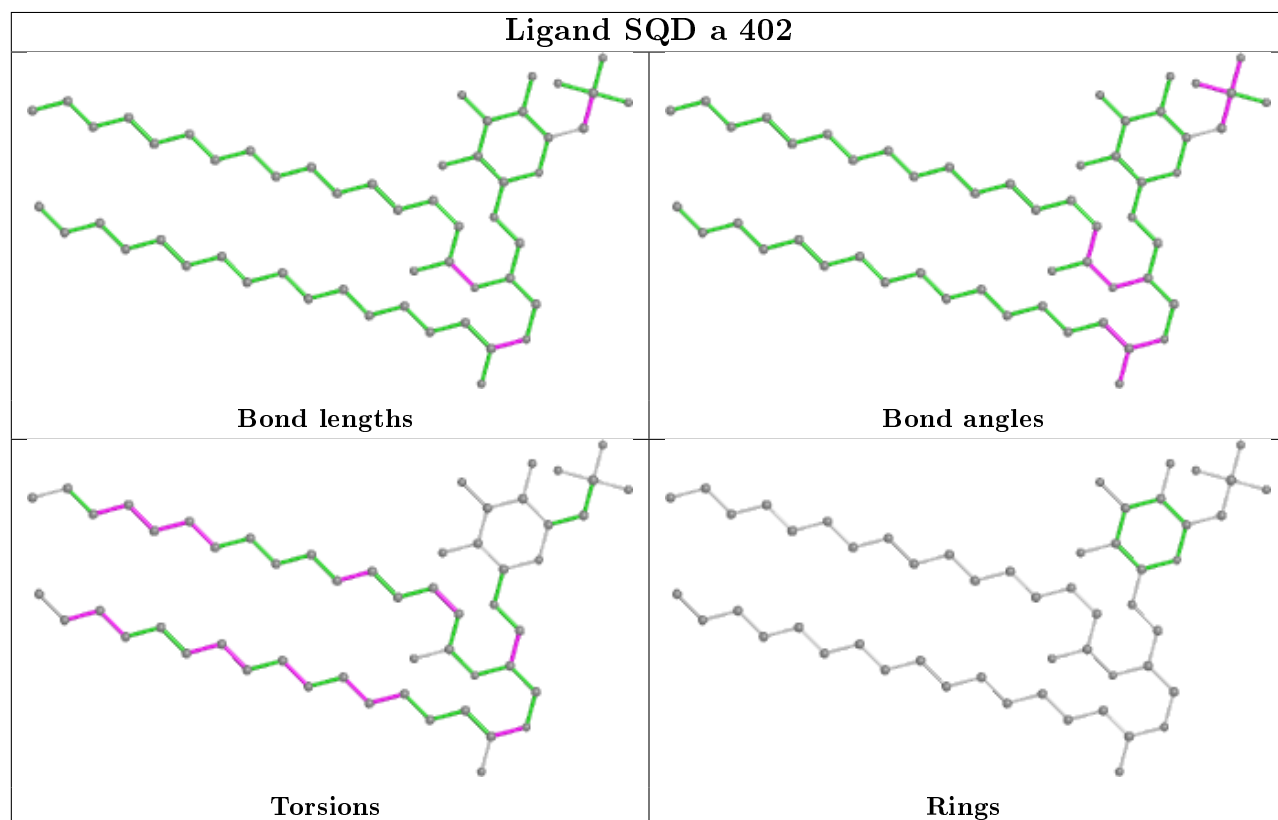


Ligand LMG c 521**Ligand SQD F 101**

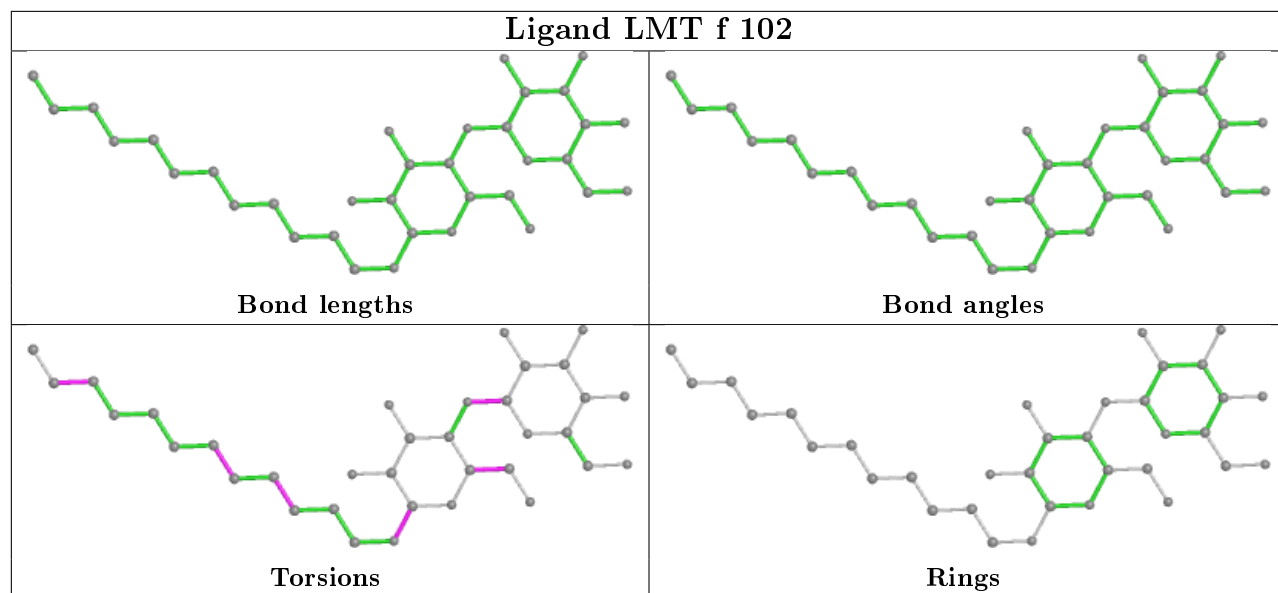
Ligand CLA c 506



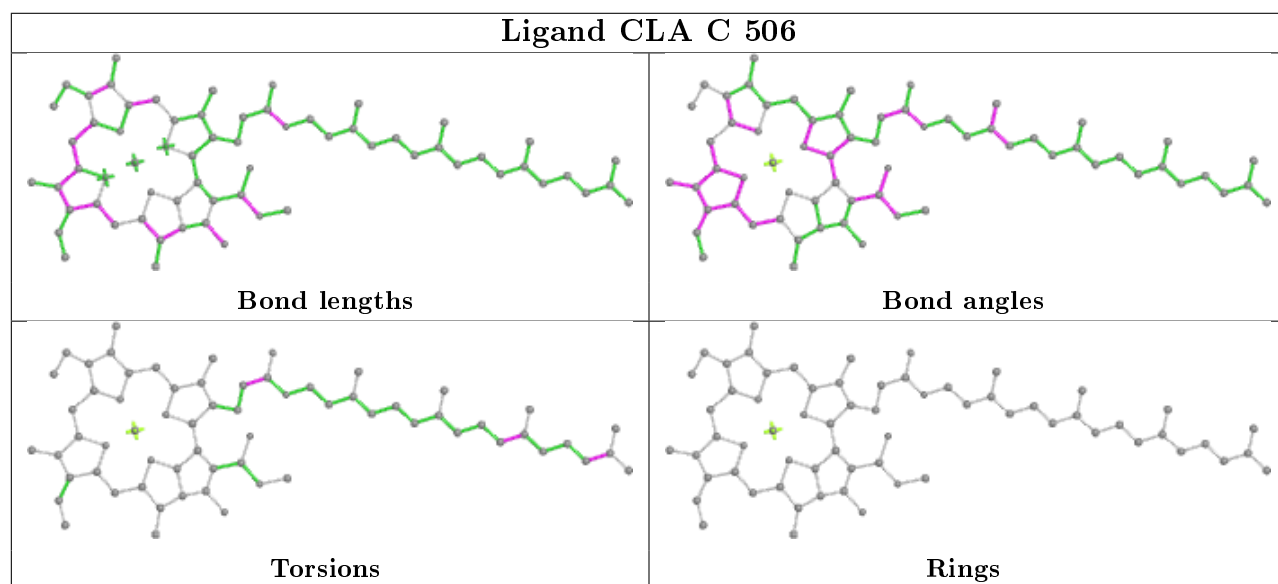
Ligand SQD a 402



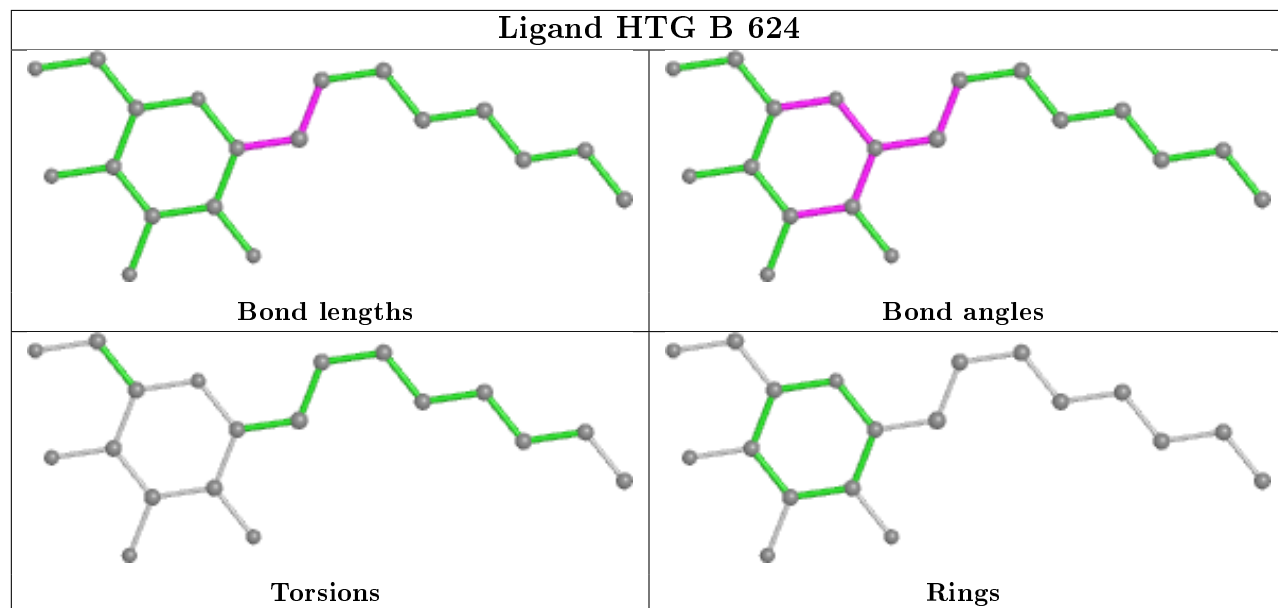
Ligand LMT f 102

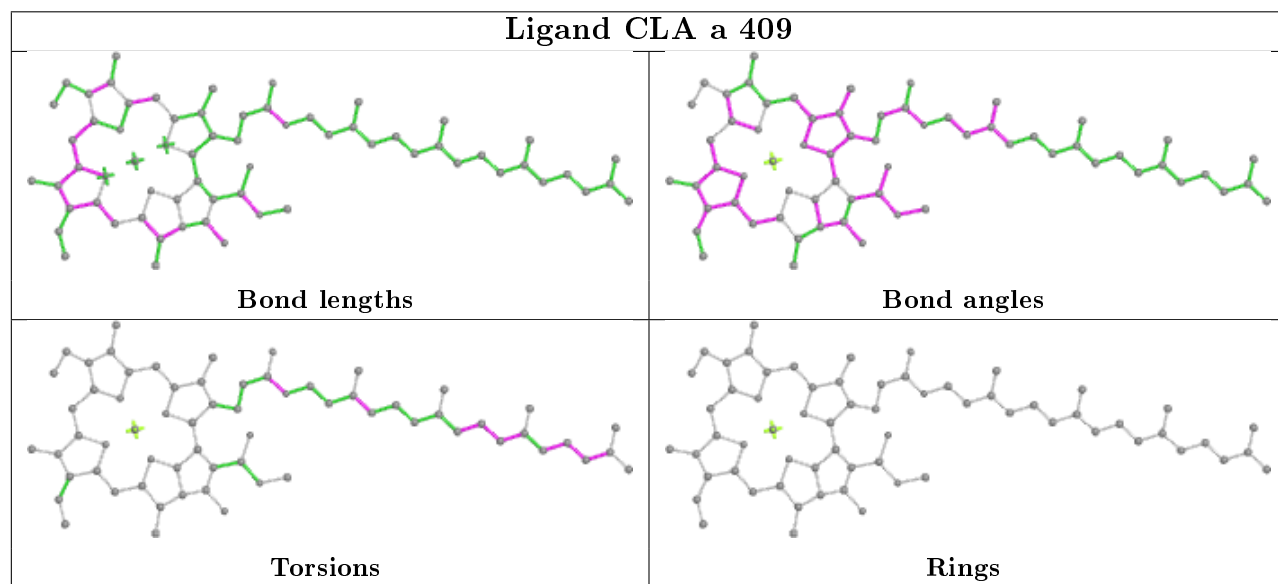
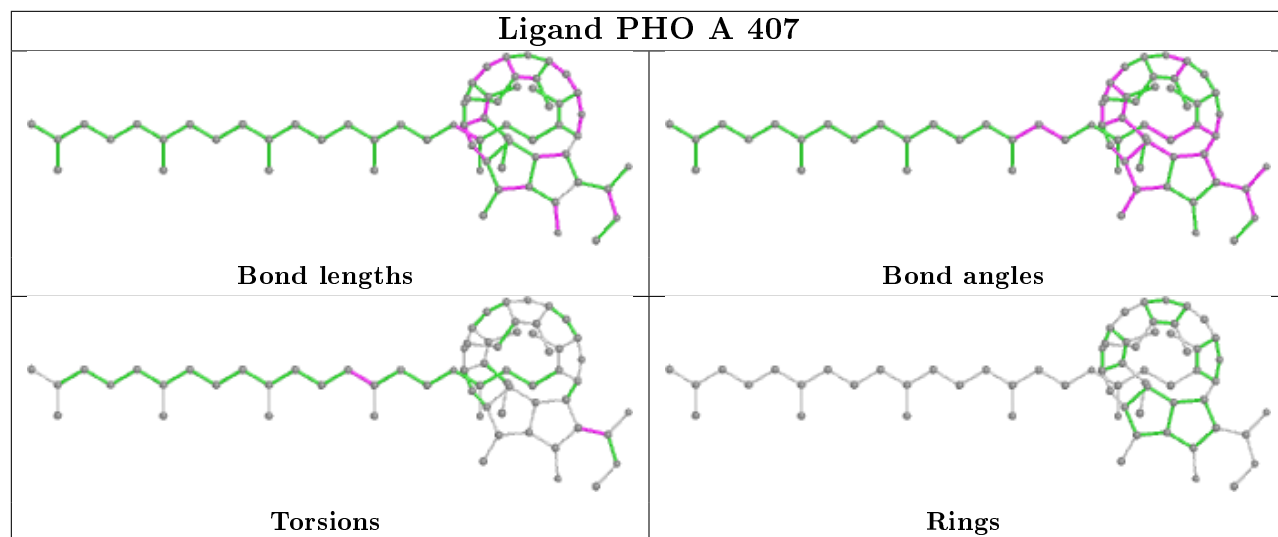
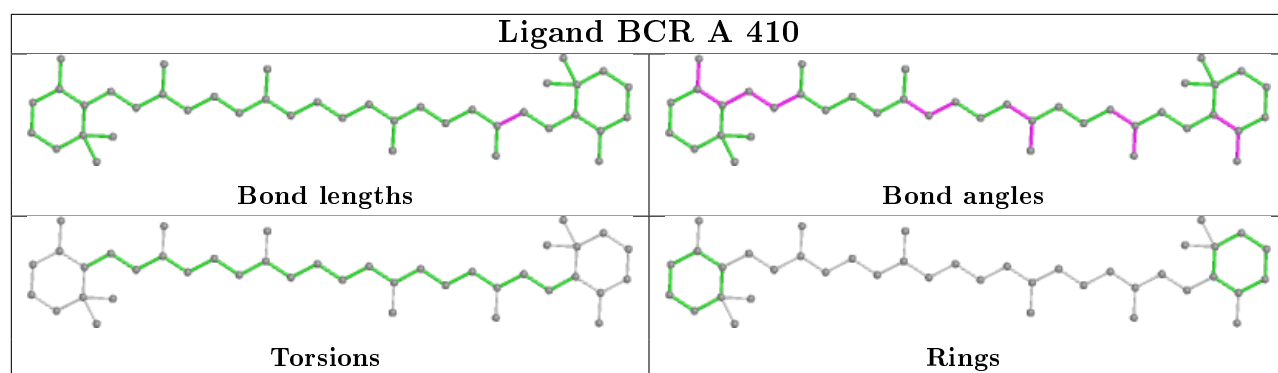


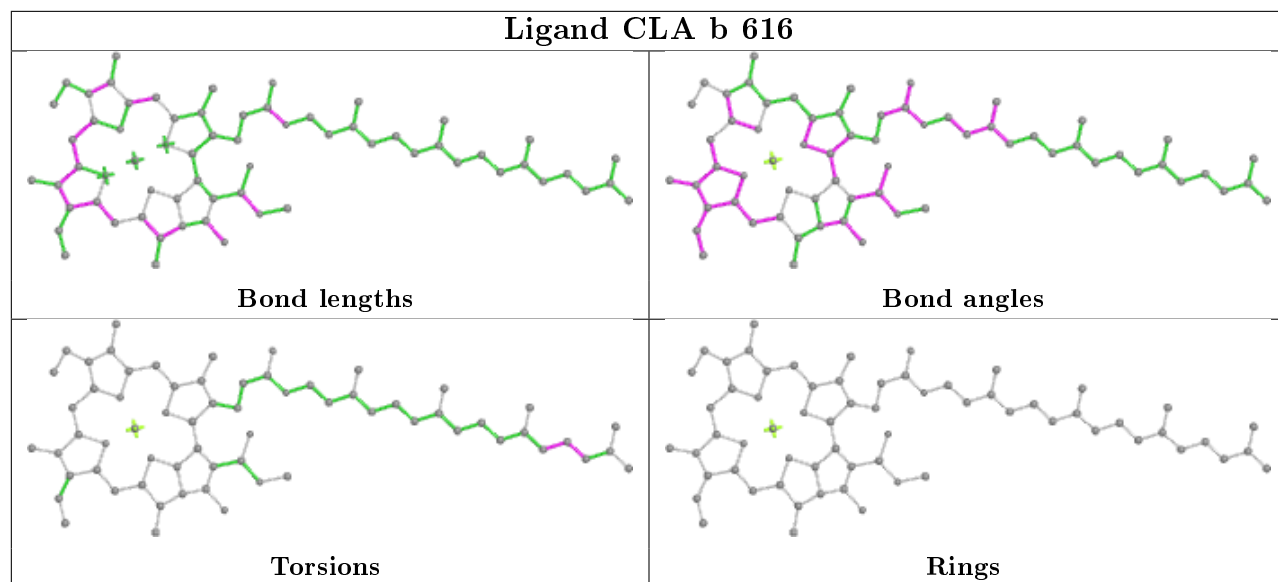
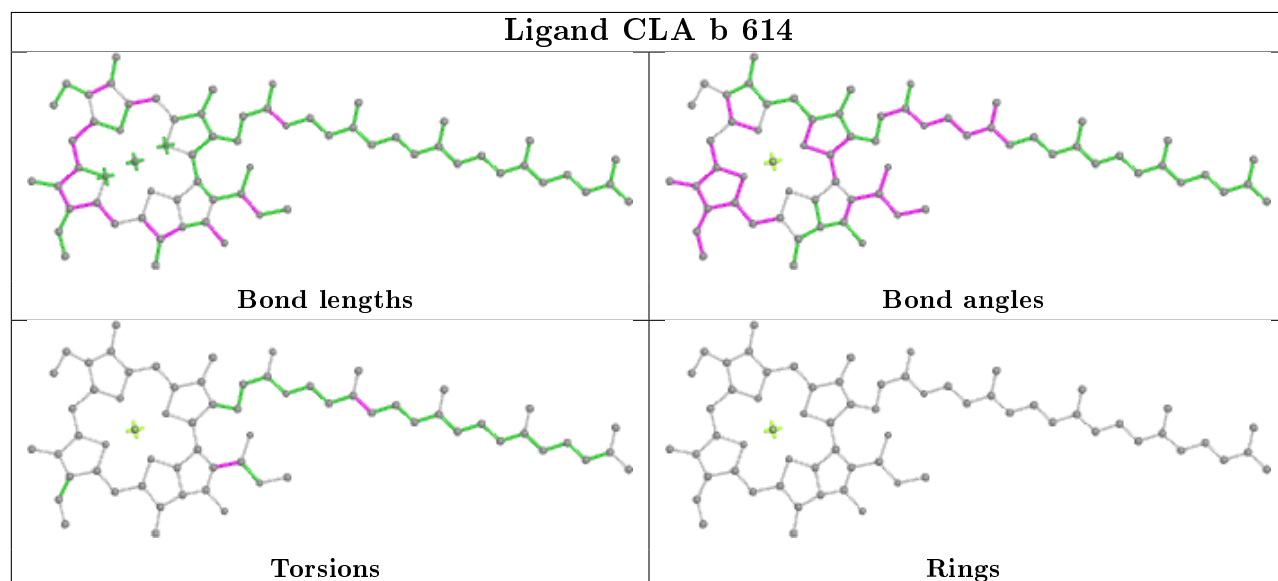
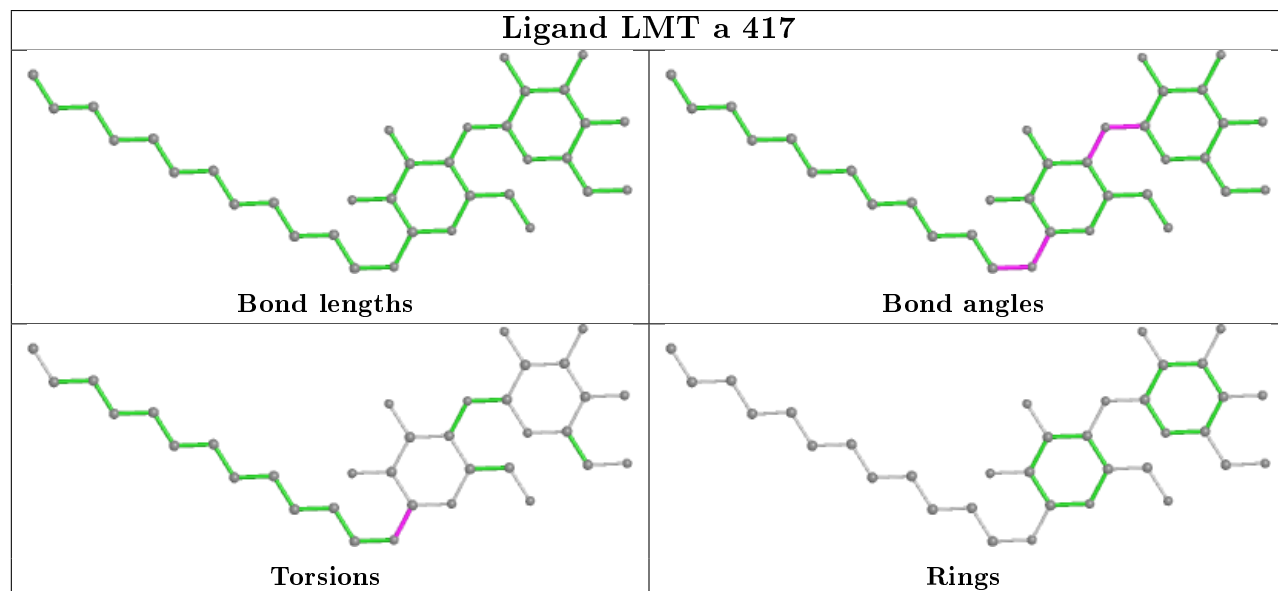
Ligand CLA C 506

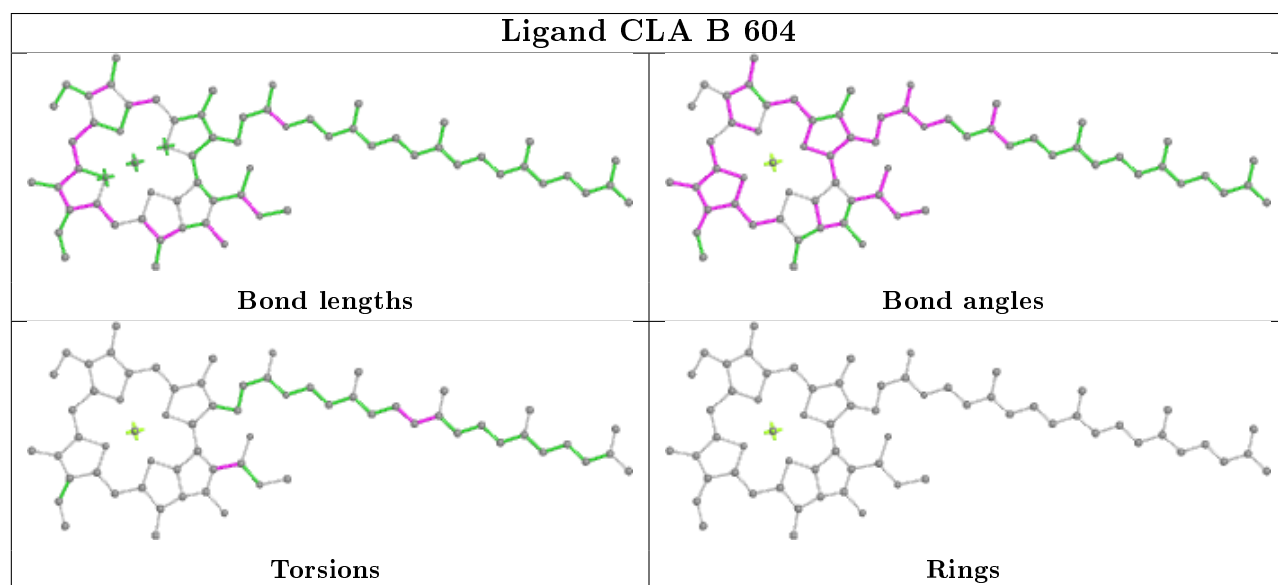
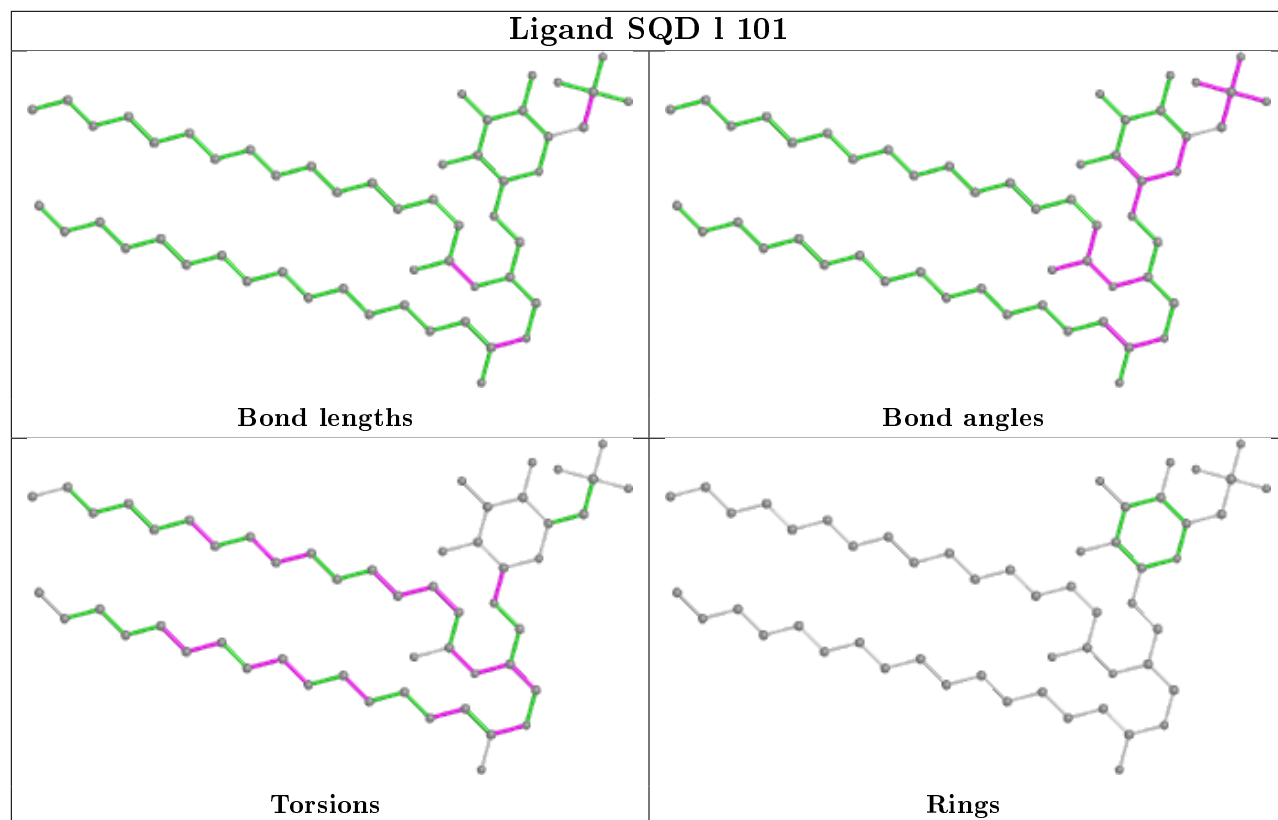
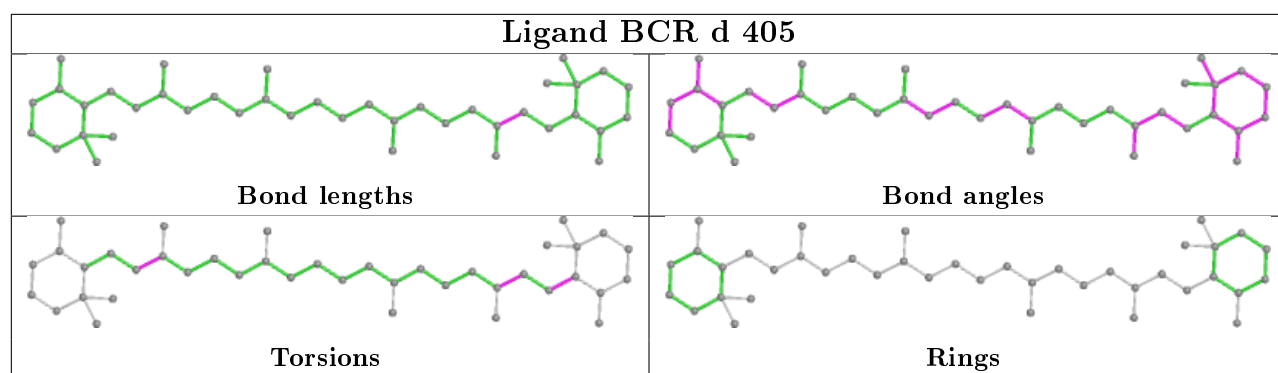


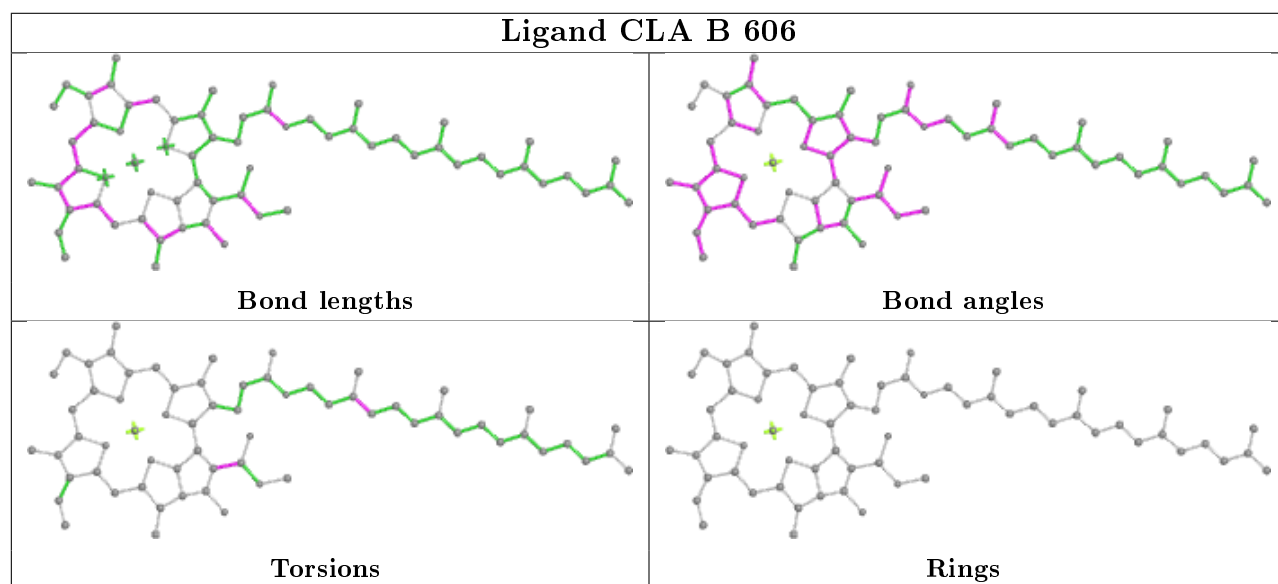
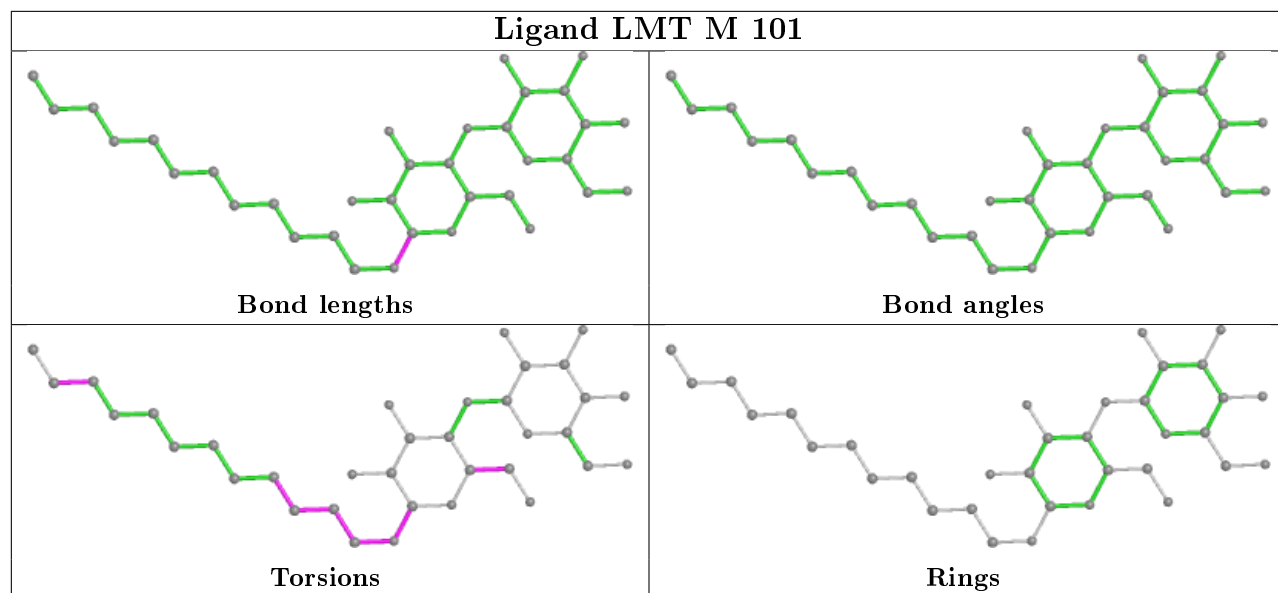
Ligand HTG B 624

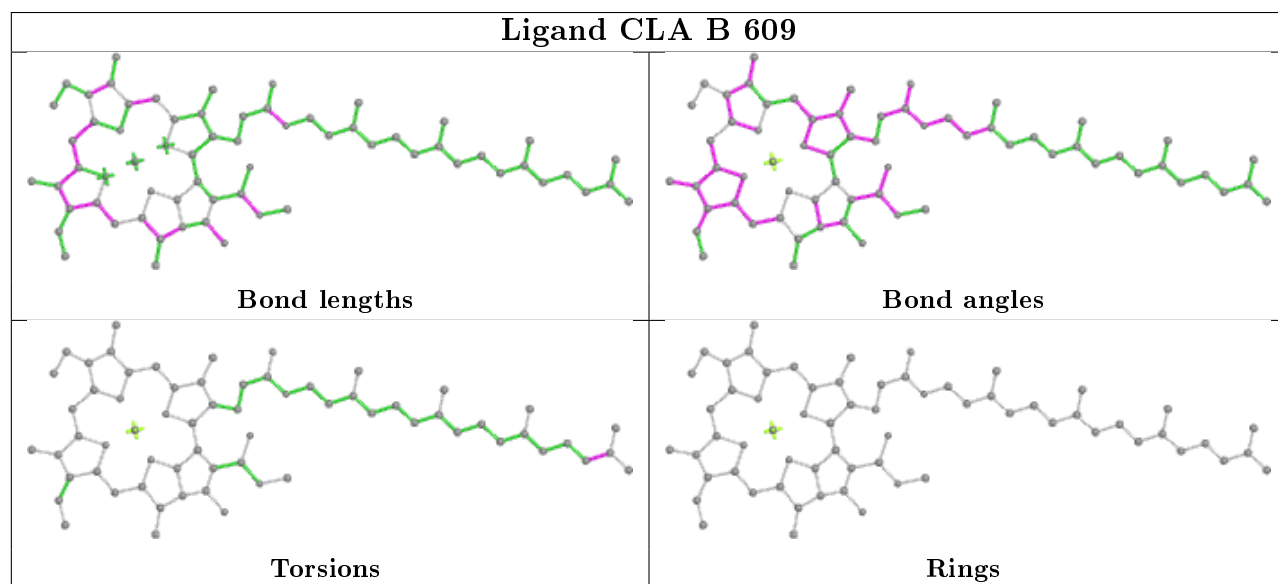
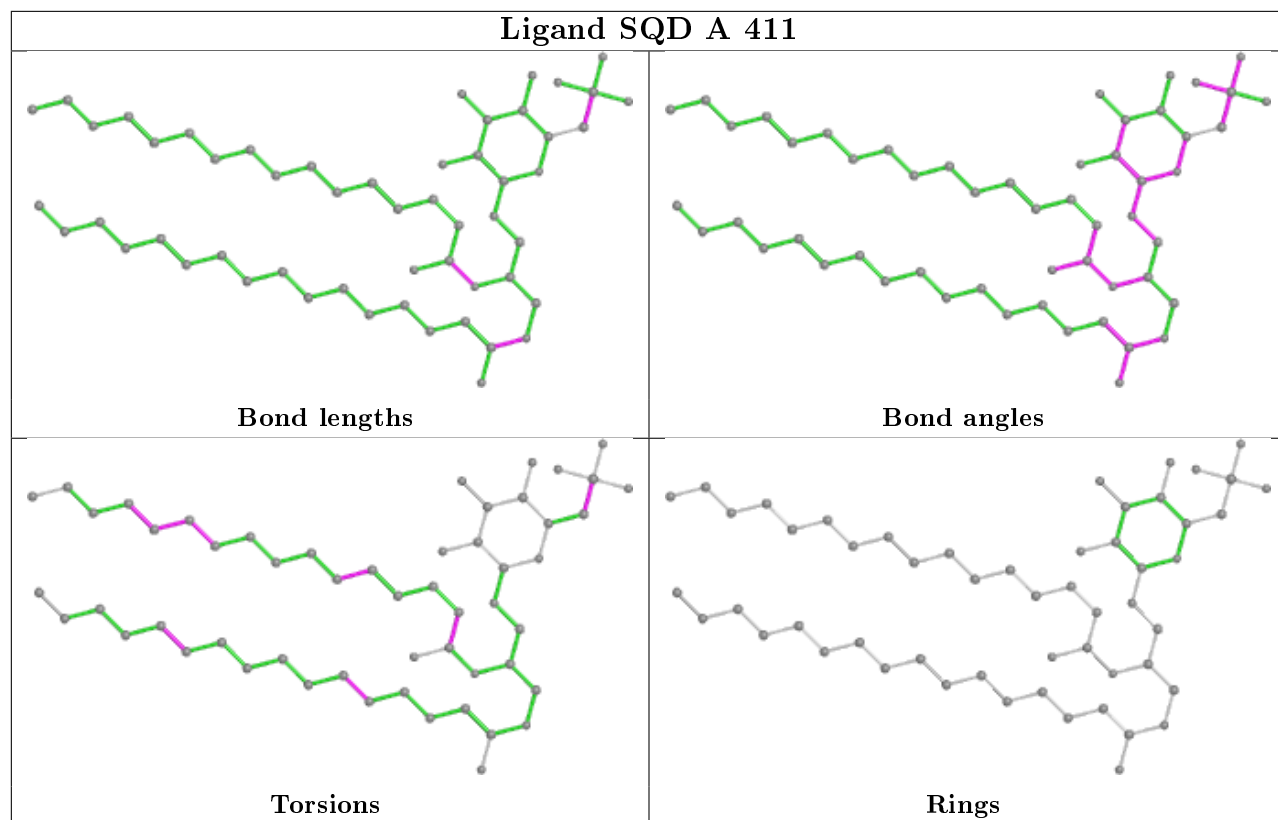


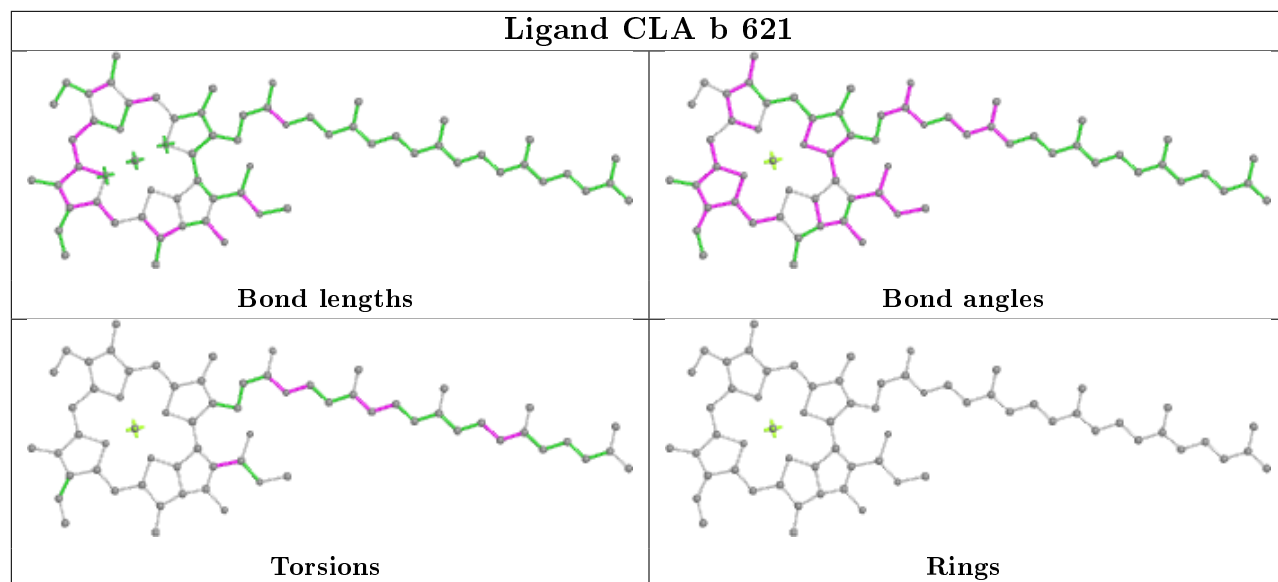
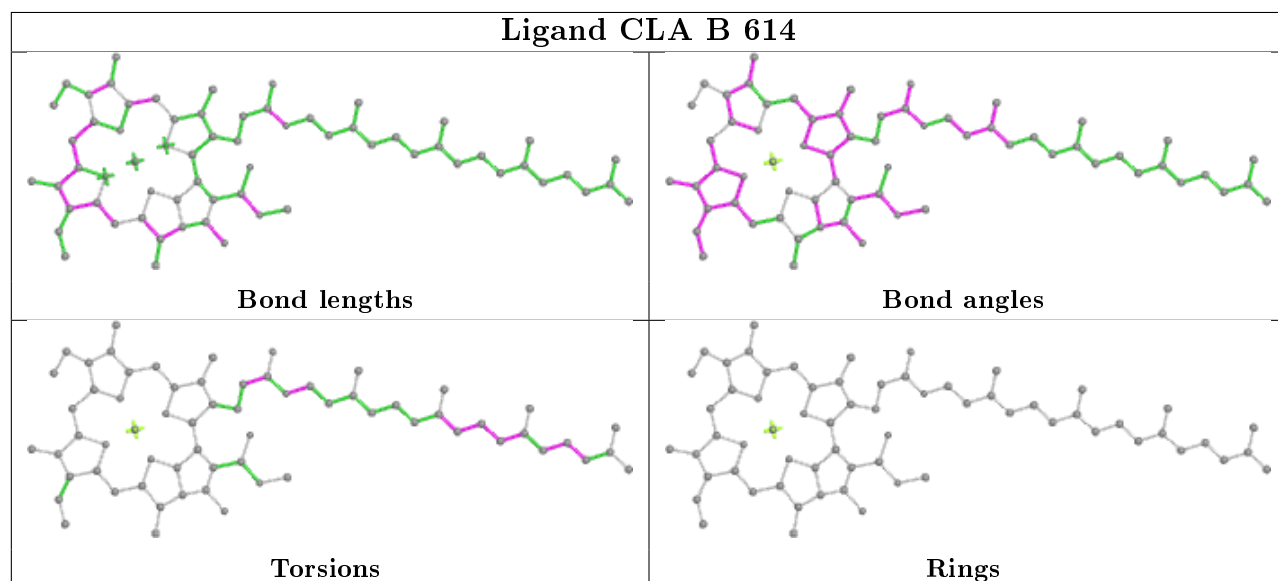
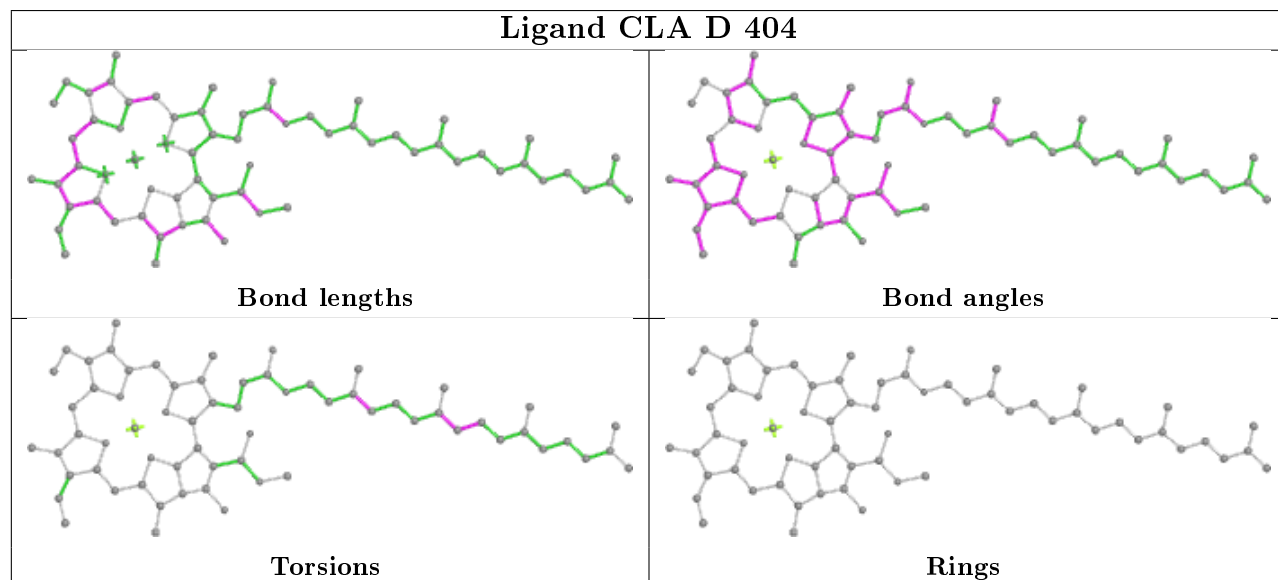


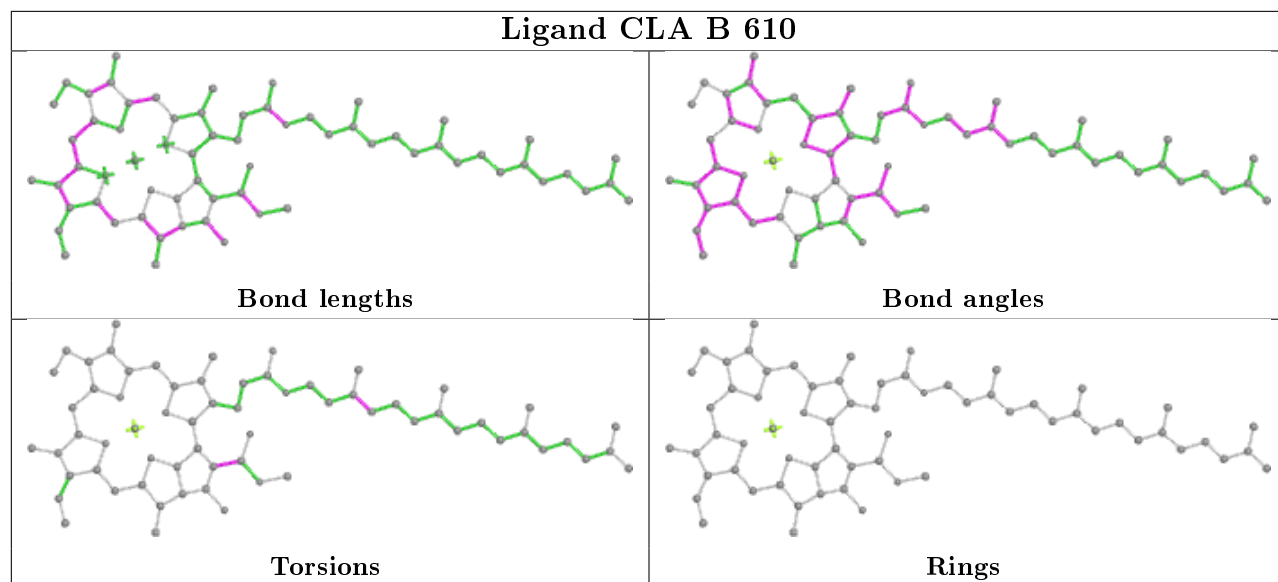
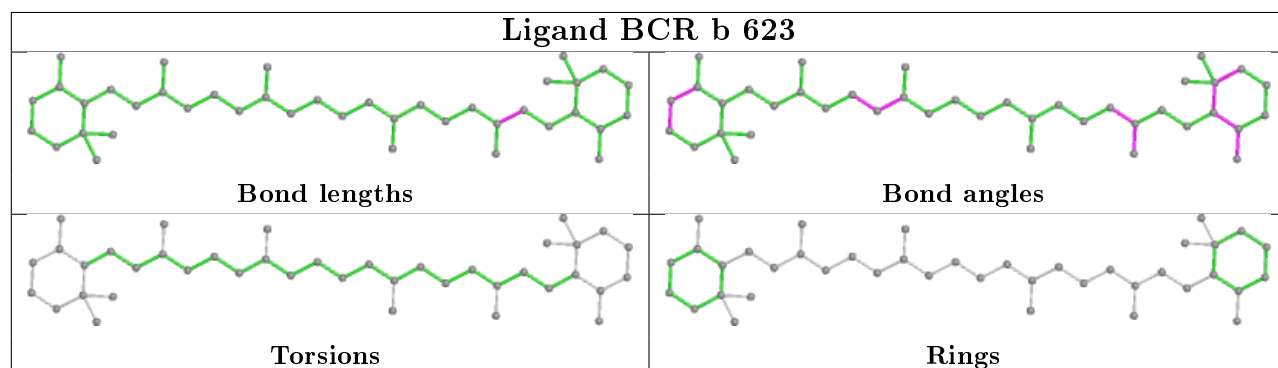
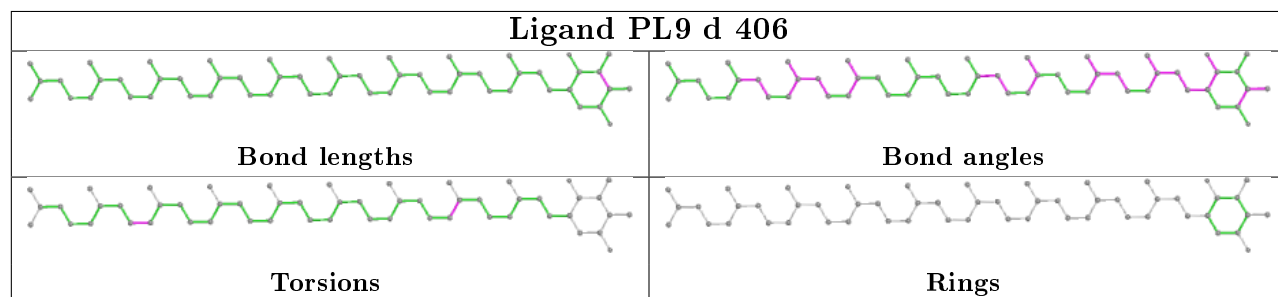
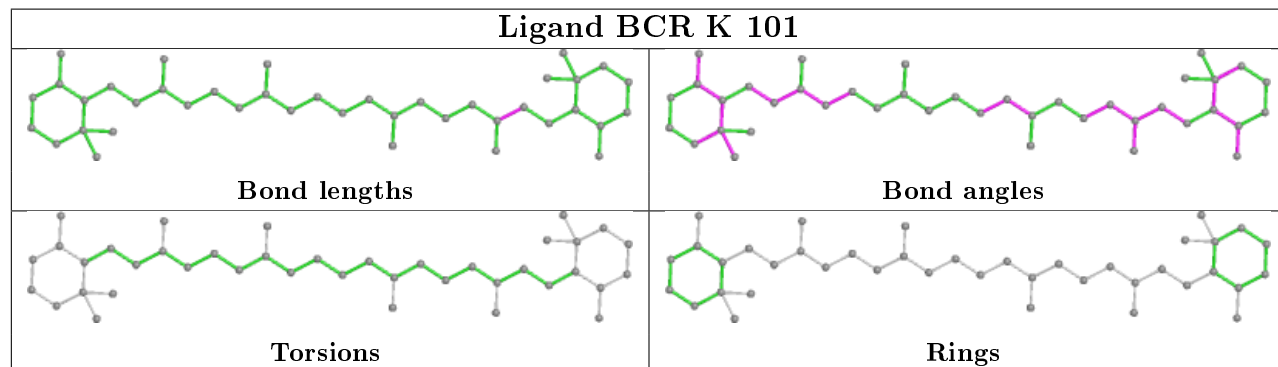
Ligand CLA b 616**Ligand CLA b 614****Ligand LMT a 417**

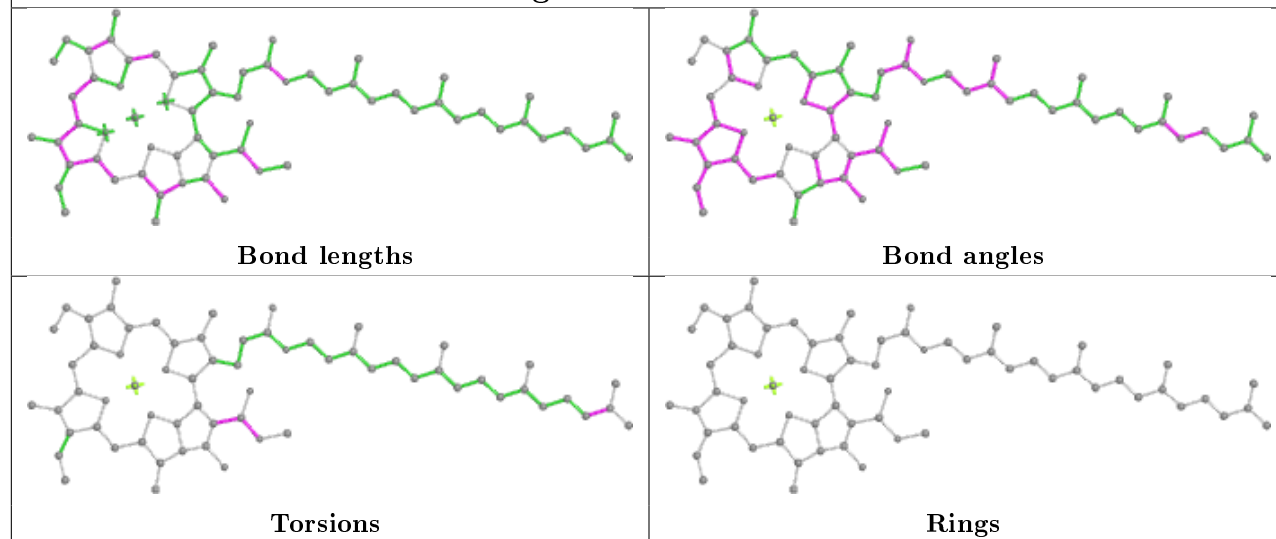
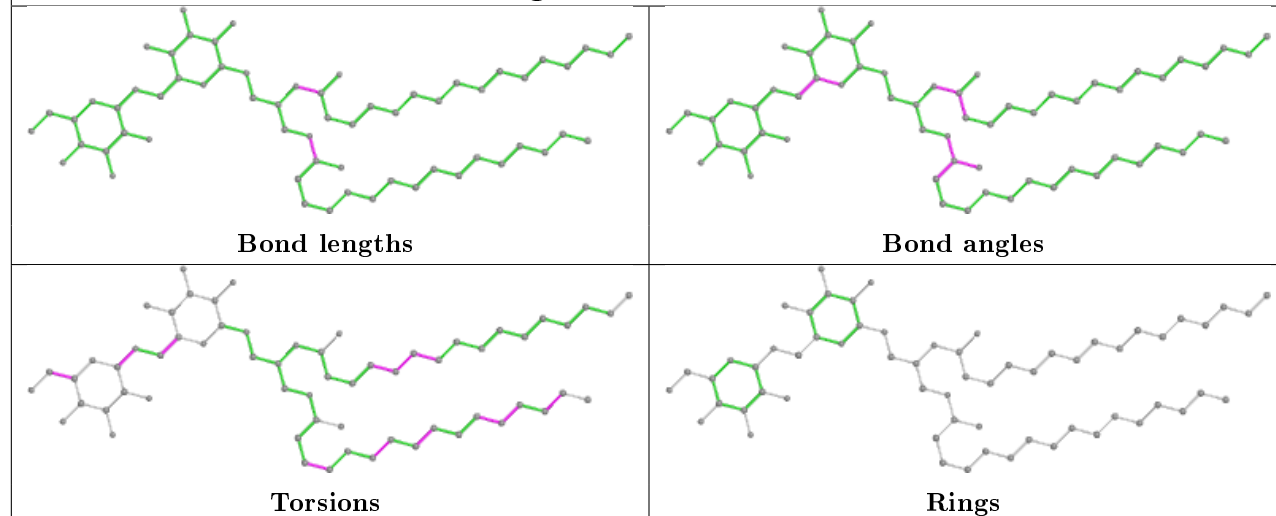
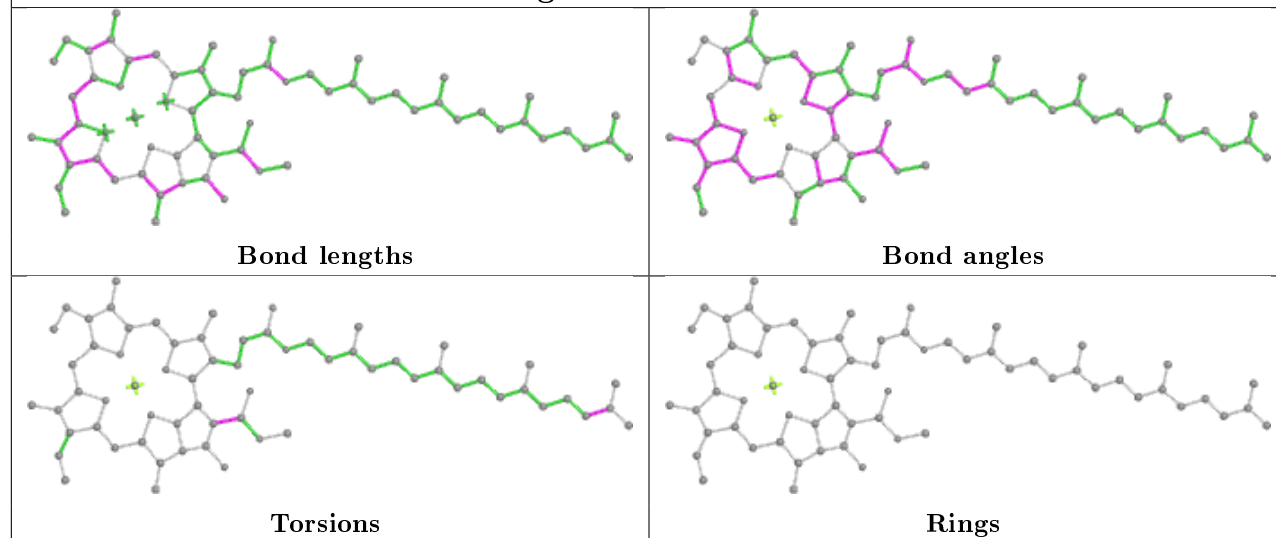


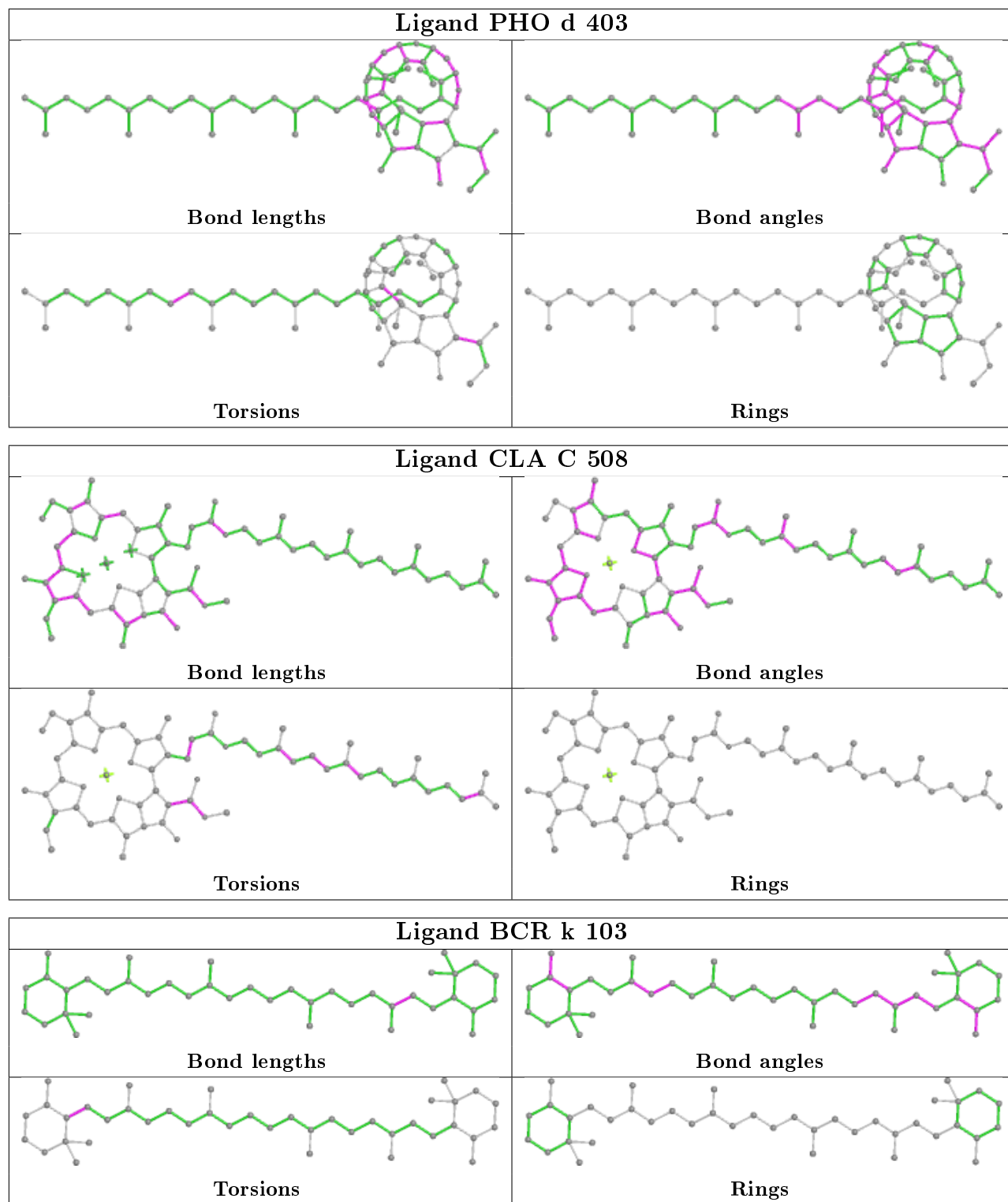


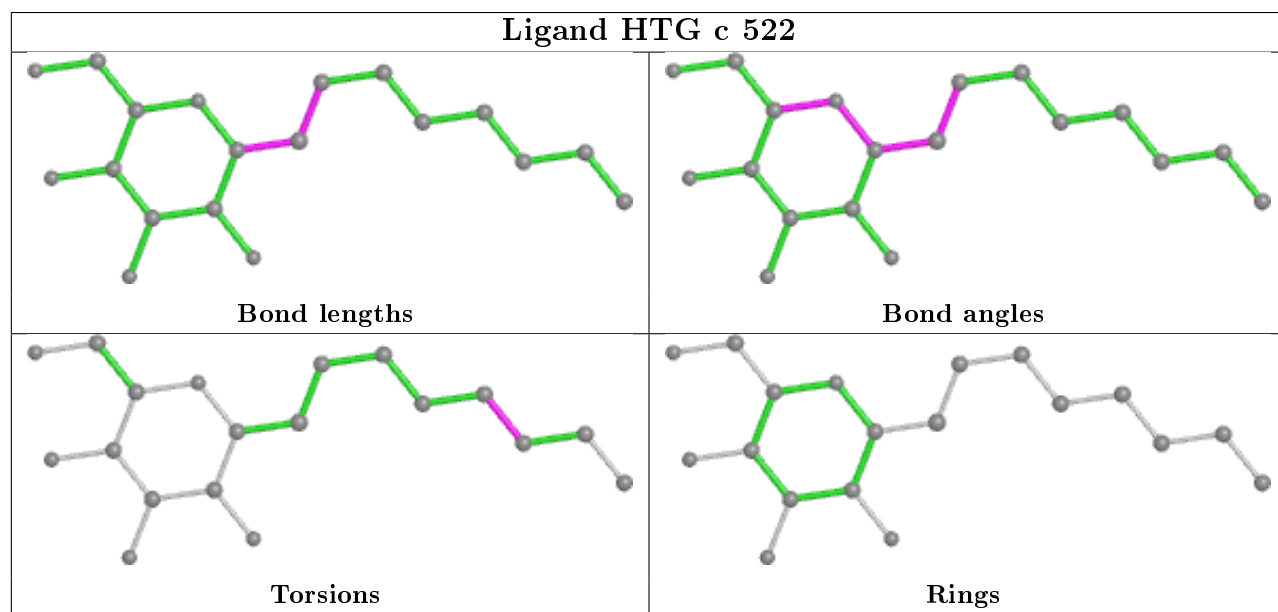
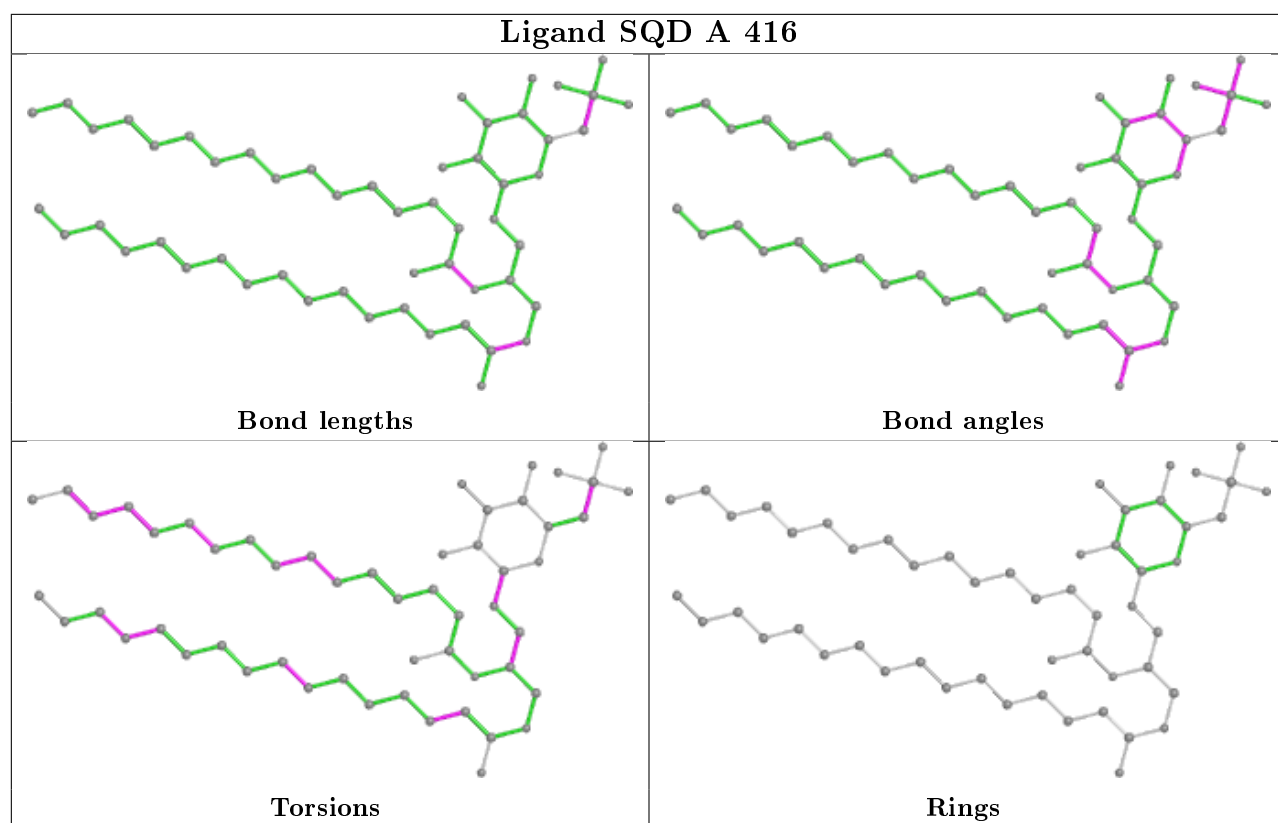


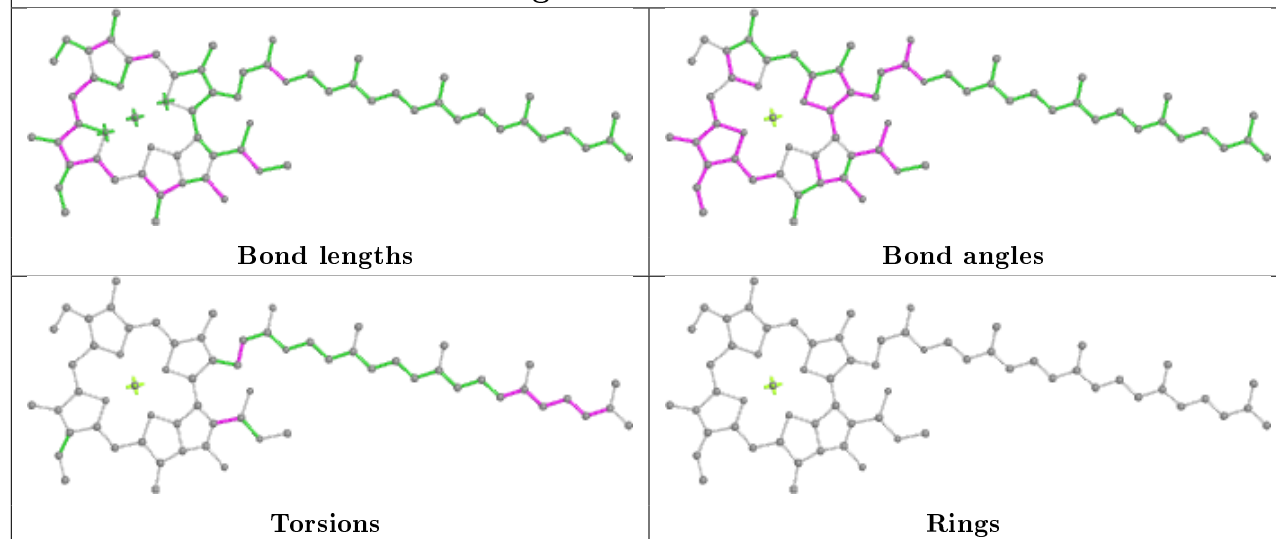
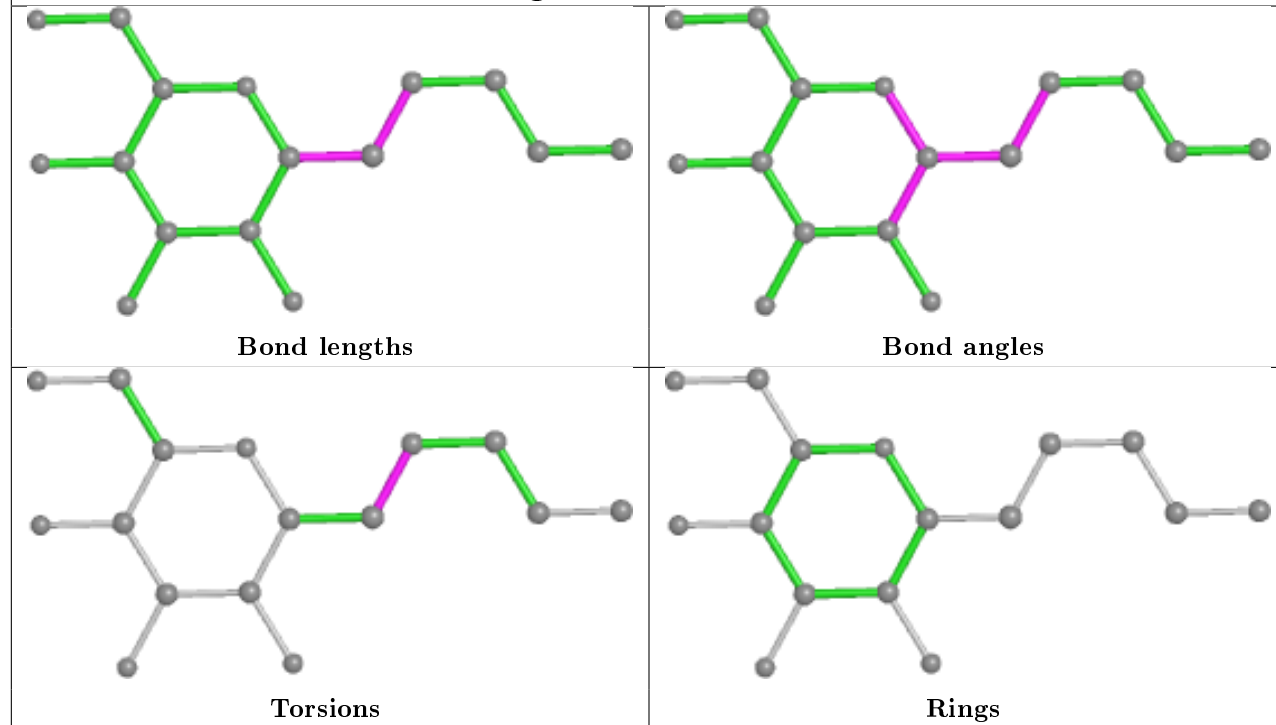
Ligand CLA b 621**Ligand CLA B 614****Ligand CLA D 404**

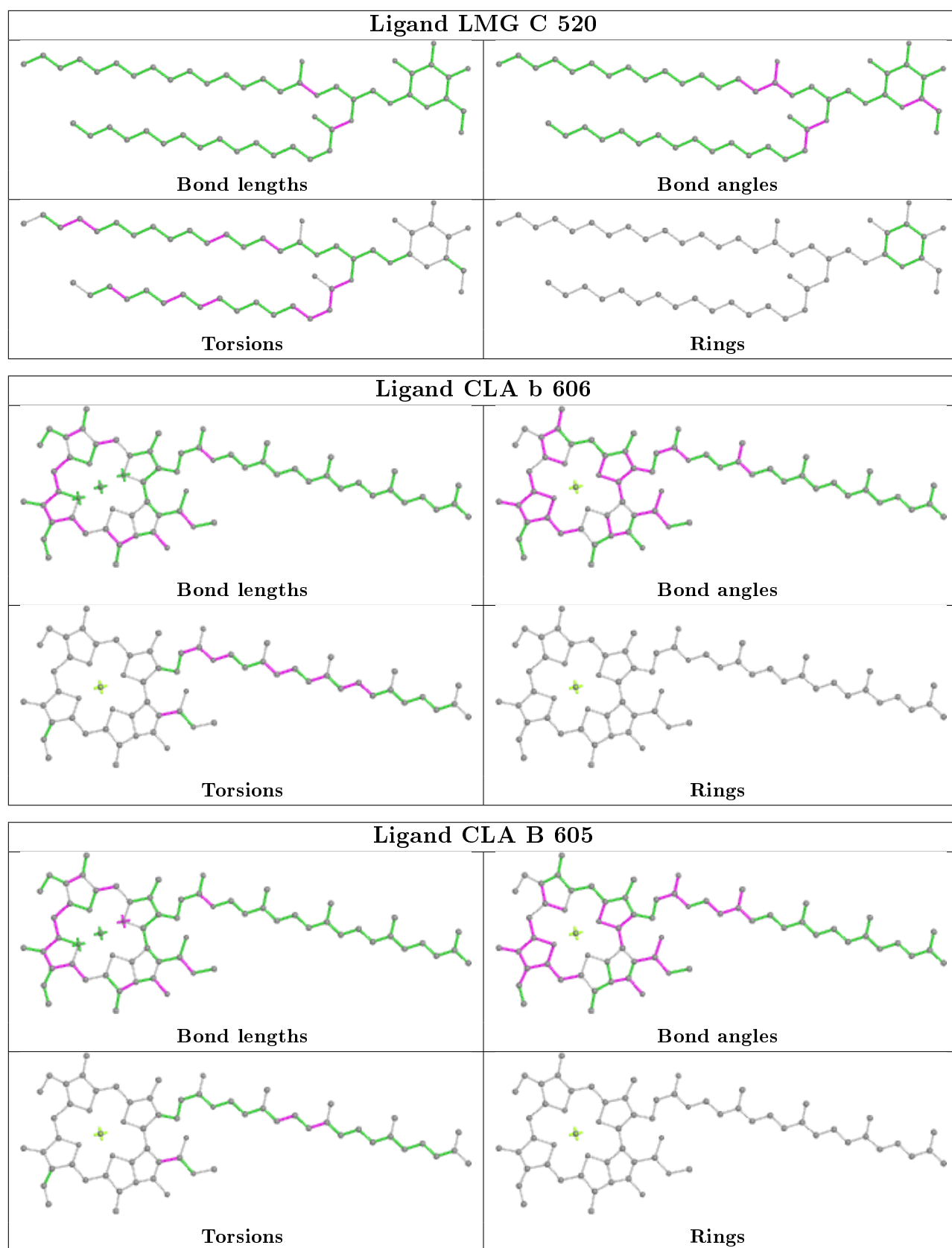
Ligand CLA B 610**Ligand BCR b 623****Ligand PL9 d 406****Ligand BCR K 101**

Ligand CLA C 503**Ligand DGD C 517****Ligand CLA c 504**

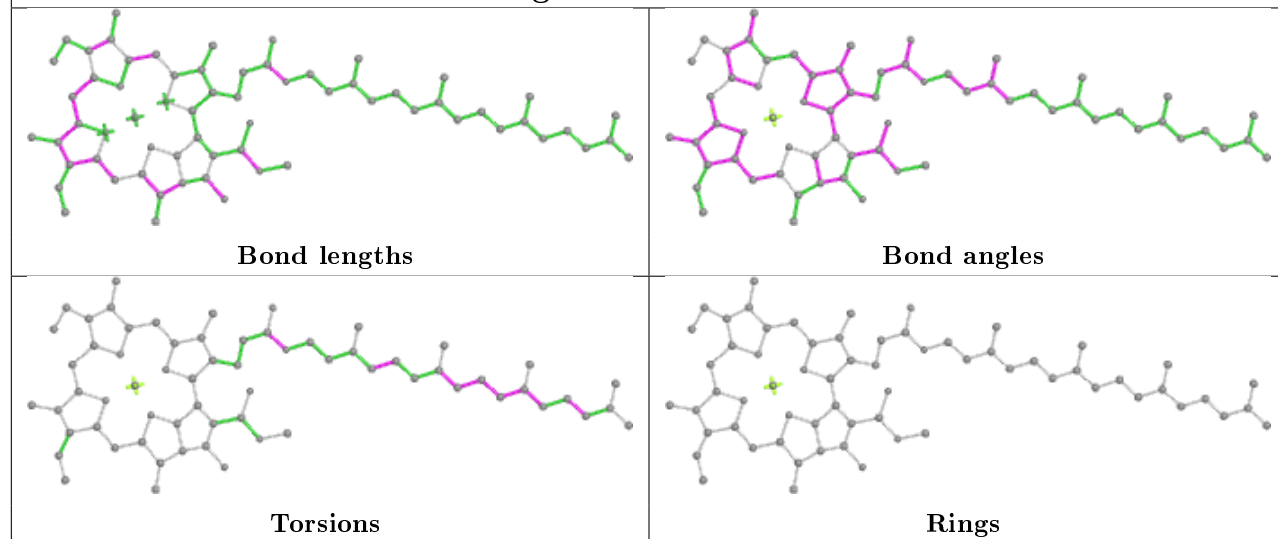




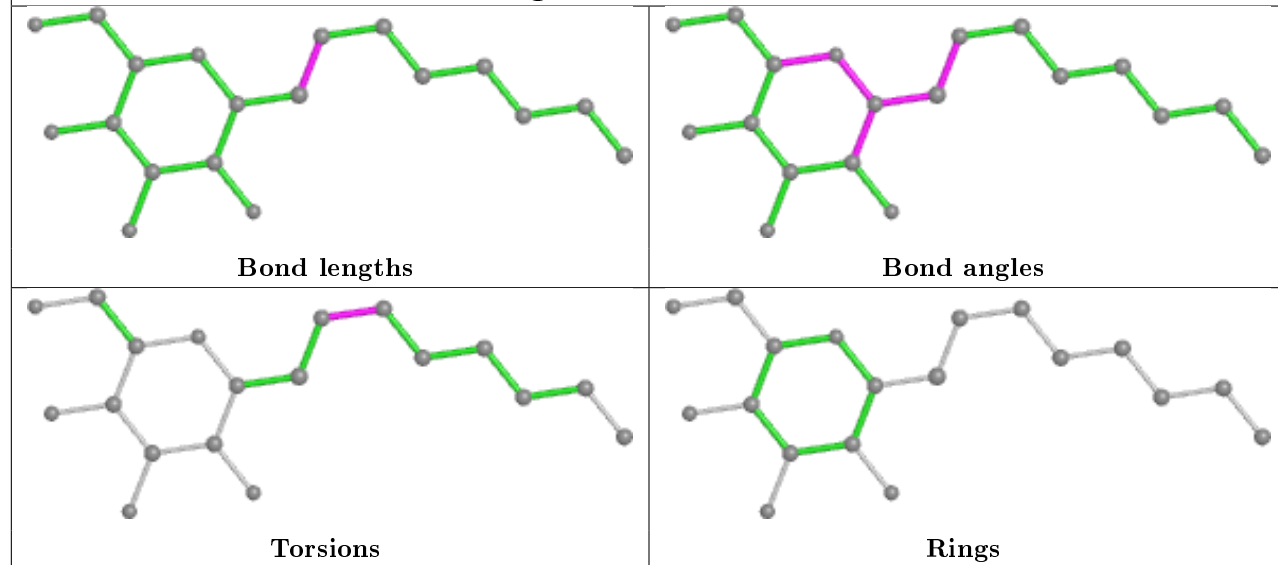
Ligand CLA C 502**Ligand HTG D 411**

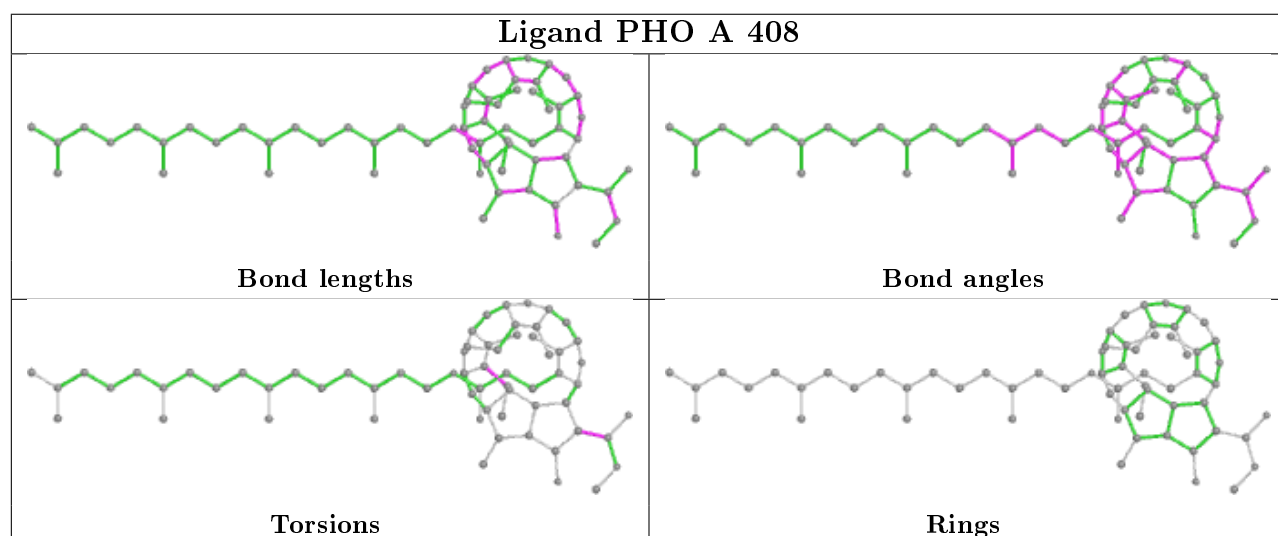
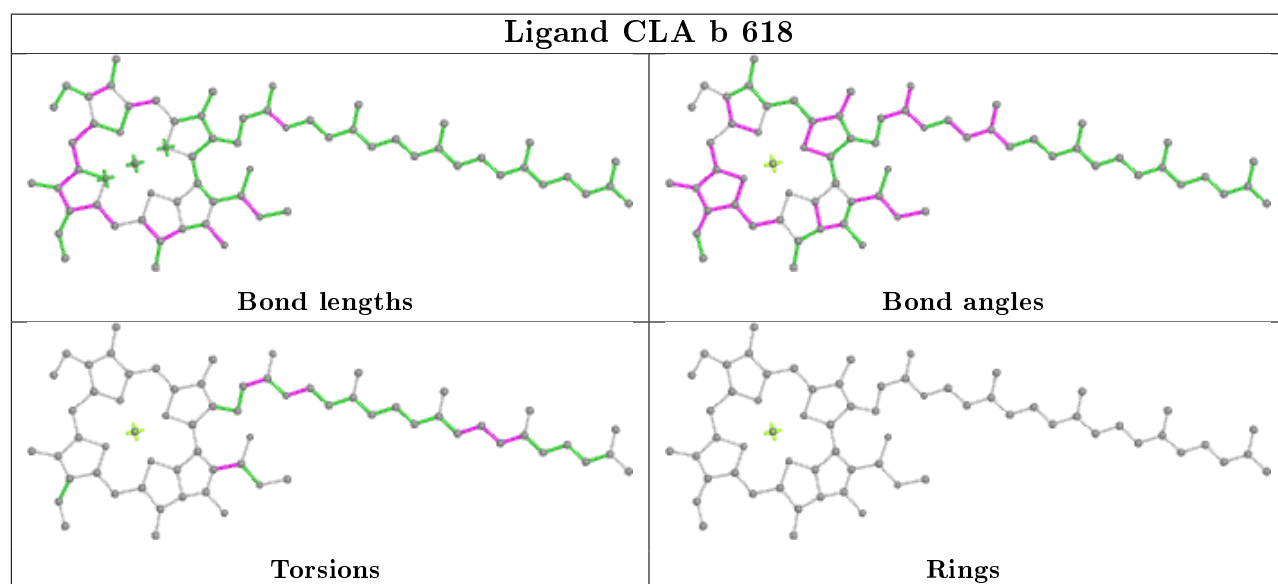
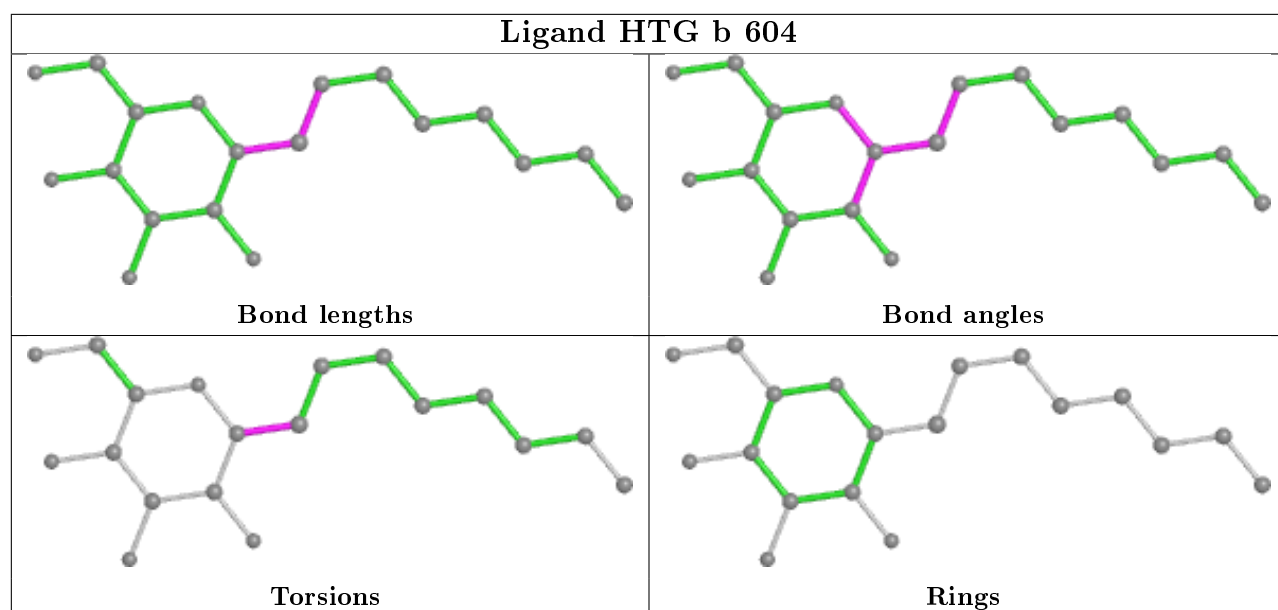


