



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 09:34 PM BST

PDB ID : 4UB6
Title : Native structure of photosystem II (dataset-1) 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

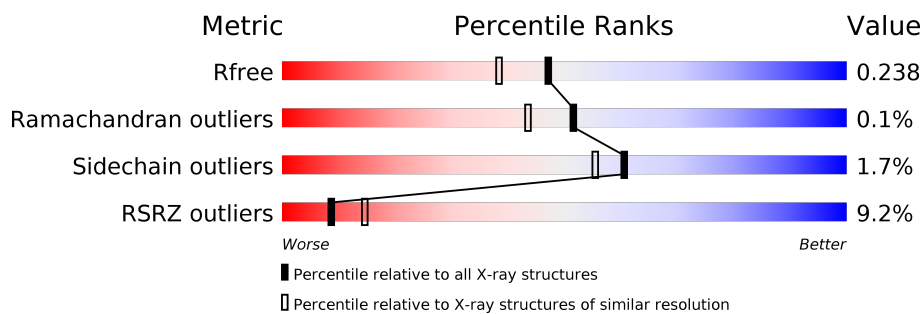
1 Overall quality at a glance

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>6%</div> <div>97%</div> </div>
1	a	344	<div> <div>10%</div> <div>96%</div> </div>
2	B	505	<div> <div>5%</div> <div>98%</div> </div>
2	b	505	<div> <div>7%</div> <div>98%</div> </div>
3	C	455	<div> <div>4%</div> <div>98%</div> </div>
3	c	455	<div> <div>6%</div> <div>99%</div> </div>
4	D	342	<div> <div>9%</div> <div>99%</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	32	
14	t	32	
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	407	X	-	-	-
24	CLA	A	410	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	409	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	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	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	403	X	-	-	-
28	GOL	V	203	-	-	-	X
36	DGD	d	406	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54195 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
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	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	11	0
			4027	2643	668	703	13			
2	b	504	Total	C	N	O	S	0	12	0
			4033	2650	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	4	0
			3501	2291	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	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

- 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
			280	187	43	48	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	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	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	0	0
			287	191	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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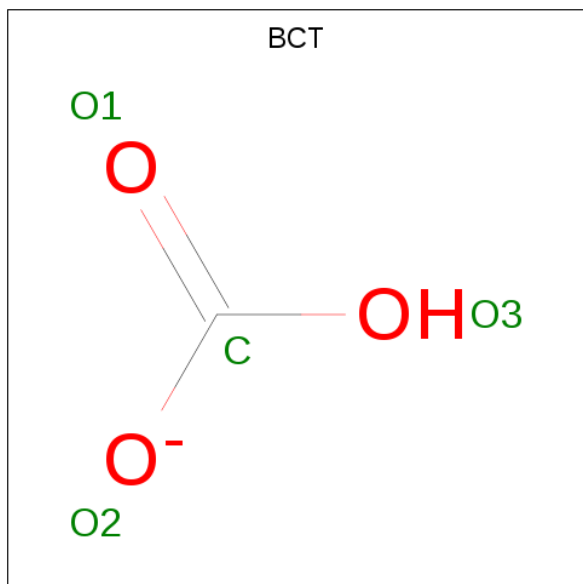
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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	v	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
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: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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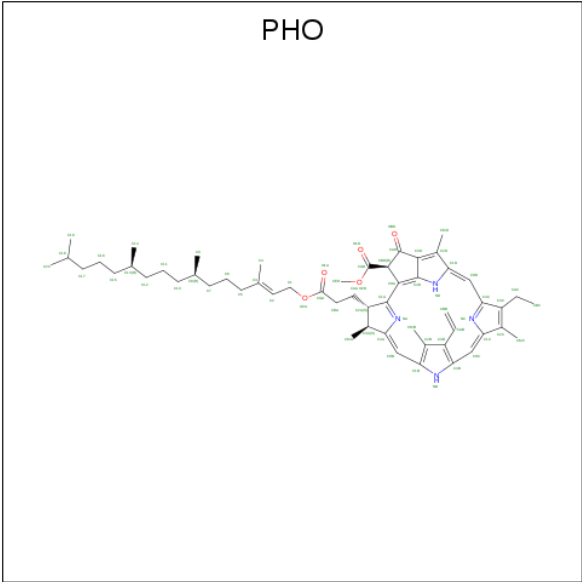
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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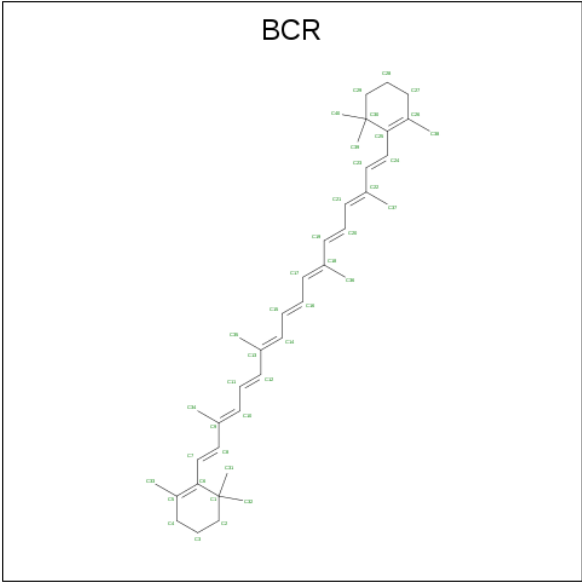
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



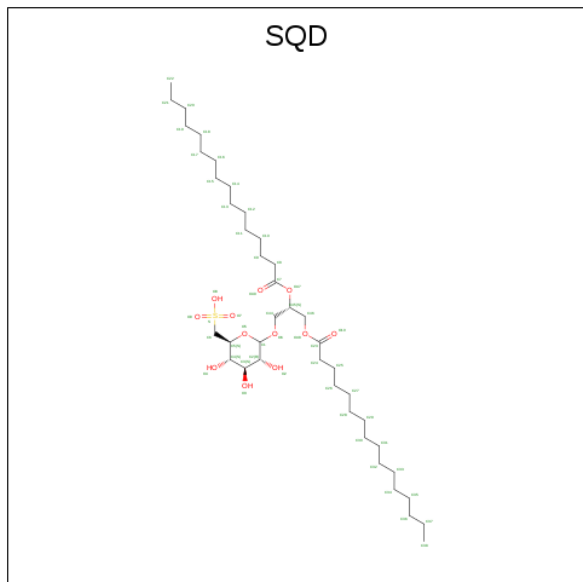
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- 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	K	1	Total C 40 40	0	0
26	T	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	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	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	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		
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		

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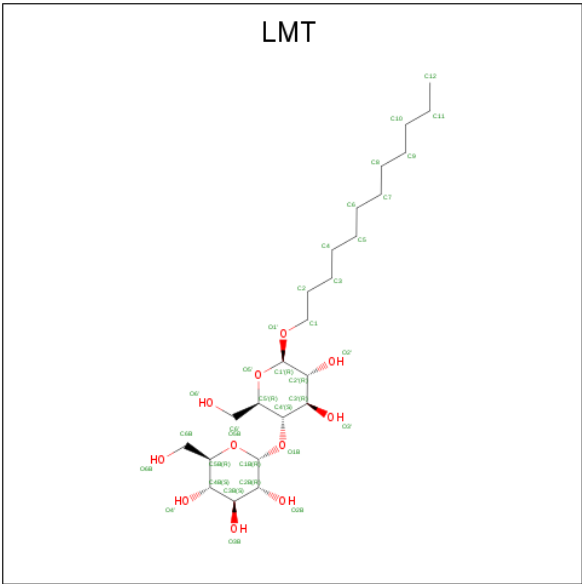
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28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

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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 DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



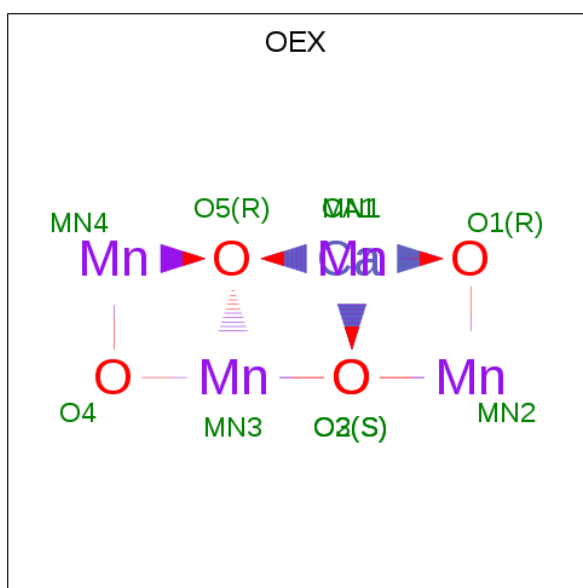
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	b	1	Total	C	O	0	0
			25	19	6		

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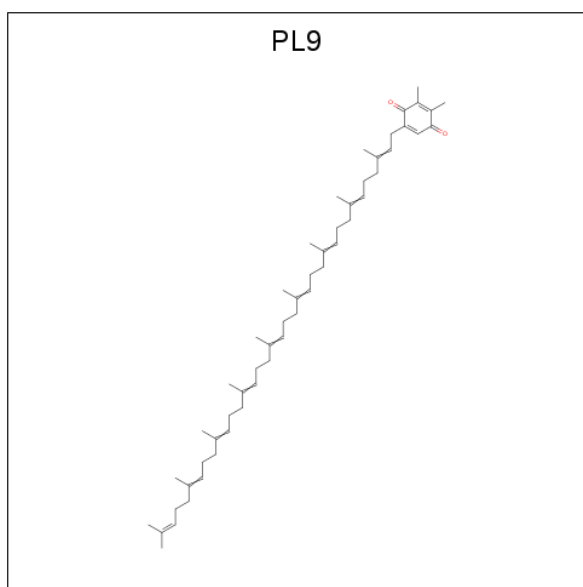
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			35	24	11		
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	a	1	Total	C	O	0	0
			30	25	5		

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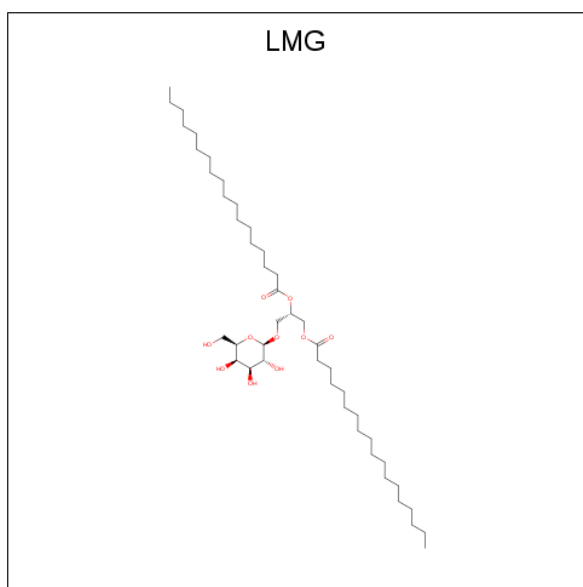
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	j	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	d	3	Total C O 71 63 8	0	0
32	m	1	Total C 10 10	0	0
32	b	1	Total C O 33 28 5	0	0
32	M	1	Total C 10 10	0	0

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

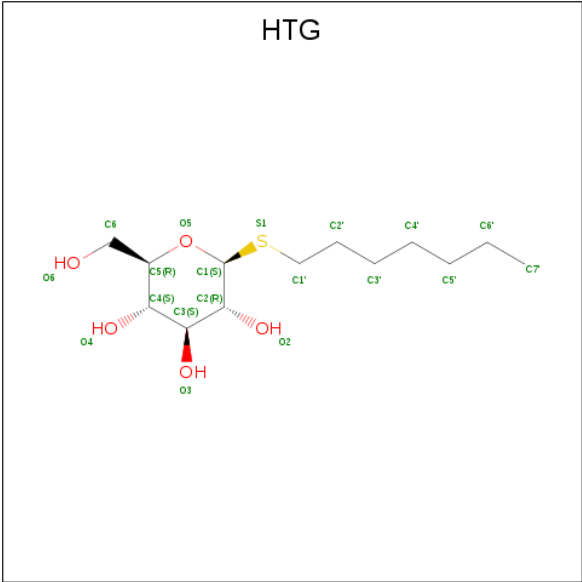
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0

- 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	a	1	Total	C	O	0	0
			51	41	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	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: C₁₃H₂₆O₅S).



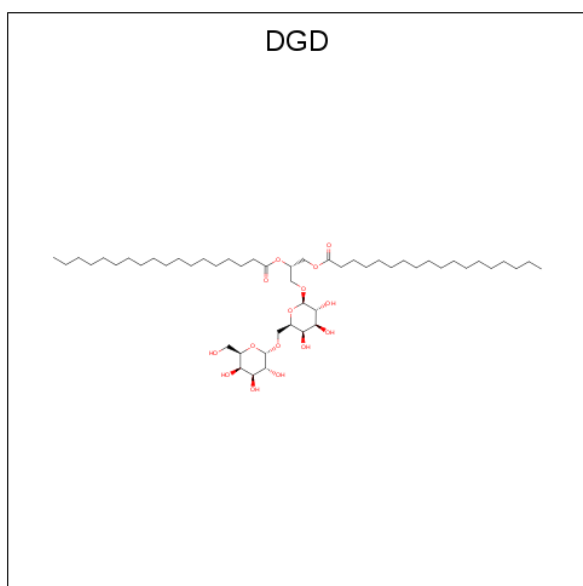
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	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: $C_{51}H_{96}O_{15}$).



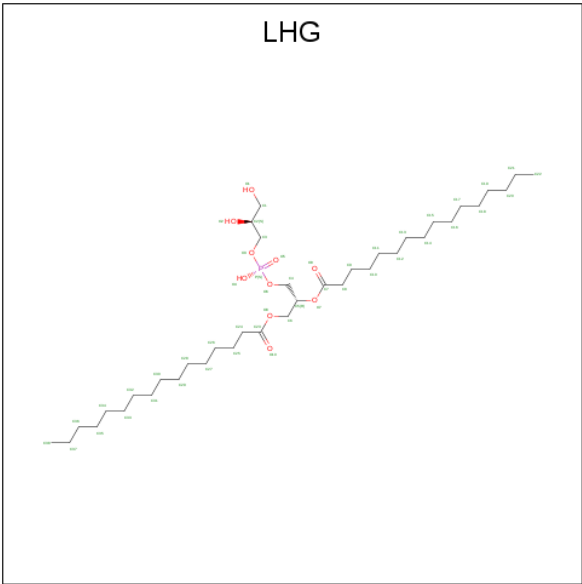
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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



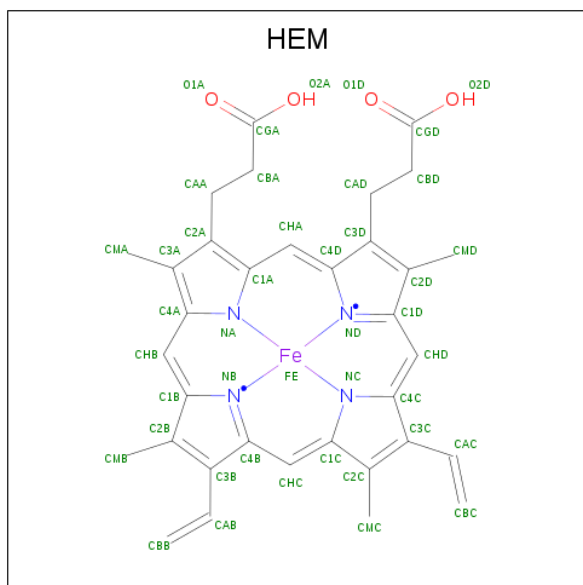
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

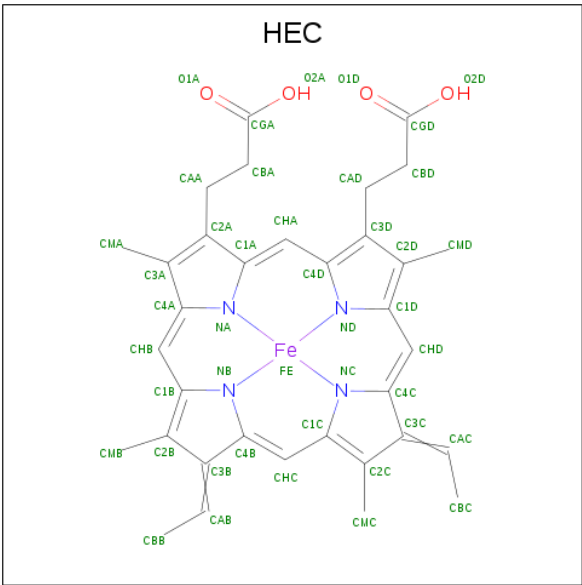


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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	165	Total	O	0	2
			167	167		
41	B	289	Total	O	0	4
			293	293		
41	C	233	Total	O	0	2
			235	235		
41	D	138	Total	O	0	5
			143	143		
41	E	31	Total	O	0	0
			31	31		
41	F	9	Total	O	0	0
			9	9		
41	H	48	Total	O	0	1
			49	49		
41	I	4	Total	O	0	0
			4	4		
41	J	13	Total	O	0	0
			13	13		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	16	Total 17	O 17	0	1
41	M	8	Total 8	O 8	0	0
41	O	188	Total 191	O 191	0	3
41	T	16	Total 17	O 17	0	1
41	U	81	Total 81	O 81	0	0
41	V	116	Total 118	O 118	0	2
41	Y	4	Total 4	O 4	0	0
41	X	9	Total 9	O 9	0	0
41	Z	1	Total 1	O 1	0	0
41	a	153	Total 154	O 154	0	1
41	b	261	Total 264	O 264	0	3
41	c	197	Total 199	O 199	0	2
41	d	132	Total 137	O 137	0	5
41	e	17	Total 17	O 17	0	0
41	f	5	Total 5	O 5	0	0
41	h	41	Total 41	O 41	0	0
41	i	6	Total 6	O 6	0	0
41	j	7	Total 7	O 7	0	0
41	k	6	Total 6	O 6	0	0
41	l	10	Total 10	O 10	0	0
41	m	18	Total 18	O 18	0	0

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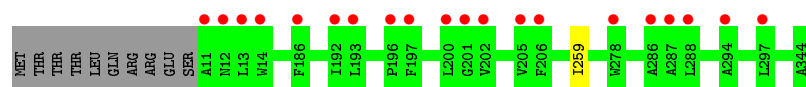
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	154	Total 155	O 155	0	1
41	t	12	Total 12	O 12	0	0
41	u	97	Total 97	O 97	0	0
41	v	89	Total 90	O 90	0	1
41	y	4	Total 4	O 4	0	0
41	x	4	Total 4	O 4	0	0

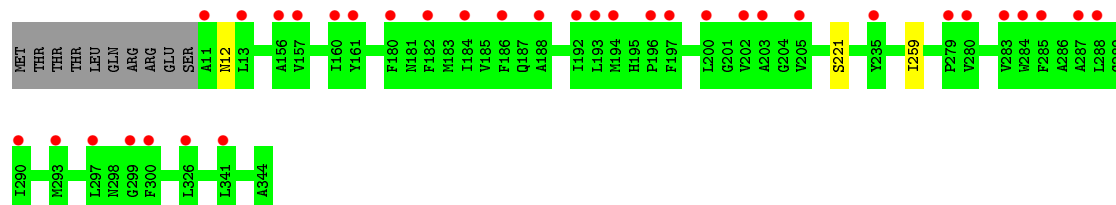
3 Residue-property plots

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

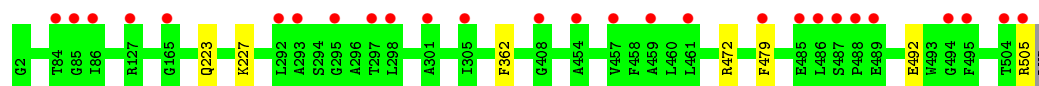
- Molecule 1: Photosystem Q(B) protein



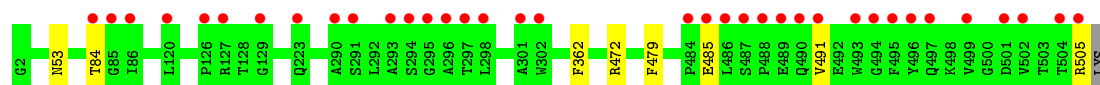
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

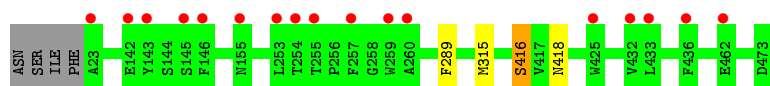


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

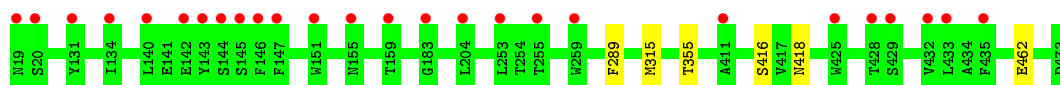


- Molecule 3: Photosystem II 44 kDa reaction center protein

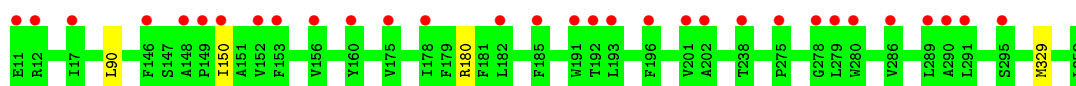




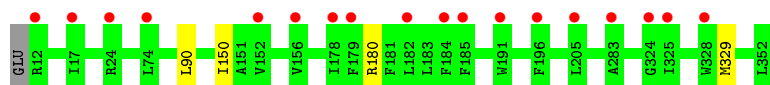
- Molecule 3: Photosystem II 44 kDa reaction center protein



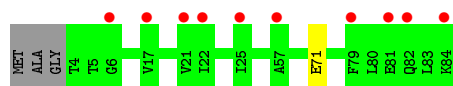
- Molecule 4: Photosystem II D2 protein



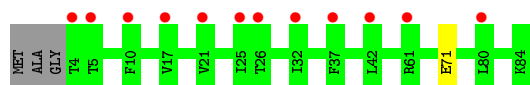
- Molecule 4: Photosystem II D2 protein



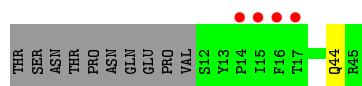
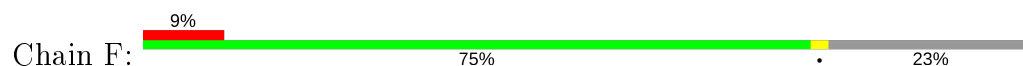
- Molecule 5: Cytochrome b559 subunit alpha



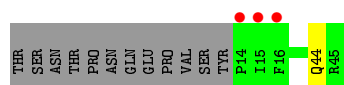
- Molecule 5: Cytochrome b559 subunit alpha



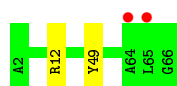
- Molecule 6: Cytochrome b559 subunit beta



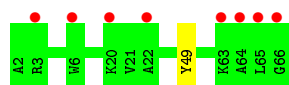
- Molecule 6: Cytochrome b559 subunit beta



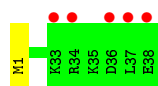
- Molecule 7: Photosystem II reaction center protein H



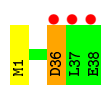
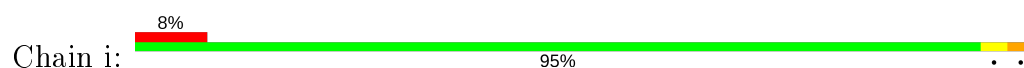
- Molecule 7: Photosystem II reaction center protein H



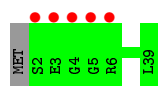
- Molecule 8: Photosystem II reaction center protein I



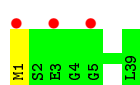
- Molecule 8: Photosystem II reaction center protein I



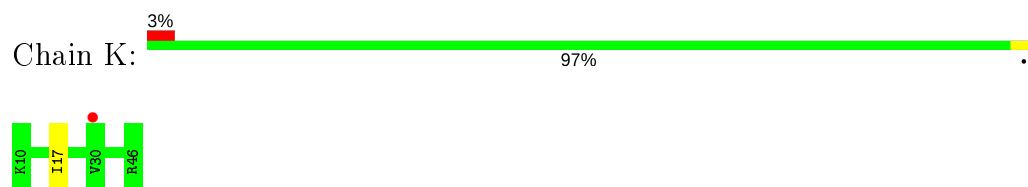
- Molecule 9: Photosystem II reaction center protein J



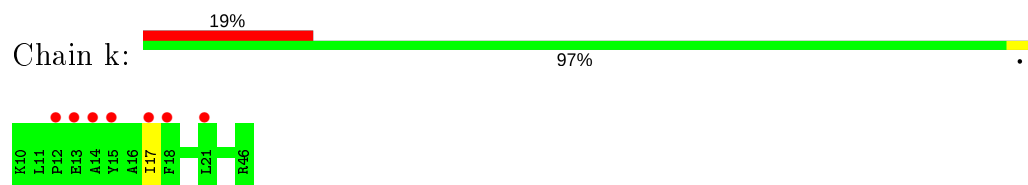
- Molecule 9: Photosystem II reaction center protein J



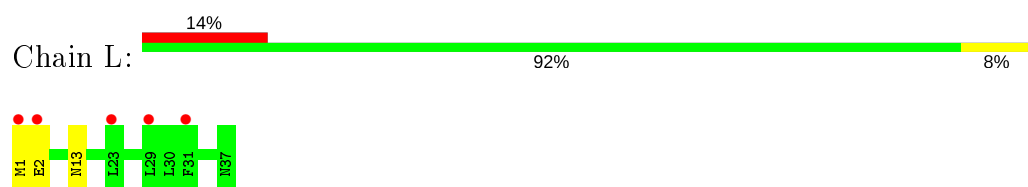
- Molecule 10: Photosystem II reaction center protein K



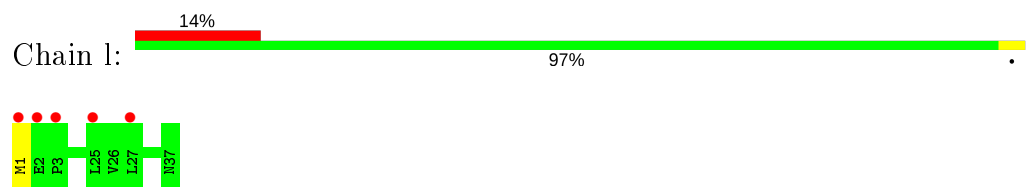
- Molecule 10: Photosystem II reaction center protein K



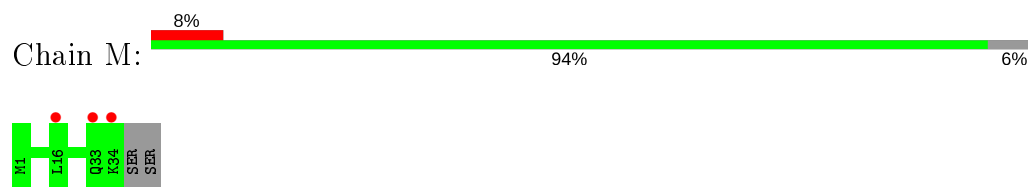
- Molecule 11: Photosystem II reaction center protein L



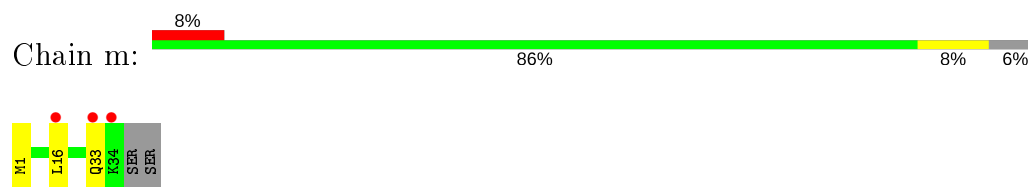
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

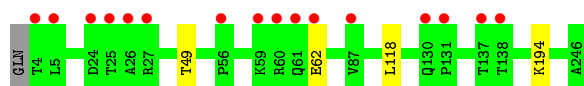


- Molecule 12: Photosystem II reaction center protein M

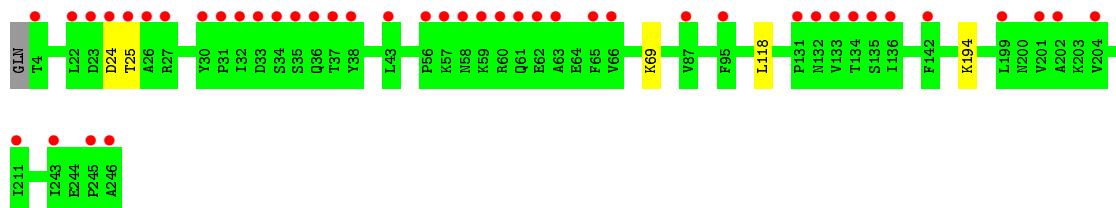


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

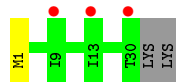
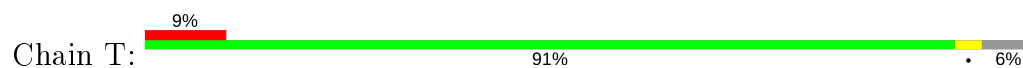




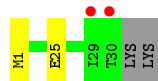
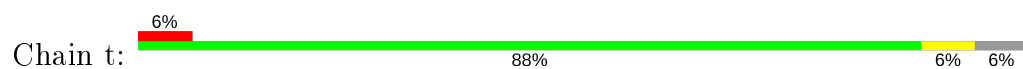
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



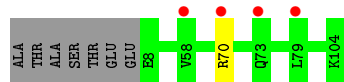
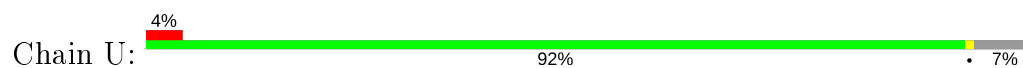
- Molecule 14: Photosystem II reaction center protein T



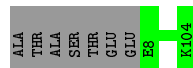
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



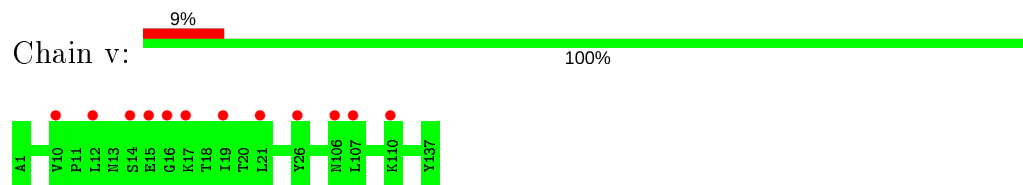
- Molecule 15: Photosystem II 12 kDa extrinsic protein



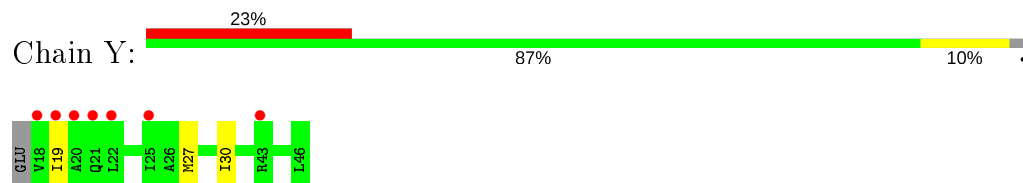
- Molecule 16: Cytochrome c-550



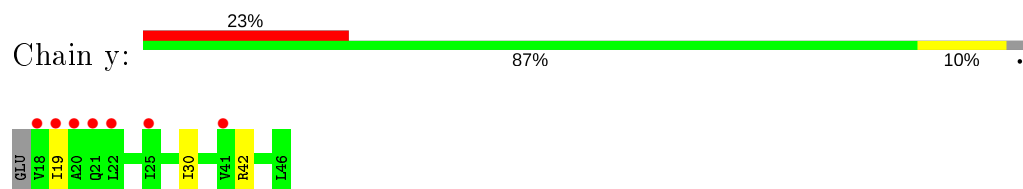
- Molecule 16: Cytochrome c-550



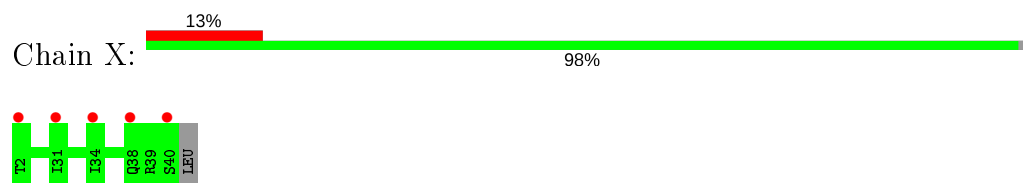
- Molecule 17: Photosystem II reaction center protein Ycf12



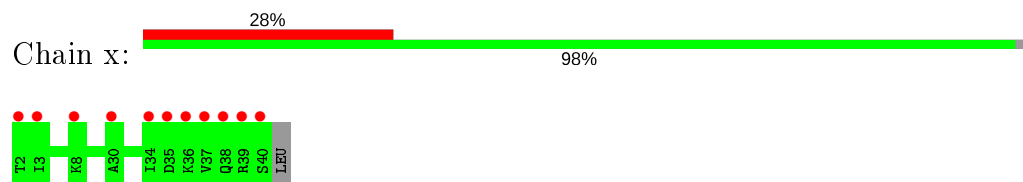
- Molecule 17: Photosystem II reaction center protein Ycf12



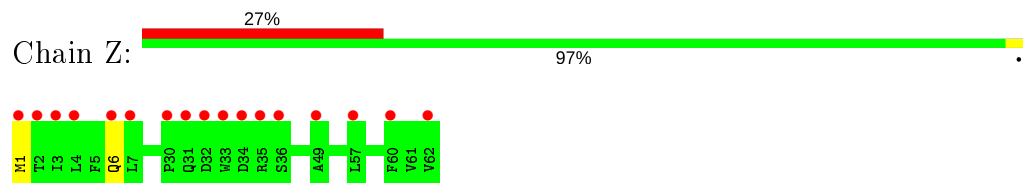
- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X

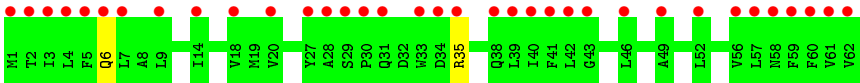


- Molecule 19: Photosystem II reaction center protein Z

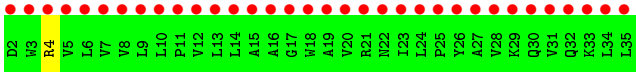


- Molecule 19: Photosystem II reaction center protein Z





● 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	123.74Å 229.99Å 288.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.29 – 1.95 62.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.29-1.95) 92.0 (62.29-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	29338 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54195	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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	0.52	0/2728	0.59	0/3719
1	a	0.52	0/2748	0.57	0/3746
2	B	0.49	0/4200	0.56	0/5721
2	b	0.47	0/4209	0.56	0/5734
3	C	0.45	0/3626	0.54	0/4936
3	c	0.45	0/3676	0.53	0/5004
4	D	0.53	0/2827	0.57	0/3852
4	d	0.51	0/2818	0.56	0/3840
5	E	0.37	0/693	0.54	0/944
5	e	0.35	0/695	0.50	0/948
6	F	0.40	0/284	0.52	0/387
6	f	0.39	0/265	0.52	0/360
7	H	0.37	0/535	0.53	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.38	0/311	0.55	0/419
8	i	0.38	0/311	0.51	0/419
9	J	0.42	0/278	0.47	0/376
9	j	0.41	0/286	0.47	0/386
10	K	0.33	0/303	0.52	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.47	0/319	0.51	0/433
11	l	0.45	0/319	0.50	0/433
12	M	0.45	0/270	0.58	0/368
12	m	0.55	0/262	0.63	0/357
13	O	0.40	0/1958	0.58	0/2654
13	o	0.39	0/1937	0.58	0/2625
14	T	0.55	0/266	0.54	0/362
14	t	0.56	0/266	0.57	0/362
15	U	0.45	0/785	0.58	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.42	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.39	0/1085	0.52	0/1473
17	Y	0.32	0/216	0.46	0/289
17	y	0.33	0/216	0.51	0/289
18	X	0.37	0/290	0.42	0/392
18	x	0.35	0/290	0.46	0/392
19	Z	0.33	0/490	0.43	0/669
19	z	0.33	0/490	0.45	0/669
20	R	0.26	0/279	0.38	0/383
All	All	0.46	0/43239	0.55	0/58829

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%)	331 (99%)	3 (1%)	1 (0%)	41	30
1	a	338/344 (98%)	333 (98%)	4 (1%)	1 (0%)	41	30
2	B	513/505 (102%)	506 (99%)	7 (1%)	0	100	100
2	b	514/505 (102%)	506 (98%)	8 (2%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	34	22
3	c	459/455 (101%)	445 (97%)	12 (3%)	2 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	79 (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%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	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	249/244 (102%)	240 (96%)	8 (3%)	1 (0%)	34	22
13	o	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	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%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5290/5384 (98%)	5170 (98%)	112 (2%)	8 (0%)	51	38

5 of 8 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
13	O	62	GLU

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	275/279 (99%)	272 (99%)	3 (1%)	73	71
2	B	413/403 (102%)	405 (98%)	8 (2%)	57	50
2	b	414/403 (103%)	406 (98%)	8 (2%)	57	50
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	62
3	c	362/356 (102%)	356 (98%)	6 (2%)	60	55
4	D	278/277 (100%)	274 (99%)	4 (1%)	67	62
4	d	277/277 (100%)	273 (99%)	4 (1%)	67	62
5	E	74/73 (101%)	73 (99%)	1 (1%)	67	62
5	e	74/73 (101%)	73 (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	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	22
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	26
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	26
11	L	36/35 (103%)	33 (92%)	3 (8%)	11	3
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%)	28 (93%)	2 (7%)	16	5
13	O	214/207 (103%)	210 (98%)	4 (2%)	57	50
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	40
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	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%)	117 (100%)	0	100	100
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3	0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	0
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	21
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	21
20	R	29/29 (100%)	28 (97%)	1 (3%)	37	25
All	All	4395/4403 (100%)	4315 (98%)	80 (2%)	60	53

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	6	GLN
2	b	472	ARG
14	t	25[A]	GLU

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Mol	Chain	Res	Type
20	R	4	ARG
1	a	221[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	315	ASN
2	b	331	ASN
16	v	118	HIS
2	b	53	ASN
2	b	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.69	0	7,9,11	1.37	1 (14%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.11	0
12	FME	m	1	12	8,9,10	0.72	0	7,9,11	1.11	1 (14%)
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.56	1 (14%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.32	2 (28%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	2.10	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.07	115.27	109.73
14	T	1	FME	C-CA-N	2.67	114.55	109.73
14	t	1	FME	O-C-CA	-2.63	117.88	124.78
14	t	1	FME	CA-N-CN	-2.56	118.89	122.82
8	I	1	FME	O-C-CA	-2.36	118.59	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 18 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$
35	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.18	2 (8%)
36	DGD	D	405	-	63,63,67	0.98	3 (4%)	77,77,81	1.24	7 (9%)
24	CLA	c	904	-	59,73,73	1.96	13 (22%)	67,113,113	2.18	21 (31%)
24	CLA	C	506	-	59,73,73	2.02	14 (23%)	67,113,113	2.20	19 (28%)
27	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.45	8 (15%)
26	BCR	A	411	-	41,41,41	1.02	1 (2%)	56,56,56	1.22	5 (8%)
24	CLA	C	503	-	59,73,73	2.00	13 (22%)	67,113,113	2.22	23 (34%)
27	SQD	A	412	-	53,54,54	0.99	3 (5%)	62,65,65	1.77	12 (19%)
28	GOL	b	629	-	5,5,5	0.34	0	5,5,5	0.15	0
24	CLA	b	609	-	59,73,73	1.98	12 (20%)	67,113,113	2.30	22 (32%)
24	CLA	D	401	-	59,73,73	1.95	13 (22%)	67,113,113	2.23	21 (31%)
36	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	1.22	6 (7%)
24	CLA	a	407	41	59,73,73	1.98	13 (22%)	67,113,113	2.28	26 (38%)
24	CLA	A	410	-	59,73,73	2.05	12 (20%)	67,113,113	2.10	24 (35%)
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	618	-	59,73,73	1.97	13 (22%)	67,113,113	2.34	23 (34%)
25	PHO	a	408	-	67,69,69	2.02	15 (22%)	85,99,99	1.90	20 (23%)
26	BCR	c	915	-	41,41,41	1.07	1 (2%)	56,56,56	1.43	9 (16%)
26	BCR	T	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.38	11 (19%)
29	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.86	0
24	CLA	C	513	-	59,73,73	2.00	12 (20%)	67,113,113	2.25	26 (38%)
24	CLA	b	605	41	59,73,73	2.04	12 (20%)	67,113,113	2.14	19 (28%)
28	GOL	b	630	-	5,5,5	0.32	0	5,5,5	0.52	0
25	PHO	a	420	-	67,69,69	2.19	17 (25%)	85,99,99	1.98	20 (23%)
24	CLA	C	505	41	59,73,73	2.04	13 (22%)	67,113,113	2.20	22 (32%)
24	CLA	B	615	-	59,73,73	1.98	13 (22%)	67,113,113	2.33	25 (37%)
28	GOL	b	632	-	5,5,5	0.37	0	5,5,5	0.56	0
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.46	7 (14%)
24	CLA	B	602	41	59,73,73	2.00	14 (23%)	67,113,113	2.18	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	621	-	41,41,41	1.12	1 (2%)	56,56,56	1.19	2 (3%)
29	LMT	c	921	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
24	CLA	B	607	-	59,73,73	2.04	14 (23%)	67,113,113	2.37	23 (34%)
24	CLA	B	612	-	59,73,73	2.02	13 (22%)	67,113,113	2.15	22 (32%)
28	GOL	b	631	-	5,5,5	0.33	0	5,5,5	0.46	0
38	HEM	e	102	5,6	27,50,50	0.83	1 (3%)	17,82,82	2.15	3 (17%)
28	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.35	0
24	CLA	b	619	-	59,73,73	2.03	12 (20%)	67,113,113	2.26	23 (34%)
24	CLA	d	402	-	59,73,73	1.92	14 (23%)	67,113,113	2.36	22 (32%)
28	GOL	b	628	-	5,5,5	0.36	0	5,5,5	0.30	0
24	CLA	c	914	-	59,73,73	2.00	13 (22%)	67,113,113	2.06	22 (32%)
24	CLA	c	911	-	59,73,73	2.02	13 (22%)	67,113,113	2.15	22 (32%)
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
36	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	0.93	4 (5%)
27	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.48	9 (14%)
31	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.55	14 (20%)
24	CLA	B	608	41	59,73,73	2.04	13 (22%)	67,113,113	2.13	20 (29%)
28	GOL	B	629	-	5,5,5	0.41	0	5,5,5	0.56	0
28	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.61	0
28	GOL	C	526	-	5,5,5	0.22	0	5,5,5	0.43	0
29	LMT	C	522	-	36,36,36	0.48	0	47,47,47	1.27	5 (10%)
26	BCR	k	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.46	10 (17%)
37	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	4 (7%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
28	GOL	A	413	-	5,5,5	0.25	0	5,5,5	0.52	0
24	CLA	B	606	-	59,73,73	1.98	12 (20%)	67,113,113	2.27	21 (31%)
36	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	2 (2%)
24	CLA	B	604	-	59,73,73	2.04	13 (22%)	67,113,113	2.33	22 (32%)
28	GOL	V	205	-	5,5,5	0.36	0	5,5,5	0.38	0
24	CLA	a	409	-	59,73,73	1.99	13 (22%)	67,113,113	2.26	26 (38%)
25	PHO	A	409	-	67,69,69	2.14	16 (23%)	85,99,99	1.84	21 (24%)
26	BCR	B	618	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	8 (14%)
35	HTG	b	602	-	19,19,19	1.14	2 (10%)	23,24,24	1.22	1 (4%)
29	LMT	B	636	-	25,25,36	0.43	0	30,30,47	0.65	0
30	OEX	A	418	1,3,41	0,15,15	0.00	-	-	-	-
24	CLA	d	403	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	22 (32%)
31	PL9	D	404	-	55,55,55	0.73	2 (3%)	68,69,69	1.58	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.96	10 (19%)
28	GOL	B	637	-	5,5,5	0.40	0	5,5,5	0.30	0
23	BCT	a	419	21	0,3,3	0.00	-	0,3,3	0.00	-
26	BCR	b	623	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	9 (16%)
28	GOL	B	630	-	5,5,5	0.33	0	5,5,5	0.36	0
28	GOL	a	414	-	5,5,5	0.39	0	5,5,5	0.43	0
28	GOL	a	415	-	5,5,5	0.40	0	5,5,5	0.46	0
24	CLA	c	912	3	59,73,73	2.03	13 (22%)	67,113,113	2.08	21 (31%)
37	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
28	GOL	F	103	33	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	B	610	-	59,73,73	1.94	13 (22%)	67,113,113	2.22	24 (35%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.00	1 (5%)
24	CLA	c	905	41	59,73,73	2.04	13 (22%)	67,113,113	2.16	25 (37%)
24	CLA	C	514	-	59,73,73	2.02	13 (22%)	67,113,113	2.16	23 (34%)
24	CLA	b	613	-	59,73,73	1.96	13 (22%)	67,113,113	2.25	24 (35%)
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.57	11 (17%)
28	GOL	f	101	33	5,5,5	0.37	0	5,5,5	0.40	0
24	CLA	b	616	-	59,73,73	1.96	11 (18%)	67,113,113	2.20	20 (29%)
28	GOL	V	203	-	5,5,5	0.38	0	5,5,5	0.15	0
24	CLA	c	913	-	59,73,73	1.96	13 (22%)	67,113,113	2.20	24 (35%)
26	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.37	7 (12%)
35	HTG	b	603	-	19,19,19	1.03	2 (10%)	23,24,24	1.47	3 (13%)
24	CLA	C	511	-	59,73,73	2.03	13 (22%)	67,113,113	2.23	22 (32%)
35	HTG	B	624	-	19,19,19	1.13	1 (5%)	23,24,24	1.39	1 (4%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.07	4 (6%)
29	LMT	A	417	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	2 (4%)
24	CLA	b	607	-	59,73,73	2.01	13 (22%)	67,113,113	2.40	26 (38%)
35	HTG	d	412	-	16,16,19	1.11	2 (12%)	20,21,24	1.38	1 (5%)
24	CLA	B	603	-	59,73,73	2.00	13 (22%)	67,113,113	2.30	28 (41%)
34	LMG	B	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.16	3 (5%)
24	CLA	B	609	-	59,73,73	2.10	13 (22%)	67,113,113	2.24	25 (37%)
24	CLA	d	401	41	59,73,73	2.01	12 (20%)	67,113,113	2.20	24 (35%)
24	CLA	C	512	3	59,73,73	2.01	15 (25%)	67,113,113	2.10	21 (31%)
28	GOL	c	925	-	5,5,5	0.36	0	5,5,5	0.56	0
26	BCR	D	403	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	14 (25%)
24	CLA	D	402	-	59,73,73	1.98	13 (22%)	67,113,113	2.03	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	507	-	59,73,73	2.02	13 (22%)	67,113,113	2.17	24 (35%)
24	CLA	B	614	-	59,73,73	2.06	13 (22%)	67,113,113	2.15	22 (32%)
28	GOL	v	205	-	5,5,5	0.39	0	5,5,5	0.35	0
28	GOL	V	206	-	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	c	903	-	59,73,73	1.97	13 (22%)	67,113,113	2.15	20 (29%)
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.27	0
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	B	627	-	5,5,5	0.41	0	5,5,5	0.57	0
37	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	4 (7%)
26	BCR	b	622	-	41,41,41	1.06	1 (2%)	56,56,56	1.27	5 (8%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	2 (3%)
35	HTG	c	922	-	19,19,19	0.90	1 (5%)	23,24,24	1.34	1 (4%)
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
24	CLA	b	620	-	59,73,73	2.03	14 (23%)	67,113,113	2.26	20 (29%)
35	HTG	B	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	2 (8%)
30	OEX	a	416	1,3,41	0,15,15	0.00	-	-	-	-
27	SQD	a	402	-	53,54,54	1.06	3 (5%)	62,65,65	1.16	7 (11%)
26	BCR	K	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
24	CLA	b	614	41	59,73,73	2.04	13 (22%)	67,113,113	2.22	26 (38%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
24	CLA	B	613	-	59,73,73	2.03	13 (22%)	67,113,113	2.19	17 (25%)
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.23	5 (8%)
34	LMG	a	412	-	51,51,55	0.91	2 (3%)	59,59,63	1.15	6 (10%)
28	GOL	B	631	-	5,5,5	0.42	0	5,5,5	0.47	0
29	LMT	b	601	-	25,25,36	0.46	0	30,30,47	1.35	3 (10%)
24	CLA	B	616	-	59,73,73	1.93	13 (22%)	67,113,113	2.28	26 (38%)
36	DGD	c	918	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
29	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.40	5 (10%)
31	PL9	a	417	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	18 (26%)
29	LMT	a	401	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
24	CLA	b	611	41	59,73,73	2.05	14 (23%)	67,113,113	2.23	23 (34%)
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.31	0
28	GOL	V	204	-	5,5,5	0.43	0	5,5,5	0.44	0
28	GOL	T	103	-	5,5,5	0.39	0	5,5,5	0.19	0
28	GOL	T	101	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	a	406	-	59,73,73	2.05	13 (22%)	67,113,113	2.22	27 (40%)
35	HTG	B	633	-	19,19,19	1.12	2 (10%)	23,24,24	1.30	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	b	625	-	25,25,36	0.52	1 (4%)	30,30,47	0.60	0
29	LMT	f	103	-	36,36,36	0.54	1 (2%)	47,47,47	0.93	4 (8%)
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	6 (7%)
24	CLA	A	405	-	59,73,73	1.98	13 (22%)	67,113,113	2.22	18 (26%)
24	CLA	c	909	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	21 (31%)
35	HTG	B	634	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
24	CLA	b	617	-	59,73,73	2.02	14 (23%)	67,113,113	2.21	26 (38%)
35	HTG	C	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.64	4 (17%)
34	LMG	j	101	39	51,51,55	0.89	2 (3%)	59,59,63	0.99	4 (6%)
35	HTG	b	626	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	3 (13%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.90	1 (2%)
24	CLA	b	615	-	59,73,73	1.97	13 (22%)	67,113,113	2.24	20 (29%)
26	BCR	d	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	16 (28%)
34	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
34	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.31	6 (13%)
24	CLA	b	610	-	59,73,73	1.96	12 (20%)	67,113,113	2.33	23 (34%)
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.34	0
34	LMG	b	624	-	51,51,55	0.91	3 (5%)	59,59,63	1.05	3 (5%)
36	DGD	C	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
24	CLA	c	910	-	59,73,73	2.06	13 (22%)	67,113,113	2.21	23 (34%)
37	LHG	e	101	-	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
24	CLA	b	612	-	59,73,73	2.02	13 (22%)	67,113,113	2.19	22 (32%)
24	CLA	c	906	-	59,73,73	1.93	12 (20%)	67,113,113	2.17	18 (26%)
24	CLA	C	504	-	59,73,73	2.01	13 (22%)	67,113,113	2.15	20 (29%)
40	HEC	V	201	16	26,50,50	1.55	4 (15%)	18,82,82	1.53	6 (33%)
40	HEC	v	202	16	26,50,50	1.56	4 (15%)	18,82,82	1.36	4 (22%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)
24	CLA	c	908	41	59,73,73	1.99	13 (22%)	67,113,113	2.26	24 (35%)
24	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	23 (34%)
28	GOL	B	632	-	5,5,5	0.35	0	5,5,5	0.36	0
25	PHO	A	408	-	67,69,69	2.16	16 (23%)	85,99,99	1.97	20 (23%)
35	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.37	2 (8%)
24	CLA	b	608	-	59,73,73	2.01	13 (22%)	67,113,113	2.20	19 (28%)
28	GOL	O	302	-	5,5,5	0.32	0	5,5,5	0.44	0
31	PL9	A	419	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	605	-	59,73,73	1.90	12 (20%)	67,113,113	2.10	19 (28%)
24	CLA	B	611	41	59,73,73	2.02	13 (22%)	67,113,113	2.28	25 (37%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.29	5 (8%)
28	GOL	t	102	-	5,5,5	0.40	0	5,5,5	0.23	0
34	LMG	c	919	-	51,51,55	0.97	3 (5%)	59,59,63	1.01	2 (3%)
24	CLA	b	606	-	59,73,73	2.00	14 (23%)	67,113,113	2.31	24 (35%)
26	BCR	t	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
24	CLA	C	508	41	59,73,73	1.97	13 (22%)	67,113,113	2.14	20 (29%)
24	CLA	B	617	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	20 (29%)
28	GOL	o	302	-	5,5,5	0.39	0	5,5,5	0.48	0
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	7 (12%)
37	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	A	407	41	59,73,73	2.02	13 (22%)	67,113,113	2.25	25 (37%)
34	LMG	C	501	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.06	4 (7%)
38	HEM	E	103	5,6	27,50,50	0.80	1 (3%)	17,82,82	2.34	3 (17%)
29	LMT	m	104	-	36,36,36	0.51	0	47,47,47	1.01	2 (4%)
28	GOL	B	628	-	5,5,5	0.27	0	5,5,5	0.42	0
24	CLA	C	510	-	59,73,73	2.08	13 (22%)	67,113,113	2.21	27 (40%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	12 (21%)
35	HTG	O	303	-	19,19,19	0.95	1 (5%)	23,24,24	0.71	0
29	LMT	m	103	-	36,36,36	0.48	0	47,47,47	0.99	1 (2%)
28	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.61	0
29	LMT	m	102	-	36,36,36	0.48	0	47,47,47	0.91	1 (2%)
28	GOL	a	413	-	5,5,5	0.31	0	5,5,5	0.65	0
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.37	0
24	CLA	A	406	41	59,73,73	1.98	11 (18%)	67,113,113	2.42	27 (40%)
27	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.60	10 (16%)
37	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.09	3 (6%)
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.21	6 (9%)
35	HTG	V	202	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	3 (13%)
24	CLA	c	902	-	59,73,73	1.98	12 (20%)	67,113,113	2.18	22 (32%)
26	BCR	B	620	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	4 (7%)
35	HTG	b	627	-	19,19,19	1.09	2 (10%)	23,24,24	1.97	4 (17%)
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	4 (7%)
24	CLA	c	907	-	59,73,73	1.99	14 (23%)	67,113,113	2.26	25 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	J	101	39	51,51,55	0.88	2 (3%)	59,59,63	0.89	3 (5%)
35	HTG	c	923	-	19,19,19	1.14	2 (10%)	23,24,24	1.84	5 (21%)
36	DGD	C	519	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	5 (6%)
24	CLA	C	509	-	59,73,73	2.05	13 (22%)	67,113,113	2.41	25 (37%)
36	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	6 (7%)
26	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	7 (12%)

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
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
36	DGD	D	405	-	-	22/51/91/95	0/2/2/2
24	CLA	c	904	-	3/3/20/25	3/37/135/135	-
24	CLA	C	506	-	1/1/20/25	6/37/135/135	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
24	CLA	C	503	-	2/2/20/25	4/37/135/135	-
27	SQD	A	412	-	-	11/49/69/69	0/1/1/1
28	GOL	b	629	-	-	0/4/4/4	-
24	CLA	b	609	-	3/3/20/25	9/37/135/135	-
24	CLA	D	401	-	2/2/20/25	0/37/135/135	-
36	DGD	d	406	-	-	28/51/91/95	0/2/2/2
24	CLA	a	407	41	2/2/20/25	6/37/135/135	-
24	CLA	A	410	-	2/2/20/25	9/37/135/135	-
36	DGD	C	518	-	-	15/51/91/95	0/2/2/2
24	CLA	d	403	-	2/2/20/25	7/37/135/135	-
25	PHO	a	408	-	-	2/53/103/103	0/5/6/6
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
29	LMT	E	102	-	-	7/21/61/61	0/2/2/2
24	CLA	C	513	-	3/3/20/25	10/37/135/135	-
24	CLA	b	605	41	3/3/20/25	12/37/135/135	-
28	GOL	b	630	-	-	0/4/4/4	-
25	PHO	a	420	-	-	4/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	505	41	3/3/20/25	5/37/135/135	-
24	CLA	B	615	-	2/2/20/25	18/37/135/135	-
28	GOL	b	632	-	-	2/4/4/4	-
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
24	CLA	B	602	41	3/3/20/25	16/37/135/135	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	B	607	-	2/2/20/25	7/37/135/135	-
24	CLA	B	612	-	3/3/20/25	2/37/135/135	-
28	GOL	b	631	-	-	2/4/4/4	-
38	HEM	e	102	5,6	-	0/6/54/54	-
29	LMT	c	921	-	-	4/21/61/61	0/2/2/2
24	CLA	b	619	-	3/3/20/25	4/37/135/135	-
24	CLA	d	402	-	1/1/20/25	0/37/135/135	-
28	GOL	b	628	-	-	2/4/4/4	-
24	CLA	c	914	-	3/3/20/25	10/37/135/135	-
24	CLA	c	911	-	3/3/20/25	9/37/135/135	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	9/51/91/95	0/2/2/2
28	GOL	V	205	-	-	1/4/4/4	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
24	CLA	B	608	41	3/3/20/25	2/37/135/135	-
28	GOL	a	415	-	-	2/4/4/4	-
28	GOL	v	203	-	-	4/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
29	LMT	C	522	-	-	9/21/61/61	0/2/2/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
37	LHG	d	407	-	-	9/53/53/53	-
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	B	606	-	3/3/20/25	7/37/135/135	-
36	DGD	c	917	-	-	14/51/91/95	0/2/2/2
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2
24	CLA	B	604	-	2/2/20/25	6/37/135/135	-
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	409	-	3/3/20/25	7/37/135/135	-
25	PHO	A	409	-	-	2/53/103/103	0/5/6/6
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
35	HTG	b	602	-	-	1/10/30/30	0/1/1/1
29	LMT	B	636	-	-	8/17/37/61	0/1/1/2
24	CLA	b	618	-	2/2/20/25	17/37/135/135	-
31	PL9	D	404	-	-	3/53/73/73	0/1/1/1
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
28	GOL	B	637	-	-	2/4/4/4	-
26	BCR	b	623	-	-	3/29/63/63	0/2/2/2
28	GOL	B	630	-	-	0/4/4/4	-
28	GOL	a	414	-	-	2/4/4/4	-
28	GOL	B	629	-	-	2/4/4/4	-
24	CLA	c	912	3	3/3/20/25	5/37/135/135	-
37	LHG	D	406	-	-	6/53/53/53	-
24	CLA	C	511	-	3/3/20/25	9/37/135/135	-
24	CLA	B	610	-	2/2/20/25	3/37/135/135	-
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
24	CLA	c	905	41	3/3/20/25	5/37/135/135	-
24	CLA	C	514	-	2/2/20/25	2/37/135/135	-
24	CLA	b	613	-	3/3/20/25	2/37/135/135	-
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
28	GOL	f	101	33	-	4/4/4/4	-
24	CLA	b	616	-	3/3/20/25	1/37/135/135	-
28	GOL	V	203	-	-	4/4/4/4	-
24	CLA	c	913	-	3/3/20/25	7/37/135/135	-
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
34	LMG	c	920	-	-	4/46/66/70	0/1/1/1
35	HTG	B	624	-	-	1/10/30/30	0/1/1/1
34	LMG	C	521	-	-	12/46/66/70	0/1/1/1
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
24	CLA	b	607	-	2/2/20/25	8/37/135/135	-
35	HTG	d	412	-	-	0/7/27/30	0/1/1/1
24	CLA	B	603	-	2/2/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
24	CLA	B	609	-	2/2/20/25	0/37/135/135	-
24	CLA	d	401	41	2/2/20/25	7/37/135/135	-
24	CLA	C	512	3	3/3/20/25	2/37/135/135	-
28	GOL	c	925	-	-	0/4/4/4	-
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2
24	CLA	D	402	-	3/3/20/25	9/37/135/135	-
24	CLA	C	507	-	3/3/20/25	11/37/135/135	-
24	CLA	B	614	-	3/3/20/25	9/37/135/135	-
28	GOL	v	205	-	-	2/4/4/4	-
28	GOL	V	206	-	-	1/4/4/4	-
24	CLA	c	903	-	3/3/20/25	4/37/135/135	-
28	GOL	A	415	-	-	2/4/4/4	-
28	GOL	B	627	-	-	1/4/4/4	-
37	LHG	d	409	-	-	12/53/53/53	-
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
37	LHG	D	407	-	-	5/53/53/53	-
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
37	LHG	d	408	-	-	11/53/53/53	-
24	CLA	b	620	-	3/3/20/25	8/37/135/135	-
35	HTG	B	626	-	-	4/10/30/30	0/1/1/1
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
26	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	CLA	b	614	41	3/3/20/25	3/37/135/135	-
37	LHG	l	101	-	-	15/53/53/53	-
24	CLA	B	613	-	3/3/20/25	4/37/135/135	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
34	LMG	a	412	-	-	10/46/66/70	0/1/1/1
28	GOL	B	631	-	-	4/4/4/4	-
29	LMT	b	601	-	-	8/17/37/61	0/1/1/2
24	CLA	B	616	-	3/3/20/25	10/37/135/135	-
36	DGD	c	918	-	-	17/51/91/95	0/2/2/2
29	LMT	B	623	-	-	7/21/61/61	0/2/2/2
28	GOL	F	103	33	-	2/4/4/4	-
29	LMT	a	401	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	611	41	2/2/20/25	2/37/135/135	-
28	GOL	c	924	-	-	0/4/4/4	-
28	GOL	V	204	-	-	2/4/4/4	-
28	GOL	T	103	-	-	4/4/4/4	-
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	a	406	-	3/3/20/25	2/37/135/135	-
35	HTG	B	633	-	-	3/10/30/30	0/1/1/1
29	LMT	b	625	-	-	4/17/37/61	0/1/1/2
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
24	CLA	A	405	-	2/2/20/25	2/37/135/135	-
24	CLA	c	909	-	3/3/20/25	3/37/135/135	-
35	HTG	B	634	-	-	2/10/30/30	0/1/1/1
24	CLA	b	617	-	3/3/20/25	4/37/135/135	-
35	HTG	C	524	-	-	2/10/30/30	0/1/1/1
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
35	HTG	b	626	-	-	1/10/30/30	0/1/1/1
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
24	CLA	b	615	-	2/2/20/25	5/37/135/135	-
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
34	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
24	CLA	b	610	-	3/3/20/25	16/37/135/135	-
28	GOL	A	414	-	-	2/4/4/4	-
34	LMG	b	624	-	-	14/46/66/70	0/1/1/1
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
24	CLA	c	910	-	3/3/20/25	9/37/135/135	-
37	LHG	e	101	-	-	10/46/46/53	-
24	CLA	b	612	-	2/2/20/25	4/37/135/135	-
24	CLA	c	906	-	1/1/20/25	4/37/135/135	-
24	CLA	C	504	-	3/3/20/25	5/37/135/135	-
40	HEC	V	201	16	-	0/6/54/54	-
40	HEC	v	202	16	-	0/6/54/54	-
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
24	CLA	c	908	41	3/3/20/25	2/37/135/135	-
24	CLA	C	502	-	3/3/20/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	632	-	-	2/4/4/4	-
25	PHO	A	408	-	-	4/53/103/103	0/5/6/6
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
24	CLA	b	608	-	3/3/20/25	7/37/135/135	-
28	GOL	O	302	-	-	2/4/4/4	-
31	PL9	A	419	-	-	7/53/73/73	0/1/1/1
24	CLA	B	605	-	3/3/20/25	4/37/135/135	-
24	CLA	B	611	41	3/3/20/25	7/37/135/135	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
28	GOL	t	102	-	-	0/4/4/4	-
34	LMG	c	919	-	-	16/46/66/70	0/1/1/1
24	CLA	b	606	-	2/2/20/25	3/37/135/135	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	508	41	3/3/20/25	6/37/135/135	-
24	CLA	B	617	-	3/3/20/25	9/37/135/135	-
28	GOL	o	302	-	-	2/4/4/4	-
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
37	LHG	L	101	-	-	15/53/53/53	-
24	CLA	A	407	41	2/2/20/25	2/37/135/135	-
34	LMG	C	501	-	-	19/46/66/70	0/1/1/1
37	LHG	D	408	-	-	11/53/53/53	-
38	HEM	E	103	5,6	-	0/6/54/54	-
29	LMT	m	104	-	-	7/21/61/61	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
24	CLA	C	510	-	3/3/20/25	7/37/135/135	-
31	PL9	a	417	-	-	12/53/73/73	0/1/1/1
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
29	LMT	m	103	-	-	3/21/61/61	0/2/2/2
28	GOL	C	525	-	-	0/4/4/4	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
28	GOL	a	413	-	-	0/4/4/4	-
28	GOL	v	204	-	-	3/4/4/4	-
24	CLA	A	406	41	3/3/20/25	4/37/135/135	-
27	SQD	a	411	-	-	11/49/69/69	0/1/1/1
37	LHG	E	101	-	-	21/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
35	HTG	V	202	-	-	5/10/30/30	0/1/1/1
24	CLA	c	902	-	3/3/20/25	4/37/135/135	-
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	CLA	c	907	-	3/3/20/25	9/37/135/135	-
34	LMG	J	101	39	-	13/46/66/70	0/1/1/1
35	HTG	c	923	-	-	0/10/30/30	0/1/1/1
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
24	CLA	C	509	-	2/2/20/25	7/37/135/135	-
36	DGD	c	916	-	-	10/51/91/95	0/2/2/2
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2

The worst 5 of 1140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-C2B	6.98	1.50	1.40
24	b	620	CLA	C3B-C2B	6.75	1.49	1.40
24	a	406	CLA	C3B-C2B	6.74	1.49	1.40
24	B	617	CLA	C3B-C2B	6.73	1.49	1.40
24	c	910	CLA	C3B-C2B	6.65	1.49	1.40

The worst 5 of 2191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C4A-NA-C1A	-7.78	103.21	106.71
24	d	402	CLA	C4A-NA-C1A	-7.52	103.33	106.71
25	A	408	PHO	CMD-C2D-C1D	7.42	136.50	125.06
24	b	613	CLA	C4A-NA-C1A	-7.29	103.43	106.71
24	B	616	CLA	C4A-NA-C1A	-7.09	103.52	106.71

5 of 182 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	c	904	CLA	NC
24	c	904	CLA	ND
24	c	904	CLA	NA
24	C	506	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	503	CLA	NC

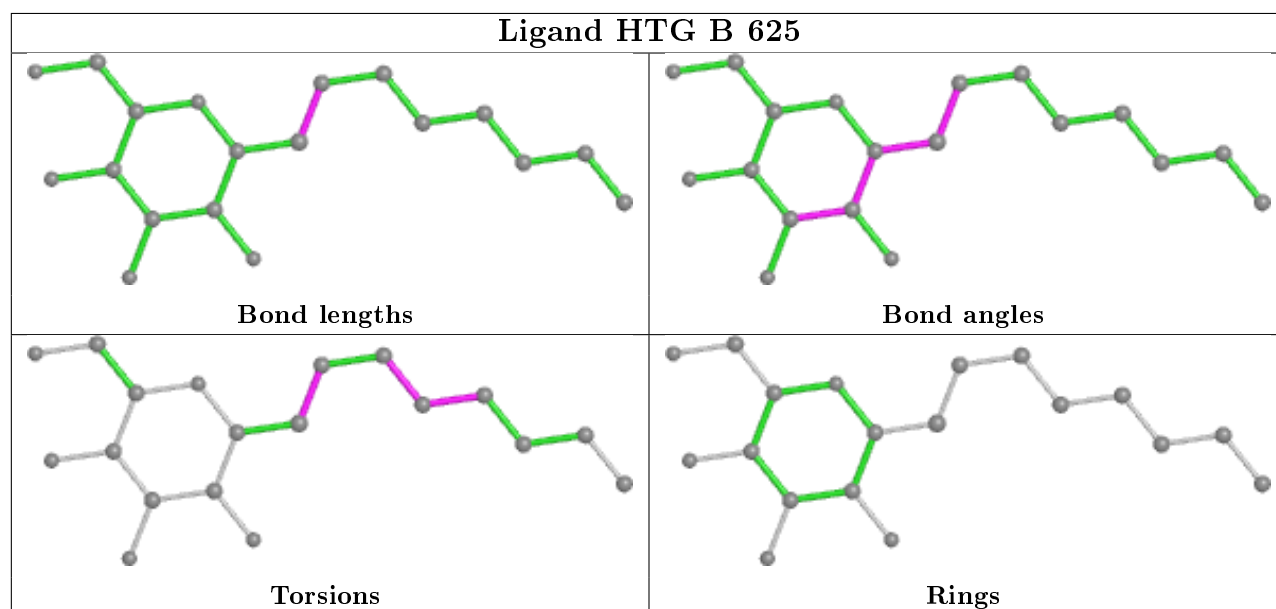
5 of 1245 torsion outliers are listed below:

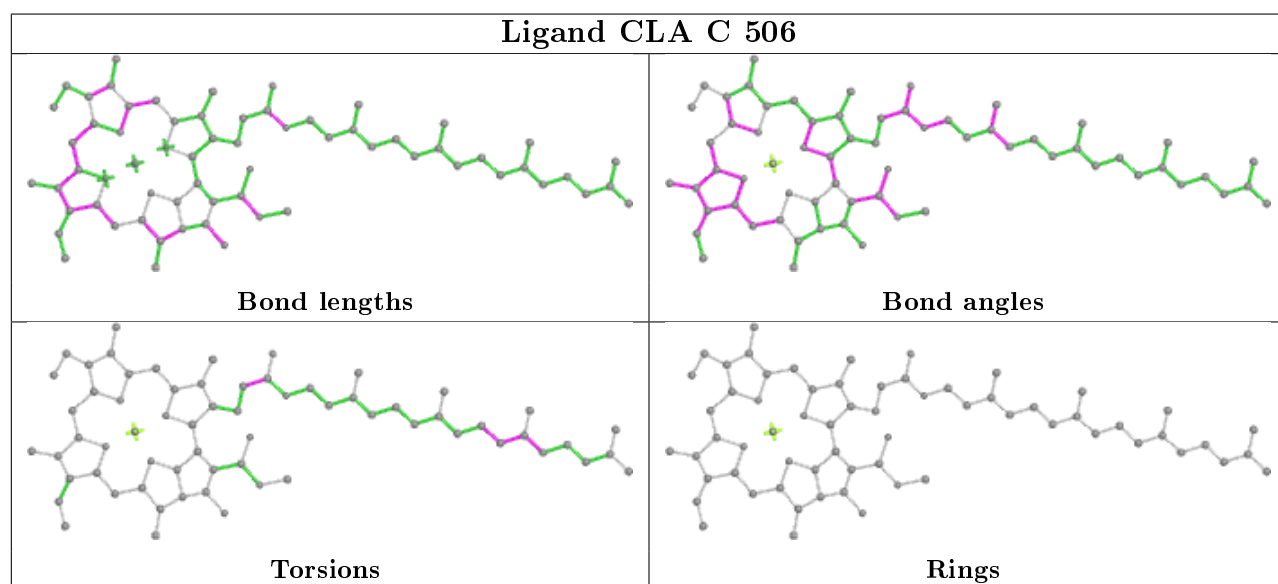
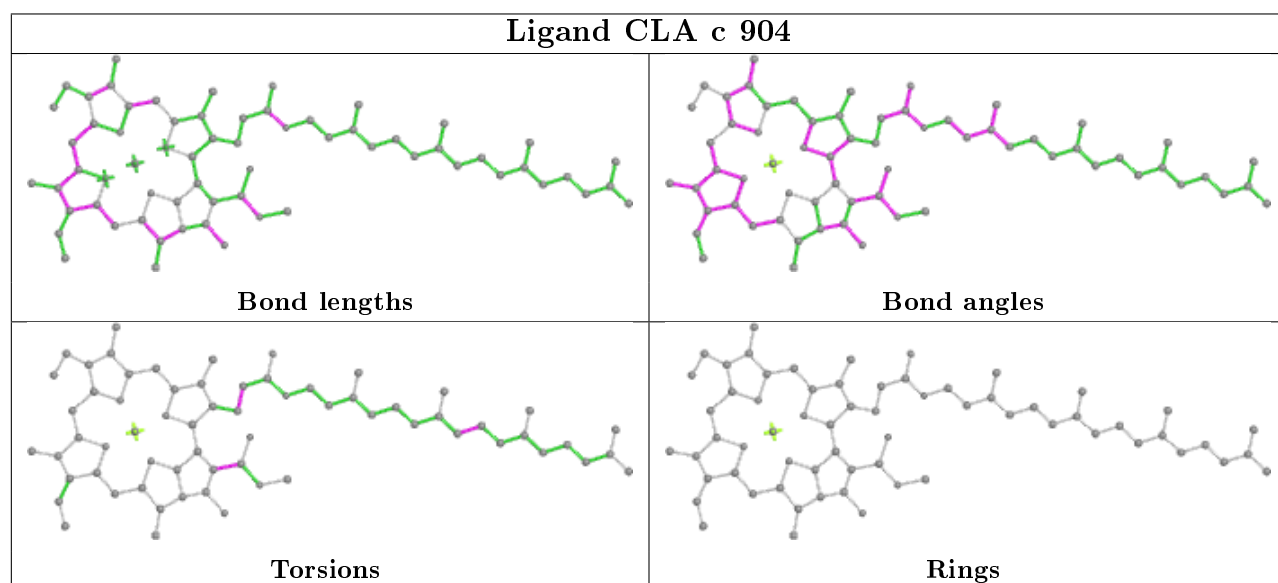
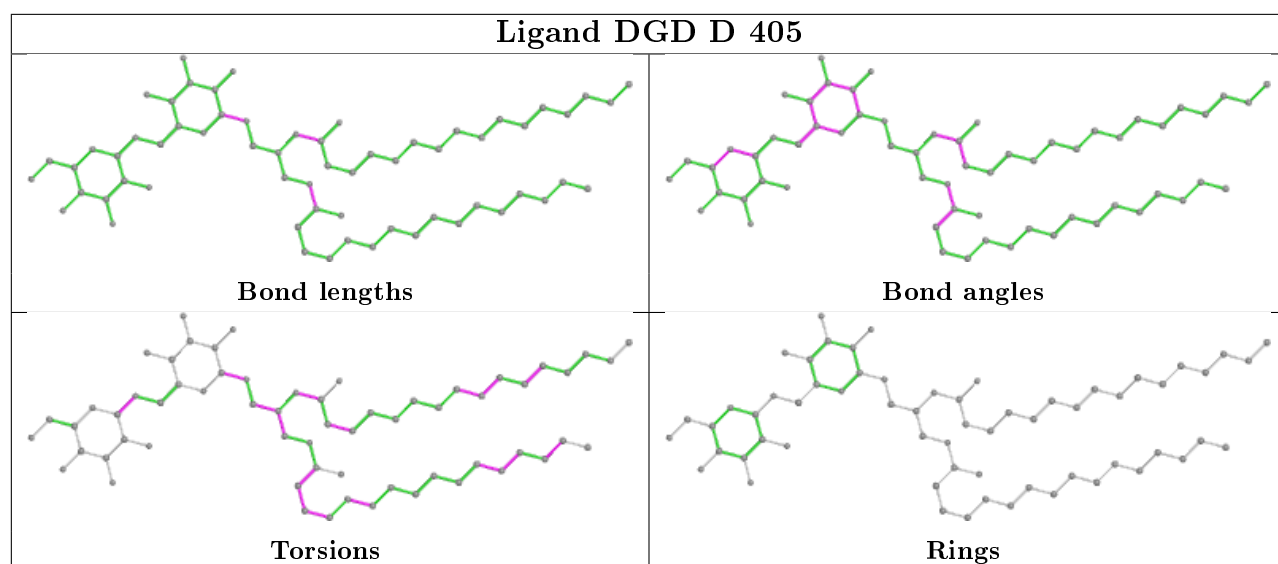
Mol	Chain	Res	Type	Atoms
35	B	625	HTG	C2'-C1'-S1-C1
36	D	405	DGD	C2B-C1B-O2G-C2G
36	D	405	DGD	C2D-C1D-O3G-C3G
36	D	405	DGD	O6D-C1D-O3G-C3G
36	D	405	DGD	O6E-C1E-O5D-C6D

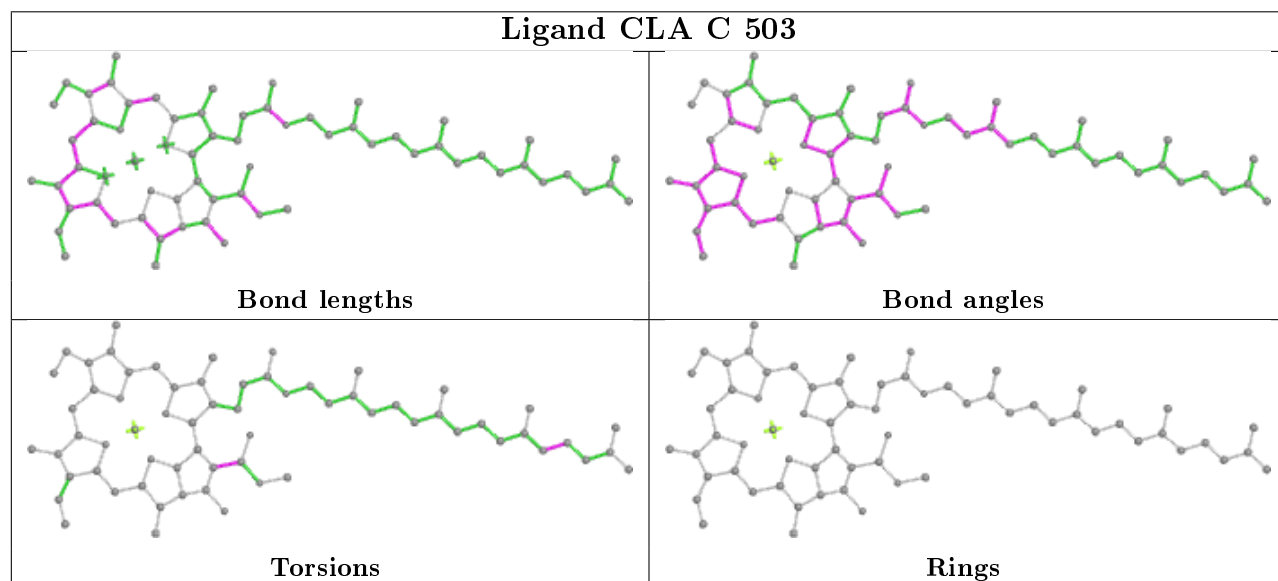
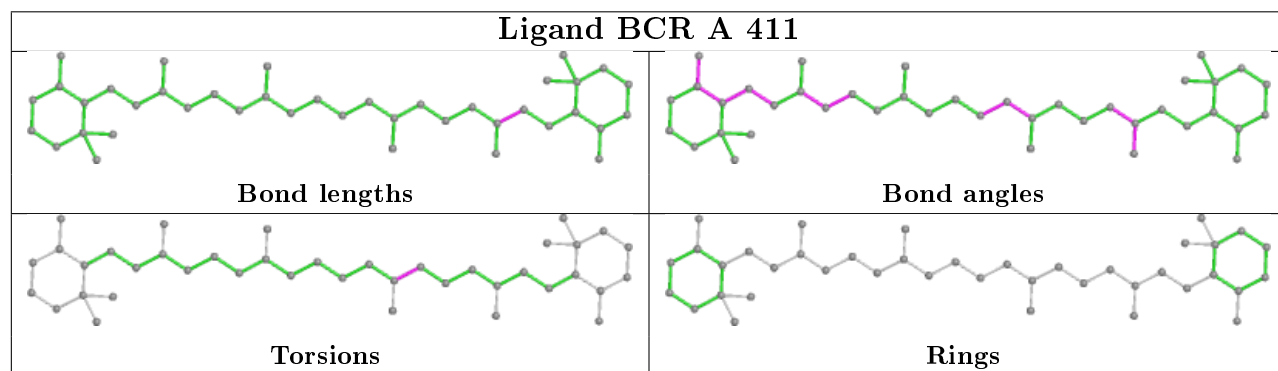
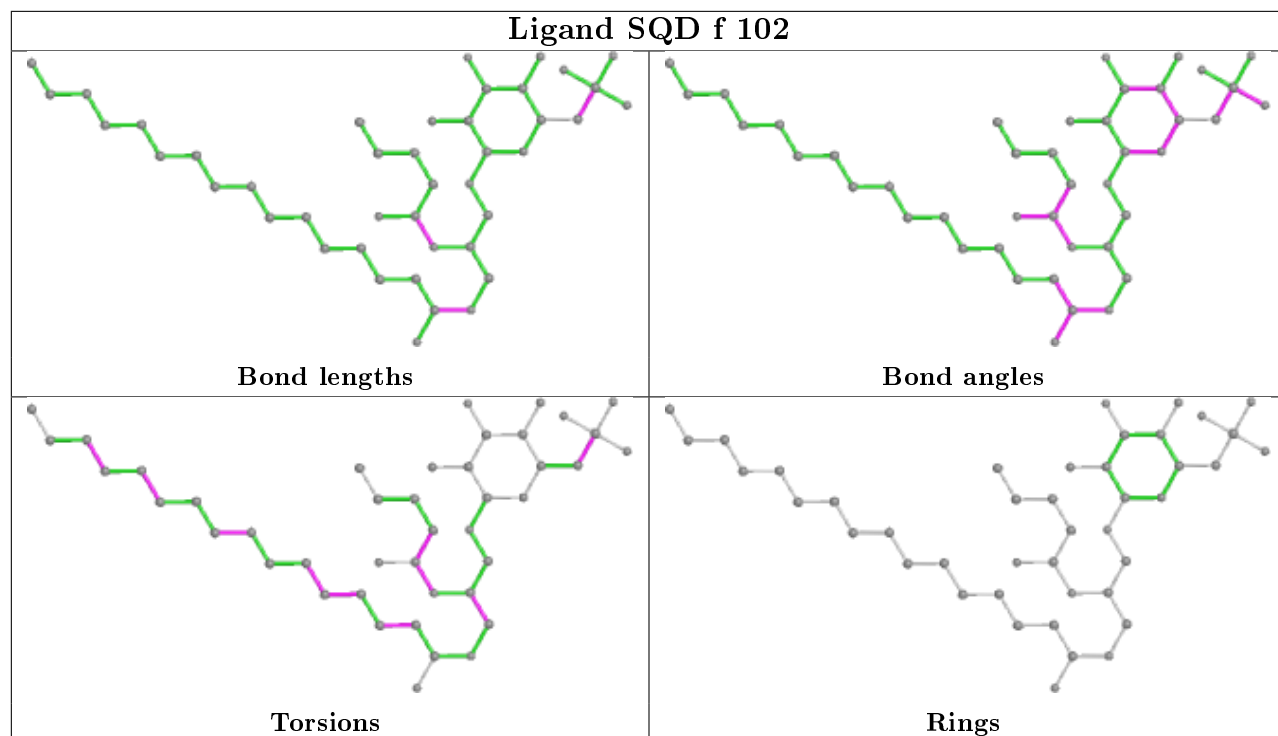
There are no ring outliers.

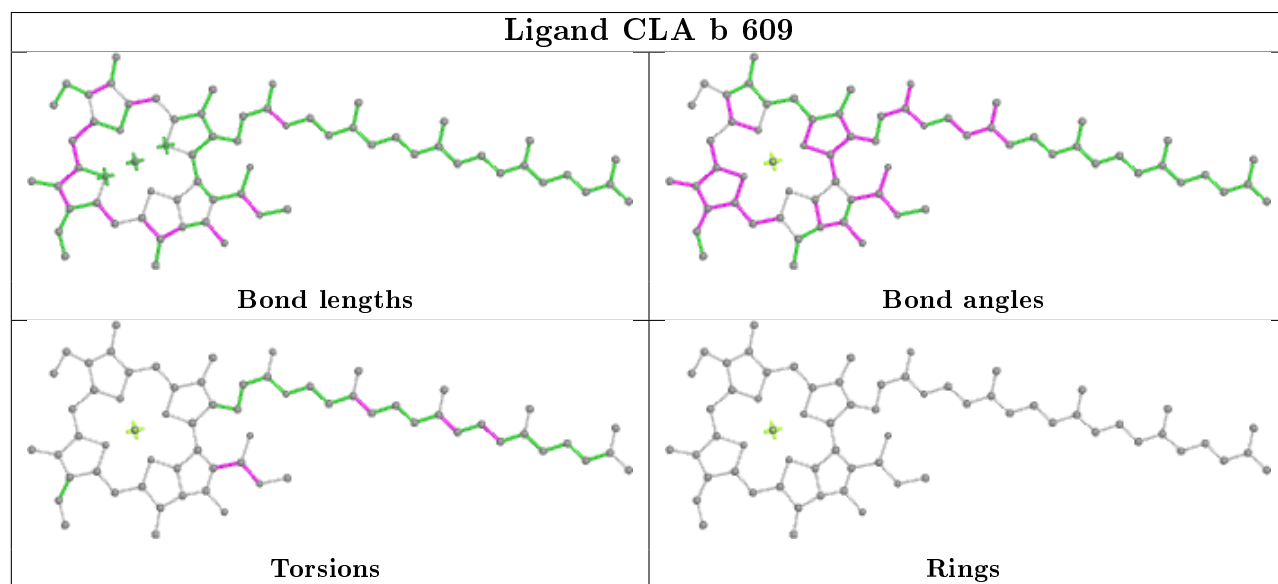
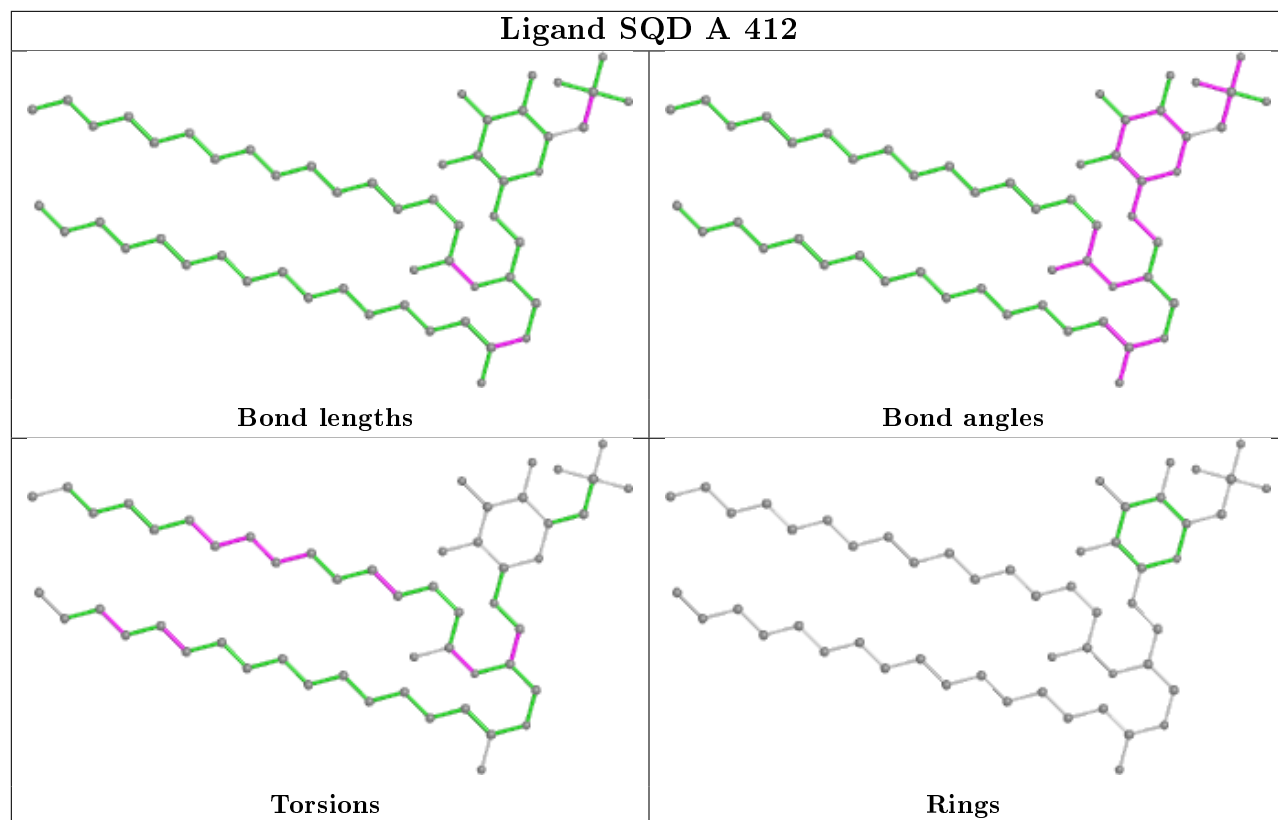
No monomer is involved in short contacts.

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.

