



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 02:24 PM BST

PDB ID : 3WU2  
Title : Crystal structure analysis of Photosystem II complex  
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.  
Deposited on : 2014-04-21  
Resolution : 1.90 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](mailto: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.

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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

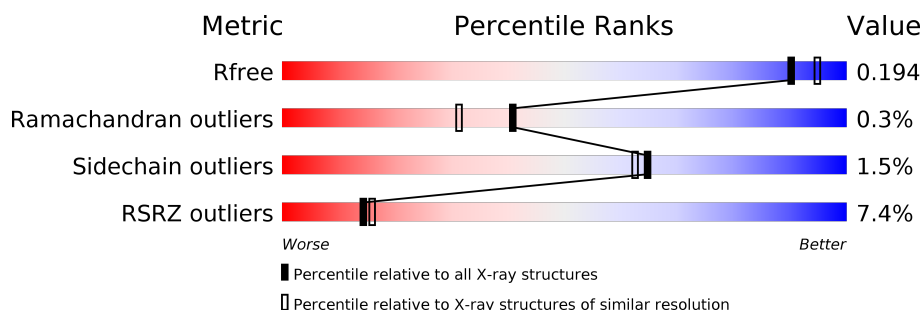
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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>0%</div> <div>94%</div> <div>0%</div> </div>
1	a	344	<div> <div>4%</div> <div>93%</div> <div>0%</div> </div>
2	B	504	<div> <div>8%</div> <div>97%</div> <div>0%</div> </div>
2	b	504	<div> <div>9%</div> <div>97%</div> <div>0%</div> </div>
3	C	455	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
3	c	455	<div> <div>5%</div> <div>97%</div> <div>0%</div> </div>
4	D	342	<div> <div>2%</div> <div>96%</div> <div>0%</div> </div>

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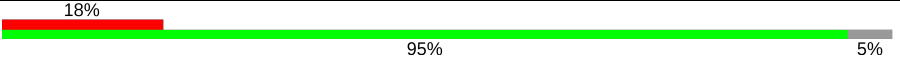
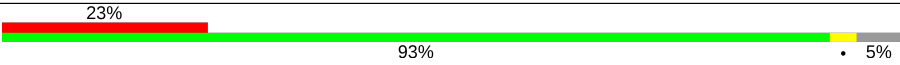
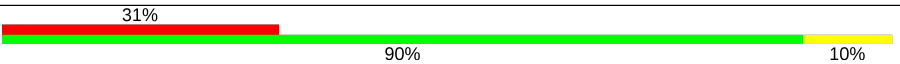



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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	a	414	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	904	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	909	X	-	-	-
23	CLA	c	910	X	-	-	-
23	CLA	c	911	X	-	-	-
23	CLA	c	912	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	c	914	X	-	-	-
23	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
29	UNL	T	102	-	-	-	X
29	UNL	t	103	-	-	-	X
33	HTG	B	626	-	-	-	X
33	HTG	c	924	-	-	-	X

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54036 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	4	0
			2633	1729	429	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2625	1722	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4009	2633	668	695	13			
2	b	501	Total	C	N	O	S	0	11	0
			3964	2605	658	688	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	3	0
			3502	2291	588	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	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	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			639	419	103	117				

- 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
			274	187	45	41	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	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	48	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	UNP P19054

- 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	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	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
			770	489	129	152				
15	u	97	Total	C	N	O		0	1	0
			772	490	129	153				

- 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	2	0
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

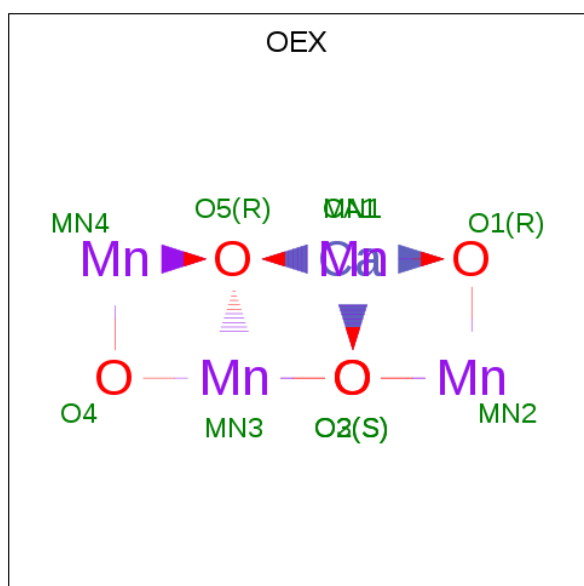
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O	S	0	1	0
			280	190	44	46				

- 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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

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

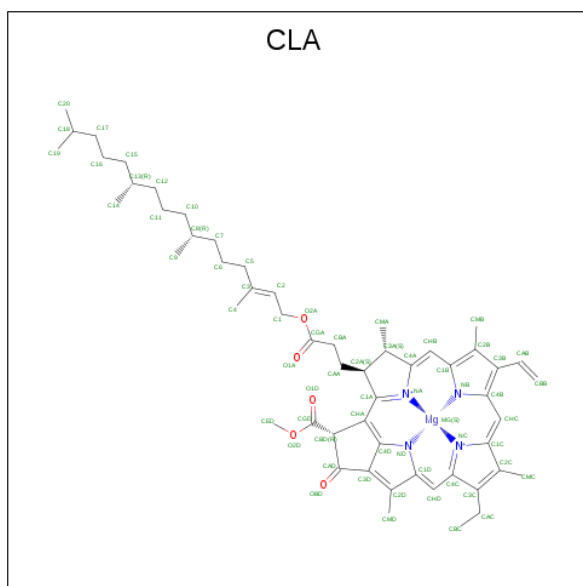
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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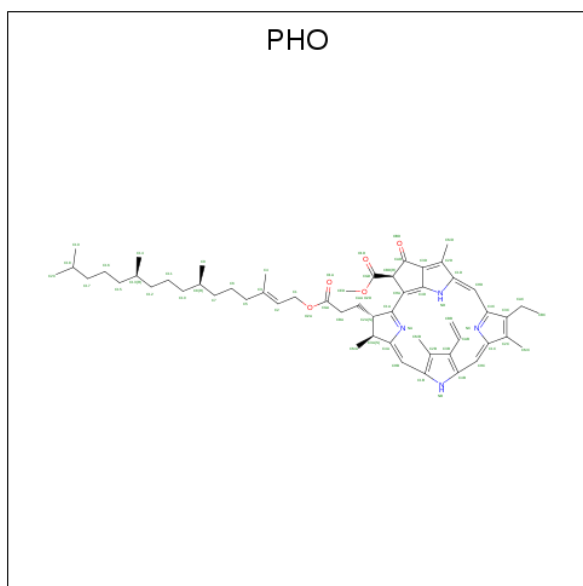
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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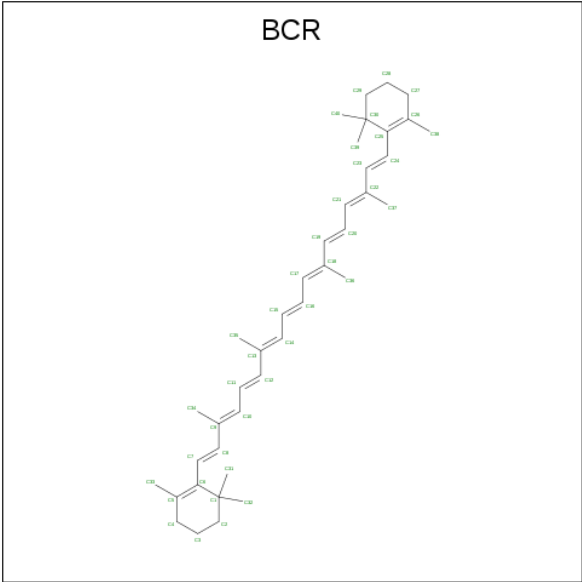
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



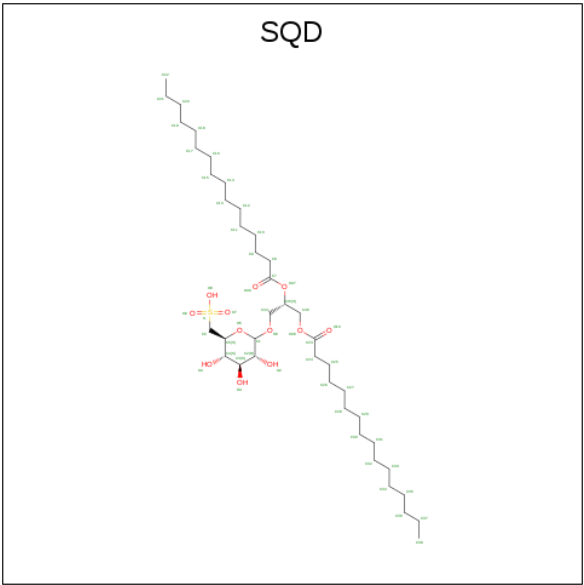
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

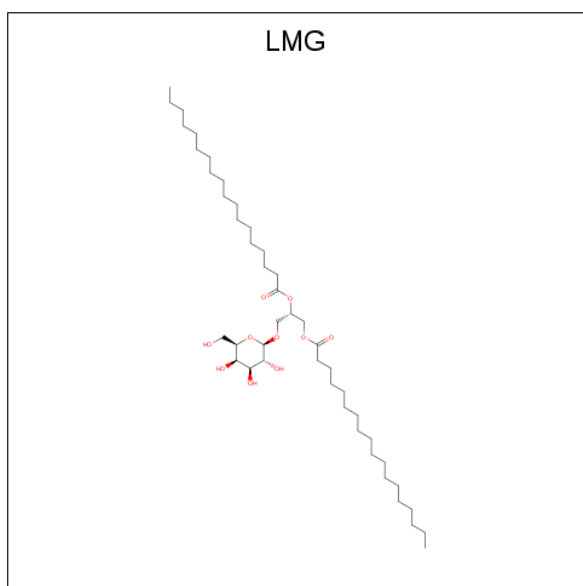
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			33	23	9	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



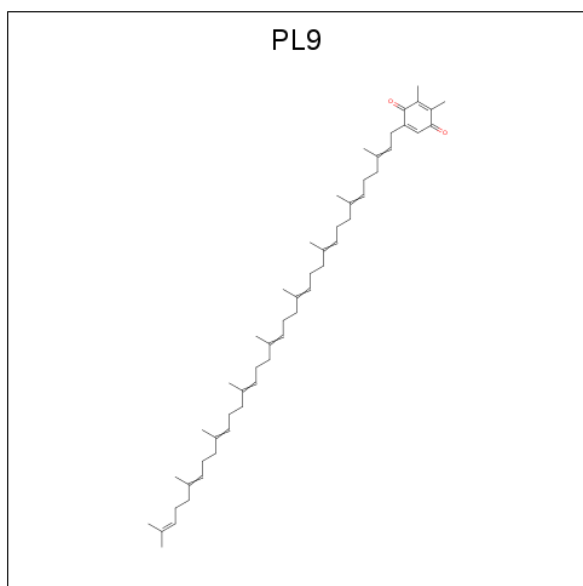
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			51	41	10			
27	B	1	Total	C	O		0	0
			51	41	10			
27	C	1	Total	C	O		0	0
			51	41	10			
27	D	1	Total	C	O		0	0
			51	41	10			
27	Z	1	Total	C	O		0	0
			51	41	10			
27	a	1	Total	C	O		0	0
			51	41	10			
27	b	1	Total	C	O		0	0
			51	41	10			
27	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			51	41	10		
27	d	1	Total	C	O	0	0
			51	41	10		

- Molecule 28 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:  $C_{53}H_{80}O_2$ ).



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

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

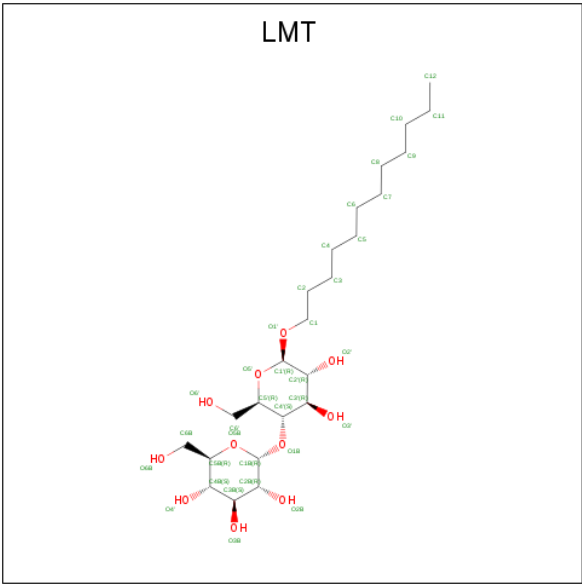
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	4	Total	C		0	0
			56	56			
29	c	2	Total	C	O	0	0
			40	35	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	2	Total C 26 26	0	0
29	E	2	Total C 27 27	0	0
29	b	4	Total C O 84 79 5	0	0
29	A	4	Total C O 69 64 5	0	0
29	x	1	Total C 16 16	0	0
29	M	1	Total C 16 16	0	0
29	j	2	Total C 28 28	0	0
29	D	2	Total C O 56 51 5	0	0
29	e	1	Total C 11 11	0	0
29	I	2	Total C 24 24	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	L	1	Total C 14 14	0	0
29	d	1	Total C 16 16	0	0
29	H	1	Total C 10 10	0	0
29	i	4	Total C 55 55	0	0
29	C	1	Total C O 34 29 5	0	0
29	z	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	C	1	Total	C	O	0	0
			35	24	11		
30	F	1	Total	C	O	0	0
			35	24	11		
30	J	1	Total	C	O	0	0
			24	18	6		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	b	1	Total	C	O	0	0
			24	18	6		
30	c	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	t	1	Total	C	O	0	0
			24	18	6		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	D	1	Total	C	O	0	0
			6	3	3		
31	L	1	Total	C	O	0	0
			6	3	3		
31	O	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		

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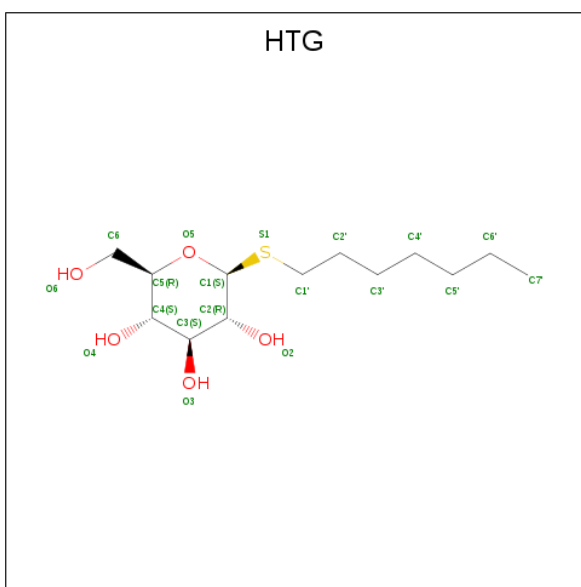
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	f	1	Total	C	O	0	0
			6	3	3		
31	h	1	Total	C	O	0	0
			6	3	3		
31	l	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	D	1	Total 19	C 13	O 5	S 1	0	0
33	O	1	Total 19	C 13	O 5	S 1	0	0
33	U	1	Total 9	C 8	S 1		0	0
33	V	1	Total 13	C 7	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0

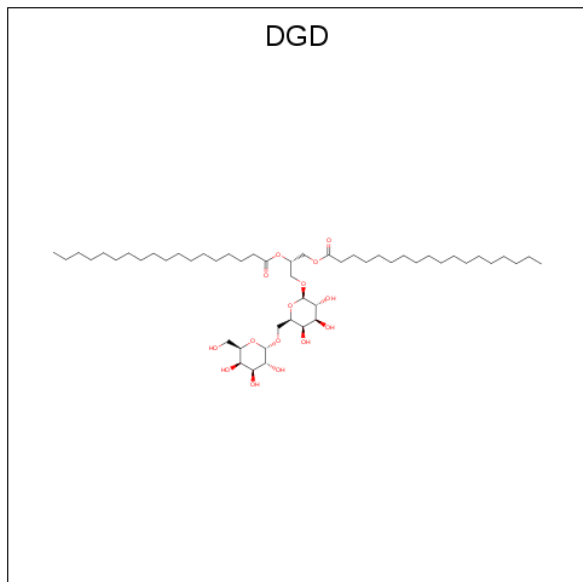
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	d	1	Total	C	O	S	0	0
			19	13	5	1		
33	u	1	Total	C	O	S	0	0
			14	10	3	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



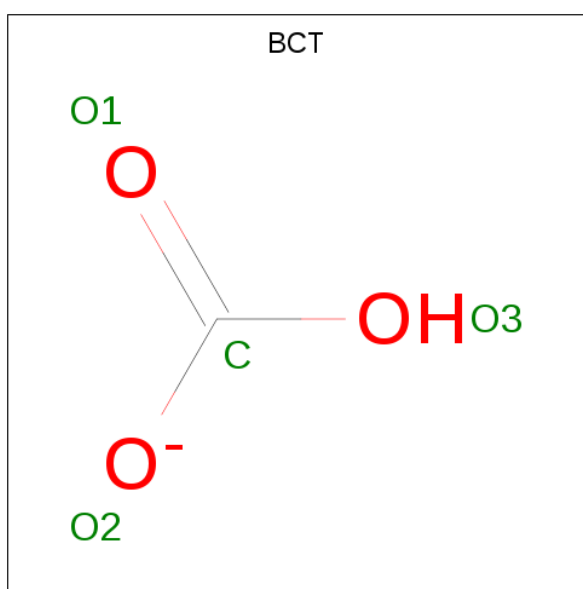
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	D	1	Total	C	O		0	0
			53	42	11			
34	H	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15			

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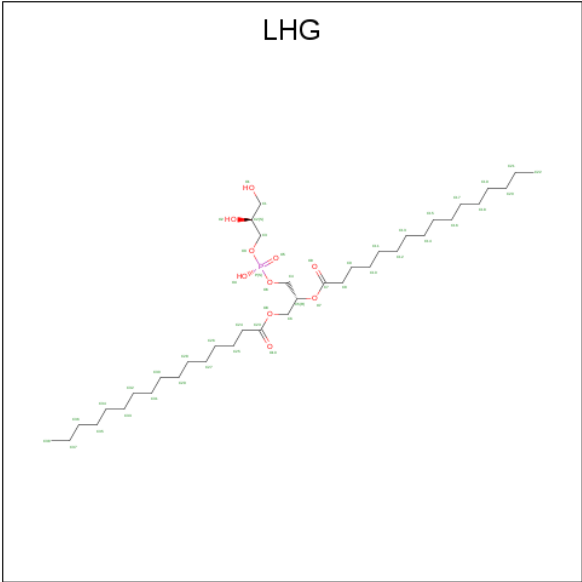
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$ ).



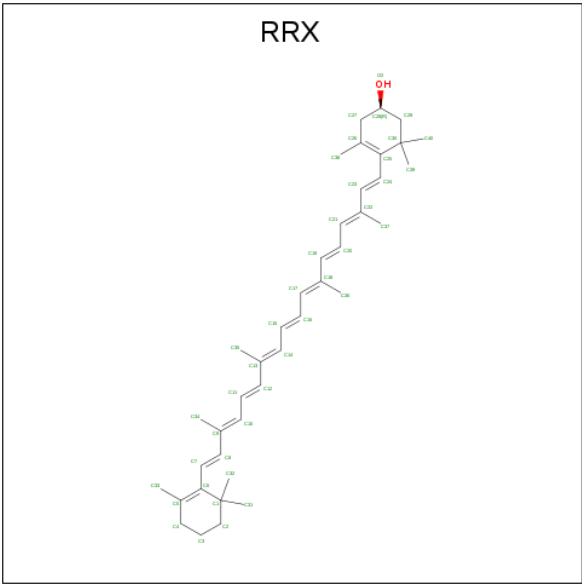
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			46	35	10	1		
36	E	1	Total	C	O	P	0	0
			49	38	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			40	29	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).

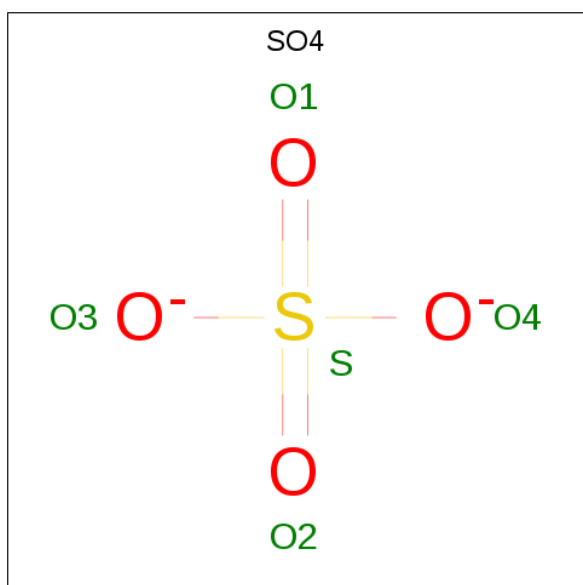


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	h	1	Total	C	O	0	0
			41	40	1		

- 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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	253	Total 263	O 263	0	10
41	D	156	Total 161	O 161	0	5
41	E	32	Total 35	O 35	0	3
41	F	12	Total 12	O 12	0	0
41	H	50	Total 52	O 52	0	2
41	I	8	Total 8	O 8	0	0
41	J	9	Total 9	O 9	0	0
41	K	8	Total 8	O 8	0	0
41	L	23	Total 24	O 24	0	1
41	M	15	Total 16	O 16	0	1
41	O	193	Total 202	O 202	0	9
41	T	10	Total 10	O 10	0	0
41	U	98	Total 100	O 100	0	2
41	V	140	Total 144	O 144	0	4
41	Y	6	Total 6	O 6	0	0
41	X	13	Total 14	O 14	0	1
41	Z	1	Total 1	O 1	0	0
41	a	153	Total 155	O 155	0	2
41	b	295	Total 306	O 306	0	11
41	c	238	Total 245	O 245	0	7
41	d	156	Total 160	O 160	0	4

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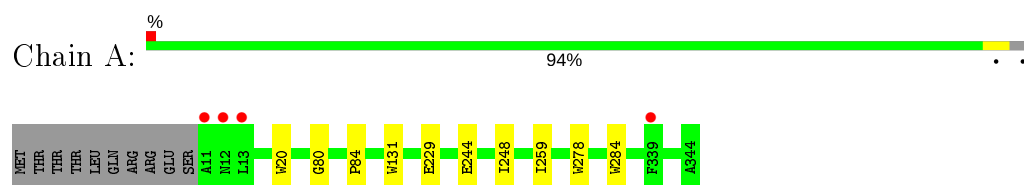
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	e	22	Total 22	O 22	0	0
41	f	13	Total 14	O 14	0	1
41	h	48	Total 53	O 53	0	5
41	i	13	Total 14	O 14	0	1
41	j	9	Total 9	O 9	0	0
41	k	5	Total 5	O 5	0	0
41	l	17	Total 18	O 18	0	1
41	m	15	Total 16	O 16	0	1
41	o	167	Total 175	O 175	0	8
41	t	12	Total 12	O 12	0	0
41	u	102	Total 106	O 106	0	4
41	v	98	Total 104	O 104	0	6
41	y	7	Total 7	O 7	0	0
41	x	6	Total 6	O 6	0	0
41	z	2	Total 2	O 2	0	0

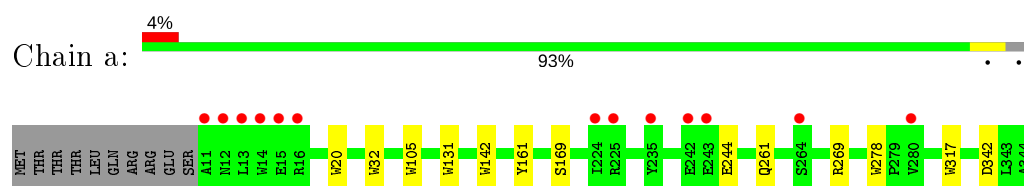
### 3 Residue-property plots [i](#)

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

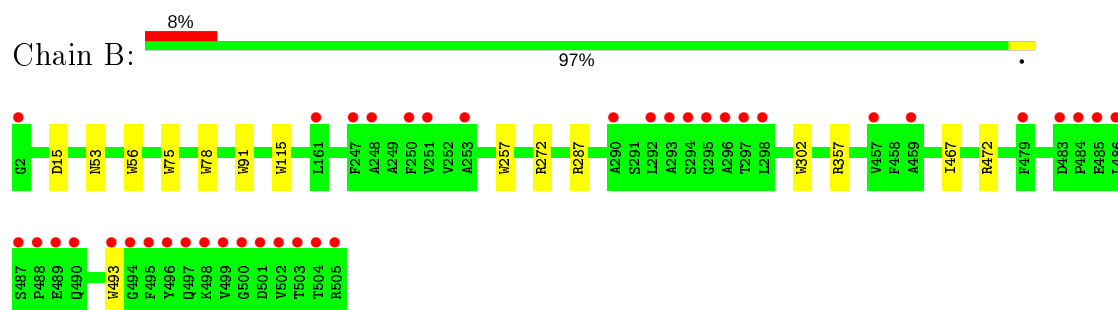
- Molecule 1: Photosystem Q(B) protein



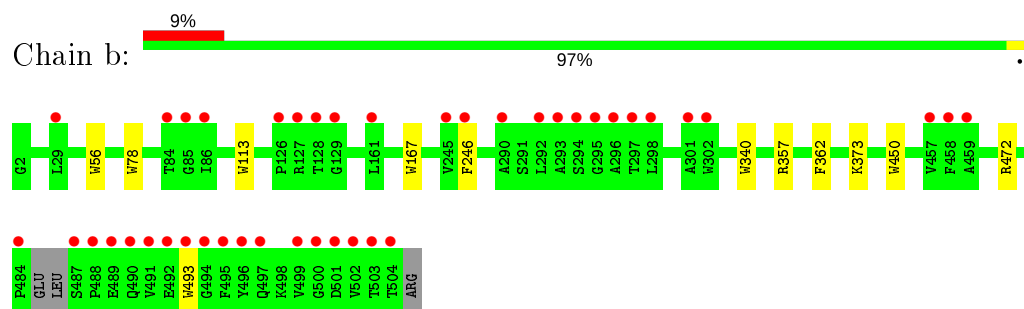
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

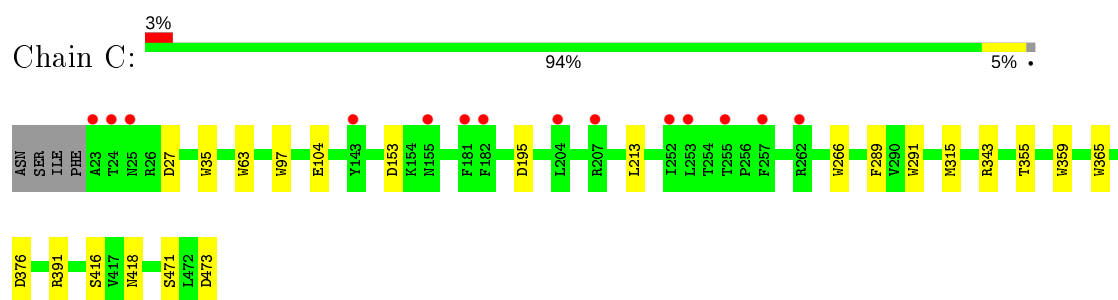


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

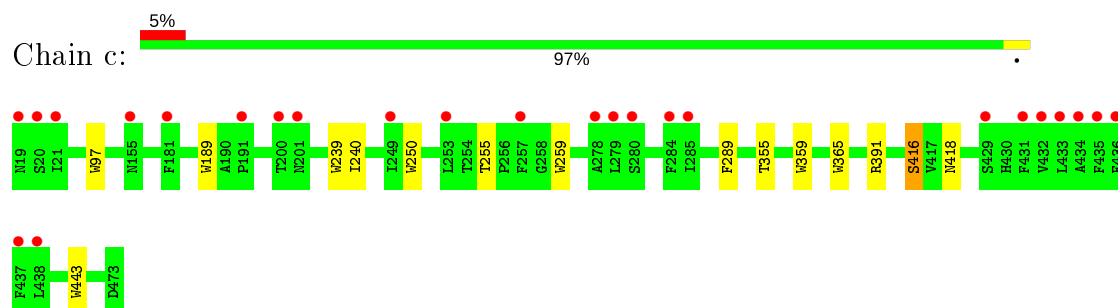


- Molecule 3: Photosystem II 44 kDa reaction center protein

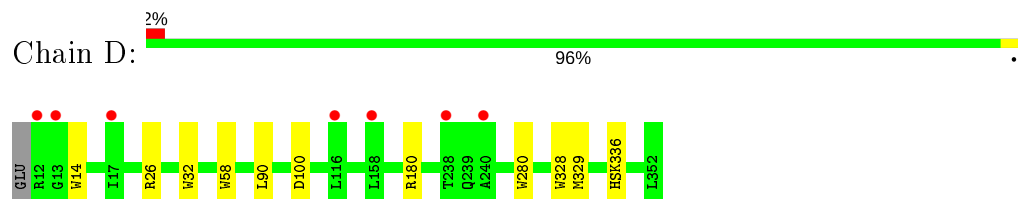




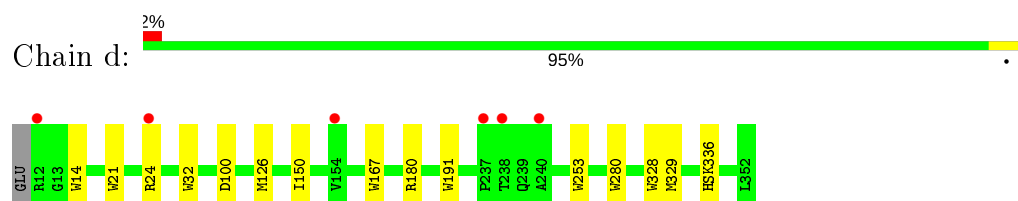
- Molecule 3: Photosystem II 44 kDa reaction center protein