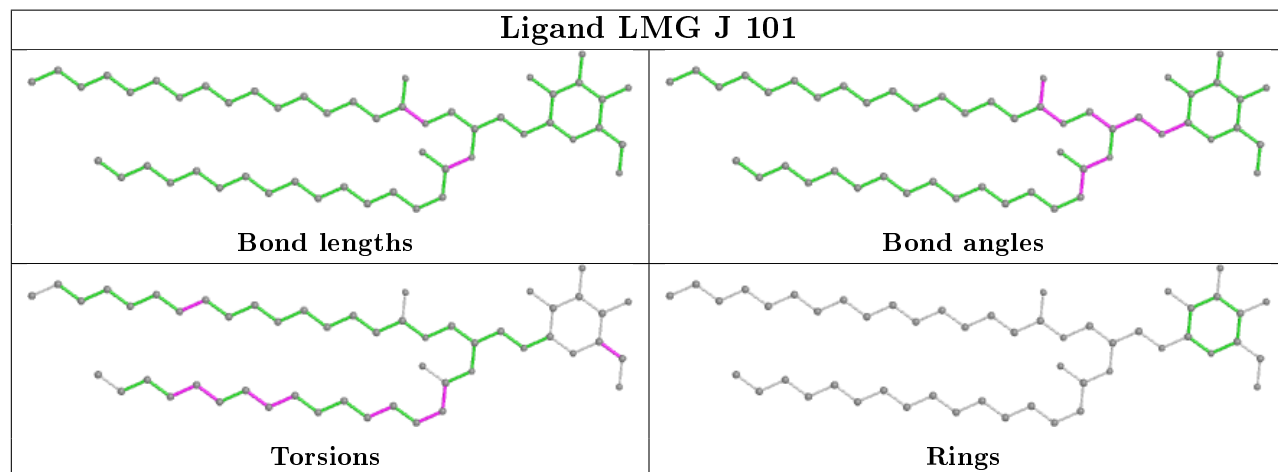
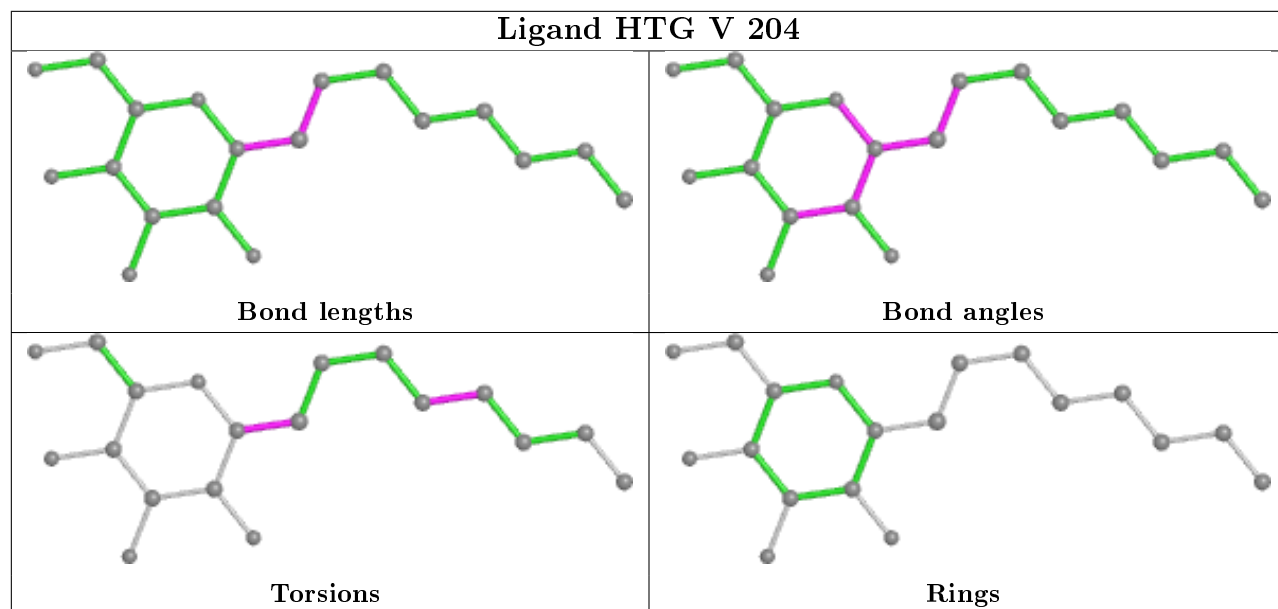
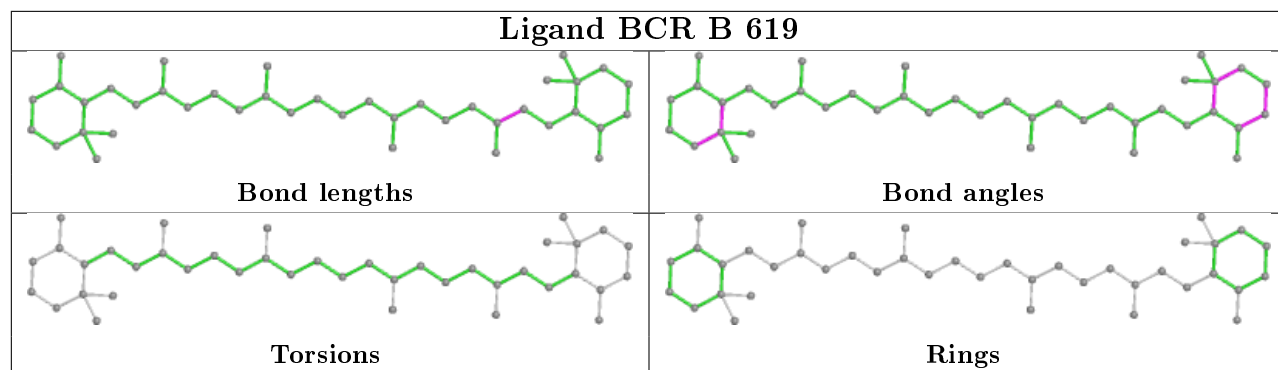
Ligand CLA A 409

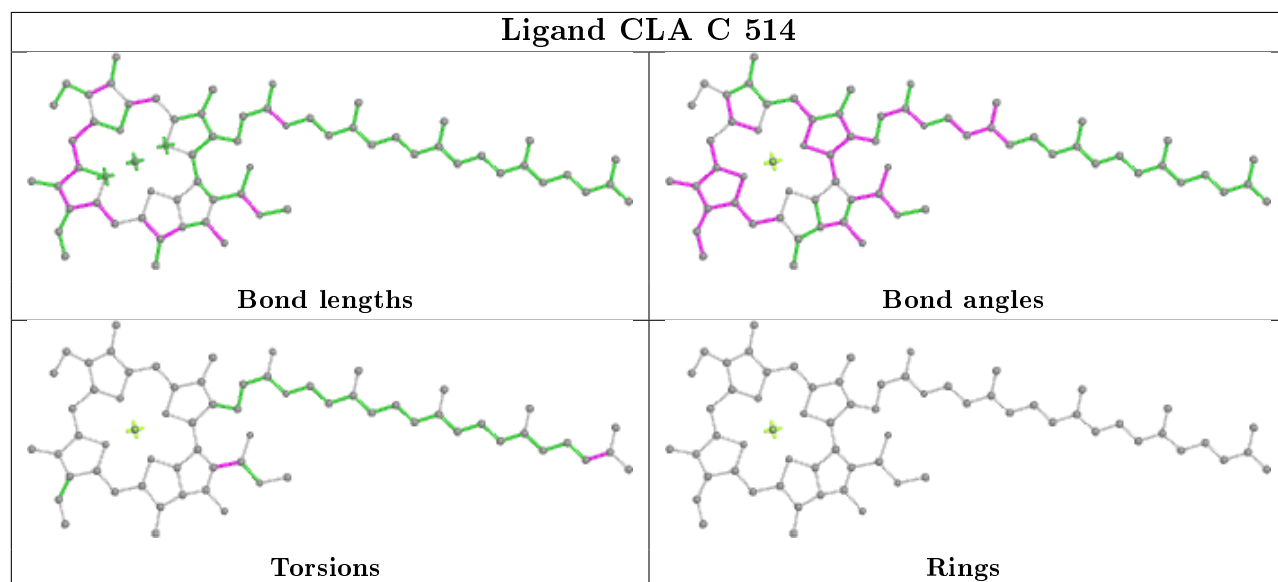
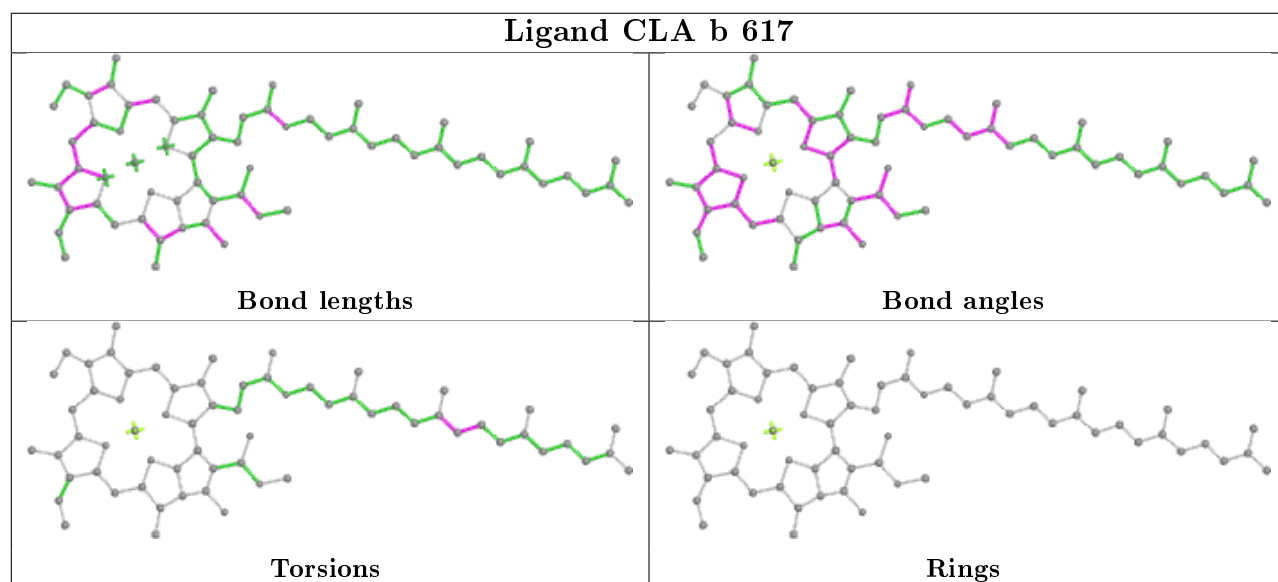
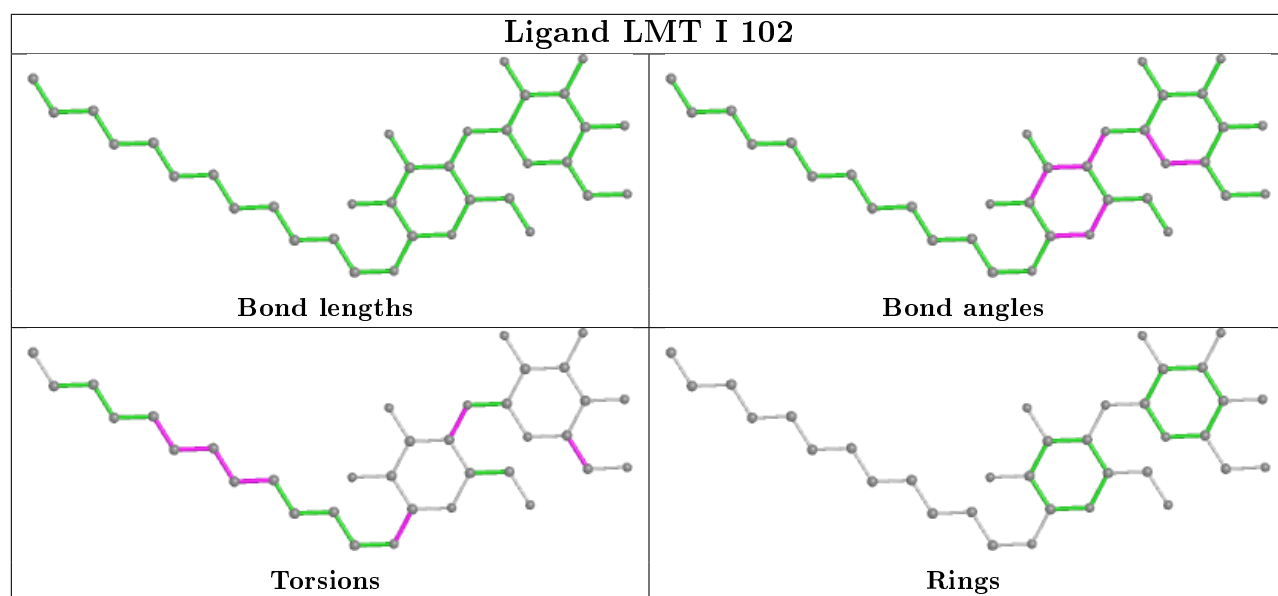


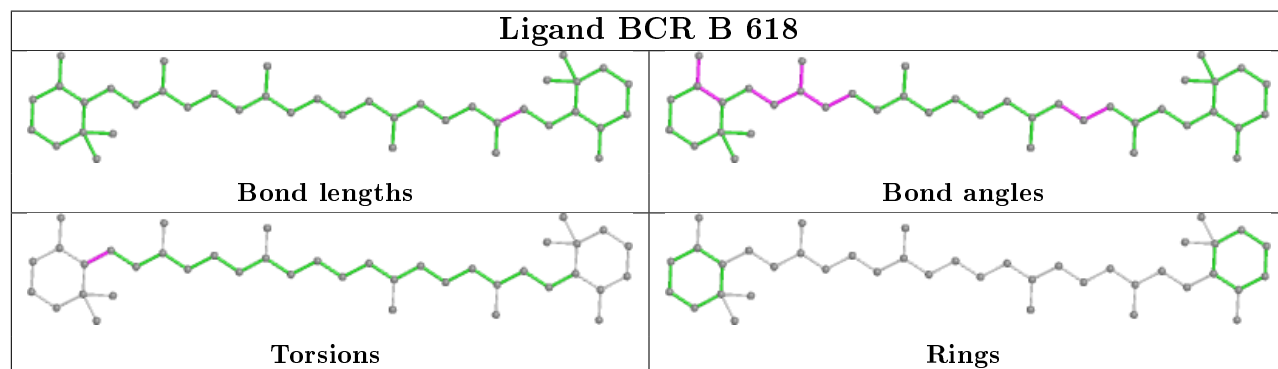
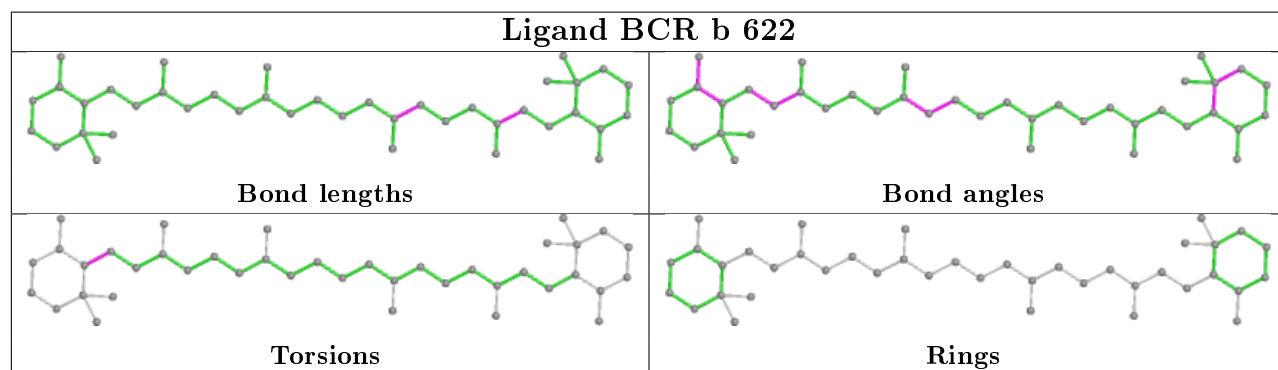
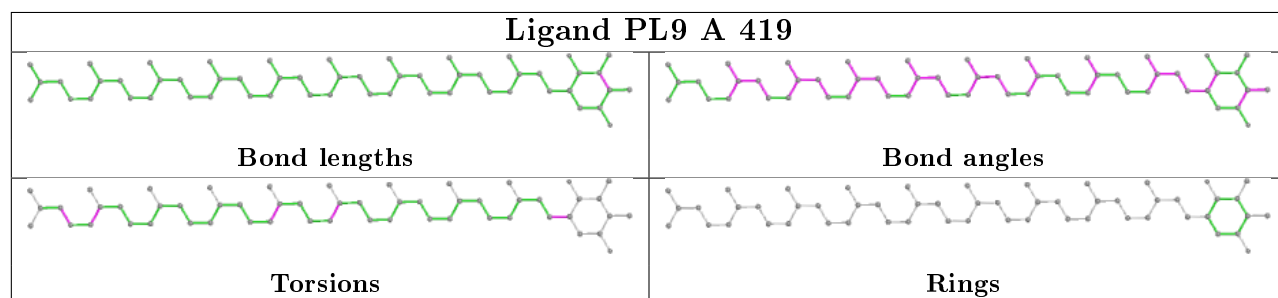
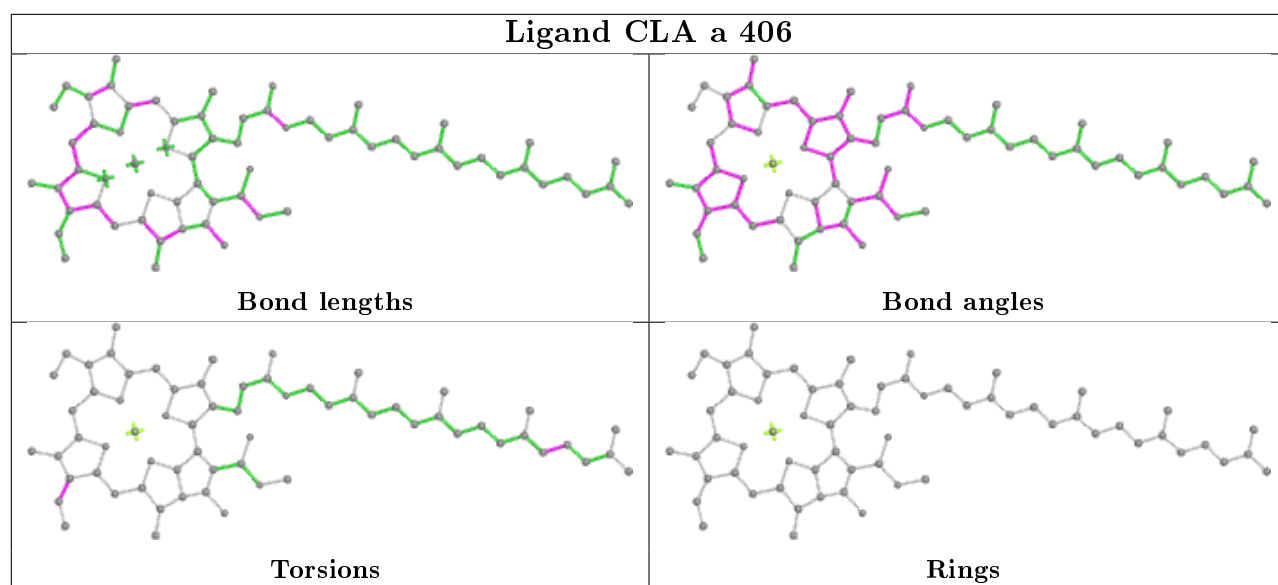
Ligand HTG B 622



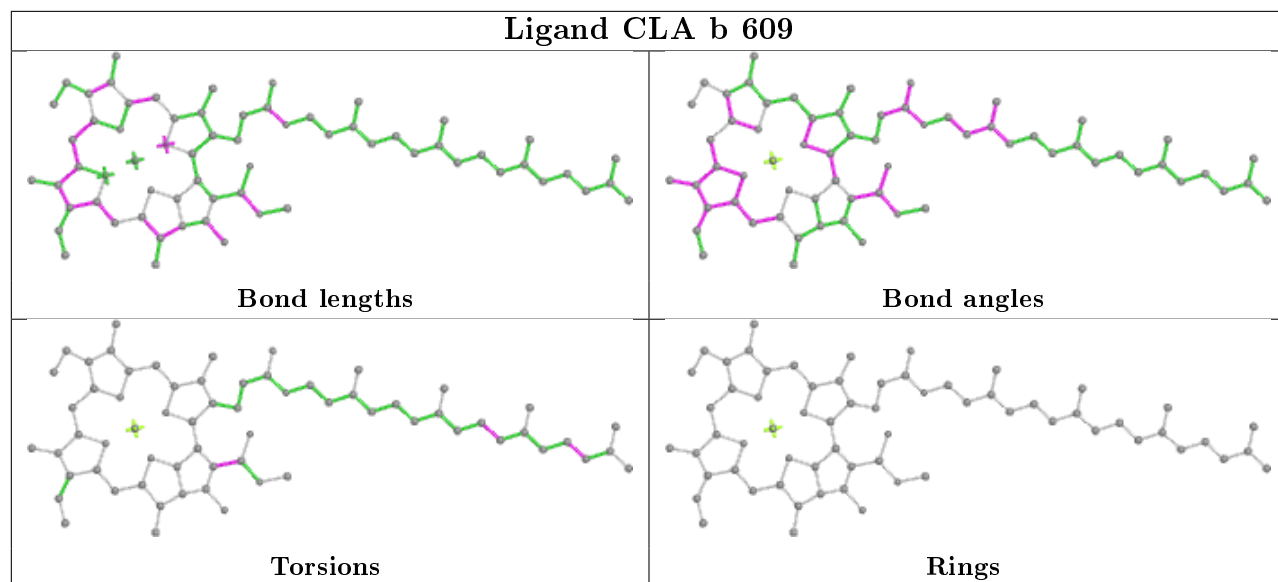




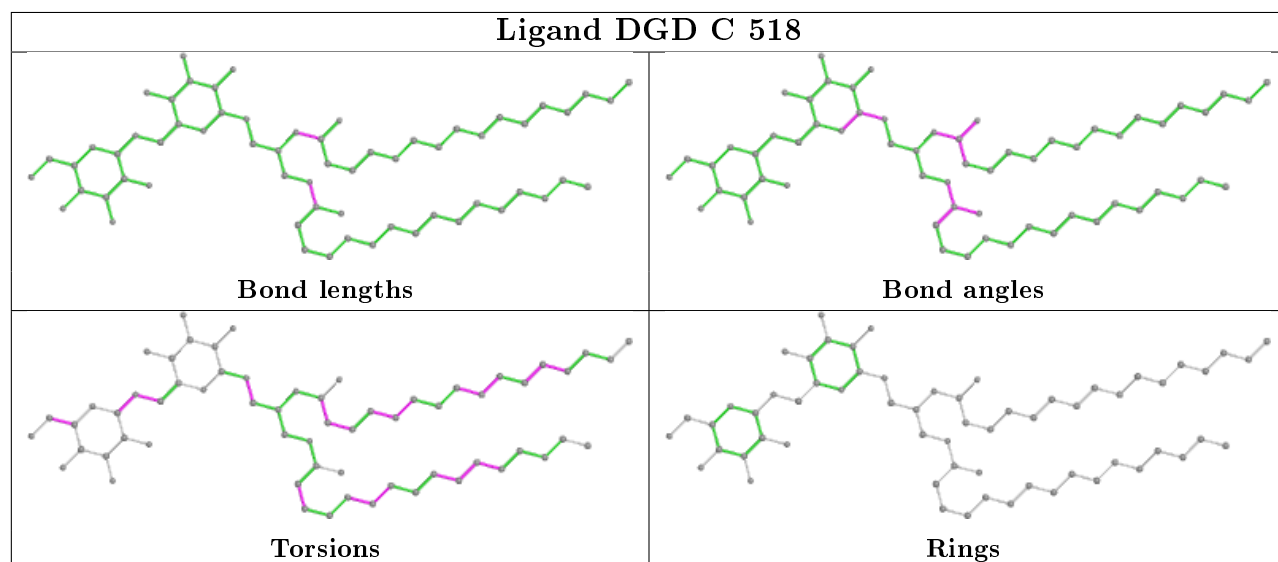




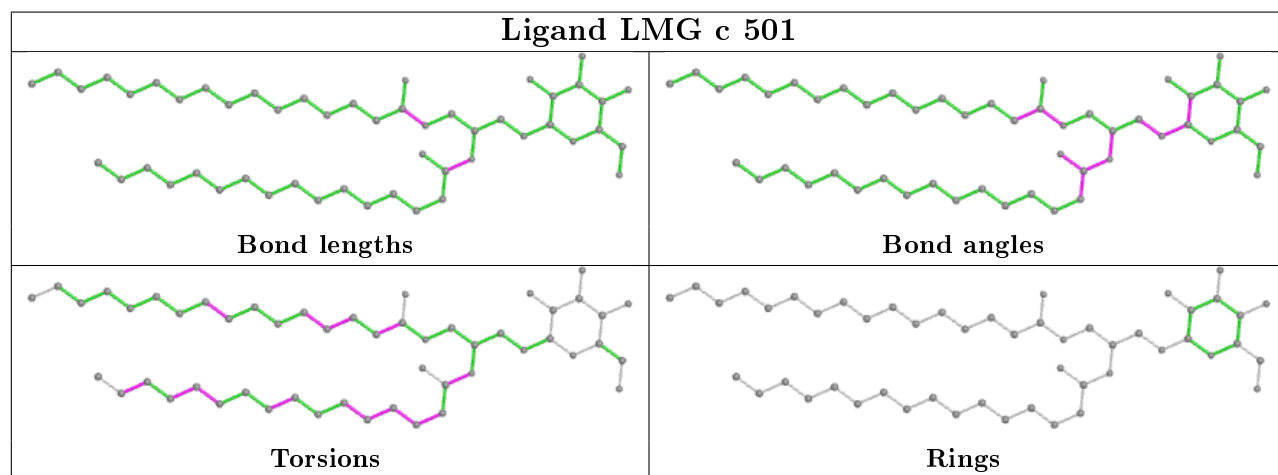
Ligand CLA b 609

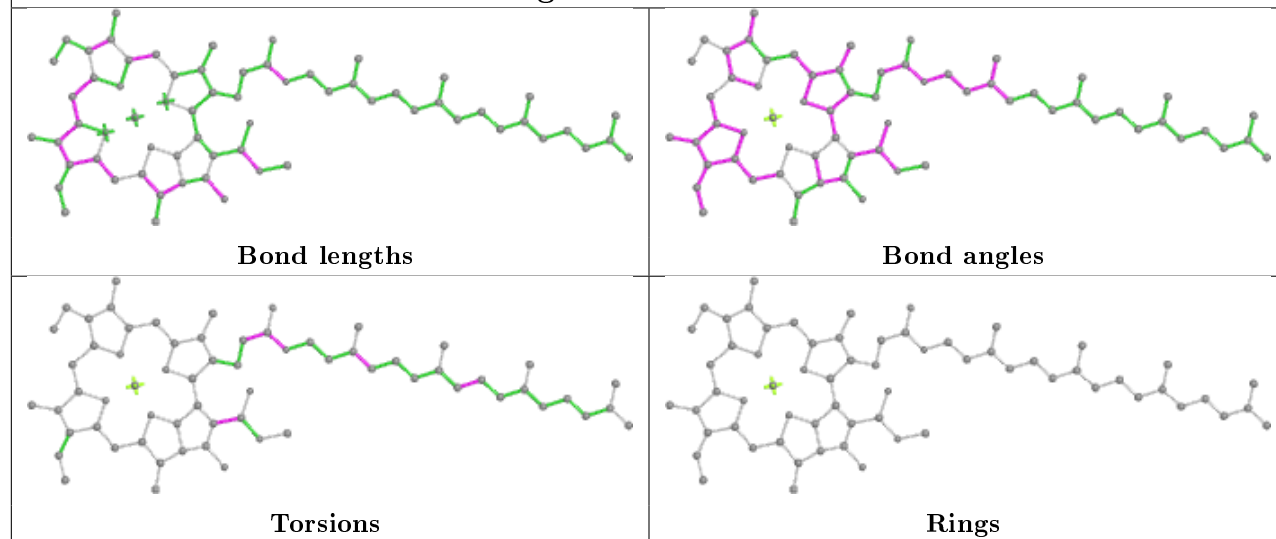
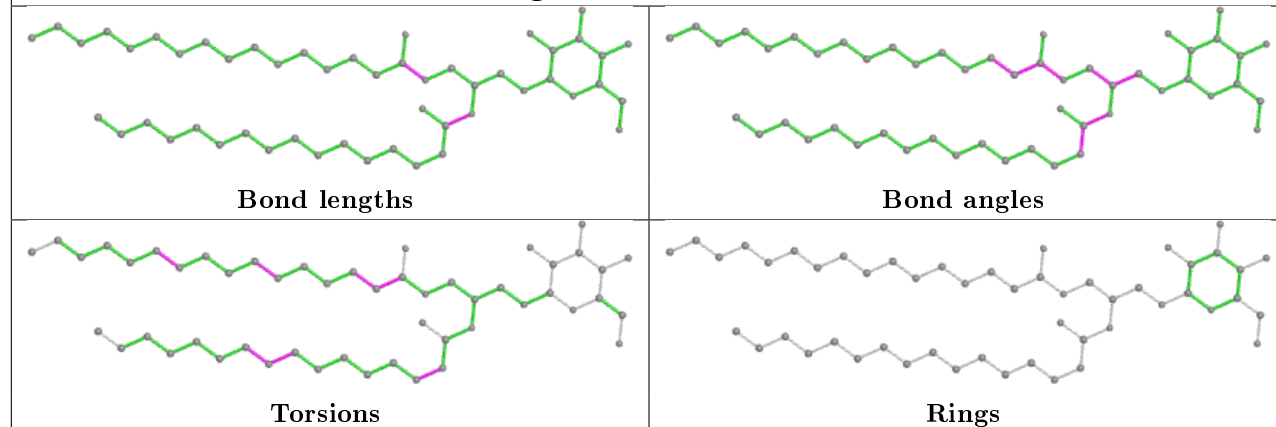
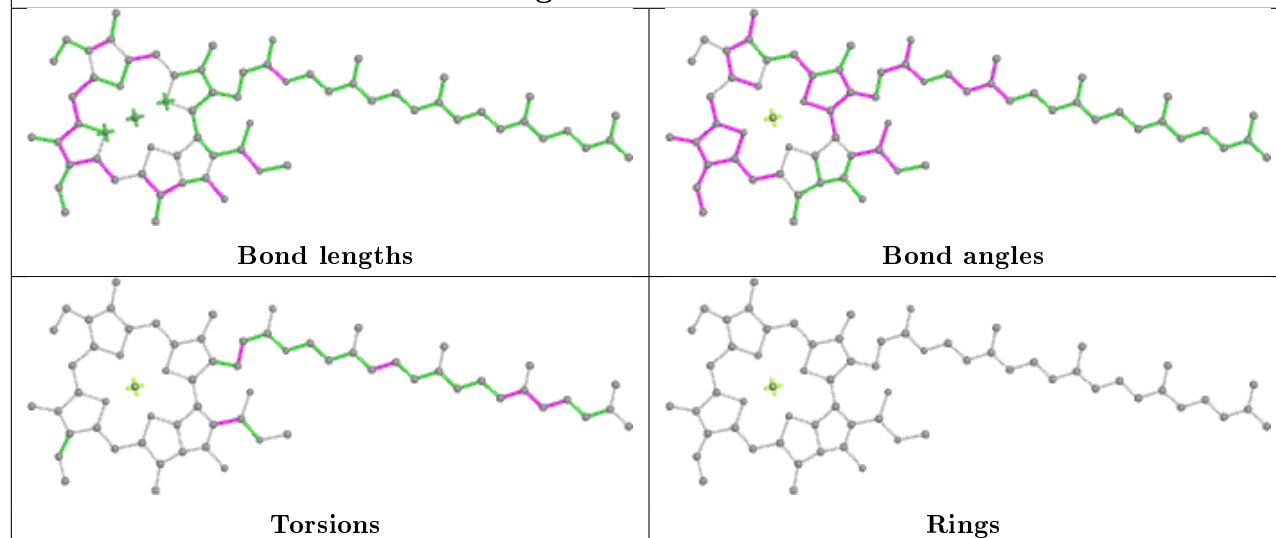


Ligand DGD C 518

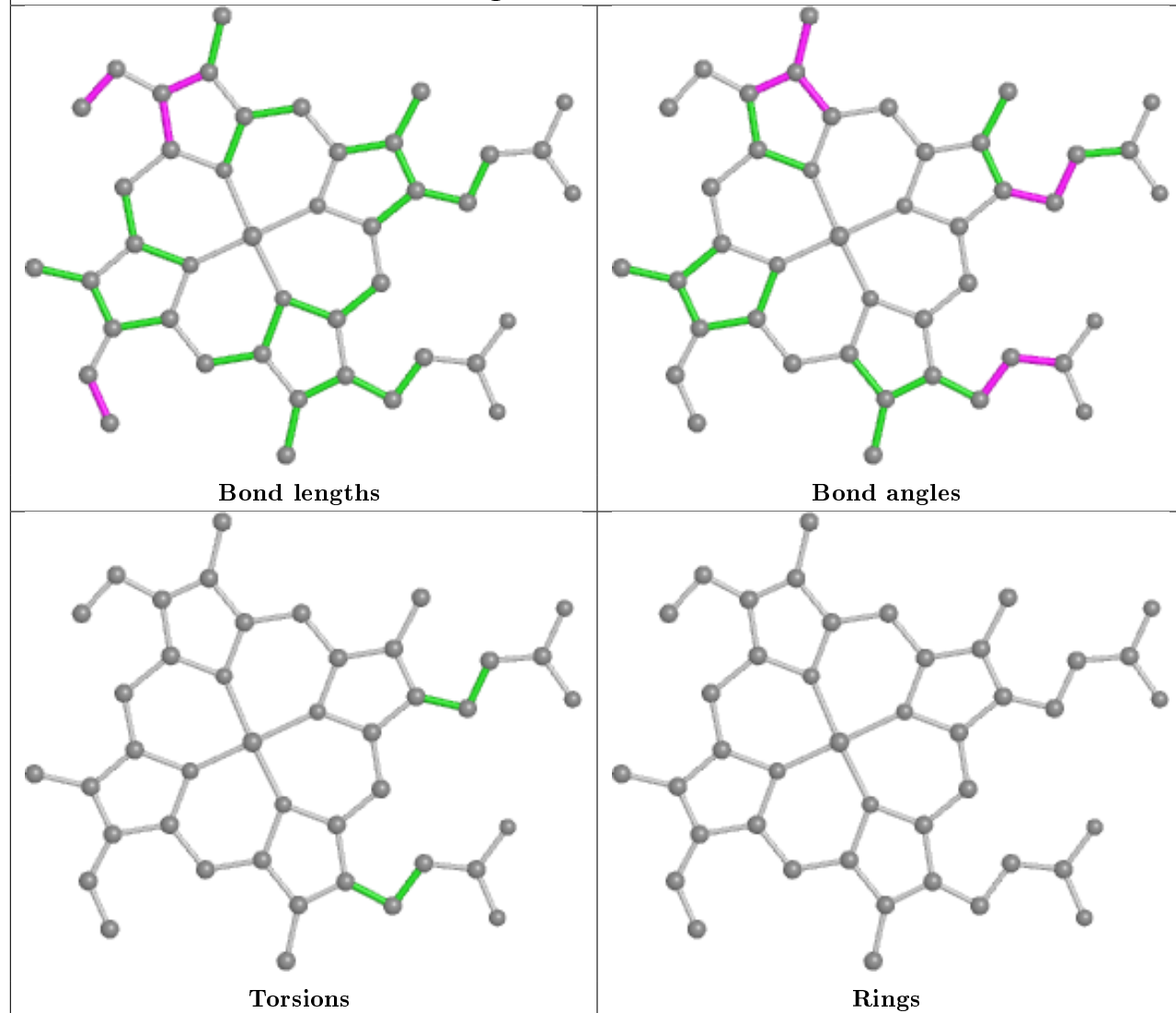


Ligand LMG c 501

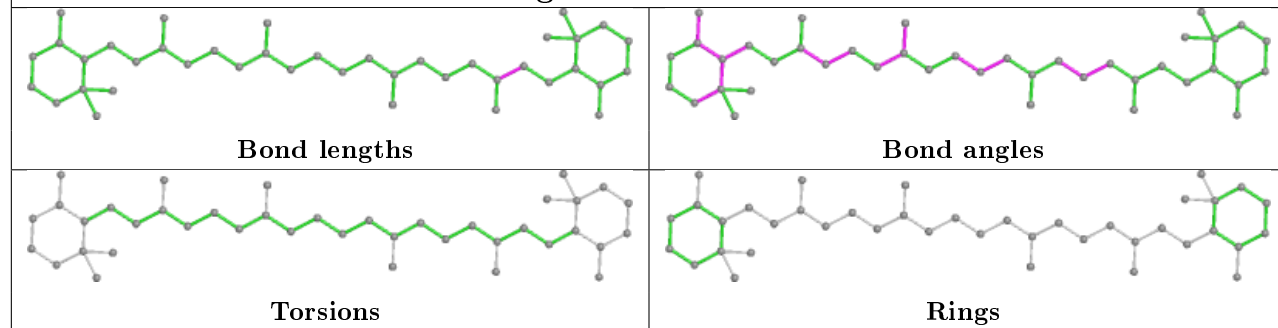


Ligand CLA c 512**Ligand LMG B 621****Ligand CLA b 611**

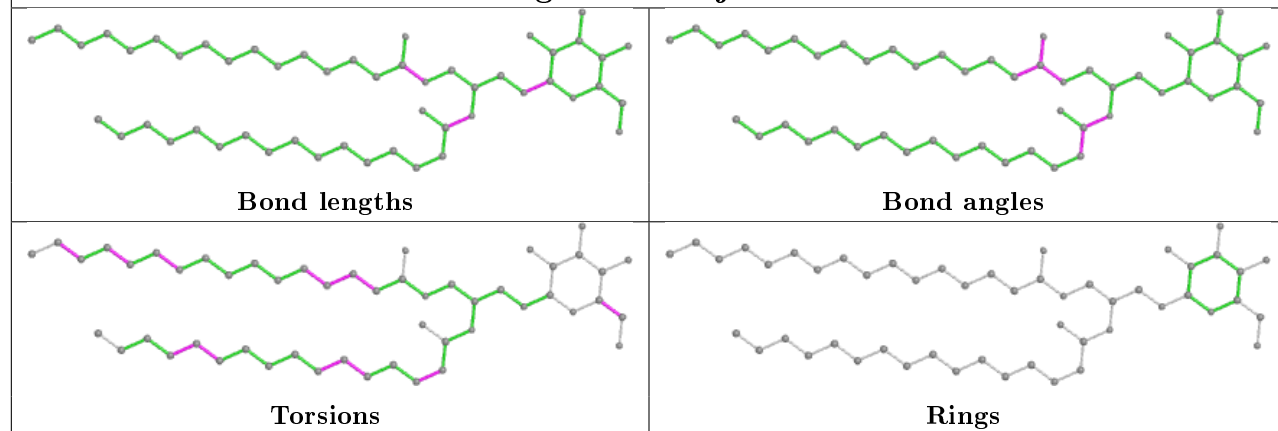
Ligand HEC V 203



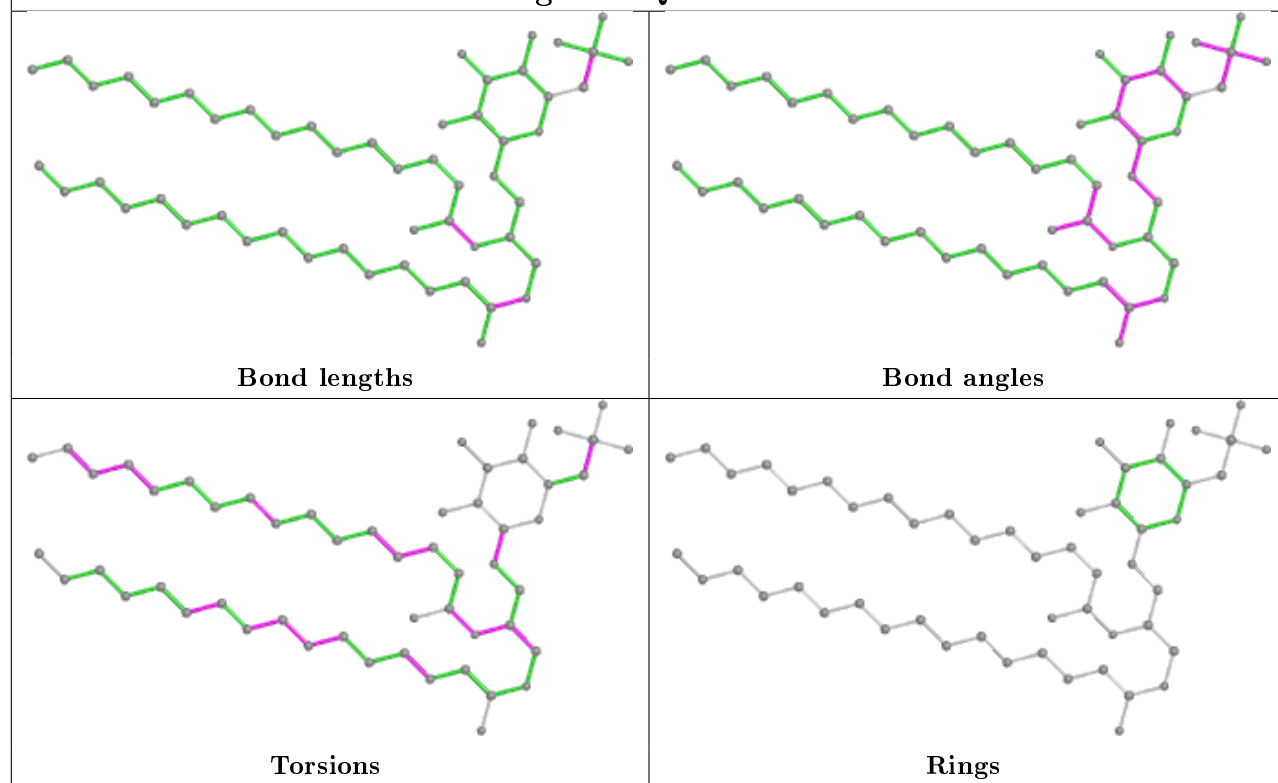
Ligand BCR t 101

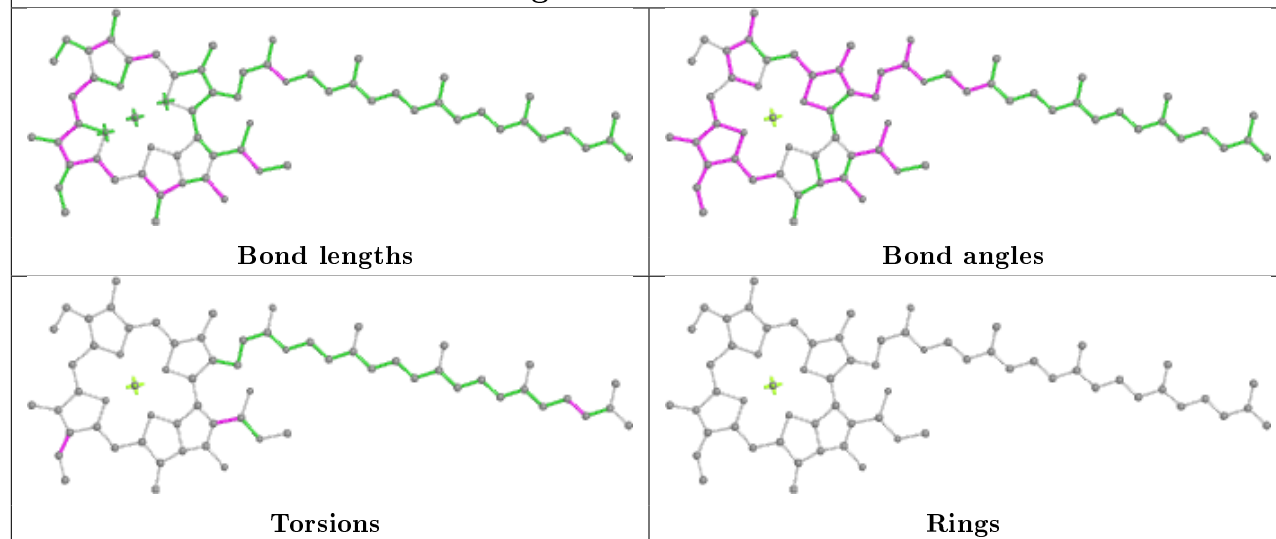
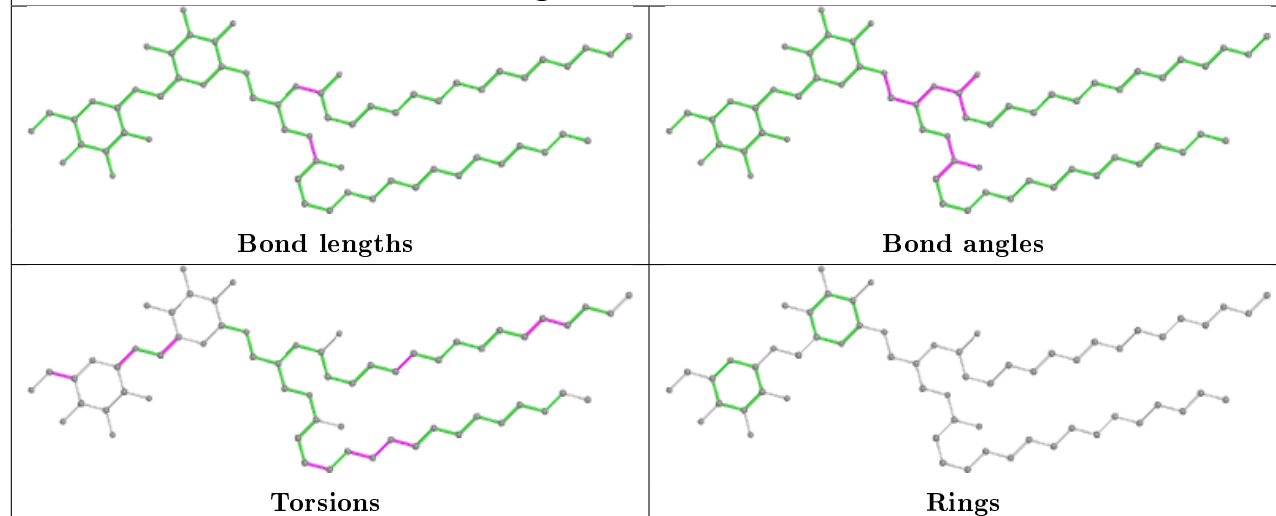


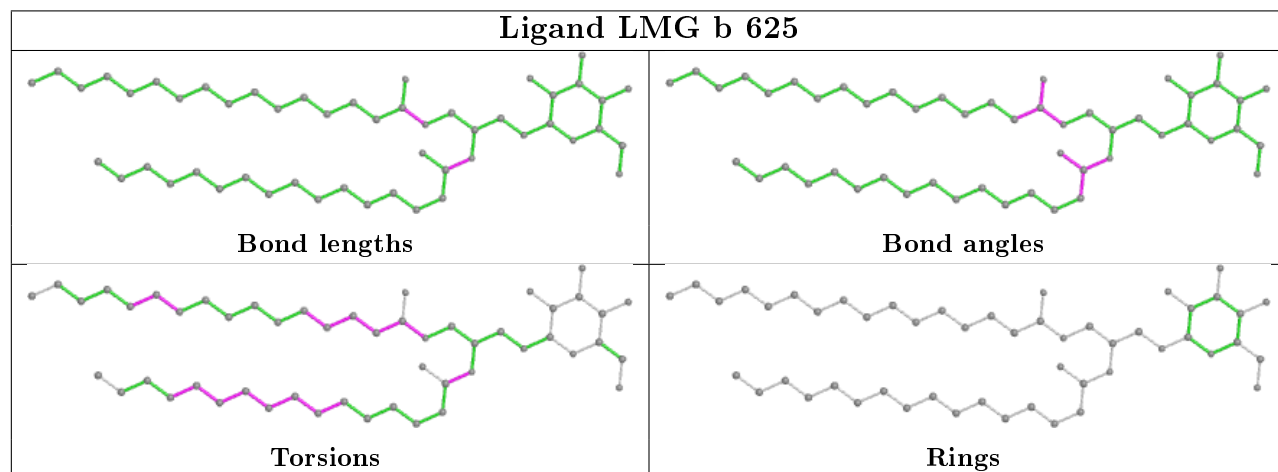
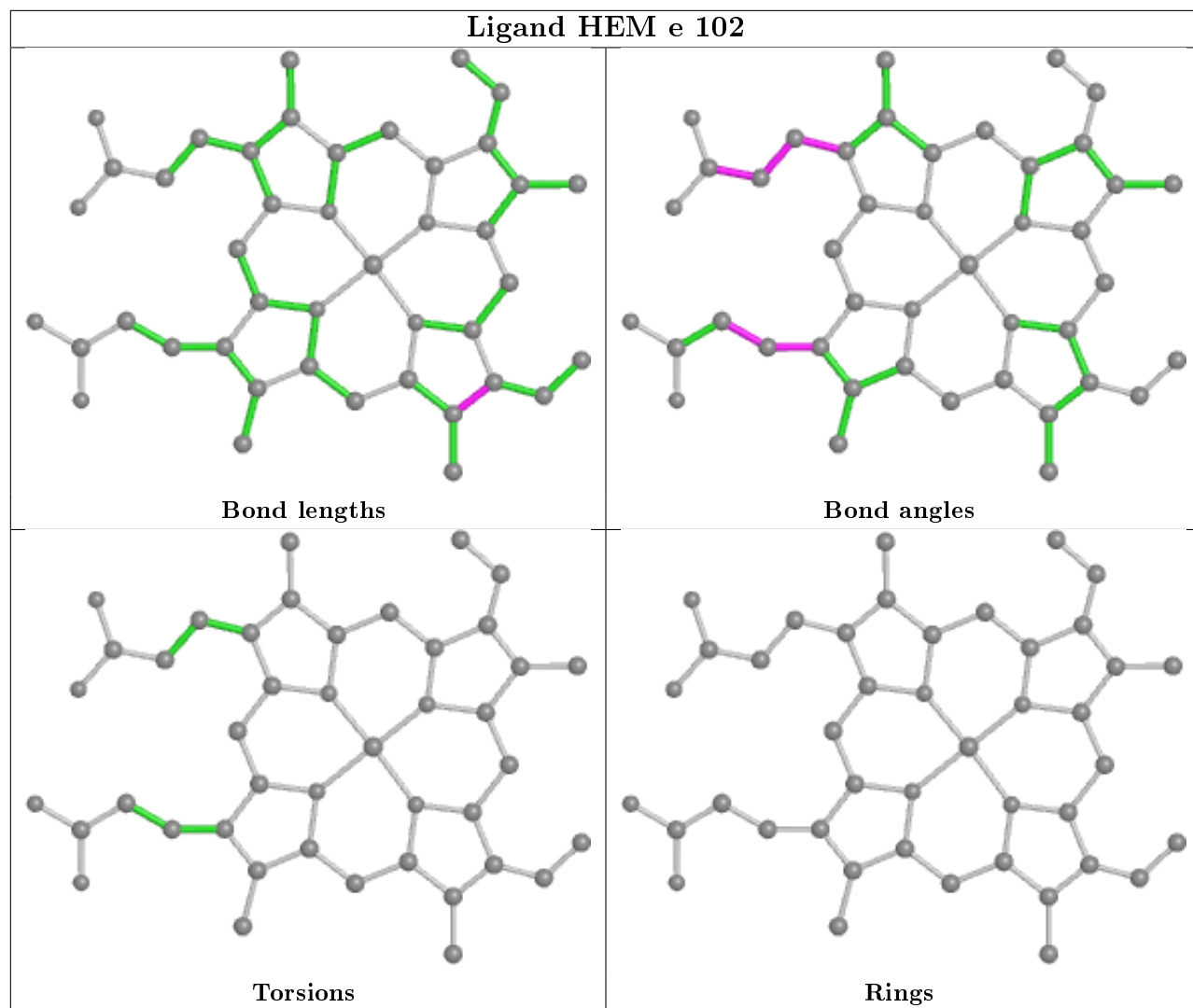
Ligand LMG j 101



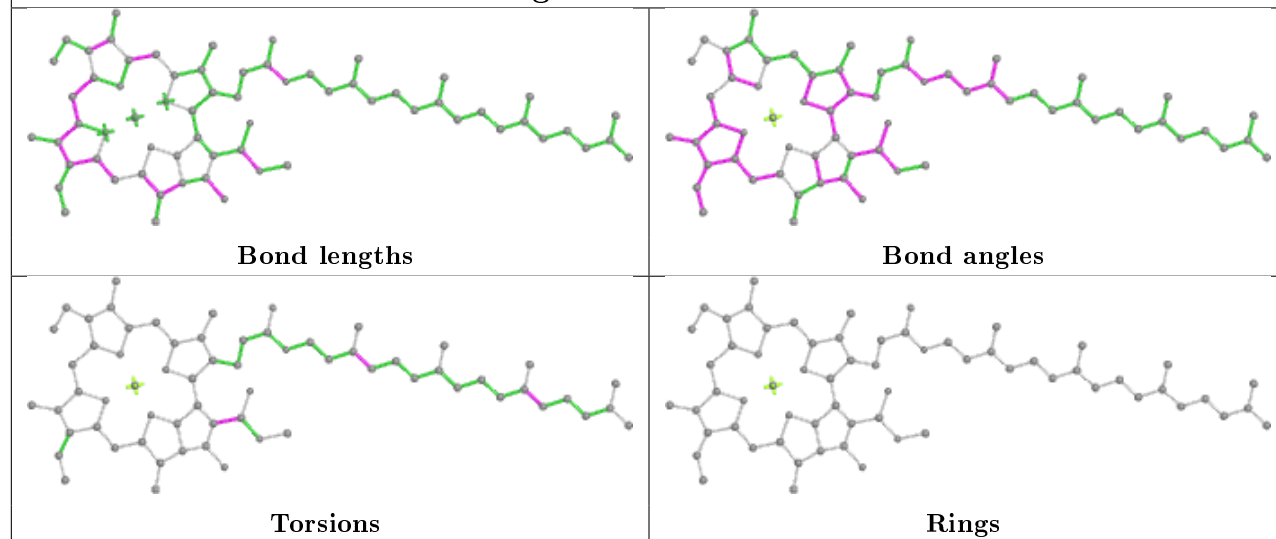
Ligand SQD b 601



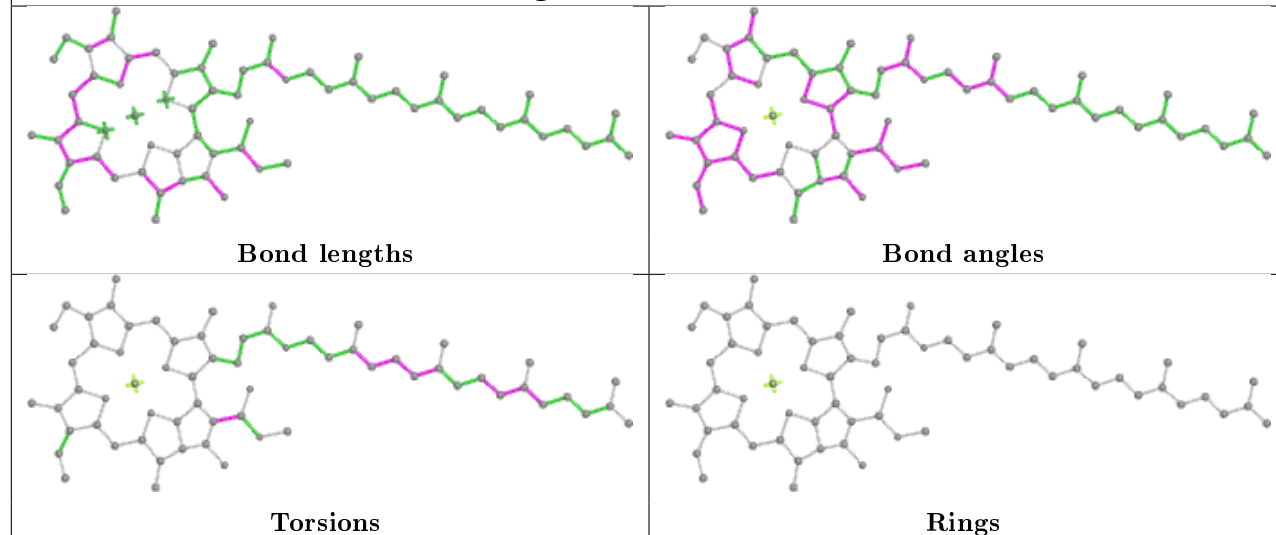
Ligand CLA D 401**Ligand DGD c 517**



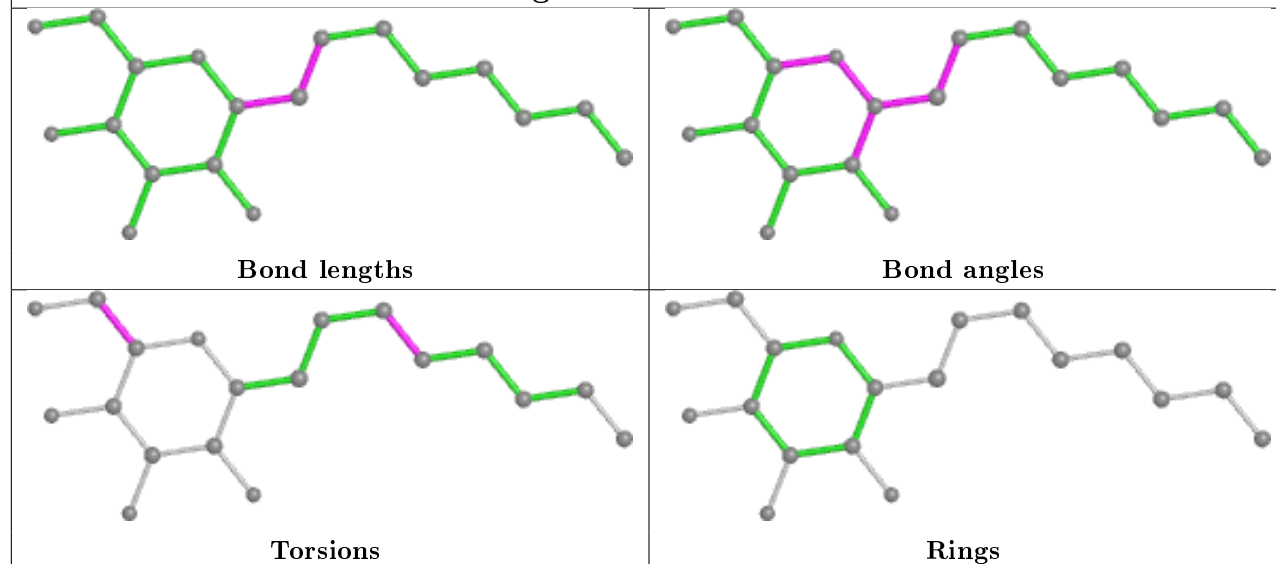
Ligand CLA C 505

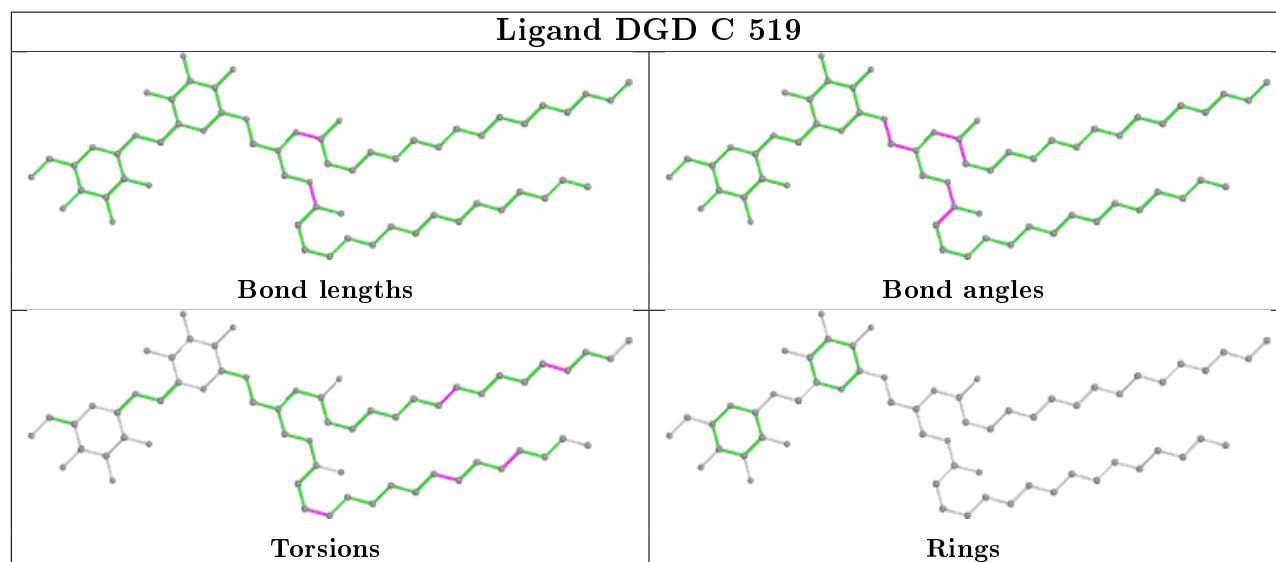
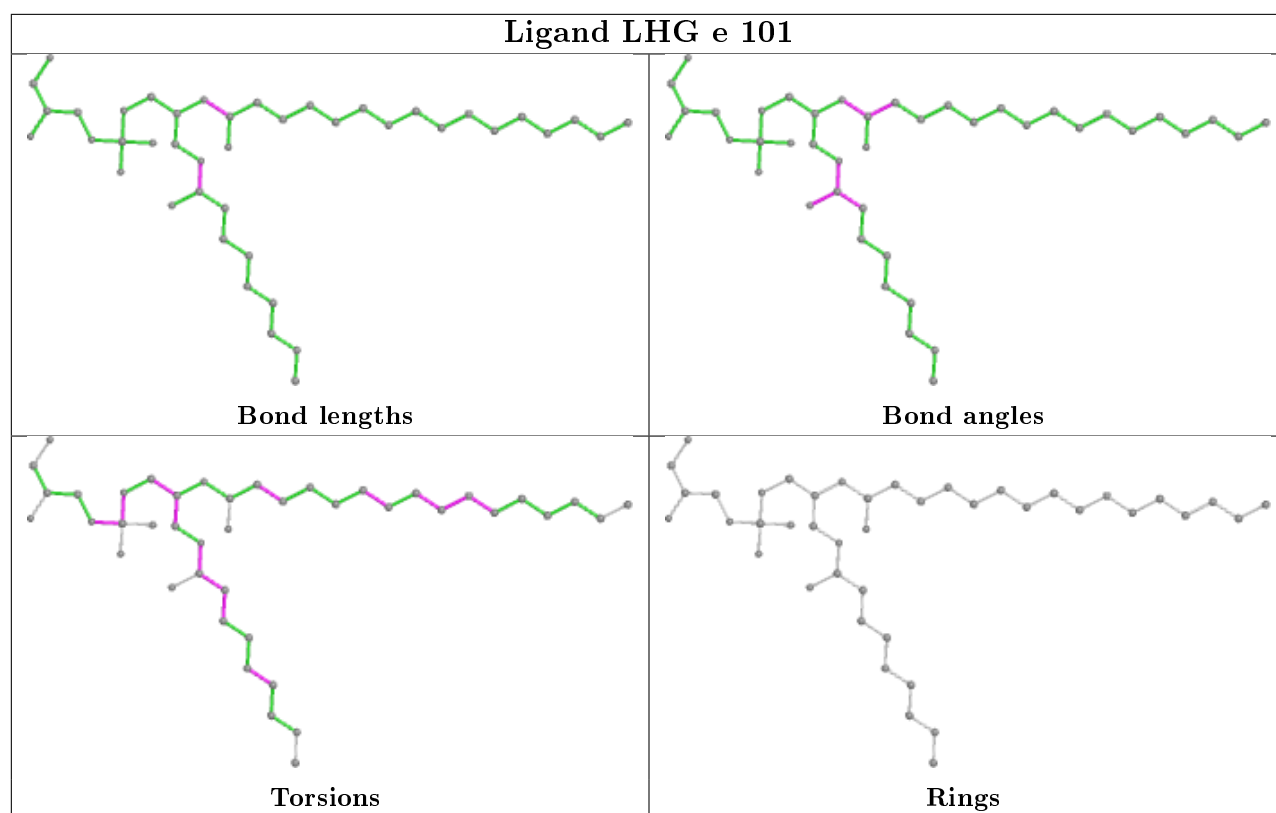


Ligand CLA B 615

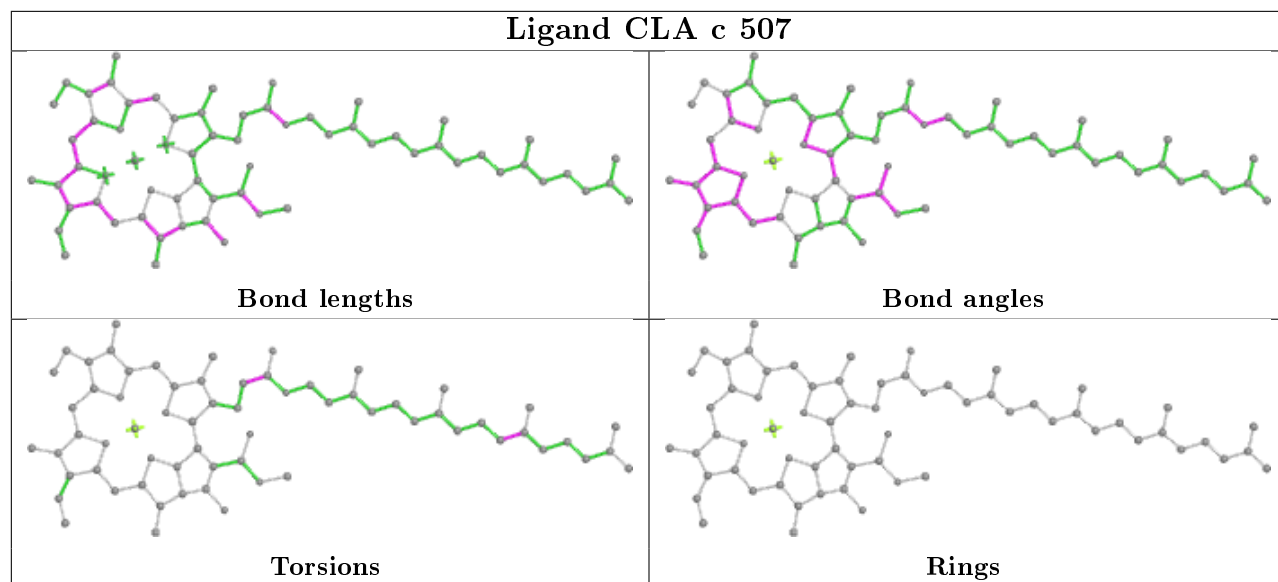


Ligand HTG b 628

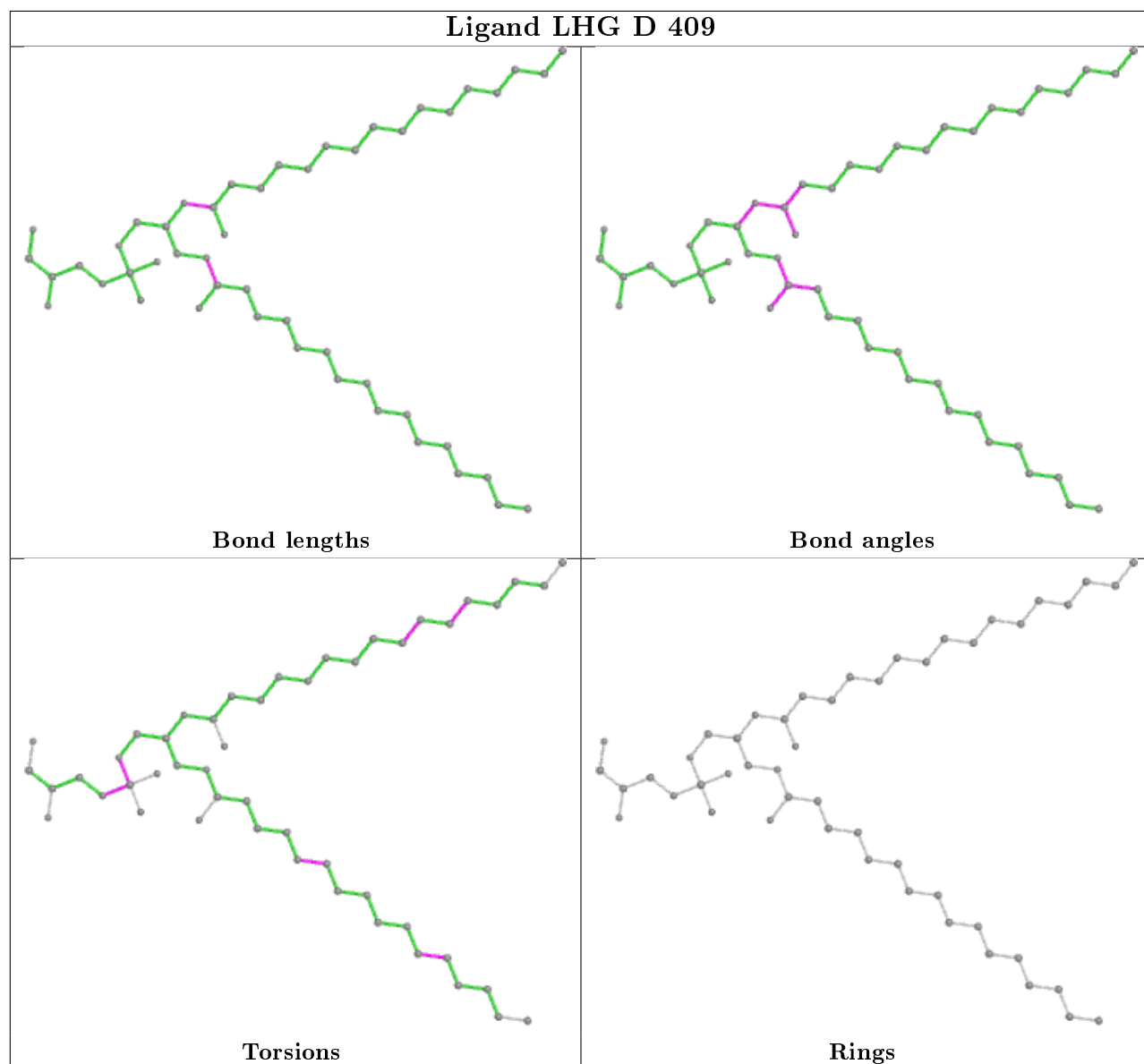


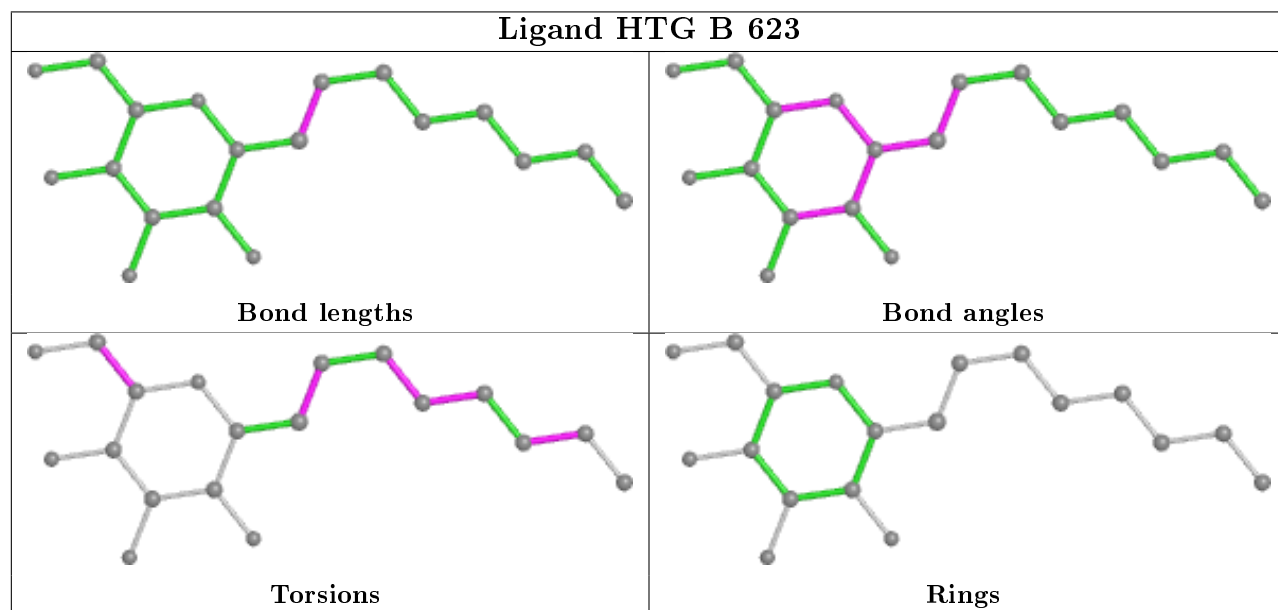
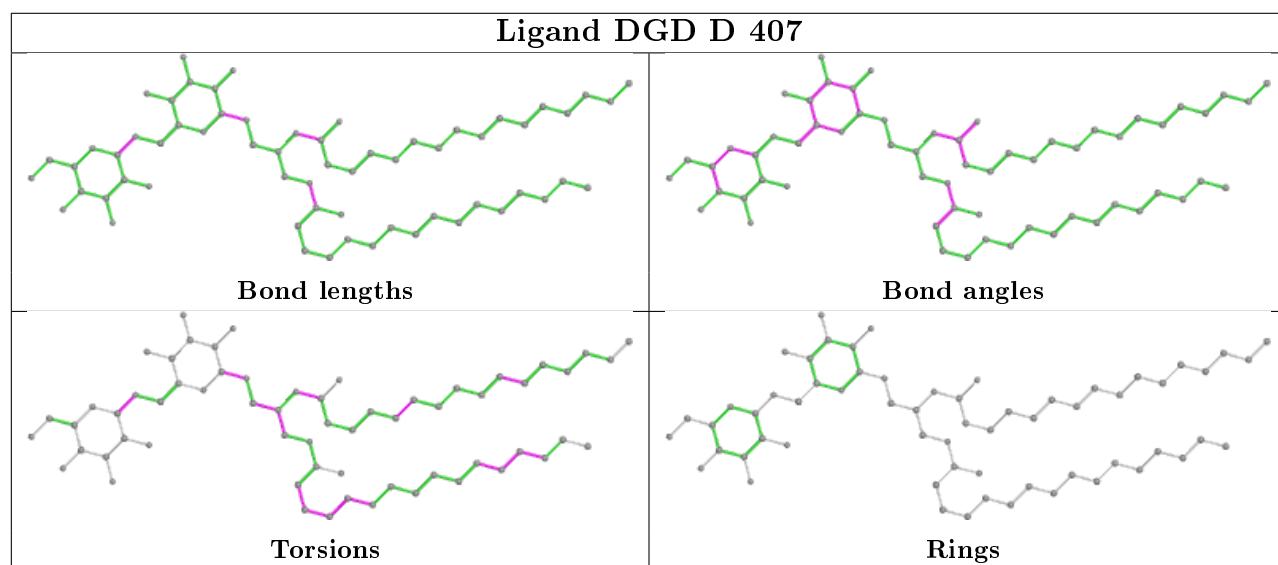
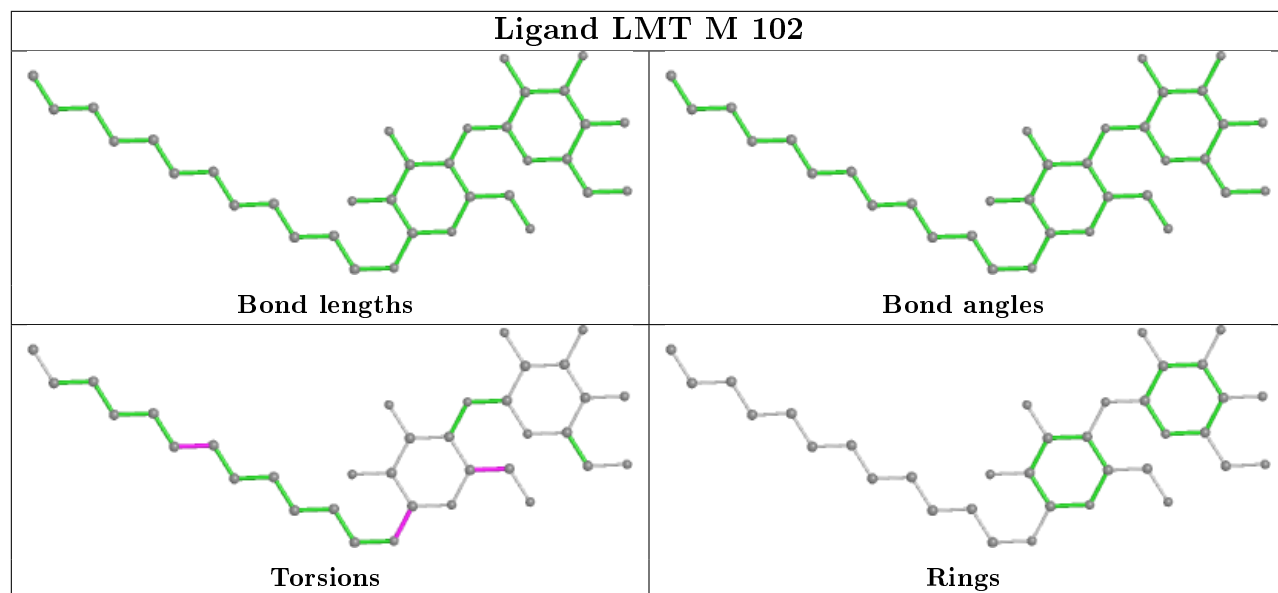


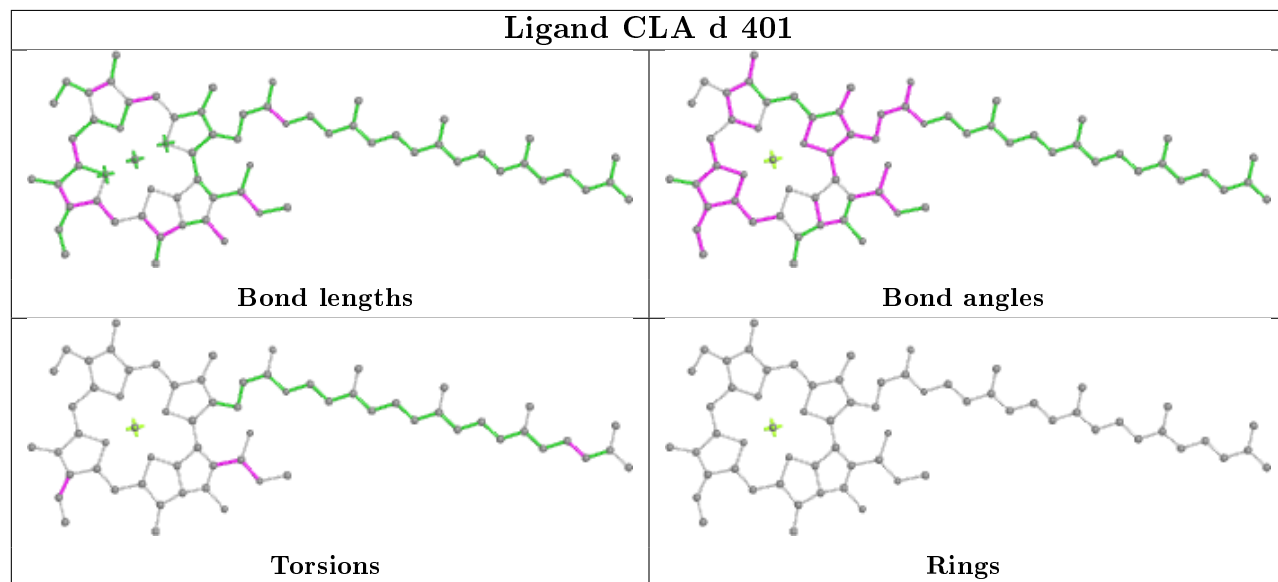
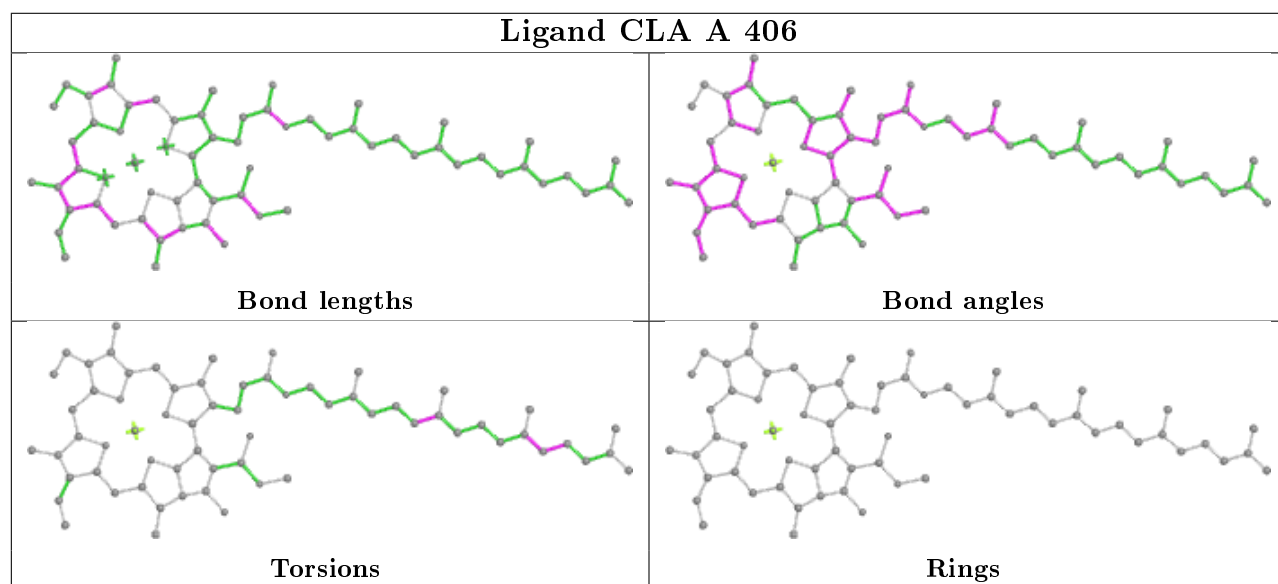
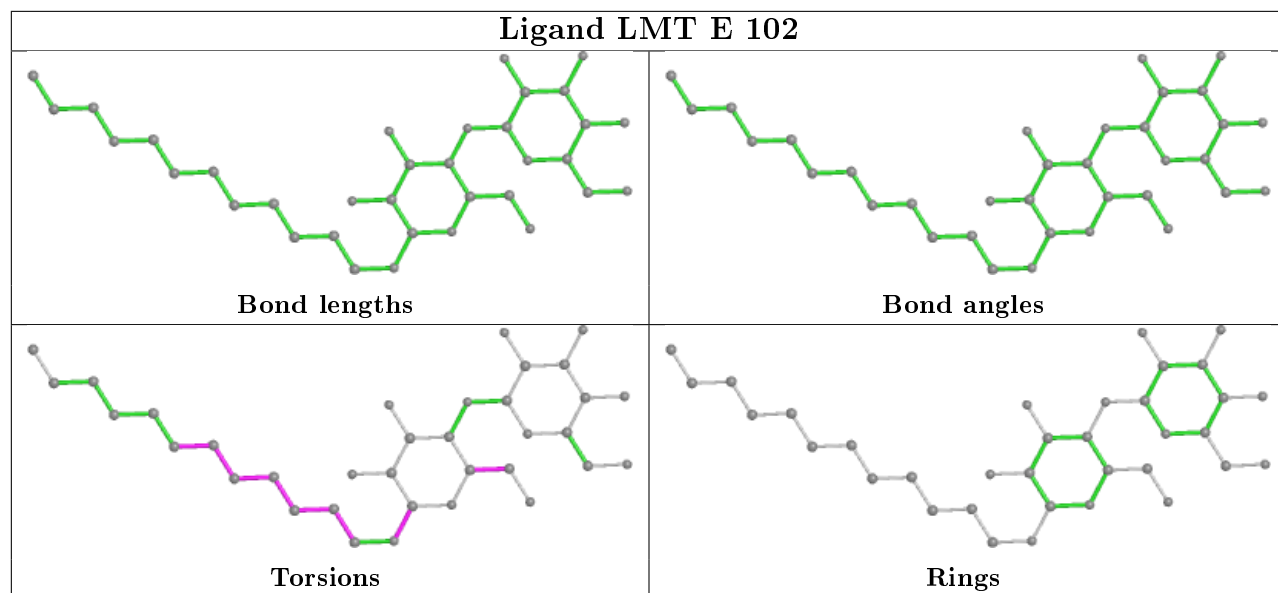
Ligand CLA c 507