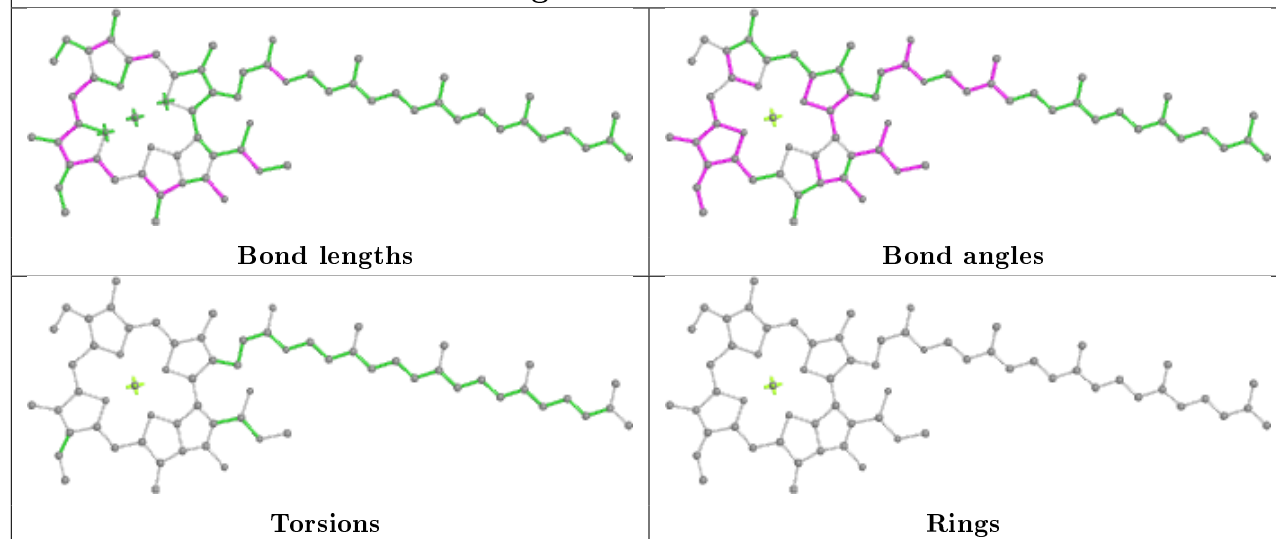




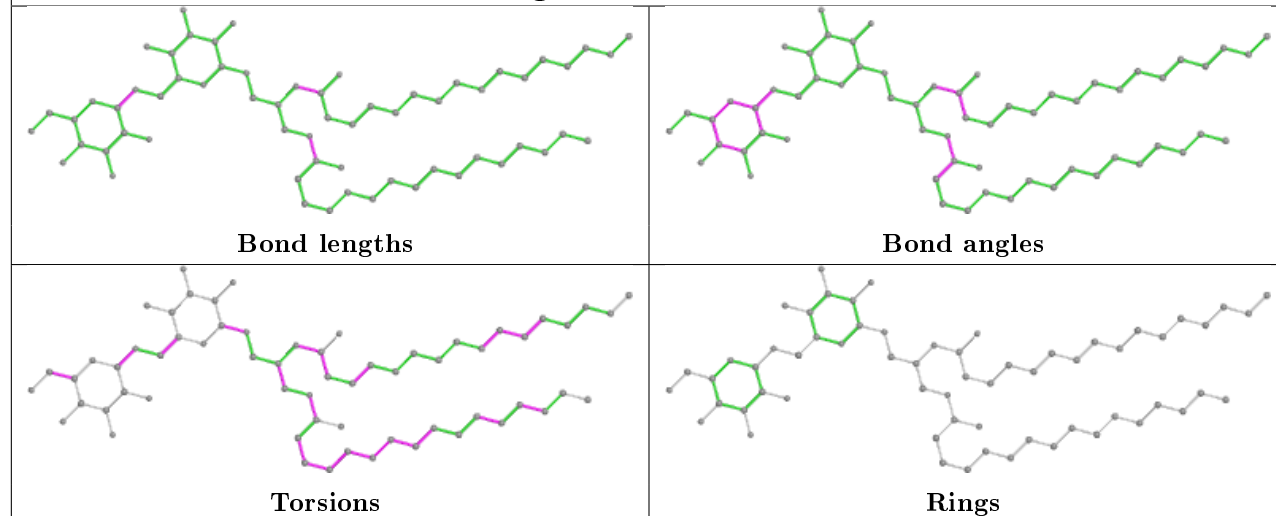




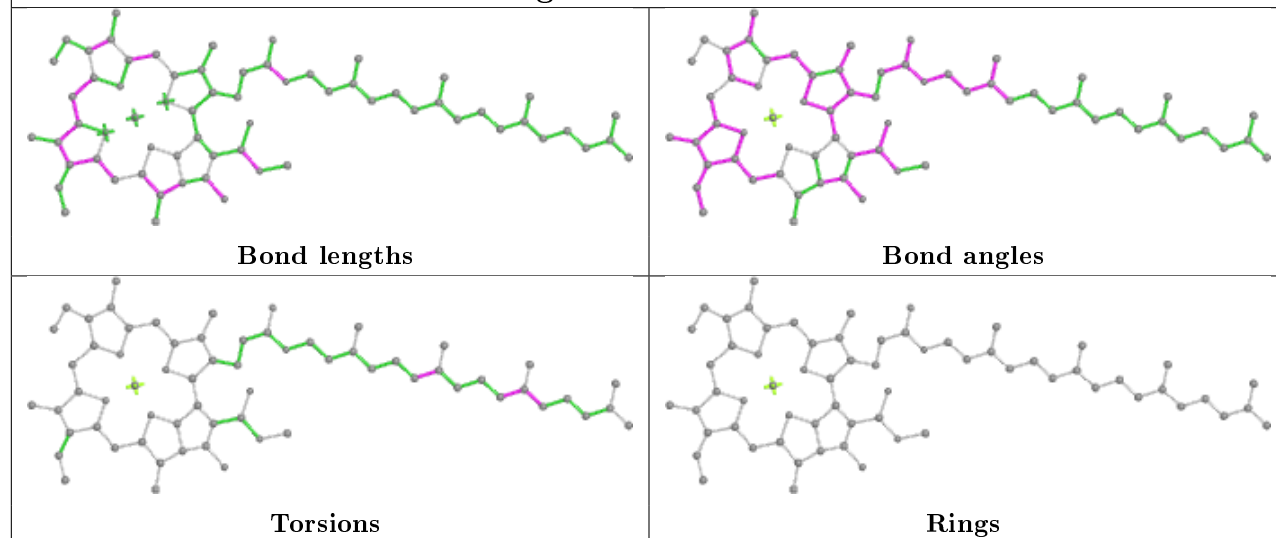
Ligand CLA D 401

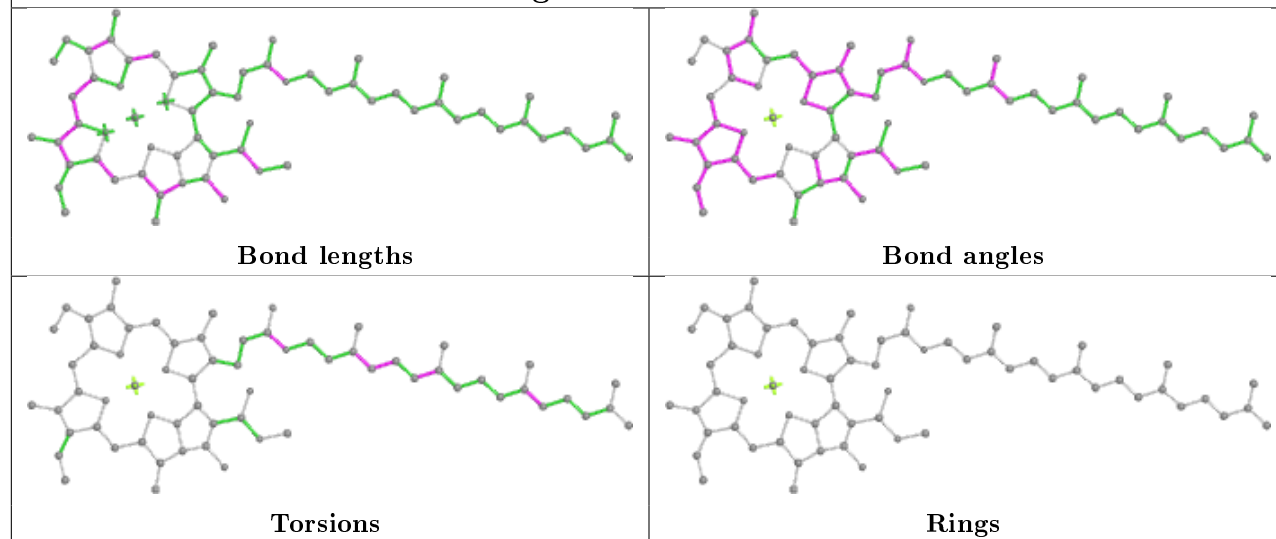
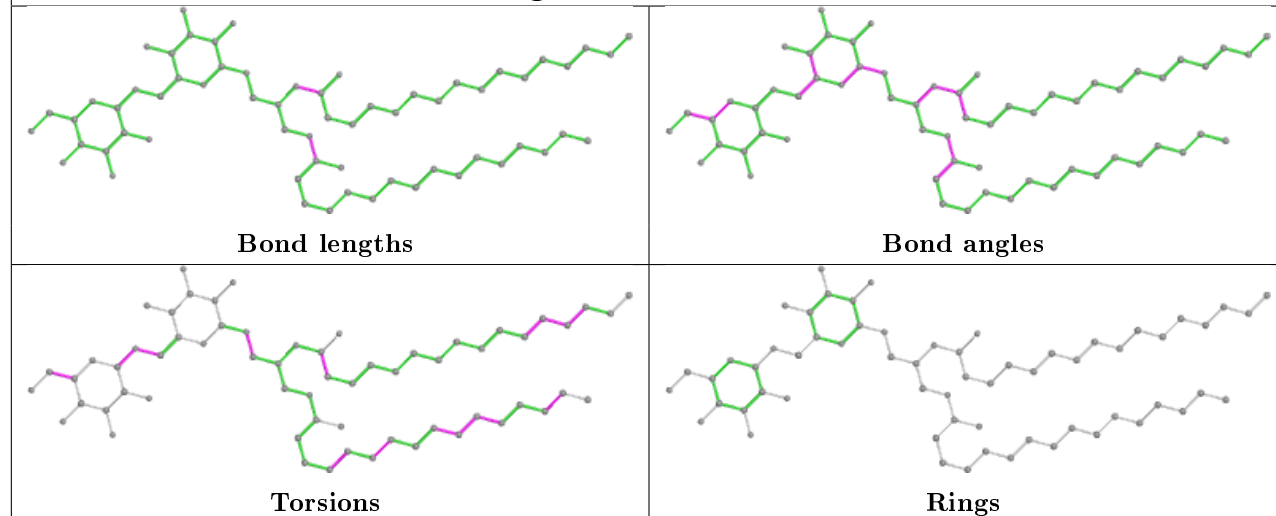
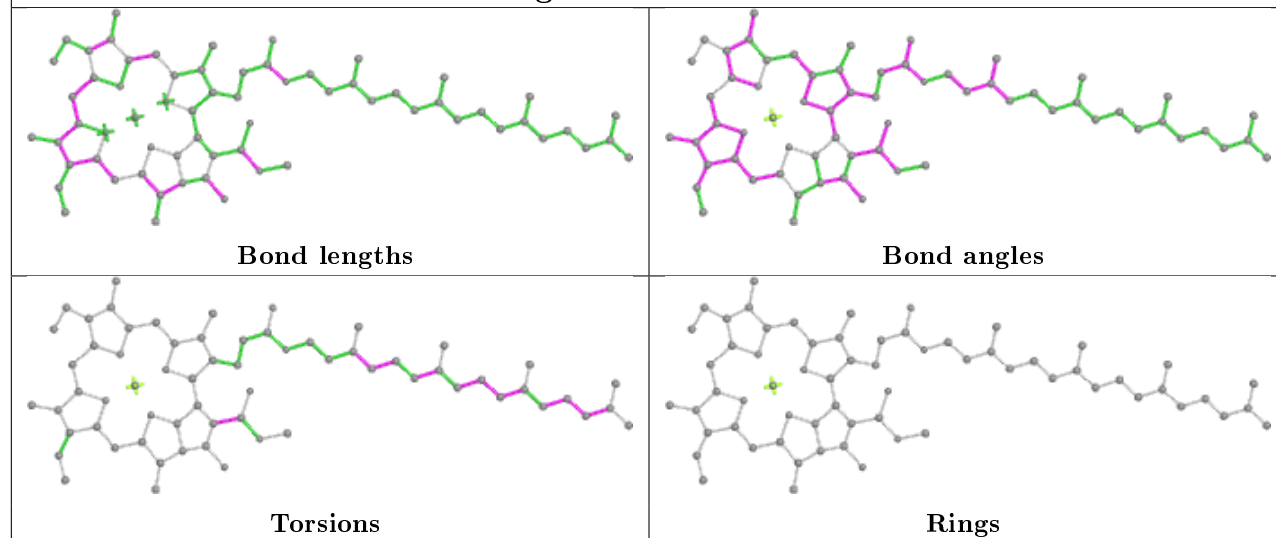


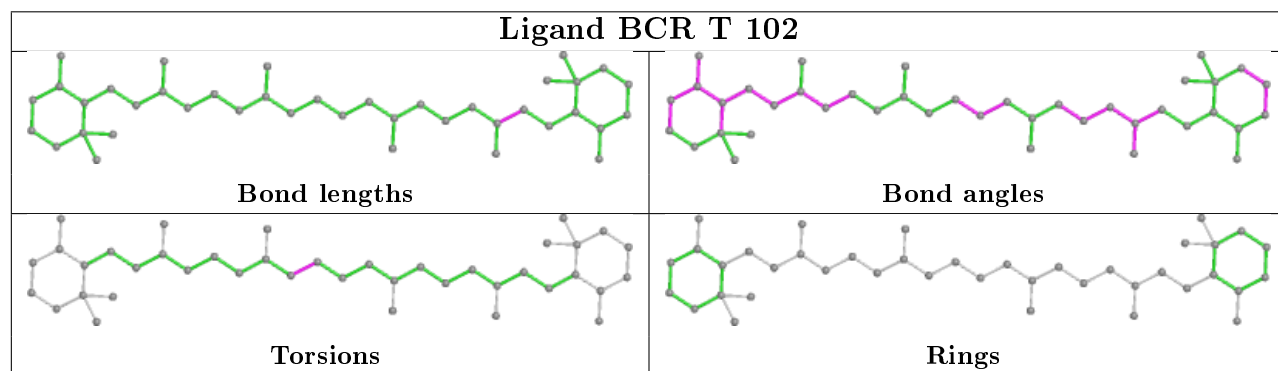
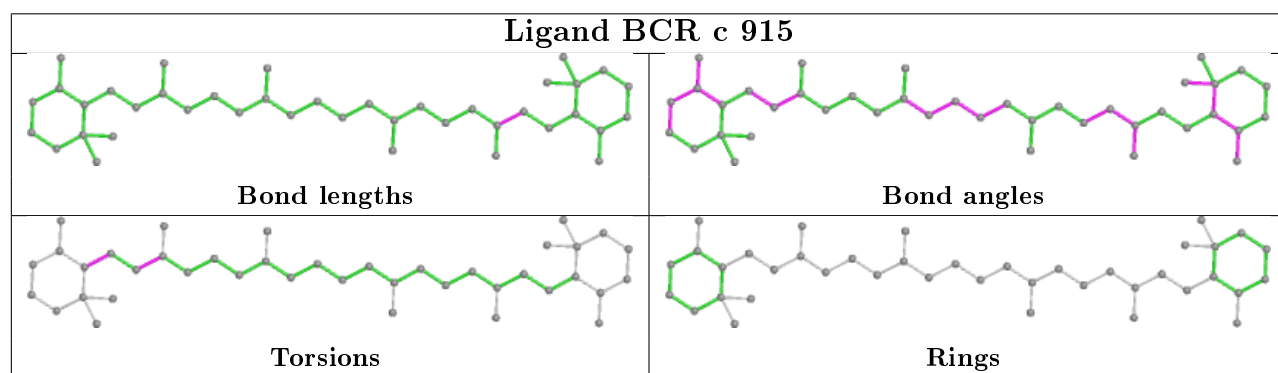
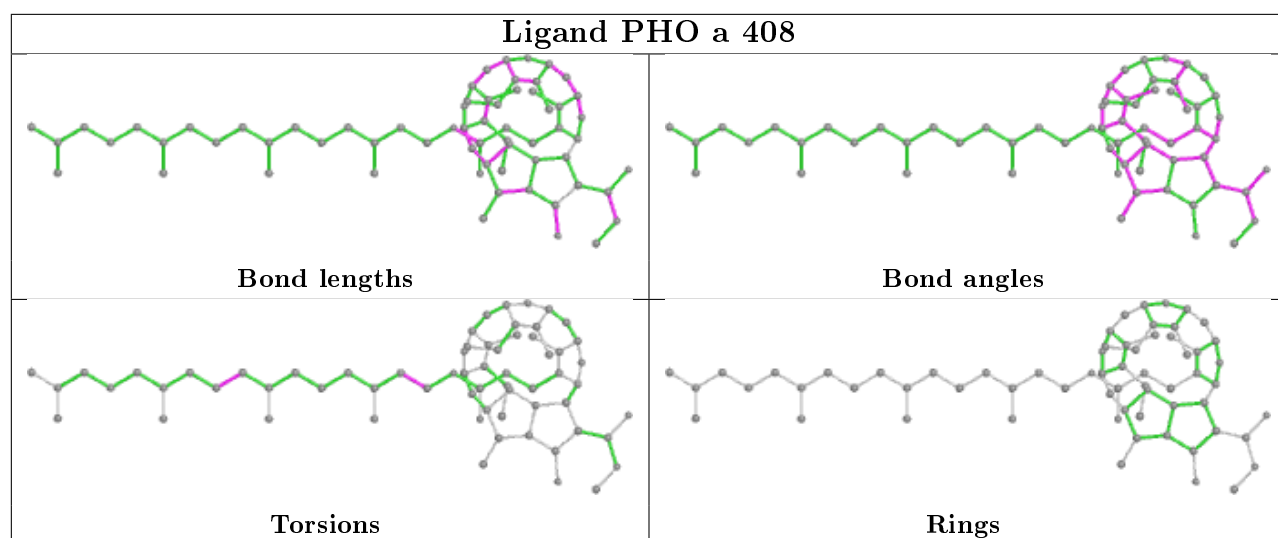
Ligand DGD d 406

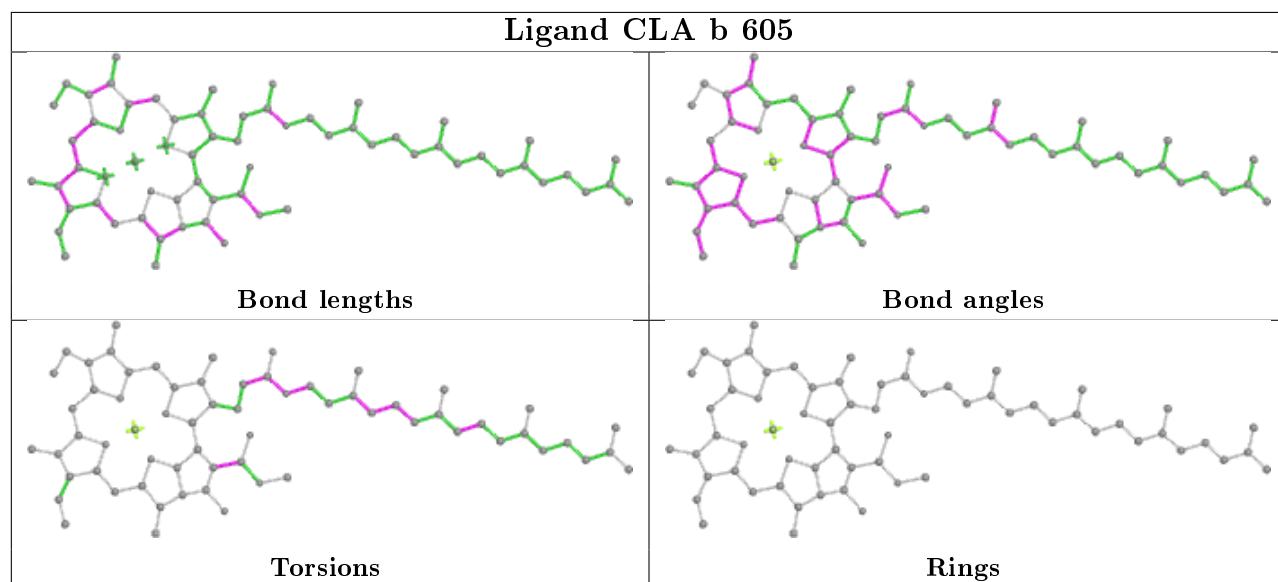
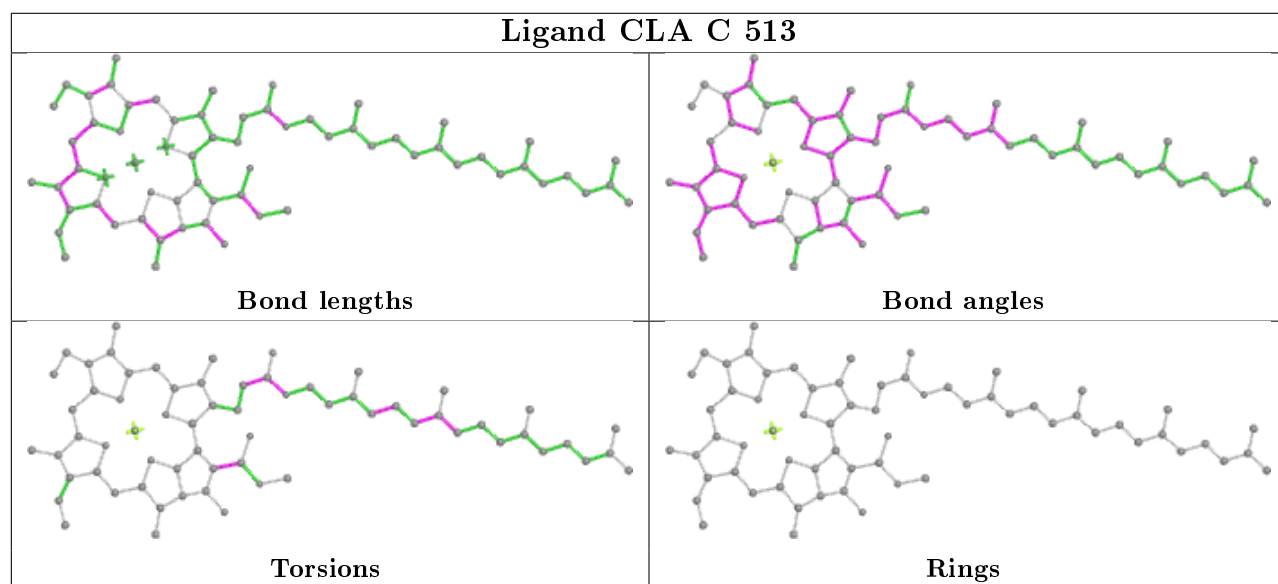
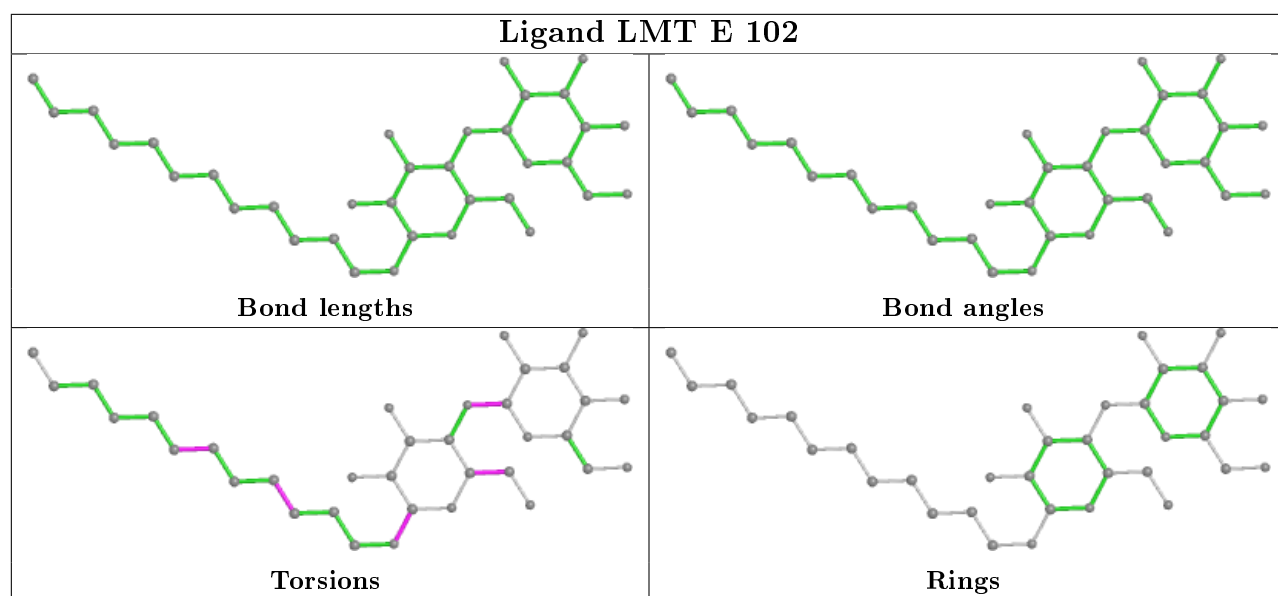


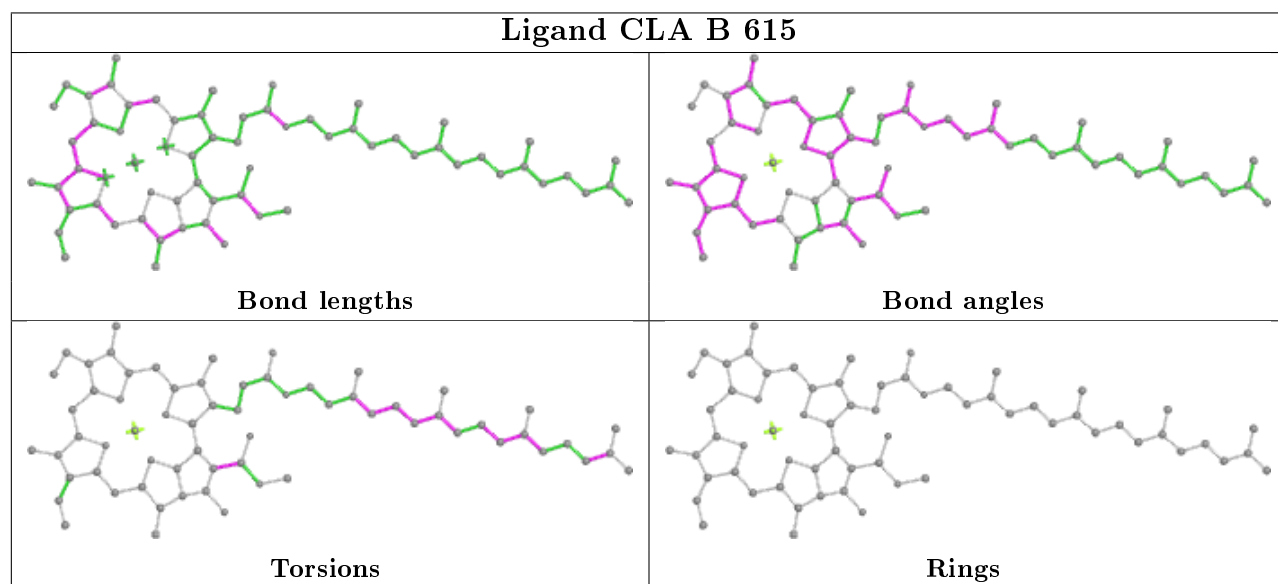
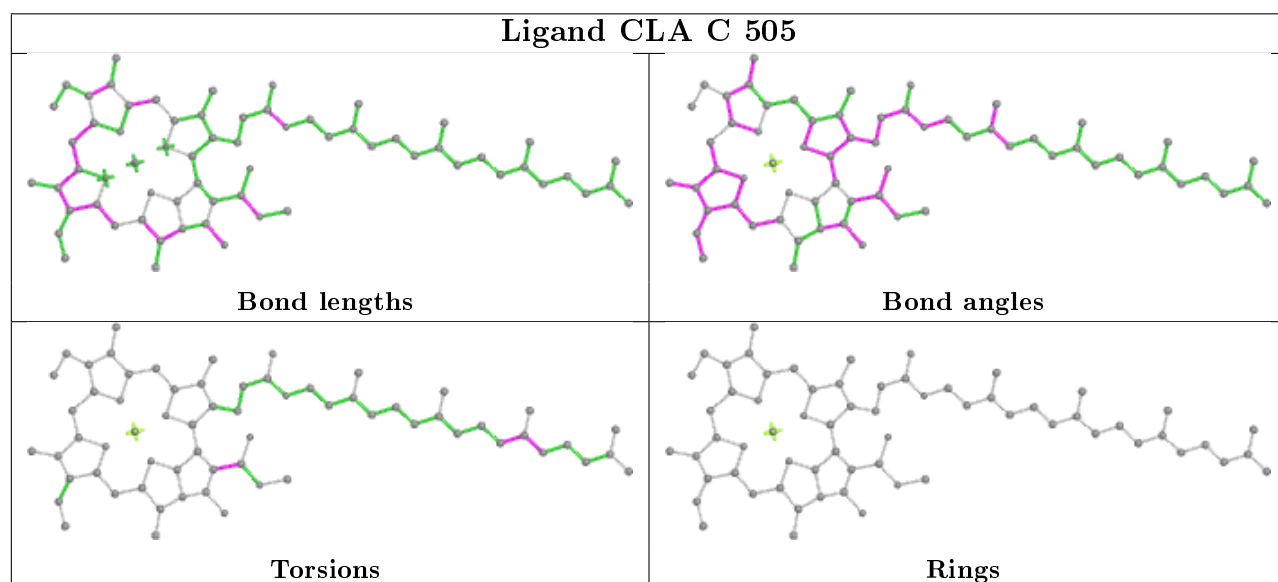
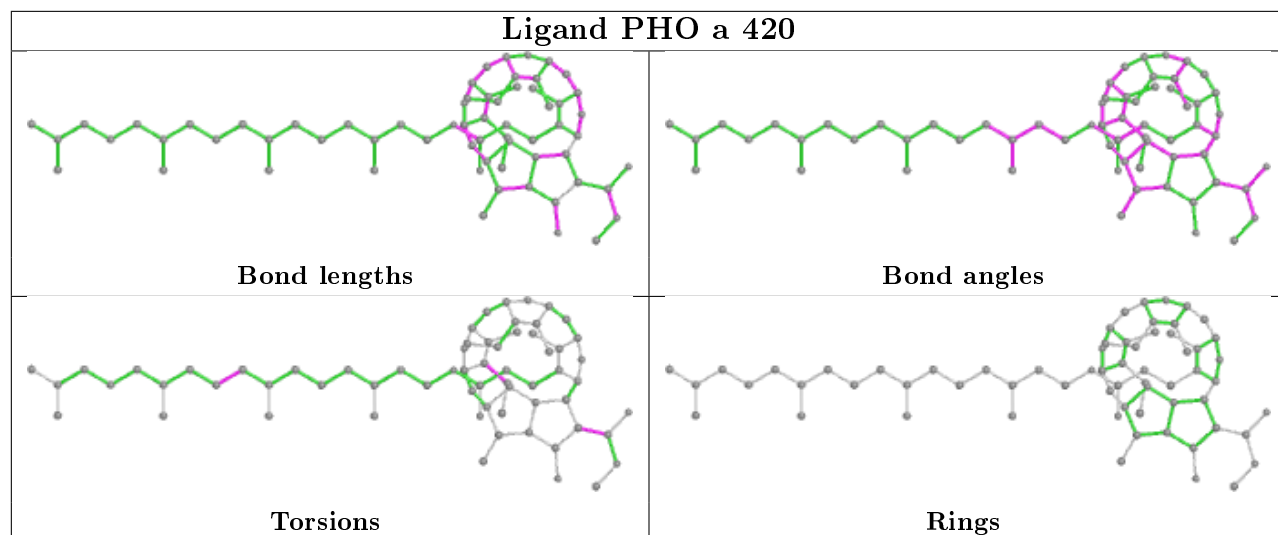
Ligand CLA a 407

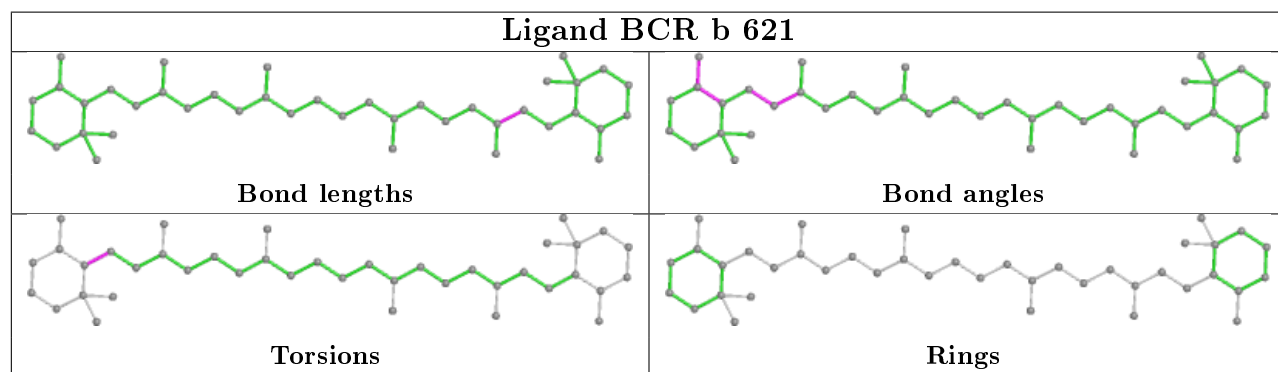
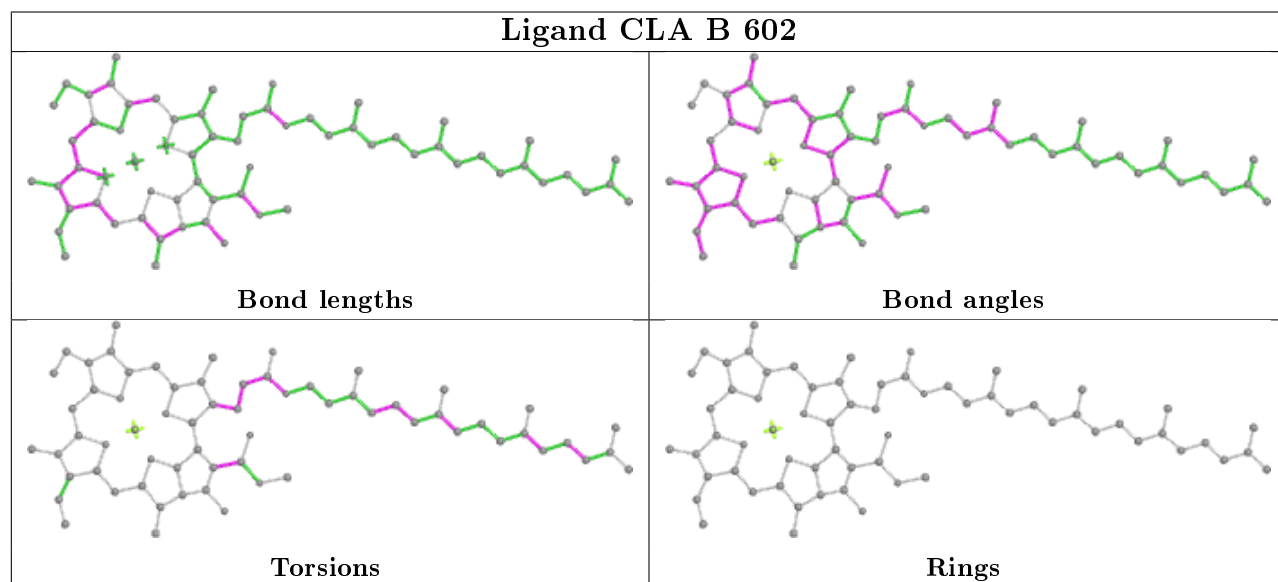
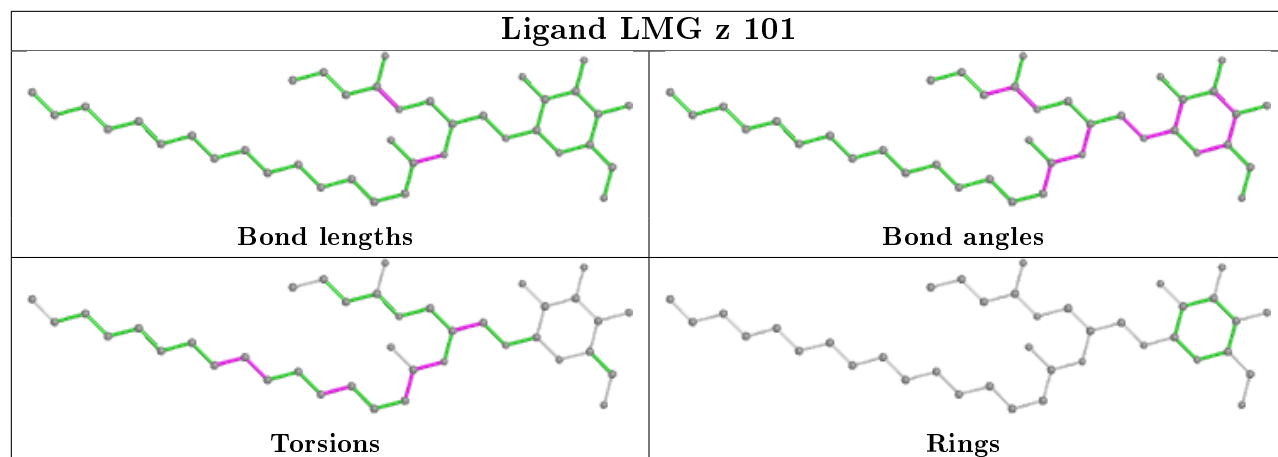


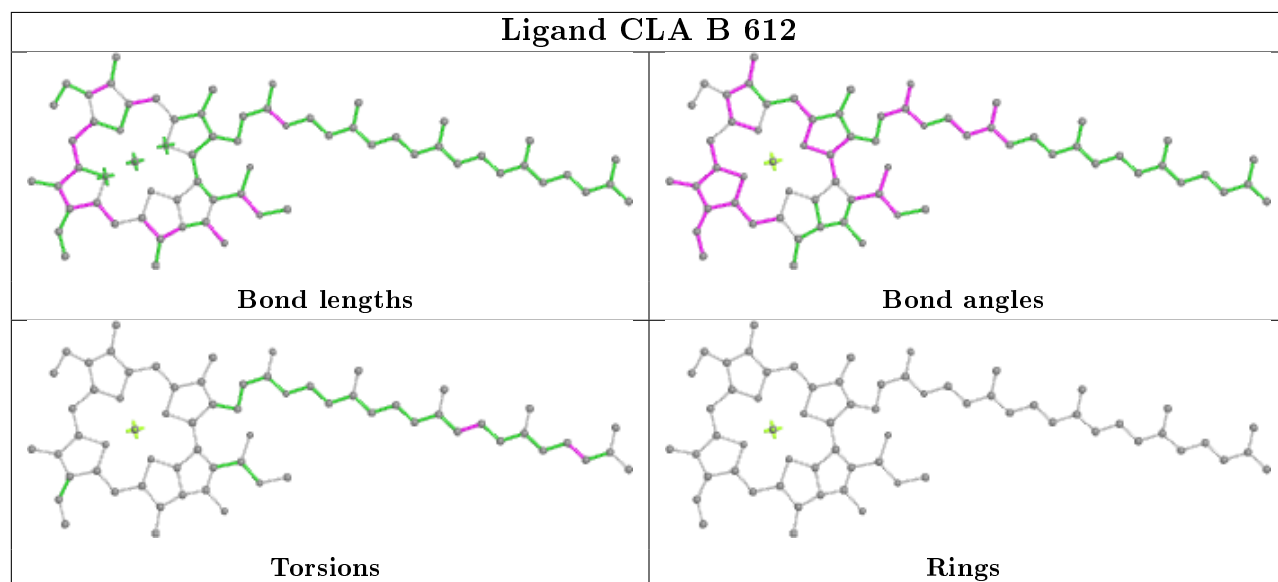
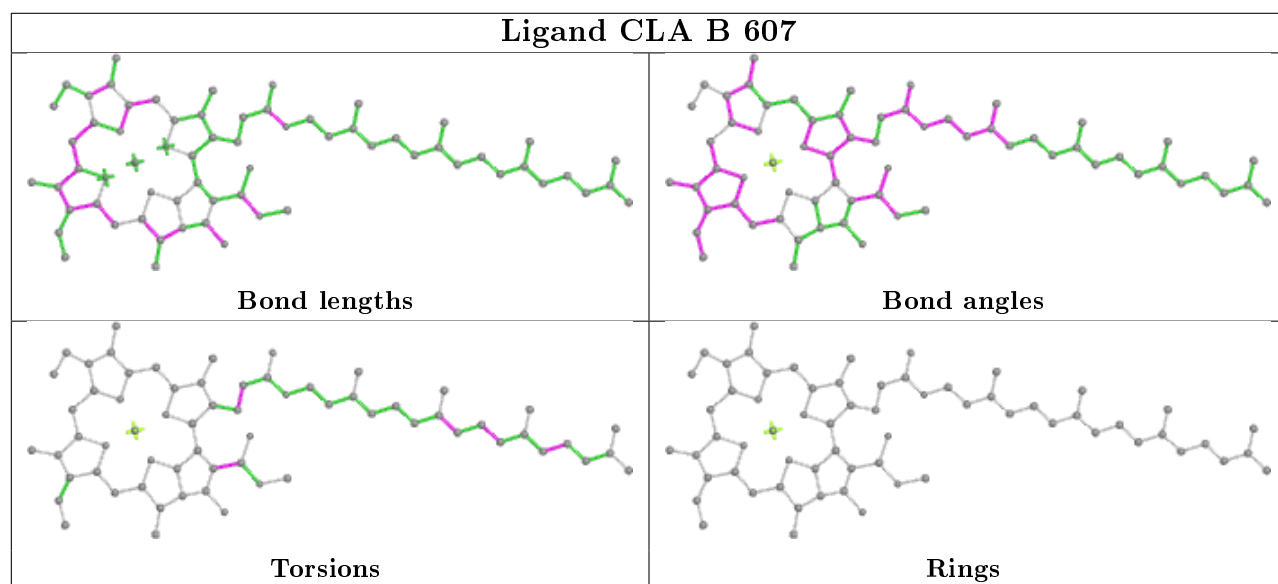
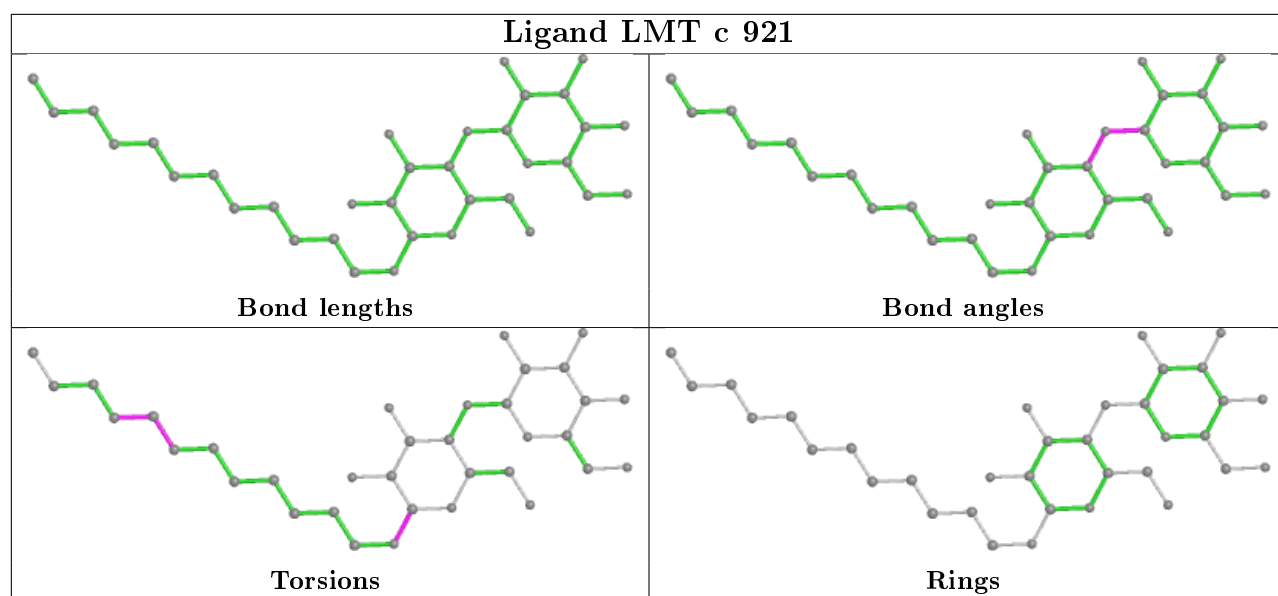
Ligand CLA A 410**Ligand DGD C 518****Ligand CLA b 618**



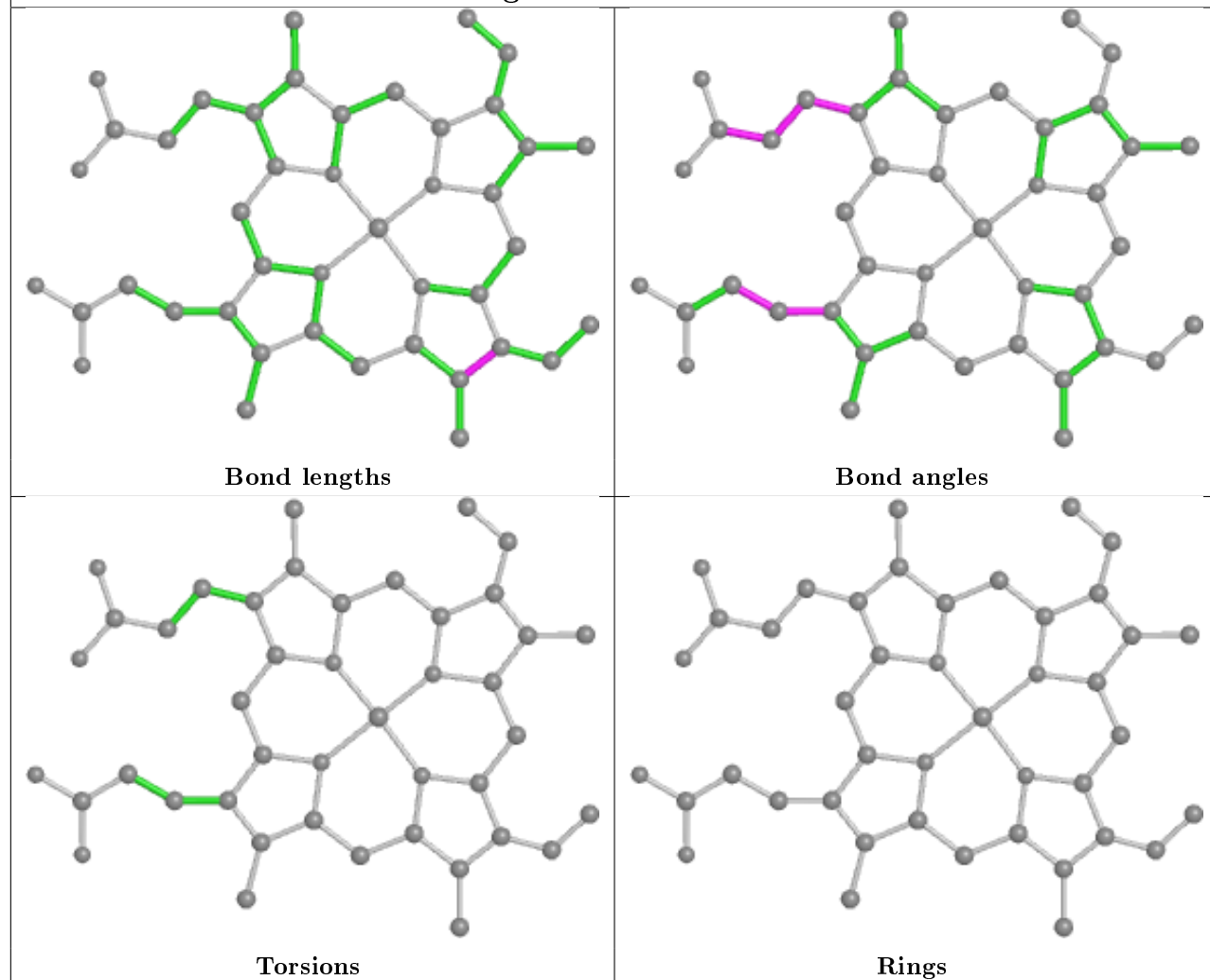




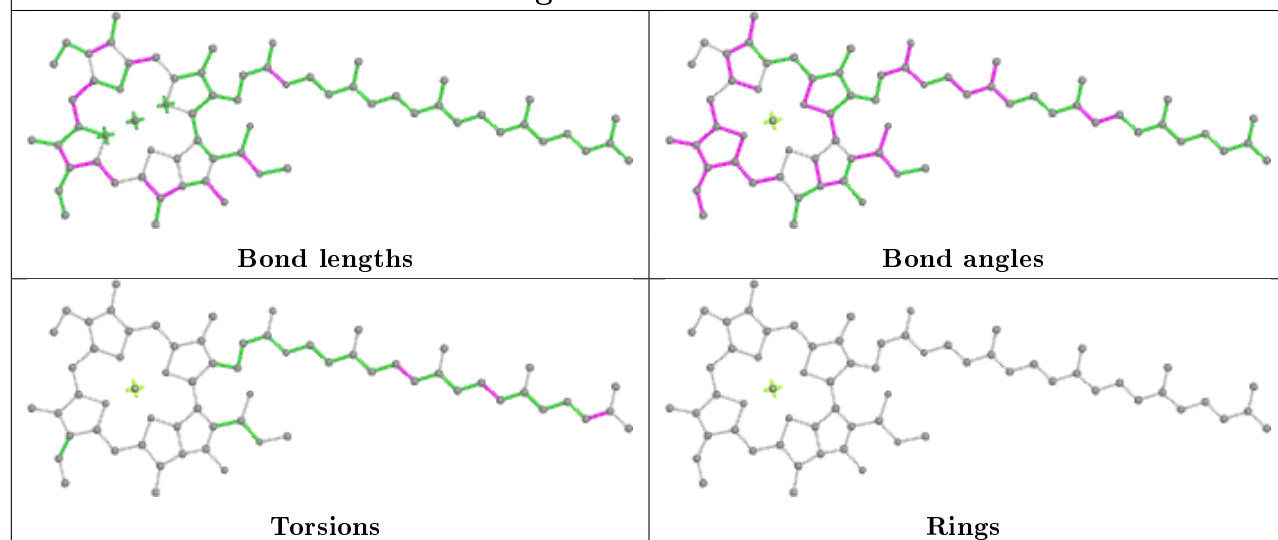




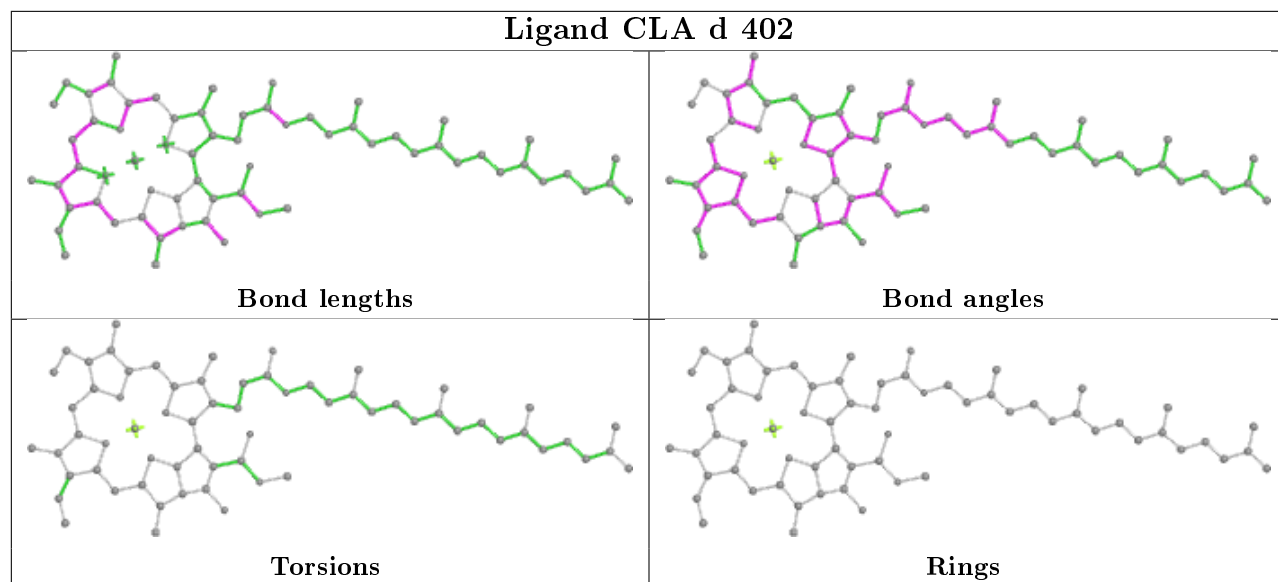
Ligand HEM e 102



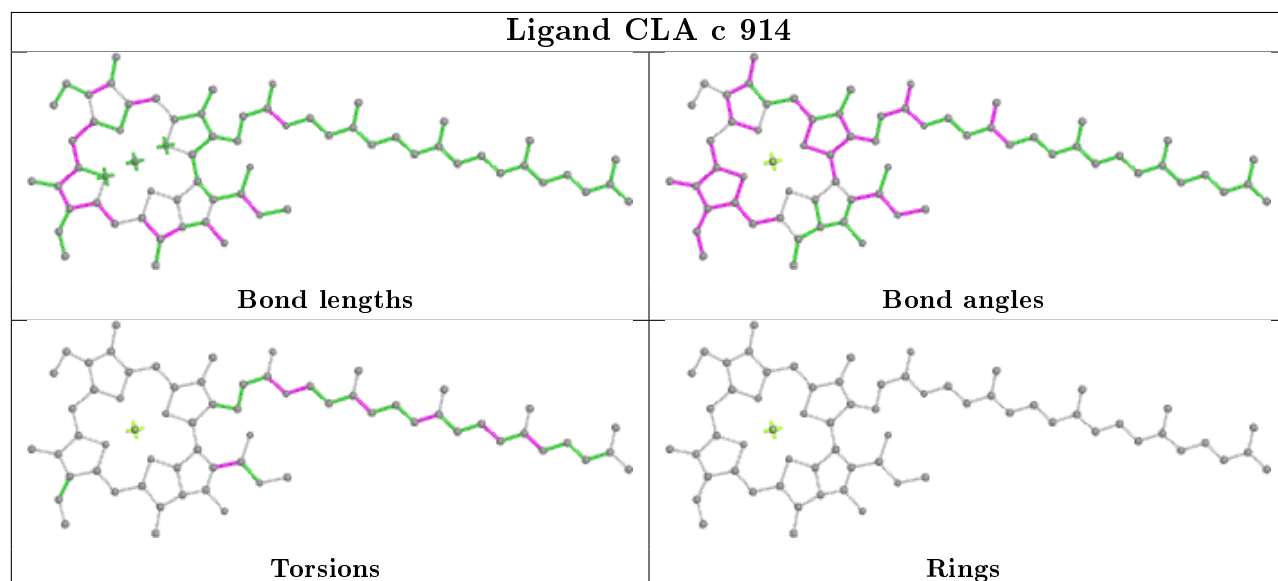
Ligand CLA b 619



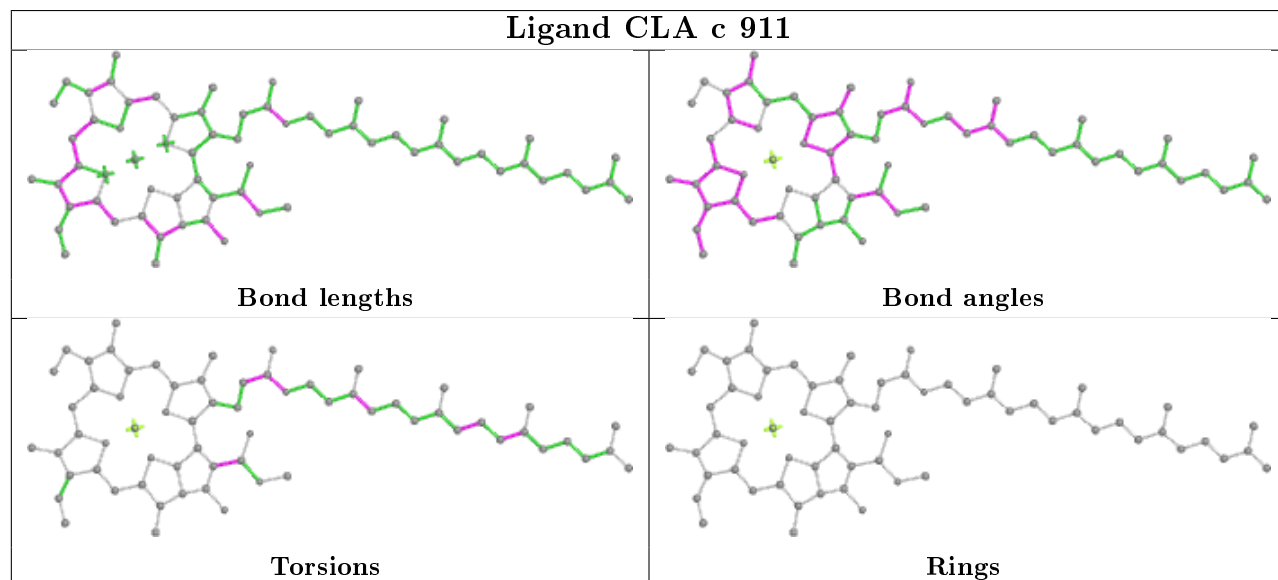
Ligand CLA d 402

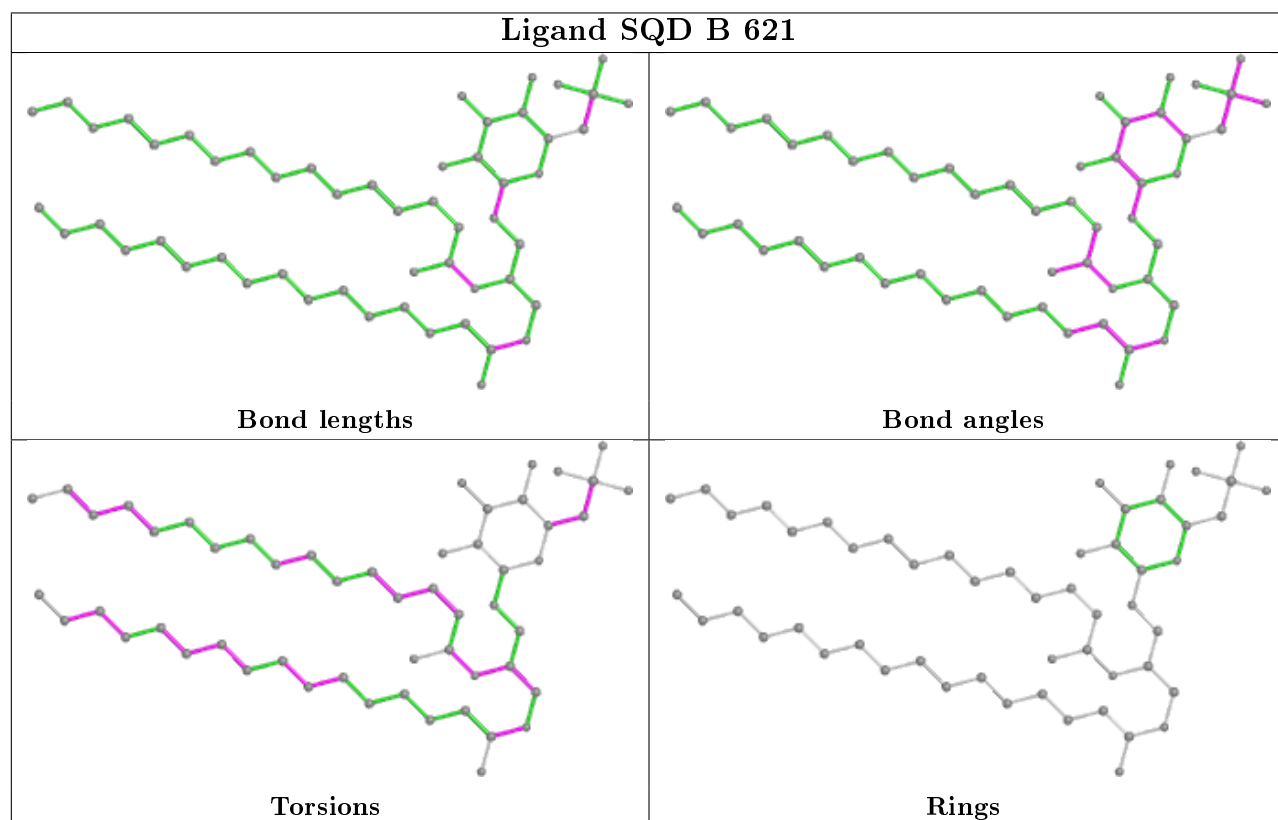
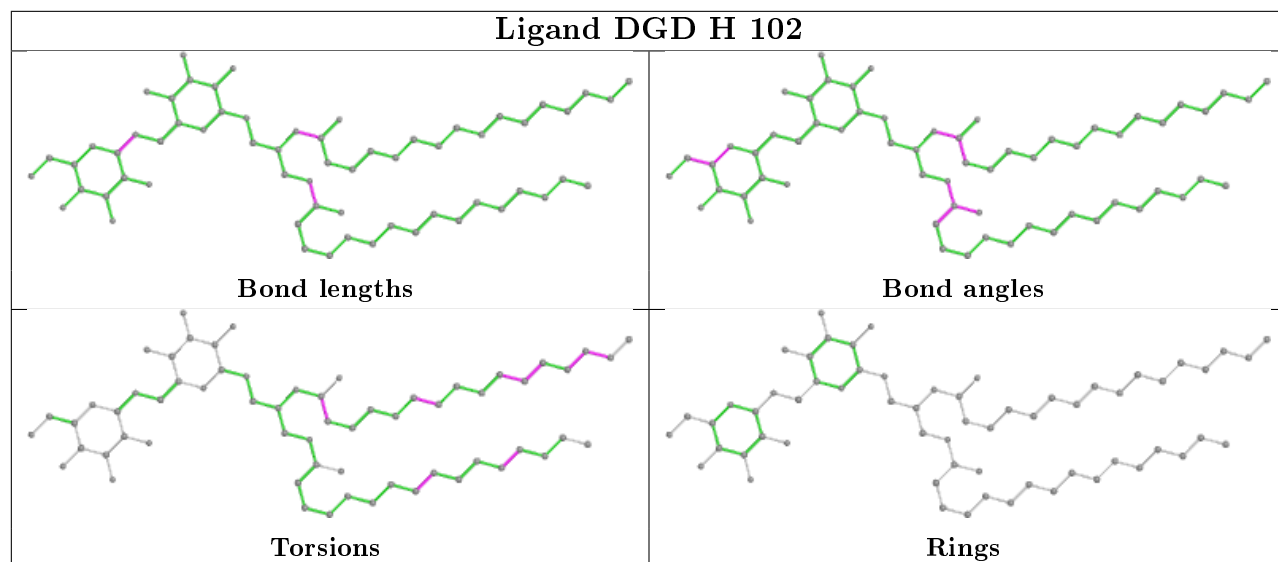
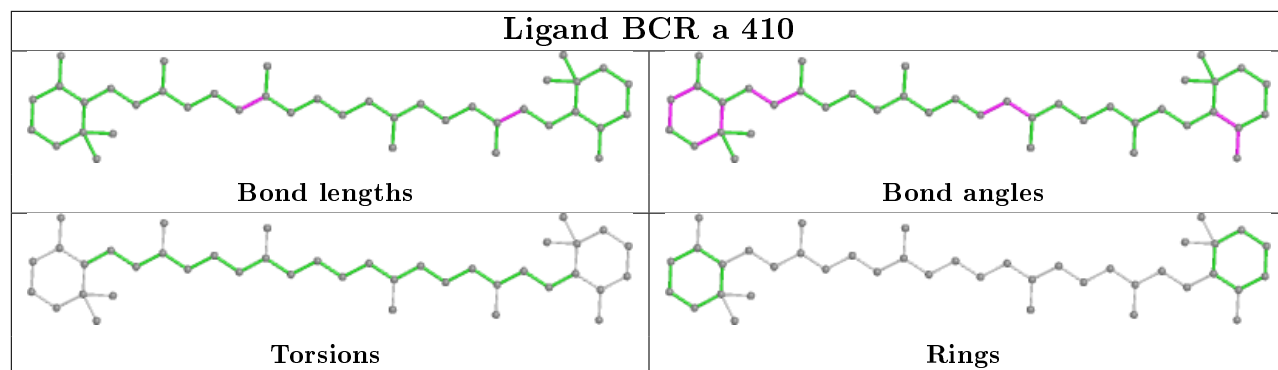


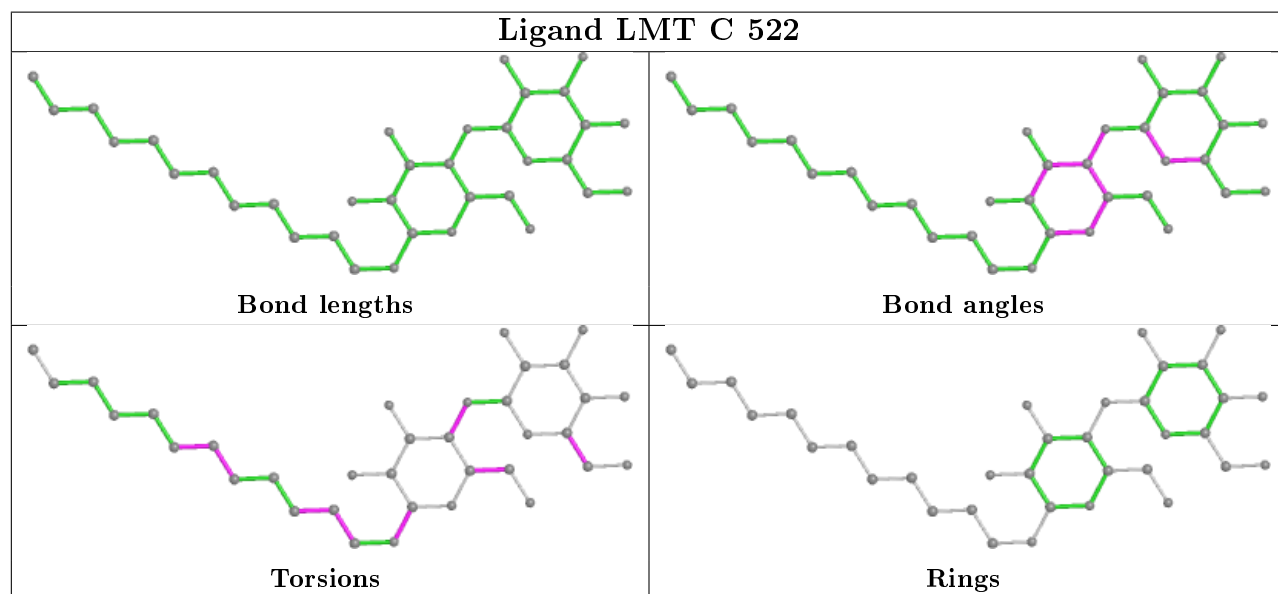
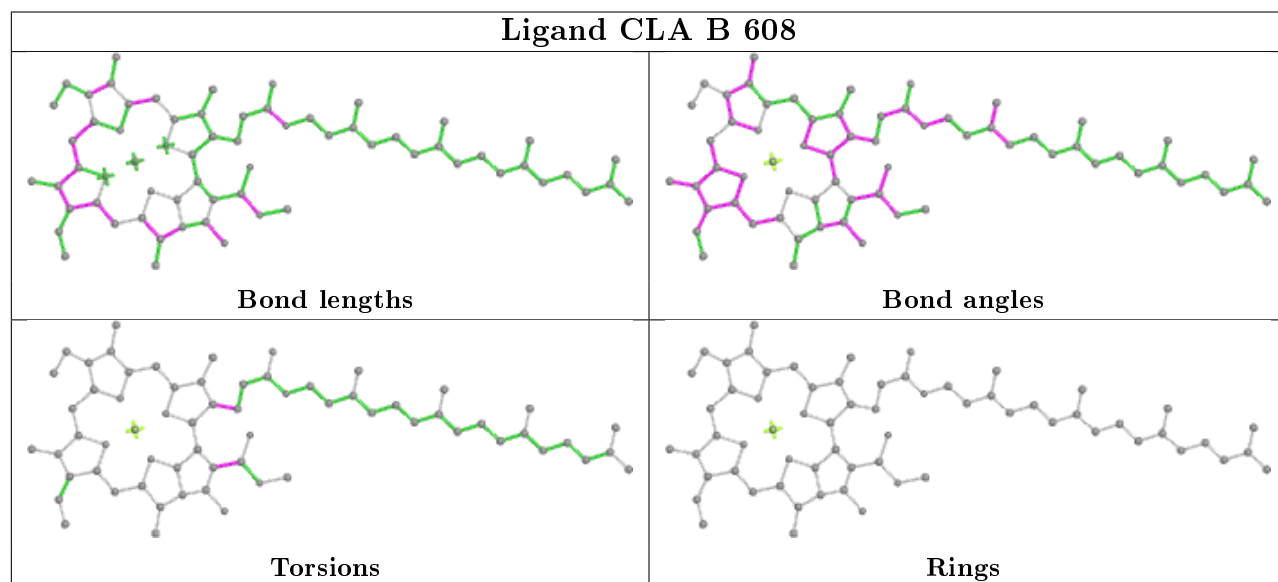
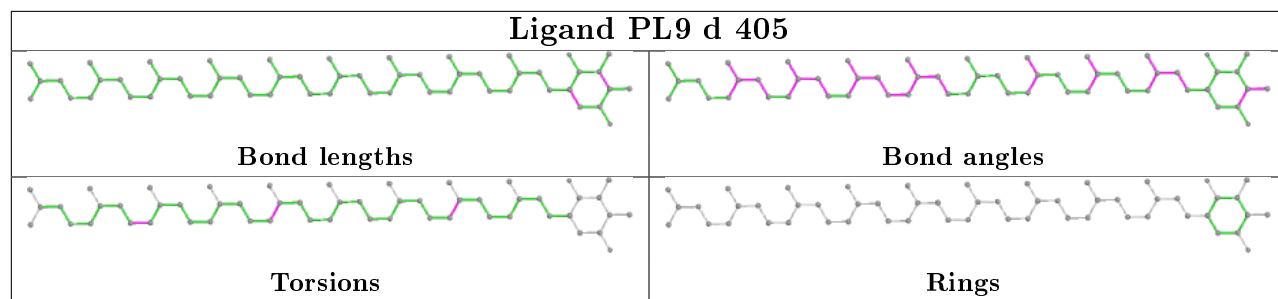
Ligand CLA c 914

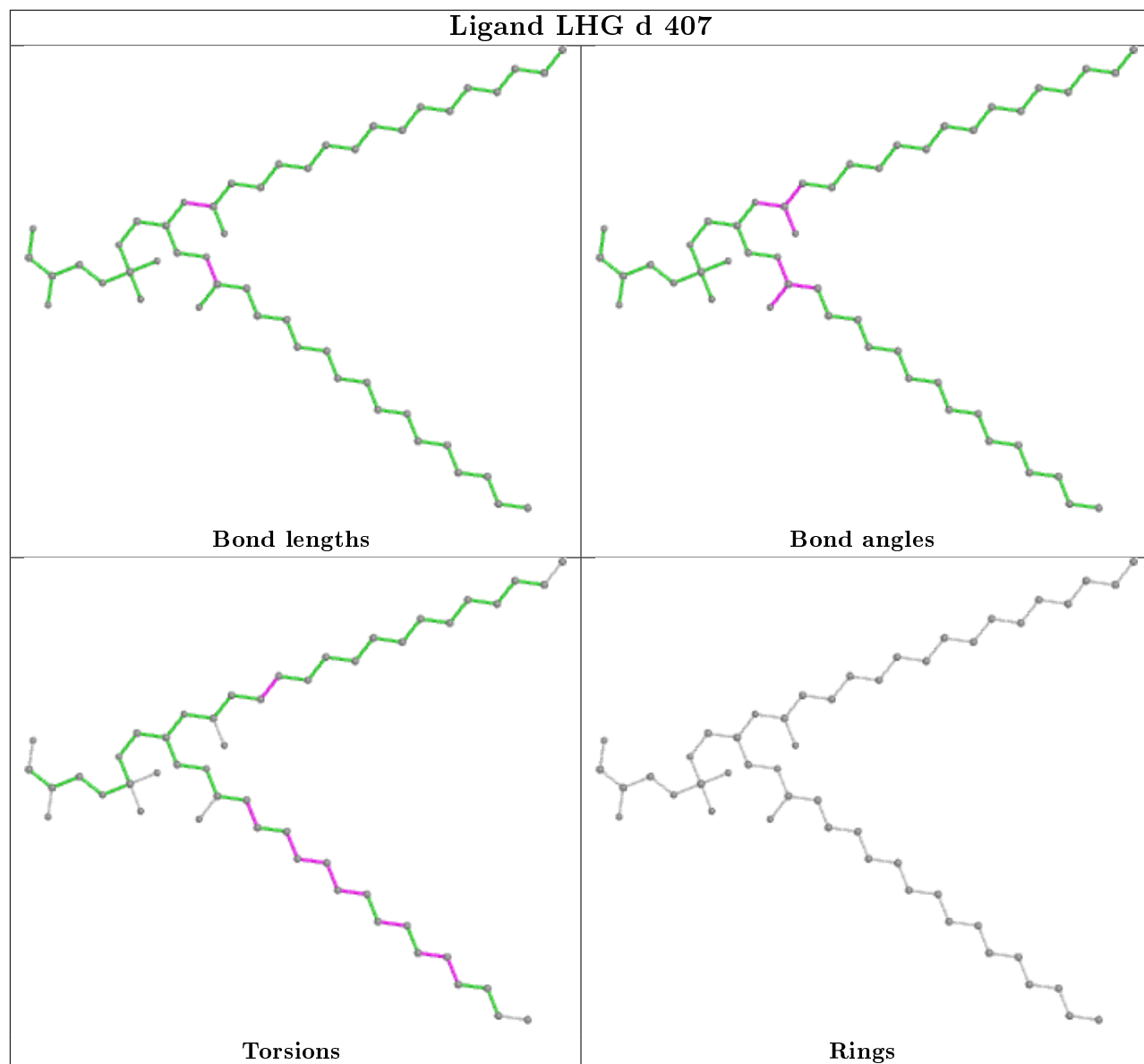
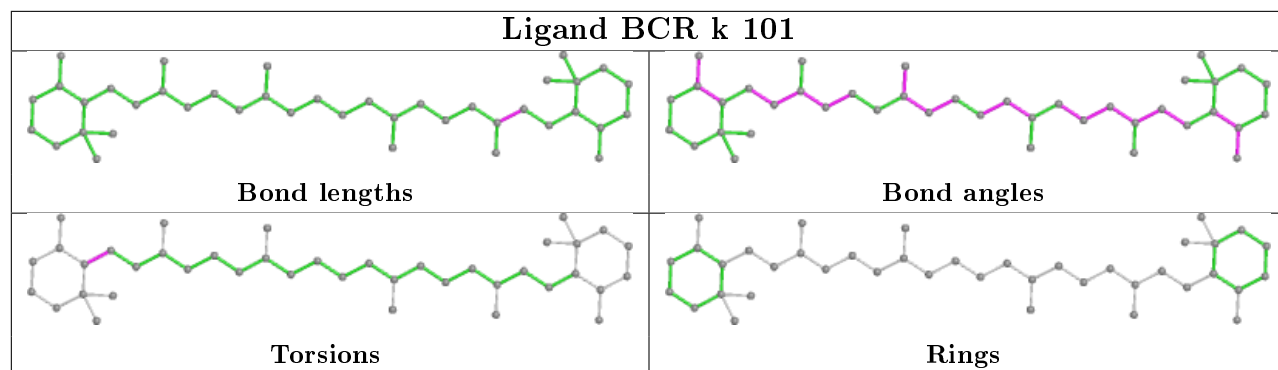


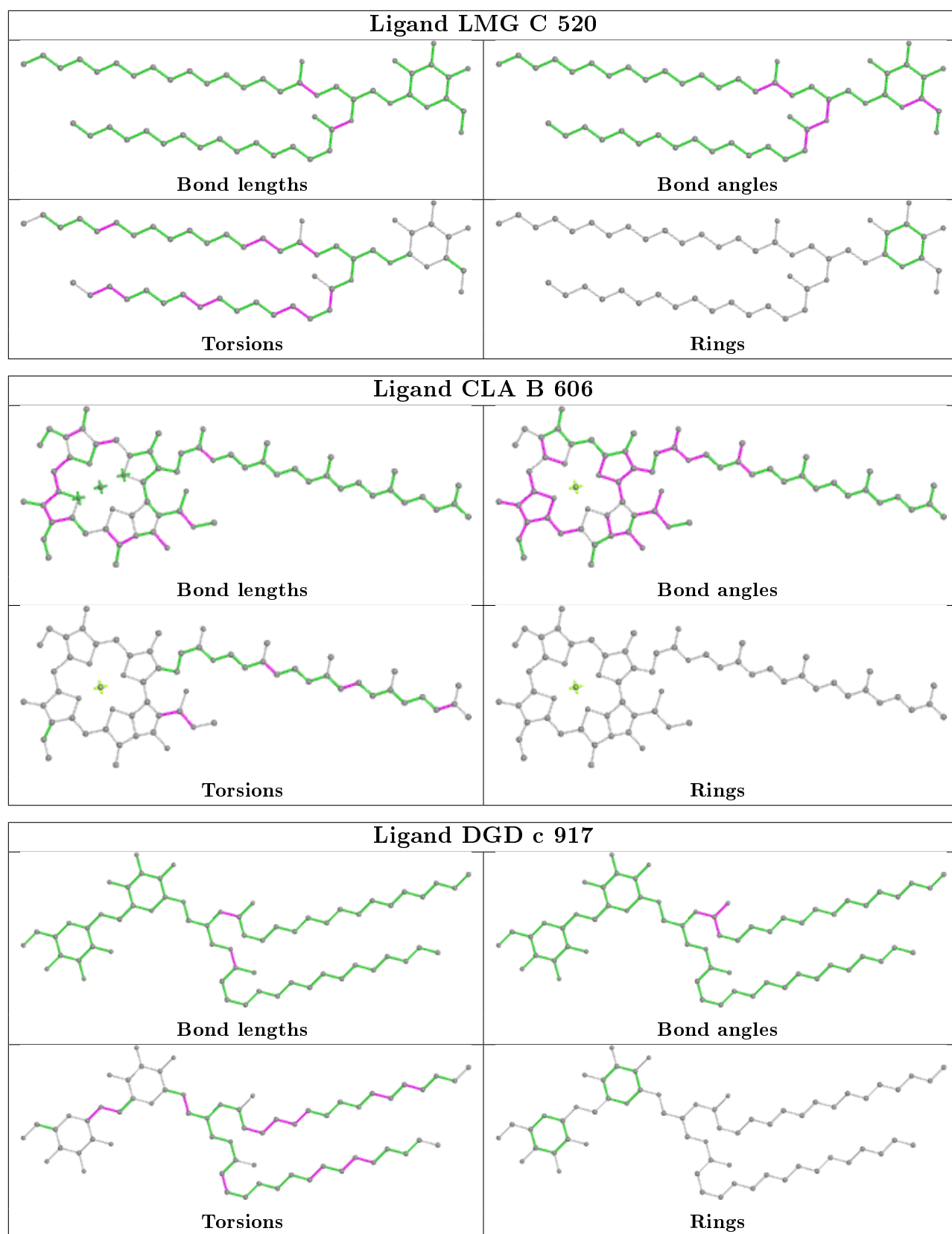
Ligand CLA c 911



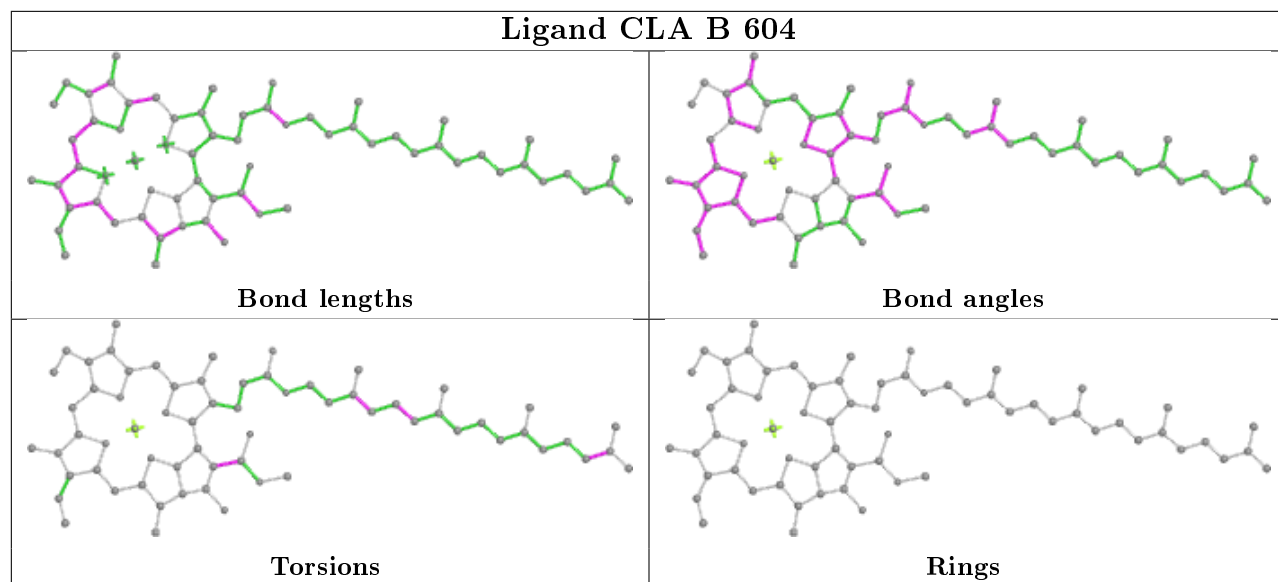




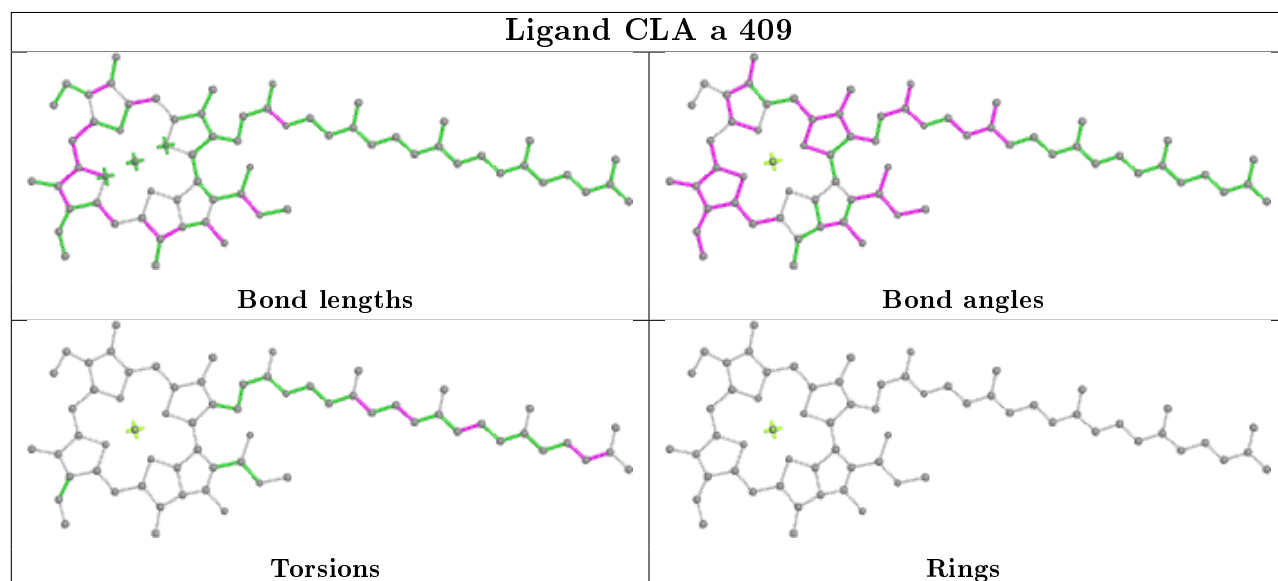




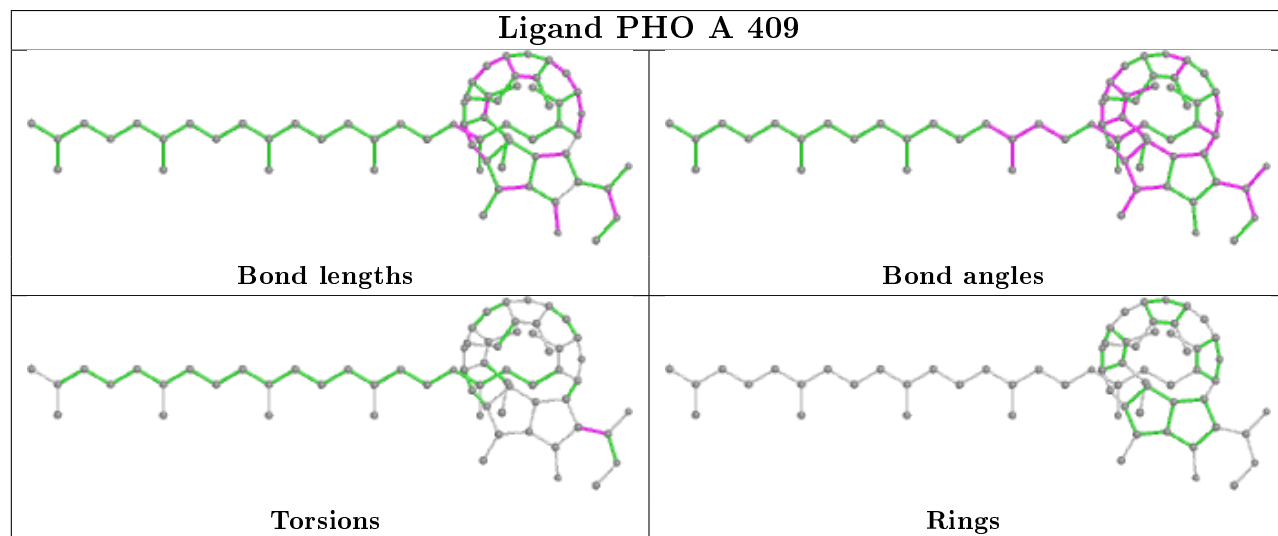
Ligand CLA B 604

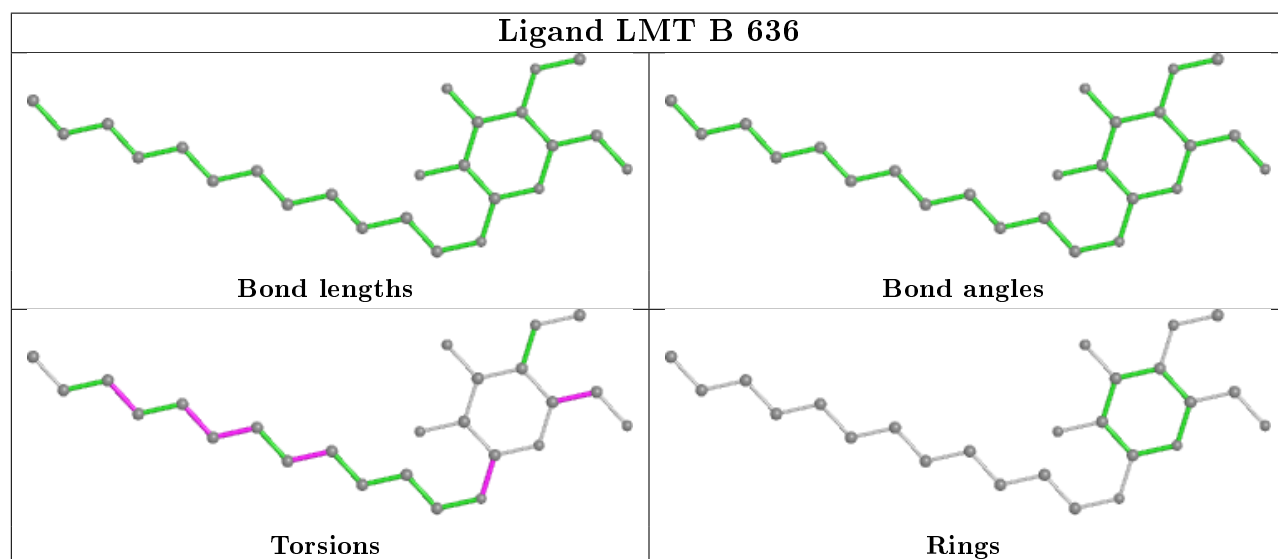
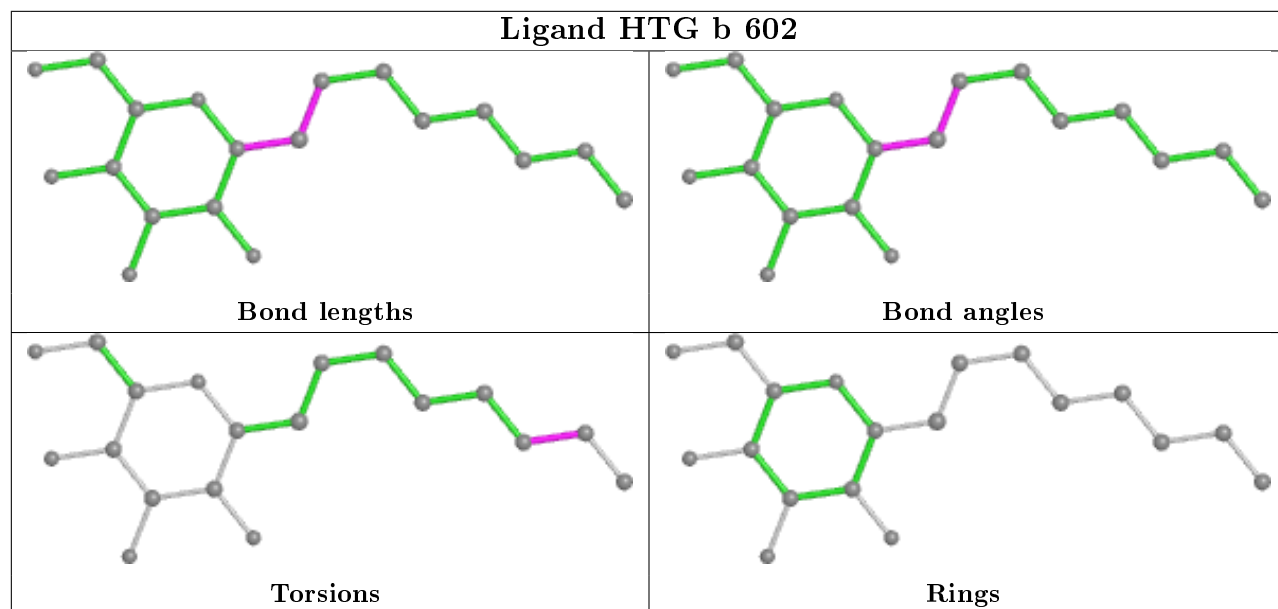
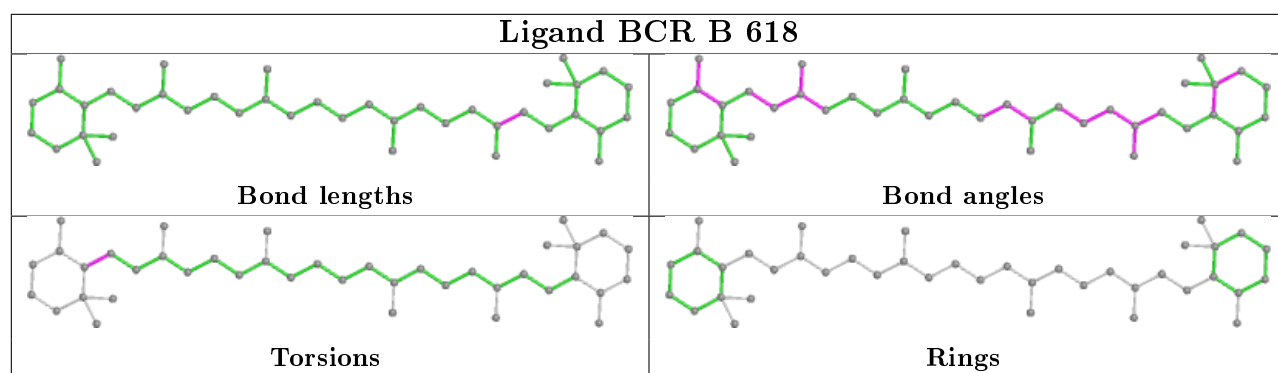


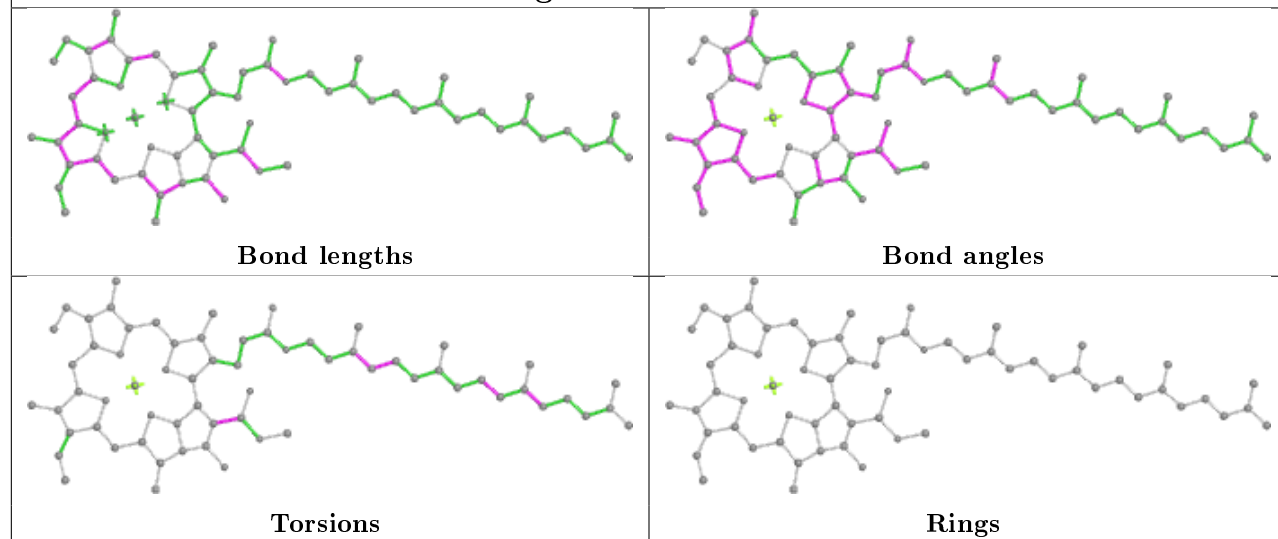
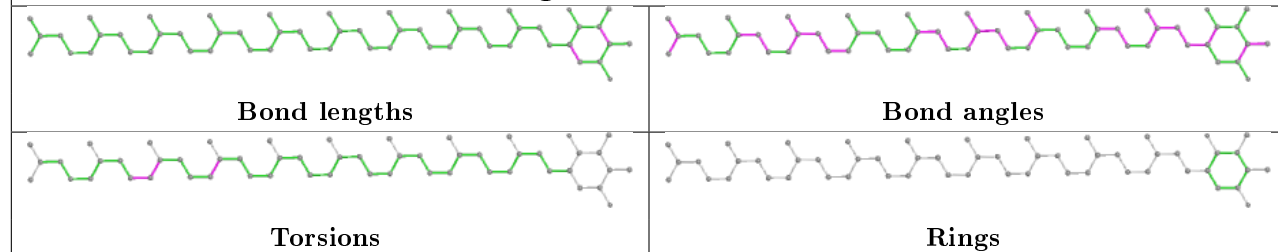
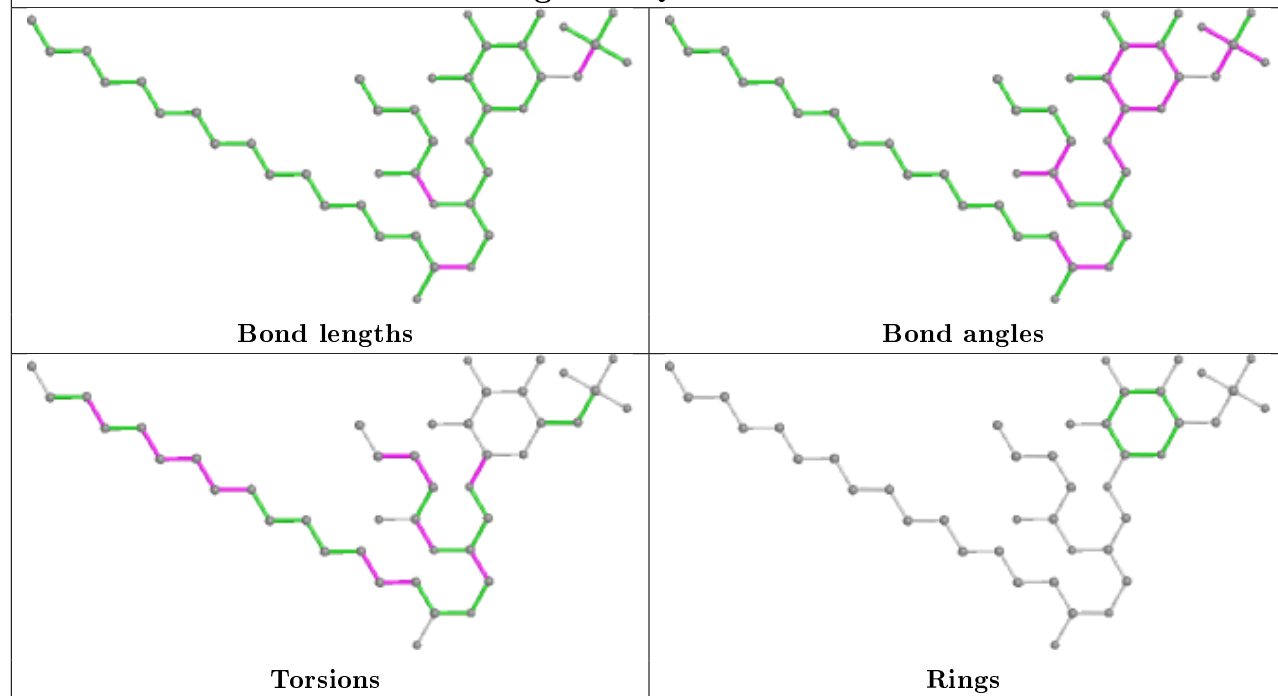
Ligand CLA a 409

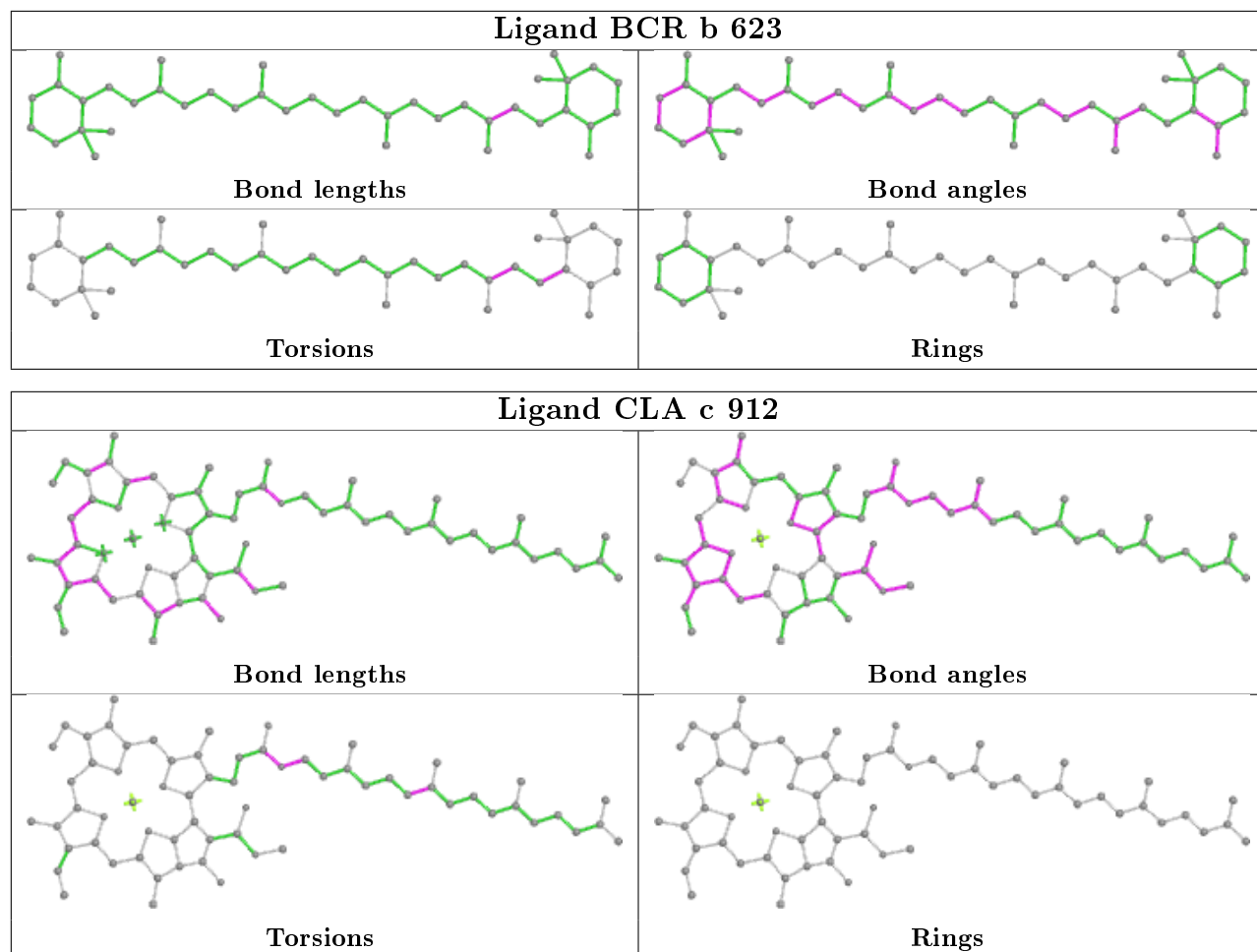


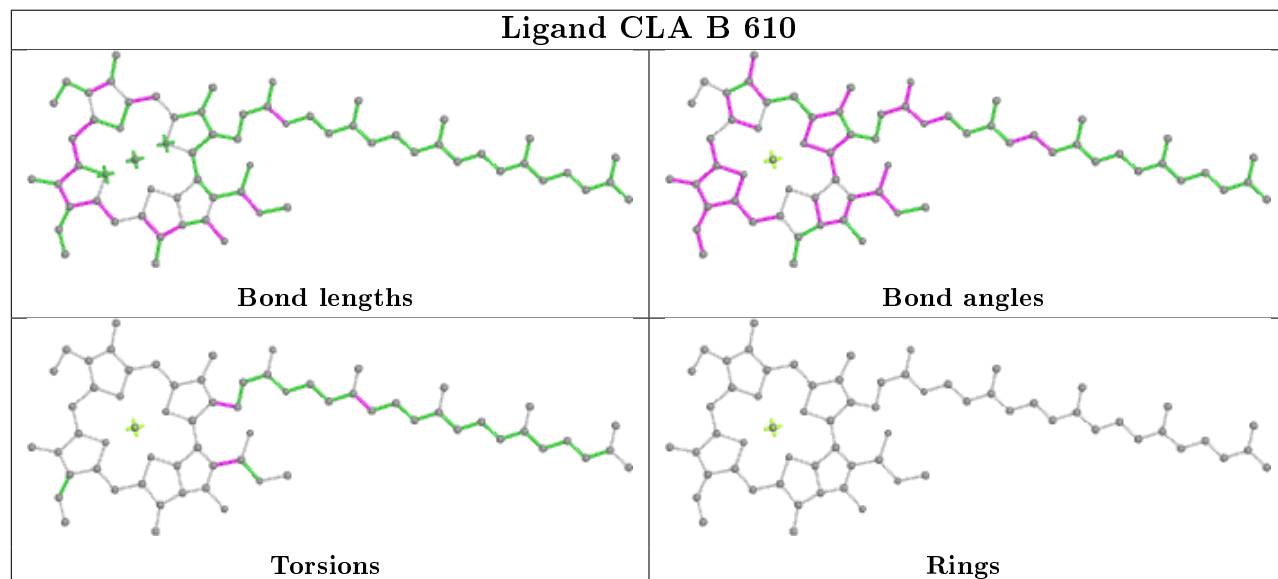
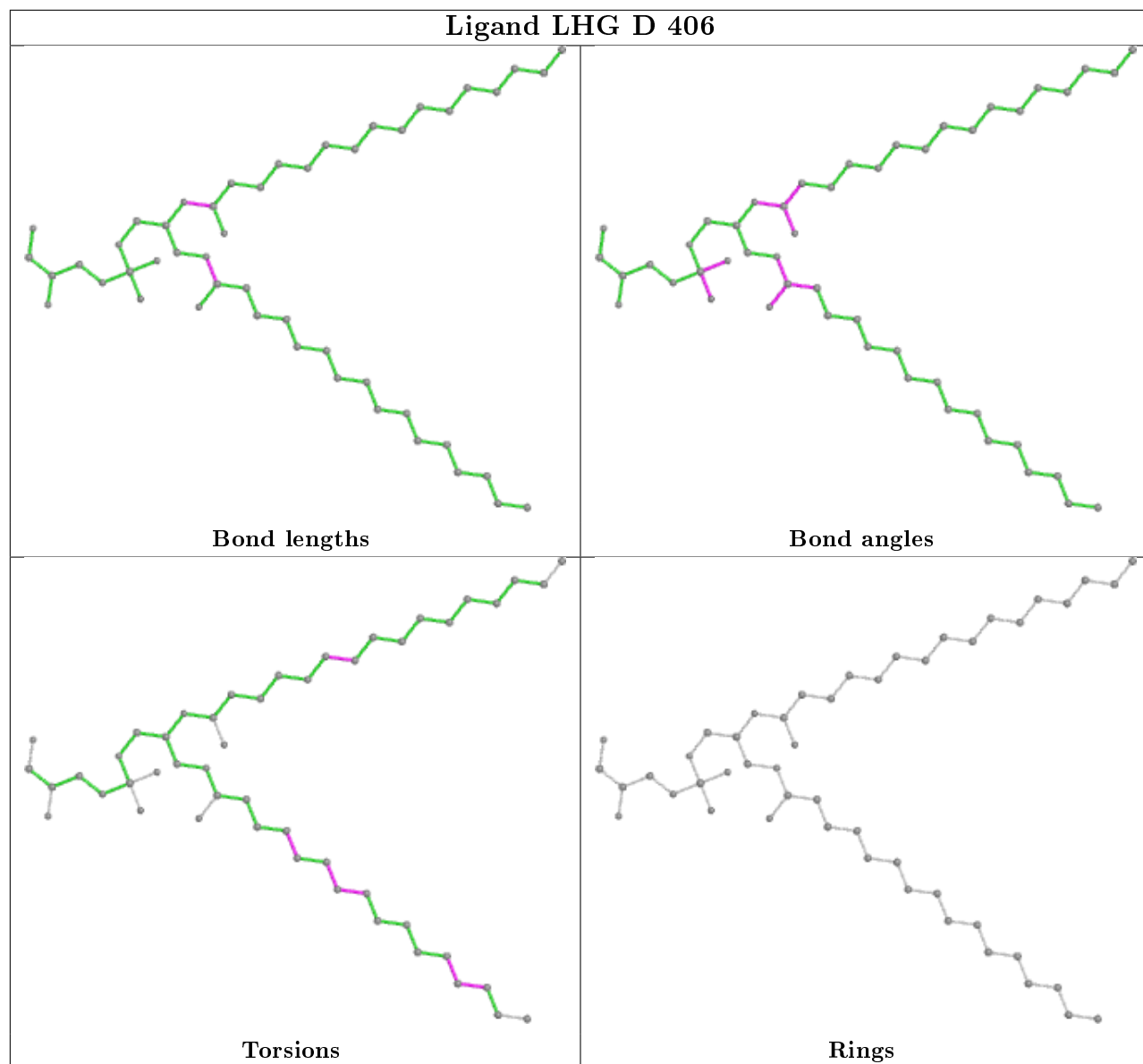
Ligand PHO A 409

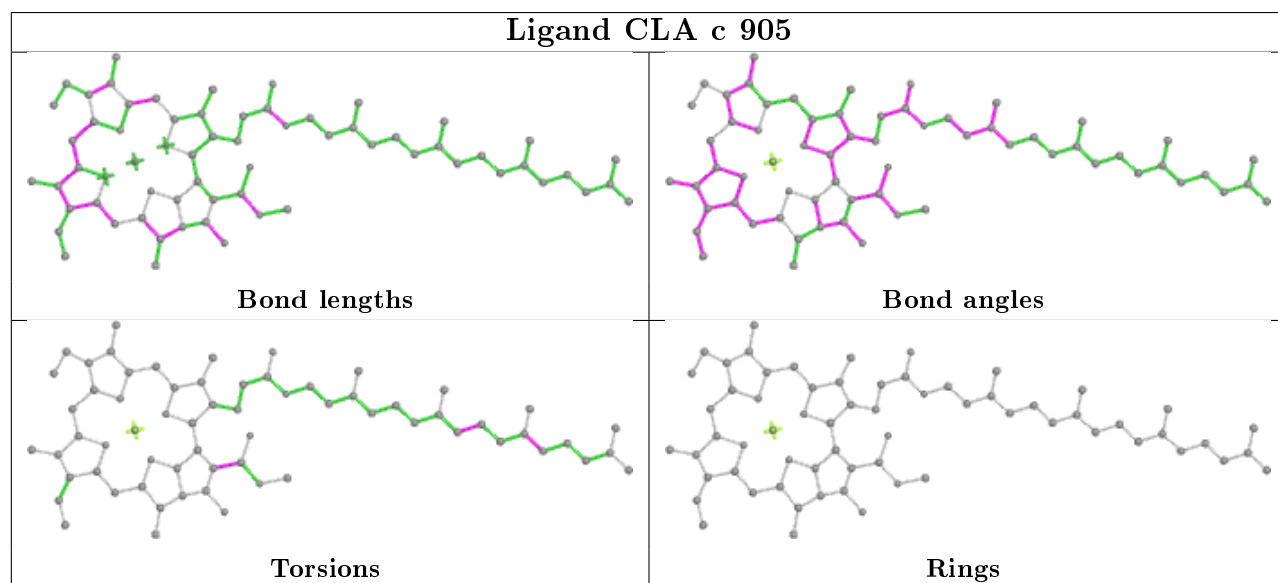
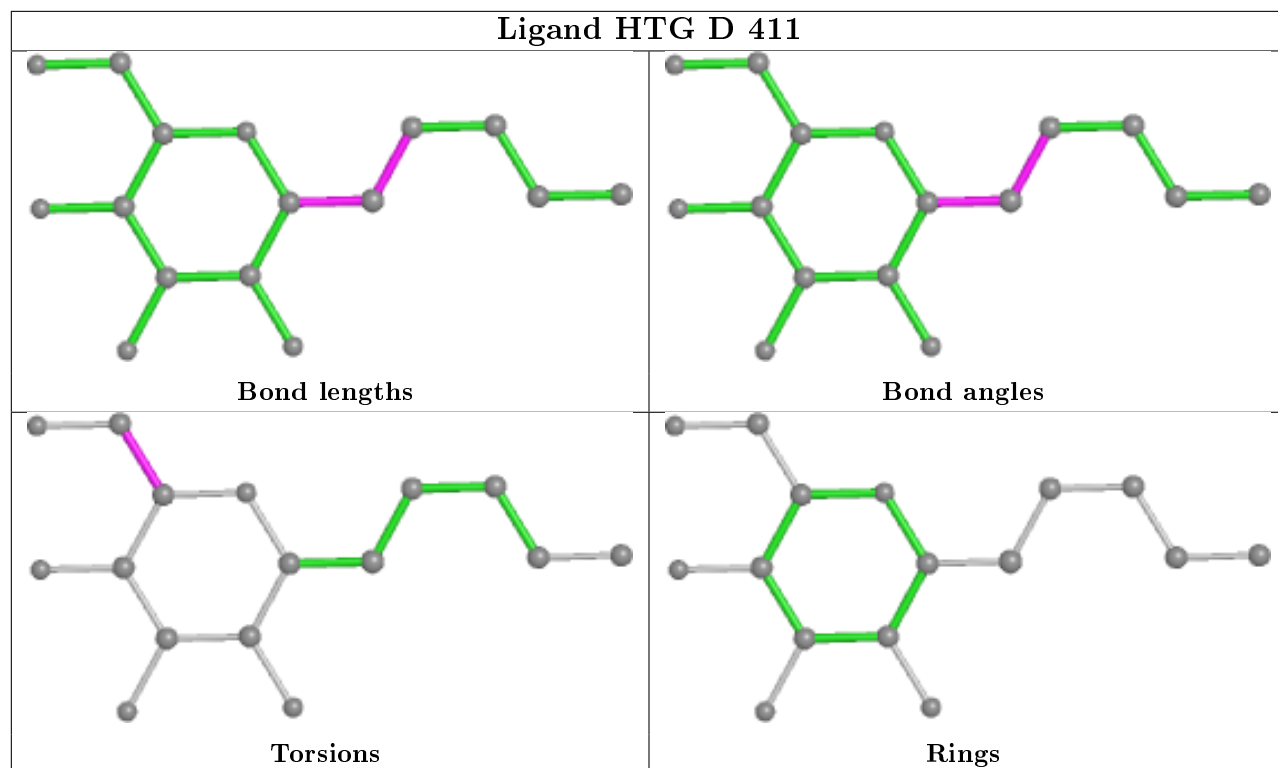


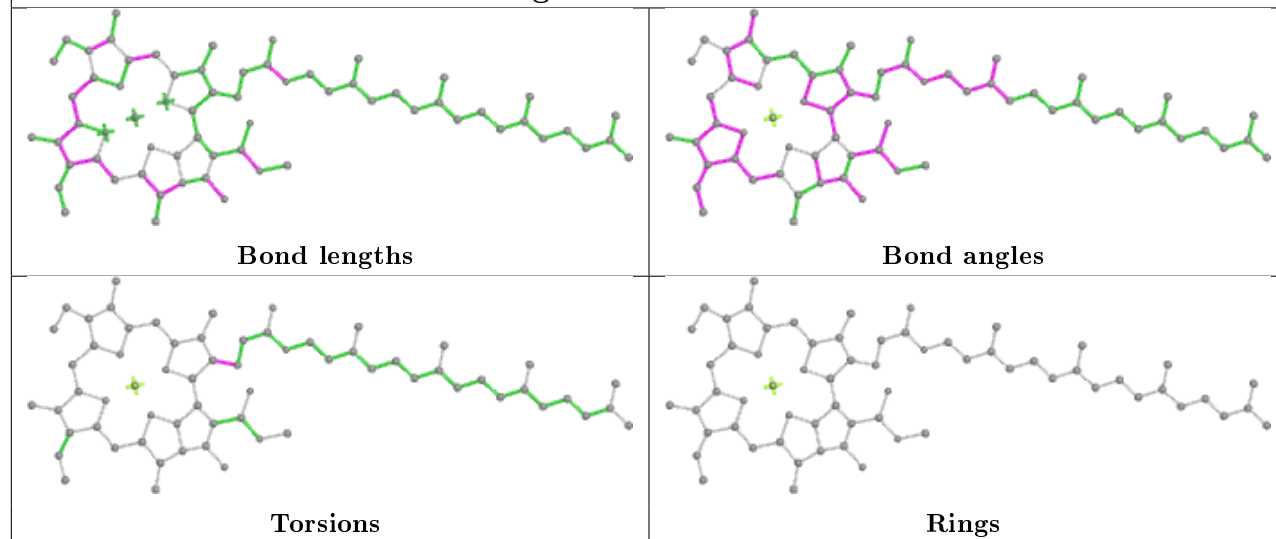
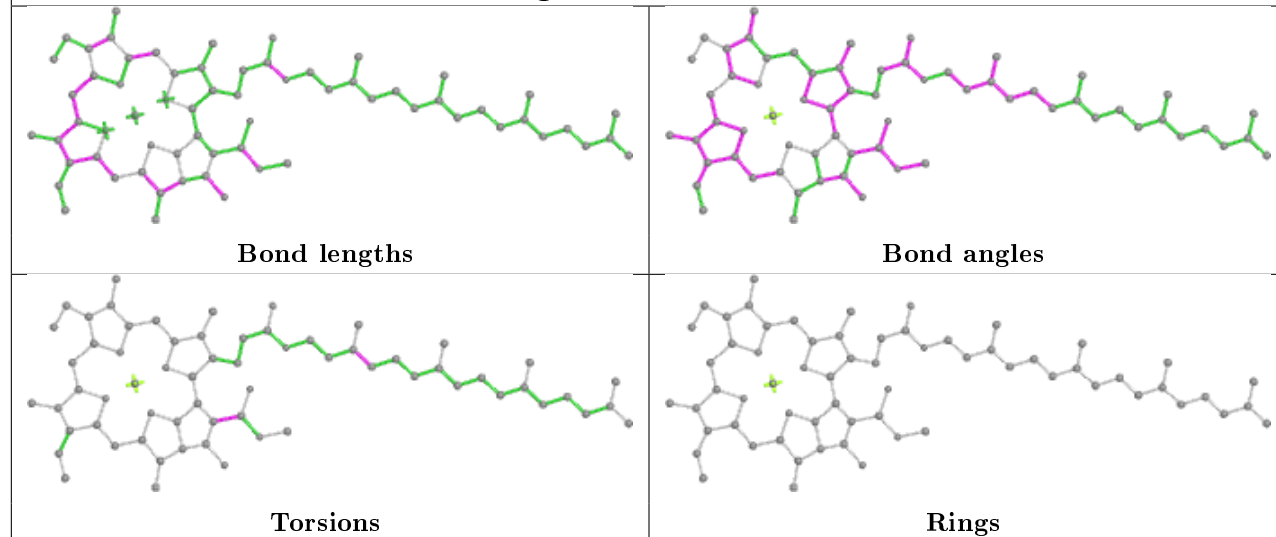