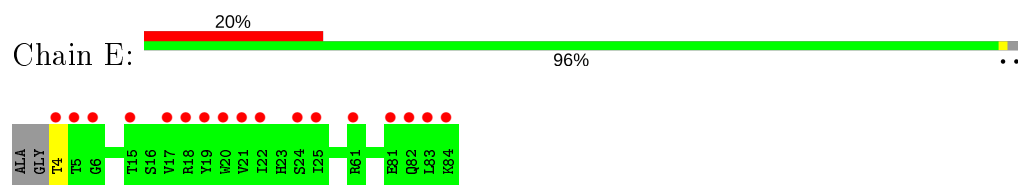
- Molecule 4: Photosystem II D2 protein



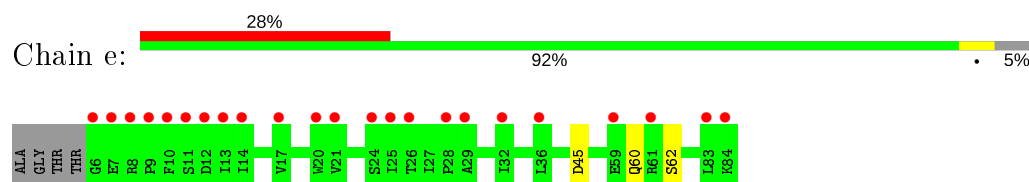
- Molecule 4: Photosystem II D2 protein



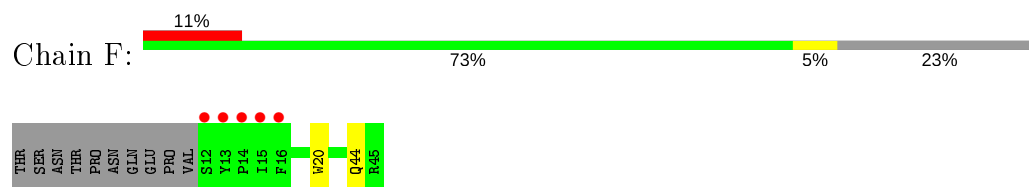
- Molecule 5: Cytochrome b559 subunit alpha



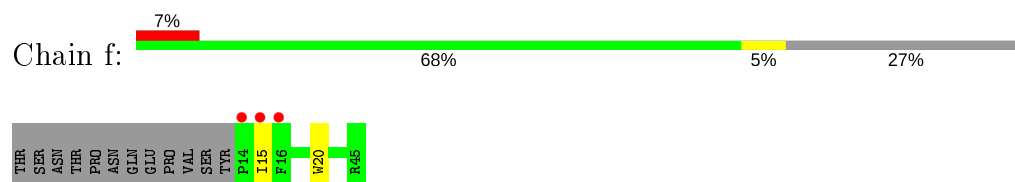
- Molecule 5: Cytochrome b559 subunit alpha



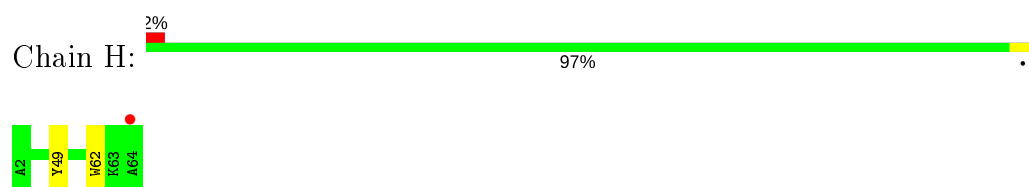
- Molecule 6: Cytochrome b559 subunit beta



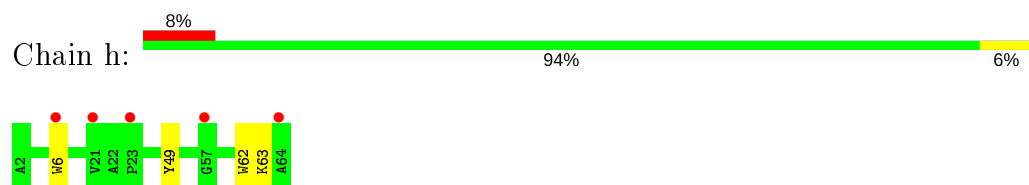
- Molecule 6: Cytochrome b559 subunit beta



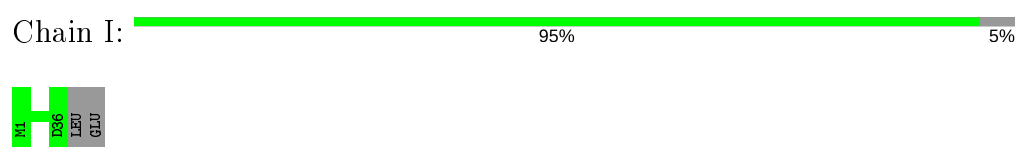
- Molecule 7: Photosystem II reaction center protein H



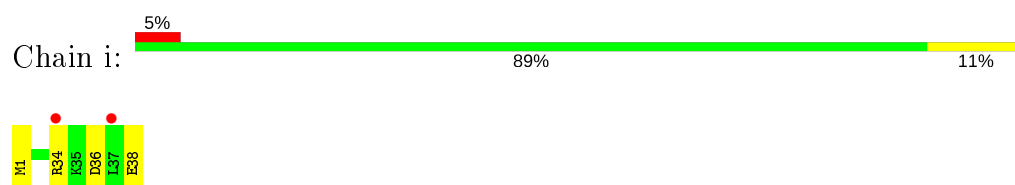
- Molecule 7: Photosystem II reaction center protein H



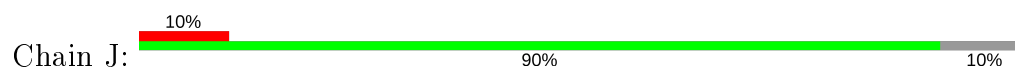
- Molecule 8: Photosystem II reaction center protein I

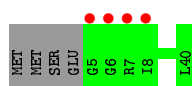


- Molecule 8: Photosystem II reaction center protein I

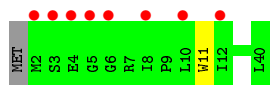
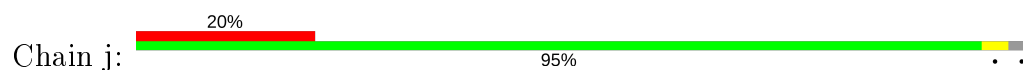


- Molecule 9: Photosystem II reaction center protein J





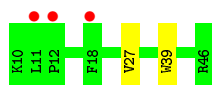
- Molecule 9: Photosystem II reaction center protein J



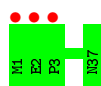
- Molecule 10: Photosystem II reaction center protein K



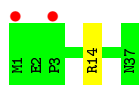
- Molecule 10: Photosystem II reaction center protein K



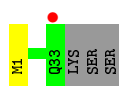
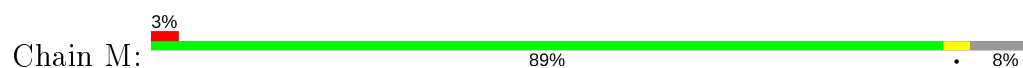
- Molecule 11: Photosystem II reaction center protein L



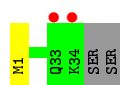
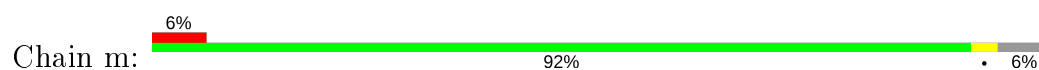
- Molecule 11: Photosystem II reaction center protein L



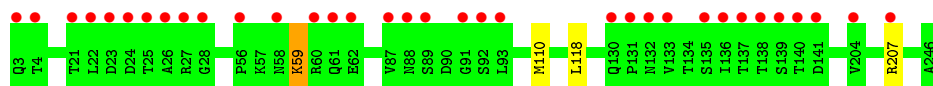
- Molecule 12: Photosystem II reaction center protein M



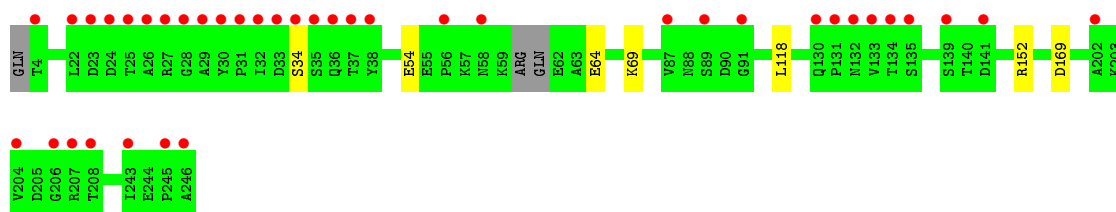
- Molecule 12: Photosystem II reaction center protein M



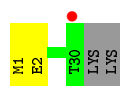
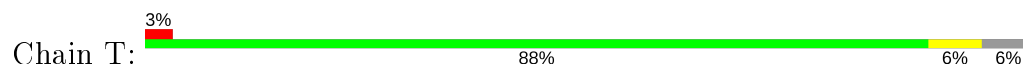
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



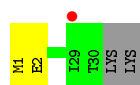
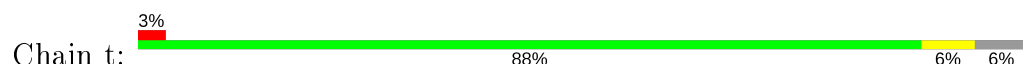
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

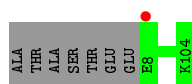


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein





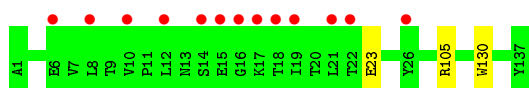
- Molecule 16: Cytochrome c-550

Chain V: 99%



- Molecule 16: Cytochrome c-550

Chain v: 9% 98%



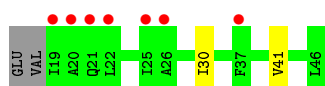
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 13% 87% 10%



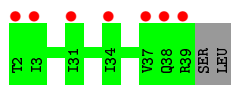
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 23% 87% 7% 7%



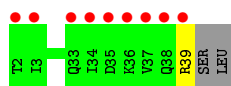
- Molecule 18: Photosystem II reaction center protein X

Chain X: 18% 95% 5%

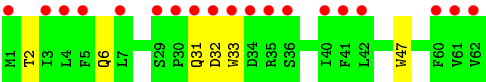
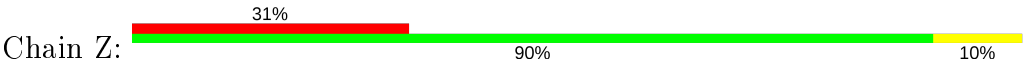


- Molecule 18: Photosystem II reaction center protein X

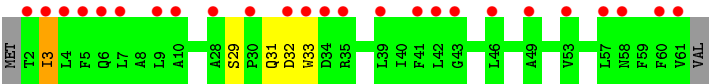
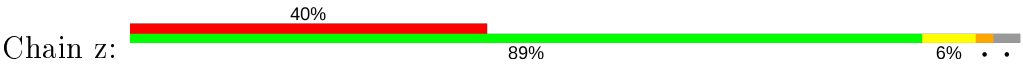
Chain x: 23% 93% 5%



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (49.02-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.156 , 0.194 0.157 , 0.194	Depositor DCC
$R_{free}$ test set	31215 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, BCT, BCR, DGD, HSK, FE2, RRX, LHG, GOL, CL, CA, CLA, SO4, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, SQD, LMG

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	1.08	4/2730 (0.1%)	0.90	1/3723 (0.0%)
1	a	1.06	9/2721 (0.3%)	0.86	4/3711 (0.1%)
2	B	1.03	9/4179 (0.2%)	0.89	5/5693 (0.1%)
2	b	1.01	7/4134 (0.2%)	0.85	2/5633 (0.0%)
3	C	1.00	7/3624 (0.2%)	0.84	9/4933 (0.2%)
3	c	0.96	8/3662 (0.2%)	0.81	0/4986
4	D	1.13	5/2804 (0.2%)	0.93	3/3820 (0.1%)
4	d	1.05	8/2825 (0.3%)	0.87	2/3847 (0.1%)
5	E	0.81	0/676	0.82	0/924
5	e	0.81	0/658	0.78	1/899 (0.1%)
6	F	0.90	1/283 (0.4%)	0.71	0/386
6	f	0.92	1/265 (0.4%)	0.69	0/360
7	H	0.98	1/511 (0.2%)	0.79	0/697
7	h	0.94	2/511 (0.4%)	0.81	0/697
8	I	0.77	0/291	0.78	0/394
8	i	0.75	0/308	0.77	0/415
9	J	0.94	0/257	0.68	0/349
9	j	0.81	1/277 (0.4%)	0.69	0/376
10	K	0.76	1/303 (0.3%)	0.75	0/418
10	k	0.79	1/296 (0.3%)	0.77	0/408
11	L	1.05	0/312	0.88	0/425
11	l	1.00	0/313	0.84	1/428 (0.2%)
12	M	0.85	0/257	0.91	0/352
12	m	0.86	0/270	0.80	0/370
13	O	0.84	0/1924	0.89	0/2610
13	o	0.79	0/1900	0.86	3/2577 (0.1%)
14	T	0.93	0/255	0.86	0/346
14	t	0.99	0/255	0.92	0/346
15	U	0.93	0/781	0.90	1/1059 (0.1%)
15	u	0.95	0/786	0.91	0/1067
16	V	0.97	0/1093	0.89	1/1485 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.88	1/1084 (0.1%)	0.85	1/1475 (0.1%)
17	Y	0.55	0/197	0.66	0/263
17	y	0.50	0/197	0.75	0/264
18	X	0.72	0/286	0.75	0/387
18	x	0.67	0/286	0.75	0/387
19	Z	0.76	2/470 (0.4%)	0.74	0/645
19	z	0.68	1/442 (0.2%)	0.71	0/608
All	All	0.97	69/42423 (0.2%)	0.85	34/57763 (0.1%)

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	TRP	CD2-CE2	7.33	1.50	1.41
7	H	62	TRP	CD2-CE2	6.81	1.49	1.41
3	c	443	TRP	CD2-CE2	6.79	1.49	1.41
1	A	284	TRP	CD2-CE2	6.79	1.49	1.41
3	C	359	TRP	CD2-CE2	6.46	1.49	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ARG	NE-CZ-NH1	-7.88	116.36	120.30
13	o	152	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	B	357	ARG	NE-CZ-NH2	-7.36	116.62	120.30
3	C	153	ASP	CB-CG-OD1	7.03	124.63	118.30
4	D	100	ASP	CB-CG-OD2	7.02	124.62	118.30

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	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	31
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	47	38
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	34	24
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	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	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	2
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	0
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	34	24
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	34	24
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (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%)	55 (92%)	2 (3%)	3 (5%)	2	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	2	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	41	31

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN

### 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%)	267 (98%)	5 (2%)	59	55
1	a	271/279 (97%)	269 (99%)	2 (1%)	84	84
2	B	407/402 (101%)	404 (99%)	3 (1%)	84	84
2	b	399/402 (99%)	393 (98%)	6 (2%)	65	62
3	C	355/356 (100%)	347 (98%)	8 (2%)	50	45
3	c	358/356 (101%)	349 (98%)	9 (2%)	47	41
4	D	275/276 (100%)	273 (99%)	2 (1%)	84	84
4	d	278/276 (101%)	274 (99%)	4 (1%)	67	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	71/72 (99%)	70 (99%)	1 (1%)	67	65
5	e	68/72 (94%)	66 (97%)	2 (3%)	42	35
6	F	27/38 (71%)	26 (96%)	1 (4%)	34	25
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	24
7	H	53/53 (100%)	52 (98%)	1 (2%)	57	53
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	53
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	33/34 (97%)	32 (97%)	1 (3%)	41	33
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	35	26
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	203 (98%)	4 (2%)	57	53
13	o	206/207 (100%)	203 (98%)	3 (2%)	65	62
14	T	25/28 (89%)	24 (96%)	1 (4%)	31	22
14	t	25/28 (89%)	24 (96%)	1 (4%)	31	22
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	43
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	78	79
17	Y	19/23 (83%)	18 (95%)	1 (5%)	22	13
17	y	18/23 (78%)	16 (89%)	2 (11%)	6	2
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	38	29
19	Z	47/52 (90%)	46 (98%)	1 (2%)	53	48
19	z	40/52 (77%)	38 (95%)	2 (5%)	24	15
All	All	4253/4368 (97%)	4186 (98%)	67 (2%)	65	60

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	244	GLU
2	b	479	PHE
16	v	23	GLU
1	a	261	GLN
2	b	373	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
16	V	34	GLN
2	b	53	ASN
4	d	332	GLN
13	O	104	GLN
13	o	36	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
4	HSK	D	336[B]	-	7,11,12	1.38	1 (14%)	3,14,16	1.69	1 (33%)
14	FME	T	1	14	8,9,10	0.50	0	7,9,11	1.30	2 (28%)
12	FME	M	1	12	8,9,10	0.83	0	7,9,11	1.95	3 (42%)
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	1.44	2 (28%)
8	FME	I	1	8	8,9,10	0.64	0	7,9,11	1.12	0
4	HSK	D	336[A]	-	7,10,12	1.05	1 (14%)	3,12,16	2.05	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	m	1	12	8,9,10	0.85	0	7,9,11	1.80	2 (28%)
8	FME	i	1	8	8,9,10	0.43	0	7,9,11	1.34	2 (28%)
4	HSK	d	336[A]	-	7,10,12	1.05	1 (14%)	3,12,16	1.51	0
4	HSK	d	336[B]	-	7,11,12	1.28	1 (14%)	3,14,16	1.52	1 (33%)

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
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	5/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	CE1-ND1	-3.25	1.32	1.36
4	d	336[B]	HSK	CE1-ND1	-2.98	1.33	1.36
4	D	336[A]	HSK	CE1-ND1	-2.46	1.33	1.36
4	d	336[A]	HSK	CE1-ND1	-2.37	1.33	1.36

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CE-SD-CG	2.94	110.49	100.40
12	M	1	FME	CG-CB-CA	2.82	120.80	112.95
12	m	1	FME	CG-CB-CA	2.79	120.69	112.95
12	M	1	FME	C-CA-N	-2.64	104.97	109.73
4	D	336[B]	HSK	CD2-NE2-CE1	2.46	109.62	105.78