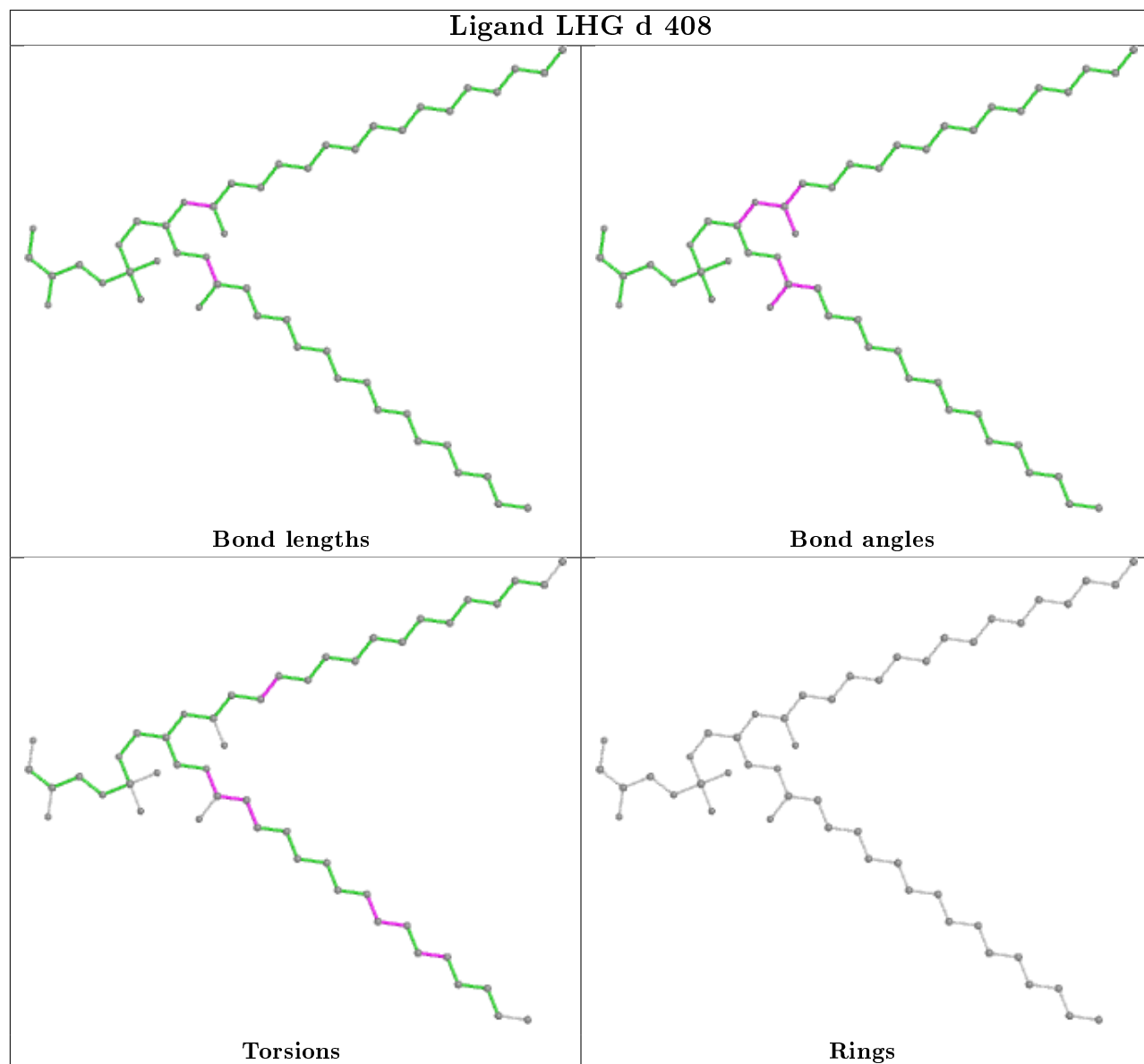
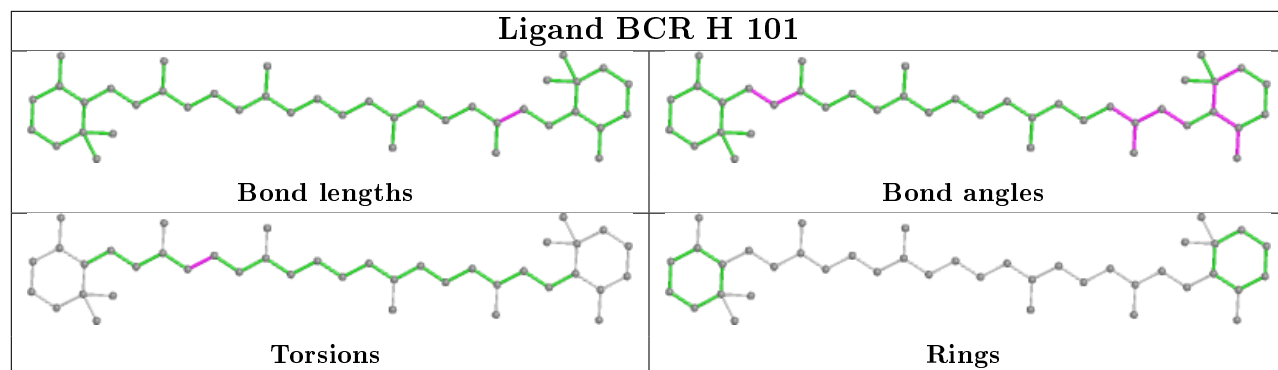


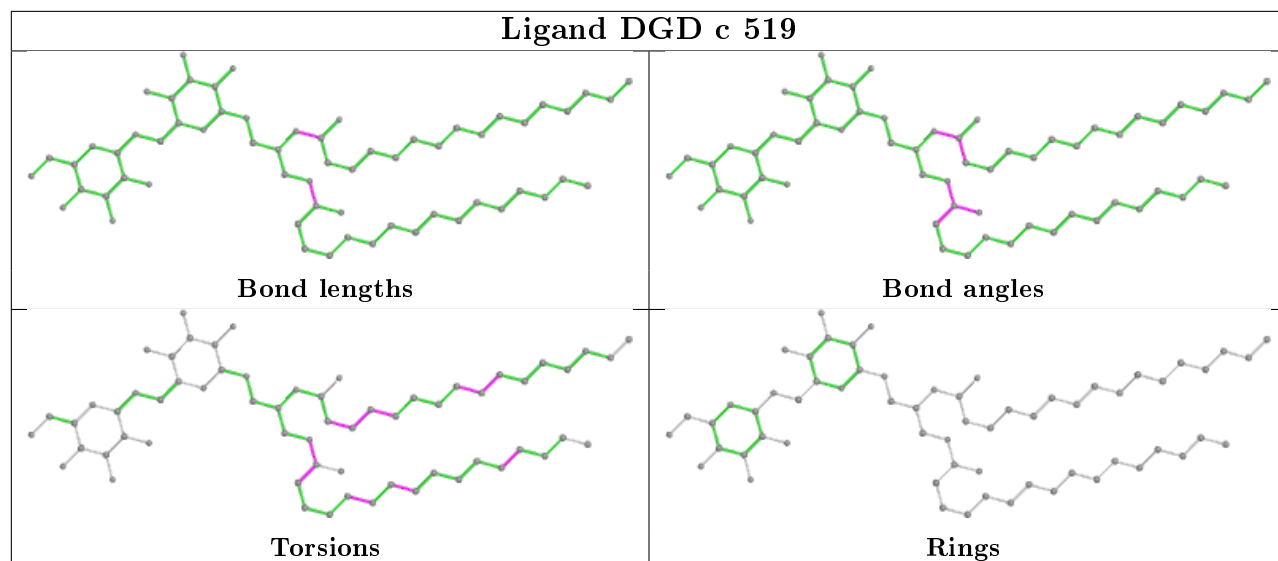
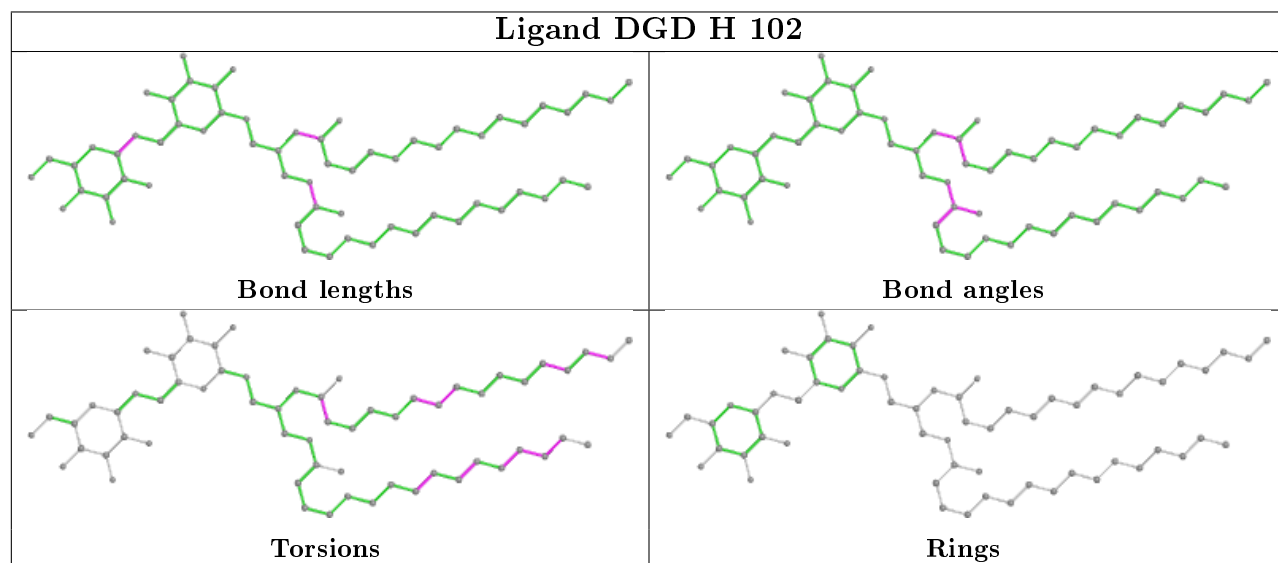
Ligand LHG D 409



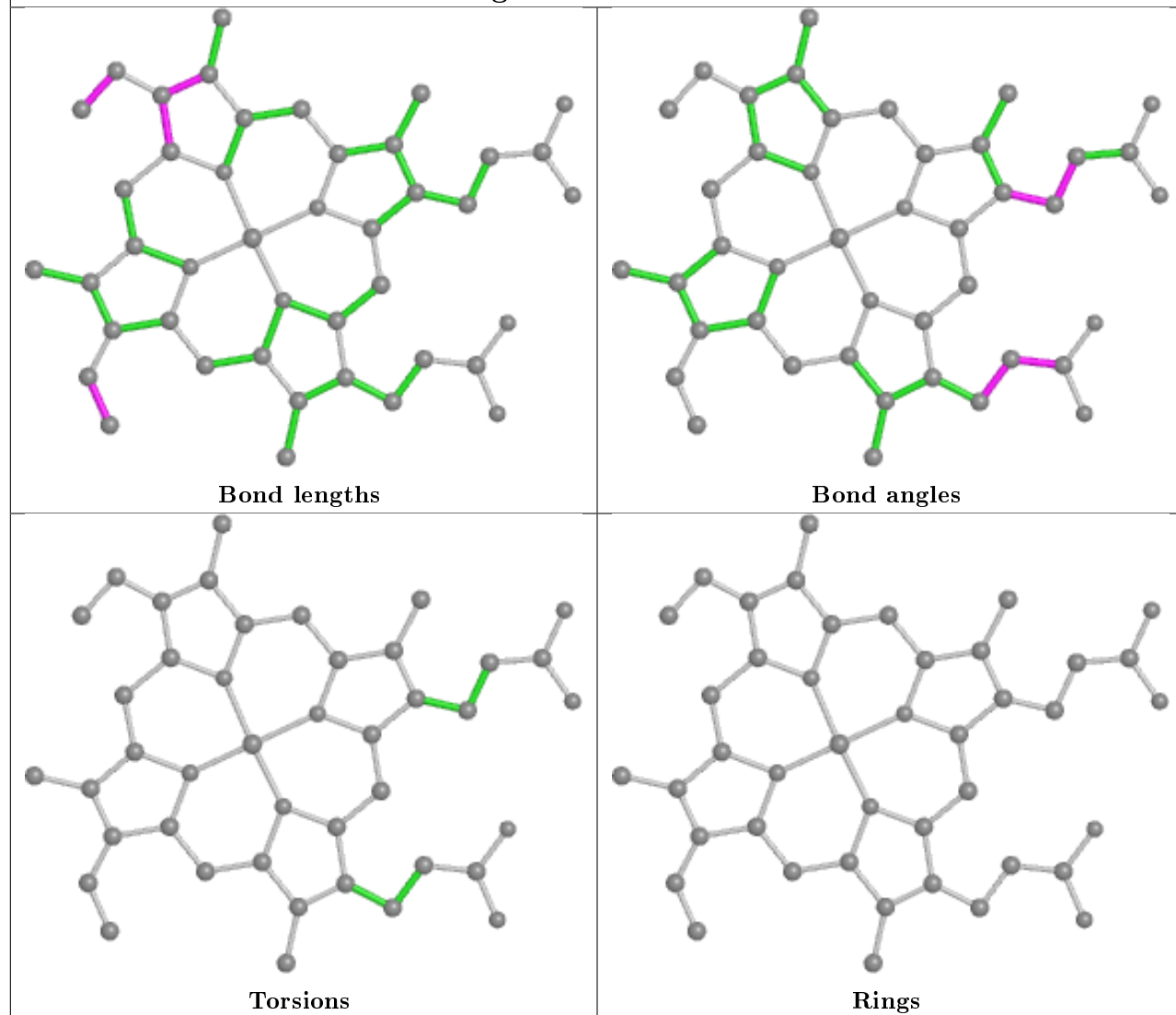




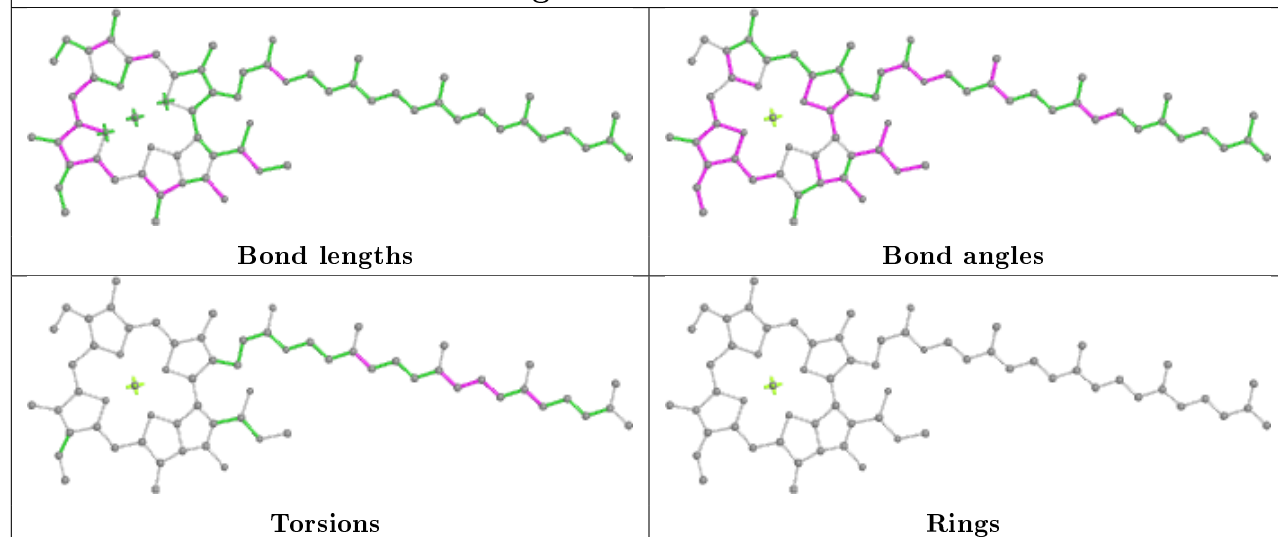


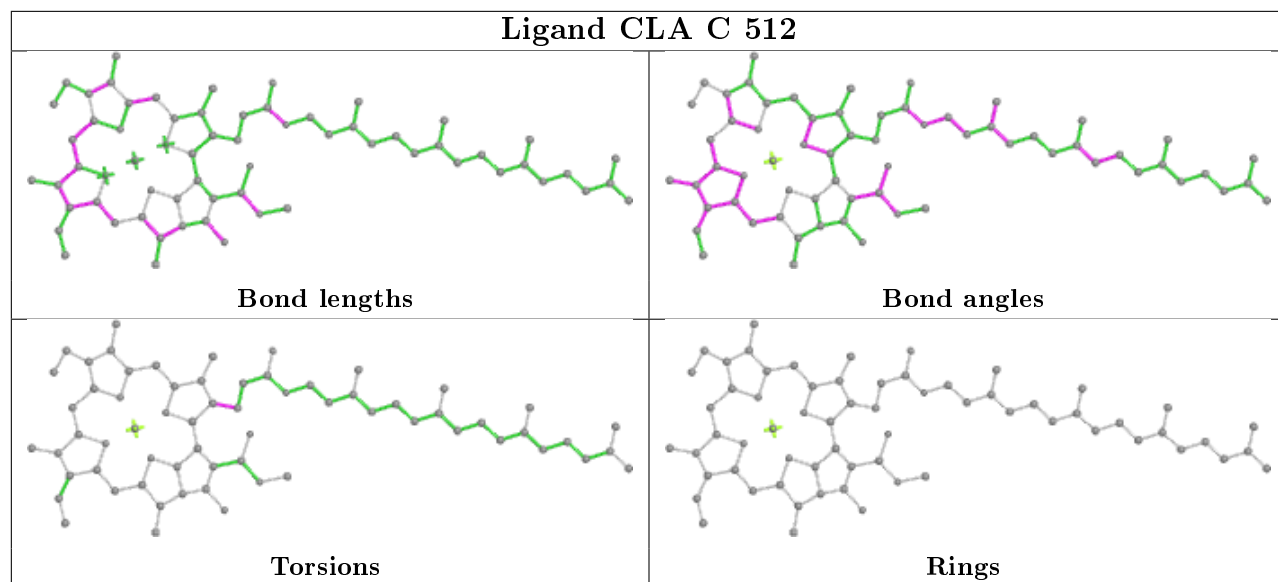
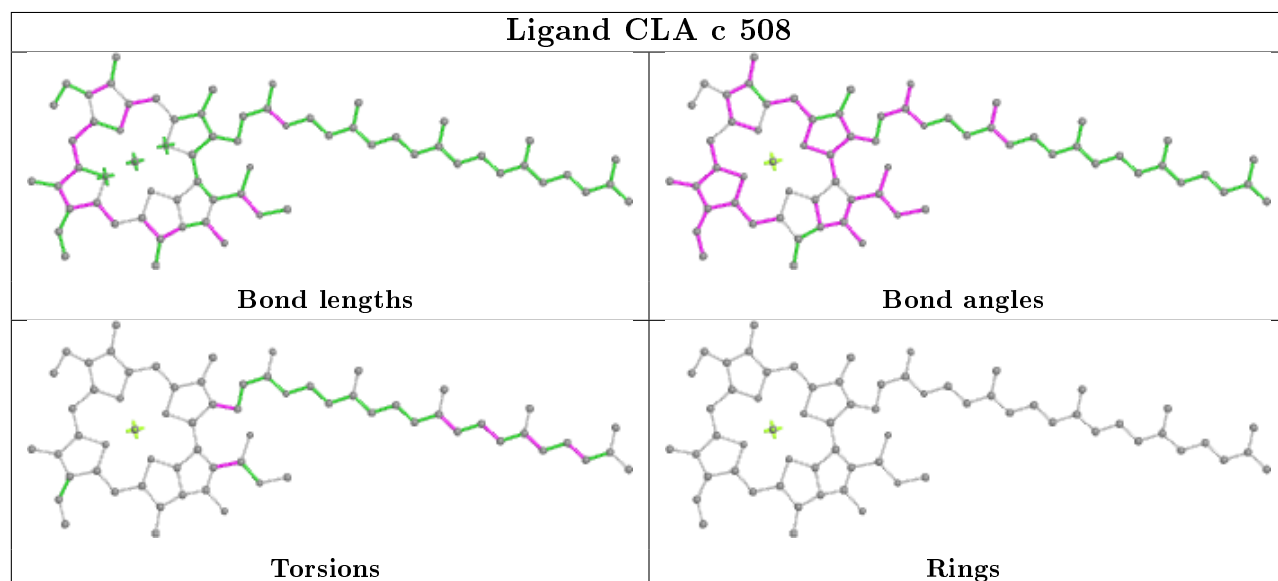
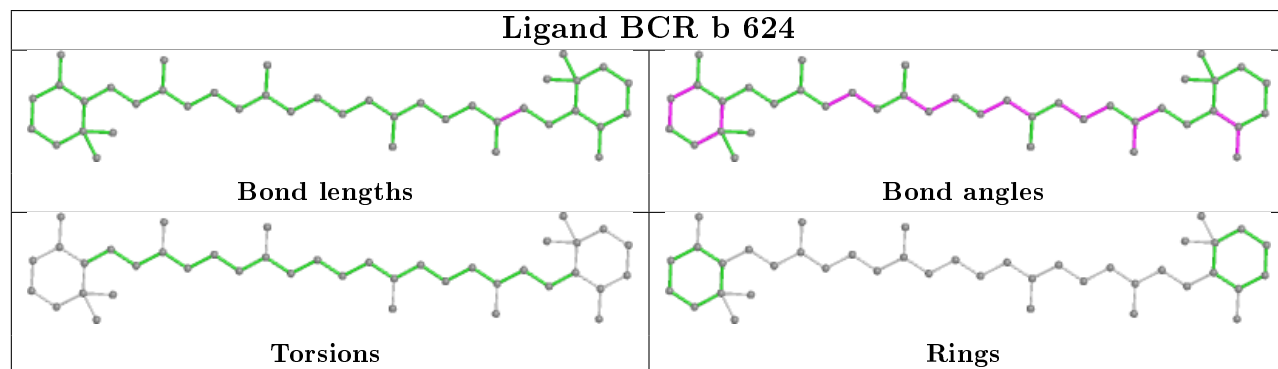
Ligand DGD c 519**Ligand DGD H 102**

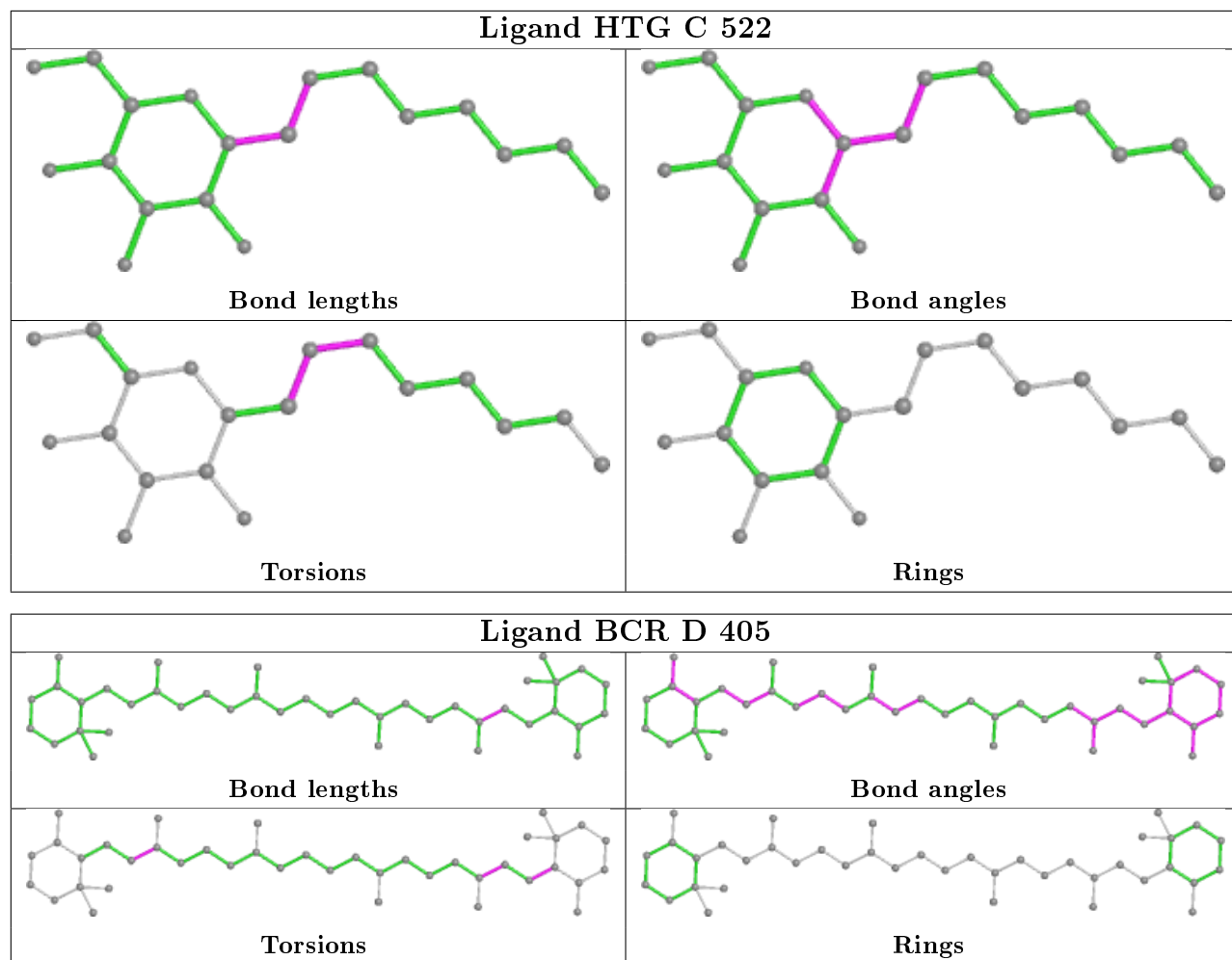
Ligand HEC v 202

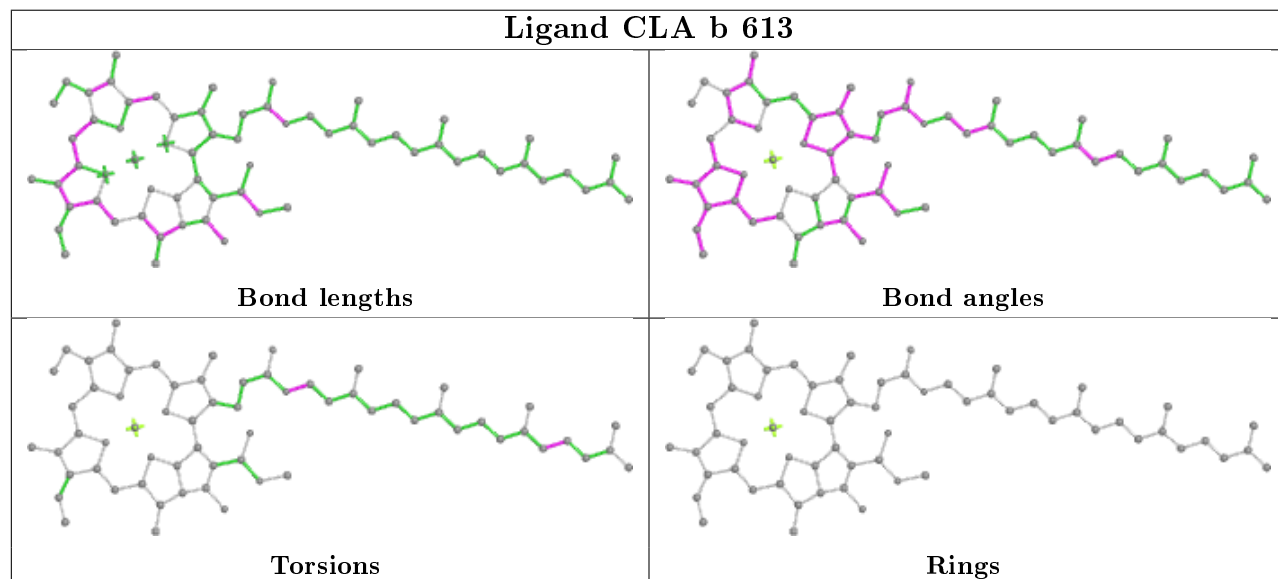
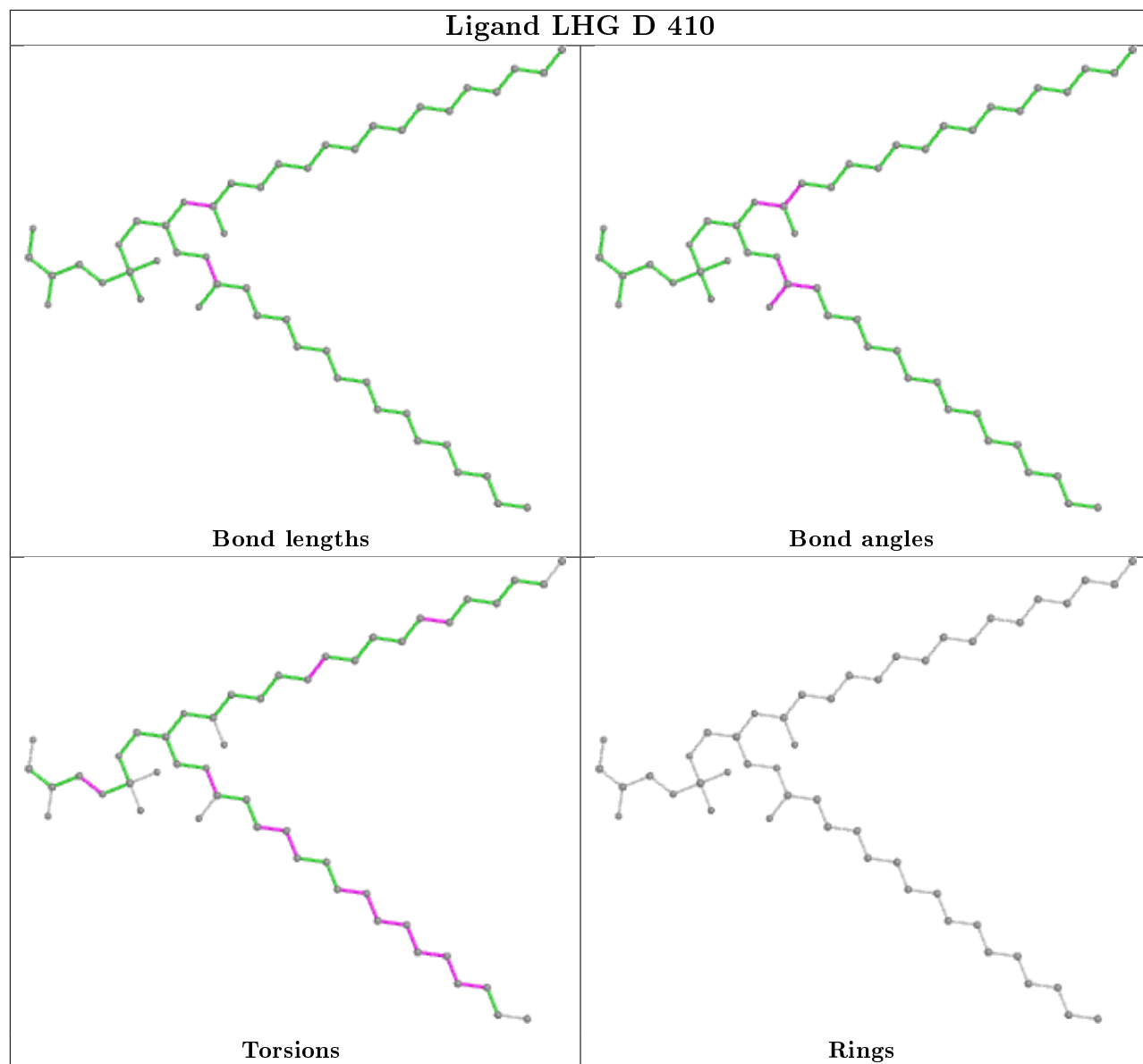


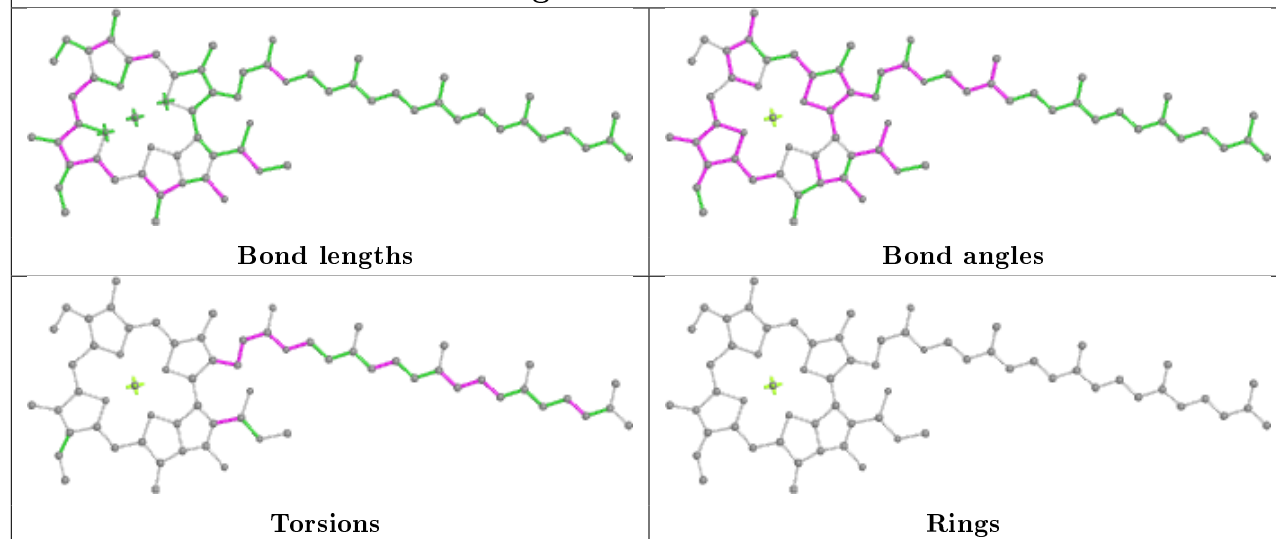
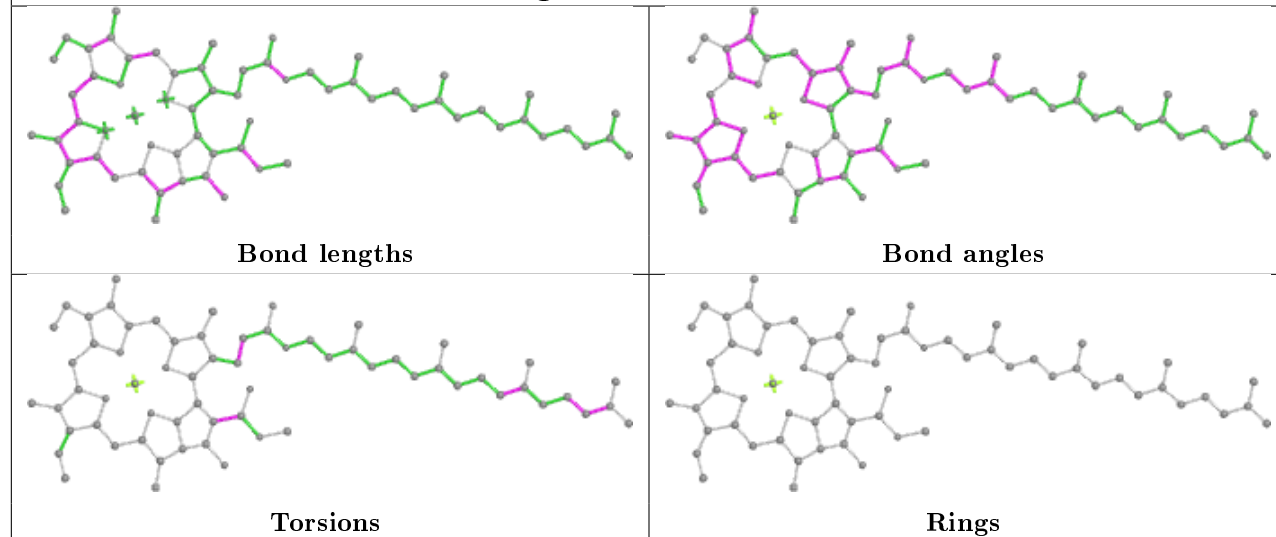
Ligand CLA B 616

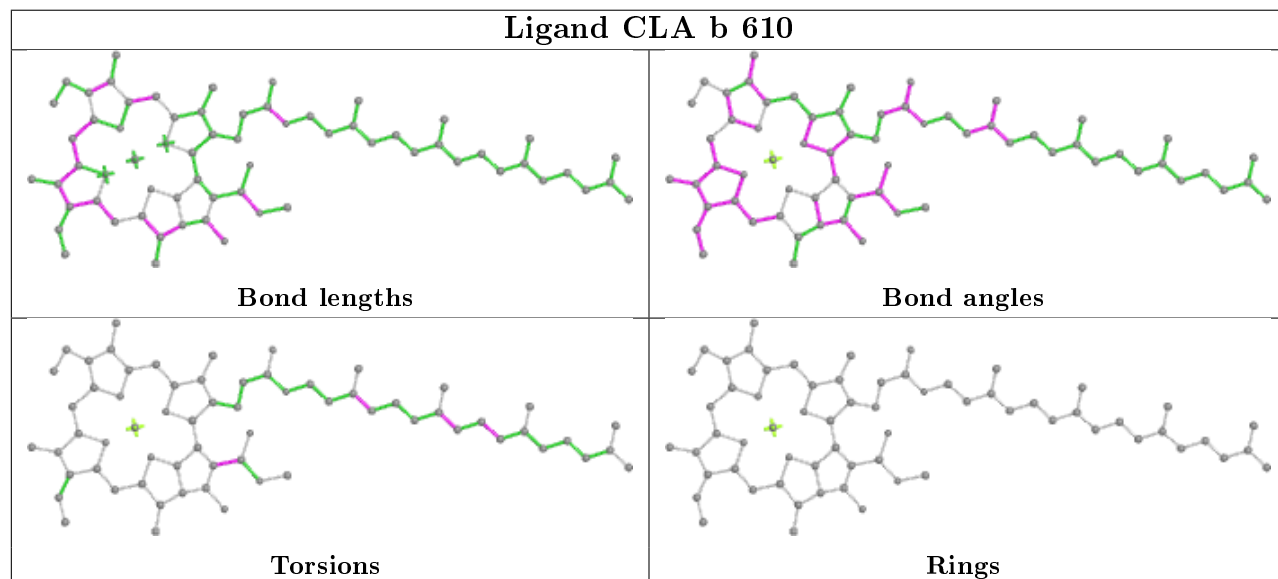
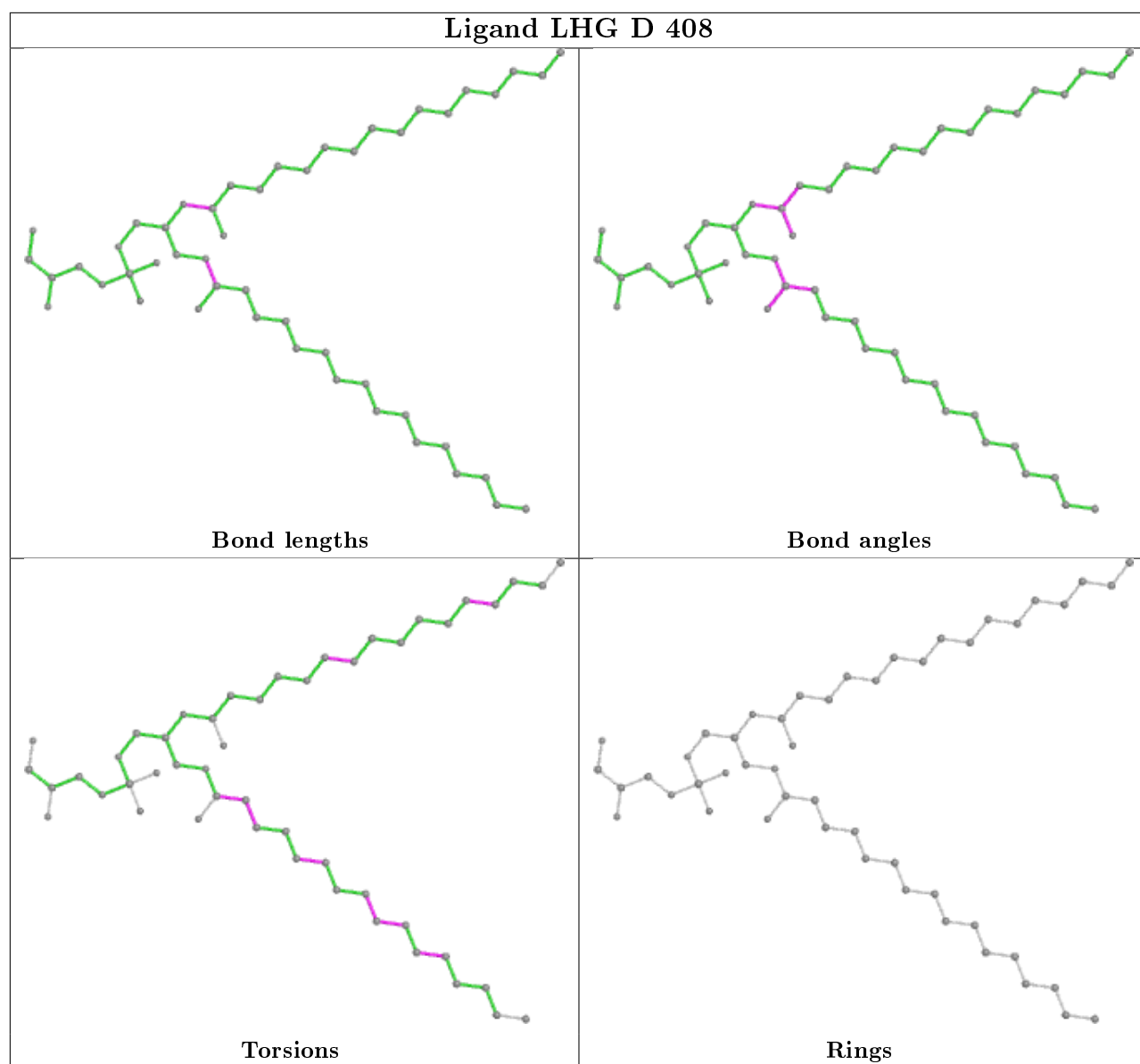


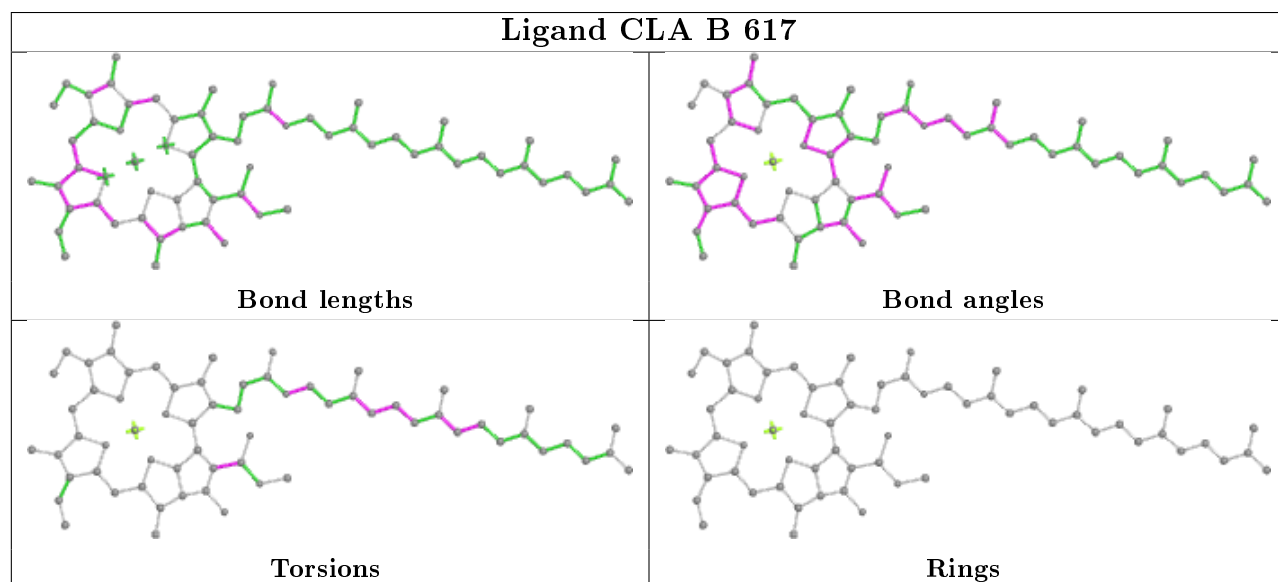
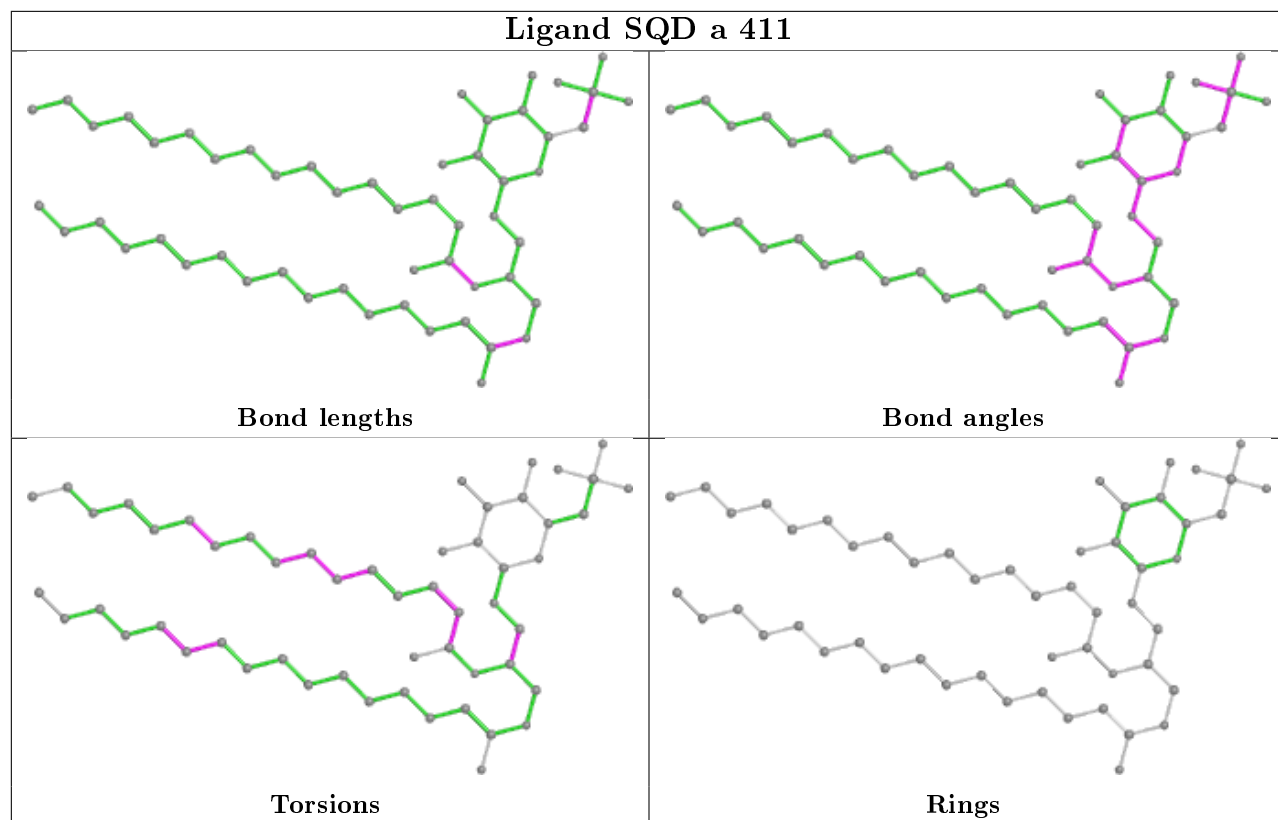
Ligand CLA C 512**Ligand CLA c 508****Ligand BCR b 624**

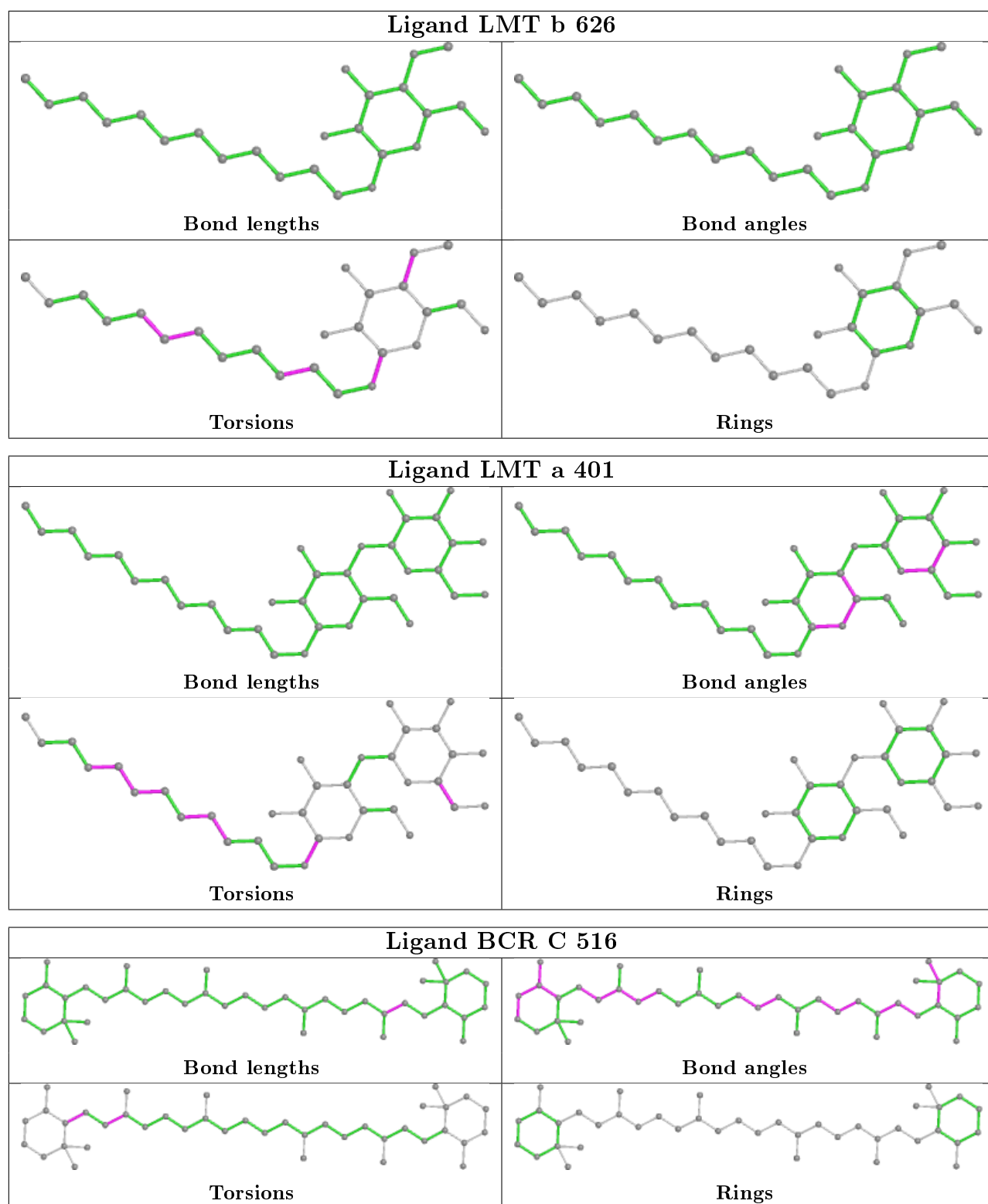


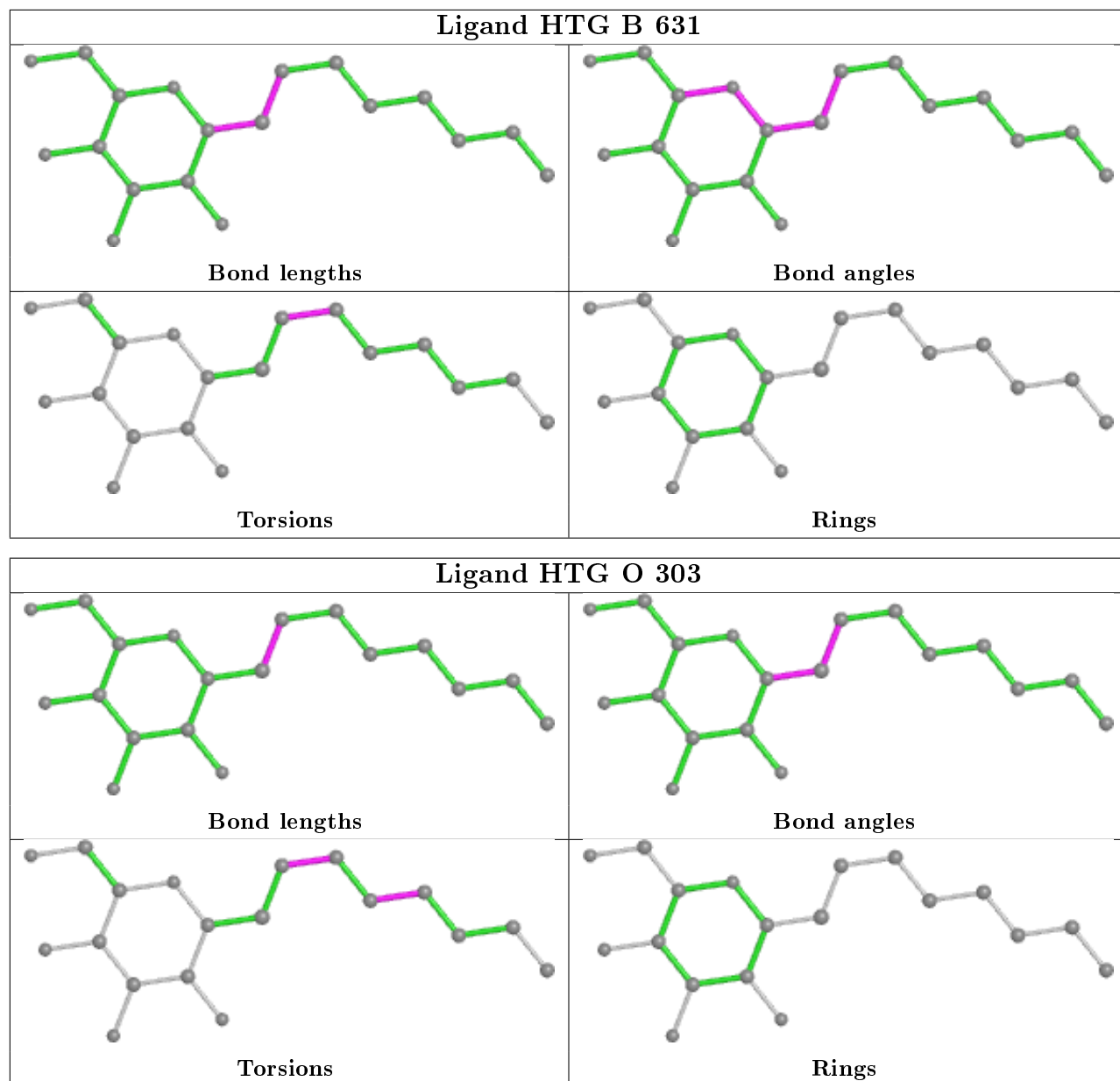


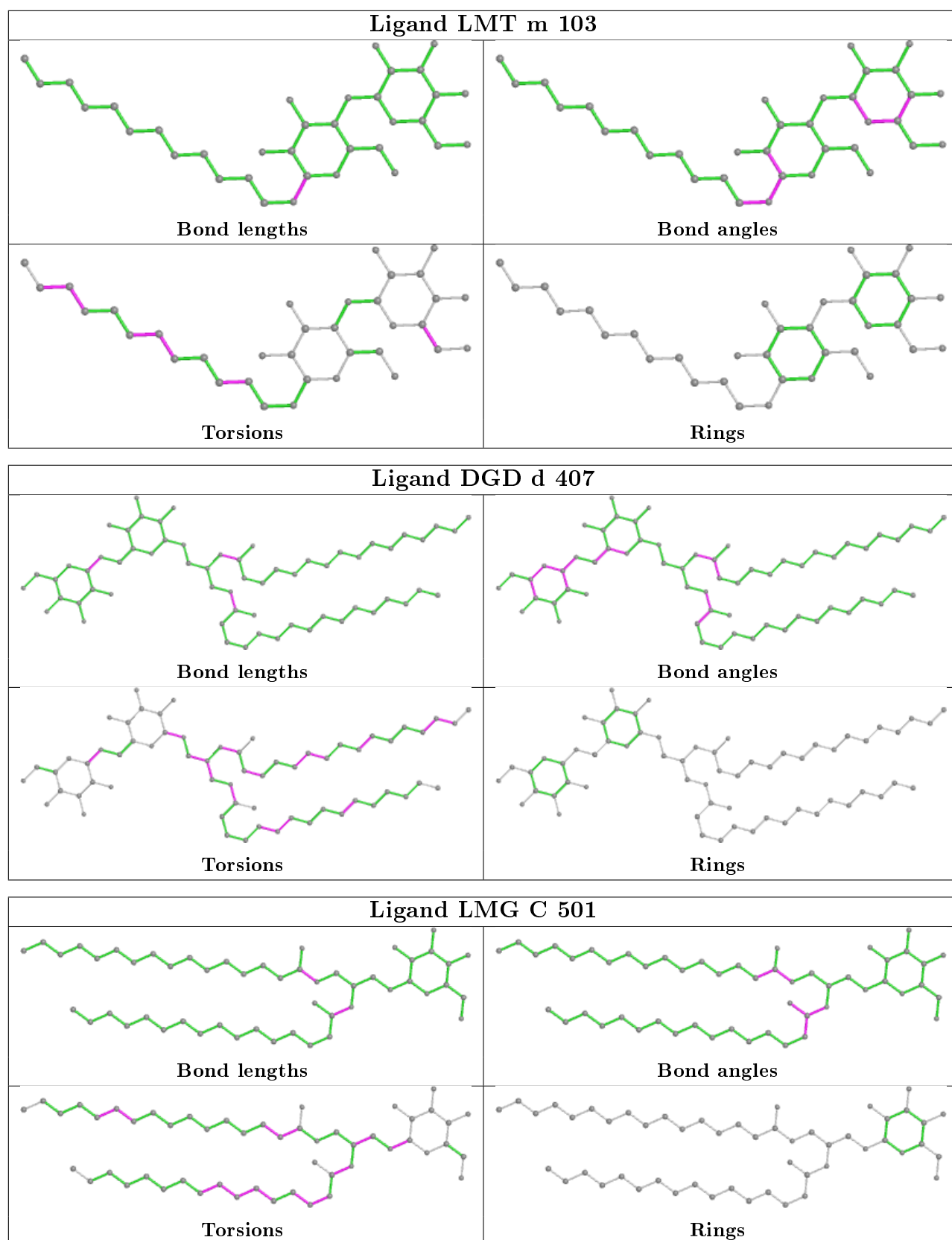
Ligand CLA B 602**Ligand CLA b 615**

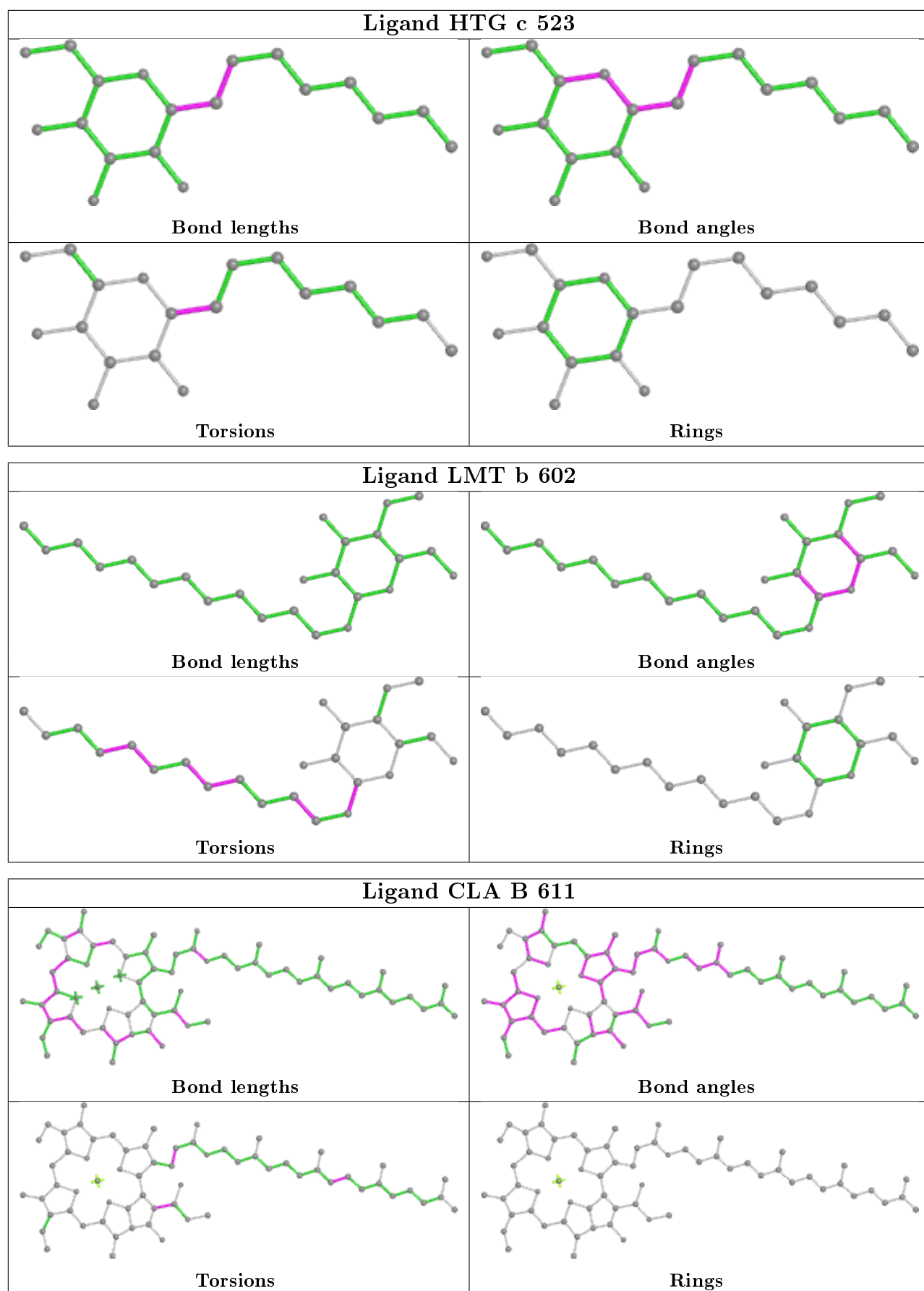




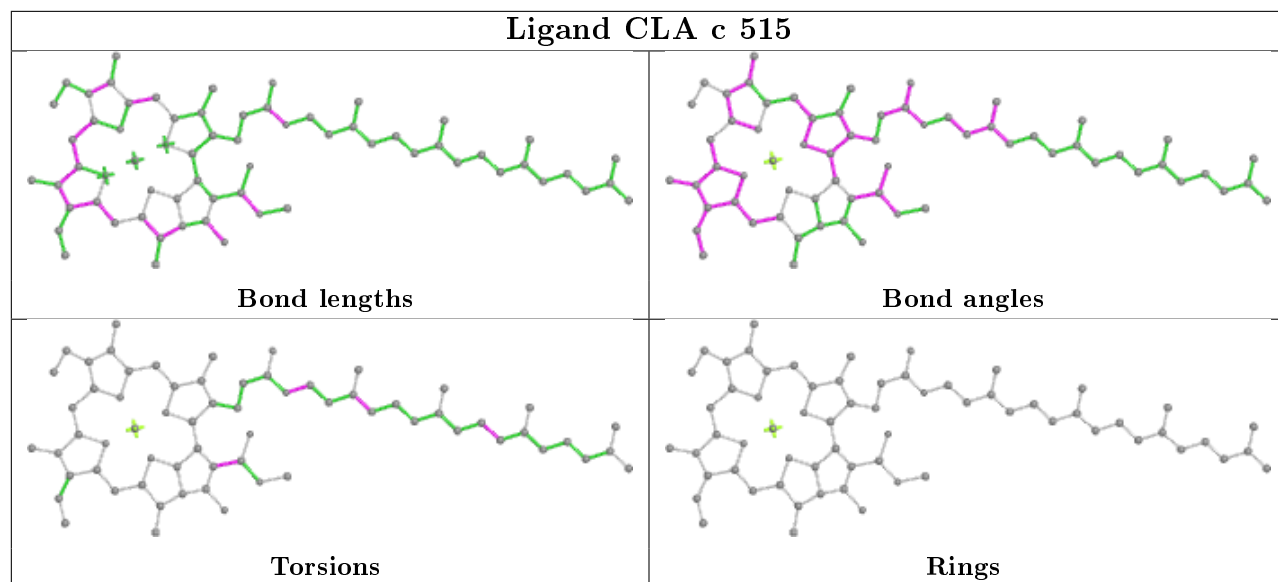




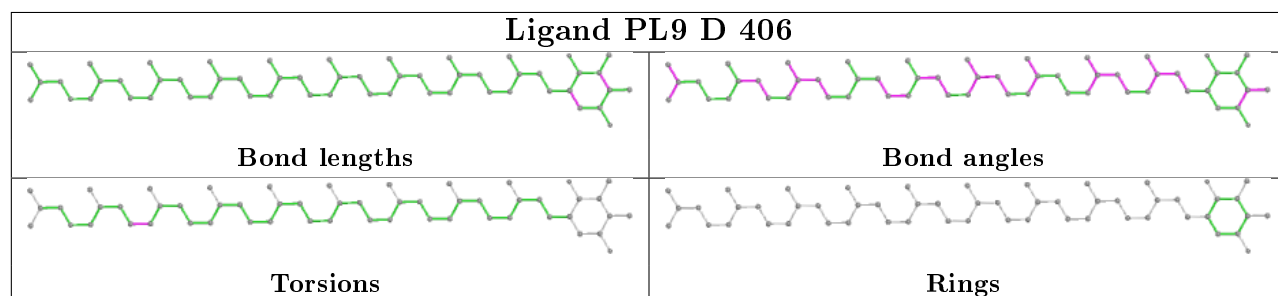




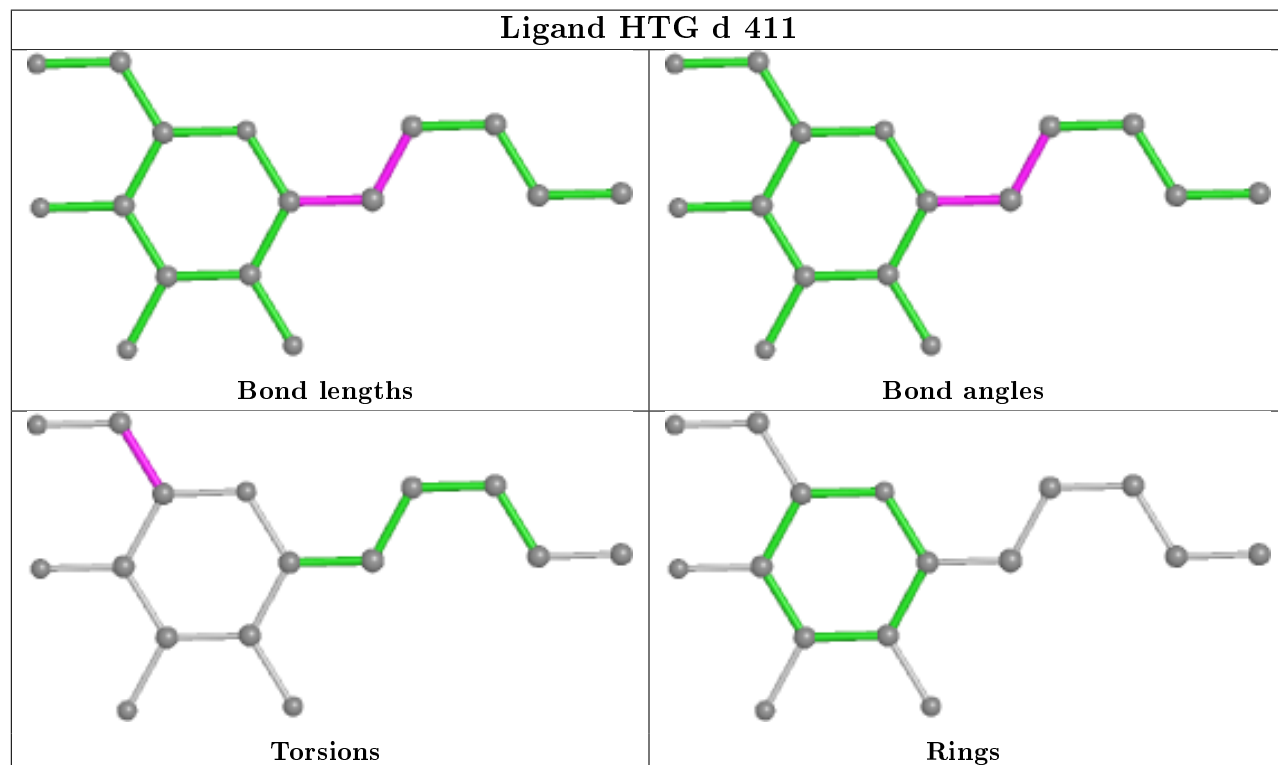
Ligand CLA c 515



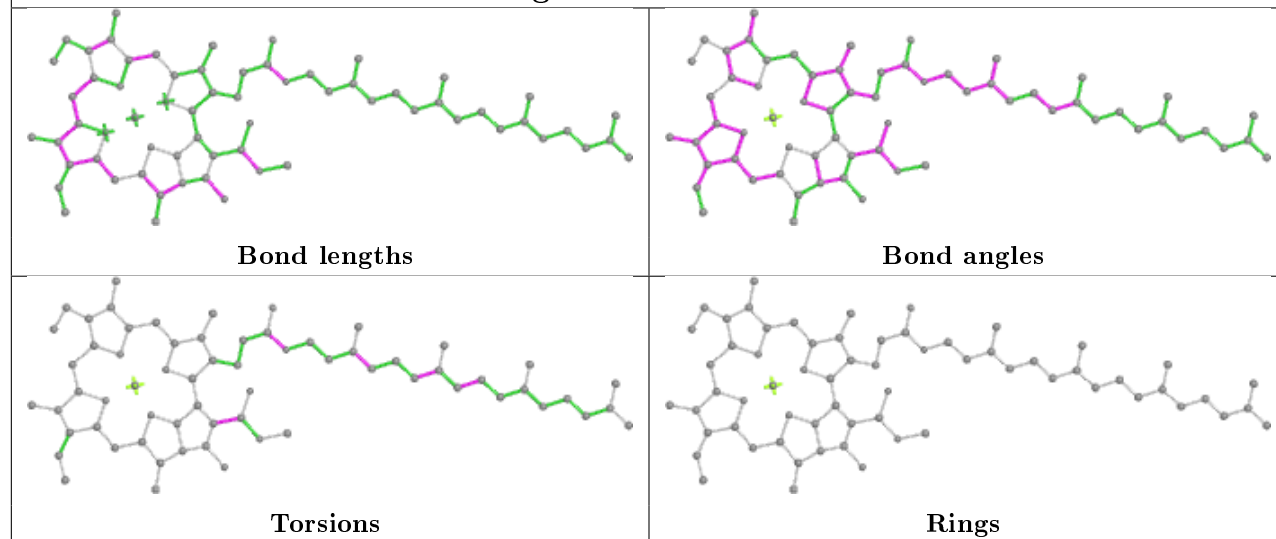
Ligand PL9 D 406



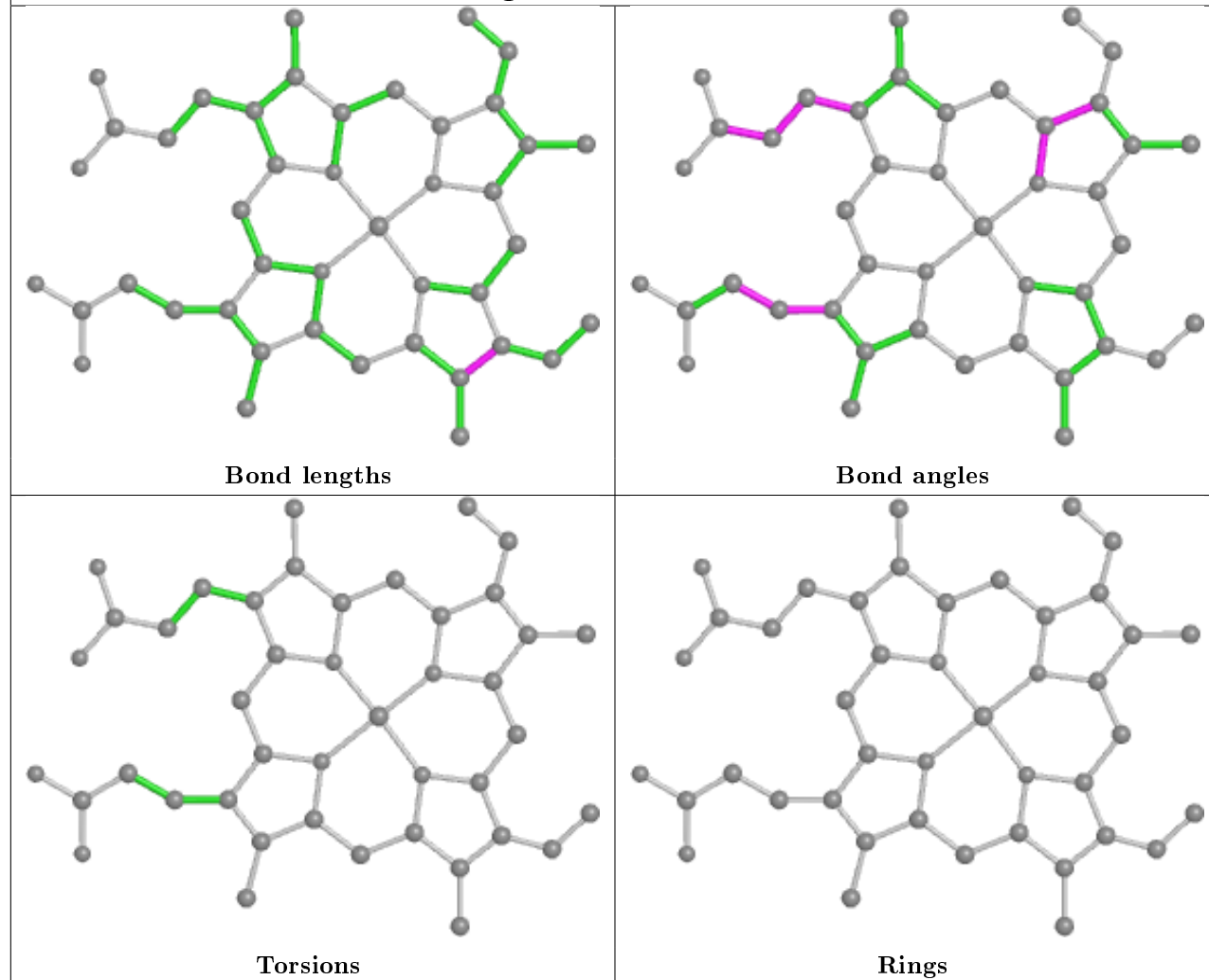
Ligand HTG d 411

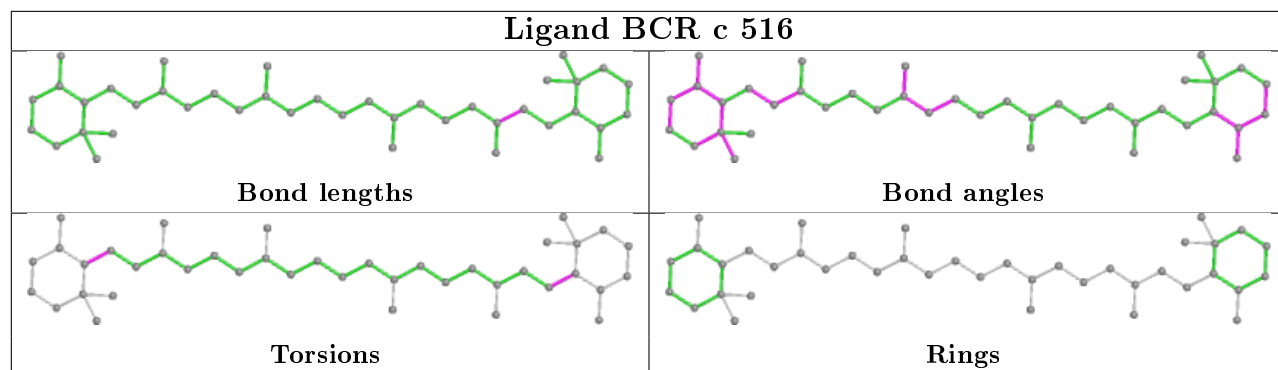
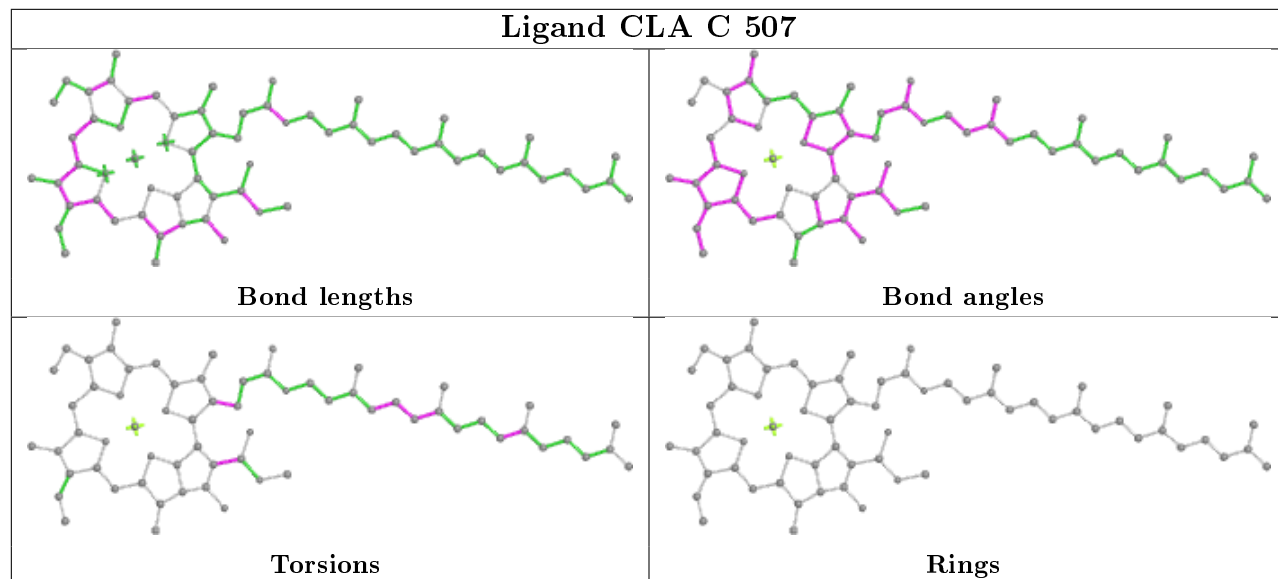
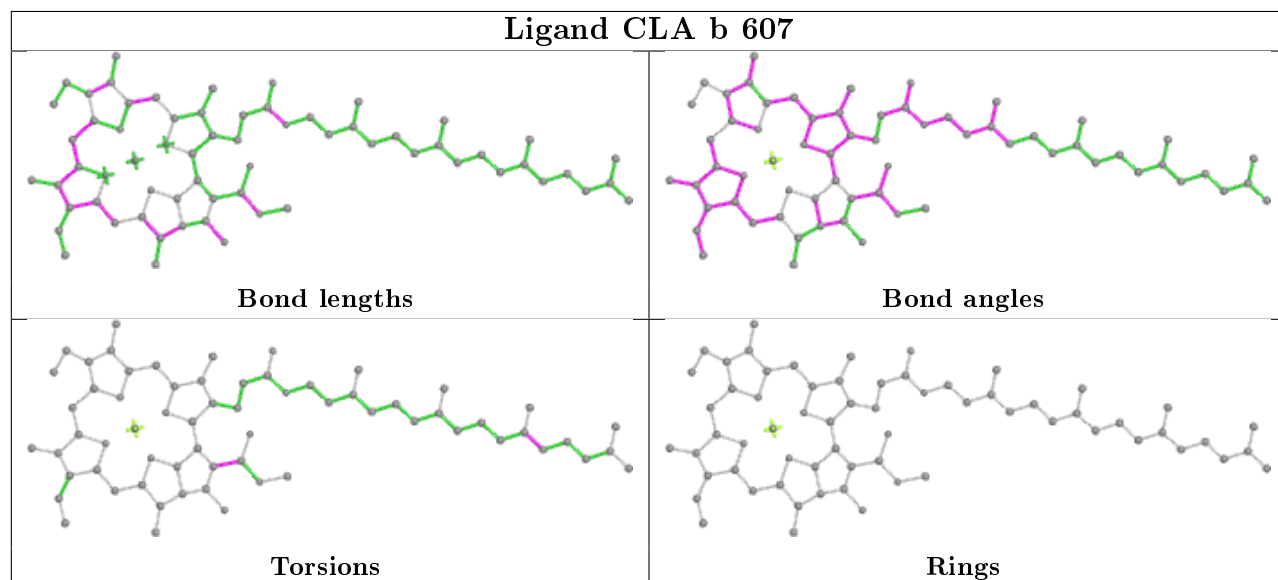


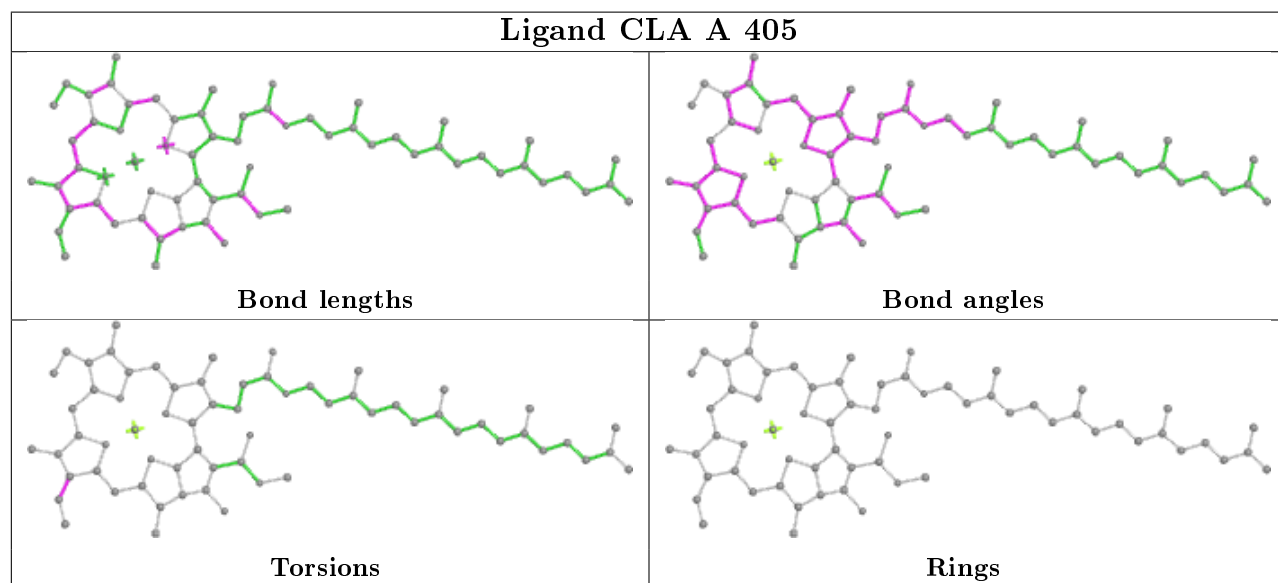
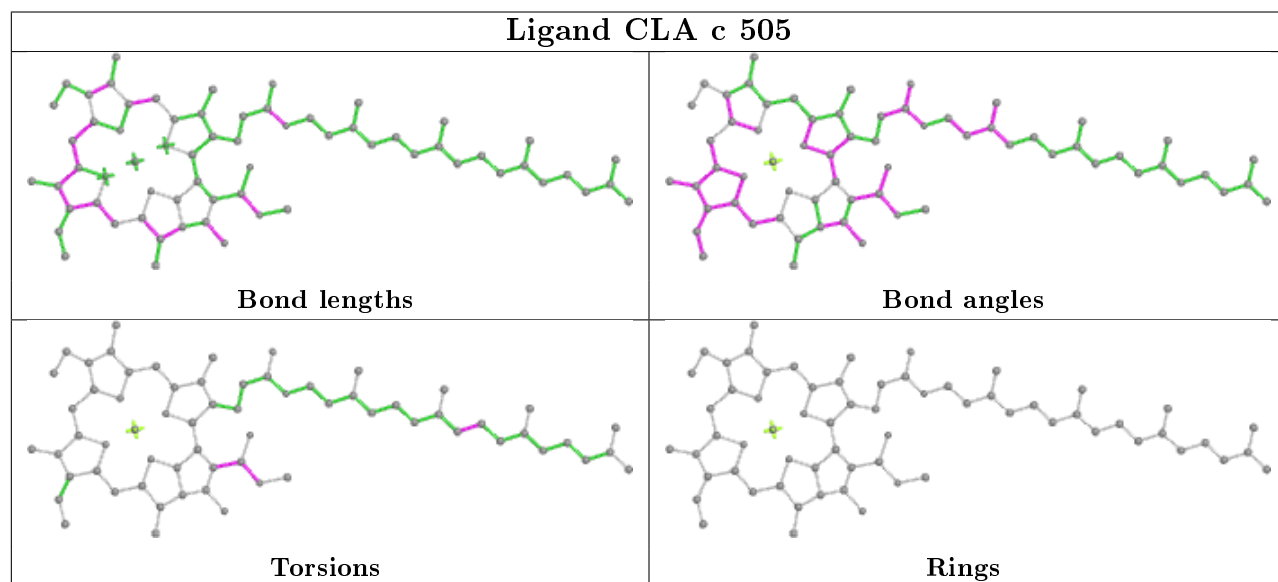
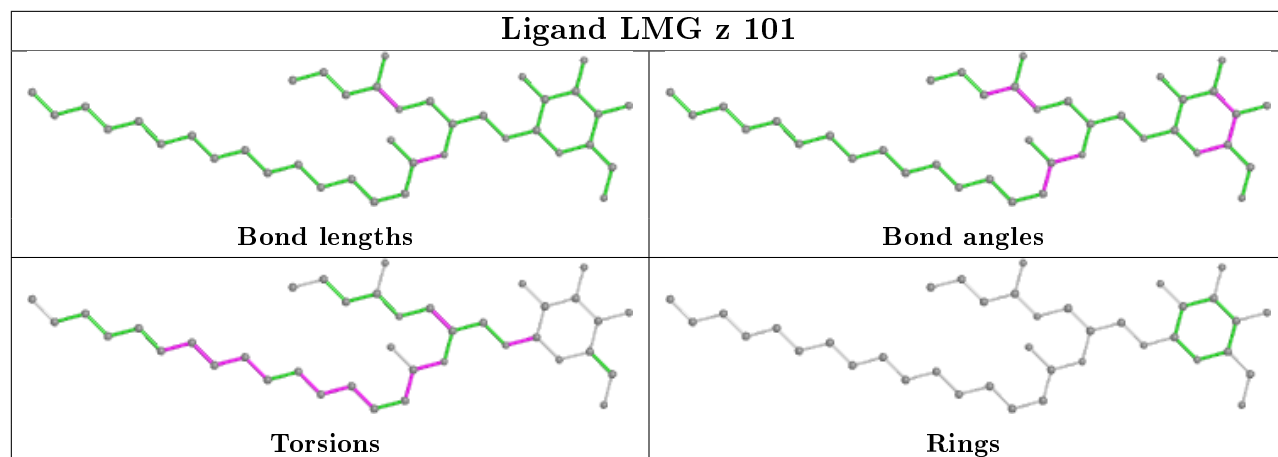
Ligand CLA C 511