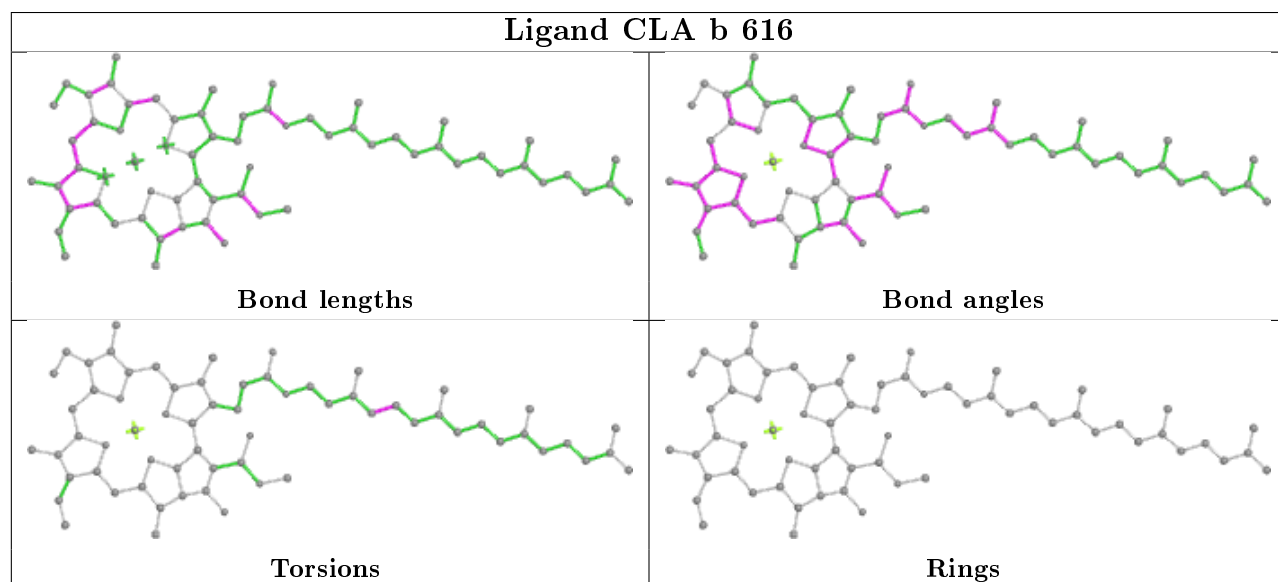
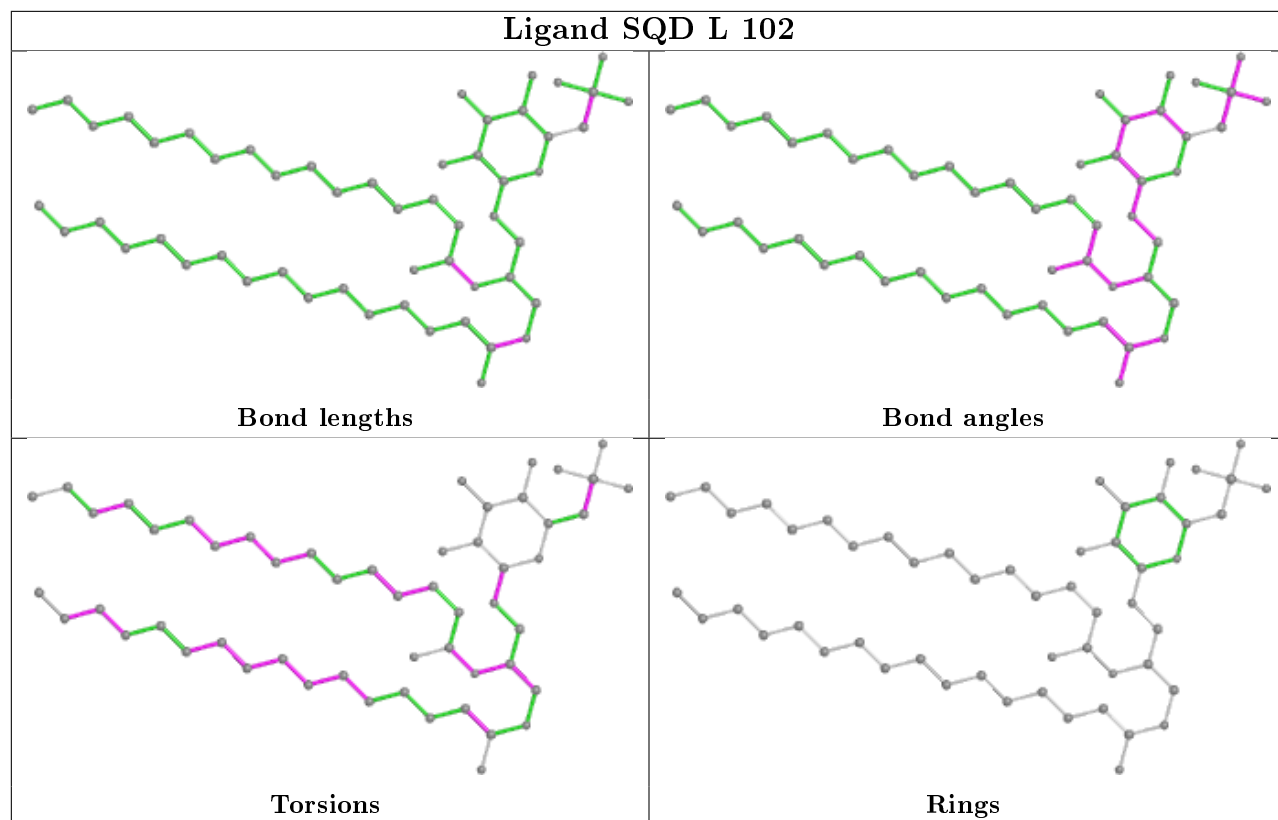
Ligand CLA d 403**Ligand PL9 D 404****Ligand SQD F 101**



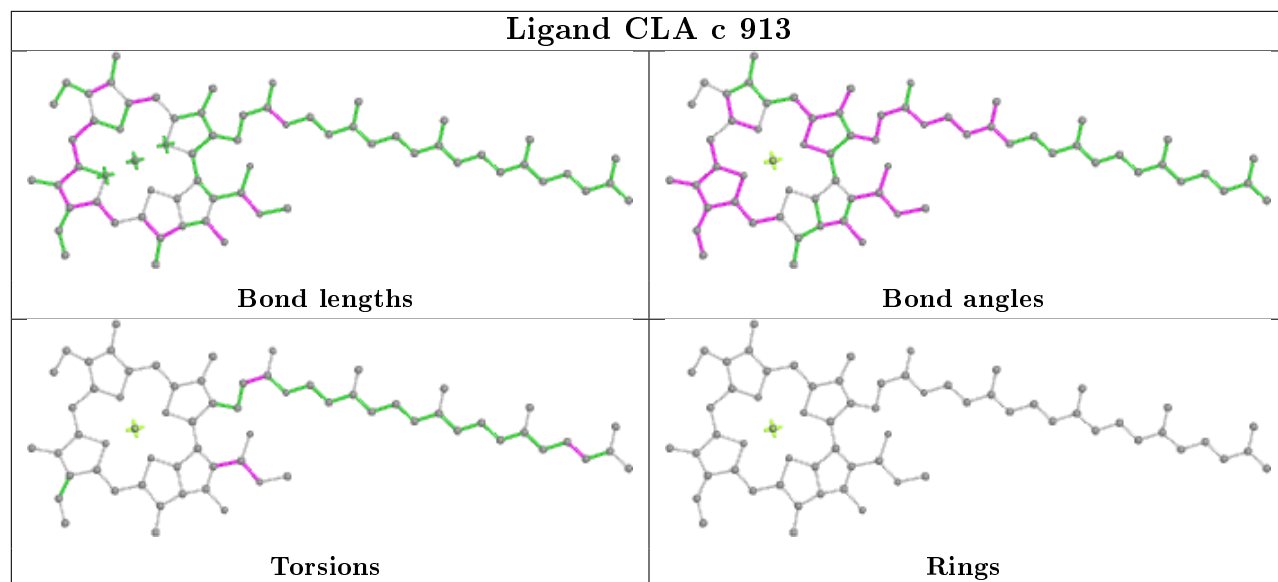




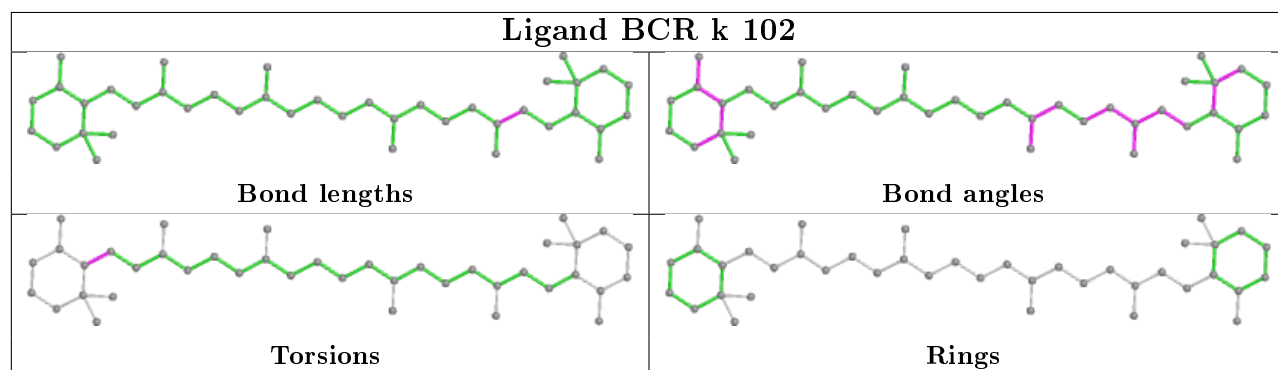
Ligand CLA C 514**Ligand CLA b 613**



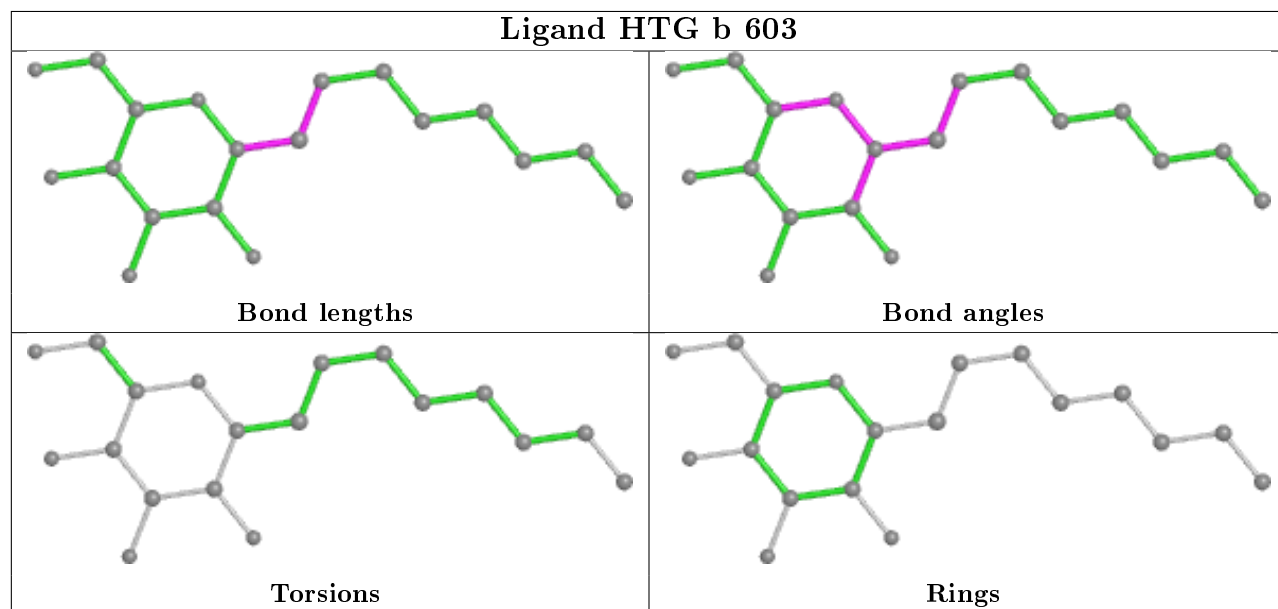
Ligand CLA c 913



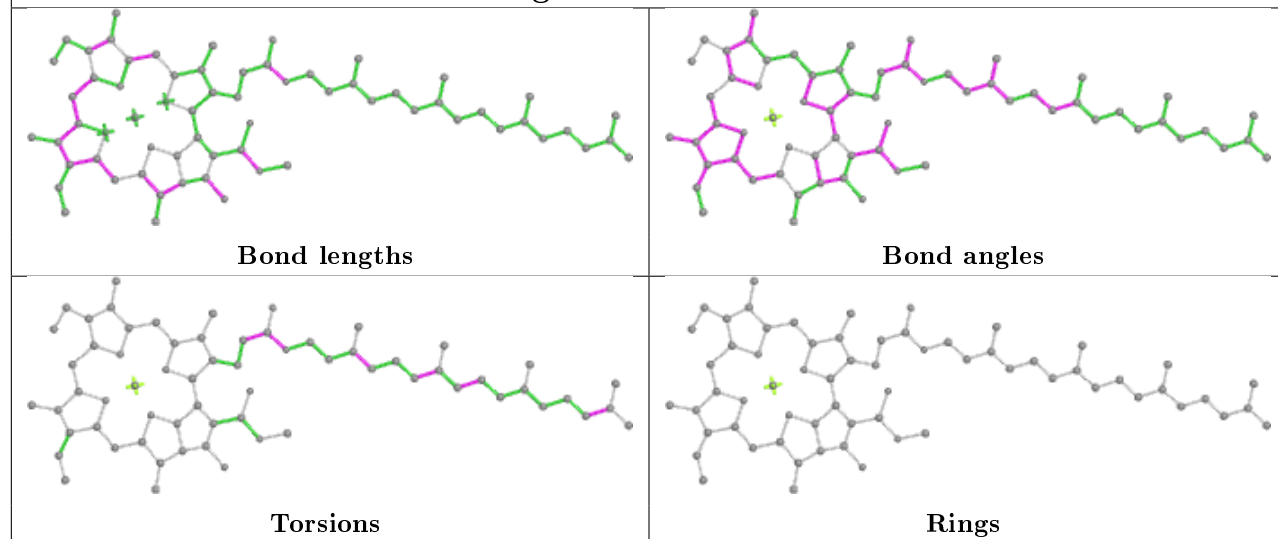
Ligand BCR k 102



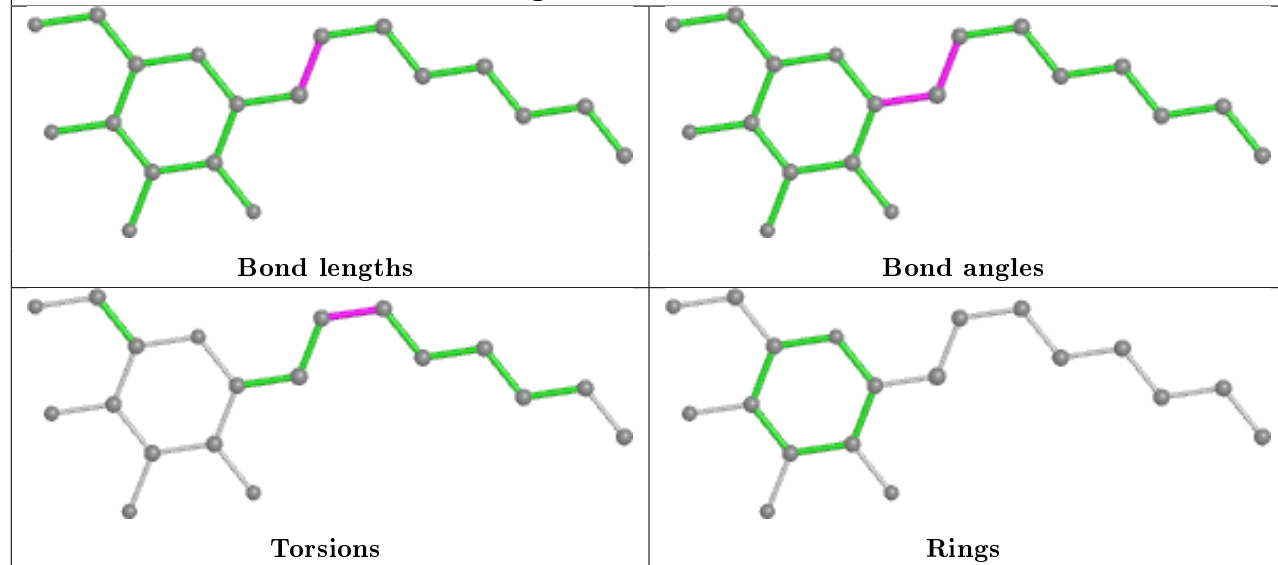
Ligand HTG b 603



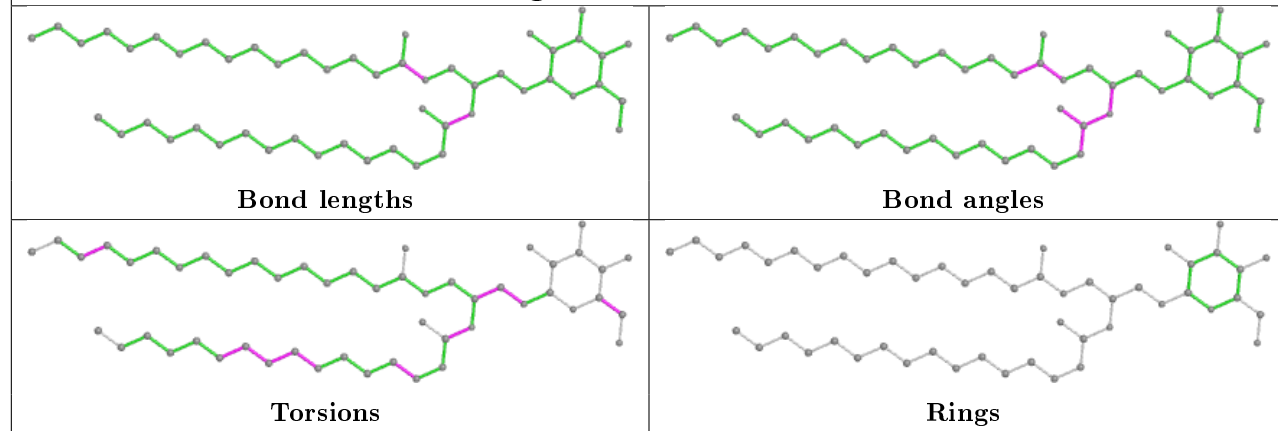
Ligand CLA C 511

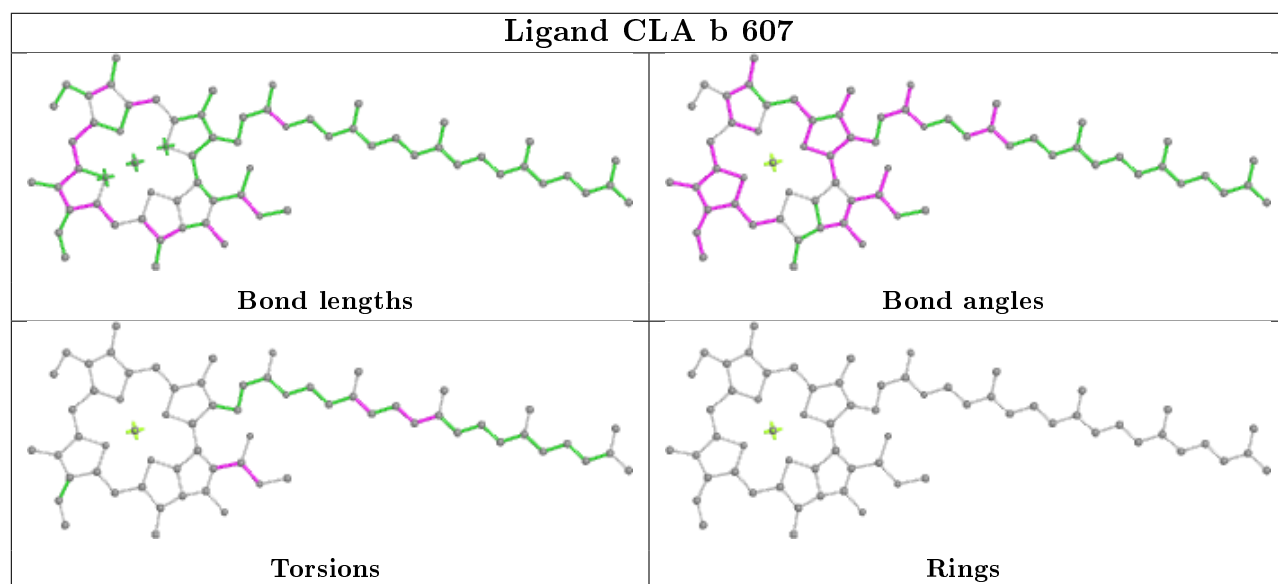
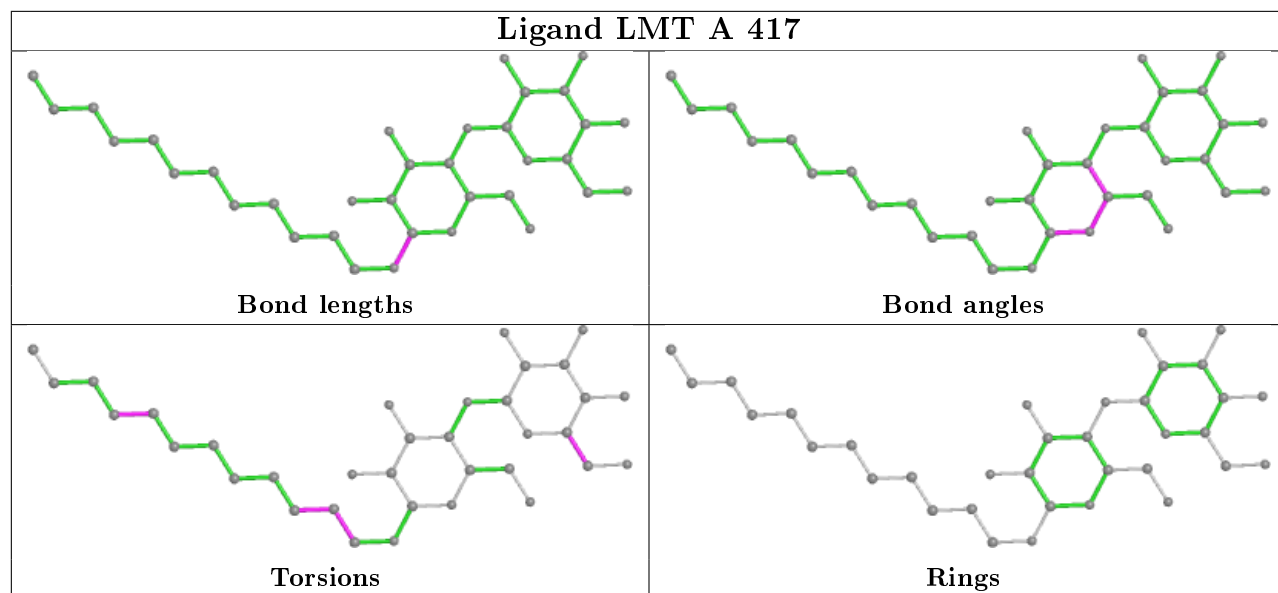


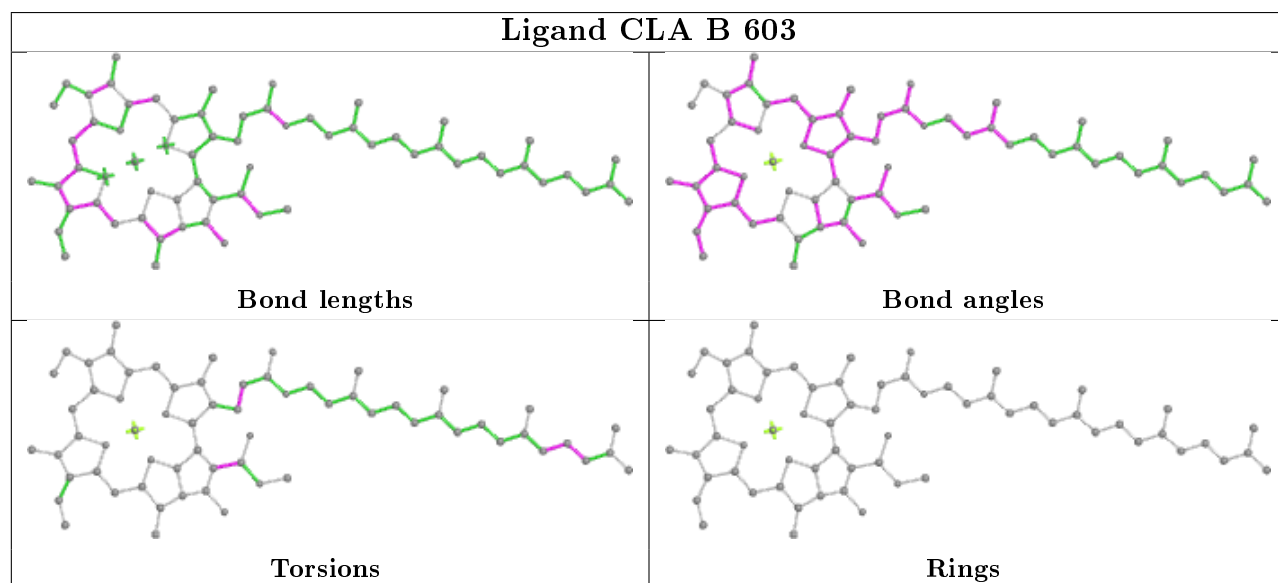
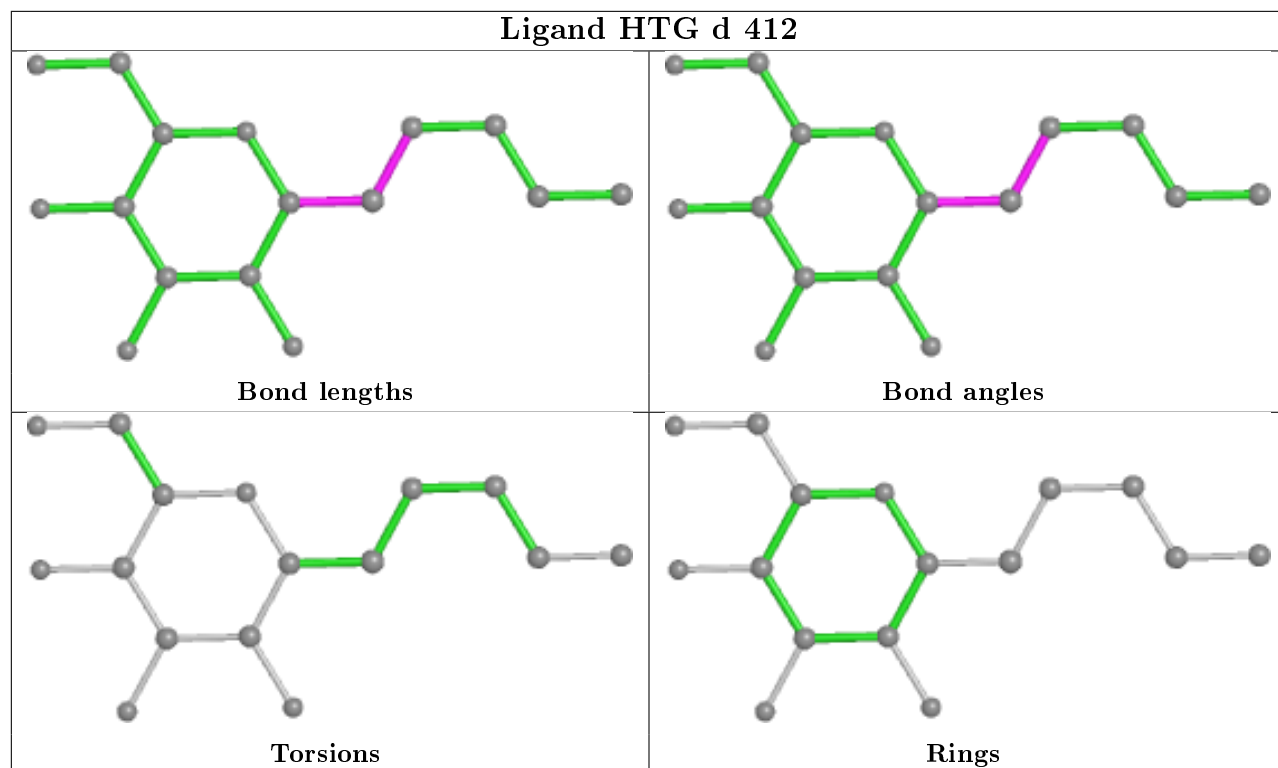
Ligand HTG B 624

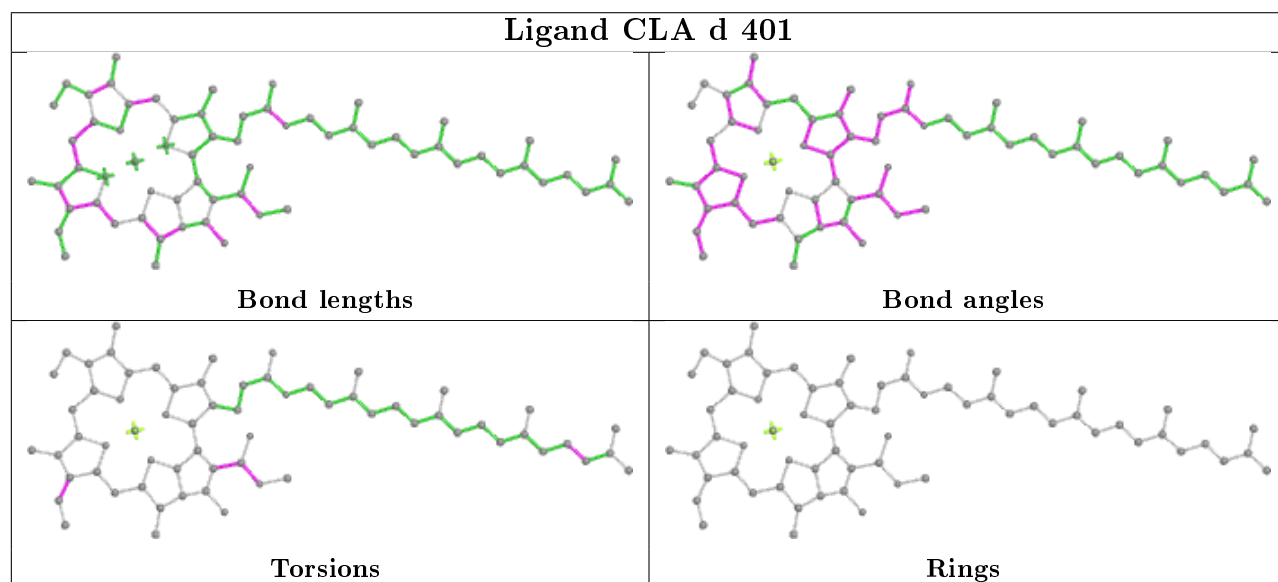
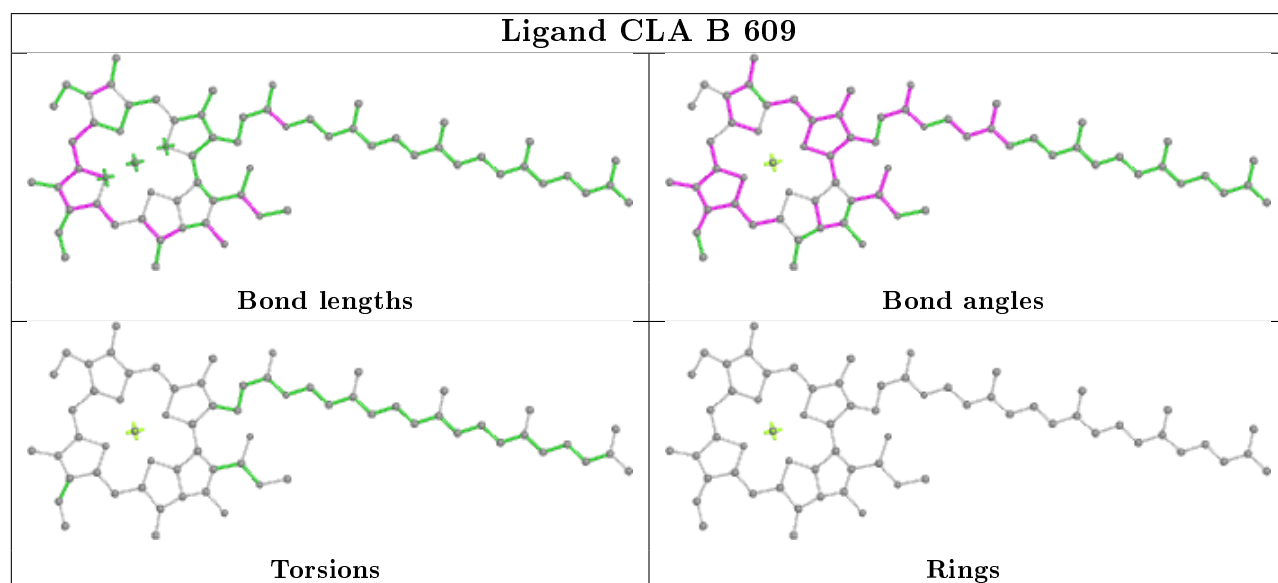
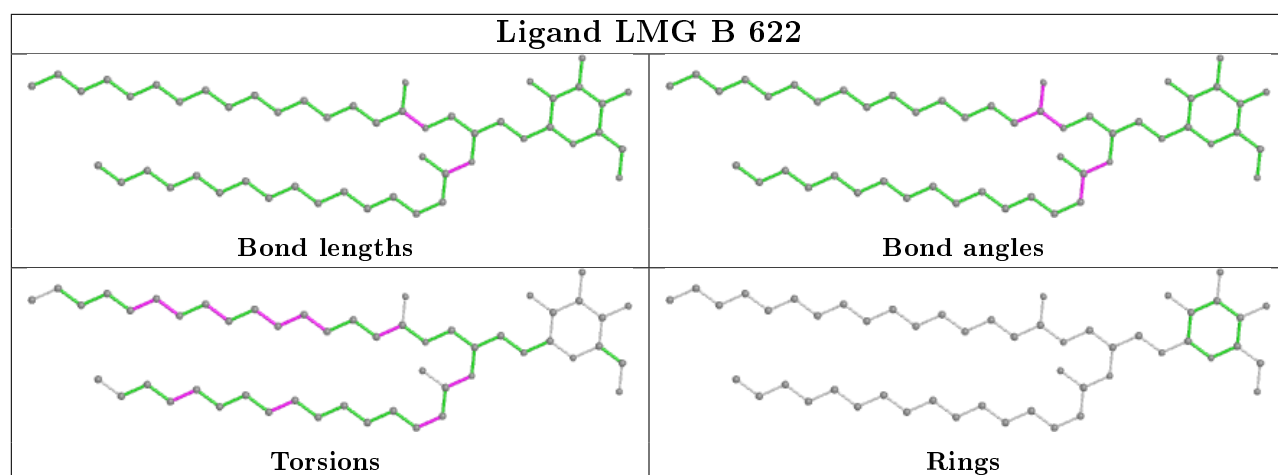


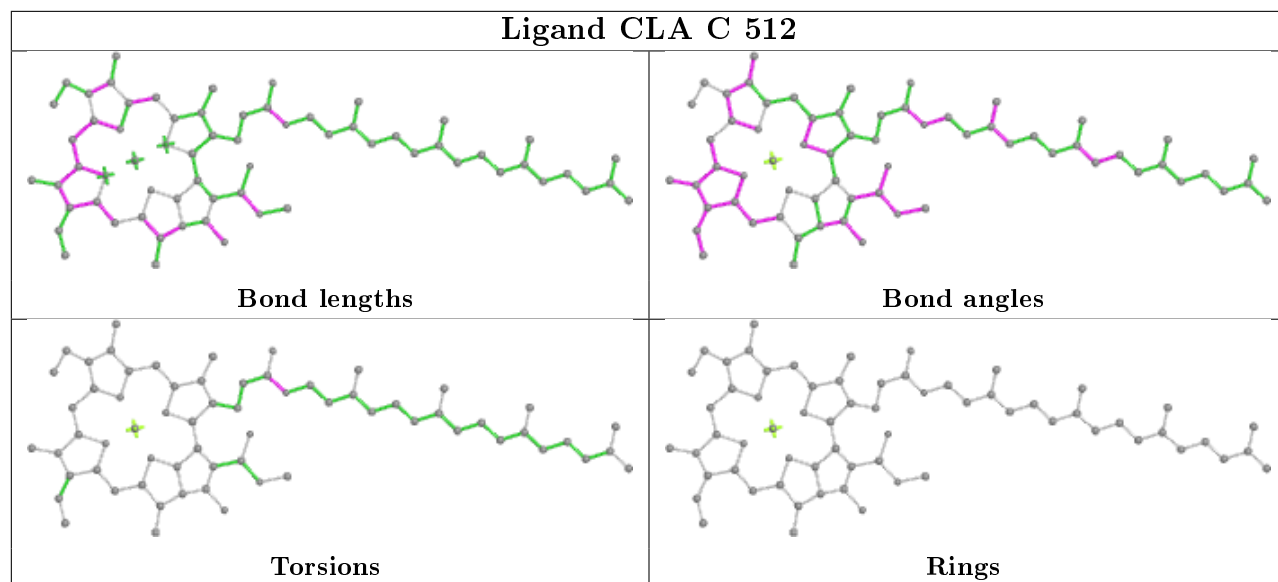
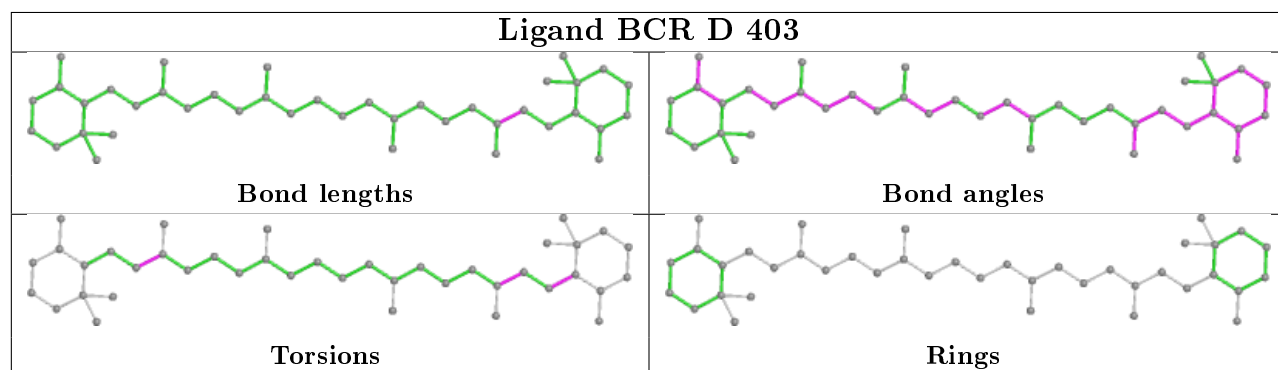
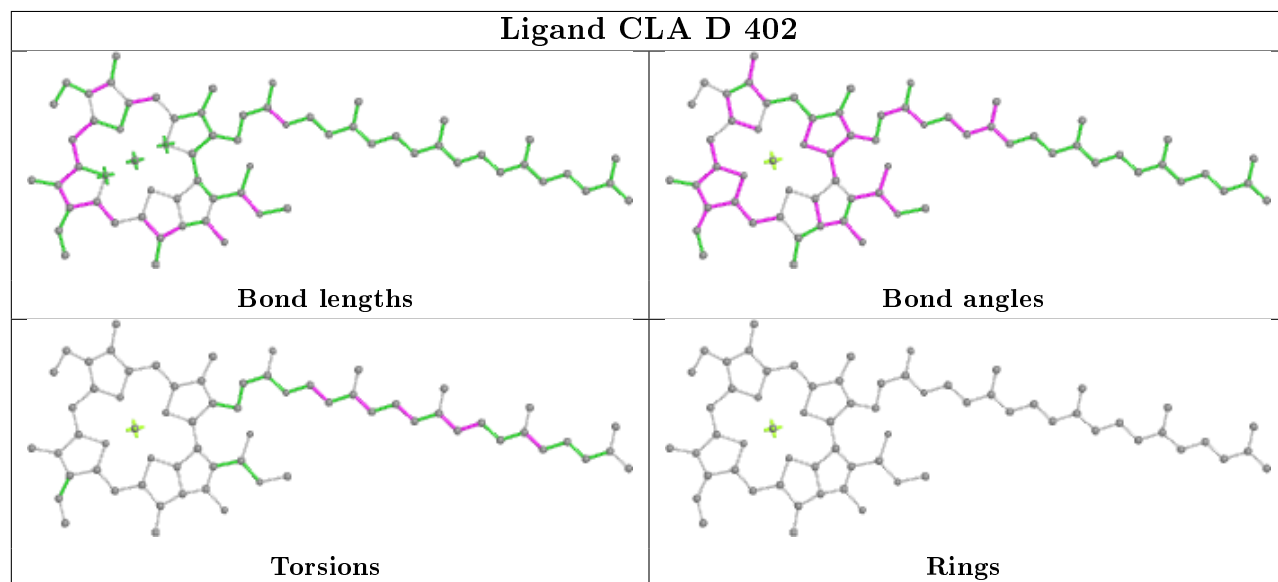
Ligand LMG C 521

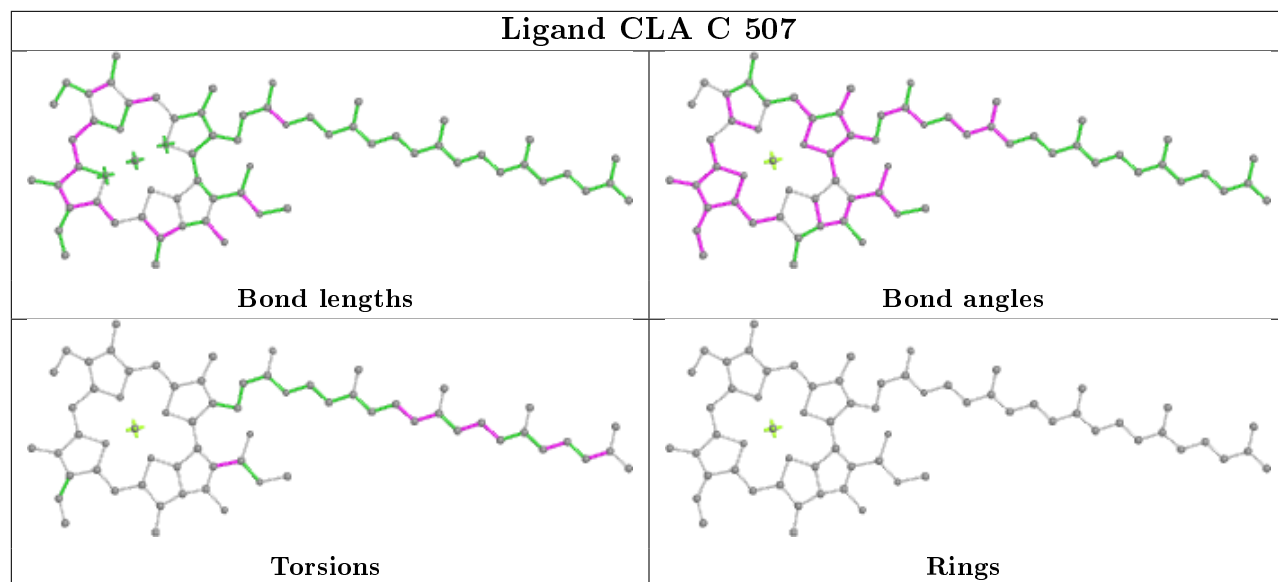
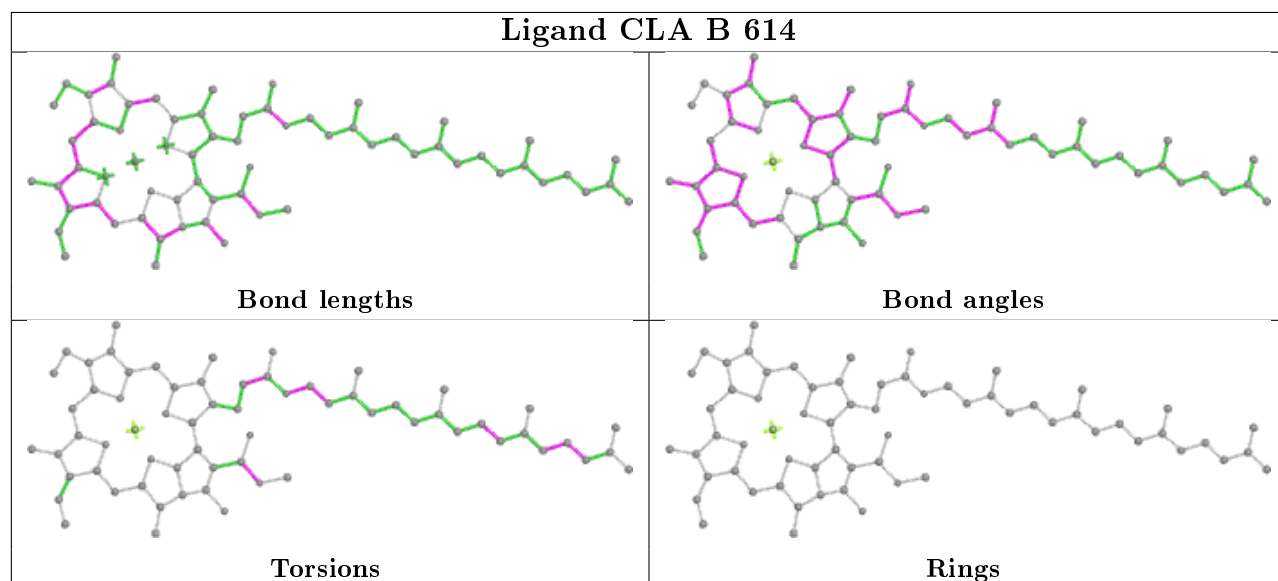
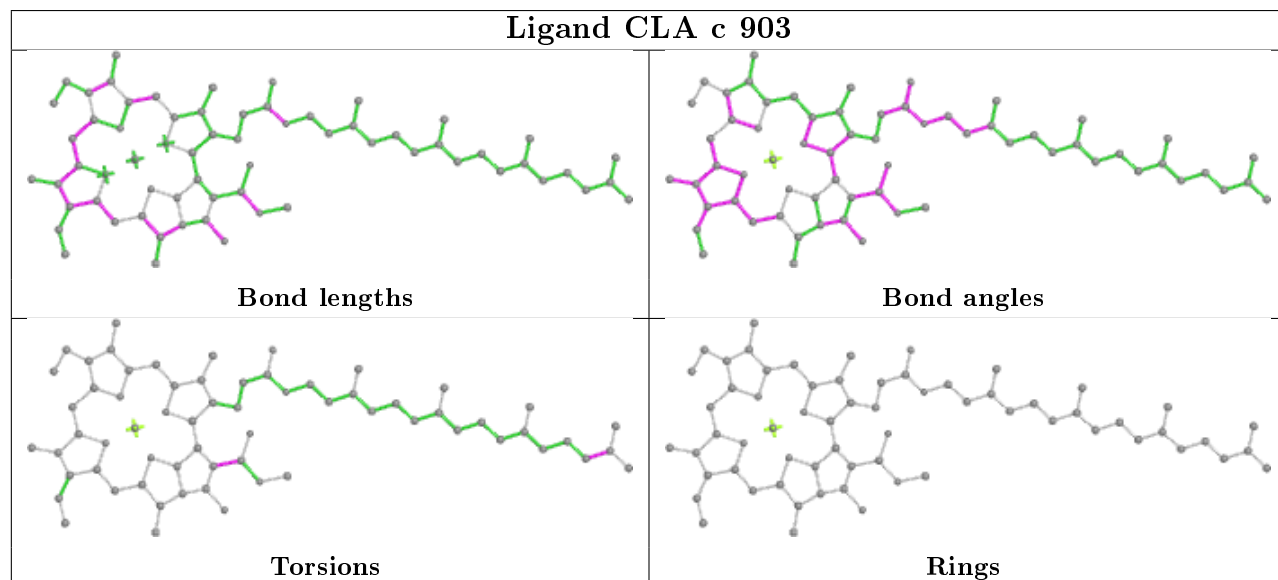




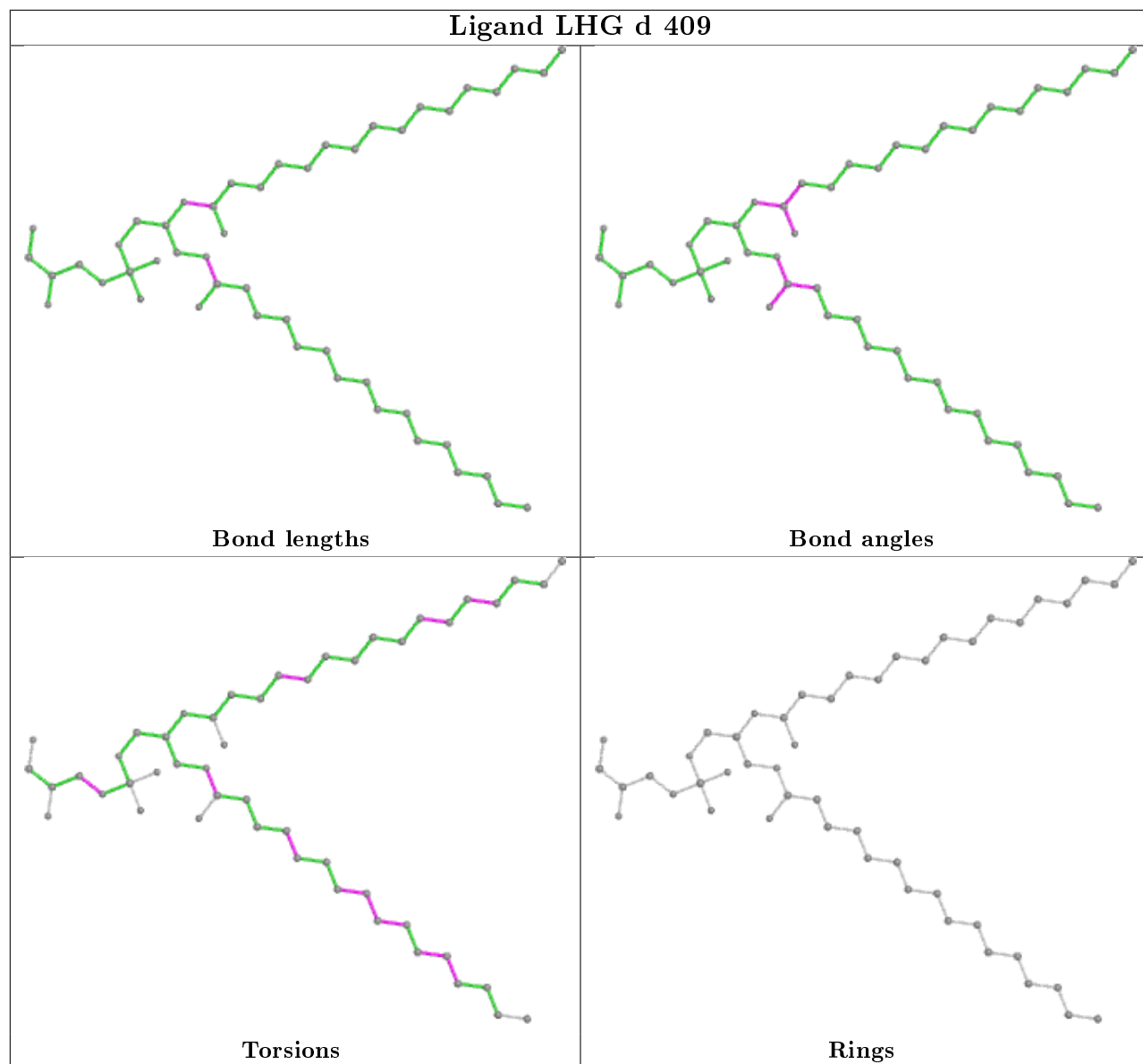




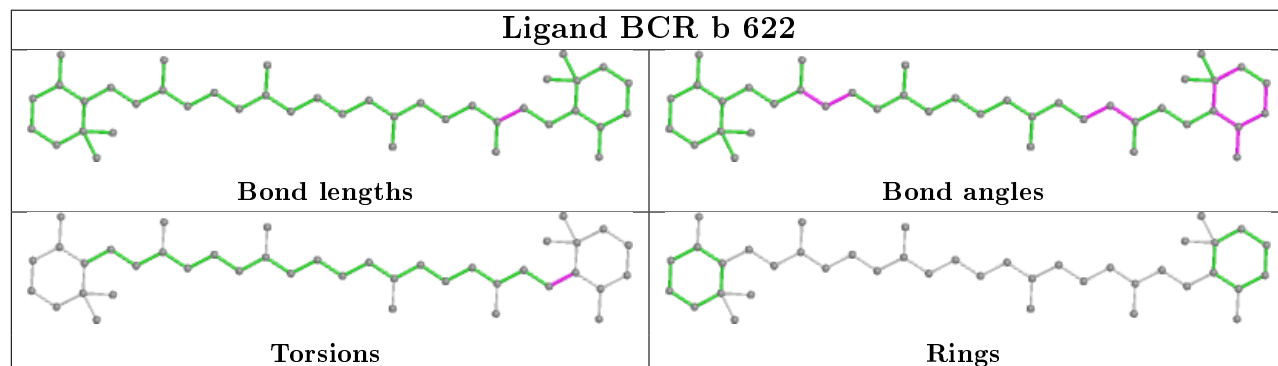
Ligand CLA C 512**Ligand BCR D 403****Ligand CLA D 402**

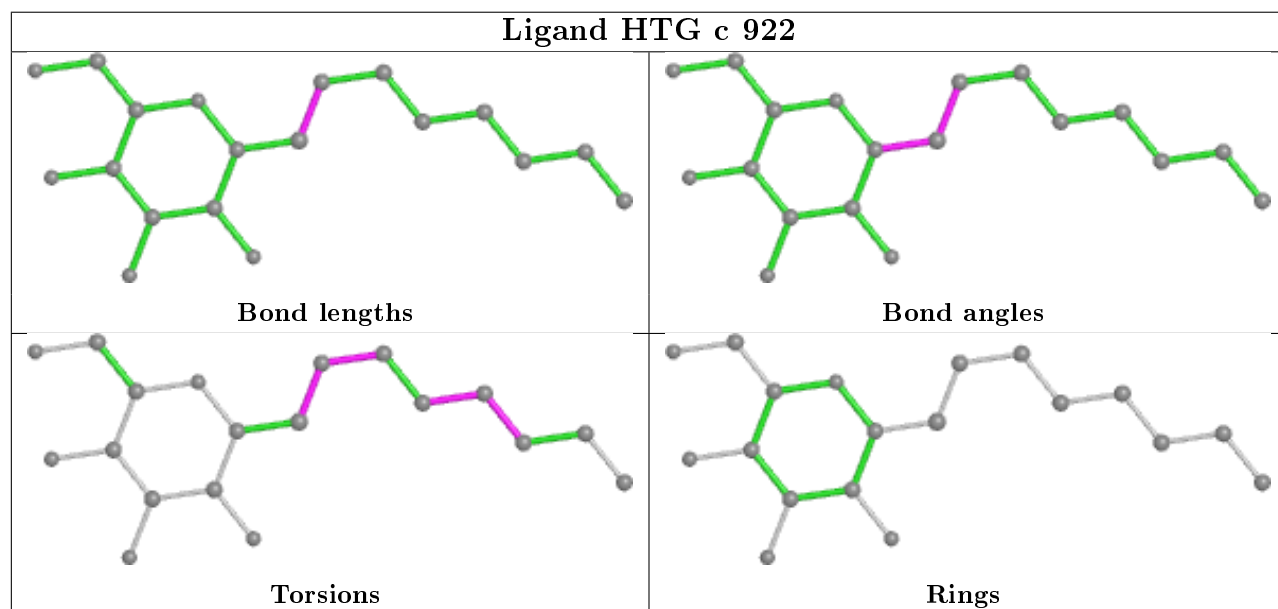
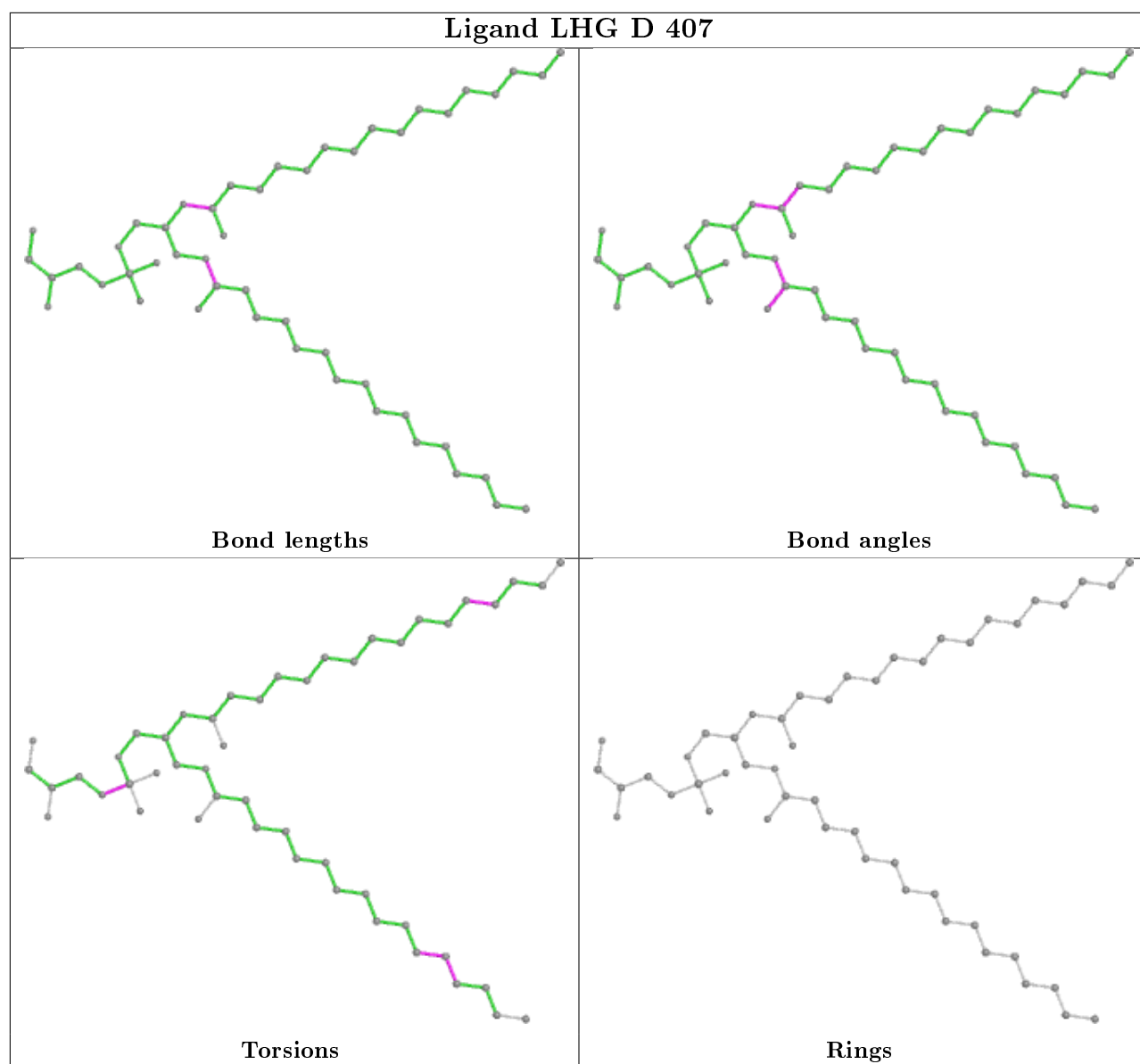
Ligand CLA C 507**Ligand CLA B 614****Ligand CLA c 903**

Ligand LHG d 409

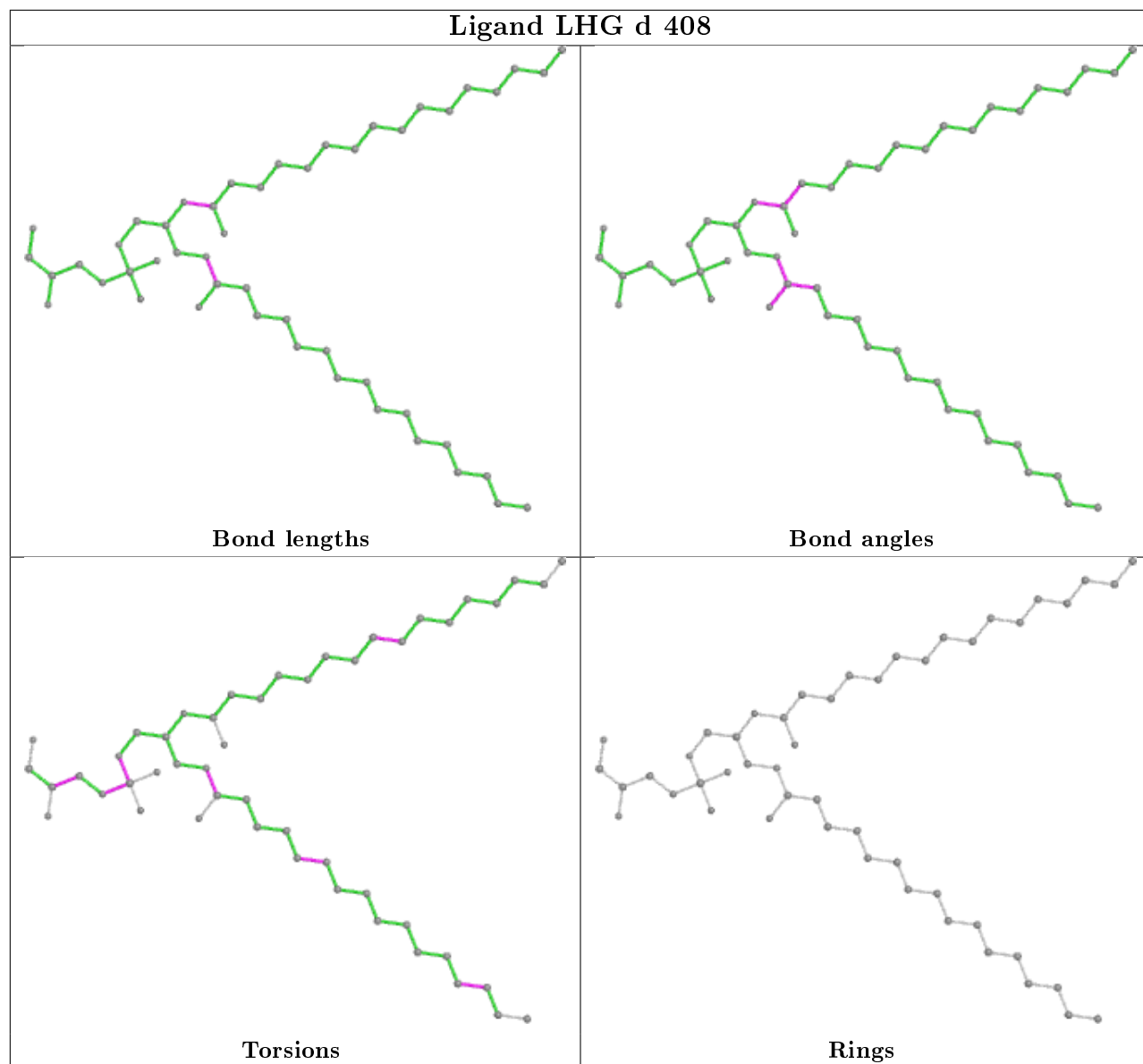


Ligand BCR b 622

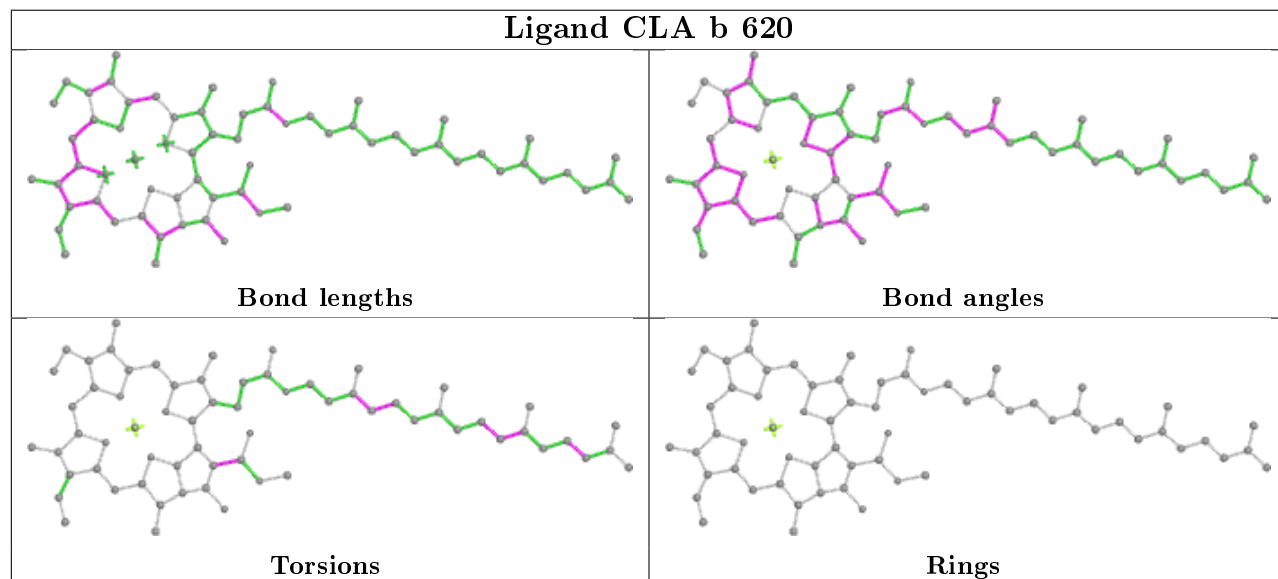


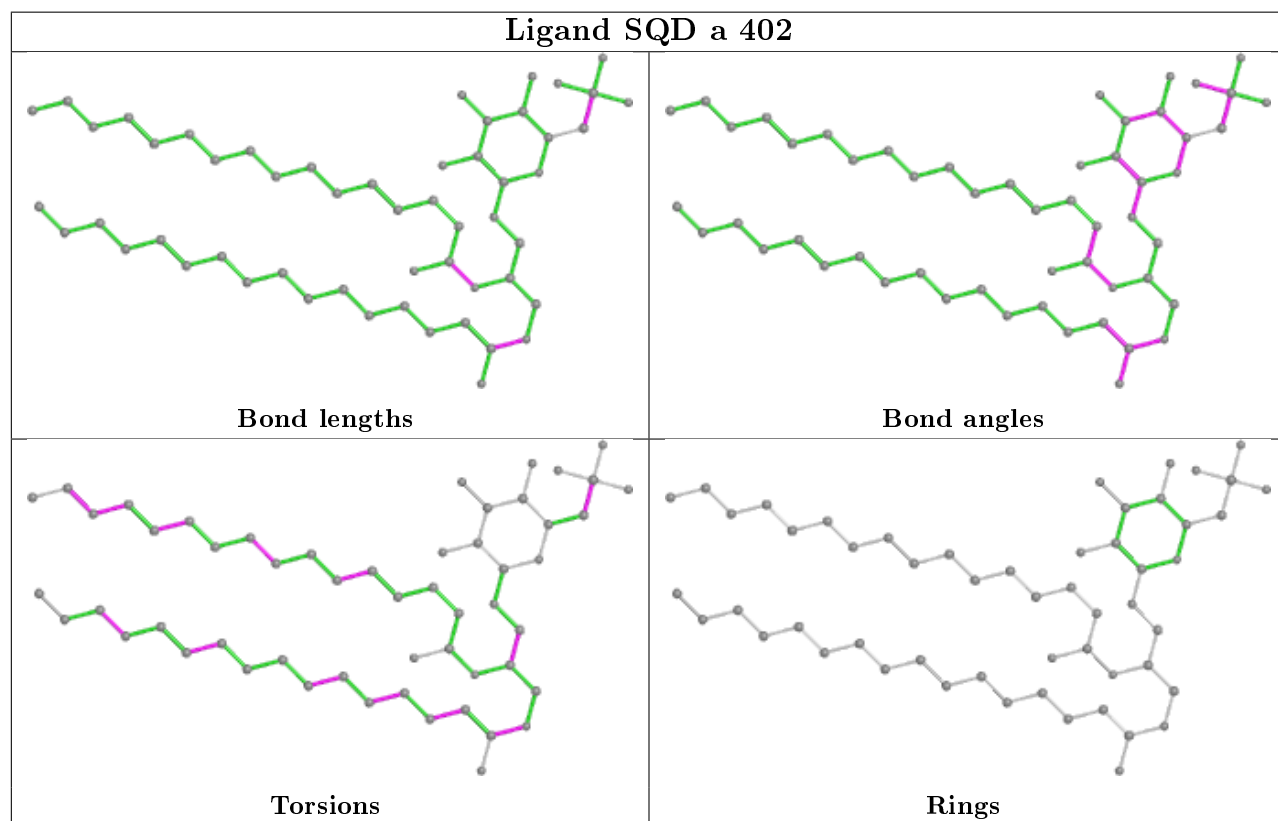
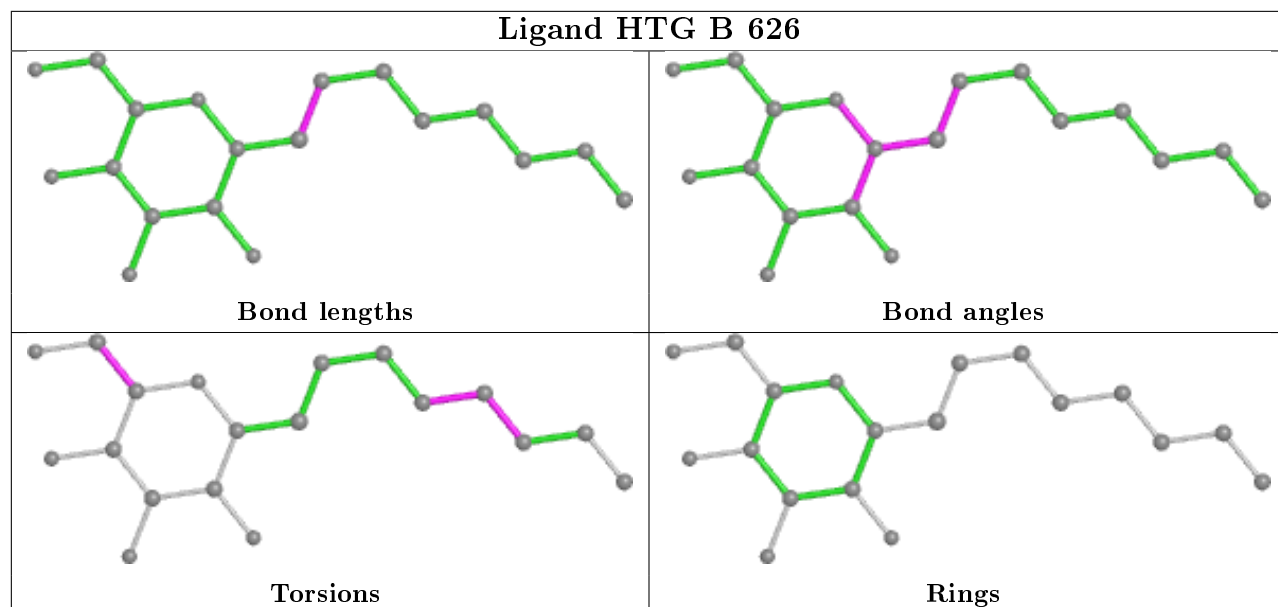


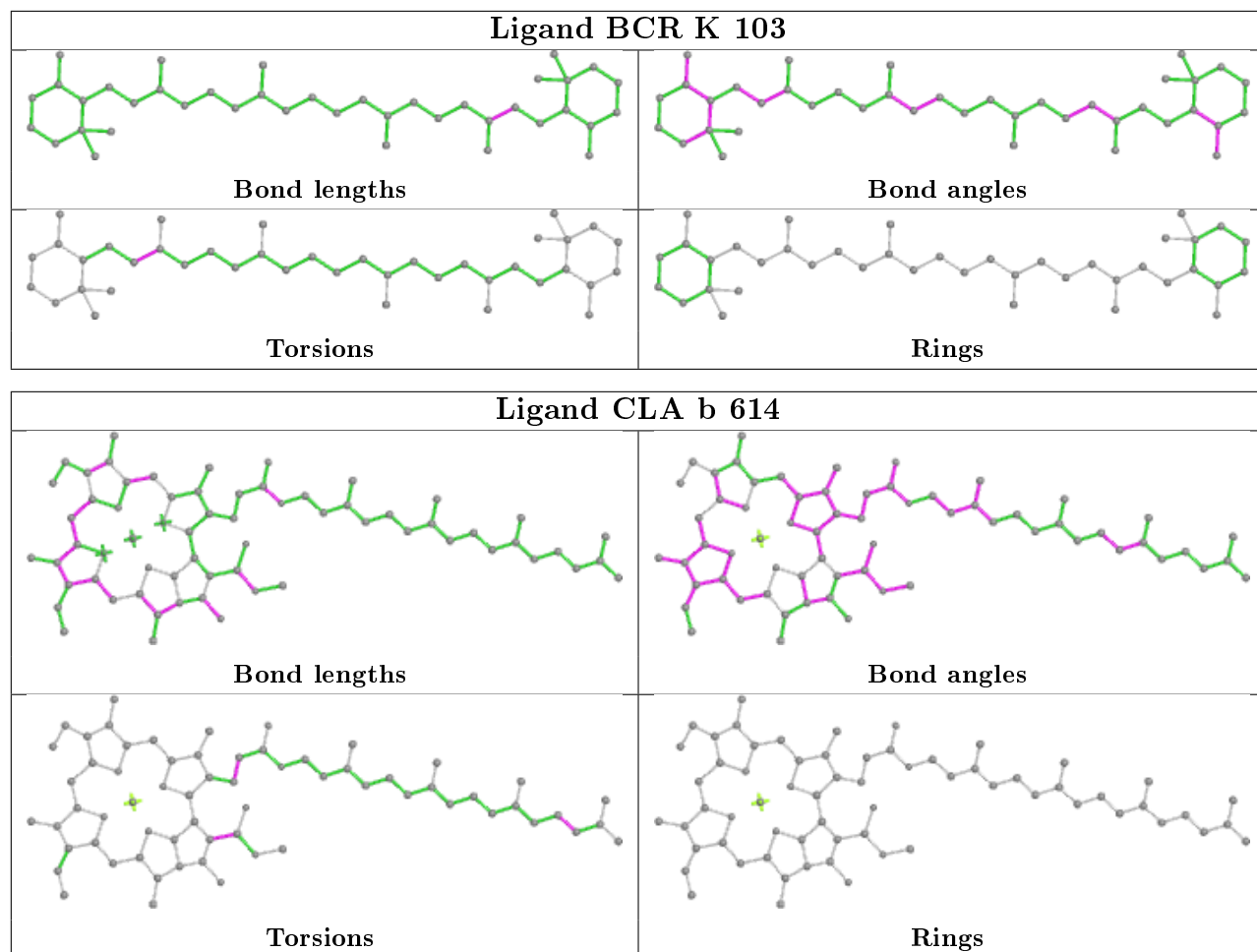
Ligand LHG d 408



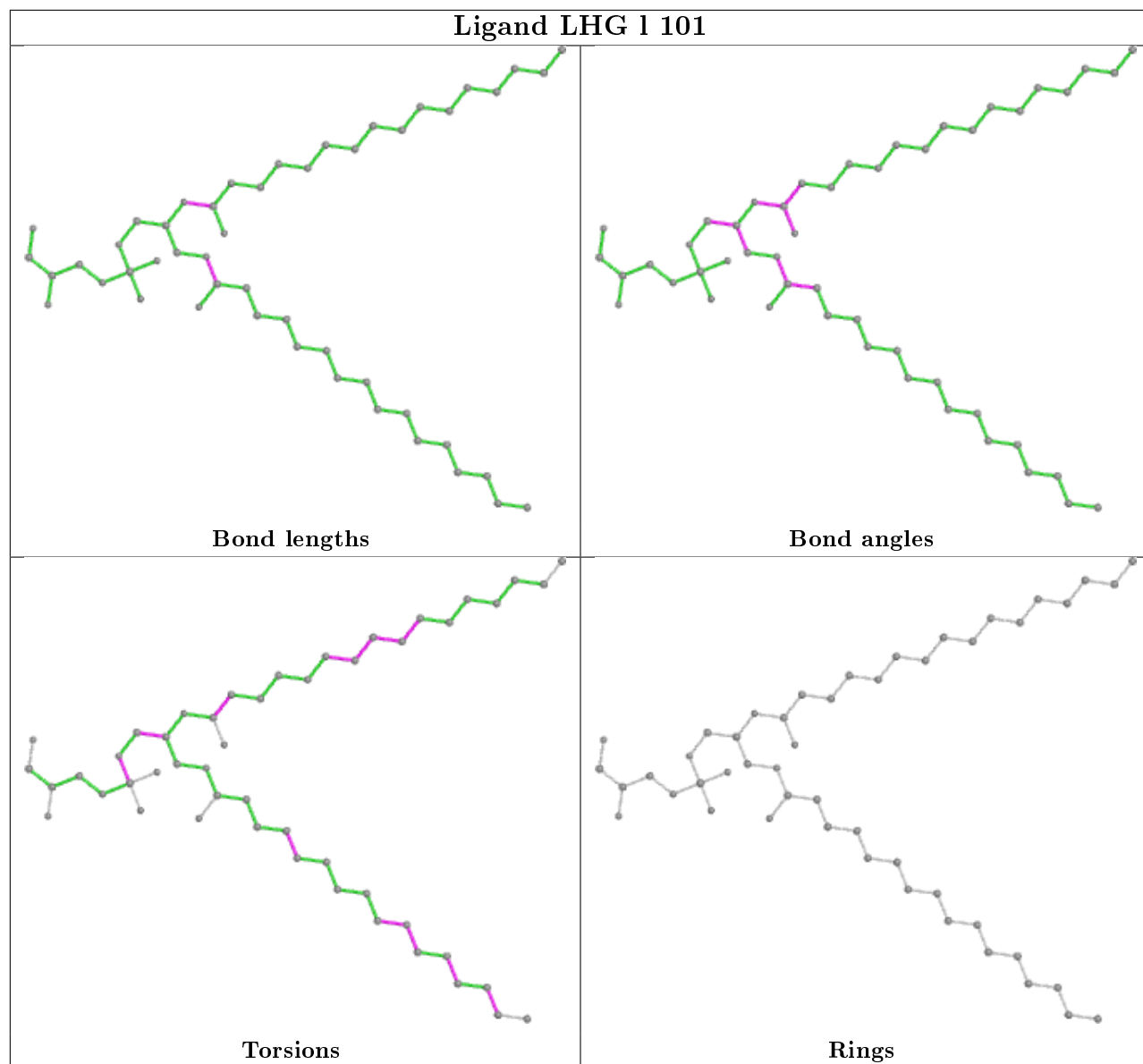
Ligand CLA b 620



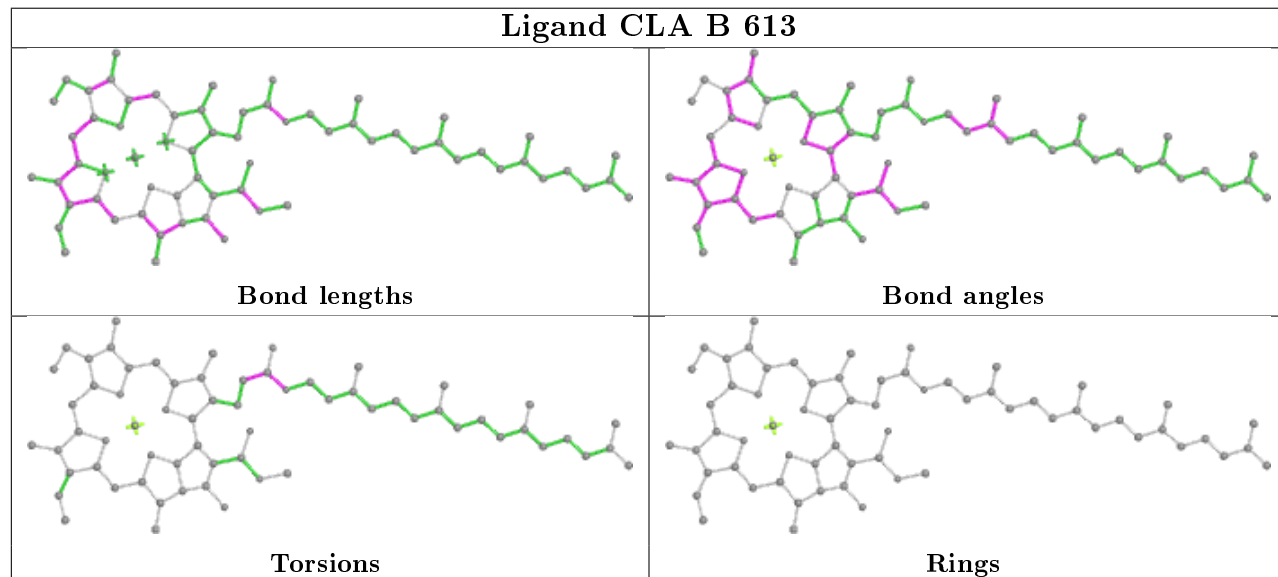


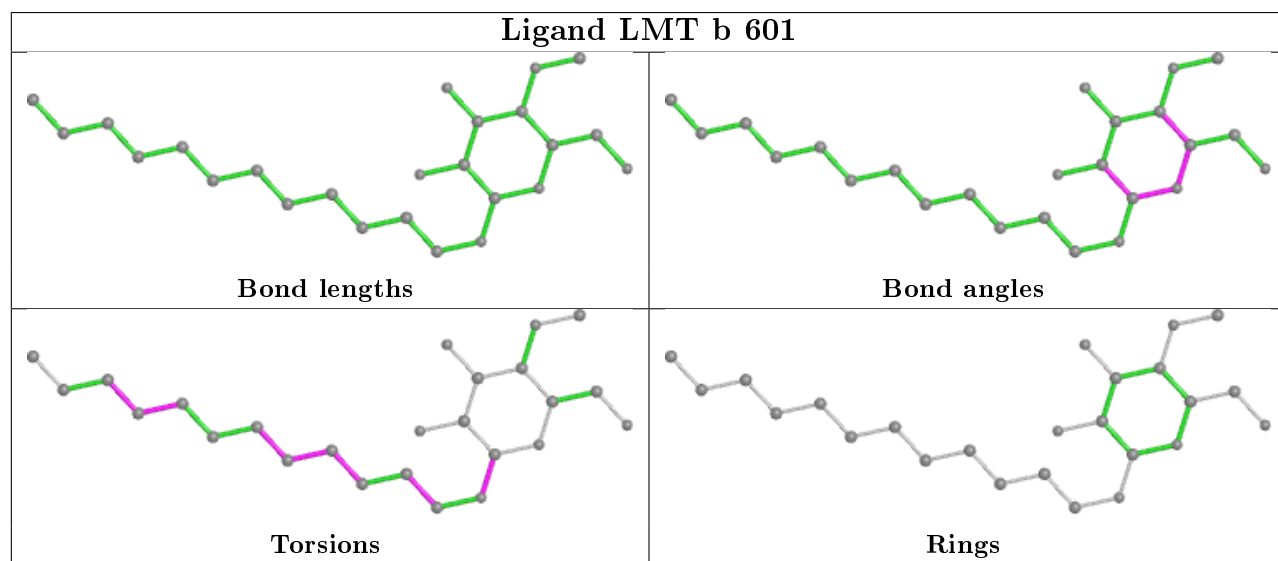
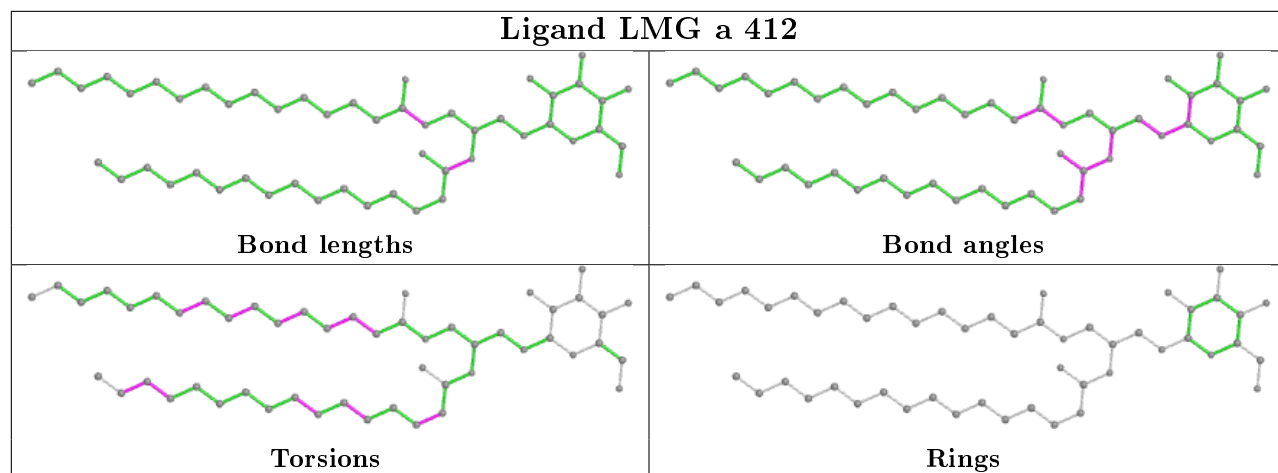
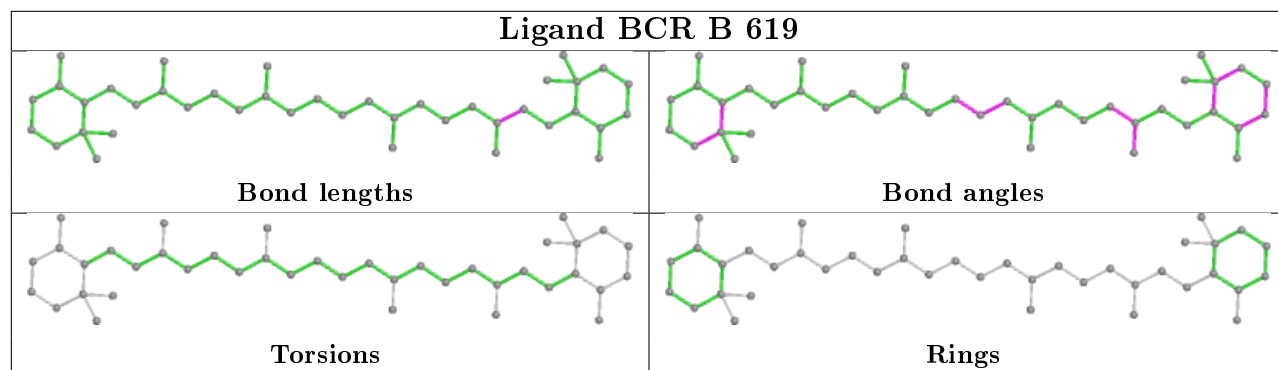


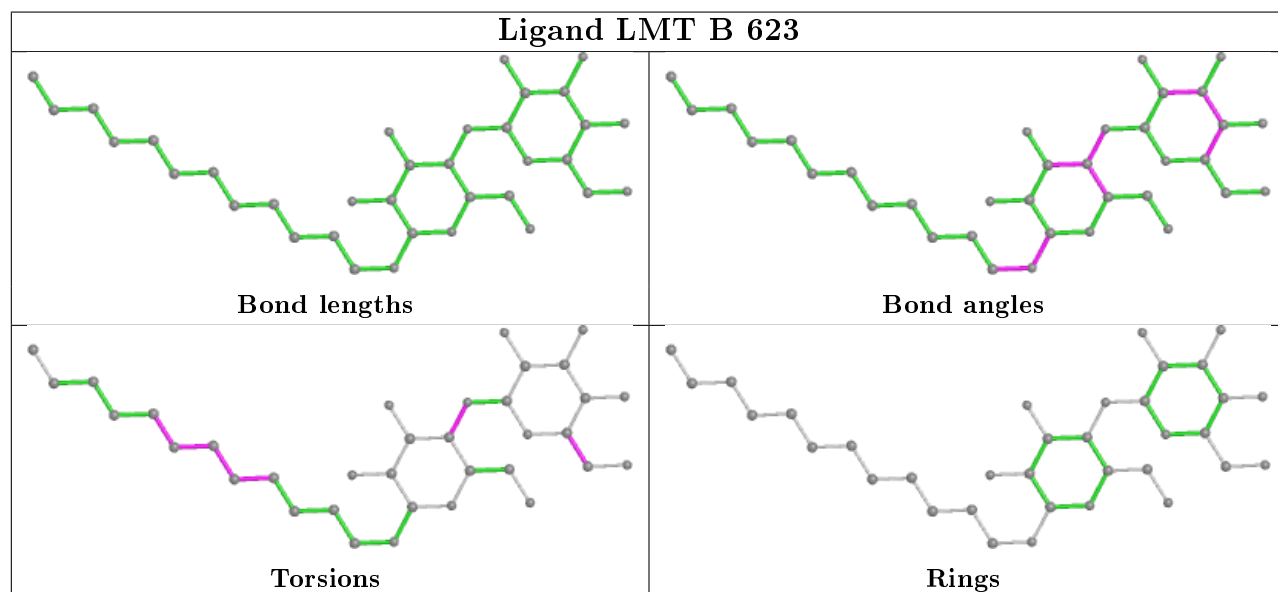
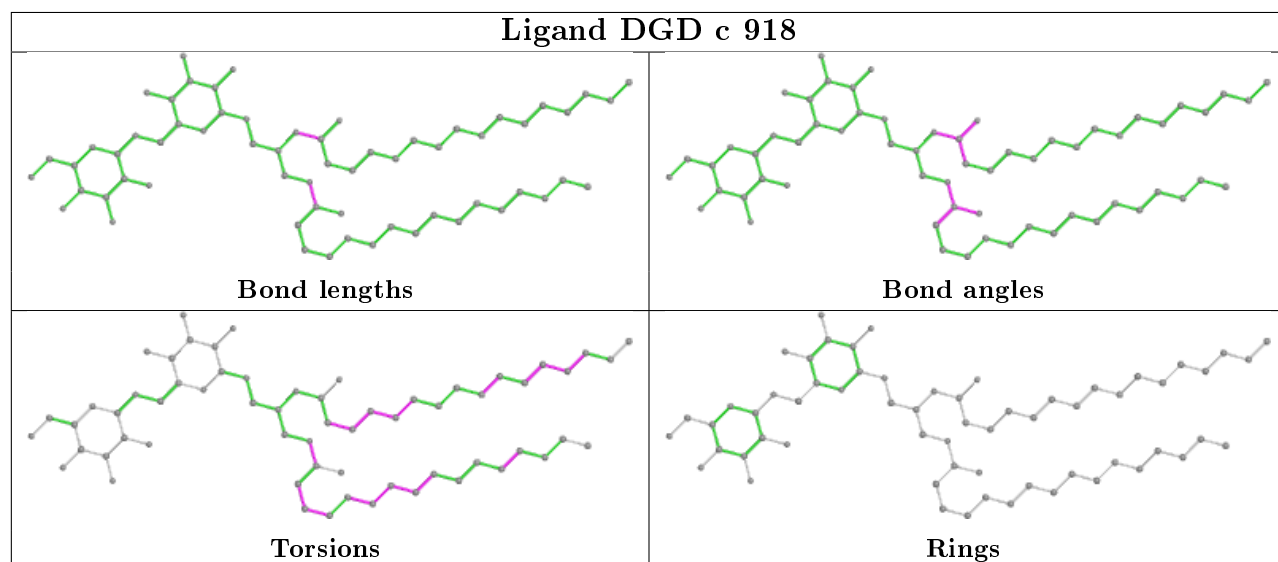
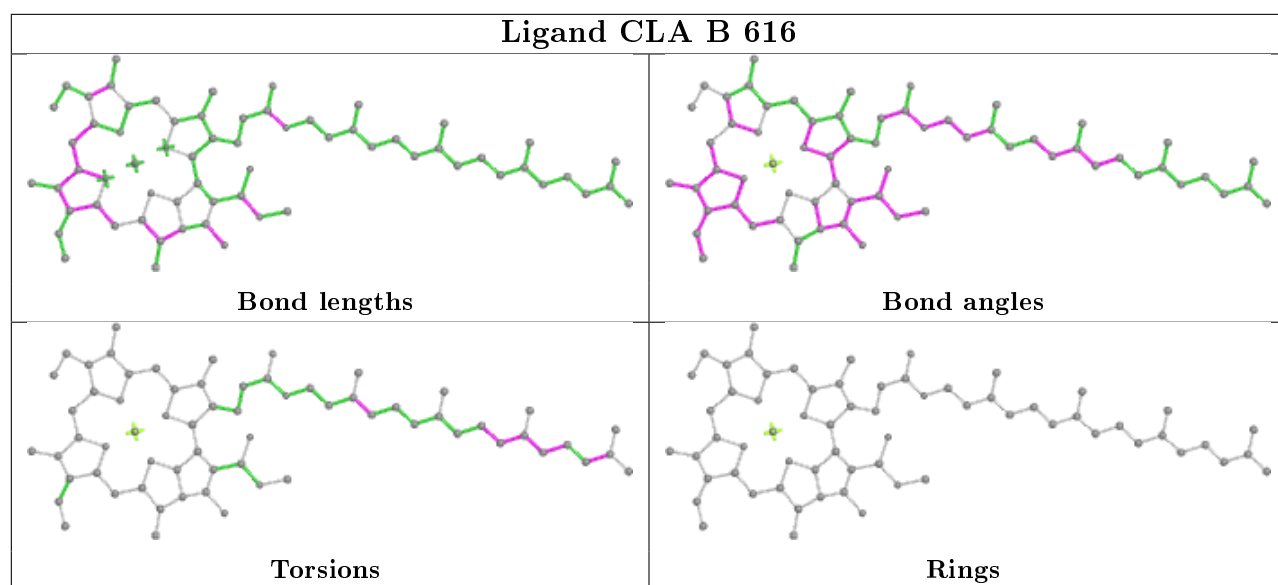
Ligand LHG 1 101

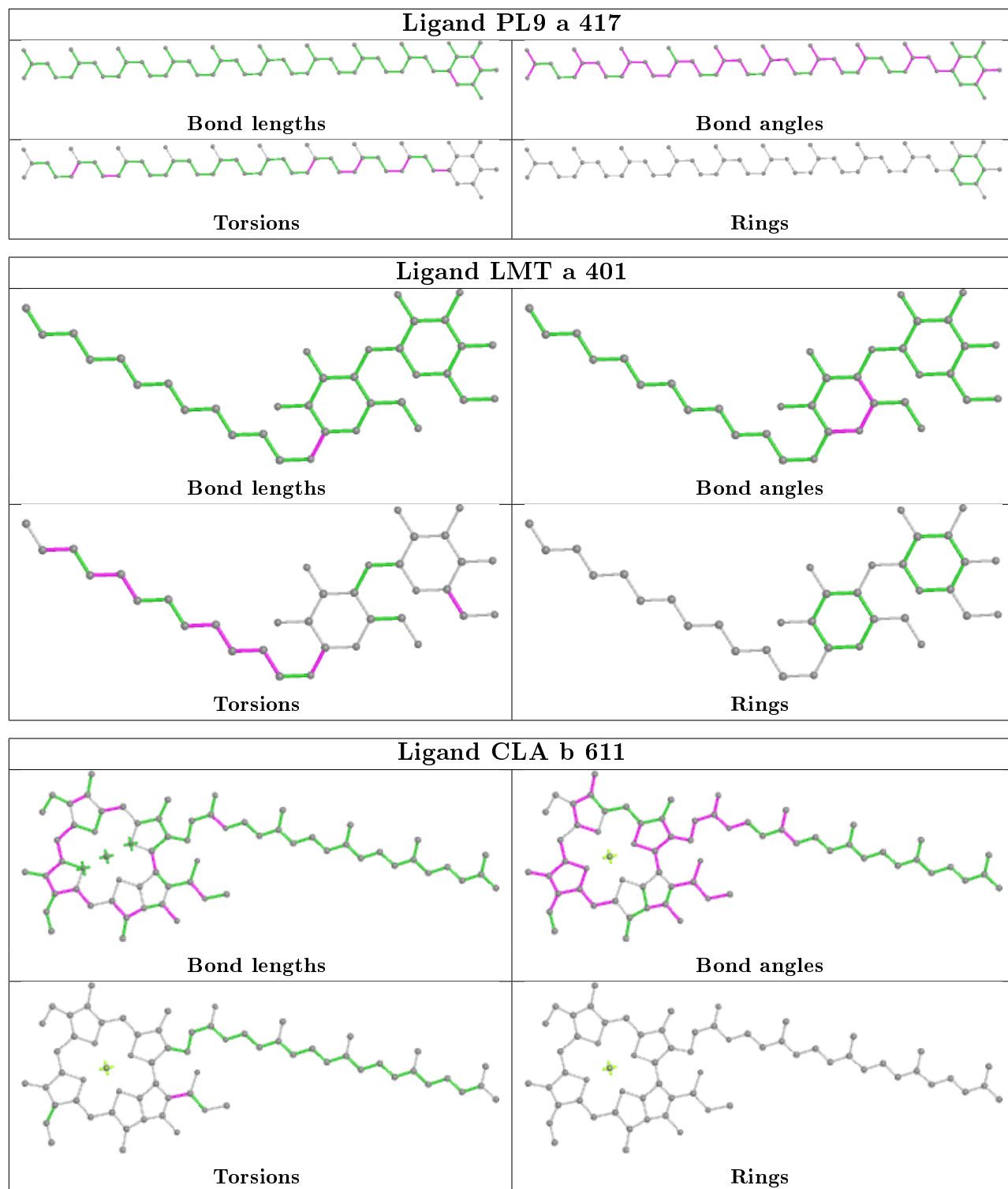


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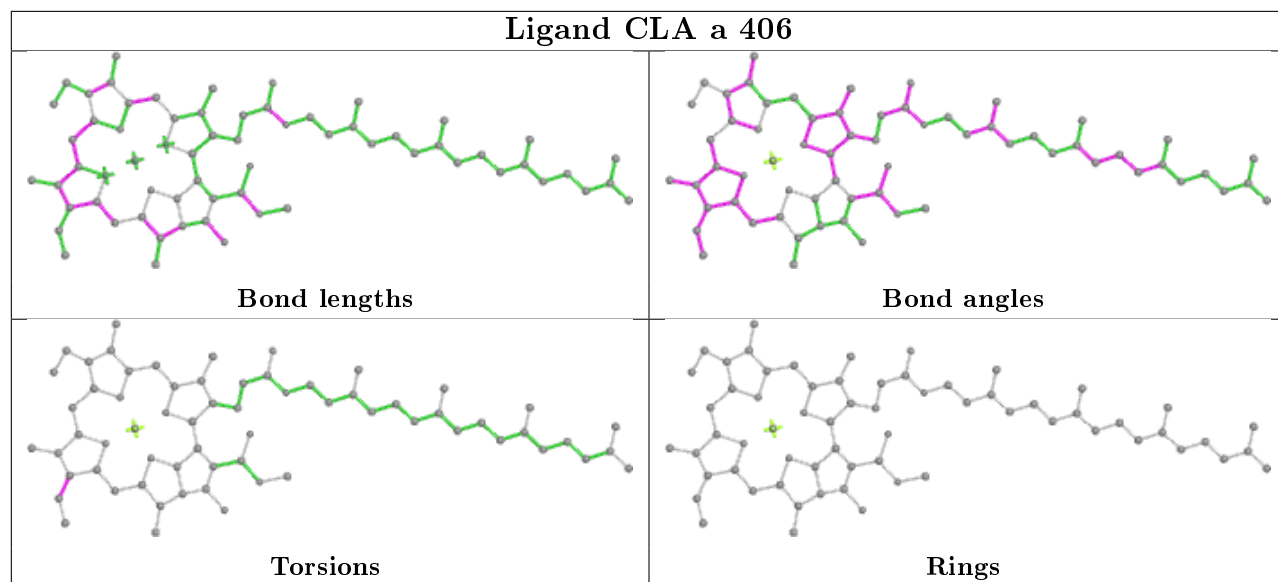