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

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 276 ligands modelled in this entry, 43 are unknown and 15 are monoatomic - leaving 218 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	$\# Z  > 2$
27	LMG	A	413	-	51,51,55	0.99	2 (3%)	59,59,63	1.21	4 (6%)
25	BCR	a	415	-	41,41,41	1.22	3 (7%)	56,56,56	1.45	8 (14%)
30	LMT	M	102	-	36,36,36	0.63	0	47,47,47	1.34	6 (12%)
27	LMG	c	921	-	51,51,55	1.10	3 (5%)	59,59,63	1.22	6 (10%)
31	GOL	v	202	-	5,5,5	0.59	0	5,5,5	0.51	0
23	CLA	c	914	-	59,73,73	2.57	14 (23%)	67,113,113	1.88	18 (26%)
23	CLA	A	406	41	59,73,73	1.87	14 (23%)	67,113,113	2.51	27 (40%)
25	BCR	c	916	-	41,41,41	0.98	1 (2%)	56,56,56	1.40	7 (12%)
31	GOL	f	104	32	5,5,5	0.54	0	5,5,5	0.43	0
23	CLA	d	402	-	59,73,73	1.85	11 (18%)	67,113,113	2.20	19 (28%)
33	HTG	V	202	-	12,13,19	0.75	0	16,18,24	3.09	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DGD	c	918	-	63,63,67	1.00	4 (6%)	77,77,81	1.24	10 (12%)
23	CLA	b	618	-	59,73,73	2.17	13 (22%)	67,113,113	2.42	23 (34%)
33	HTG	D	414	-	19,19,19	1.08	2 (10%)	23,24,24	1.16	1 (4%)
31	GOL	a	422	-	5,5,5	0.67	0	5,5,5	0.78	0
30	LMT	B	623	-	36,36,36	1.00	2 (5%)	47,47,47	1.37	8 (17%)
31	GOL	l	102	-	5,5,5	0.48	0	5,5,5	1.00	0
25	BCR	K	101	-	41,41,41	0.90	0	56,56,56	1.68	12 (21%)
31	GOL	B	635	-	5,5,5	0.52	0	5,5,5	1.05	0
33	HTG	b	601	-	19,19,19	0.99	2 (10%)	23,24,24	1.31	3 (13%)
25	BCR	c	915	-	41,41,41	0.87	1 (2%)	56,56,56	1.25	6 (10%)
25	BCR	B	618	-	41,41,41	1.13	4 (9%)	56,56,56	1.58	10 (17%)
27	LMG	Z	101	-	51,51,55	1.10	3 (5%)	59,59,63	1.37	7 (11%)
28	PL9	D	405	-	55,55,55	1.34	7 (12%)	68,69,69	1.56	14 (20%)
23	CLA	d	403	-	59,73,73	2.14	16 (27%)	67,113,113	1.94	18 (26%)
26	SQD	B	621	-	53,54,54	1.13	4 (7%)	62,65,65	1.88	11 (17%)
30	LMT	z	101	-	32,32,36	0.70	1 (3%)	42,42,47	0.99	2 (4%)
25	BCR	b	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.74	14 (25%)
23	CLA	C	508	-	59,73,73	2.48	15 (25%)	67,113,113	1.88	18 (26%)
40	SO4	O	302	-	4,4,4	0.52	0	6,6,6	0.38	0
25	BCR	T	101	-	41,41,41	0.90	0	56,56,56	1.66	14 (25%)
25	BCR	k	102	-	41,41,41	0.99	2 (4%)	56,56,56	1.31	5 (8%)
23	CLA	b	617	-	59,73,73	1.78	13 (22%)	67,113,113	2.36	21 (31%)
33	HTG	d	401	-	19,19,19	1.08	2 (10%)	23,24,24	1.41	2 (8%)
34	DGD	C	518	-	63,63,67	0.78	3 (4%)	77,77,81	1.31	9 (11%)
36	LHG	L	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.53	7 (13%)
23	CLA	B	606	-	59,73,73	2.03	12 (20%)	67,113,113	1.95	17 (25%)
23	CLA	b	612	-	59,73,73	2.24	14 (23%)	67,113,113	1.88	15 (22%)
28	PL9	d	405	-	55,55,55	1.28	9 (16%)	68,69,69	1.59	14 (20%)
23	CLA	b	607	-	59,73,73	2.04	12 (20%)	67,113,113	2.38	18 (26%)
23	CLA	B	609	-	59,73,73	1.64	12 (20%)	67,113,113	2.23	19 (28%)
23	CLA	B	603	-	59,73,73	2.31	16 (27%)	67,113,113	1.86	21 (31%)
31	GOL	D	415	-	5,5,5	0.70	0	5,5,5	1.24	0
26	SQD	D	407	-	44,45,54	1.26	3 (6%)	53,56,65	2.15	15 (28%)
33	HTG	c	923	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	2 (8%)
31	GOL	V	203	-	5,5,5	1.00	0	5,5,5	0.81	0
27	LMG	c	920	-	51,51,55	1.12	4 (7%)	59,59,63	1.27	9 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	513	-	59,73,73	2.60	14 (23%)	67,113,113	2.09	19 (28%)
36	LHG	D	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.12	5 (9%)
31	GOL	A	422	-	5,5,5	0.43	0	5,5,5	0.48	0
38	RRX	h	101	-	42,42,42	0.97	0	57,58,58	1.31	8 (14%)
23	CLA	a	411	41	59,73,73	1.74	11 (18%)	67,113,113	2.28	24 (35%)
23	CLA	D	402	-	59,73,73	1.87	13 (22%)	67,113,113	2.25	25 (37%)
23	CLA	B	612	-	59,73,73	1.73	11 (18%)	67,113,113	2.39	20 (29%)
23	CLA	C	506	-	59,73,73	2.22	13 (22%)	67,113,113	2.20	19 (28%)
23	CLA	A	405	-	59,73,73	1.87	13 (22%)	67,113,113	2.03	22 (32%)
23	CLA	c	912	3	59,73,73	2.23	13 (22%)	67,113,113	2.40	22 (32%)
37	HEM	f	101	5,6	27,50,50	2.05	7 (25%)	17,82,82	2.66	6 (35%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.36	1 (20%)
31	GOL	A	423	32	5,5,5	0.32	0	5,5,5	0.77	0
34	DGD	c	919	-	63,63,67	1.05	6 (9%)	77,77,81	1.37	10 (12%)
23	CLA	C	511	3	59,73,73	2.40	15 (25%)	67,113,113	2.46	17 (25%)
23	CLA	c	908	41	59,73,73	2.24	18 (30%)	67,113,113	2.33	21 (31%)
25	BCR	K	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.68	11 (19%)
25	BCR	C	514	-	41,41,41	0.91	0	56,56,56	1.30	8 (14%)
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.07	4 (7%)
30	LMT	t	102	-	24,24,36	0.69	0	29,29,47	1.31	4 (13%)
23	CLA	b	608	-	59,73,73	1.79	11 (18%)	67,113,113	2.33	21 (31%)
24	PHO	a	413	-	67,69,69	1.97	15 (22%)	85,99,99	2.04	22 (25%)
23	CLA	B	616	-	59,73,73	2.35	13 (22%)	67,113,113	2.20	18 (26%)
23	CLA	b	611	-	59,73,73	2.06	15 (25%)	67,113,113	1.96	17 (25%)
33	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	2.16	3 (13%)
24	PHO	a	412	-	67,69,69	1.88	12 (17%)	85,99,99	1.92	19 (22%)
28	PL9	a	419	-	55,55,55	0.88	3 (5%)	68,69,69	1.77	17 (25%)
27	LMG	a	418	-	51,51,55	0.94	2 (3%)	59,59,63	1.33	5 (8%)
31	GOL	c	927	-	5,5,5	0.63	0	5,5,5	0.41	0
23	CLA	C	503	-	59,73,73	2.19	15 (25%)	67,113,113	1.92	15 (22%)
30	LMT	b	625	-	24,24,36	0.54	0	29,29,47	1.24	4 (13%)
23	CLA	C	512	-	59,73,73	2.38	13 (22%)	67,113,113	2.11	20 (29%)
25	BCR	B	619	-	41,41,41	1.19	4 (9%)	56,56,56	1.23	6 (10%)
31	GOL	h	103	-	5,5,5	0.37	0	5,5,5	0.26	0
23	CLA	B	604	-	59,73,73	2.00	12 (20%)	67,113,113	2.50	21 (31%)
35	BCT	a	408	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LMT	Z	102	-	36,36,36	0.68	1 (2%)	47,47,47	0.89	0
31	GOL	c	928	-	5,5,5	0.21	0	5,5,5	0.80	0
24	PHO	A	409	-	67,69,69	1.90	14 (20%)	85,99,99	2.16	23 (27%)
23	CLA	b	605	-	59,73,73	2.07	11 (18%)	67,113,113	2.16	22 (32%)
23	CLA	A	410	-	59,73,73	1.84	12 (20%)	67,113,113	2.07	15 (22%)
31	GOL	b	634	-	5,5,5	0.50	0	5,5,5	0.22	0
23	CLA	a	409	-	59,73,73	1.96	12 (20%)	67,113,113	1.98	19 (28%)
31	GOL	v	203	-	5,5,5	0.73	0	5,5,5	0.48	0
23	CLA	B	602	41	59,73,73	2.31	15 (25%)	67,113,113	2.44	20 (29%)
31	GOL	L	104	-	5,5,5	0.51	0	5,5,5	0.59	0
23	CLA	c	902	-	59,73,73	2.10	15 (25%)	67,113,113	2.27	17 (25%)
31	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.68	0
30	LMT	m	102	-	36,36,36	0.73	1 (2%)	47,47,47	1.06	3 (6%)
23	CLA	C	502	-	59,73,73	1.92	11 (18%)	67,113,113	2.02	19 (28%)
30	LMT	a	402	-	36,36,36	0.77	1 (2%)	47,47,47	1.59	9 (19%)
23	CLA	a	414	-	59,73,73	1.86	12 (20%)	67,113,113	2.37	23 (34%)
23	CLA	B	605	-	59,73,73	1.84	10 (16%)	67,113,113	2.13	20 (29%)
36	LHG	D	408	-	48,48,48	0.79	1 (2%)	51,54,54	1.47	6 (11%)
23	CLA	c	904	-	59,73,73	2.51	15 (25%)	67,113,113	2.23	22 (32%)
26	SQD	L	103	-	53,54,54	1.10	2 (3%)	62,65,65	1.74	12 (19%)
23	CLA	b	619	-	59,73,73	2.09	13 (22%)	67,113,113	2.22	20 (29%)
23	CLA	B	607	-	59,73,73	2.32	12 (20%)	67,113,113	2.29	20 (29%)
23	CLA	b	616	-	59,73,73	1.96	11 (18%)	67,113,113	2.17	19 (28%)
33	HTG	U	201	-	8,8,19	0.29	0	7,7,24	1.26	1 (14%)
31	GOL	C	526	-	5,5,5	0.67	0	5,5,5	0.49	0
31	GOL	B	636	-	5,5,5	0.47	0	5,5,5	0.72	0
25	BCR	k	101	-	41,41,41	0.85	0	56,56,56	1.47	11 (19%)
31	GOL	V	205	-	5,5,5	0.65	0	5,5,5	0.31	0
33	HTG	b	602	-	19,19,19	0.78	1 (5%)	23,24,24	1.18	2 (8%)
23	CLA	A	407	41	59,73,73	2.10	11 (18%)	67,113,113	2.17	18 (26%)
30	LMT	m	101	-	36,36,36	0.75	0	47,47,47	1.37	8 (17%)
31	GOL	A	421	-	5,5,5	0.89	0	5,5,5	0.51	0
23	CLA	c	911	-	59,73,73	2.08	14 (23%)	67,113,113	1.82	18 (26%)
34	DGD	c	917	-	63,63,67	0.90	4 (6%)	77,77,81	1.28	9 (11%)
23	CLA	C	507	41	59,73,73	2.36	14 (23%)	67,113,113	2.17	16 (23%)
36	LHG	d	407	-	48,48,48	0.80	2 (4%)	51,54,54	1.39	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	LHG	l	101	-	48,48,48	0.84	2 (4%)	51,54,54	1.11	5 (9%)
26	SQD	A	412	-	53,54,54	0.94	3 (5%)	62,65,65	2.24	17 (27%)
28	PL9	A	414	-	55,55,55	0.94	3 (5%)	68,69,69	1.48	11 (16%)
23	CLA	c	909	-	59,73,73	2.39	15 (25%)	67,113,113	2.05	18 (26%)
25	BCR	t	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.83	14 (25%)
23	CLA	B	613	-	59,73,73	2.19	16 (27%)	67,113,113	1.99	20 (29%)
31	GOL	c	930	-	5,5,5	0.45	0	5,5,5	0.68	0
24	PHO	A	408	-	67,69,69	1.72	11 (16%)	85,99,99	2.14	21 (24%)
23	CLA	B	608	41	59,73,73	2.13	17 (28%)	67,113,113	2.00	22 (32%)
33	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.79	3 (13%)
23	CLA	b	606	-	59,73,73	1.94	11 (18%)	67,113,113	2.29	20 (29%)
34	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.05	3 (3%)
34	DGD	H	102	-	63,63,67	1.12	3 (4%)	77,77,81	1.37	13 (16%)
23	CLA	b	609	-	59,73,73	2.43	17 (28%)	67,113,113	2.29	18 (26%)
30	LMT	c	922	-	36,36,36	0.75	1 (2%)	47,47,47	0.96	3 (6%)
26	SQD	a	401	-	53,54,54	1.17	3 (5%)	62,65,65	1.59	9 (14%)
30	LMT	b	624	-	25,25,36	0.75	1 (4%)	30,30,47	1.38	5 (16%)
31	GOL	b	635	-	5,5,5	0.79	0	5,5,5	0.88	0
27	LMG	d	410	39	51,51,55	1.01	3 (5%)	59,59,63	1.14	7 (11%)
27	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.61	9 (15%)
26	SQD	A	418	-	53,54,54	1.13	3 (5%)	62,65,65	1.66	12 (19%)
36	LHG	d	408	-	48,48,48	0.78	2 (4%)	51,54,54	1.32	9 (17%)
23	CLA	c	907	-	59,73,73	1.91	13 (22%)	67,113,113	2.04	19 (28%)
34	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.37	12 (15%)
33	HTG	B	630	-	19,19,19	1.07	2 (10%)	23,24,24	1.54	3 (13%)
23	CLA	c	910	-	59,73,73	2.33	14 (23%)	67,113,113	2.24	24 (35%)
25	BCR	d	404	-	41,41,41	1.01	3 (7%)	56,56,56	1.81	16 (28%)
34	DGD	D	406	-	53,53,67	1.20	3 (5%)	60,61,81	1.39	8 (13%)
23	CLA	c	906	-	59,73,73	1.98	16 (27%)	67,113,113	2.12	20 (29%)
31	GOL	b	633	-	5,5,5	0.38	0	5,5,5	0.89	0
23	CLA	b	613	41	59,73,73	2.05	13 (22%)	67,113,113	2.13	15 (22%)
23	CLA	b	614	-	59,73,73	2.02	12 (20%)	67,113,113	2.17	21 (31%)
33	HTG	B	624	-	19,19,19	1.15	1 (5%)	23,24,24	1.44	5 (21%)
33	HTG	B	631	-	19,19,19	0.84	2 (10%)	23,24,24	1.88	3 (13%)
30	LMT	F	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.18	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	617	-	59,73,73	1.86	14 (23%)	67,113,113	2.05	16 (23%)
23	CLA	a	410	41	59,73,73	1.87	13 (22%)	67,113,113	2.00	17 (25%)
25	BCR	D	404	-	41,41,41	1.17	3 (7%)	56,56,56	2.05	18 (32%)
31	GOL	B	634	-	5,5,5	0.84	0	5,5,5	0.66	0
26	SQD	a	416	-	53,54,54	0.96	3 (5%)	62,65,65	2.26	14 (22%)
25	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
35	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	615	-	59,73,73	2.11	13 (22%)	67,113,113	2.09	18 (26%)
36	LHG	D	410	-	45,45,48	1.02	2 (4%)	48,51,54	1.05	3 (6%)
20	OEX	A	401	1,3,41	0,15,15	0.00	-	-	-	-
27	LMG	b	623	-	51,51,55	0.86	2 (3%)	59,59,63	1.46	7 (11%)
25	BCR	A	411	-	41,41,41	1.04	0	56,56,56	1.49	11 (19%)
25	BCR	b	622	-	41,41,41	0.97	2 (4%)	56,56,56	1.26	6 (10%)
20	OEX	a	404	1,3,41	0,15,15	0.00	-	-	-	-
30	LMT	M	101	-	36,36,36	0.87	1 (2%)	47,47,47	1.22	6 (12%)
25	BCR	C	515	-	41,41,41	0.94	1 (2%)	56,56,56	1.45	5 (8%)
31	GOL	B	638	-	5,5,5	0.51	0	5,5,5	0.86	0
23	CLA	D	403	-	59,73,73	2.21	14 (23%)	67,113,113	1.99	18 (26%)
33	HTG	B	625	-	19,19,19	0.98	1 (5%)	23,24,24	1.46	4 (17%)
37	HEM	v	201	16	27,50,50	2.26	7 (25%)	17,82,82	2.14	6 (35%)
37	HEM	F	101	5,6	27,50,50	2.14	9 (33%)	17,82,82	2.72	6 (35%)
31	GOL	V	204	-	5,5,5	0.31	0	5,5,5	0.43	0
23	CLA	b	610	41	59,73,73	2.16	11 (18%)	67,113,113	1.89	18 (26%)
31	GOL	a	423	-	5,5,5	0.57	0	5,5,5	0.58	0
30	LMT	A	419	-	36,36,36	0.84	1 (2%)	47,47,47	1.33	5 (10%)
33	HTG	C	521	-	19,19,19	0.91	2 (10%)	23,24,24	1.37	1 (4%)
23	CLA	c	903	-	59,73,73	2.06	11 (18%)	67,113,113	2.16	20 (29%)
31	GOL	b	632	-	5,5,5	0.53	0	5,5,5	1.30	0
33	HTG	b	627	-	19,19,19	1.14	2 (10%)	23,24,24	1.60	1 (4%)
23	CLA	C	510	-	59,73,73	2.10	12 (20%)	67,113,113	2.10	15 (22%)
31	GOL	C	525	-	5,5,5	0.81	0	5,5,5	0.88	0
38	RRX	H	101	-	42,42,42	1.10	3 (7%)	57,58,58	1.63	11 (19%)
23	CLA	C	505	-	59,73,73	1.96	13 (22%)	67,113,113	1.92	16 (23%)
31	GOL	c	929	-	5,5,5	0.53	0	5,5,5	0.85	0
23	CLA	b	604	41	59,73,73	2.34	15 (25%)	67,113,113	2.23	16 (23%)
31	GOL	B	637	-	5,5,5	0.47	0	5,5,5	1.09	0
36	LHG	a	417	-	39,39,48	1.17	2 (5%)	42,45,54	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	610	-	59,73,73	1.81	12 (20%)	67,113,113	2.15	18 (26%)
23	CLA	C	509	-	59,73,73	2.15	13 (22%)	67,113,113	2.10	18 (26%)
31	GOL	O	304	-	5,5,5	0.54	0	5,5,5	0.59	0
26	SQD	f	102	-	31,32,54	1.97	4 (12%)	34,36,65	1.64	5 (14%)
33	HTG	u	201	-	10,13,19	0.81	1 (10%)	13,14,24	1.92	2 (15%)
25	BCR	b	621	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
27	LMG	D	411	39	51,51,55	0.86	2 (3%)	59,59,63	1.03	2 (3%)
33	HTG	b	626	-	19,19,19	1.01	1 (5%)	23,24,24	1.38	3 (13%)
33	HTG	O	303	-	19,19,19	1.17	2 (10%)	23,24,24	1.32	1 (4%)
34	DGD	h	102	-	63,63,67	0.99	3 (4%)	77,77,81	1.28	11 (14%)
31	GOL	C	524	-	5,5,5	0.34	0	5,5,5	1.56	1 (20%)
23	CLA	C	501	-	59,73,73	1.86	14 (23%)	67,113,113	2.53	18 (26%)
33	HTG	c	924	-	19,19,19	1.00	1 (5%)	23,24,24	2.28	5 (21%)
23	CLA	b	615	-	59,73,73	2.17	12 (20%)	67,113,113	2.45	17 (25%)
31	GOL	a	424	-	5,5,5	0.65	0	5,5,5	0.76	0
23	CLA	C	504	41	59,73,73	2.06	14 (23%)	67,113,113	2.09	17 (25%)
23	CLA	B	611	41	59,73,73	2.01	13 (22%)	67,113,113	2.17	19 (28%)
31	GOL	b	636	-	5,5,5	0.57	0	5,5,5	0.98	0
27	LMG	C	519	-	51,51,55	1.02	3 (5%)	59,59,63	1.47	9 (15%)
37	HEM	V	201	16	27,50,50	2.27	11 (40%)	17,82,82	2.34	7 (41%)
23	CLA	c	905	41	59,73,73	2.34	15 (25%)	67,113,113	2.12	18 (26%)
30	LMT	J	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.13	2 (6%)
34	DGD	d	406	-	50,50,67	1.19	3 (6%)	58,58,81	1.37	8 (13%)
30	LMT	C	520	-	36,36,36	0.62	1 (2%)	47,47,47	1.46	6 (12%)
23	CLA	c	913	-	59,73,73	2.44	15 (25%)	67,113,113	2.00	19 (28%)
36	LHG	E	101	-	48,48,48	1.01	2 (4%)	51,54,54	0.93	1 (1%)
23	CLA	B	614	-	59,73,73	1.92	14 (23%)	67,113,113	1.76	17 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	A	413	-	-	26/46/66/70	0/1/1/1
25	BCR	a	415	-	-	1/29/63/63	0/2/2/2
30	LMT	M	102	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	921	-	-	13/46/66/70	0/1/1/1
31	GOL	v	202	-	-	0/4/4/4	-
23	CLA	c	914	-	2/2/20/25	11/37/135/135	-
23	CLA	A	406	41	1/1/20/25	6/37/135/135	-
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
31	GOL	f	104	32	-	2/4/4/4	-
23	CLA	d	402	-	2/2/20/25	2/37/135/135	-
33	HTG	V	202	-	-	2/4/24/30	0/1/1/1
34	DGD	c	918	-	-	22/51/91/95	0/2/2/2
23	CLA	b	618	-	3/3/20/25	9/37/135/135	-
33	HTG	D	414	-	-	2/10/30/30	0/1/1/1
31	GOL	a	422	-	-	0/4/4/4	-
30	LMT	B	623	-	-	12/21/61/61	0/2/2/2
31	GOL	l	102	-	-	0/4/4/4	-
25	BCR	K	101	-	-	3/29/63/63	0/2/2/2
31	GOL	B	635	-	-	4/4/4/4	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
25	BCR	c	915	-	-	6/29/63/63	0/2/2/2
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
27	LMG	Z	101	-	-	25/46/66/70	0/1/1/1
28	PL9	D	405	-	-	1/53/73/73	0/1/1/1
23	CLA	C	512	-	3/3/20/25	9/37/135/135	-
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
23	CLA	C	508	-	2/2/20/25	7/37/135/135	-
30	LMT	t	102	-	-	8/15/35/61	0/1/1/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
23	CLA	b	617	-	3/3/20/25	18/37/135/135	-
33	HTG	d	401	-	-	5/10/30/30	0/1/1/1
34	DGD	C	518	-	-	14/51/91/95	0/2/2/2
36	LHG	L	101	-	-	10/53/53/53	-
23	CLA	B	606	-	3/3/20/25	6/37/135/135	-
23	CLA	b	612	-	1/1/20/25	0/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	d	405	-	-	5/53/73/73	0/1/1/1
23	CLA	b	607	-	3/3/20/25	7/37/135/135	-
23	CLA	B	609	-	1/1/20/25	1/37/135/135	-
23	CLA	B	603	-	2/2/20/25	4/37/135/135	-
31	GOL	D	415	-	-	2/4/4/4	-
26	SQD	D	407	-	-	13/40/60/69	0/1/1/1
33	HTG	c	923	-	-	4/10/30/30	0/1/1/1
31	GOL	V	203	-	-	2/4/4/4	-
27	LMG	c	920	-	-	18/46/66/70	0/1/1/1
23	CLA	C	513	-	1/1/20/25	13/37/135/135	-
36	LHG	D	409	-	-	13/53/53/53	-
31	GOL	A	422	-	-	0/4/4/4	-
38	RRX	h	101	-	-	2/29/65/65	0/2/2/2
23	CLA	a	411	41	2/2/20/25	6/37/135/135	-
23	CLA	D	402	-	1/1/20/25	7/37/135/135	-
23	CLA	B	612	-	2/2/20/25	2/37/135/135	-
23	CLA	C	506	-	2/2/20/25	13/37/135/135	-
23	CLA	A	405	-	3/3/20/25	3/37/135/135	-
23	CLA	c	912	3	1/1/20/25	7/37/135/135	-
37	HEM	f	101	5,6	-	0/6/54/54	-
31	GOL	B	633	-	-	2/4/4/4	-
31	GOL	A	423	32	-	0/4/4/4	-
34	DGD	c	919	-	-	16/51/91/95	0/2/2/2
23	CLA	C	511	3	3/3/20/25	0/37/135/135	-
23	CLA	c	908	41	3/3/20/25	7/37/135/135	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	c	911	-	3/3/20/25	9/37/135/135	-
36	LHG	d	409	-	-	16/53/53/53	-
23	CLA	b	613	41	3/3/20/25	4/37/135/135	-
23	CLA	b	608	-	3/3/20/25	4/37/135/135	-
24	PHO	a	413	-	-	4/53/103/103	0/5/6/6
23	CLA	B	616	-	3/3/20/25	5/37/135/135	-
23	CLA	b	611	-	1/1/20/25	1/37/135/135	-
33	HTG	C	522	-	-	4/10/30/30	0/1/1/1
24	PHO	a	412	-	-	2/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	a	419	-	-	11/53/73/73	0/1/1/1
27	LMG	a	418	-	-	20/46/66/70	0/1/1/1
31	GOL	c	927	-	-	2/4/4/4	-
23	CLA	C	503	-	3/3/20/25	1/37/135/135	-
30	LMT	b	625	-	-	11/15/35/61	0/1/1/2
23	CLA	d	403	-	1/1/20/25	9/37/135/135	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	GOL	h	103	-	-	1/4/4/4	-
23	CLA	B	604	-	3/3/20/25	5/37/135/135	-
30	LMT	Z	102	-	-	13/21/61/61	0/2/2/2
31	GOL	c	928	-	-	1/4/4/4	-
24	PHO	A	409	-	-	5/53/103/103	0/5/6/6
23	CLA	b	605	-	3/3/20/25	4/37/135/135	-
25	BCR	B	620	-	-	1/29/63/63	0/2/2/2
23	CLA	A	410	-	1/1/20/25	14/37/135/135	-
31	GOL	b	634	-	-	0/4/4/4	-
23	CLA	a	409	-	3/3/20/25	5/37/135/135	-
31	GOL	v	203	-	-	2/4/4/4	-
23	CLA	B	602	41	2/2/20/25	20/37/135/135	-
31	GOL	L	104	-	-	2/4/4/4	-
23	CLA	c	902	-	3/3/20/25	4/37/135/135	-
31	GOL	v	204	-	-	0/4/4/4	-
30	LMT	m	102	-	-	6/21/61/61	0/2/2/2
23	CLA	C	502	-	2/2/20/25	7/37/135/135	-
30	LMT	a	402	-	-	11/21/61/61	0/2/2/2
23	CLA	a	414	-	1/1/20/25	12/37/135/135	-
23	CLA	B	605	-	3/3/20/25	7/37/135/135	-
36	LHG	D	408	-	-	9/53/53/53	-
23	CLA	c	904	-	1/1/20/25	2/37/135/135	-
26	SQD	L	103	-	-	28/49/69/69	0/1/1/1
23	CLA	b	619	-	3/3/20/25	7/37/135/135	-
23	CLA	C	505	-	1/1/20/25	4/37/135/135	-
23	CLA	b	616	-	3/3/20/25	2/37/135/135	-
33	HTG	U	201	-	-	4/6/6/30	-
31	GOL	C	526	-	-	0/4/4/4	-
31	GOL	B	636	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
31	GOL	V	205	-	-	0/4/4/4	-
23	CLA	A	407	41	2/2/20/25	7/37/135/135	-
30	LMT	m	101	-	-	3/21/61/61	0/2/2/2
31	GOL	A	421	-	-	0/4/4/4	-
25	BCR	C	514	-	-	3/29/63/63	0/2/2/2
34	DGD	c	917	-	-	14/51/91/95	0/2/2/2
36	LHG	d	407	-	-	6/53/53/53	-
36	LHG	l	101	-	-	17/53/53/53	-
26	SQD	A	412	-	-	18/49/69/69	0/1/1/1
28	PL9	A	414	-	-	12/53/73/73	0/1/1/1
23	CLA	c	909	-	2/2/20/25	3/37/135/135	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/20/25	3/37/135/135	-
31	GOL	c	930	-	-	4/4/4/4	-
24	PHO	A	408	-	-	3/53/103/103	0/5/6/6
23	CLA	B	608	41	3/3/20/25	1/37/135/135	-
33	HTG	B	626	-	-	5/10/30/30	0/1/1/1
23	CLA	b	606	-	3/3/20/25	4/37/135/135	-
34	DGD	C	517	-	-	23/51/91/95	0/2/2/2
34	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	b	609	-	2/2/20/25	12/37/135/135	-
30	LMT	c	922	-	-	4/21/61/61	0/2/2/2
26	SQD	a	401	-	-	23/49/69/69	0/1/1/1
30	LMT	b	624	-	-	10/17/37/61	0/1/1/2
31	GOL	b	635	-	-	1/4/4/4	-
27	LMG	d	410	39	-	10/46/66/70	0/1/1/1
27	LMG	B	622	-	-	15/46/66/70	0/1/1/1
26	SQD	A	418	-	-	17/49/69/69	0/1/1/1
36	LHG	d	408	-	-	10/53/53/53	-
23	CLA	c	907	-	2/2/20/25	14/37/135/135	-
34	DGD	C	516	-	-	16/51/91/95	0/2/2/2
33	HTG	B	630	-	-	4/10/30/30	0/1/1/1
23	CLA	c	910	-	3/3/20/25	13/37/135/135	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	D	406	-	-	26/47/68/95	0/1/1/2
23	CLA	c	906	-	1/1/20/25	7/37/135/135	-
31	GOL	b	633	-	-	3/4/4/4	-
23	CLA	b	614	-	2/2/20/25	6/37/135/135	-
33	HTG	B	624	-	-	2/10/30/30	0/1/1/1
33	HTG	B	631	-	-	5/10/30/30	0/1/1/1
30	LMT	F	102	-	-	11/21/61/61	0/2/2/2
23	CLA	B	617	-	3/3/20/25	16/37/135/135	-
23	CLA	a	410	41	3/3/20/25	5/37/135/135	-
25	BCR	D	404	-	-	2/29/63/63	0/2/2/2
31	GOL	B	634	-	-	0/4/4/4	-
26	SQD	a	416	-	-	20/49/69/69	0/1/1/1
23	CLA	C	507	41	3/3/20/25	11/37/135/135	-
23	CLA	B	615	-	3/3/20/25	13/37/135/135	-
36	LHG	D	410	-	-	13/50/50/53	-
33	HTG	b	602	-	-	1/10/30/30	0/1/1/1
31	GOL	B	637	-	-	0/4/4/4	-
27	LMG	b	623	-	-	19/46/66/70	0/1/1/1
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
30	LMT	M	101	-	-	7/21/61/61	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	GOL	B	638	-	-	2/4/4/4	-
23	CLA	D	403	-	3/3/20/25	15/37/135/135	-
33	HTG	B	625	-	-	4/10/30/30	0/1/1/1
37	HEM	v	201	16	-	0/6/54/54	-
37	HEM	F	101	5,6	-	0/6/54/54	-
31	GOL	V	204	-	-	0/4/4/4	-
23	CLA	b	610	41	3/3/20/25	2/37/135/135	-
31	GOL	a	423	-	-	2/4/4/4	-
23	CLA	b	604	41	2/2/20/25	15/37/135/135	-
33	HTG	C	521	-	-	3/10/30/30	0/1/1/1
23	CLA	c	903	-	3/3/20/25	7/37/135/135	-
31	GOL	b	632	-	-	4/4/4/4	-
33	HTG	b	627	-	-	5/10/30/30	0/1/1/1
23	CLA	C	510	-	3/3/20/25	2/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	C	525	-	-	0/4/4/4	-
38	RRX	H	101	-	-	2/29/65/65	0/2/2/2
23	CLA	B	607	-	3/3/20/25	8/37/135/135	-
31	GOL	c	929	-	-	0/4/4/4	-
30	LMT	A	419	-	-	5/21/61/61	0/2/2/2
23	CLA	B	611	41	3/3/20/25	8/37/135/135	-
36	LHG	a	417	-	-	28/44/44/53	-
23	CLA	B	610	-	2/2/20/25	4/37/135/135	-
23	CLA	C	509	-	3/3/20/25	7/37/135/135	-
31	GOL	O	304	-	-	3/4/4/4	-
26	SQD	f	102	-	-	13/33/33/69	-
33	HTG	u	201	-	-	6/12/14/30	-
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	LMG	D	411	39	-	9/46/66/70	0/1/1/1
33	HTG	b	626	-	-	4/10/30/30	0/1/1/1
33	HTG	O	303	-	-	3/10/30/30	0/1/1/1
34	DGD	h	102	-	-	9/51/91/95	0/2/2/2
31	GOL	C	524	-	-	2/4/4/4	-
23	CLA	C	501	-	3/3/20/25	4/37/135/135	-
33	HTG	c	924	-	-	1/10/30/30	0/1/1/1
23	CLA	b	615	-	3/3/20/25	7/37/135/135	-
31	GOL	a	424	-	-	3/4/4/4	-
23	CLA	C	504	41	3/3/20/25	11/37/135/135	-
31	GOL	b	636	-	-	2/4/4/4	-
27	LMG	C	519	-	-	22/46/66/70	0/1/1/1
37	HEM	V	201	16	-	0/6/54/54	-
23	CLA	c	905	41	3/3/20/25	11/37/135/135	-
30	LMT	J	102	-	-	7/15/35/61	0/1/1/2
34	DGD	d	406	-	-	27/44/64/95	0/1/1/2
30	LMT	C	520	-	-	10/21/61/61	0/2/2/2
23	CLA	c	913	-	3/3/20/25	10/37/135/135	-
36	LHG	E	101	-	-	27/53/53/53	-
23	CLA	B	614	-	3/3/20/25	7/37/135/135	-

The worst 5 of 1219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NA	12.57	2.36	2.06
23	c	914	CLA	MG-NC	11.74	2.34	2.06
23	C	512	CLA	MG-NA	11.26	2.33	2.06
23	C	511	CLA	MG-NA	11.02	2.32	2.06
23	B	616	CLA	MG-NA	10.89	2.32	2.06

The worst 5 of 2148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	13.25	112.67	106.71
23	b	609	CLA	C4A-NA-C1A	11.92	112.06	106.71
23	c	904	CLA	C4A-NA-C1A	10.61	111.48	106.71
23	C	501	CLA	O2D-CGD-O1D	-10.49	103.33	123.84
23	c	902	CLA	C4A-NA-C1A	10.12	111.25	106.71

5 of 168 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	914	CLA	NC
23	c	914	CLA	NA
23	A	406	CLA	NA
23	d	402	CLA	ND
23	d	402	CLA	NA

5 of 1486 torsion outliers are listed below:

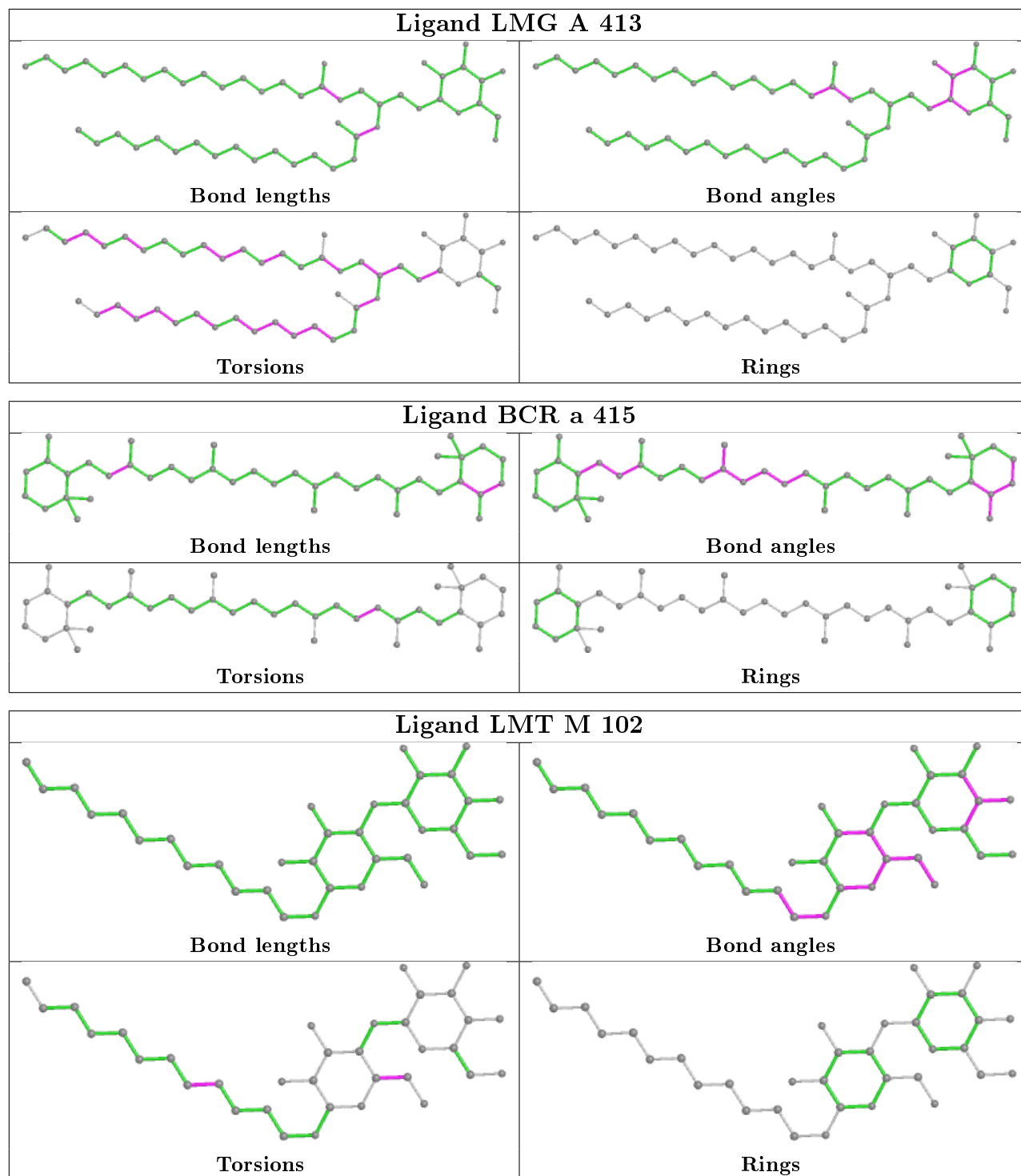
Mol	Chain	Res	Type	Atoms
33	V	202	HTG	C2-C1-S1-C1'
33	V	202	HTG	O5-C1-S1-C1'
30	B	623	LMT	C2-C1-O1'-C1'
36	L	101	LHG	C4-O6-P-O4
26	B	621	SQD	C5-C6-S-O8