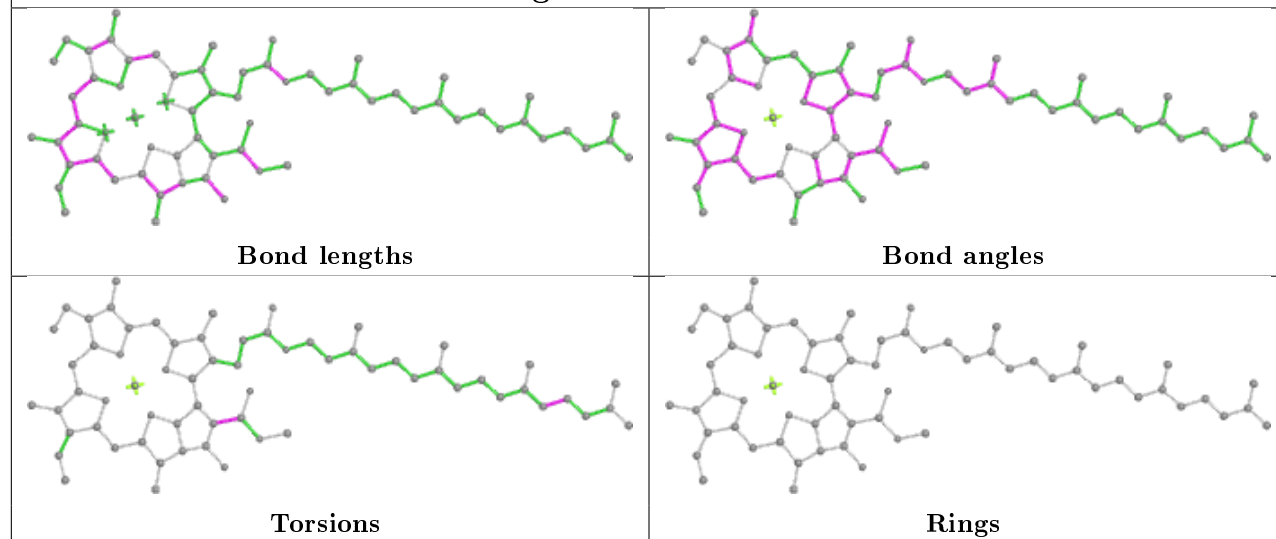
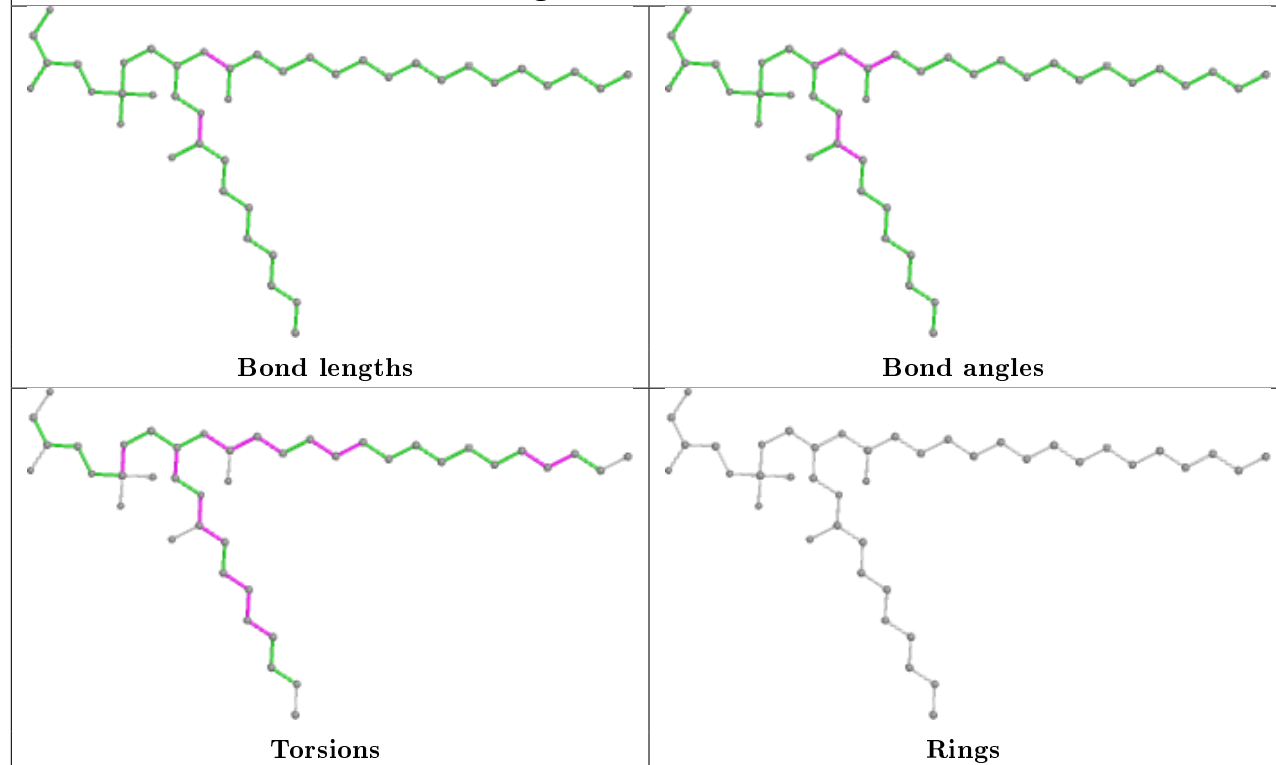


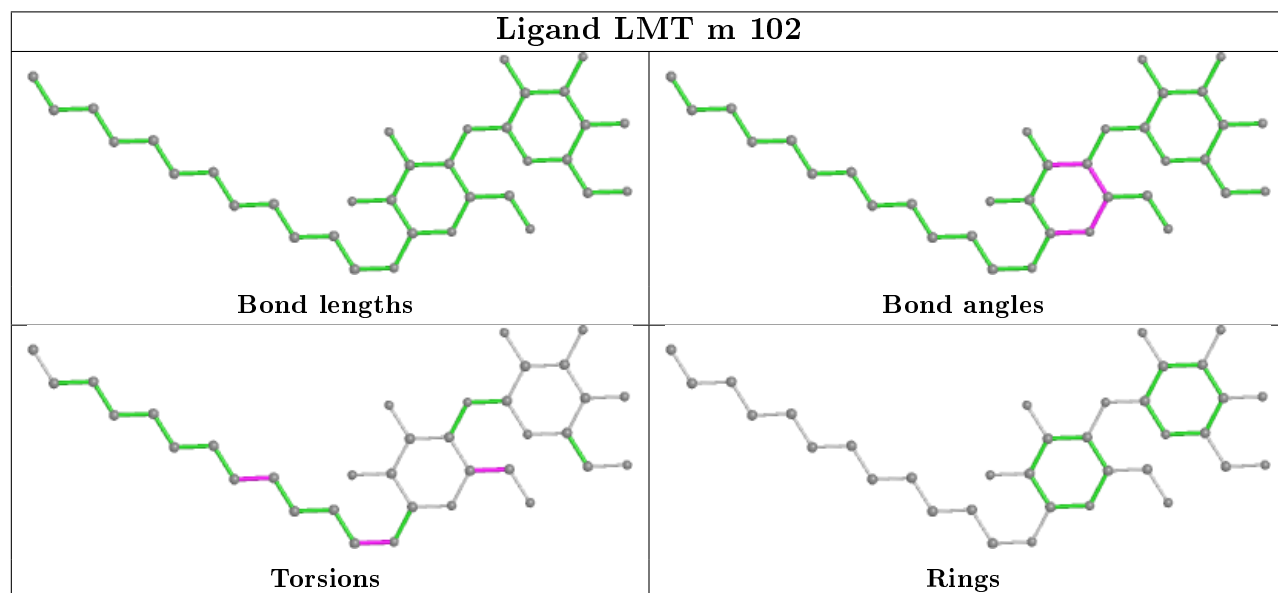
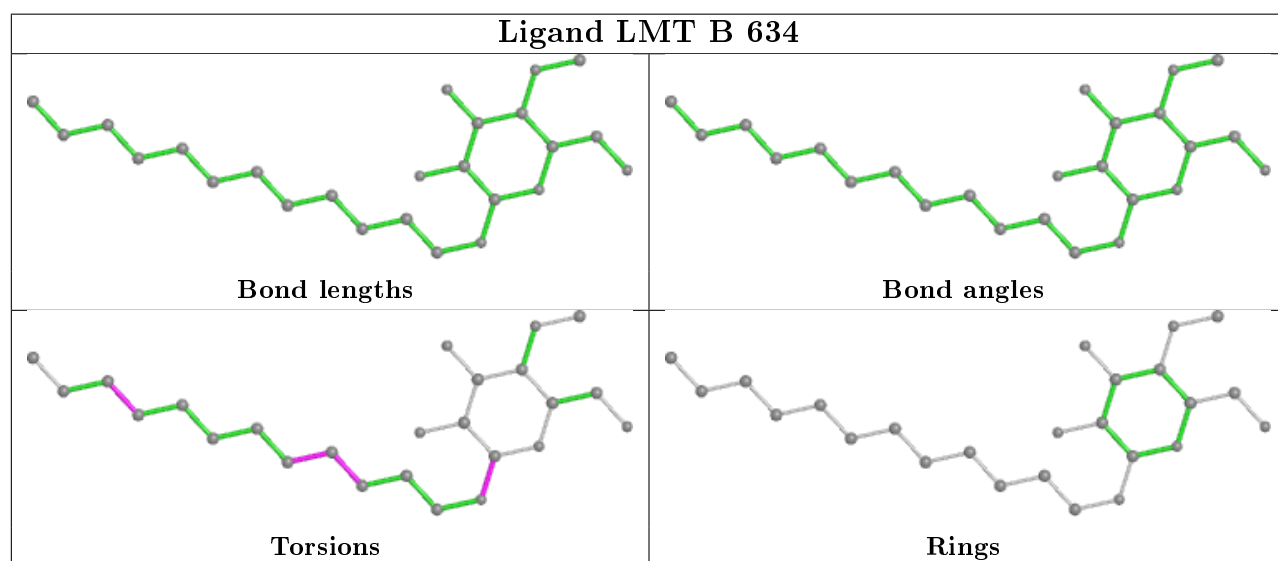
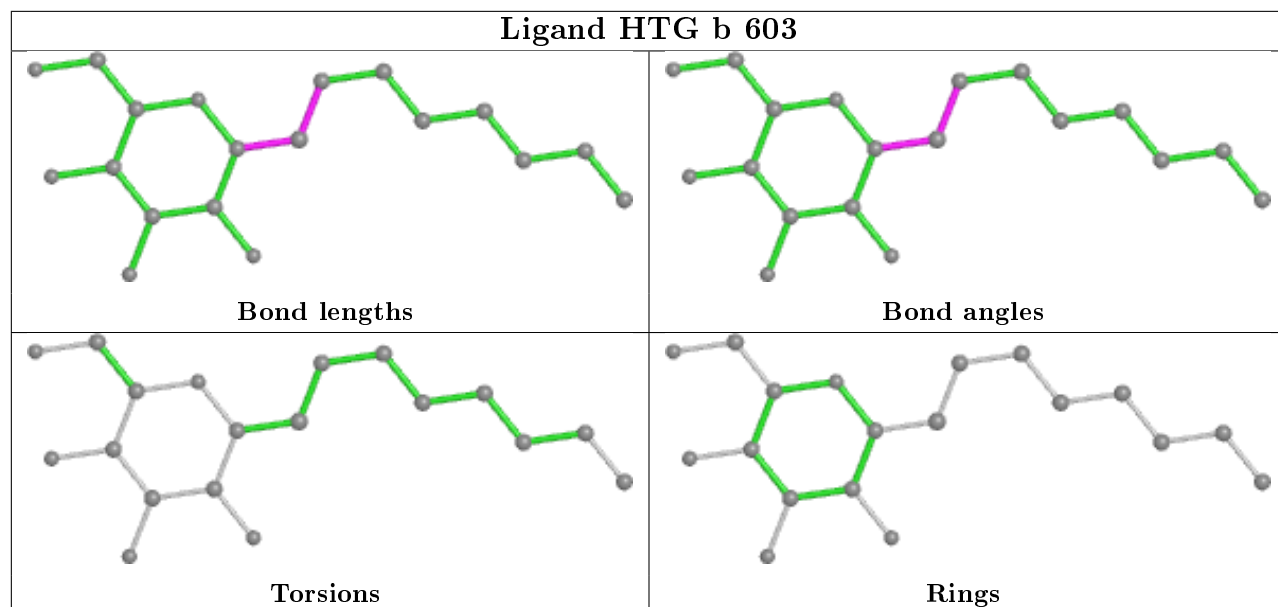
Ligand HEM E 103



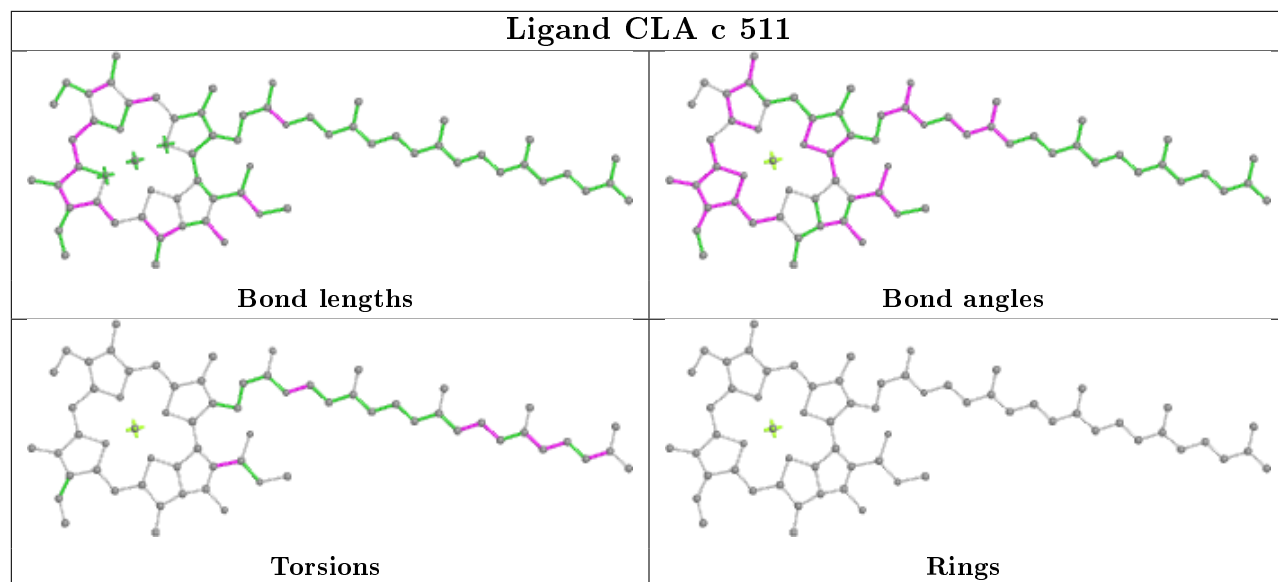
Ligand BCR c 516**Ligand CLA C 507****Ligand CLA b 607**



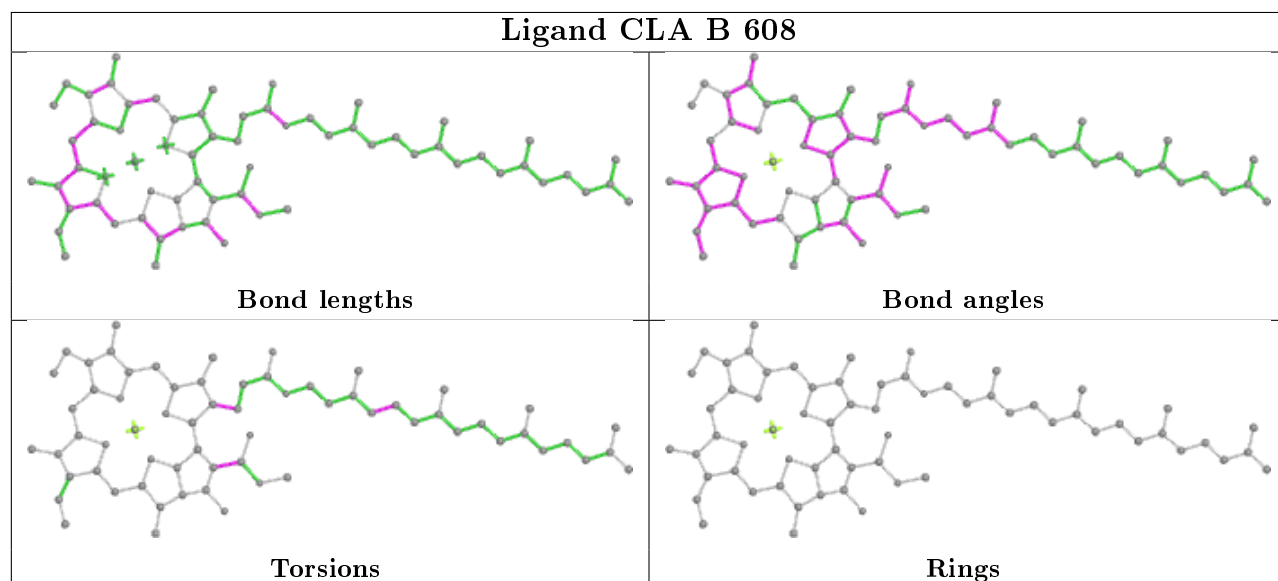
Ligand CLA C 509**Ligand LHG E 101**



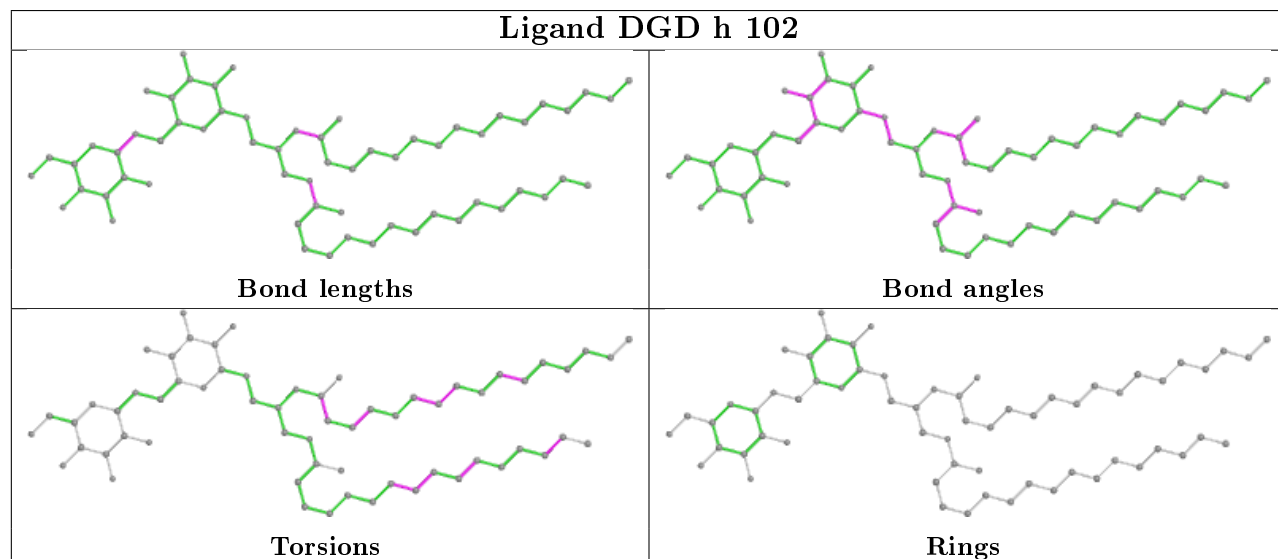
Ligand CLA c 511

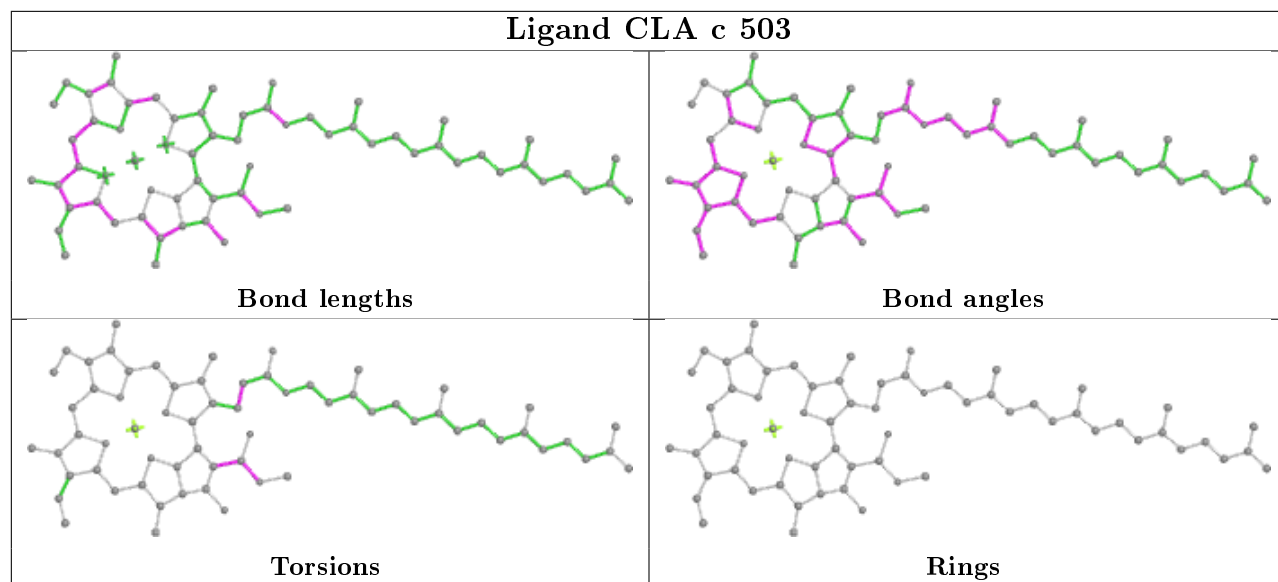
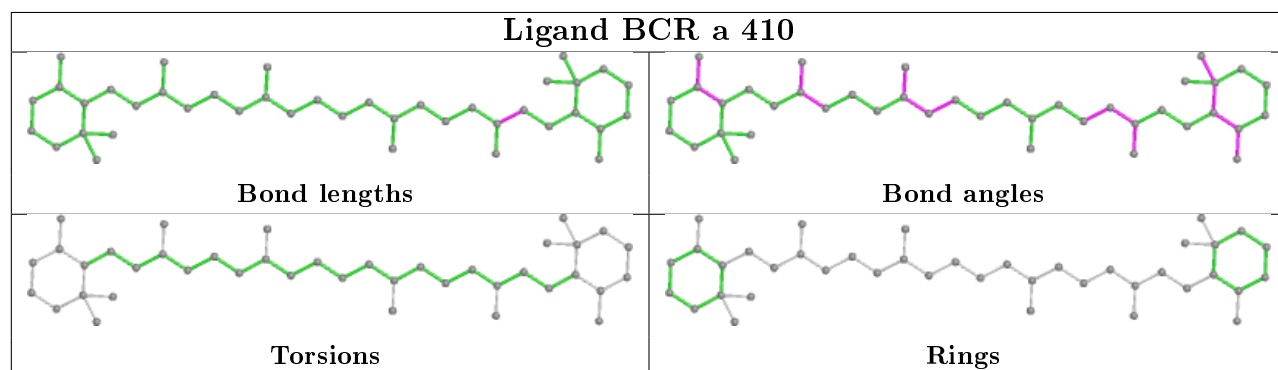
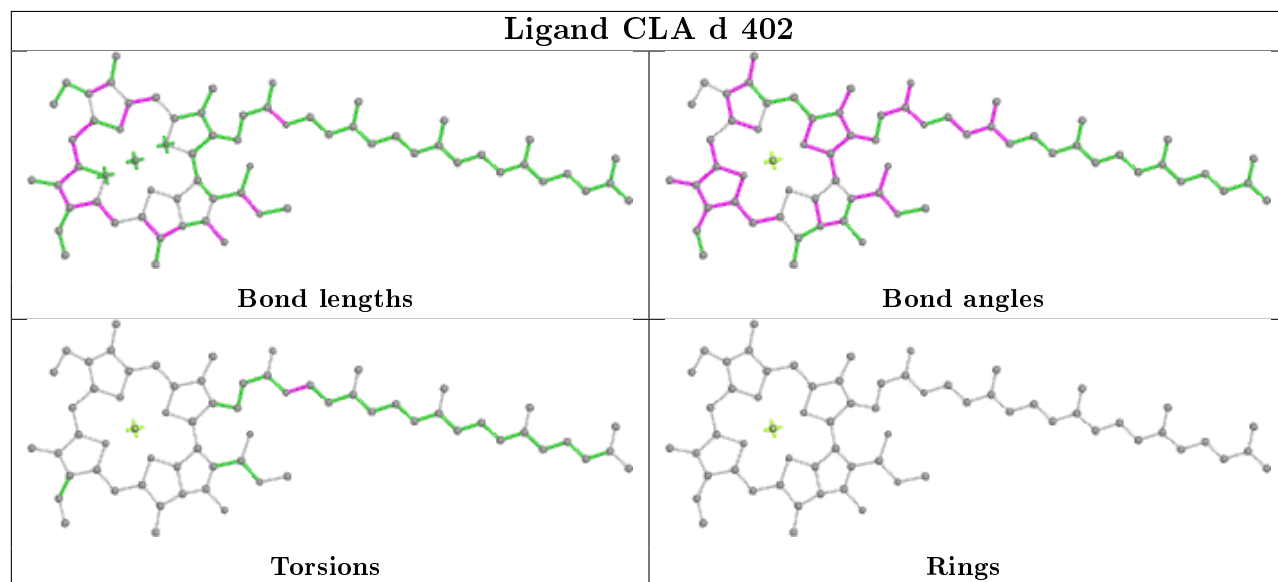


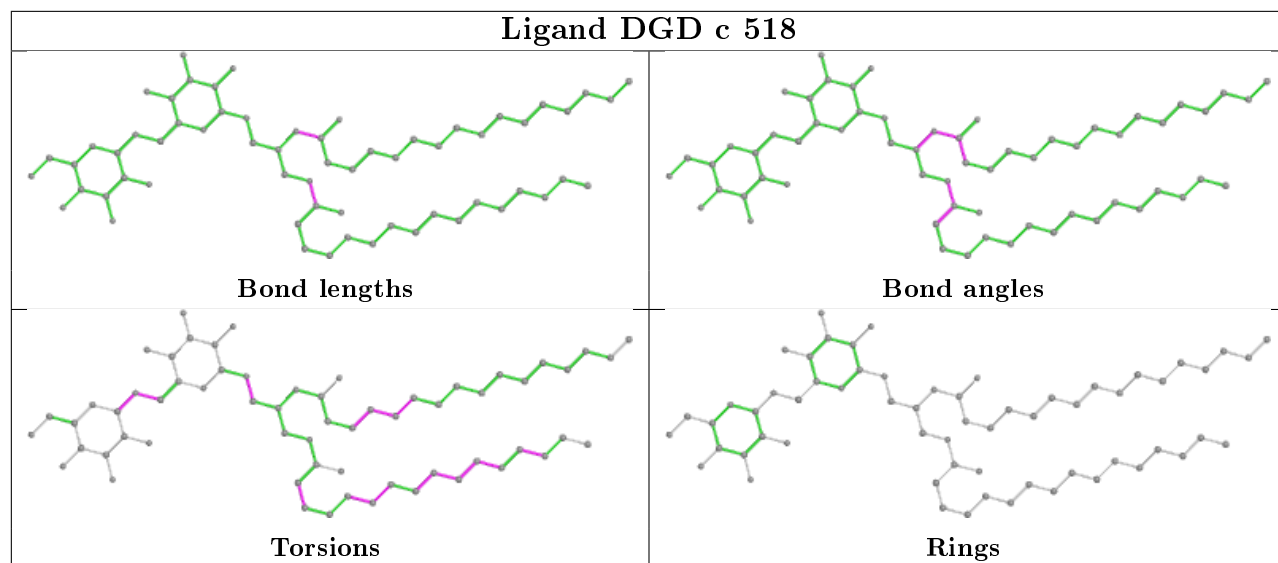
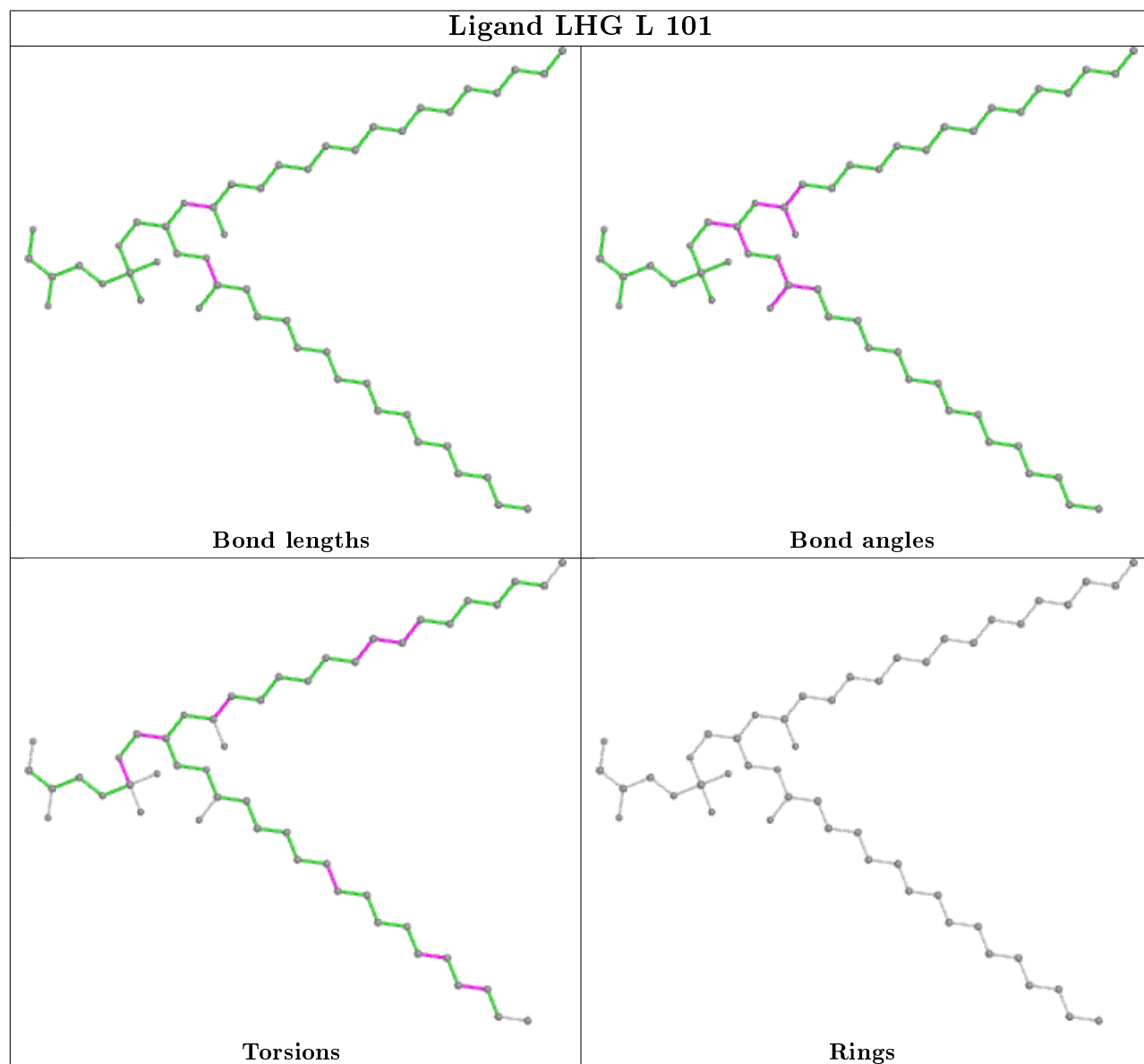
Ligand CLA B 608

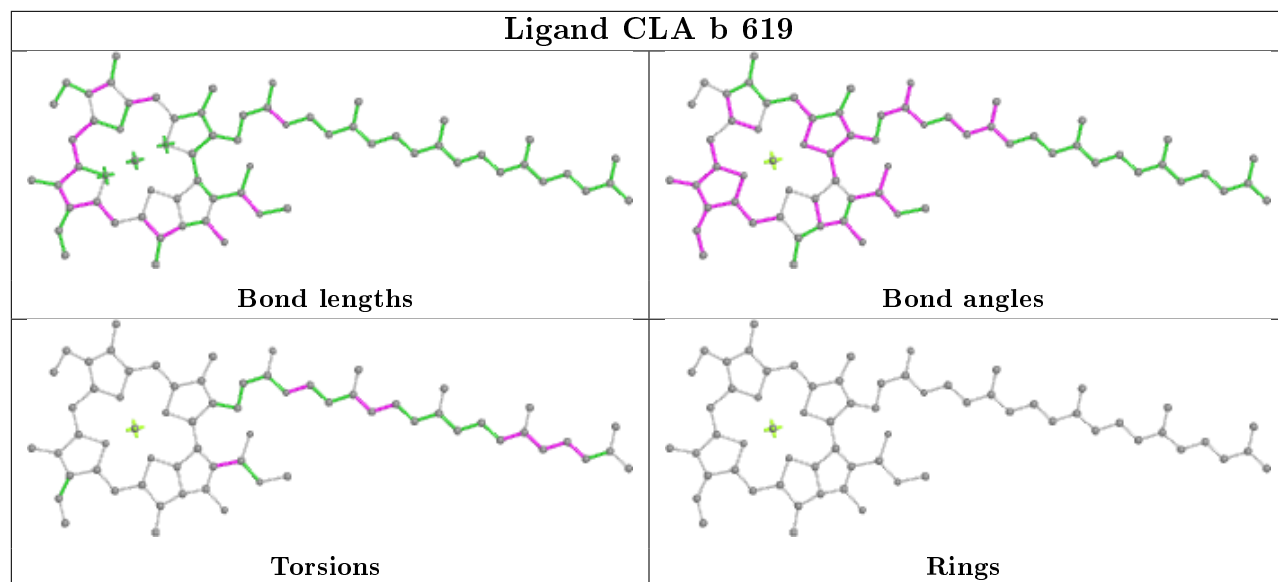
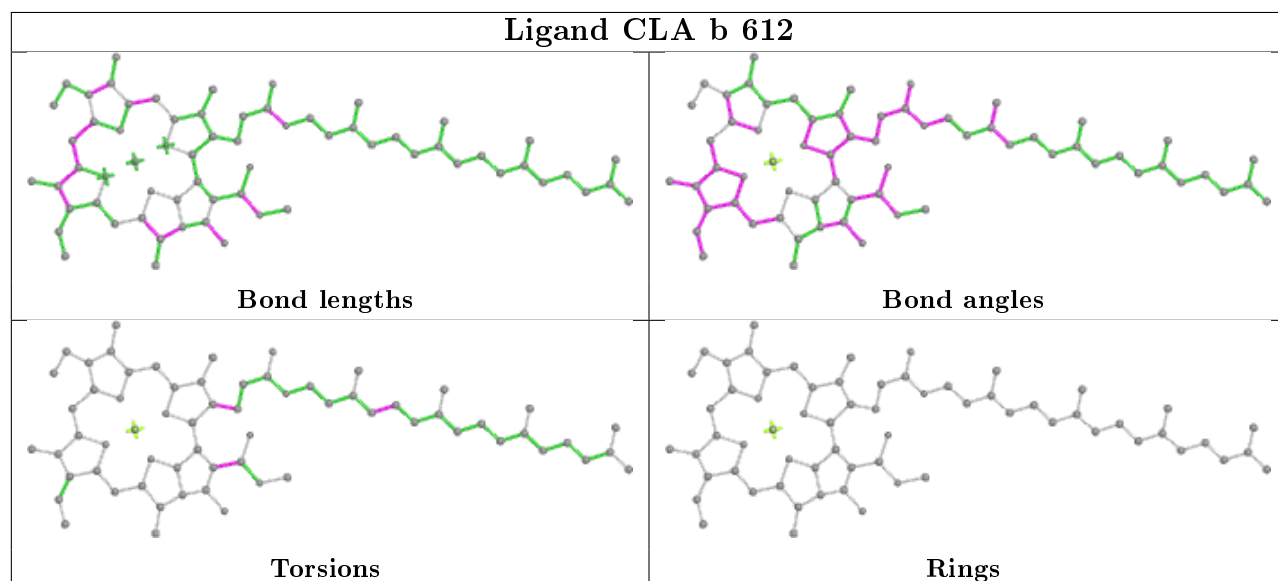
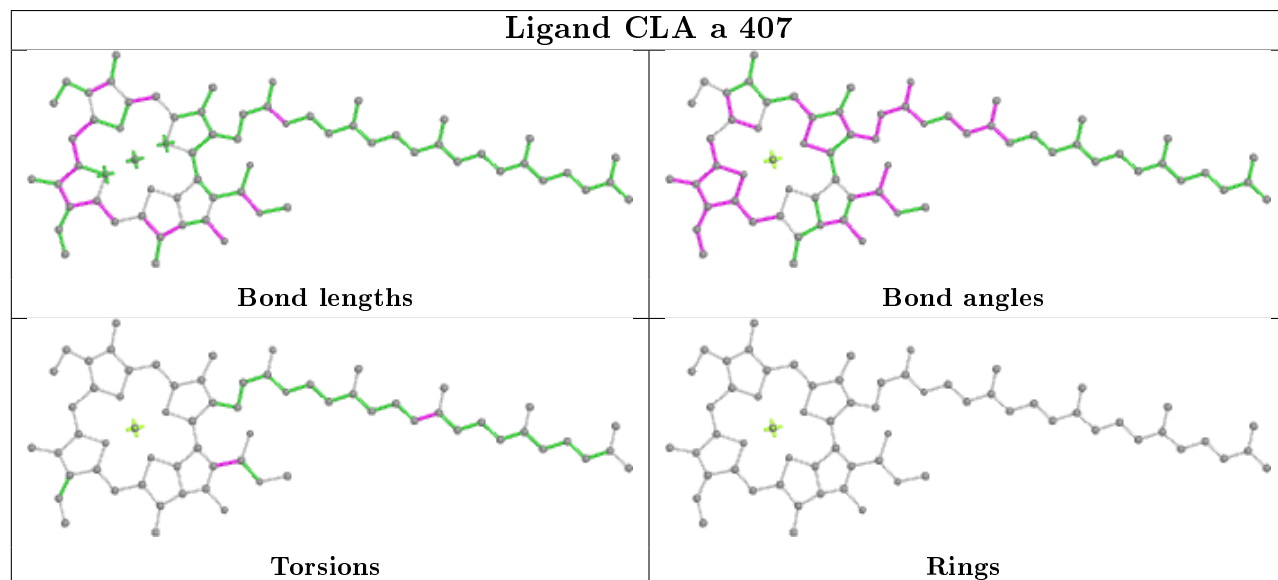


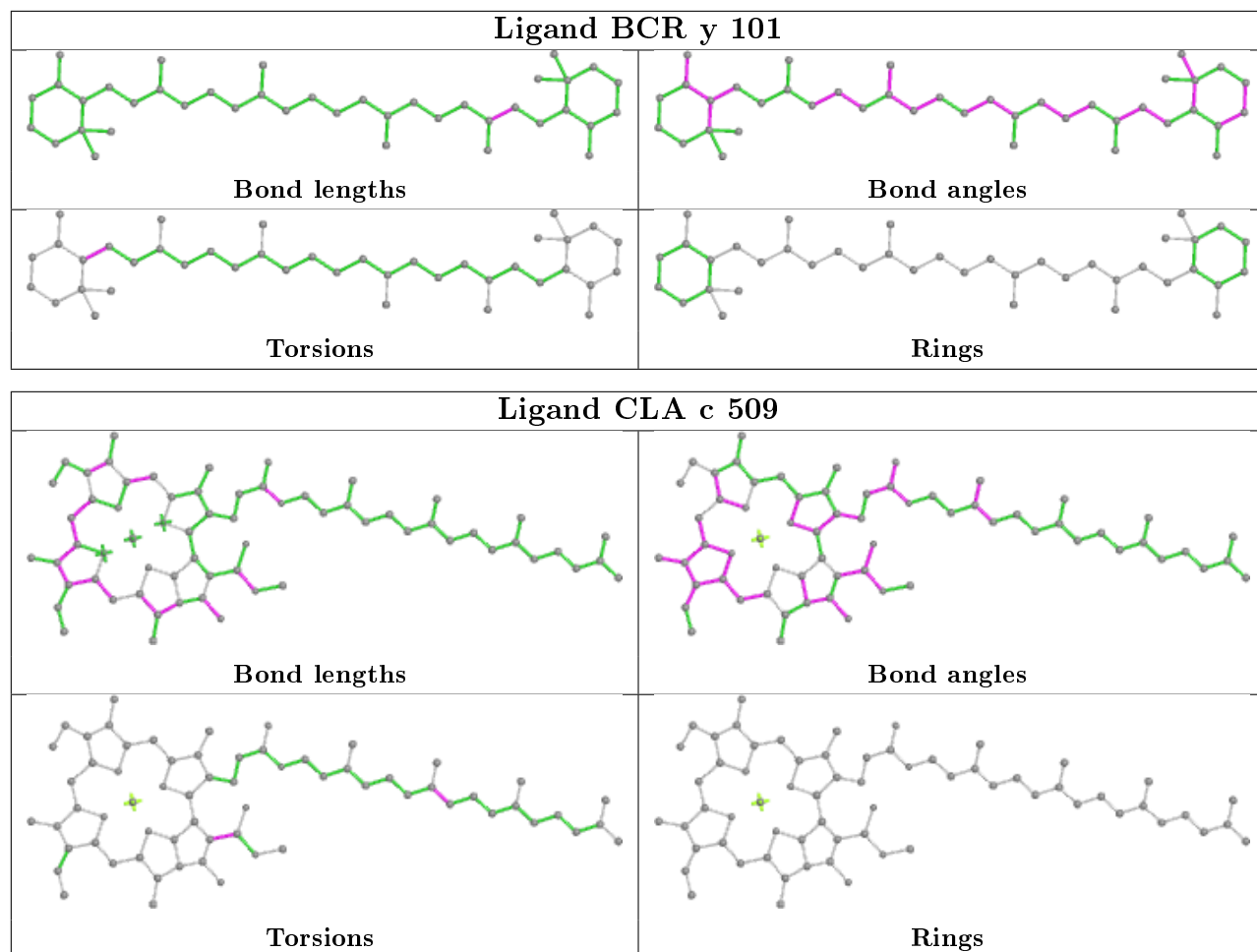
Ligand DGD h 102



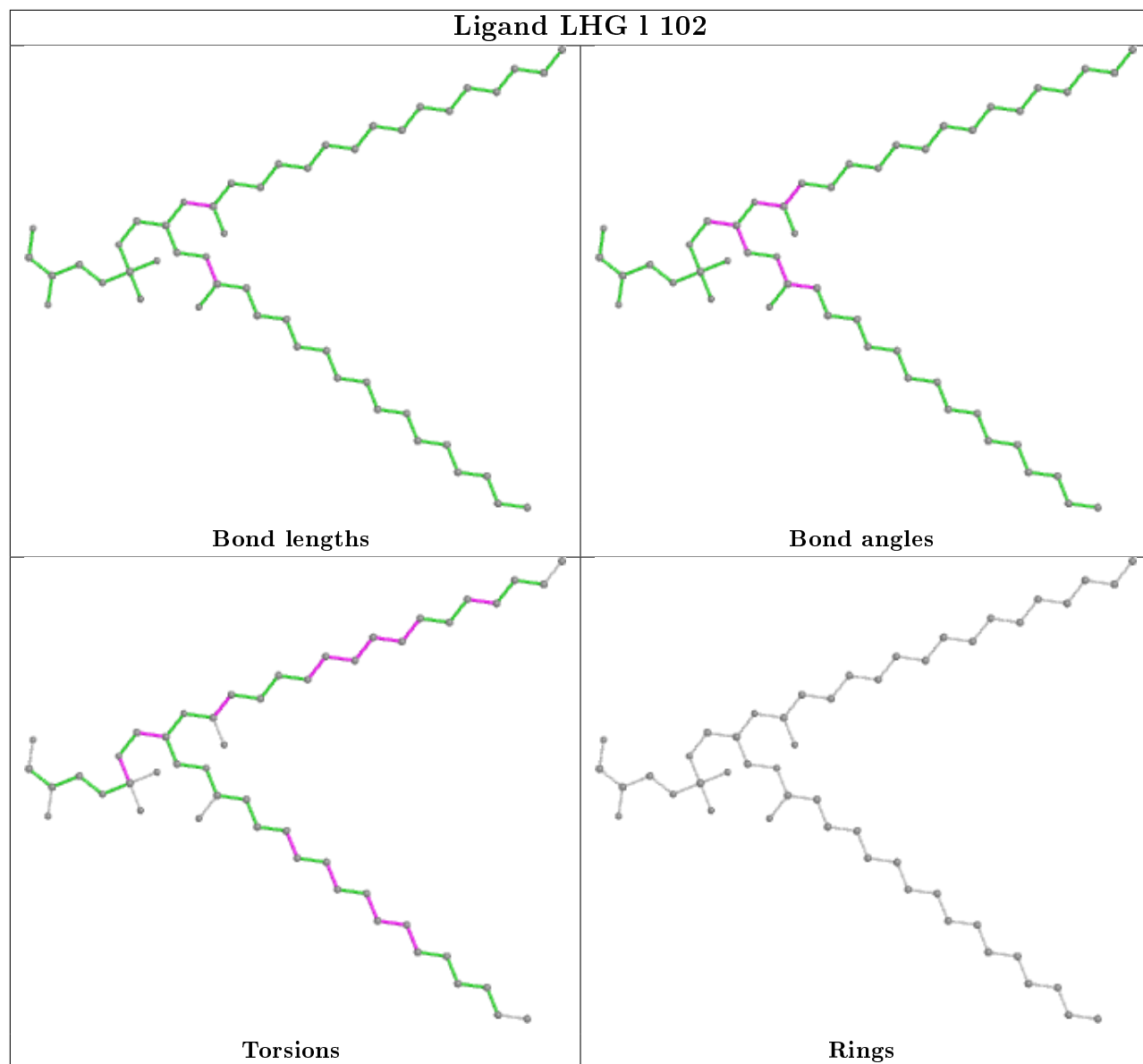
Ligand CLA c 503**Ligand BCR a 410****Ligand CLA d 402**

Ligand DGD c 518**Ligand LHG L 101**

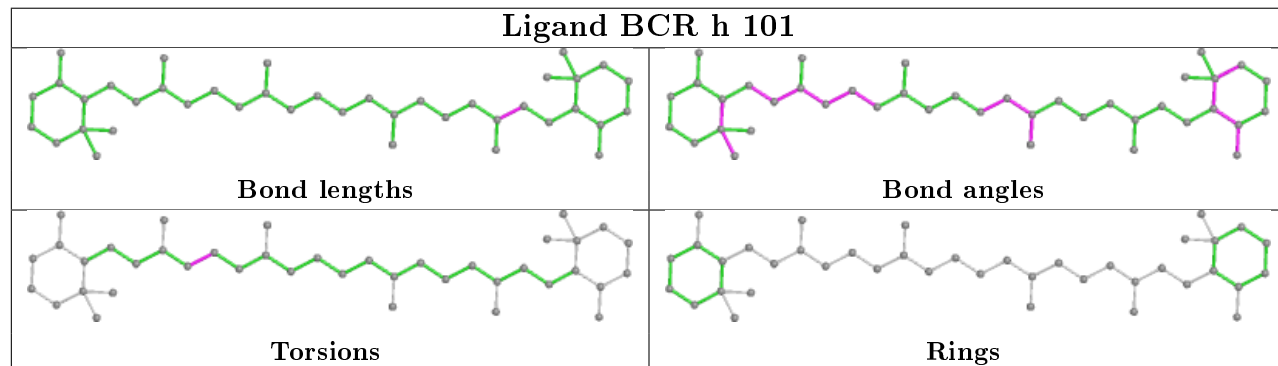
Ligand CLA b 619**Ligand CLA b 612****Ligand CLA a 407**

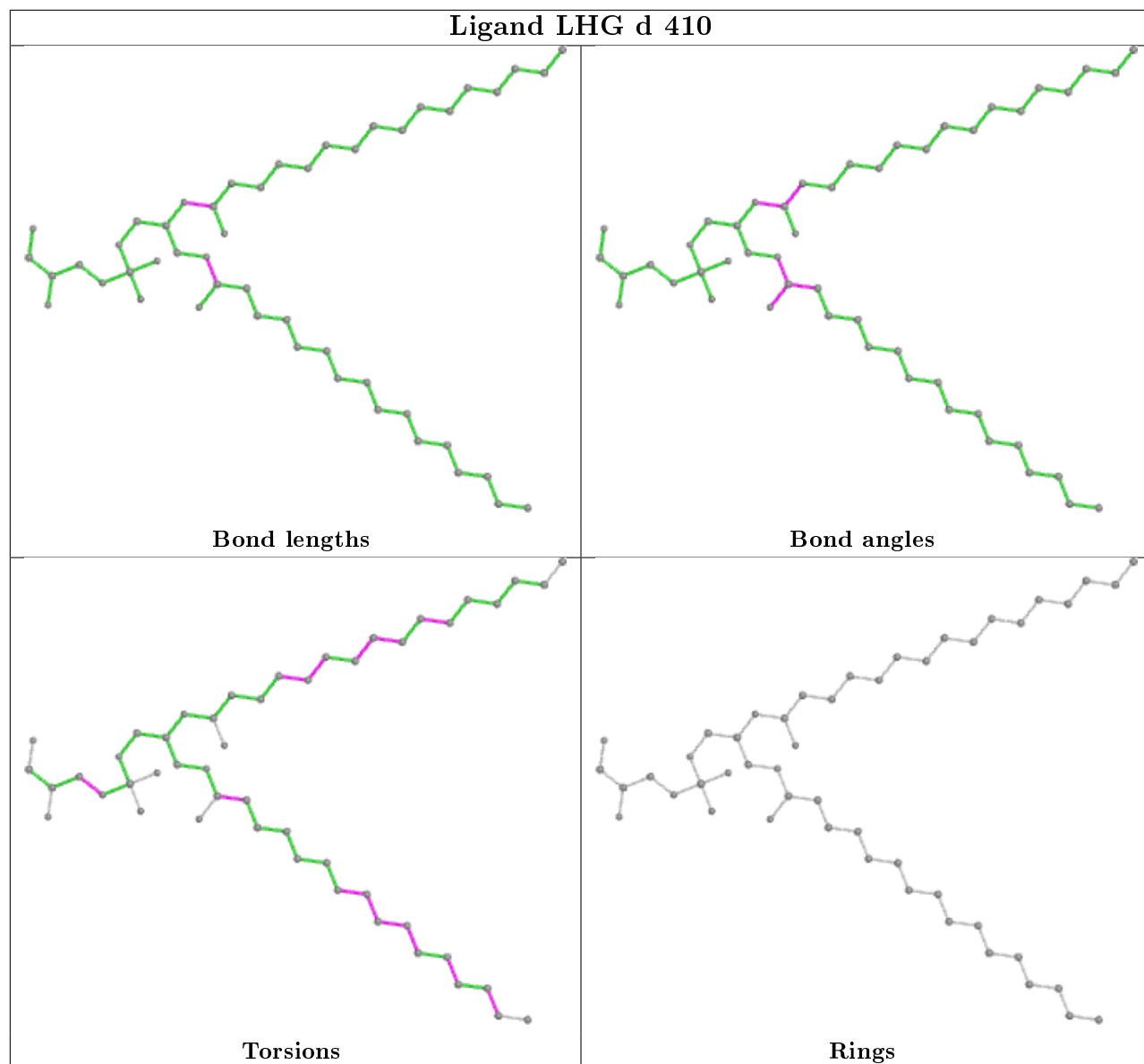
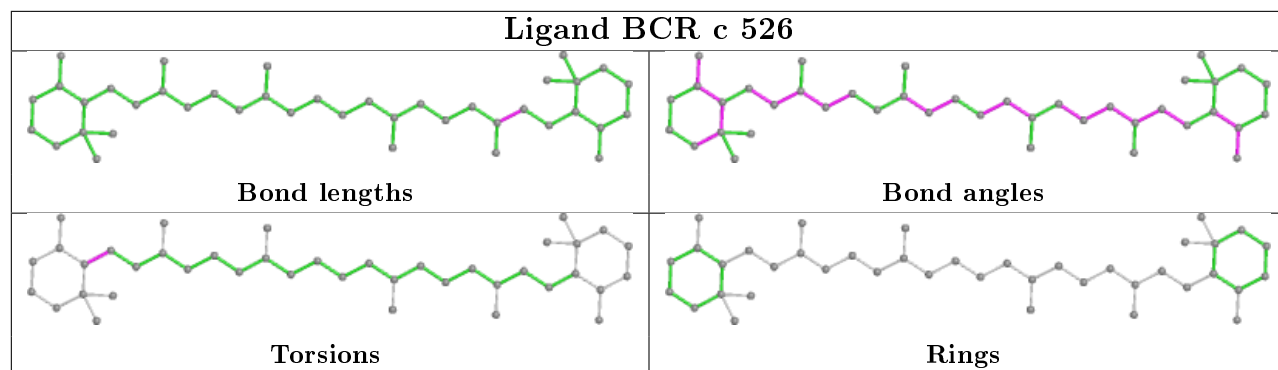


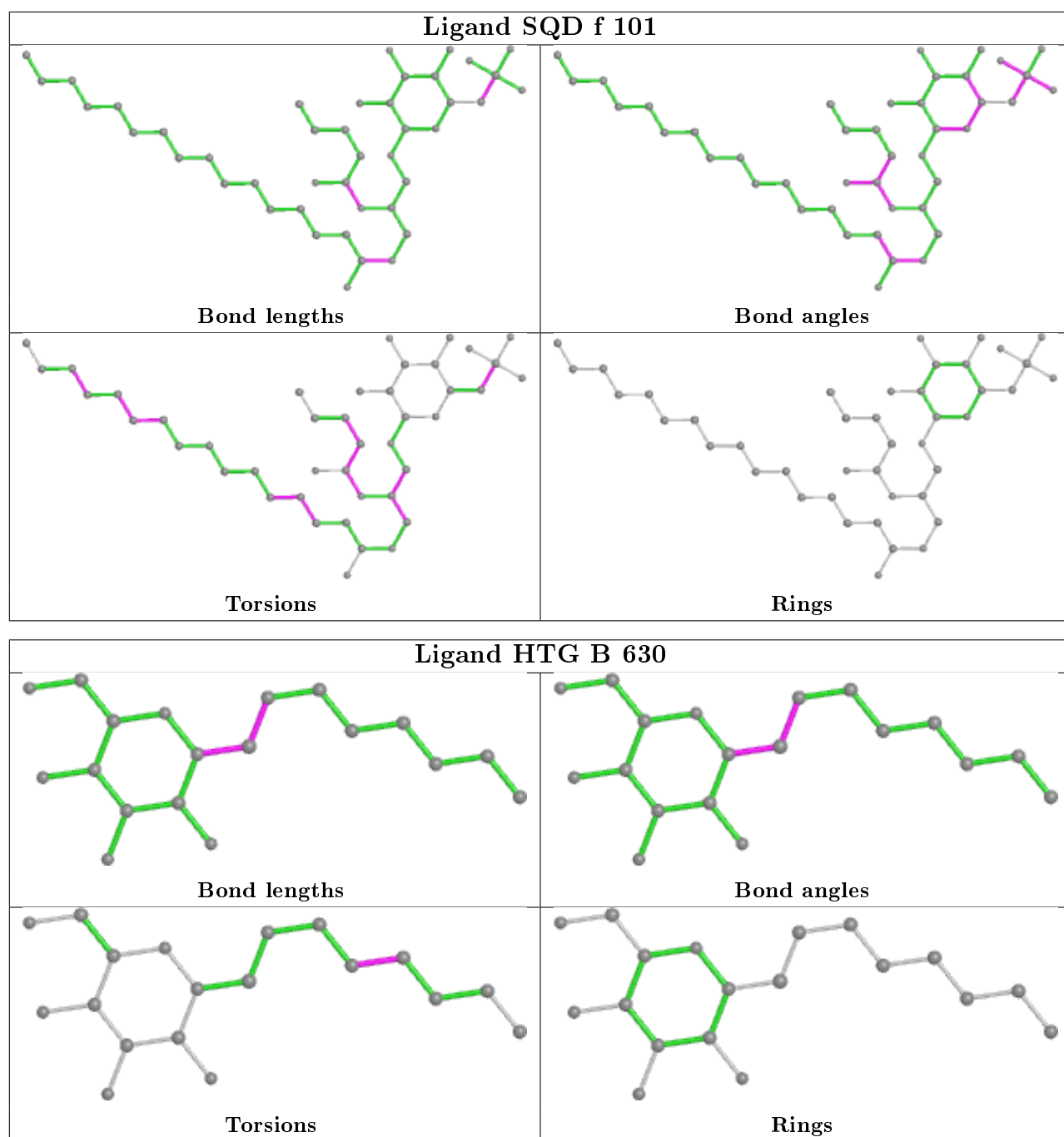
Ligand LHG 1 102

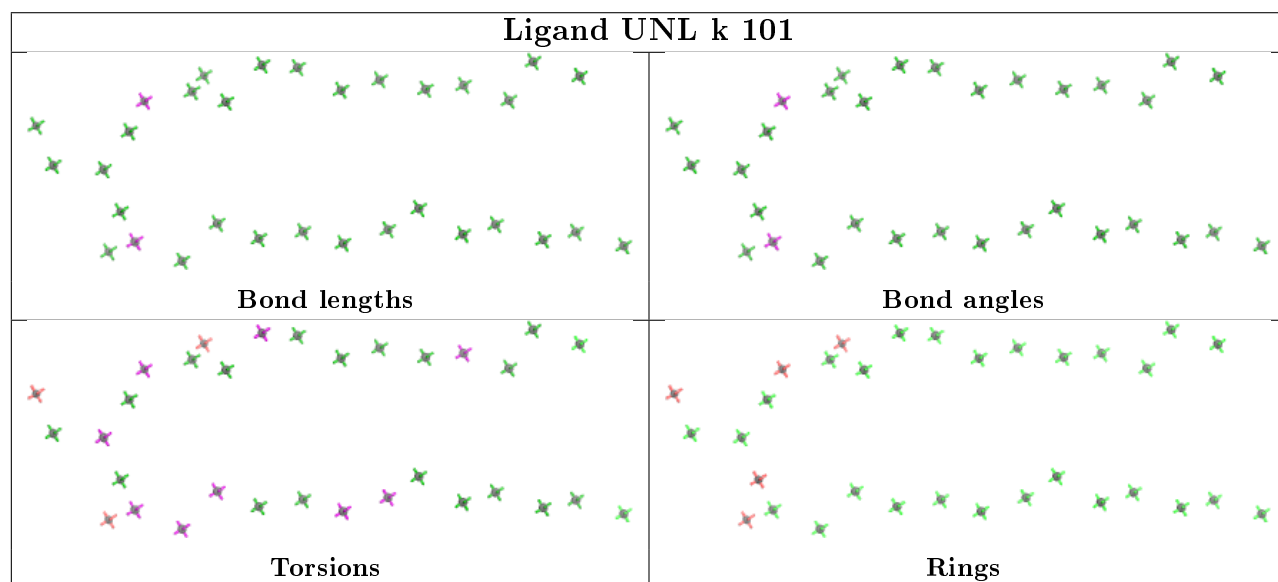
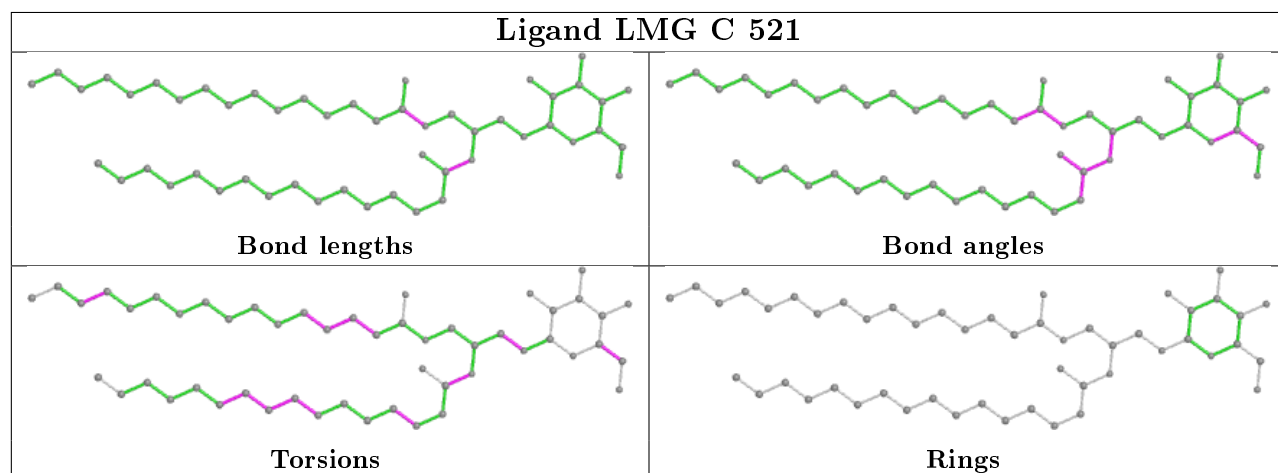
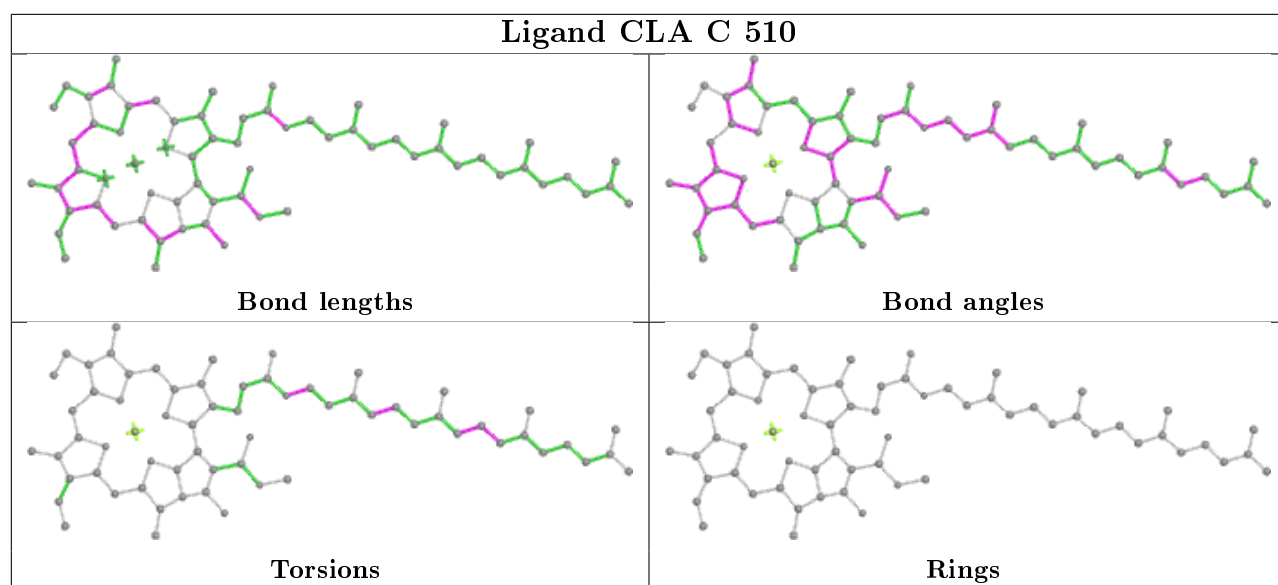


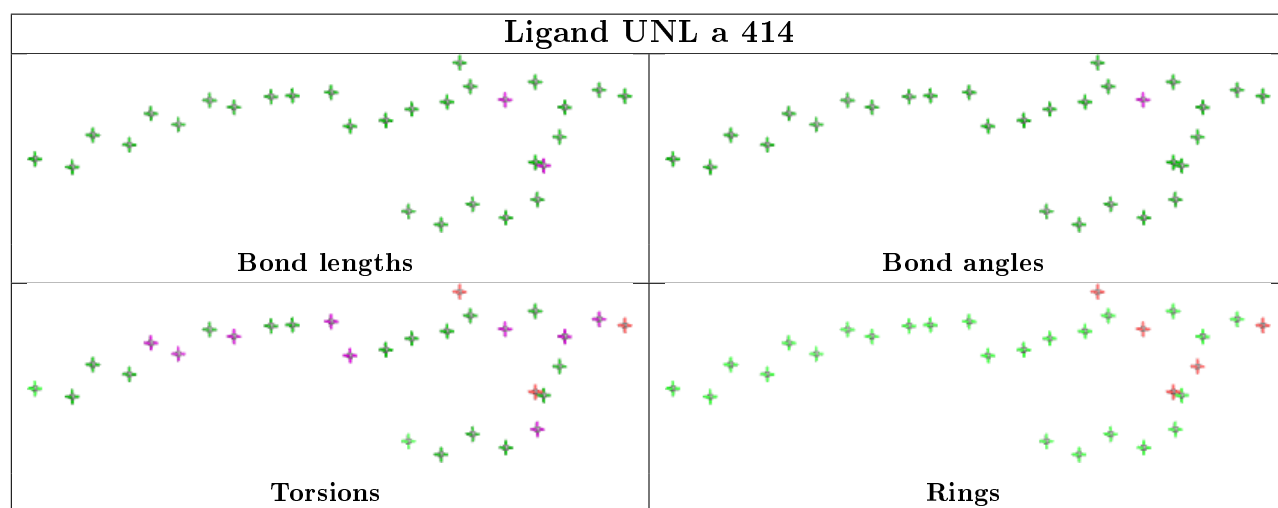
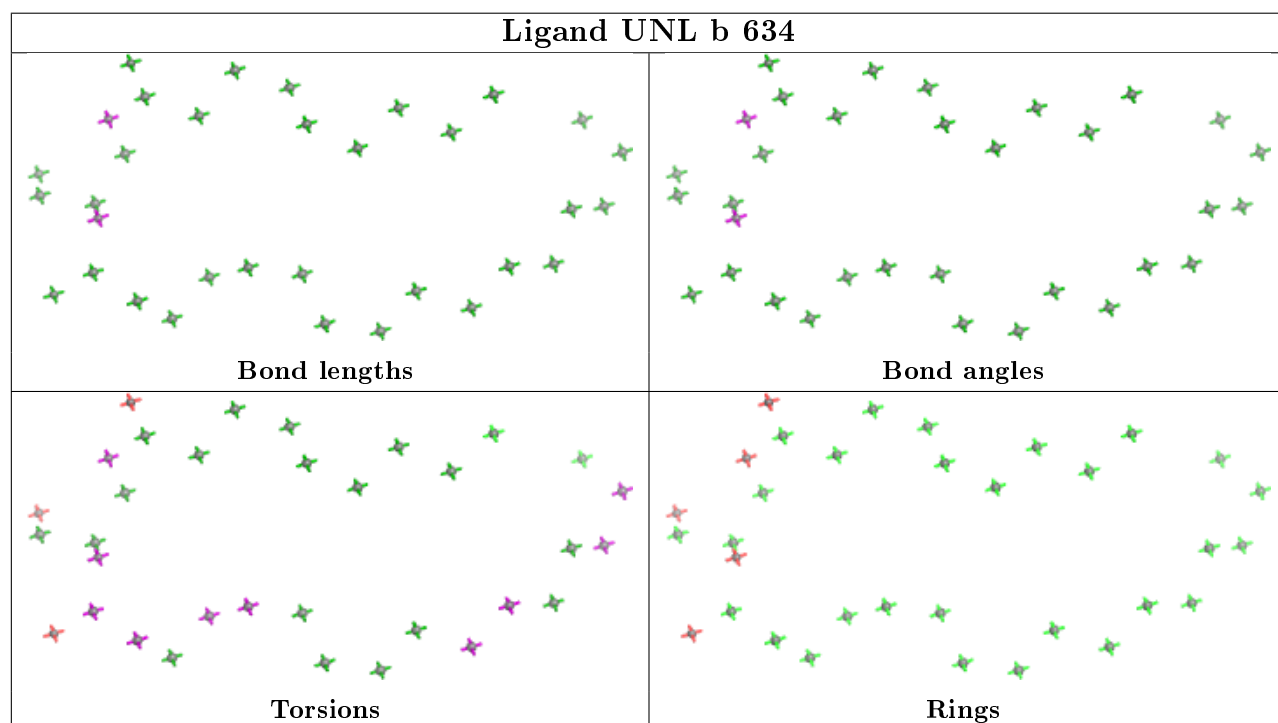
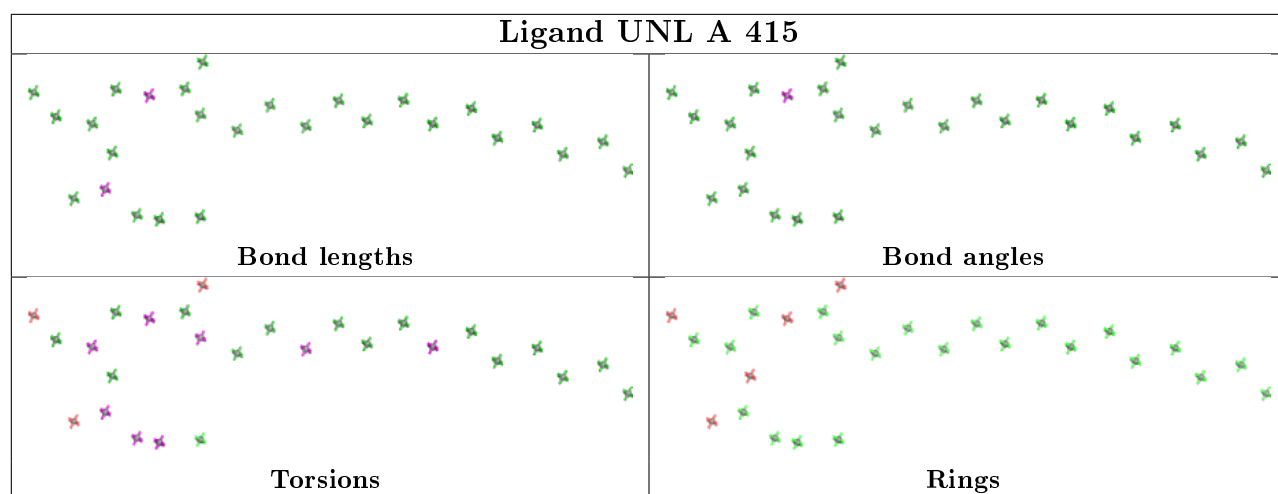
Ligand BCR h 101

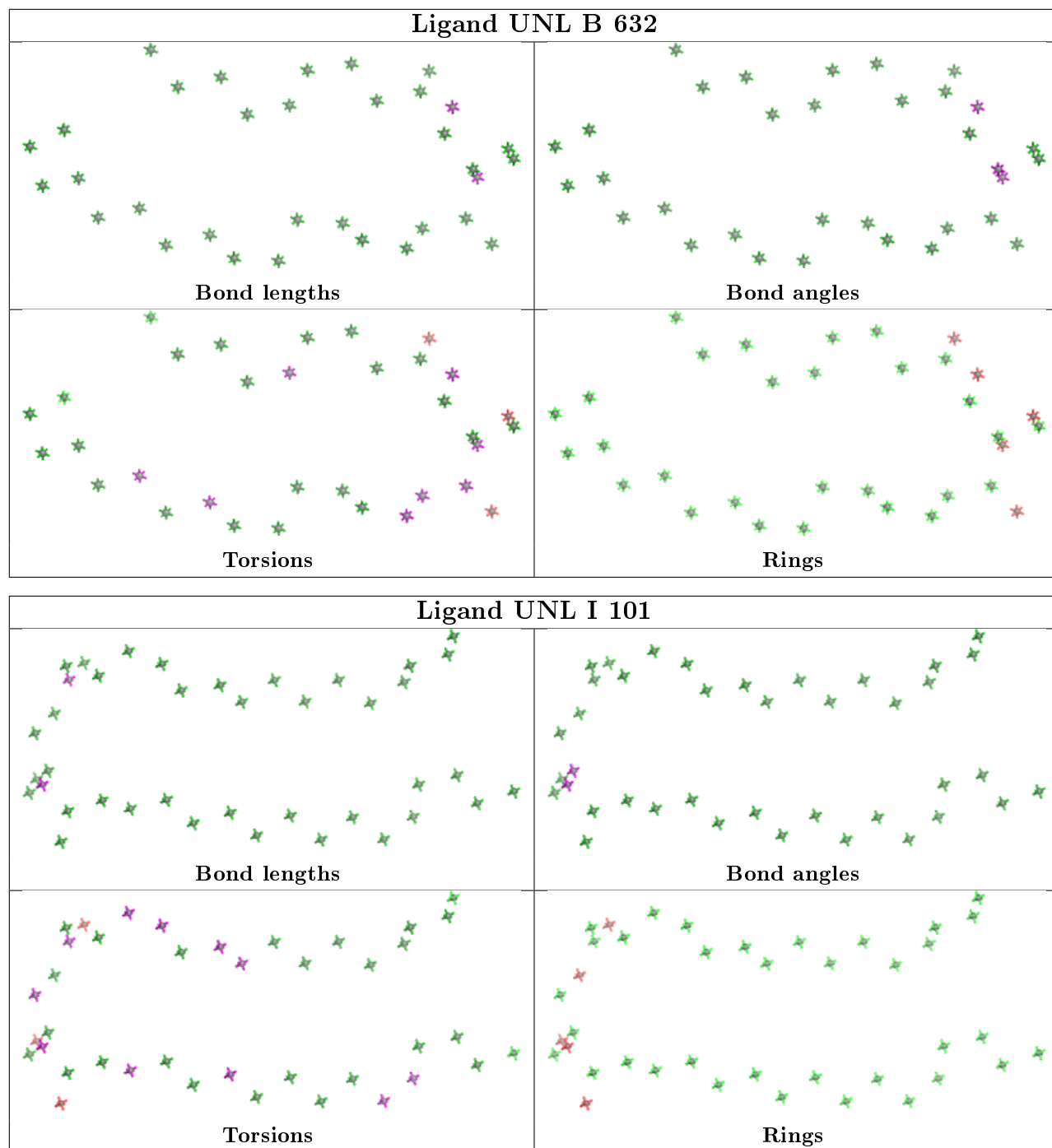


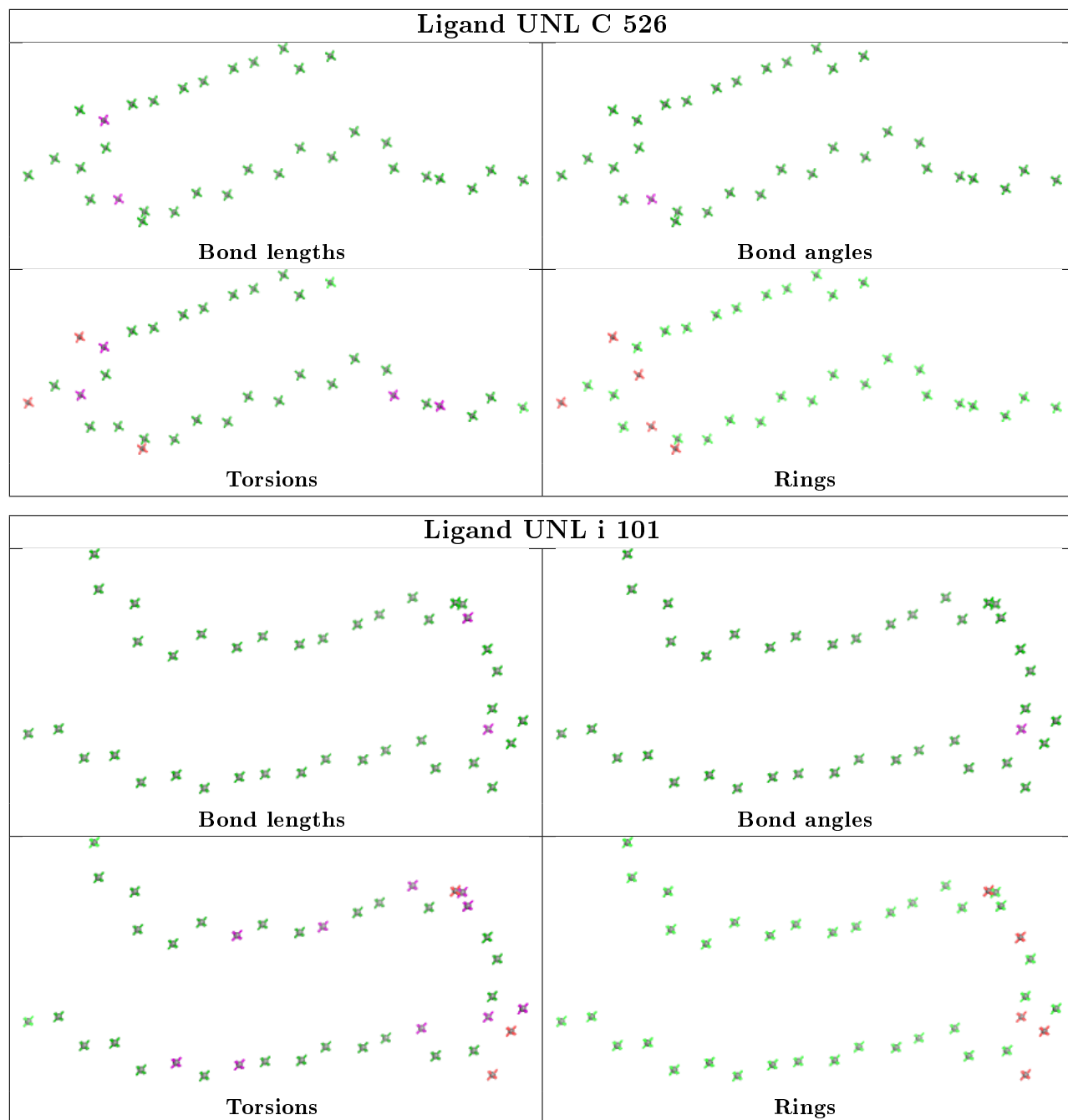


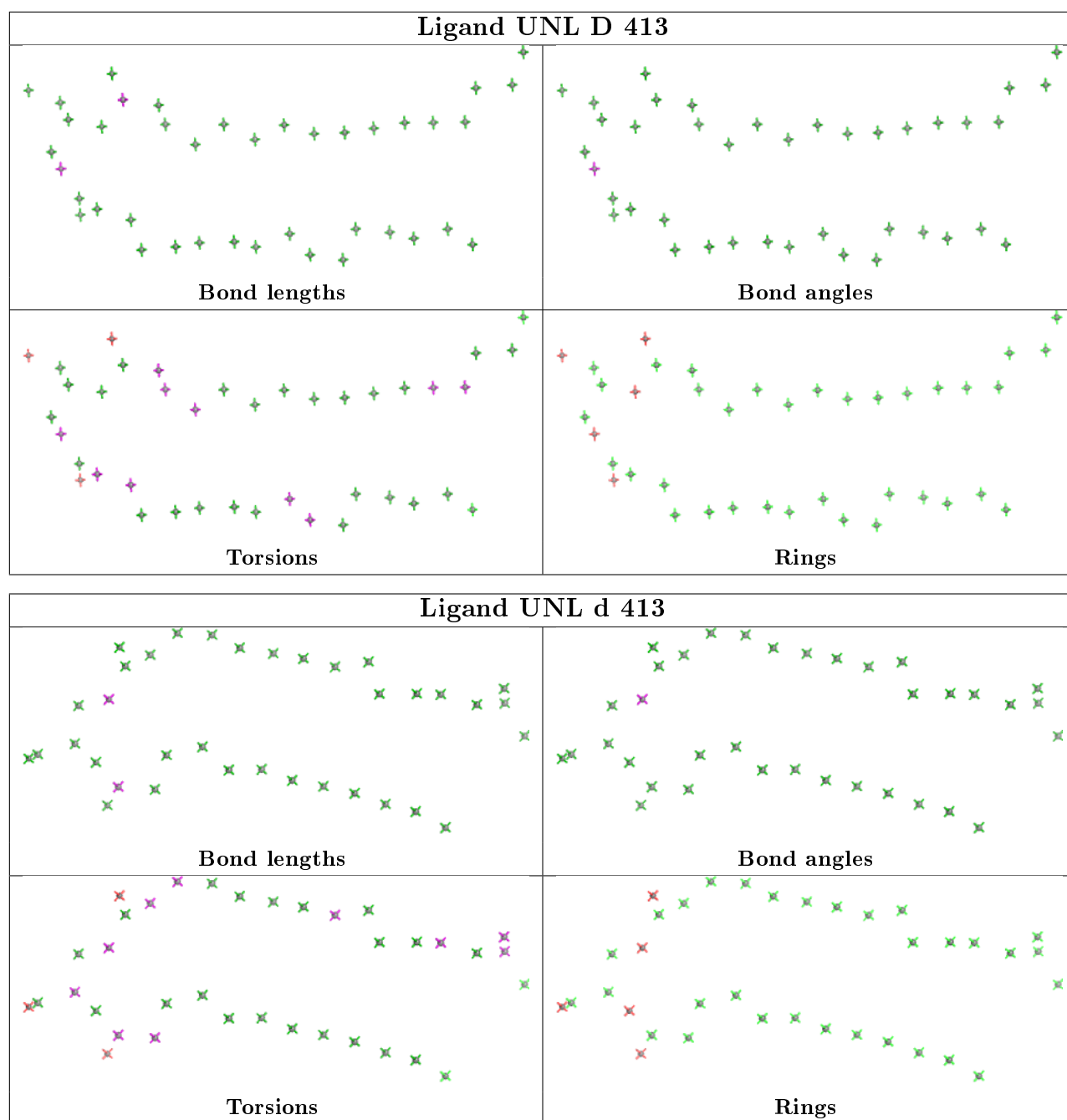












5.7 Other polymers [i](#)

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%)	0.67	44 (13%) 3 5	16, 23, 42, 79	0
1	a	334/344 (97%)	0.83	59 (17%) 1 1	17, 25, 48, 82	0
2	B	504/505 (99%)	0.27	42 (8%) 11 17	18, 27, 52, 90	0
2	b	504/505 (99%)	0.46	50 (9%) 7 12	19, 29, 60, 108	0
3	C	451/455 (99%)	0.24	28 (6%) 20 29	20, 32, 49, 89	0
3	c	455/455 (100%)	0.43	38 (8%) 11 17	23, 35, 50, 87	0
4	D	342/342 (100%)	0.88	63 (18%) 1 1	15, 24, 40, 114	0
4	d	341/342 (99%)	0.59	39 (11%) 5 8	18, 26, 42, 90	0
5	E	81/84 (96%)	1.20	15 (18%) 1 1	27, 40, 68, 97	0
5	e	81/84 (96%)	1.09	15 (18%) 1 1	32, 45, 77, 97	0
6	F	34/44 (77%)	0.35	6 (17%) 1 1	26, 35, 56, 64	0
6	f	32/44 (72%)	0.40	4 (12%) 3 6	31, 37, 84, 99	0
7	H	65/65 (100%)	0.34	3 (4%) 32 42	24, 34, 52, 97	0
7	h	65/65 (100%)	0.55	6 (9%) 9 14	28, 37, 58, 113	0
8	I	37/38 (97%)	0.83	5 (13%) 3 5	30, 34, 91, 101	0
8	i	37/38 (97%)	0.73	5 (13%) 3 5	29, 34, 79, 102	0
9	J	38/39 (97%)	0.73	8 (21%) 1 1	26, 38, 85, 109	0
9	j	38/39 (97%)	0.25	3 (7%) 12 19	30, 41, 84, 85	0
10	K	37/37 (100%)	0.16	0 100 100	31, 38, 55, 64	0
10	k	37/37 (100%)	0.86	8 (21%) 0 1	33, 42, 56, 66	0
11	L	37/37 (100%)	1.17	11 (29%) 0 0	16, 20, 66, 91	0
11	l	37/37 (100%)	1.04	6 (16%) 1 2	17, 21, 61, 91	0
12	M	33/36 (91%)	0.89	6 (18%) 1 1	18, 23, 44, 100	0
12	m	33/36 (91%)	0.76	5 (15%) 2 3	19, 23, 44, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.38	21 (8%) 10 16	16, 34, 65, 113	0
13	o	243/244 (99%)	0.89	52 (21%) 0 1	18, 35, 75, 122	0
14	T	29/31 (93%)	0.98	4 (13%) 2 4	17, 23, 48, 85	0
14	t	29/31 (93%)	0.55	2 (6%) 16 25	17, 23, 49, 85	0
15	U	97/104 (93%)	0.26	5 (5%) 27 37	22, 33, 53, 85	0
15	u	97/104 (93%)	-0.11	0 100 100	25, 34, 51, 85	0
16	V	137/137 (100%)	-0.03	0 100 100	23, 33, 54, 70	0
16	v	137/137 (100%)	0.49	13 (9%) 8 13	26, 38, 57, 72	0
17	Y	29/30 (96%)	2.05	9 (31%) 0 0	38, 50, 91, 107	0
17	y	29/30 (96%)	1.91	9 (31%) 0 0	41, 54, 91, 107	0
18	X	39/40 (97%)	0.77	8 (20%) 1 1	32, 42, 80, 92	0
18	x	39/40 (97%)	1.59	11 (28%) 0 0	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.28	18 (29%) 0 0	40, 52, 87, 98	0
19	z	62/62 (100%)	2.95	36 (58%) 0 0	44, 53, 87, 98	0
20	R	34/34 (100%)	9.29	34 (100%) 0 0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.65	691 (13%) 3 5	15, 31, 63, 122	0

The worst 5 of 691 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	18.4
20	R	6	LEU	14.1
20	R	14	LEU	13.2
20	R	31	VAL	13.0
20	R	20	VAL	12.0