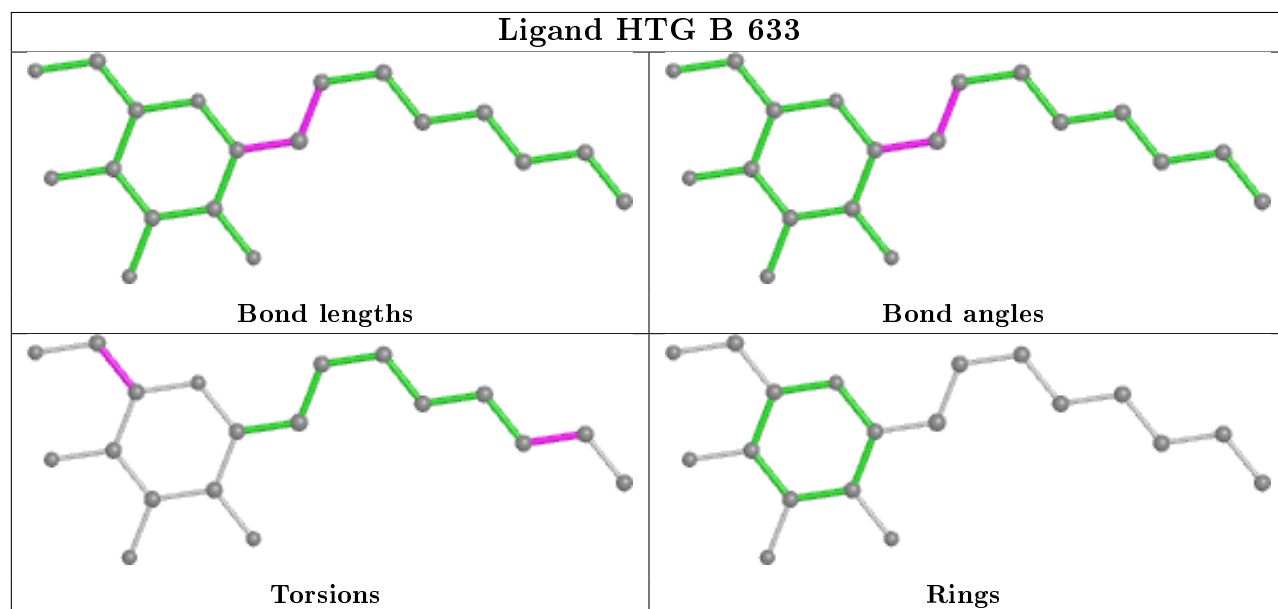




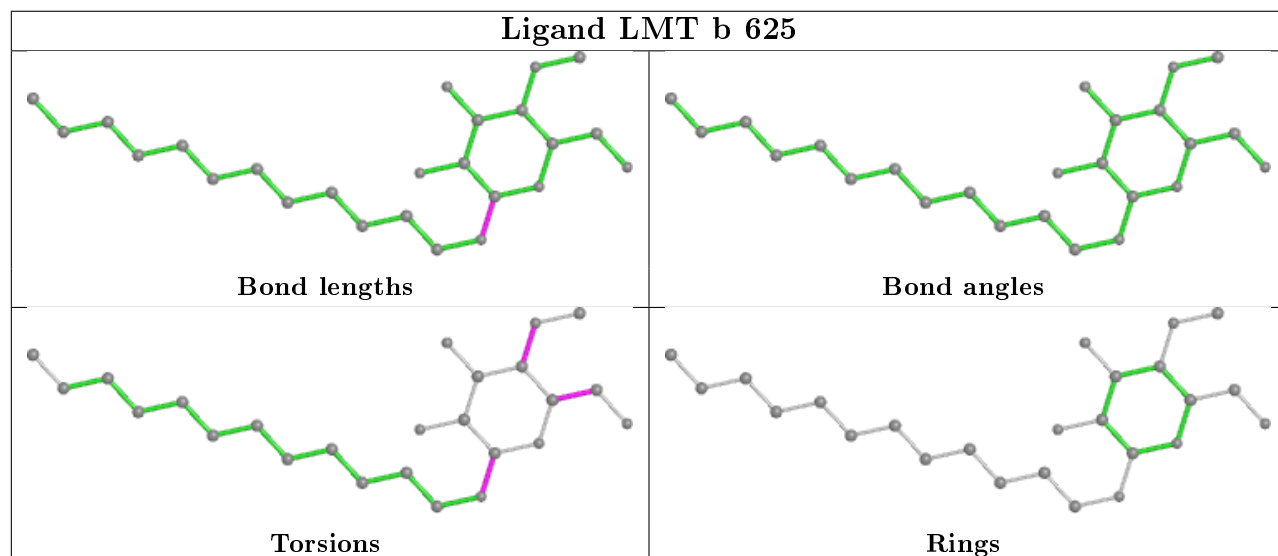
Ligand CLA a 406

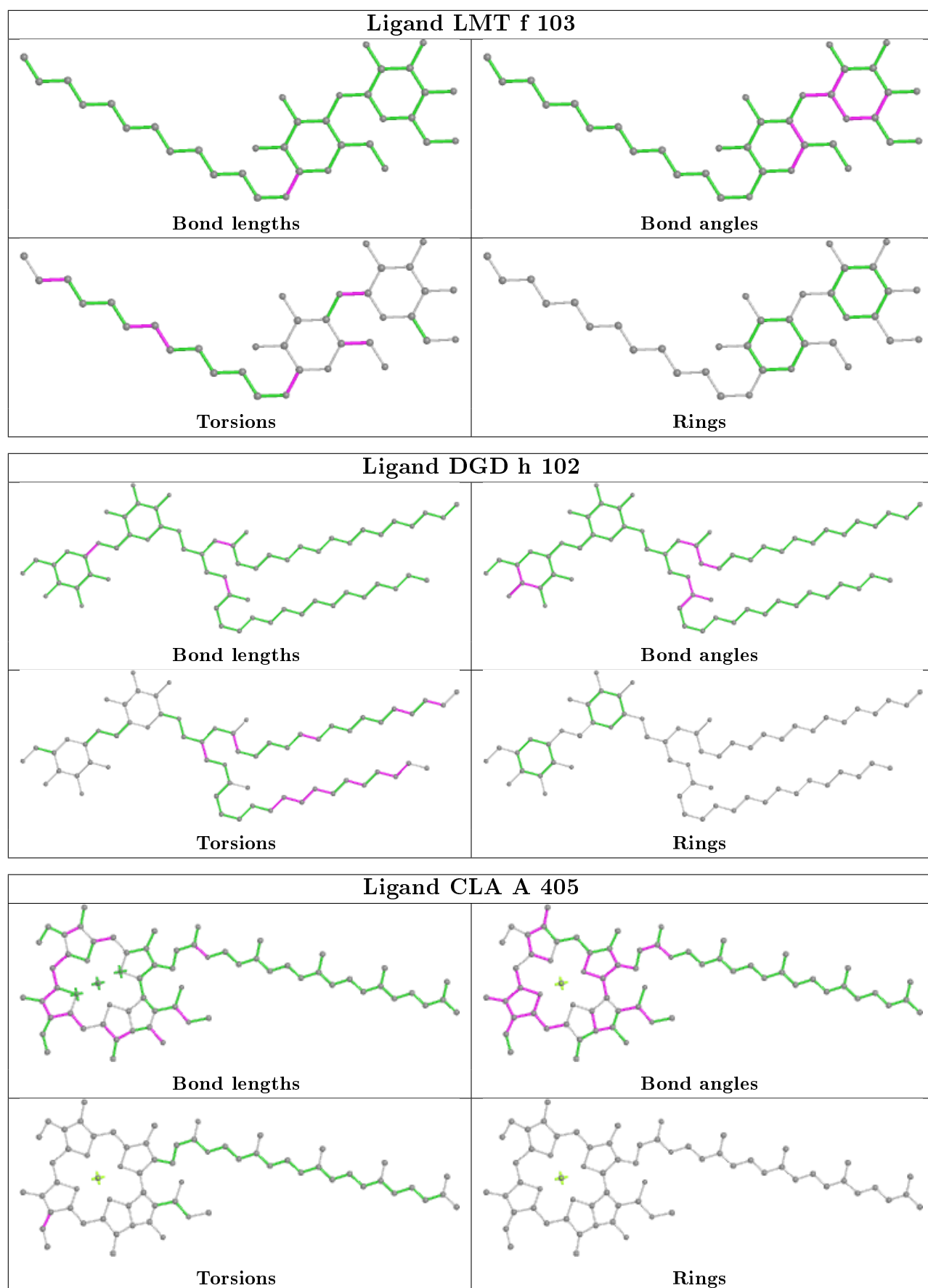


Ligand HTG B 633

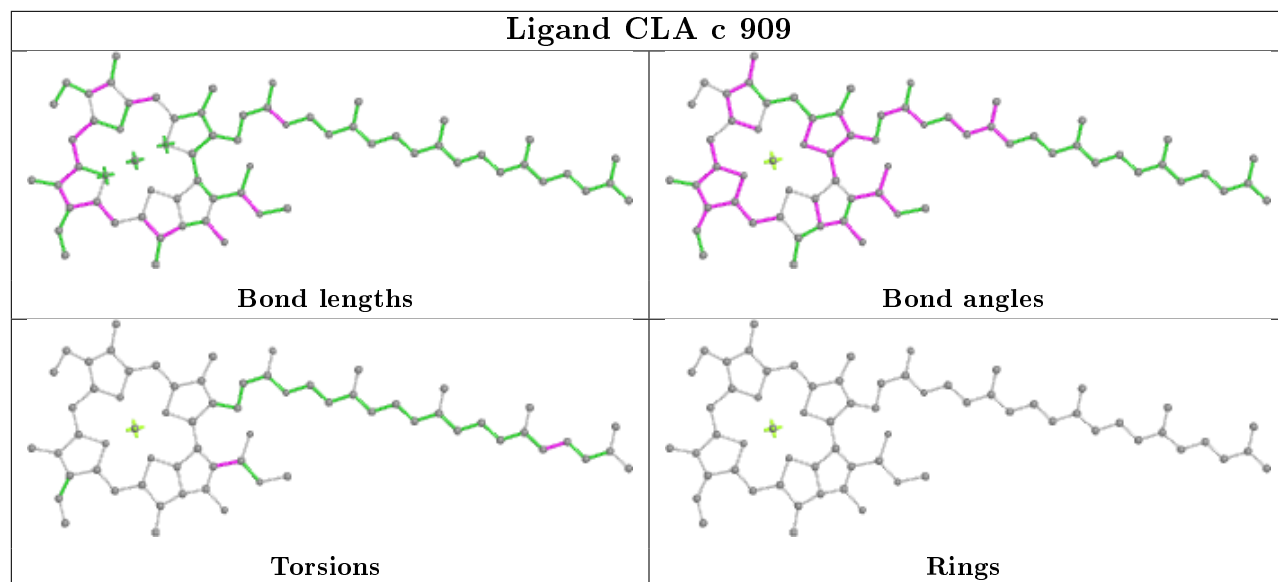


Ligand LMT b 625

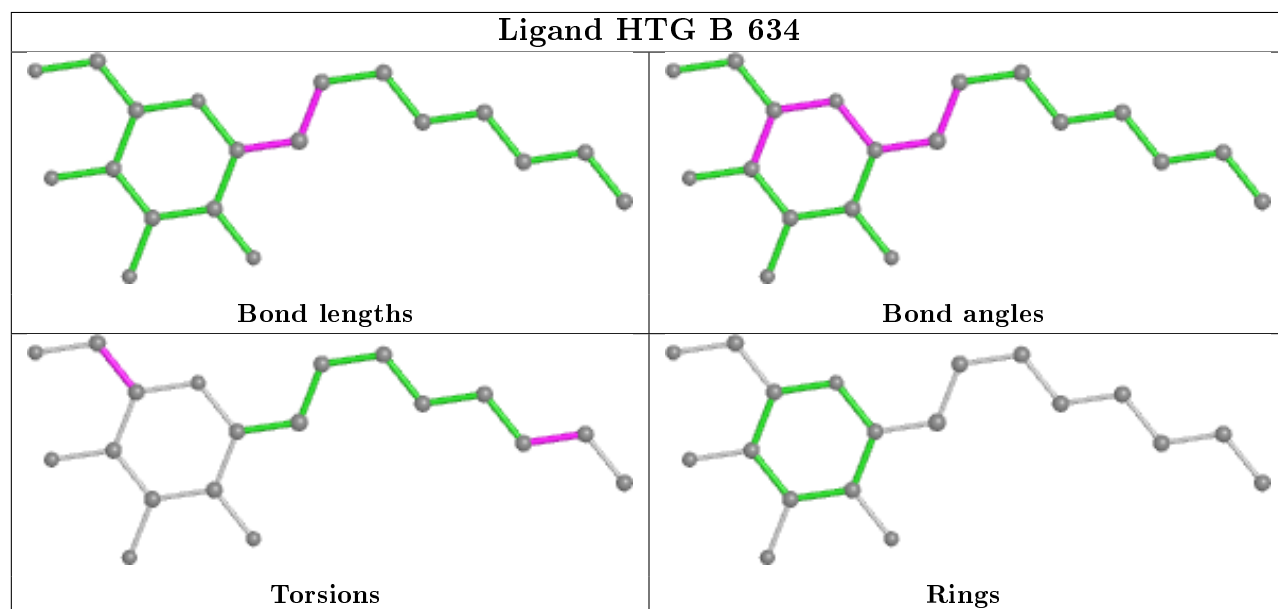




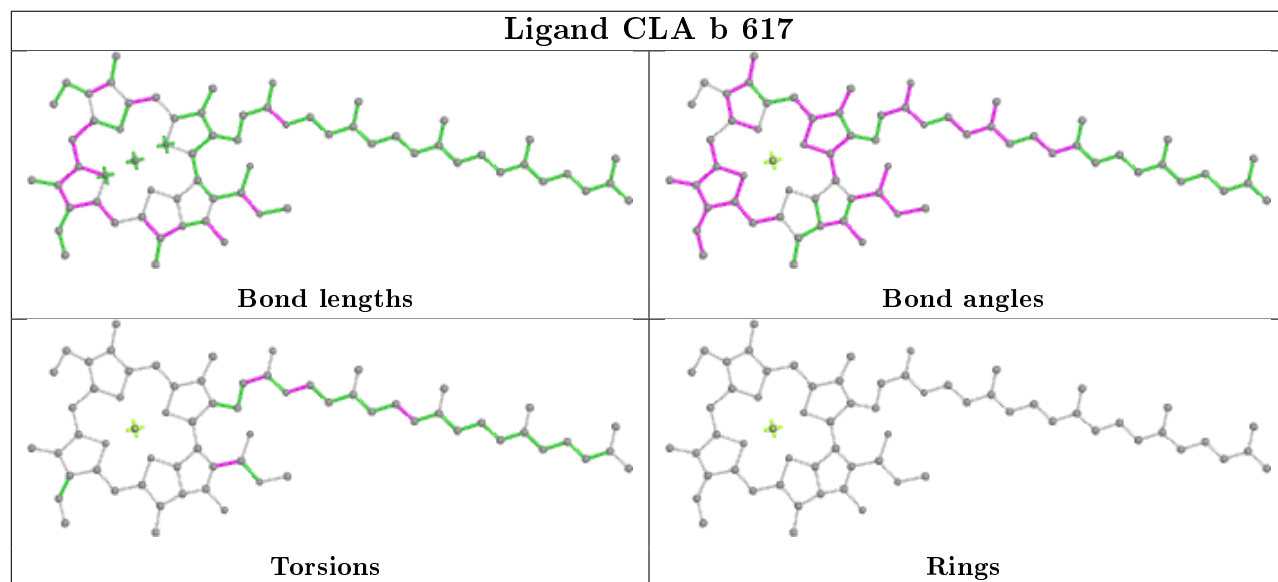
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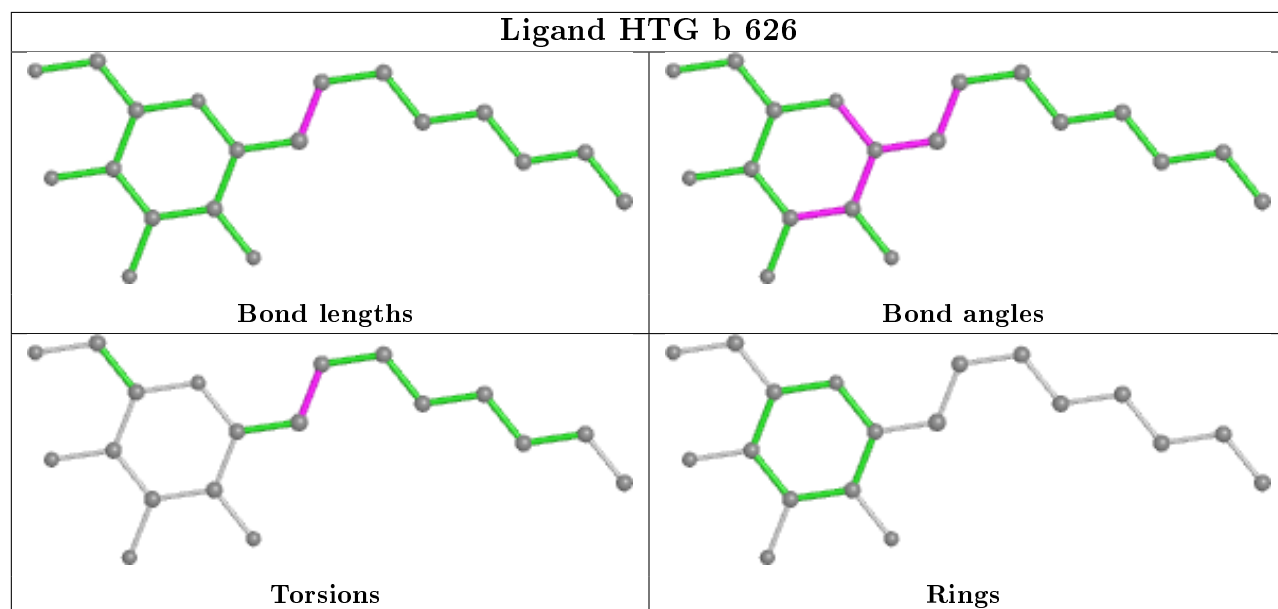
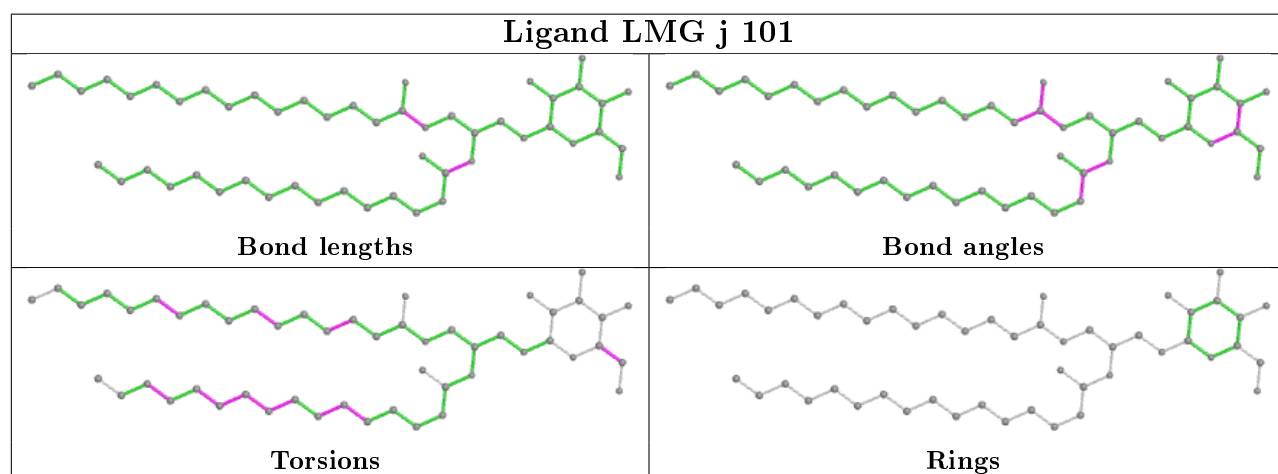
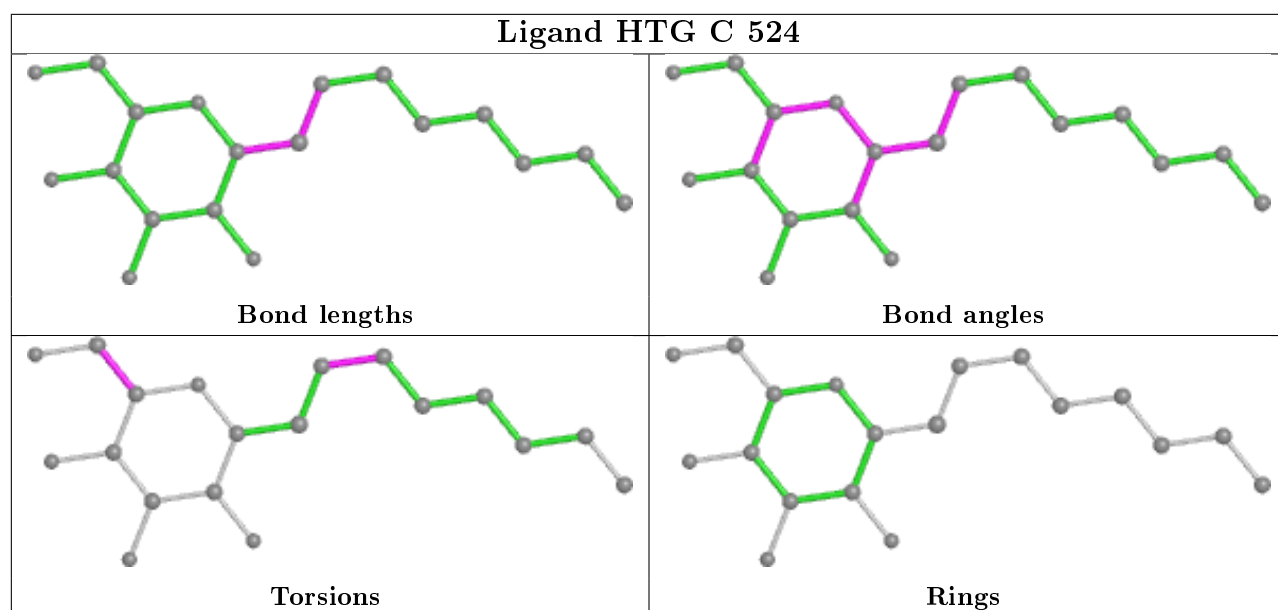


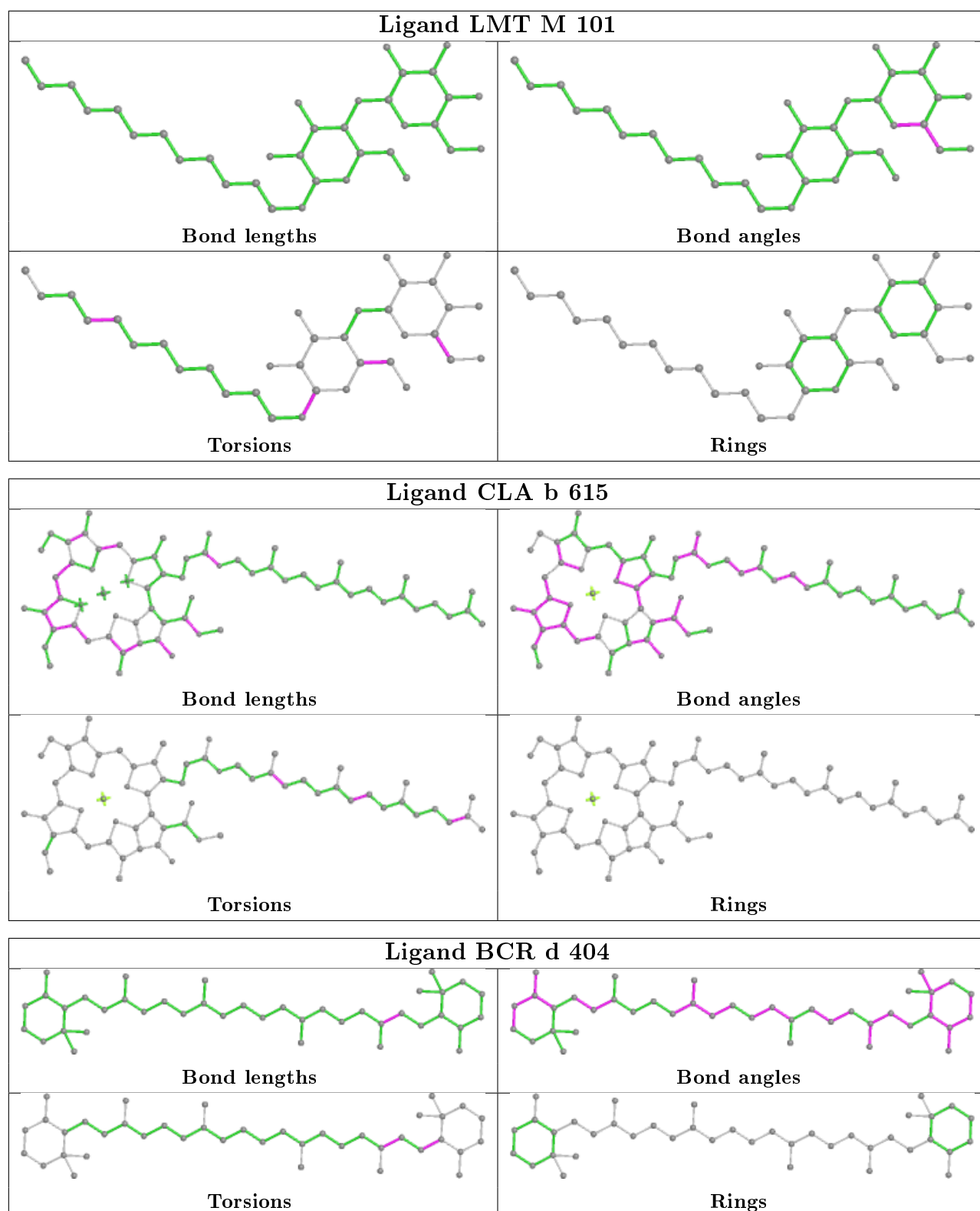
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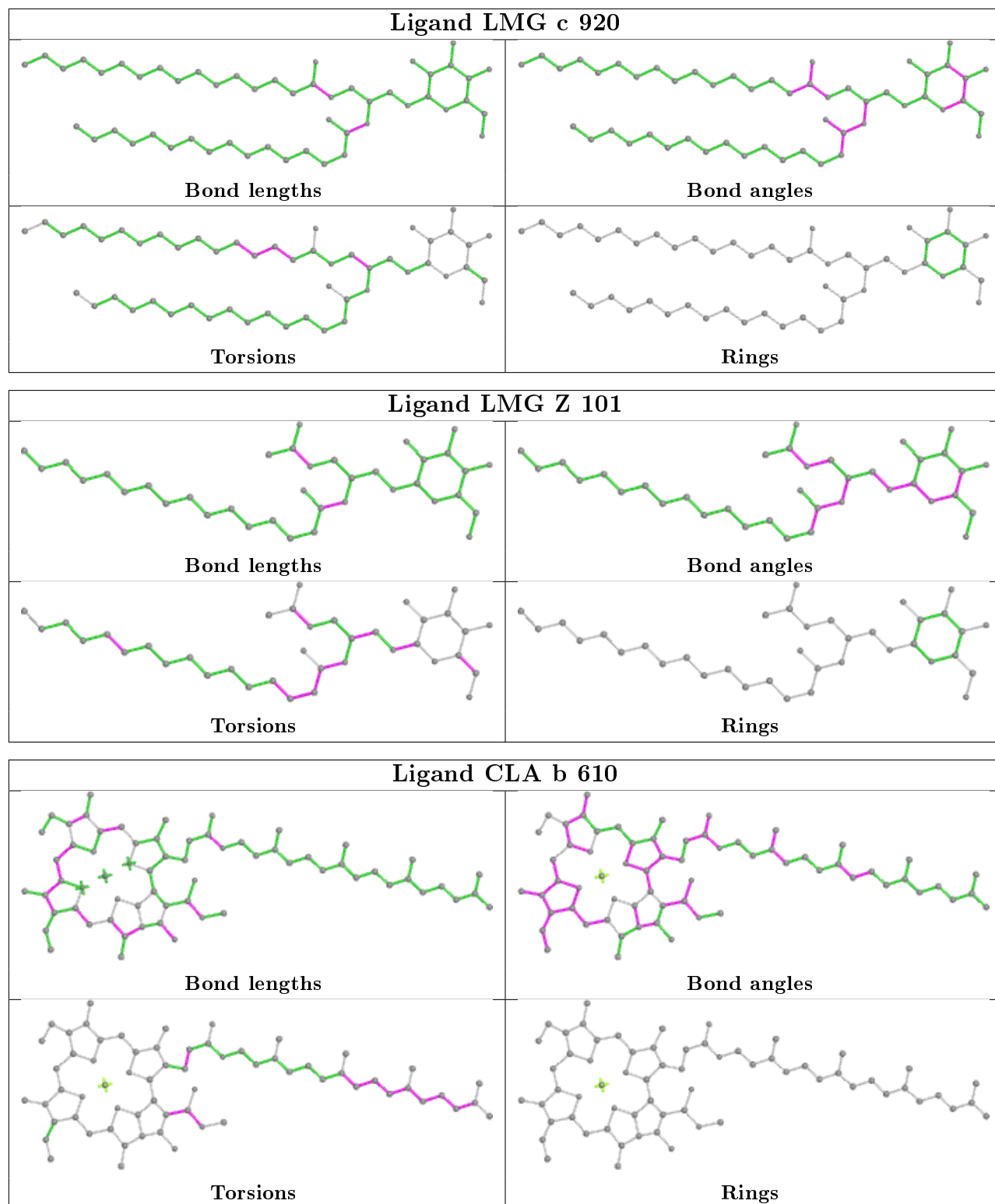


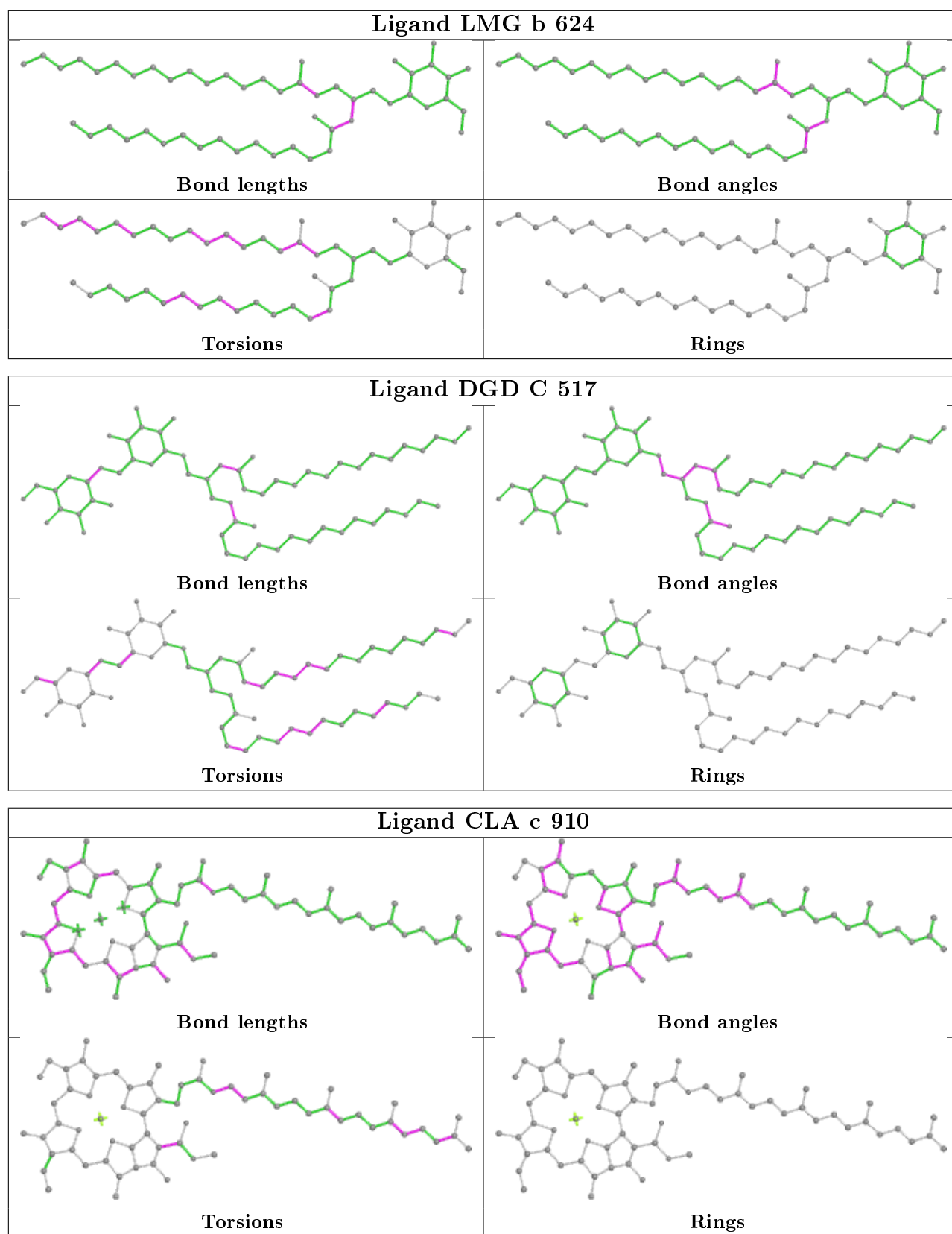
Ligand CLA b 617

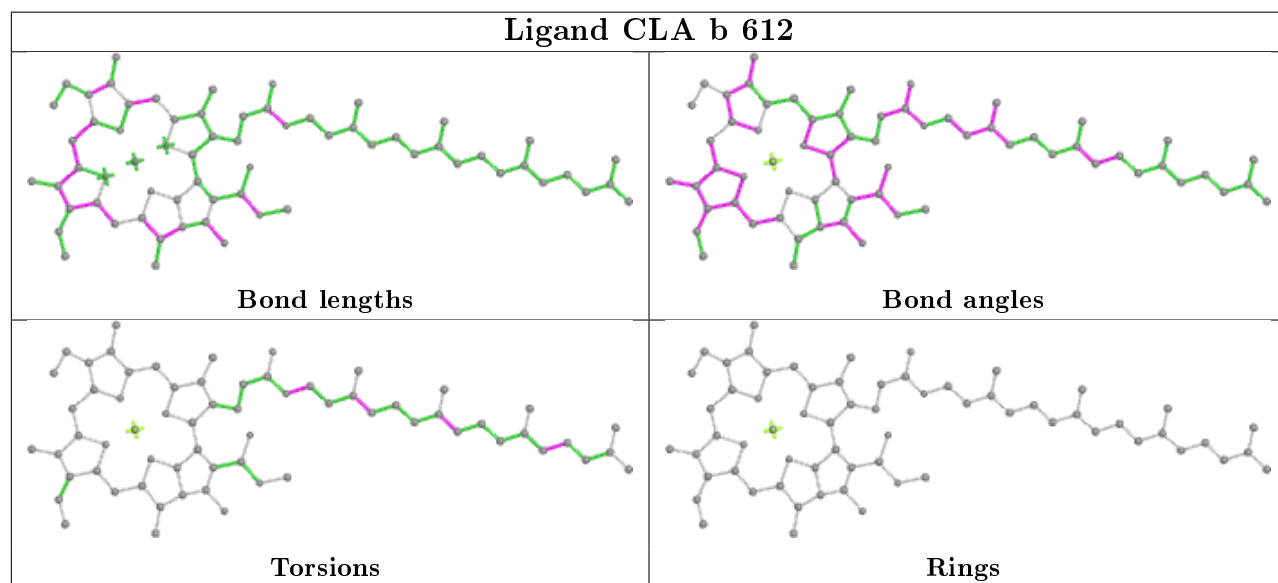
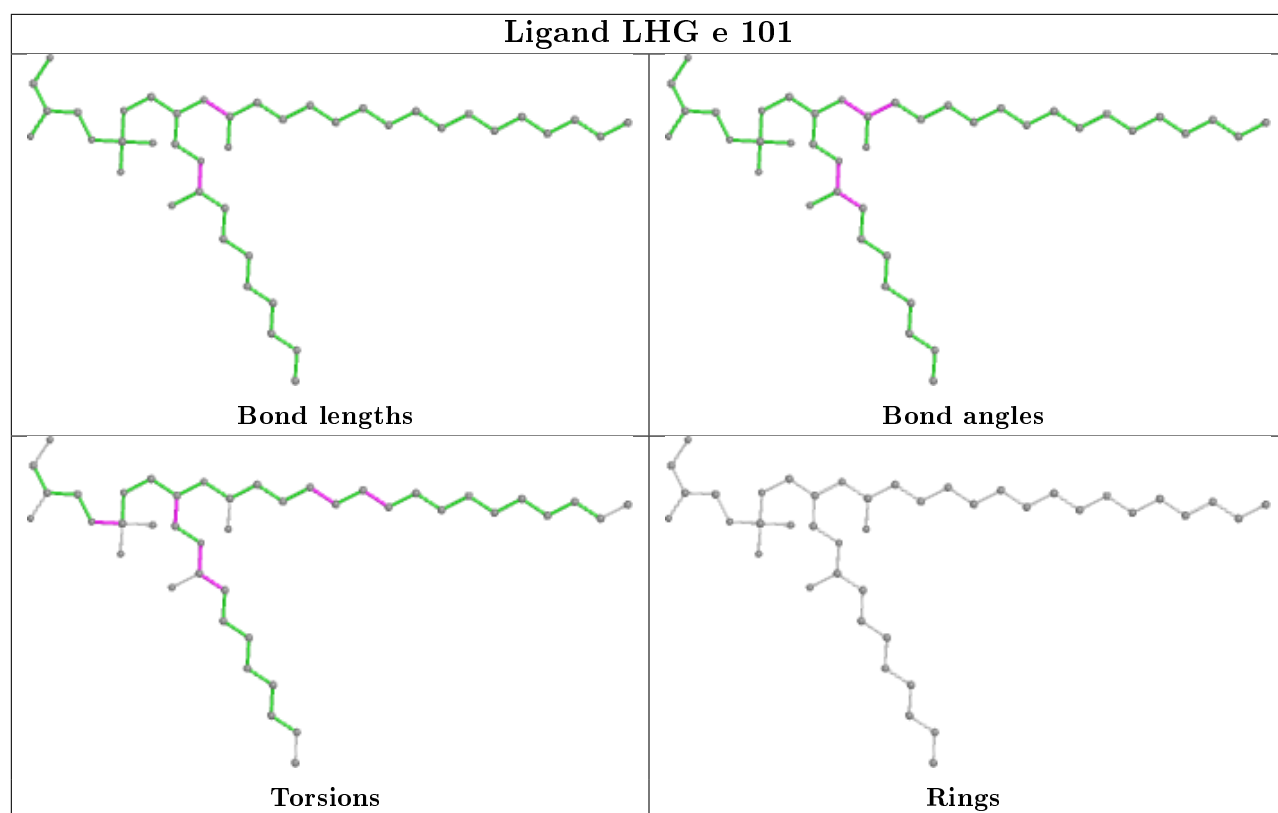


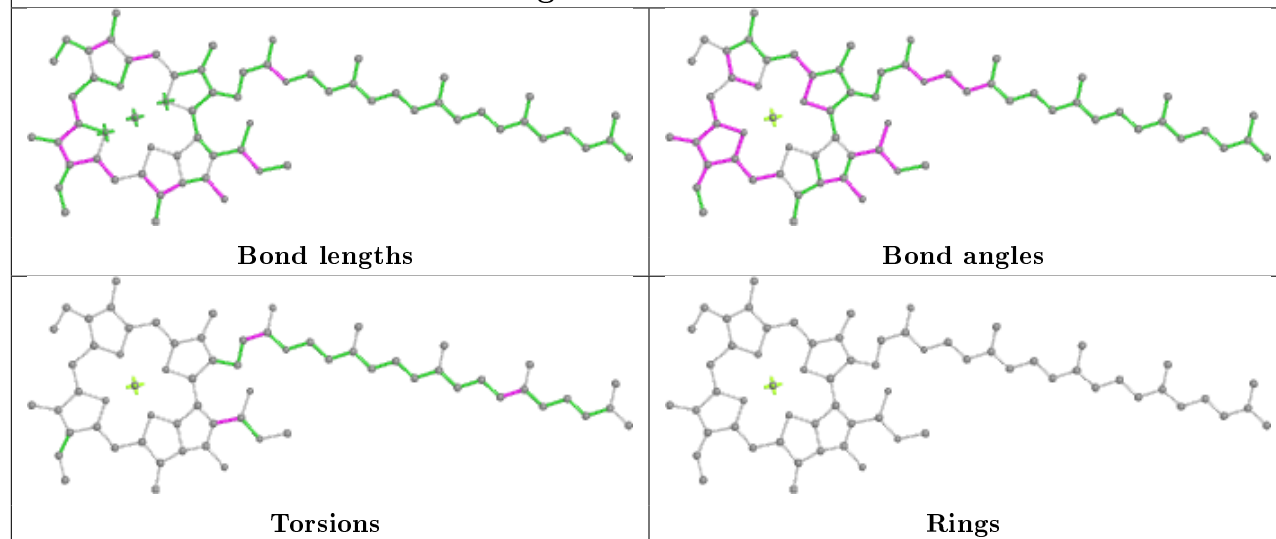
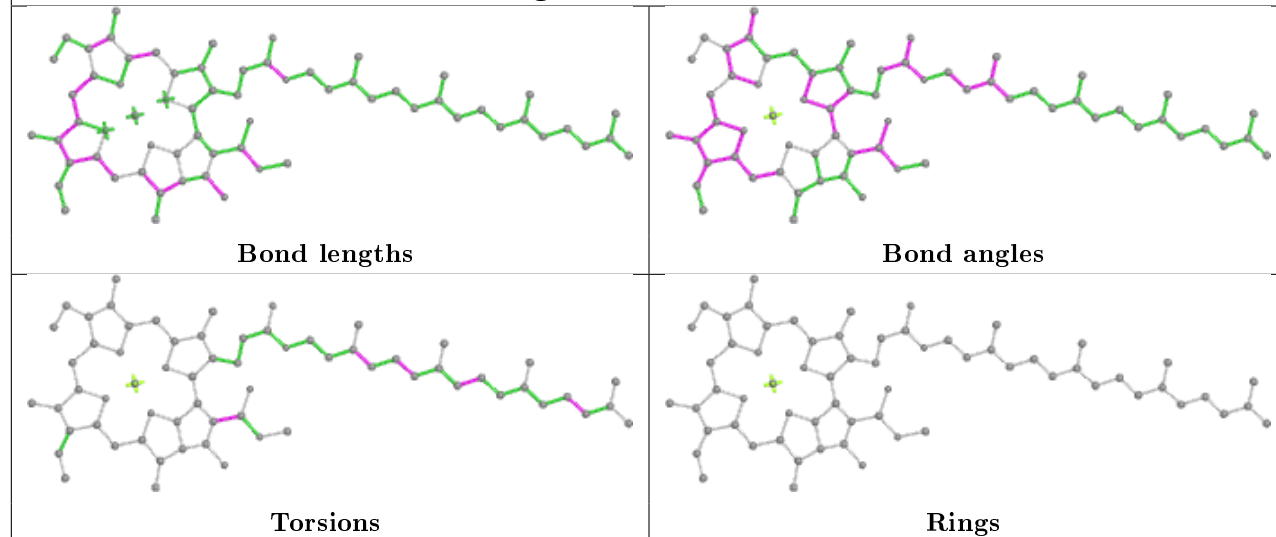


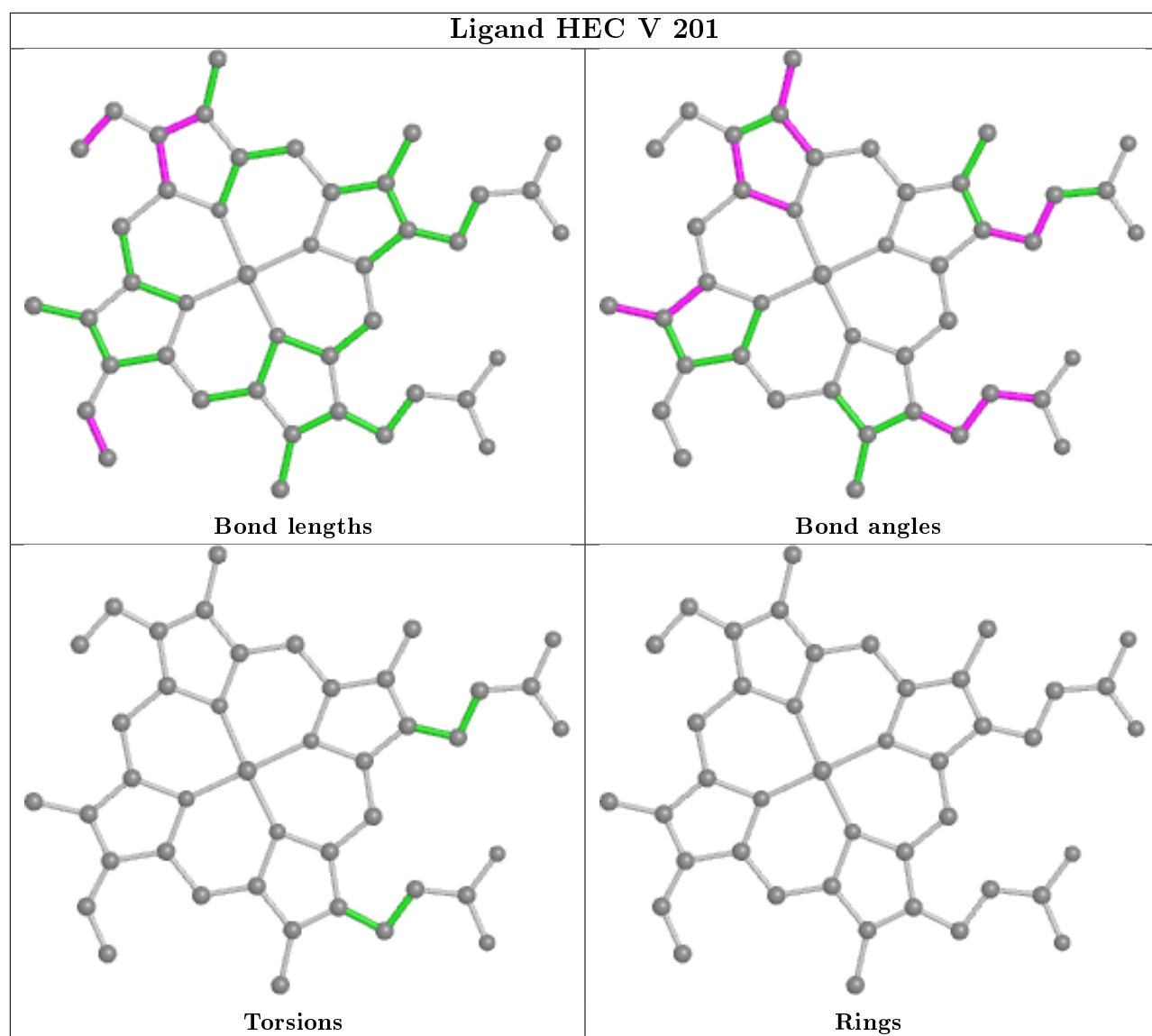




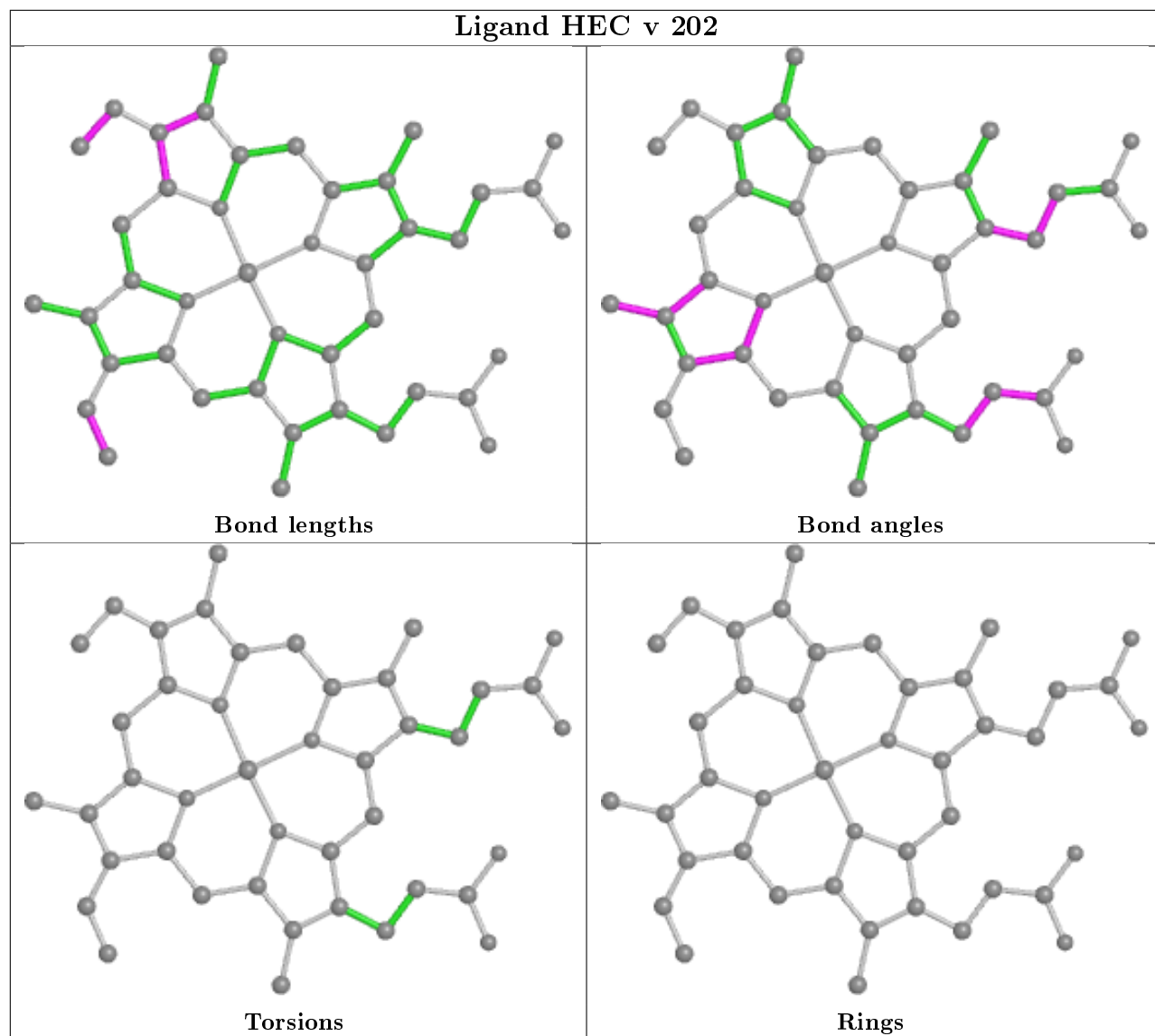




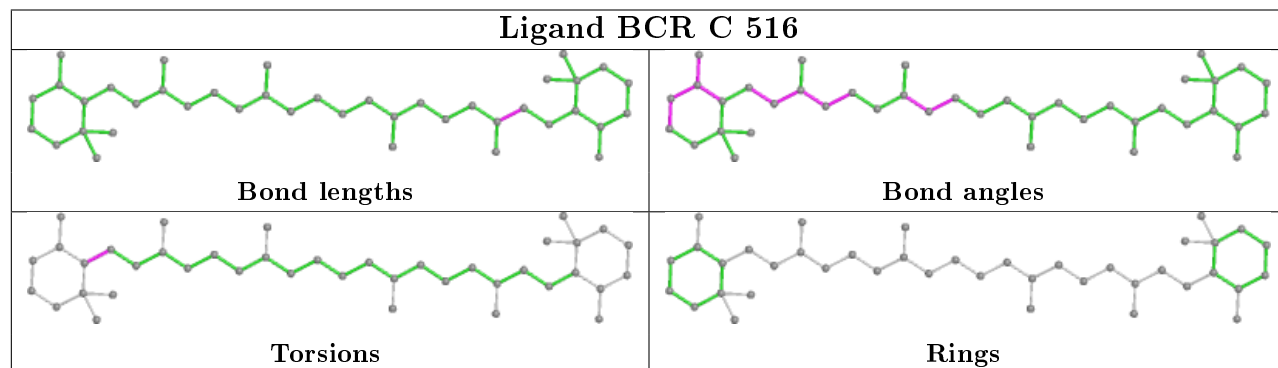
Ligand CLA c 906**Ligand CLA C 504**



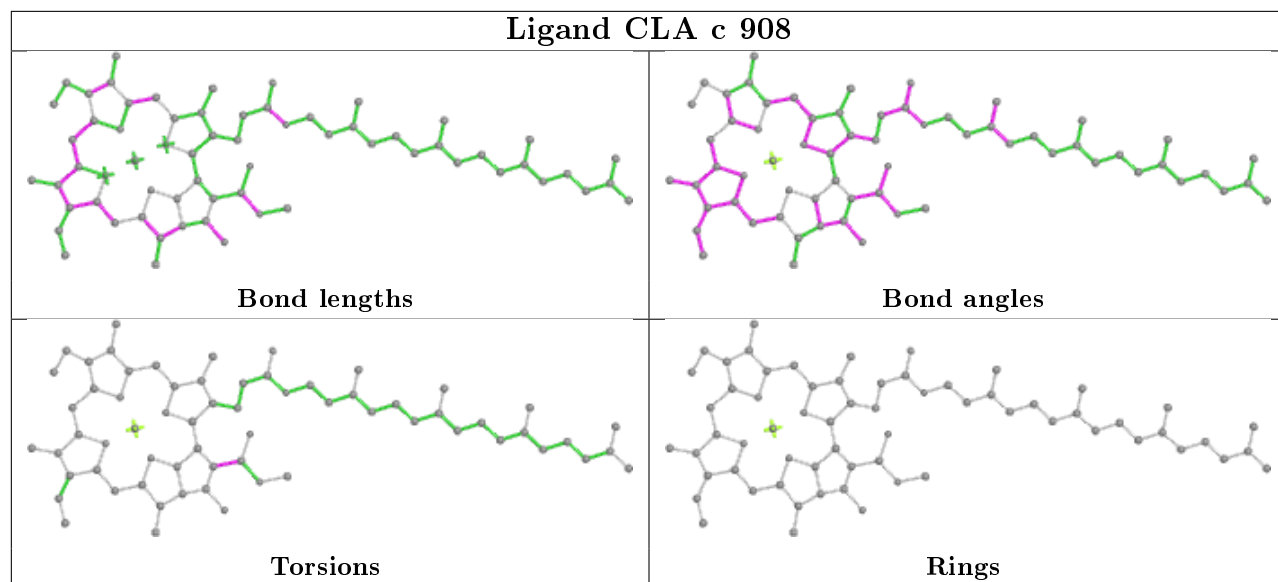
Ligand HEC v 202



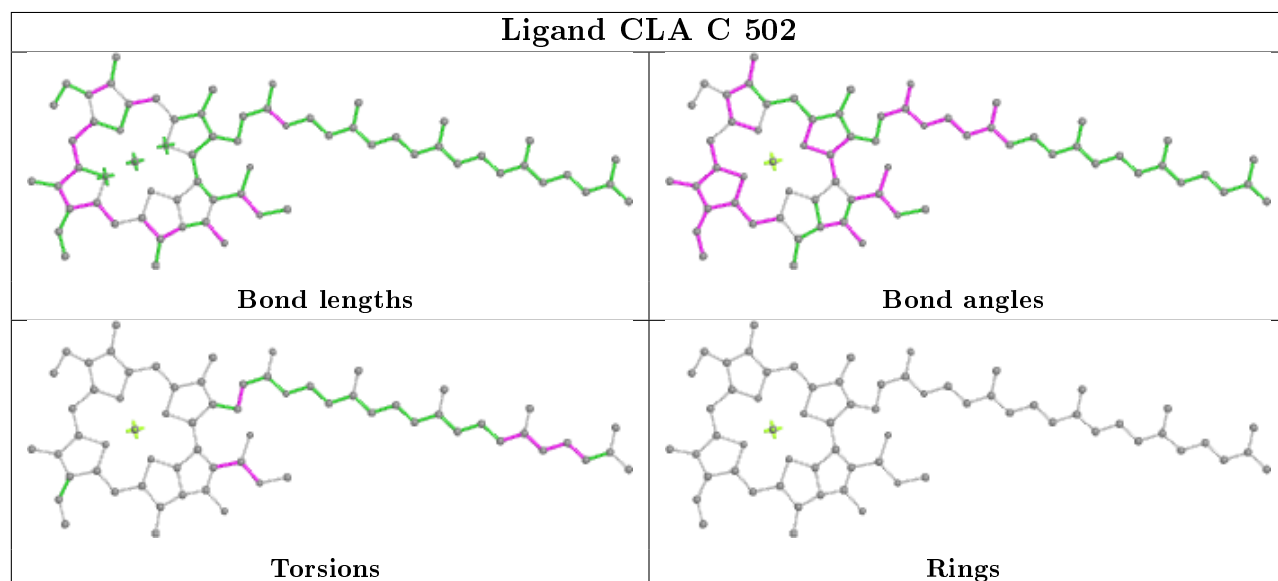
Ligand BCR C 516



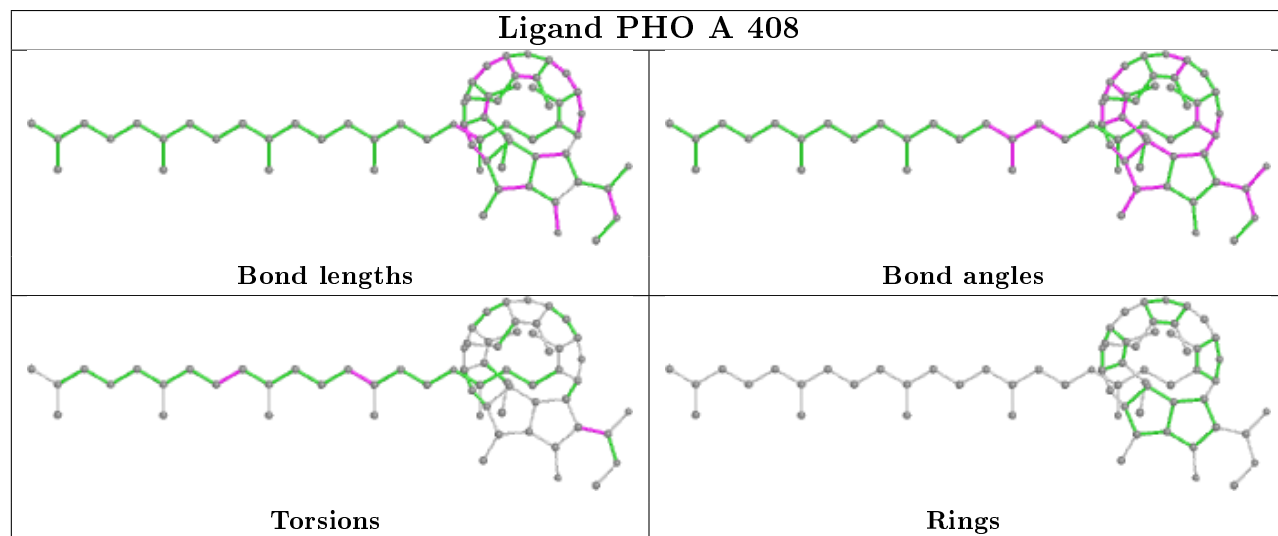
Ligand CLA c 908

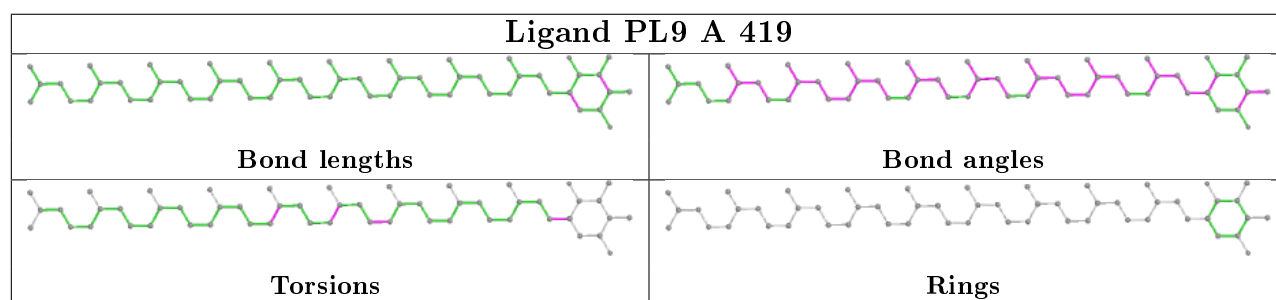
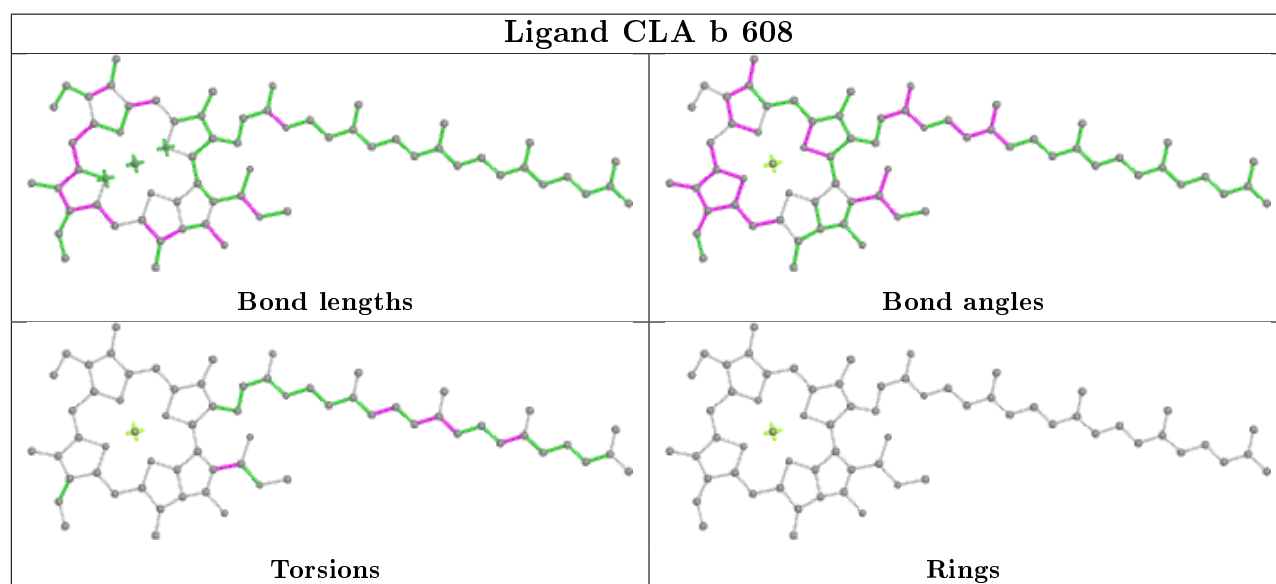
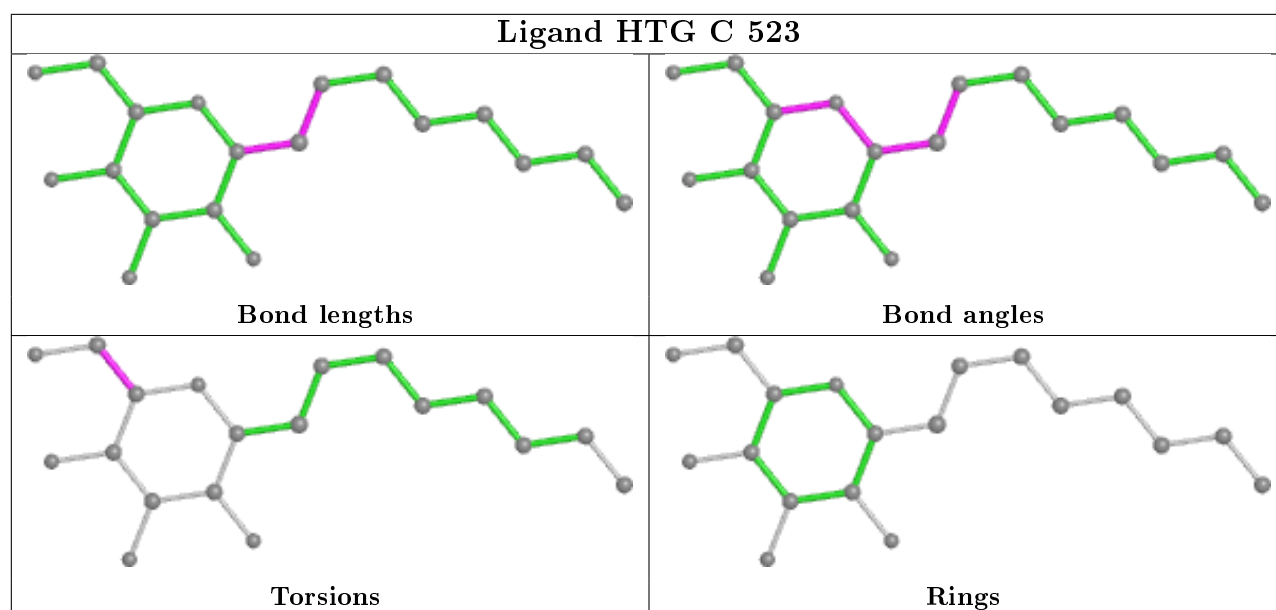


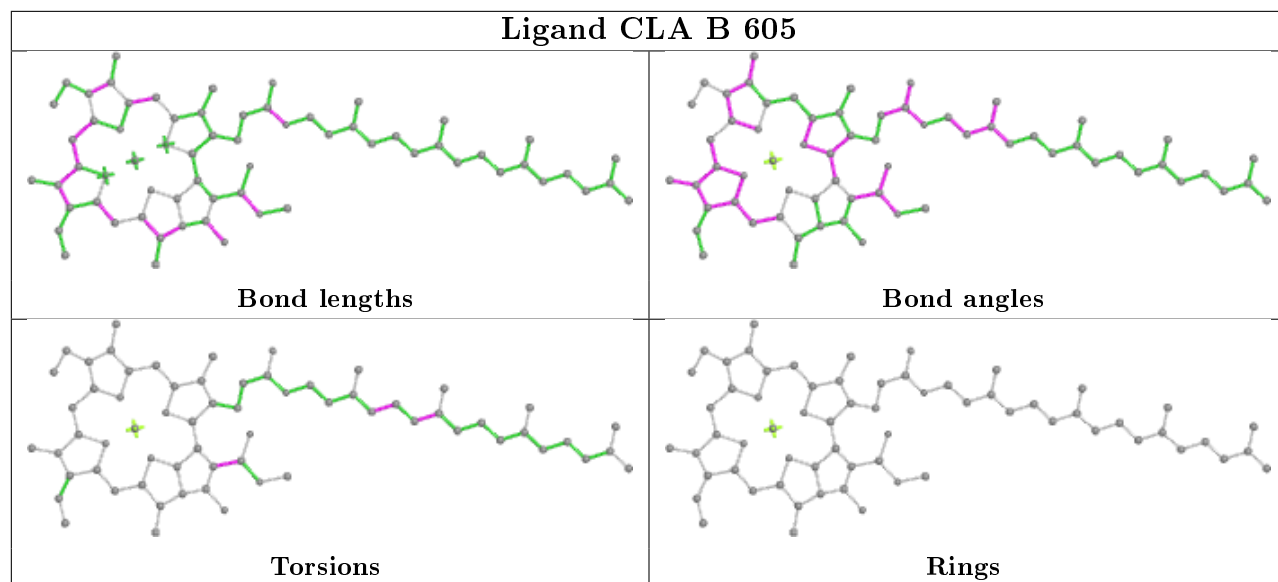
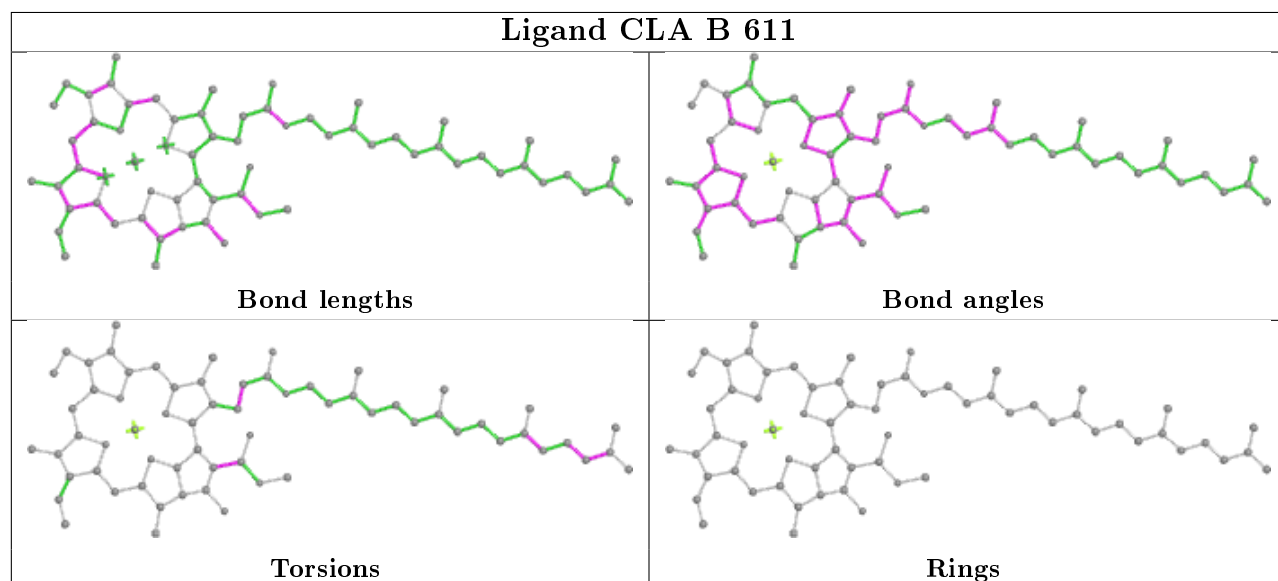
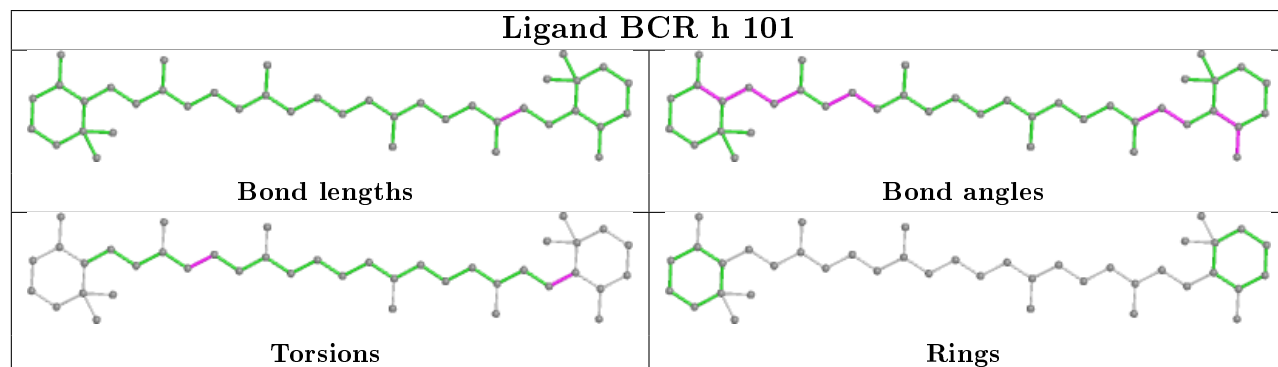
Ligand CLA C 502

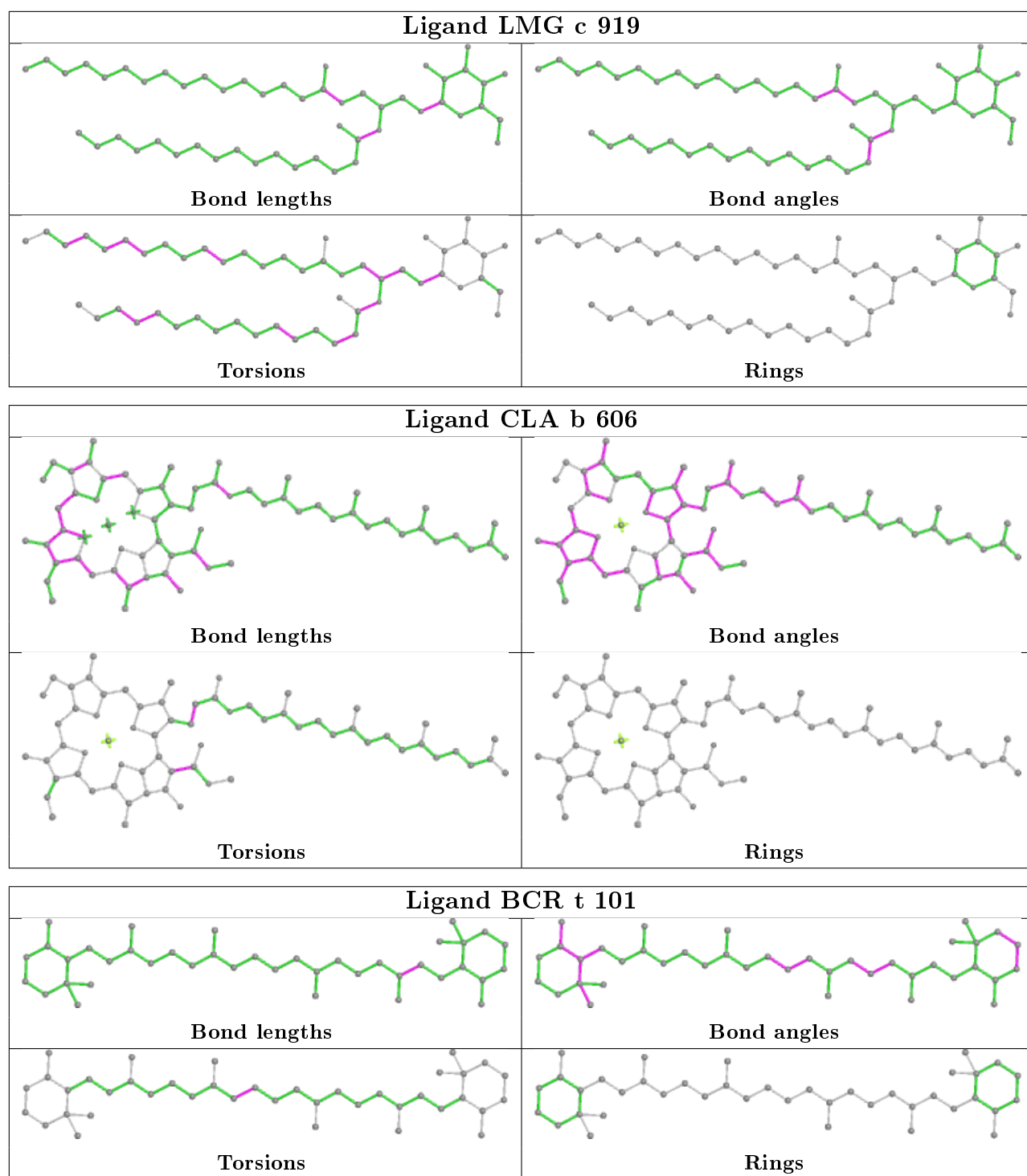


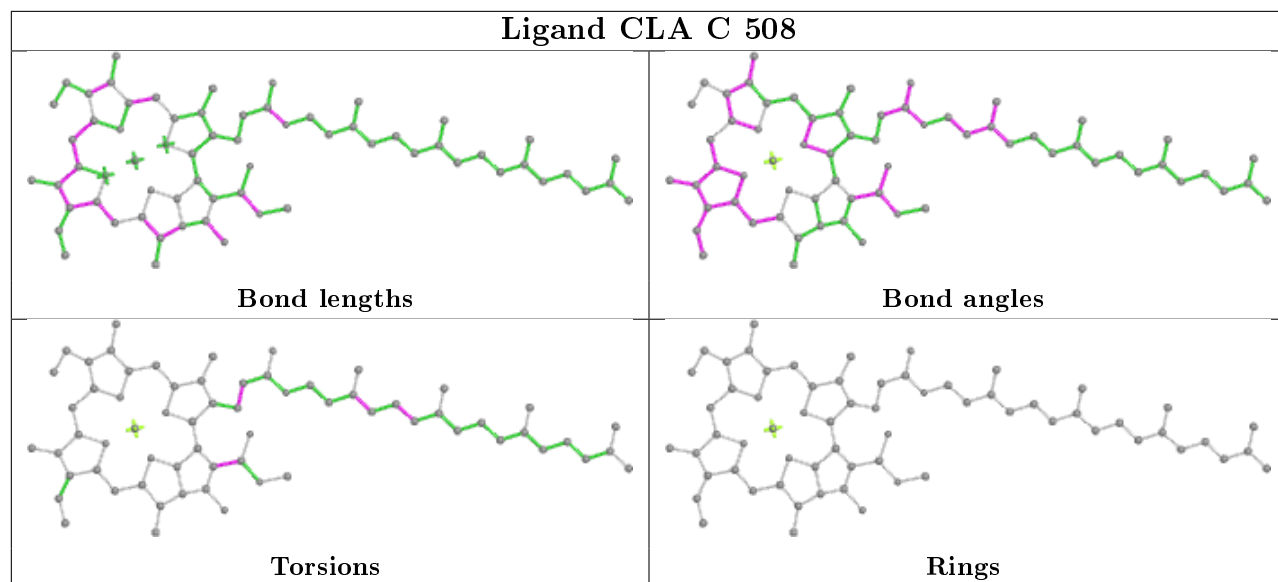
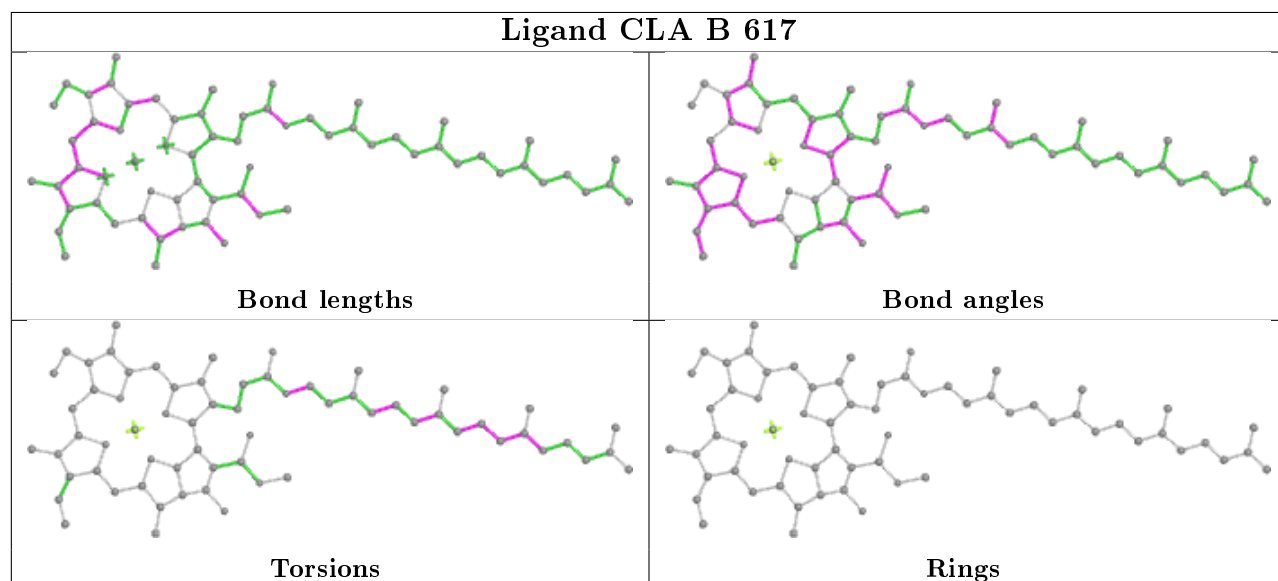
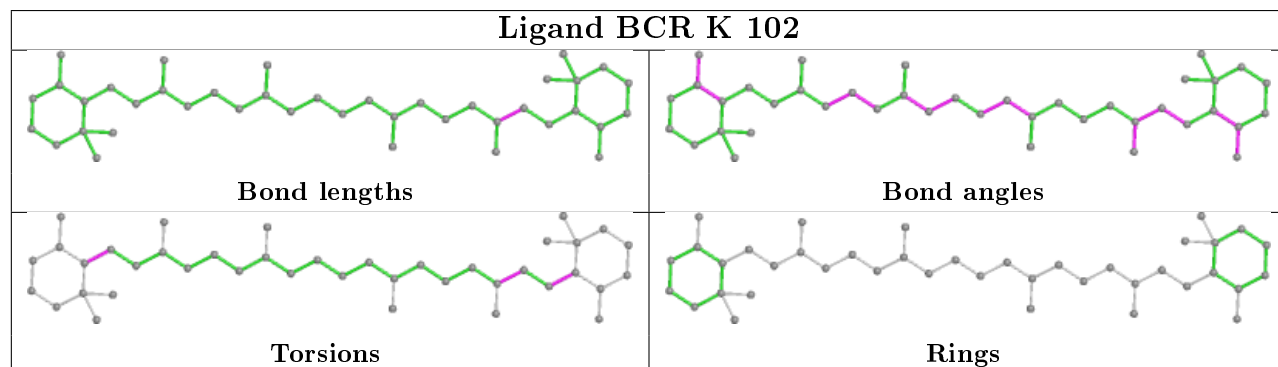
Ligand PHO A 408



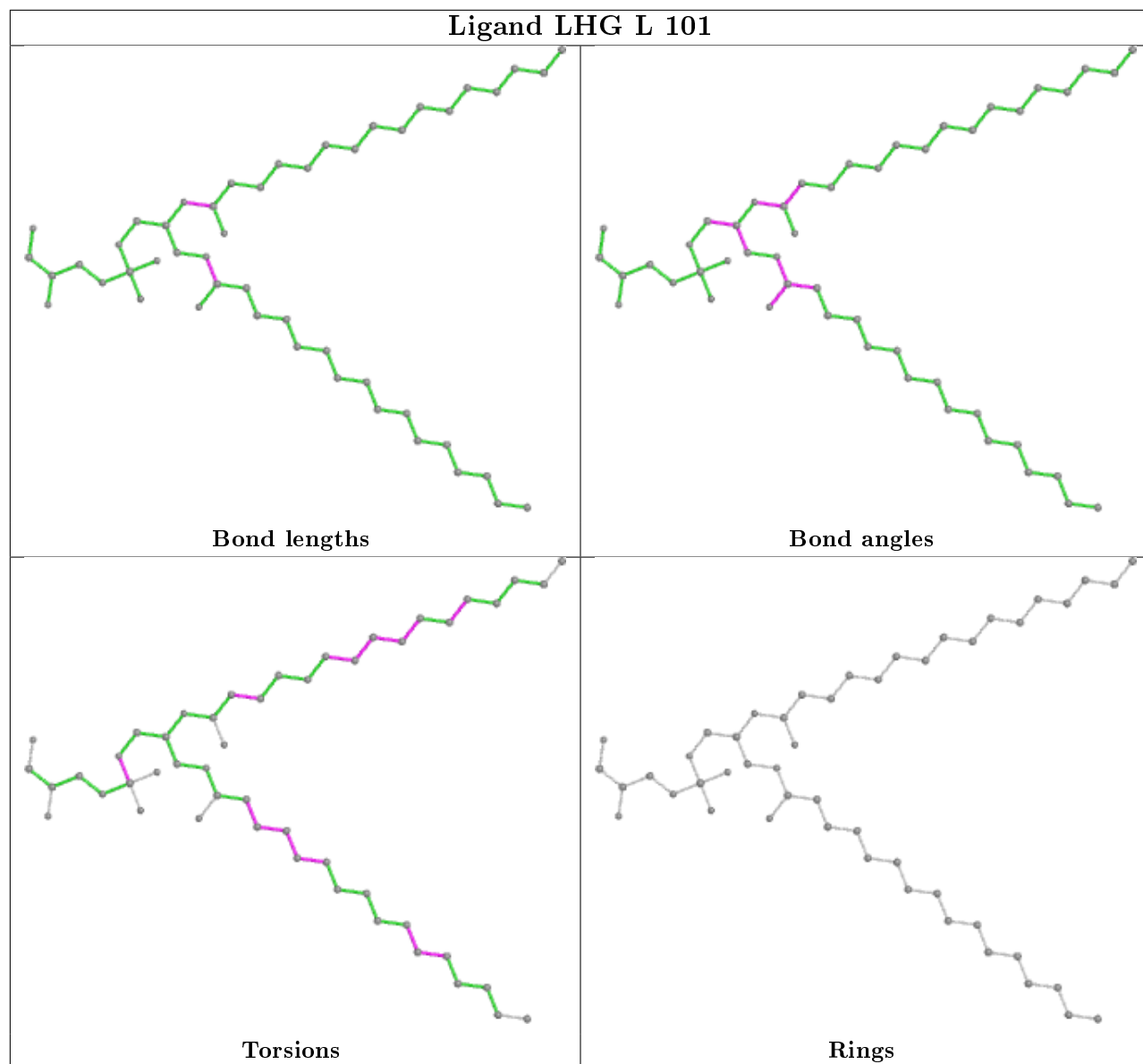


Ligand CLA B 605**Ligand CLA B 611****Ligand BCR h 101**

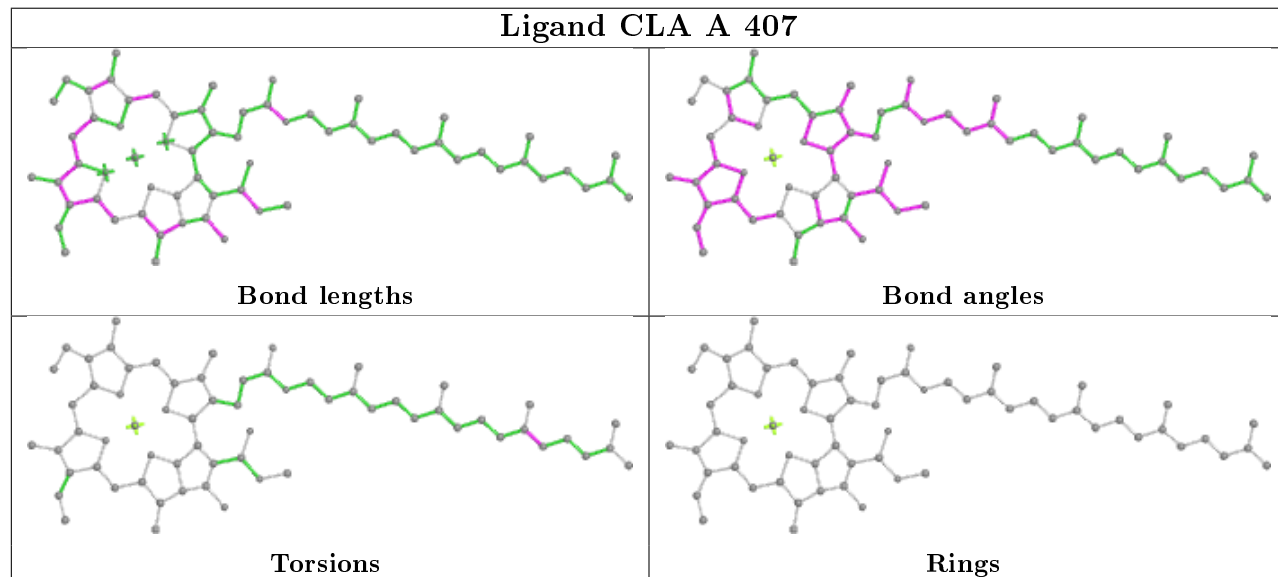


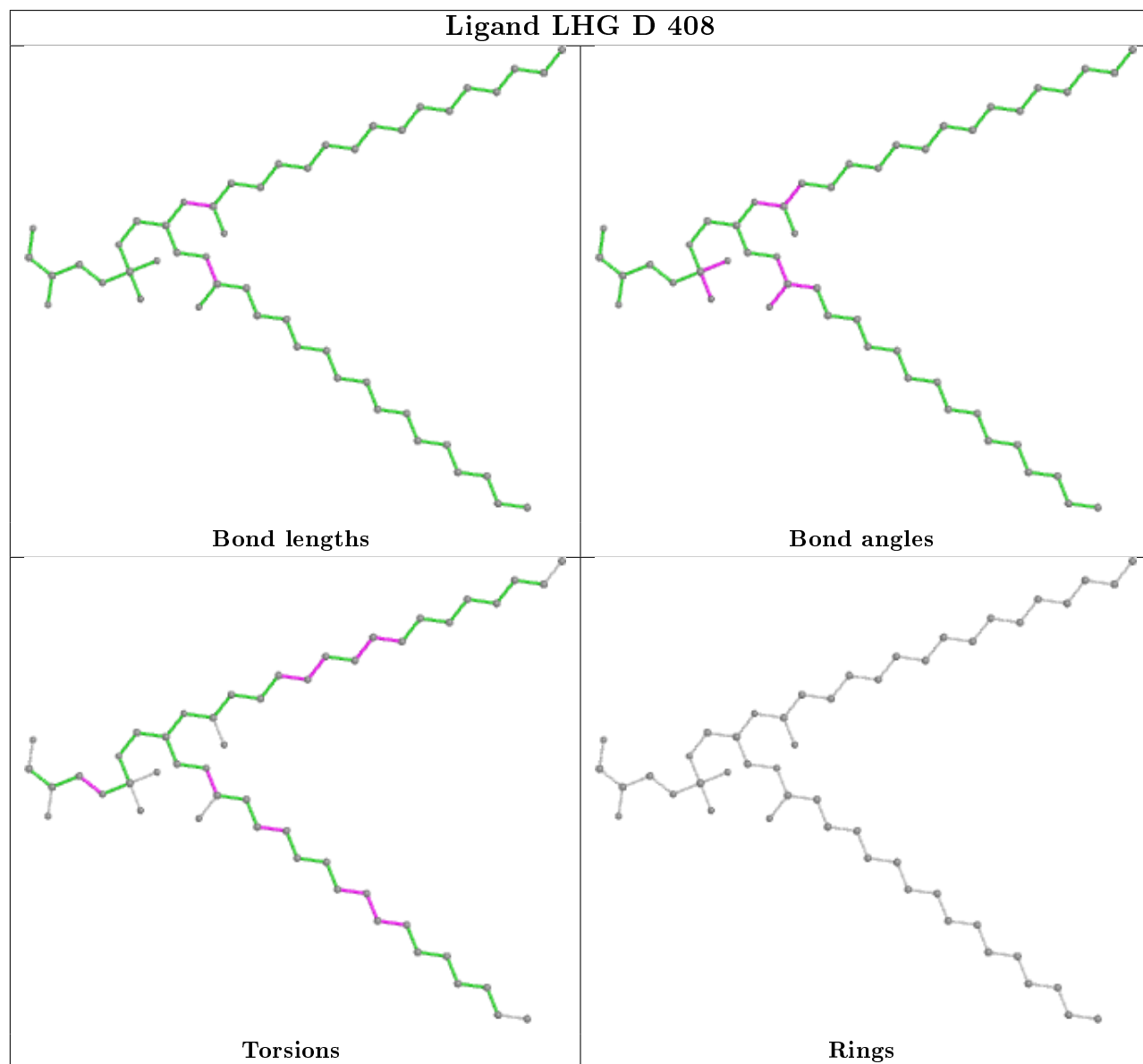
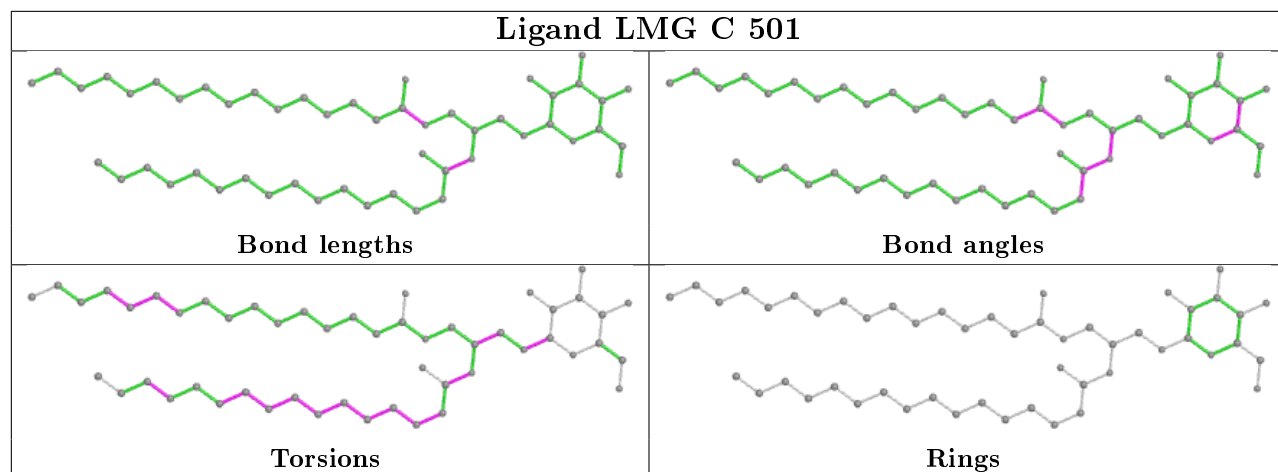
Ligand CLA C 508**Ligand CLA B 617****Ligand BCR K 102**

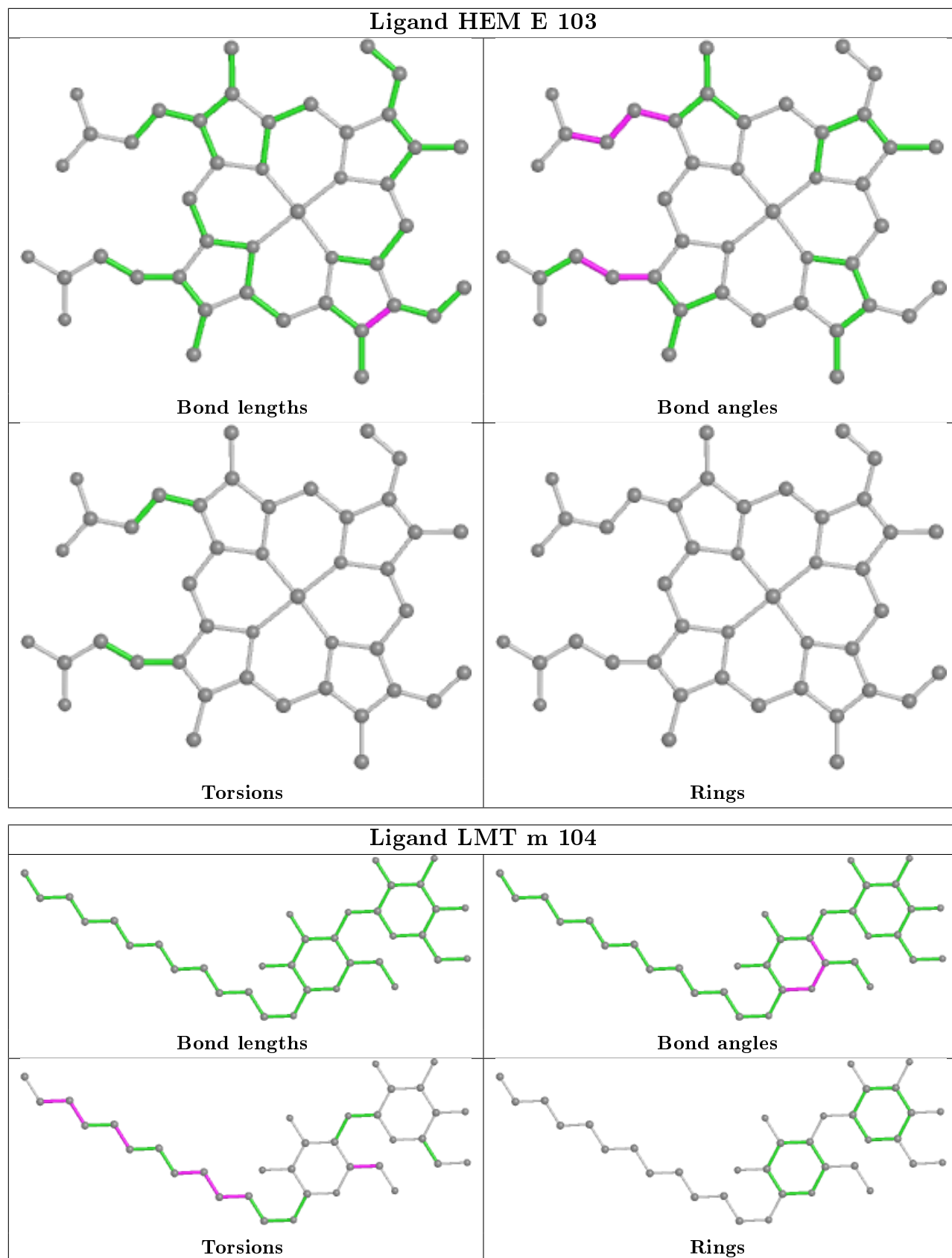
Ligand LHG L 101



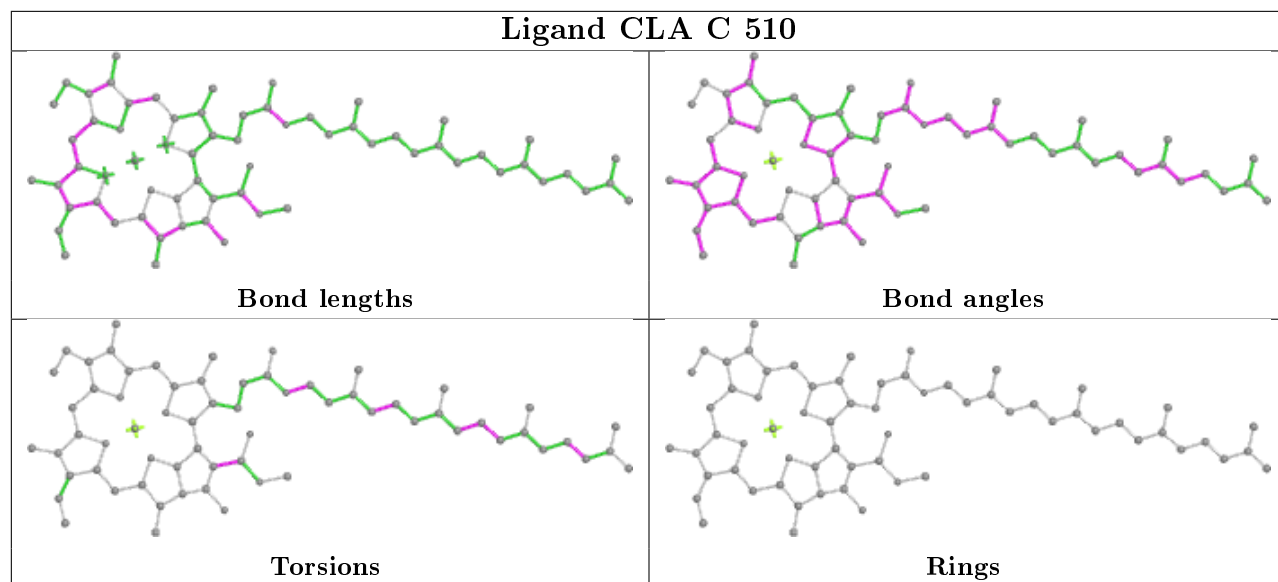
Ligand CLA A 407



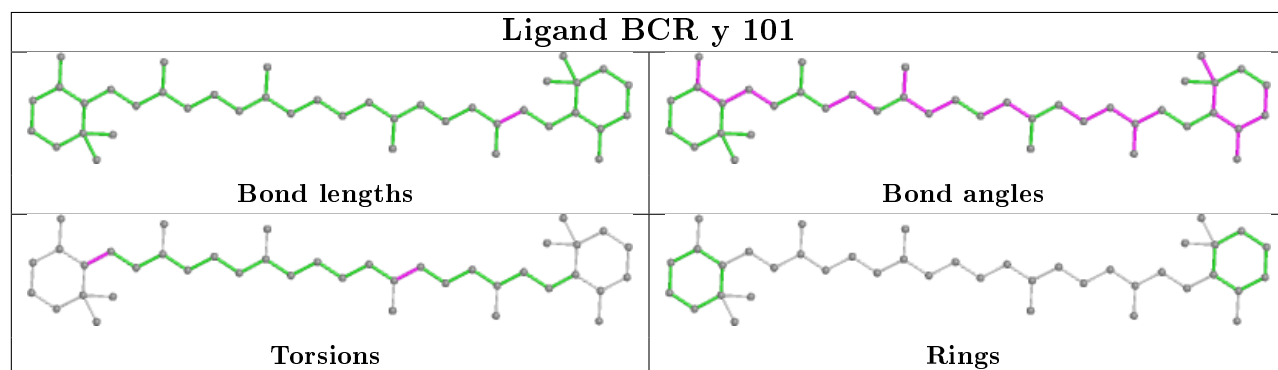




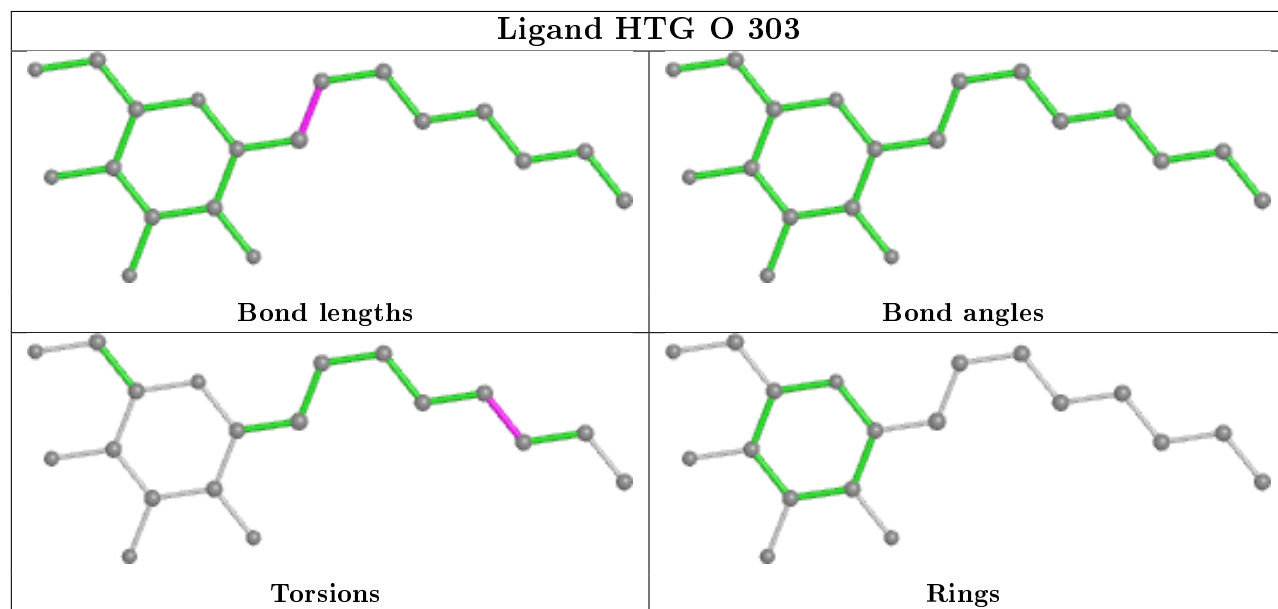
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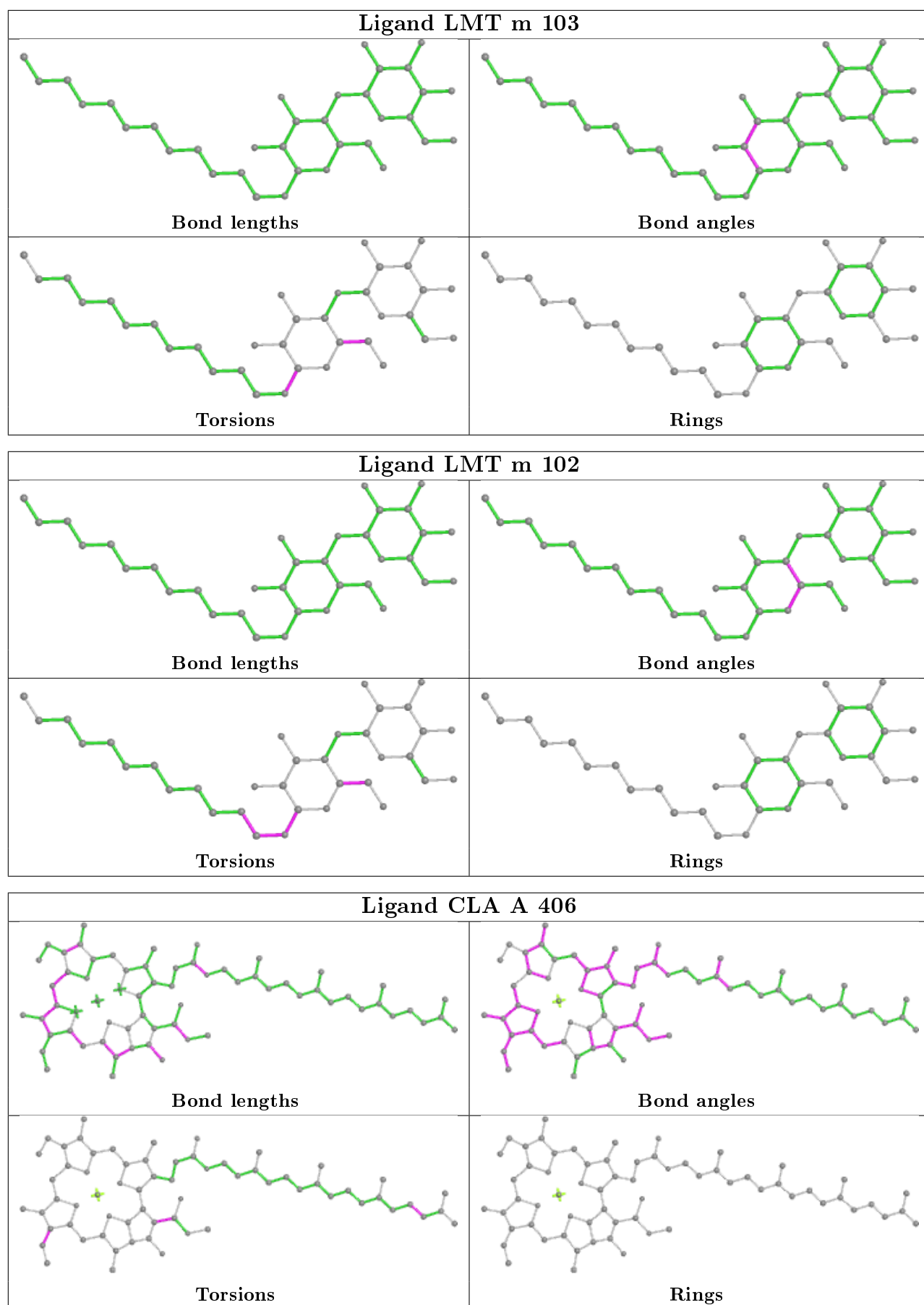