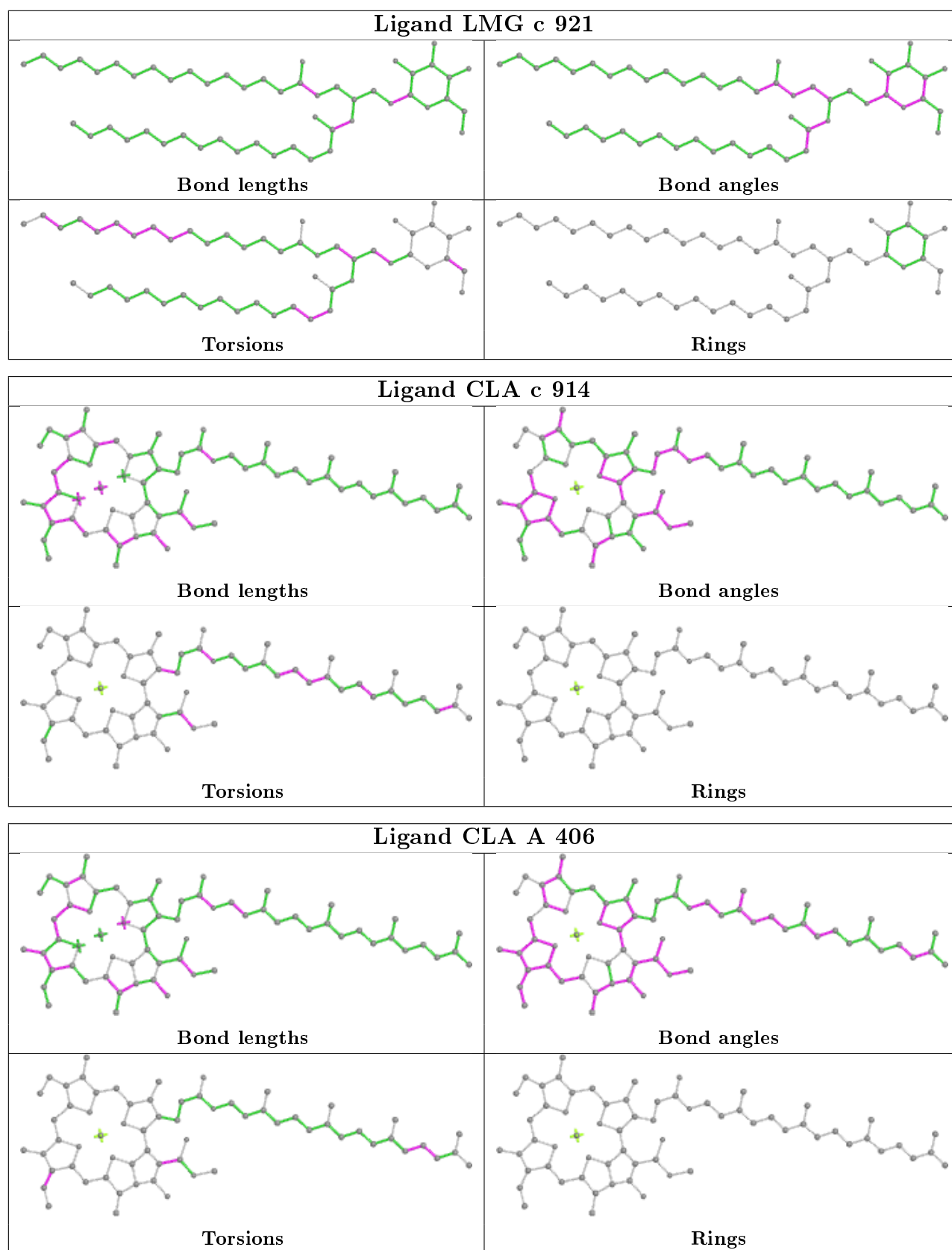
There are no ring outliers.

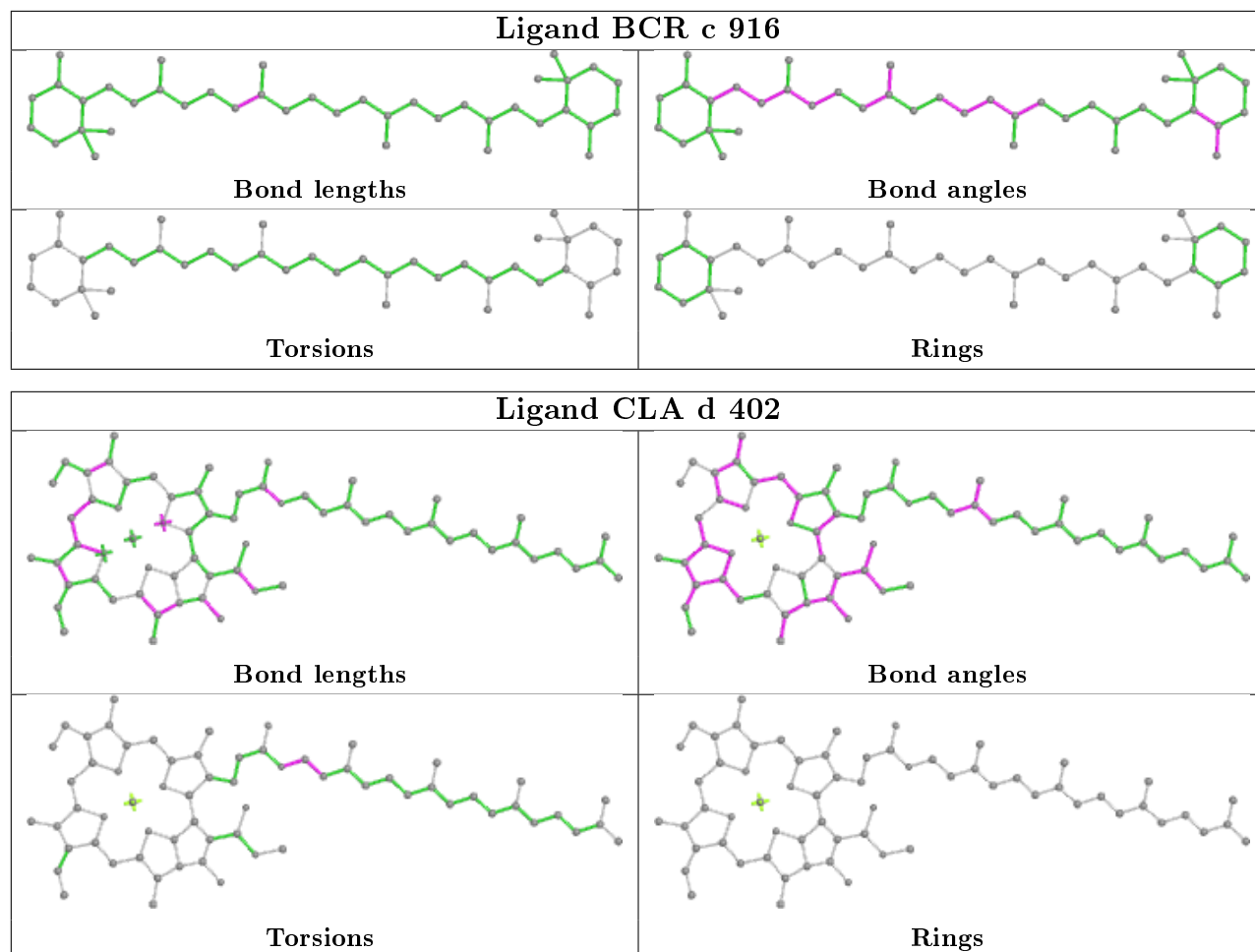
No monomer is involved in short contacts.

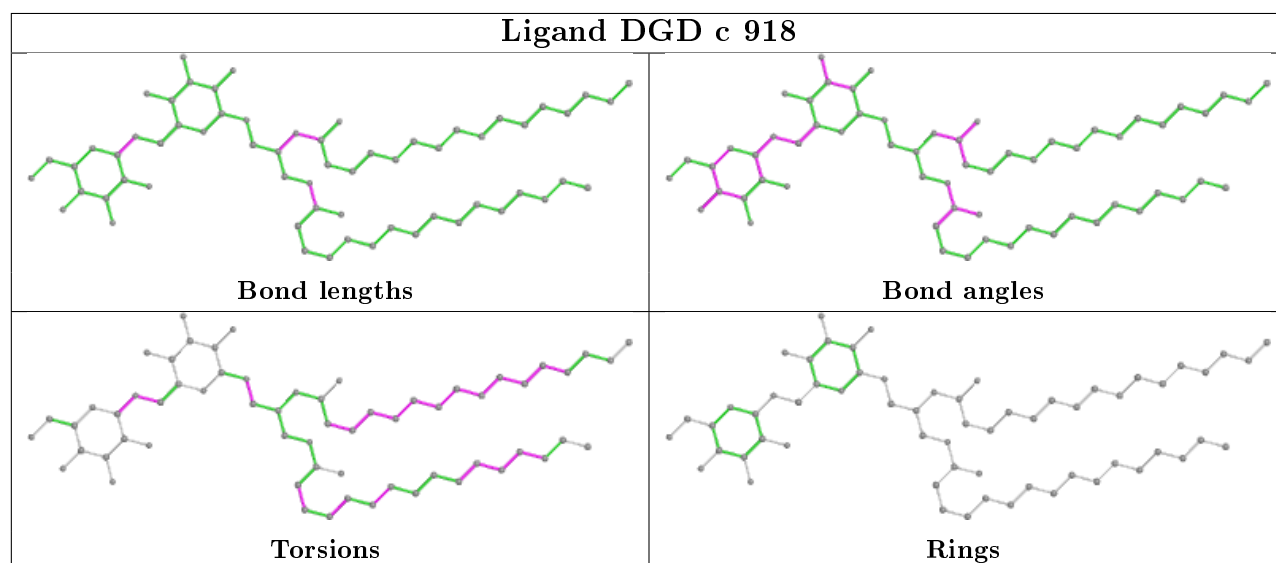
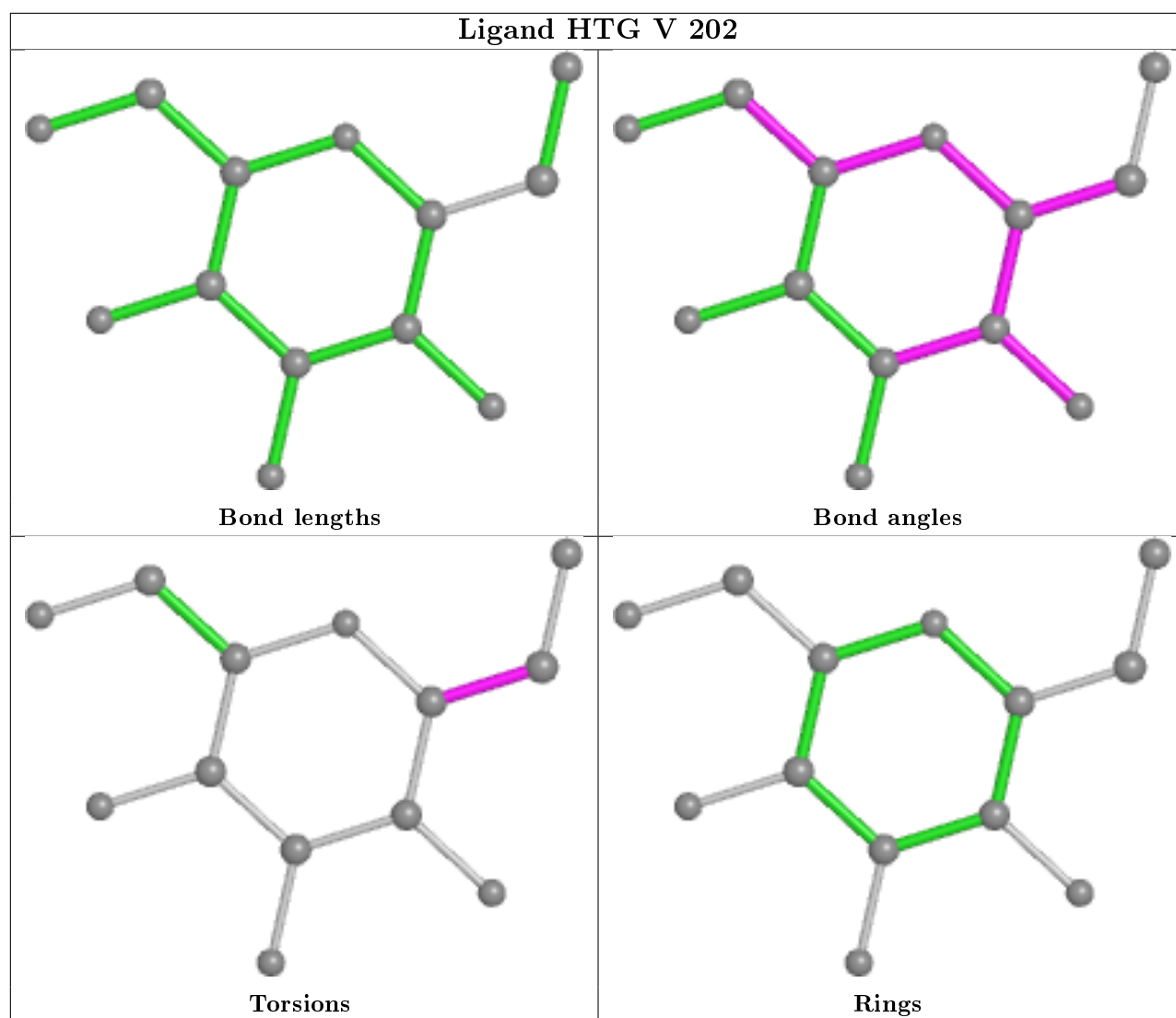
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



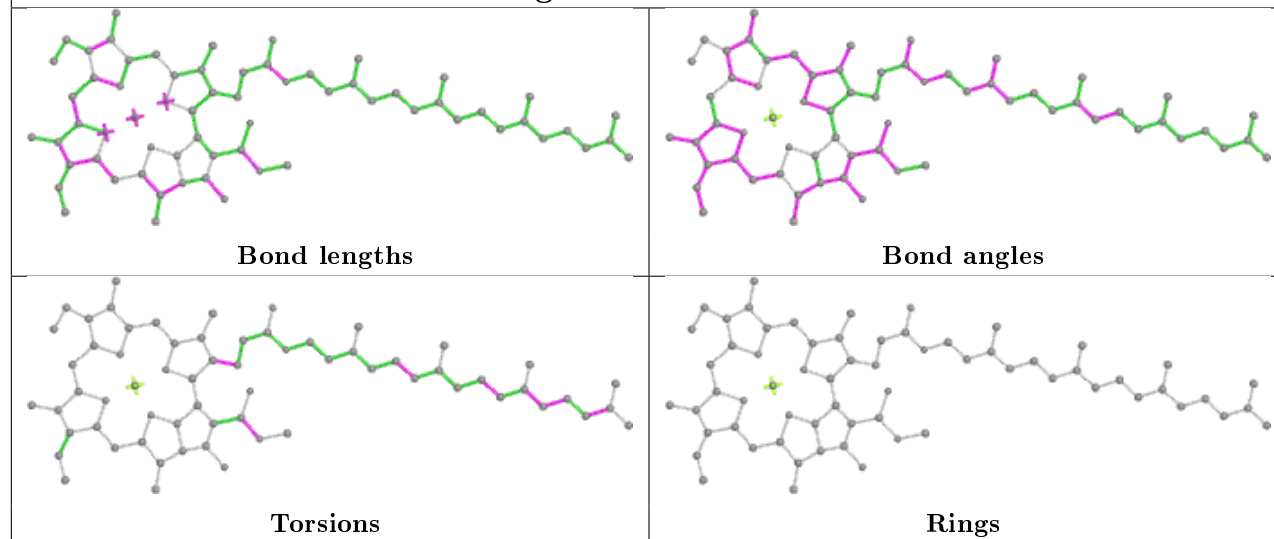




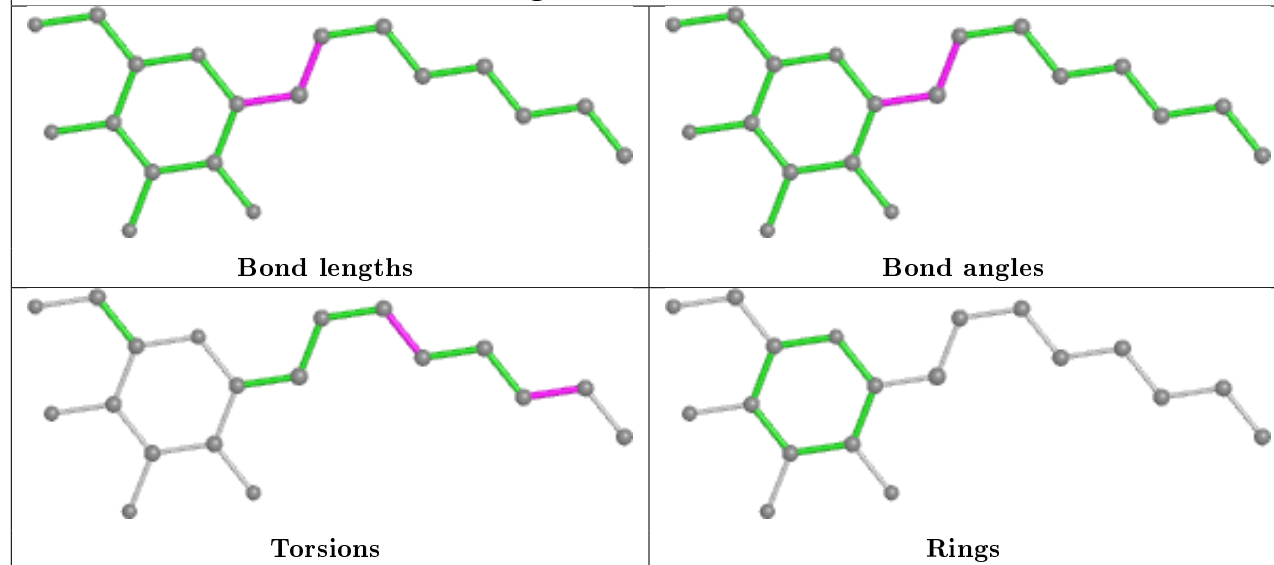




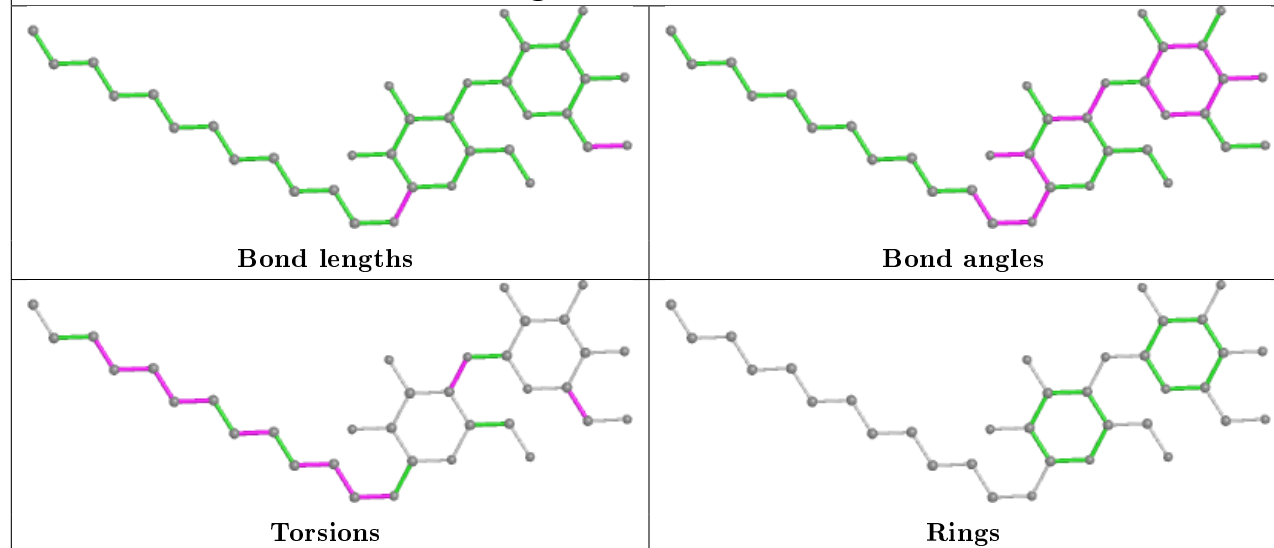
## Ligand CLA b 618

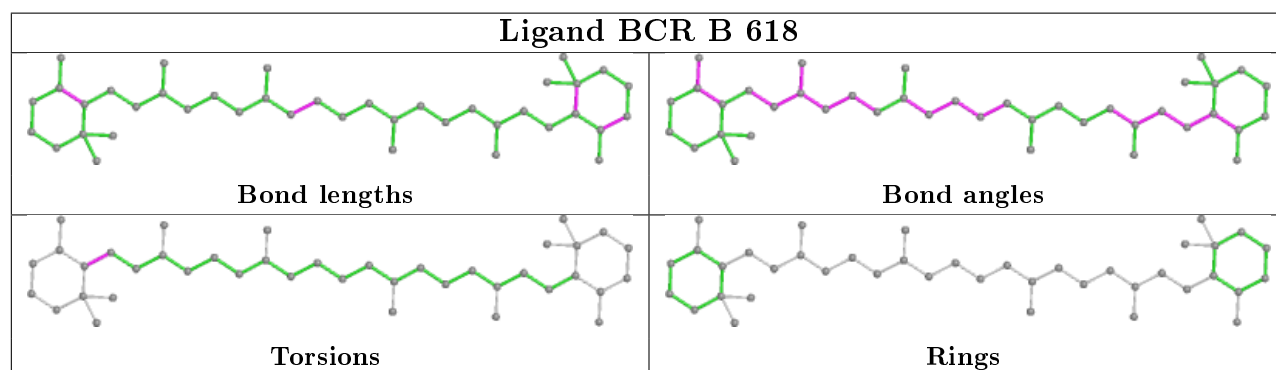
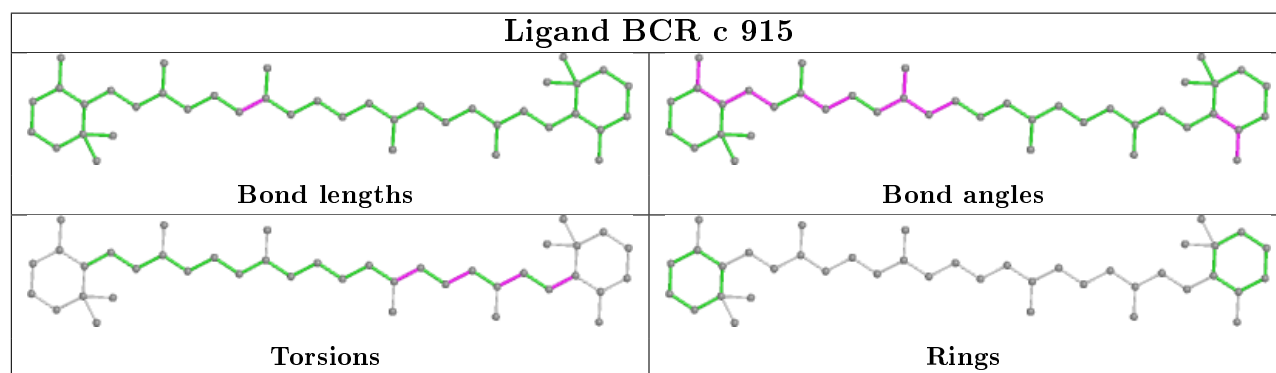
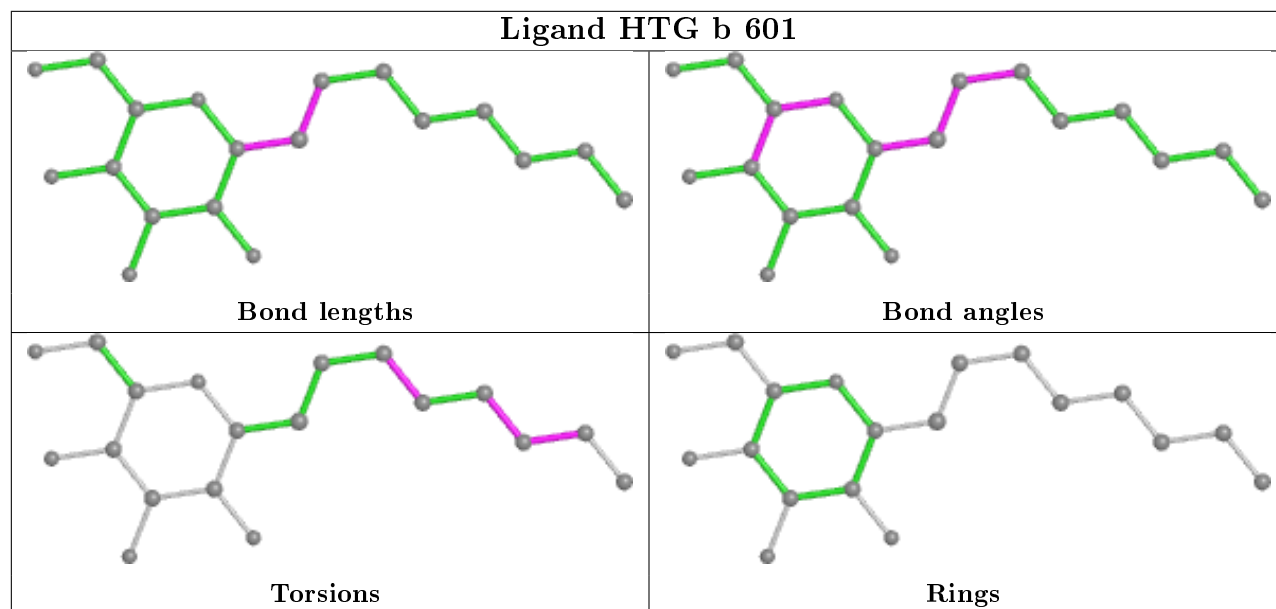
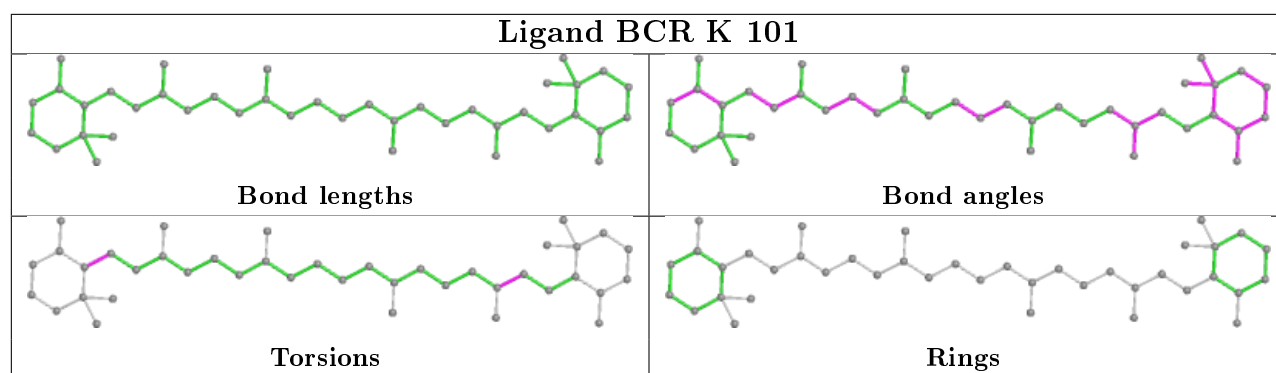


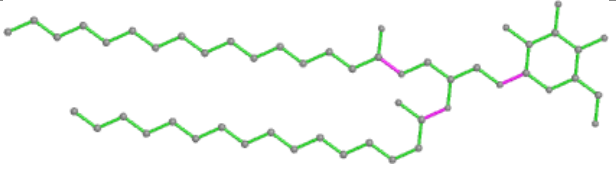
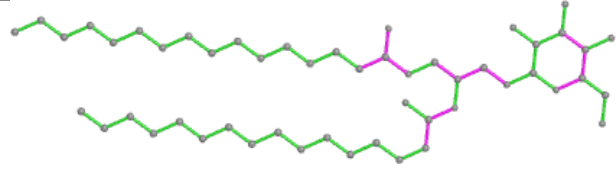
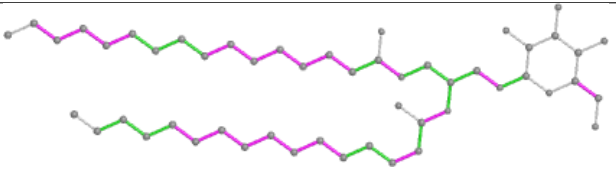
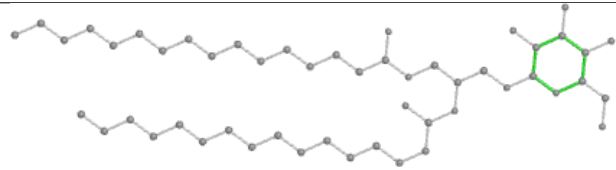
## Ligand HTG D 414