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
9	FME	j	1	10/11	0.76	0.35	53,71,94,136	0
12	FME	m	1	10/11	0.93	0.15	25,31,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	FME	t	1	10/11	0.95	0.11	13,22,33,65	0
14	FME	T	1	10/11	0.96	0.15	21,27,45,56	0
12	FME	M	1	10/11	0.96	0.14	23,34,56,61	0
8	FME	i	1	10/11	0.97	0.15	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.11	22,34,37,40	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
28	GOL	B	635	6/6	0.22	0.43	82,91,97,98	0
36	DGD	D	407	62/66	0.51	0.49	44,89,114,119	0
29	UNL	k	102	10/-	0.58	0.61	54,83,94,102	0
36	DGD	d	407	62/66	0.59	0.44	41,88,117,122	0
29	UNL	j	103	10/-	0.60	0.32	44,61,67,73	0
30	LMT	f	102	35/35	0.60	0.36	56,83,109,113	0
35	HTG	b	628	19/19	0.61	0.31	48,90,106,124	0
30	LMT	E	102	35/35	0.61	0.34	43,81,105,107	0
35	HTG	b	604	19/19	0.62	0.19	50,80,106,112	0
34	LMG	Z	101	37/55	0.62	0.32	32,81,104,105	0
29	UNL	A	415	28/-	0.62	0.30	55,65,84,90	0
29	UNL	a	414	30/-	0.64	0.28	45,65,86,89	0
29	UNL	b	634	33/-	0.65	0.26	42,71,112,116	0
30	LMT	m	103	35/35	0.65	0.27	30,60,86,90	0
29	UNL	C	526	34/-	0.65	0.34	46,71,82,84	0
30	LMT	M	101	35/35	0.66	0.28	35,60,79,85	0
33	CA	b	605	1/1	0.67	0.14	95,95,95,95	0
35	HTG	d	411	16/19	0.67	0.27	54,73,84,87	0
28	GOL	O	302	6/6	0.68	0.18	52,61,64,70	0
27	SQD	l	101	54/54	0.68	0.25	31,67,98,101	0
30	LMT	b	626	25/35	0.69	0.29	33,67,110,115	0
32	PL9	A	419	55/55	0.69	0.29	38,66,87,92	0
28	GOL	T	103	6/6	0.69	0.31	63,76,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	LMT	D	402	35/35	0.69	0.25	32,75,96,97	0
35	HTG	D	411	16/19	0.70	0.24	38,100,111,113	0
29	UNL	k	101	32/-	0.70	0.38	42,75,105,108	0
37	LHG	E	101	42/49	0.70	0.25	38,73,93,103	0
30	LMT	m	102	35/35	0.70	0.22	16,51,73,79	0
35	HTG	B	624	19/19	0.71	0.36	38,95,102,121	0
29	UNL	J	103	10/-	0.71	0.44	38,53,73,75	0
34	LMG	z	101	39/55	0.72	0.39	47,74,94,101	0
29	UNL	i	101	40/-	0.73	0.24	36,64,96,108	0
27	SQD	b	601	54/54	0.73	0.23	36,58,91,95	0
37	LHG	e	101	42/49	0.74	0.23	49,87,117,128	0
29	UNL	B	632	33/-	0.74	0.24	32,70,105,113	0
28	GOL	v	203	6/6	0.75	0.29	50,69,71,78	0
30	LMT	I	102	35/35	0.75	0.34	59,81,95,100	0
32	PL9	a	416	55/55	0.75	0.27	50,76,94,95	0
27	SQD	a	402	54/54	0.76	0.23	34,61,79,100	0
35	HTG	B	631	19/19	0.76	0.21	25,84,104,120	0
29	UNL	x	101	10/-	0.76	0.17	35,44,57,58	0
35	HTG	C	523	19/19	0.76	0.28	46,75,97,109	0
29	UNL	I	101	40/-	0.76	0.29	27,63,114,119	0
33	CA	B	601	1/1	0.76	0.09	79,79,79,79	0
30	LMT	a	417	35/35	0.77	0.41	52,76,90,94	0
34	LMG	C	520	51/55	0.77	0.28	26,61,82,87	0
28	GOL	t	102	6/6	0.77	0.33	29,60,65,69	0
34	LMG	c	521	51/55	0.77	0.28	35,79,91,98	0
28	GOL	A	414	6/6	0.78	0.19	40,60,69,70	0
30	LMT	M	102	35/35	0.78	0.20	22,50,66,76	0
30	LMT	B	634	25/35	0.78	0.27	32,63,105,111	0
30	LMT	b	602	25/35	0.79	0.30	22,63,102,106	0
34	LMG	C	521	51/55	0.79	0.23	31,74,90,96	0
28	GOL	a	413	6/6	0.80	0.22	38,67,69,71	0
29	UNL	d	413	36/-	0.80	0.19	35,58,94,99	0
28	GOL	V	205	6/6	0.80	0.39	37,54,59,72	0
34	LMG	c	501	51/55	0.80	0.21	39,60,77,85	0
27	SQD	A	416	54/54	0.80	0.18	28,52,75,76	0
28	GOL	b	632	6/6	0.81	0.29	40,46,68,69	0
29	UNL	D	413	40/-	0.81	0.20	33,55,105,108	0
30	LMT	a	401	35/35	0.82	0.19	28,61,79,86	0
27	SQD	f	101	43/54	0.83	0.30	55,82,109,117	0
35	HTG	c	523	19/19	0.83	0.32	60,84,93,98	0
34	LMG	B	621	51/55	0.83	0.25	20,35,52,64	0
34	LMG	c	520	51/55	0.84	0.22	33,63,86,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	GOL	v	204	6/6	0.84	0.20	47,64,70,92	0
34	LMG	C	501	51/55	0.84	0.19	37,54,74,82	0
29	UNL	d	412	17/-	0.84	0.16	31,48,79,85	0
28	GOL	B	627	6/6	0.85	0.22	31,35,43,44	0
29	UNL	M	103	10/-	0.85	0.18	34,42,59,64	0
30	LMT	A	417	33/35	0.85	0.19	27,65,78,85	0
35	HTG	B	623	19/19	0.85	0.16	29,42,64,71	0
29	UNL	X	101	10/-	0.85	0.15	29,37,41,42	0
35	HTG	c	522	19/19	0.86	0.17	63,69,80,85	0
24	CLA	c	515	65/65	0.86	0.27	37,51,79,88	0
35	HTG	B	630	19/19	0.86	0.17	30,54,78,81	0
36	DGD	H	102	62/66	0.86	0.19	20,29,42,58	0
26	BCR	k	103	40/40	0.86	0.17	32,40,48,52	0
29	UNL	m	101	10/-	0.86	0.26	37,51,60,62	0
28	GOL	A	413	6/6	0.86	0.19	35,38,41,42	0
28	GOL	V	208	6/6	0.86	0.26	41,56,62,63	0
26	BCR	h	101	40/40	0.87	0.12	27,35,46,49	0
28	GOL	V	206	6/6	0.87	0.20	21,38,44,48	0
36	DGD	h	102	62/66	0.87	0.17	23,35,52,69	0
26	BCR	d	405	40/40	0.87	0.16	29,35,63,64	0
34	LMG	b	625	51/55	0.87	0.28	24,39,59,71	0
35	HTG	V	204	19/19	0.88	0.26	40,65,99,175	0
28	GOL	B	628	6/6	0.88	0.22	35,46,67,70	0
28	GOL	C	524	6/6	0.88	0.21	39,45,57,60	0
27	SQD	F	101	43/54	0.88	0.30	39,70,96,105	0
33	CA	F	102	1/1	0.88	0.14	72,72,72,72	0
26	BCR	H	101	40/40	0.88	0.13	21,32,48,52	0
24	CLA	b	614	65/65	0.89	0.12	24,31,41,50	0
28	GOL	c	527	6/6	0.89	0.21	36,57,61,63	0
24	CLA	c	505	65/65	0.89	0.13	29,35,46,60	0
35	HTG	b	627	19/19	0.89	0.23	27,44,80,80	0
33	CA	f	103	1/1	0.89	0.12	72,72,72,72	0
37	LHG	d	408	49/49	0.89	0.23	26,34,46,50	0
32	PL9	d	406	55/55	0.89	0.21	16,23,35,47	0
28	GOL	T	101	6/6	0.89	0.18	35,60,64,65	0
28	GOL	b	631	6/6	0.90	0.11	39,46,48,60	0
35	HTG	b	603	19/19	0.90	0.14	34,44,64,67	0
26	BCR	B	619	40/40	0.90	0.17	17,25,44,46	0
37	LHG	D	408	49/49	0.90	0.25	16,31,43,54	0
34	LMG	j	101	51/55	0.90	0.19	26,39,70,82	0
24	CLA	c	514	65/65	0.90	0.18	34,43,67,76	0
26	BCR	Y	101	40/40	0.90	0.12	28,35,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	DGD	c	518	62/66	0.90	0.19	24,35,79,94	0
28	GOL	c	525	6/6	0.90	0.24	43,46,61,62	0
27	SQD	A	411	54/54	0.90	0.21	26,51,71,78	0
28	GOL	B	626	6/6	0.90	0.21	32,37,40,59	0
37	LHG	l	102	49/49	0.90	0.19	19,30,48,57	0
26	BCR	c	526	40/40	0.90	0.16	39,48,59,63	0
27	SQD	a	411	54/54	0.90	0.22	32,56,75,78	0
24	CLA	c	506	65/65	0.90	0.17	26,33,51,61	0
24	CLA	C	509	65/65	0.90	0.16	21,29,78,80	0
28	GOL	a	412	6/6	0.91	0.16	22,37,41,45	0
29	UNL	D	412	17/-	0.91	0.16	24,45,74,78	0
26	BCR	T	102	40/40	0.91	0.16	14,28,36,42	0
24	CLA	c	507	65/65	0.91	0.12	22,31,52,62	0
24	CLA	C	514	65/65	0.91	0.16	32,42,69,72	0
26	BCR	D	405	40/40	0.91	0.14	22,31,61,77	0
35	HTG	C	522	19/19	0.91	0.18	53,65,89,95	0
26	BCR	b	622	40/40	0.91	0.18	16,26,33,36	0
24	CLA	c	513	65/65	0.91	0.13	30,39,50,54	0
32	PL9	D	406	55/55	0.91	0.24	14,23,36,43	0
24	CLA	B	604	65/65	0.91	0.12	18,25,32,40	0
26	BCR	c	516	40/40	0.91	0.12	29,36,47,57	0
28	GOL	F	103	6/6	0.91	0.18	52,59,65,68	0
24	CLA	B	610	65/65	0.91	0.12	19,26,36,40	0
24	CLA	B	603	65/65	0.91	0.12	18,25,32,38	0
26	BCR	b	623	40/40	0.91	0.21	15,27,40,46	0
24	CLA	b	620	65/65	0.91	0.12	22,31,51,74	0
24	CLA	B	602	65/65	0.92	0.16	24,39,82,104	0
35	HTG	B	622	19/19	0.92	0.11	26,30,44,56	0
28	GOL	V	201	6/6	0.92	0.11	27,29,40,41	0
28	GOL	B	625	6/6	0.92	0.14	28,43,48,55	0
36	DGD	C	518	62/66	0.92	0.23	22,32,76,92	0
28	GOL	A	412	6/6	0.92	0.10	29,31,34,37	0
24	CLA	B	612	65/65	0.92	0.17	15,21,37,41	0
28	GOL	b	629	6/6	0.92	0.13	32,40,48,57	0
26	BCR	t	101	40/40	0.92	0.12	15,24,45,49	0
24	CLA	C	504	65/65	0.92	0.11	24,33,42,48	0
36	DGD	c	519	62/66	0.92	0.20	26,34,65,72	0
24	CLA	B	608	65/65	0.92	0.18	13,20,31,35	0
28	GOL	b	630	6/6	0.92	0.16	37,48,50,52	0
28	GOL	f	104	6/6	0.92	0.22	45,51,59,61	0
24	CLA	b	607	65/65	0.92	0.12	23,30,38,41	0
24	CLA	b	621	65/65	0.92	0.15	21,35,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	505	65/65	0.92	0.21	22,29,59,77	0
26	BCR	y	101	40/40	0.92	0.12	31,40,53,60	0
24	CLA	c	509	65/65	0.92	0.12	27,34,49,58	0
24	CLA	B	615	65/65	0.92	0.14	15,24,67,78	0
26	BCR	b	624	40/40	0.92	0.10	20,32,46,52	0
34	LMG	J	101	51/55	0.92	0.22	20,37,78,86	0
26	BCR	C	515	40/40	0.92	0.11	31,42,49,53	0
28	GOL	B	633	6/6	0.92	0.10	27,36,40,41	0
24	CLA	C	507	65/65	0.92	0.16	28,42,81,88	0
37	LHG	L	101	49/49	0.93	0.23	15,29,47,58	0
36	DGD	c	517	62/66	0.93	0.17	23,32,68,76	0
24	CLA	c	512	65/65	0.93	0.17	26,32,44,59	0
28	GOL	v	205	6/6	0.93	0.17	25,39,52,58	0
36	DGD	C	519	62/66	0.93	0.23	20,30,58,63	0
24	CLA	c	510	65/65	0.93	0.16	24,31,70,87	0
24	CLA	c	503	65/65	0.93	0.11	29,34,45,54	0
24	CLA	C	511	65/65	0.93	0.15	23,29,41,62	0
28	GOL	v	201	6/6	0.93	0.13	31,40,49,50	0
24	CLA	B	607	65/65	0.93	0.11	18,26,51,75	0
24	CLA	b	619	65/65	0.93	0.14	15,25,72,77	0
24	CLA	b	612	65/65	0.93	0.21	14,23,30,36	0
24	CLA	b	606	65/65	0.93	0.18	30,46,82,98	0
24	CLA	b	616	65/65	0.93	0.13	18,26,38,52	0
37	LHG	d	409	49/49	0.93	0.14	17,26,39,55	0
24	CLA	C	512	65/65	0.93	0.11	26,32,41,48	0
24	CLA	c	508	65/65	0.93	0.12	30,41,65,70	0
24	CLA	C	513	65/65	0.93	0.12	29,42,67,74	0
26	BCR	B	618	40/40	0.93	0.16	15,23,33,41	0
26	BCR	K	101	40/40	0.93	0.12	27,33,42,47	0
24	CLA	C	502	65/65	0.93	0.11	25,32,47,58	0
24	CLA	A	405	65/65	0.94	0.26	15,18,26,50	0
24	CLA	a	407	65/65	0.94	0.26	19,25,72,79	0
24	CLA	c	504	65/65	0.94	0.14	26,32,45,55	0
35	HTG	O	303	19/19	0.94	0.09	24,32,47,48	0
25	PHO	d	403	64/64	0.94	0.20	20,25,34,38	0
24	CLA	B	605	65/65	0.94	0.14	15,22,51,63	0
24	CLA	C	508	65/65	0.94	0.11	25,35,48,57	0
36	DGD	C	517	62/66	0.94	0.14	22,33,75,83	0
33	CA	o	301	1/1	0.94	0.07	62,62,62,62	0
37	LHG	D	409	49/49	0.94	0.18	17,27,48,60	0
24	CLA	b	618	65/65	0.94	0.18	15,23,48,56	0
22	CL	u	201	1/1	0.94	0.05	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	BCR	a	410	40/40	0.94	0.09	16,24,31,33	0
24	CLA	d	404	65/65	0.94	0.12	27,34,74,81	0
28	GOL	B	629	6/6	0.94	0.25	24,40,61,78	0
24	CLA	b	611	65/65	0.94	0.10	19,31,58,74	0
24	CLA	b	613	65/65	0.94	0.11	22,29,38,42	0
24	CLA	C	503	65/65	0.94	0.12	22,28,40,51	0
24	CLA	a	409	65/65	0.94	0.12	20,27,83,88	0
24	CLA	b	615	65/65	0.94	0.11	21,28,39,46	0
37	LHG	D	410	49/49	0.94	0.18	20,33,91,95	0
28	GOL	V	207	6/6	0.94	0.21	35,38,41,44	0
24	CLA	b	617	65/65	0.94	0.11	18,26,36,50	0
24	CLA	b	608	65/65	0.94	0.10	22,29,38,42	0
37	LHG	d	410	49/49	0.94	0.18	23,35,85,104	0
24	CLA	B	614	65/65	0.94	0.17	14,22,45,52	0
38	HEM	e	102	43/43	0.94	0.18	38,48,65,84	0
26	BCR	C	516	40/40	0.94	0.09	25,34,43,46	0
23	BCT	a	418	4/4	0.95	0.17	30,33,42,44	0
24	CLA	B	617	65/65	0.95	0.17	19,28,88,91	0
24	CLA	B	616	65/65	0.95	0.11	19,28,48,60	0
24	CLA	B	613	65/65	0.95	0.11	15,23,32,35	0
25	PHO	A	407	64/64	0.95	0.18	15,18,23,28	0
24	CLA	A	409	65/65	0.95	0.12	18,27,83,92	0
24	CLA	A	406	65/65	0.95	0.26	15,19,84,88	0
25	PHO	a	408	64/64	0.95	0.18	16,21,29,37	0
24	CLA	C	506	65/65	0.95	0.10	21,29,45,53	0
22	CL	V	202	1/1	0.95	0.05	63,63,63,63	0
24	CLA	b	609	65/65	0.95	0.15	16,25,56,66	0
24	CLA	B	606	65/65	0.95	0.09	16,22,34,38	0
25	PHO	A	408	64/64	0.95	0.26	16,22,30,32	0
24	CLA	D	404	65/65	0.95	0.12	21,28,73,84	0
26	BCR	A	410	40/40	0.95	0.10	16,26,33,35	0
26	BCR	B	620	40/40	0.95	0.10	22,29,42,47	0
24	CLA	B	611	65/65	0.95	0.12	19,26,36,39	0
28	GOL	b	633	6/6	0.95	0.29	32,54,63,71	0
24	CLA	B	609	65/65	0.95	0.14	17,22,32,36	0
24	CLA	c	511	65/65	0.95	0.10	29,36,49,55	0
28	GOL	C	525	6/6	0.95	0.13	20,24,26,27	0
24	CLA	C	510	65/65	0.95	0.11	25,32,51,57	0
24	CLA	b	610	65/65	0.95	0.11	18,24,37,42	0
24	CLA	d	401	65/65	0.96	0.21	16,19,26,42	0
23	BCT	A	404	4/4	0.96	0.10	27,30,39,40	0
38	HEM	E	103	43/43	0.96	0.17	27,38,50,56	0

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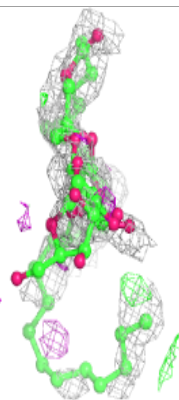
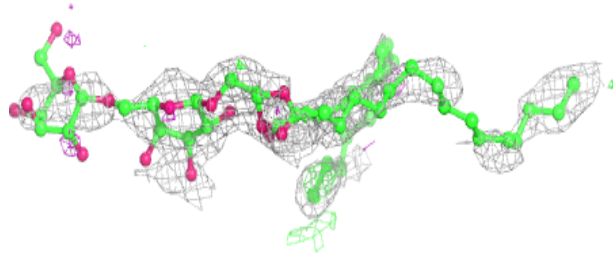
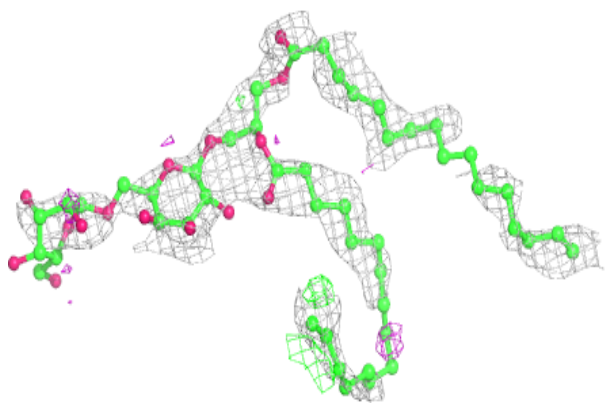
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	D	403	65/65	0.96	0.28	14,19,36,42	0
24	CLA	a	406	65/65	0.96	0.24	17,20,35,51	0
24	CLA	d	402	65/65	0.96	0.24	18,22,38,46	0
33	CA	c	502	1/1	0.96	0.04	44,44,44,44	0
24	CLA	D	401	65/65	0.96	0.24	13,18,30,32	0
40	HEC	V	203	43/43	0.97	0.08	23,26,31,36	0
33	CA	O	301	1/1	0.97	0.05	56,56,56,56	0
40	HEC	v	202	43/43	0.97	0.10	29,33,40,48	0
39	MG	J	102	1/1	0.97	0.04	28,28,28,28	0
39	MG	j	102	1/1	0.98	0.16	34,34,34,34	0
22	CL	A	403	1/1	0.98	0.07	23,23,23,23	0
28	GOL	c	524	6/6	0.98	0.15	25,28,30,34	0
31	OEX	A	418	10/10	0.99	0.09	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.11	20,24,35,37	0
21	FE2	A	401	1/1	0.99	0.10	27,27,27,27	0
22	CL	a	405	1/1	0.99	0.12	26,26,26,26	0
21	FE2	a	403	1/1	0.99	0.11	30,30,30,30	0
22	CL	A	402	1/1	0.99	0.10	19,19,19,19	0
22	CL	a	404	1/1	1.00	0.10	20,20,20,20	0

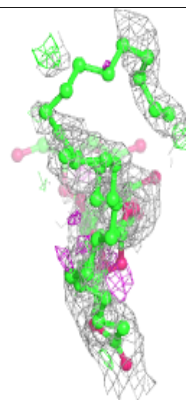
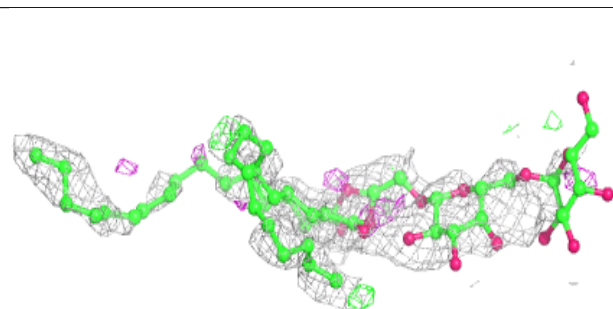
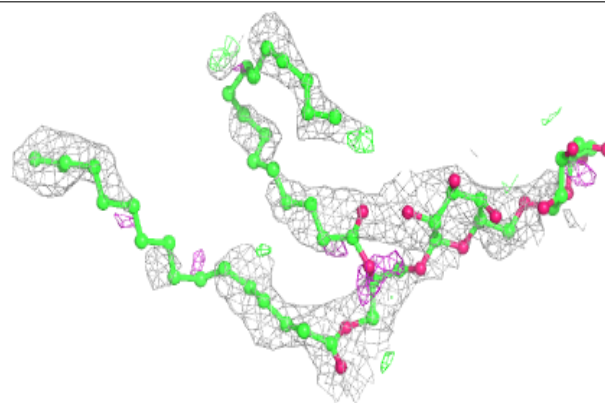
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD D 407:

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

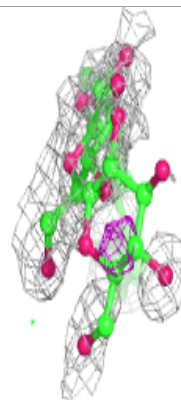
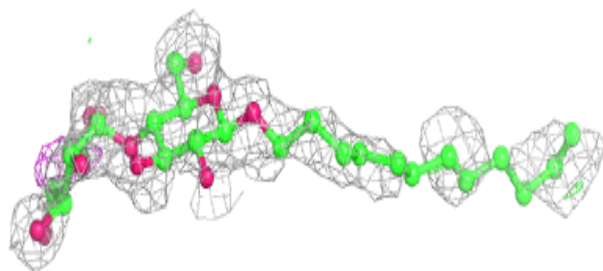
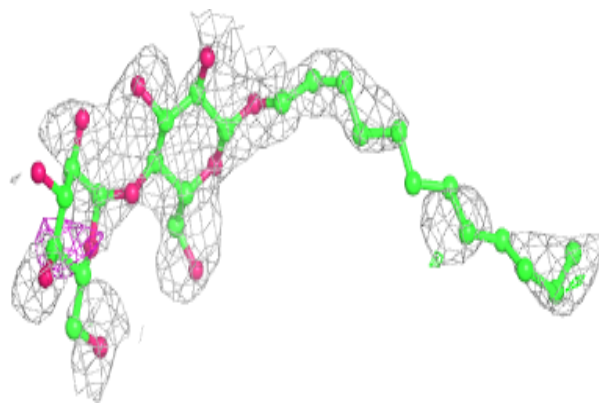
**Electron density around DGD d 407:**

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

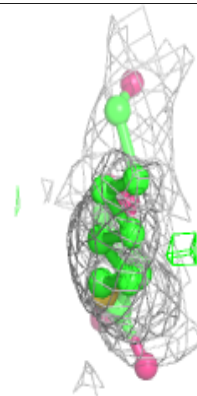
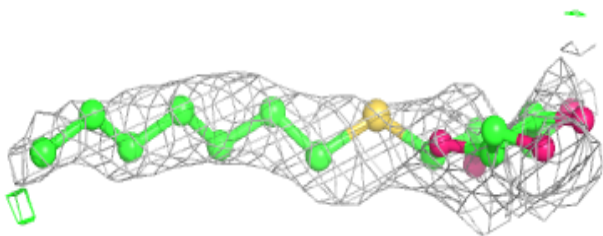
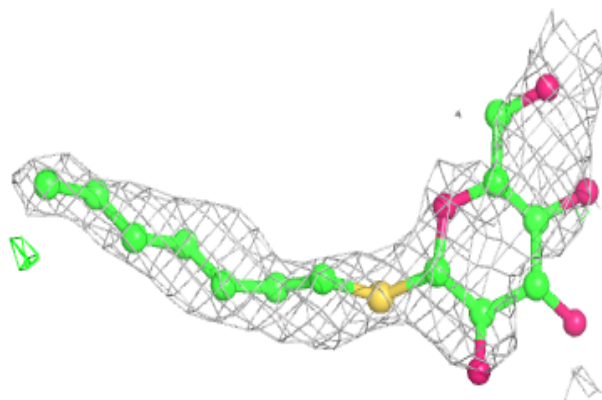


Electron density around LMT f 102:

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

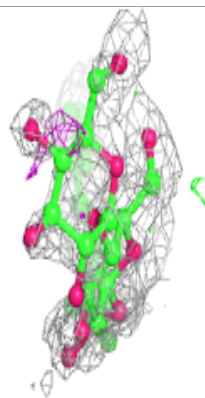
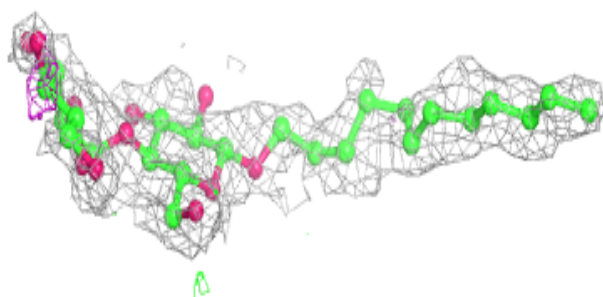
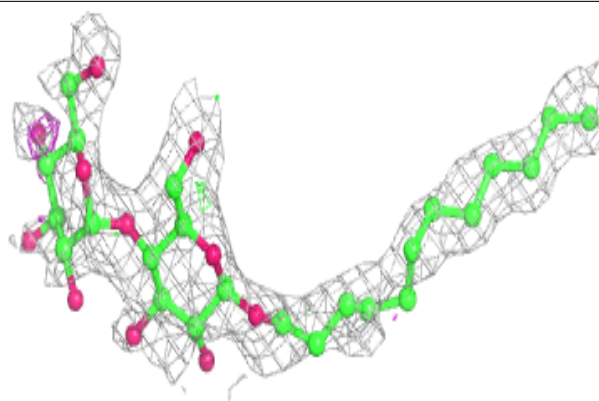
**Electron density around HTG b 628:**

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

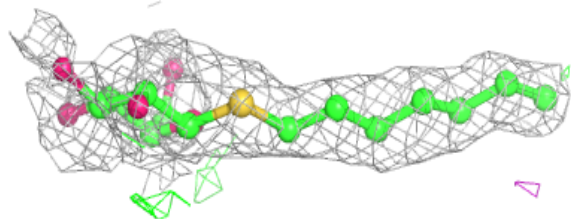
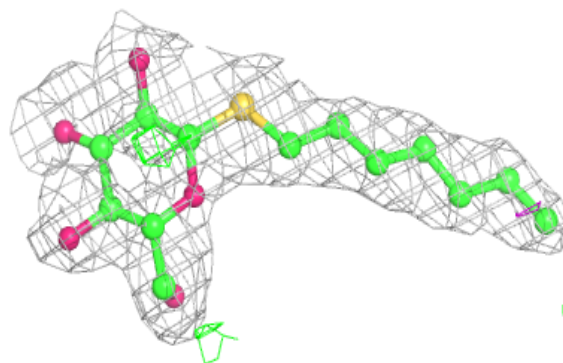


Electron density around LMT E 102:

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

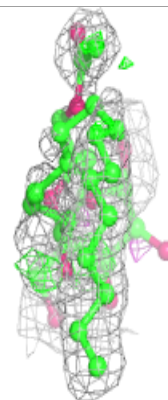
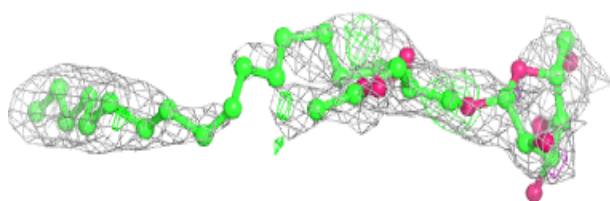
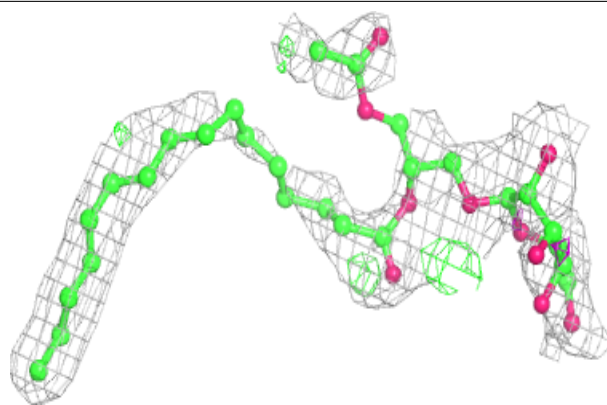
**Electron density around HTG b 604:**

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

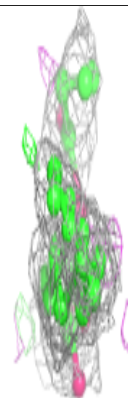
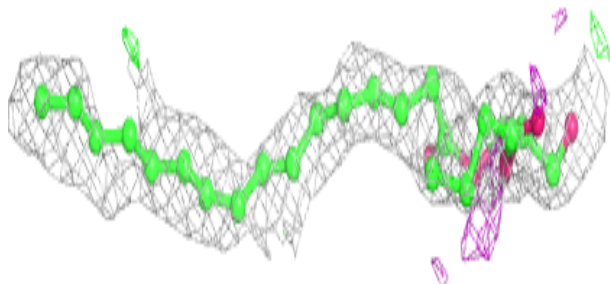
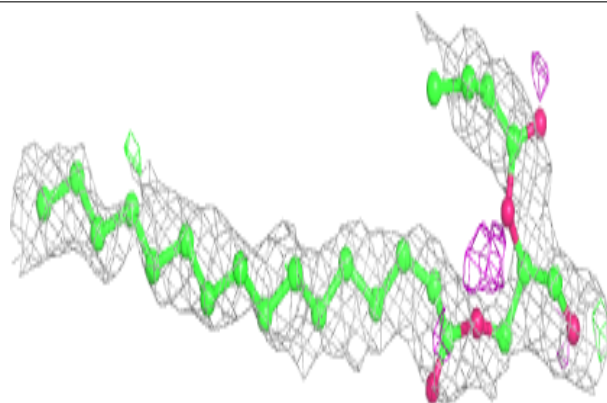


Electron density around LMG Z 101:

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

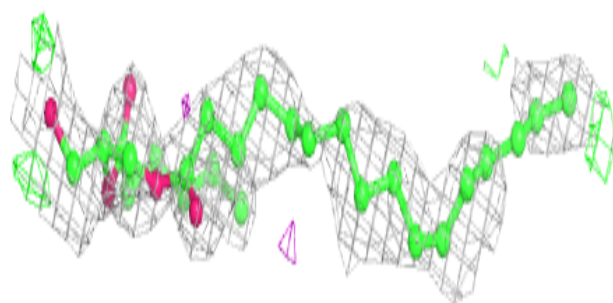
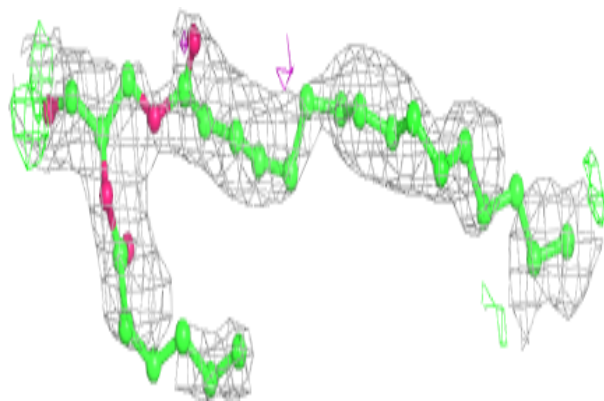
**Electron density around UNL A 415:**

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

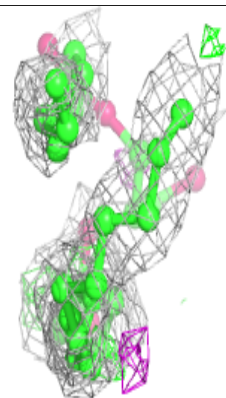
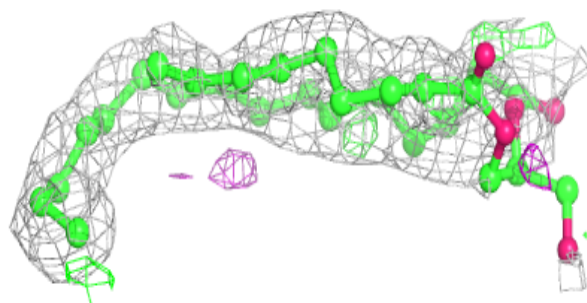
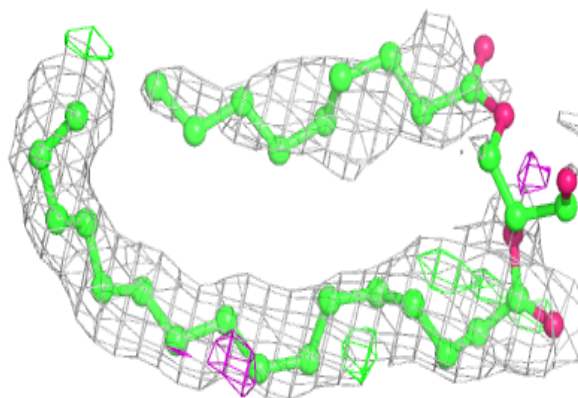


Electron density around UNL a 414:

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

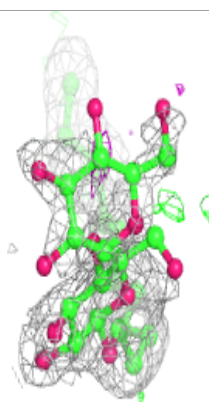
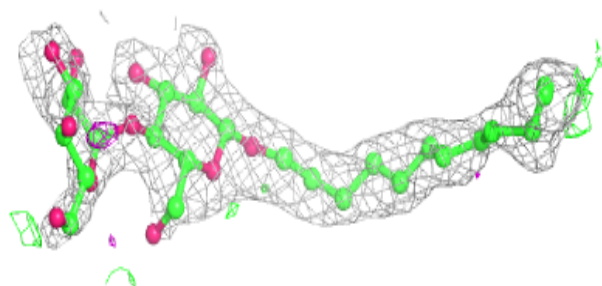
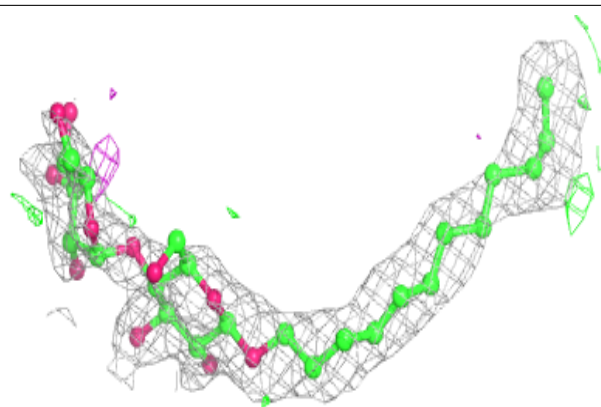
**Electron density around UNL b 634:**

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

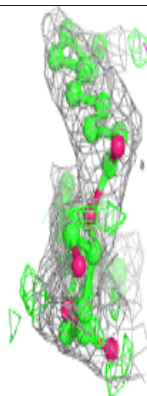
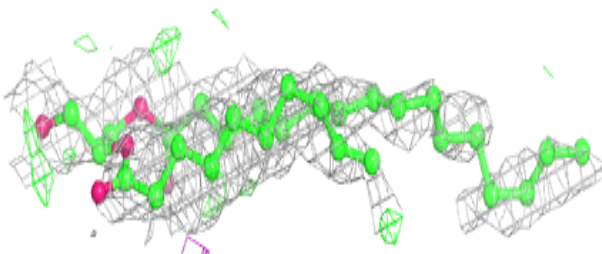
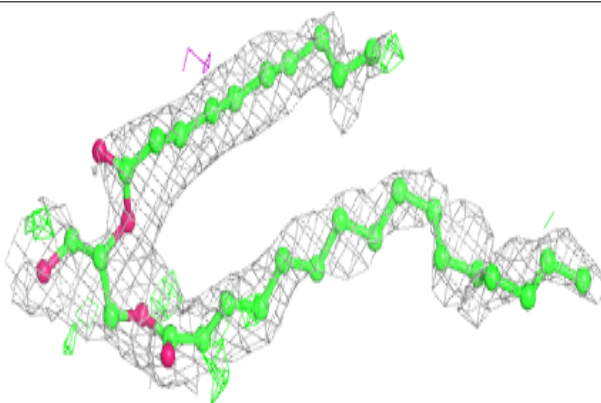


Electron density around LMT m 103:

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

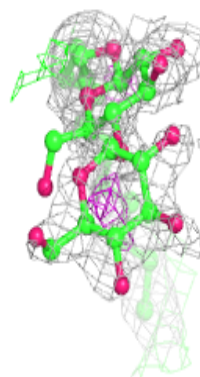
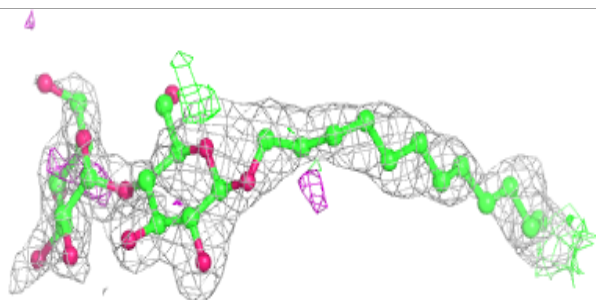
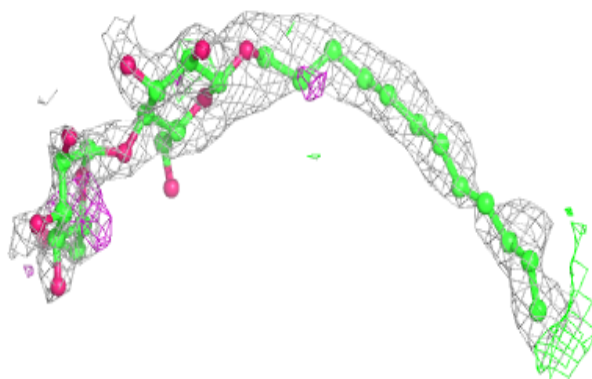
**Electron density around UNL C 526:**

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

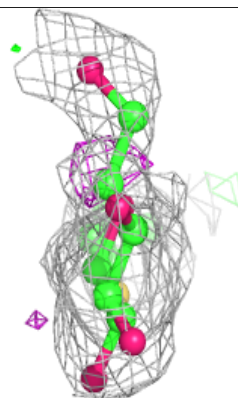
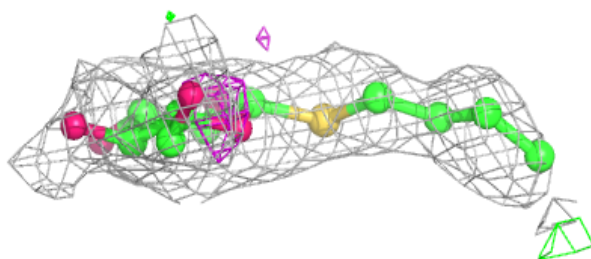
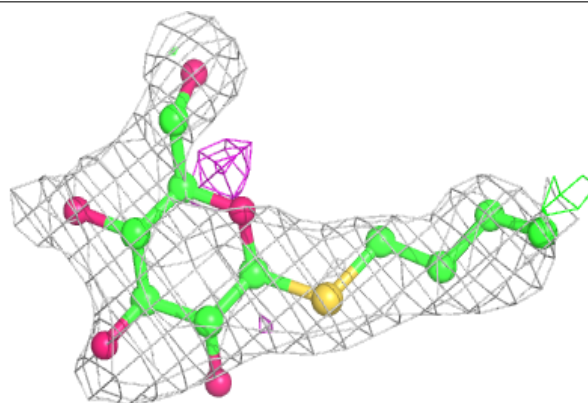


Electron density around LMT M 101:

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

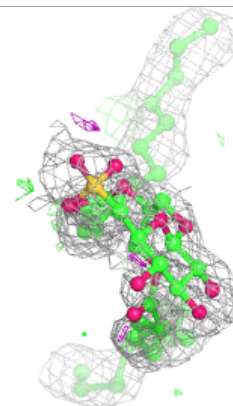
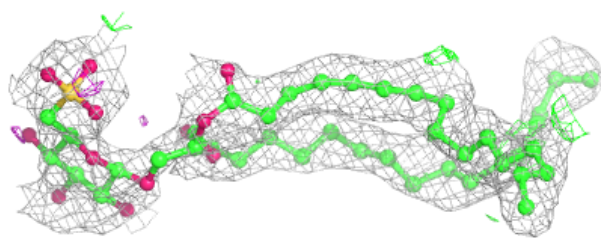
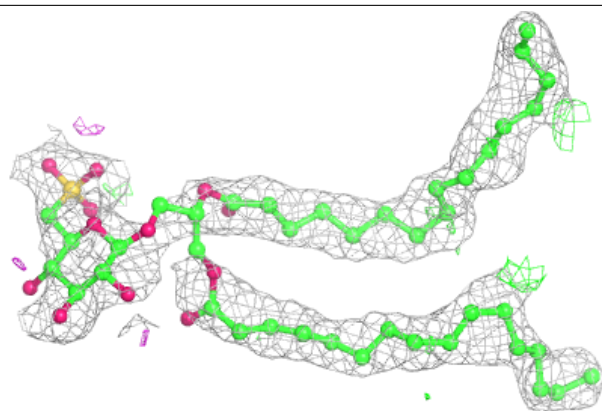
**Electron density around HTG d 411:**

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

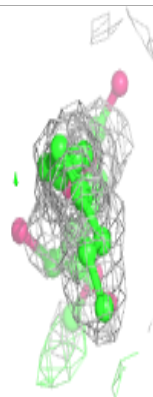
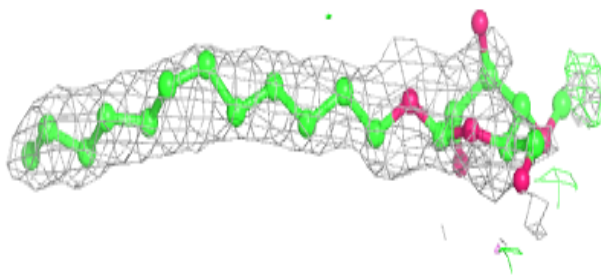
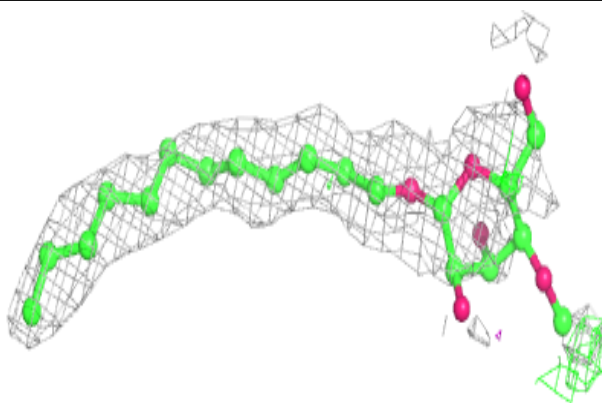


Electron density around SQD 1 101:

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

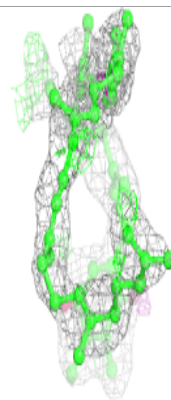
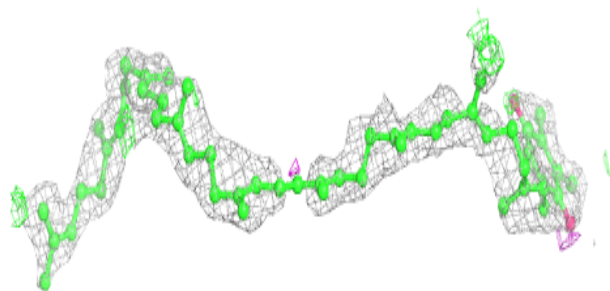
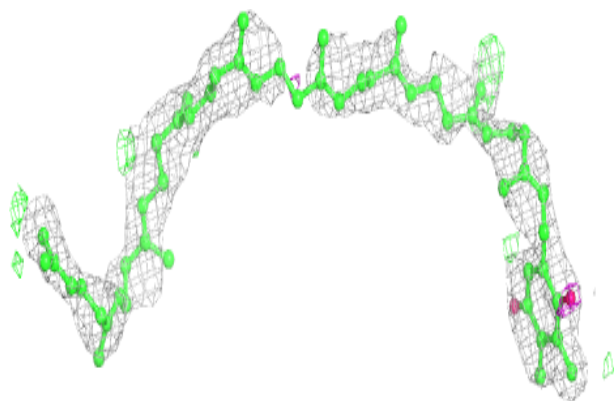
**Electron density around LMT b 626:**

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

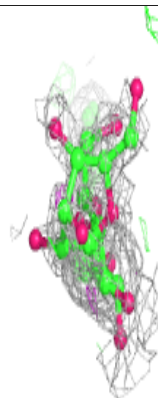
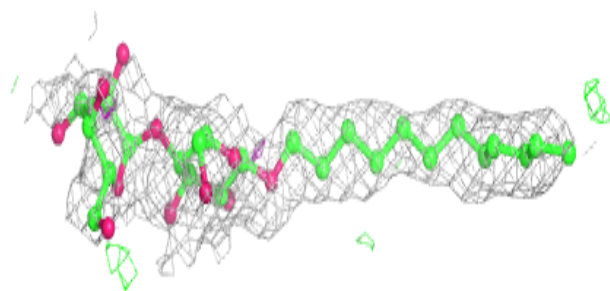
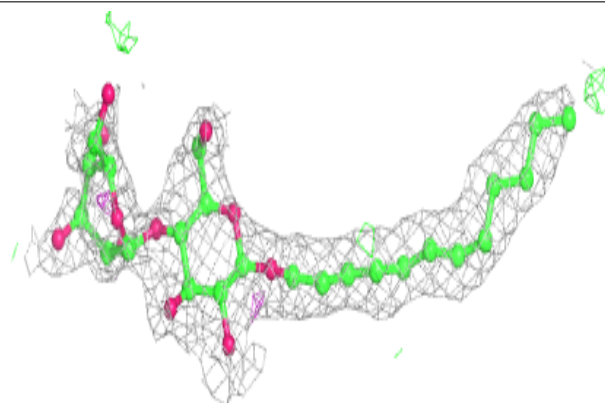


Electron density around PL9 A 419:

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

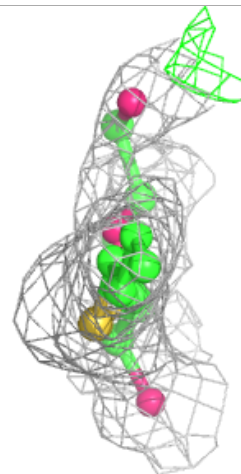
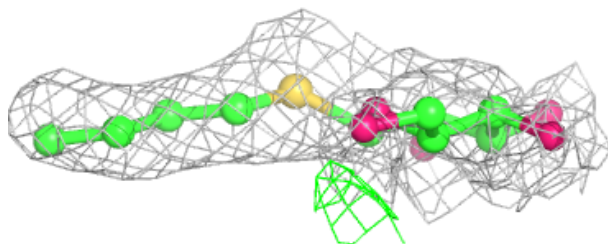
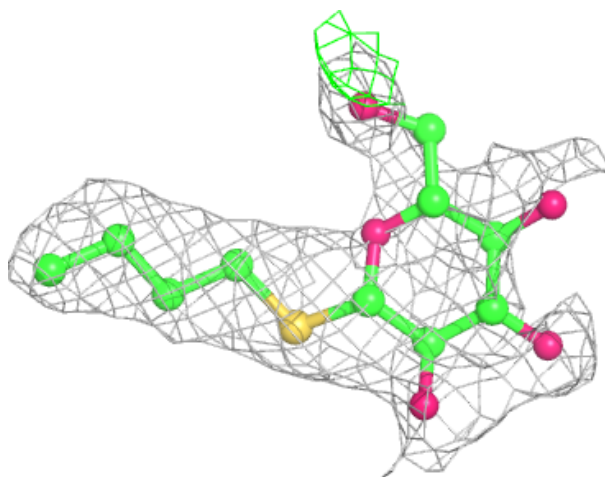
**Electron density around LMT D 402:**

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



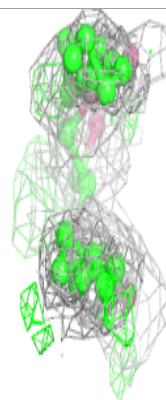
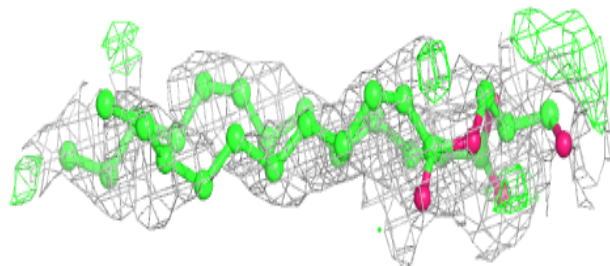
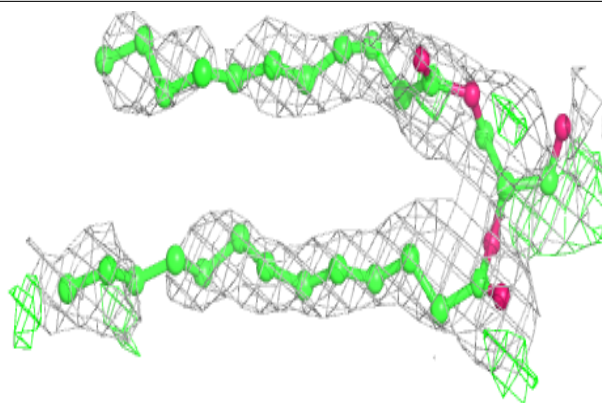
Electron density around HTG D 411:

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

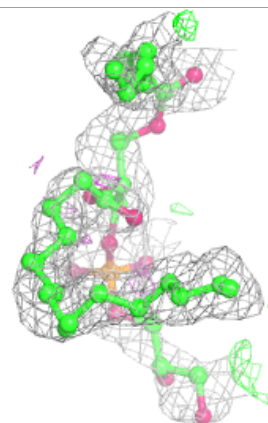
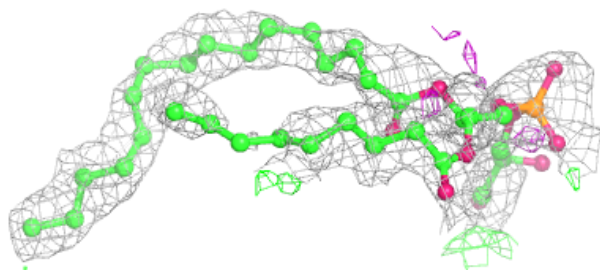
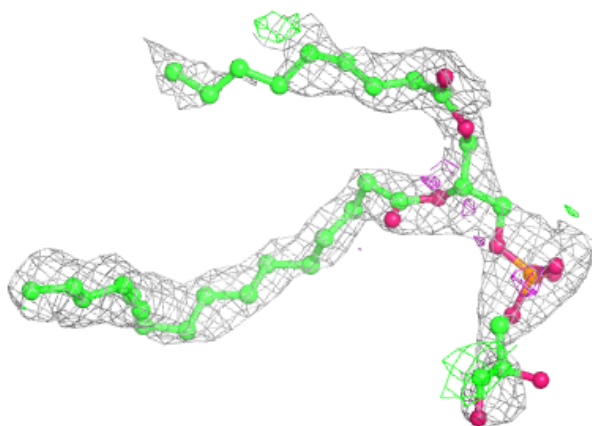


Electron density around UNL k 101:

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

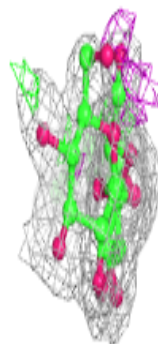
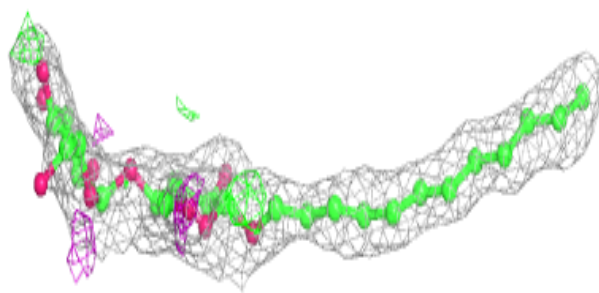
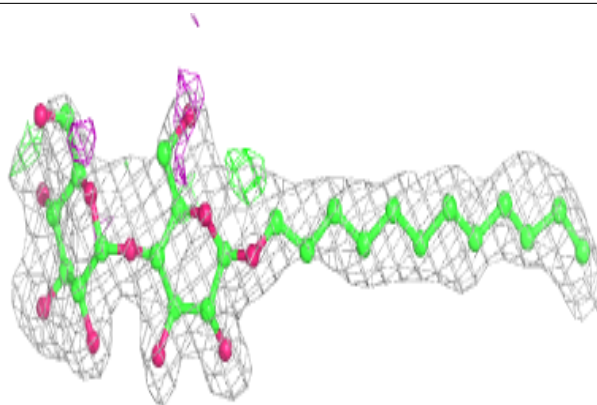
**Electron density around LHG E 101:**

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

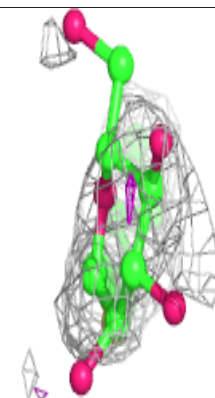
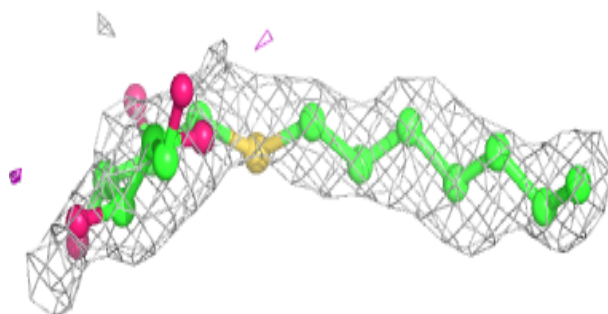
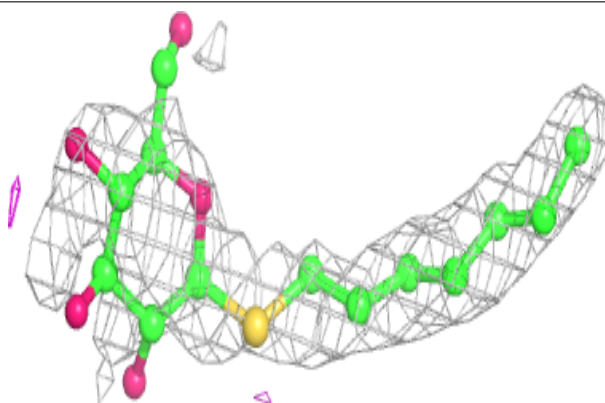


Electron density around LMT m 102:

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

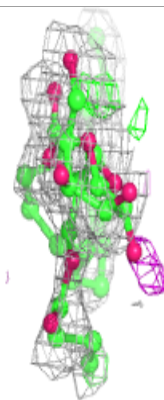
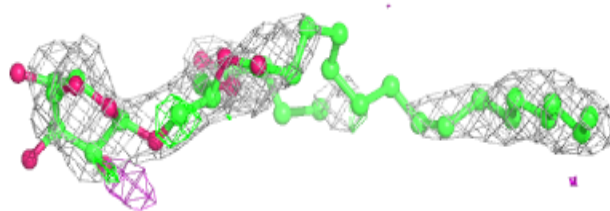
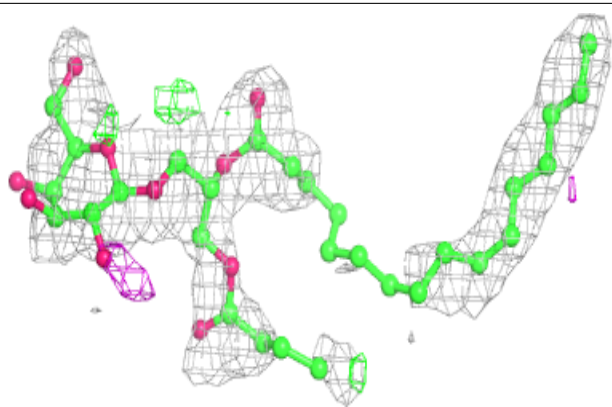
**Electron density around HTG B 624:**

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

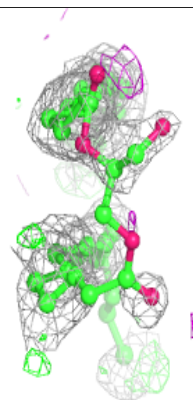
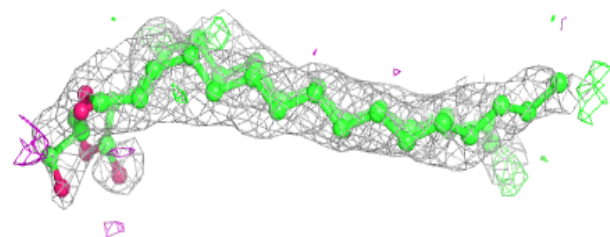
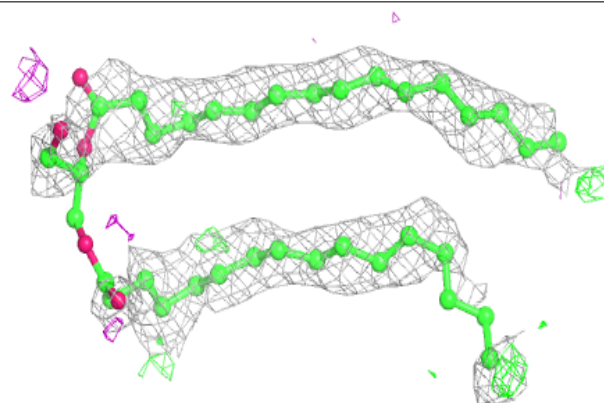


Electron density around LMG z 101:

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

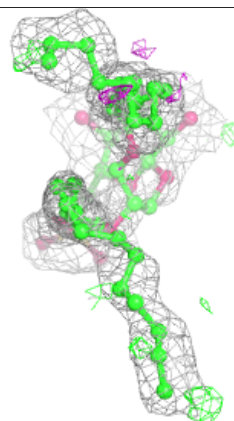
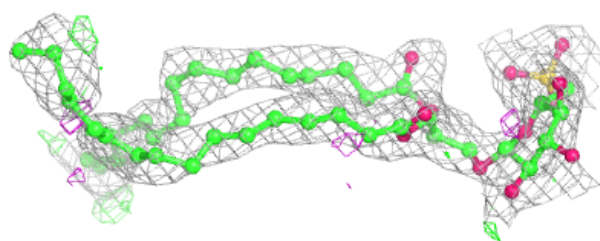
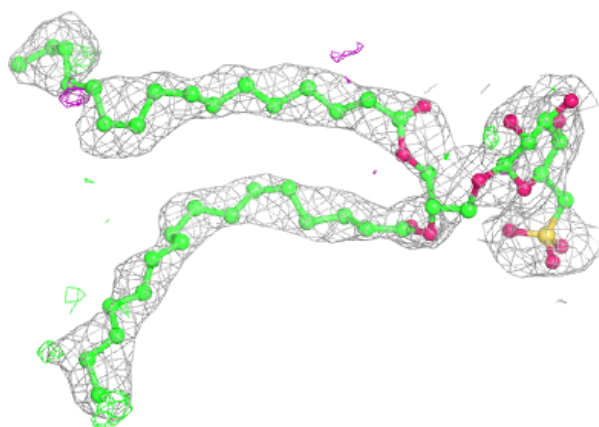
**Electron density around UNL i 101:**

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

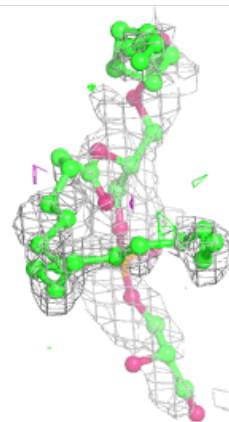
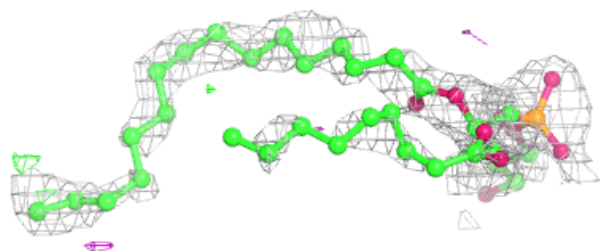
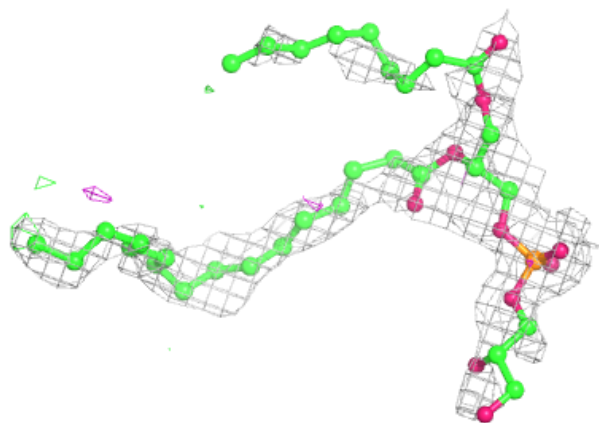


Electron density around SQD b 601:

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

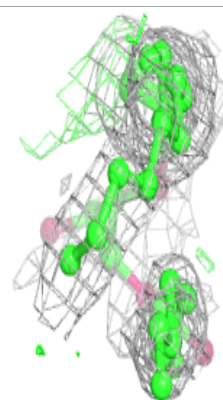
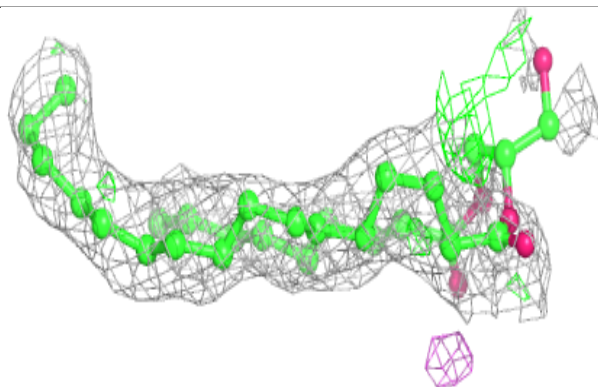
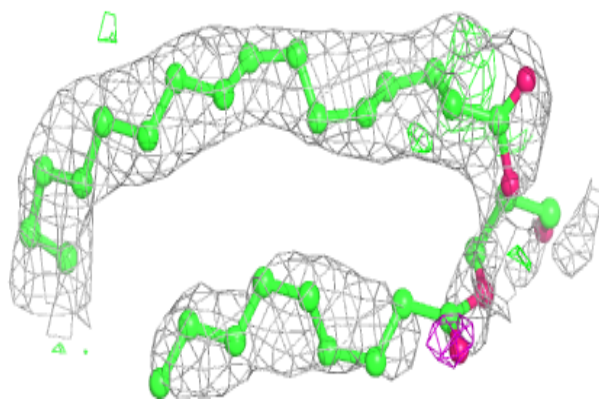
**Electron density around LHG e 101:**

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

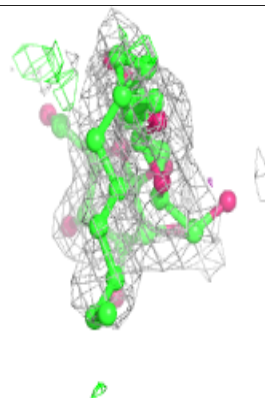
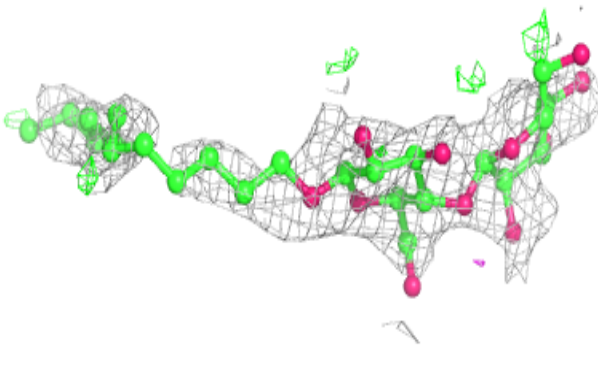
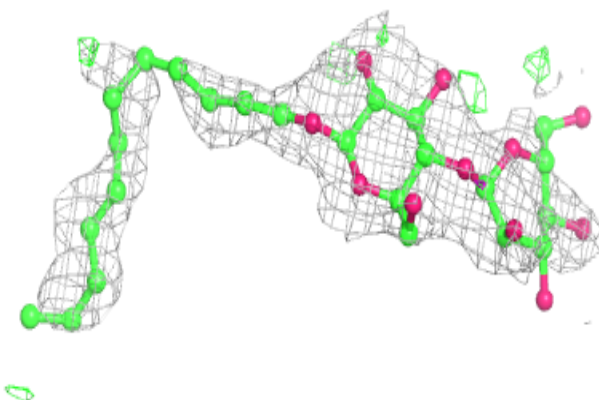


Electron density around UNL B 632:

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

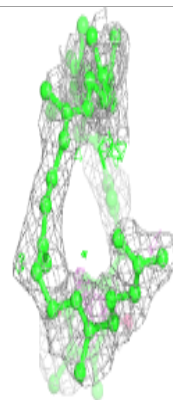
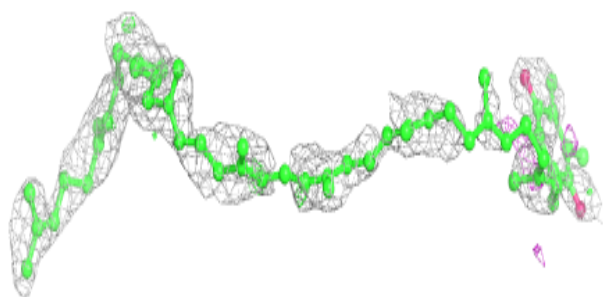
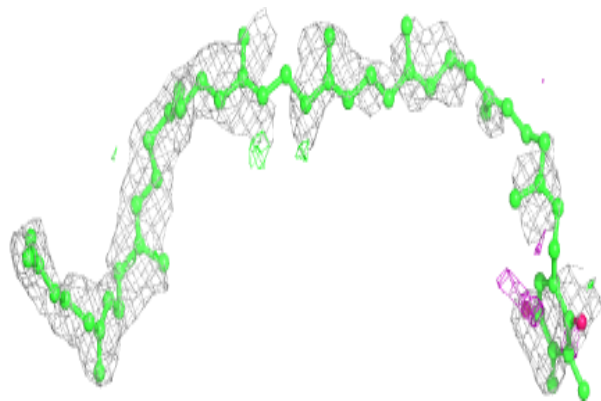
**Electron density around LMT I 102:**

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

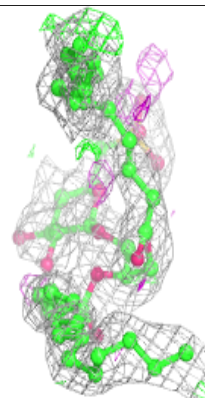
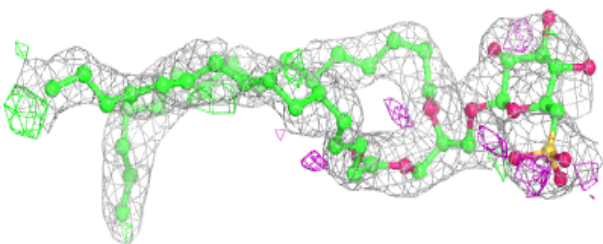
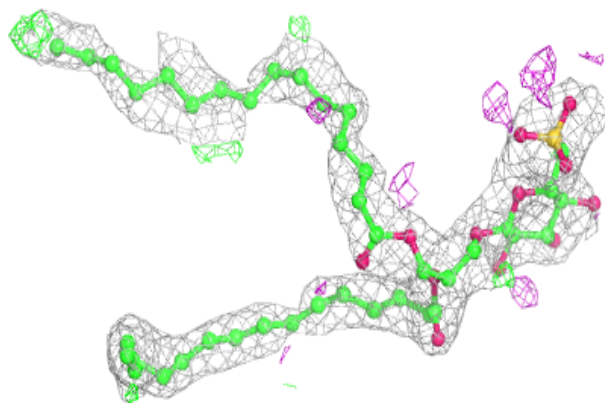


Electron density around PL9 a 416:

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

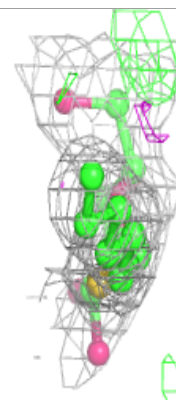
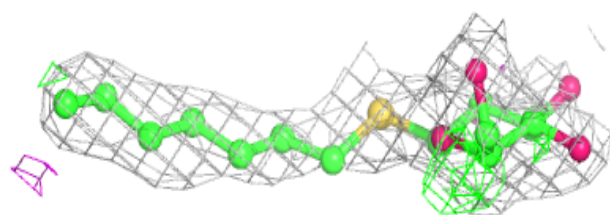
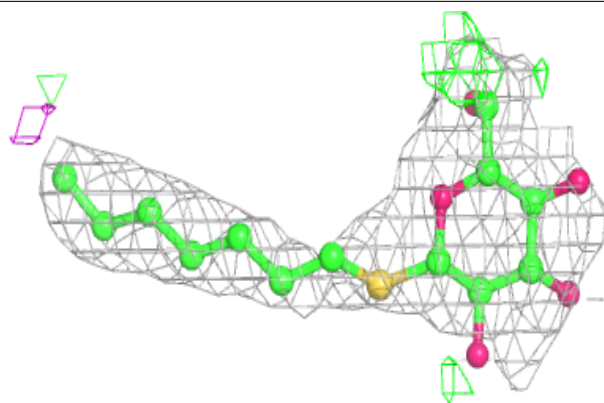
**Electron density around SQD a 402:**

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

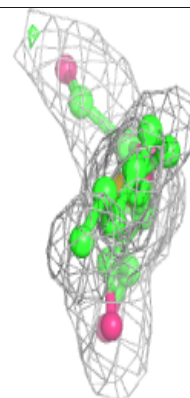
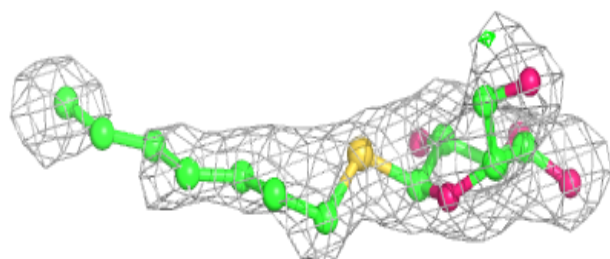
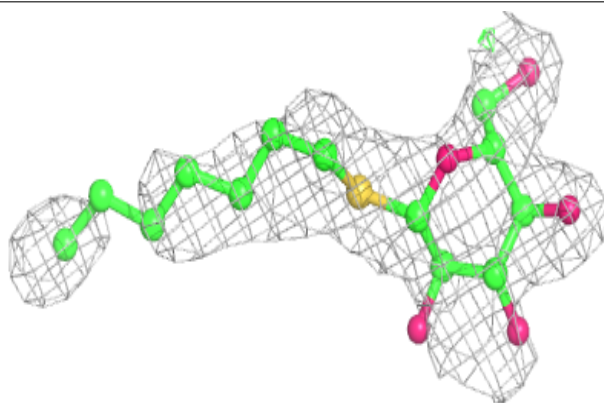


Electron density around HTG B 631:

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

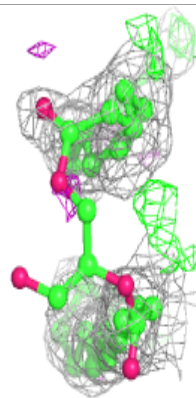
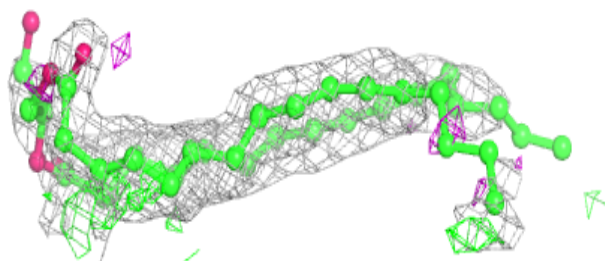
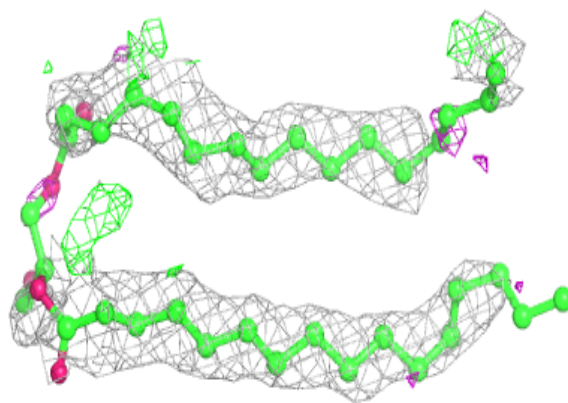
**Electron density around HTG C 523:**

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

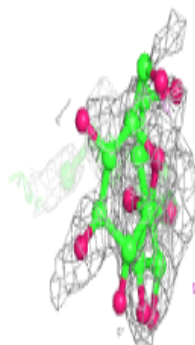
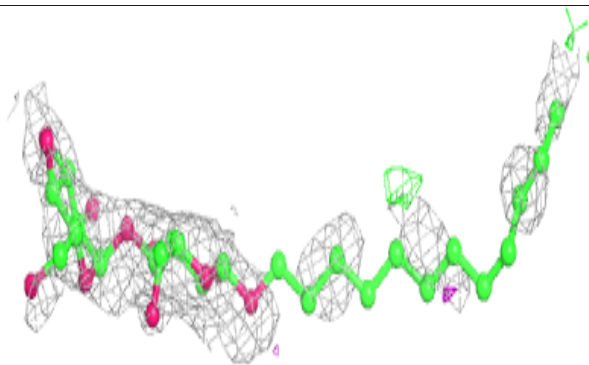
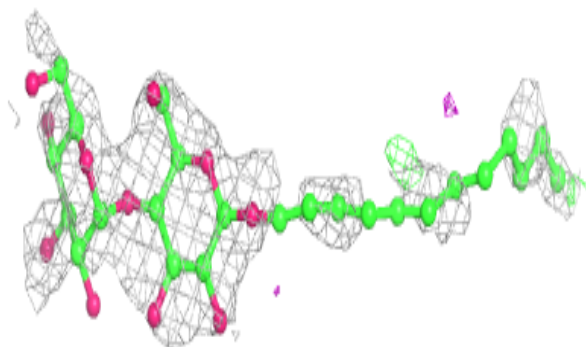


Electron density around UNL I 101:

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

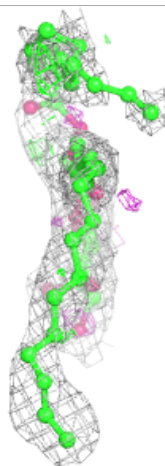
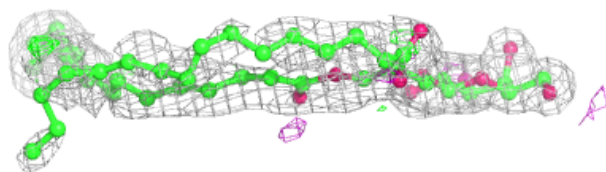
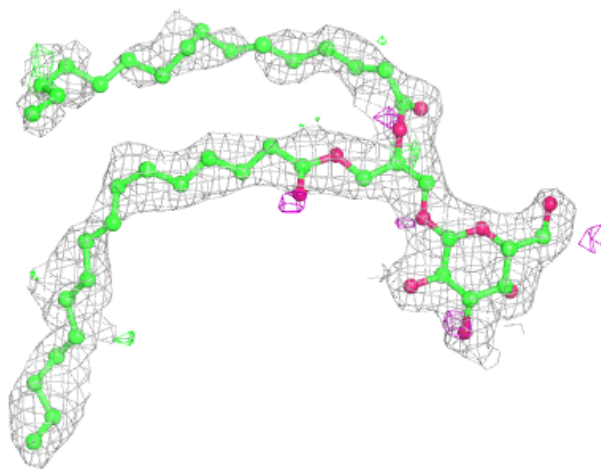
**Electron density around LMT a 417:**

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



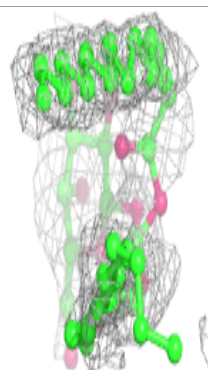
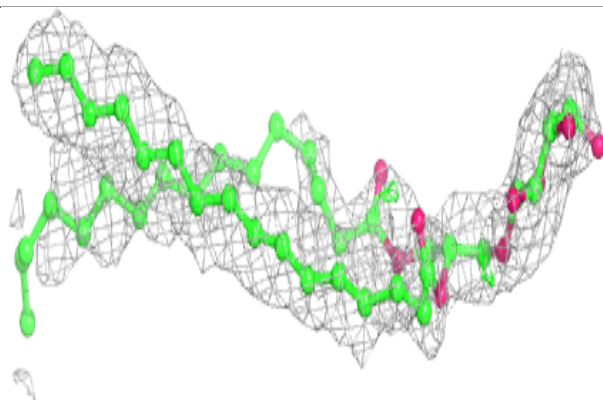
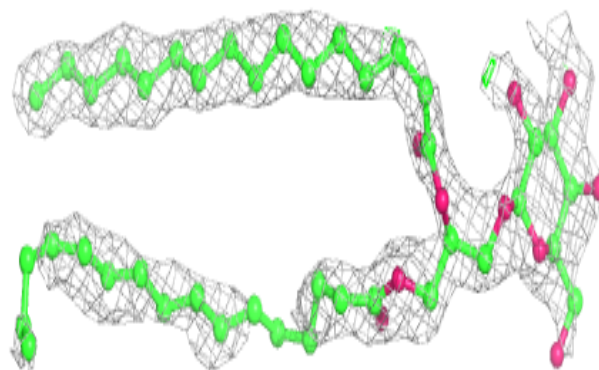
Electron density around LMG C 520:

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

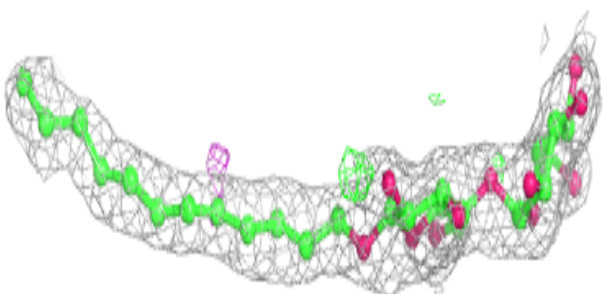
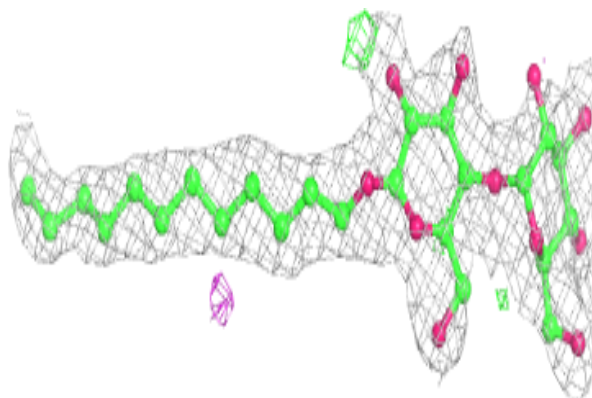


Electron density around LMG c 521:

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

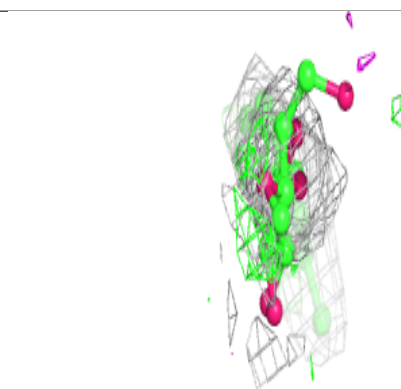
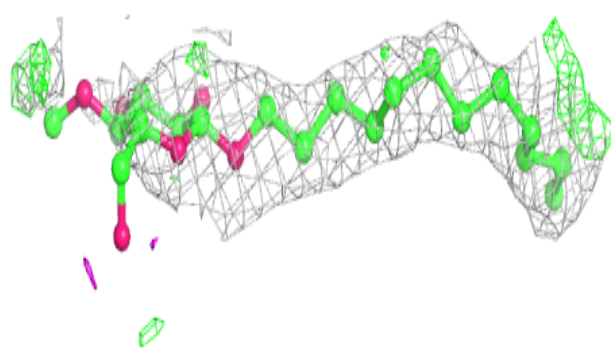
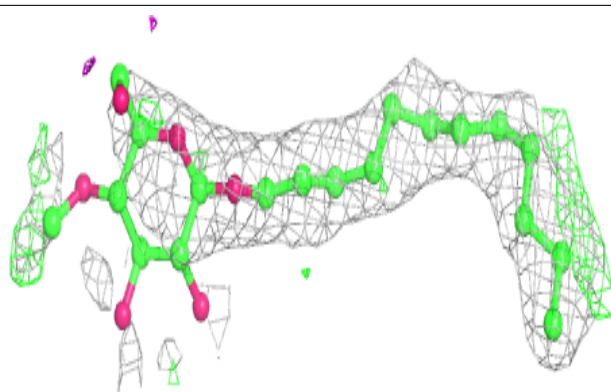
**Electron density around LMT M 102:**

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

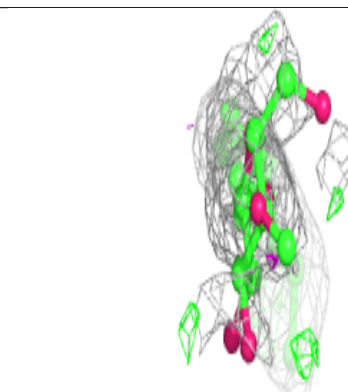
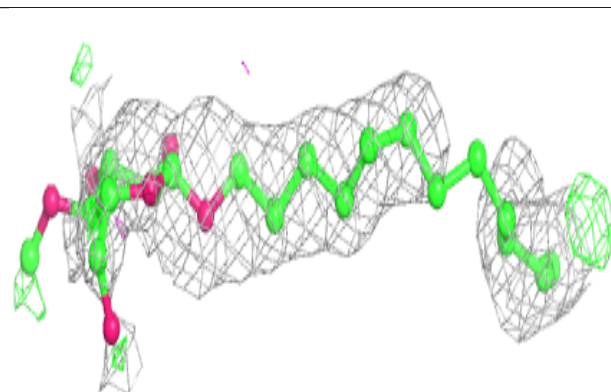
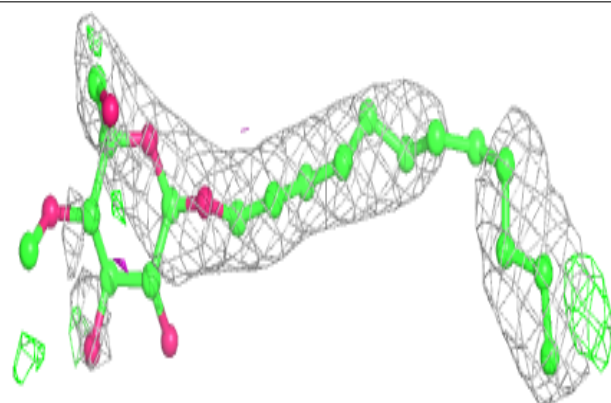


Electron density around LMT B 634:

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

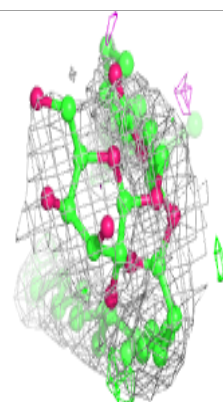
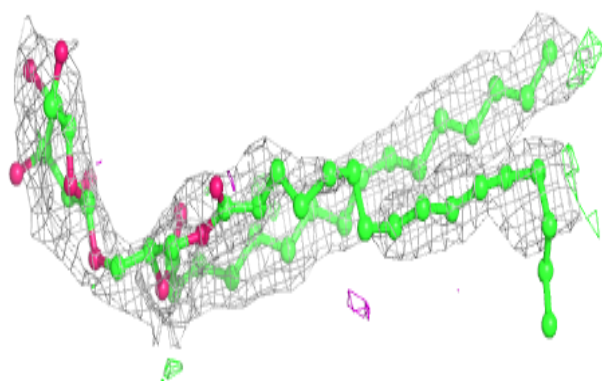
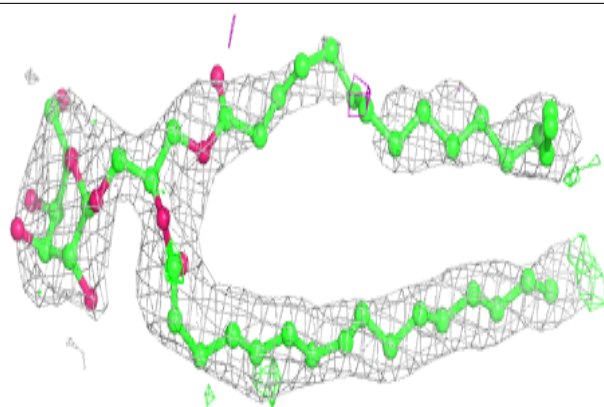
**Electron density around LMT b 602:**