Ligand BCR y 101

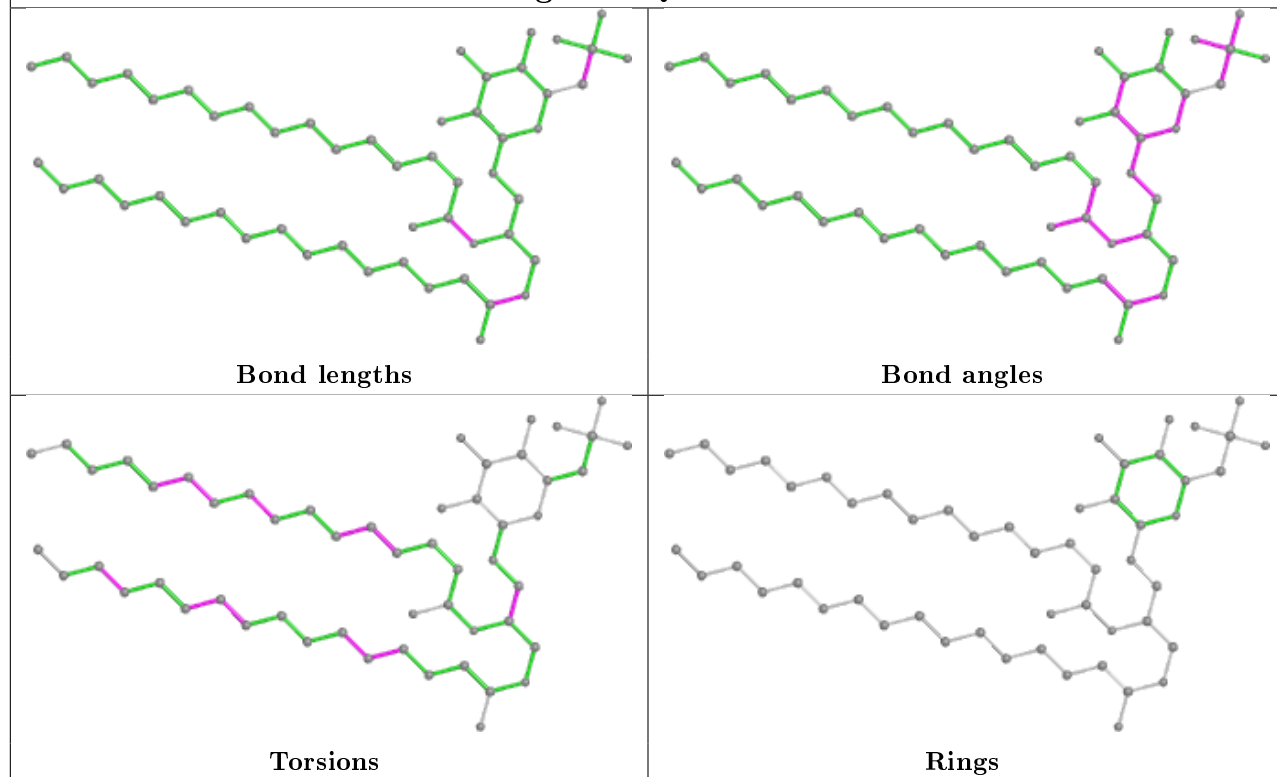


Ligand HTG O 303

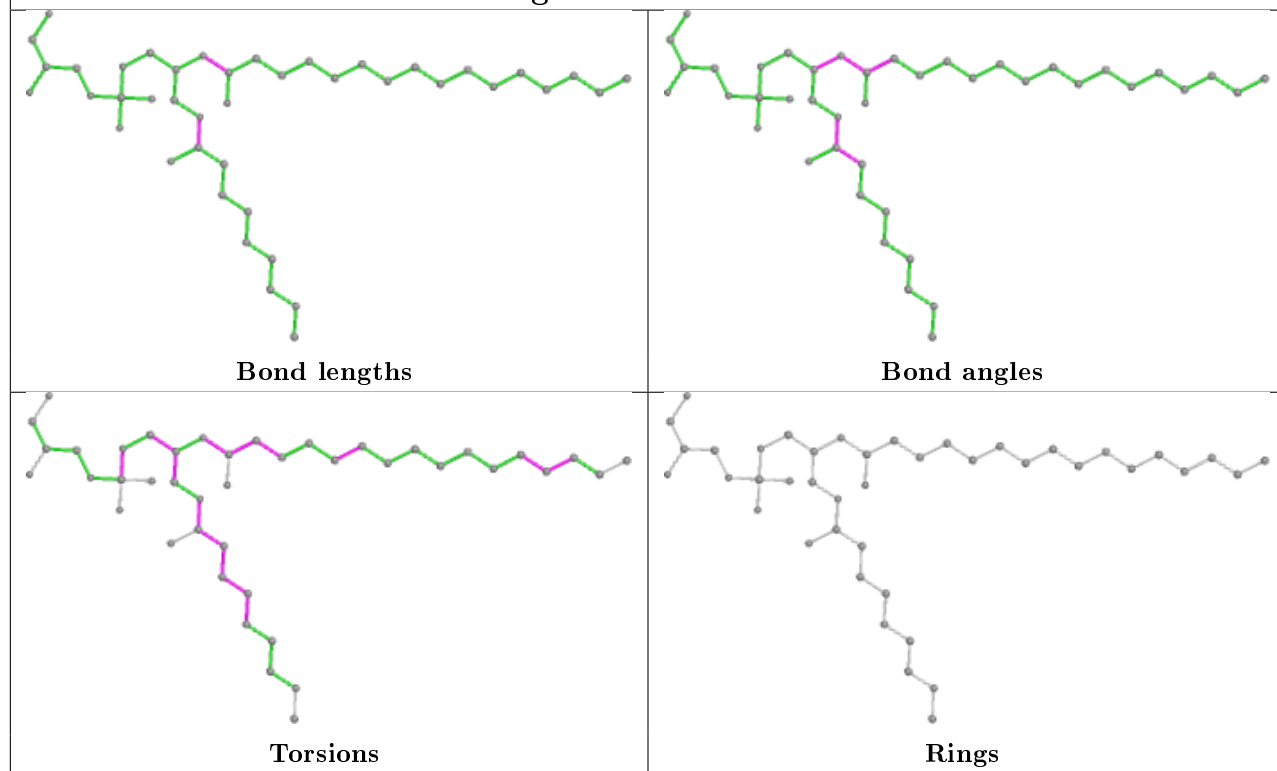


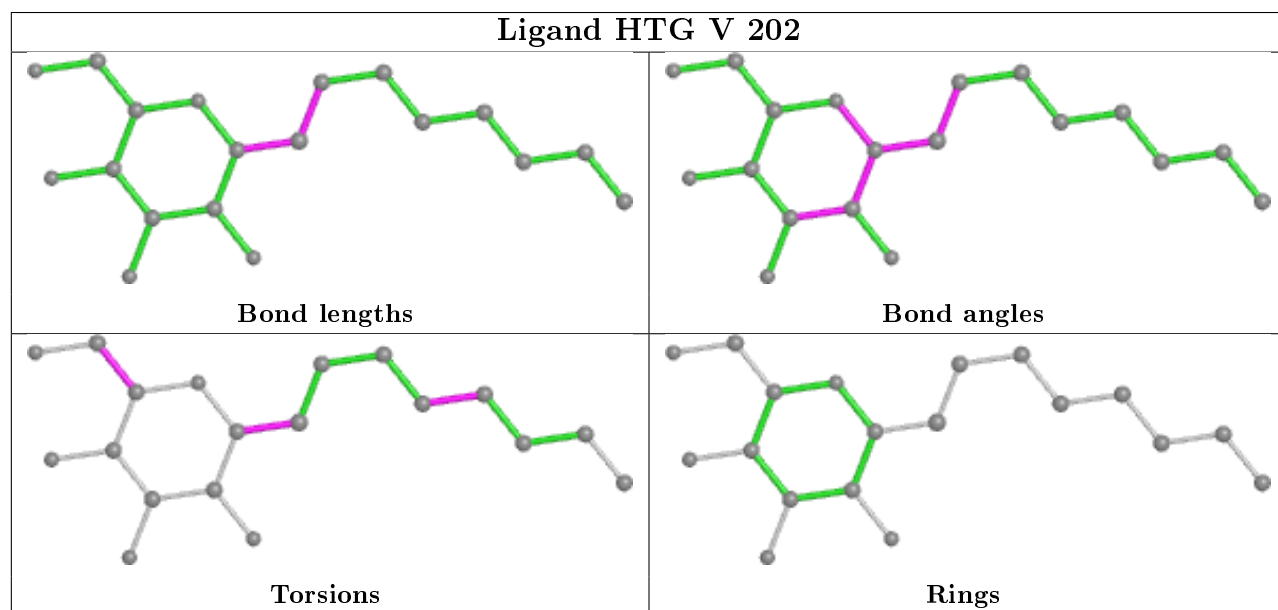
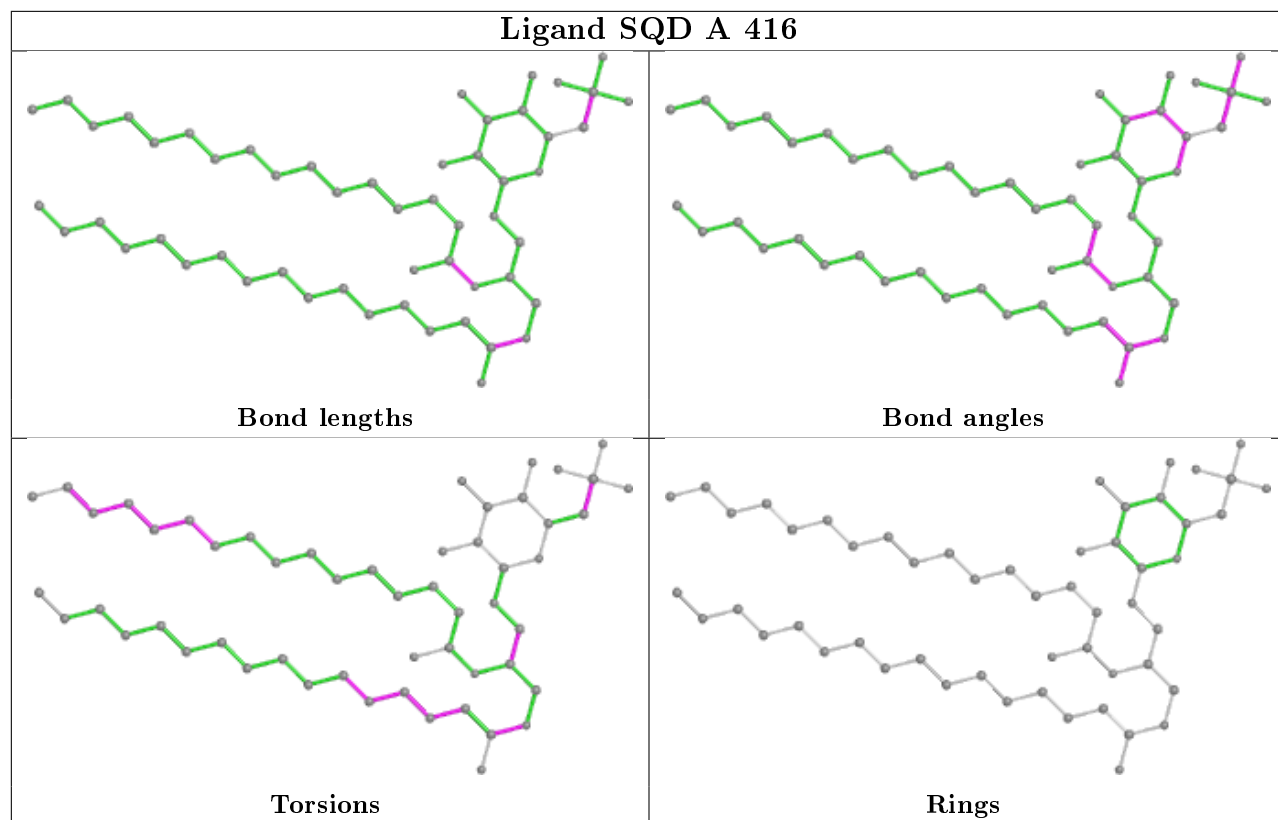


Ligand SQD a 411

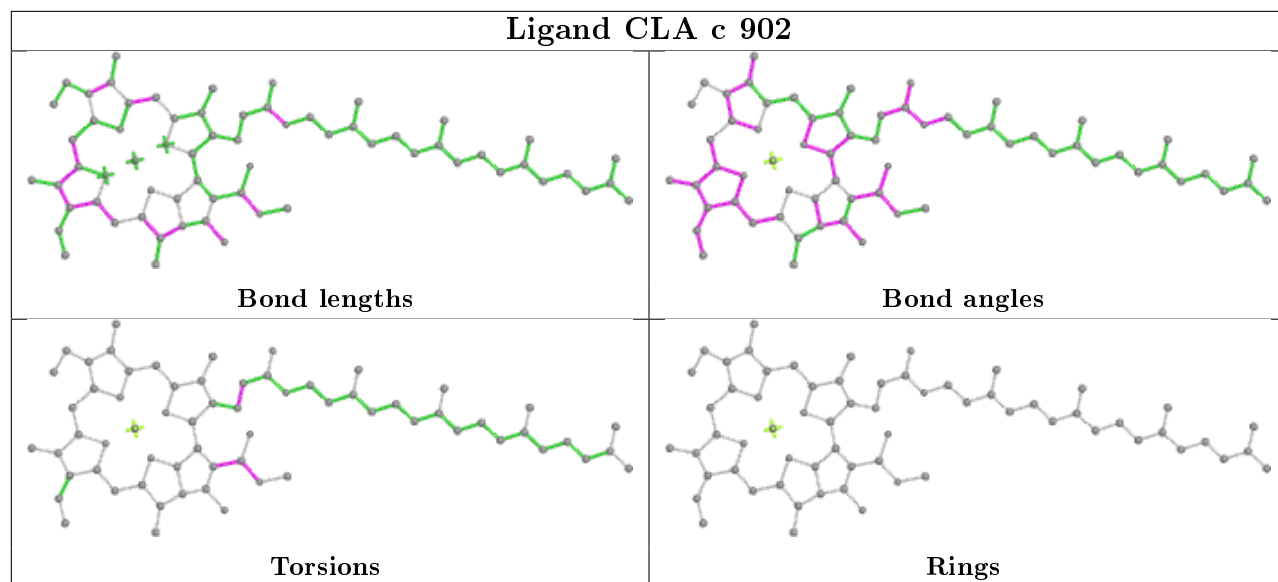


Ligand LHG E 101

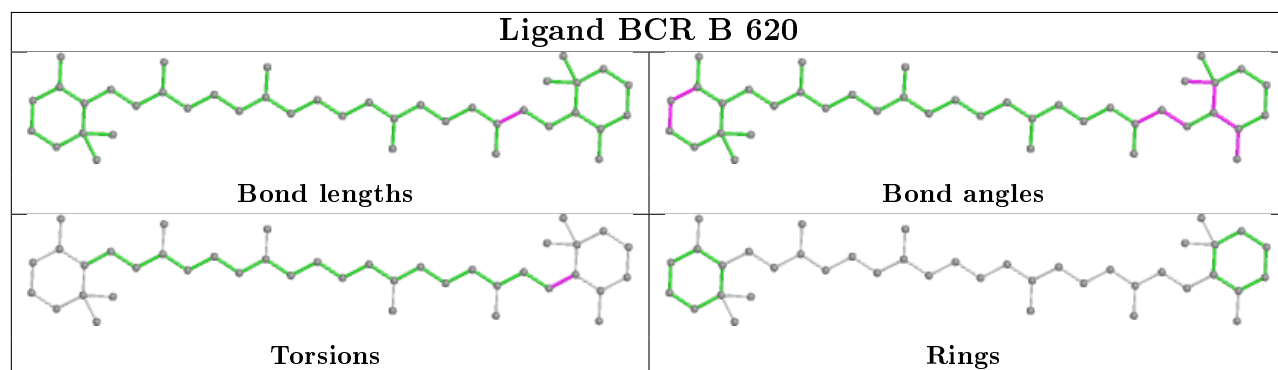




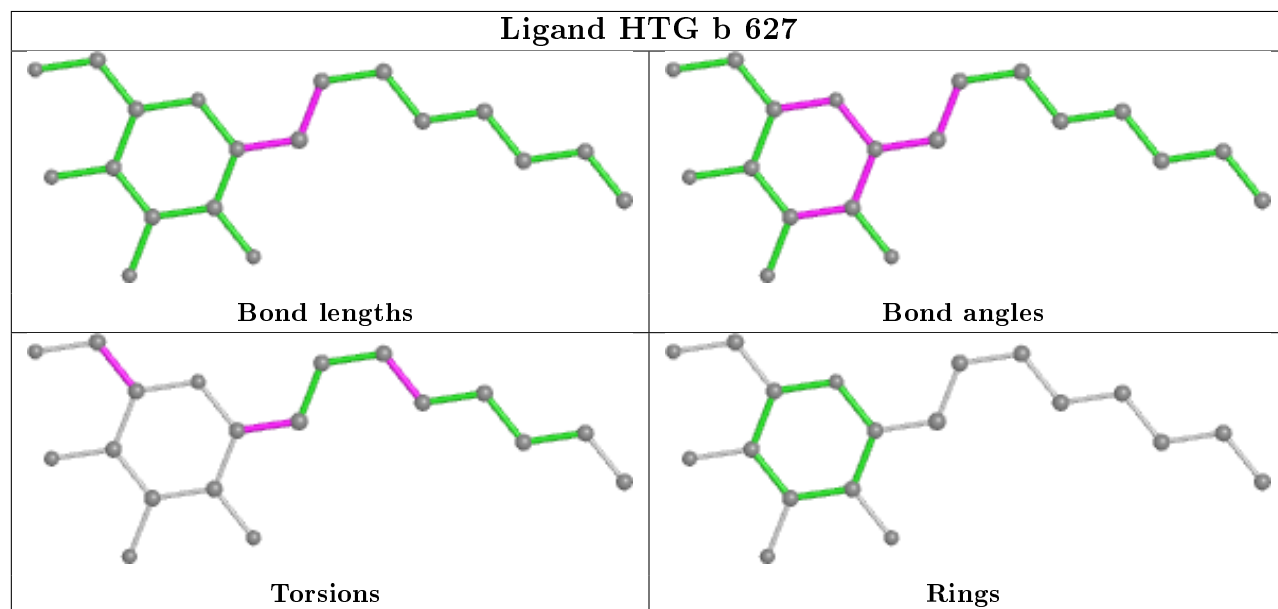
Ligand CLA c 902

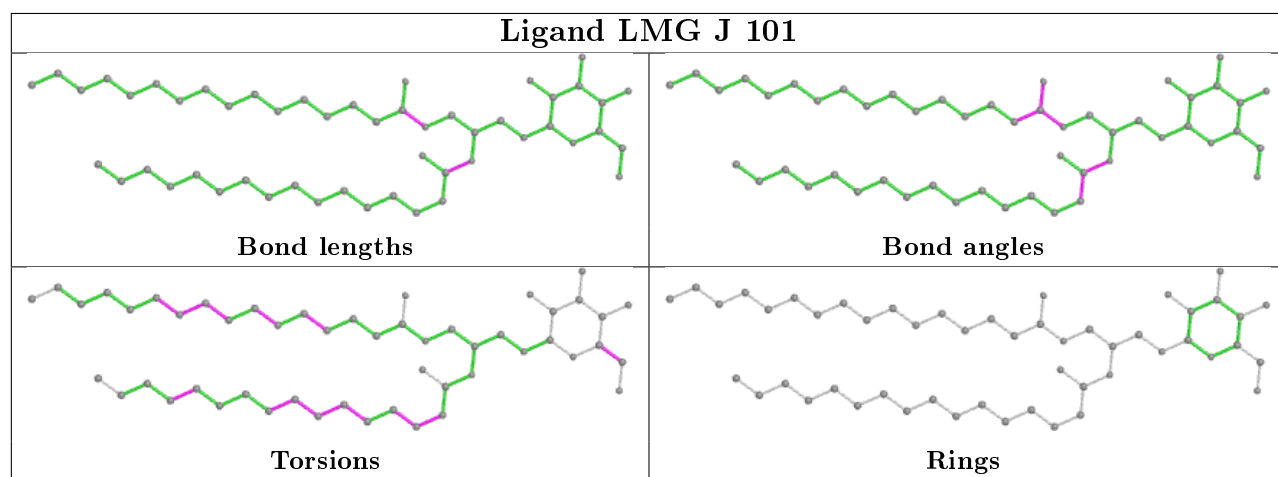
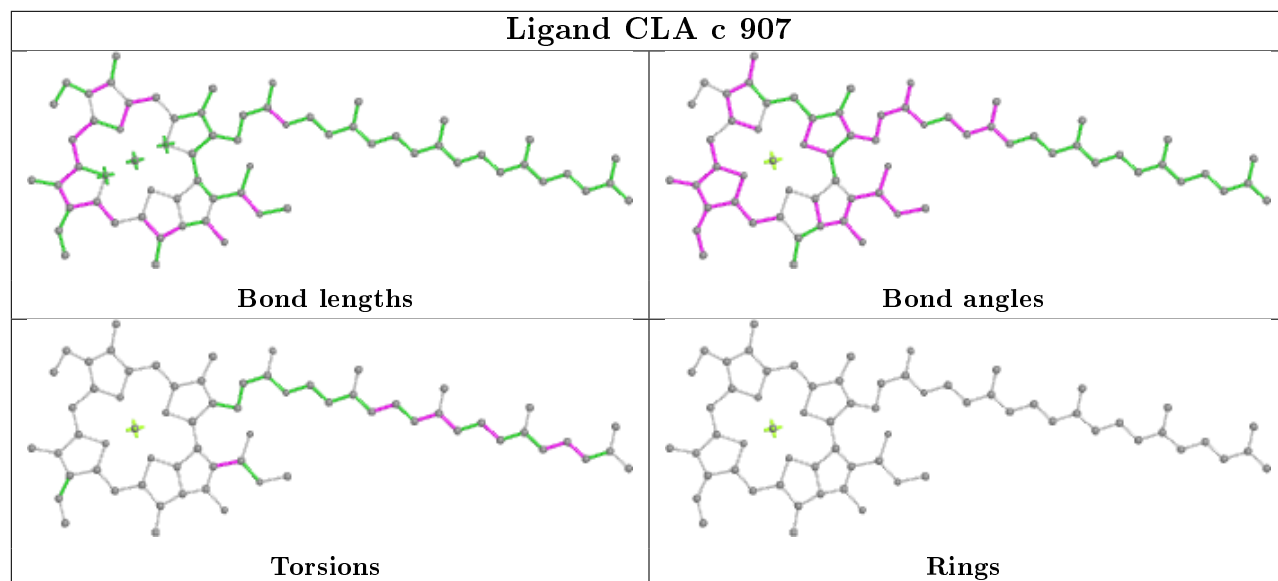
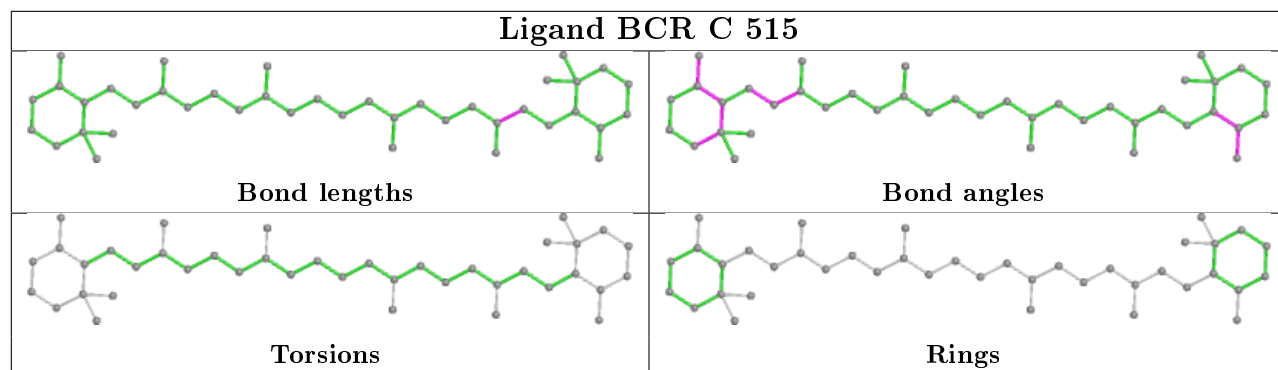


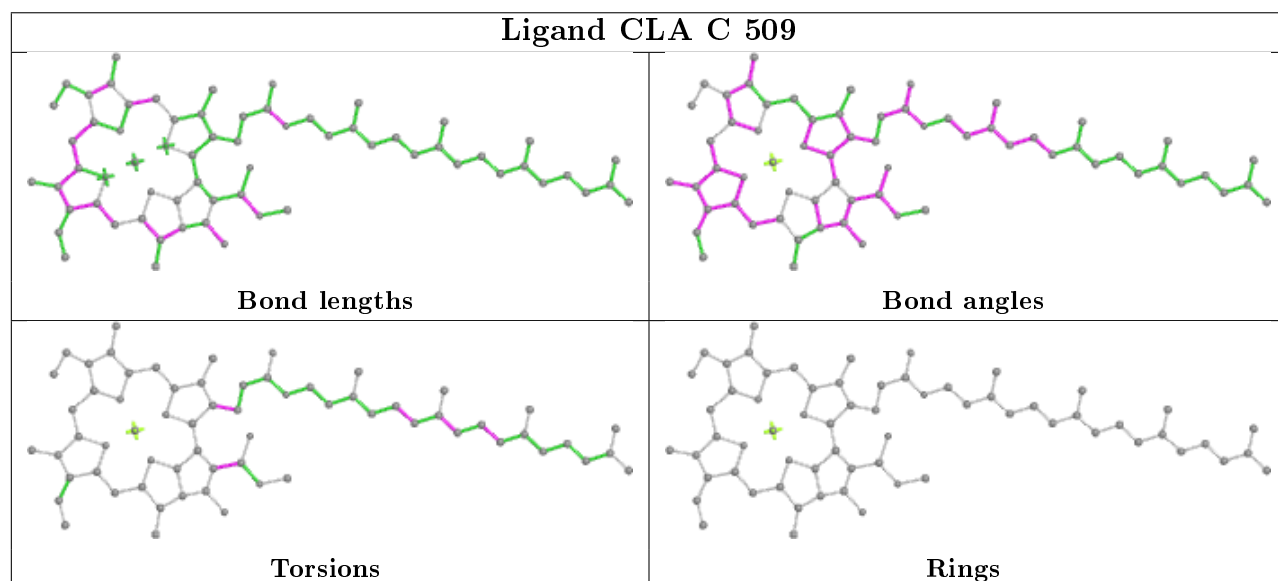
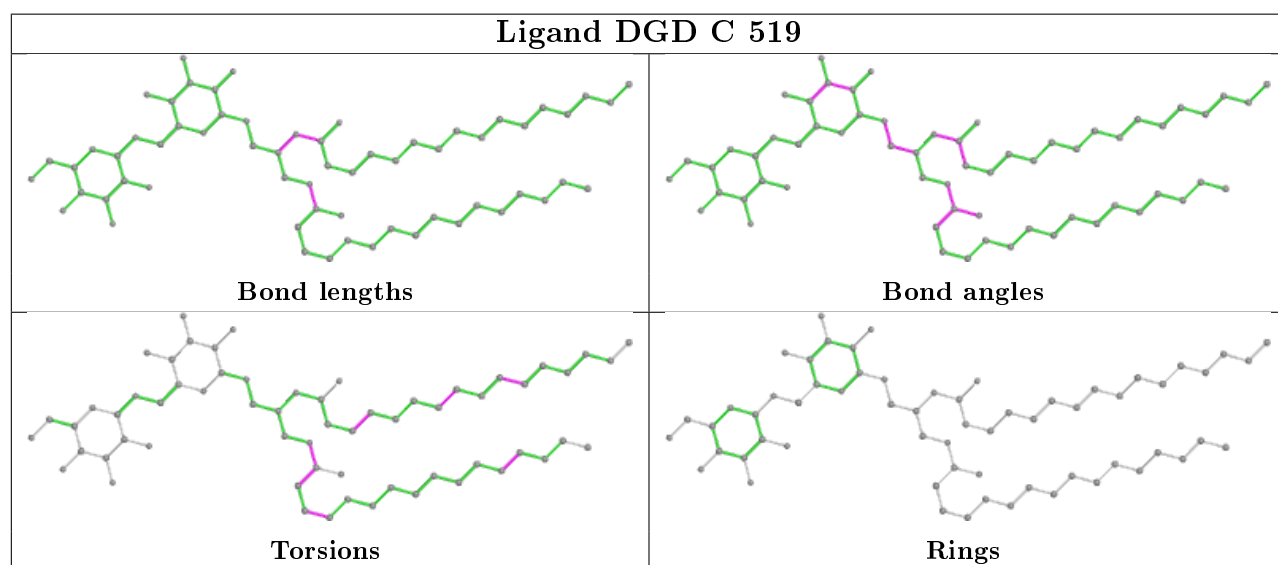
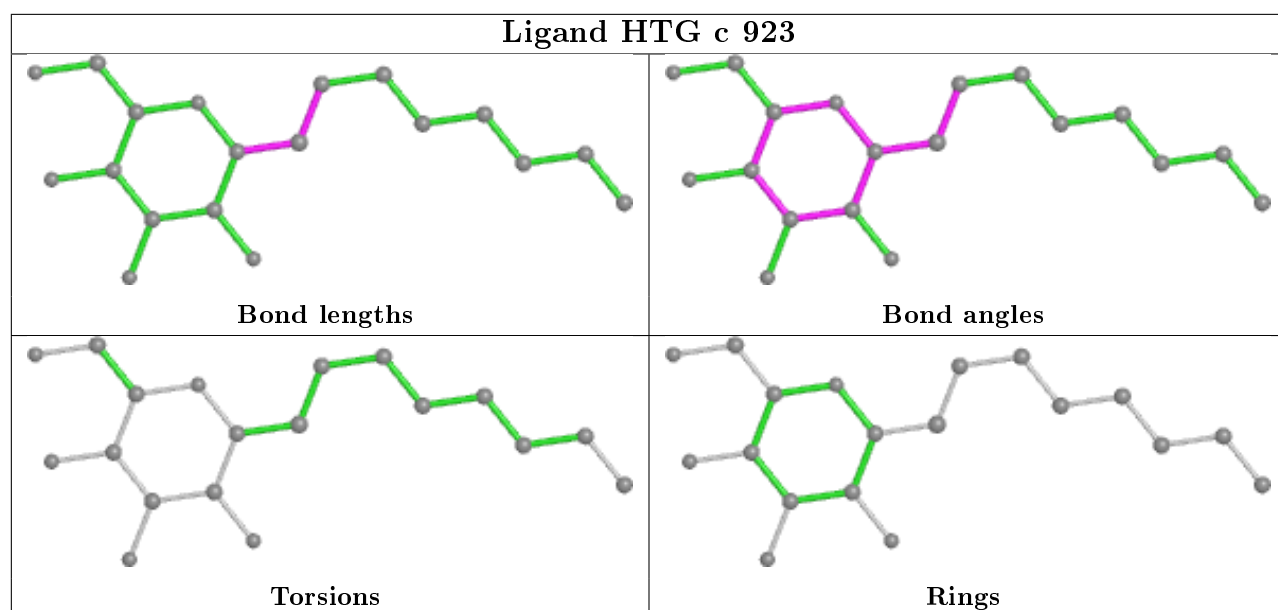
Ligand BCR B 620

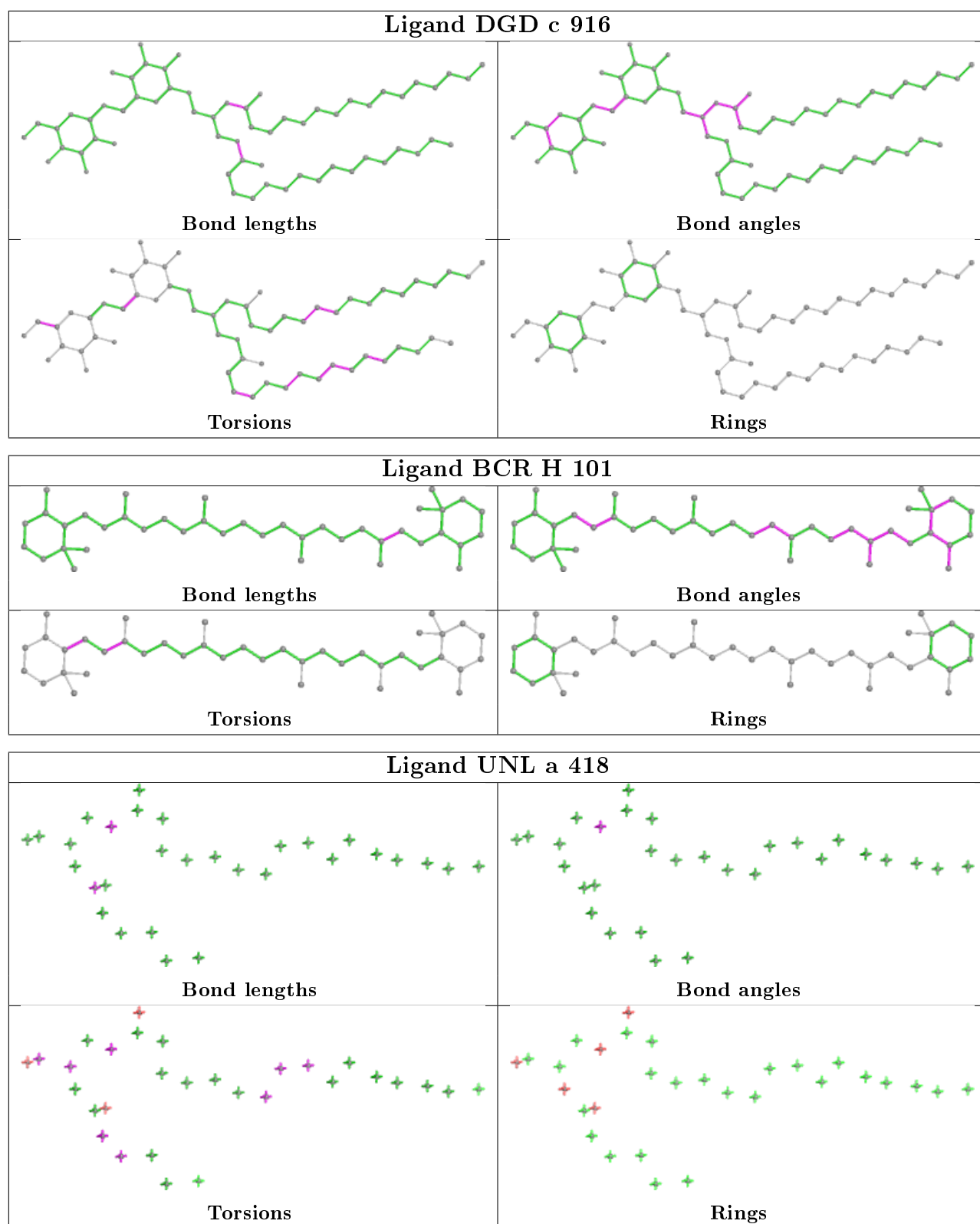


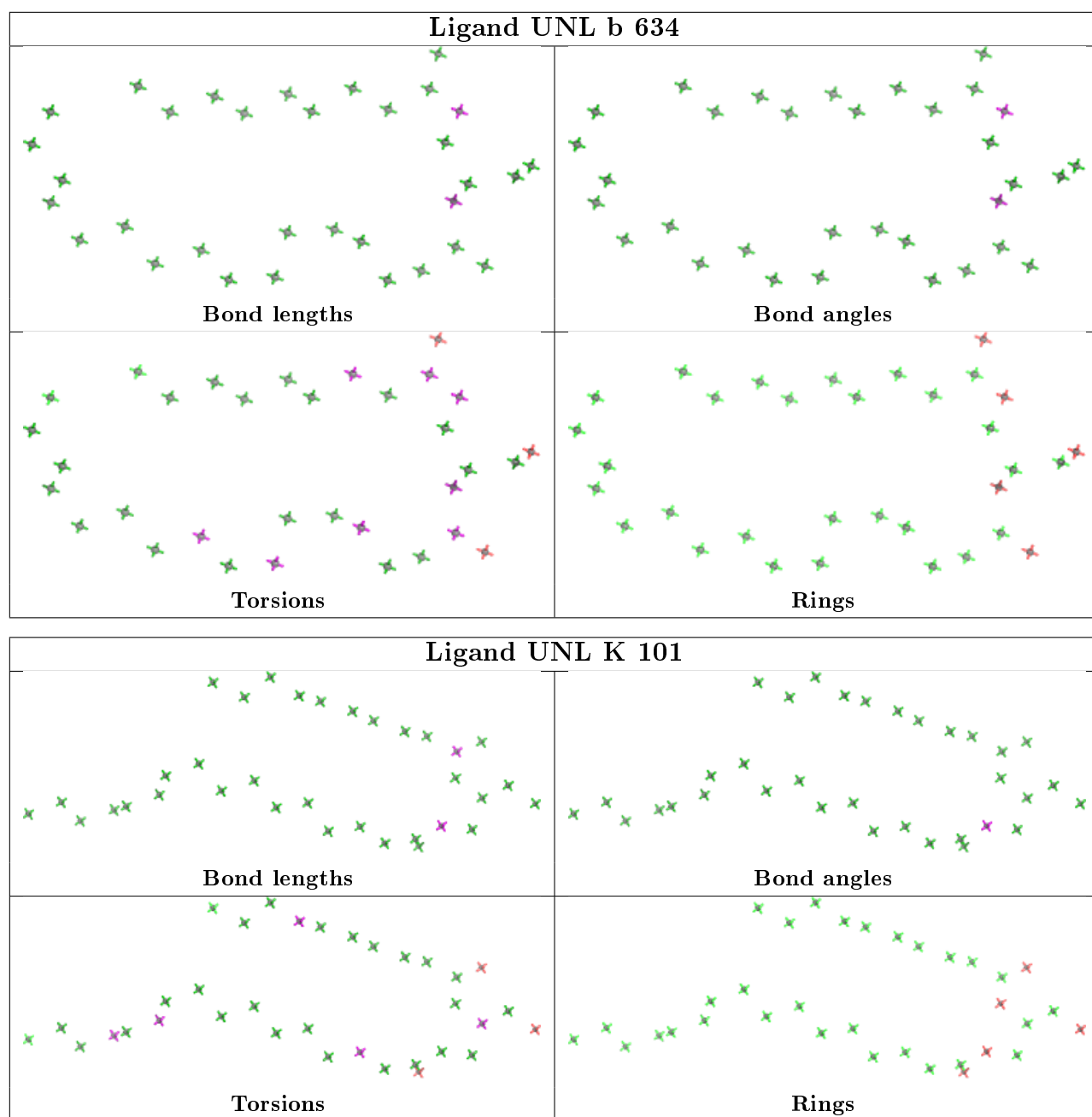
Ligand HTG b 627

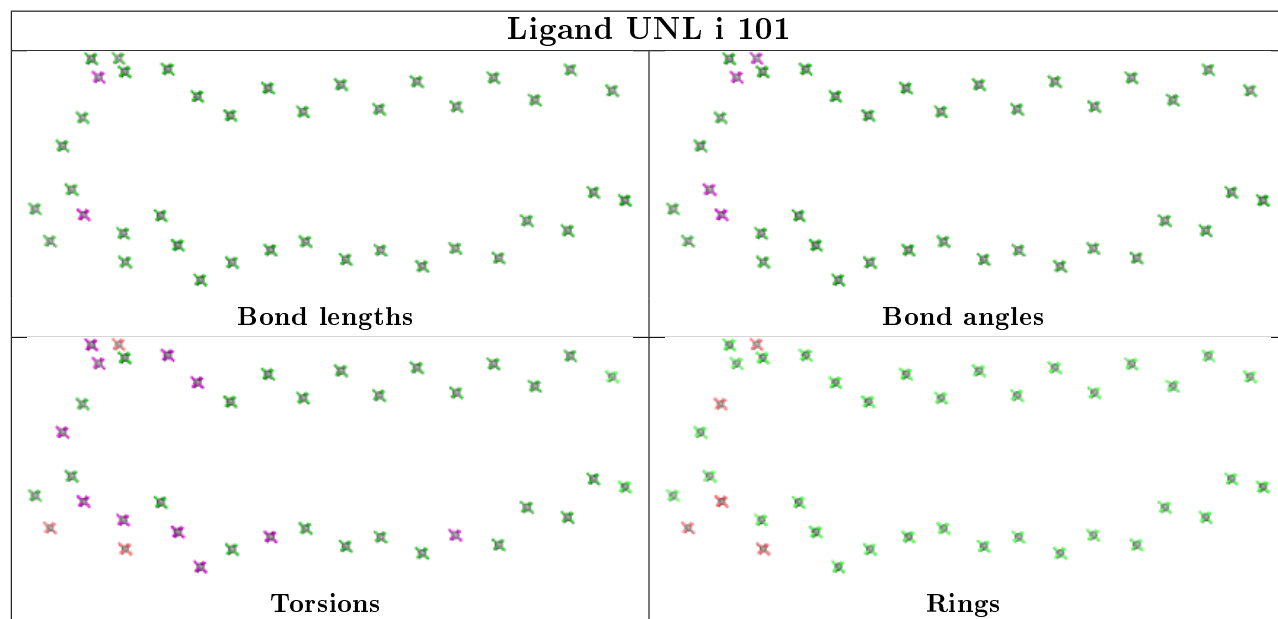
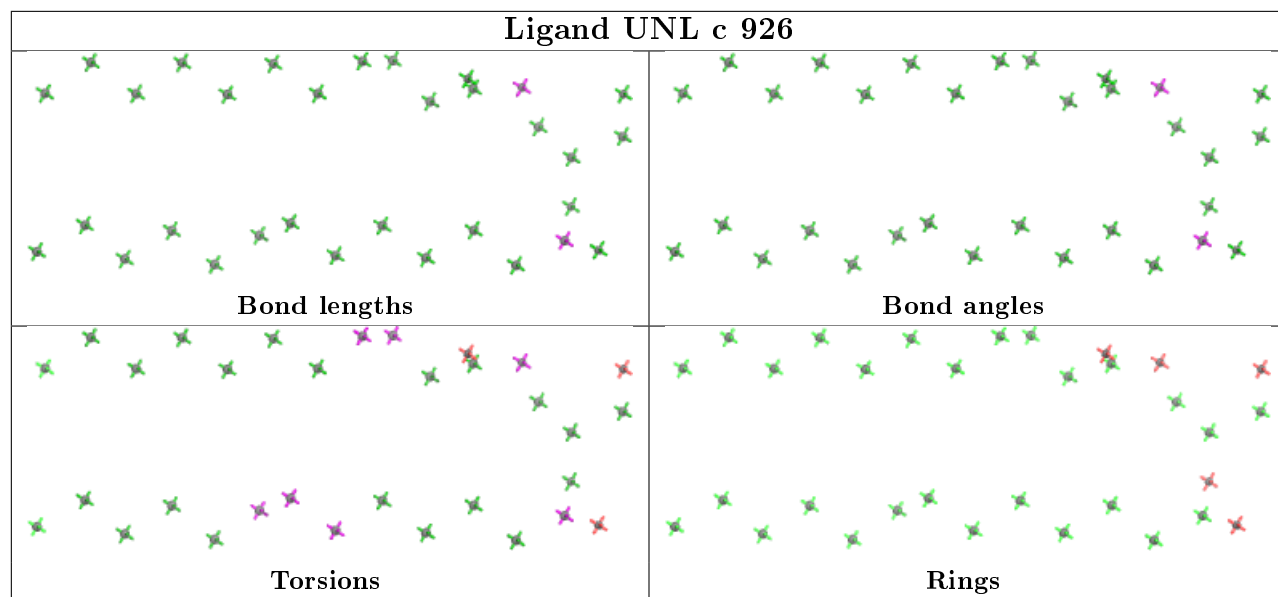


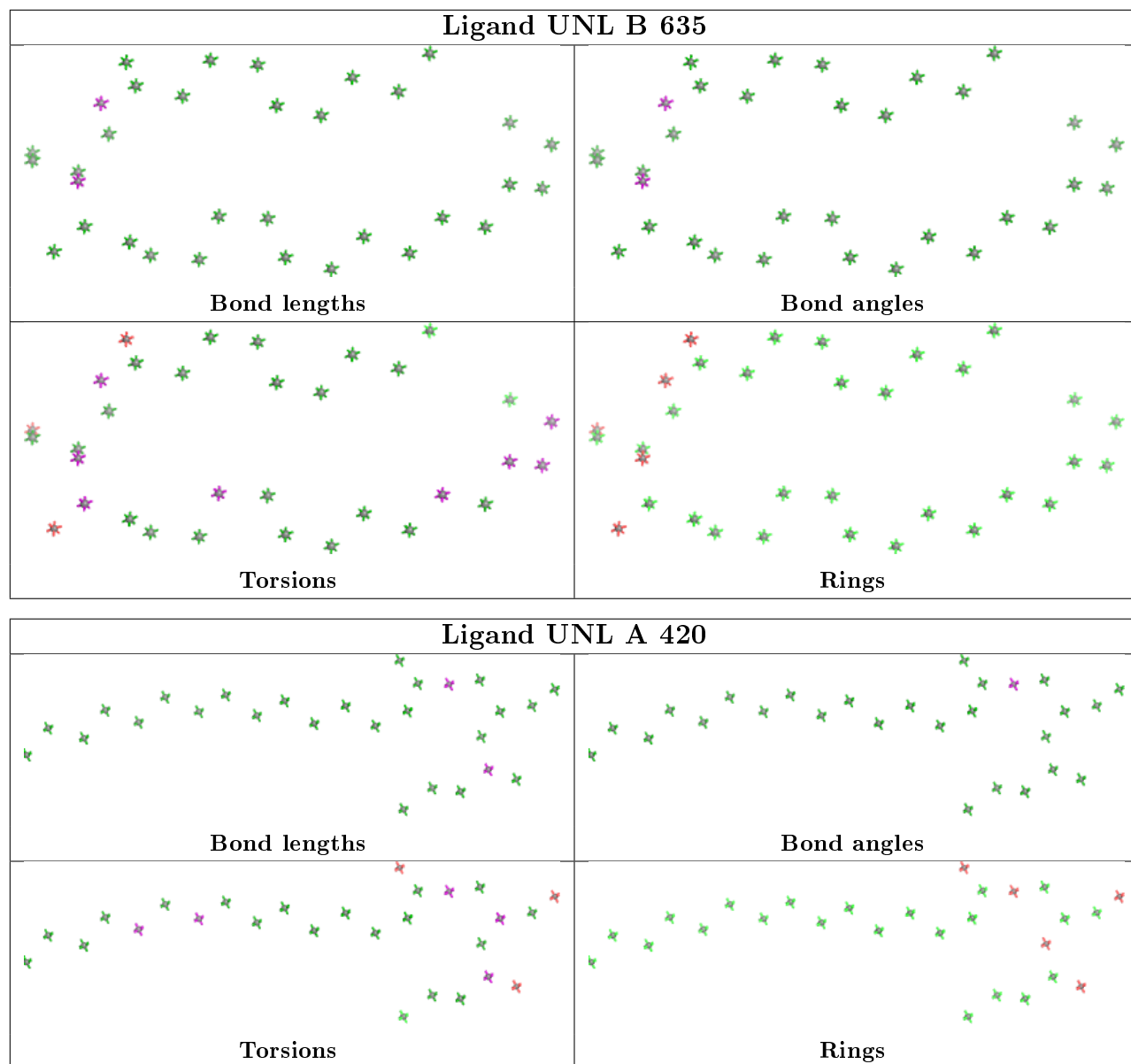


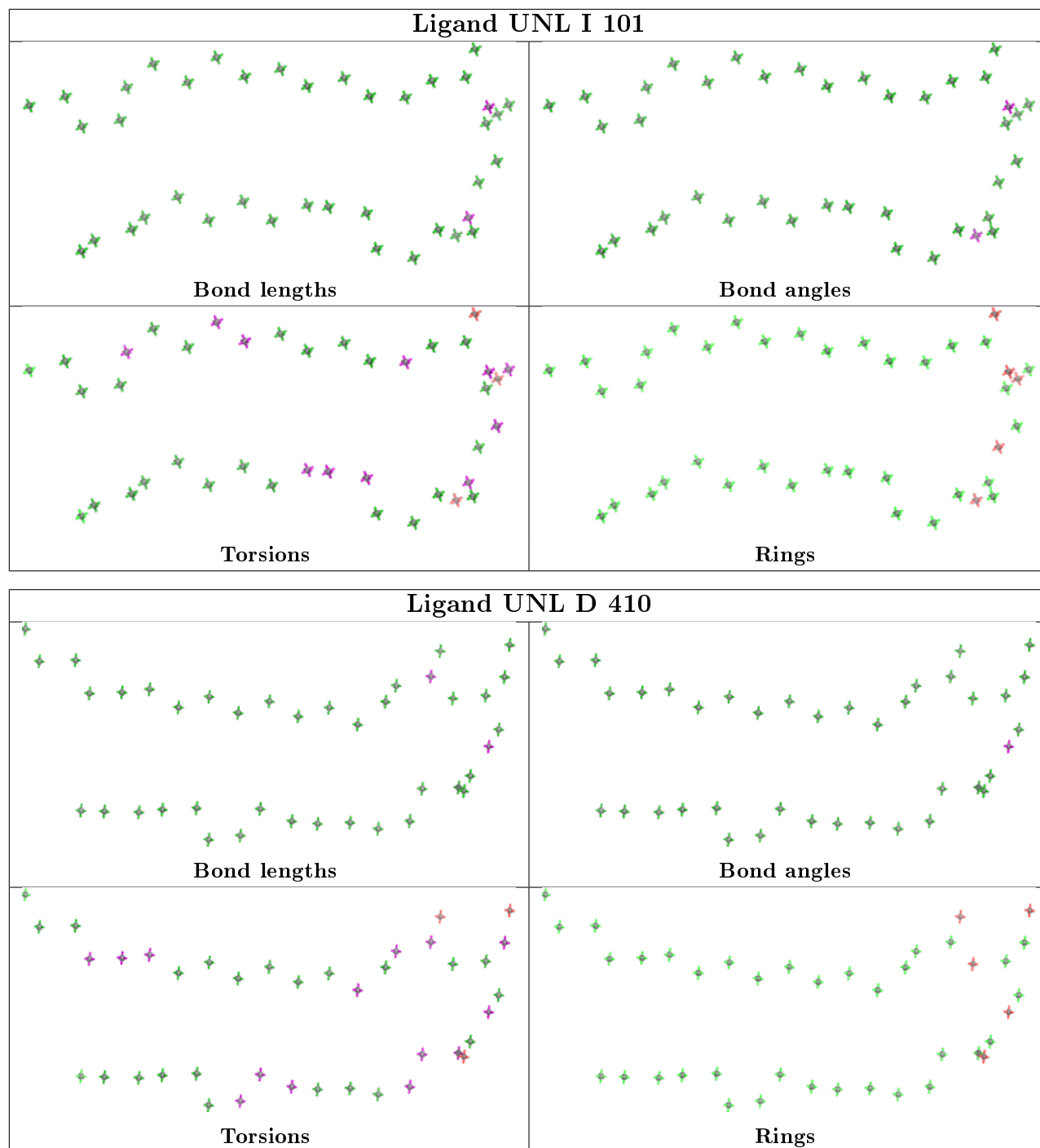


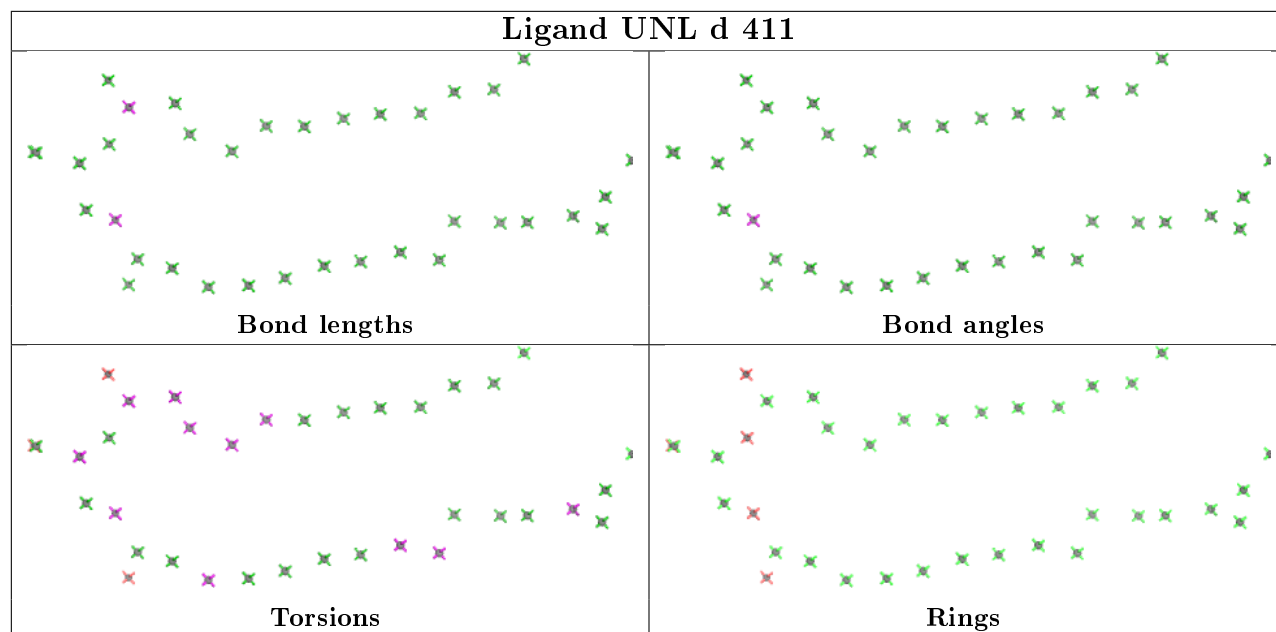












5.7 Other polymers [i](#)

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%)	0.43	20 (5%) 21 30	13, 21, 38, 73	0
1	a	334/344 (97%)	0.58	35 (10%) 6 10	15, 23, 47, 90	0
2	B	504/505 (99%)	0.17	27 (5%) 25 34	15, 25, 48, 78	0
2	b	504/505 (99%)	0.26	36 (7%) 16 24	16, 27, 59, 92	0
3	C	451/455 (99%)	0.14	17 (3%) 40 50	18, 30, 46, 73	0
3	c	455/455 (100%)	0.29	26 (5%) 23 32	21, 33, 49, 92	0
4	D	342/342 (100%)	0.56	31 (9%) 9 15	14, 22, 37, 97	0
4	d	341/342 (99%)	0.36	18 (5%) 26 35	16, 25, 39, 90	0
5	E	81/84 (96%)	0.85	10 (12%) 4 6	26, 37, 66, 92	0
5	e	81/84 (96%)	1.10	12 (14%) 2 3	30, 42, 71, 92	0
6	F	34/44 (77%)	0.34	4 (11%) 4 7	23, 30, 50, 61	0
6	f	32/44 (72%)	0.27	3 (9%) 8 13	30, 34, 79, 84	0
7	H	65/65 (100%)	0.22	2 (3%) 49 58	23, 31, 46, 110	0
7	h	65/65 (100%)	0.72	8 (12%) 4 6	27, 35, 52, 105	0
8	I	37/38 (97%)	0.58	5 (13%) 3 5	26, 33, 88, 108	0
8	i	37/38 (97%)	0.52	3 (8%) 12 18	27, 33, 73, 102	0
9	J	38/39 (97%)	0.59	5 (13%) 3 5	24, 35, 84, 98	0
9	j	39/39 (100%)	0.37	3 (7%) 13 21	29, 38, 84, 96	0
10	K	37/37 (100%)	0.22	1 (2%) 54 63	27, 35, 54, 65	0
10	k	37/37 (100%)	0.85	7 (18%) 1 1	30, 38, 55, 68	0
11	L	37/37 (100%)	0.67	5 (13%) 3 5	15, 19, 56, 82	0
11	l	37/37 (100%)	0.79	5 (13%) 3 5	16, 20, 58, 83	0
12	M	33/36 (91%)	0.75	3 (9%) 9 15	15, 21, 45, 89	0
12	m	33/36 (91%)	0.67	3 (9%) 9 15	16, 21, 41, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.27	16 (6%) 18 26	16, 32, 66, 110	0
13	o	243/244 (99%)	0.71	44 (18%) 1 1	19, 33, 71, 125	0
14	T	29/32 (90%)	0.83	3 (10%) 6 10	16, 20, 43, 89	0
14	t	29/32 (90%)	0.45	2 (6%) 16 25	16, 20, 46, 89	0
15	U	97/104 (93%)	0.34	4 (4%) 37 46	21, 31, 54, 84	0
15	u	97/104 (93%)	-0.08	0 100 100	23, 33, 51, 84	0
16	V	137/137 (100%)	-0.09	0 100 100	20, 31, 51, 69	0
16	v	137/137 (100%)	0.47	12 (8%) 10 16	24, 36, 57, 70	0
17	Y	29/30 (96%)	1.56	7 (24%) 0 0	35, 47, 82, 101	0
17	y	29/30 (96%)	1.42	7 (24%) 0 0	38, 50, 83, 100	0
18	X	39/40 (97%)	0.60	5 (12%) 3 6	31, 38, 75, 102	0
18	x	39/40 (97%)	1.50	11 (28%) 0 0	33, 41, 83, 102	0
19	Z	62/62 (100%)	1.29	17 (27%) 0 0	36, 47, 83, 96	0
19	z	62/62 (100%)	2.79	35 (56%) 0 0	42, 49, 82, 96	0
20	R	34/34 (100%)	7.13	34 (100%) 0 0	55, 75, 98, 106	0
All	All	5294/5384 (98%)	0.48	486 (9%) 9 14	13, 29, 61, 125	0

The worst 5 of 486 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	15.8
20	R	18	TRP	11.3
7	H	65	LEU	11.1
17	Y	18	VAL	10.5
20	R	23	ILE	10.4

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
12	FME	m	1	10/11	0.93	0.16	13,32,67,68	0
8	FME	I	1	10/11	0.95	0.12	22,34,38,38	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	0.96	0.17	18,26,40,49	0
14	FME	t	1	10/11	0.96	0.12	12,22,31,68	0
12	FME	M	1	10/11	0.97	0.12	23,36,70,74	0
8	FME	i	1	10/11	0.98	0.13	21,31,39,42	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
33	CA	b	604	1/1	0.47	0.25	117,117,117,117	0
36	DGD	D	405	62/66	0.55	0.40	48,79,113,122	0
29	LMT	E	102	35/35	0.57	0.34	43,80,109,115	0
29	LMT	f	103	35/35	0.59	0.37	43,86,107,111	0
36	DGD	d	406	62/66	0.61	0.45	38,89,122,130	0
35	HTG	B	626	19/19	0.61	0.36	48,81,94,95	0
28	GOL	B	637	6/6	0.61	0.26	51,72,83,86	0
35	HTG	B	634	19/19	0.65	0.29	32,76,109,127	0
32	UNL	A	420	28/-	0.66	0.28	50,71,78,86	0
35	HTG	b	603	19/19	0.67	0.24	46,84,110,111	0
32	UNL	b	634	33/-	0.68	0.29	29,62,111,117	0
29	LMT	m	102	35/35	0.68	0.25	33,61,79,95	0
37	LHG	e	101	42/49	0.69	0.28	52,89,118,129	0
32	UNL	K	101	34/-	0.70	0.30	37,61,83,88	0
35	HTG	d	412	16/19	0.70	0.31	38,78,97,98	0
29	LMT	b	625	25/35	0.71	0.29	44,67,109,119	0
32	UNL	c	926	32/-	0.71	0.36	39,79,98,105	0
32	UNL	B	635	33/-	0.72	0.25	33,58,102,102	0
29	LMT	M	101	35/35	0.72	0.21	23,52,69,77	0
35	HTG	b	627	19/19	0.72	0.27	49,86,110,116	0
31	PL9	a	417	55/55	0.73	0.26	41,73,92,99	0
32	UNL	a	418	30/-	0.73	0.31	42,66,98,106	0
34	LMG	z	101	39/55	0.73	0.33	45,82,99,107	0
29	LMT	C	522	35/35	0.74	0.40	52,81,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	GOL	v	203	6/6	0.75	0.31	39,74,86,87	0
32	UNL	j	102	10/-	0.76	0.29	47,57,63,63	0
32	UNL	J	102	10/-	0.76	0.35	39,51,64,67	0
29	LMT	m	104	35/35	0.76	0.24	29,59,85,86	0
34	LMG	Z	101	37/55	0.76	0.28	30,75,96,112	0
28	GOL	a	415	6/6	0.76	0.22	48,62,65,66	0
35	HTG	C	524	19/19	0.76	0.30	41,69,99,100	0
33	CA	B	601	1/1	0.77	0.10	83,83,83,83	0
32	UNL	i	101	40/-	0.77	0.24	28,62,105,117	0
32	UNL	d	413	18/-	0.78	0.19	30,52,81,84	0
34	LMG	C	521	51/55	0.78	0.25	32,69,88,108	0
34	LMG	a	412	51/55	0.78	0.21	33,62,84,90	0
28	GOL	O	302	6/6	0.78	0.23	49,55,57,61	0
32	UNL	I	101	40/-	0.78	0.24	27,62,110,120	0
27	SQD	B	621	54/54	0.78	0.20	26,55,94,104	0
27	SQD	L	102	54/54	0.78	0.22	24,52,86,91	0
28	GOL	V	203	6/6	0.78	0.43	50,64,71,72	0
35	HTG	D	411	16/19	0.78	0.26	38,102,111,112	0
35	HTG	c	923	19/19	0.78	0.30	45,80,94,97	0
34	LMG	C	501	51/55	0.80	0.21	34,56,76,85	0
32	UNL	d	411	36/-	0.80	0.23	32,56,104,111	0
35	HTG	c	922	19/19	0.81	0.21	43,67,84,95	0
31	PL9	A	419	55/55	0.81	0.23	28,56,91,98	0
29	LMT	B	623	35/35	0.81	0.22	26,74,96,101	0
28	GOL	A	415	6/6	0.81	0.19	36,49,64,64	0
27	SQD	a	402	54/54	0.81	0.20	29,55,76,90	0
28	GOL	f	101	6/6	0.82	0.25	44,50,62,64	0
28	GOL	T	103	6/6	0.82	0.23	52,68,70,79	0
32	UNL	m	101	10/-	0.82	0.21	35,50,55,61	0
32	UNL	M	102	10/-	0.82	0.21	28,38,57,58	0
34	LMG	c	919	51/55	0.82	0.21	29,57,78,81	0
37	LHG	E	101	42/49	0.82	0.22	22,63,78,93	0
27	SQD	A	416	54/54	0.82	0.20	26,51,78,85	0
34	LMG	c	920	51/55	0.82	0.25	33,74,88,93	0
32	UNL	D	410	40/-	0.82	0.20	24,54,93,101	0
29	LMT	c	921	35/35	0.83	0.40	46,76,97,104	0
29	LMT	a	401	35/35	0.83	0.20	21,53,74,80	0
29	LMT	b	601	25/35	0.83	0.27	18,55,104,111	0
29	LMT	m	103	35/35	0.84	0.17	19,48,62,74	0
28	GOL	V	206	6/6	0.84	0.27	47,63,66,66	0
34	LMG	C	520	51/55	0.84	0.22	22,52,72,90	0
29	LMT	B	636	25/35	0.85	0.23	24,61,106,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	LMT	A	417	35/35	0.85	0.19	22,57,79,97	0
28	GOL	B	629	6/6	0.85	0.21	28,42,50,56	0
28	GOL	b	632	6/6	0.85	0.20	38,52,59,59	0
28	GOL	B	628	6/6	0.86	0.31	33,42,54,72	0
27	SQD	f	102	43/54	0.86	0.24	41,75,103,108	0
34	LMG	B	622	51/55	0.87	0.23	19,32,49,71	0
28	GOL	B	631	6/6	0.87	0.24	30,48,62,65	0
28	GOL	v	204	6/6	0.87	0.17	54,66,71,80	0
32	UNL	X	101	18/-	0.87	0.15	29,44,62,79	0
32	UNL	D	409	17/-	0.87	0.16	30,40,63,66	0
32	UNL	d	410	17/-	0.87	0.18	34,48,82,82	0
28	GOL	A	414	6/6	0.87	0.18	30,40,43,49	0
35	HTG	B	633	19/19	0.88	0.16	28,54,70,76	0
24	CLA	c	914	65/65	0.88	0.26	35,48,81,87	0
35	HTG	b	602	19/19	0.88	0.15	29,45,65,68	0
28	GOL	t	102	6/6	0.88	0.25	22,59,67,67	0
28	GOL	T	101	6/6	0.88	0.27	54,60,61,69	0
28	GOL	c	925	6/6	0.89	0.23	34,52,63,66	0
26	BCR	d	404	40/40	0.89	0.15	27,36,54,60	0
35	HTG	V	202	19/19	0.89	0.19	40,59,77,163	0
26	BCR	k	102	40/40	0.89	0.15	30,37,50,61	0
34	LMG	b	624	51/55	0.89	0.23	21,36,57,81	0
28	GOL	o	302	6/6	0.90	0.13	44,50,53,58	0
36	DGD	H	102	62/66	0.90	0.16	16,28,46,59	0
28	GOL	F	103	6/6	0.90	0.19	60,65,71,71	0
27	SQD	F	101	43/54	0.90	0.24	34,59,81,90	0
26	BCR	h	101	40/40	0.90	0.12	25,35,48,52	0
35	HTG	b	626	19/19	0.90	0.19	30,50,86,86	0
37	LHG	l	101	49/49	0.90	0.18	15,27,39,56	0
33	CA	f	104	1/1	0.90	0.07	77,77,77,77	0
36	DGD	h	102	62/66	0.90	0.14	19,31,48,60	0
26	BCR	H	101	40/40	0.90	0.13	19,32,45,59	0
24	CLA	c	913	65/65	0.91	0.16	31,40,59,65	0
36	DGD	c	918	62/66	0.91	0.20	25,31,52,70	0
26	BCR	y	101	40/40	0.91	0.14	29,37,57,63	0
24	CLA	c	904	65/65	0.91	0.12	26,33,44,47	0
24	CLA	C	513	65/65	0.91	0.13	27,40,59,71	0
36	DGD	c	917	62/66	0.91	0.18	26,35,61,87	0
28	GOL	a	413	6/6	0.91	0.11	30,32,37,42	0
27	SQD	A	412	54/54	0.91	0.20	15,45,72,85	0
27	SQD	a	411	54/54	0.91	0.21	32,52,73,81	0
35	HTG	B	625	19/19	0.91	0.20	28,43,74,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	905	65/65	0.91	0.16	25,32,49,68	0
31	PL9	d	405	55/55	0.91	0.18	13,19,33,44	0
28	GOL	b	631	6/6	0.91	0.15	28,41,48,51	0
24	CLA	c	906	65/65	0.91	0.12	21,28,44,56	0
34	LMG	J	101	51/55	0.91	0.18	18,32,75,81	0
28	GOL	b	628	6/6	0.91	0.13	30,35,42,53	0
28	GOL	B	632	6/6	0.91	0.17	24,40,53,57	0
36	DGD	C	518	62/66	0.92	0.20	19,29,78,90	0
24	CLA	b	613	65/65	0.92	0.11	23,29,42,48	0
26	BCR	c	915	40/40	0.92	0.11	25,34,42,45	0
35	HTG	C	523	19/19	0.92	0.20	54,62,86,88	0
34	LMG	j	101	51/55	0.92	0.17	25,35,71,81	0
28	GOL	B	627	6/6	0.92	0.16	23,36,45,72	0
26	BCR	k	101	40/40	0.92	0.18	34,45,63,75	0
31	PL9	D	404	55/55	0.92	0.20	11,18,31,41	0
24	CLA	c	908	65/65	0.92	0.12	26,33,49,60	0
37	LHG	d	407	49/49	0.92	0.20	15,31,44,53	0
24	CLA	B	602	65/65	0.92	0.16	22,40,80,101	0
26	BCR	K	103	40/40	0.92	0.11	24,30,40,43	0
24	CLA	b	605	65/65	0.92	0.18	29,48,89,102	0
24	CLA	c	902	65/65	0.92	0.12	26,32,45,52	0
26	BCR	t	101	40/40	0.92	0.12	12,26,45,48	0
37	LHG	D	406	49/49	0.92	0.22	14,26,38,52	0
24	CLA	B	603	65/65	0.92	0.12	17,24,36,47	0
24	CLA	B	610	65/65	0.92	0.12	17,24,36,45	0
36	DGD	c	916	62/66	0.92	0.17	22,31,64,82	0
26	BCR	b	621	40/40	0.92	0.16	14,24,33,38	0
26	BCR	a	410	40/40	0.93	0.10	15,23,28,32	0
24	CLA	b	618	65/65	0.93	0.14	14,24,78,80	0
24	CLA	c	909	65/65	0.93	0.15	23,28,67,91	0
28	GOL	b	629	6/6	0.93	0.15	27,36,50,54	0
26	BCR	b	622	40/40	0.93	0.18	14,24,43,51	0
24	CLA	d	403	65/65	0.93	0.12	26,31,79,93	0
26	BCR	T	102	40/40	0.93	0.14	13,26,37,42	0
28	GOL	b	630	6/6	0.93	0.14	35,39,50,53	0
28	GOL	A	413	6/6	0.93	0.11	23,30,33,36	0
26	BCR	D	403	40/40	0.93	0.14	19,30,58,70	0
24	CLA	b	610	65/65	0.93	0.11	18,31,78,87	0
23	BCT	a	419	4/4	0.93	0.15	21,32,41,50	0
28	GOL	C	525	6/6	0.93	0.20	32,41,61,69	0
28	GOL	B	630	6/6	0.93	0.10	26,32,40,42	0
26	BCR	B	619	40/40	0.93	0.14	15,23,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	b	619	65/65	0.93	0.11	20,30,49,51	0
24	CLA	c	912	65/65	0.93	0.12	27,36,50,54	0
24	CLA	B	608	65/65	0.93	0.16	11,19,28,40	0
24	CLA	C	511	65/65	0.93	0.15	21,29,38,45	0
24	CLA	C	512	65/65	0.93	0.11	22,30,39,45	0
25	PHO	a	420	64/64	0.93	0.20	17,24,30,33	0
24	CLA	C	505	65/65	0.93	0.18	18,27,47,61	0
26	BCR	C	515	40/40	0.93	0.11	29,38,49,53	0
24	CLA	C	507	65/65	0.93	0.14	25,40,75,77	0
26	BCR	B	618	40/40	0.93	0.14	11,23,32,35	0
24	CLA	C	514	65/65	0.93	0.14	30,42,67,73	0
36	DGD	C	519	62/66	0.93	0.20	18,29,48,55	0
24	CLA	c	903	65/65	0.93	0.15	24,30,41,51	0
24	CLA	b	606	65/65	0.93	0.12	22,28,38,48	0
24	CLA	C	508	65/65	0.94	0.12	23,35,47,54	0
28	GOL	b	633	6/6	0.94	0.36	34,60,65,65	0
26	BCR	K	102	40/40	0.94	0.11	22,30,39,47	0
24	CLA	b	614	65/65	0.94	0.10	20,29,39,42	0
37	LHG	L	101	49/49	0.94	0.21	12,26,38,46	0
24	CLA	b	615	65/65	0.94	0.14	17,22,38,46	0
24	CLA	B	606	65/65	0.94	0.10	13,20,31,41	0
37	LHG	D	408	49/49	0.94	0.18	17,29,88,100	0
24	CLA	C	503	65/65	0.94	0.12	20,25,39,63	0
24	CLA	D	402	65/65	0.94	0.12	18,27,68,84	0
25	PHO	a	408	64/64	0.94	0.15	15,18,27,30	0
24	CLA	C	510	65/65	0.94	0.10	23,30,45,62	0
22	CL	v	201	1/1	0.94	0.08	62,62,62,62	0
24	CLA	B	614	65/65	0.94	0.16	12,20,43,55	0
24	CLA	c	910	65/65	0.94	0.11	27,34,47,53	0
24	CLA	b	616	65/65	0.94	0.10	16,23,32,44	0
26	BCR	b	623	40/40	0.94	0.09	18,31,42,48	0
24	CLA	C	504	65/65	0.94	0.11	22,28,40,45	0
24	CLA	B	604	65/65	0.94	0.11	16,25,32,38	0
24	CLA	C	502	65/65	0.94	0.11	22,30,42,54	0
28	GOL	V	204	6/6	0.94	0.14	19,26,30,37	0
28	GOL	a	414	6/6	0.94	0.14	25,34,43,53	0
23	BCT	A	404	4/4	0.94	0.17	21,24,36,47	0
37	LHG	d	408	49/49	0.94	0.13	15,23,41,54	0
26	BCR	B	620	40/40	0.94	0.09	16,26,39,49	0
28	GOL	V	205	6/6	0.94	0.16	34,41,45,52	0
24	CLA	B	605	65/65	0.94	0.13	13,19,44,57	0
24	CLA	c	911	65/65	0.94	0.16	24,31,43,53	0

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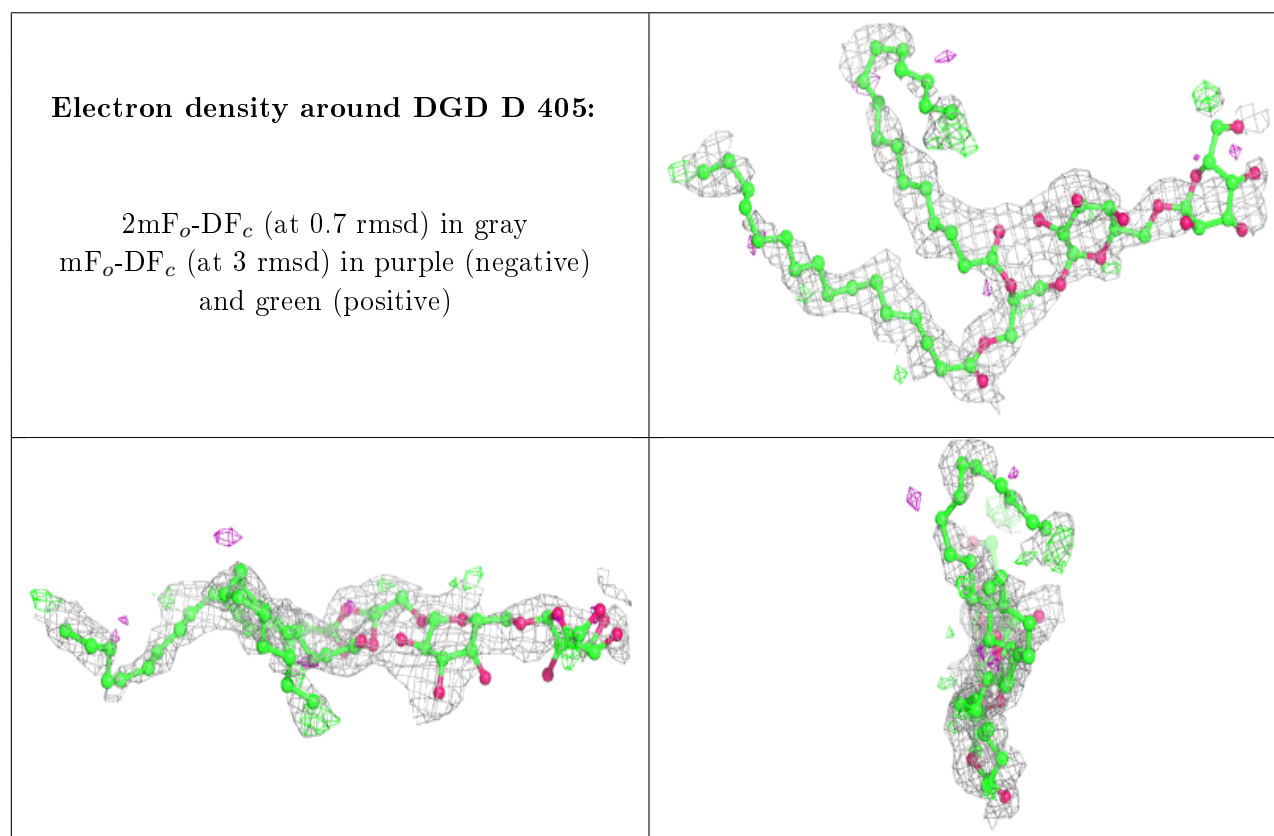
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	907	65/65	0.94	0.12	28,37,64,72	0
24	CLA	B	615	65/65	0.94	0.12	12,21,66,79	0
24	CLA	a	407	65/65	0.94	0.23	18,23,72,84	0
24	CLA	b	620	65/65	0.94	0.14	19,33,77,78	0
24	CLA	C	509	65/65	0.94	0.14	18,25,67,82	0
24	CLA	B	607	65/65	0.94	0.12	16,25,70,76	0
26	BCR	A	411	40/40	0.94	0.11	15,22,29,31	0
24	CLA	A	407	65/65	0.95	0.25	13,20,71,73	0
24	CLA	b	612	65/65	0.95	0.10	21,28,40,43	0
38	HEM	e	102	43/43	0.95	0.18	37,46,76,95	0
28	GOL	v	205	6/6	0.95	0.16	23,35,46,50	0
26	BCR	C	516	40/40	0.95	0.09	23,32,42,43	0
28	GOL	C	526	6/6	0.95	0.18	17,21,26,26	0
37	LHG	d	409	49/49	0.95	0.17	21,32,85,88	0
24	CLA	B	613	65/65	0.95	0.11	13,20,27,33	0
24	CLA	A	405	65/65	0.95	0.23	13,17,27,52	0
25	PHO	A	408	64/64	0.95	0.16	12,16,23,24	0
24	CLA	C	506	65/65	0.95	0.10	18,27,47,54	0
24	CLA	B	609	65/65	0.95	0.14	15,24,30,36	0
24	CLA	b	608	65/65	0.95	0.13	15,23,51,62	0
24	CLA	b	617	65/65	0.95	0.15	14,22,44,52	0
24	CLA	D	401	65/65	0.95	0.24	12,16,32,36	0
35	HTG	O	303	19/19	0.95	0.10	23,32,46,55	0
24	CLA	B	611	65/65	0.95	0.10	17,25,33,50	0
24	CLA	d	401	65/65	0.95	0.19	14,18,27,47	0
24	CLA	B	616	65/65	0.95	0.11	16,23,42,45	0
24	CLA	d	402	65/65	0.95	0.23	16,20,36,46	0
37	LHG	D	407	49/49	0.95	0.15	13,22,44,57	0
24	CLA	B	612	65/65	0.95	0.15	12,18,30,37	0
24	CLA	a	409	65/65	0.95	0.12	18,26,79,83	0
24	CLA	b	611	65/65	0.95	0.16	13,20,31,34	0
24	CLA	B	617	65/65	0.95	0.15	16,28,79,88	0
25	PHO	A	409	64/64	0.95	0.21	13,20,29,35	0
36	DGD	C	517	62/66	0.95	0.12	19,28,60,72	0
24	CLA	b	609	65/65	0.95	0.10	16,24,37,44	0
35	HTG	B	624	19/19	0.95	0.10	20,32,43,46	0
24	CLA	a	406	65/65	0.95	0.22	15,17,32,38	0
38	HEM	E	103	43/43	0.96	0.13	23,35,45,56	0
22	CL	U	201	1/1	0.96	0.07	50,50,50,50	0
24	CLA	b	607	65/65	0.96	0.10	21,28,38,50	0
33	CA	c	901	1/1	0.96	0.04	44,44,44,44	0
24	CLA	A	406	65/65	0.96	0.20	12,16,30,35	0

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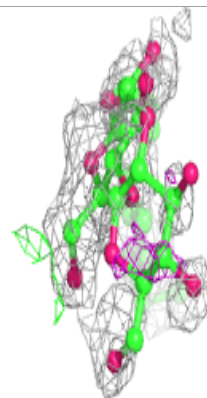
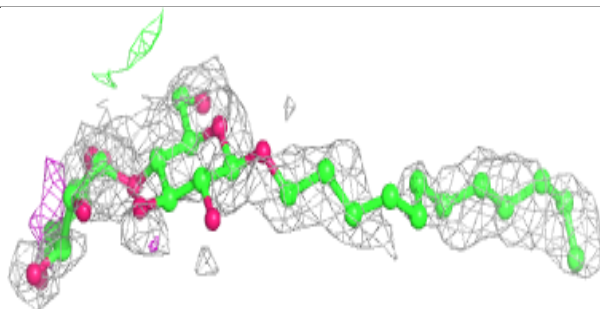
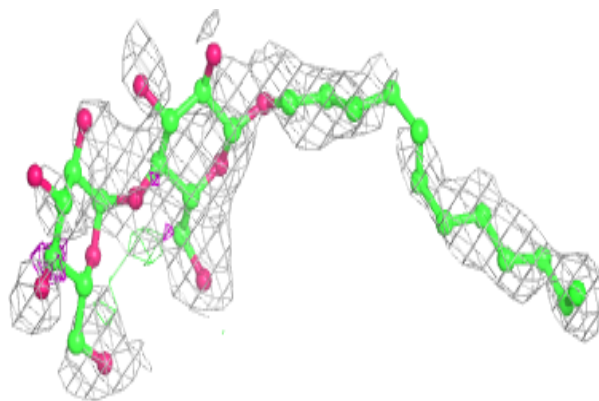
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	A	410	65/65	0.96	0.11	17,26,80,89	0
33	CA	F	102	1/1	0.96	0.09	69,69,69,69	0
40	HEC	V	201	43/43	0.97	0.09	22,25,32,39	0
39	MG	j	103	1/1	0.97	0.14	33,33,33,33	0
40	HEC	v	202	43/43	0.97	0.11	28,31,40,46	0
28	GOL	c	924	6/6	0.97	0.20	24,24,25,29	0
33	CA	O	301	1/1	0.97	0.14	53,53,53,53	0
30	OEX	a	416	10/10	0.98	0.10	18,21,24,34	0
33	CA	o	301	1/1	0.98	0.04	54,54,54,54	0
22	CL	a	404	1/1	0.98	0.07	20,20,20,20	0
39	MG	J	103	1/1	0.99	0.05	27,27,27,27	0
30	OEX	A	418	10/10	0.99	0.09	15,20,24,28	0
21	FE2	a	403	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	0.99	0.05	19,19,19,19	0
22	CL	a	405	1/1	0.99	0.09	26,26,26,26	0
22	CL	A	402	1/1	1.00	0.07	18,18,18,18	0
21	FE2	A	401	1/1	1.00	0.07	24,24,24,24	0

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

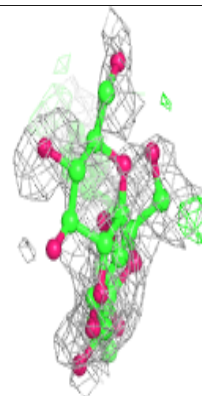
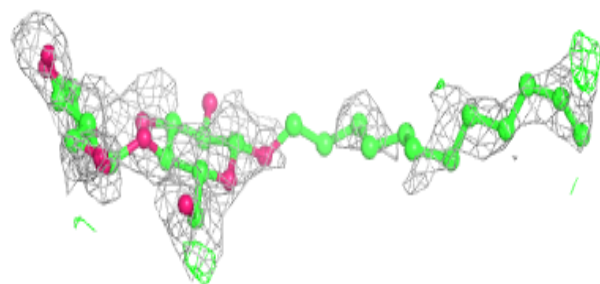
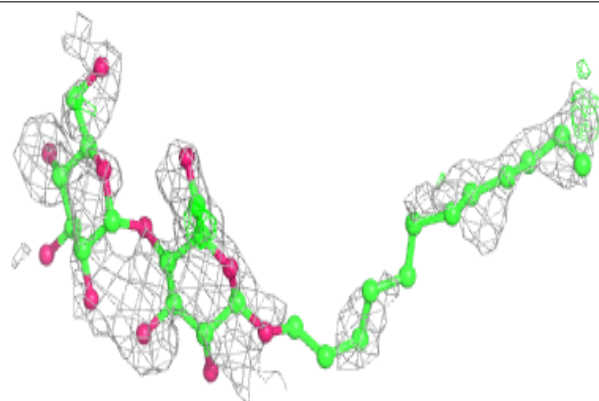


Electron density around LMT E 102:

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

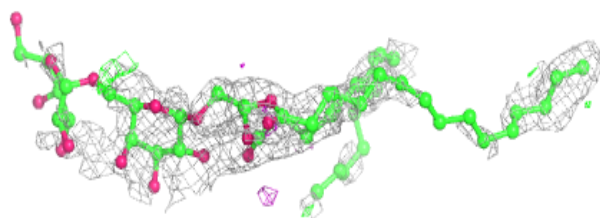
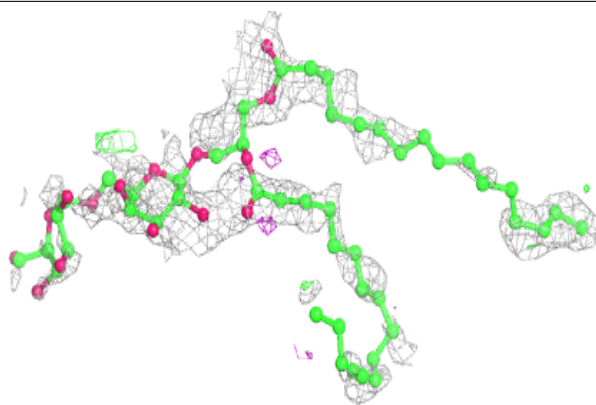
**Electron density around LMT f 103:**

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

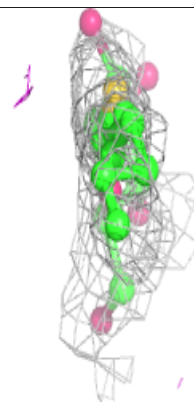
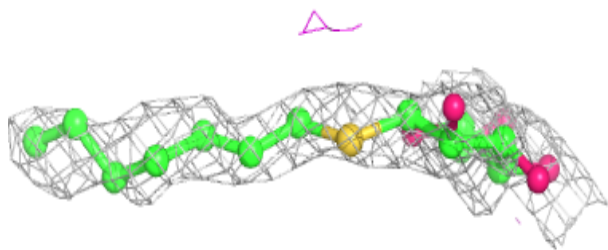
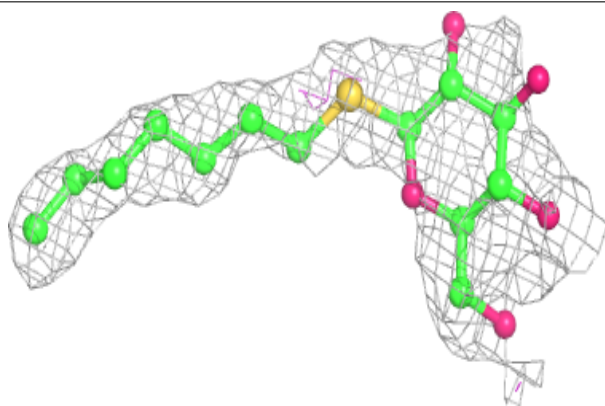


Electron density around DGD d 406:

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

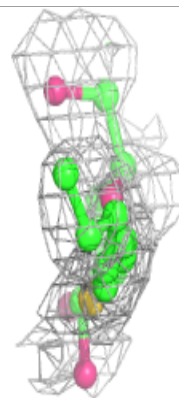
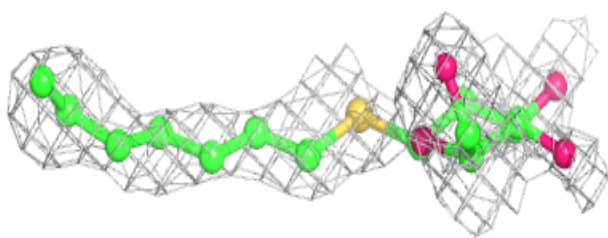
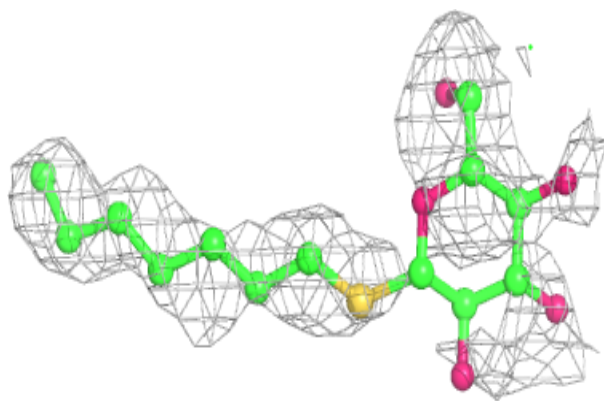
**Electron density around HTG B 626:**

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

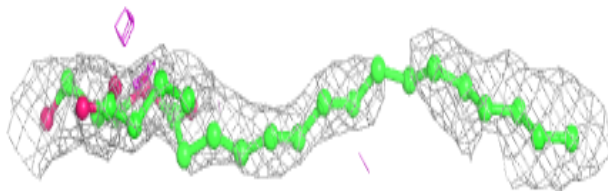
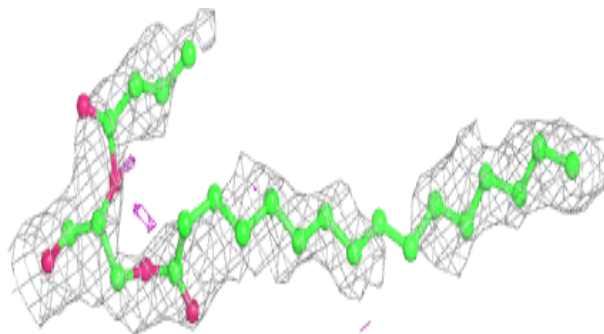


Electron density around HTG B 634:

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

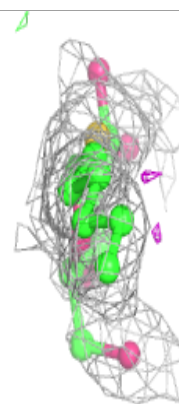
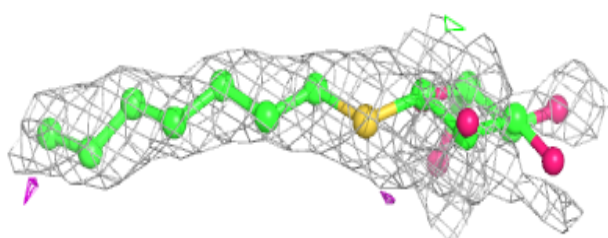
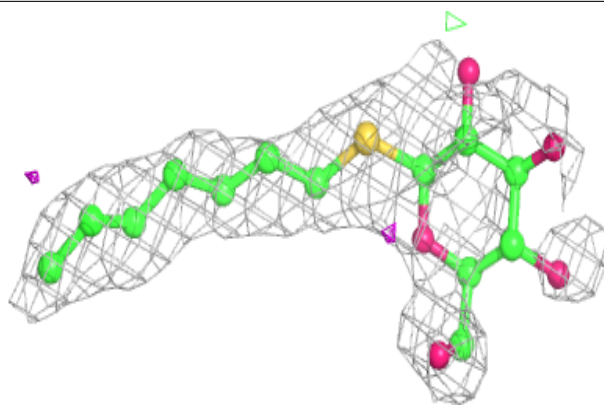
**Electron density around UNL A 420:**

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

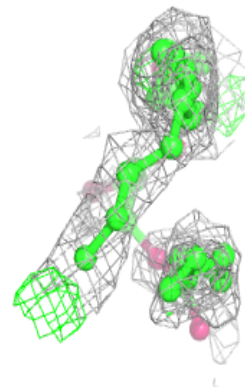
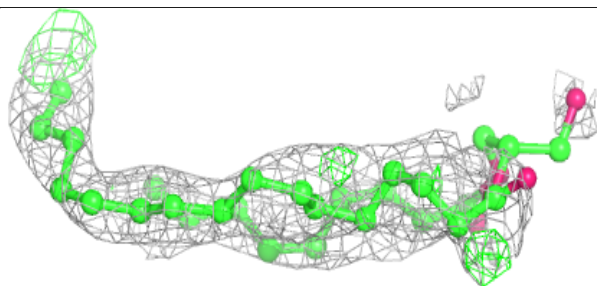
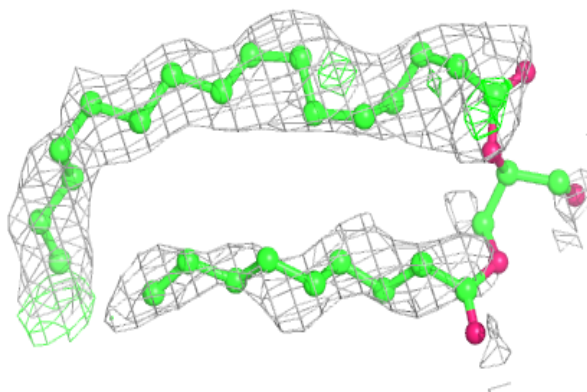


Electron density around HTG b 603:

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

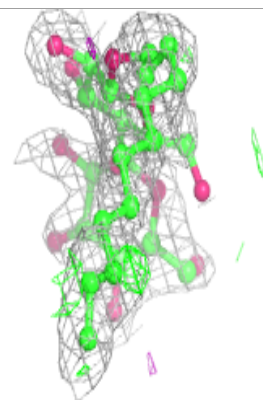
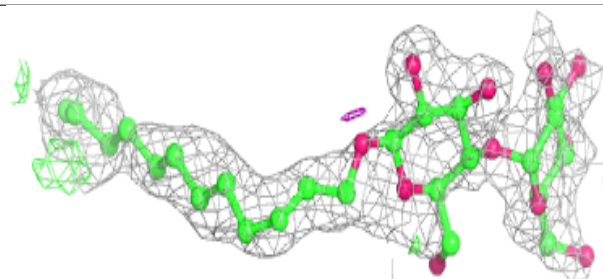
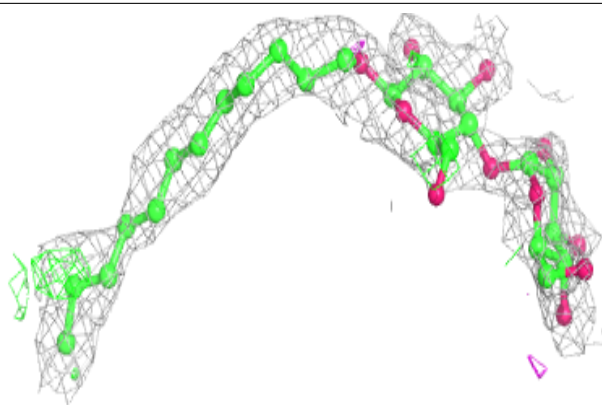
**Electron density around UNL b 634:**

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



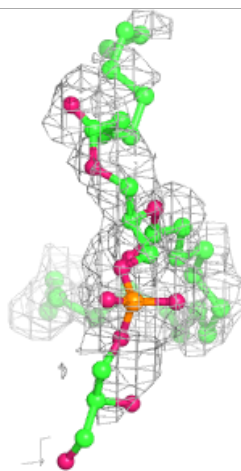
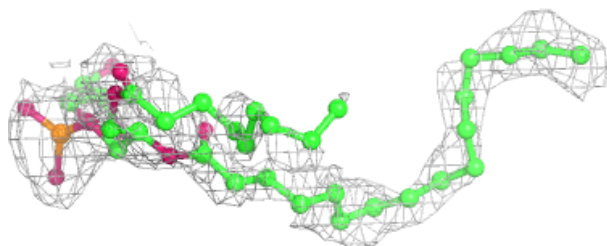
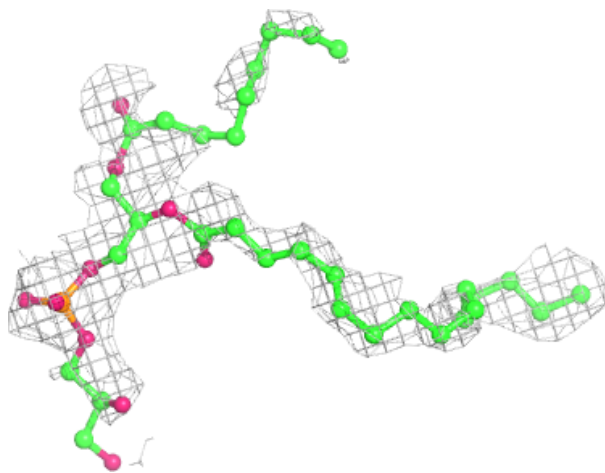
Electron density around LMT m 102:

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



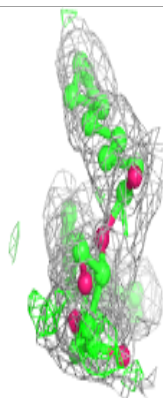
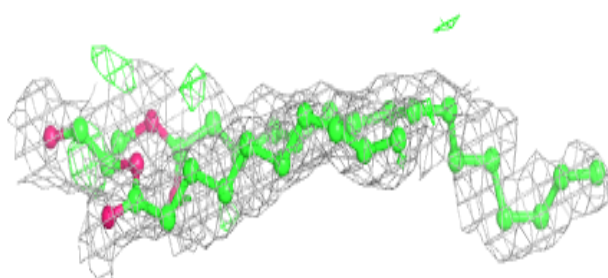
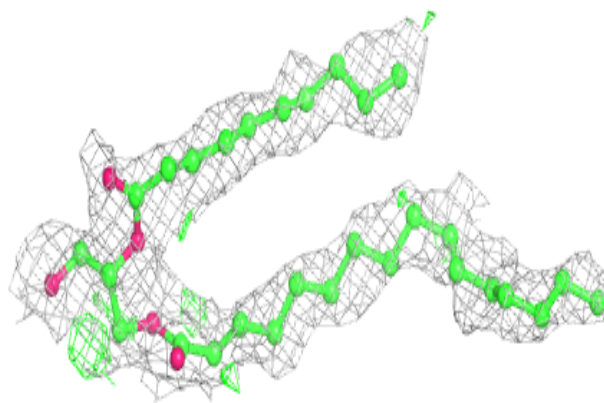
Electron density around LHG e 101:

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

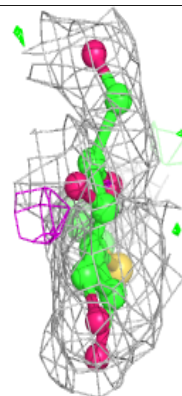
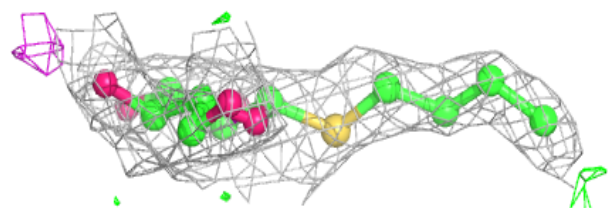
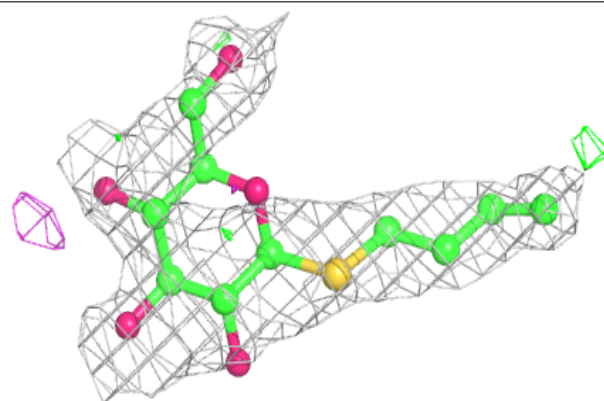


Electron density around UNL K 101:

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

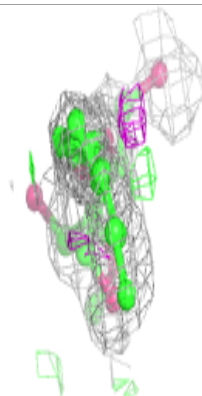
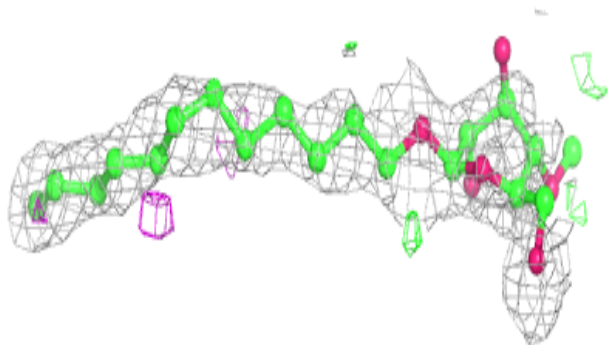
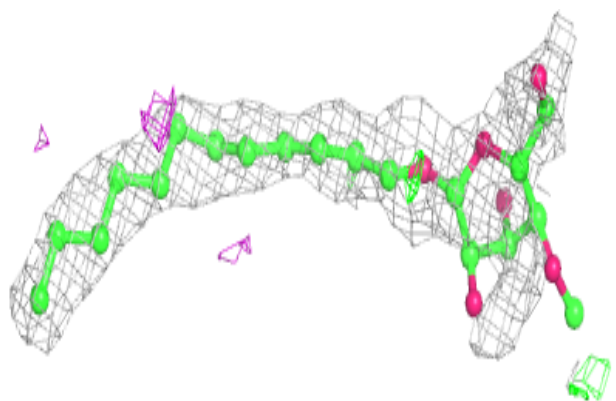
**Electron density around HTG d 412:**