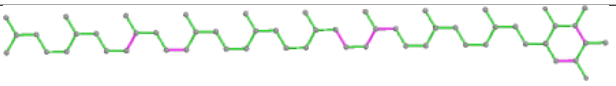
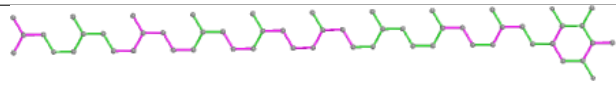
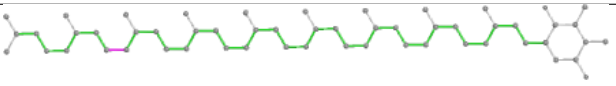
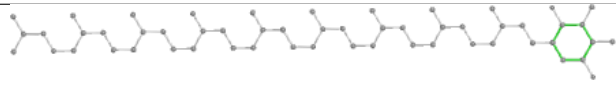


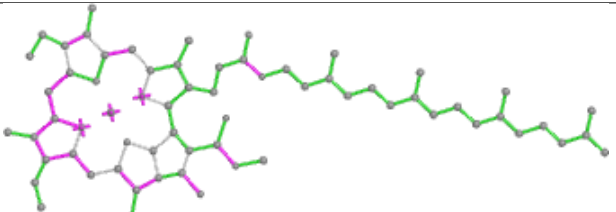
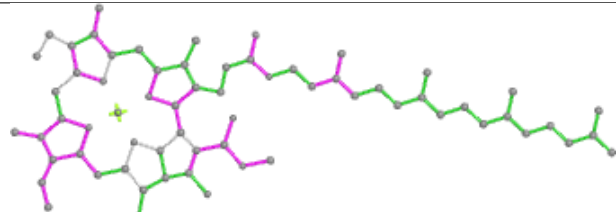
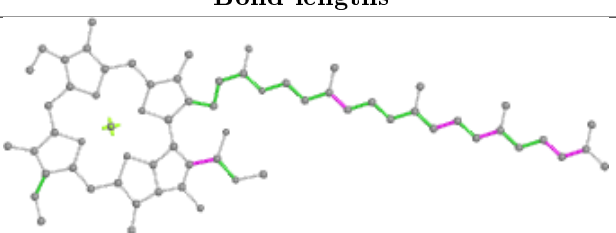
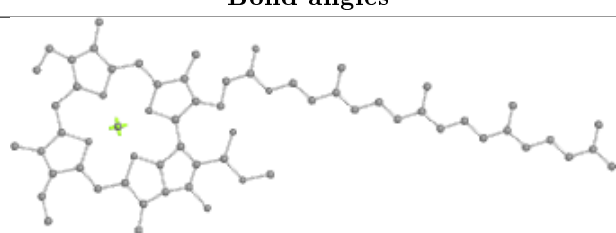
## Ligand LMT B 623

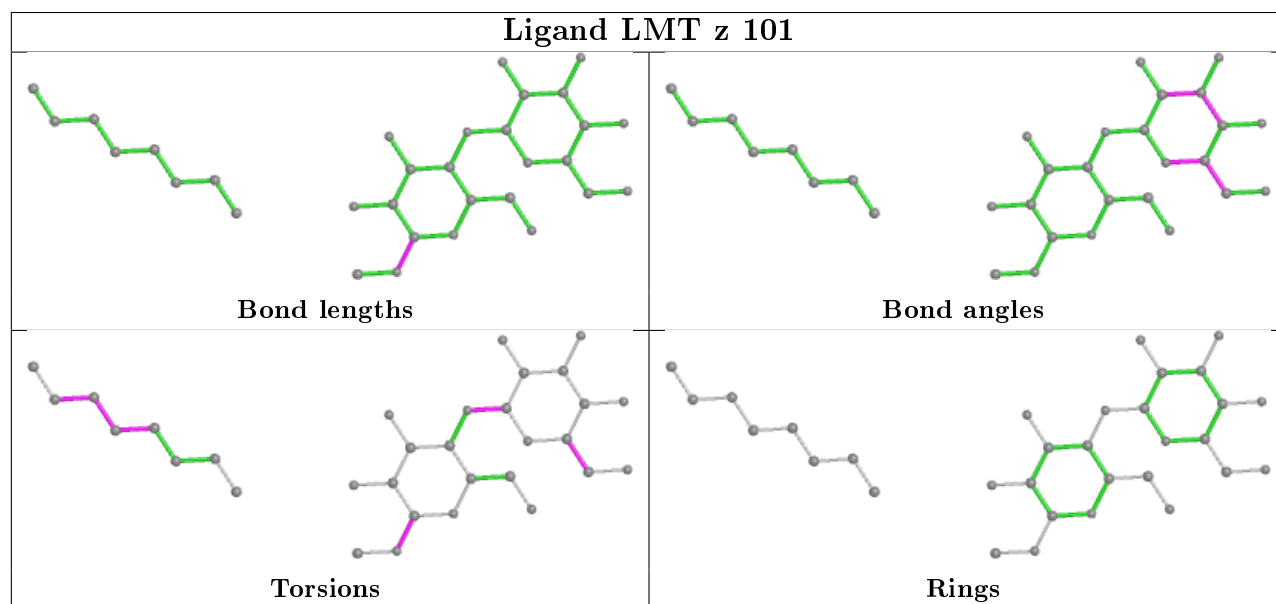
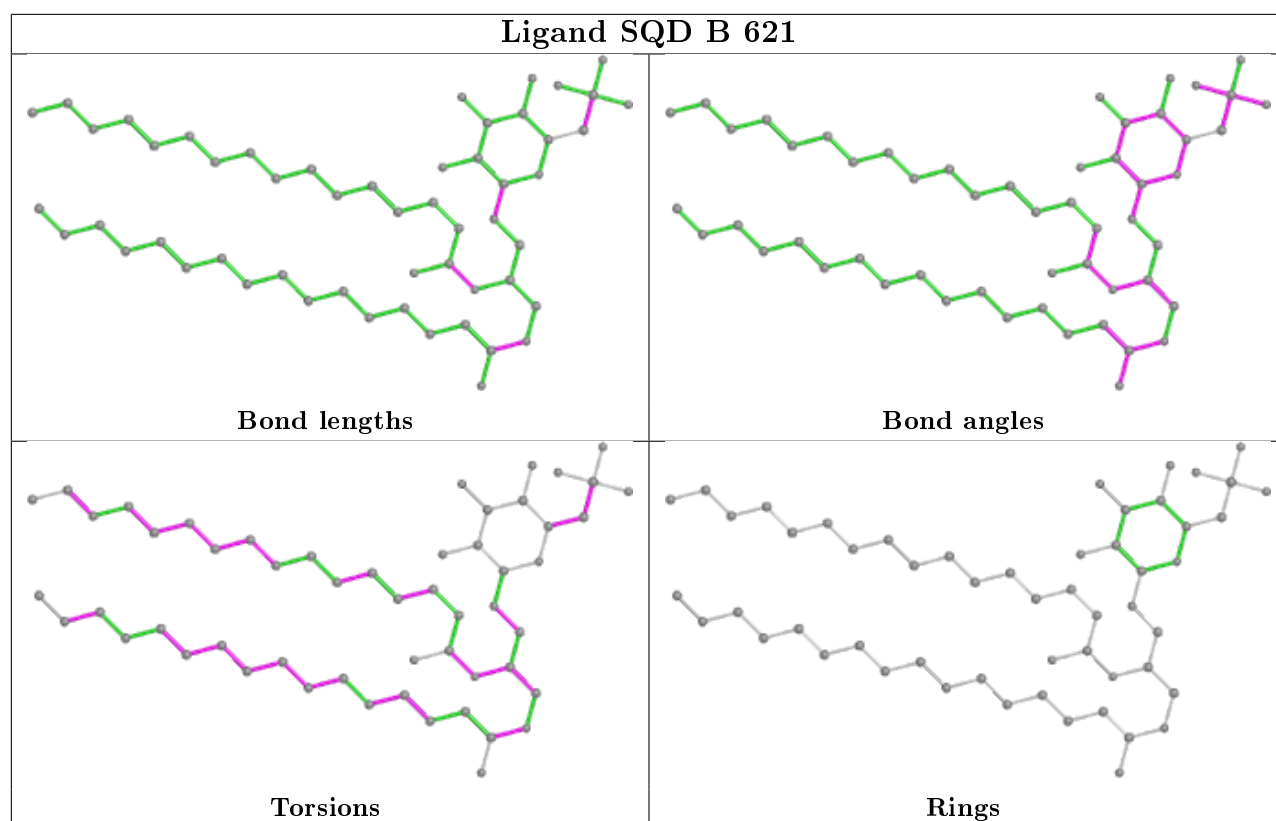


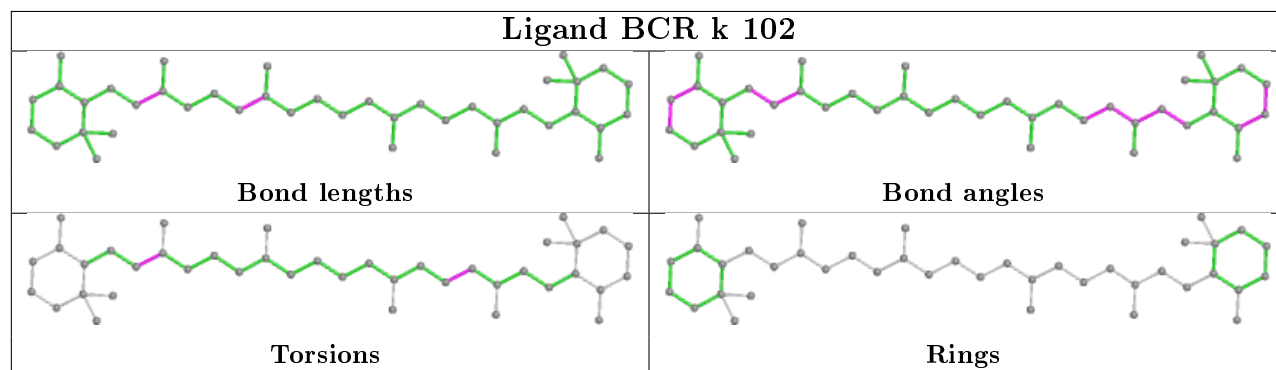
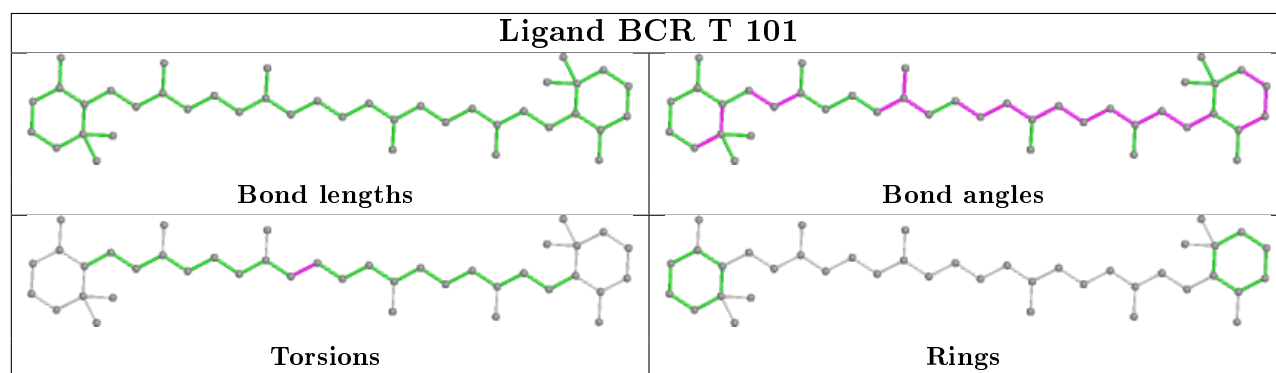
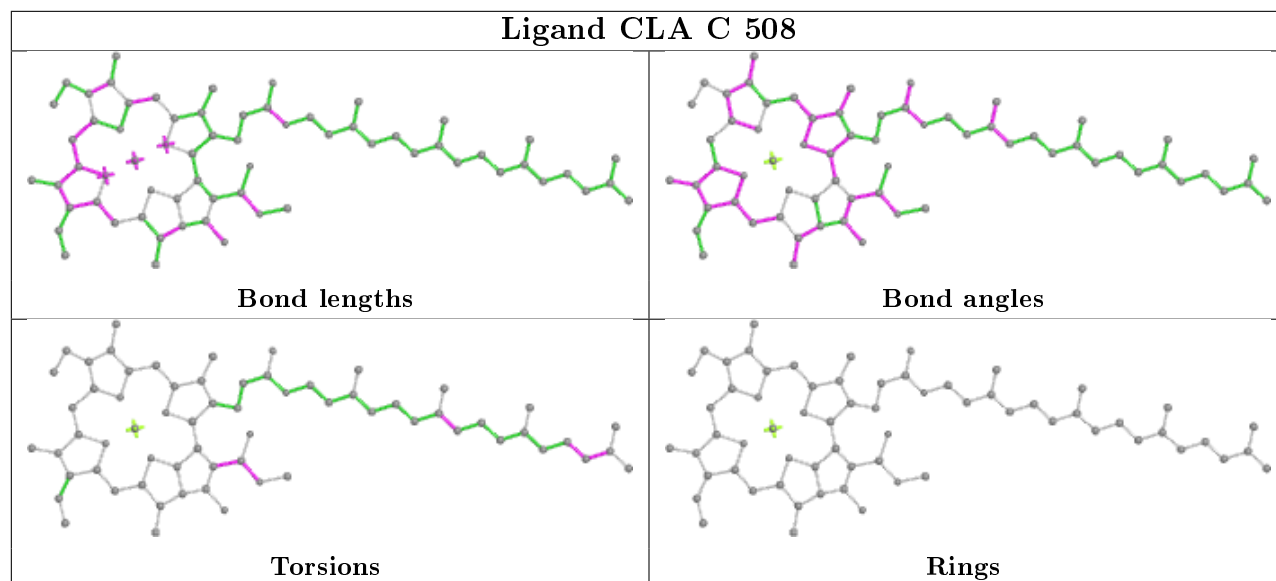
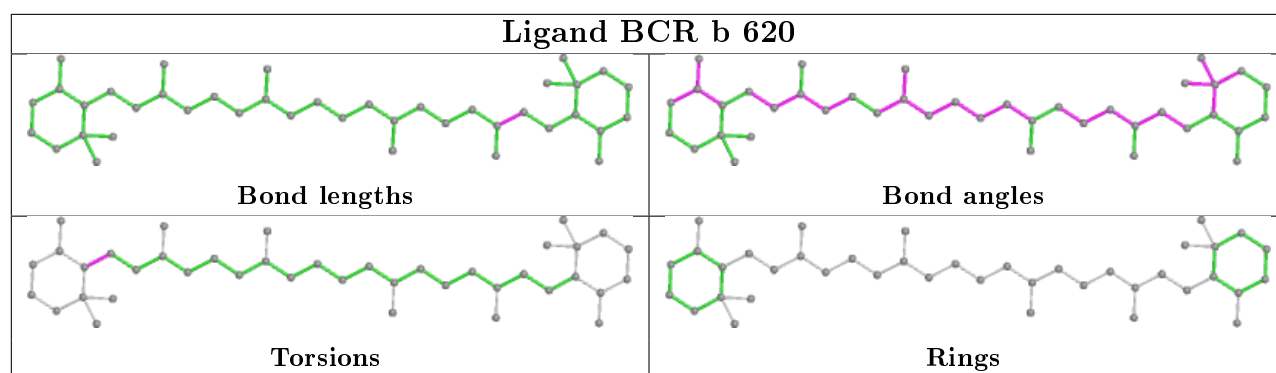


Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

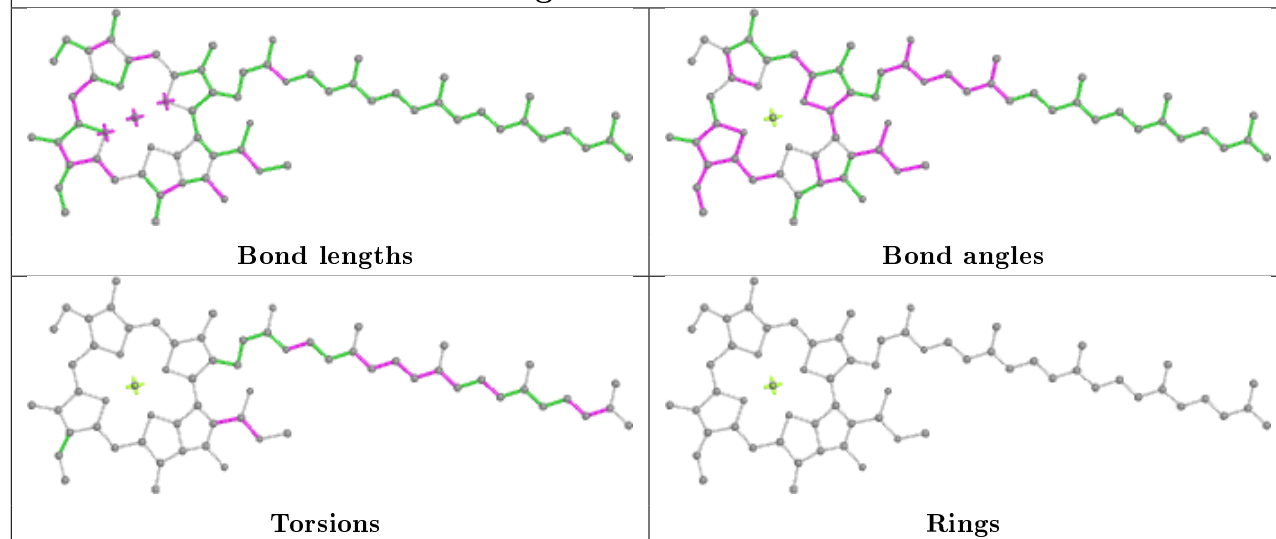
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

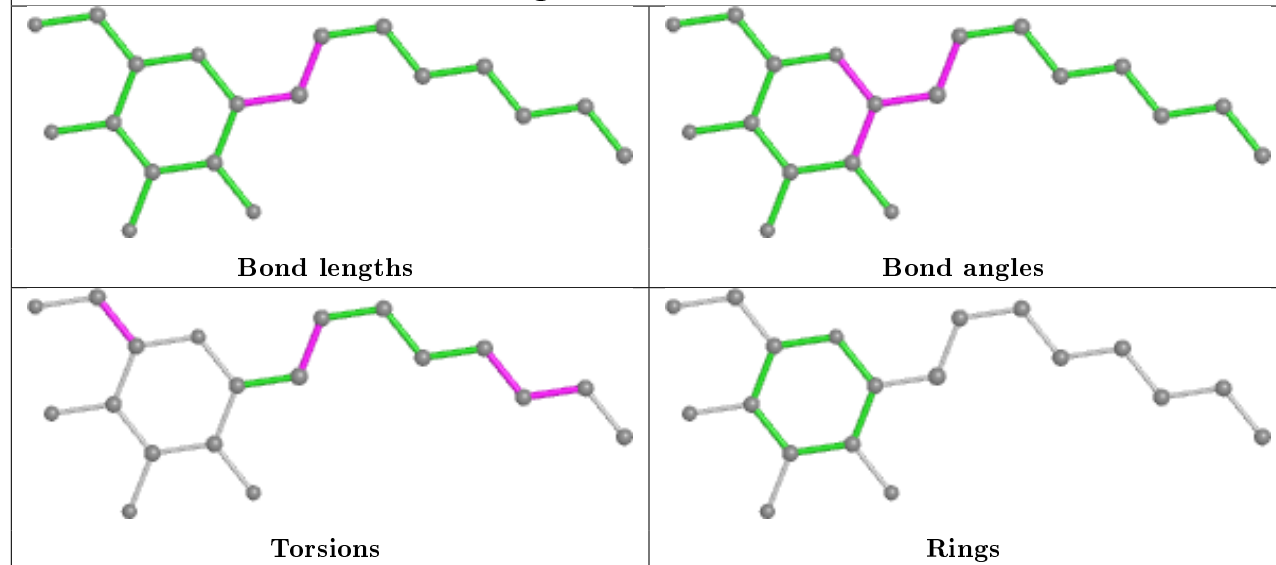




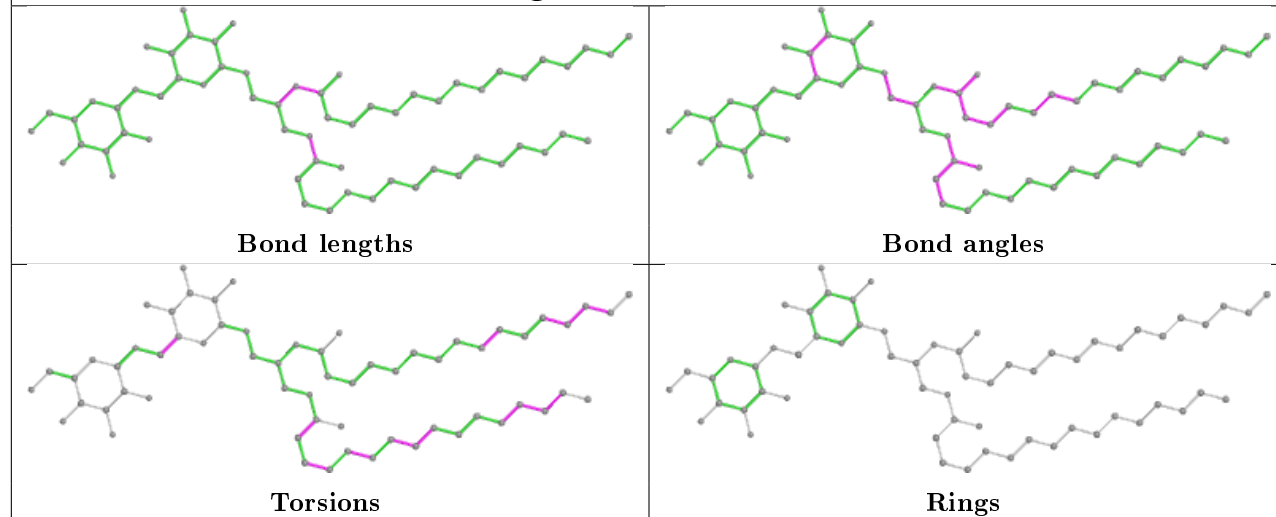
## Ligand CLA b 617

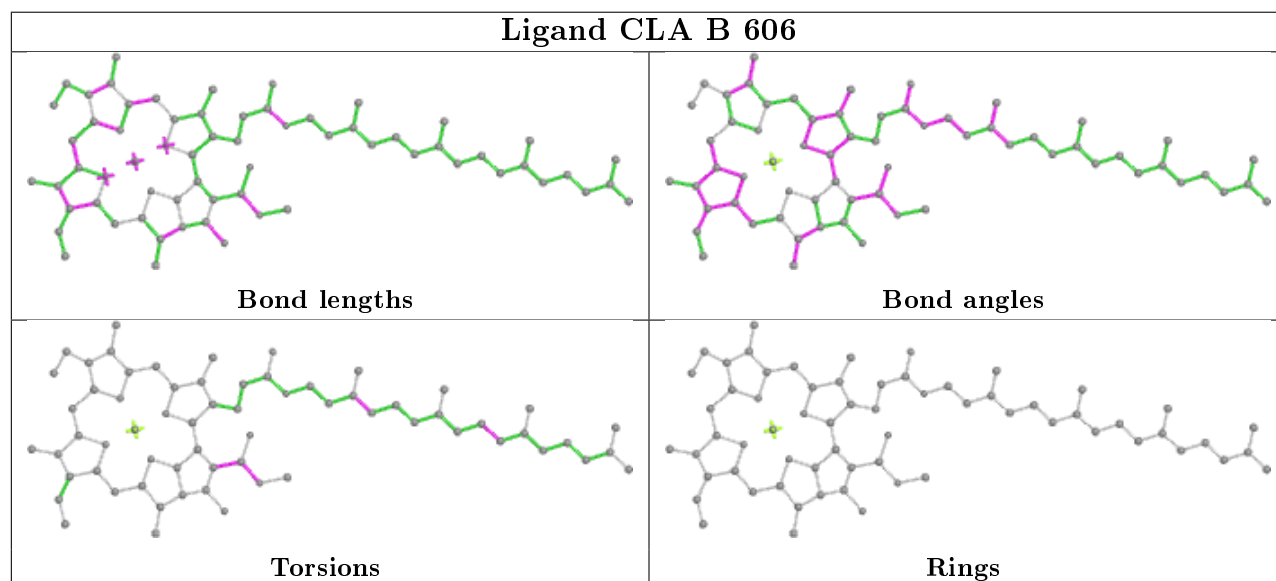
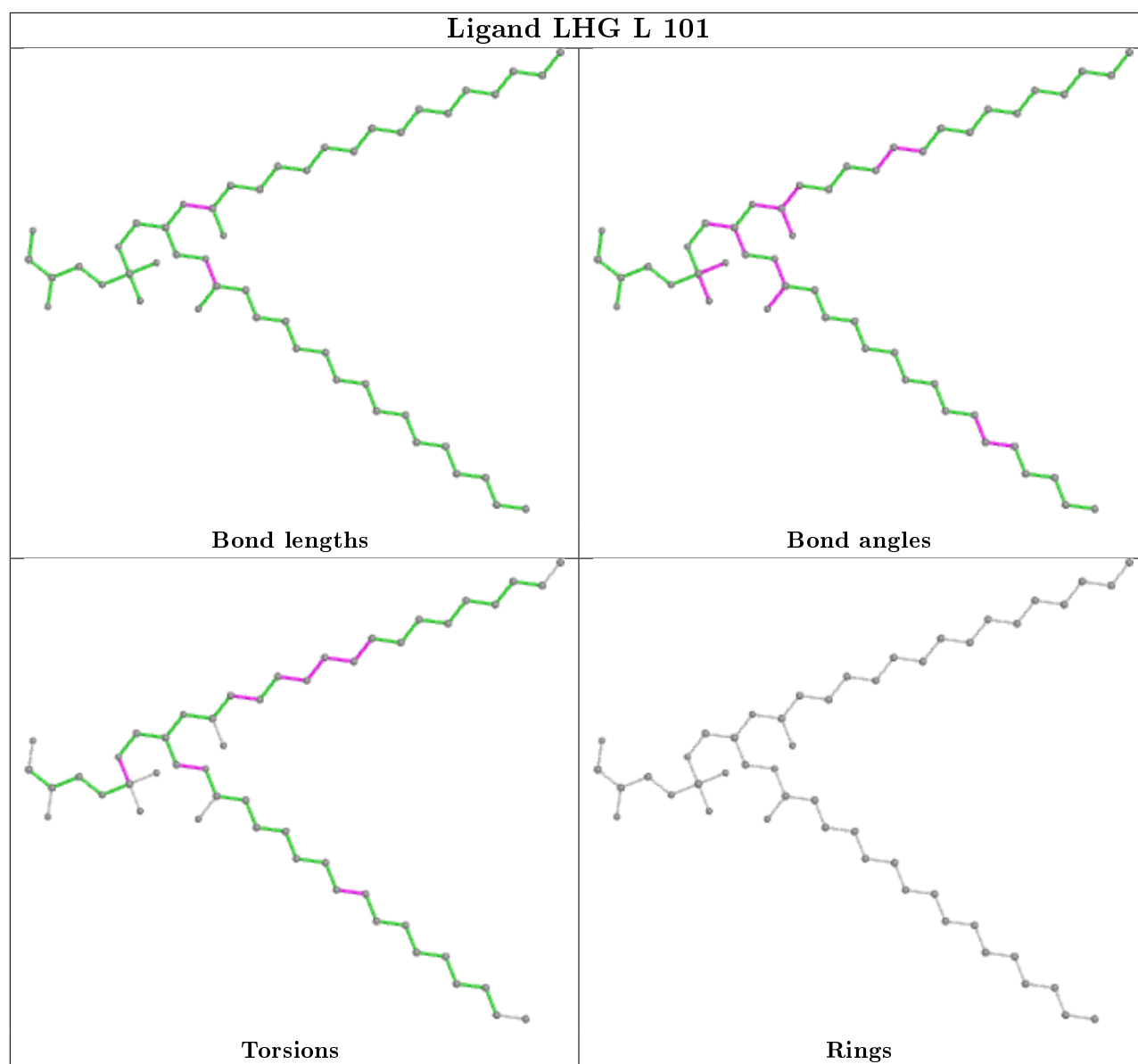