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

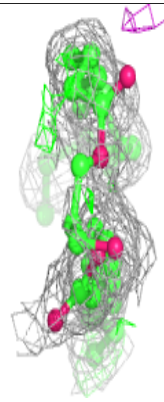
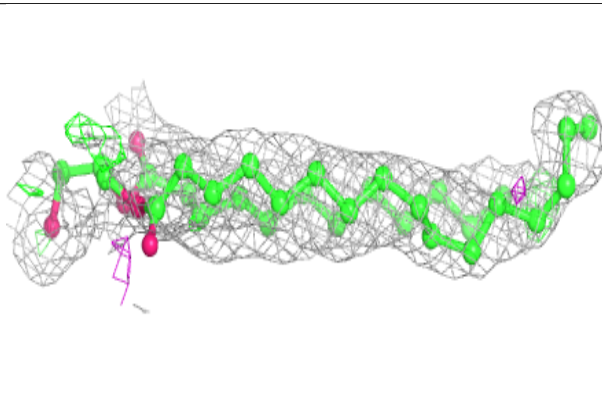
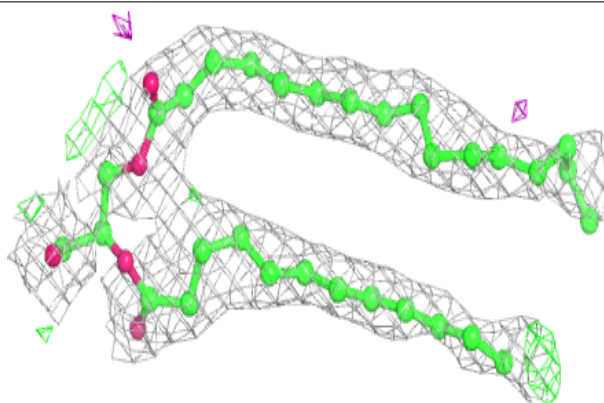


Electron density around LMG C 521:

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

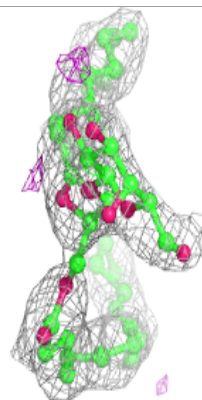
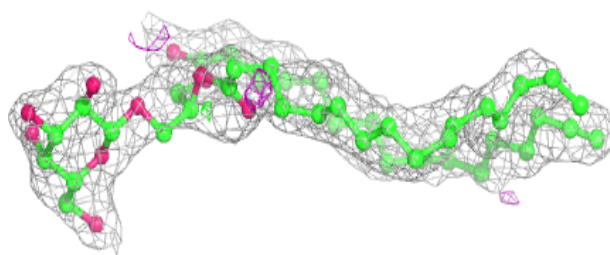
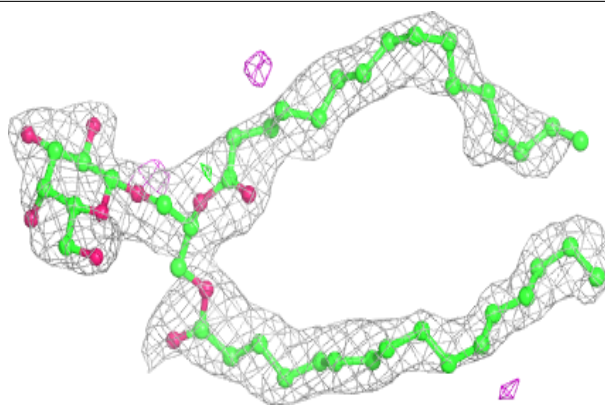
**Electron density around UNL d 413:**

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

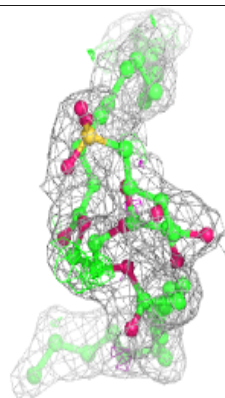
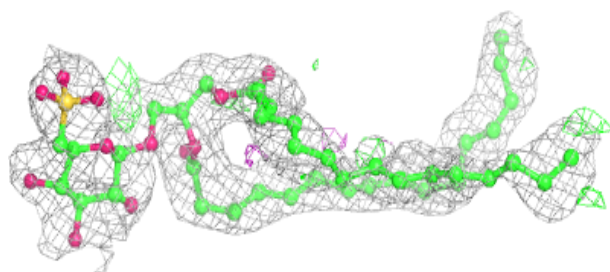
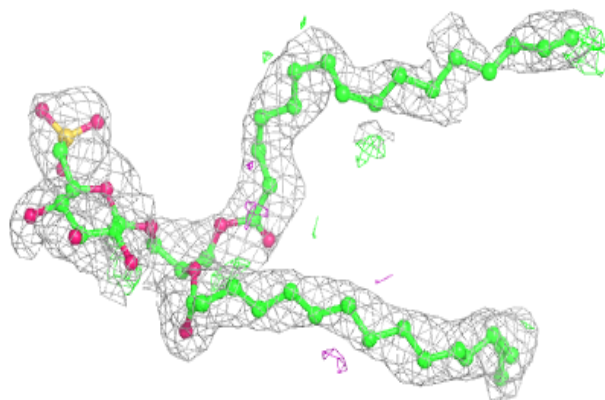


Electron density around LMG c 501:

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

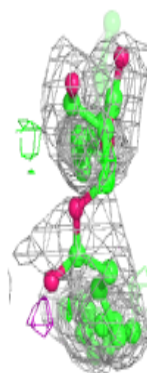
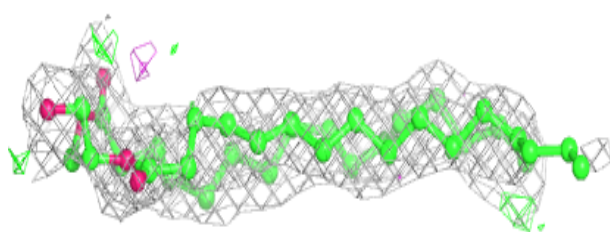
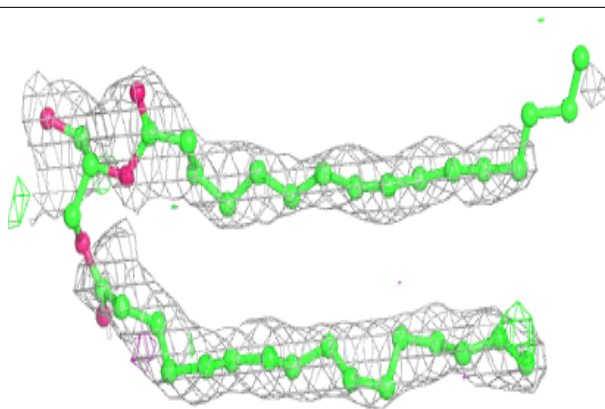
**Electron density around SQD A 416:**

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

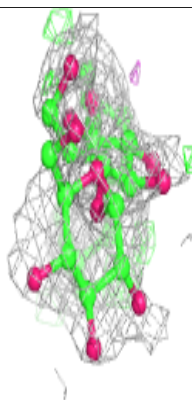
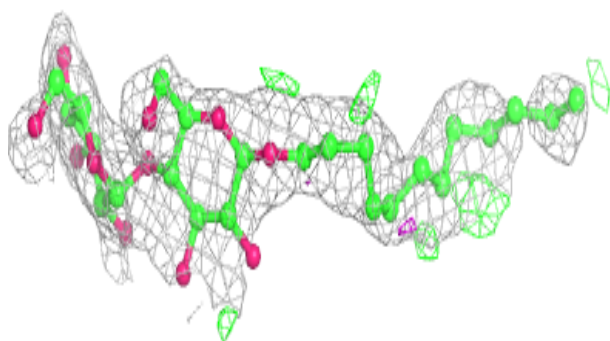
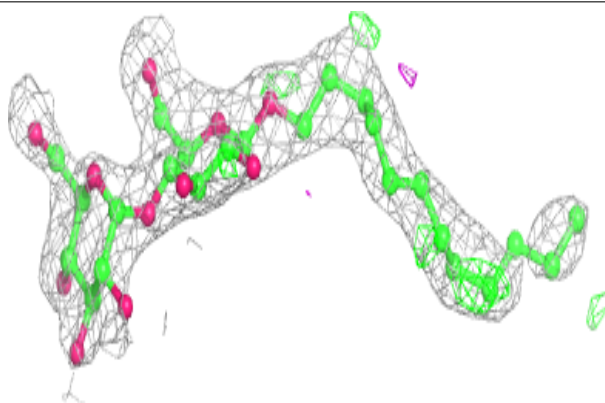


Electron density around UNL D 413:

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

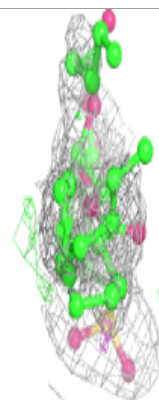
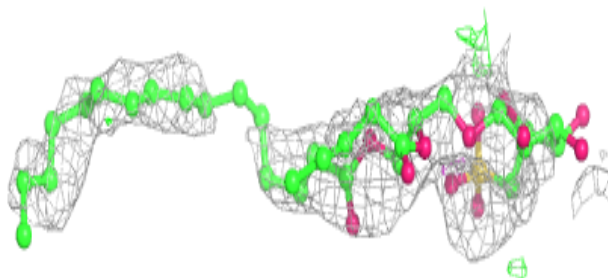
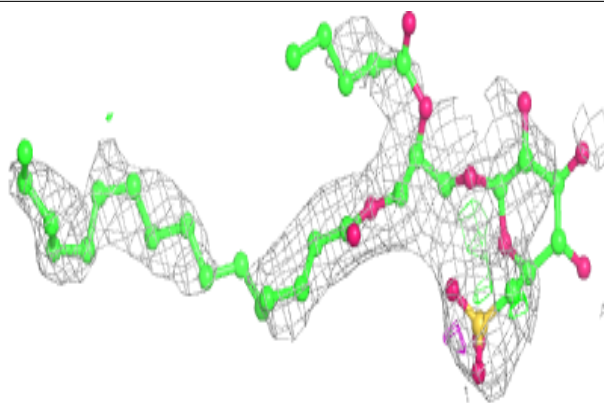
**Electron density around LMT a 401:**

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

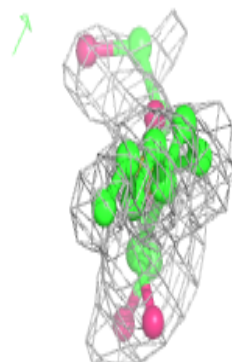
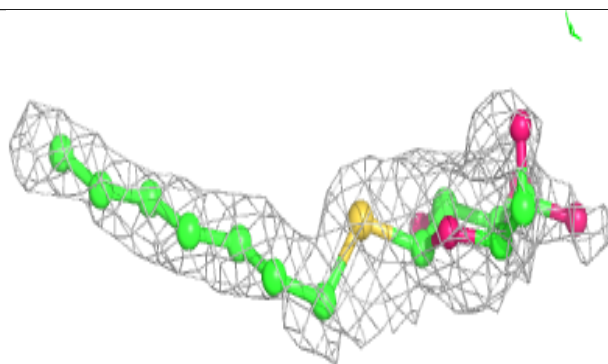
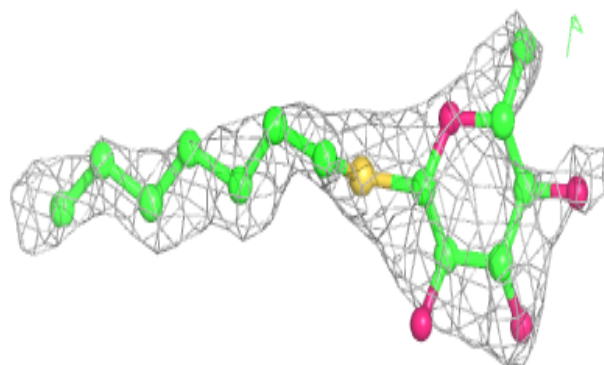


Electron density around SQD f 101:

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

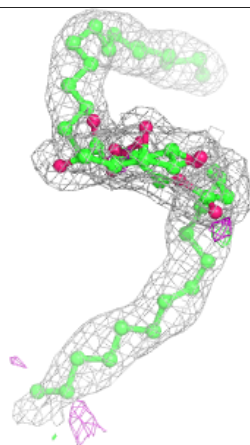
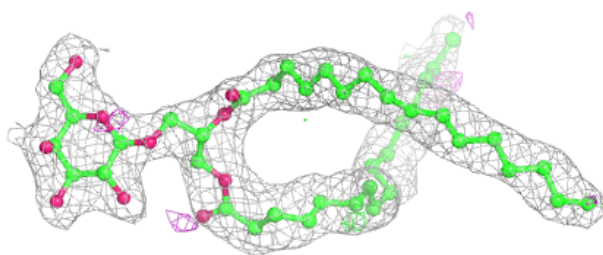
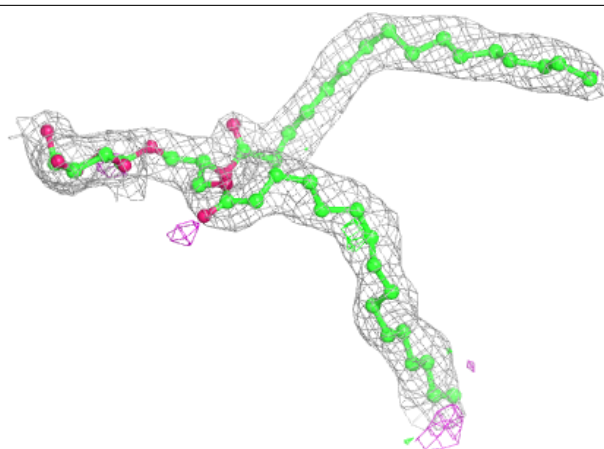
**Electron density around HTG c 523:**

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



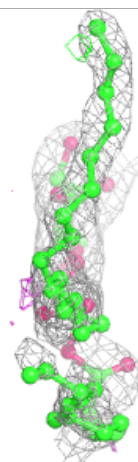
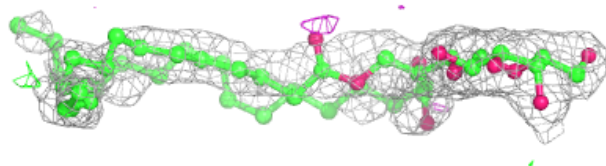
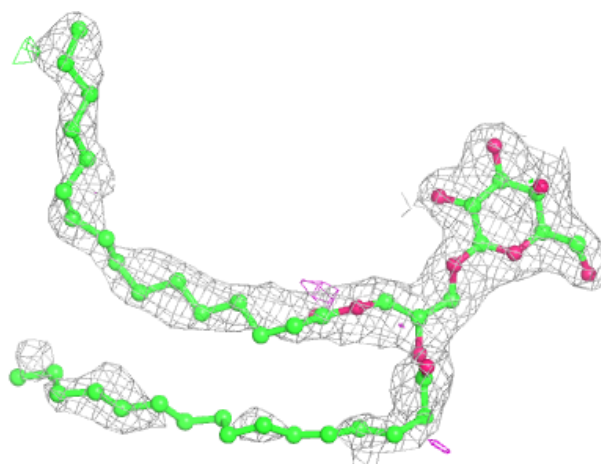
Electron density around LMG B 621:

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



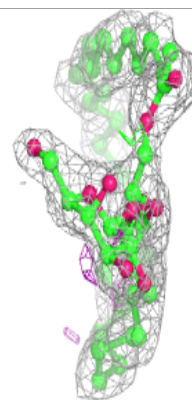
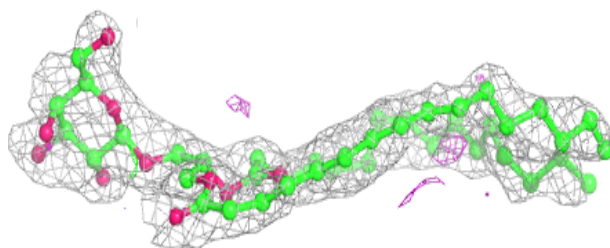
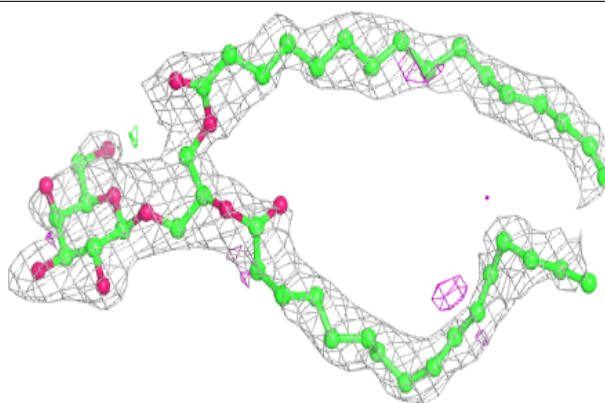
Electron density around LMG c 520:

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

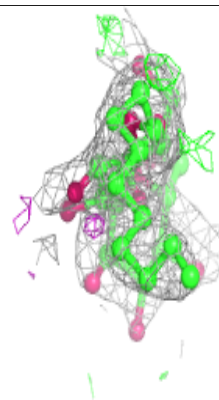
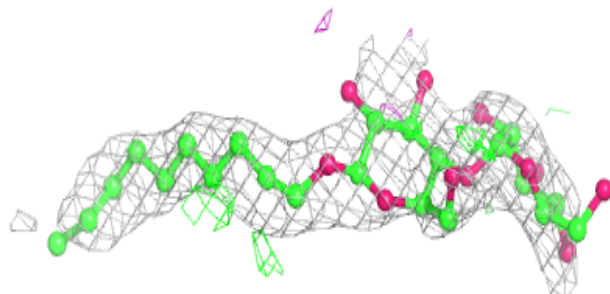
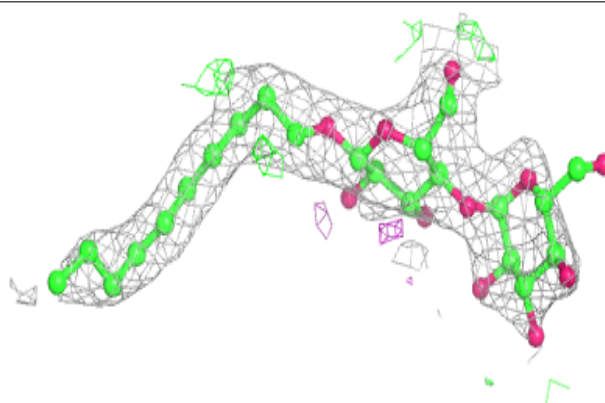


Electron density around LMG C 501:

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

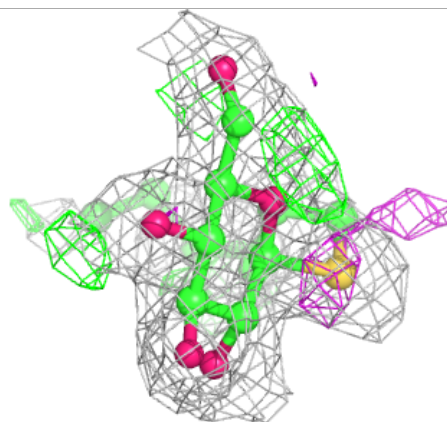
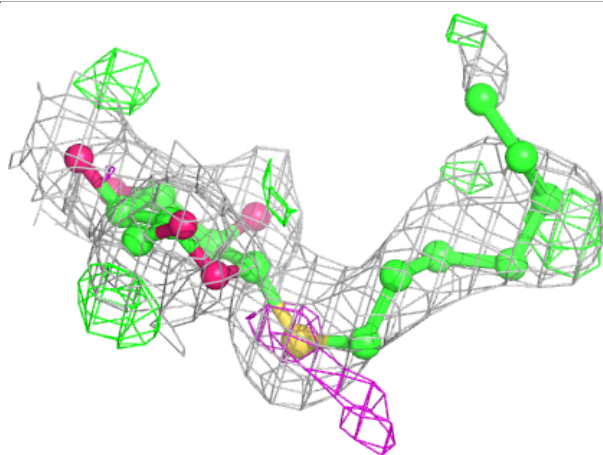
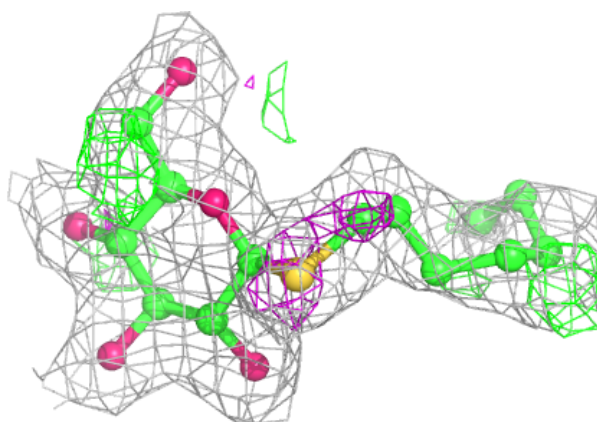
**Electron density around LMT A 417:**

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



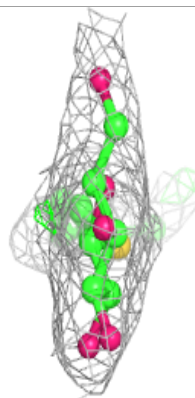
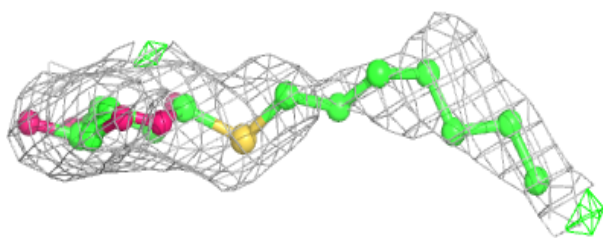
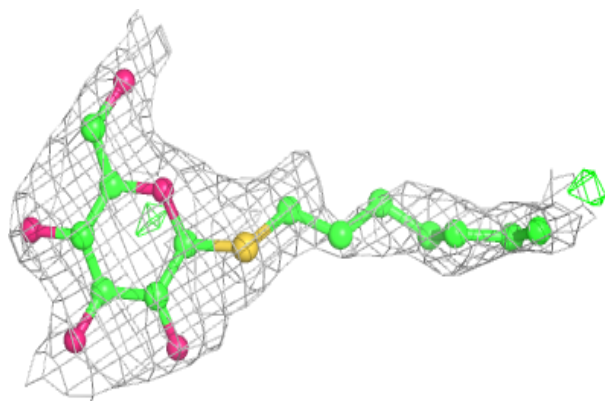
Electron density around HTG B 623:

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

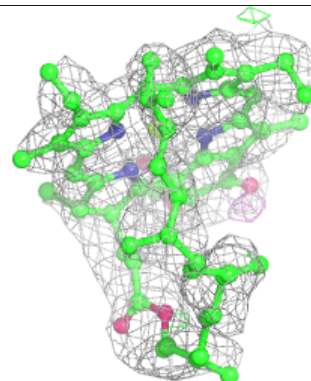
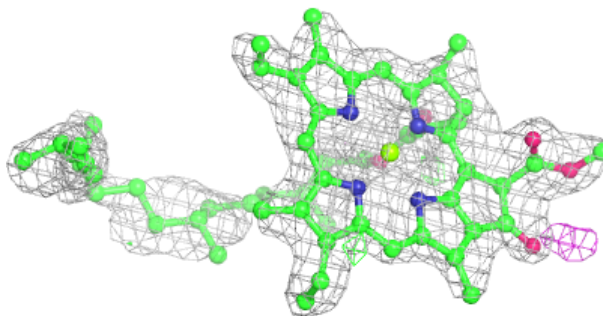
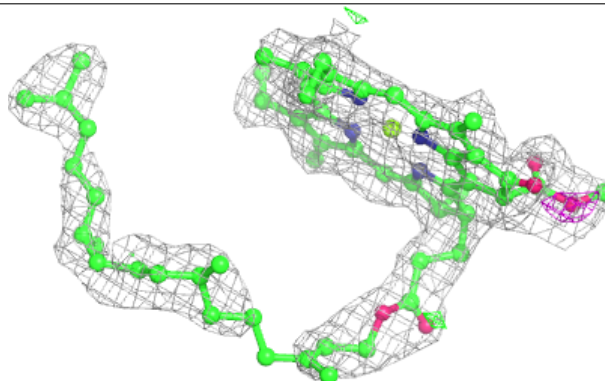


Electron density around HTG c 522:

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

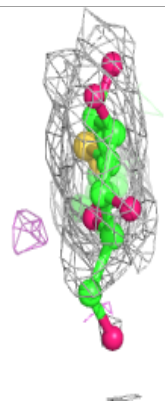
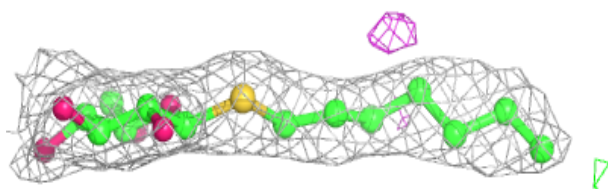
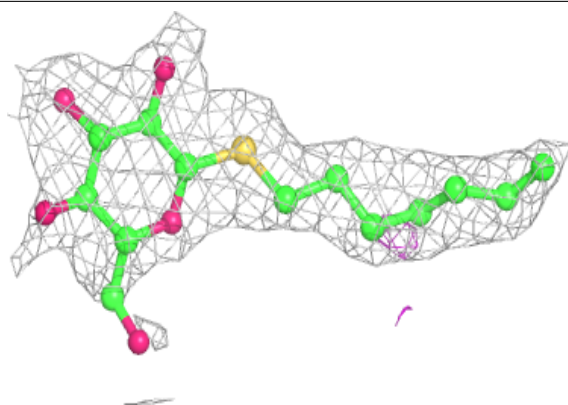
**Electron density around CLA c 515:**

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

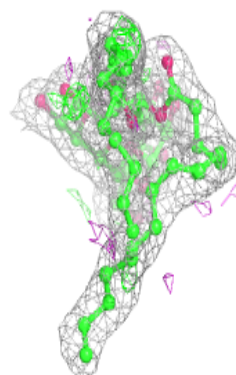
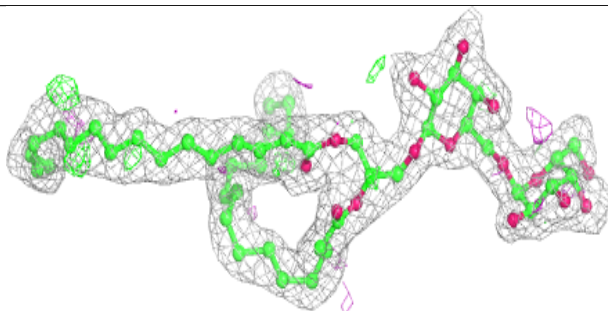
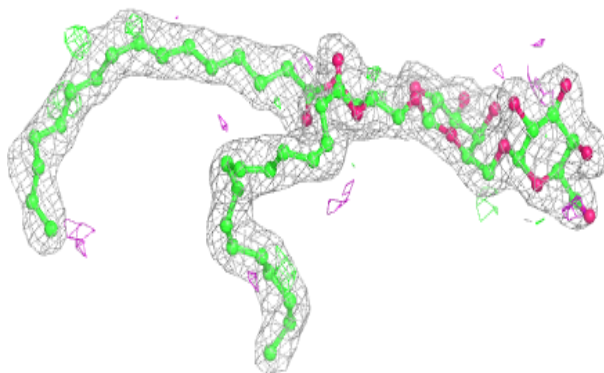


Electron density around HTG B 630:

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

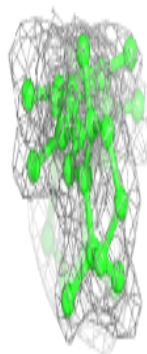
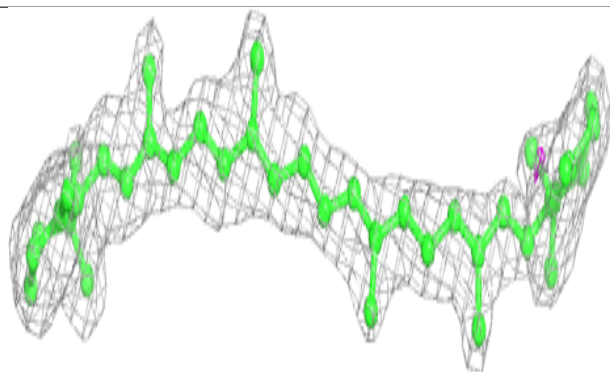
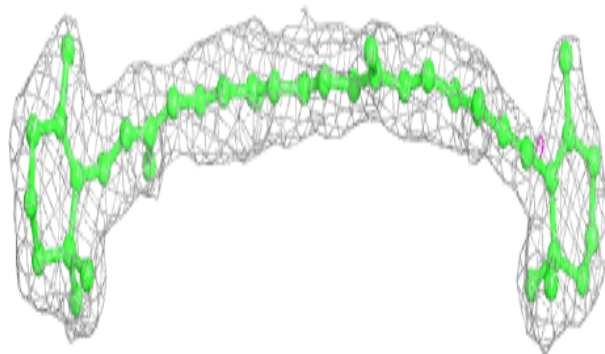
**Electron density around DGD H 102:**

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

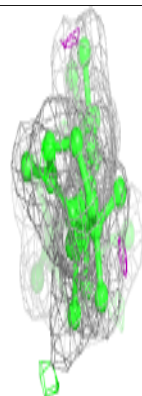
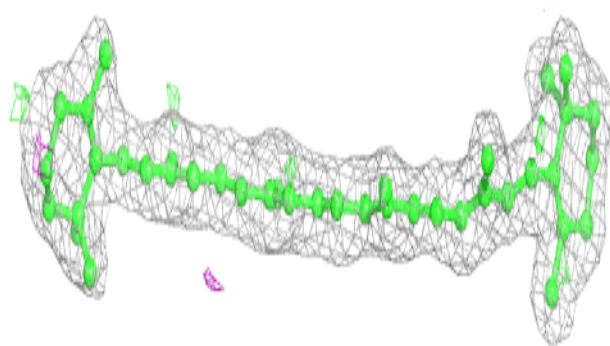
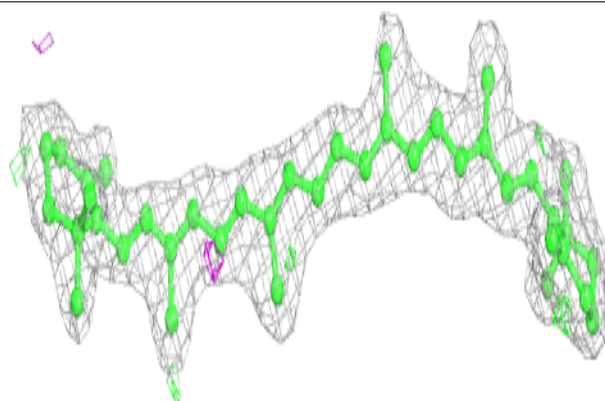


Electron density around BCR k 103:

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

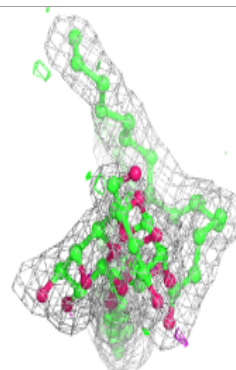
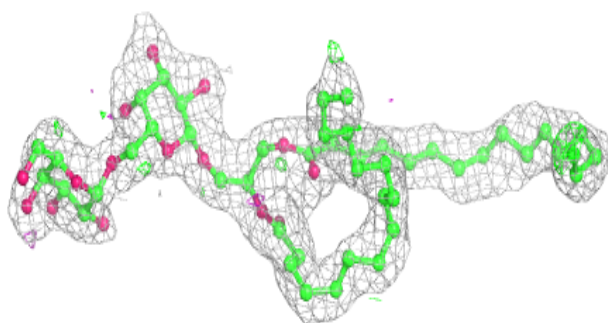
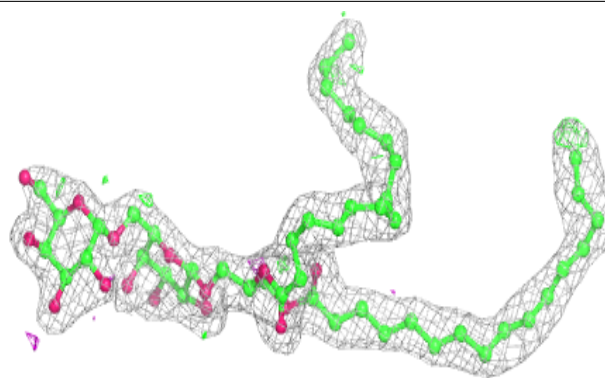
**Electron density around BCR h 101:**

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

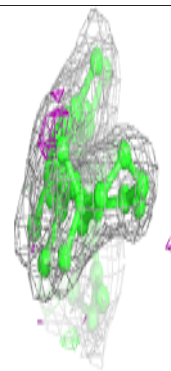
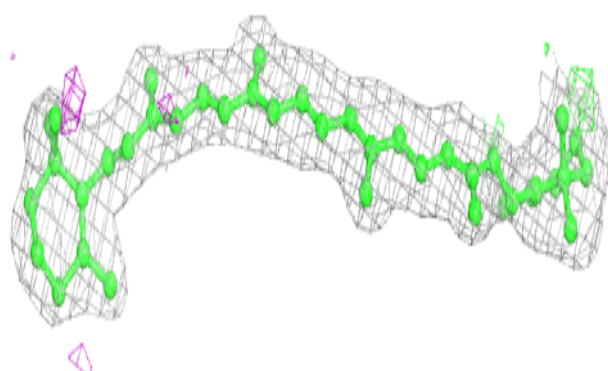
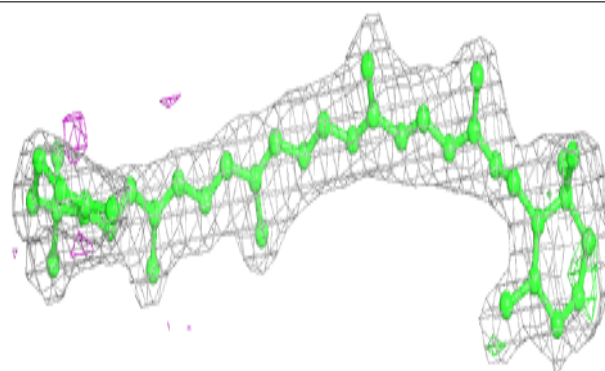


Electron density around DGD h 102:

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

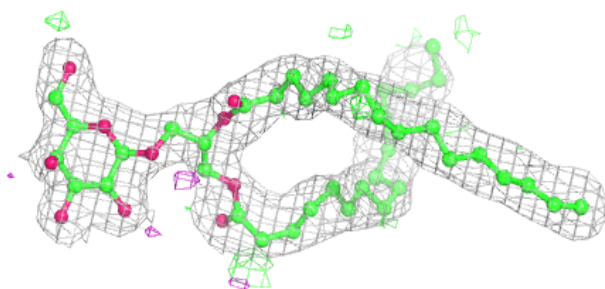
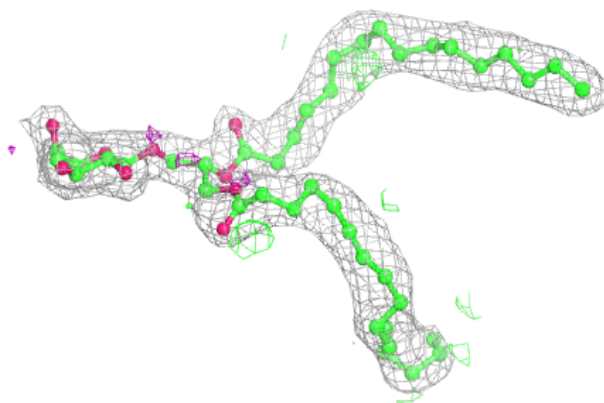
**Electron density around BCR d 405:**

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

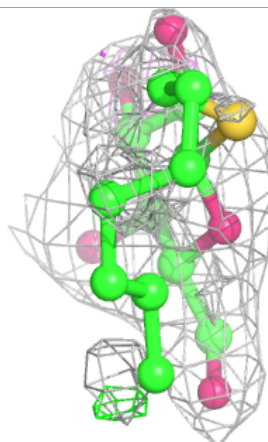
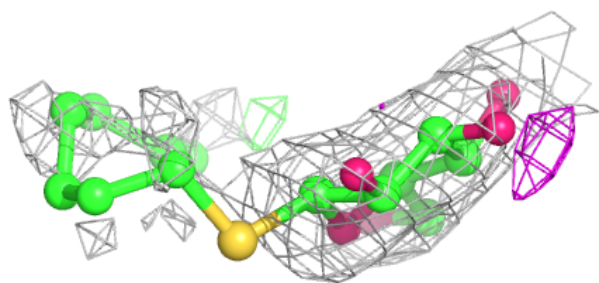
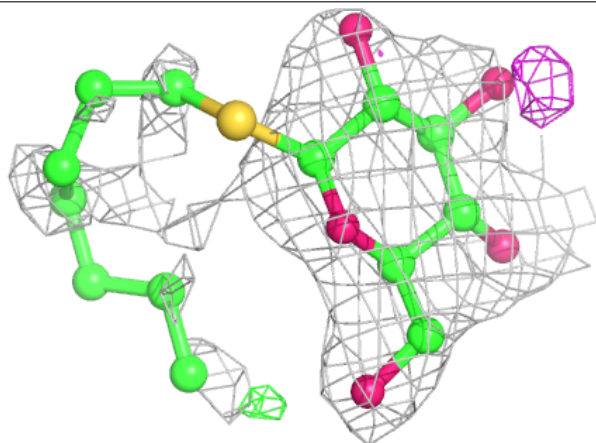


Electron density around LMG b 625:

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

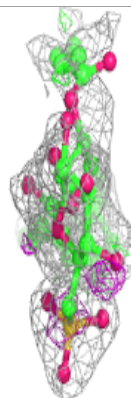
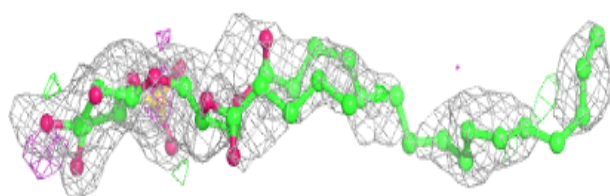
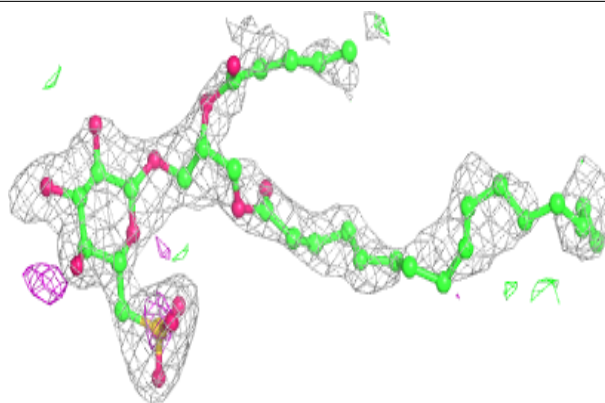
**Electron density around HTG V 204:**

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

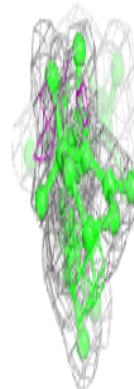
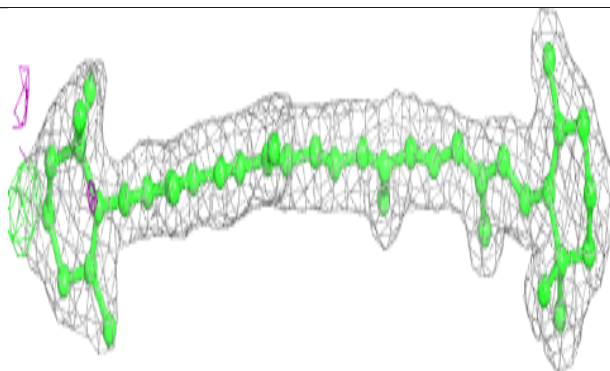
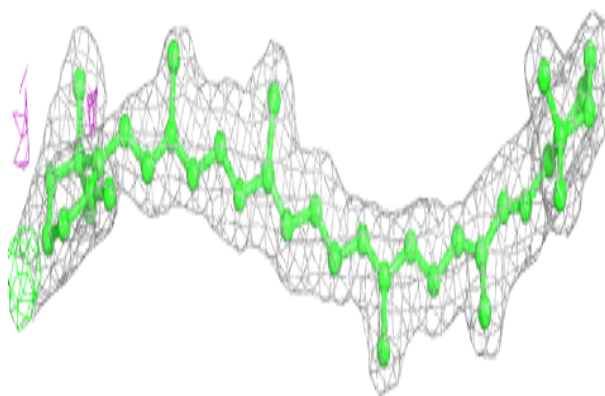


Electron density around SQD F 101:

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

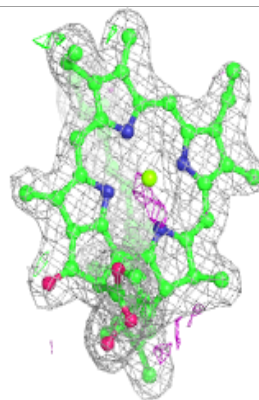
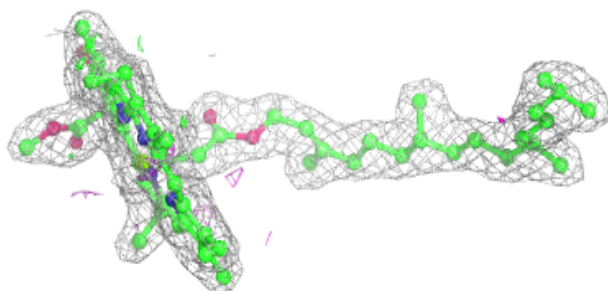
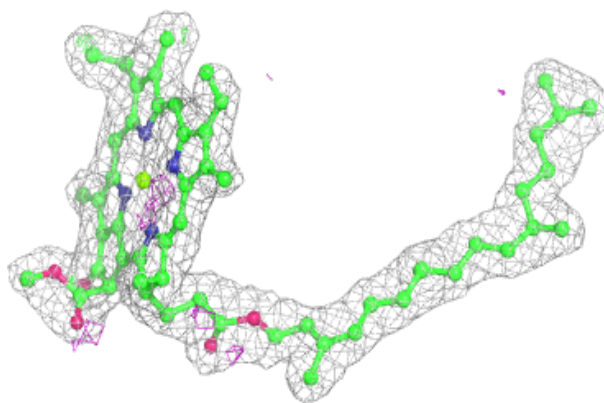
**Electron density around BCR H 101:**

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



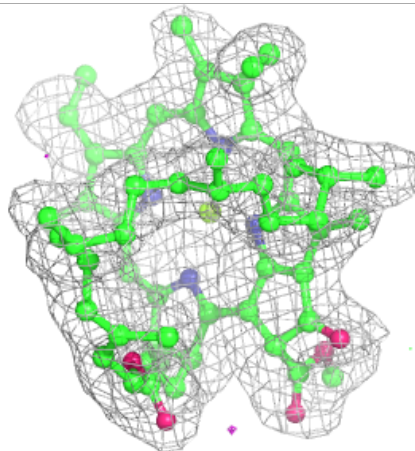
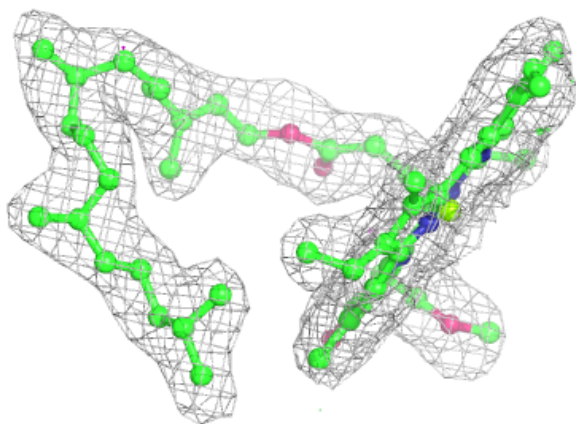
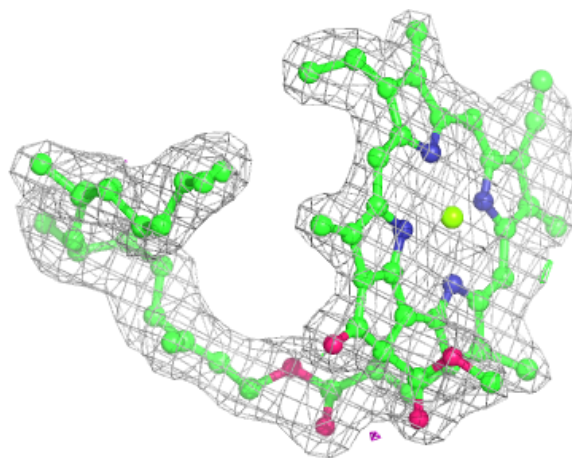
Electron density around CLA b 614:

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



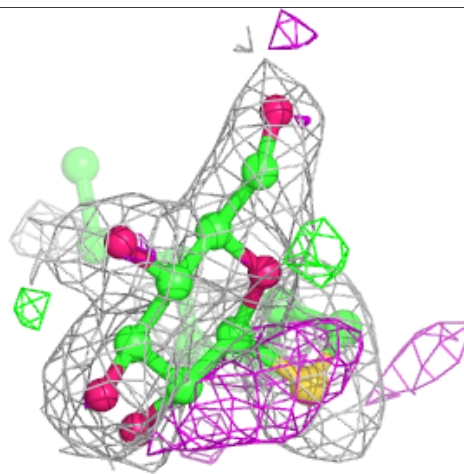
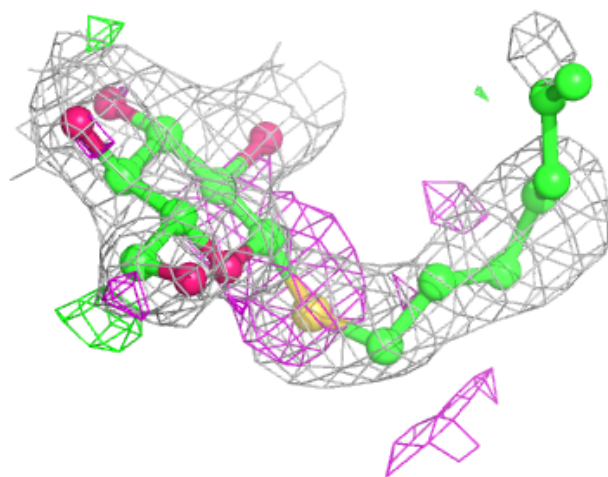
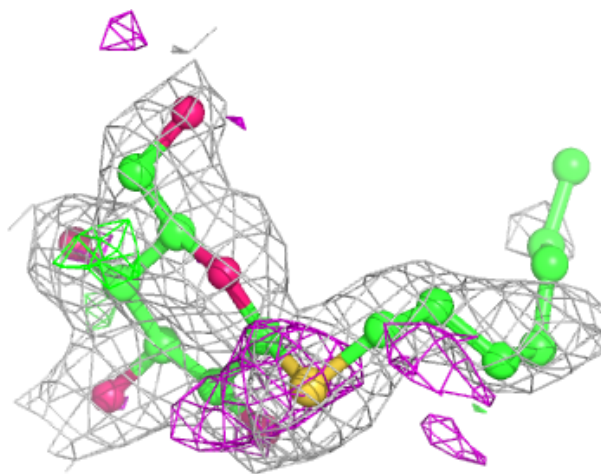
Electron density around CLA c 505:

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



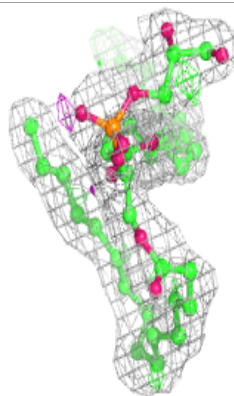
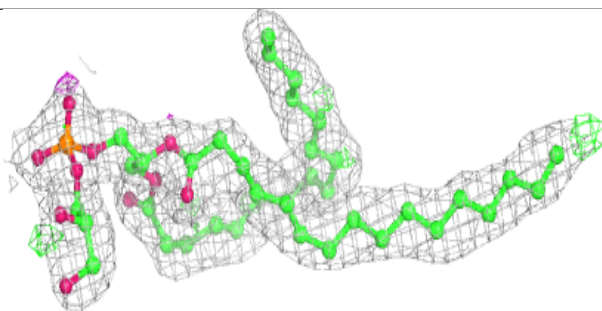
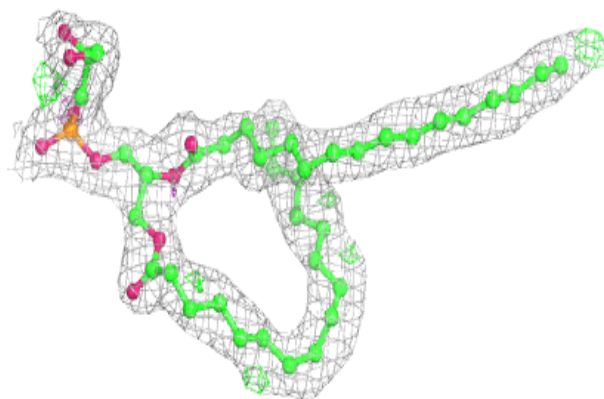
Electron density around HTG b 627:

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

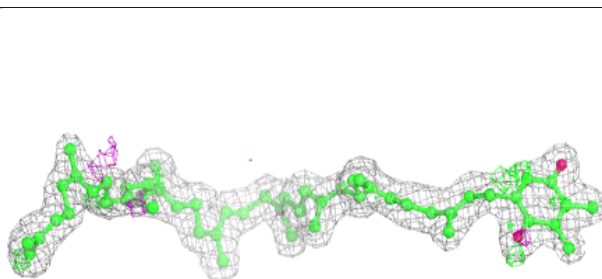
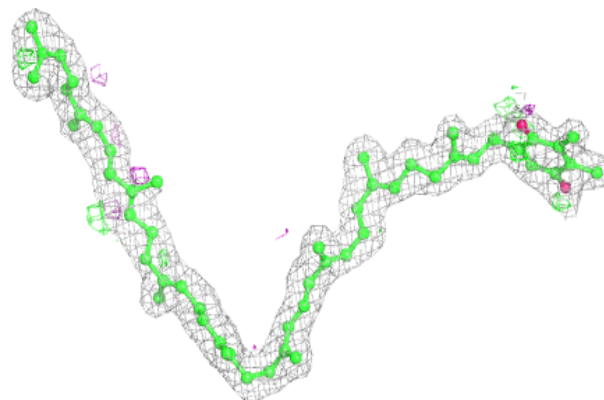


Electron density around LHG d 408:

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

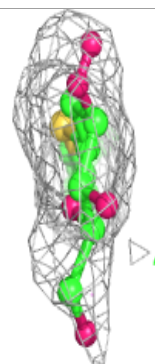
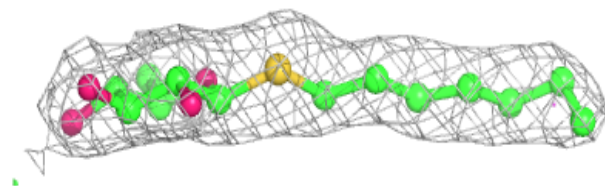
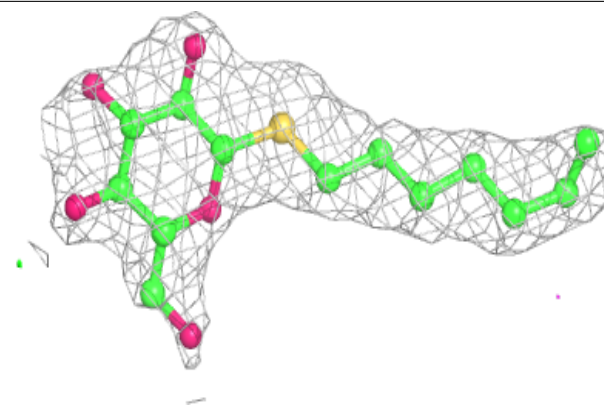
**Electron density around PL9 d 406:**

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

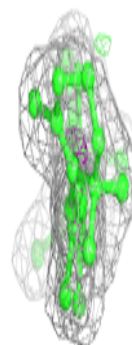
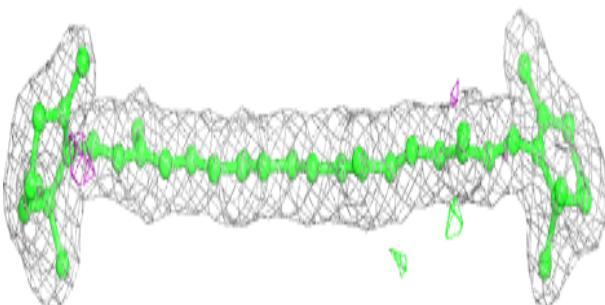
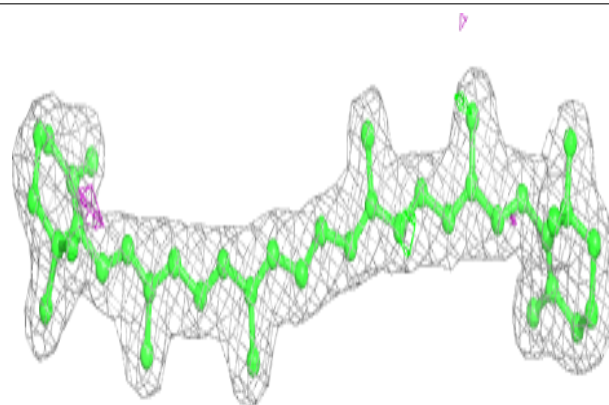


Electron density around HTG b 603:

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

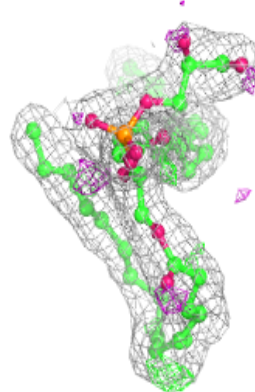
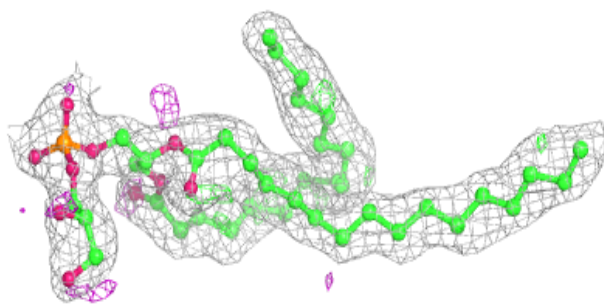
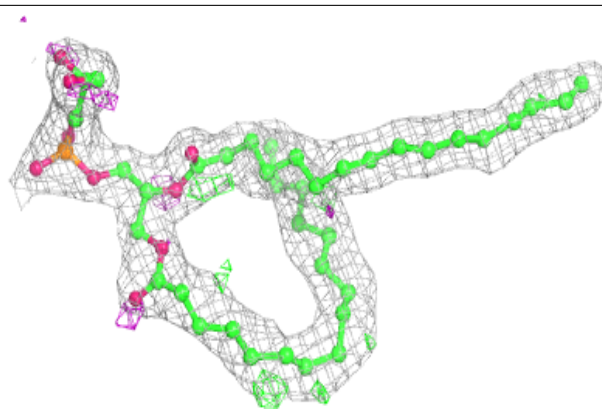
**Electron density around BCR B 619:**

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

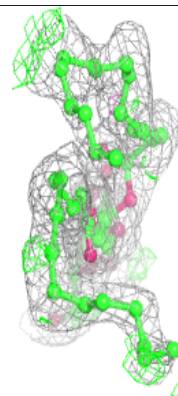
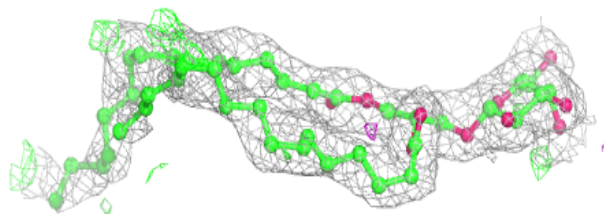
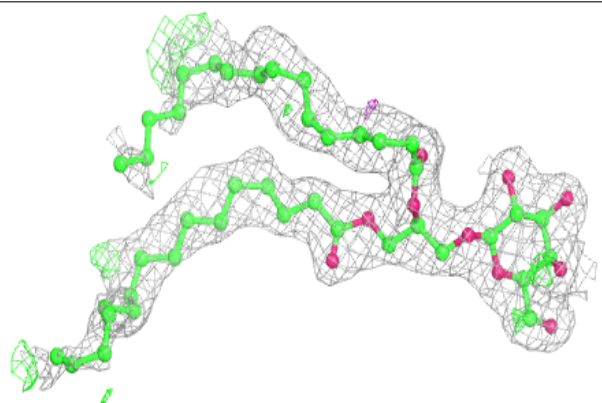


Electron density around LHG D 408:

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

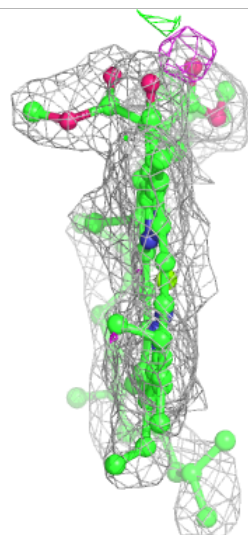
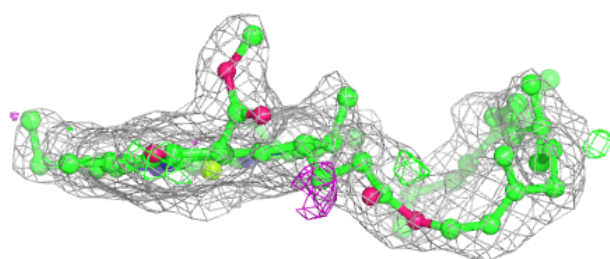
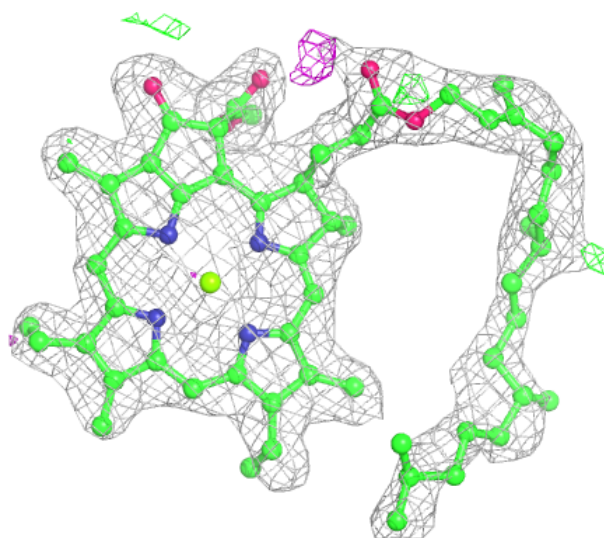
**Electron density around LMG j 101:**

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



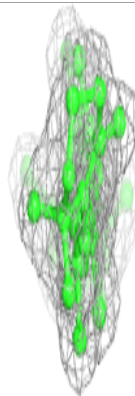
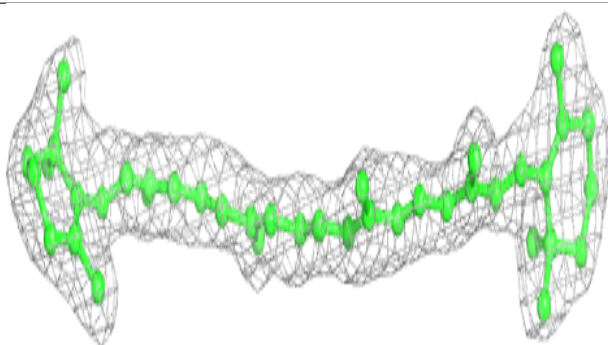
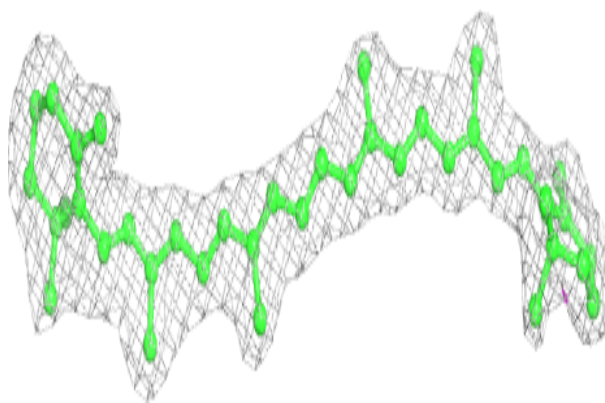
Electron density around CLA c 514:

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

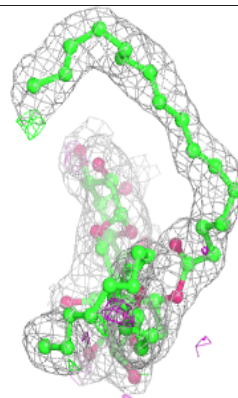
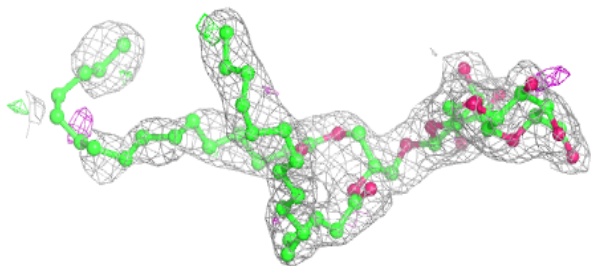
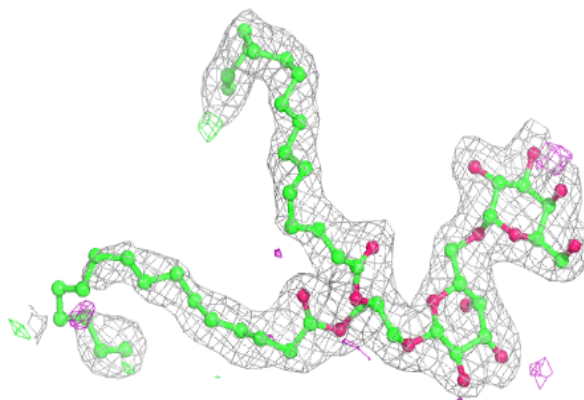


Electron density around BCR Y 101:

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

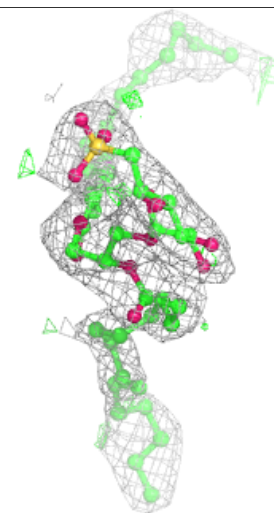
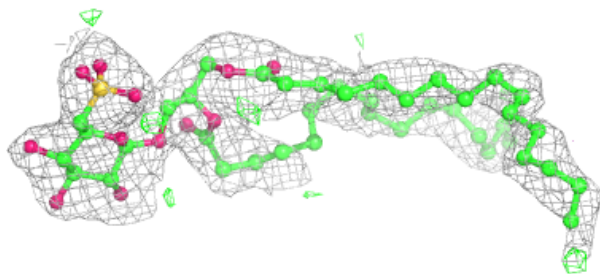
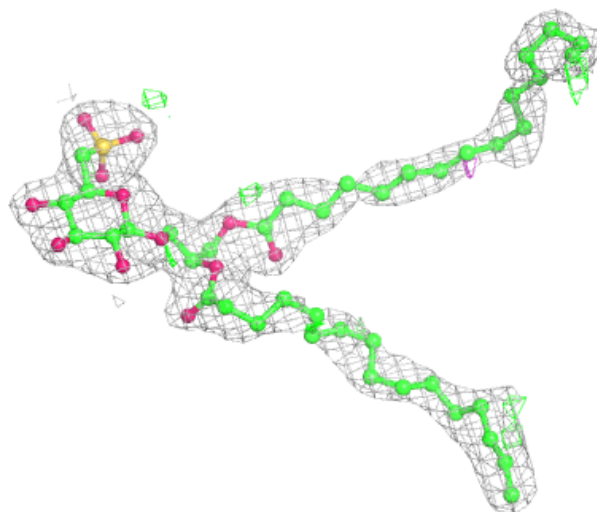
**Electron density around DGD c 518:**

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



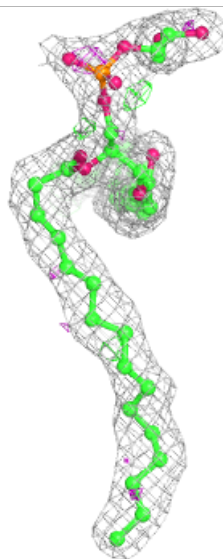
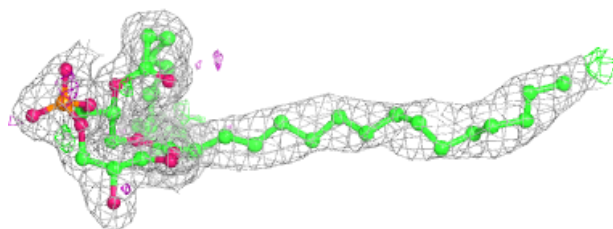
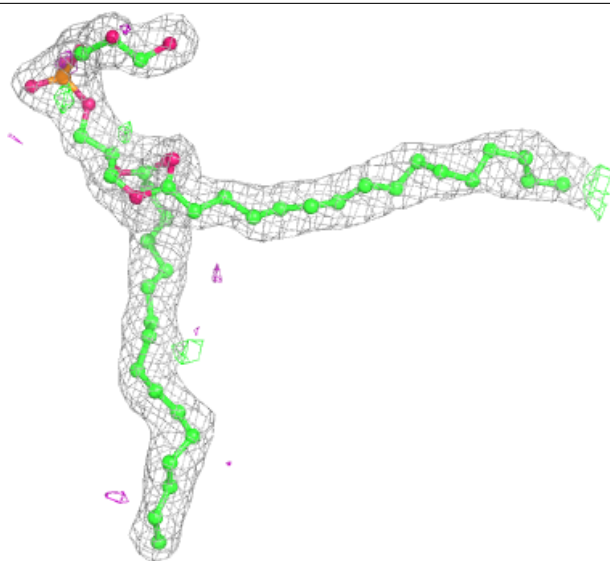
Electron density around SQD A 411:

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



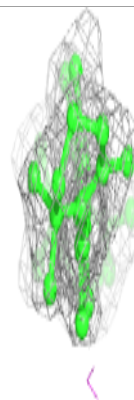
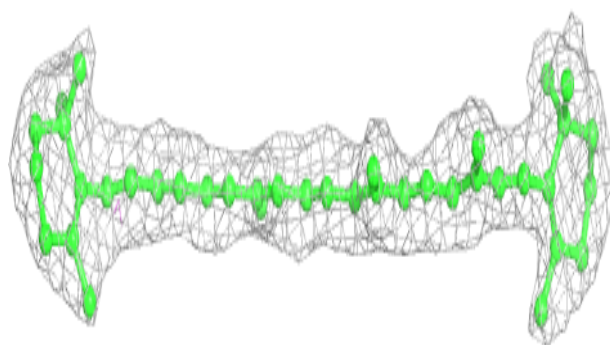
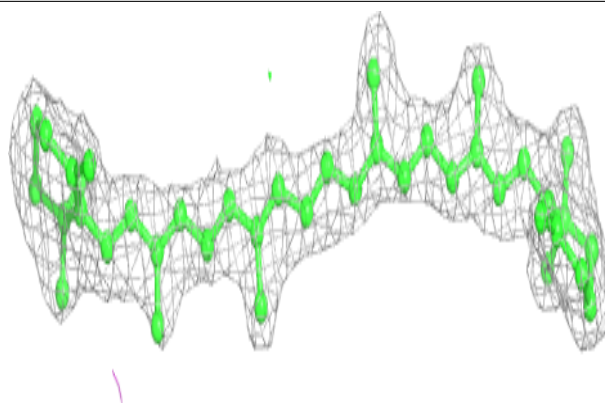
Electron density around LHG 1 102:

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



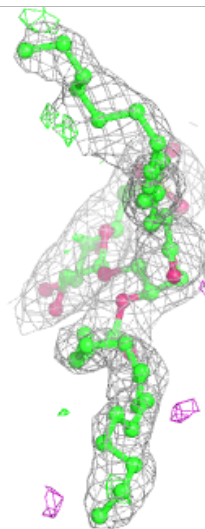
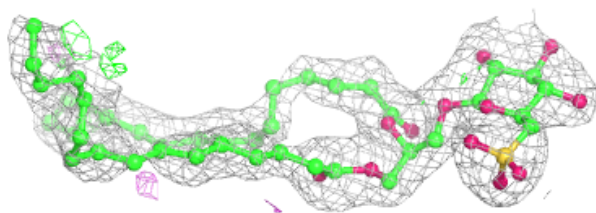
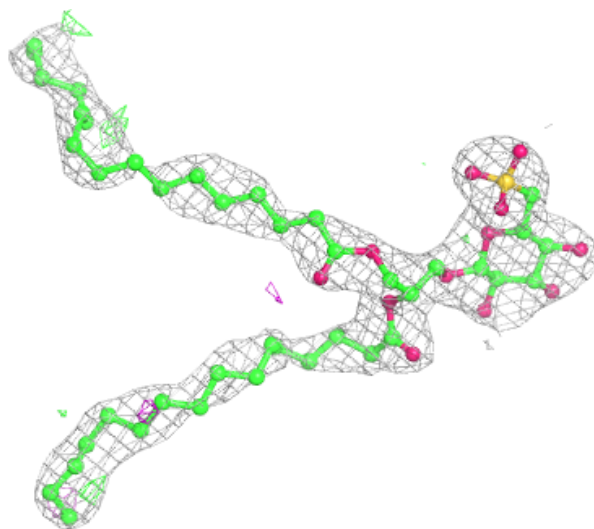
Electron density around BCR c 526:

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



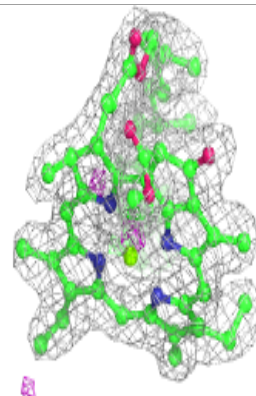
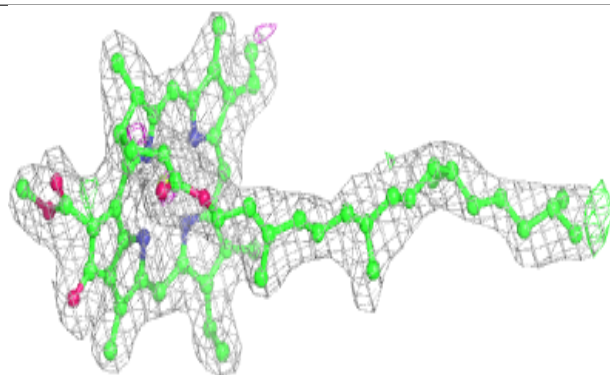
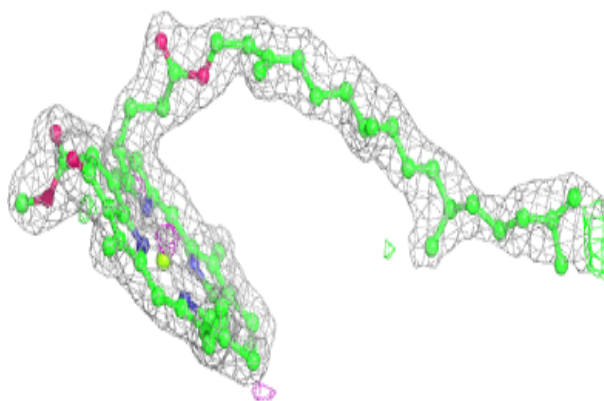
Electron density around SQD a 411:

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

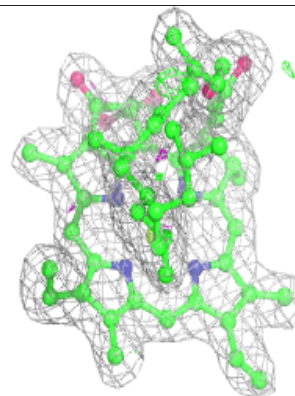
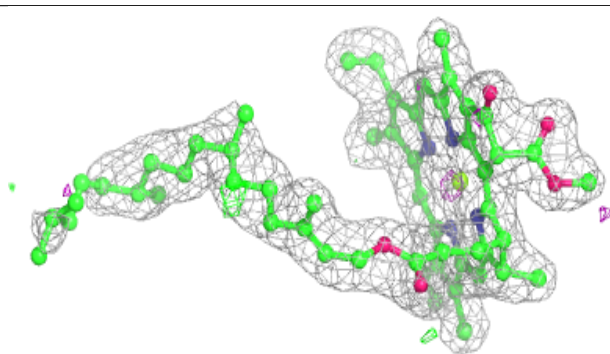
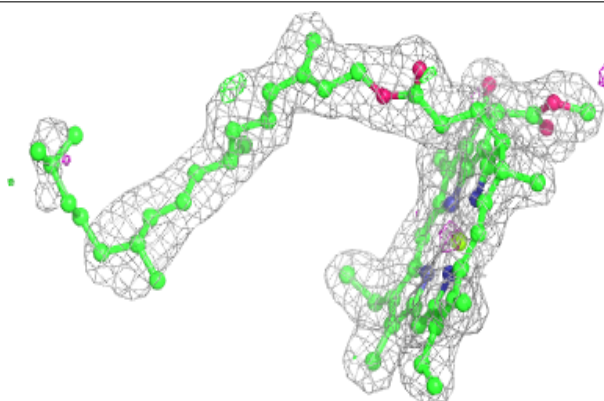


Electron density around CLA c 506:

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

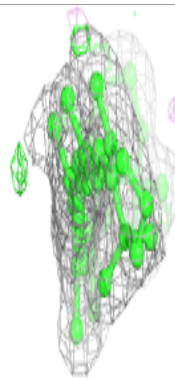
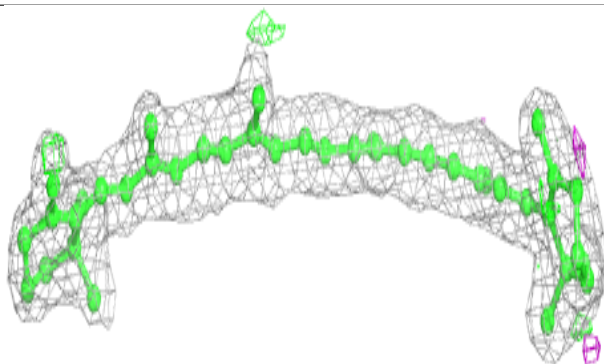
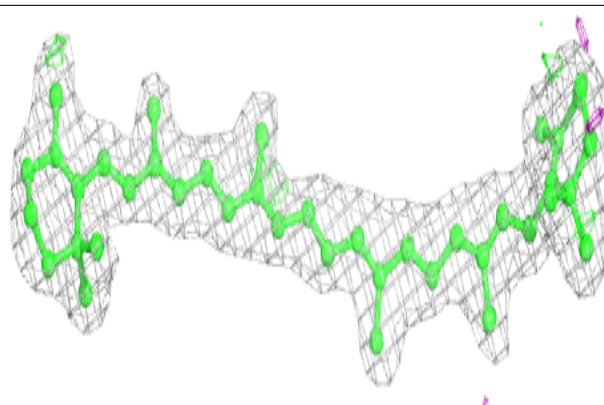
**Electron density around CLA C 509:**

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

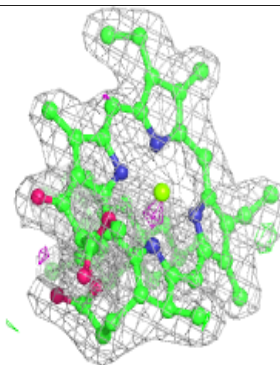
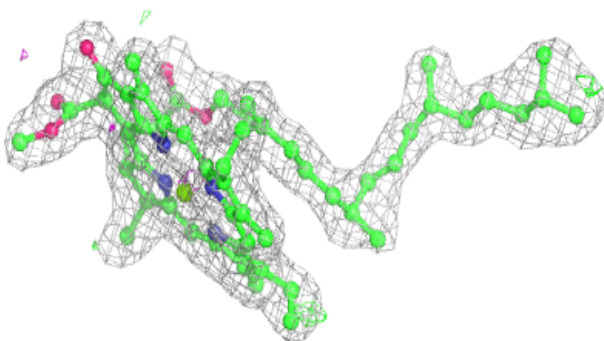
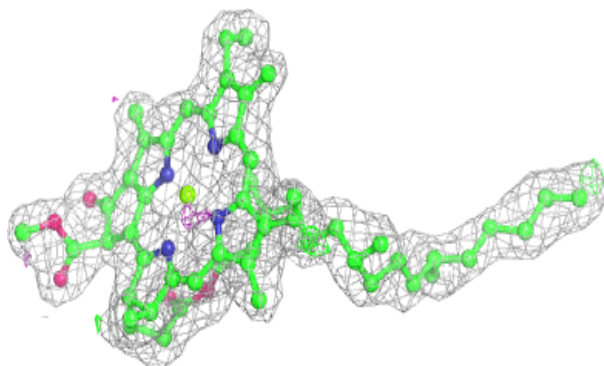


Electron density around BCR T 102:

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

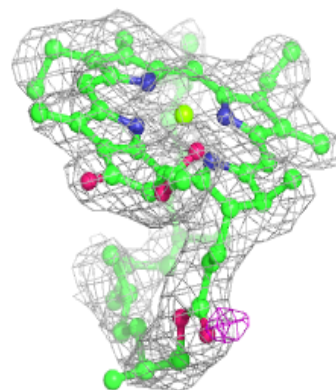
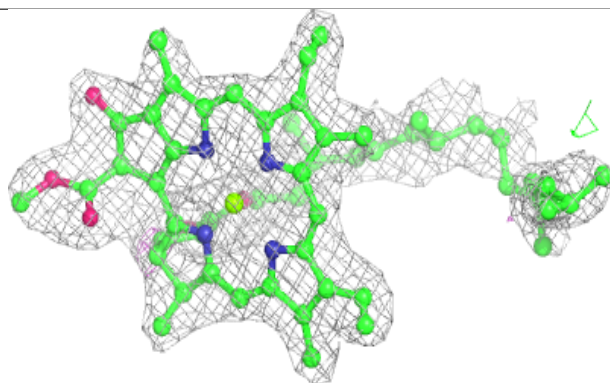
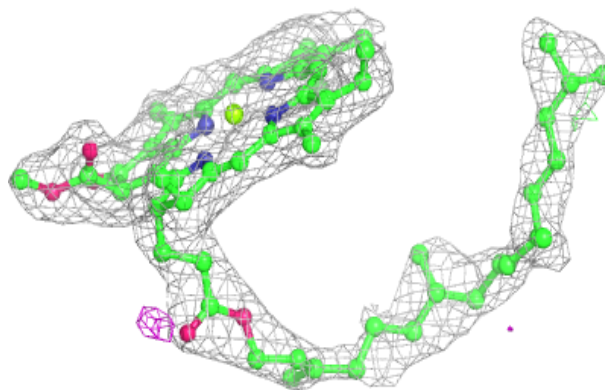
**Electron density around CLA c 507:**

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

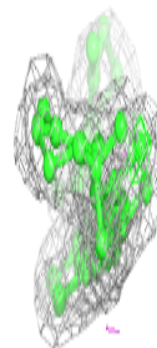
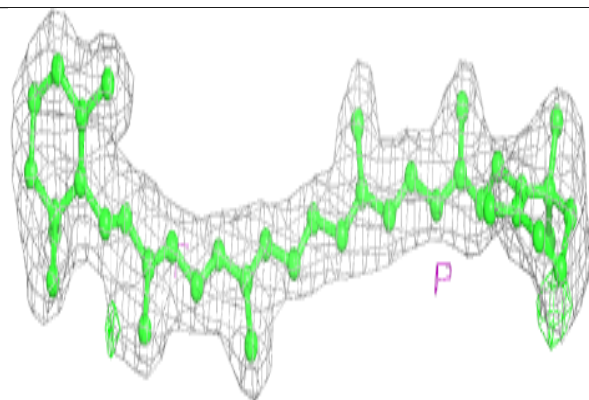
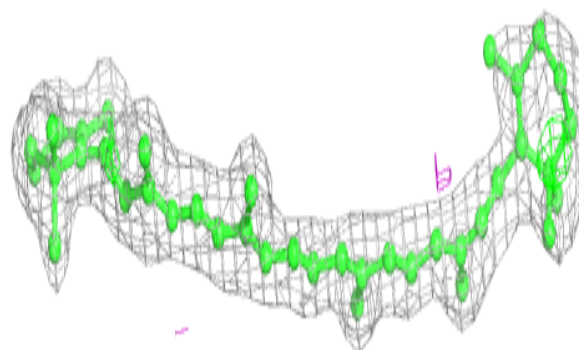


Electron density around CLA C 514:

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

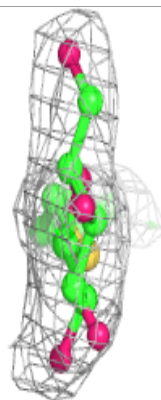
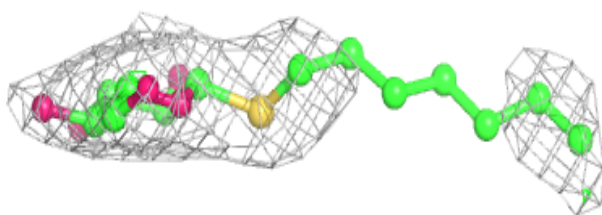
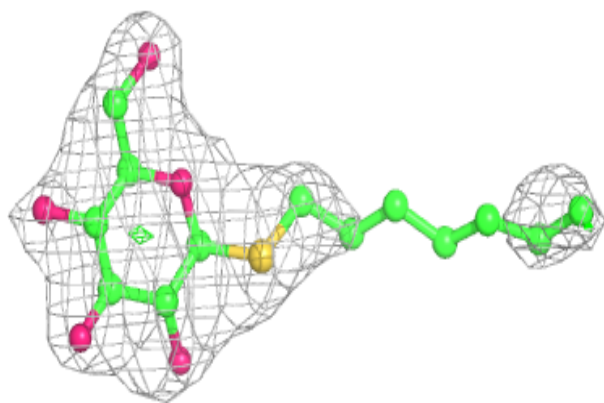
**Electron density around BCR D 405:**

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

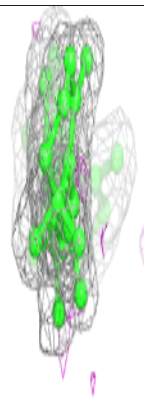
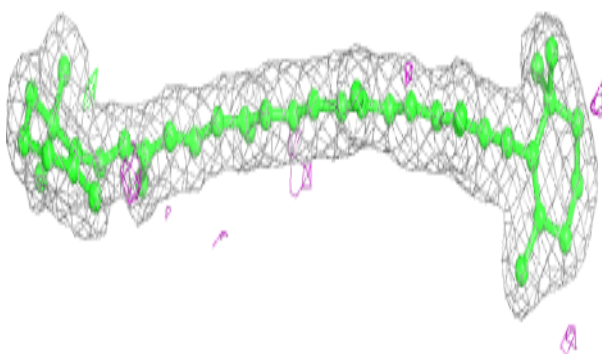
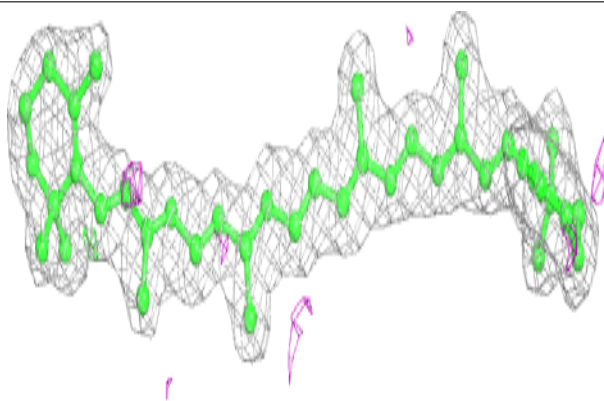


Electron density around HTG C 522:

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

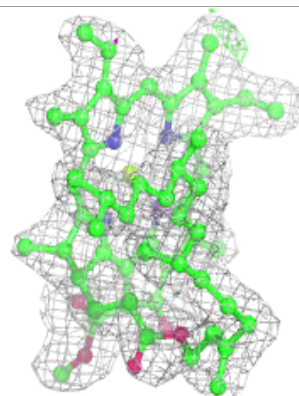
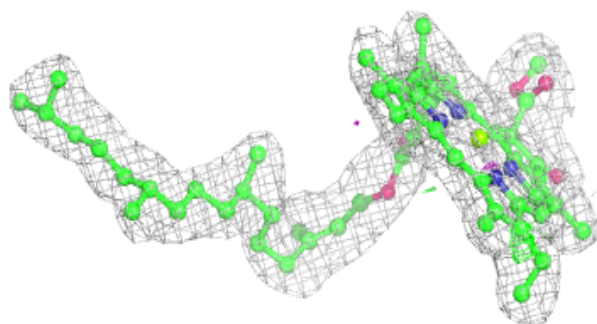
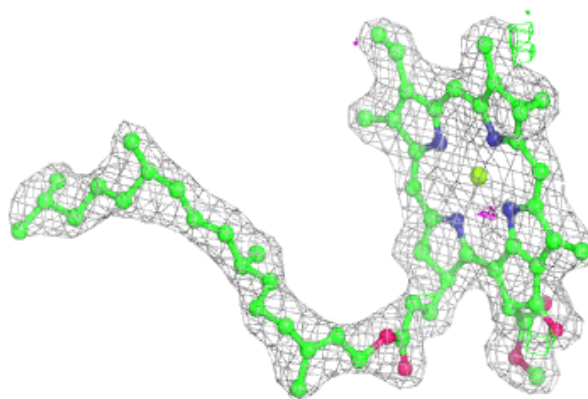
**Electron density around BCR b 622:**

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

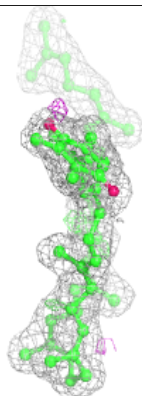
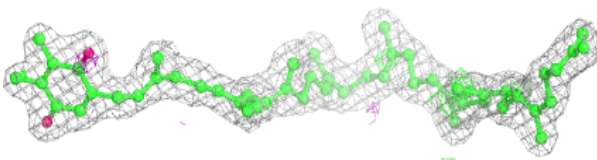
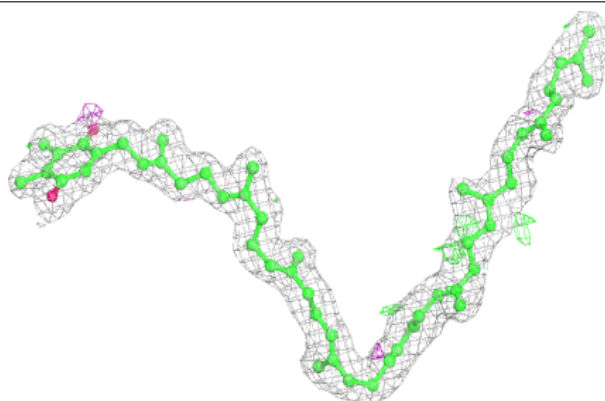


Electron density around CLA c 513:

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

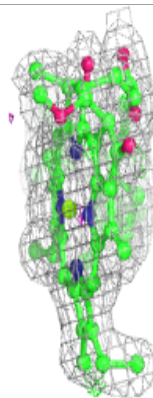
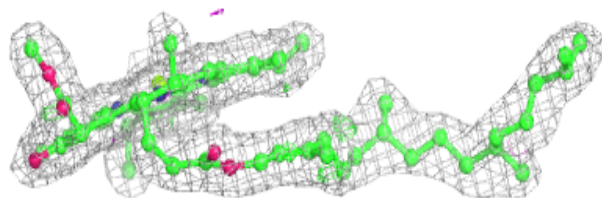
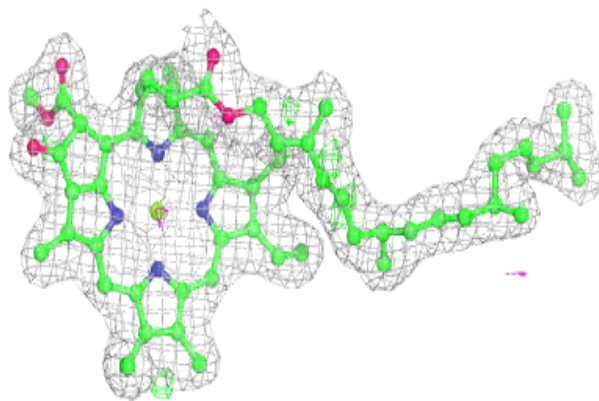
**Electron density around PL9 D 406:**