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

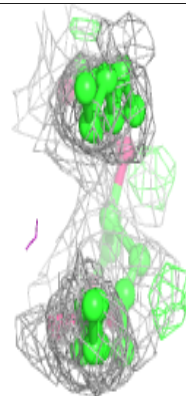
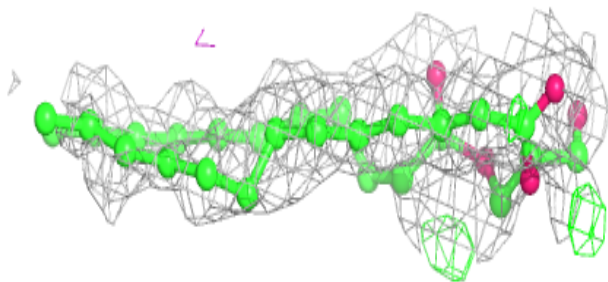
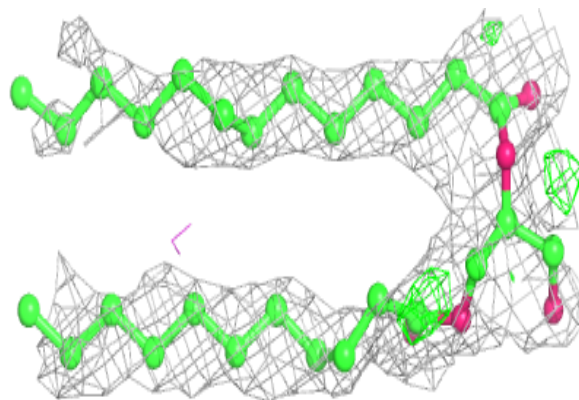


Electron density around LMT b 625:

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

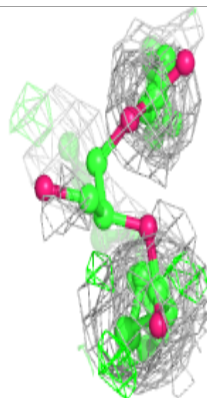
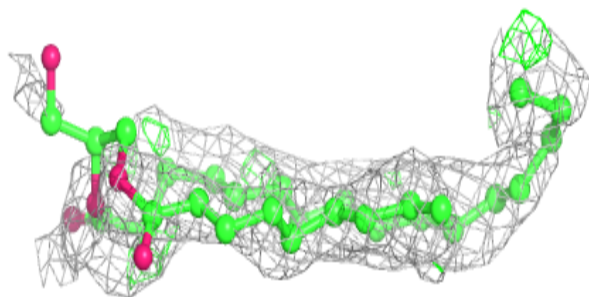
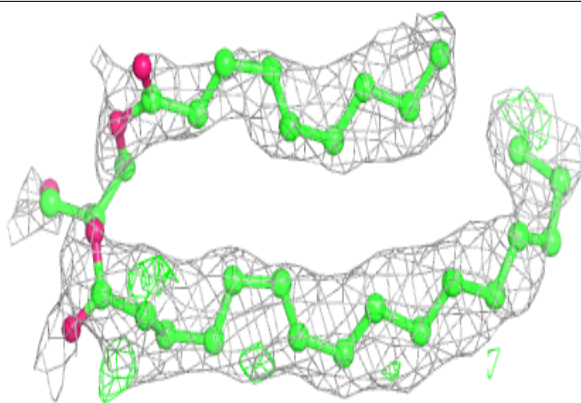
**Electron density around UNL c 926:**

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

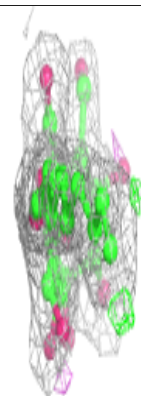
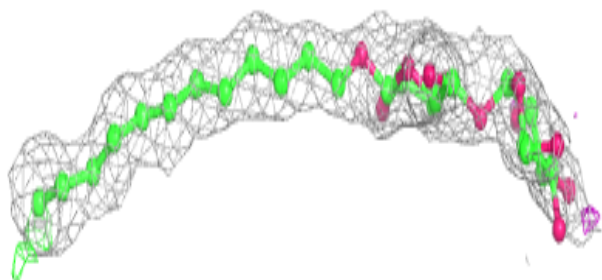
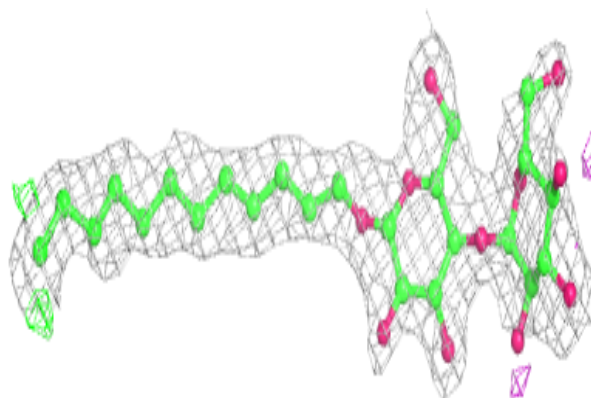


Electron density around UNL B 635:

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

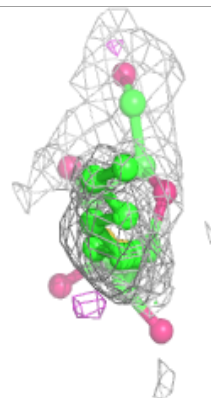
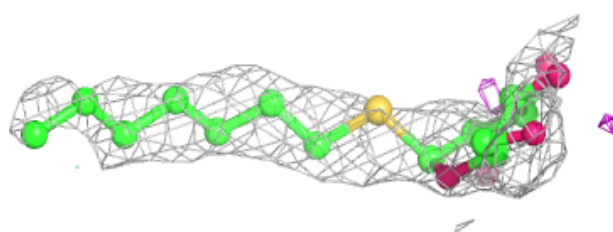
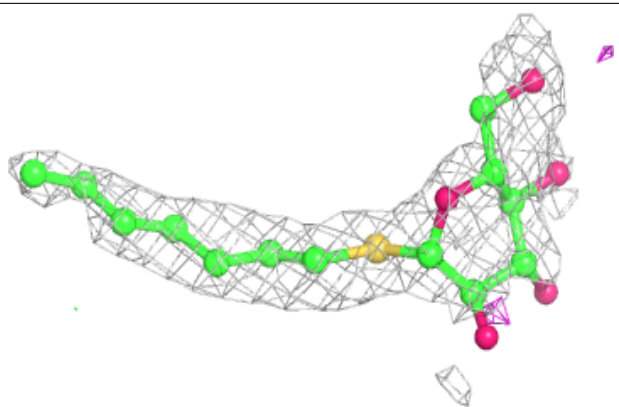
**Electron density around LMT M 101:**

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

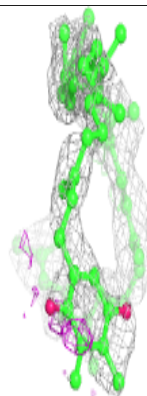
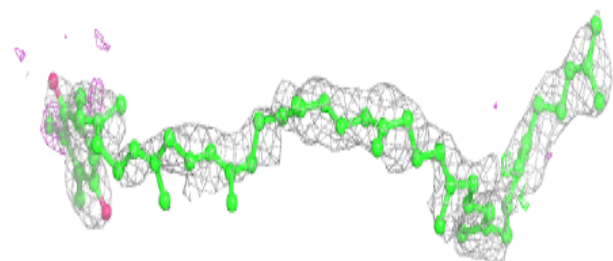
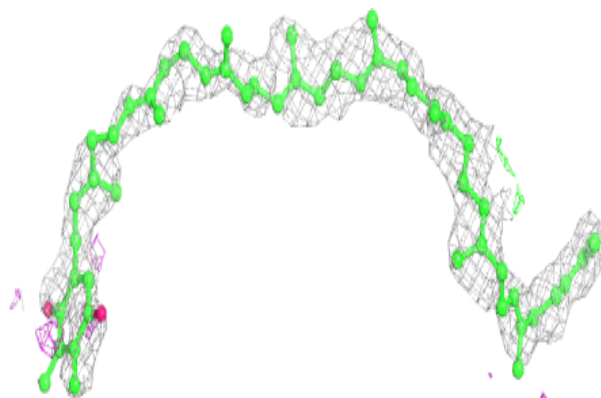


Electron density around HTG b 627:

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

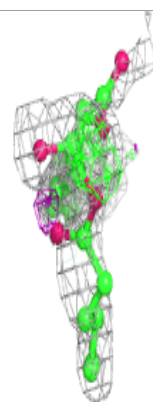
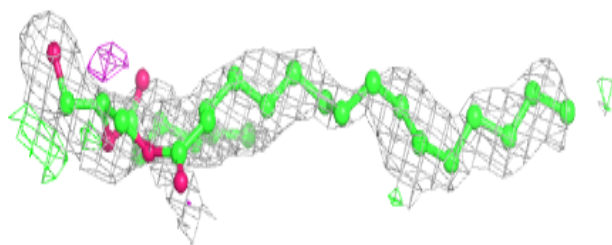
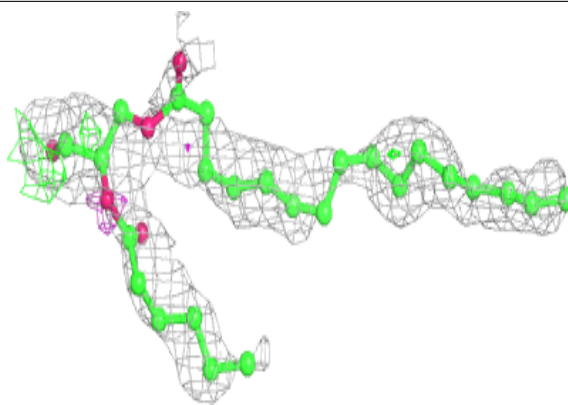
**Electron density around PL9 a 417:**

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

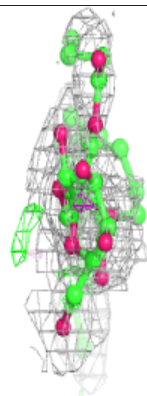
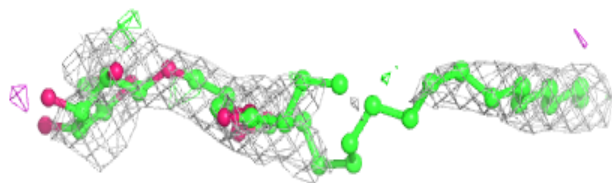
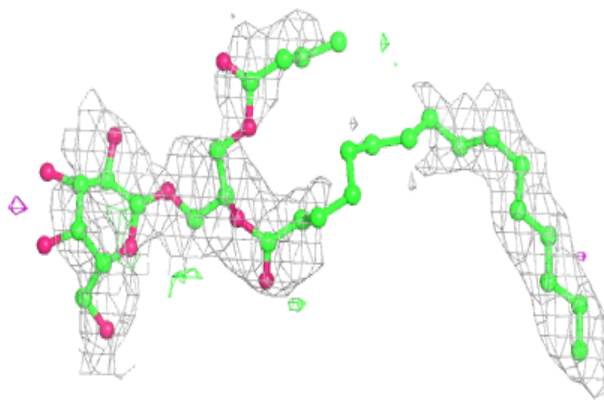


Electron density around UNL a 418:

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

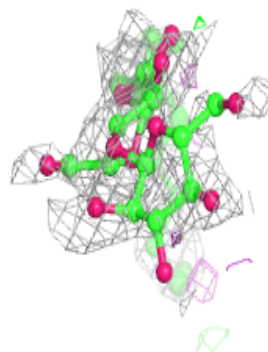
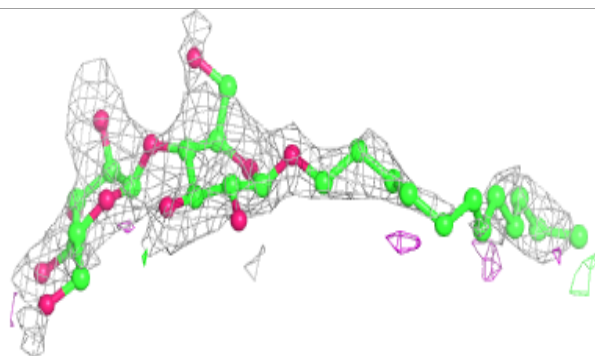
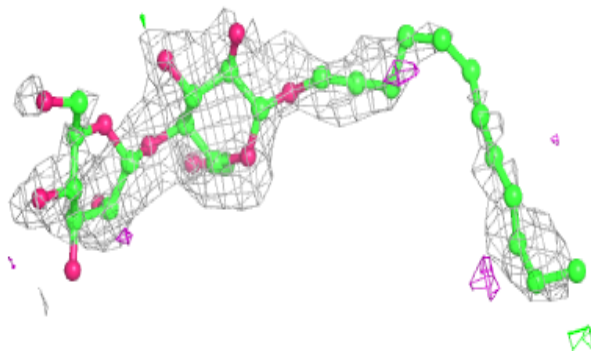
**Electron density around LMG z 101:**

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

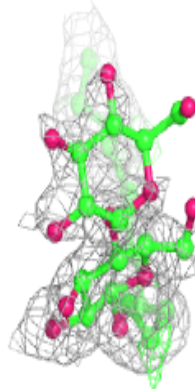
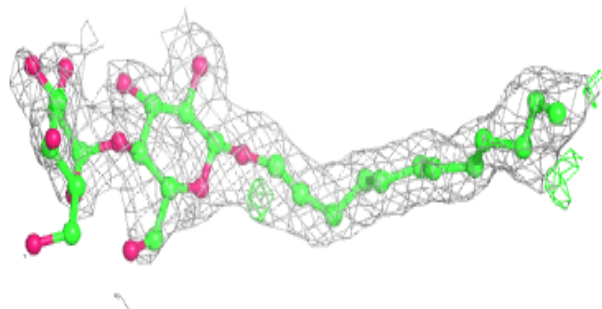
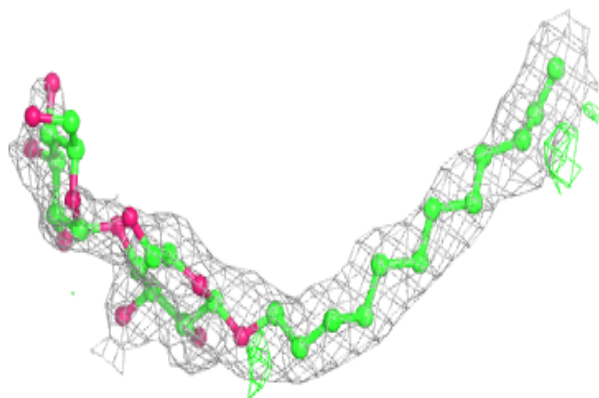


Electron density around LMT C 522:

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

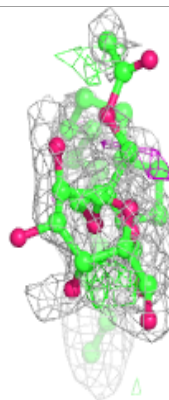
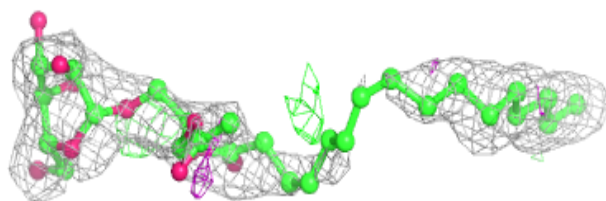
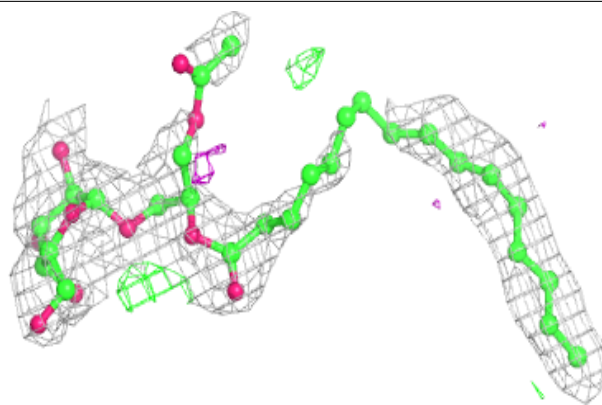
**Electron density around LMT m 104:**

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

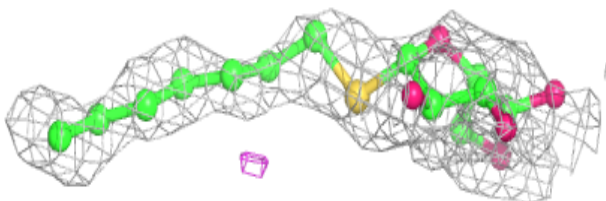
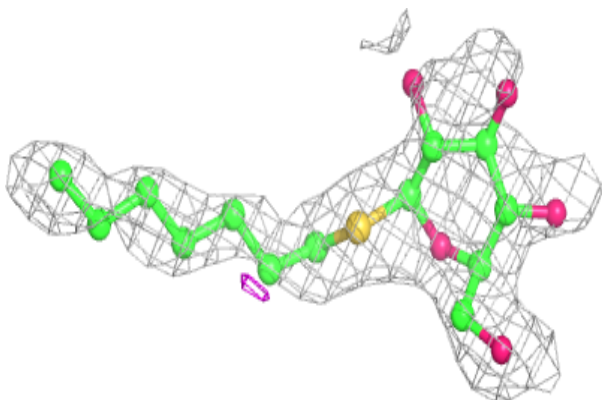


Electron density around LMG Z 101:

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

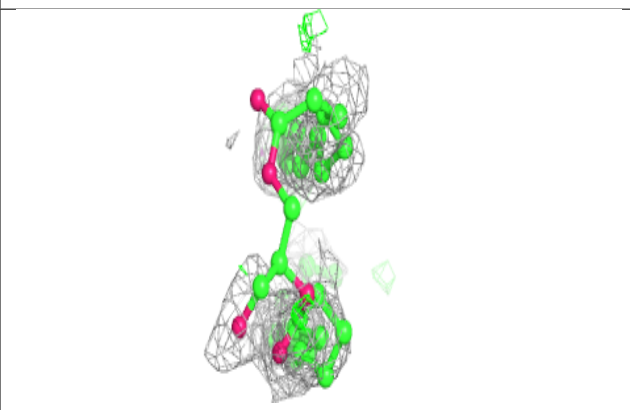
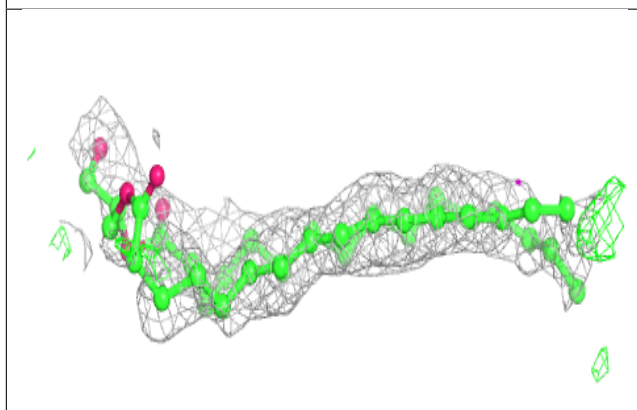
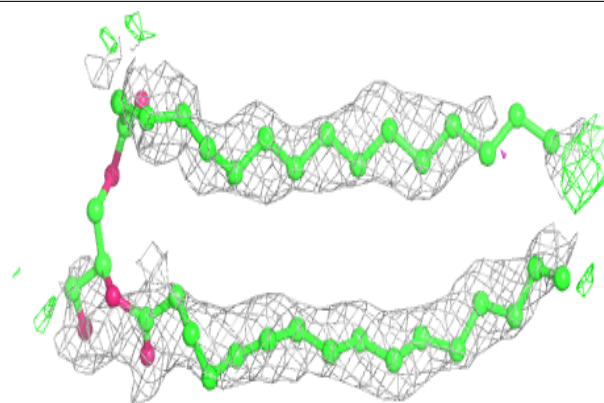
**Electron density around HTG C 524:**

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

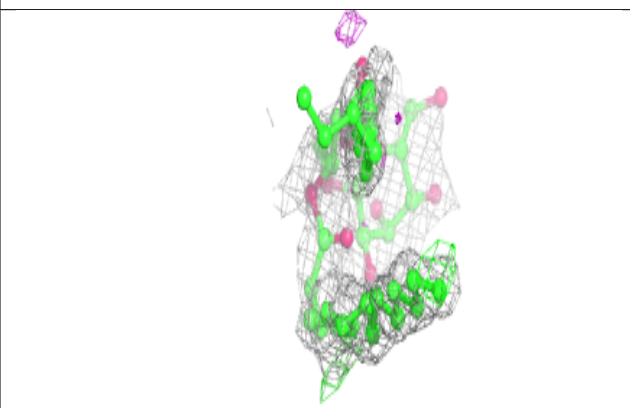
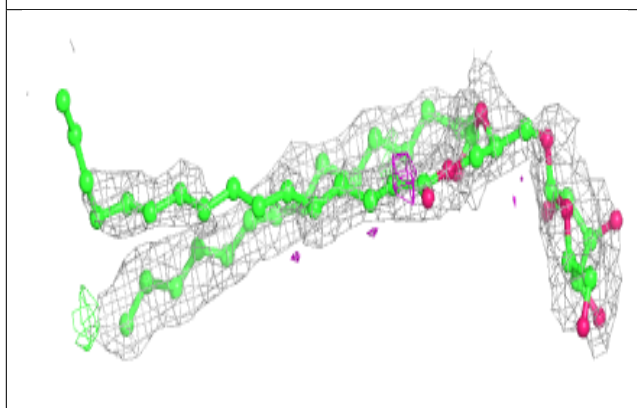
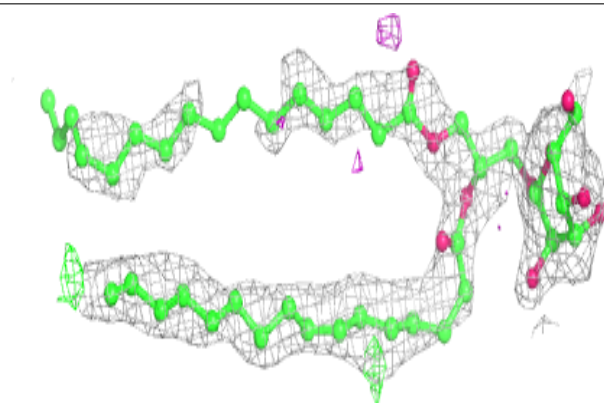


Electron density around UNL i 101:

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

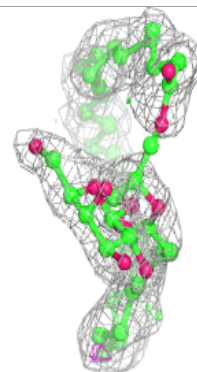
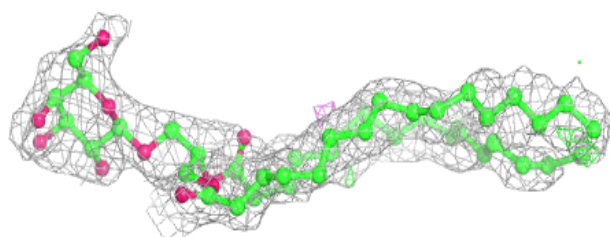
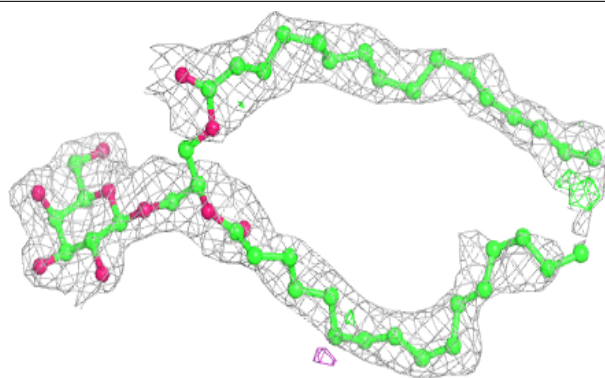
**Electron density around LMG C 521:**

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

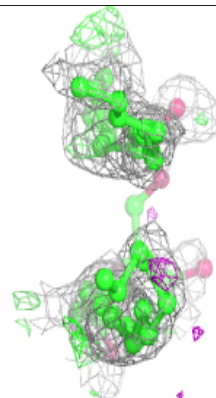
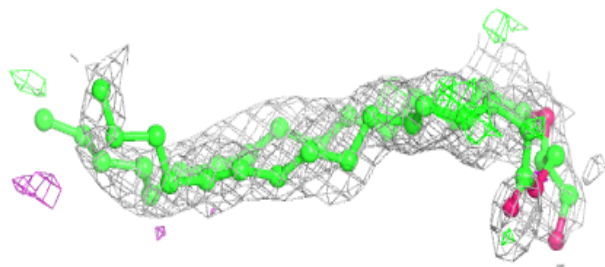
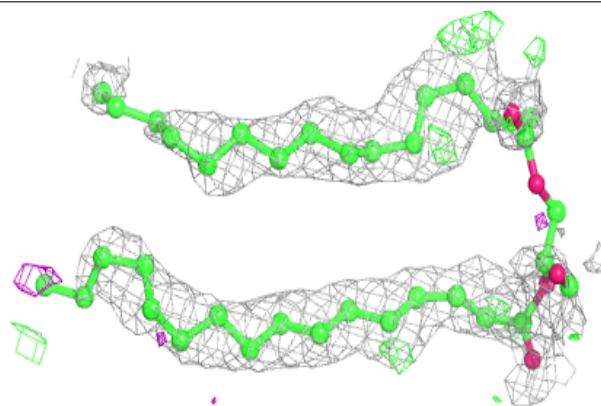


Electron density around LMG a 412:

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

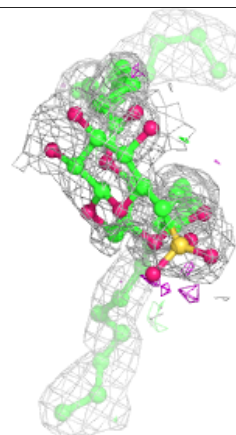
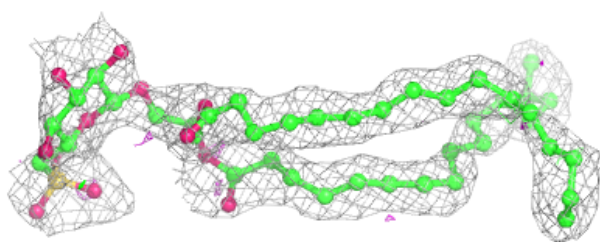
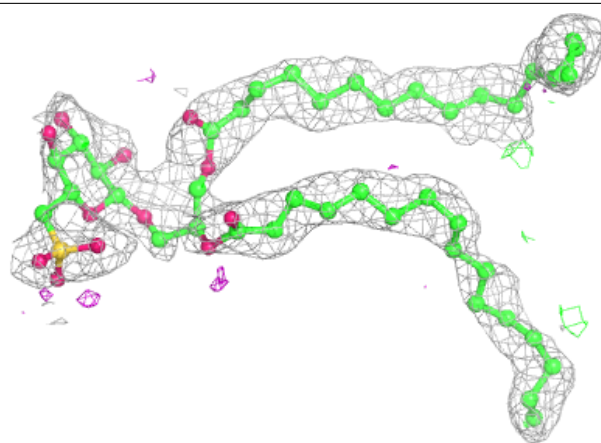
**Electron density around UNL I 101:**

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



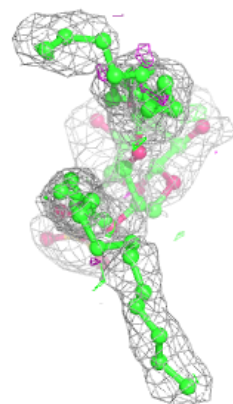
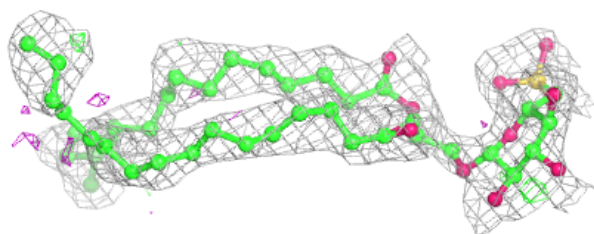
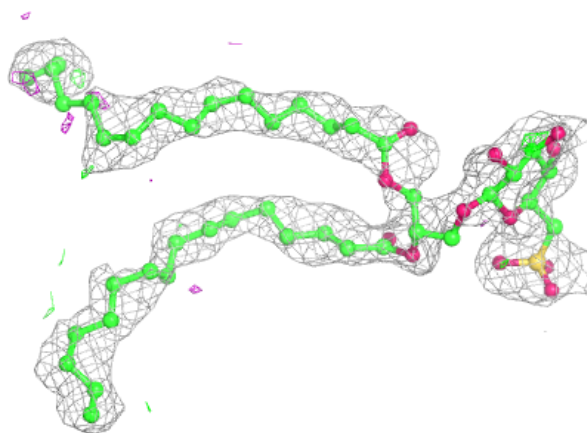
Electron density around SQD B 621:

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



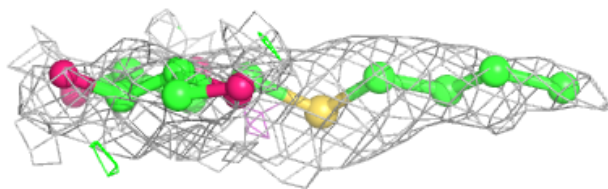
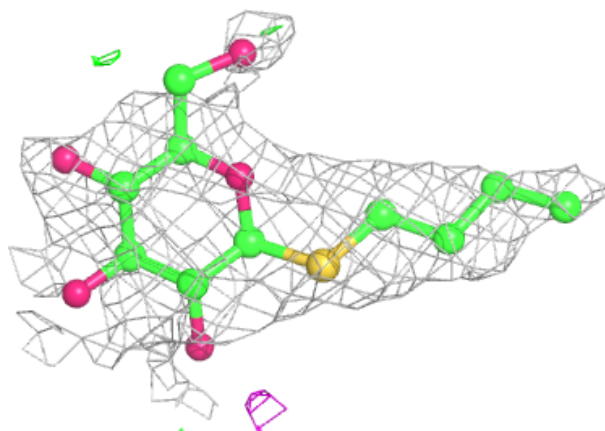
Electron density around SQD L 102:

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

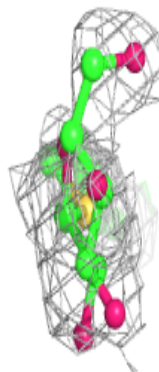
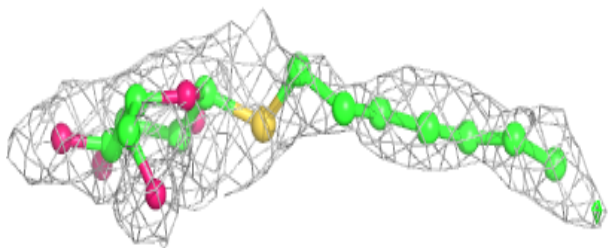
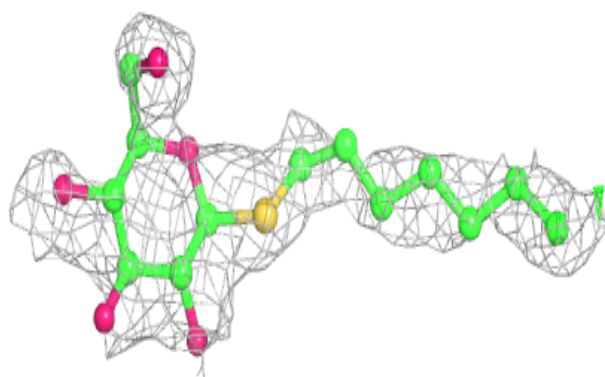


Electron density around HTG D 411:

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

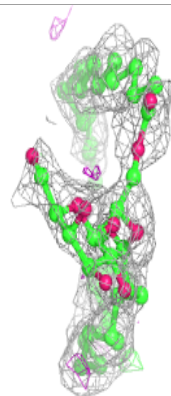
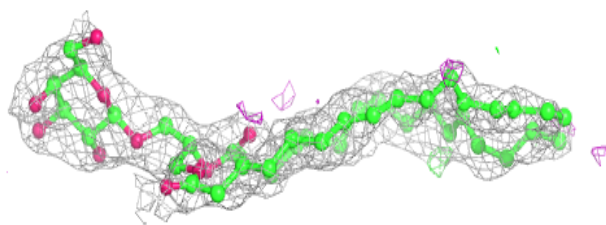
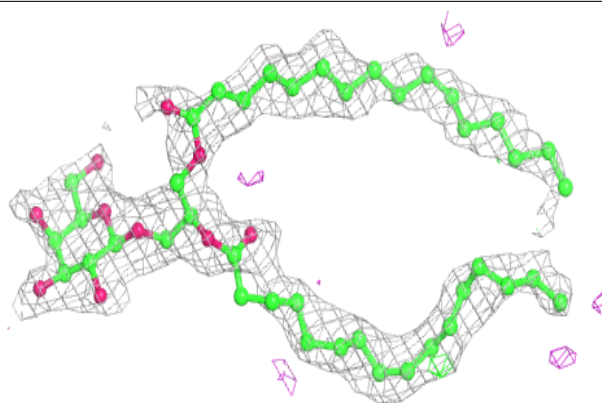
**Electron density around HTG c 923:**

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

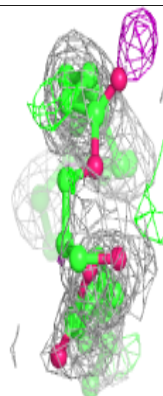
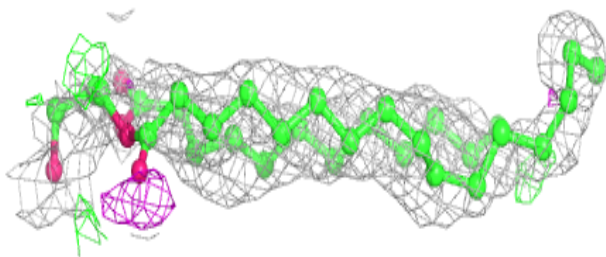
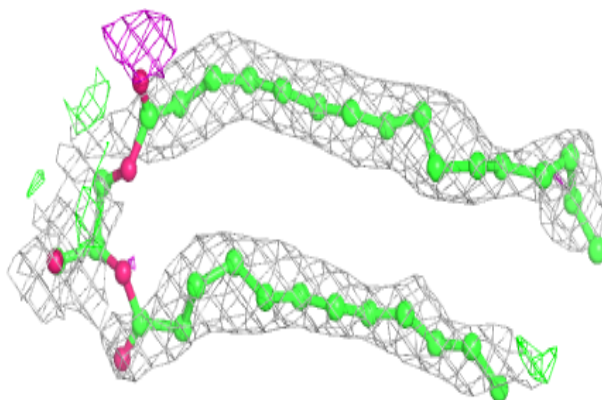


Electron density around LMG C 501:

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

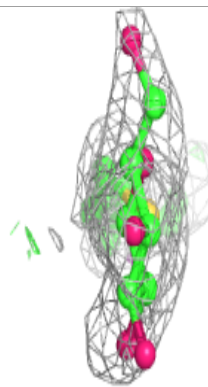
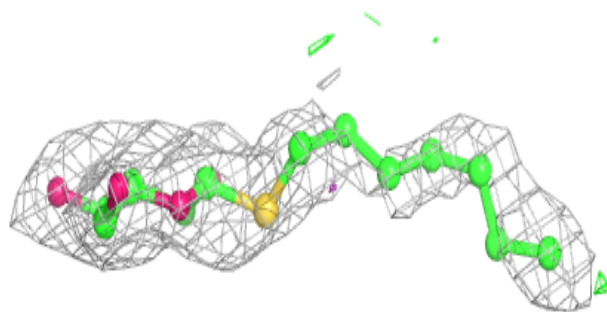
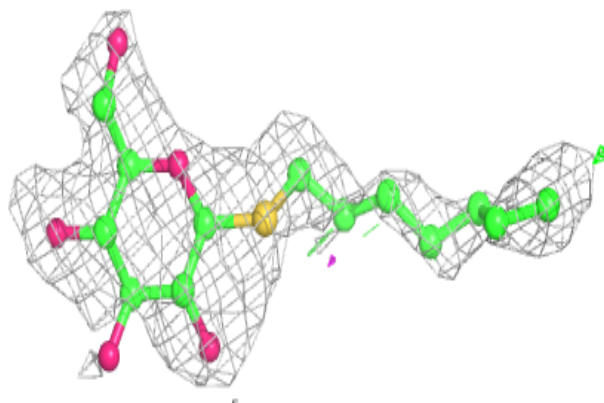
**Electron density around UNL d 411:**

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

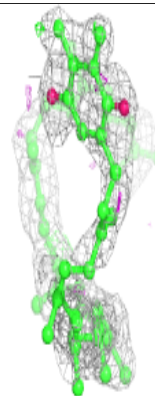
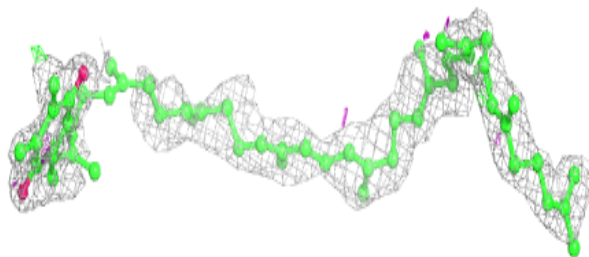
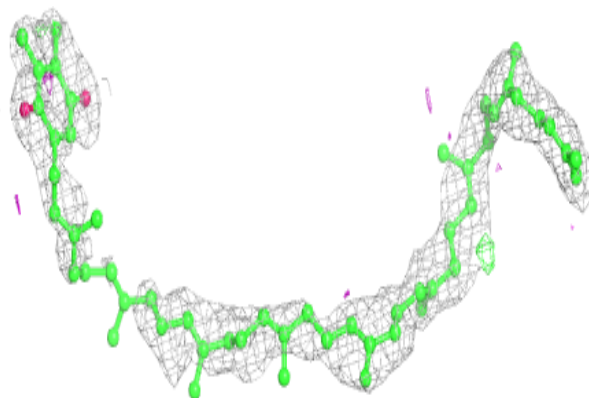


Electron density around HTG c 922:

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

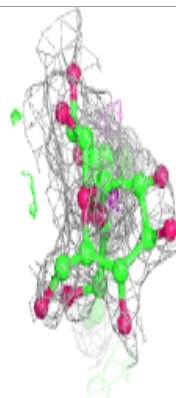
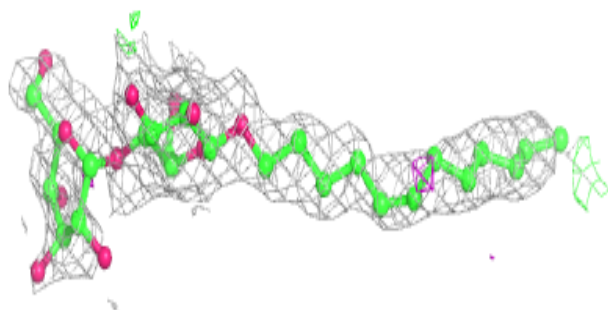
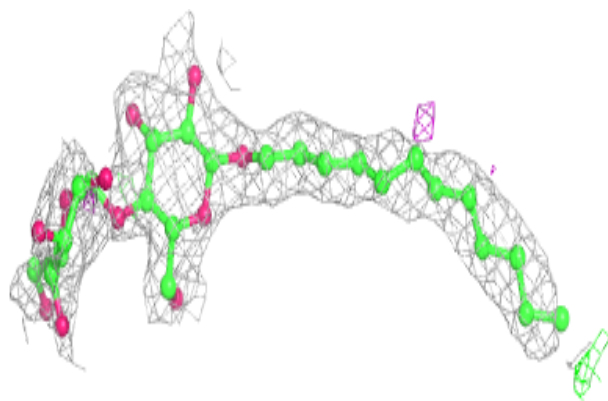
**Electron density around PL9 A 419:**

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

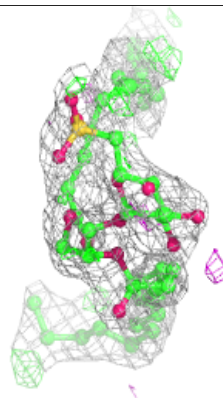
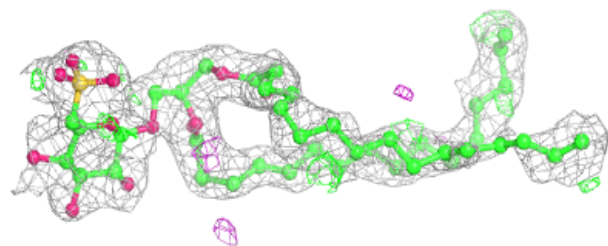
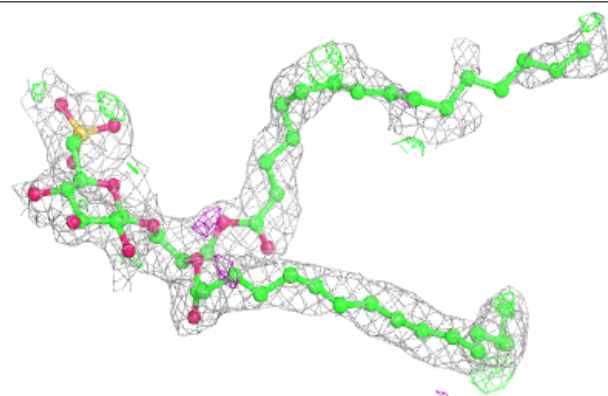


Electron density around LMT B 623:

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

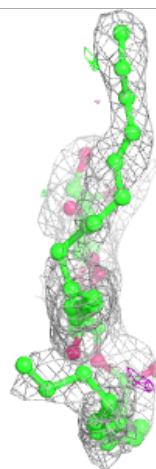
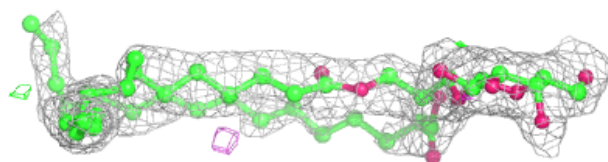
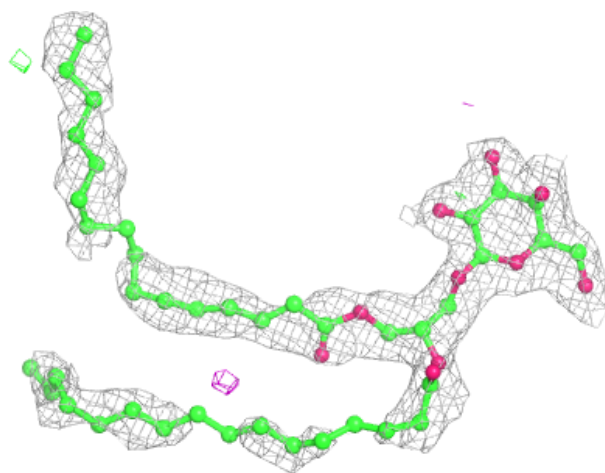
**Electron density around SQD a 402:**

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



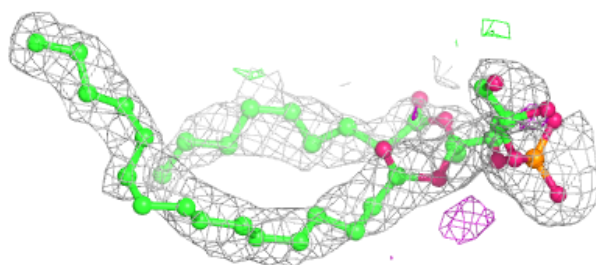
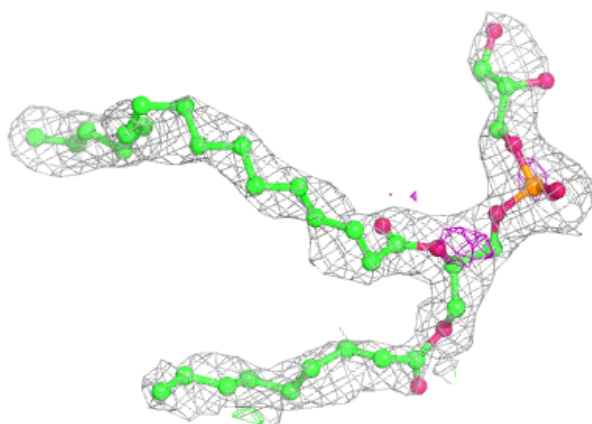
Electron density around LMG c 919:

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

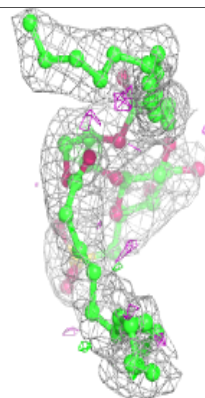
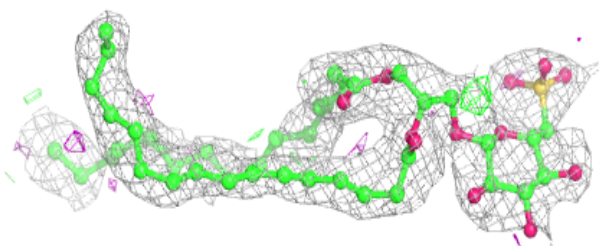
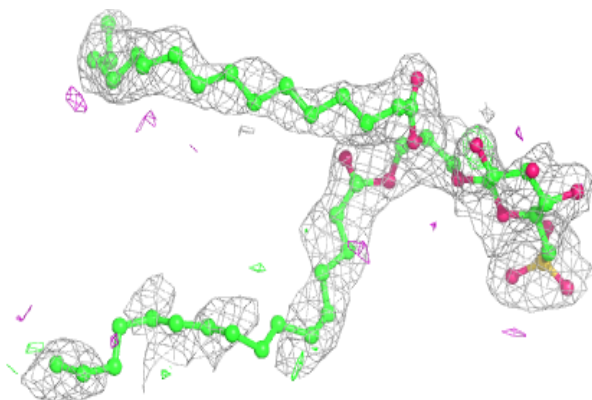


Electron density around LHG E 101:

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

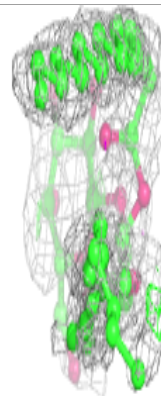
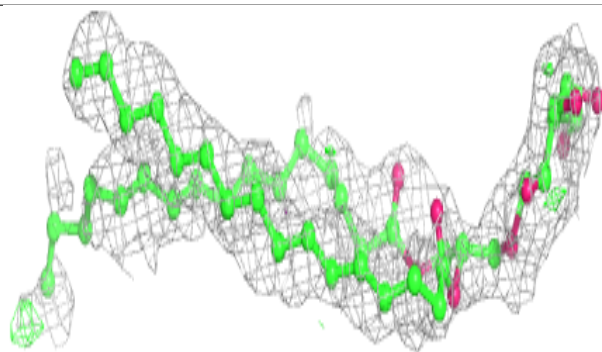
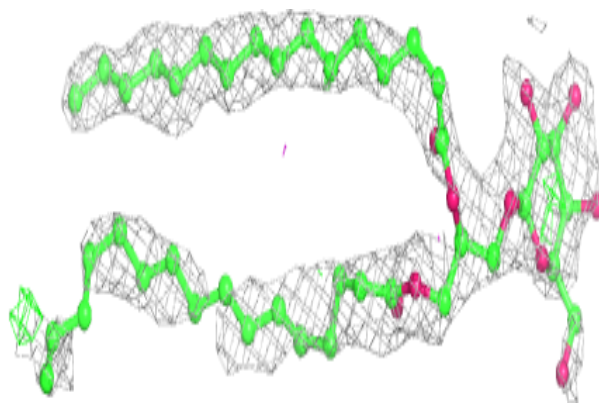
**Electron density around SQD A 416:**

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

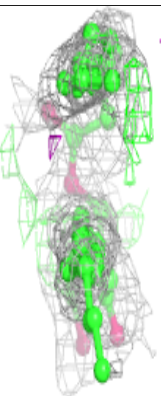
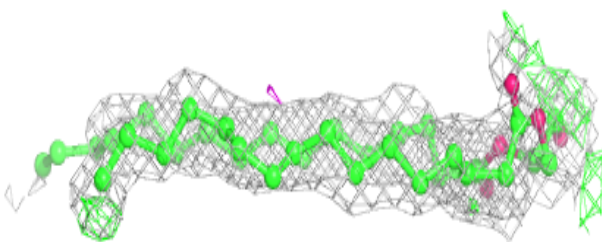
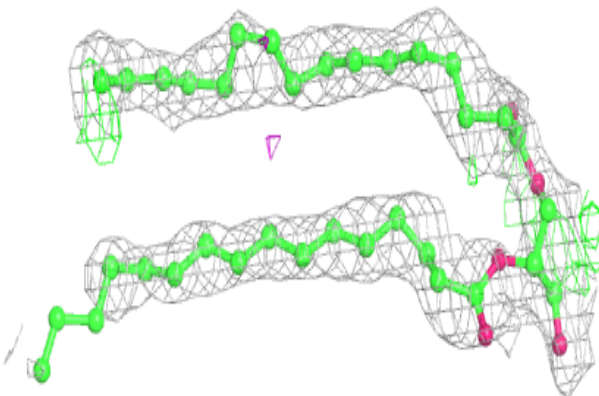


Electron density around LMG c 920:

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

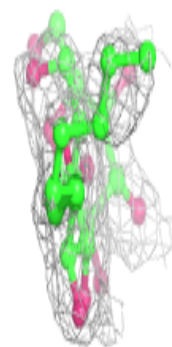
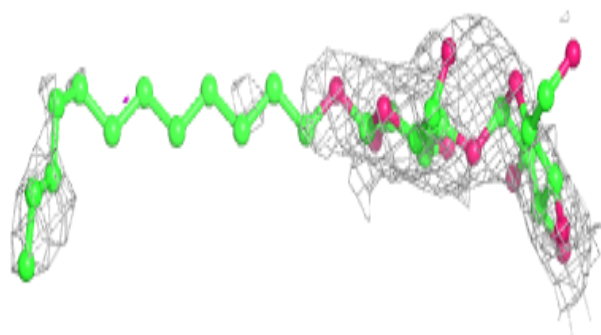
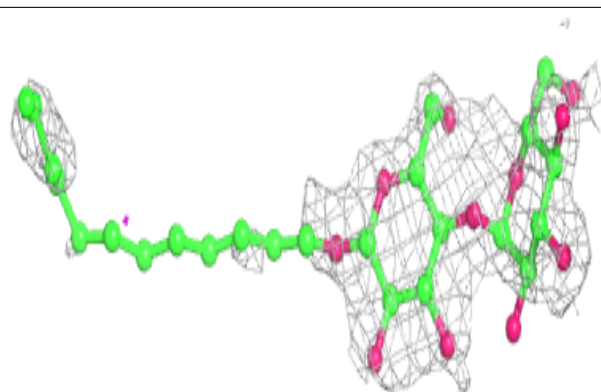
**Electron density around UNL D 410:**

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

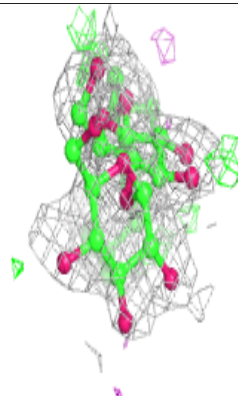
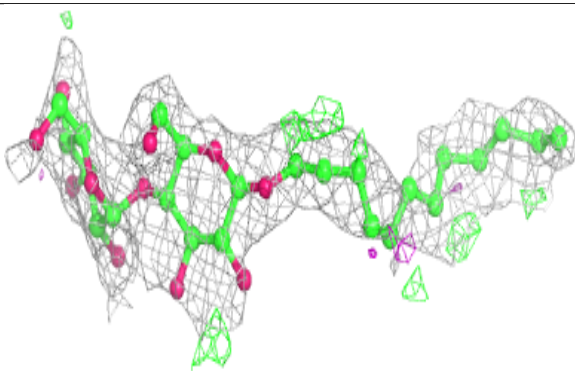
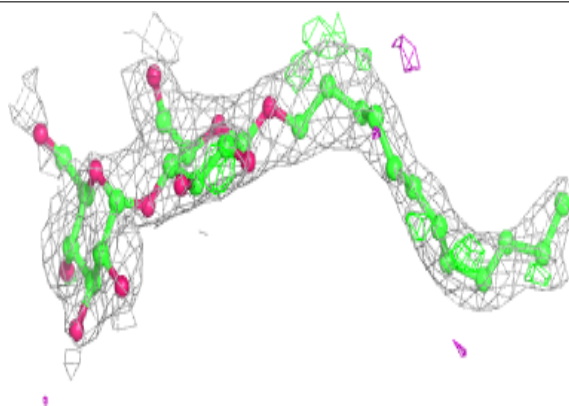


Electron density around LMT c 921:

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

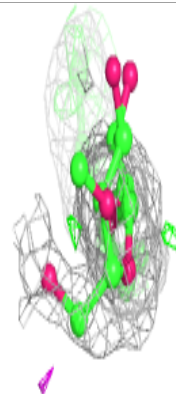
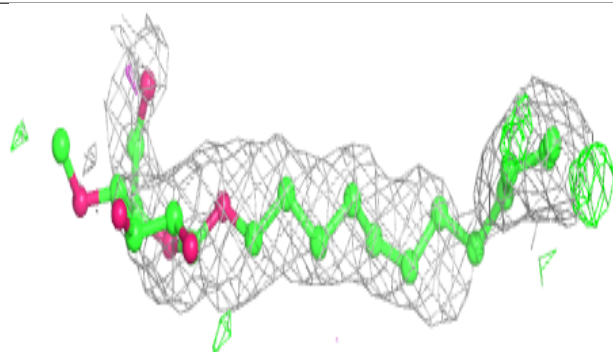
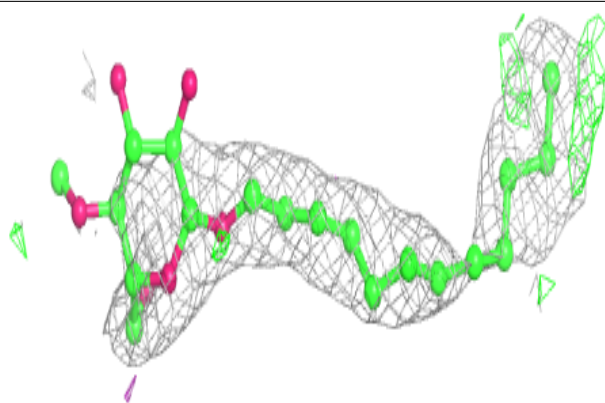
**Electron density around LMT a 401:**

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

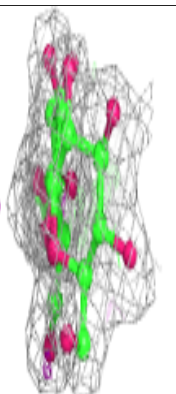
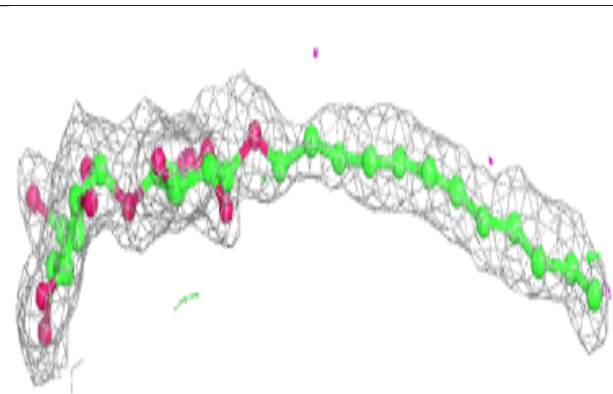
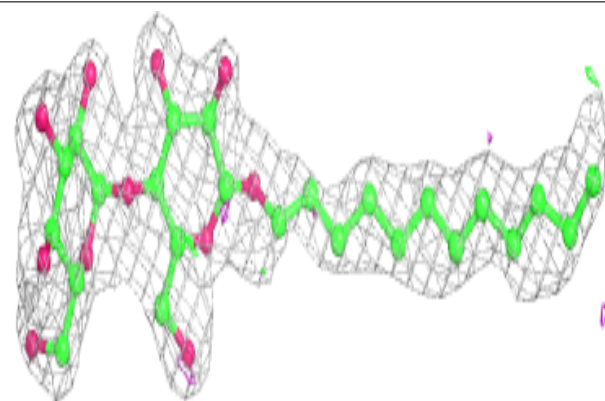


Electron density around LMT b 601:

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

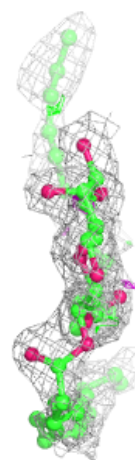
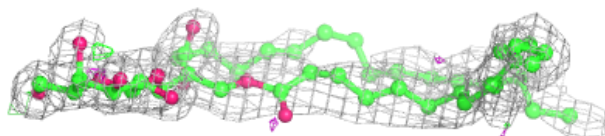
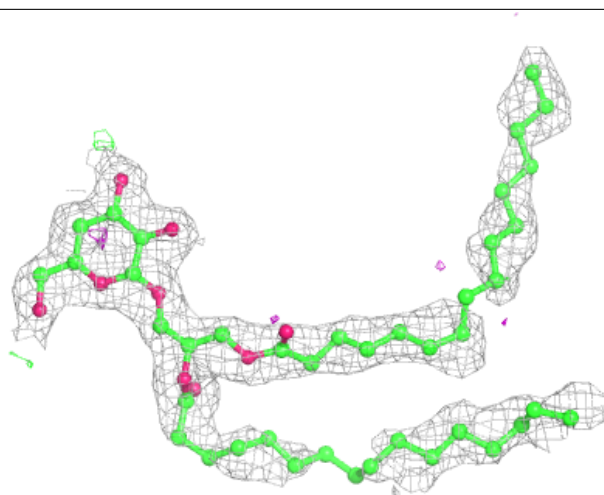
**Electron density around LMT m 103:**

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



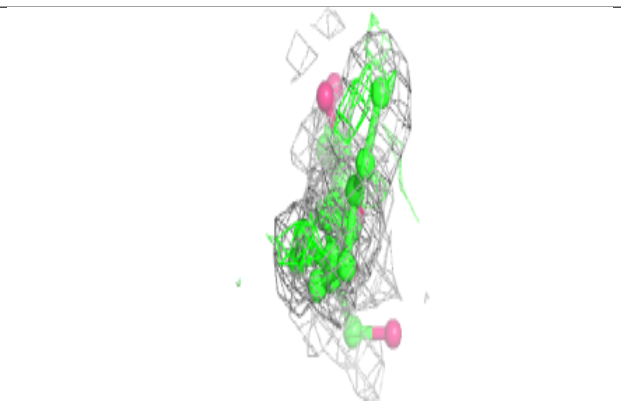
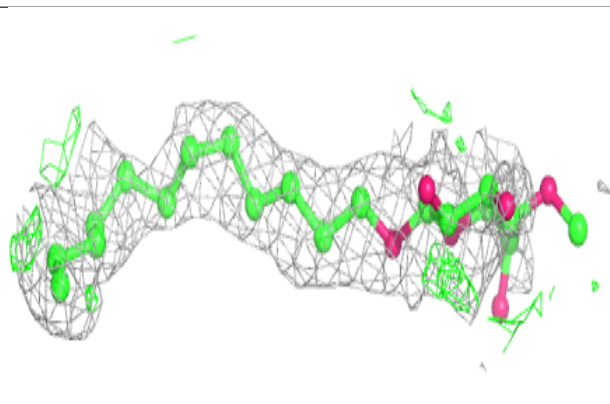
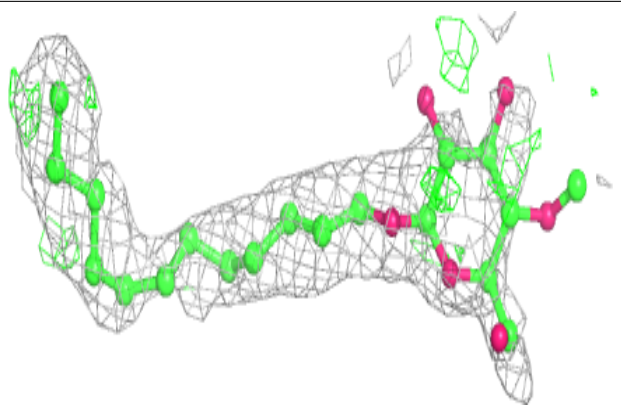
Electron density around LMG C 520:

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

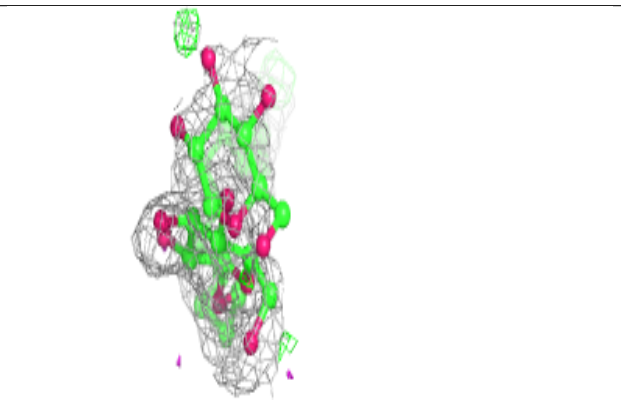
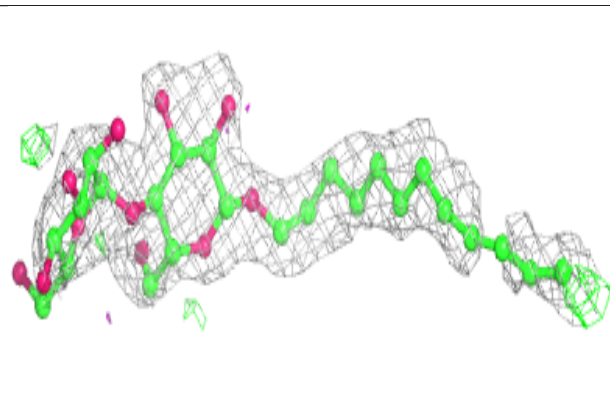
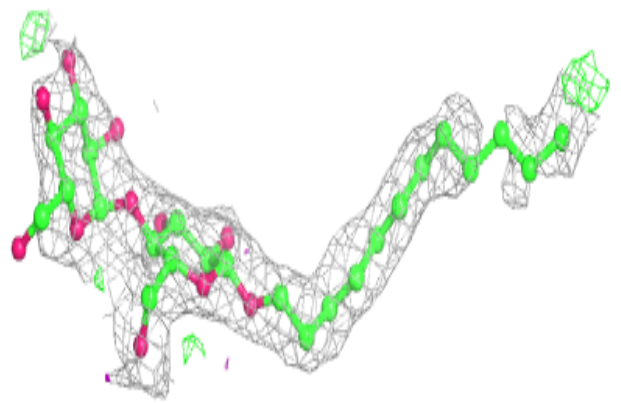


Electron density around LMT B 636:

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

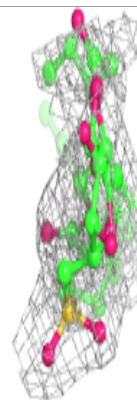
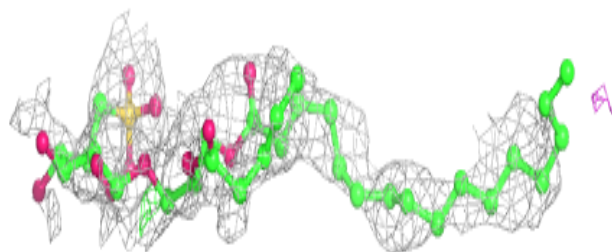
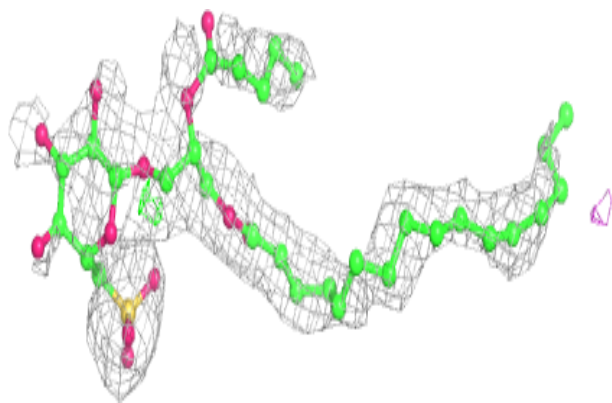
**Electron density around LMT A 417:**

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



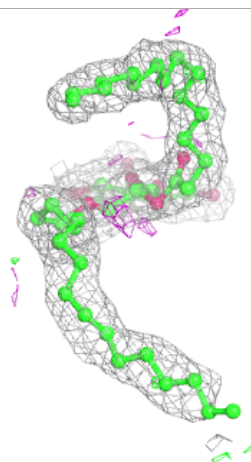
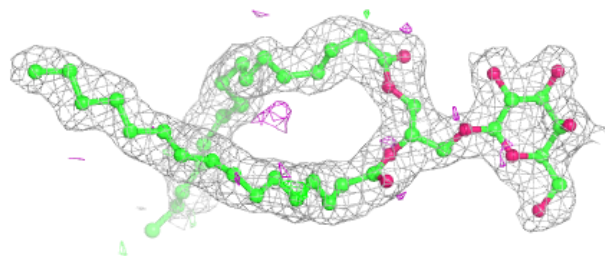
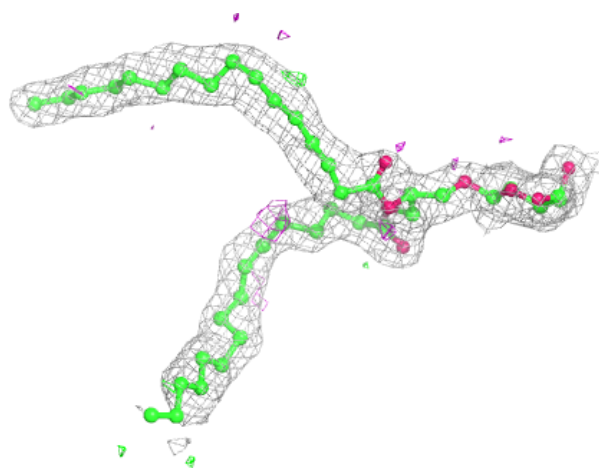
Electron density around SQD f 102:

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



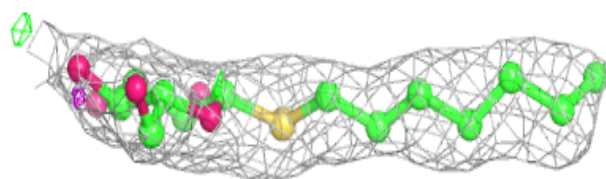
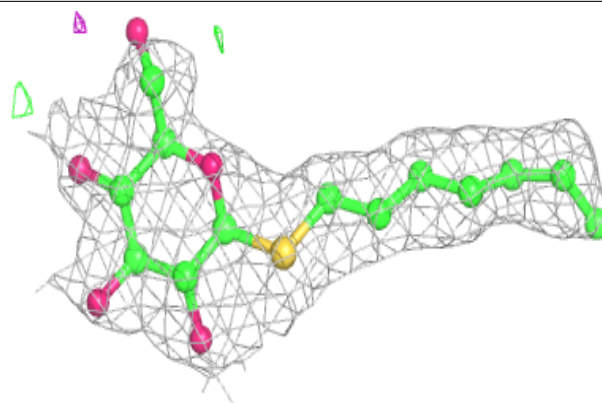
Electron density around LMG B 622:

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

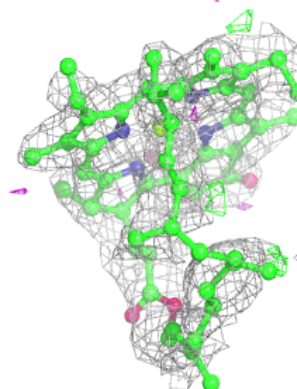
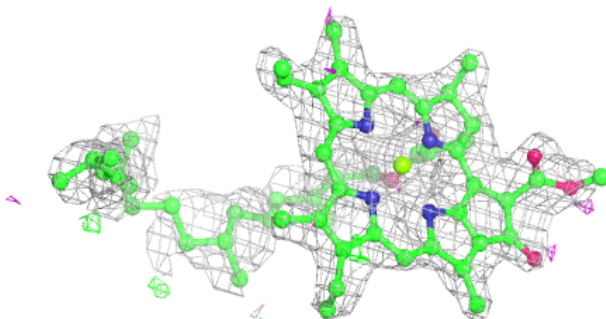
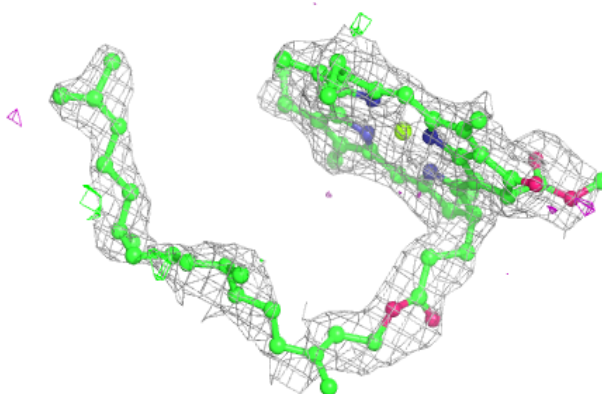


Electron density around HTG B 633:

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

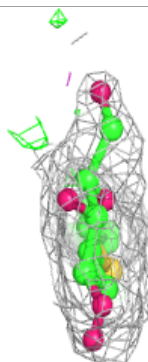
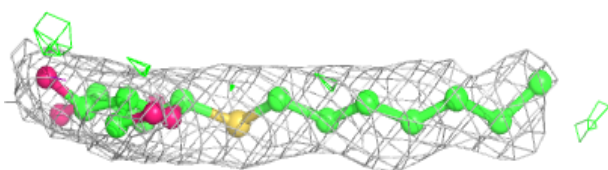
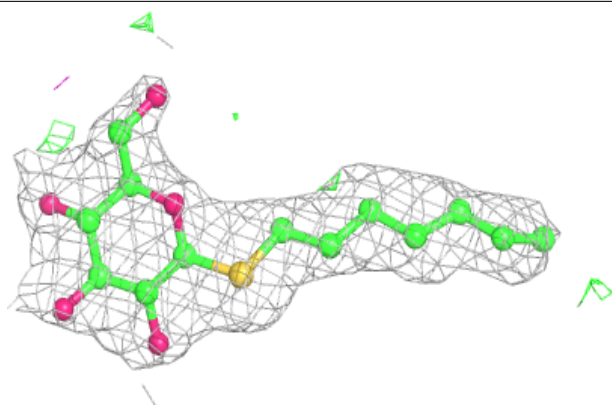
**Electron density around CLA c 914:**

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

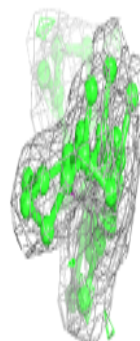
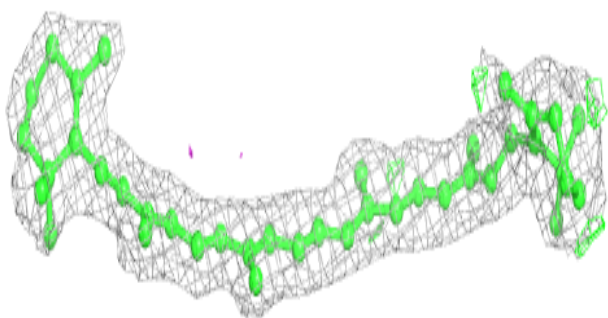
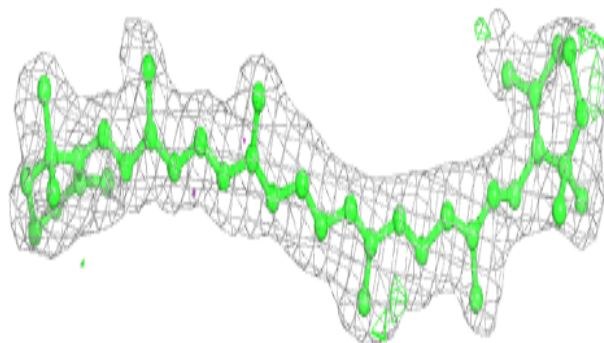


Electron density around HTG b 602:

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

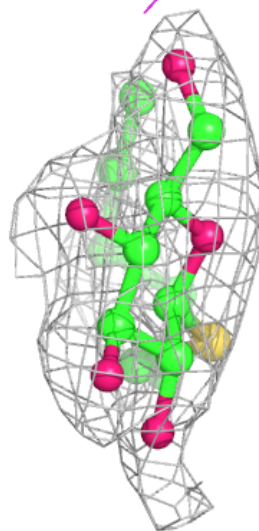
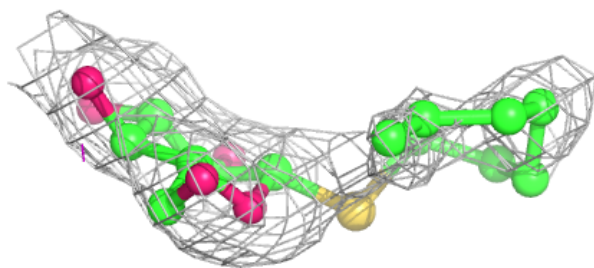
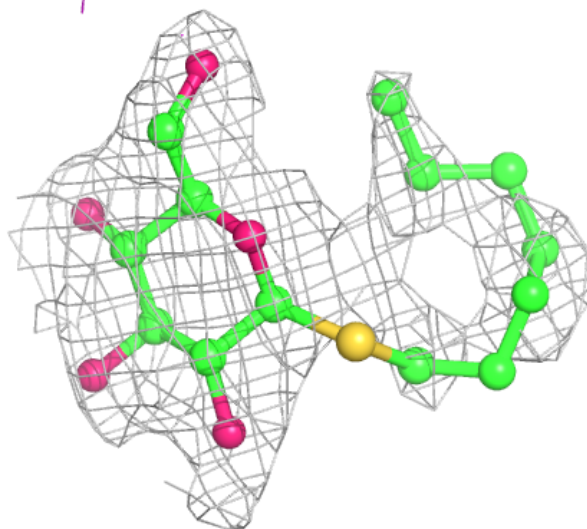
**Electron density around BCR d 404:**

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



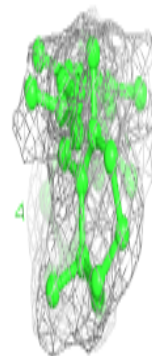
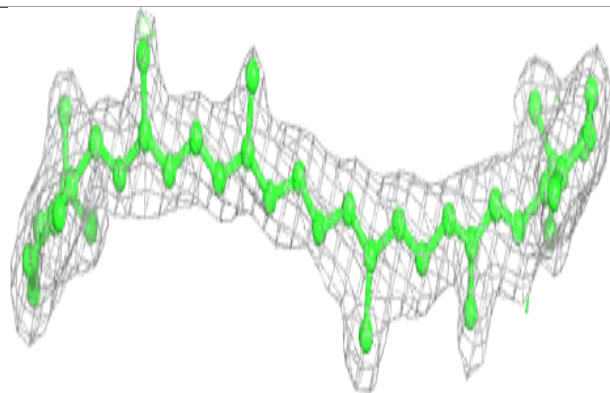
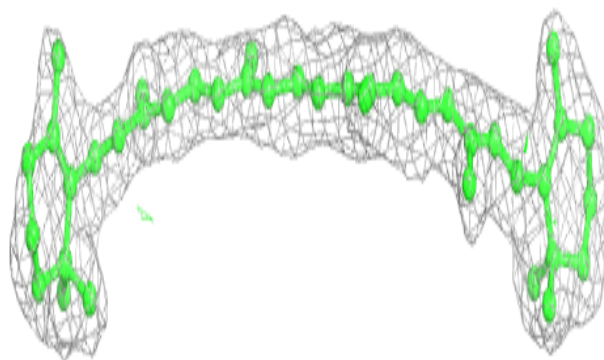
Electron density around HTG V 202:

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

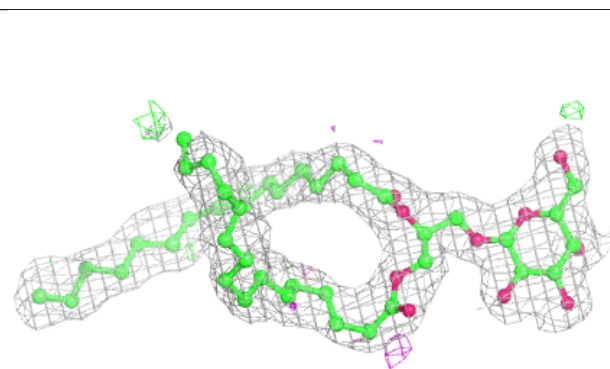
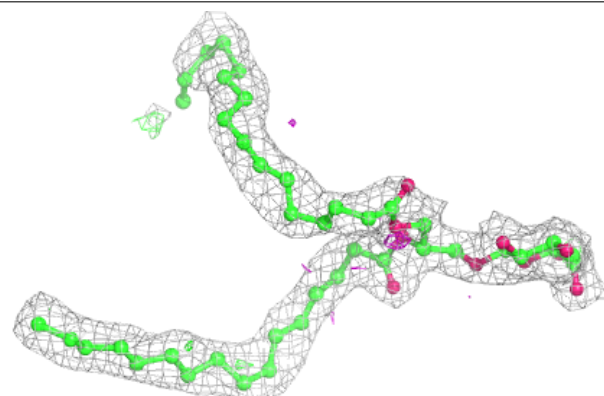


Electron density around BCR k 102:

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

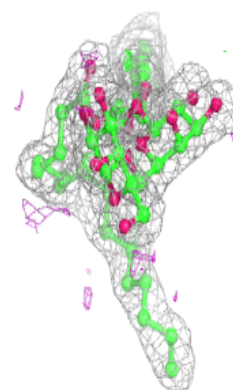
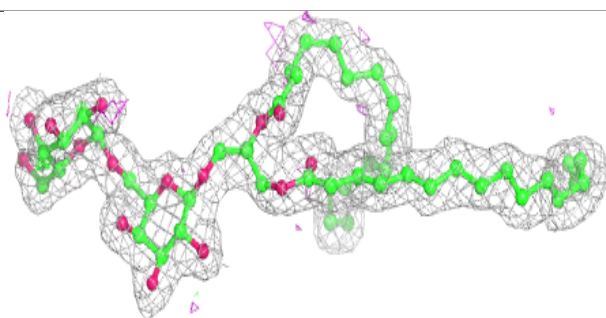
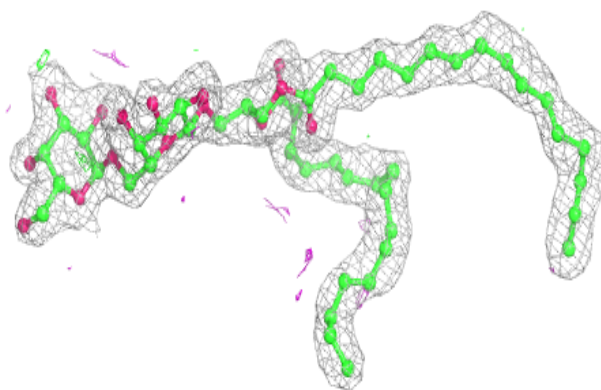
**Electron density around LMG b 624:**

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

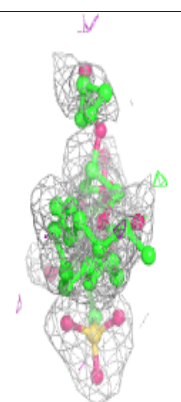
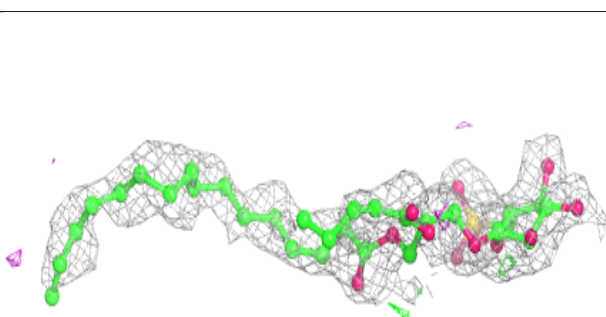
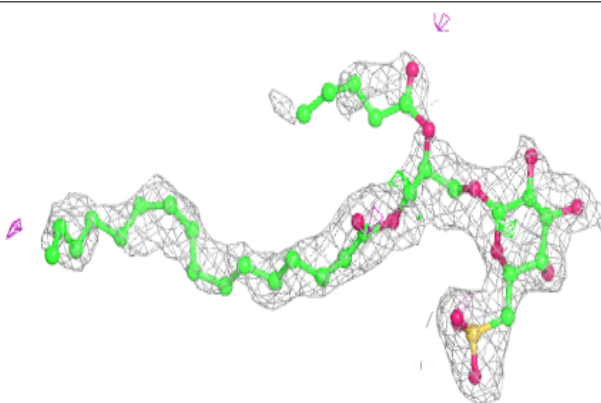


Electron density around DGD H 102:

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

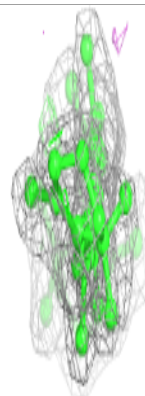
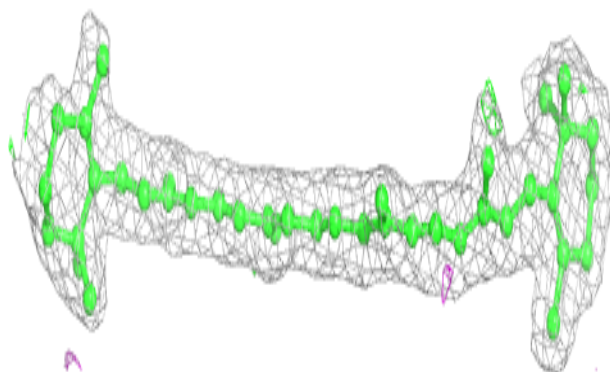
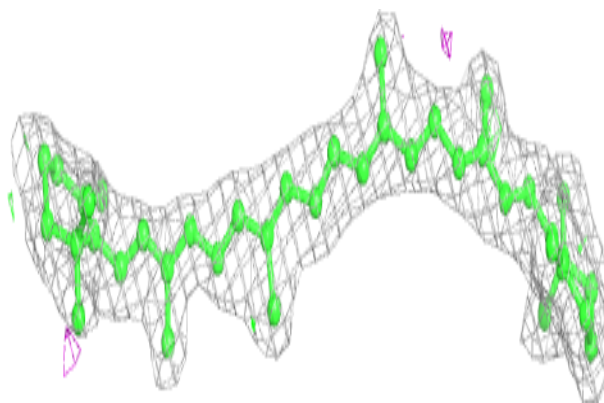
**Electron density around SQD F 101:**

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

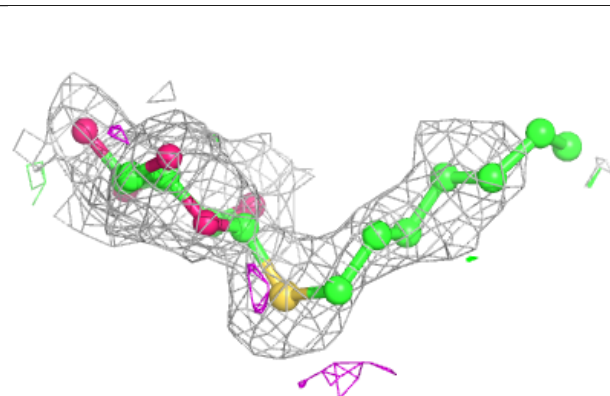
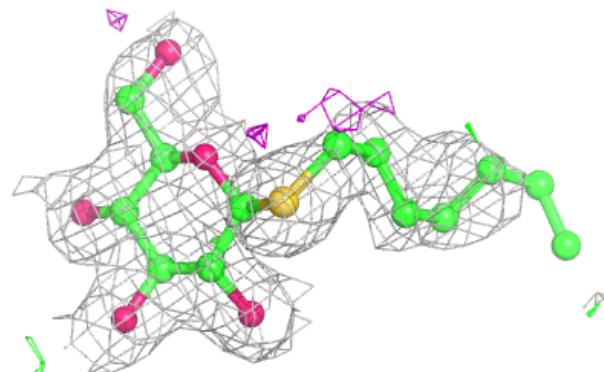


Electron density around BCR h 101:

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

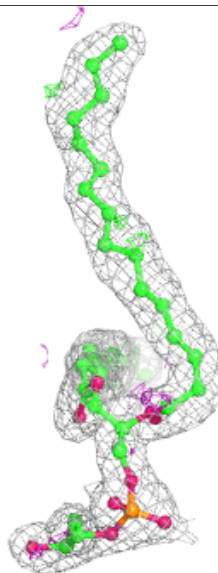
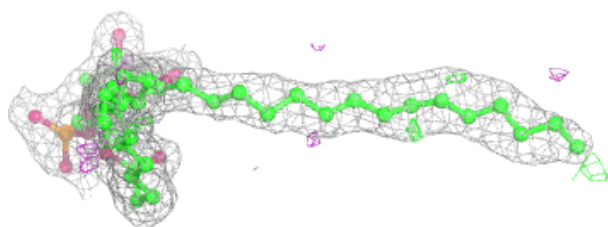
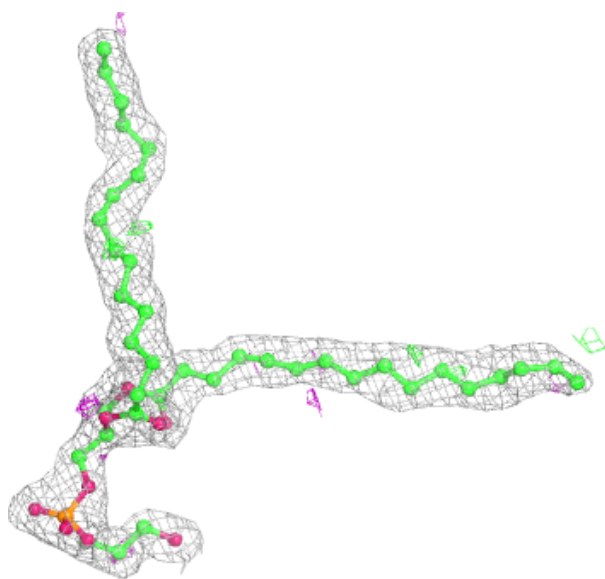
**Electron density around HTG b 626:**

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



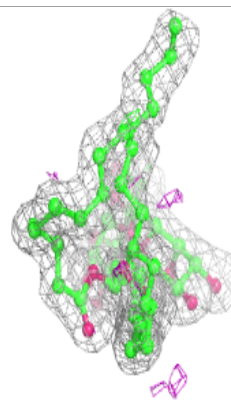
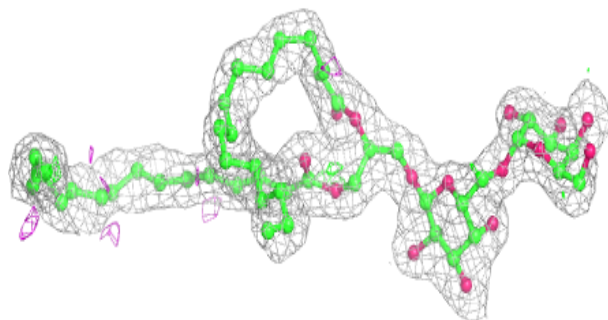
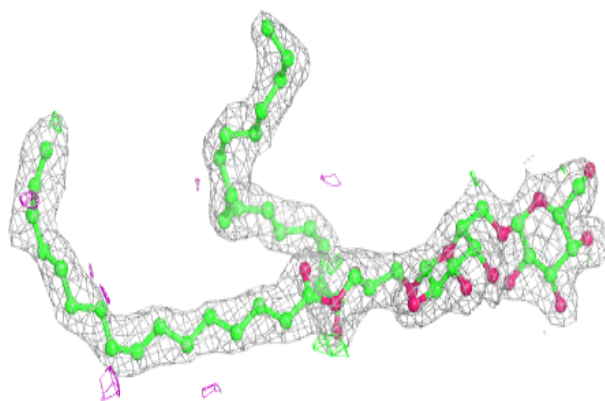
Electron density around LHG 1 101:

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

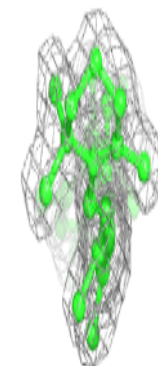
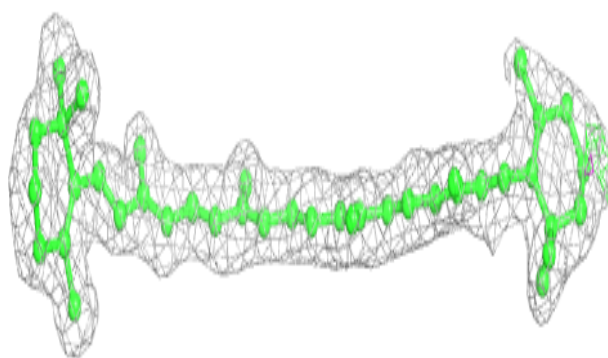
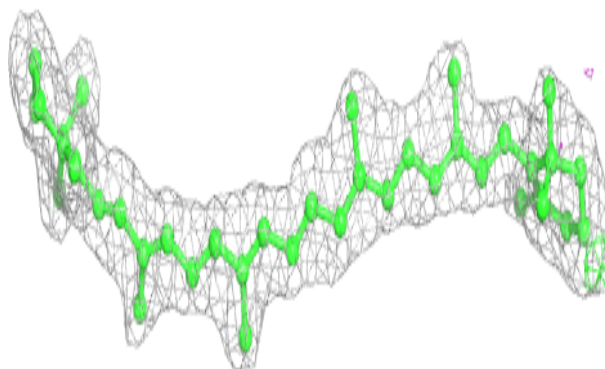


Electron density around DGD h 102:

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

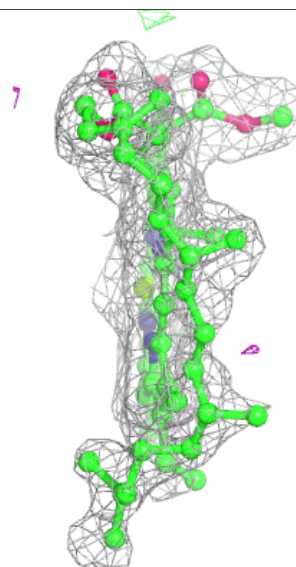
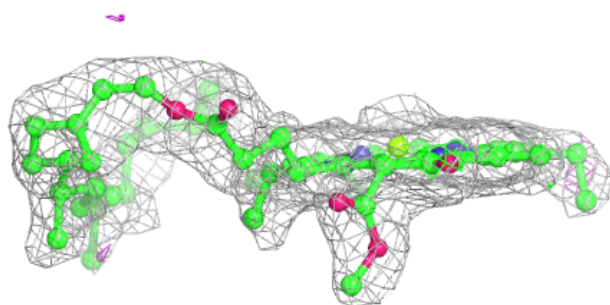
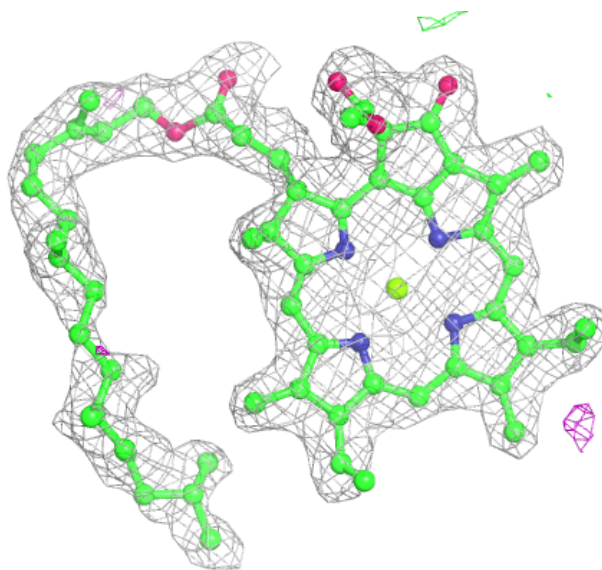
**Electron density around BCR H 101:**

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



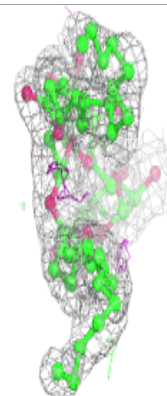
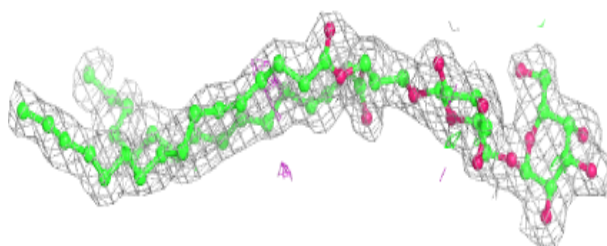
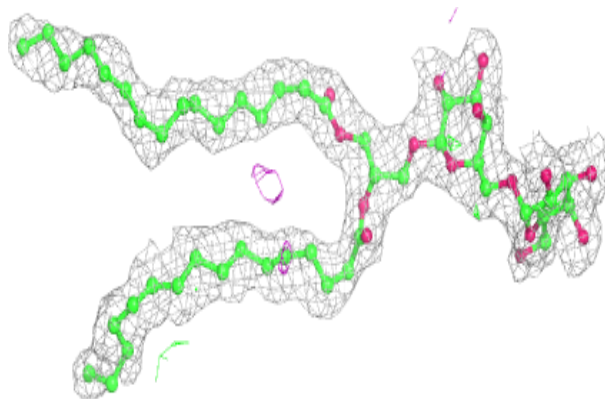
Electron density around CLA c 913:

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

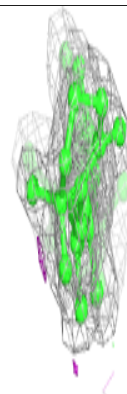
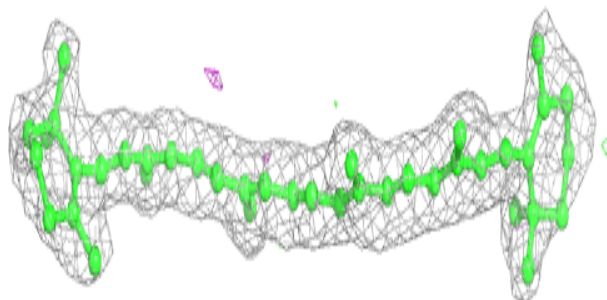
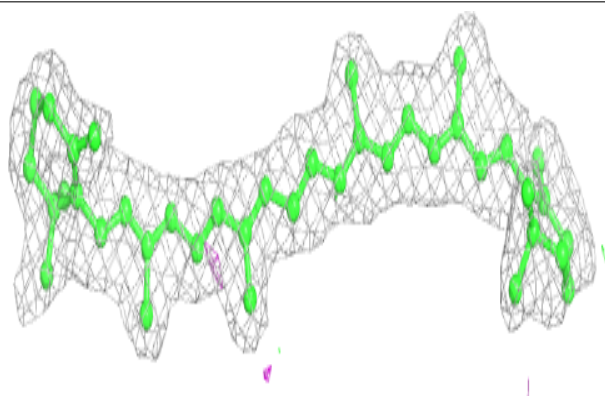


Electron density around DGD c 918:

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

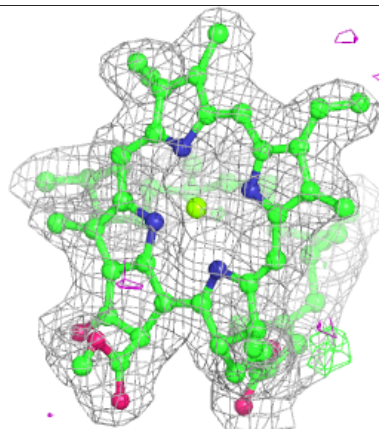
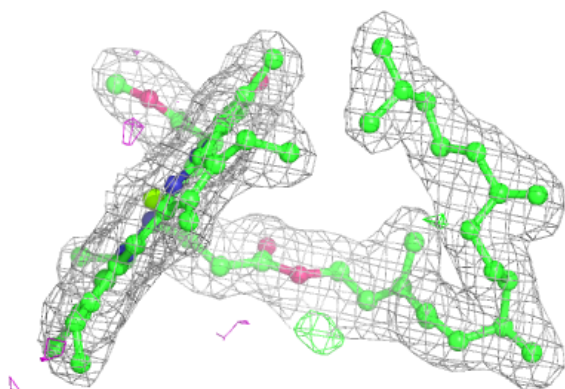
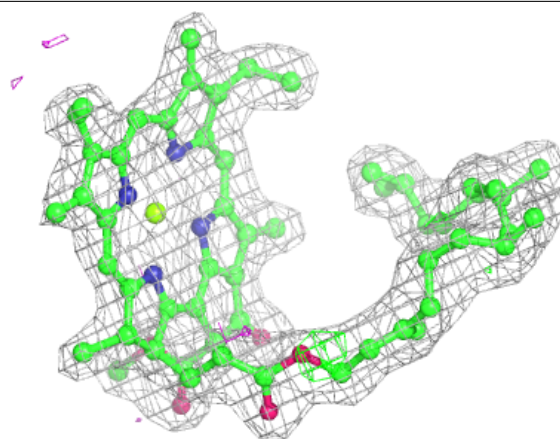
**Electron density around BCR y 101:**

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



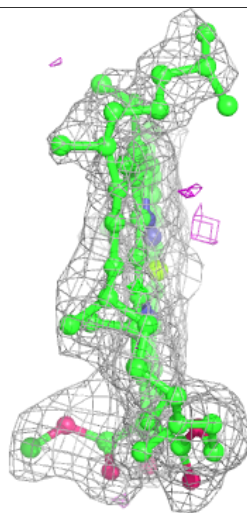
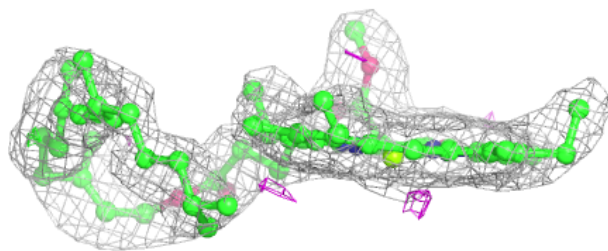
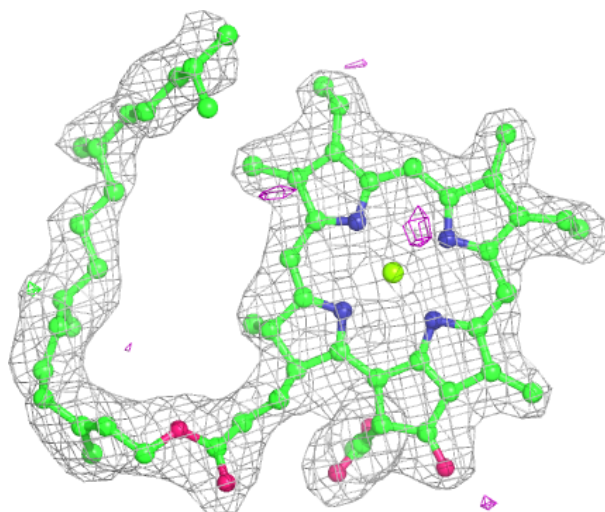
Electron density around CLA c 904:

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



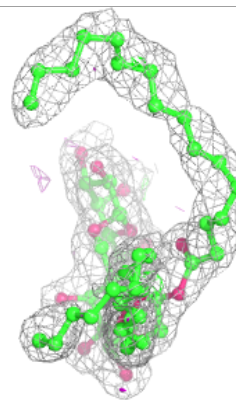
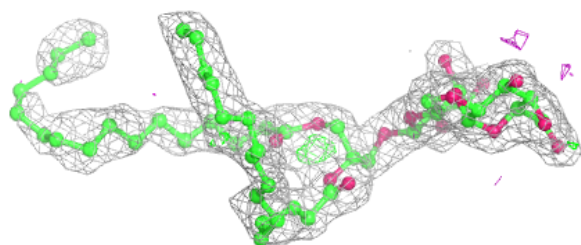
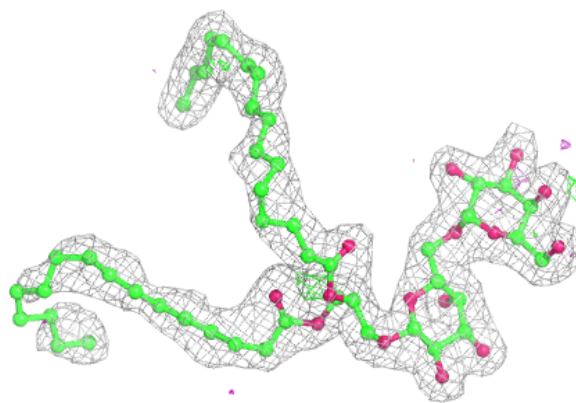
Electron density around CLA C 513:

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



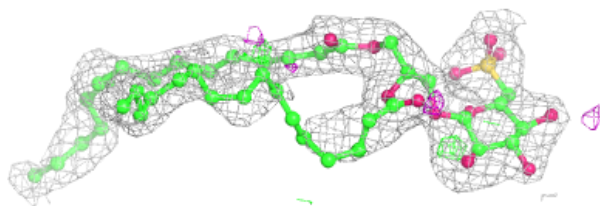
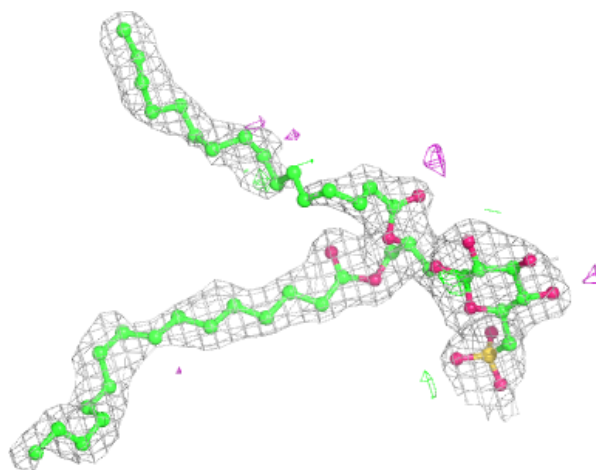
Electron density around DGD c 917:

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



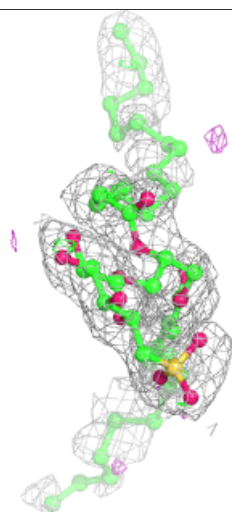
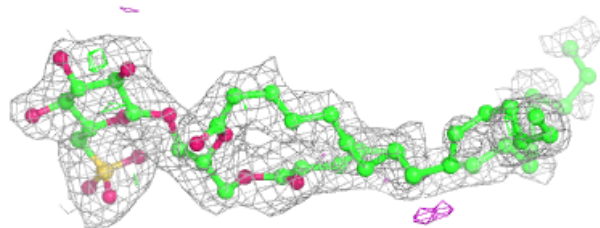
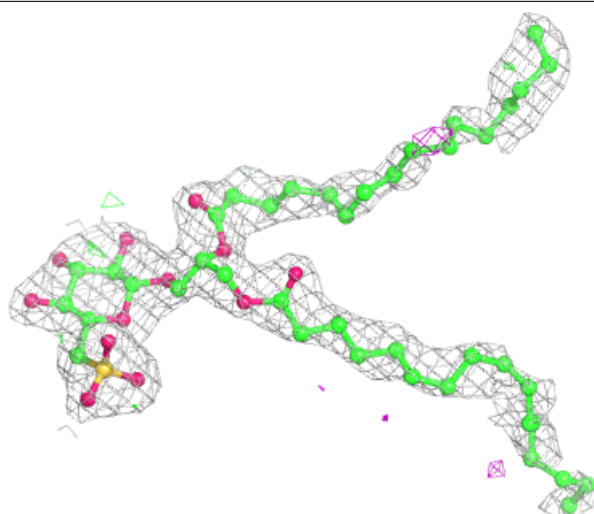
Electron density around SQD A 412:

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



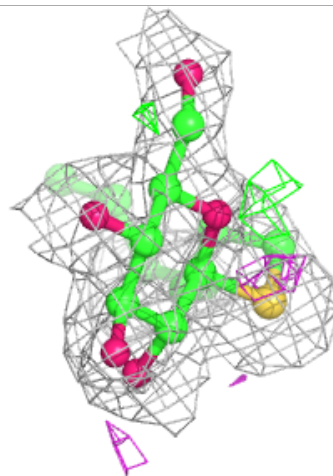
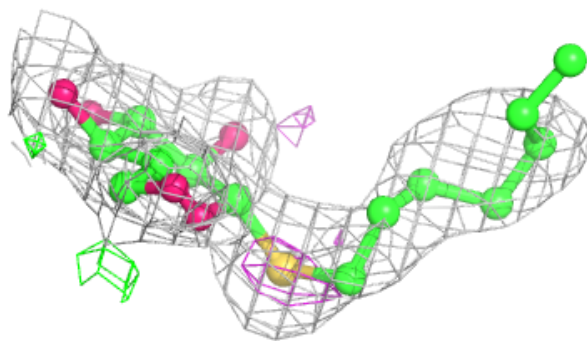
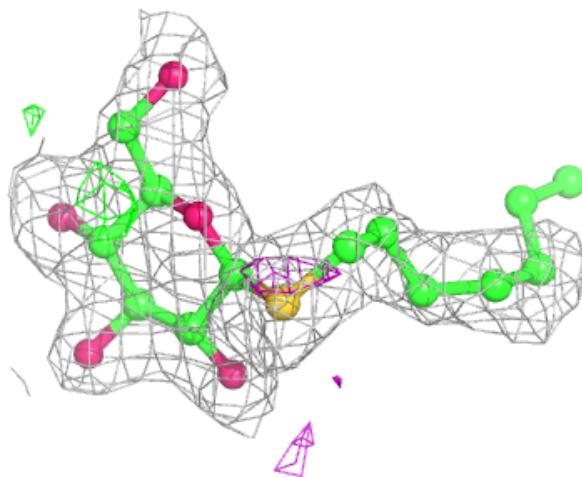
Electron density around SQD a 411:

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



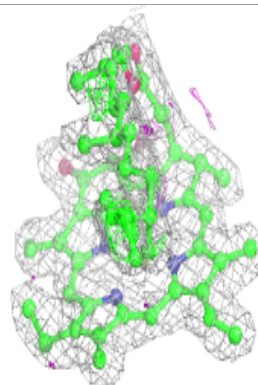
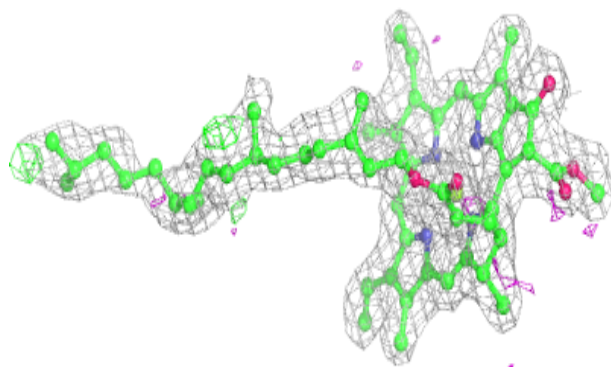
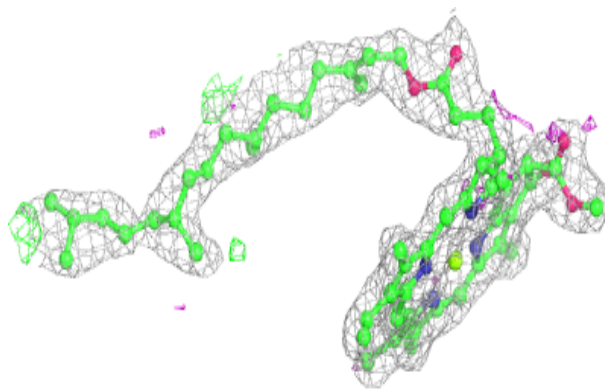
Electron density around HTG B 625:

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

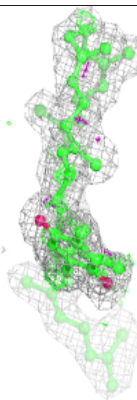
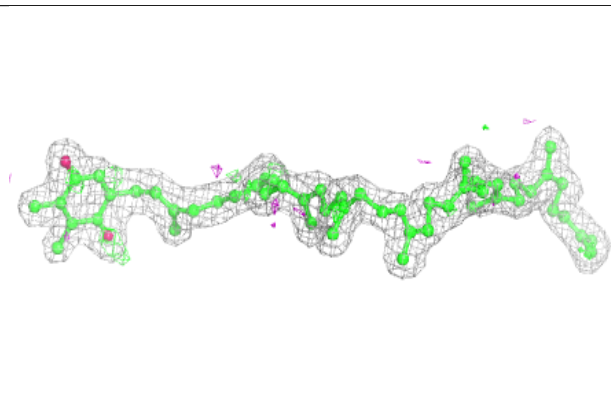
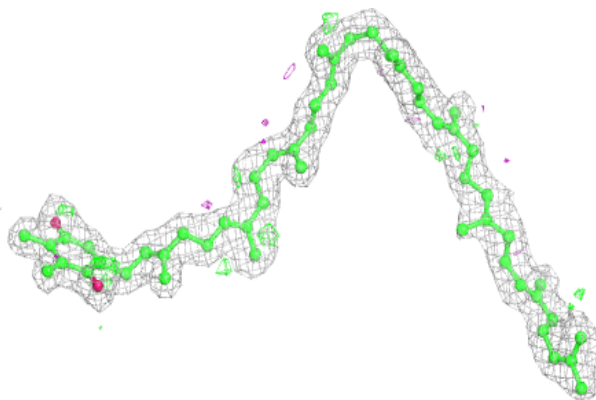


Electron density around CLA c 905:

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

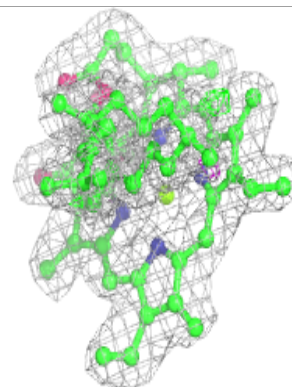
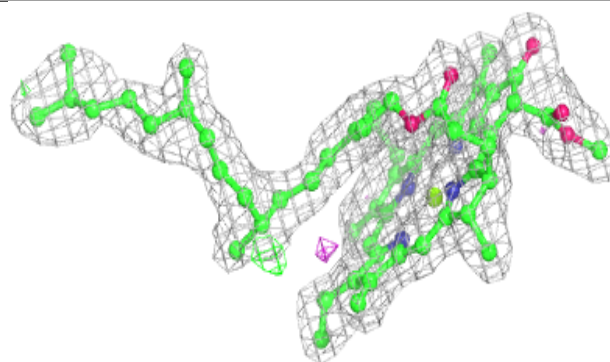
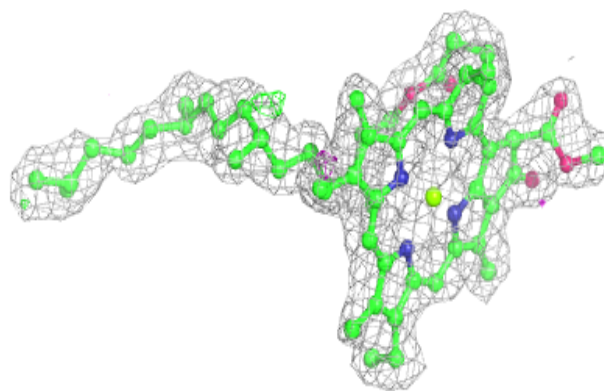
**Electron density around PL9 d 405:**

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

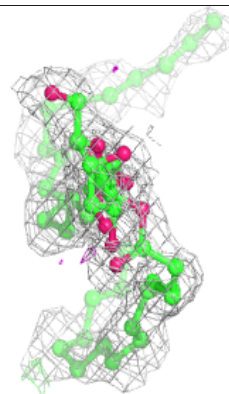
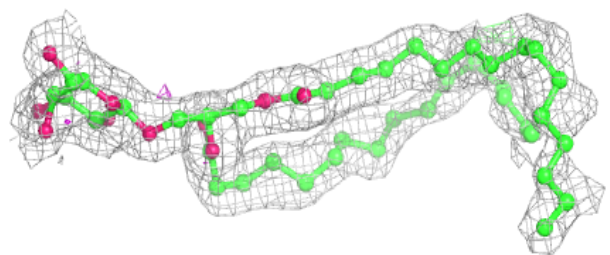
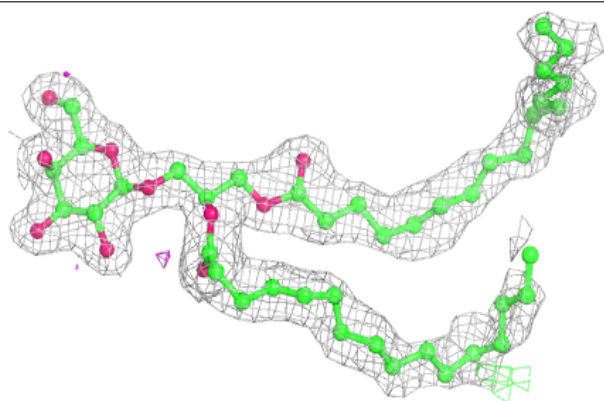


Electron density around CLA c 906:

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

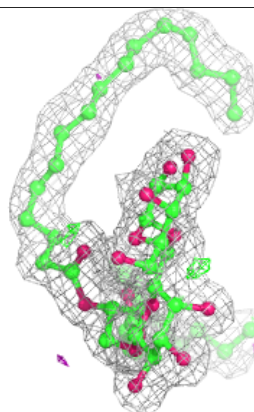
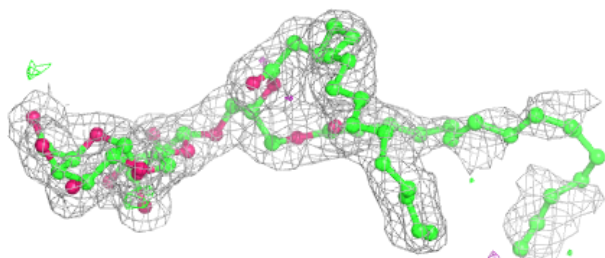
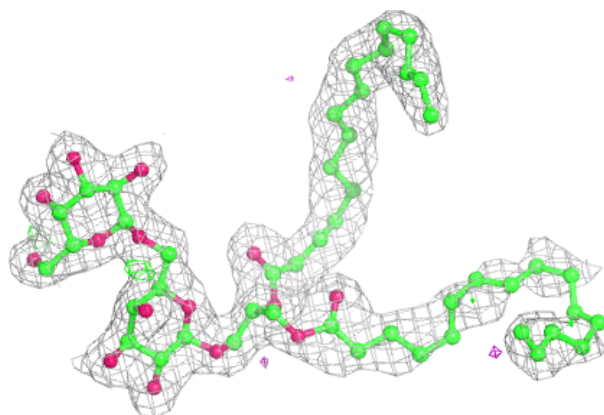
**Electron density around LMG J 101:**

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

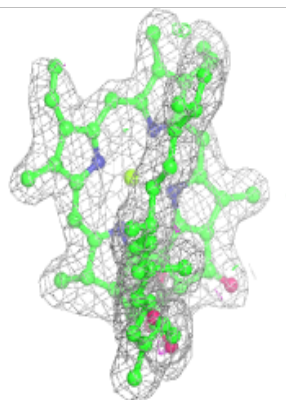
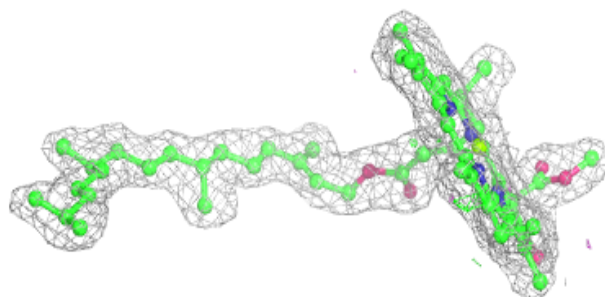
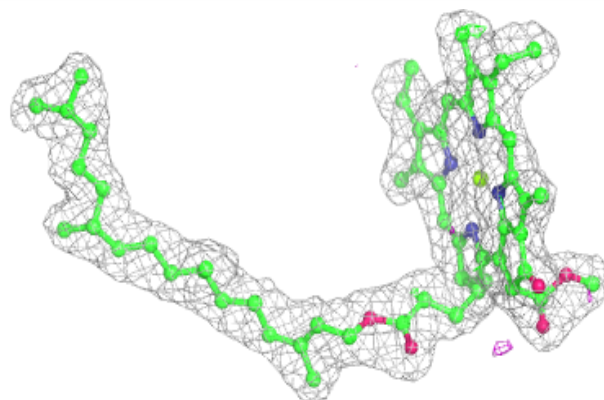


Electron density around DGD C 518:

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

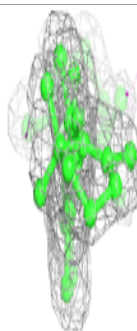
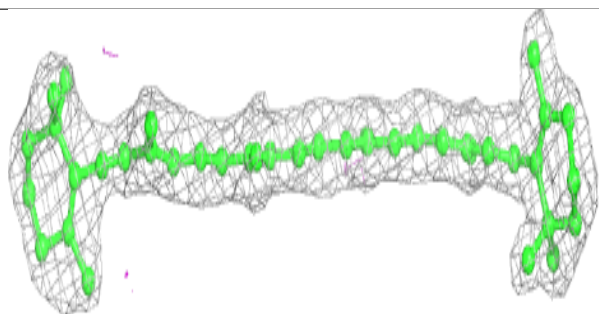
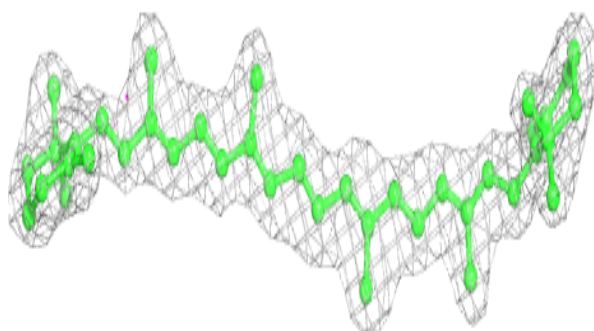
**Electron density around CLA b 613:**

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

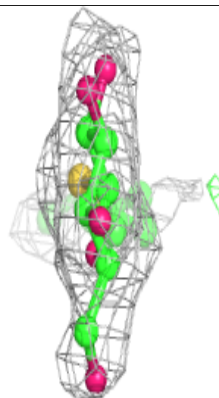
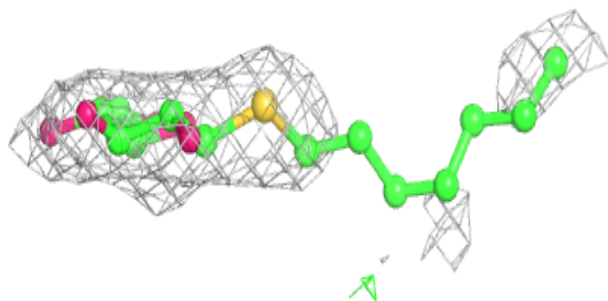
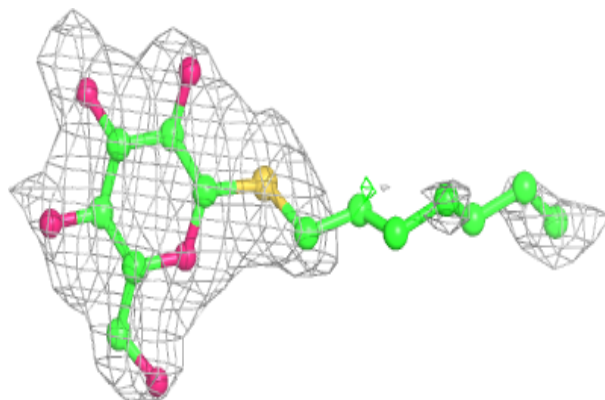


Electron density around BCR c 915:

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

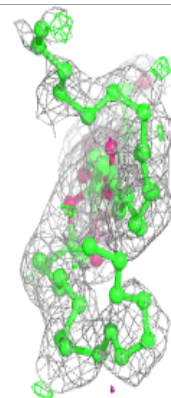
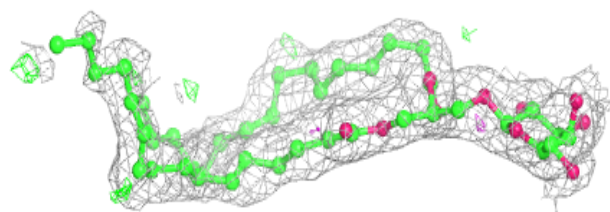
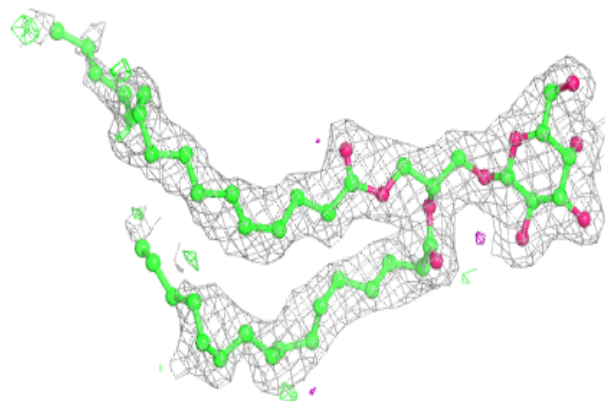
**Electron density around HTG C 523:**

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

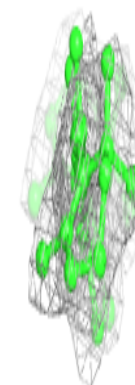
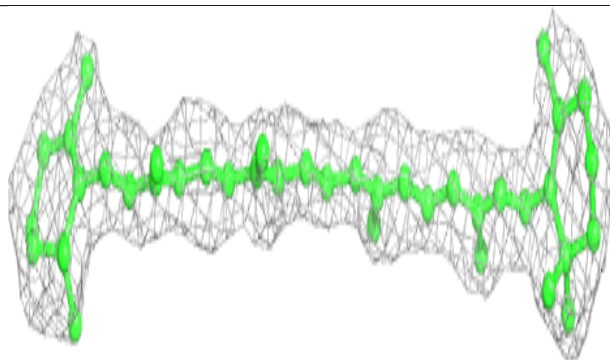
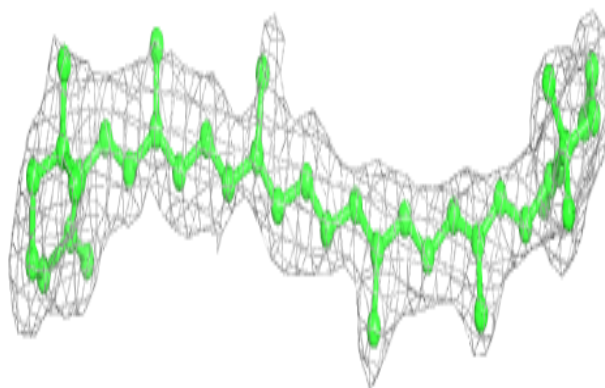


Electron density around LMG j 101:

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

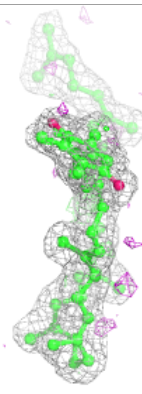
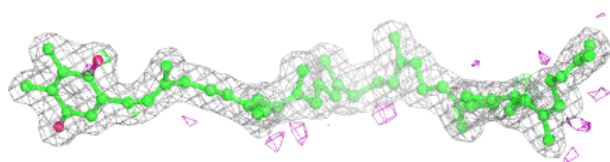
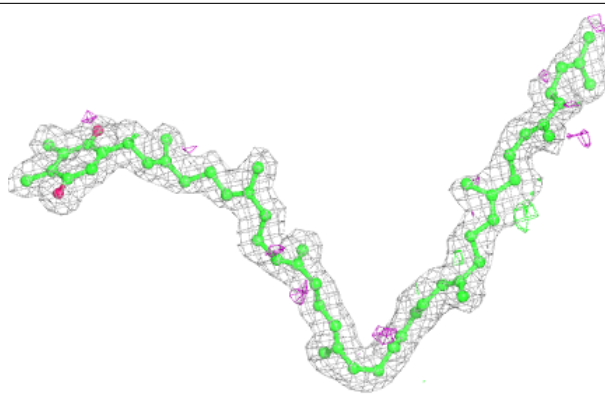
**Electron density around BCR k 101:**

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



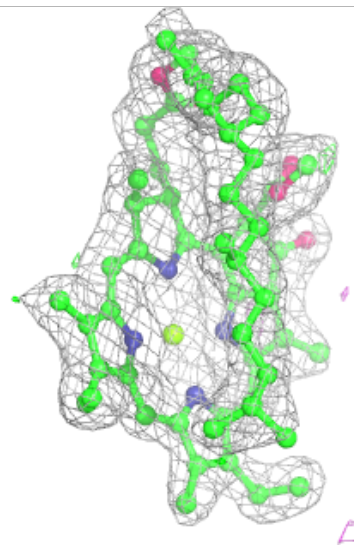
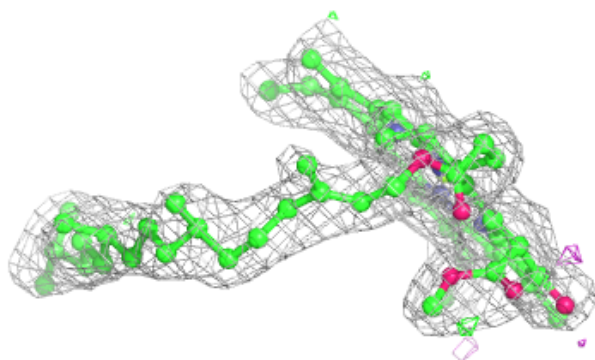
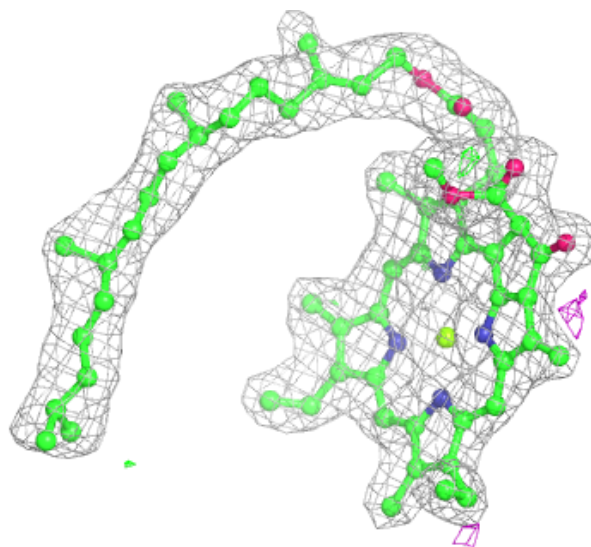
Electron density around PL9 D 404:

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



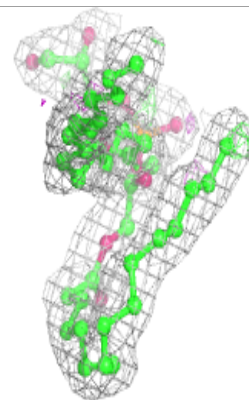
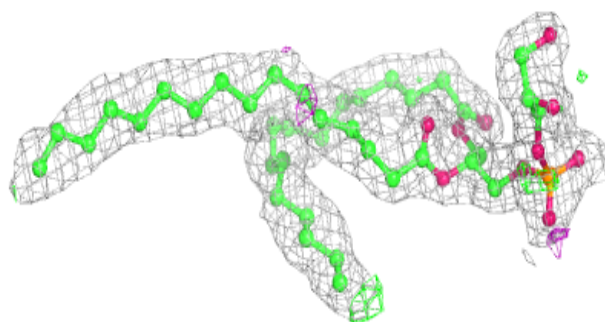
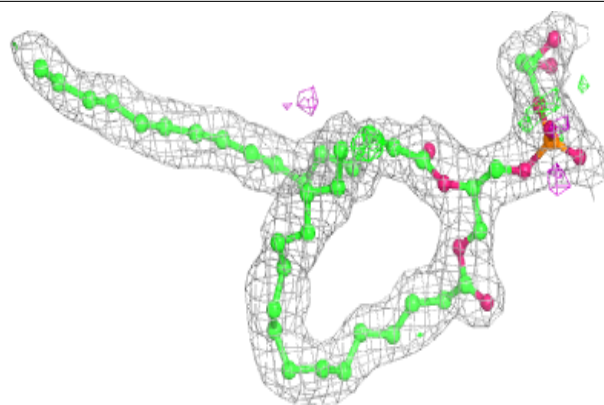
Electron density around CLA c 908:

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

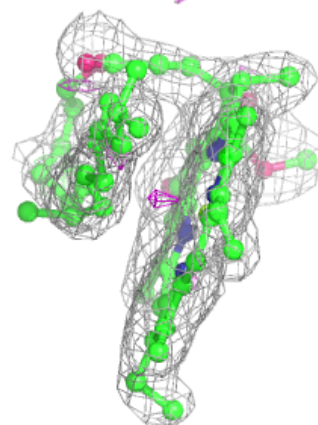
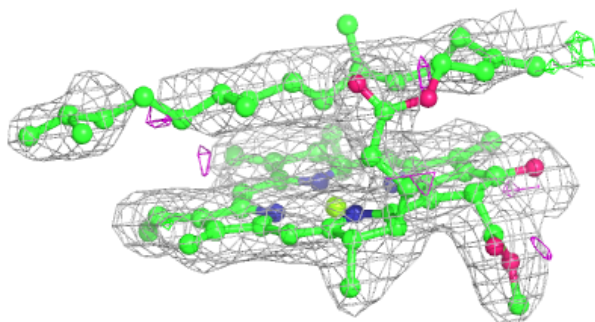
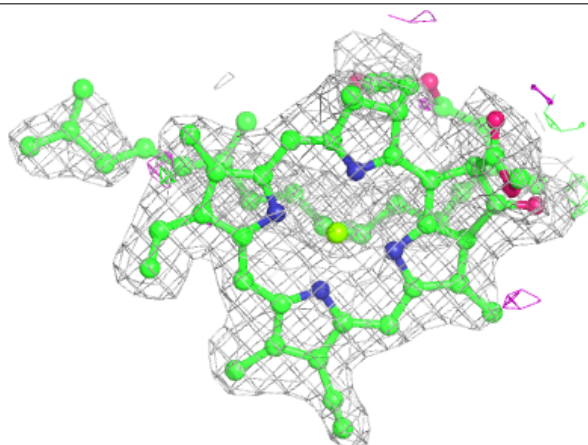


Electron density around LHG d 407:

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

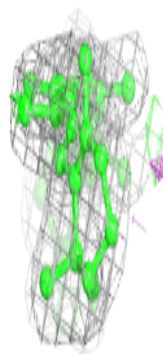
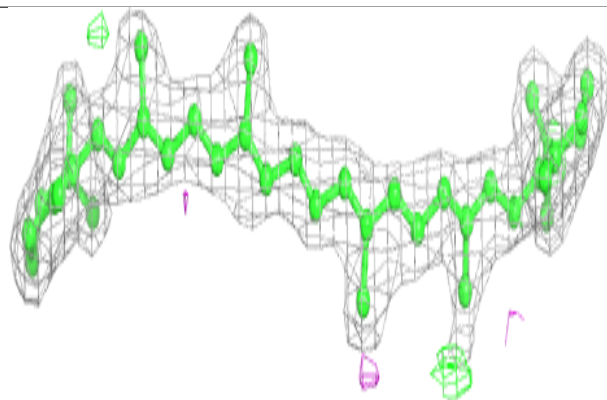
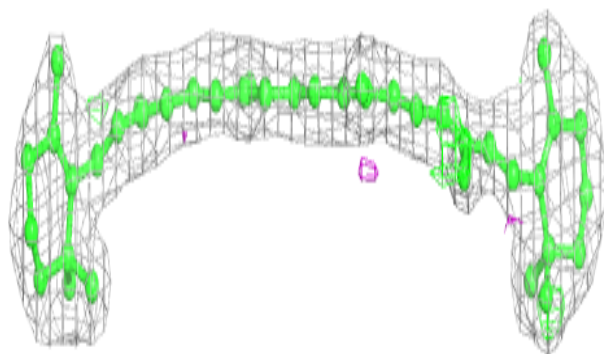
**Electron density around CLA B 602:**

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



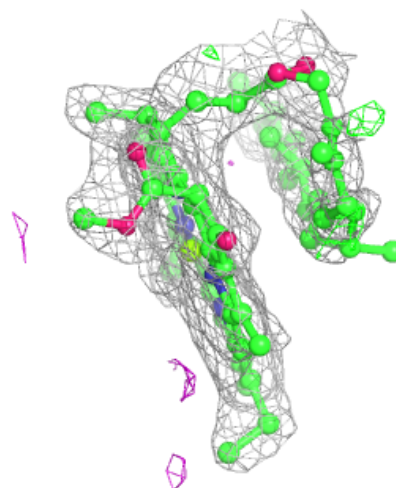
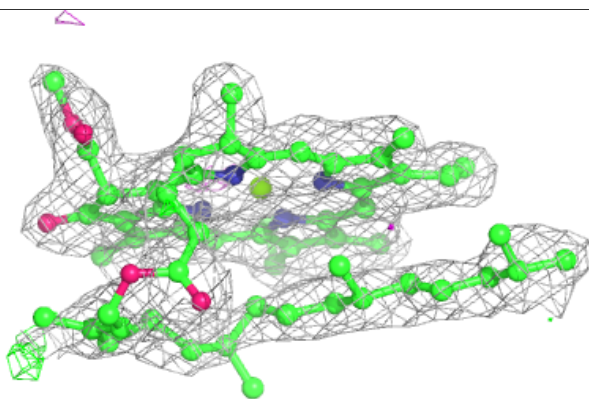
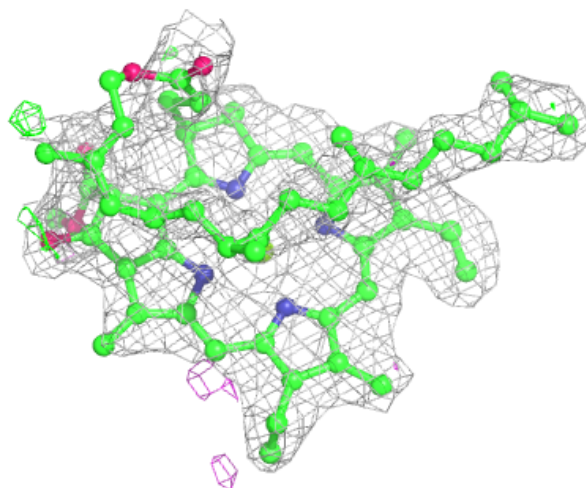
Electron density around BCR K 103:

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



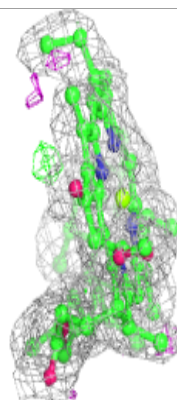
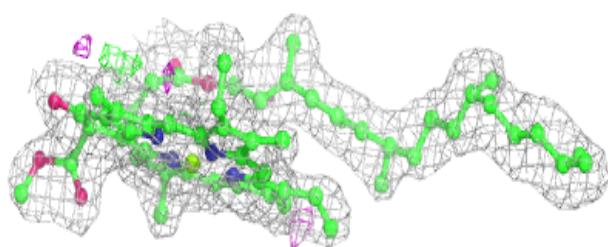
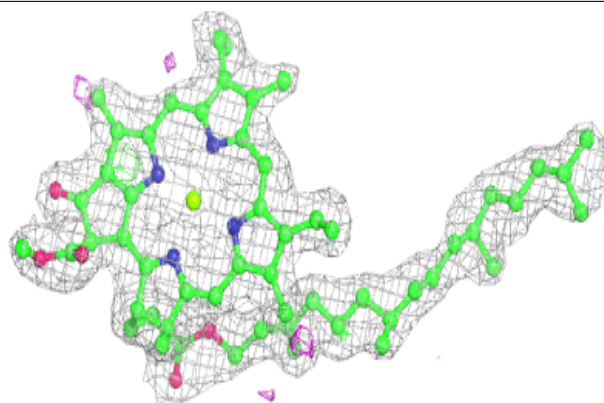
Electron density around CLA b 605:

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

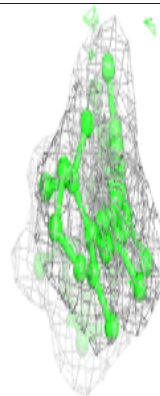
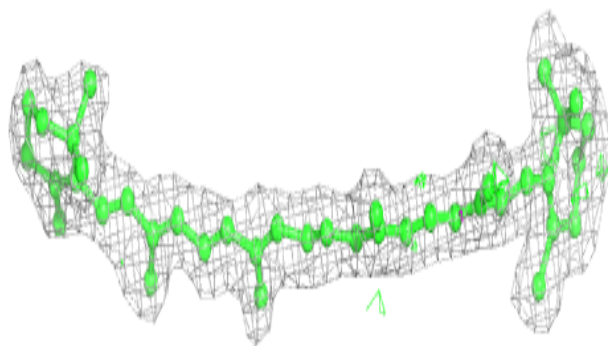
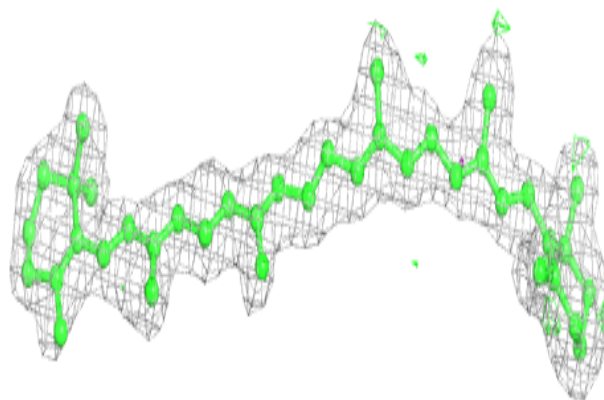


Electron density around CLA c 902:

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

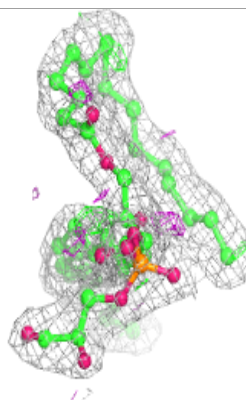
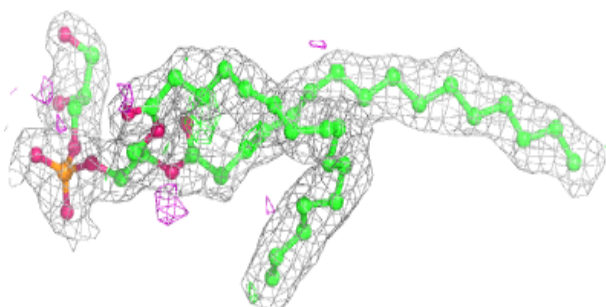
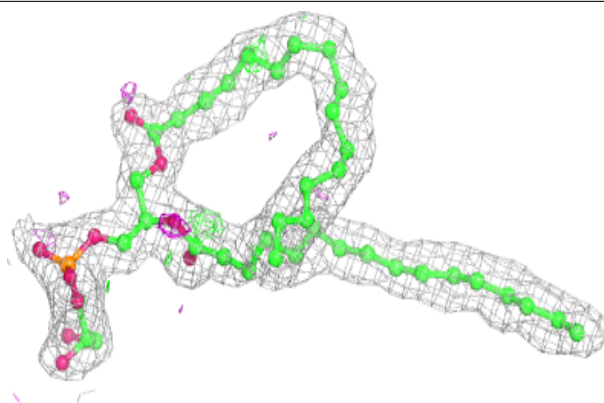
**Electron density around BCR t 101:**

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

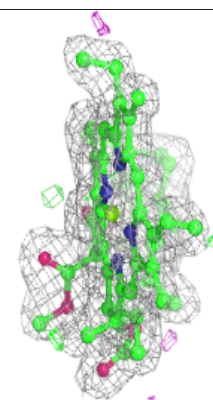
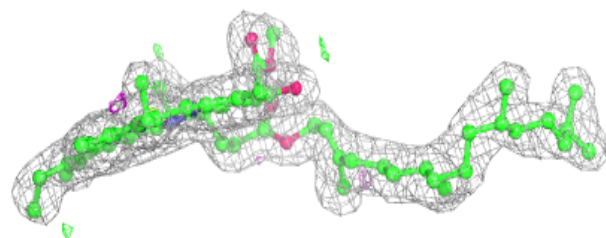
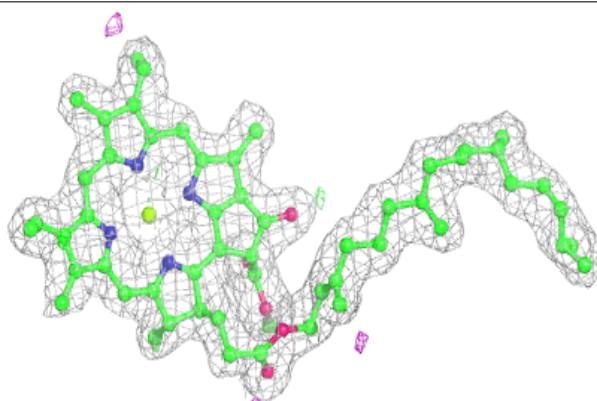


Electron density around LHG D 406:

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

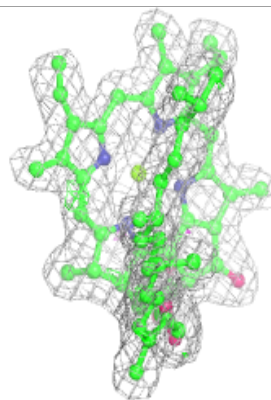
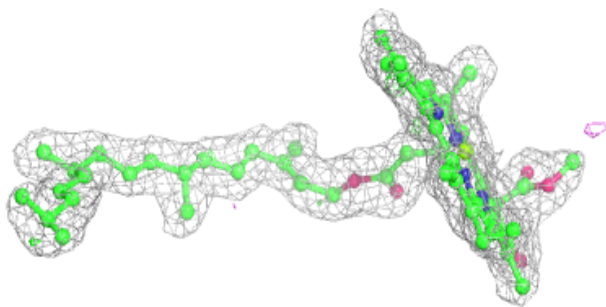
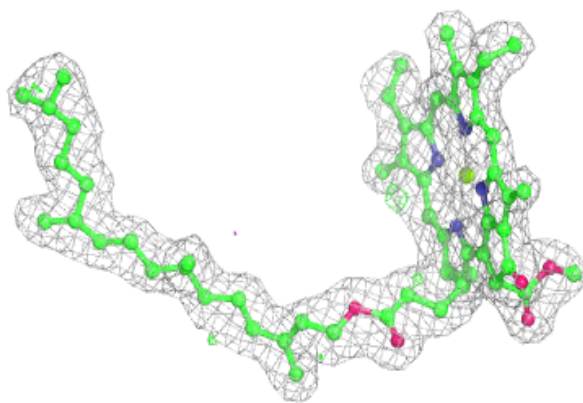
**Electron density around CLA B 603:**

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

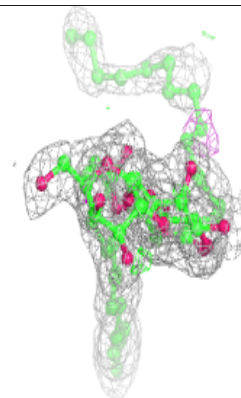
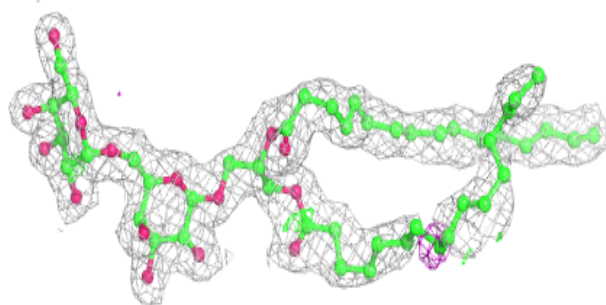
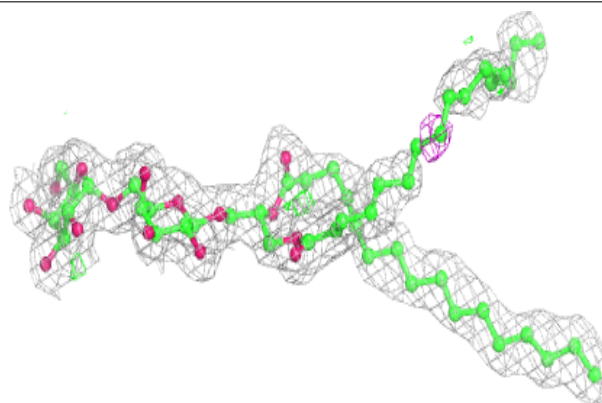


Electron density around CLA B 610:

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

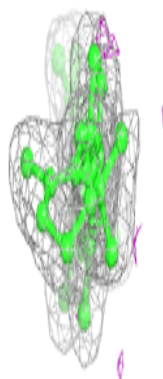
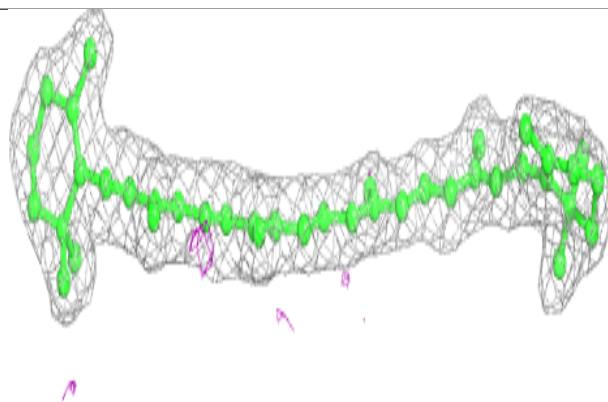
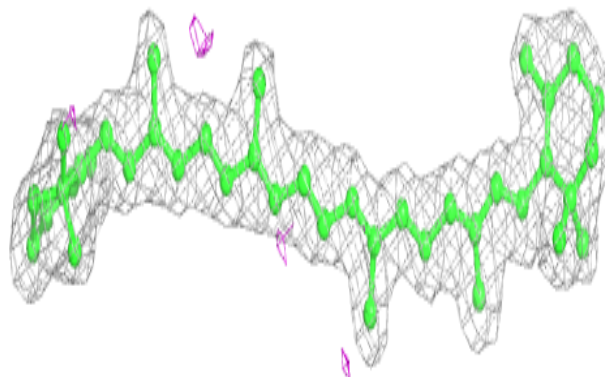
**Electron density around DGD c 916:**

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

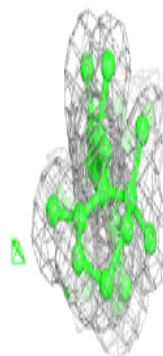
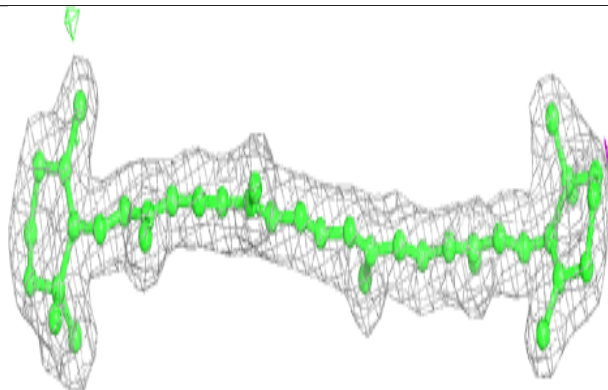
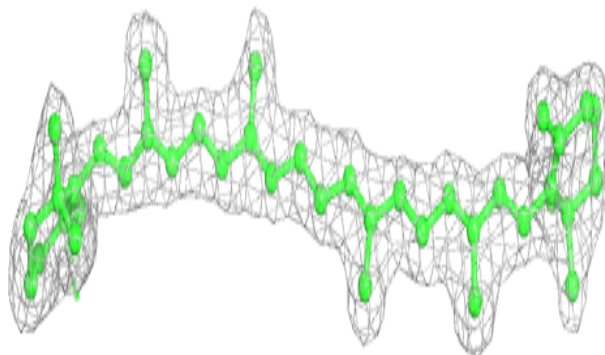


Electron density around BCR b 621:

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

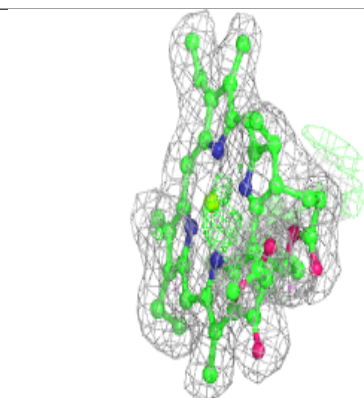
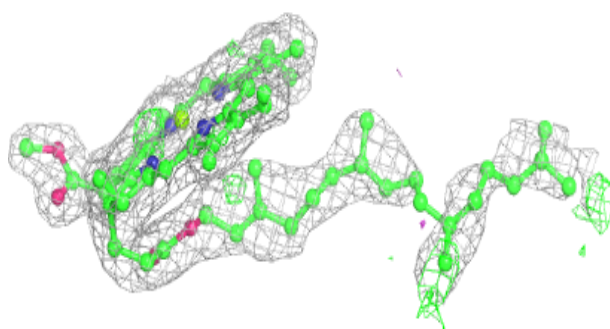
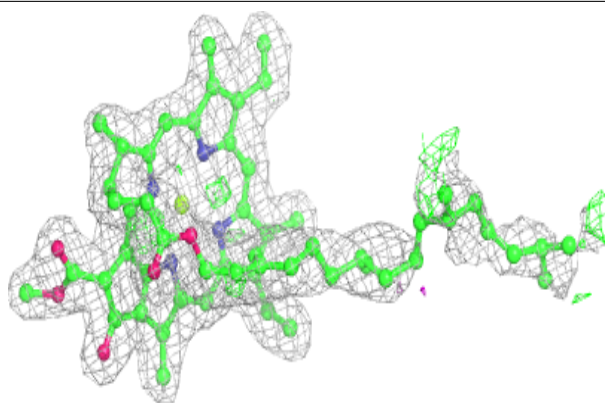
**Electron density around BCR a 410:**

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

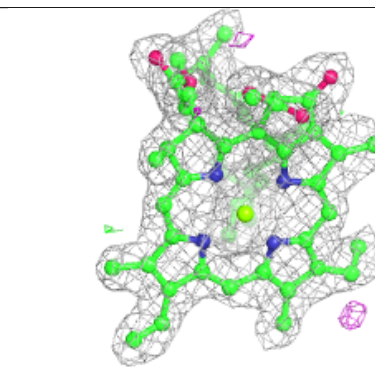
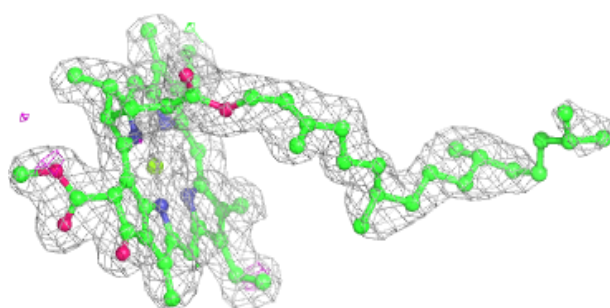
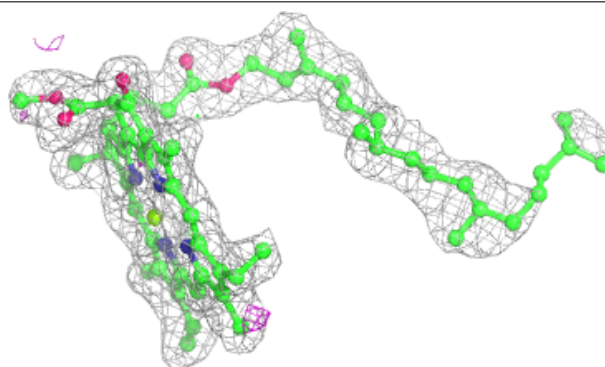


Electron density around CLA b 618:

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

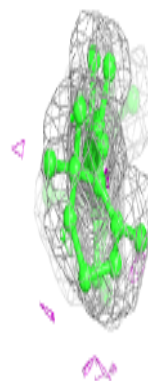
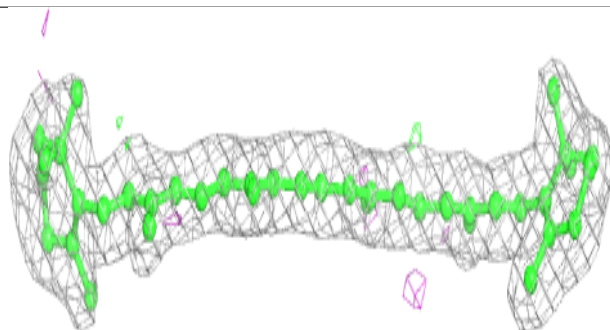
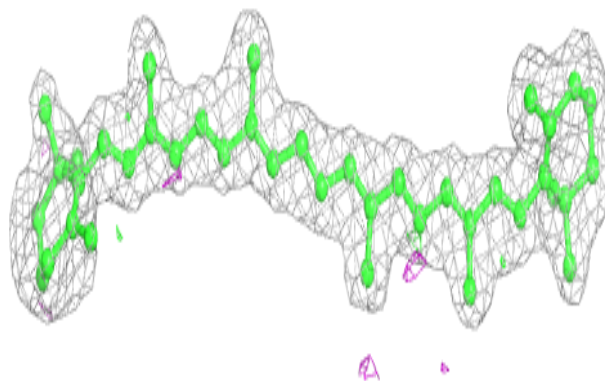
**Electron density around CLA c 909:**

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

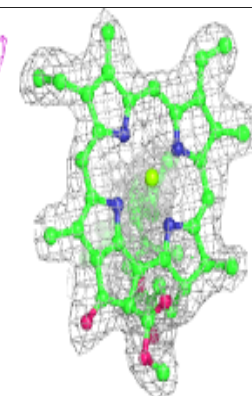
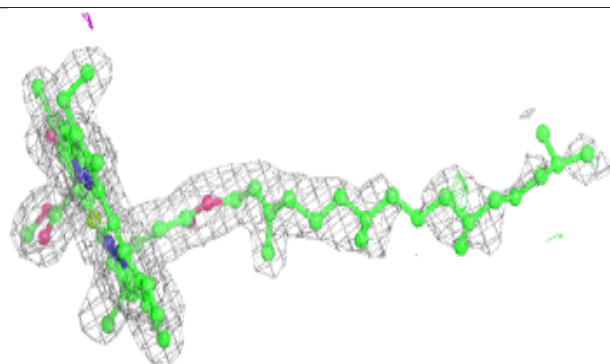
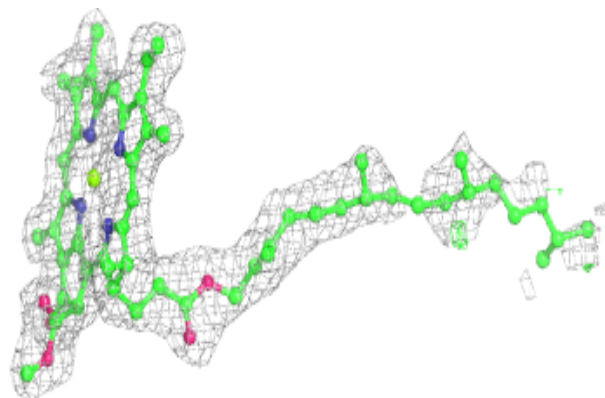


Electron density around BCR b 622:

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

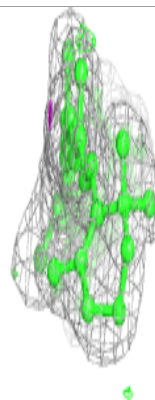
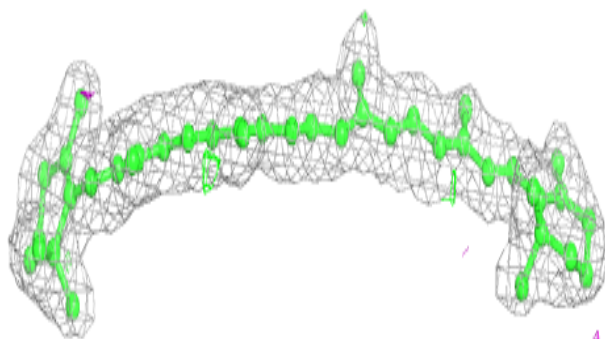
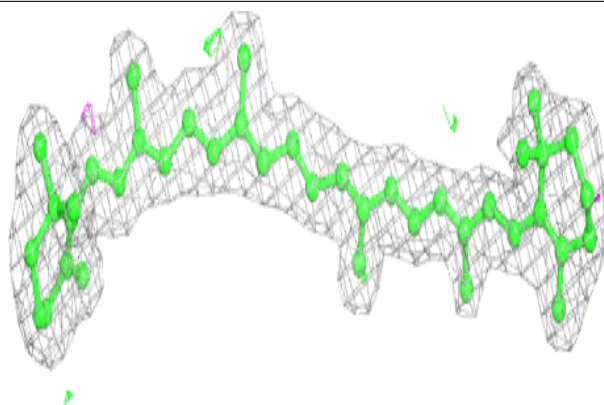
**Electron density around CLA d 403:**

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

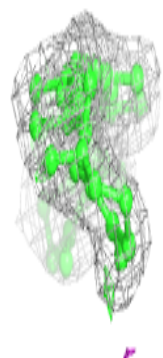
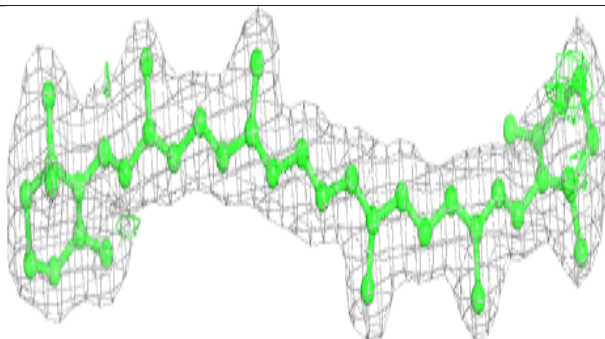
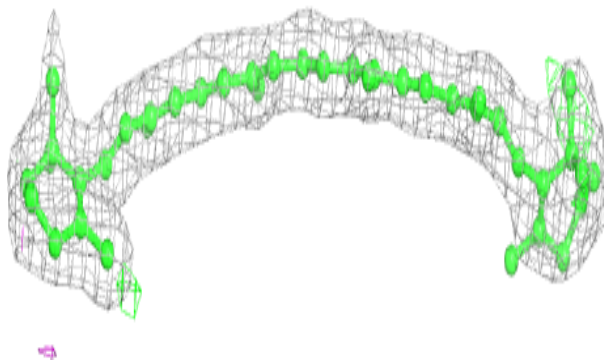


Electron density around BCR T 102:

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

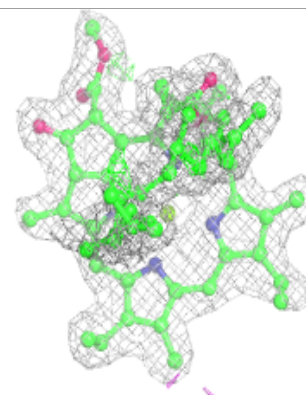
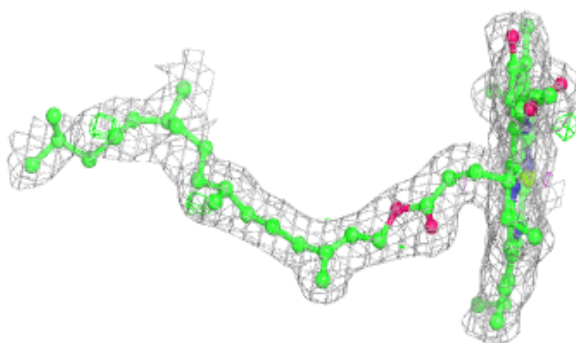
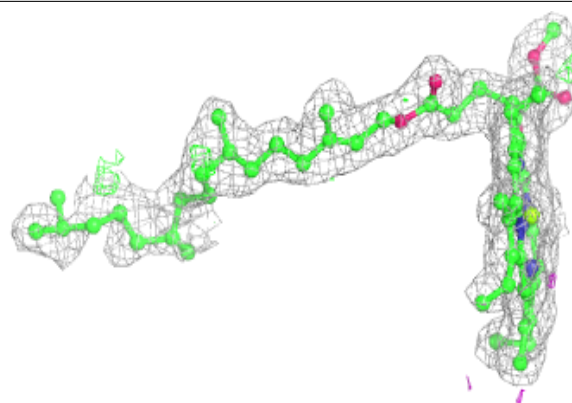
**Electron density around BCR D 403:**

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

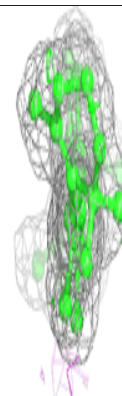
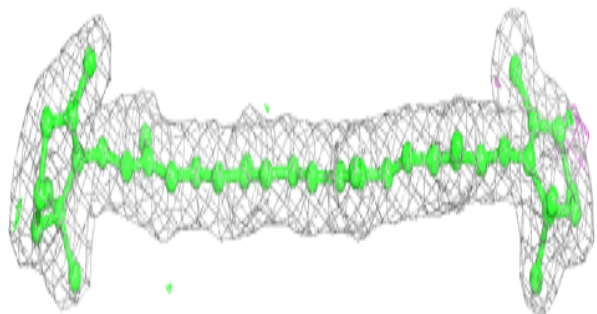
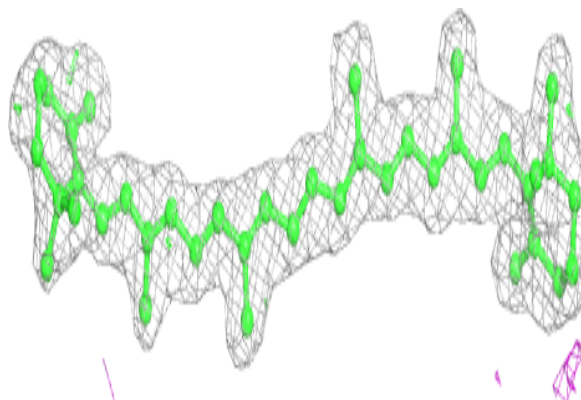


Electron density around CLA b 610:

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

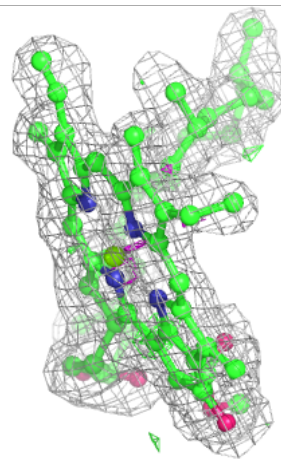
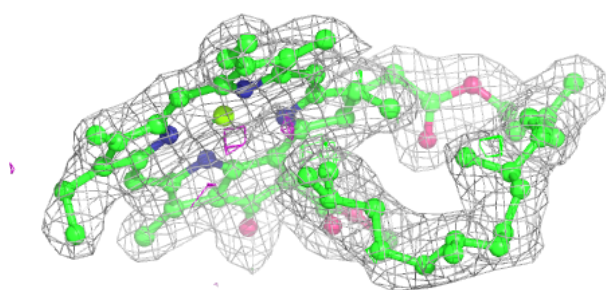
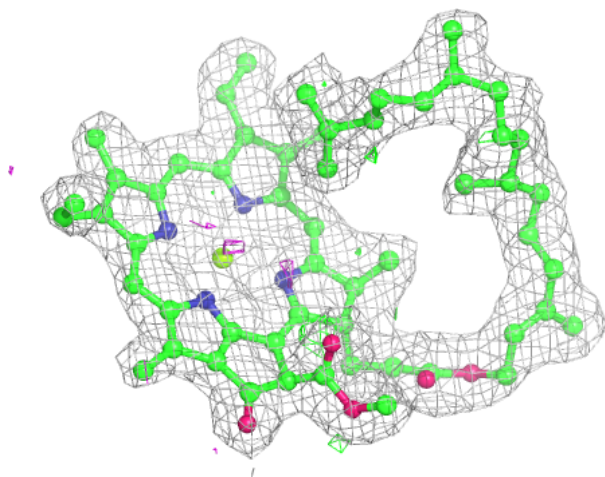
**Electron density around BCR B 619:**

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



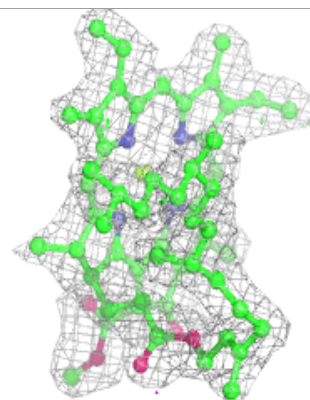
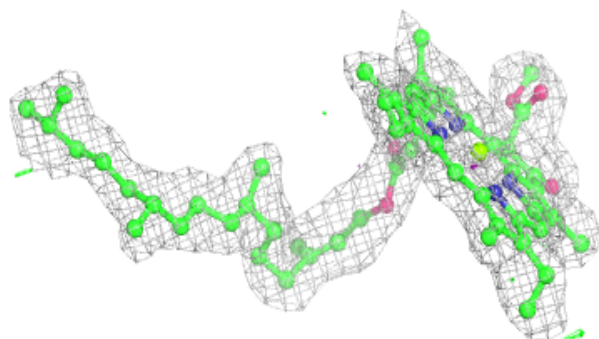
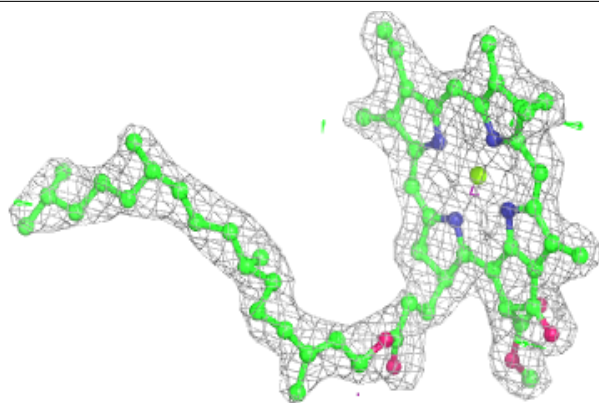
Electron density around CLA b 619:

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

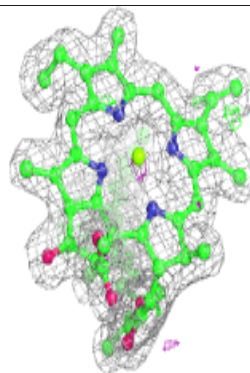
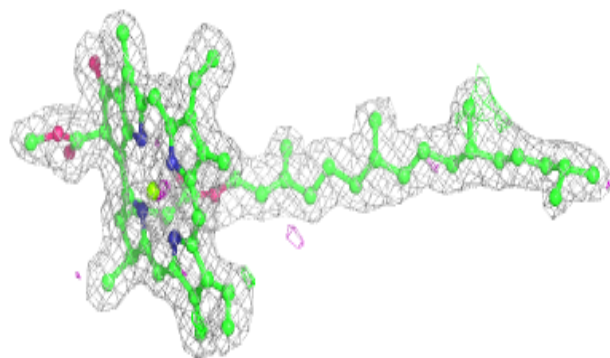
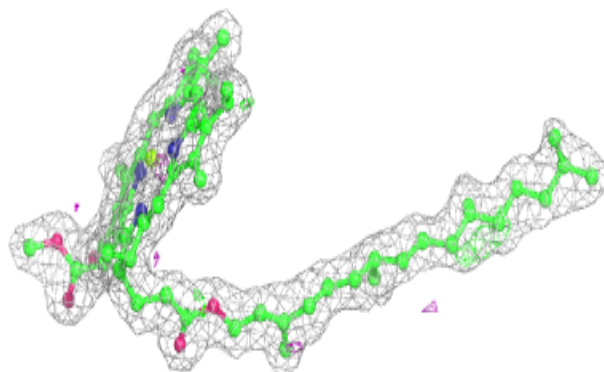


Electron density around CLA c 912:

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

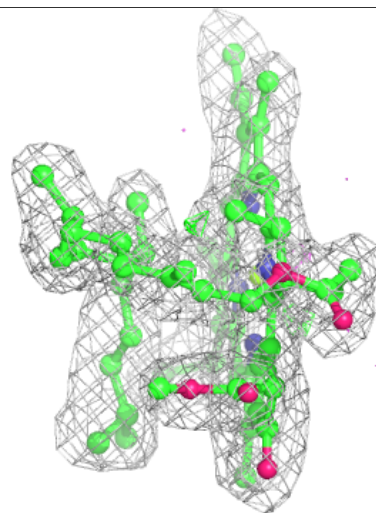
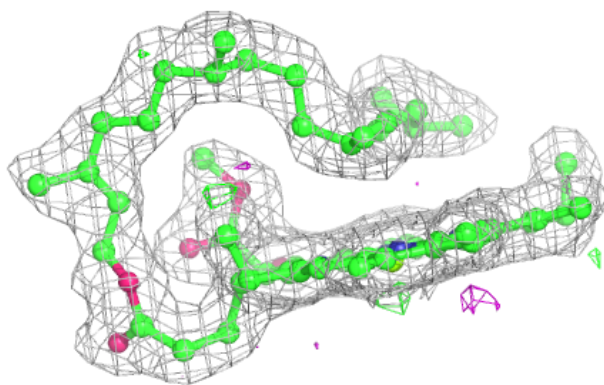
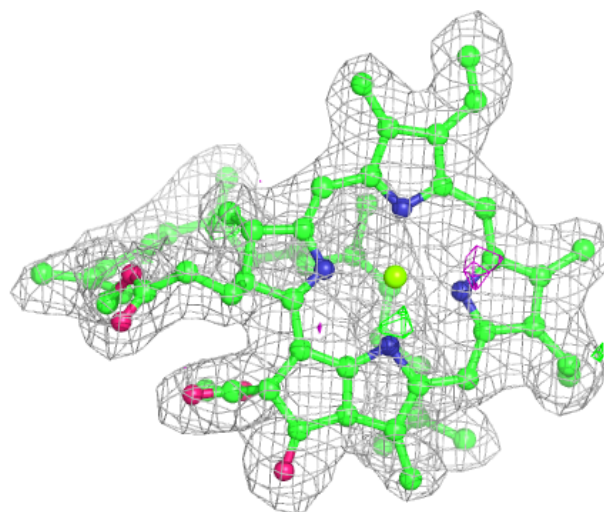
**Electron density around CLA B 608:**

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



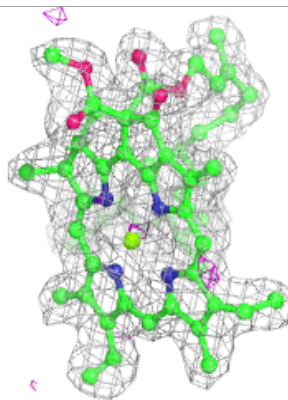
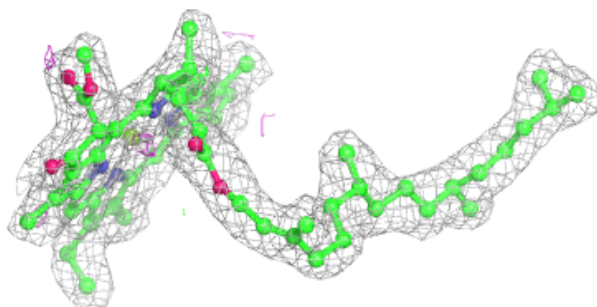
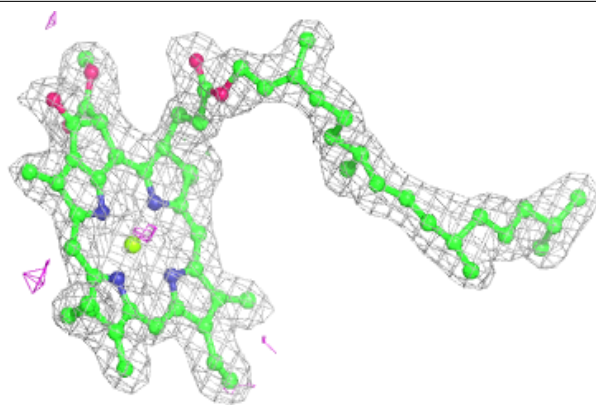
Electron density around CLA C 511:

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



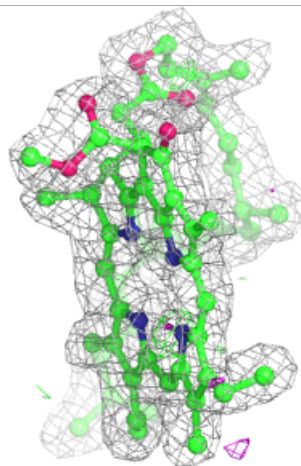
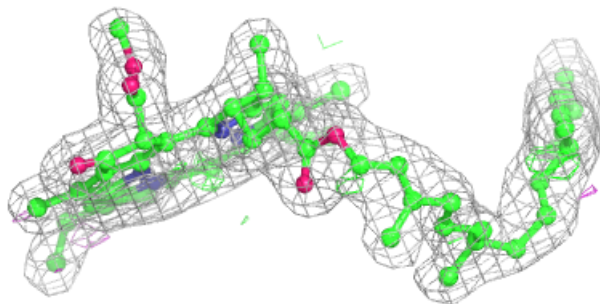
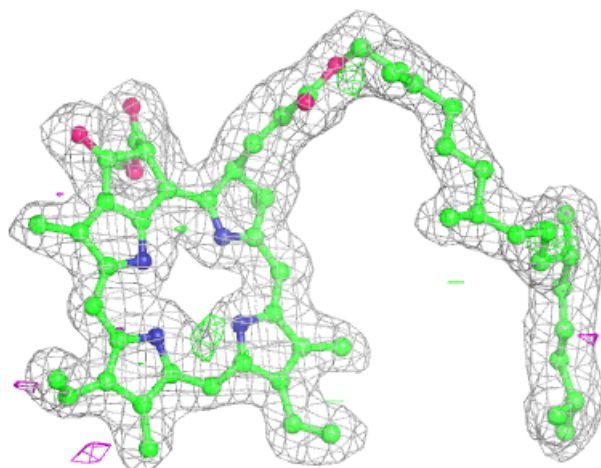
Electron density around CLA C 512:

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



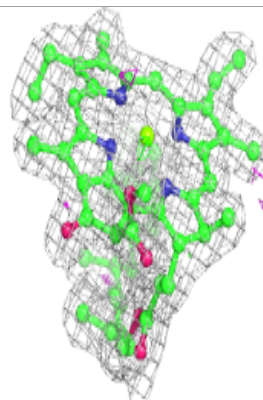
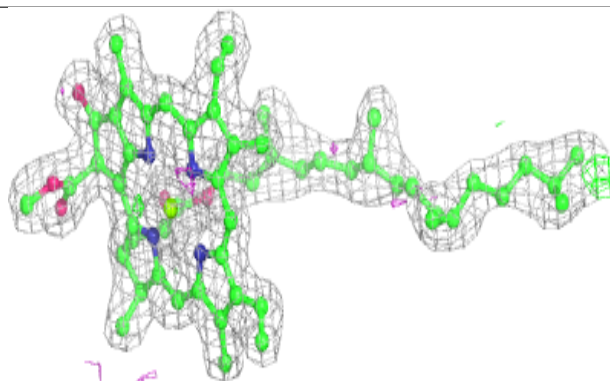
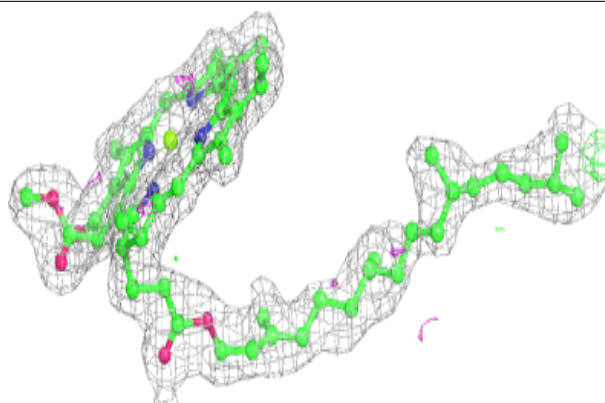
Electron density around PHO a 420:

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

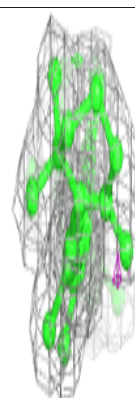
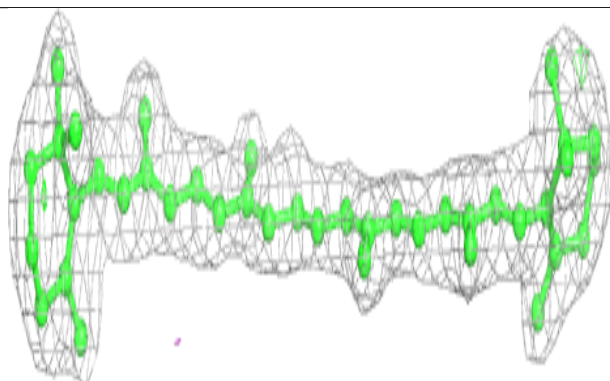
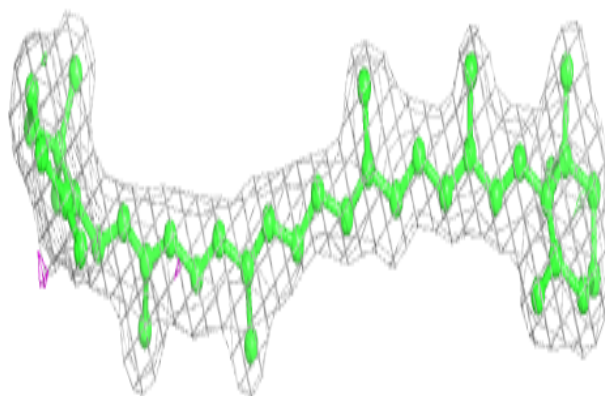


Electron density around CLA C 505:

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

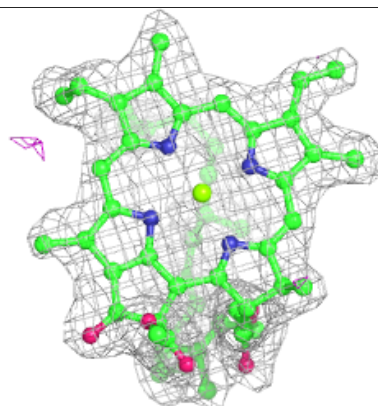
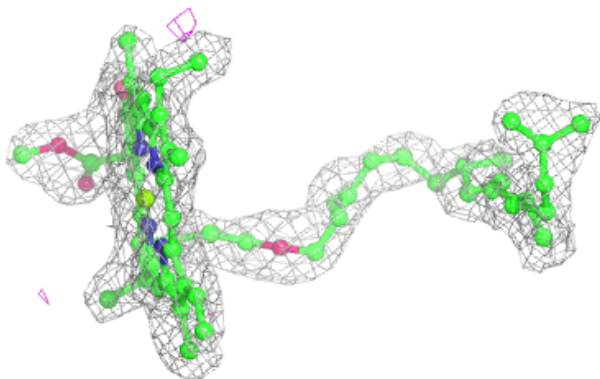
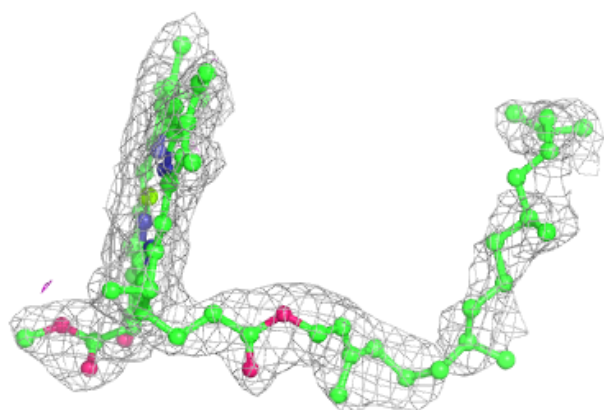
**Electron density around BCR C 515:**

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

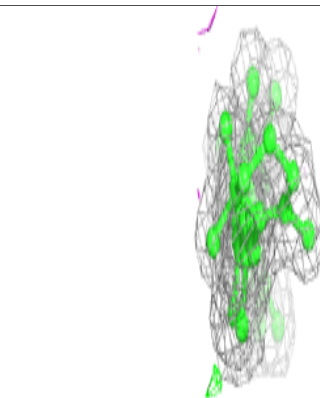
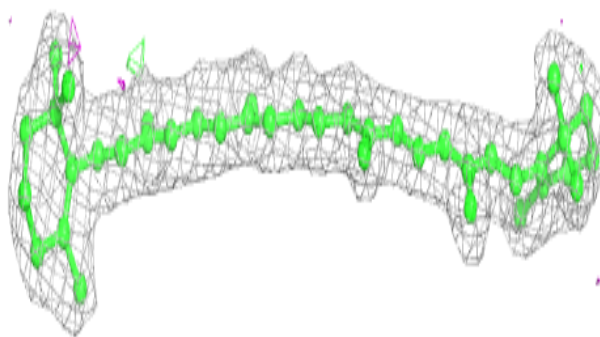
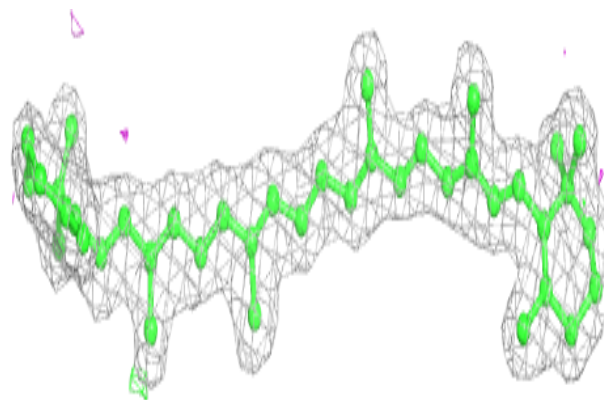


Electron density around CLA C 507:

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

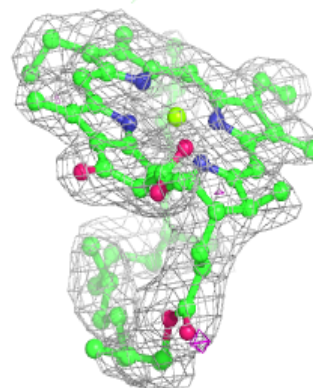
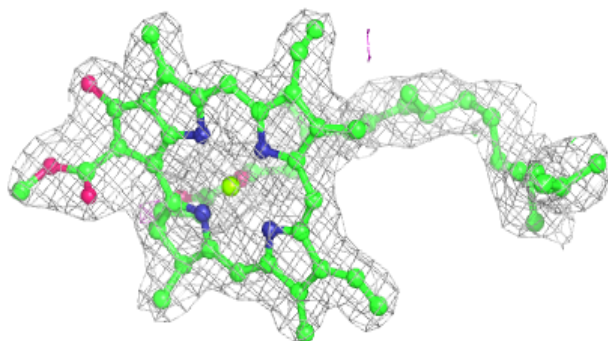
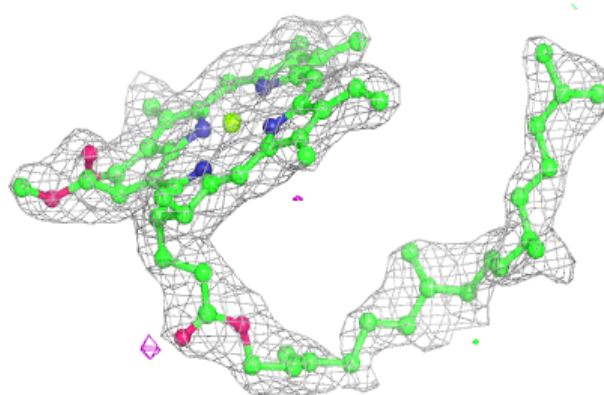
**Electron density around BCR B 618:**

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

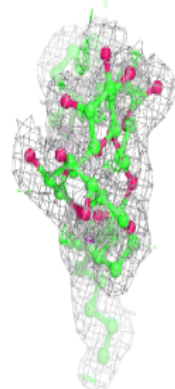
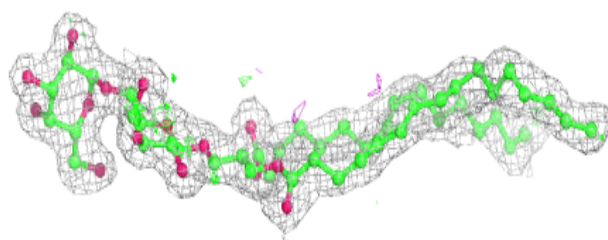
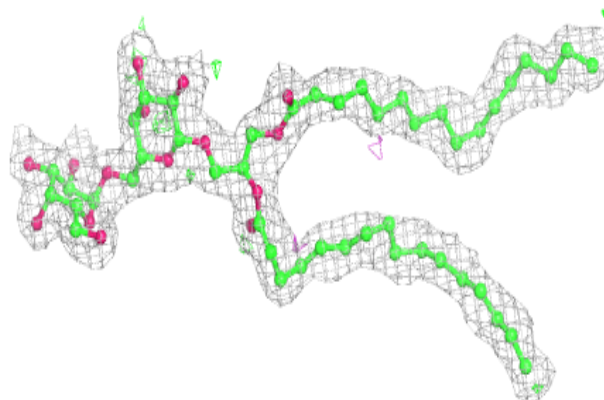


Electron density around CLA C 514:

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

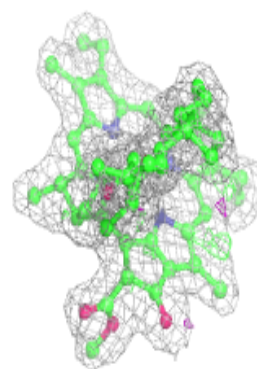
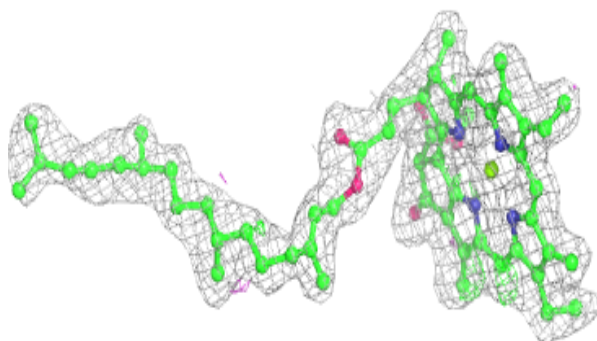
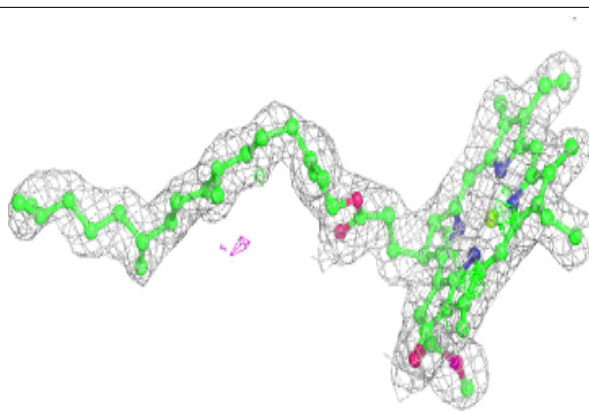
**Electron density around DGD C 519:**

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

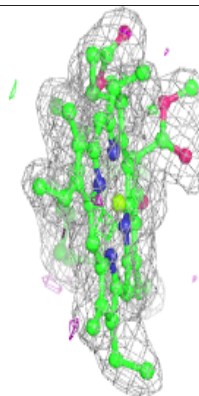
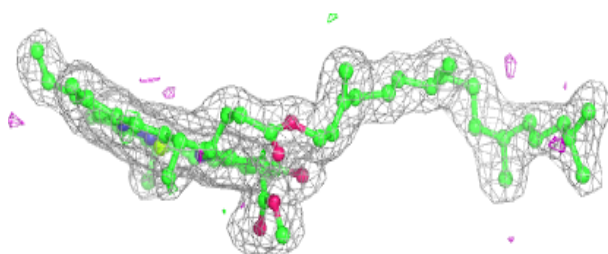
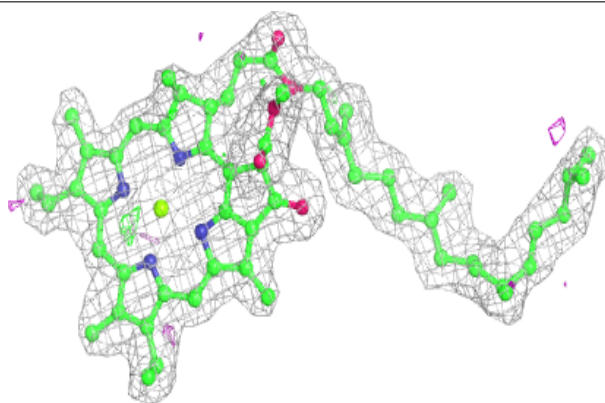


Electron density around CLA c 903:

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

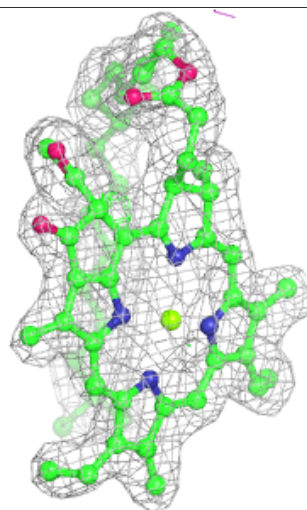
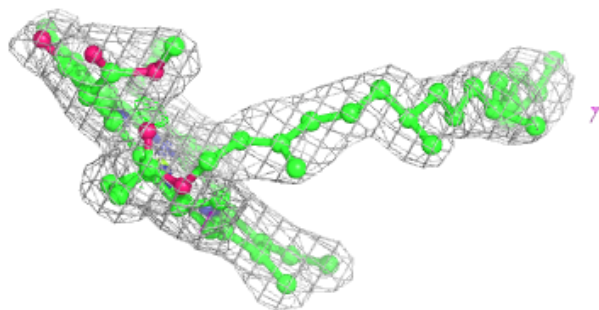
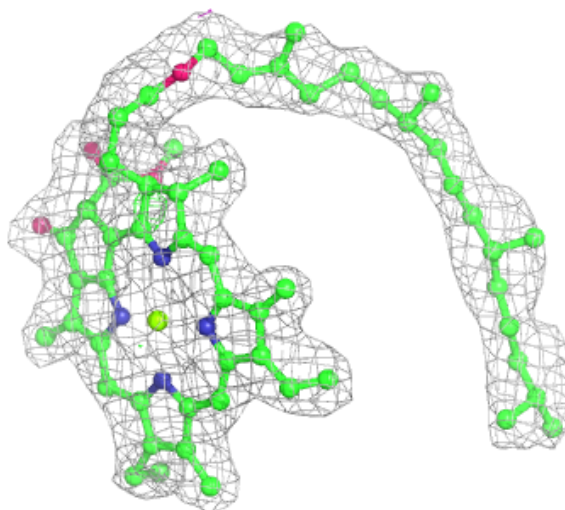
**Electron density around CLA b 606:**

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



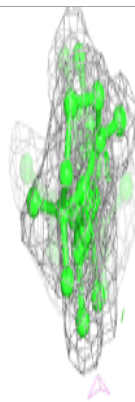
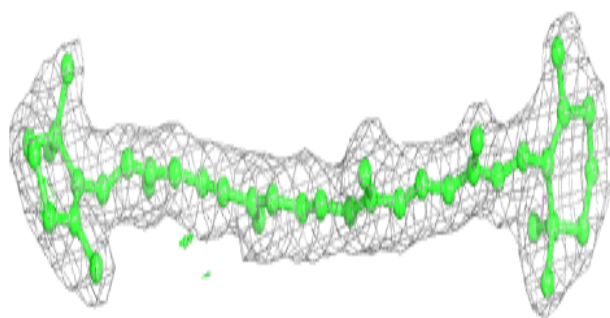
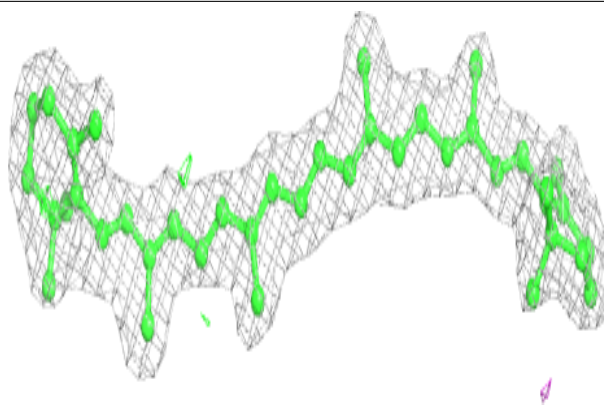
Electron density around CLA C 508:

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



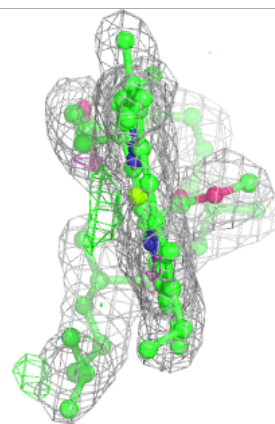
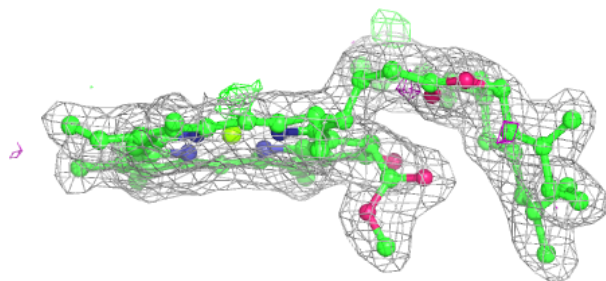
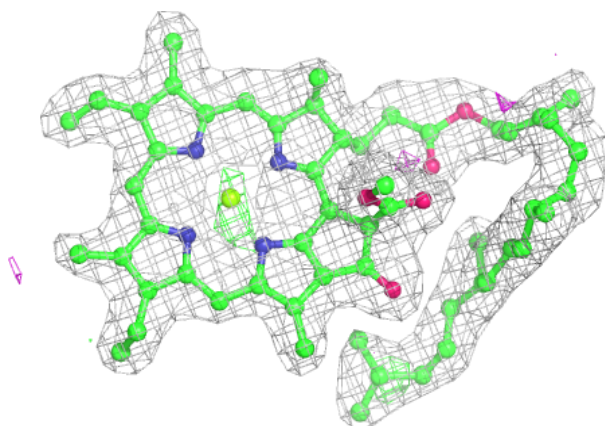
Electron density around BCR K 102:

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



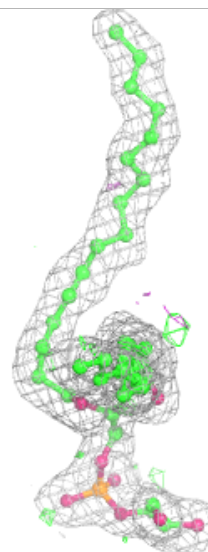
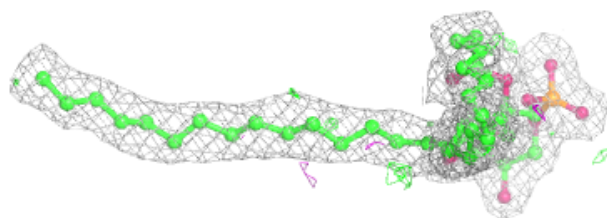
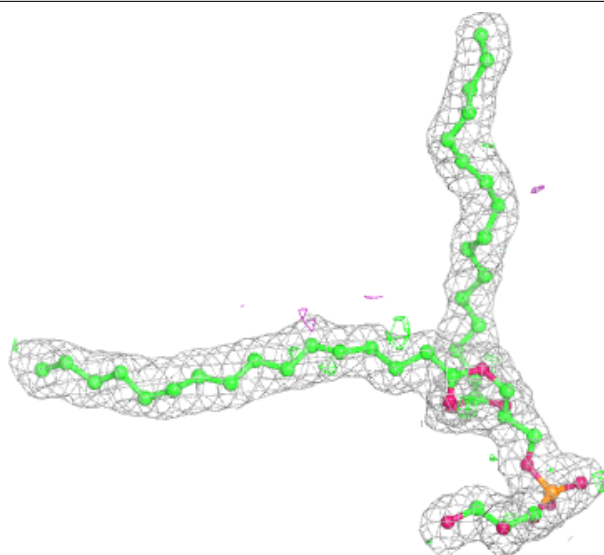
Electron density around CLA b 614:

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



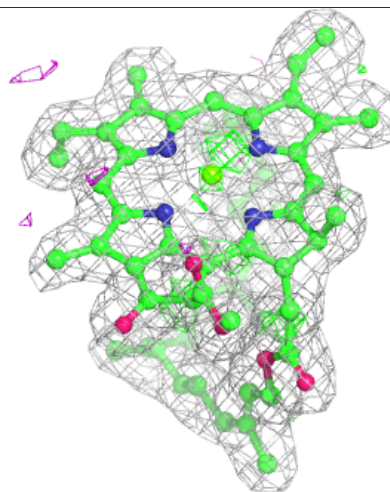
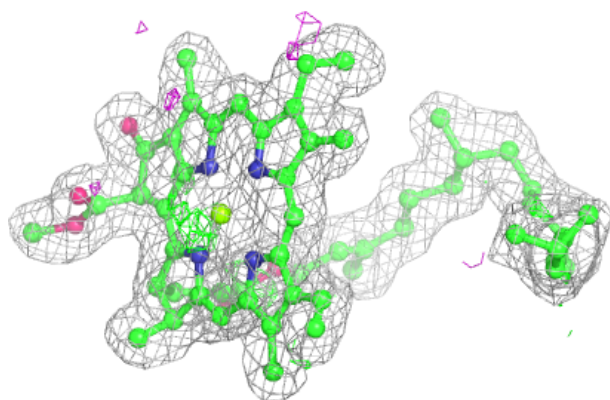
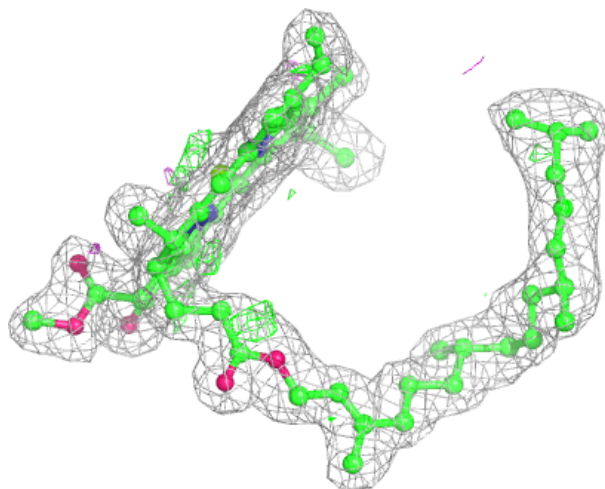
Electron density around LHG L 101:

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



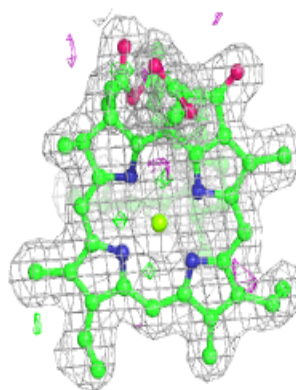
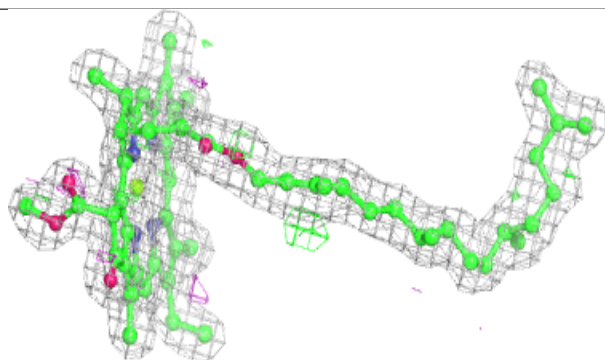
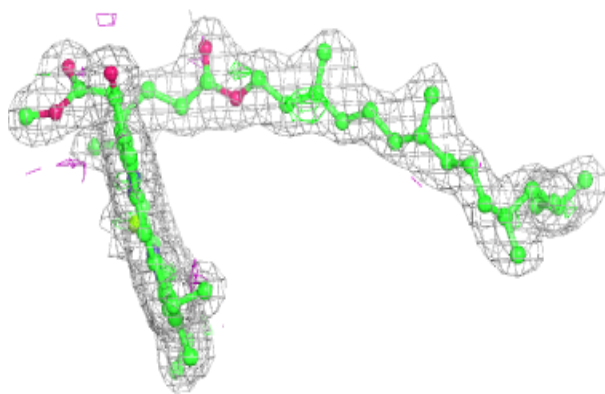
Electron density around CLA b 615:

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

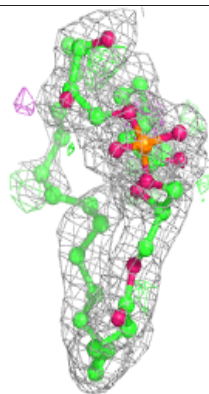
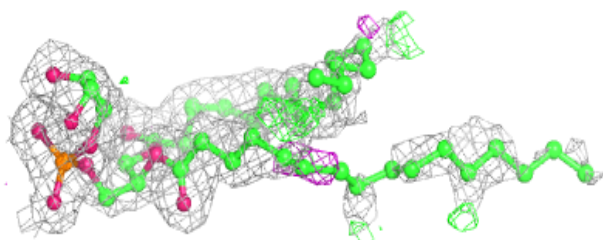
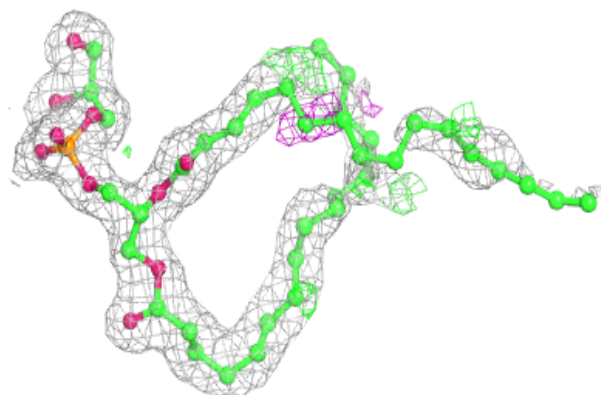


Electron density around CLA B 606:

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

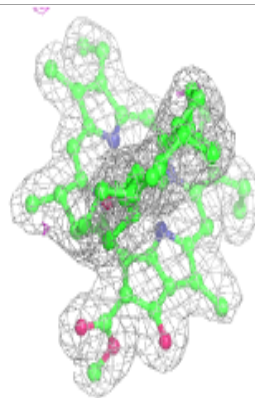
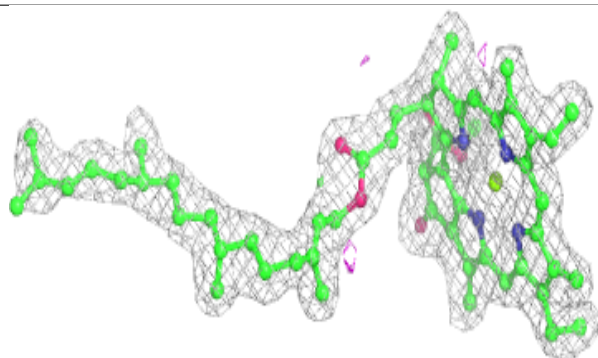
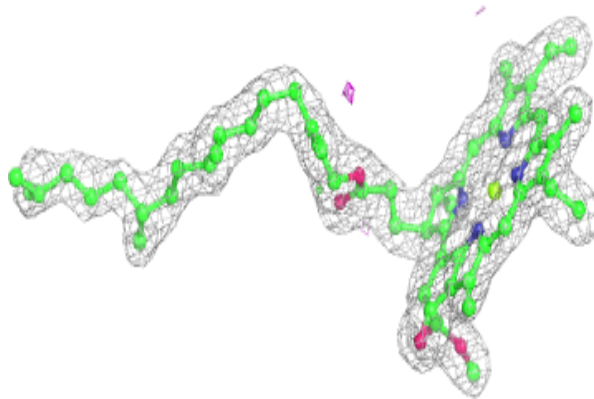
**Electron density around LHG D 408:**

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

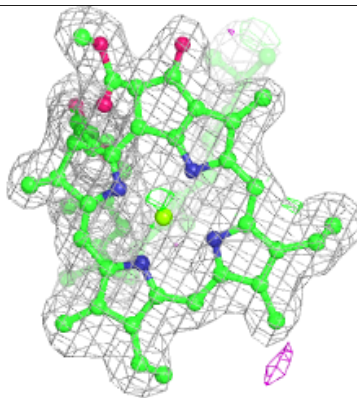
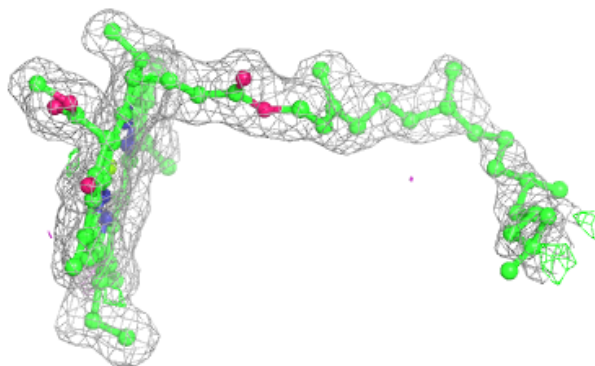
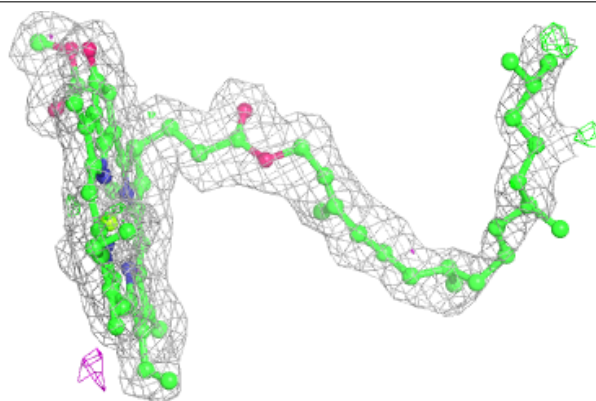