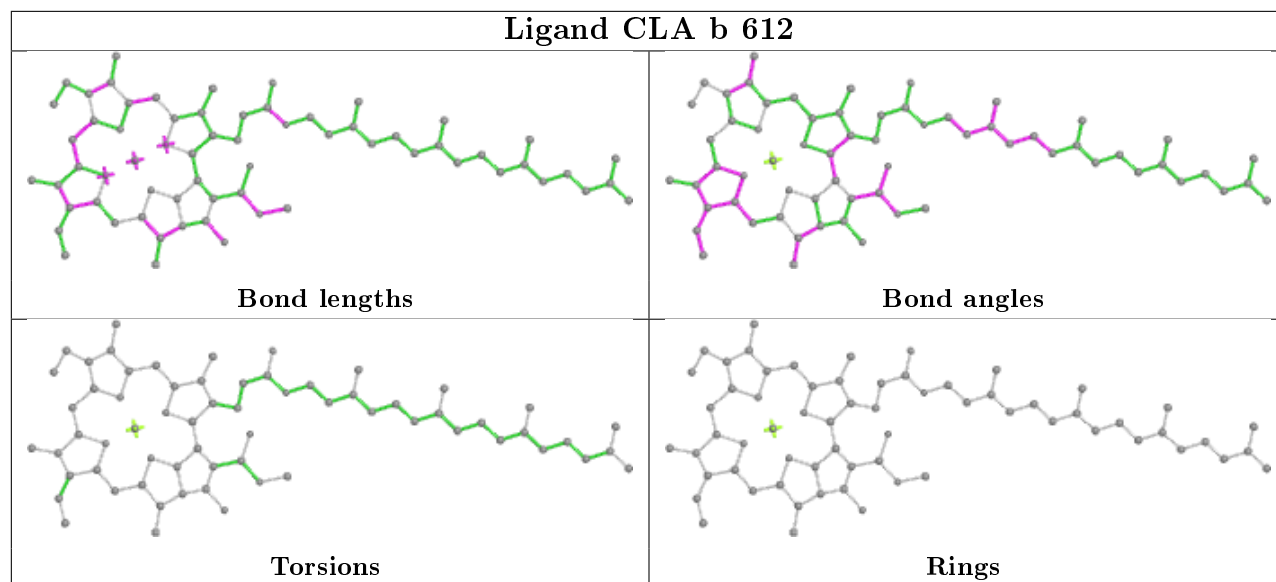
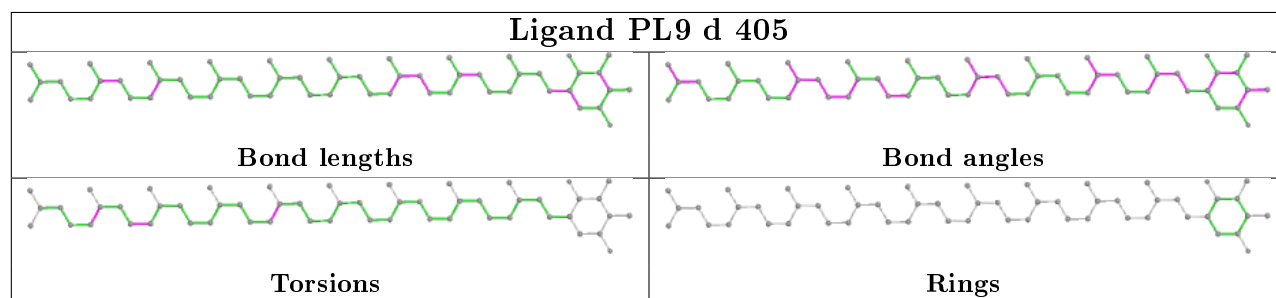
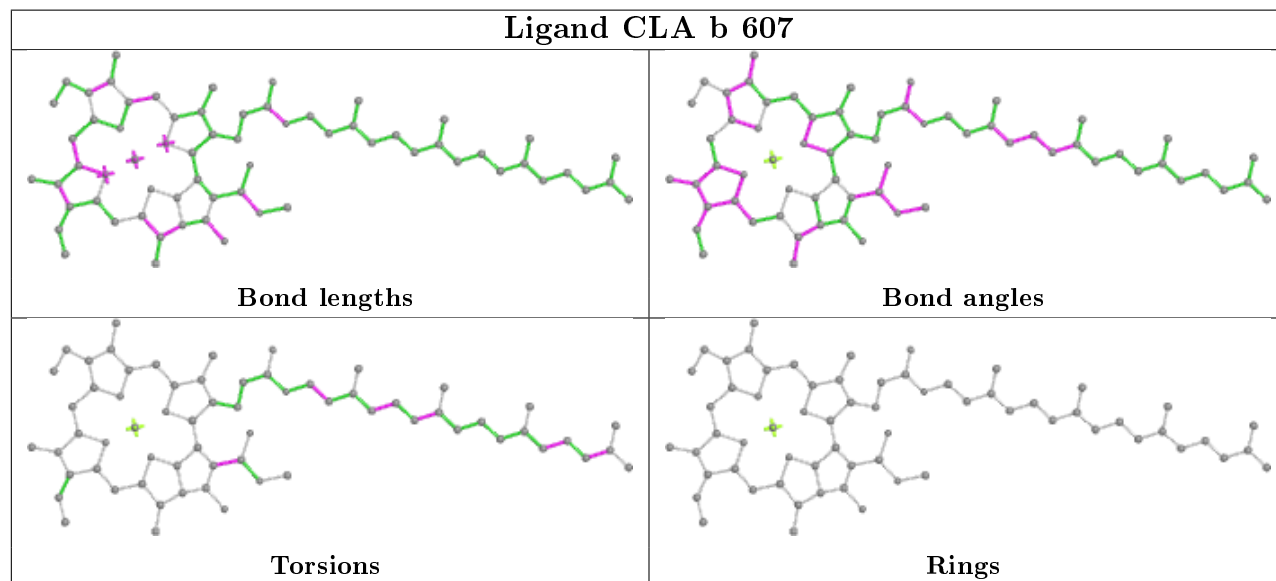
## Ligand HTG d 401



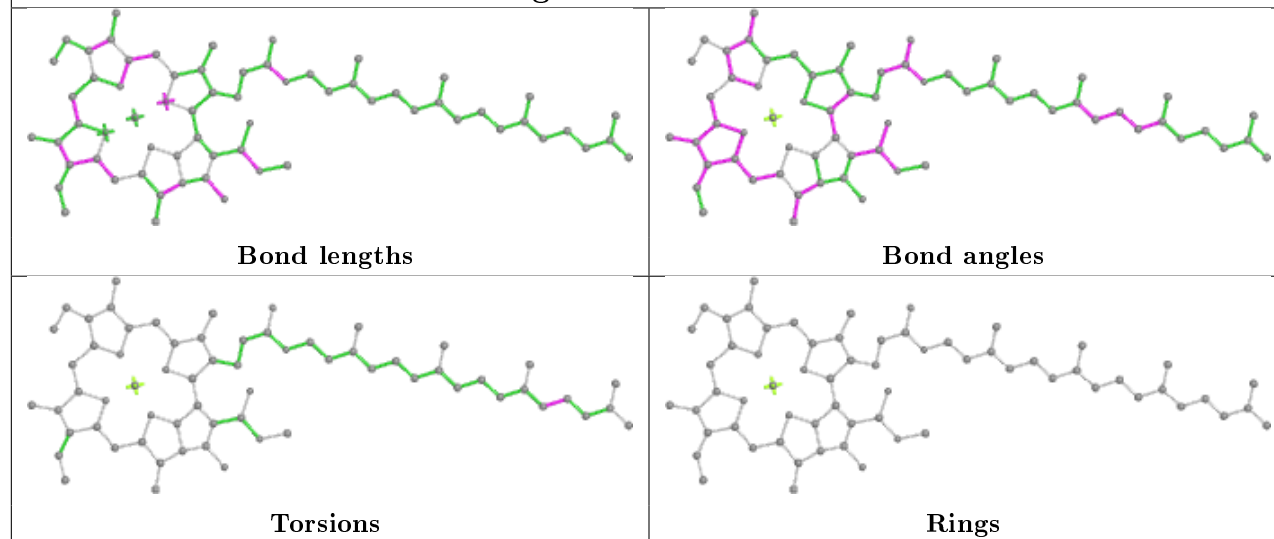
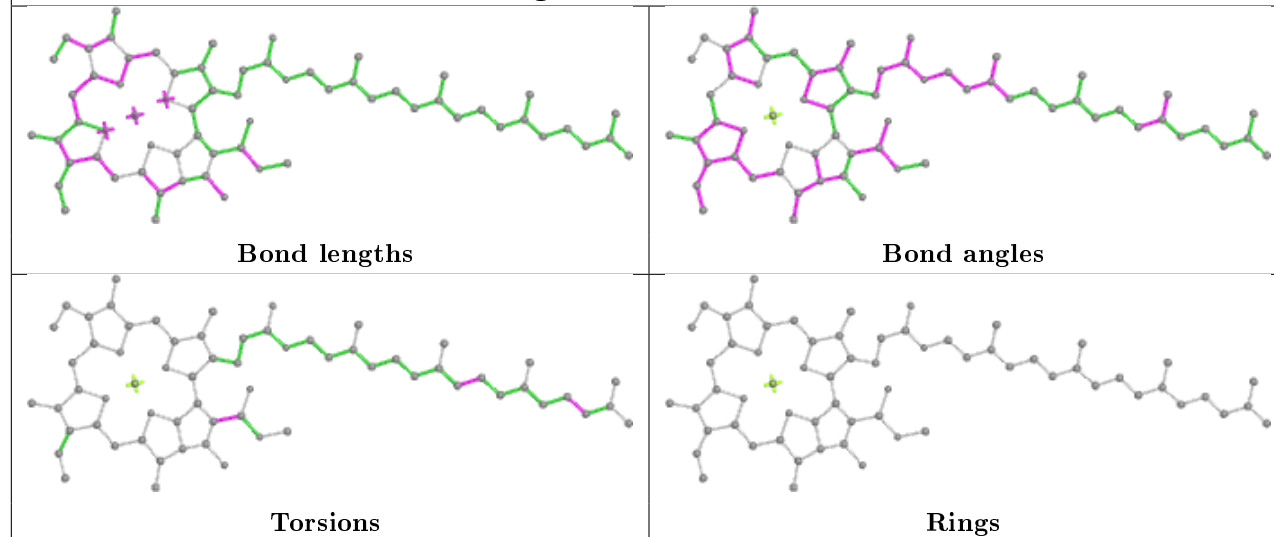
## Ligand DGD C 518

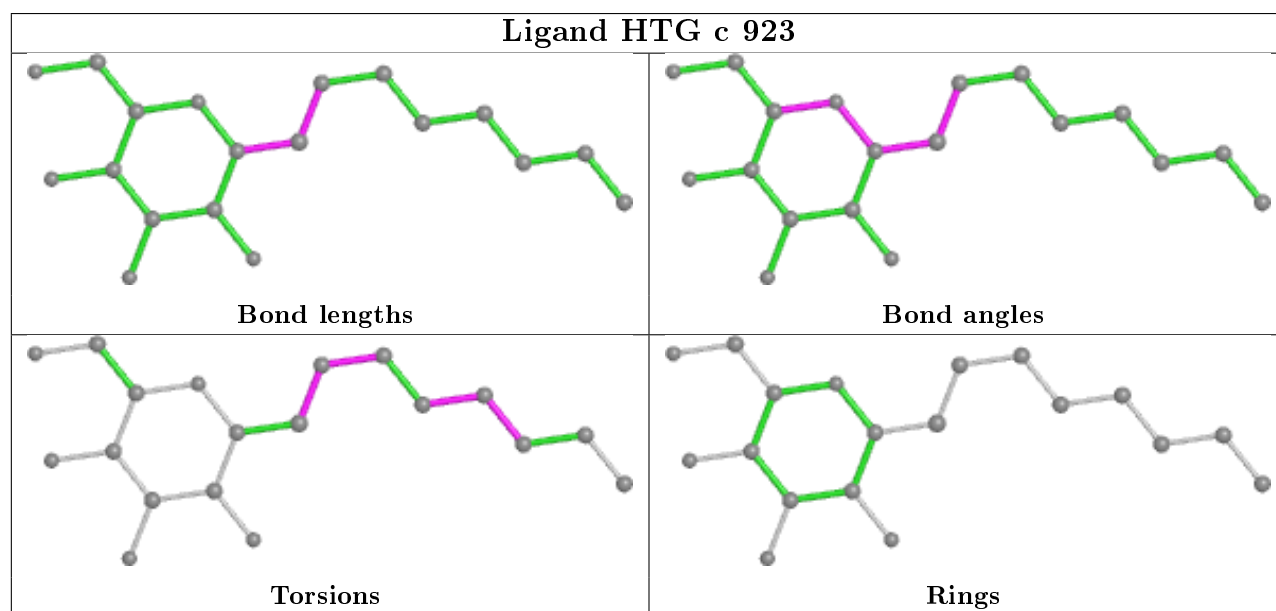
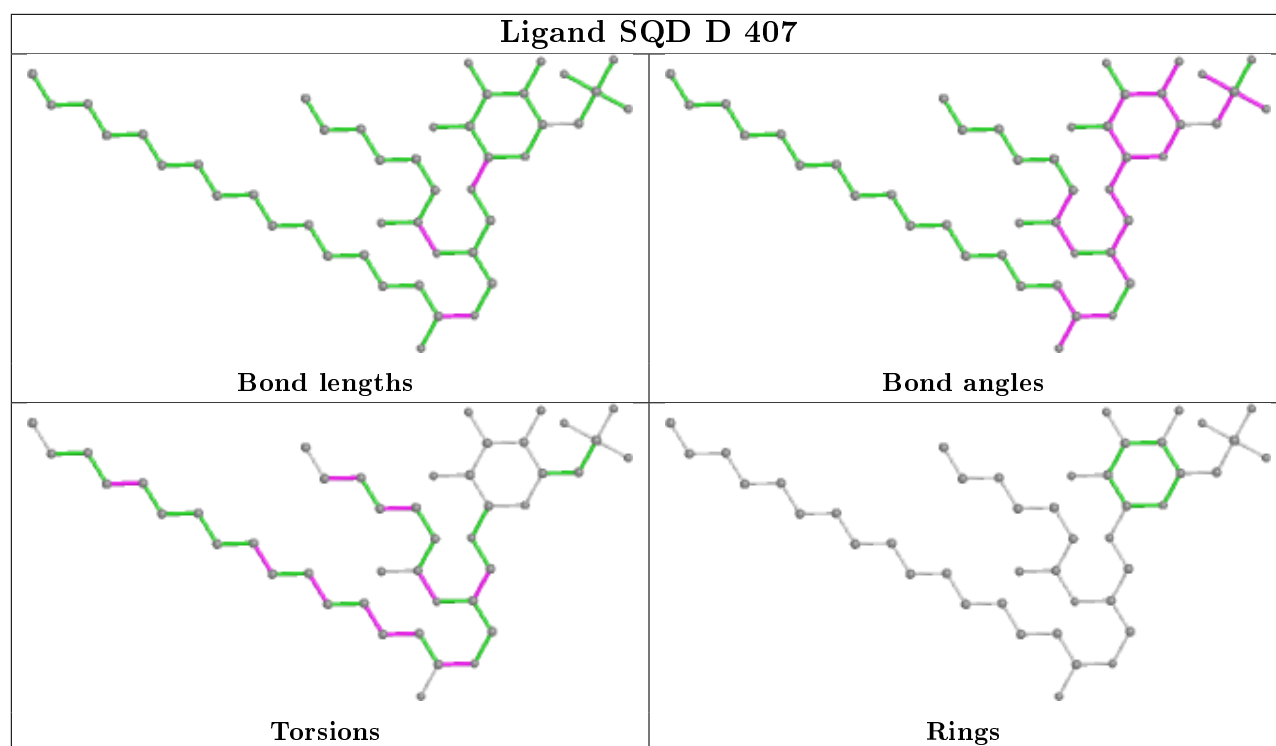


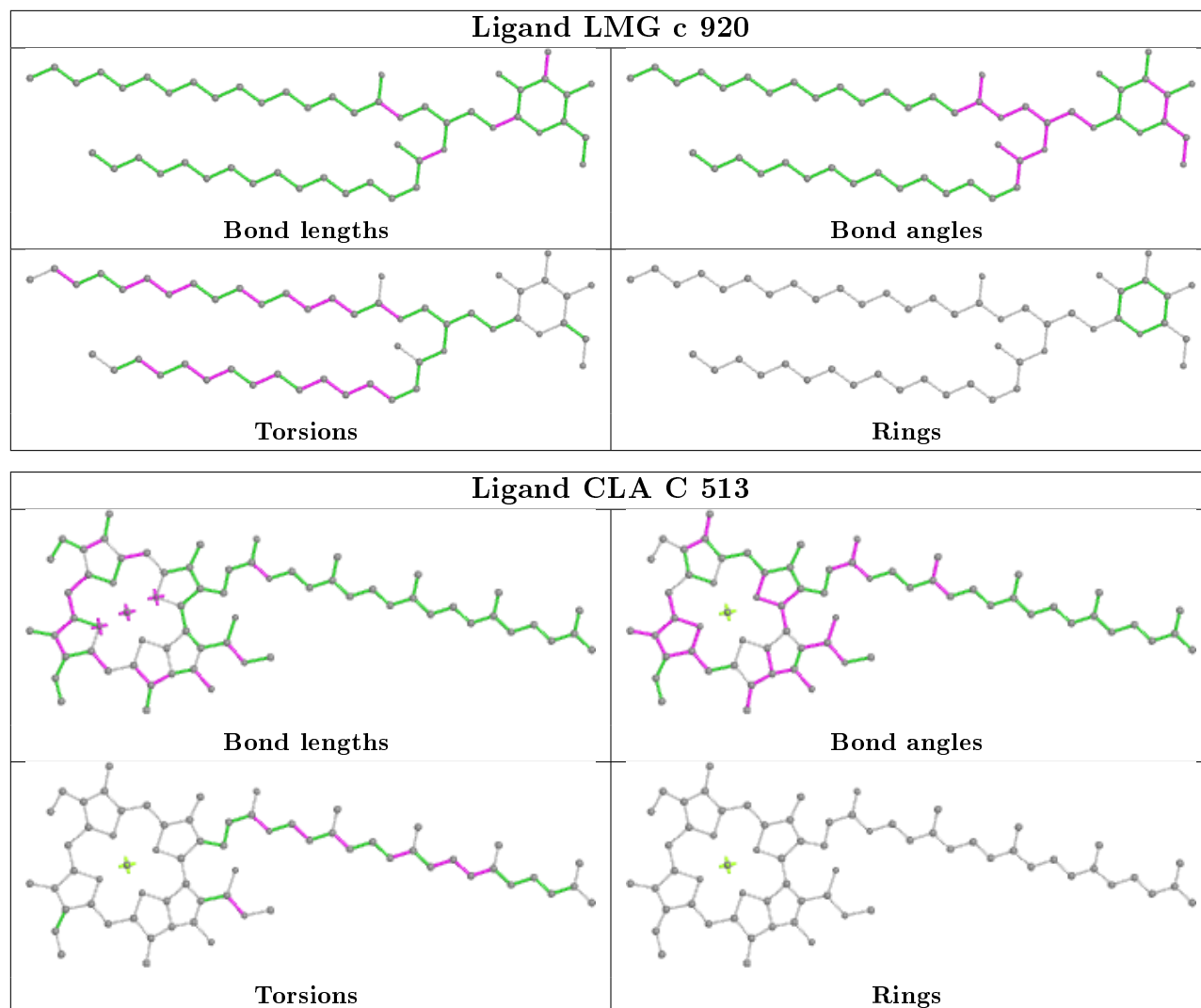


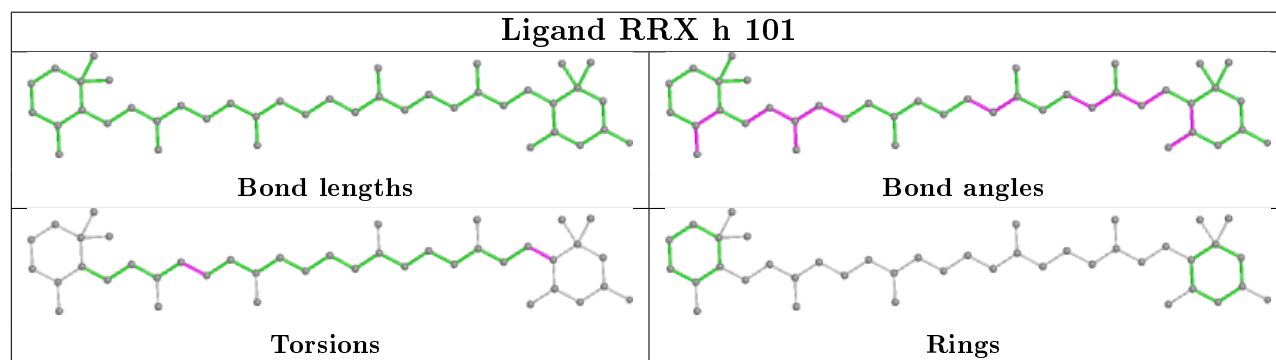
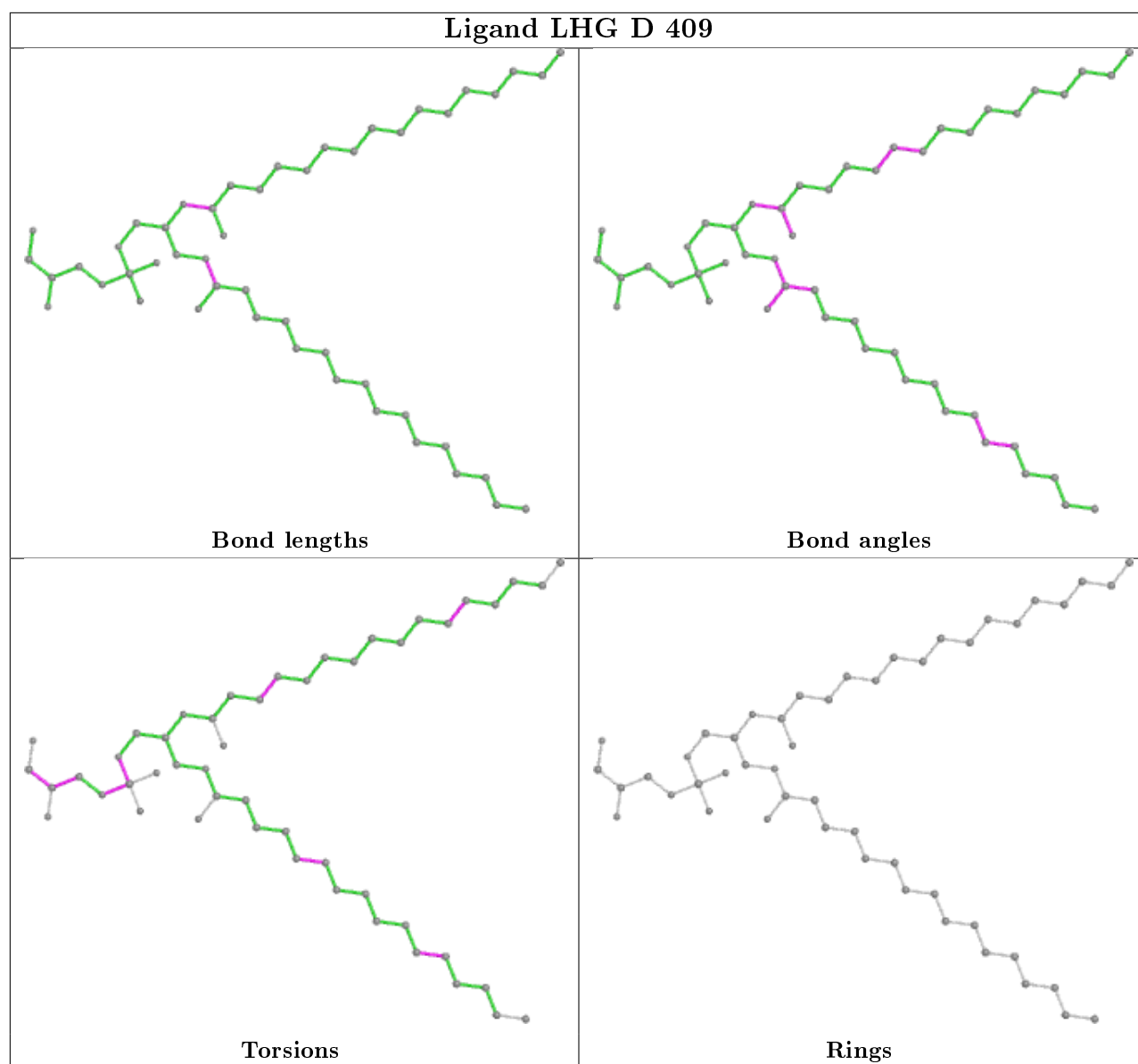
**Ligand CLA b 612****Ligand PL9 d 405****Ligand CLA b 607**

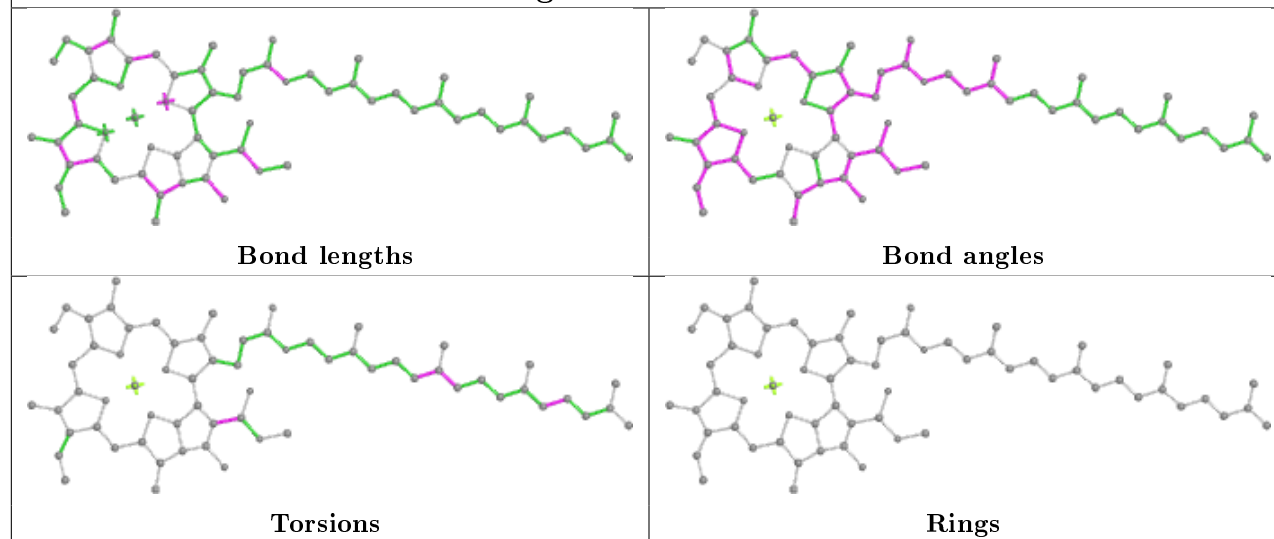
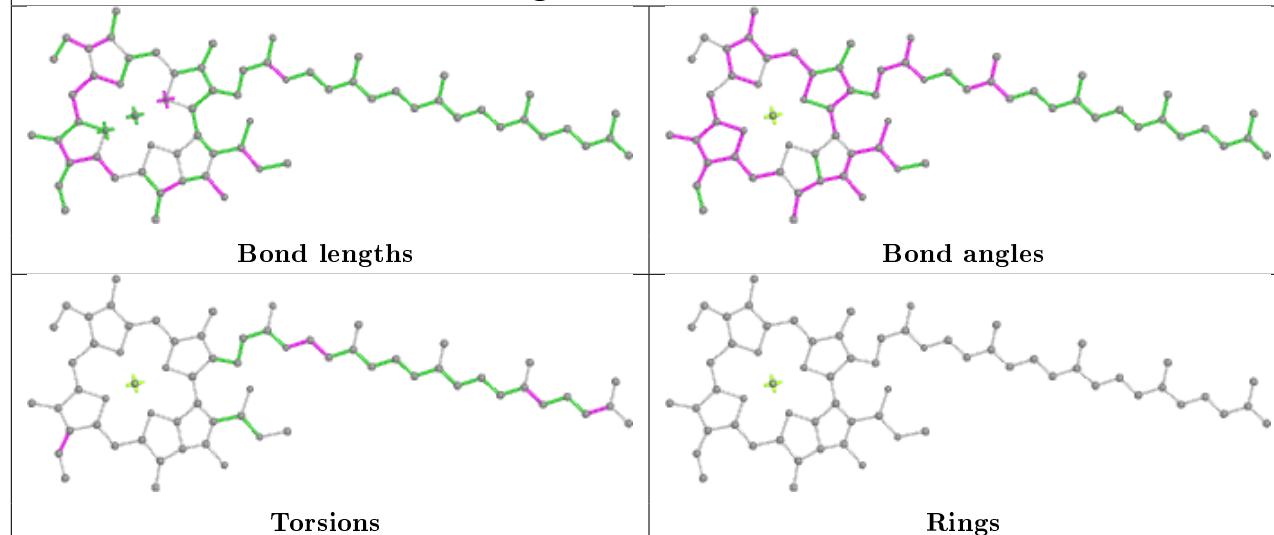
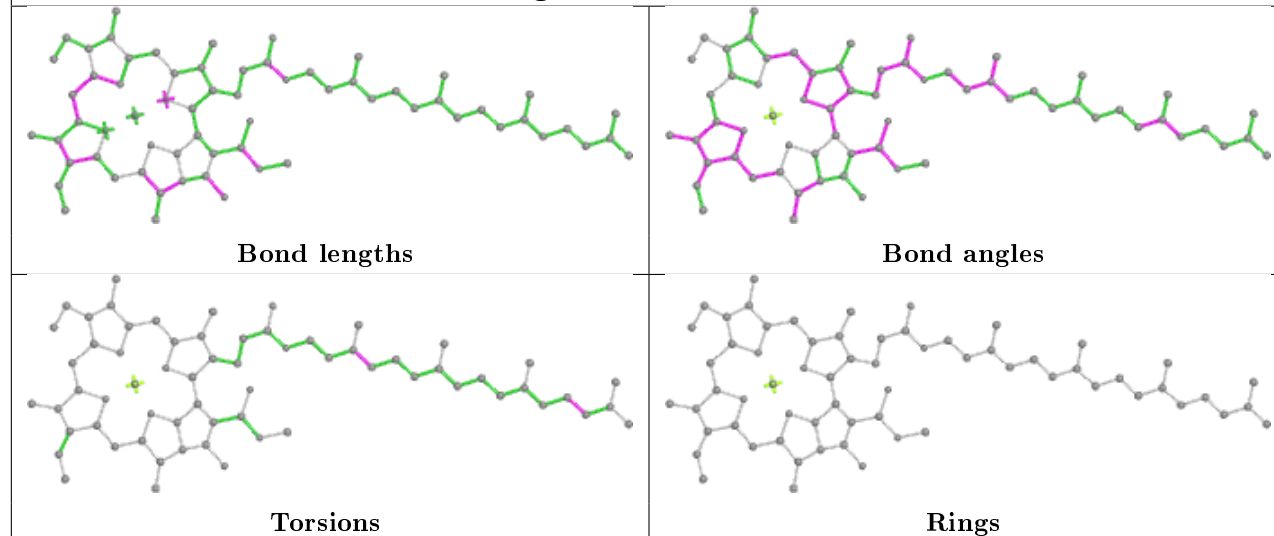