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

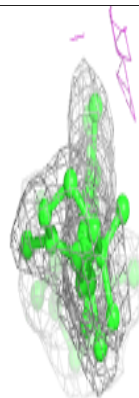
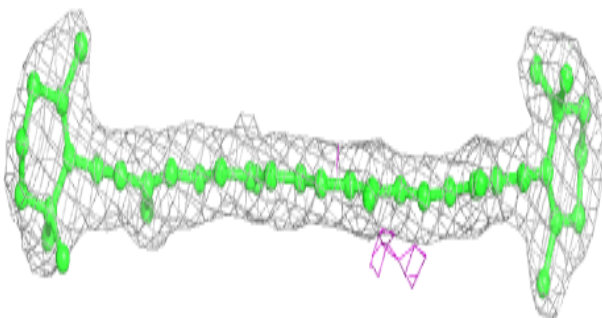
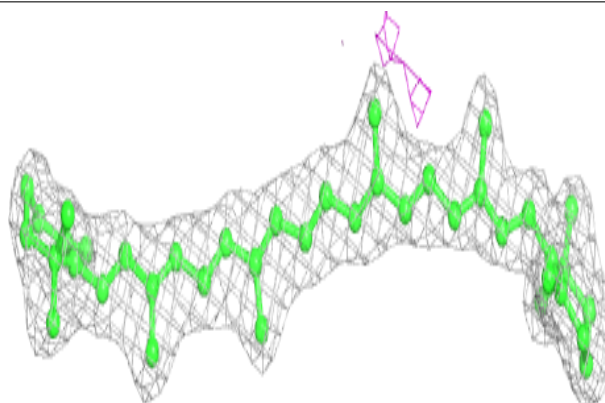


Electron density around CLA B 604:

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

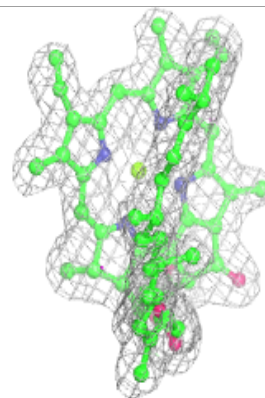
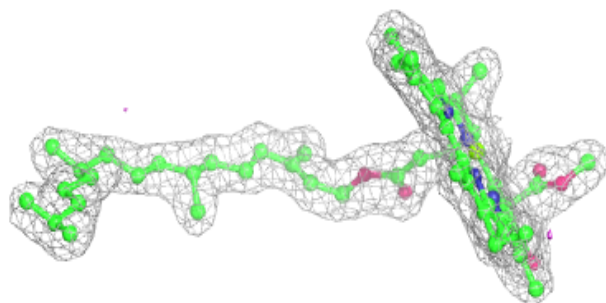
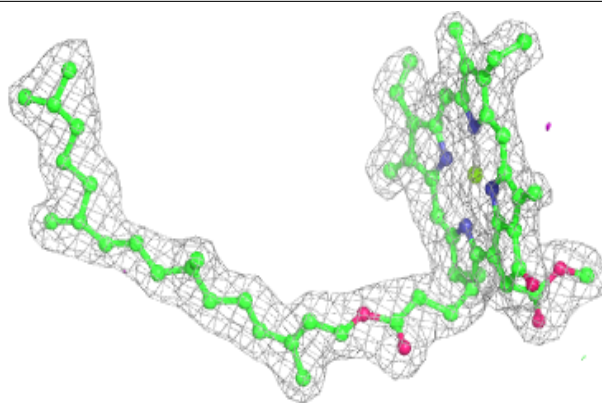
**Electron density around BCR c 516:**

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

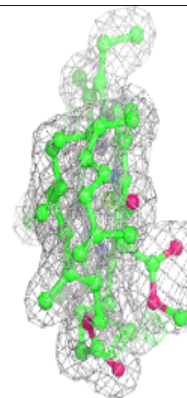
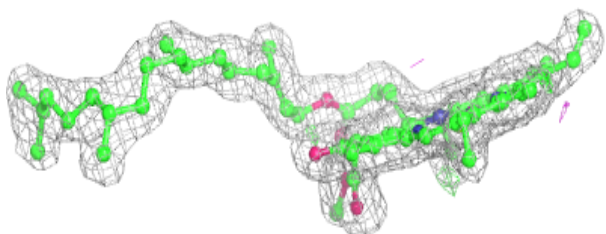
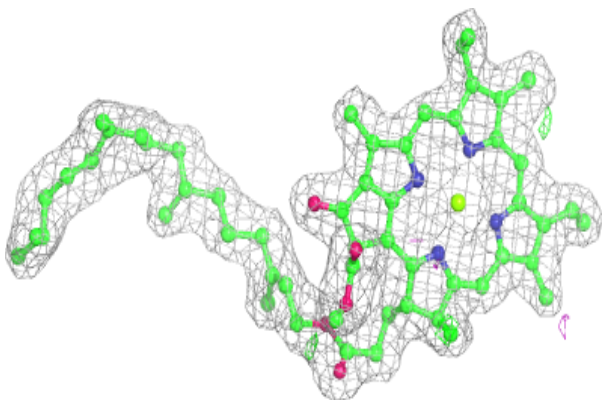


Electron density around CLA B 610:

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

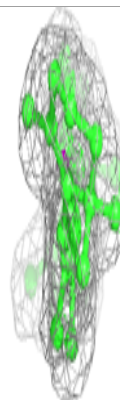
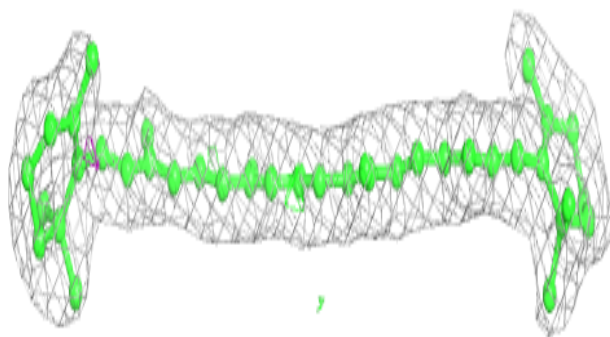
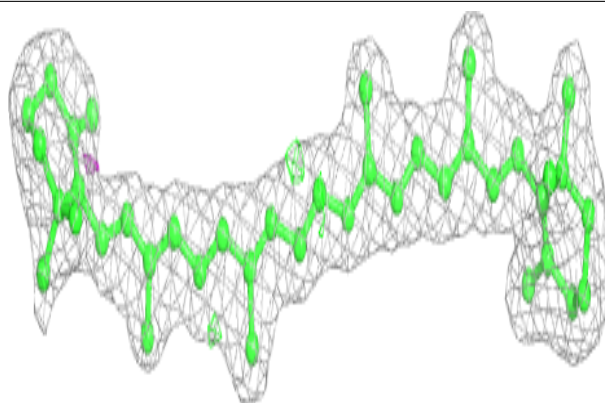
**Electron density around CLA B 603:**

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



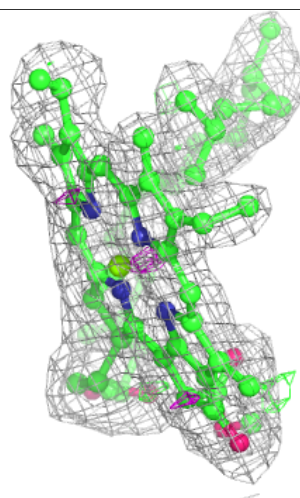
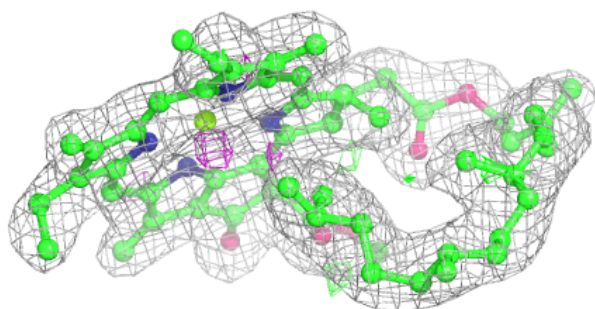
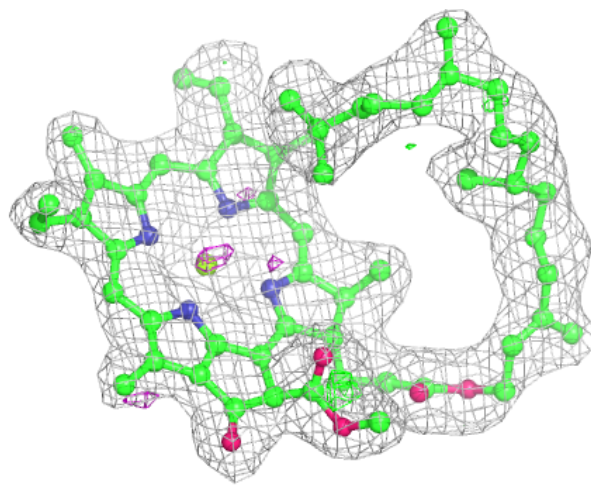
Electron density around BCR b 623:

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



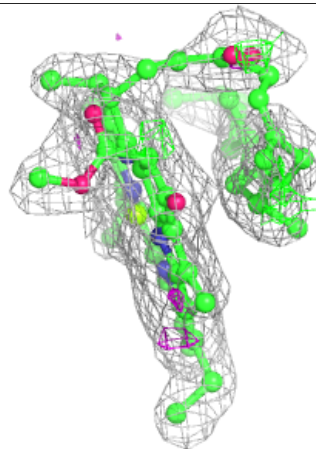
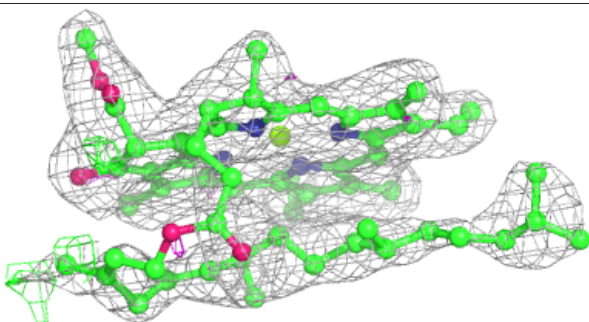
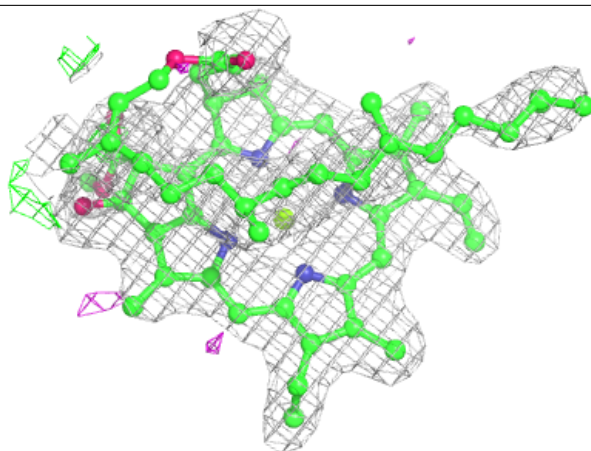
Electron density around CLA b 620:

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

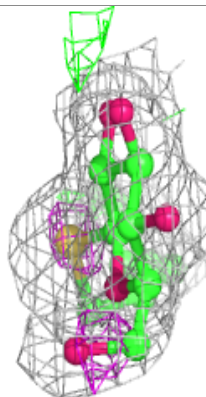
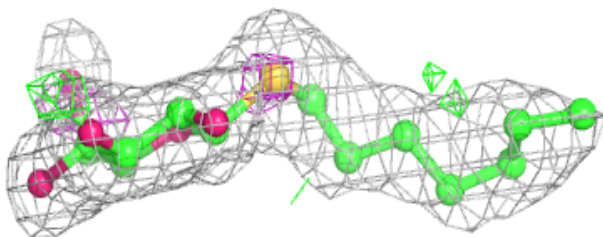
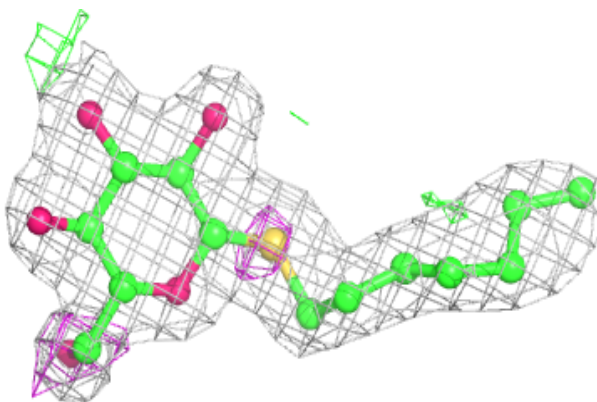


Electron density around CLA B 602:

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

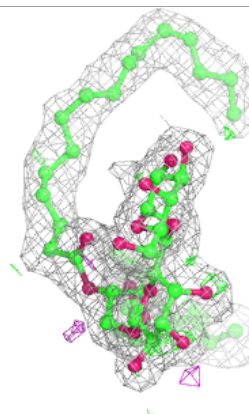
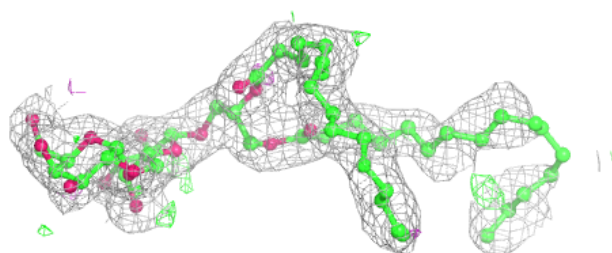
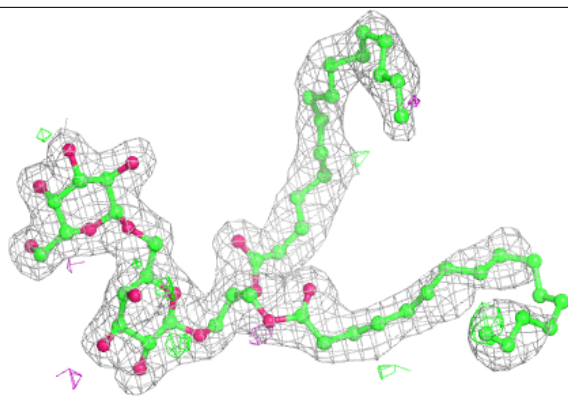
**Electron density around HTG B 622:**

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



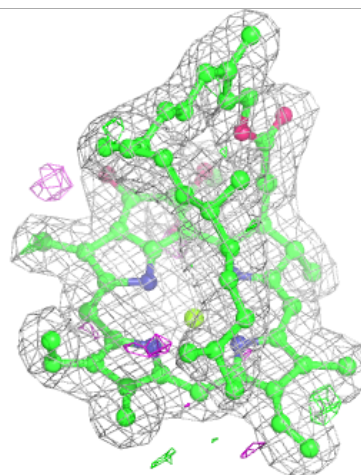
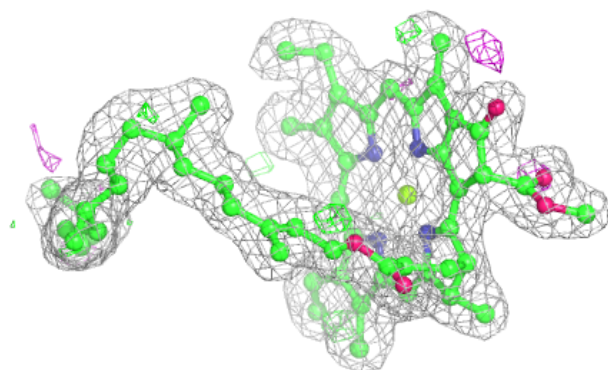
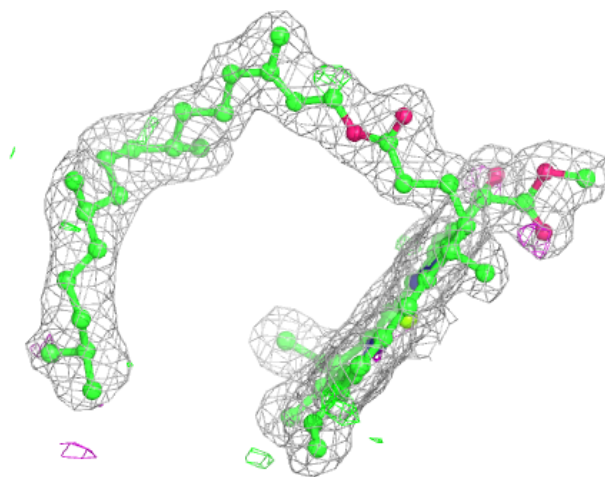
Electron density around DGD C 518:

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



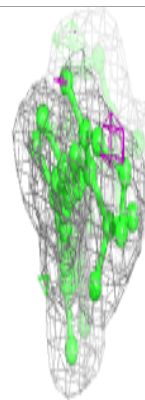
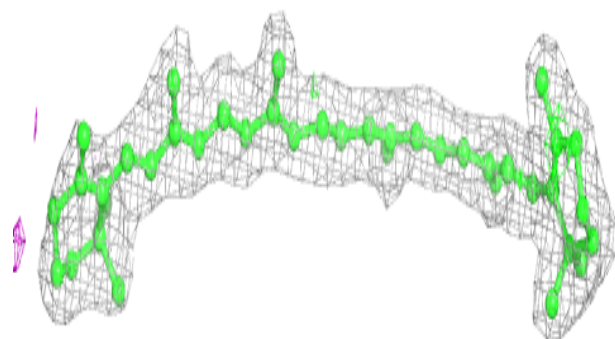
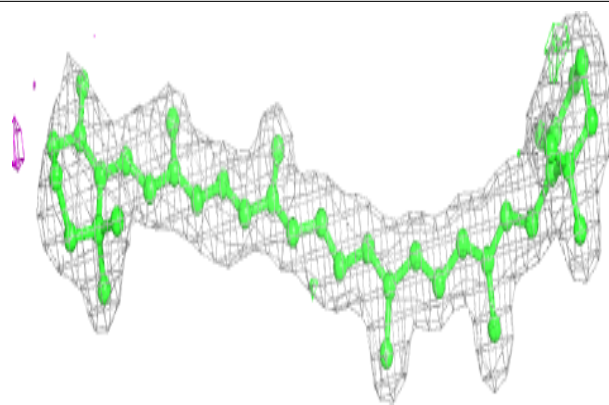
Electron density around CLA B 612:

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



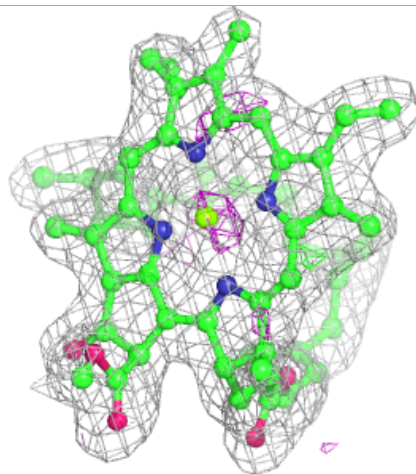
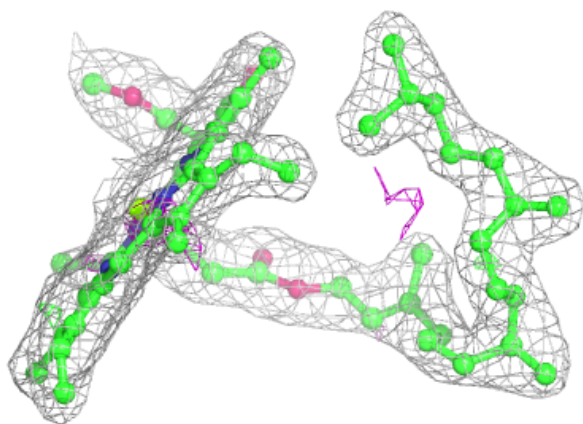
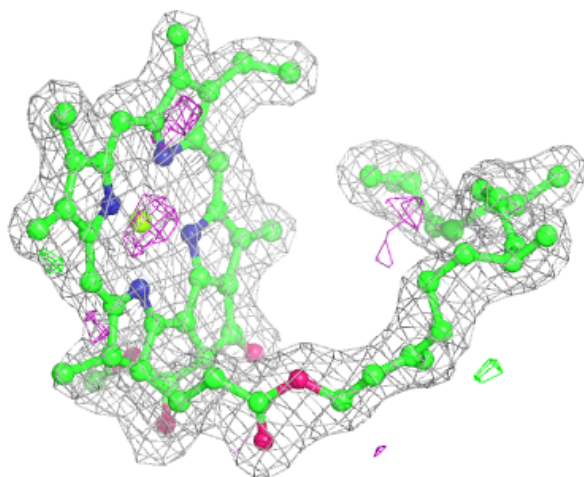
Electron density around BCR t 101:

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



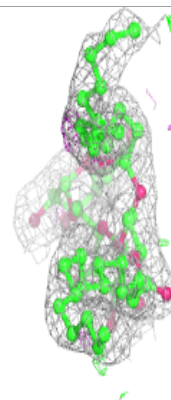
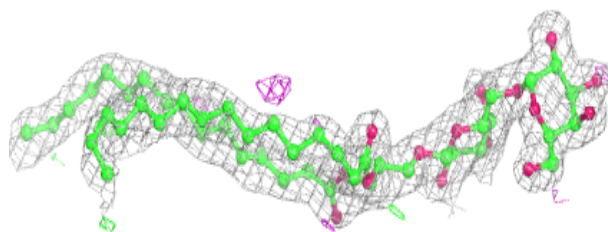
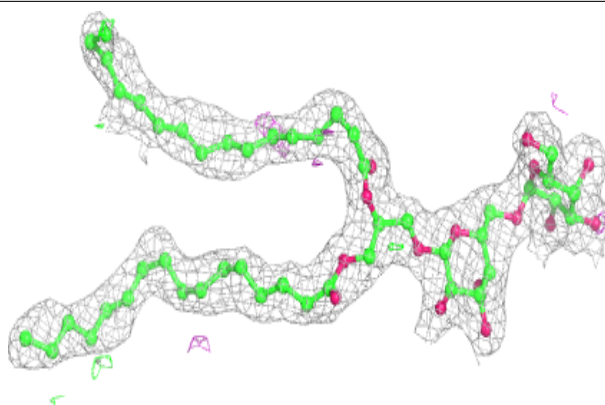
Electron density around CLA C 504:

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

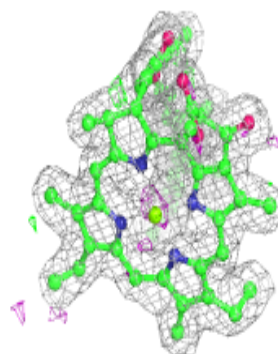
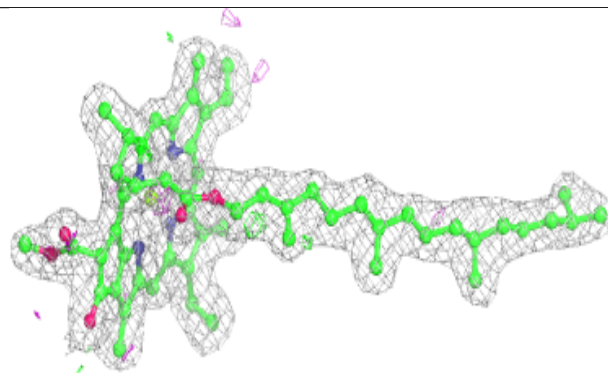
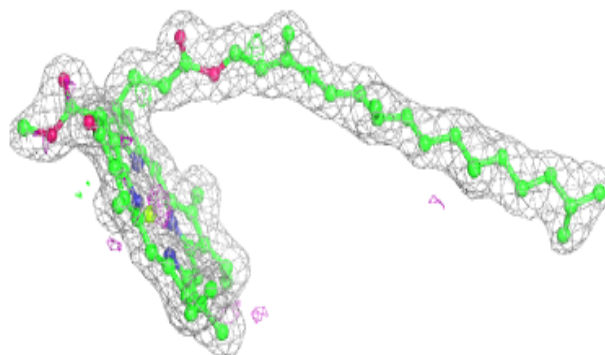


Electron density around DGD c 519:

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

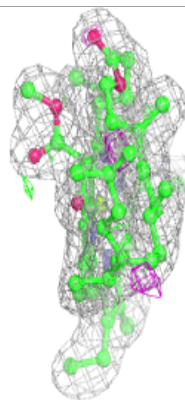
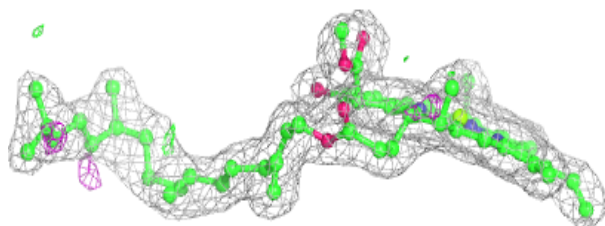
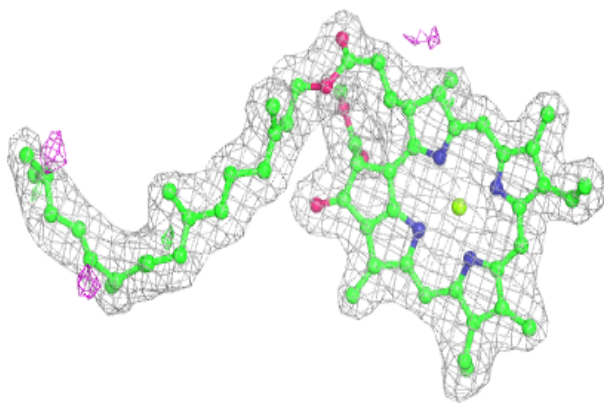
**Electron density around CLA B 608:**

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



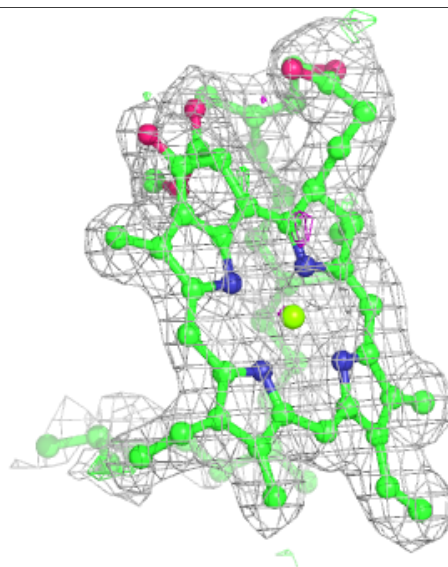
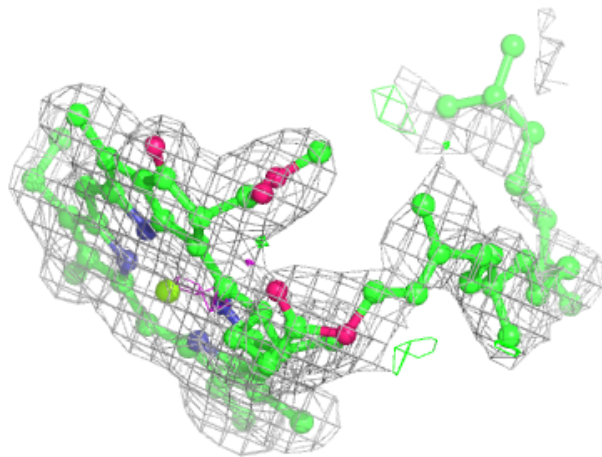
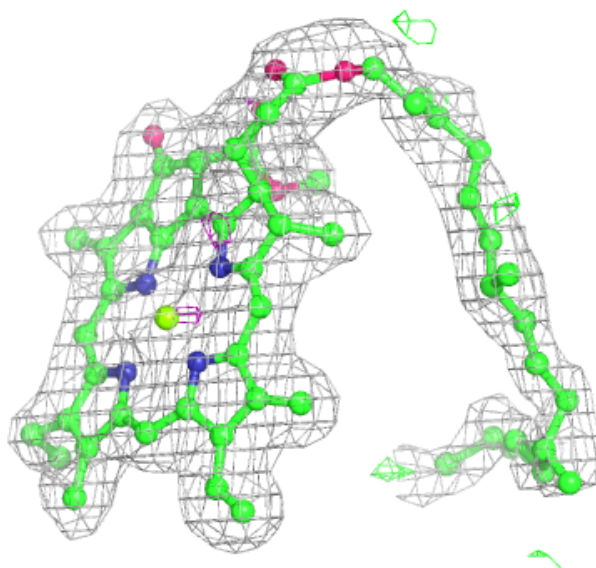
Electron density around CLA b 607:

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



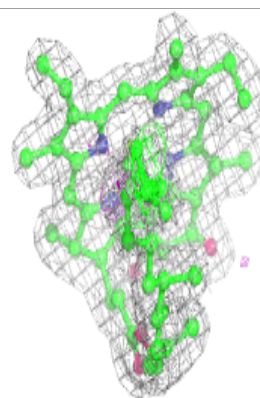
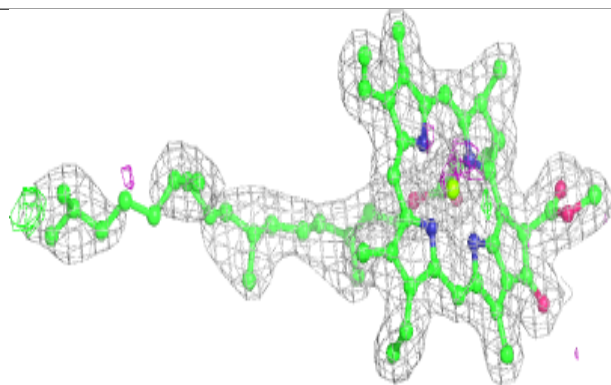
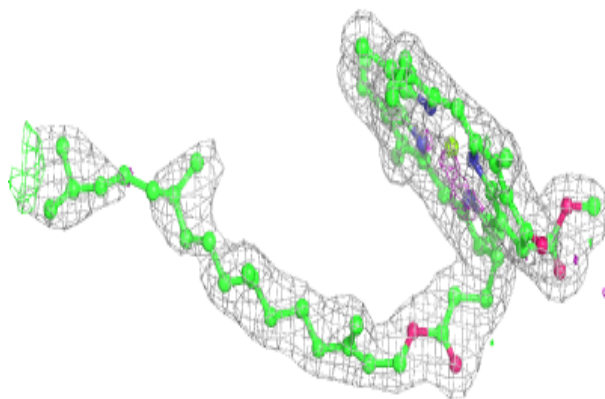
Electron density around CLA b 621:

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

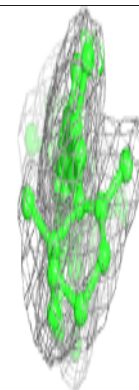
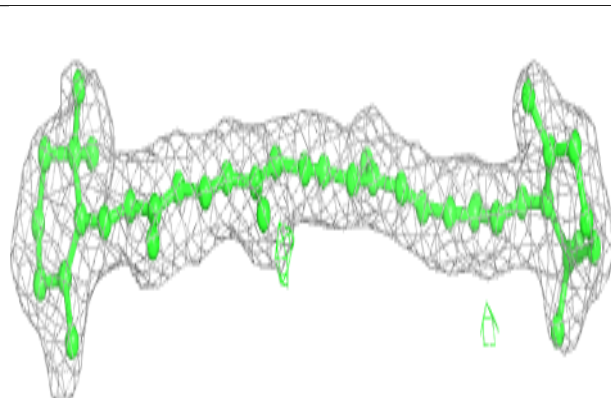
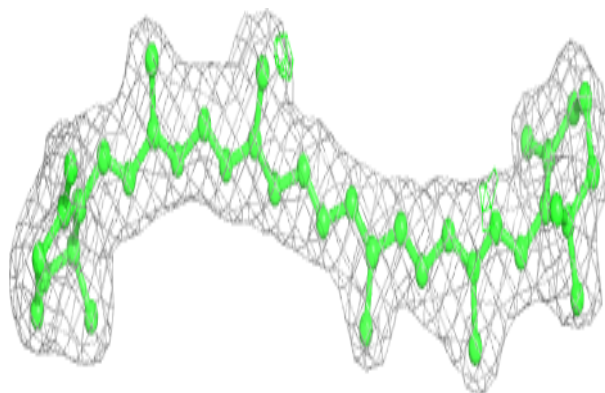


Electron density around CLA C 505:

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

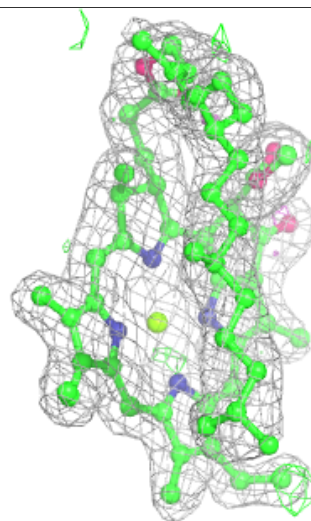
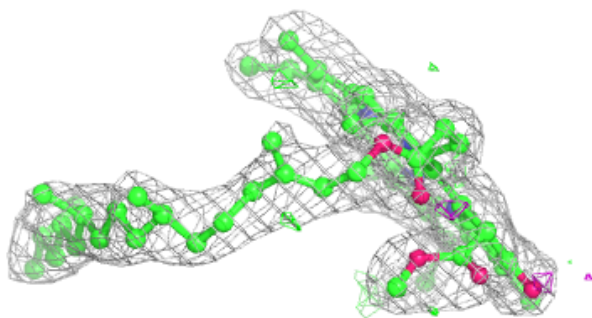
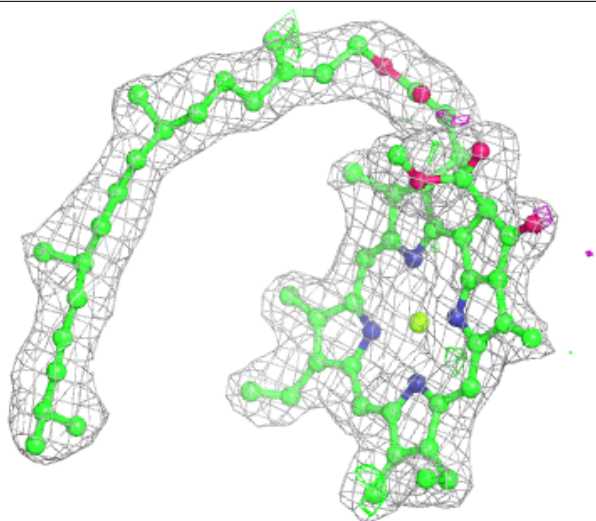
**Electron density around BCR y 101:**

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



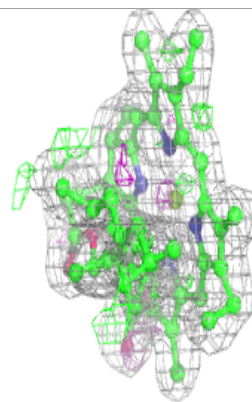
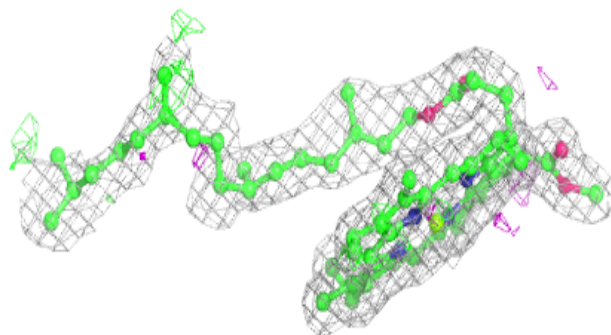
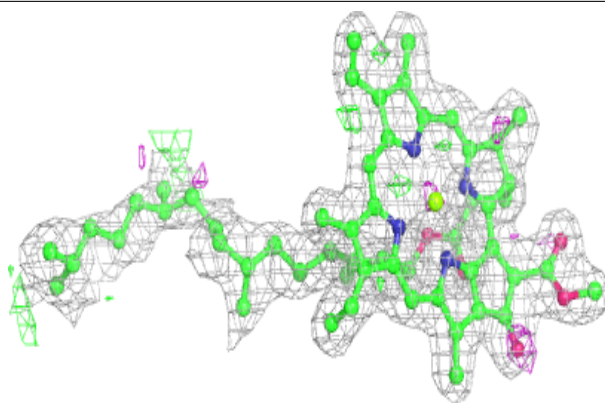
Electron density around CLA c 509:

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

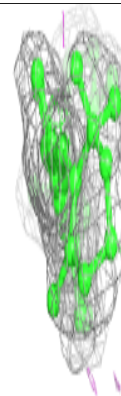
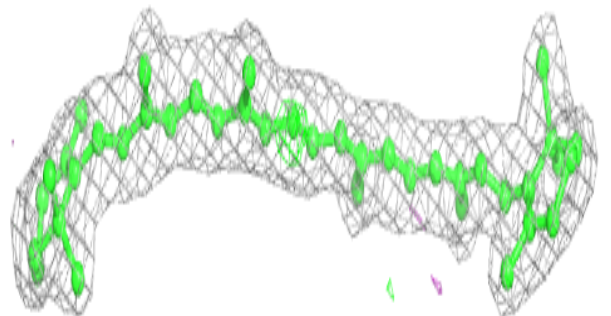
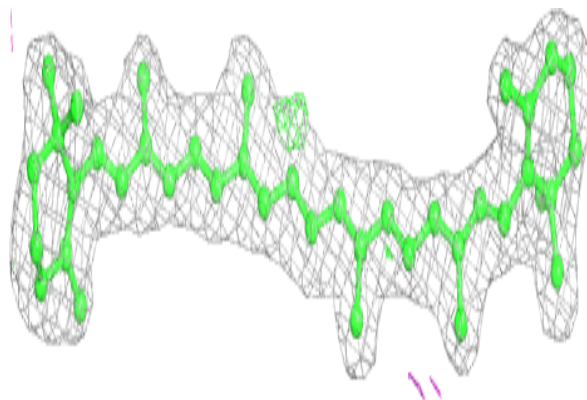


Electron density around CLA B 615:

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

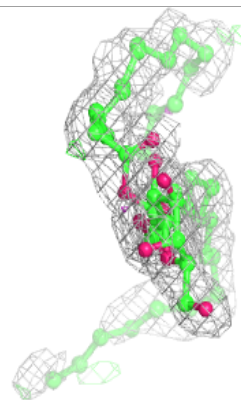
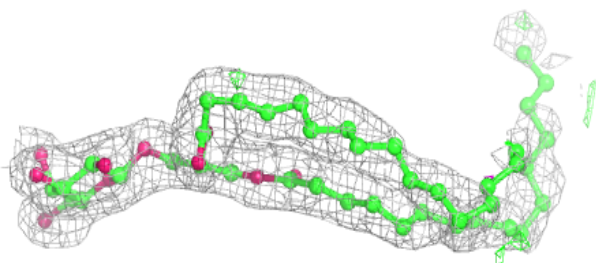
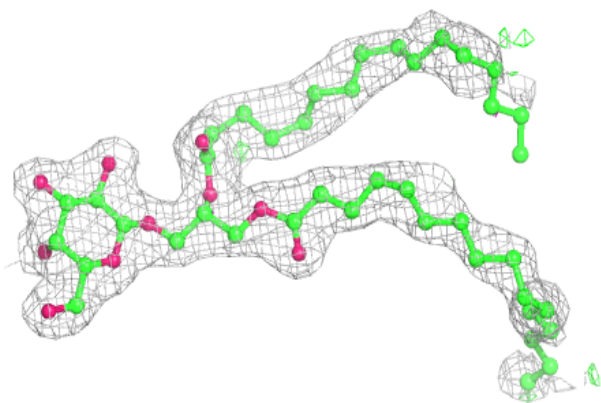
**Electron density around BCR b 624:**

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

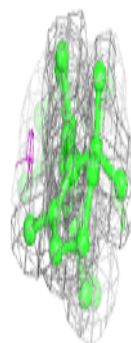
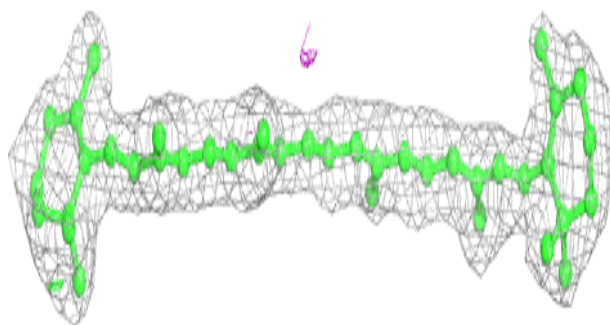
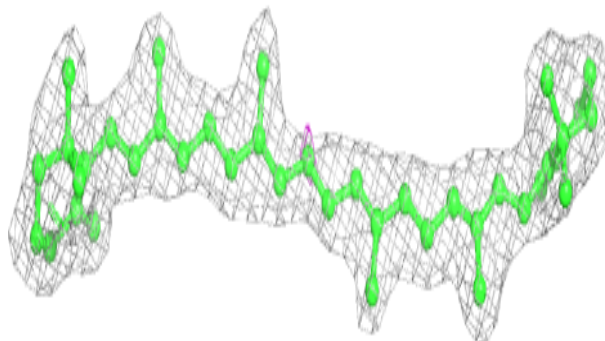


Electron density around LMG J 101:

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

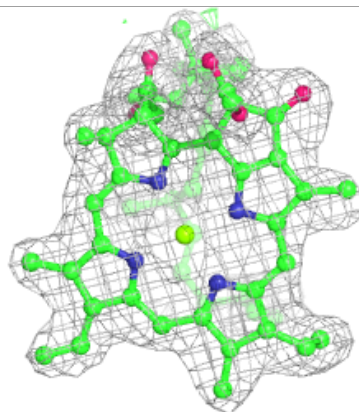
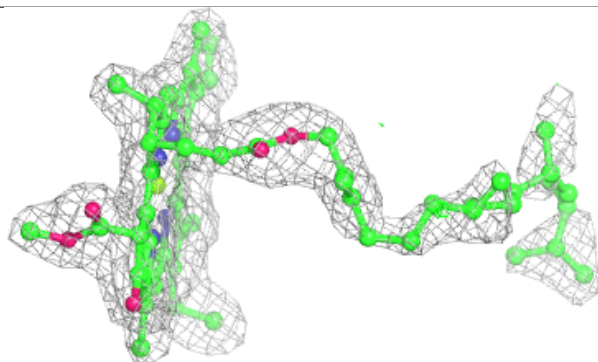
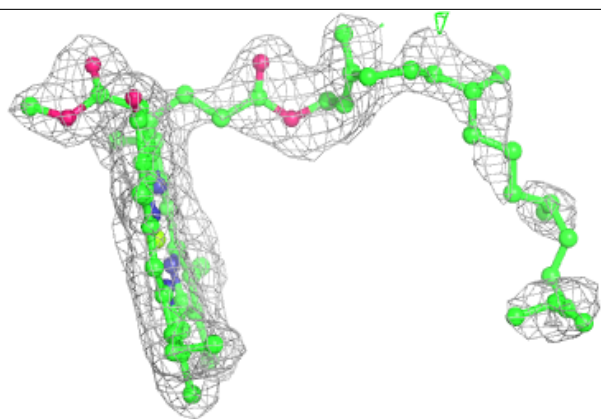
**Electron density around BCR C 515:**

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



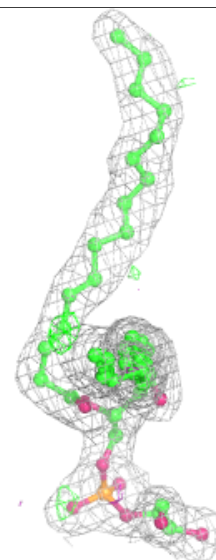
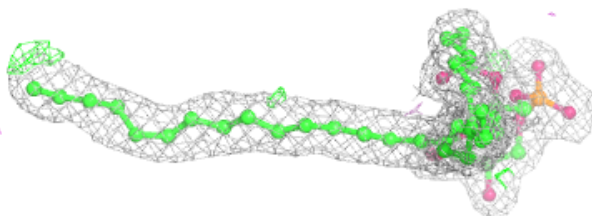
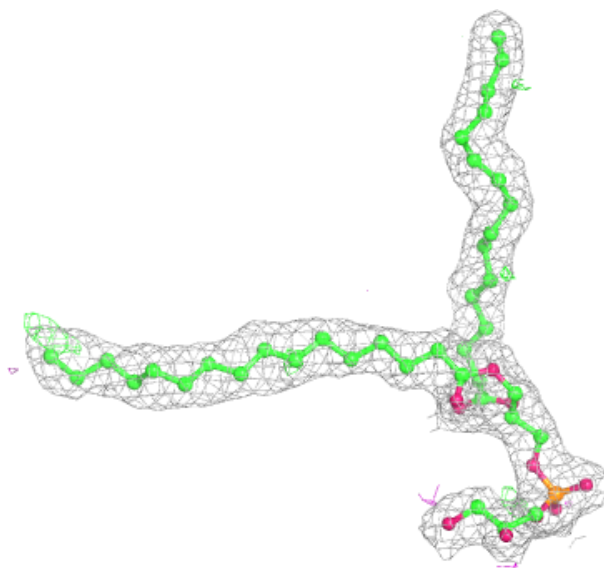
Electron density around CLA C 507:

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



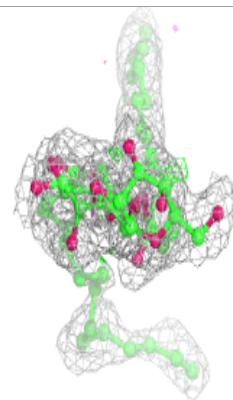
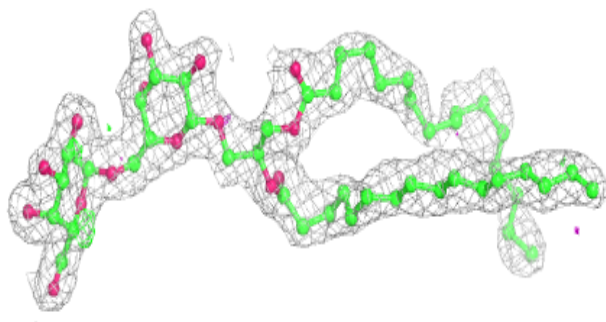
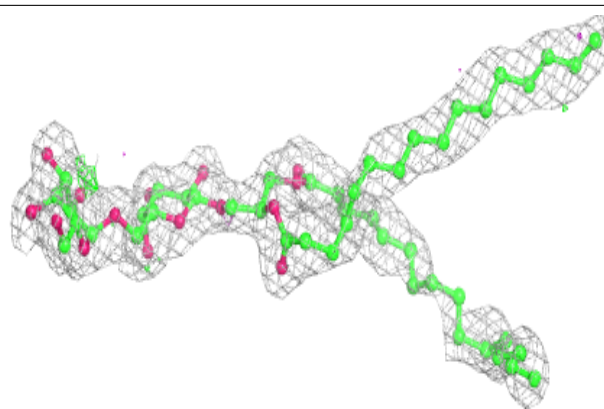
Electron density around LHG L 101:

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



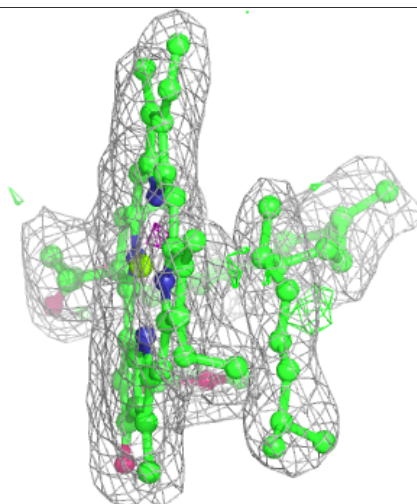
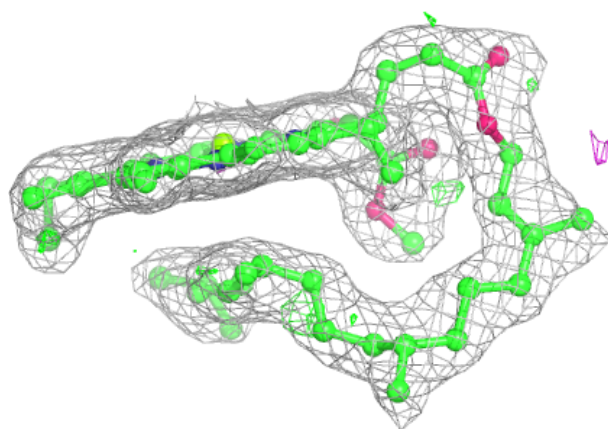
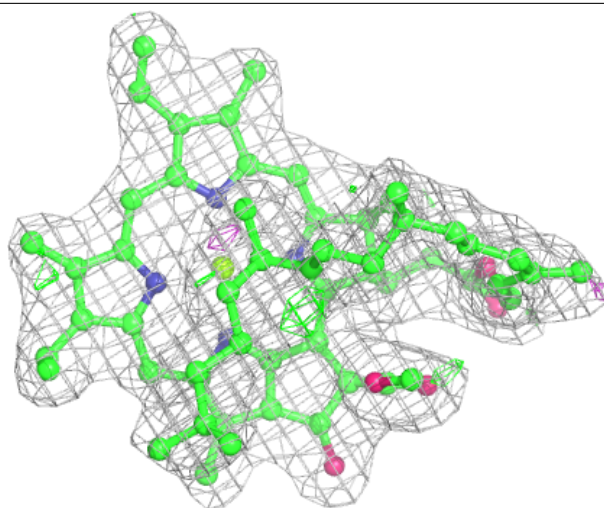
Electron density around DGD c 517:

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



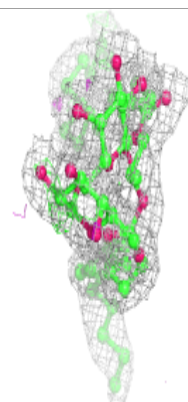
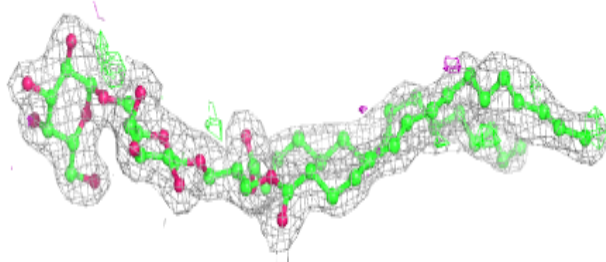
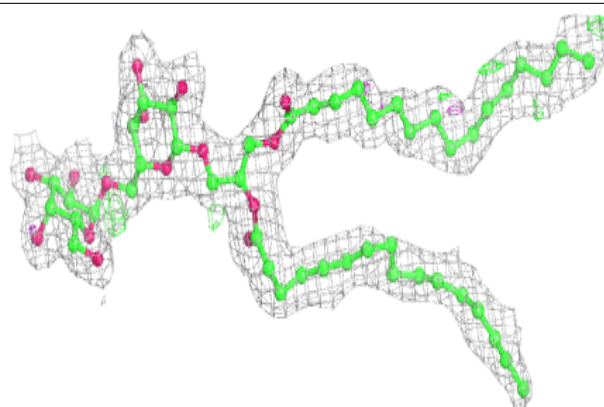
Electron density around CLA c 512:

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

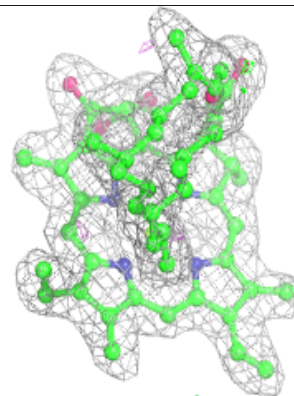
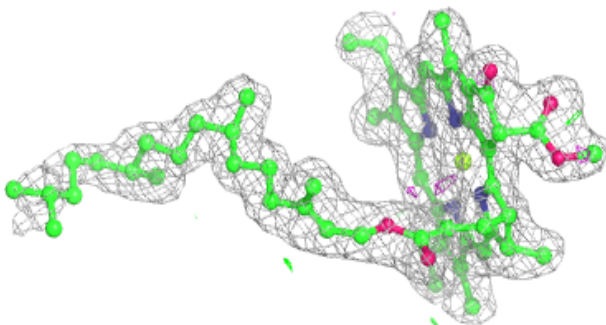
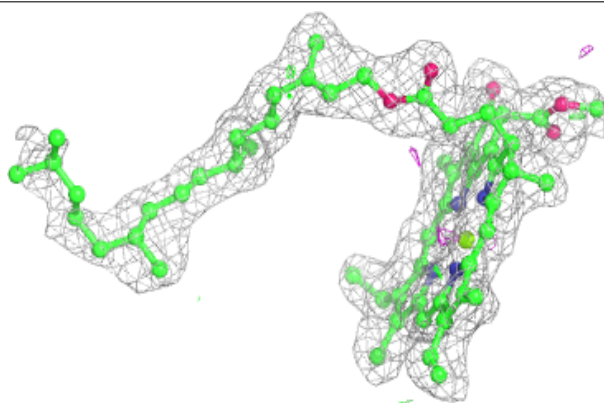


Electron density around DGD C 519:

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

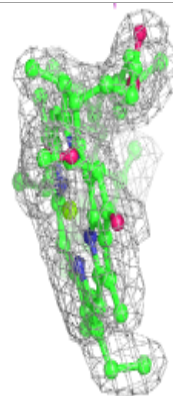
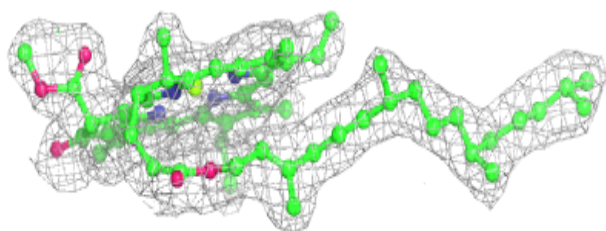
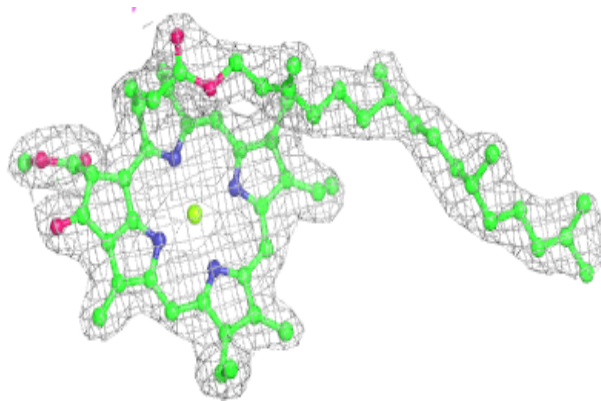
**Electron density around CLA c 510:**

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



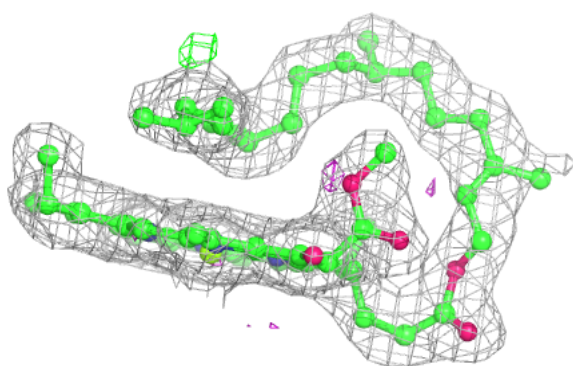
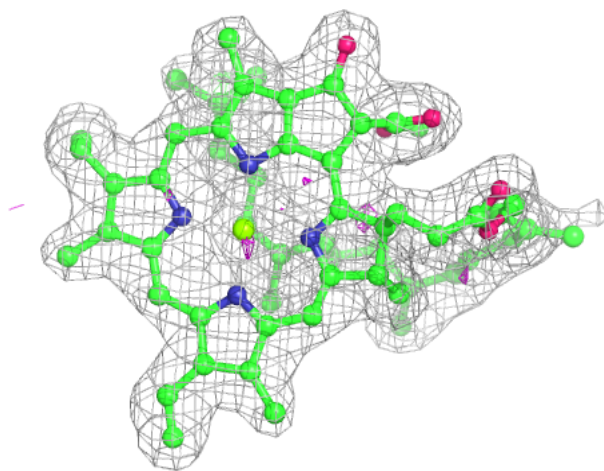
Electron density around CLA c 503:

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



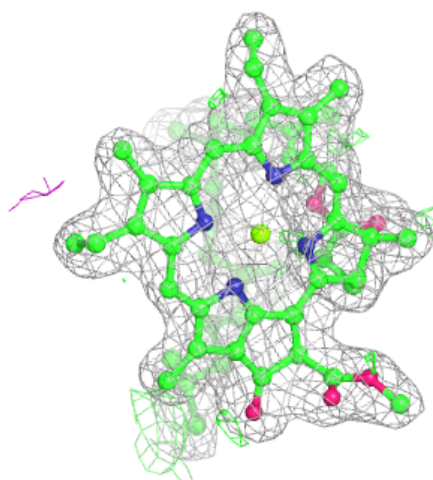
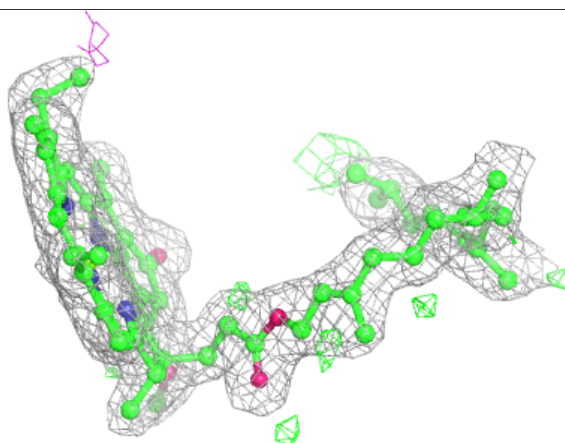
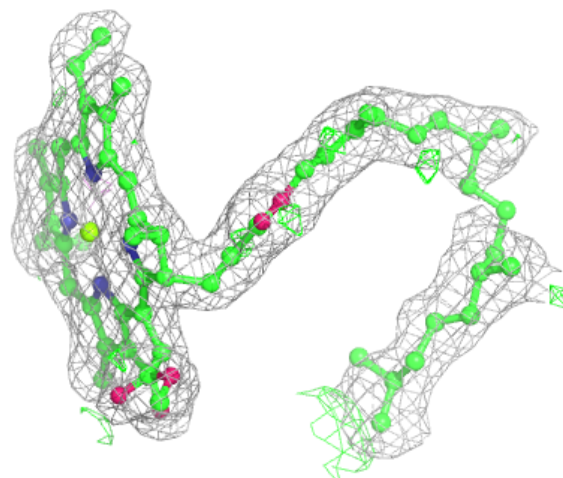
Electron density around CLA C 511:

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



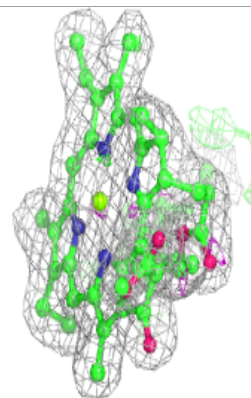
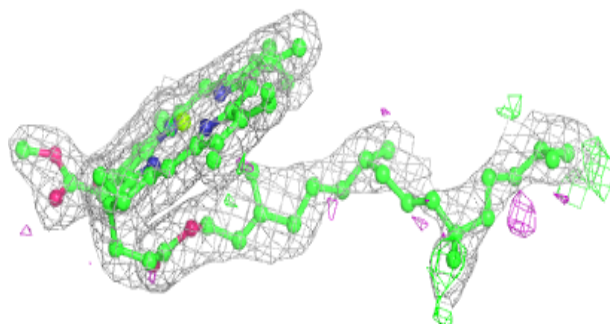
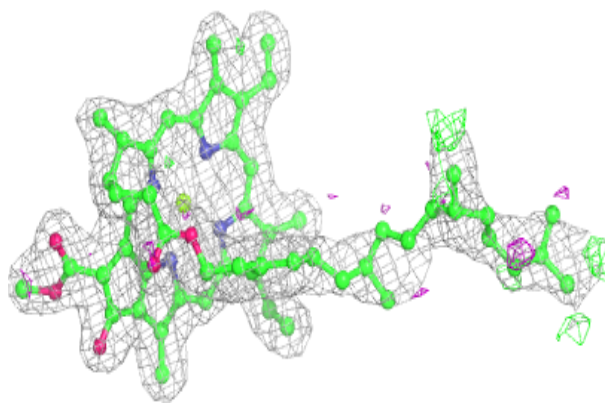
Electron density around CLA B 607:

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

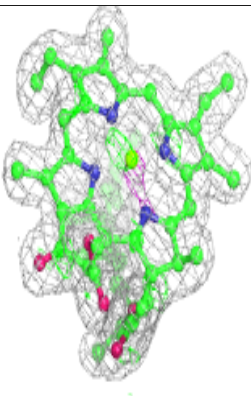
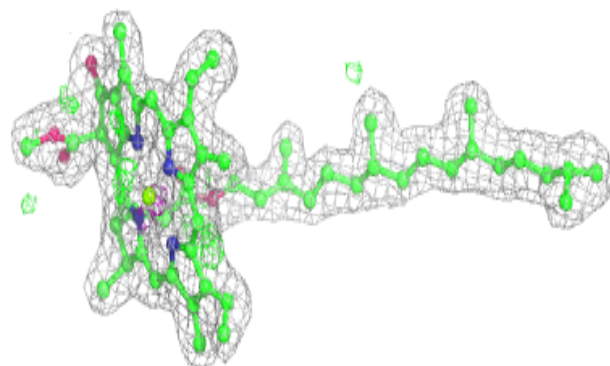
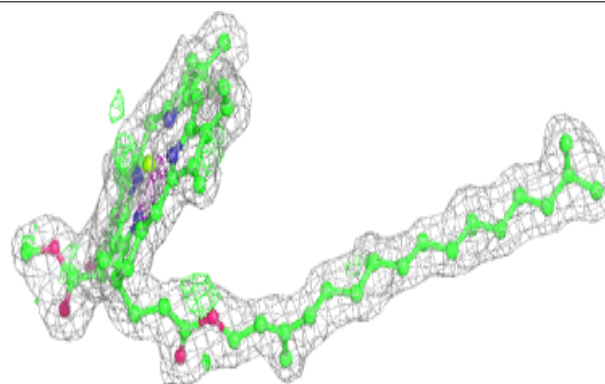


Electron density around CLA b 619:

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

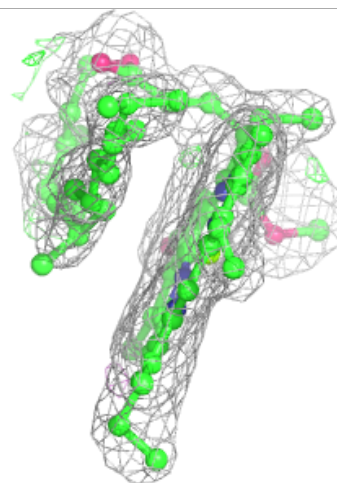
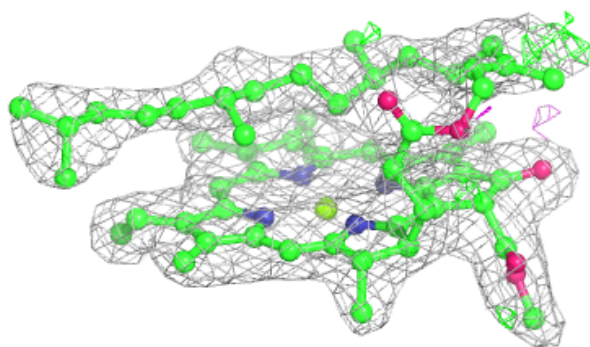
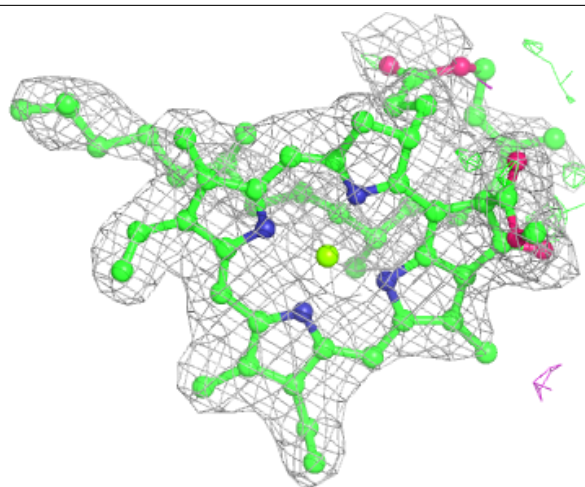
**Electron density around CLA b 612:**

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



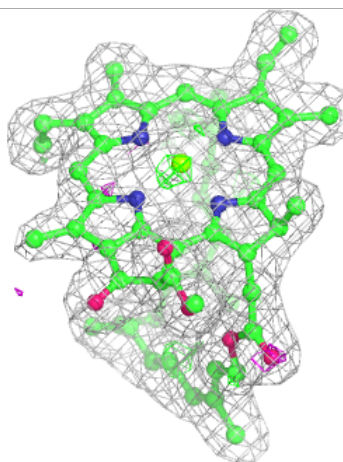
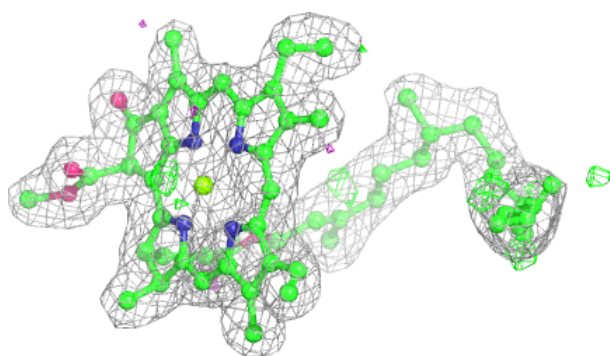
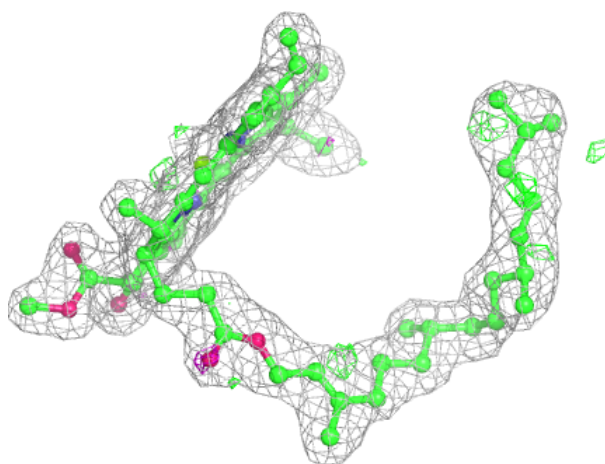
Electron density around CLA b 606:

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



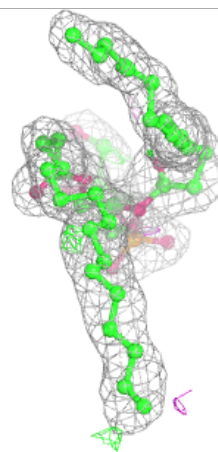
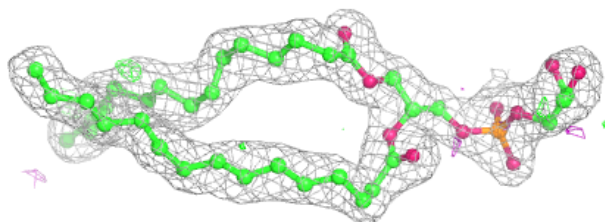
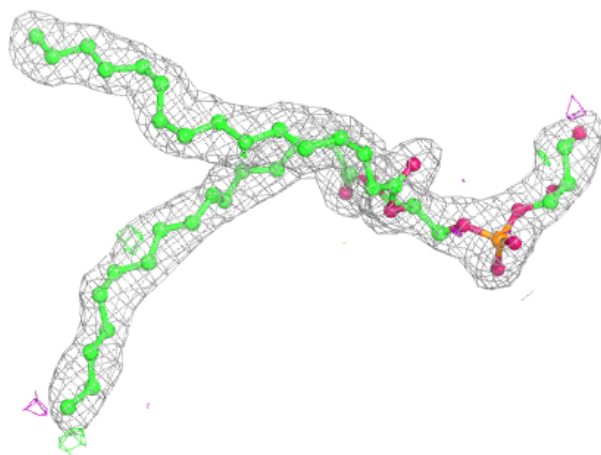
Electron density around CLA b 616:

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



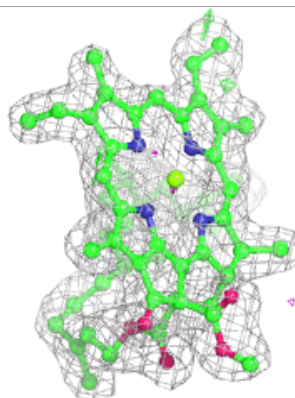
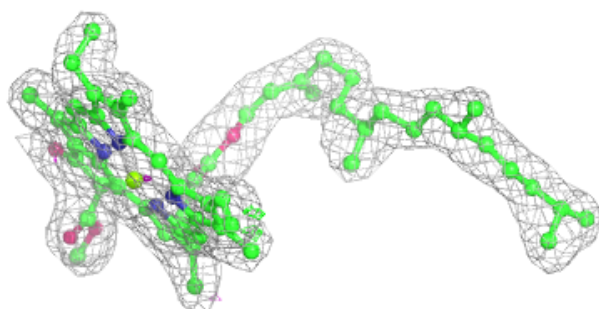
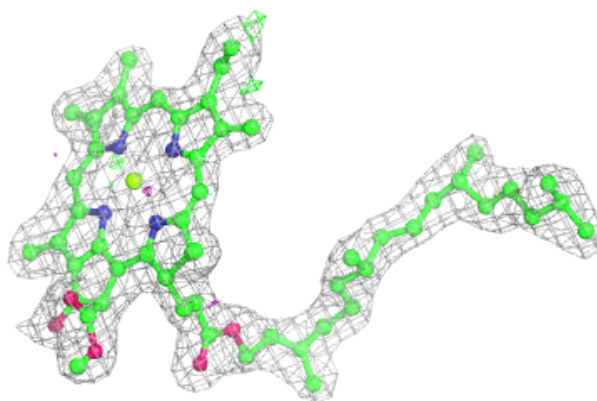
Electron density around LHG d 409:

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

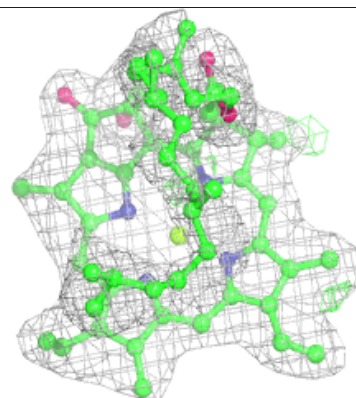
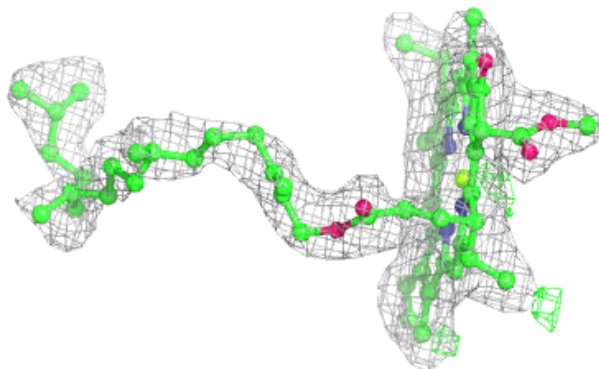
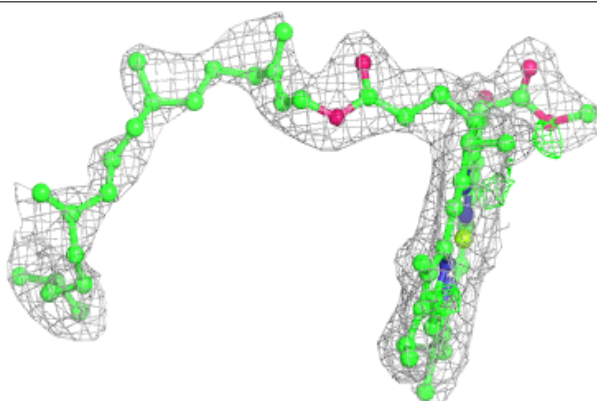


Electron density around CLA C 512:

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

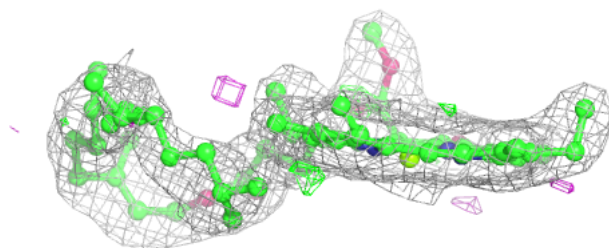
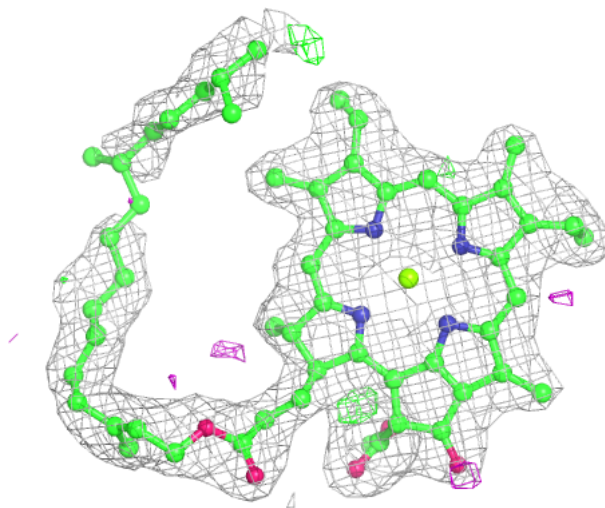
**Electron density around CLA c 508:**

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



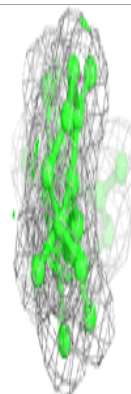
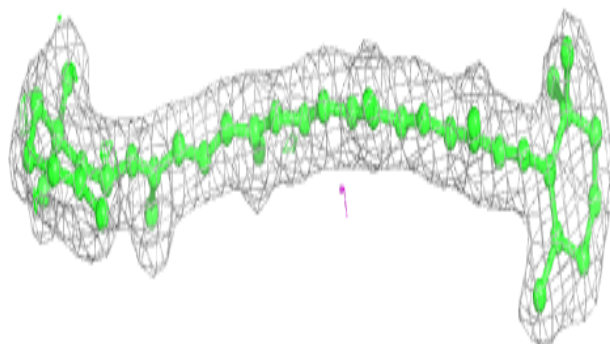
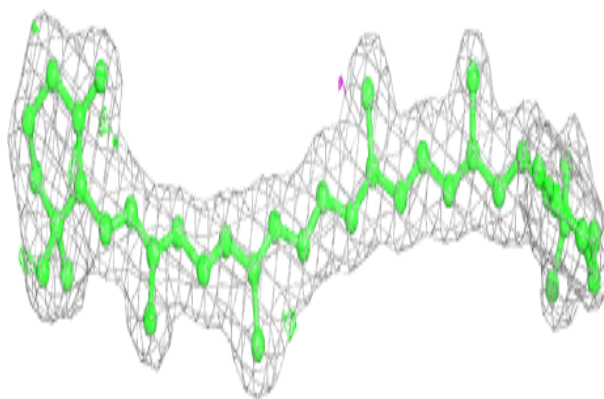
Electron density around CLA C 513:

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

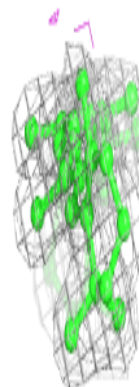
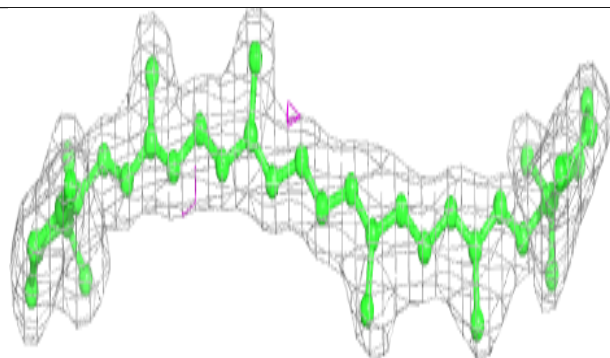
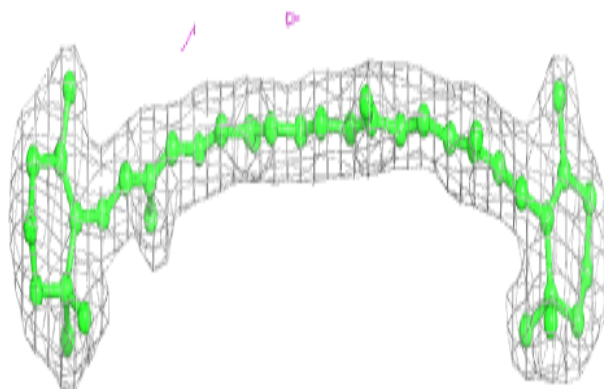


Electron density around BCR B 618:

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

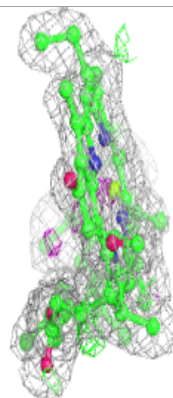
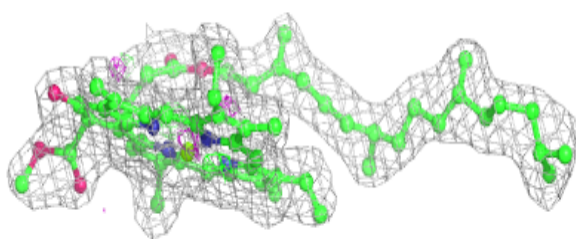
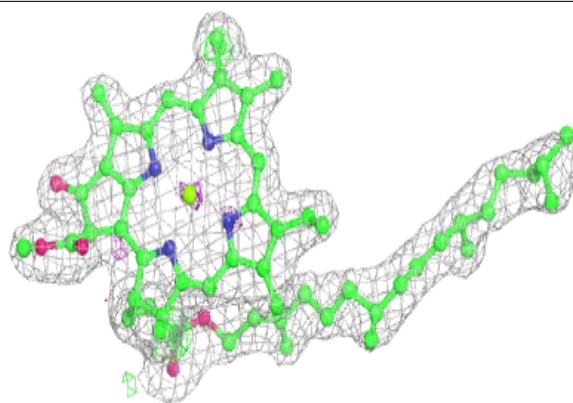
**Electron density around BCR K 101:**

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

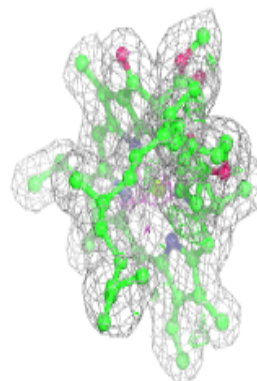
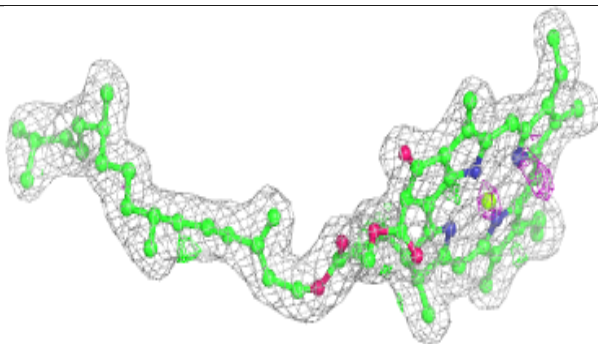
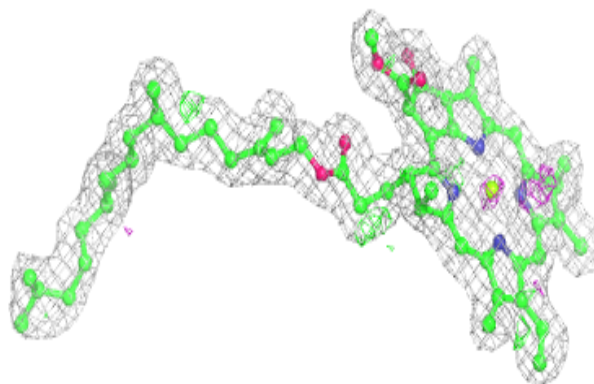


Electron density around CLA C 502:

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

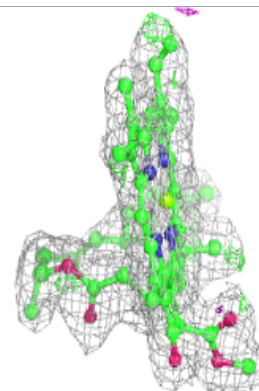
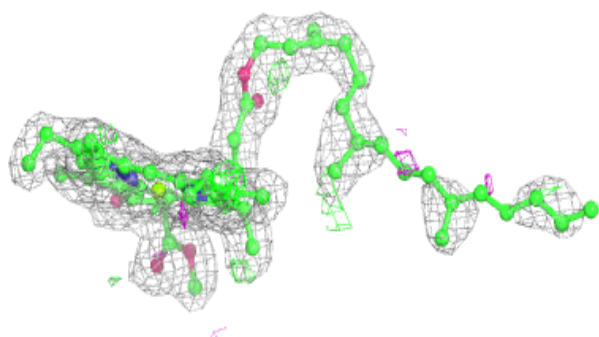
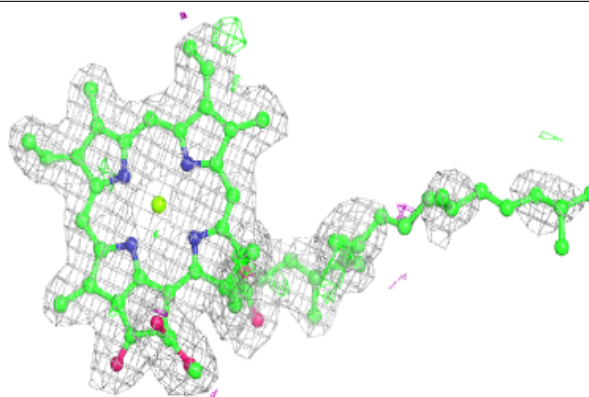
**Electron density around CLA A 405:**

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

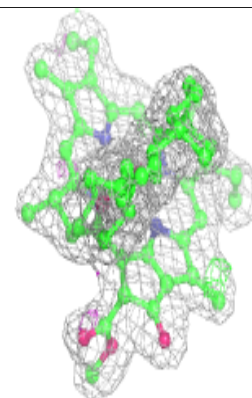
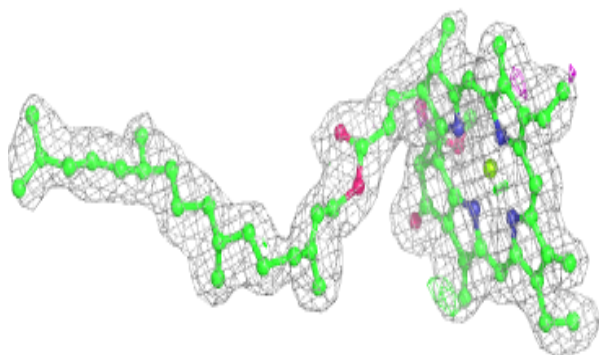
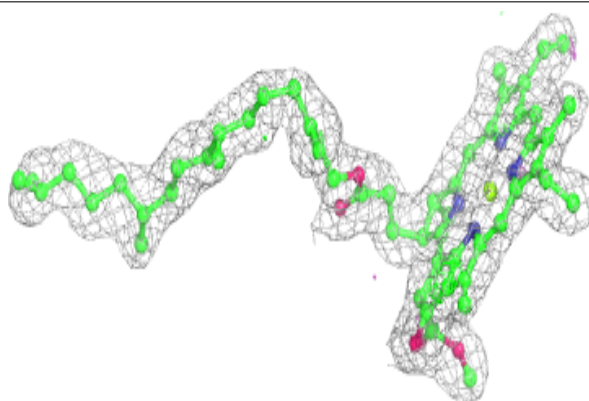


Electron density around CLA a 407:

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

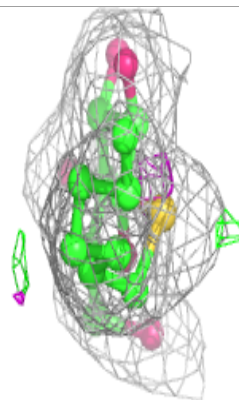
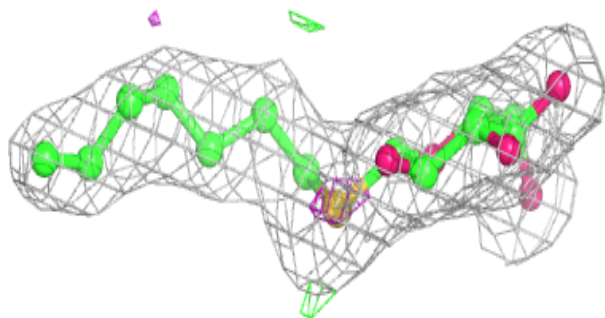
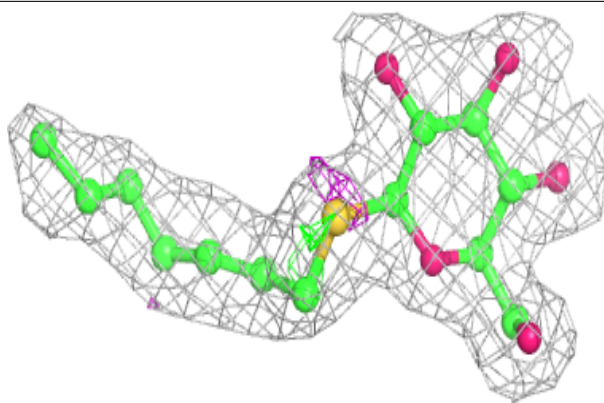
**Electron density around CLA c 504:**

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



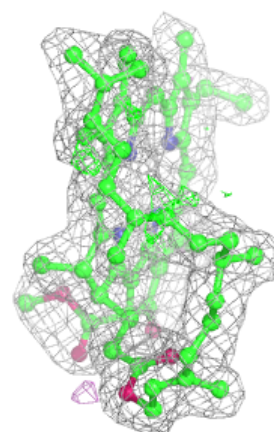
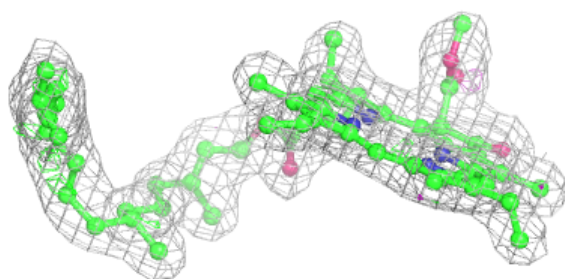
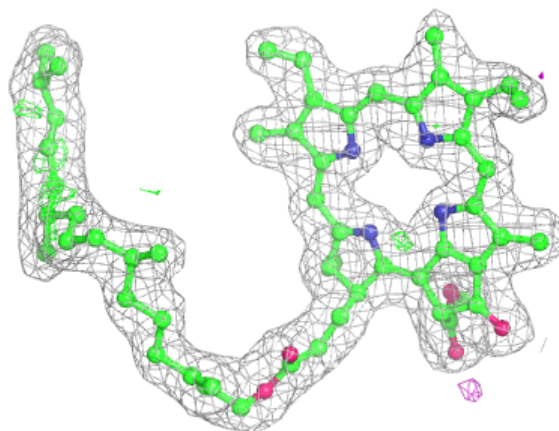
Electron density around HTG O 303:

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



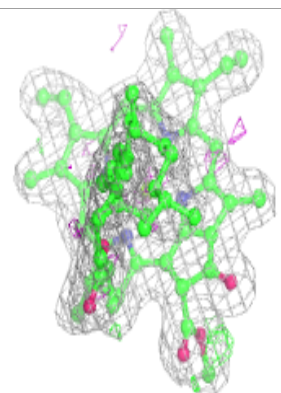
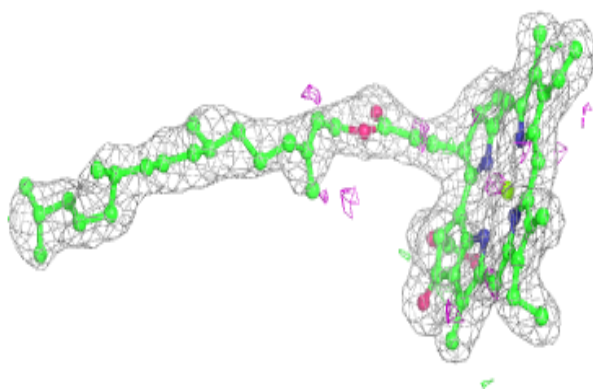
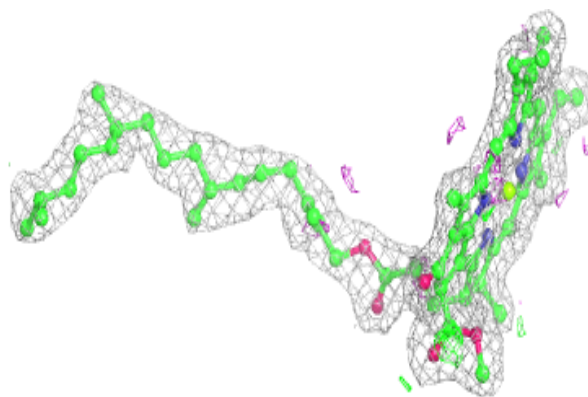
Electron density around PHO d 403:

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



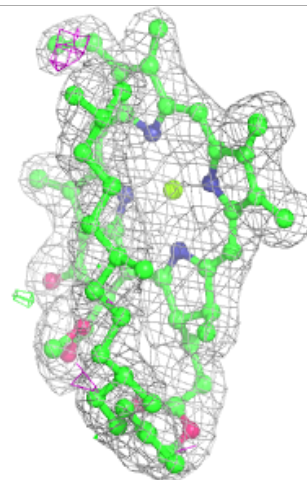
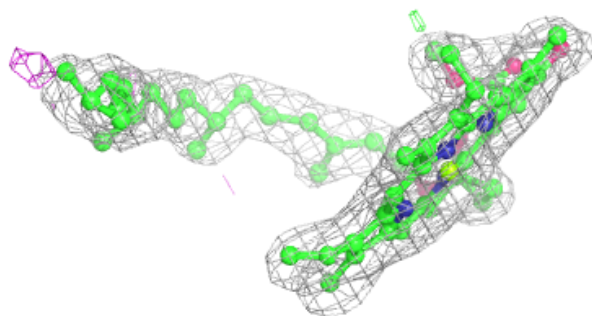
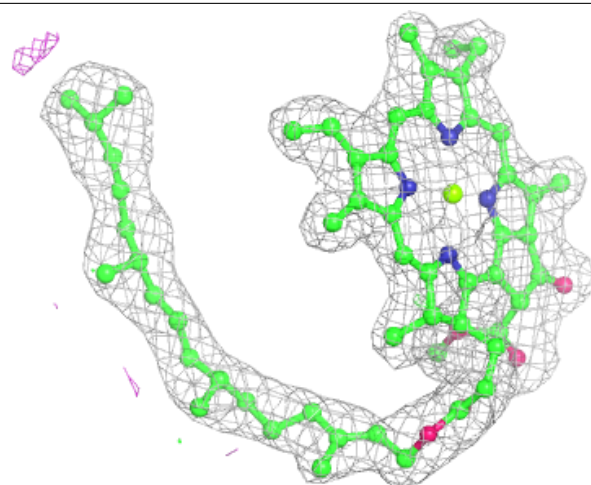
Electron density around CLA B 605:

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



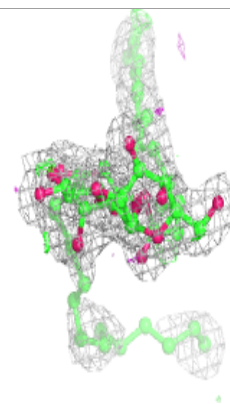
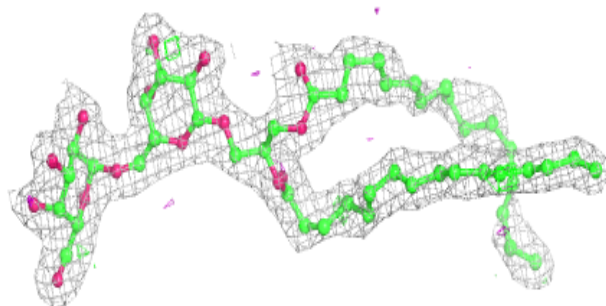
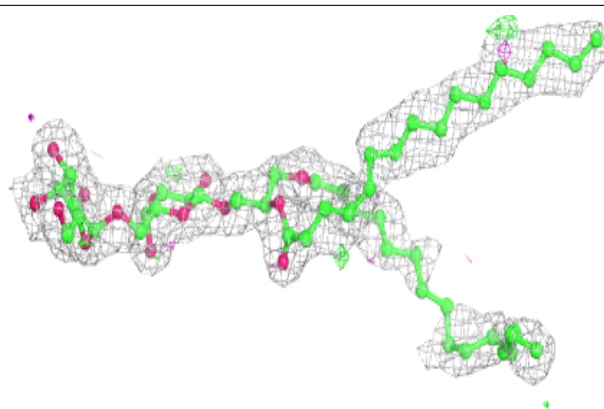
Electron density around CLA C 508:

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

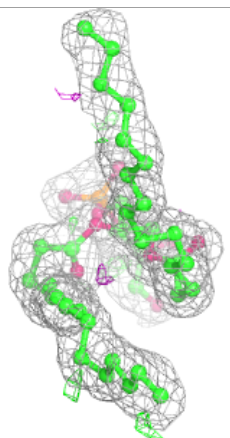
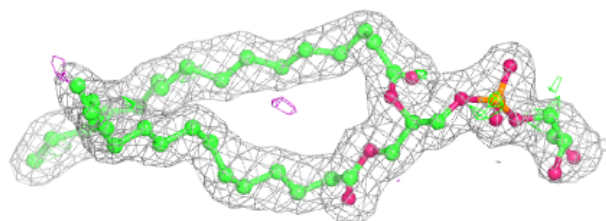
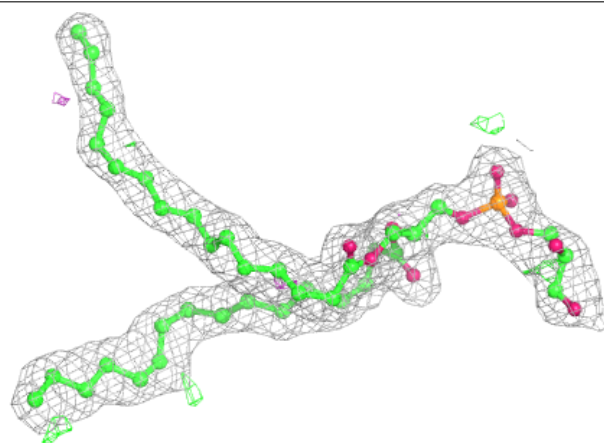


Electron density around DGD C 517:

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

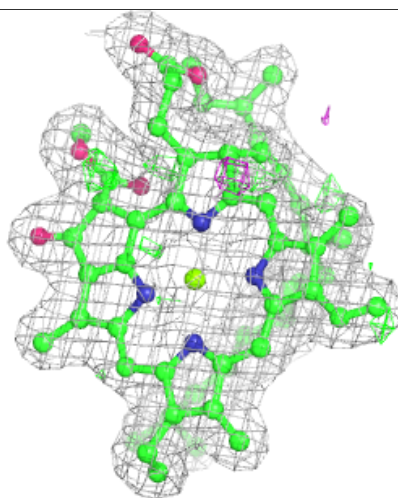
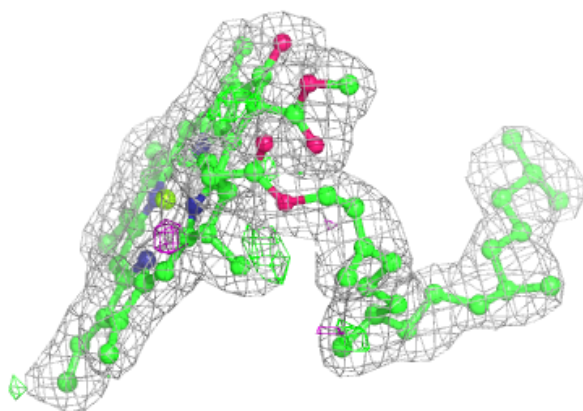
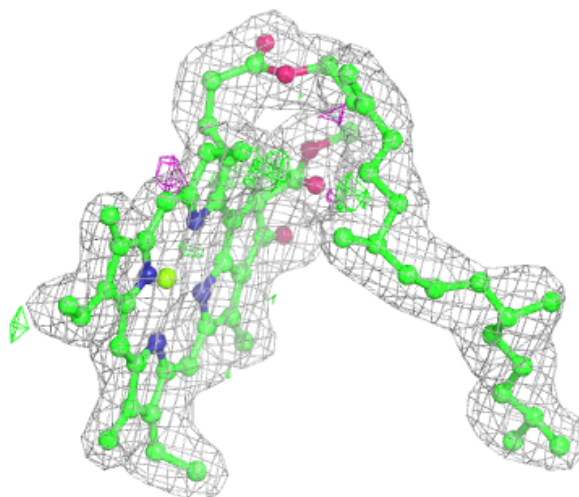
**Electron density around LHG D 409:**

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



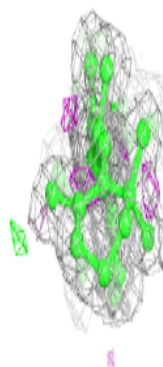
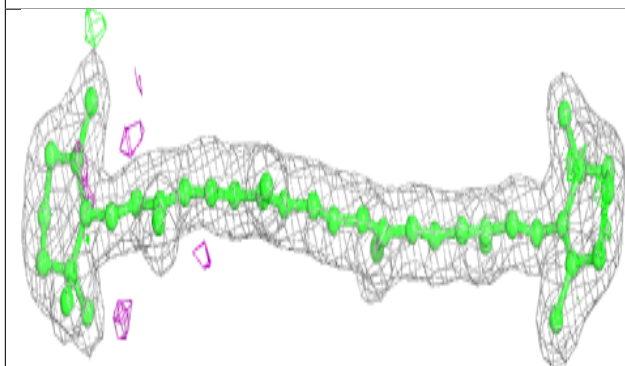
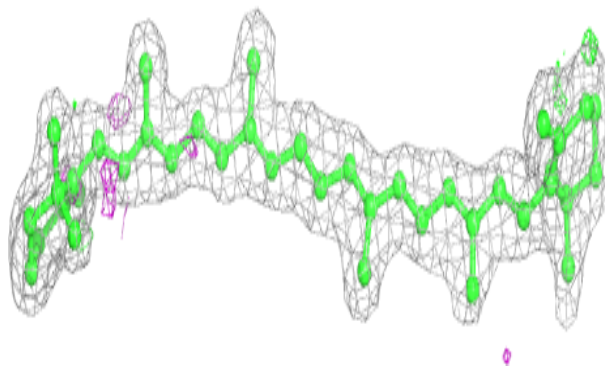
Electron density around CLA b 618:

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

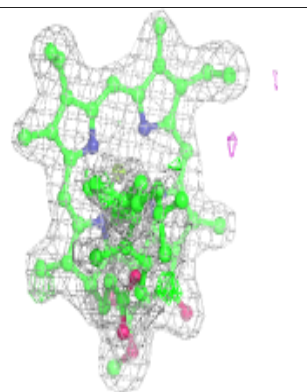
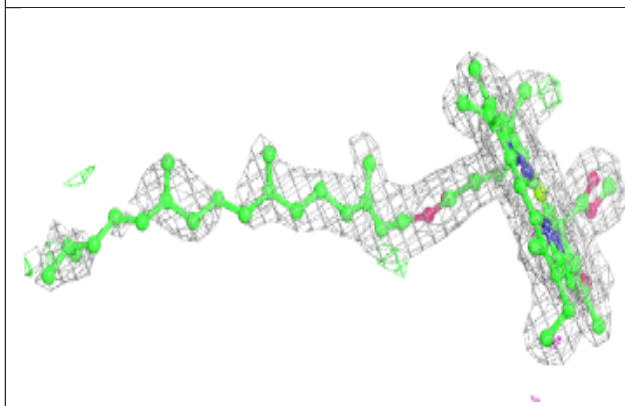
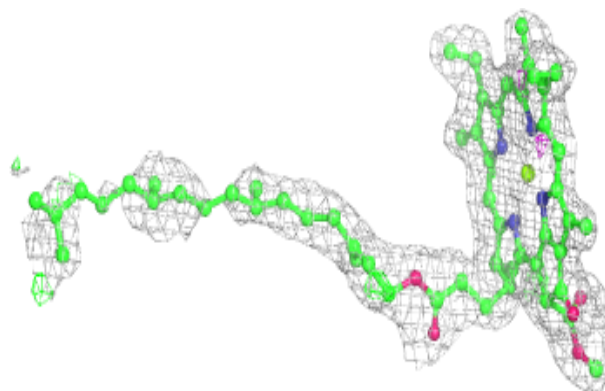


Electron density around BCR a 410:

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

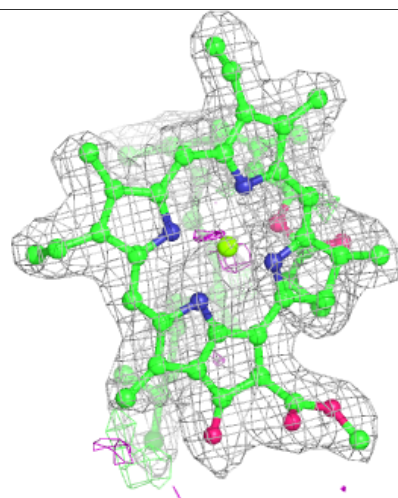
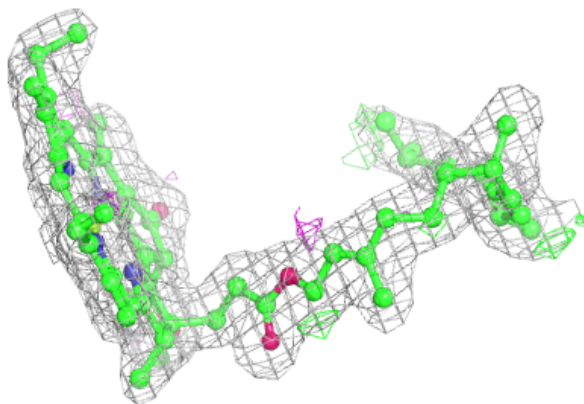
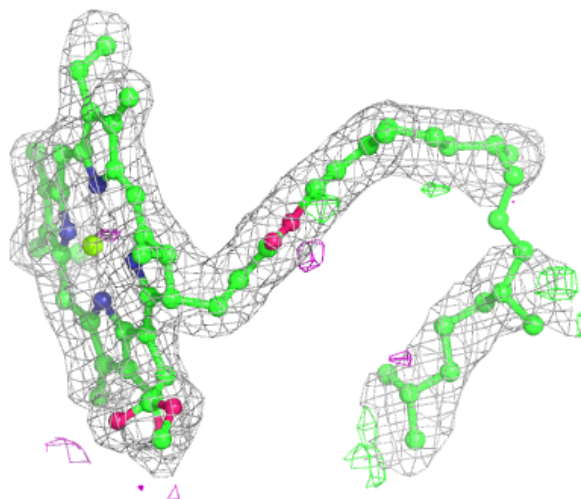
**Electron density around CLA d 404:**

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



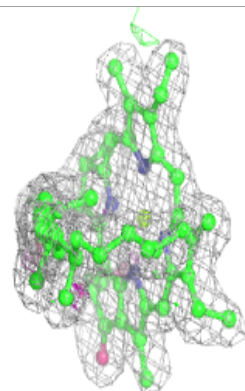
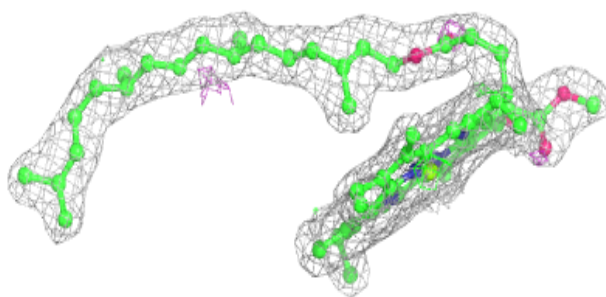
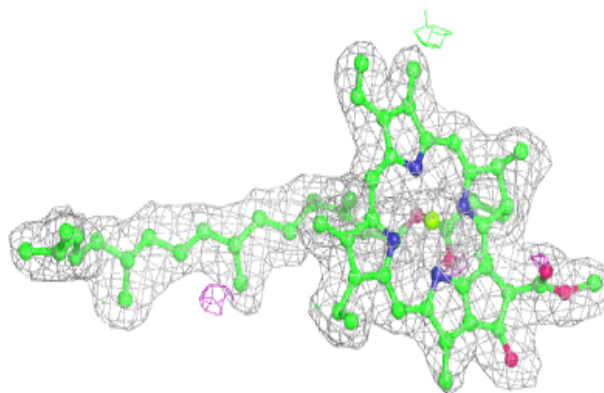
Electron density around CLA b 611:

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

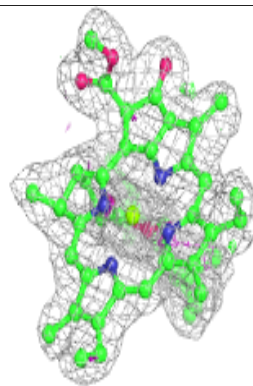
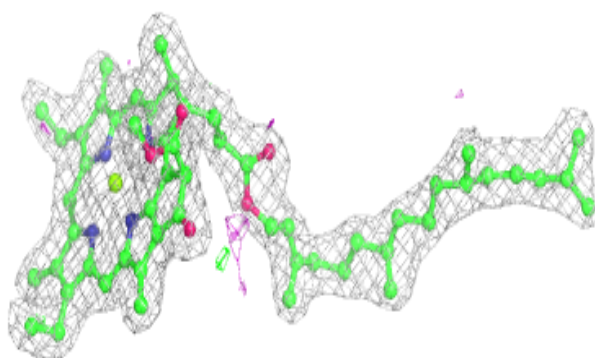
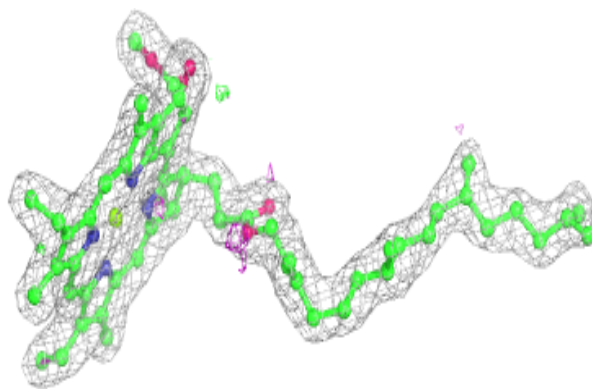


Electron density around CLA b 613:

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

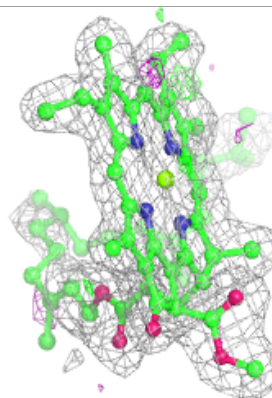
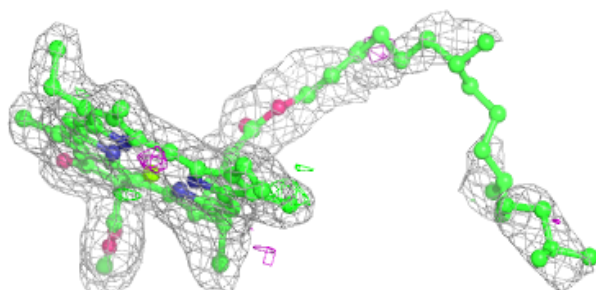
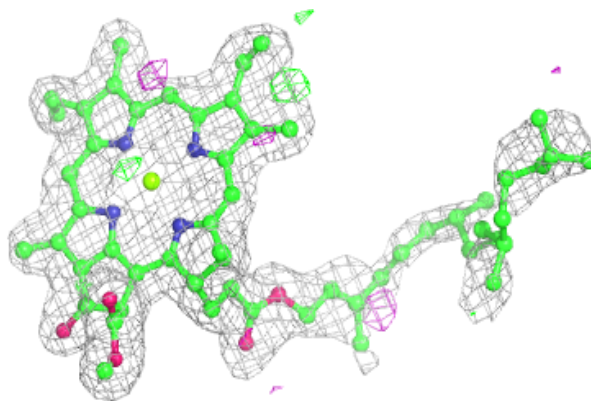
**Electron density around CLA C 503:**

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

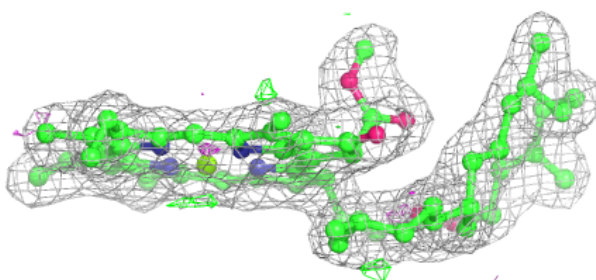
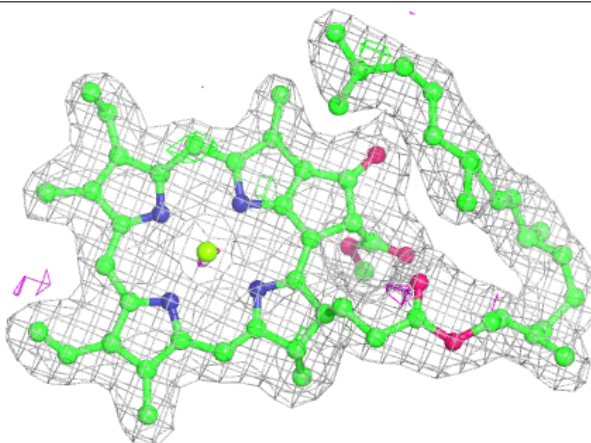


Electron density around CLA a 409:

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

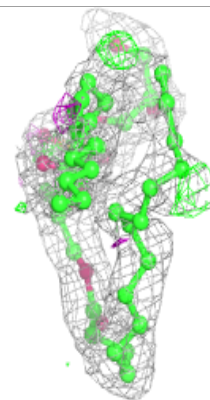
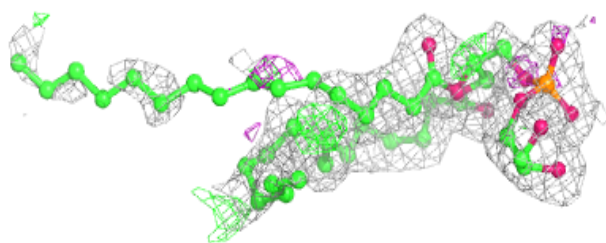
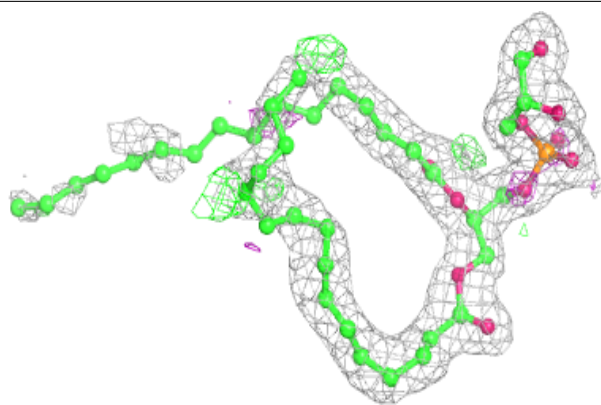
**Electron density around CLA b 615:**

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

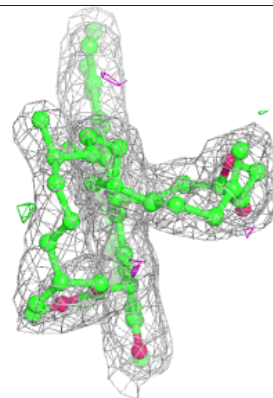
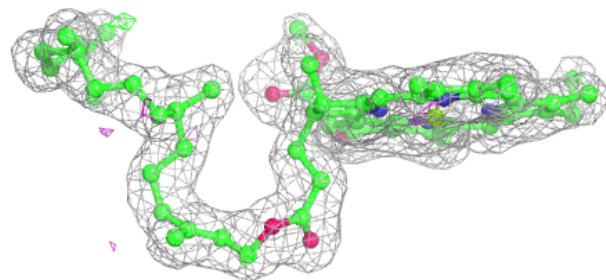
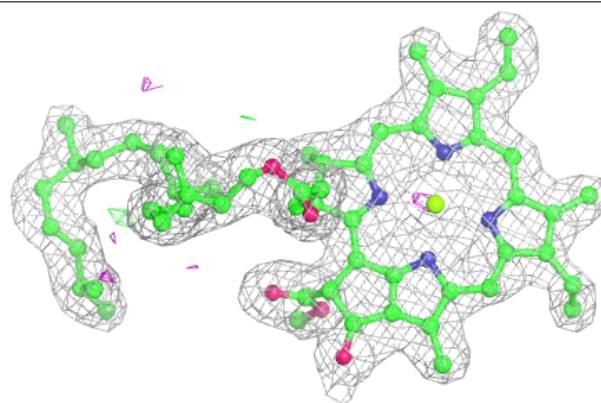


Electron density around LHG D 410:

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

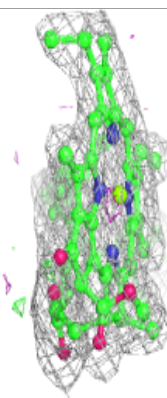
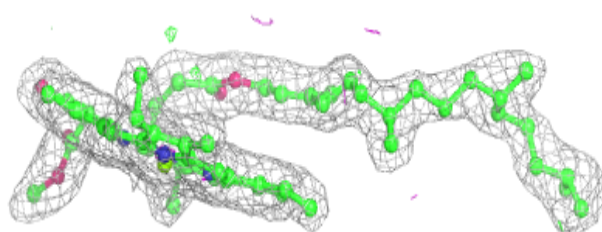
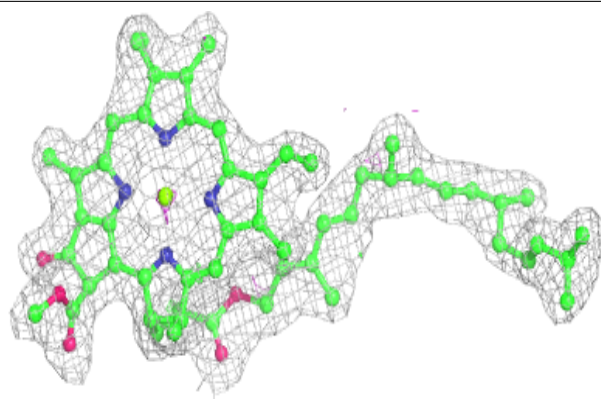
**Electron density around CLA b 617:**

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

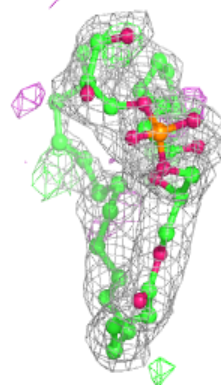
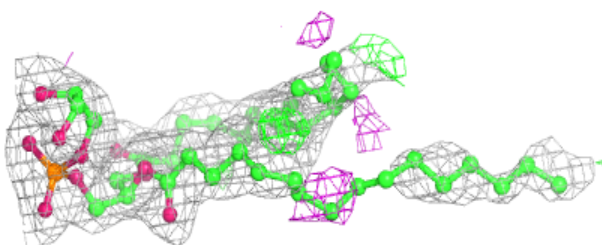
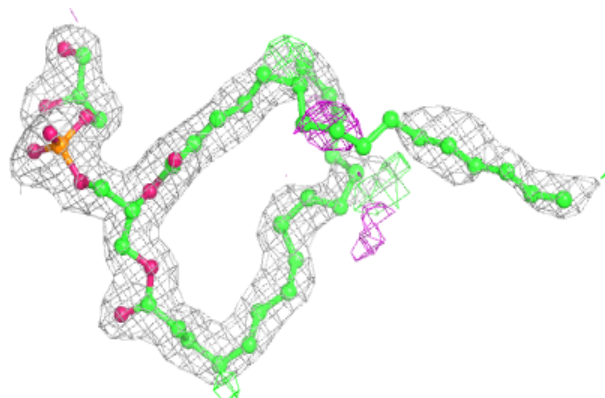


Electron density around CLA b 608:

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

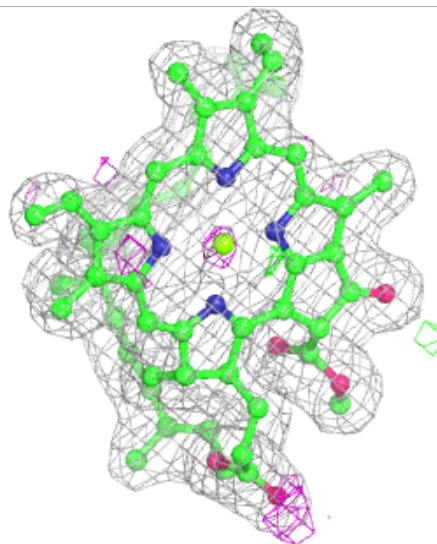
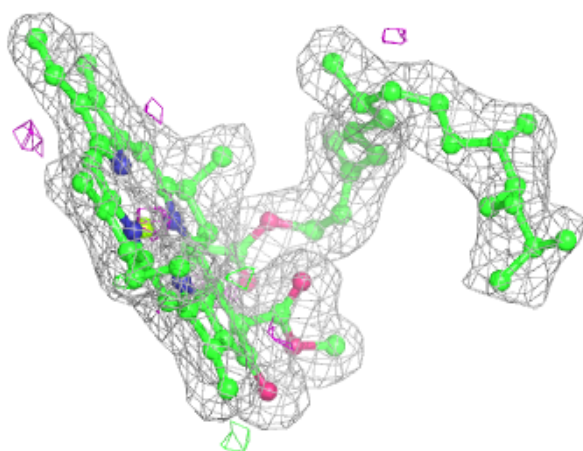
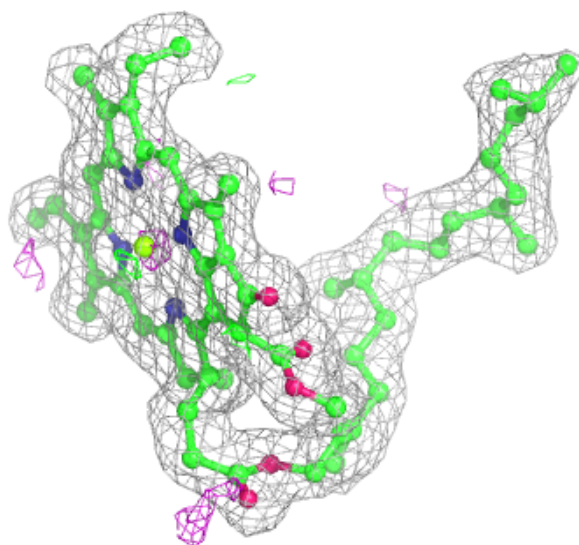
**Electron density around LHG d 410:**

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



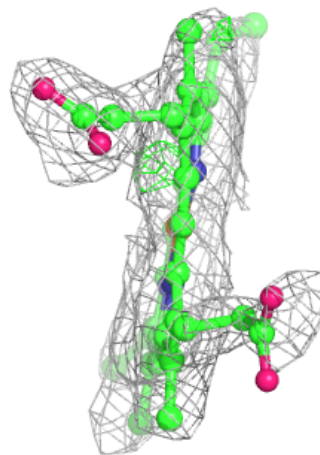
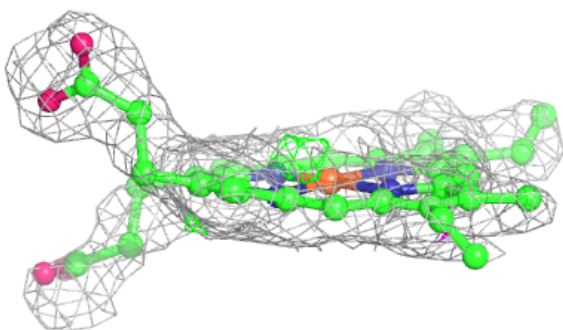
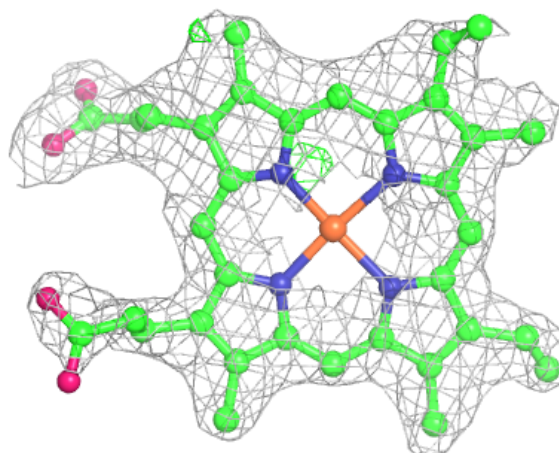
Electron density around CLA B 614:

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



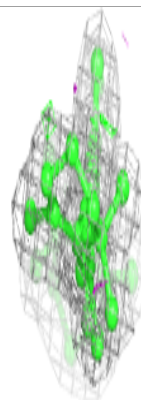
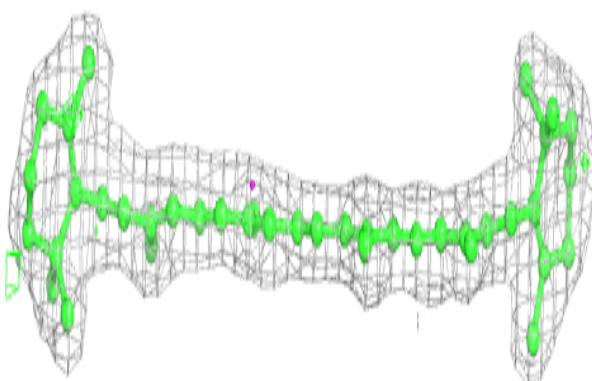
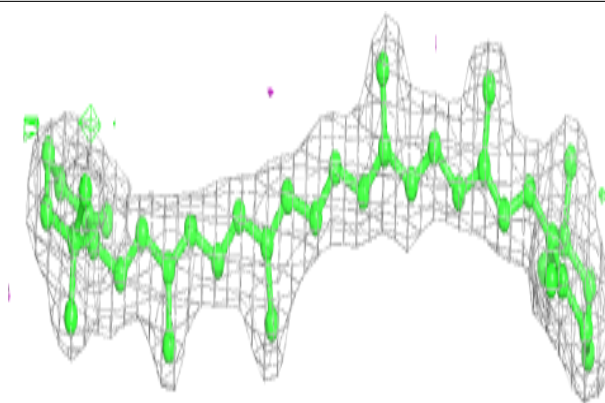
Electron density around HEM e 102:

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



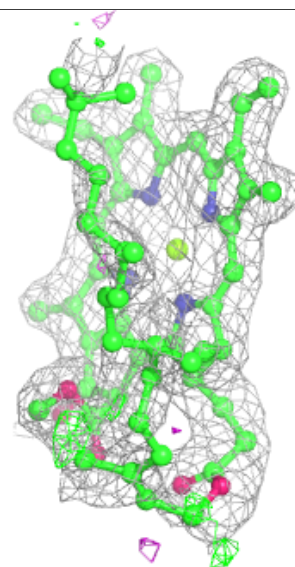
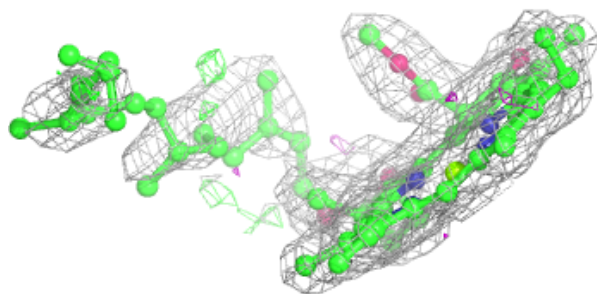
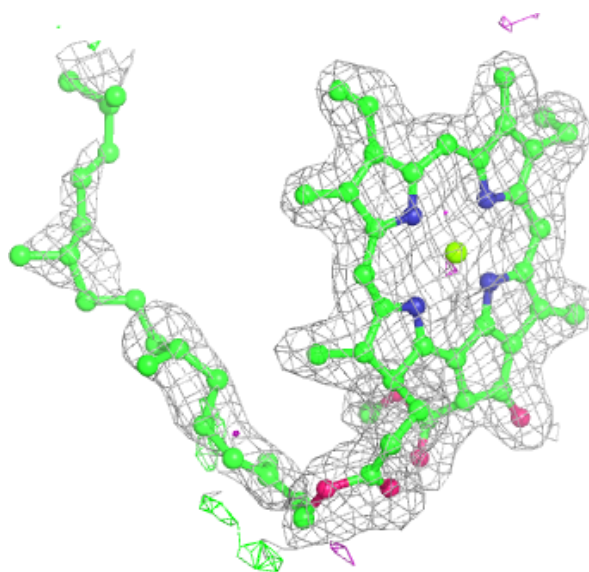
Electron density around BCR C 516:

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



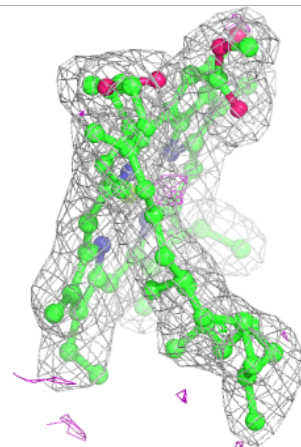
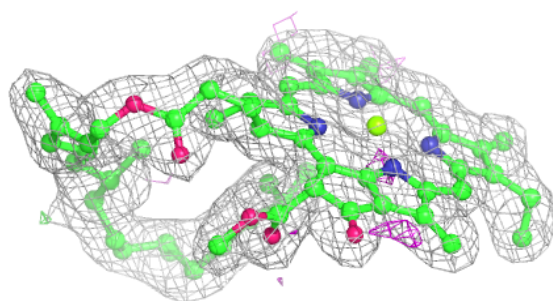
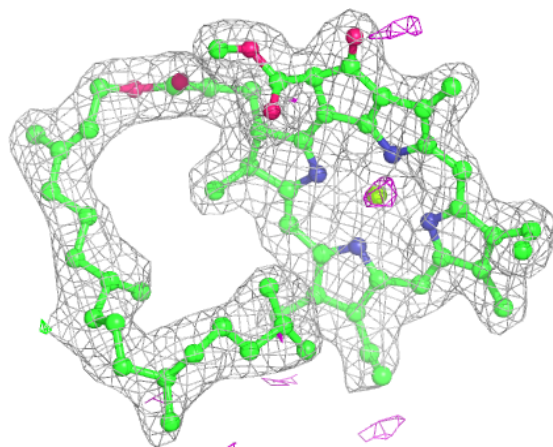
Electron density around CLA B 617:

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



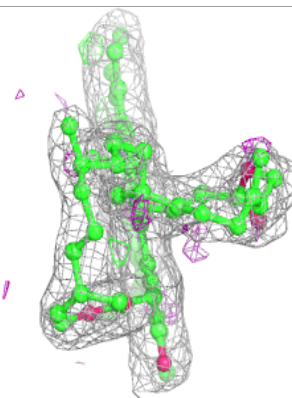
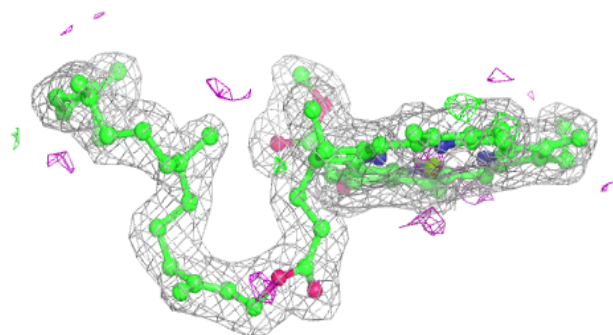
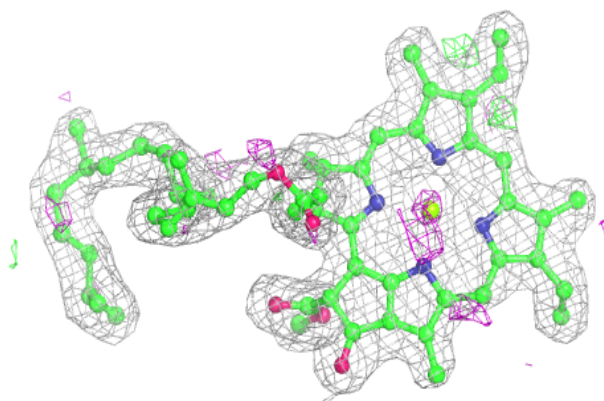
Electron density around CLA B 616:

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



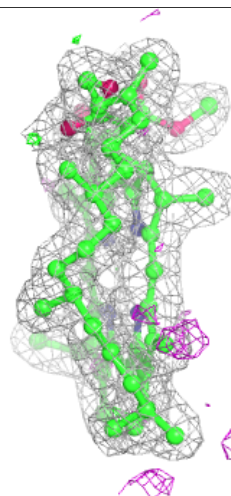
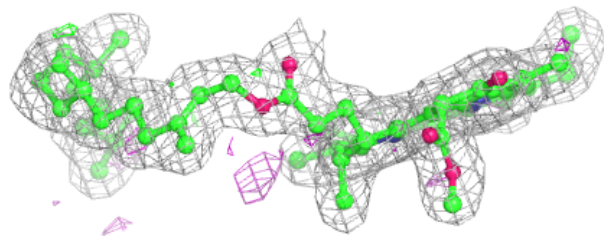
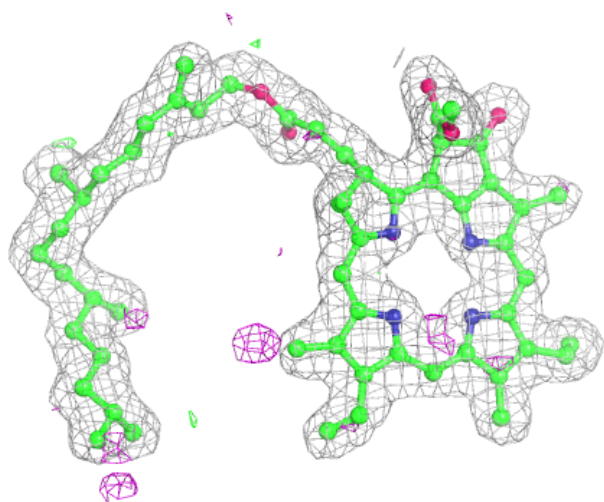
Electron density around CLA B 613:

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



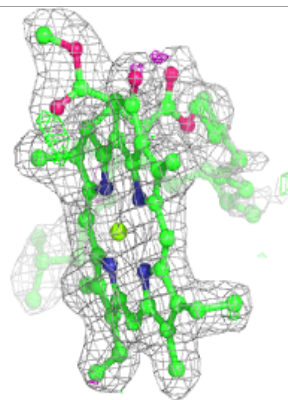
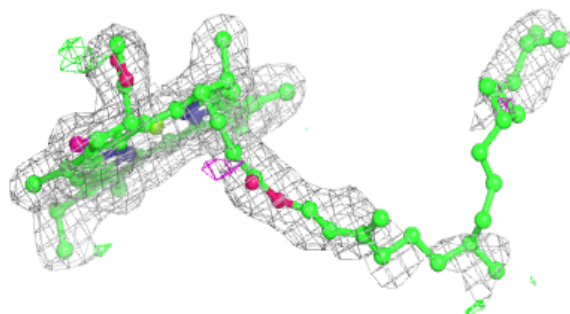
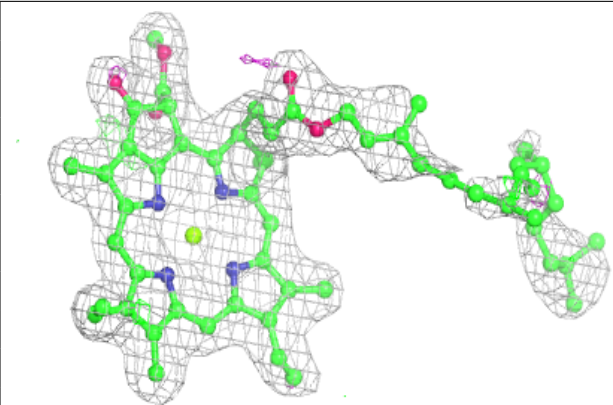
Electron density around PHO A 407:

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

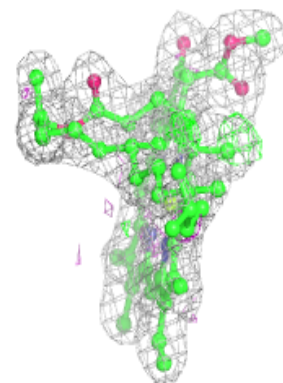
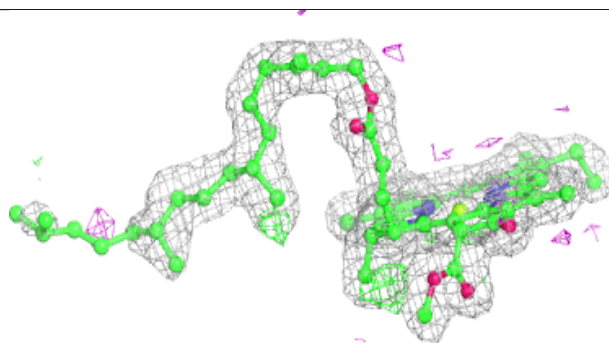
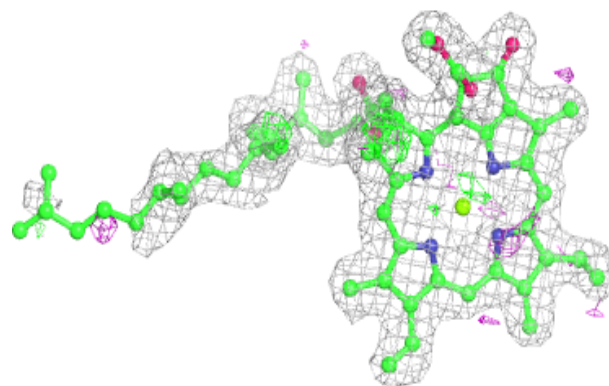


Electron density around CLA A 409:

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

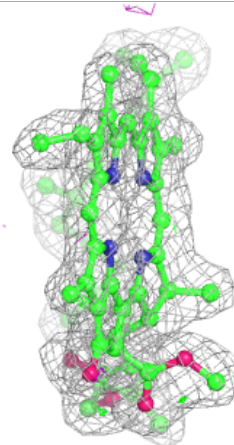
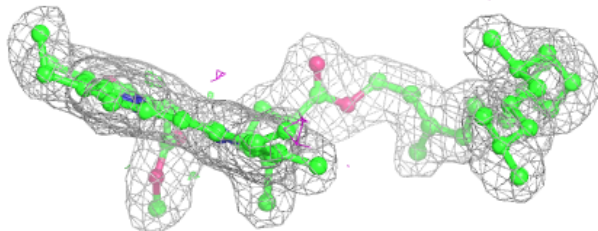
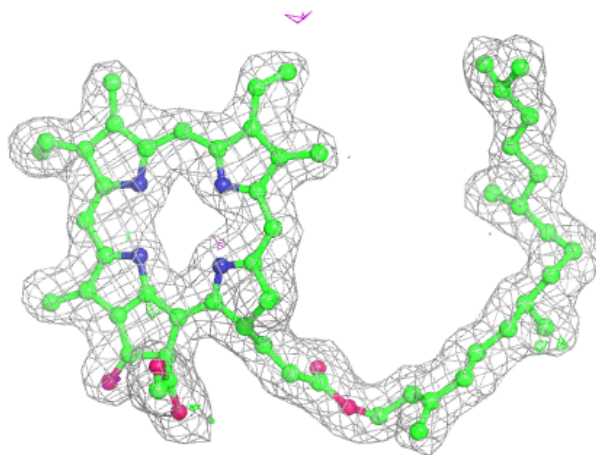
**Electron density around CLA A 406:**

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



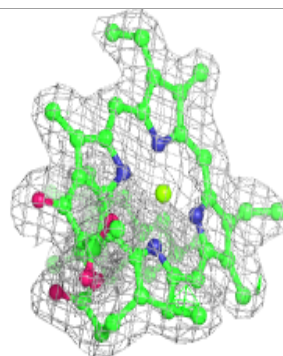
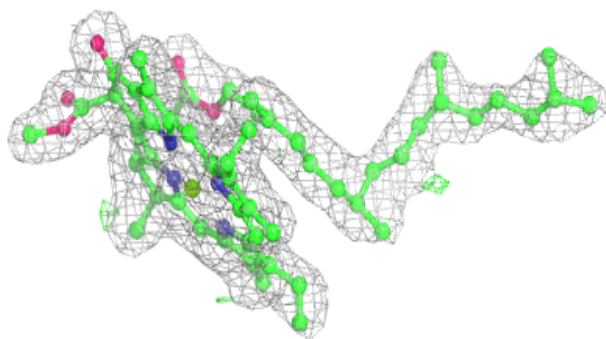
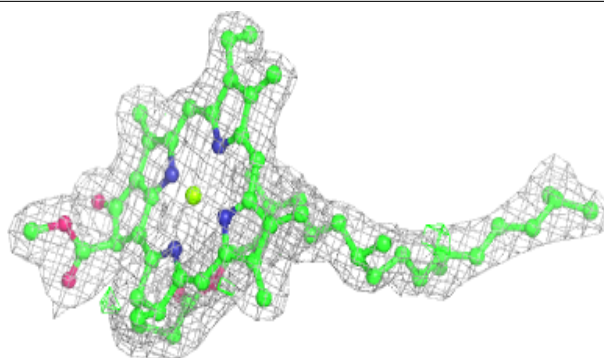
Electron density around PHO a 408:

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

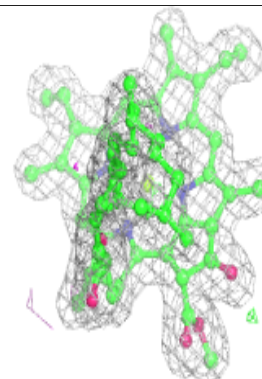
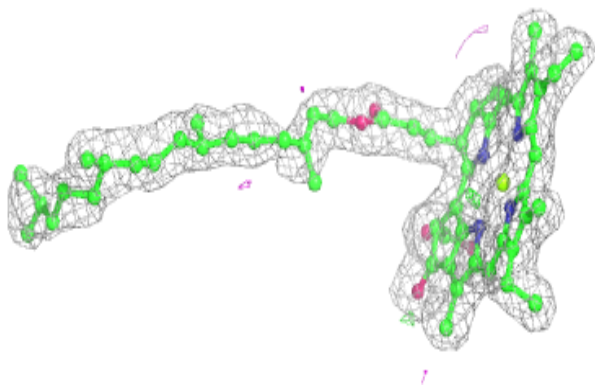
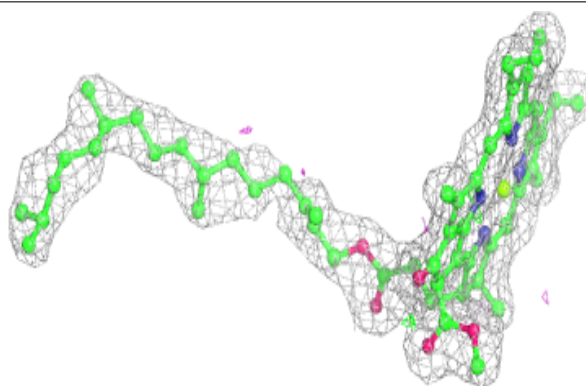


Electron density around CLA C 506:

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

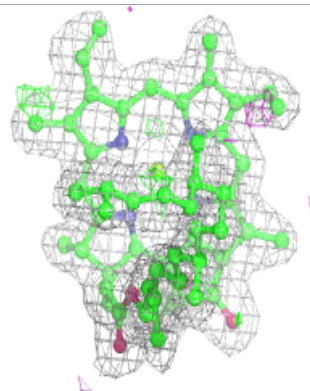
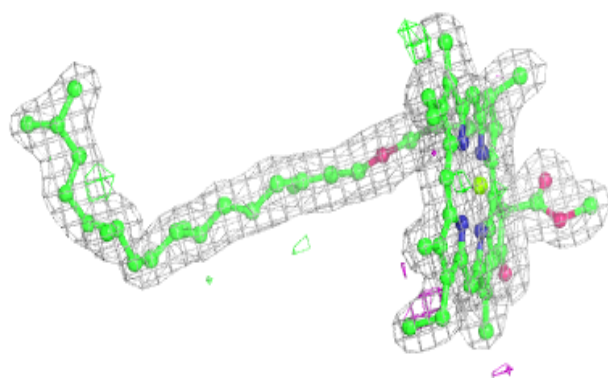
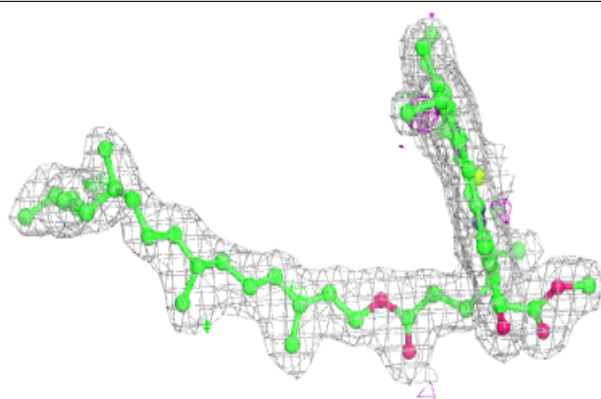
**Electron density around CLA b 609:**

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



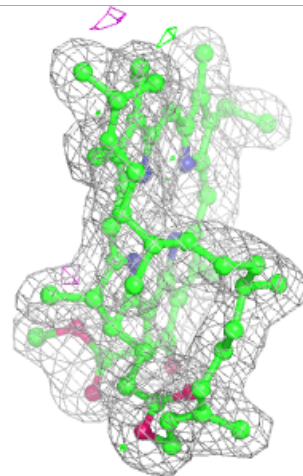
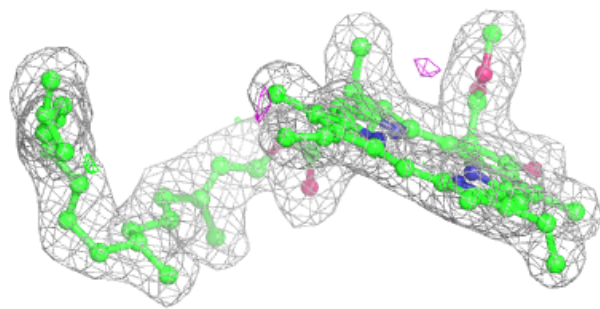
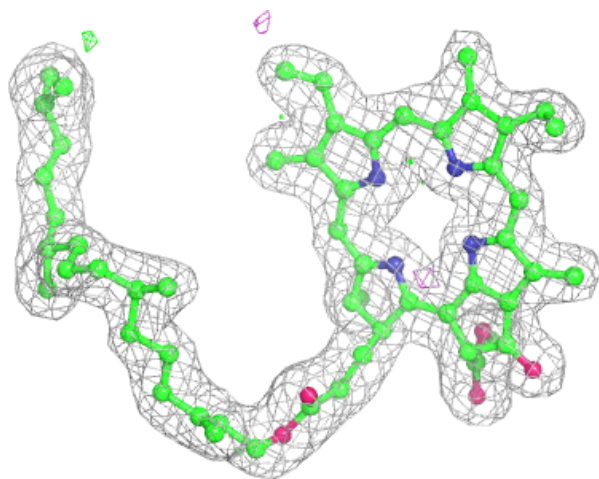
Electron density around CLA B 606:

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



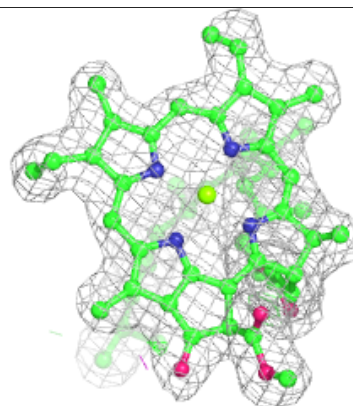
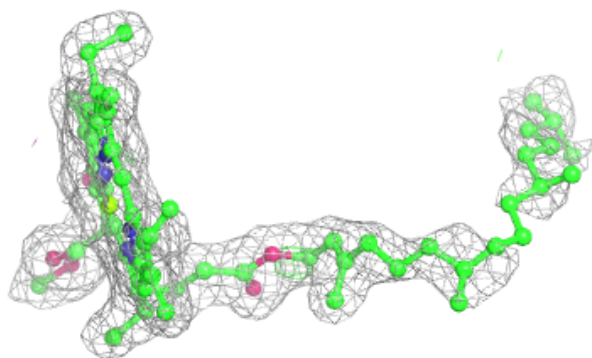
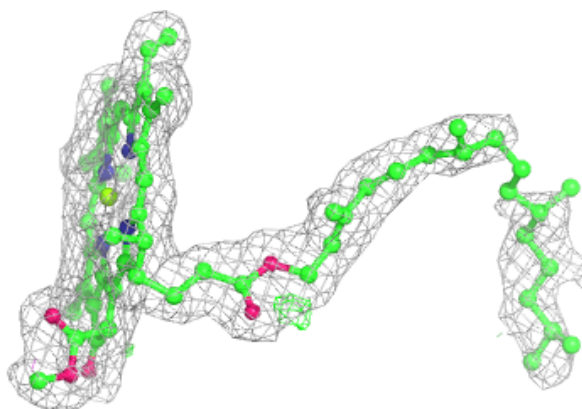
Electron density around PHO A 408:

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

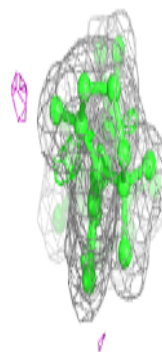
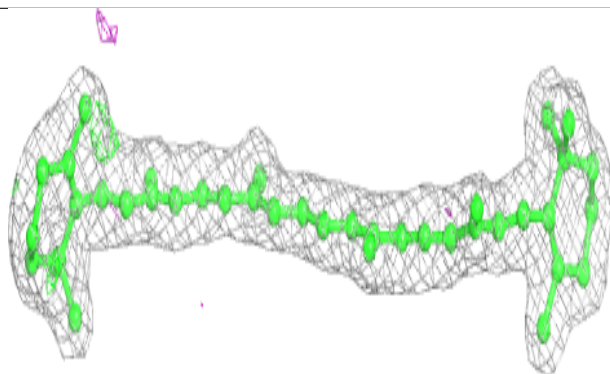
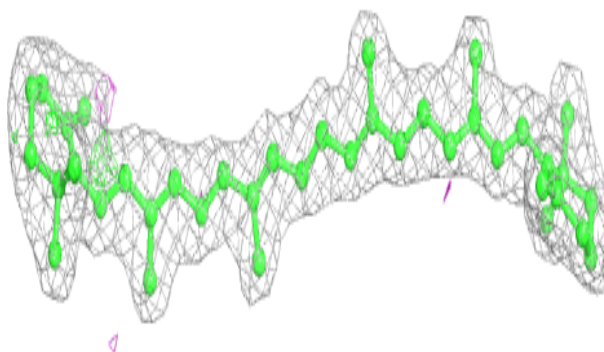


Electron density around CLA D 404:

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

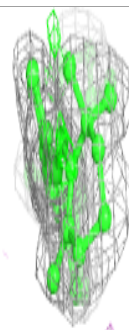
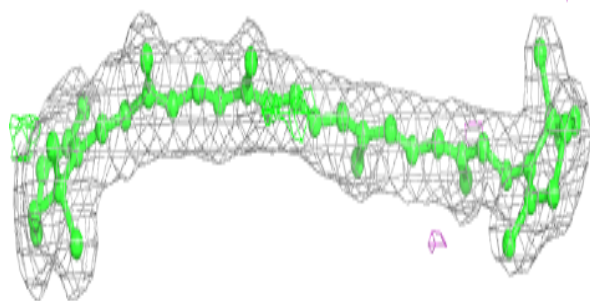
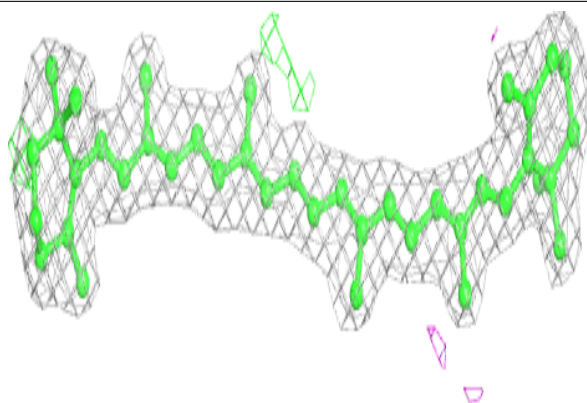
**Electron density around BCR A 410:**

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



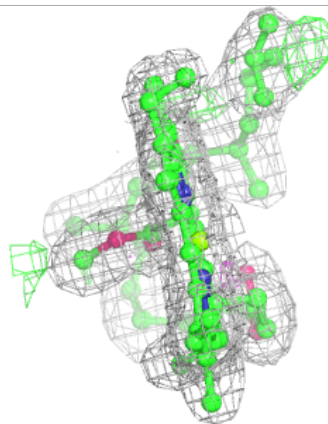
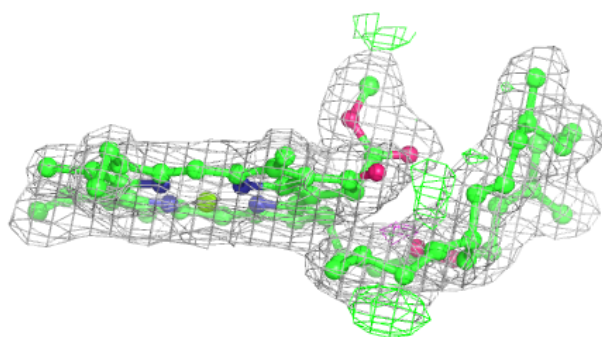
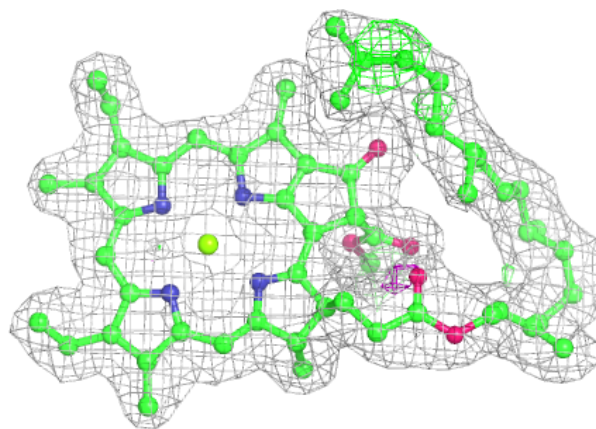
Electron density around BCR B 620:

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



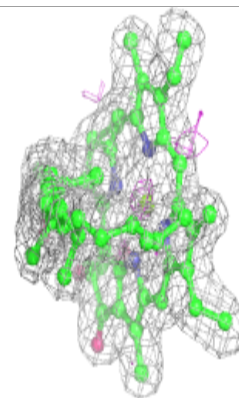
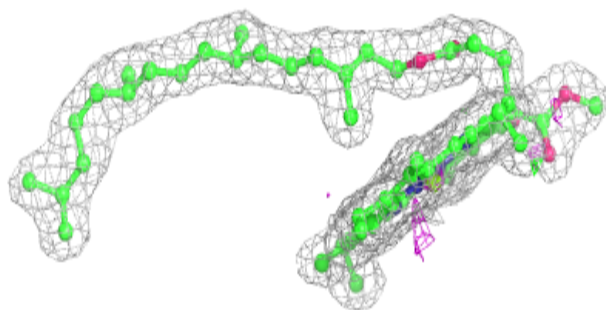
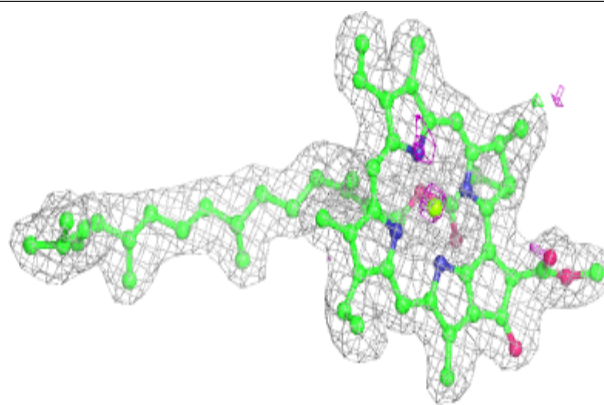
Electron density around CLA B 611:

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



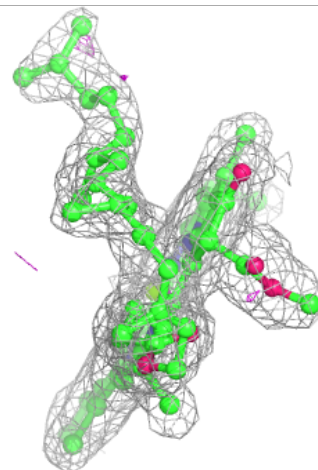
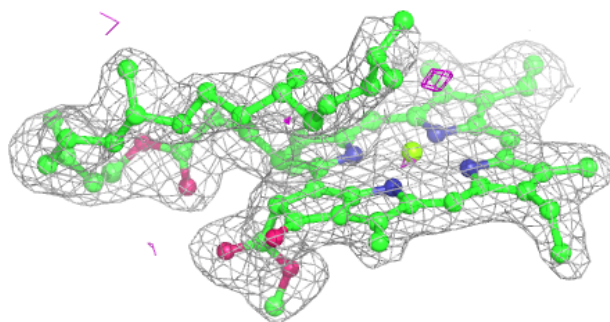
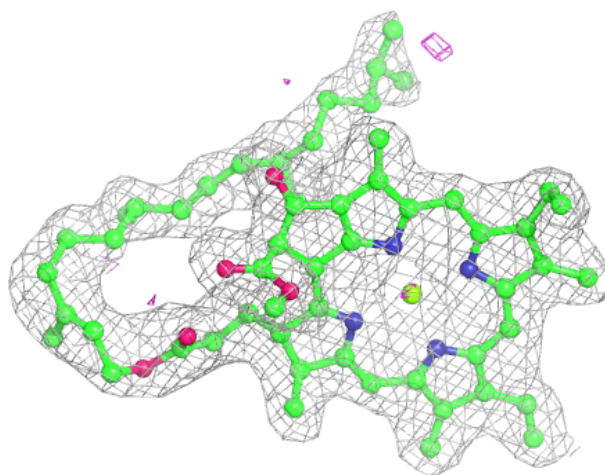
Electron density around CLA B 609:

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



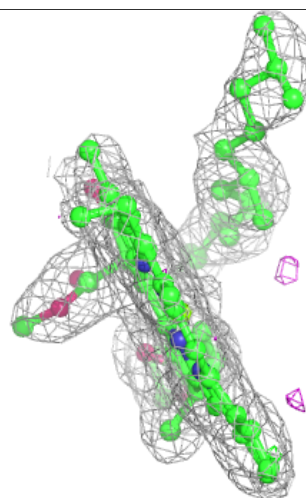
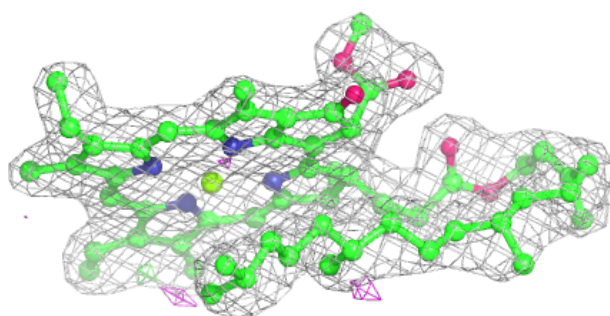
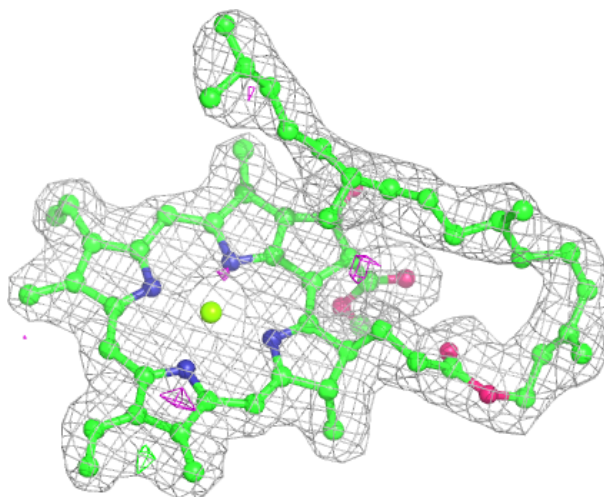
Electron density around CLA c 511:

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



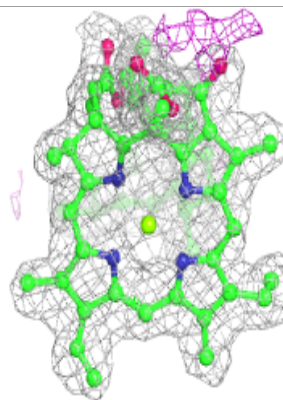
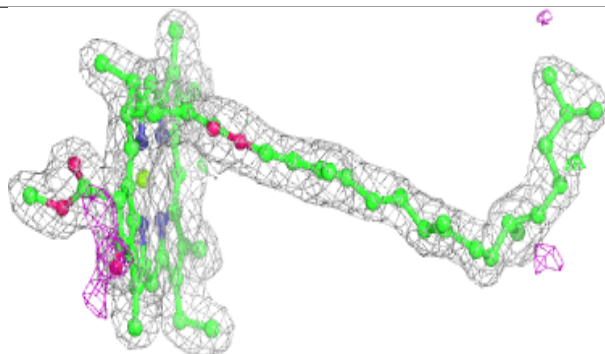
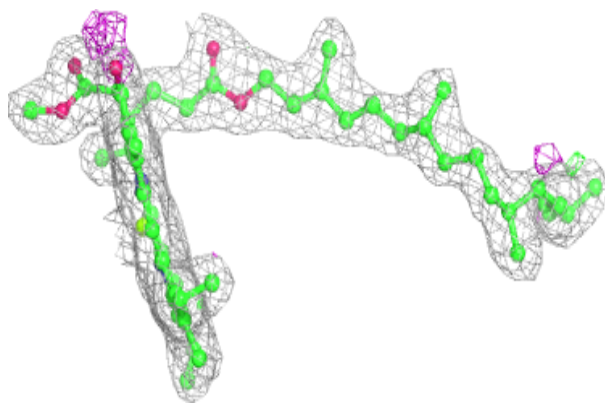
Electron density around CLA C 510:

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

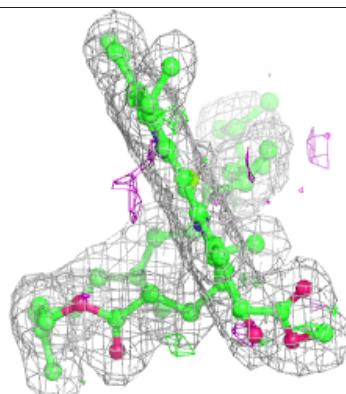
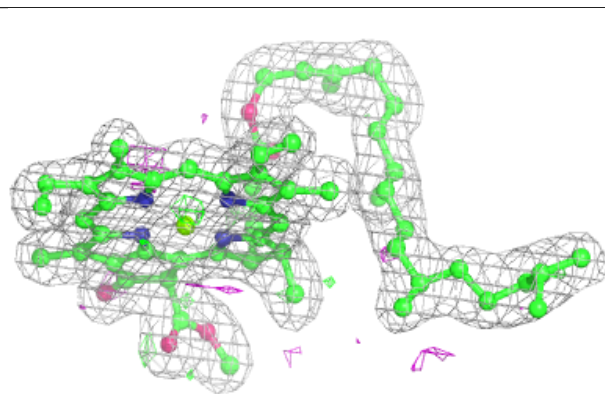
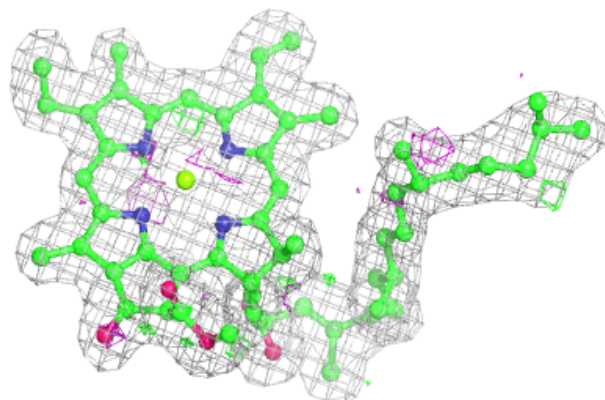


Electron density around CLA b 610:

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

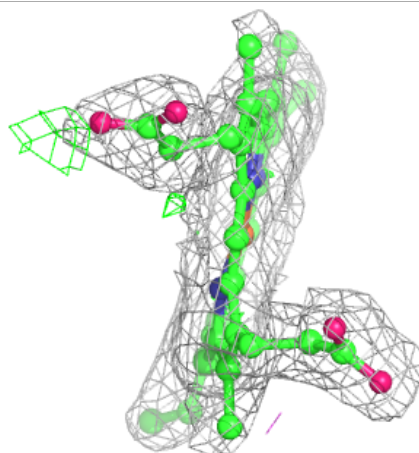
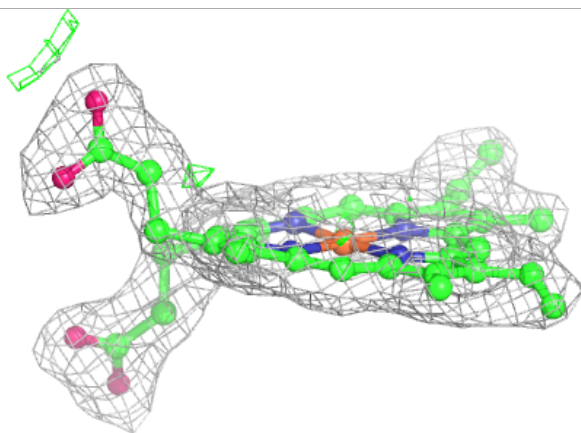
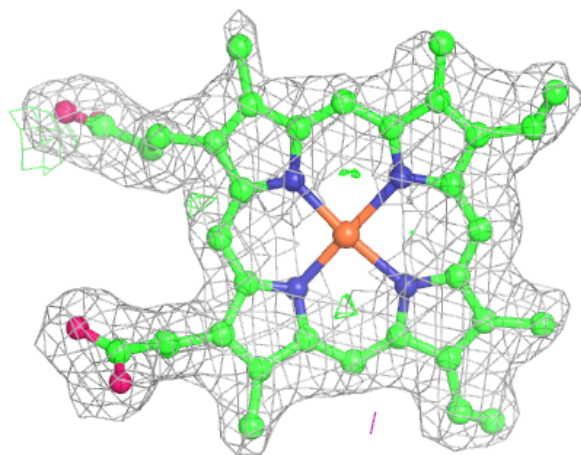
**Electron density around CLA d 401:**

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



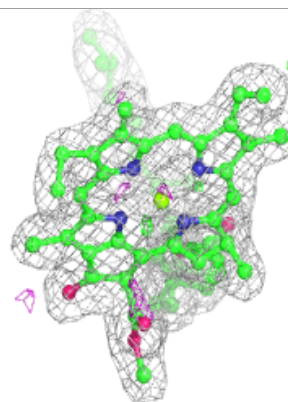
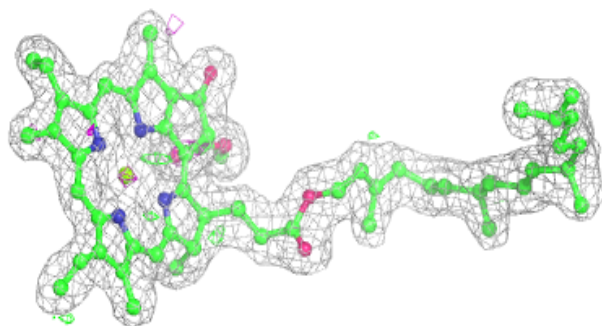
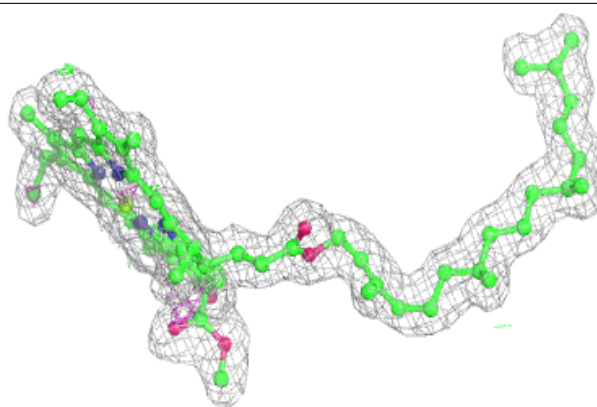
Electron density around HEM E 103:

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

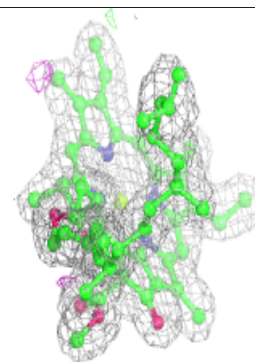
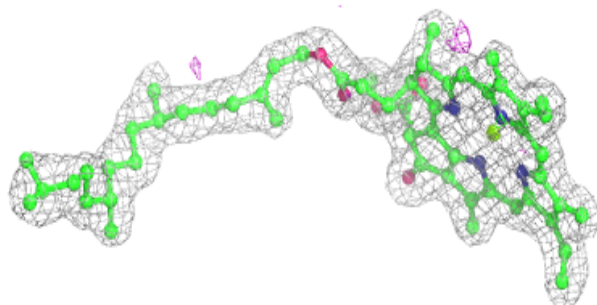
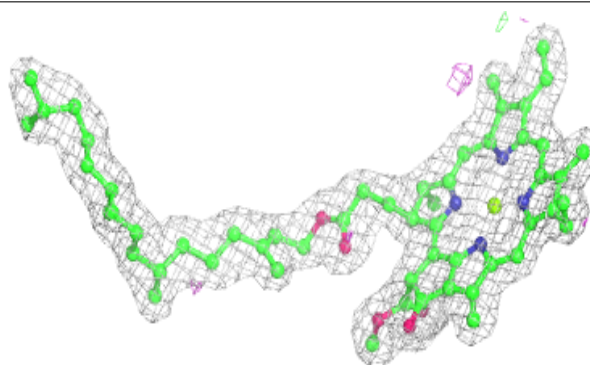


Electron density around CLA D 403:

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

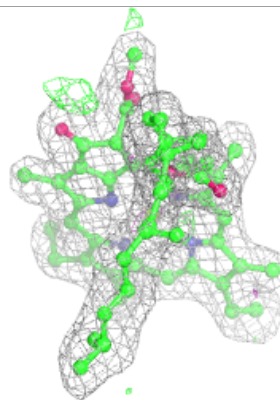
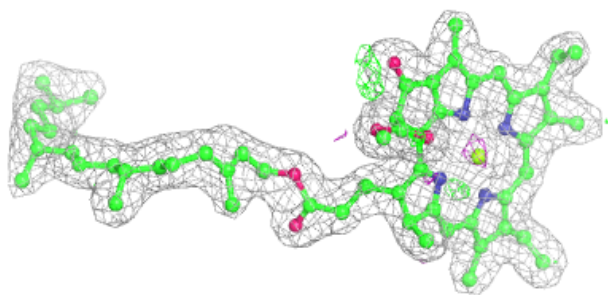
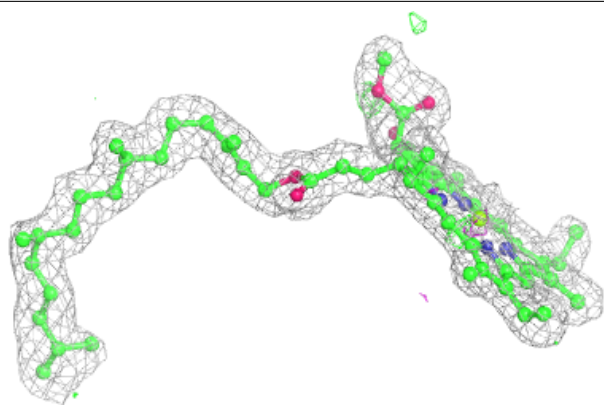
**Electron density around CLA a 406:**

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

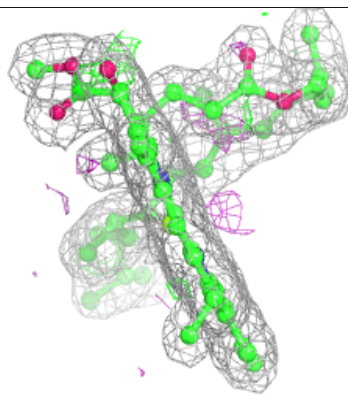
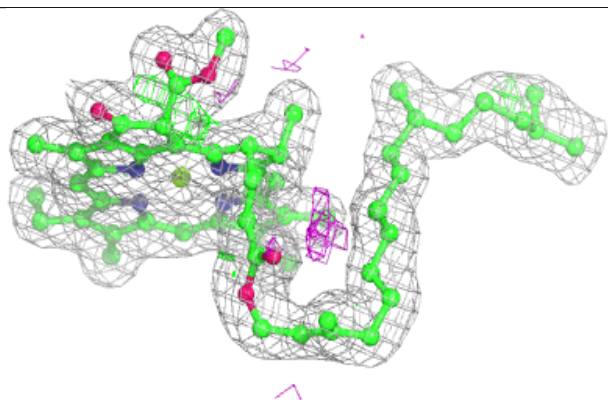
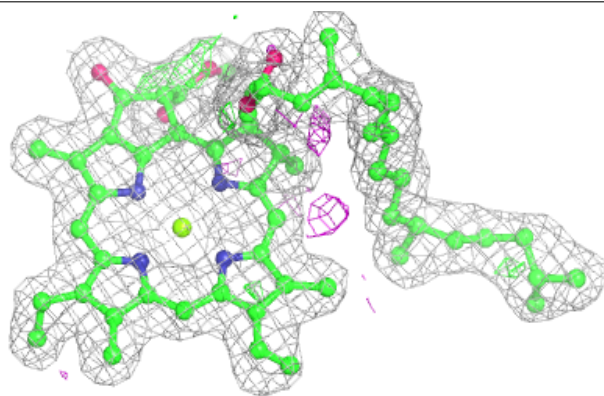


Electron density around CLA d 402:

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

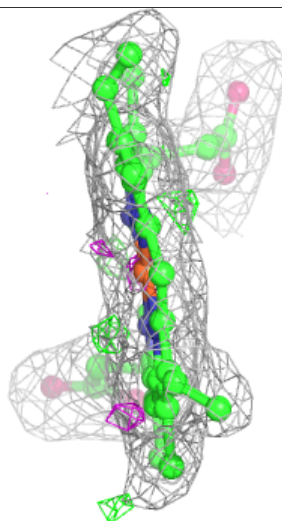
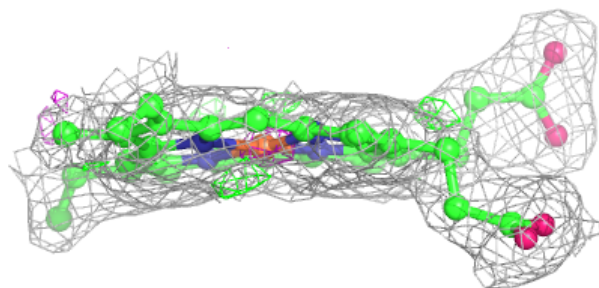
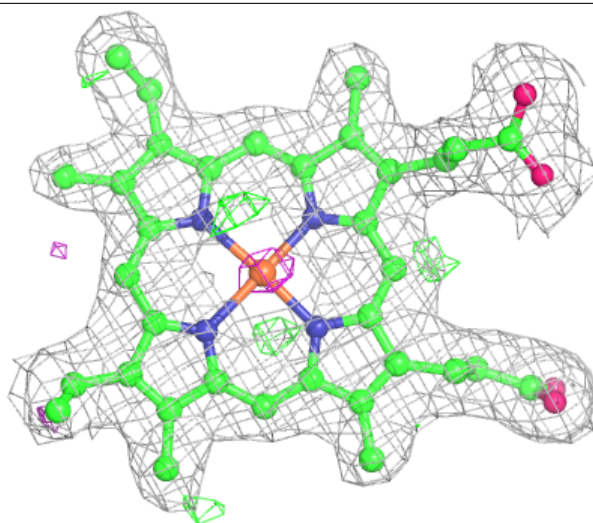
**Electron density around CLA D 401:**

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



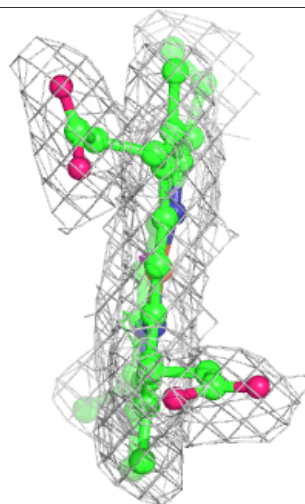
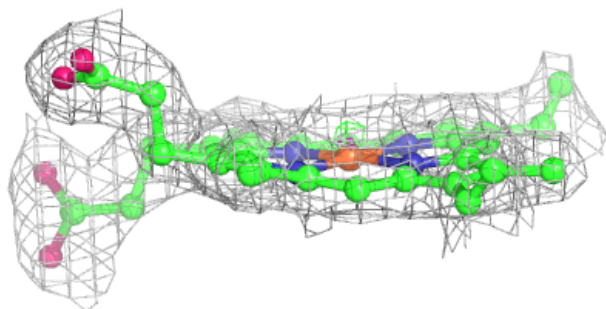
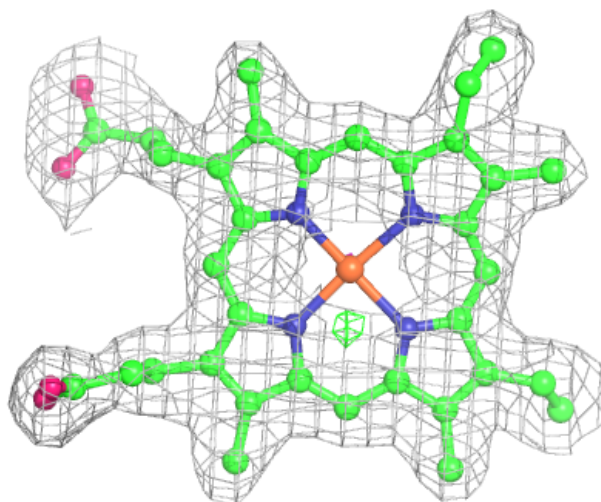
Electron density around HEC V 203:

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



Electron density around HEC v 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 [i](#)

There are no such residues in this entry.