Electron density around CLA C 503:

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

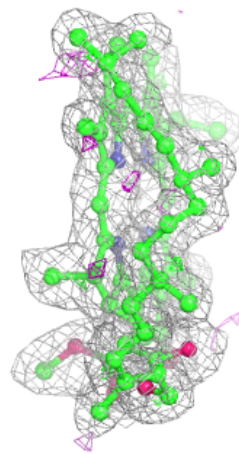
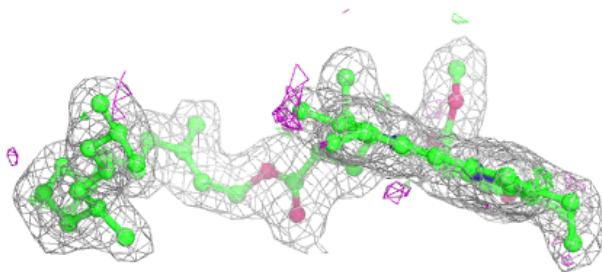
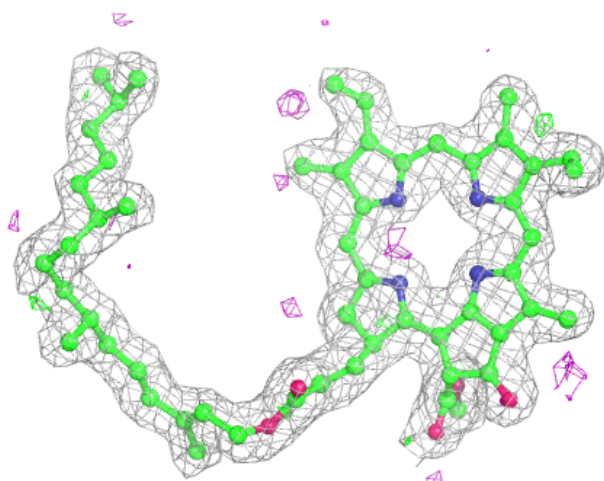
**Electron density around CLA D 402:**

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



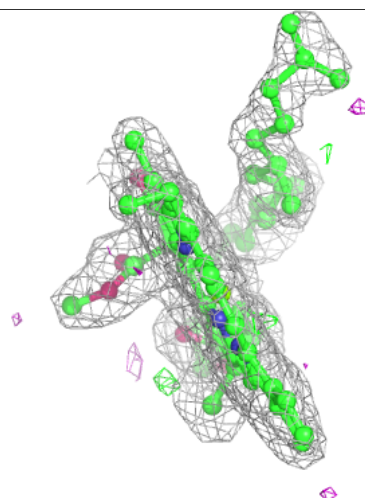
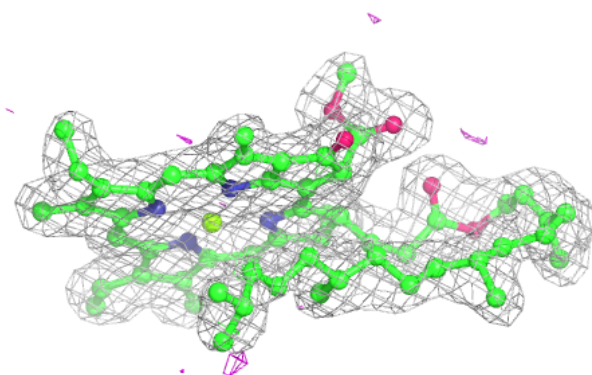
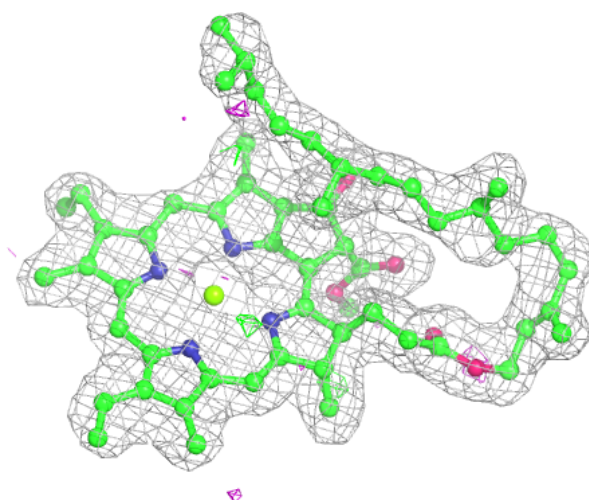
Electron density around PHO a 408:

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



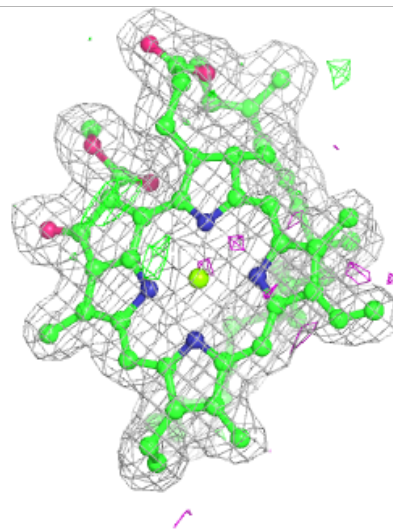
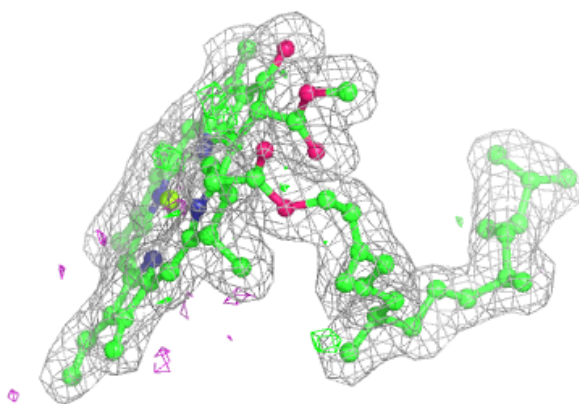
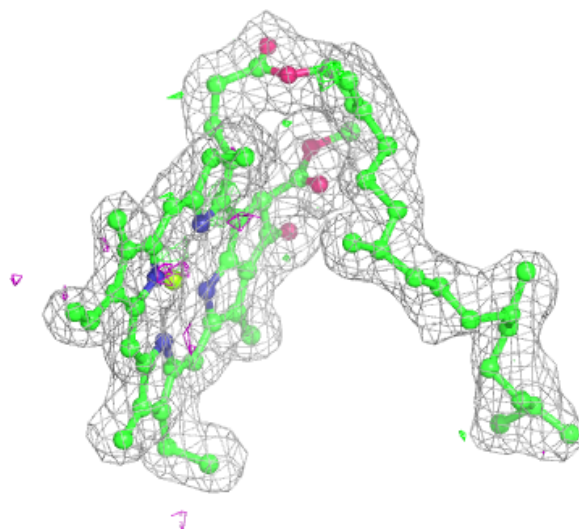
Electron density around CLA C 510:

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



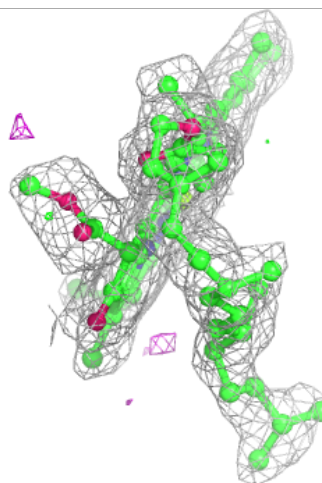
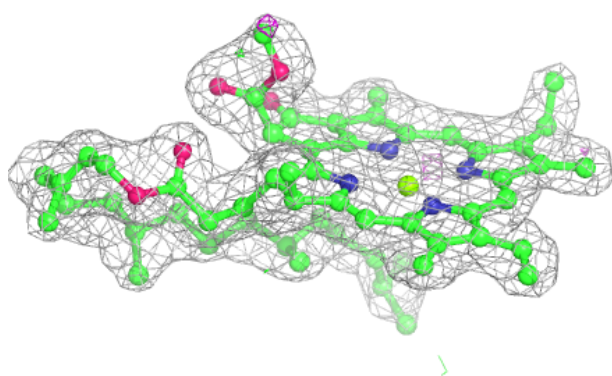
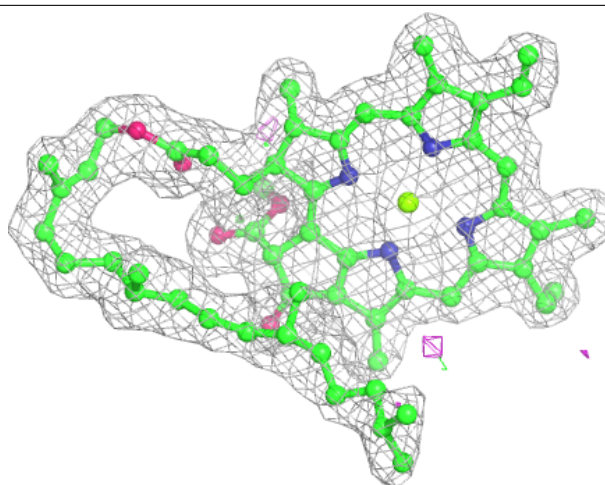
Electron density around CLA B 614:

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



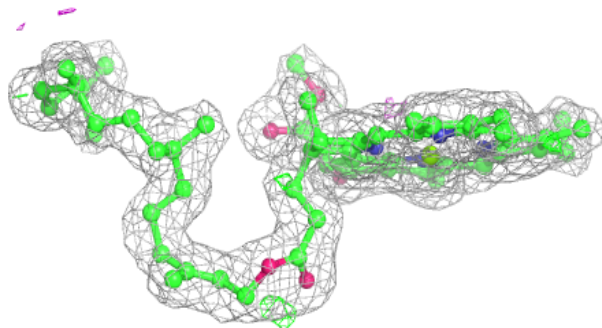
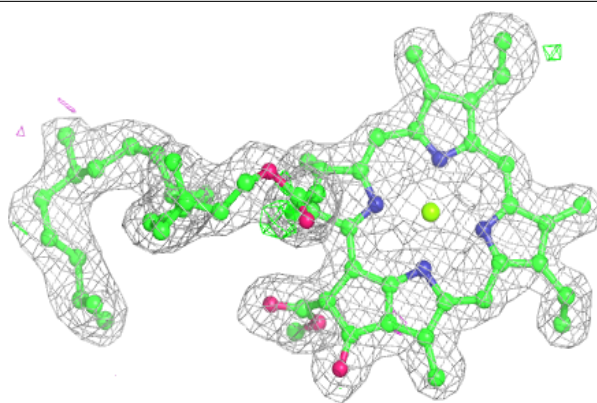
Electron density around CLA c 910:

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

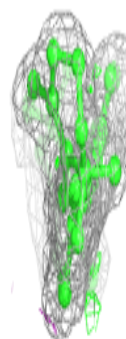
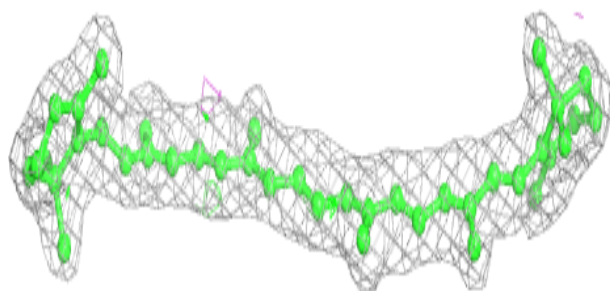
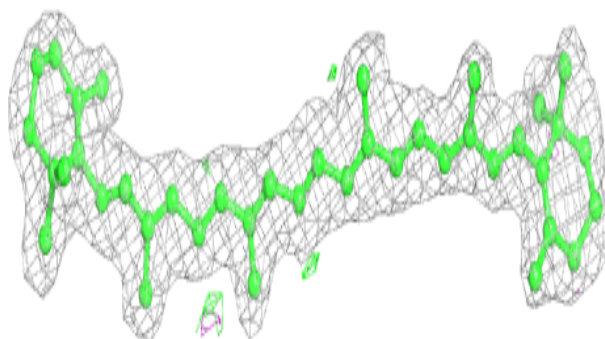


Electron density around CLA b 616:

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

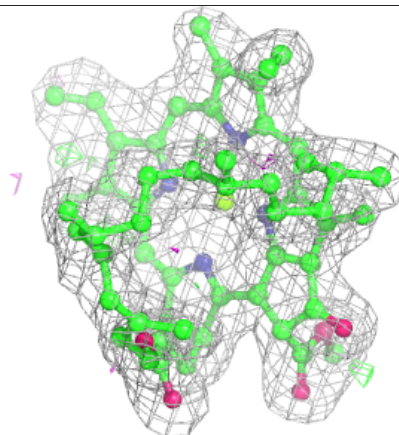
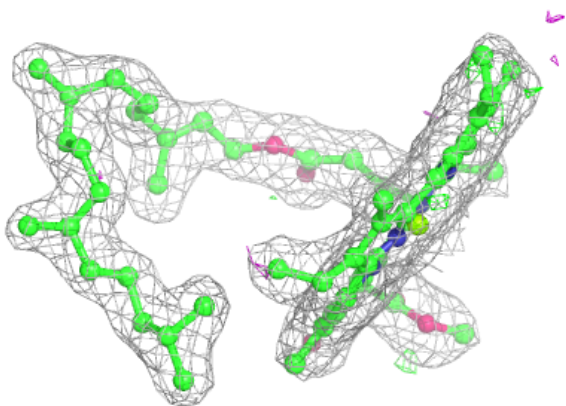
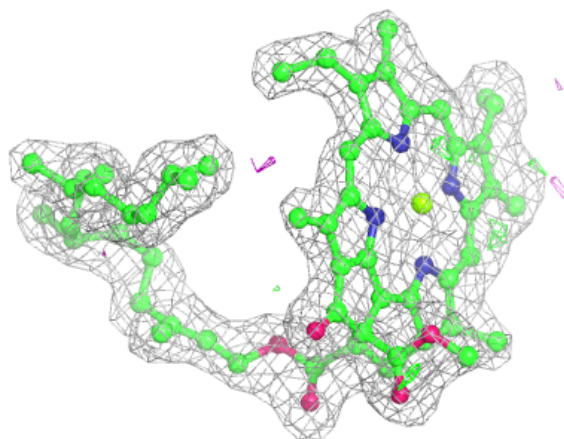
**Electron density around BCR b 623:**

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

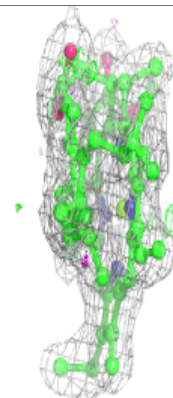
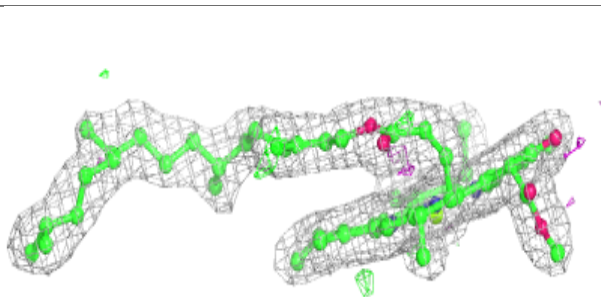
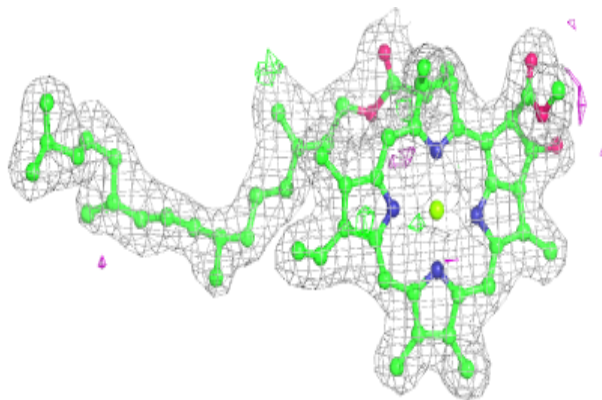


Electron density around CLA C 504:

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

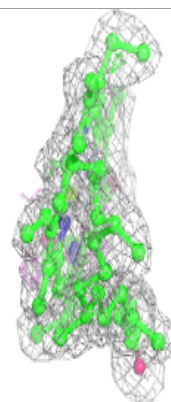
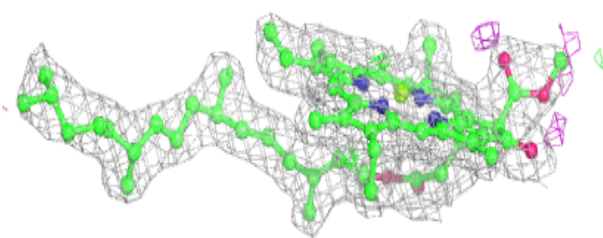
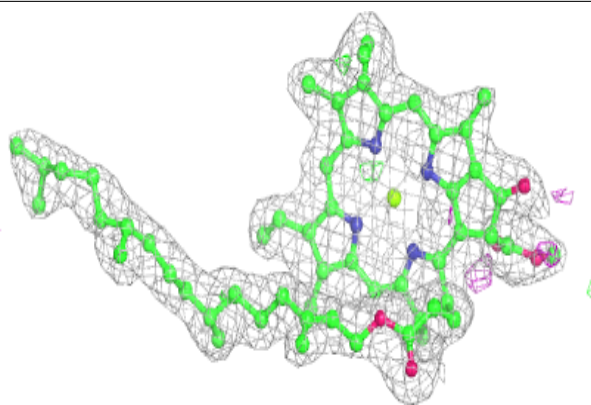
**Electron density around CLA B 604:**

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

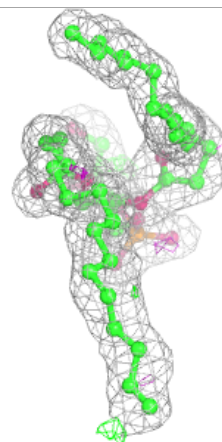
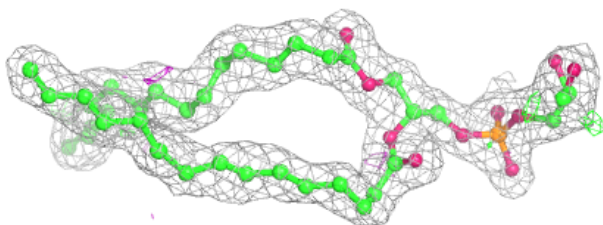
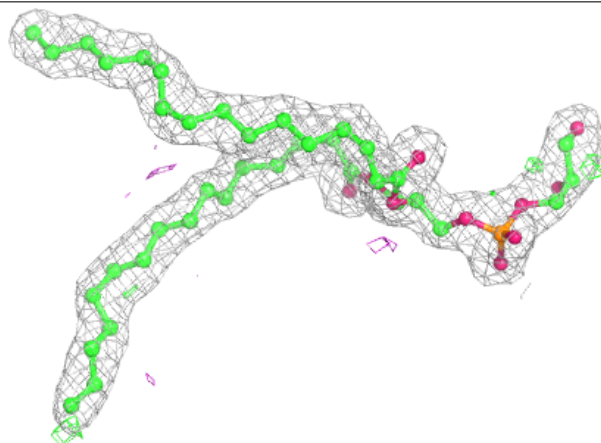


Electron density around CLA C 502:

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

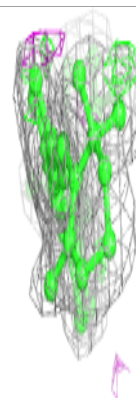
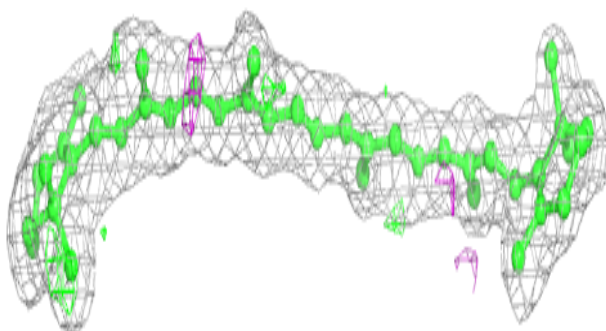
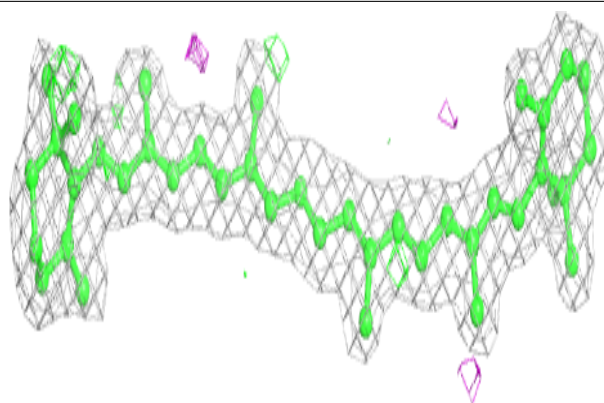
**Electron density around LHG d 408:**

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

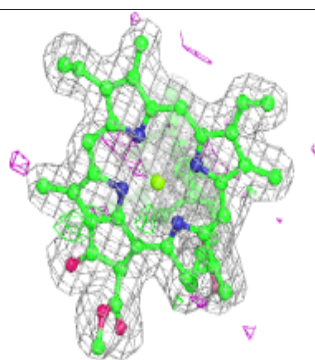
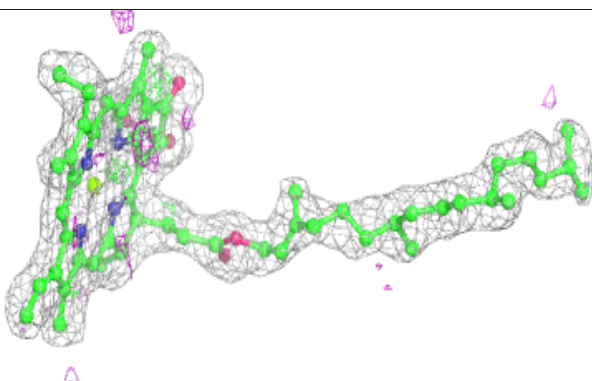
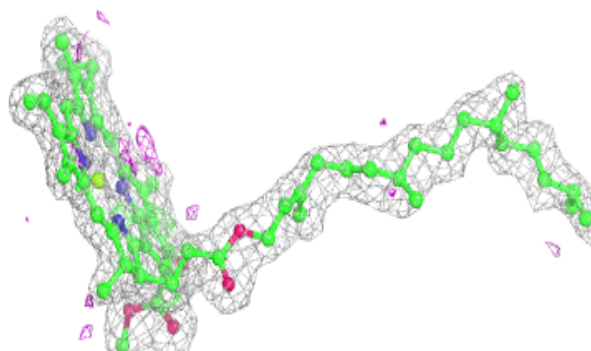


Electron density around BCR B 620:

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

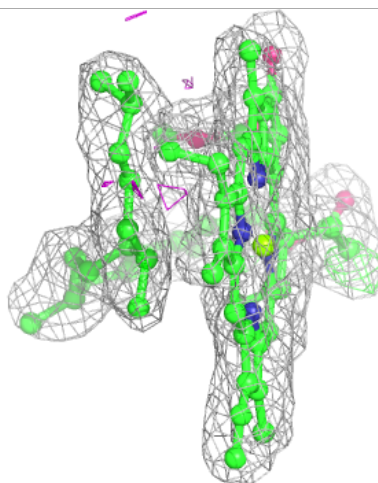
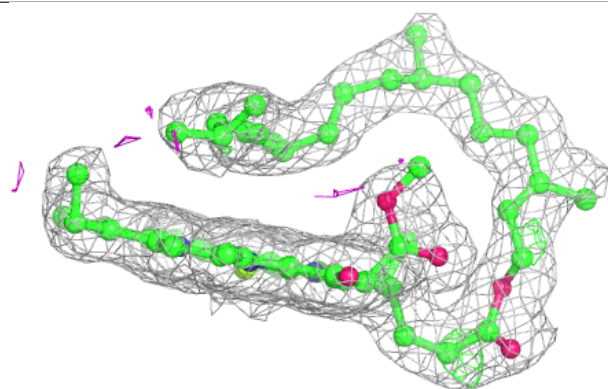
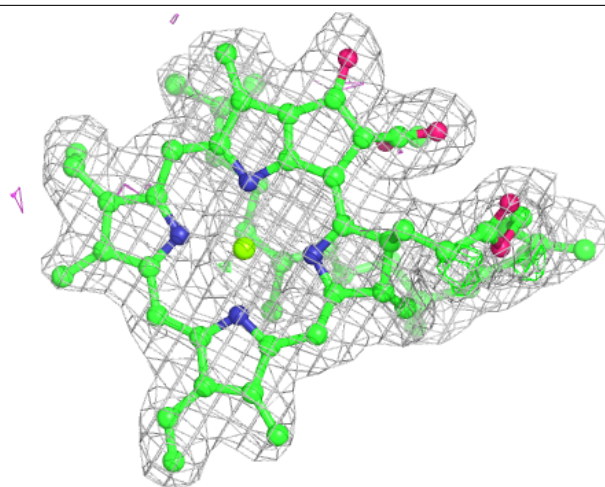
**Electron density around CLA B 605:**

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



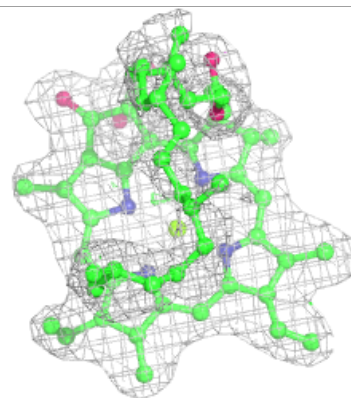
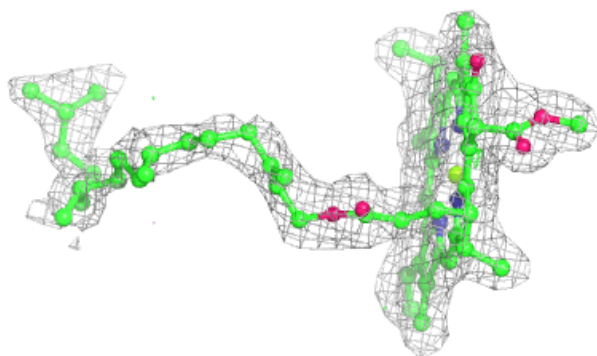
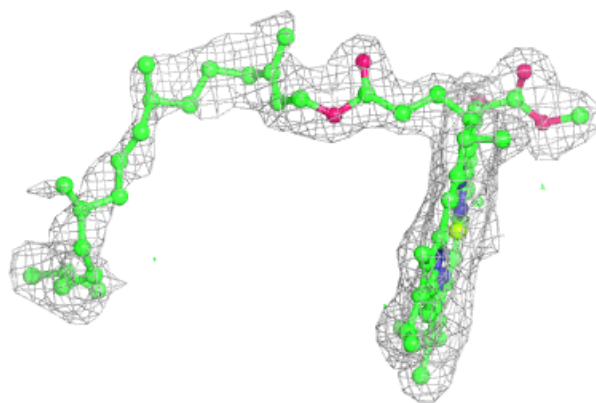
Electron density around CLA c 911:

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

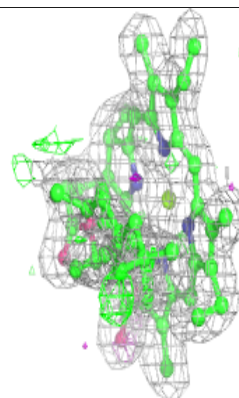
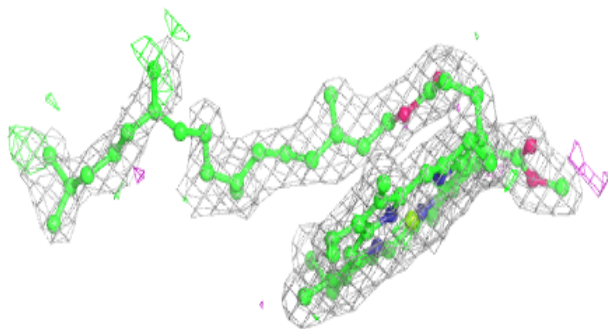
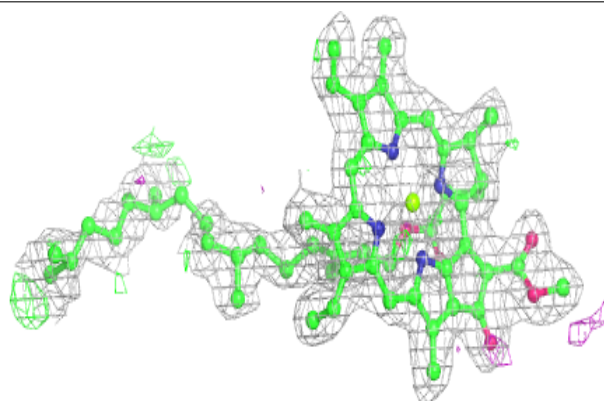


Electron density around CLA c 907:

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

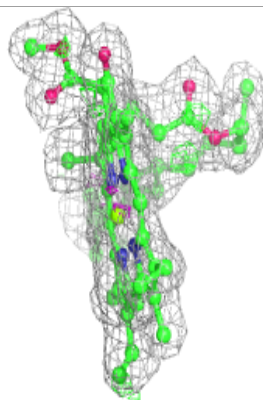
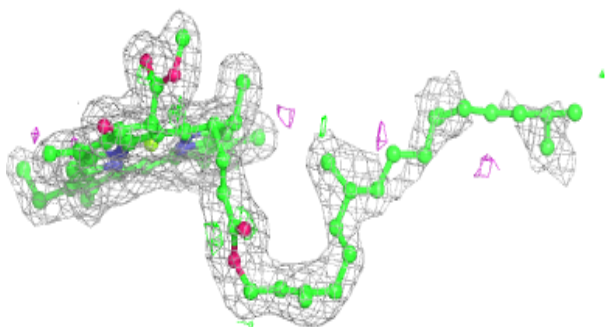
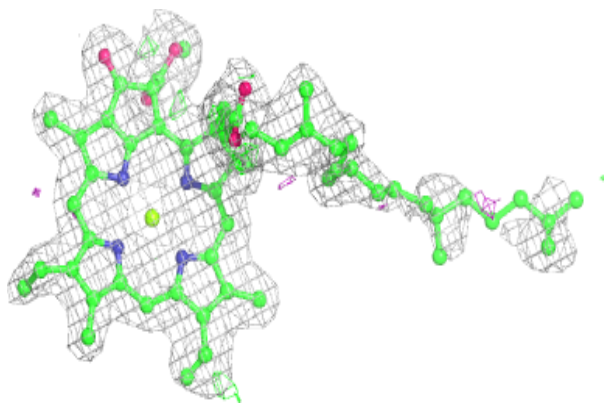
**Electron density around CLA B 615:**

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



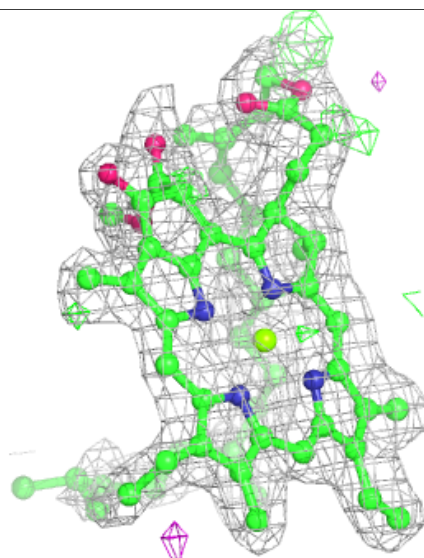
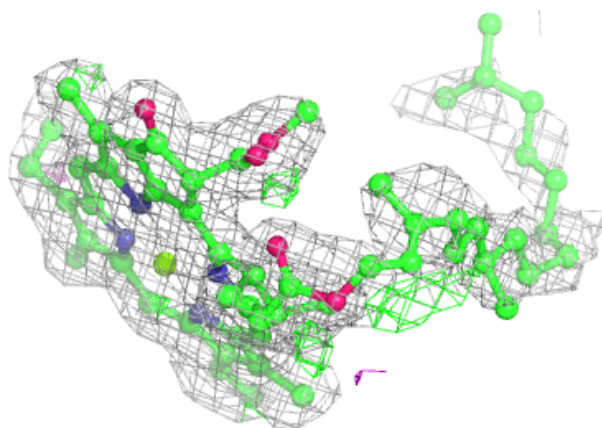
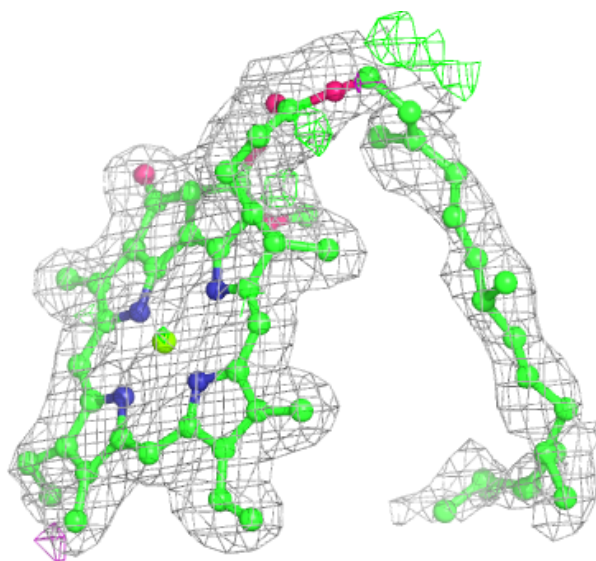
Electron density around CLA a 407:

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



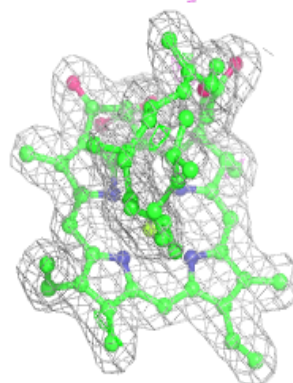
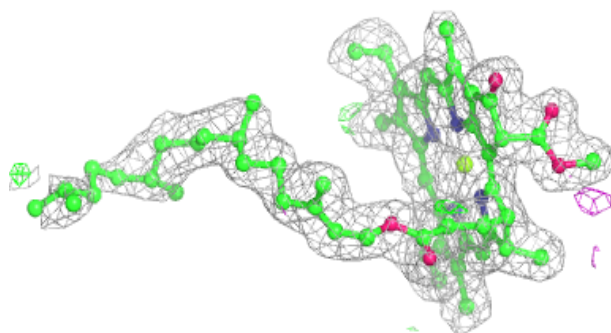
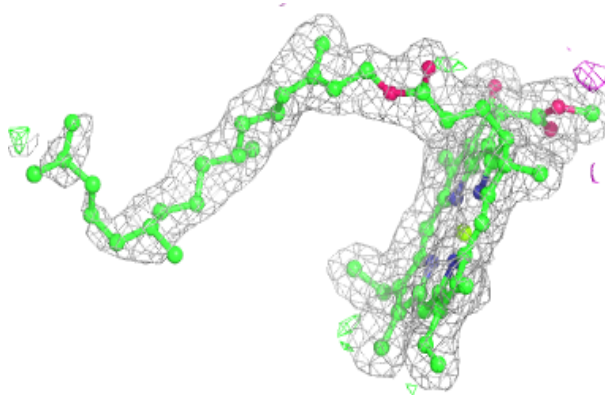
Electron density around CLA b 620:

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

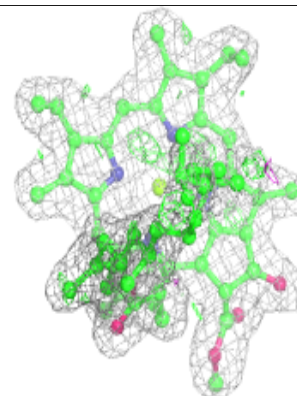
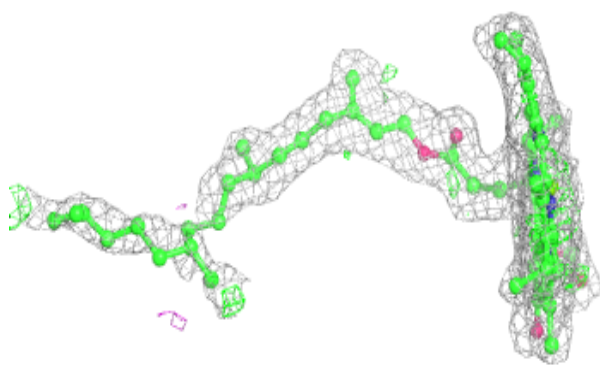
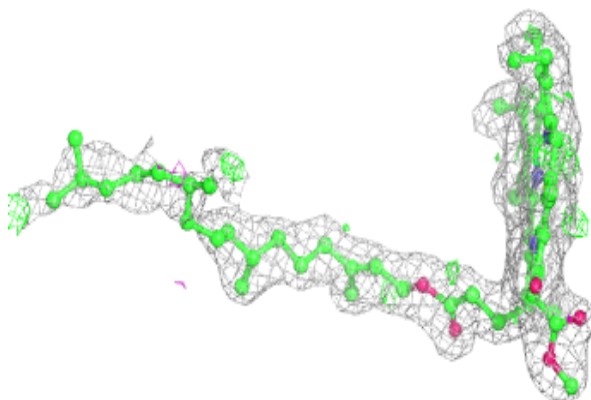


Electron density around CLA C 509:

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

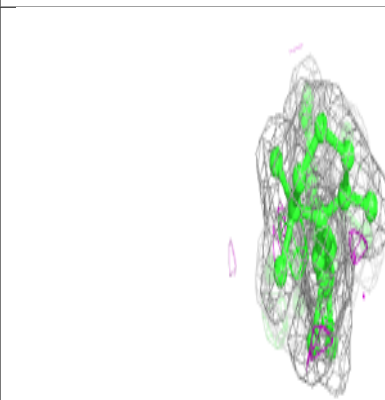
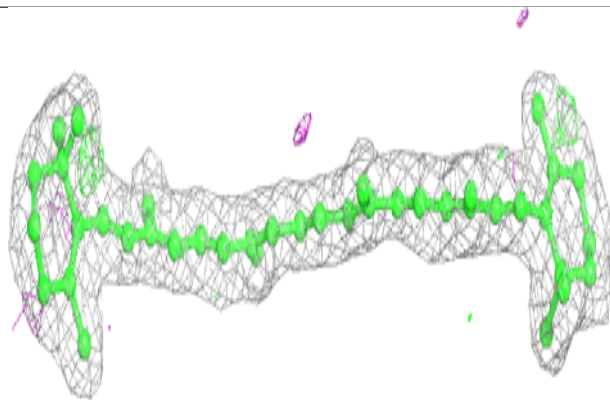
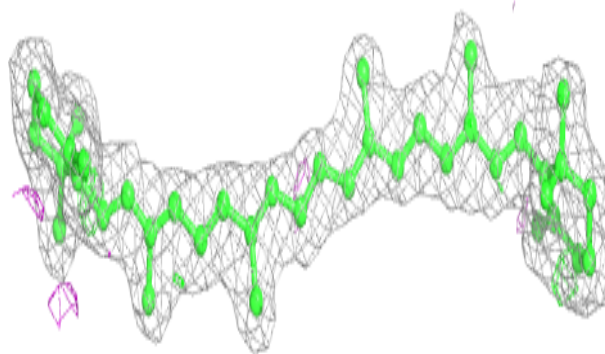
**Electron density around CLA B 607:**

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

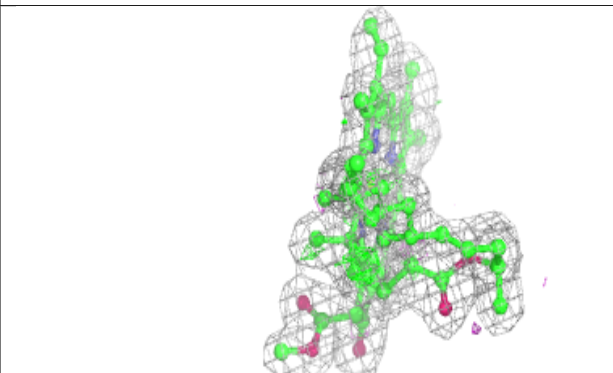
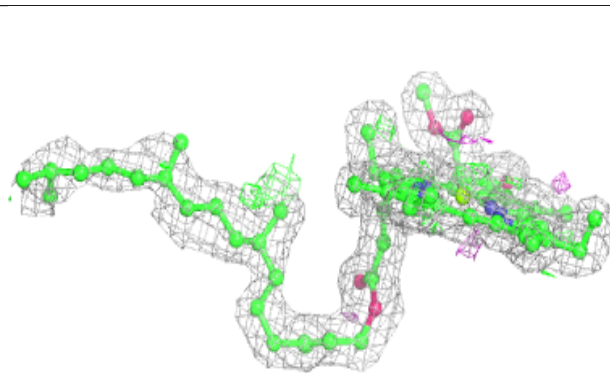
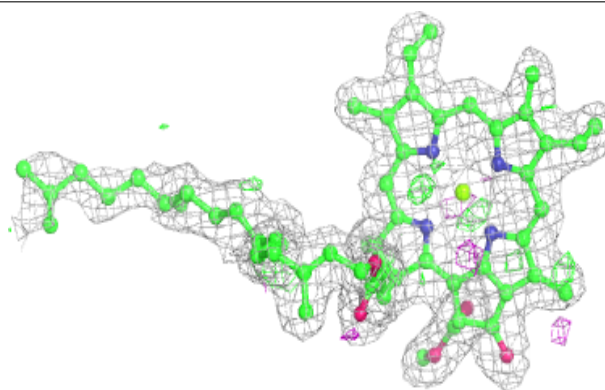


Electron density around BCR A 411:

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

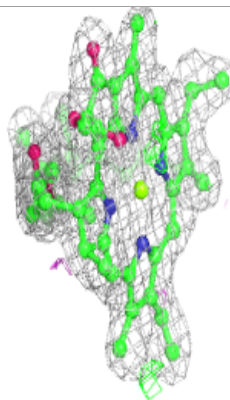
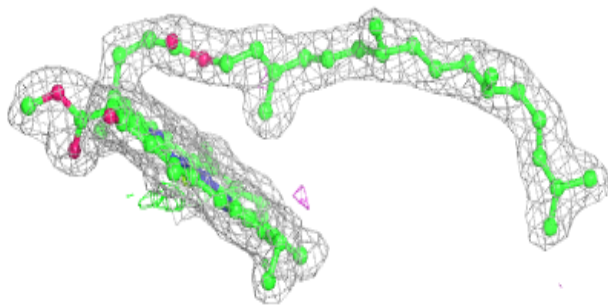
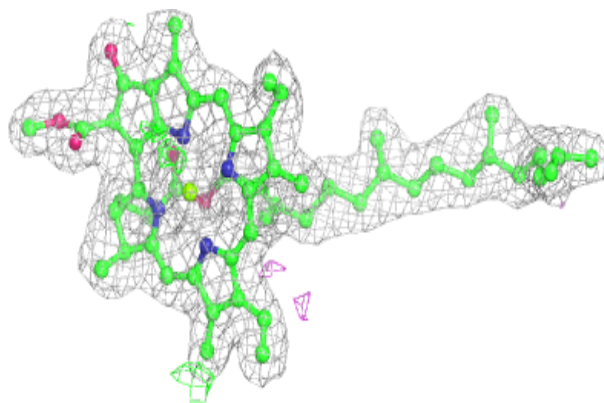
**Electron density around CLA A 407:**

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



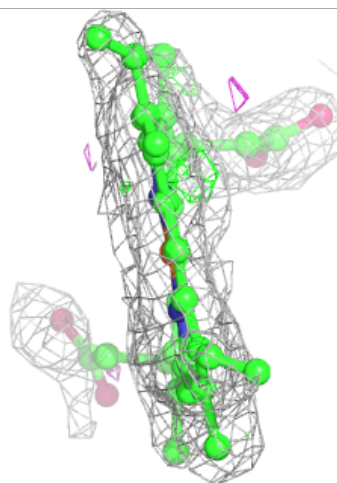
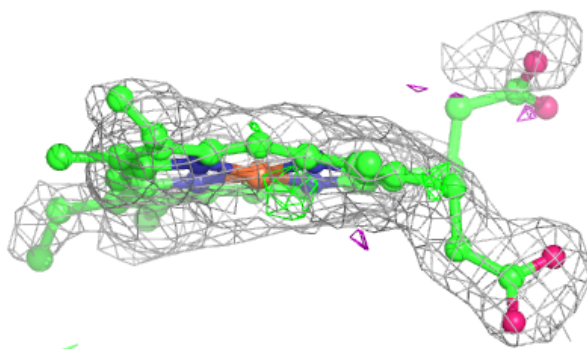
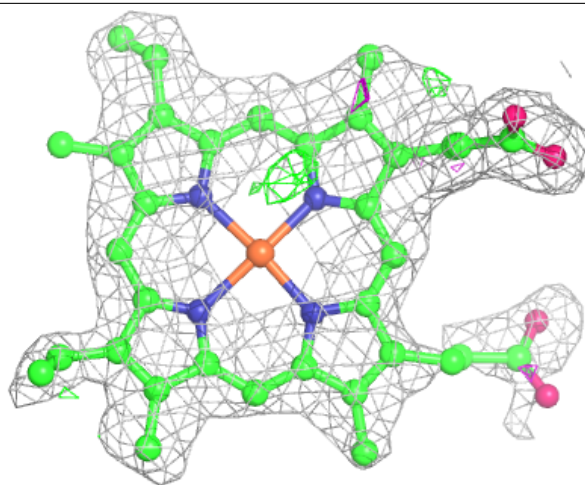
Electron density around CLA b 612:

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



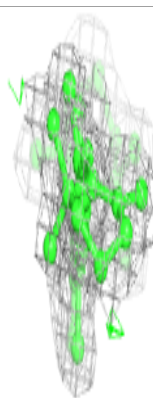
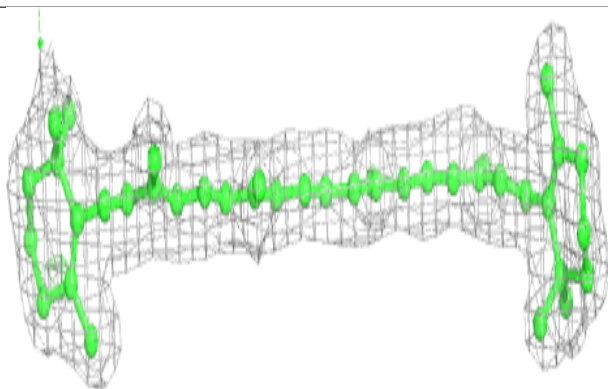
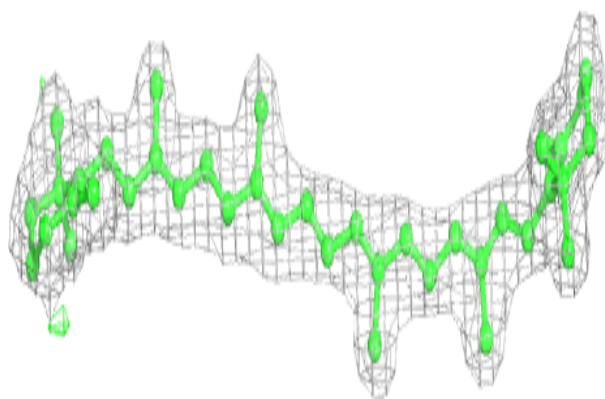
Electron density around HEM e 102:

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

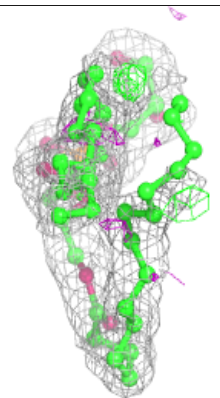
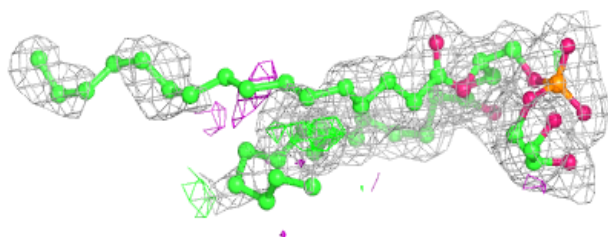
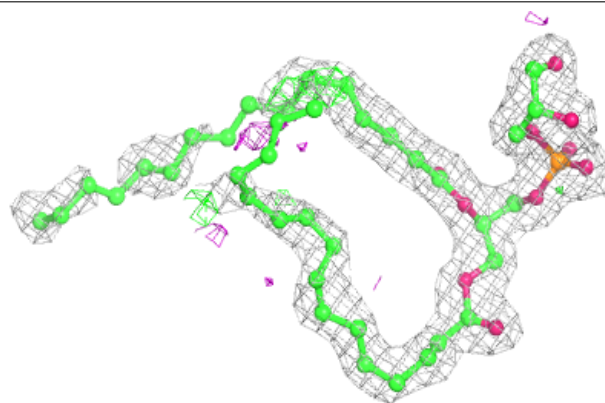


Electron density around BCR C 516:

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

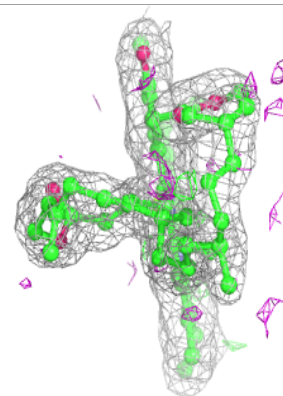
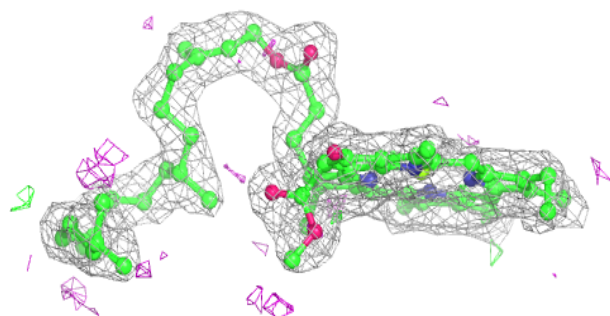
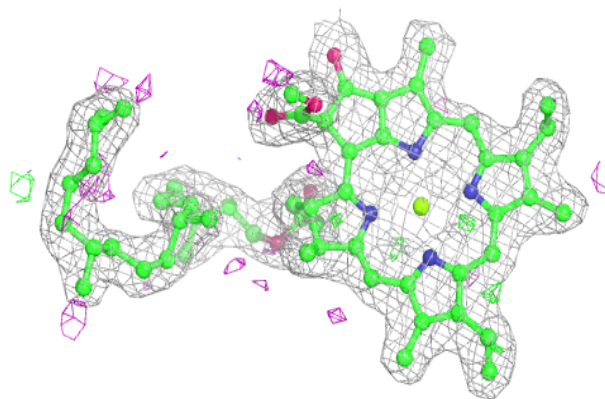
**Electron density around LHG d 409:**

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

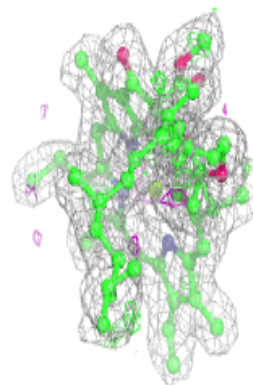
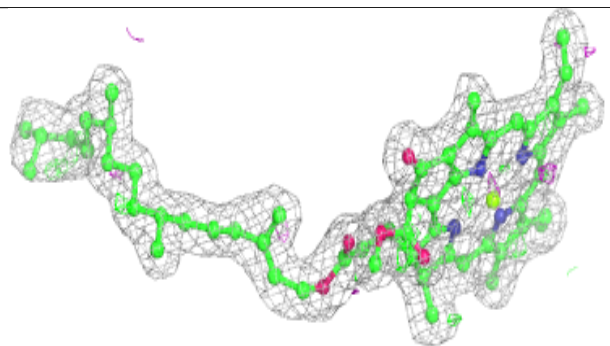
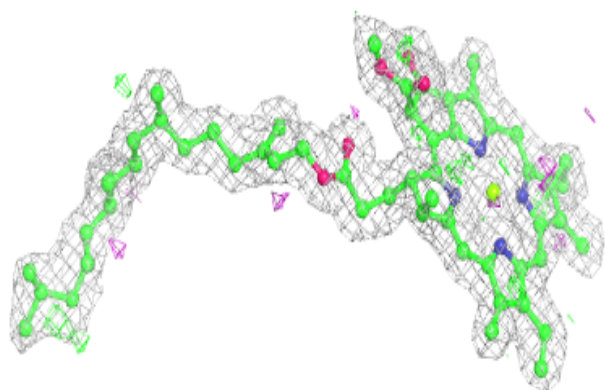


Electron density around CLA B 613:

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

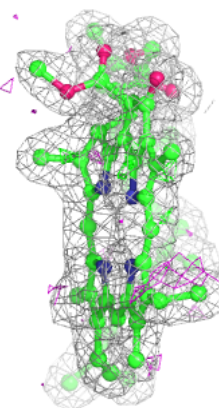
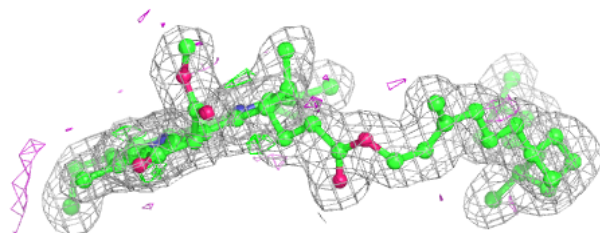
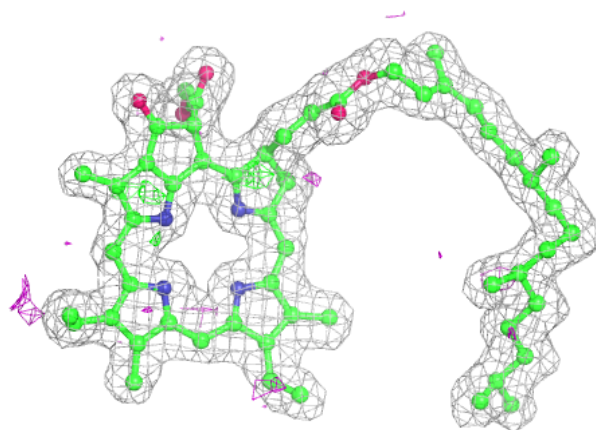
**Electron density around CLA A 405:**

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

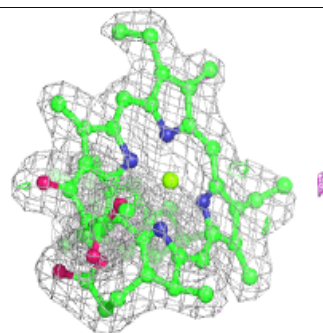
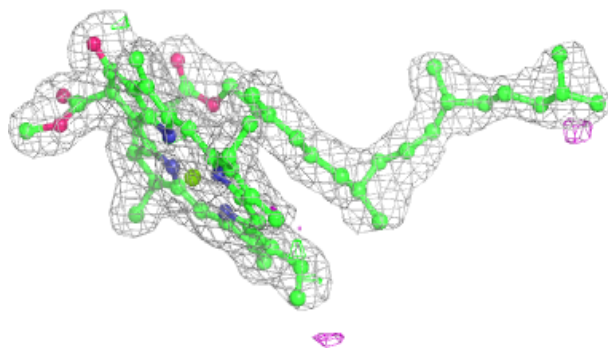
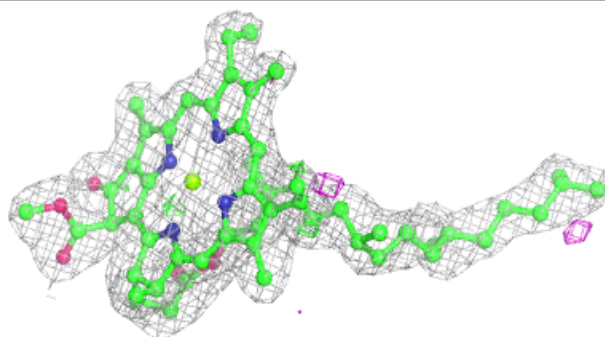


Electron density around PHO A 408:

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

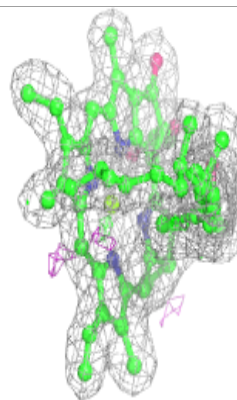
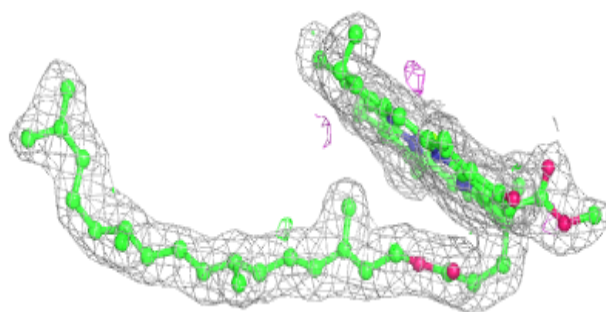
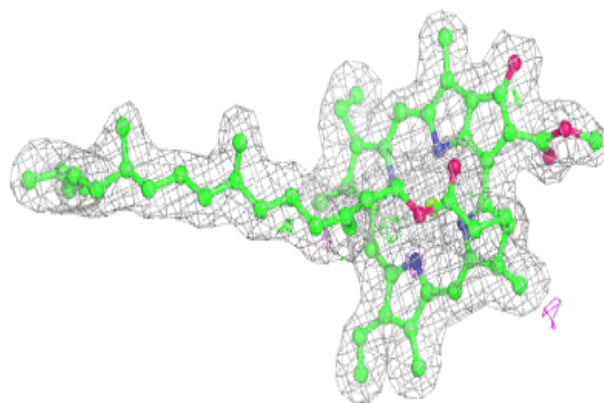
**Electron density around CLA C 506:**

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

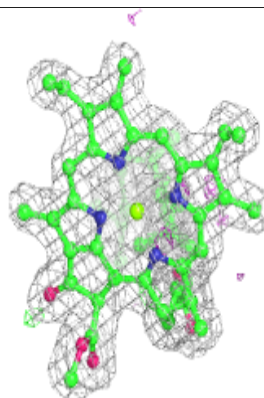
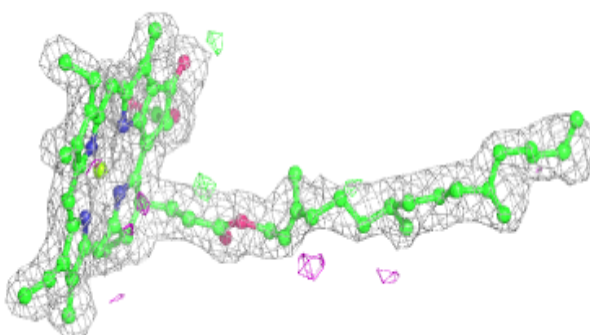
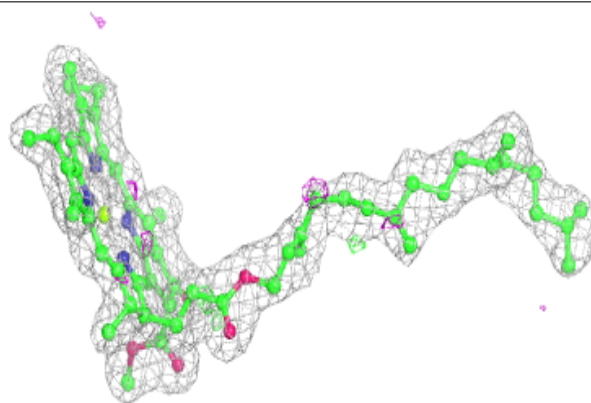


Electron density around CLA B 609:

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

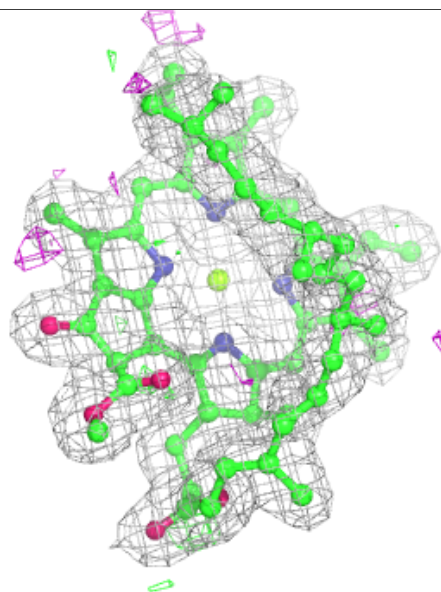
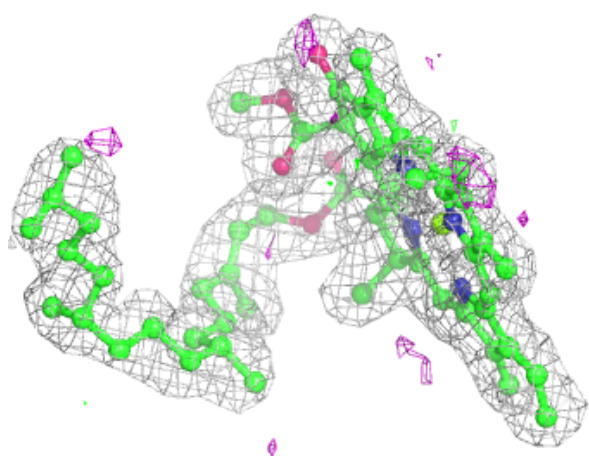
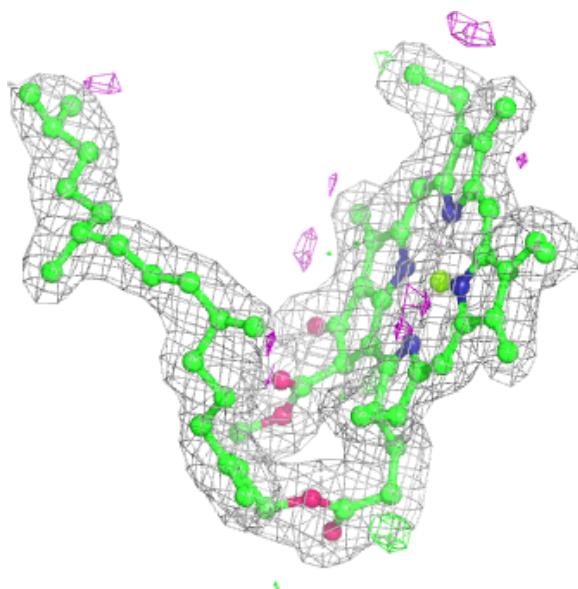
**Electron density around CLA b 608:**

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



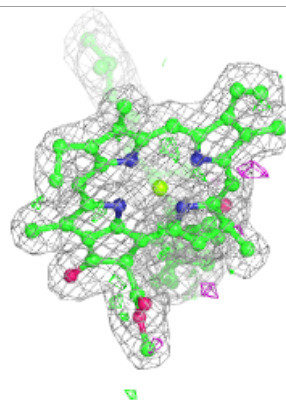
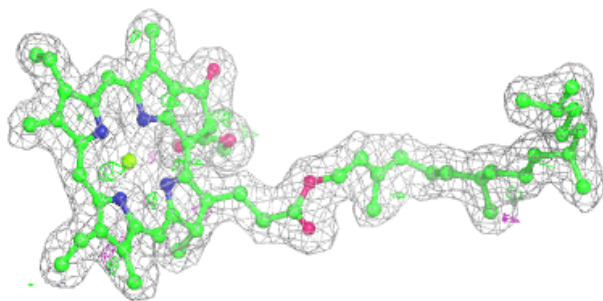
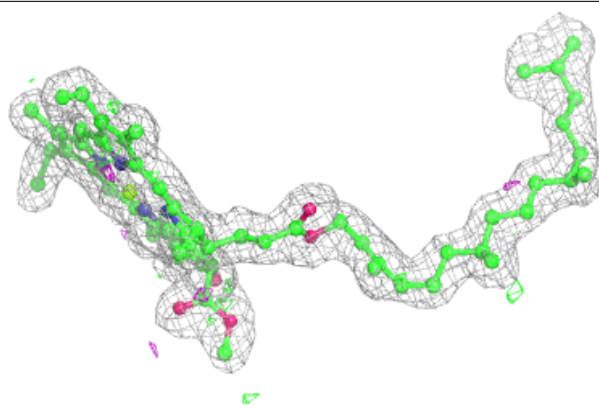
Electron density around CLA b 617:

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

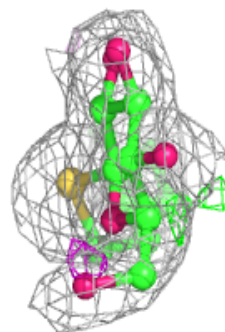
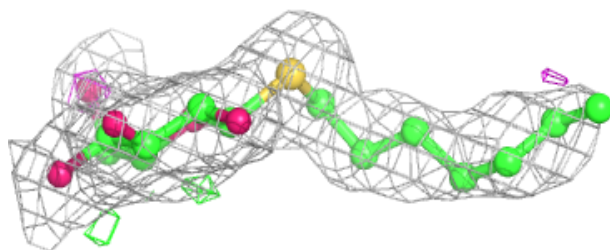
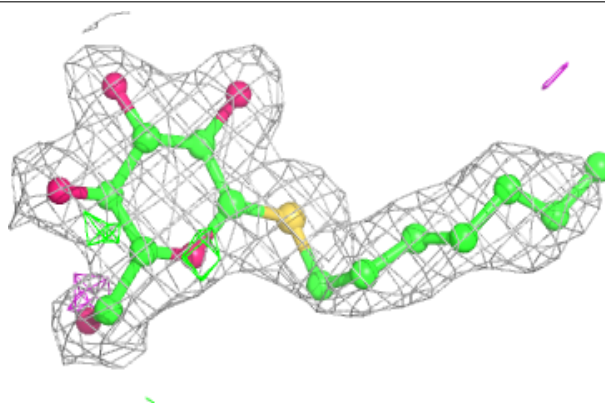


Electron density around CLA D 401:

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

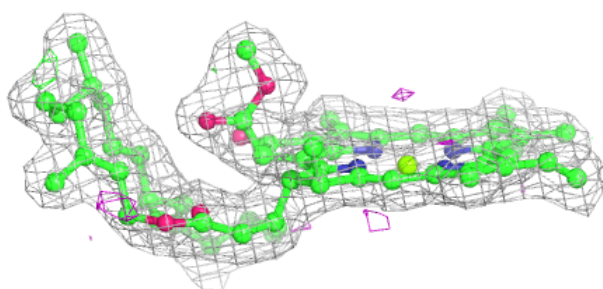
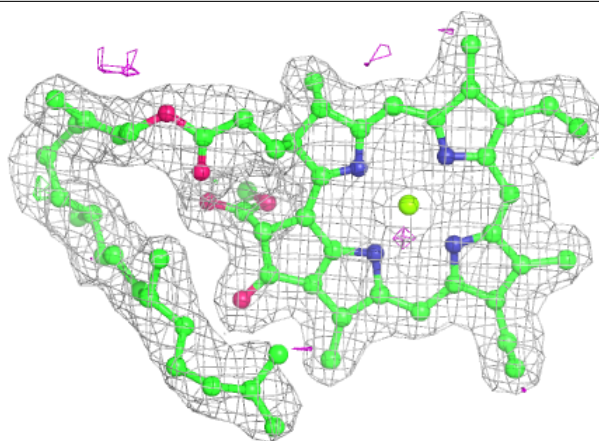
**Electron density around HTG O 303:**

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

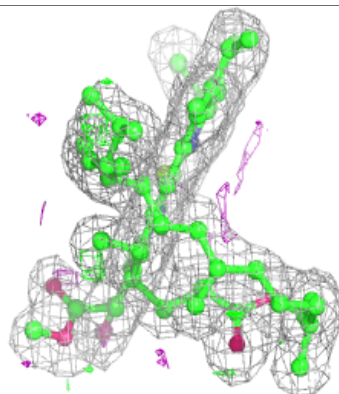
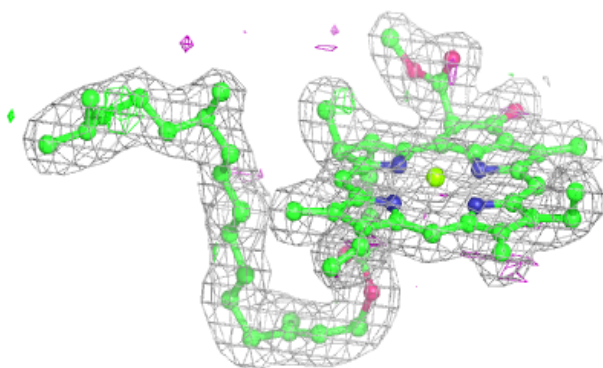
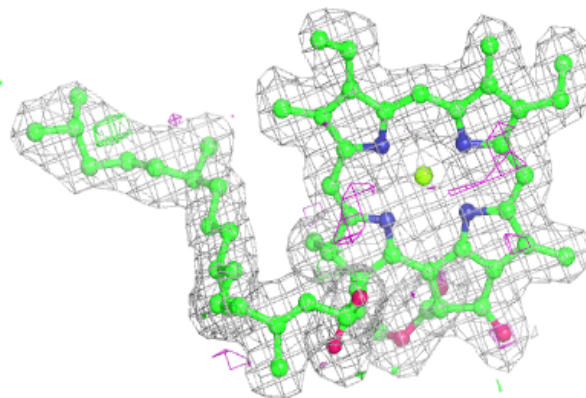


Electron density around CLA B 611:

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

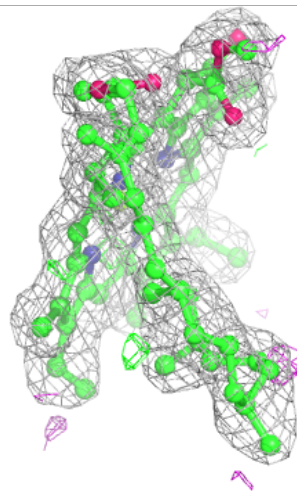
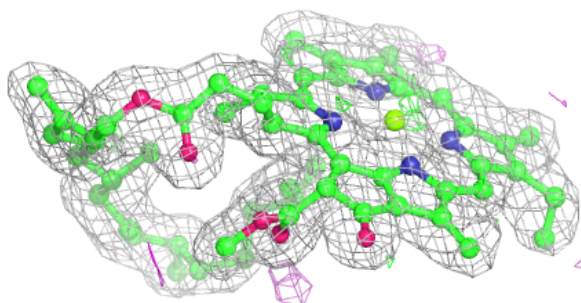
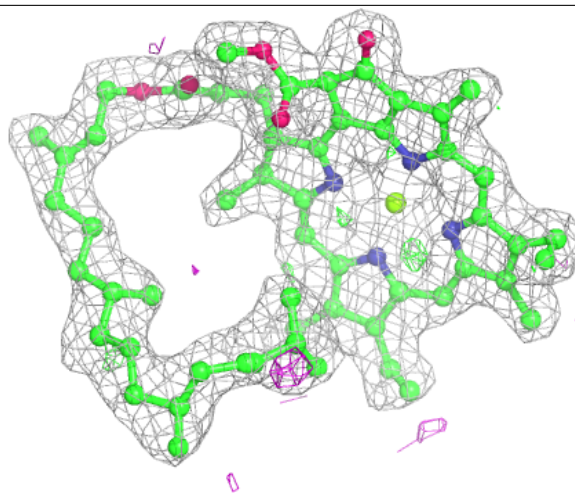
**Electron density around CLA d 401:**

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



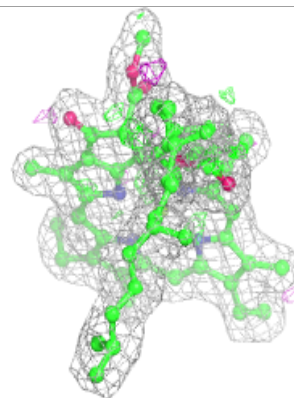
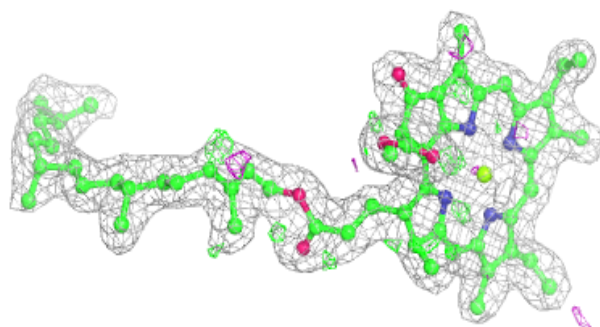
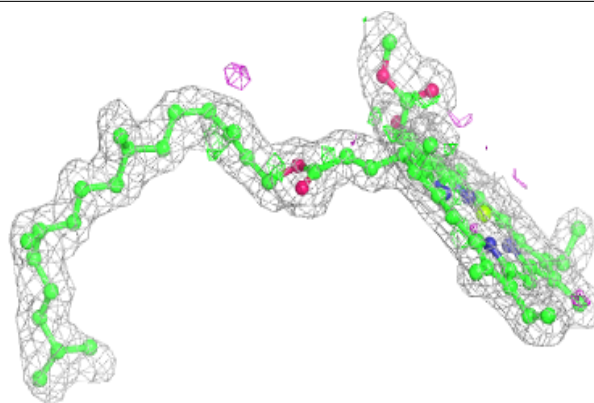
Electron density around CLA B 616:

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

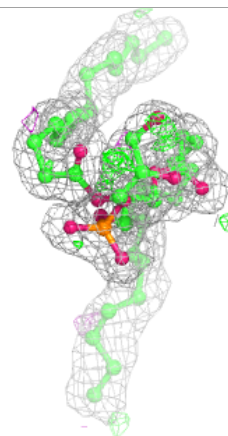
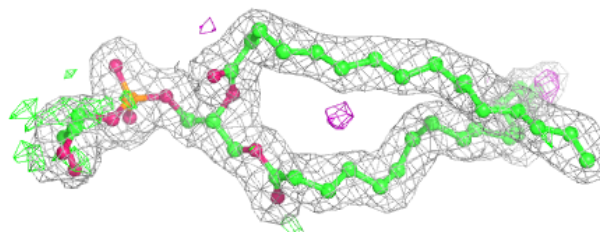
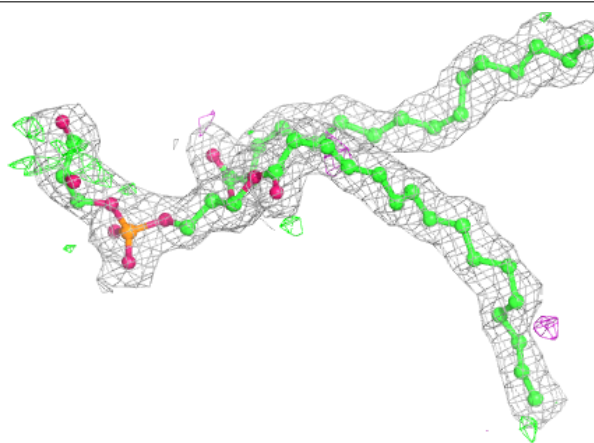


Electron density around CLA d 402:

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

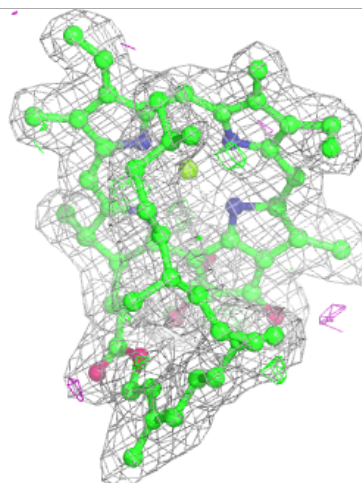
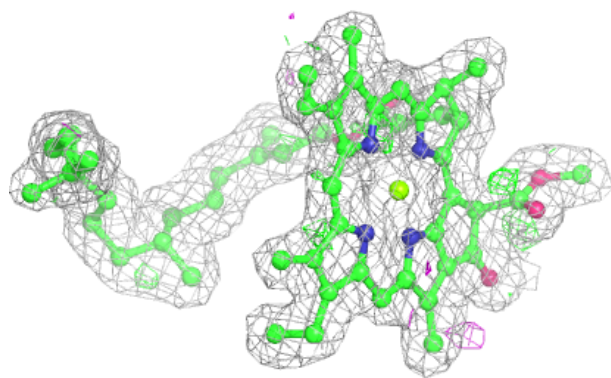
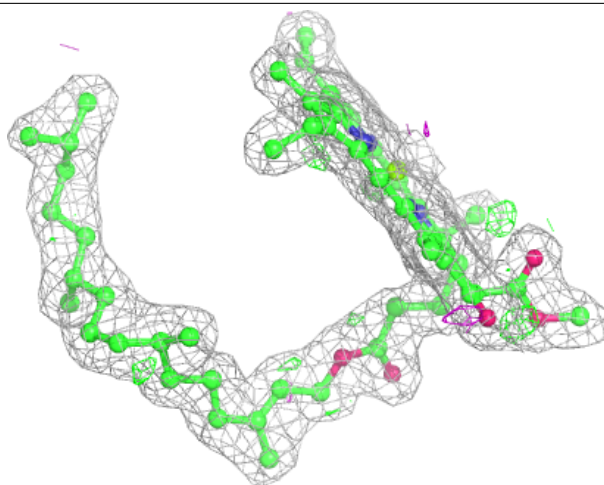
**Electron density around LHG D 407:**

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



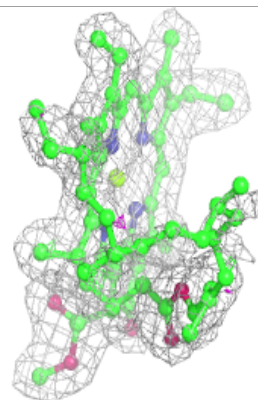
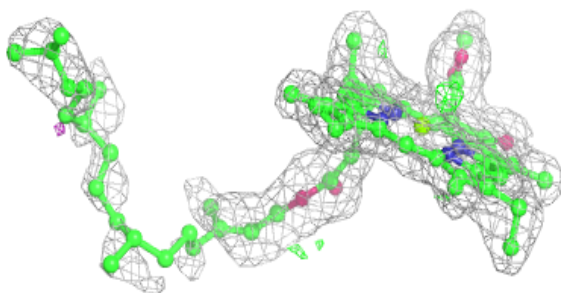
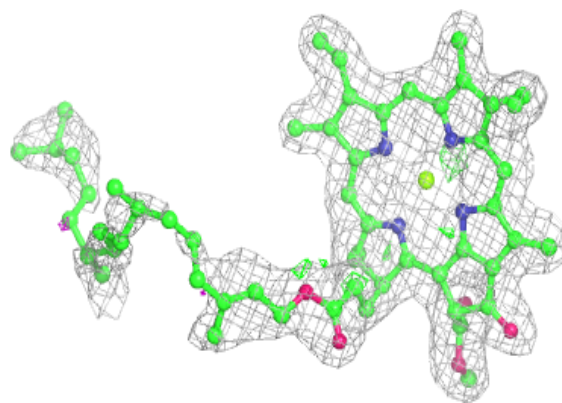
Electron density around CLA B 612:

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

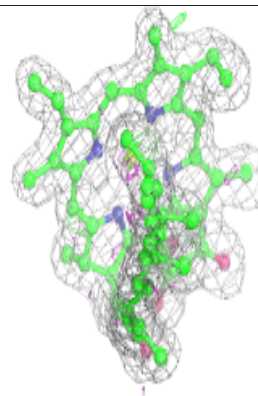
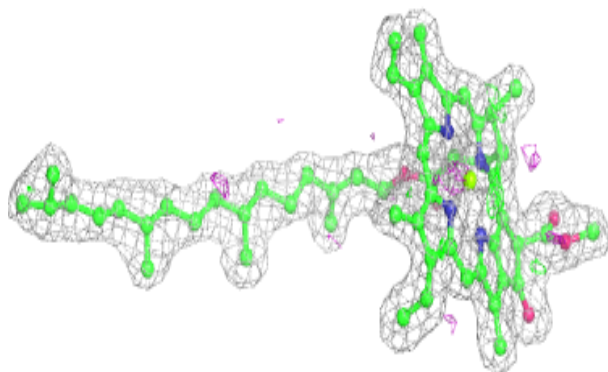
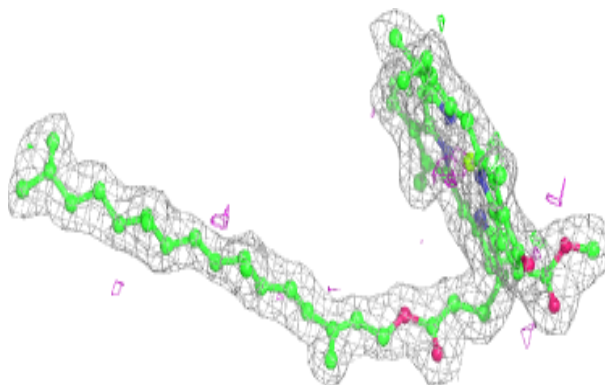


Electron density around CLA a 409:

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

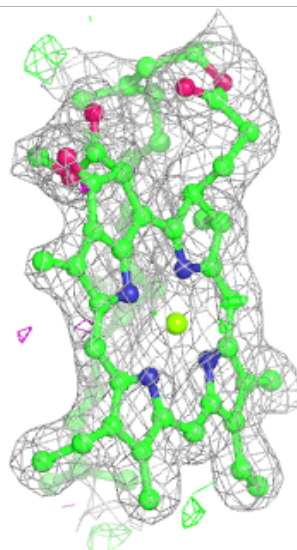
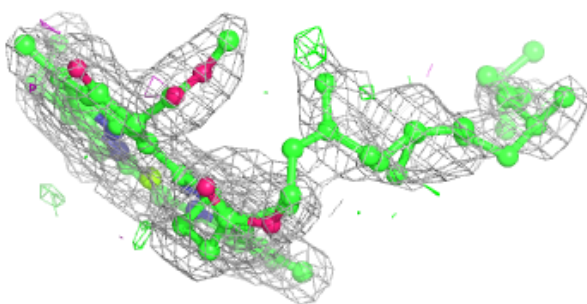
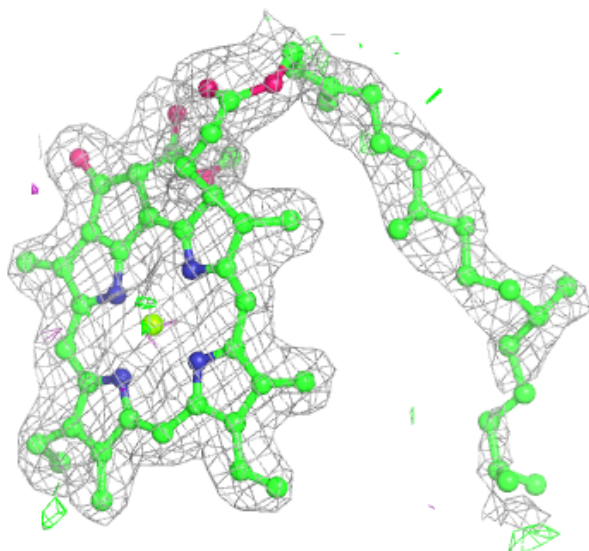
**Electron density around CLA b 611:**

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



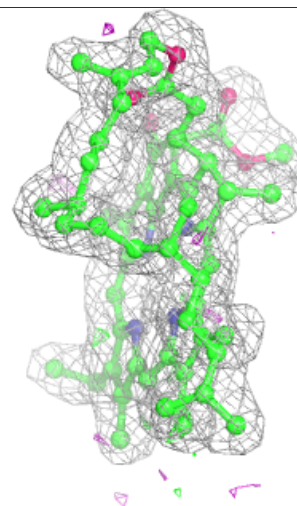
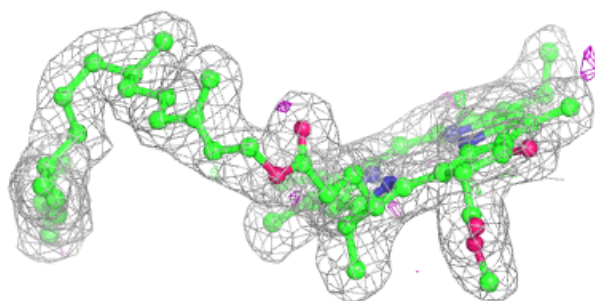
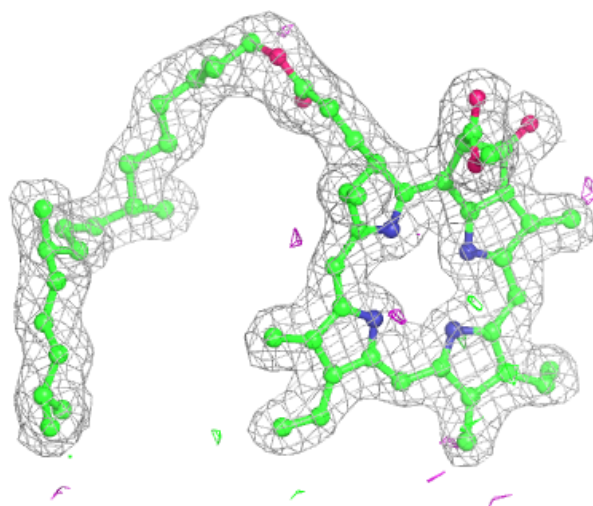
Electron density around CLA B 617:

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



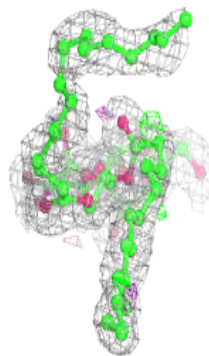
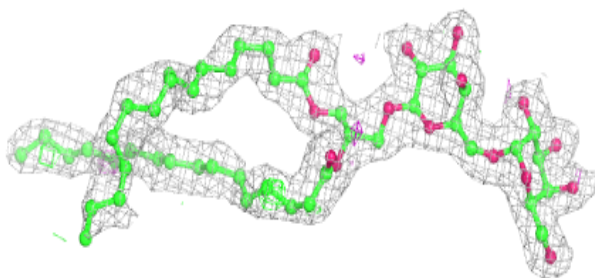
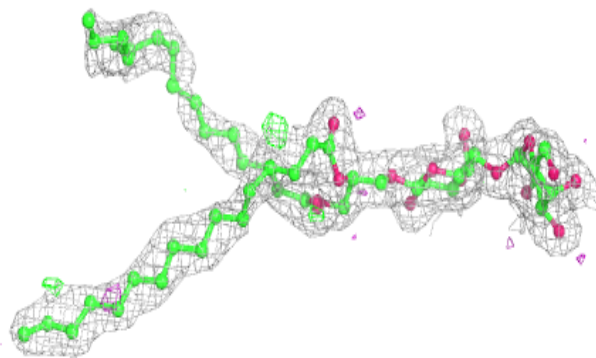
Electron density around PHO A 409:

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

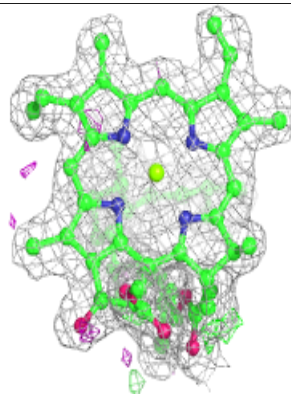
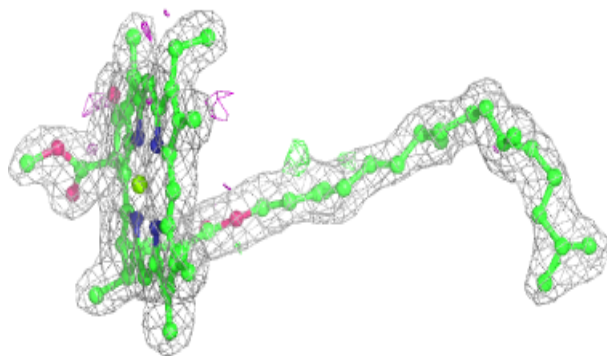
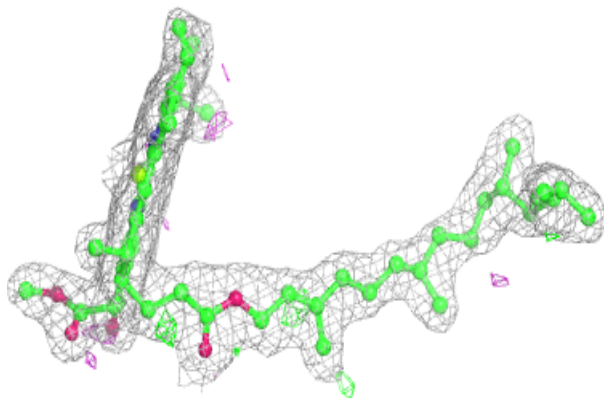


Electron density around DGD C 517:

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

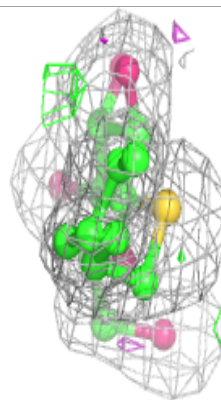
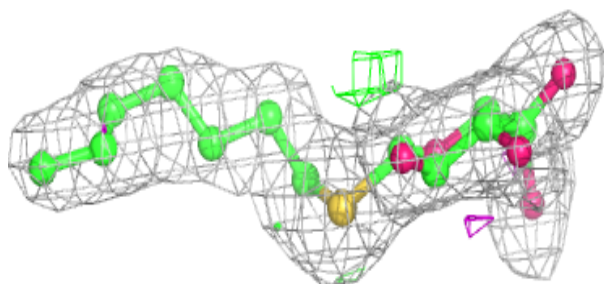
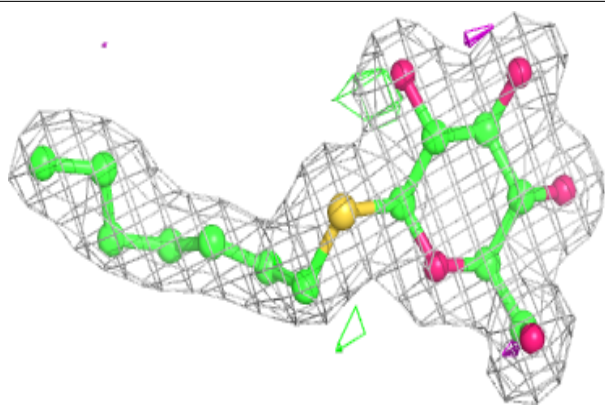
**Electron density around CLA b 609:**

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

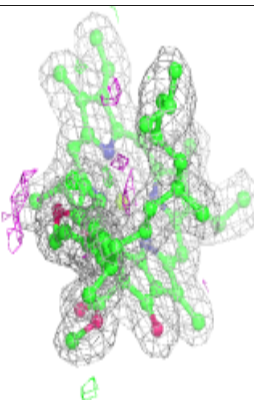
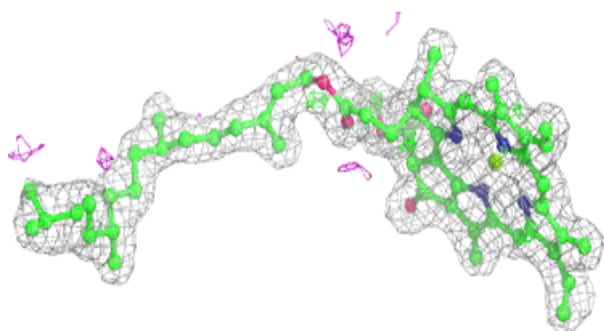
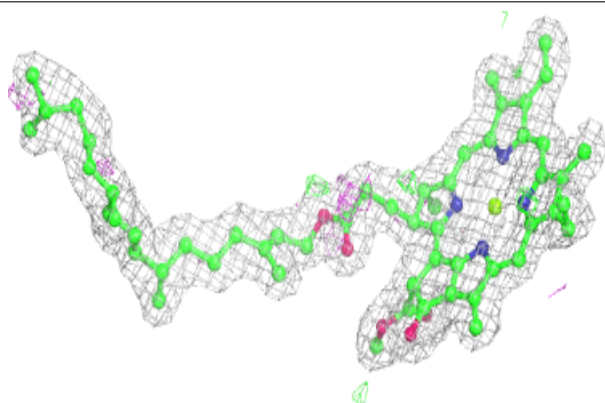


Electron density around HTG B 624:

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

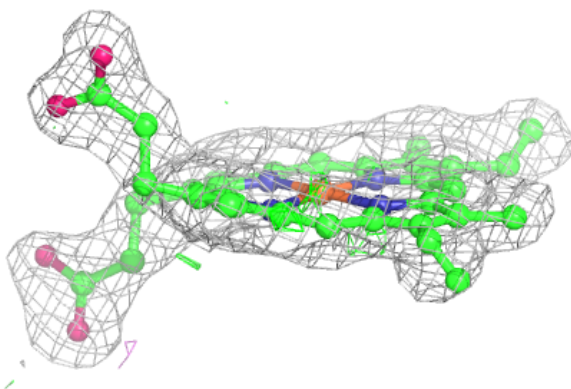
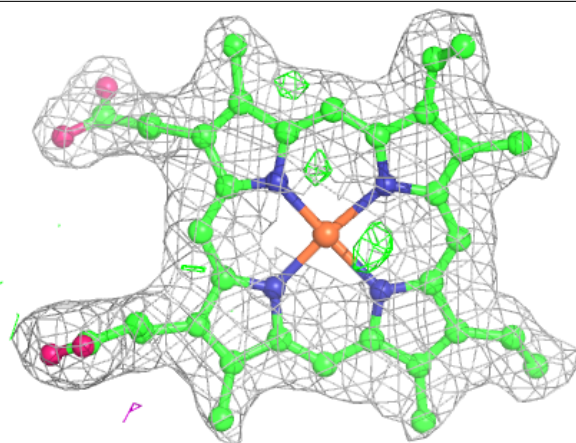
**Electron density around CLA a 406:**

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

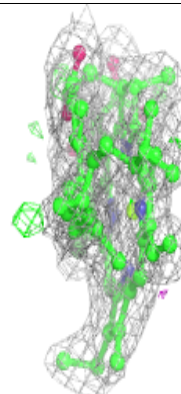
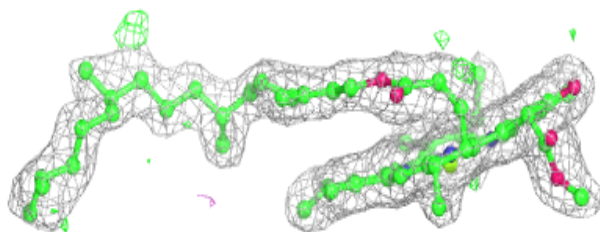
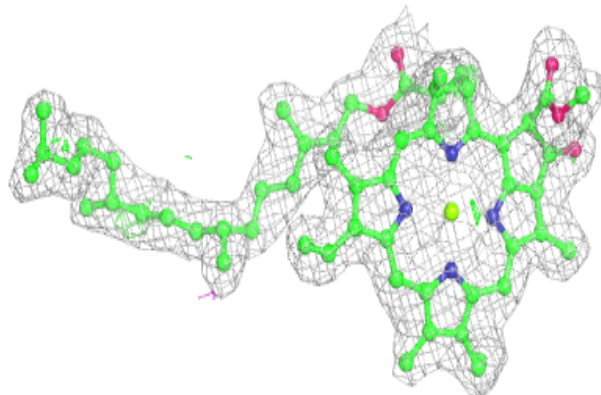


Electron density around HEM E 103:

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

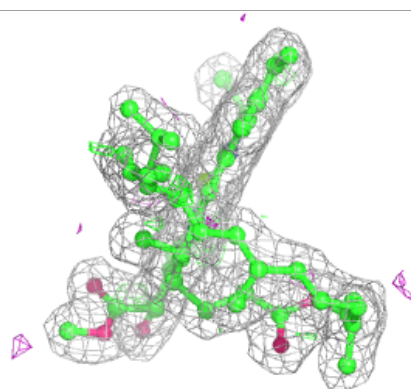
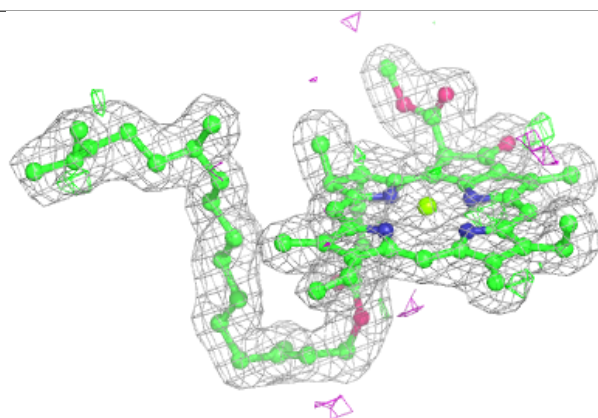
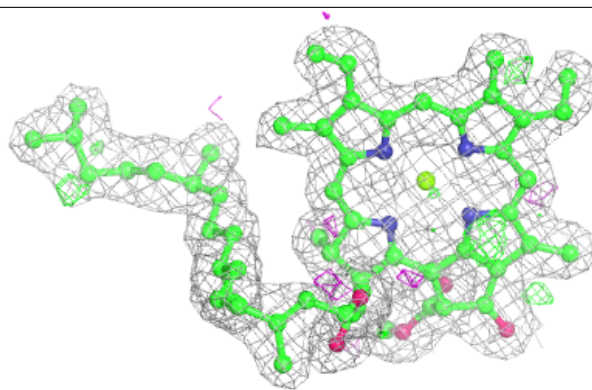
**Electron density around CLA b 607:**

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

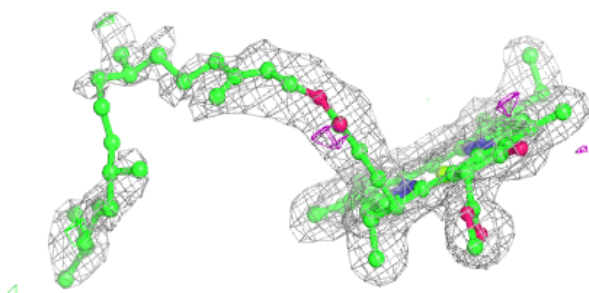
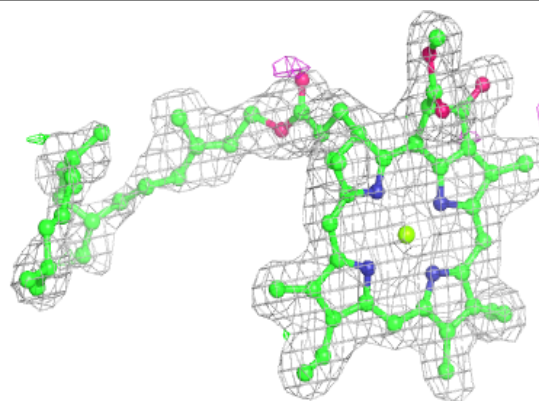


Electron density around CLA A 406:

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

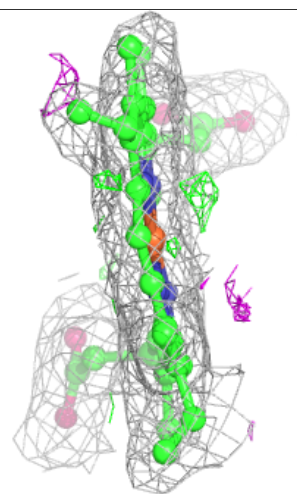
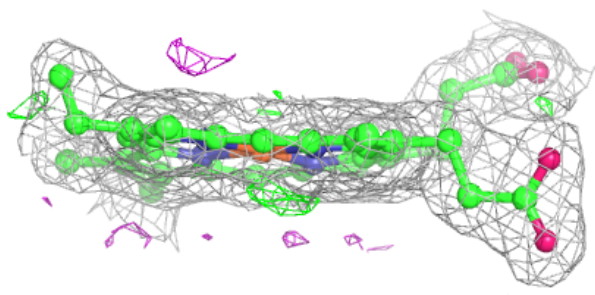
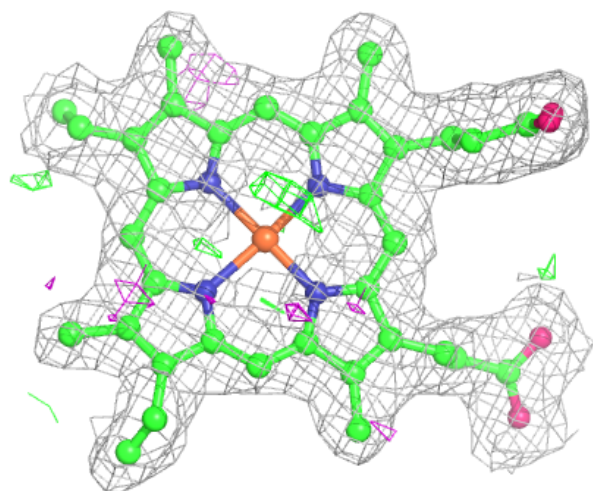
**Electron density around CLA A 410:**

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



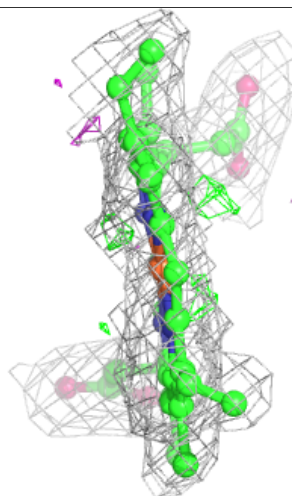
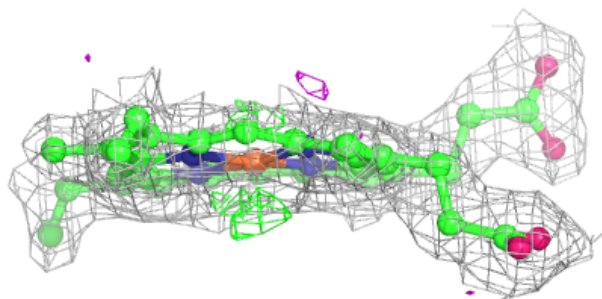
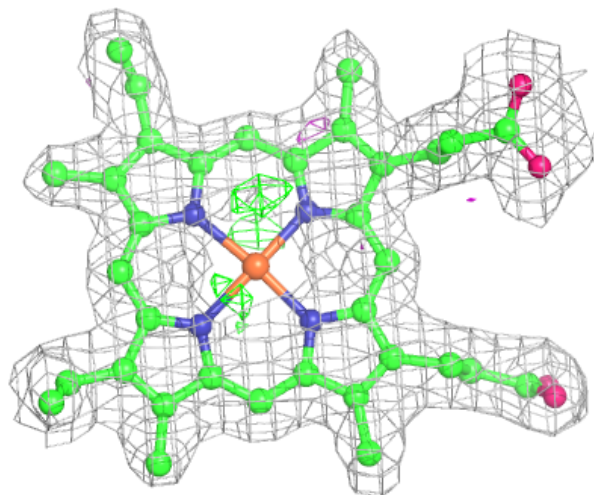
Electron density around HEC V 201:

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



Electron density around 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.