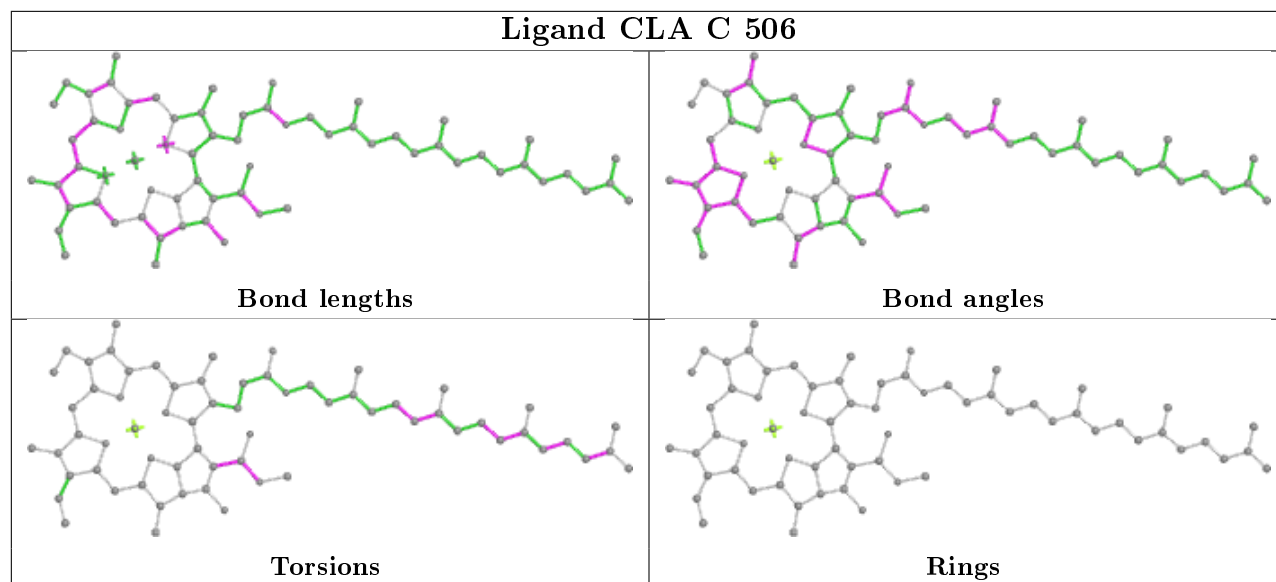
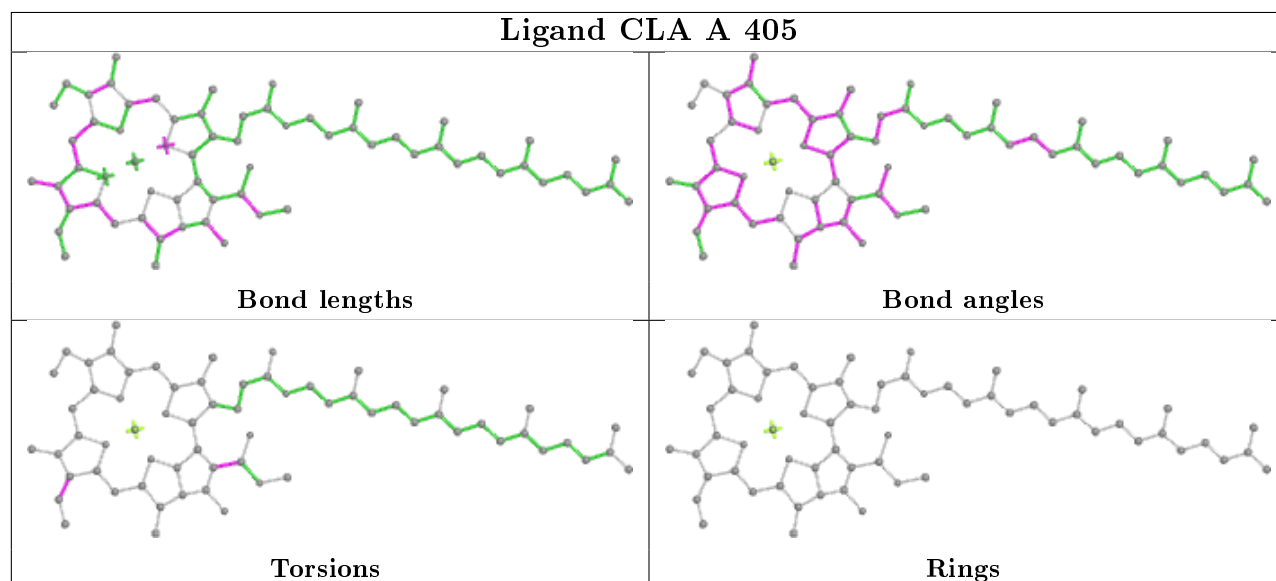
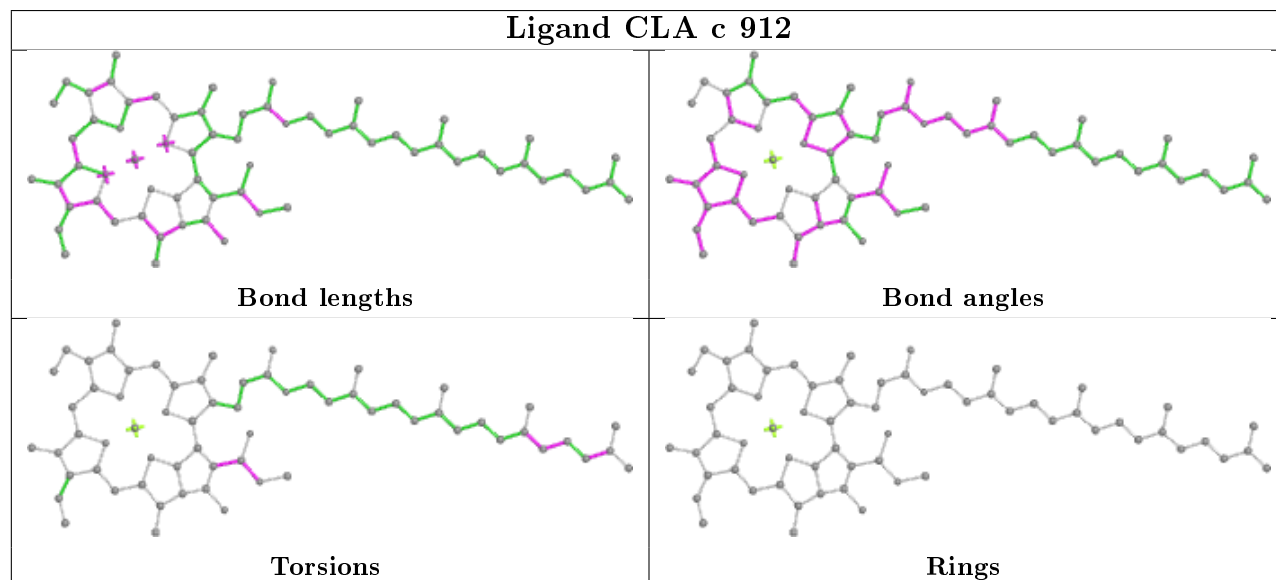
**Ligand CLA B 609****Ligand CLA B 603**



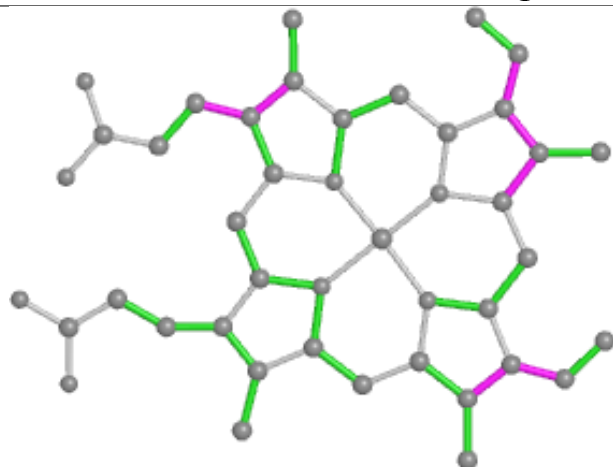




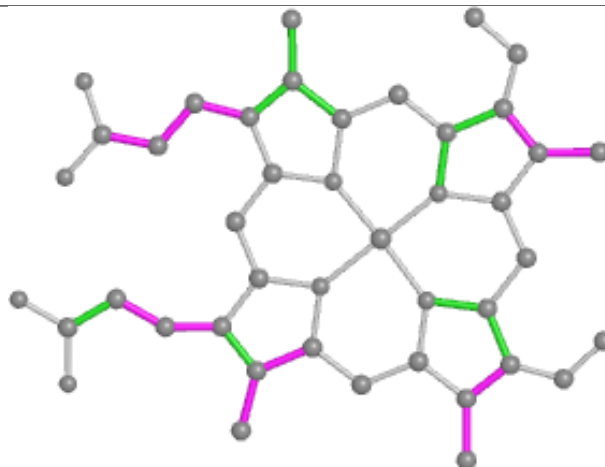
**Ligand CLA a 411****Ligand CLA D 402****Ligand CLA B 612**

**Ligand CLA C 506****Ligand CLA A 405****Ligand CLA c 912**

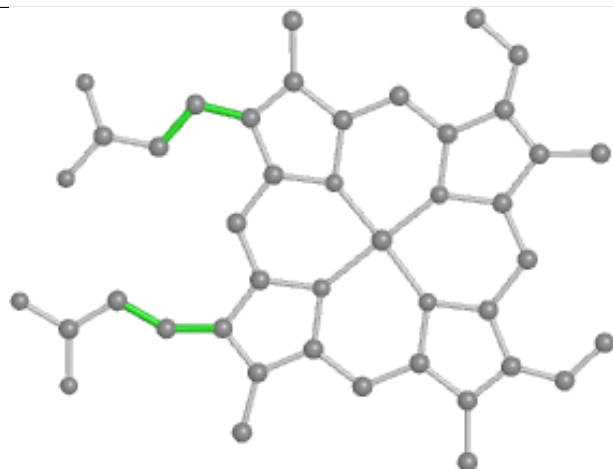
## Ligand HEM f 101



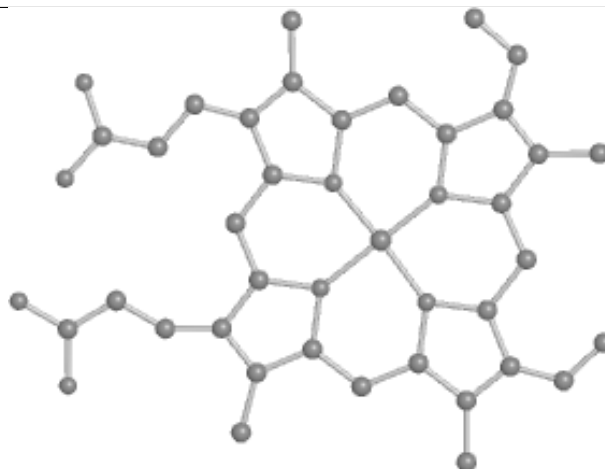
Bond lengths



Bond angles

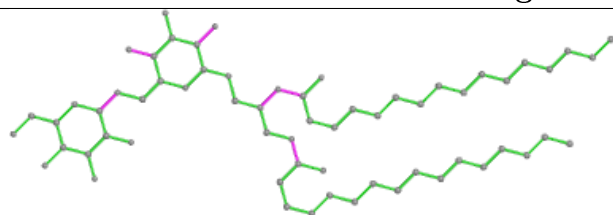


Torsions

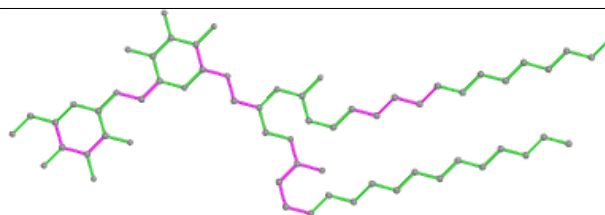


Rings

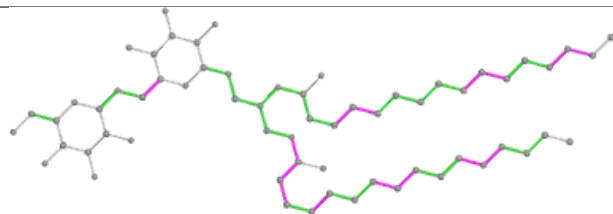
## Ligand DGD c 919



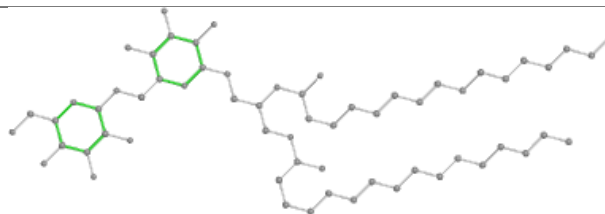
Bond lengths



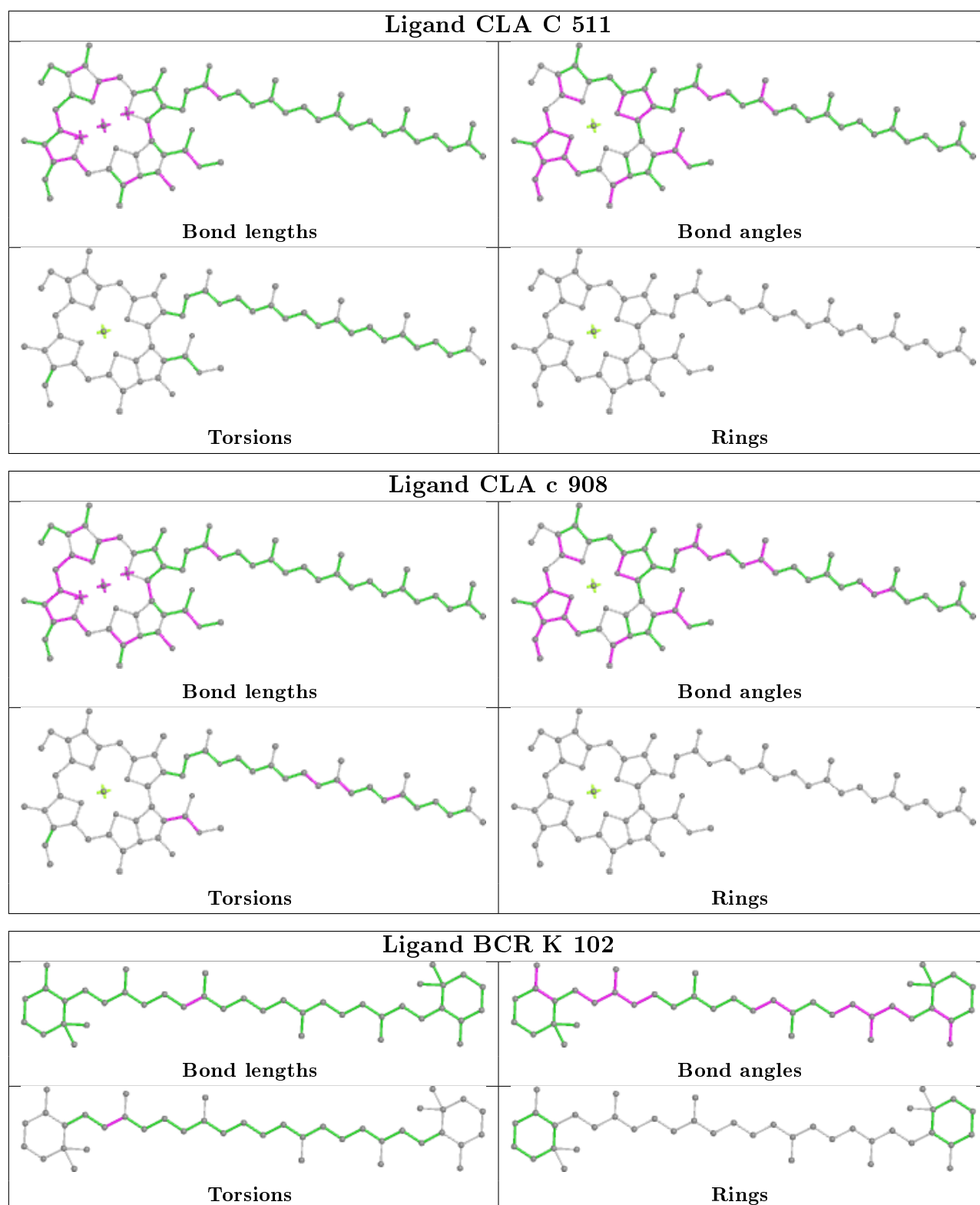
Bond angles



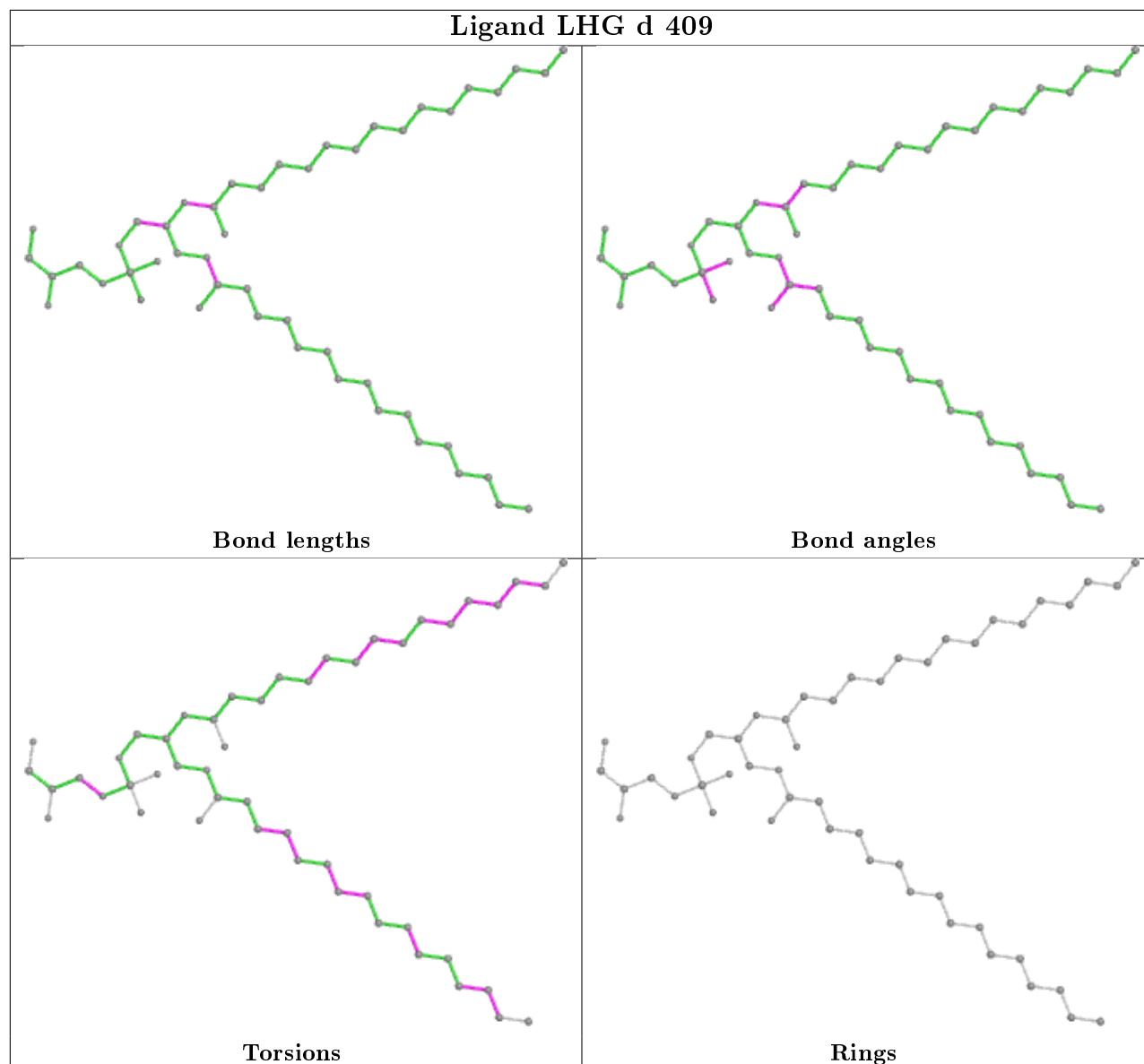
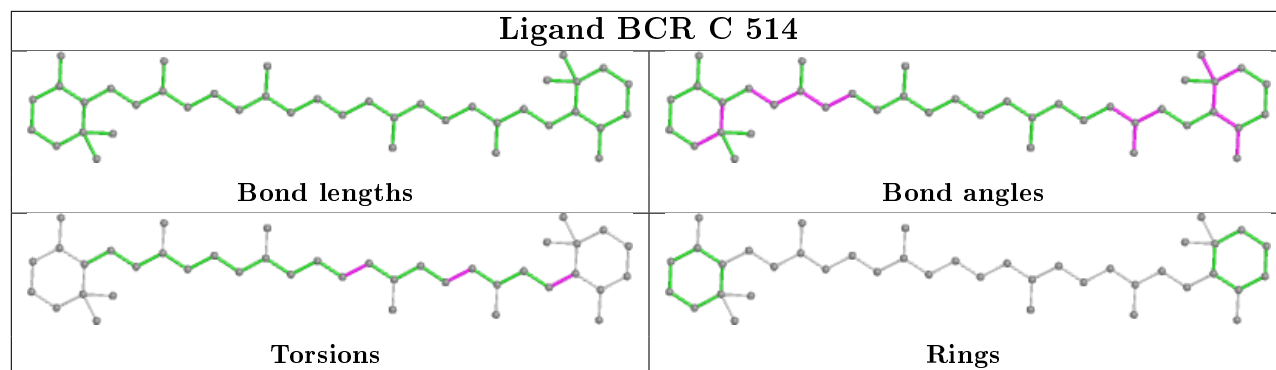
Torsions

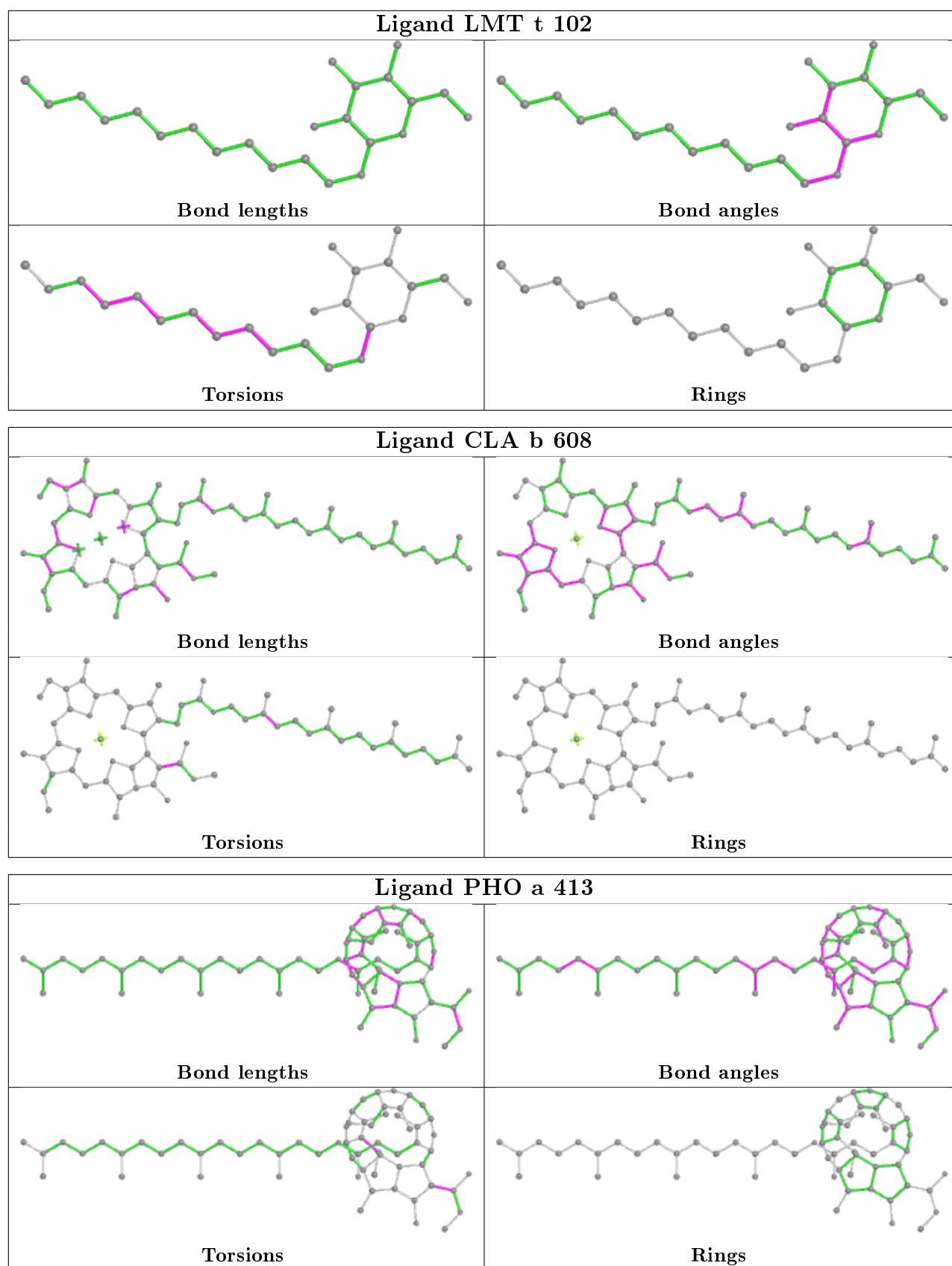


Rings

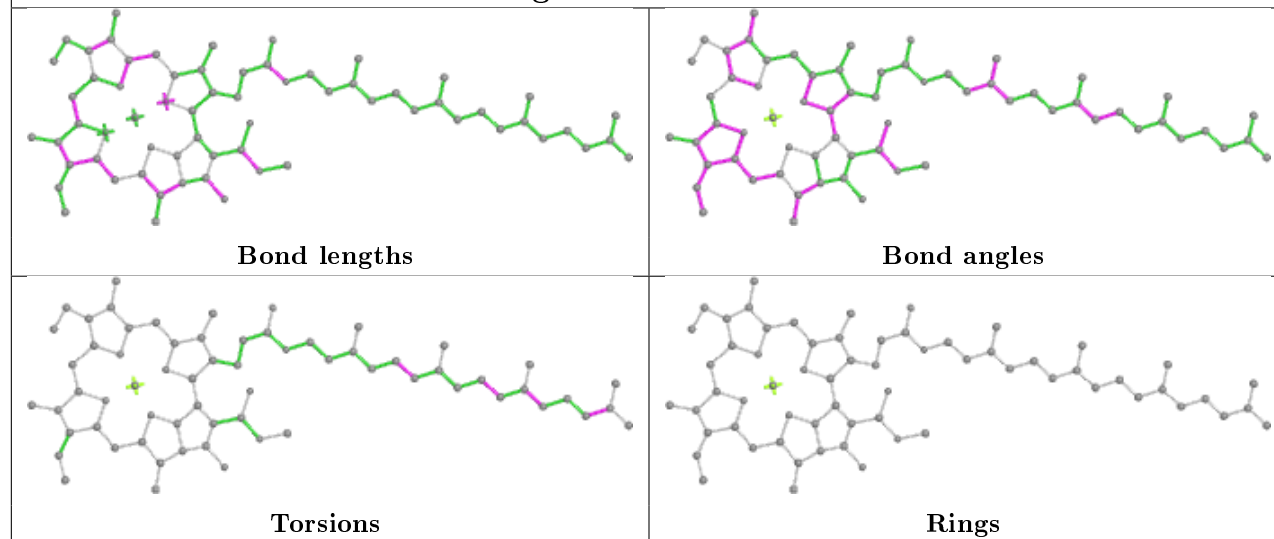




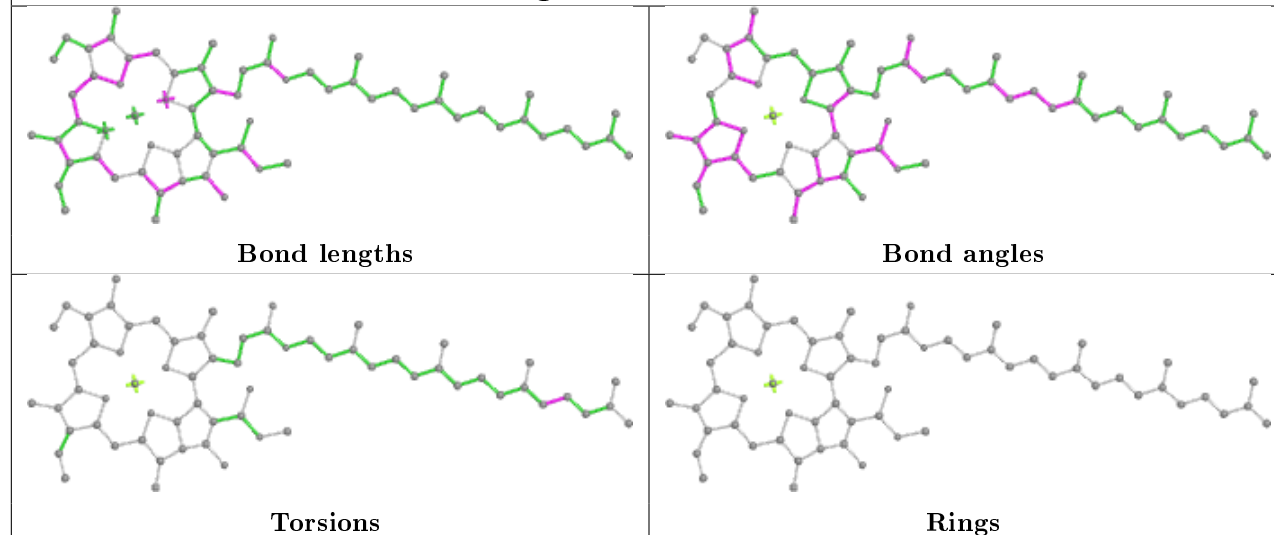




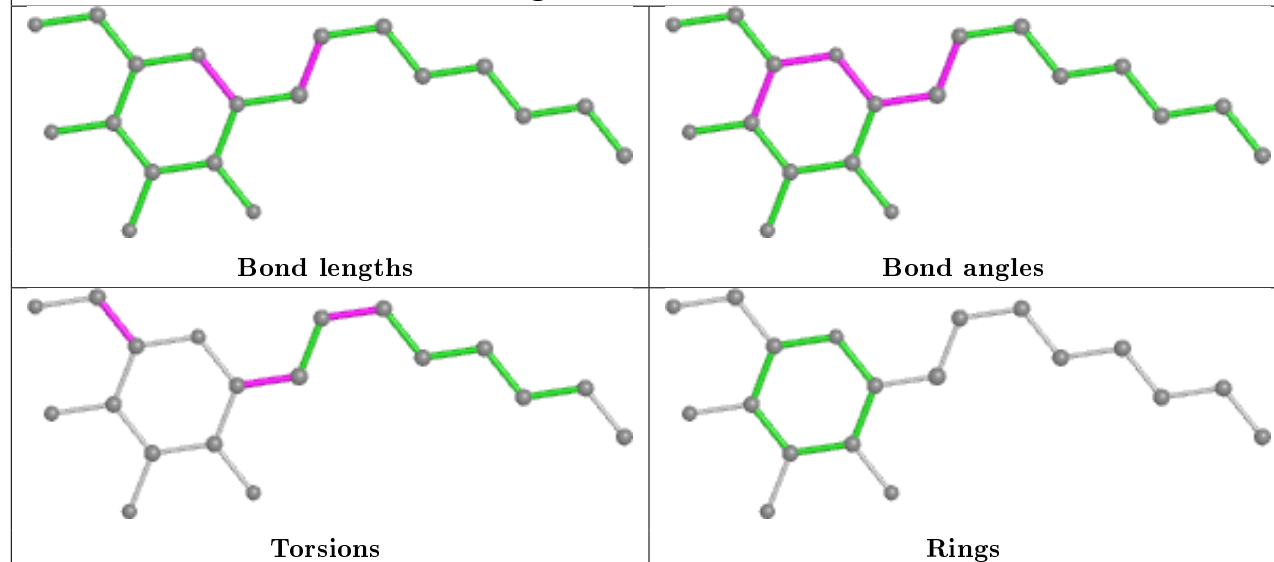
## Ligand CLA B 616

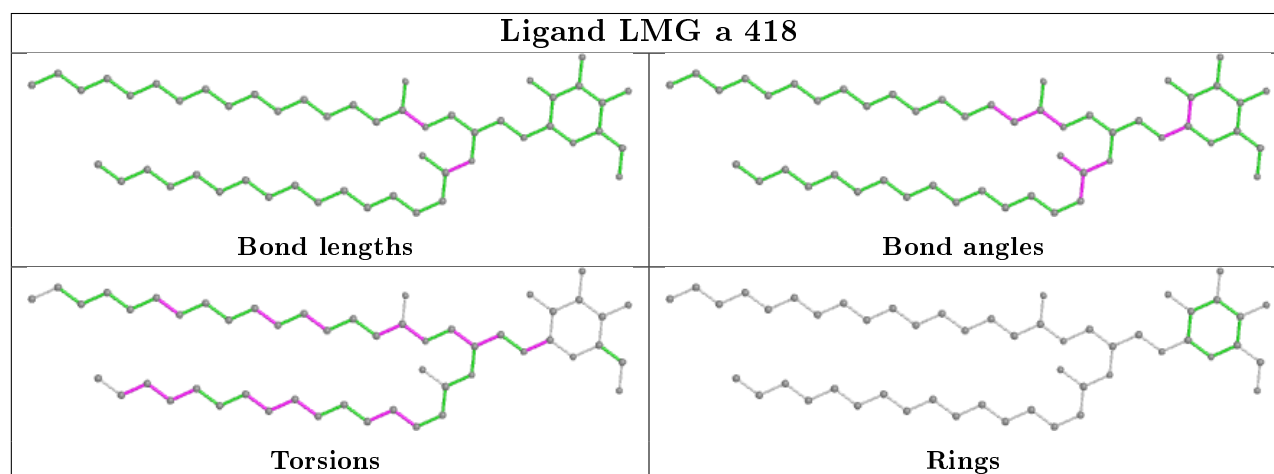
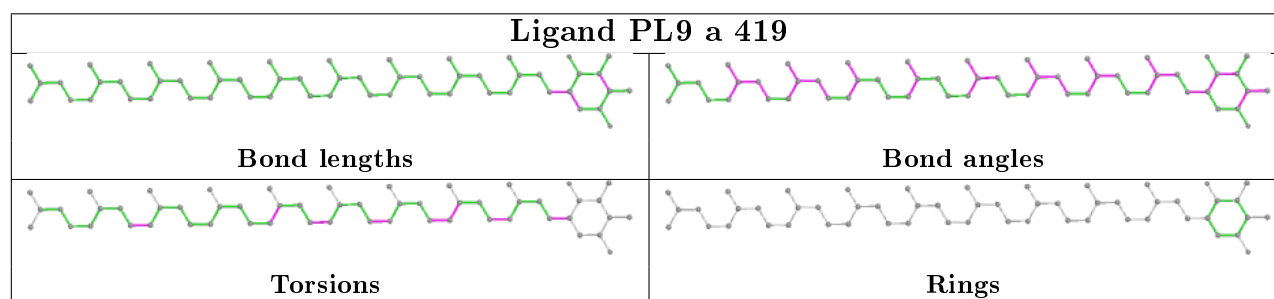
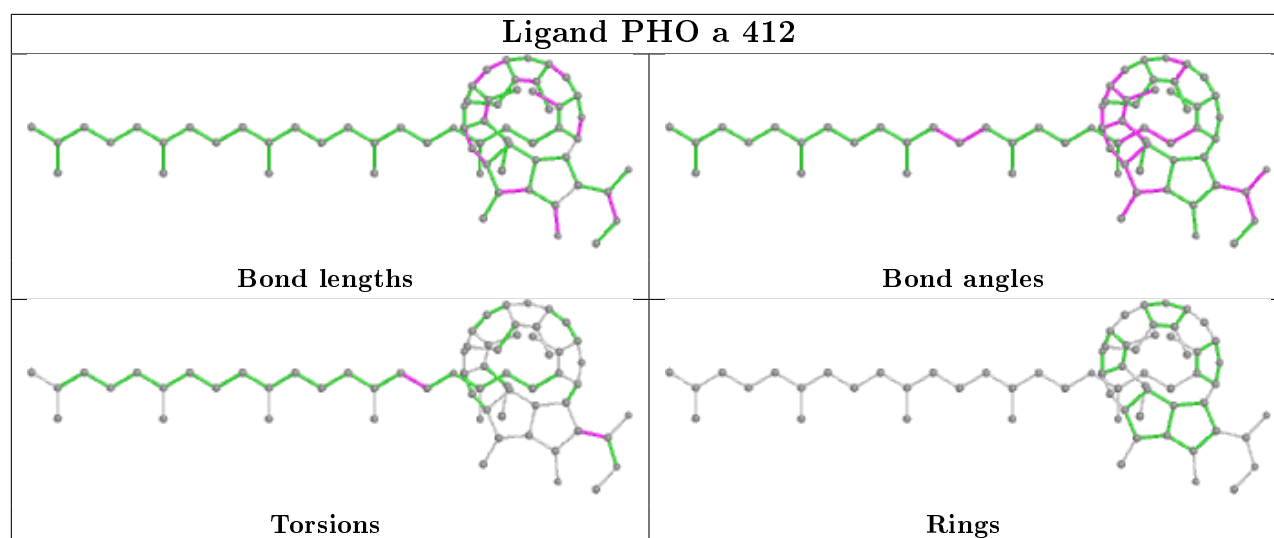


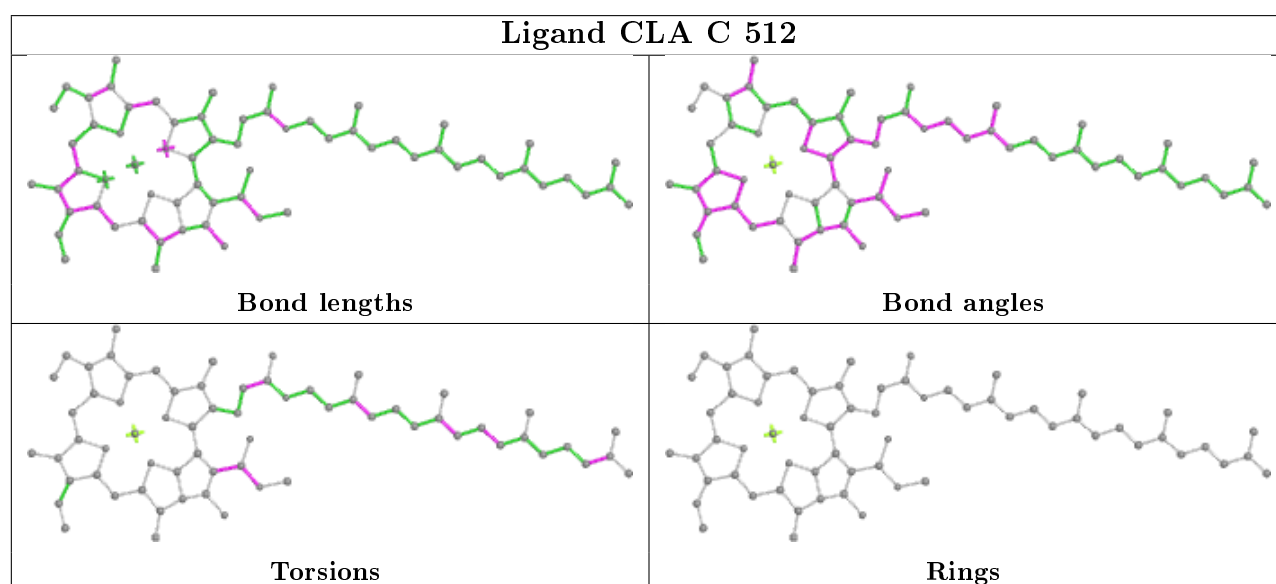
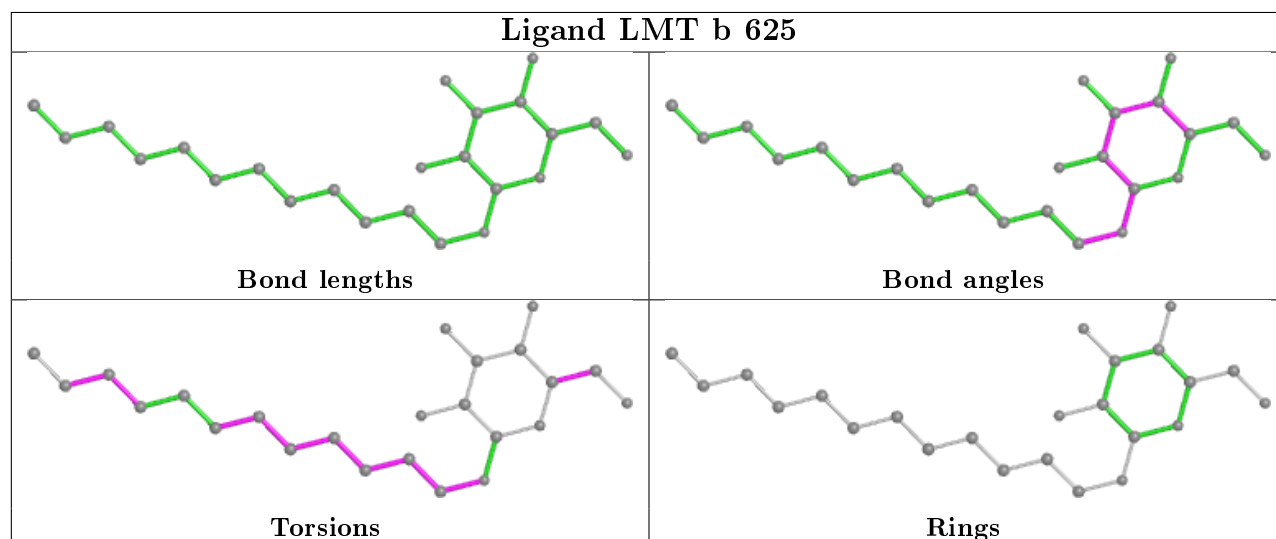
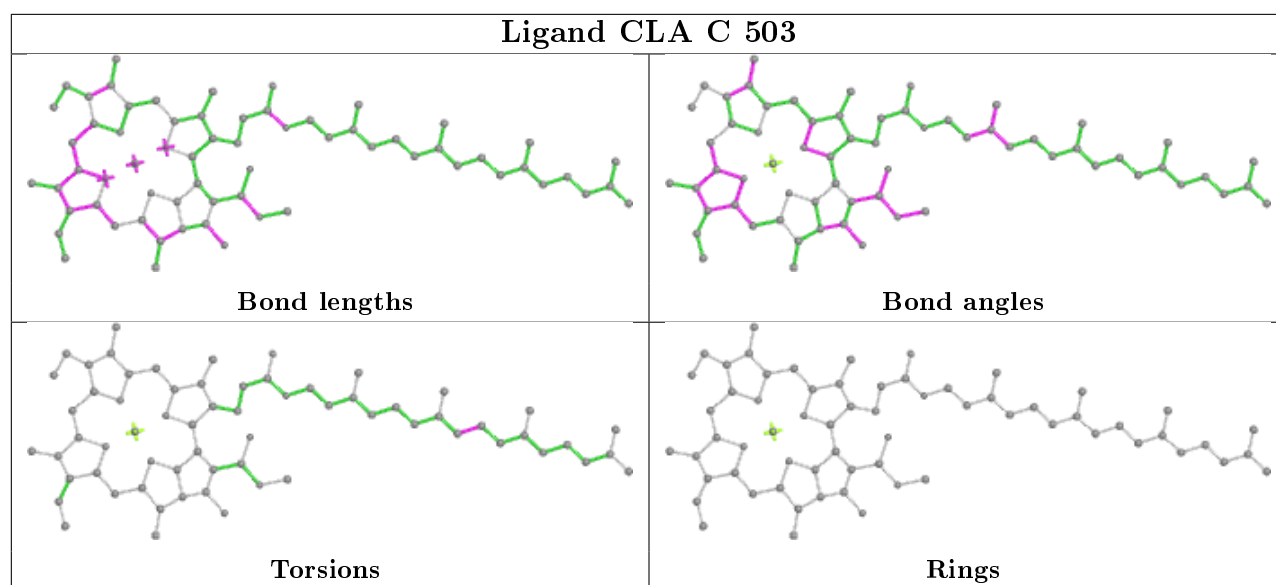
## Ligand CLA b 611

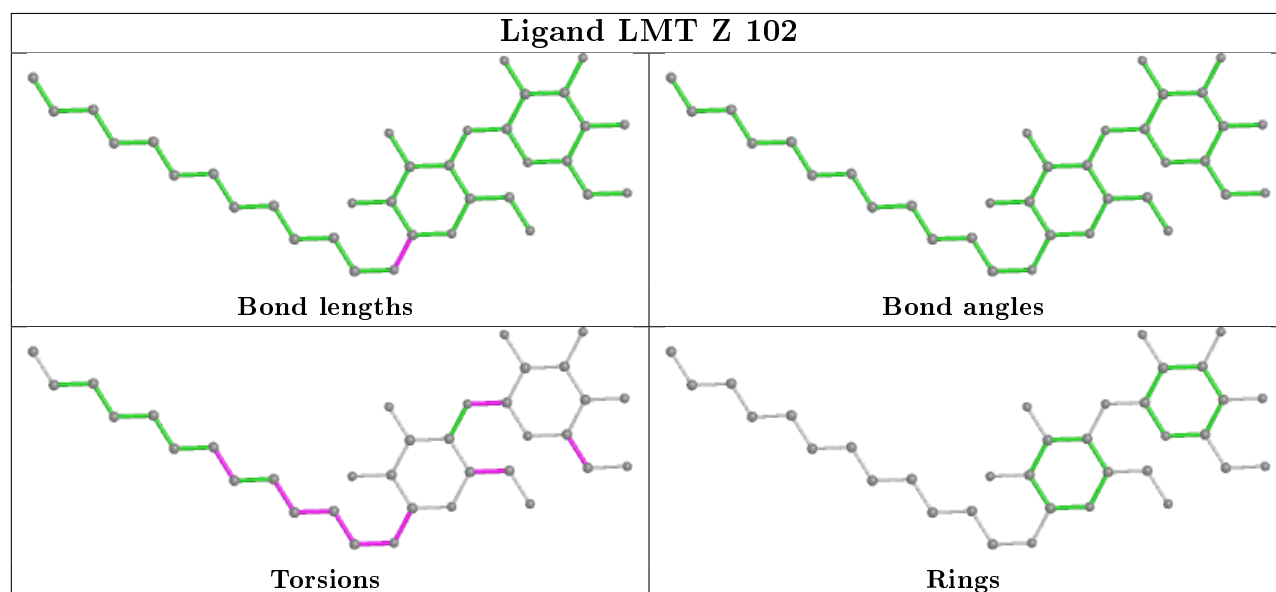
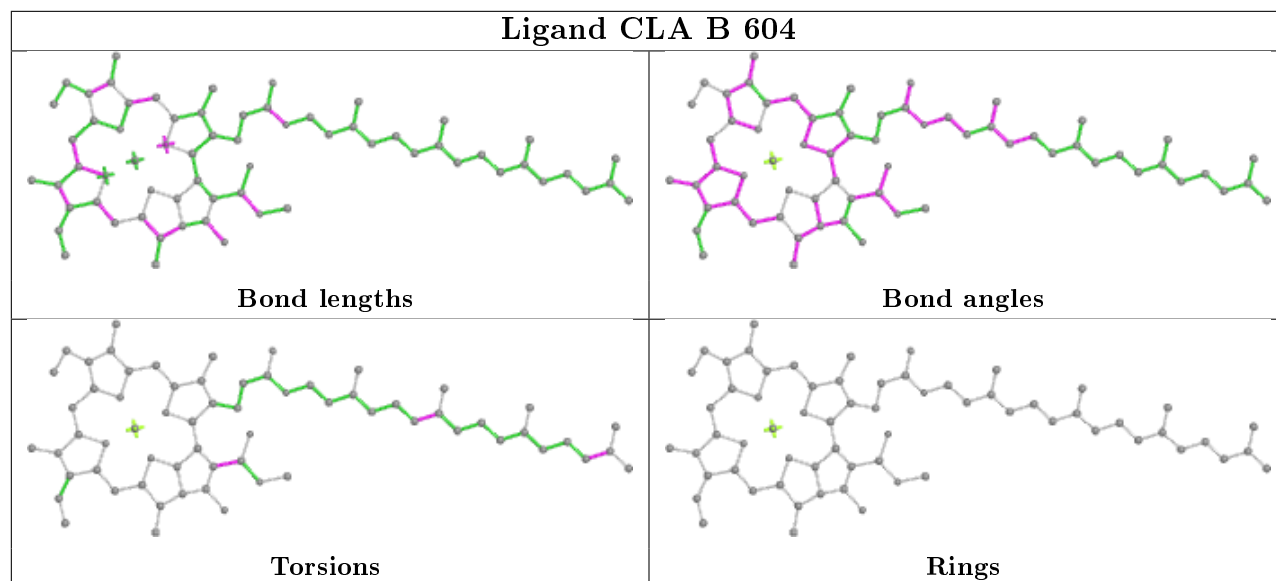
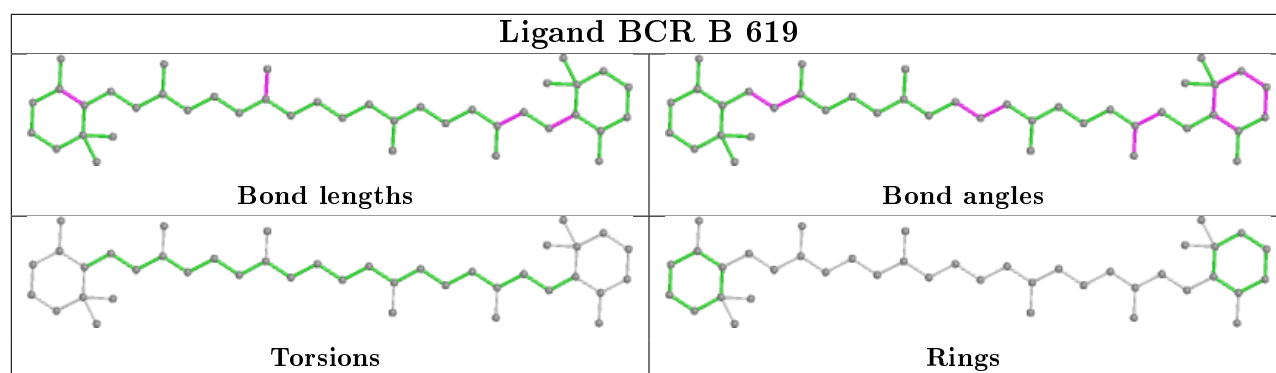


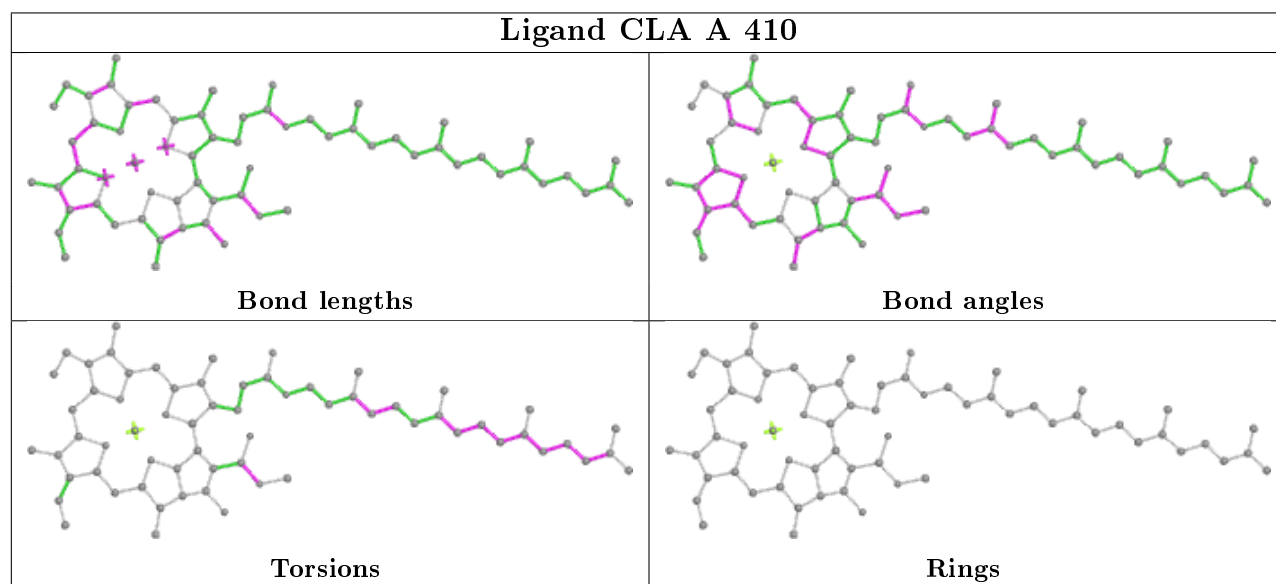
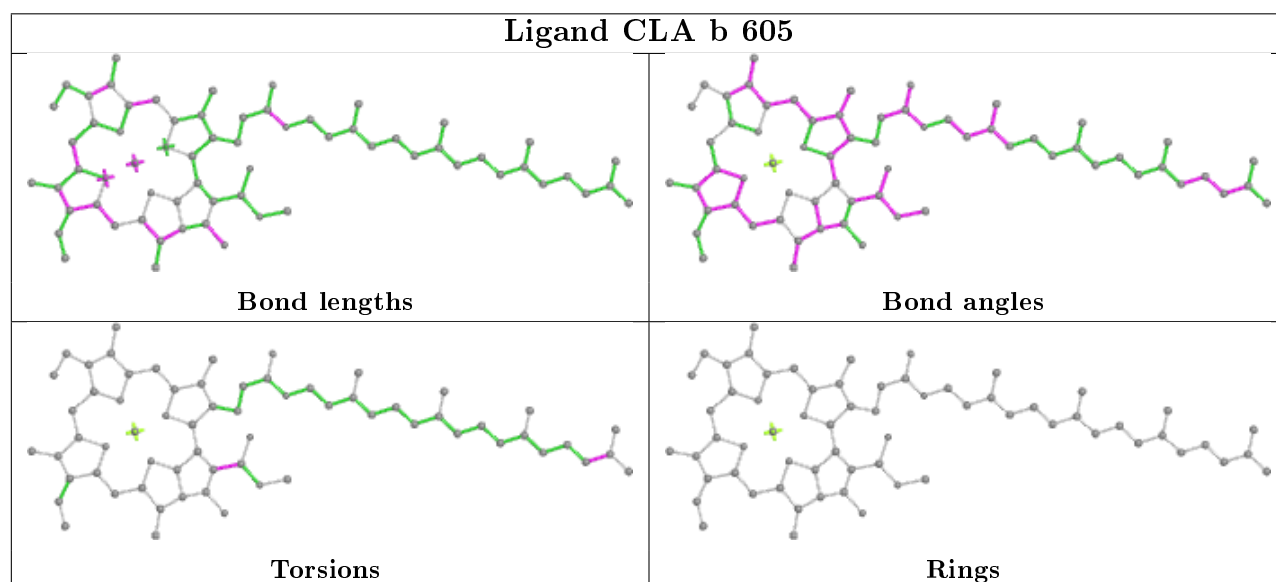
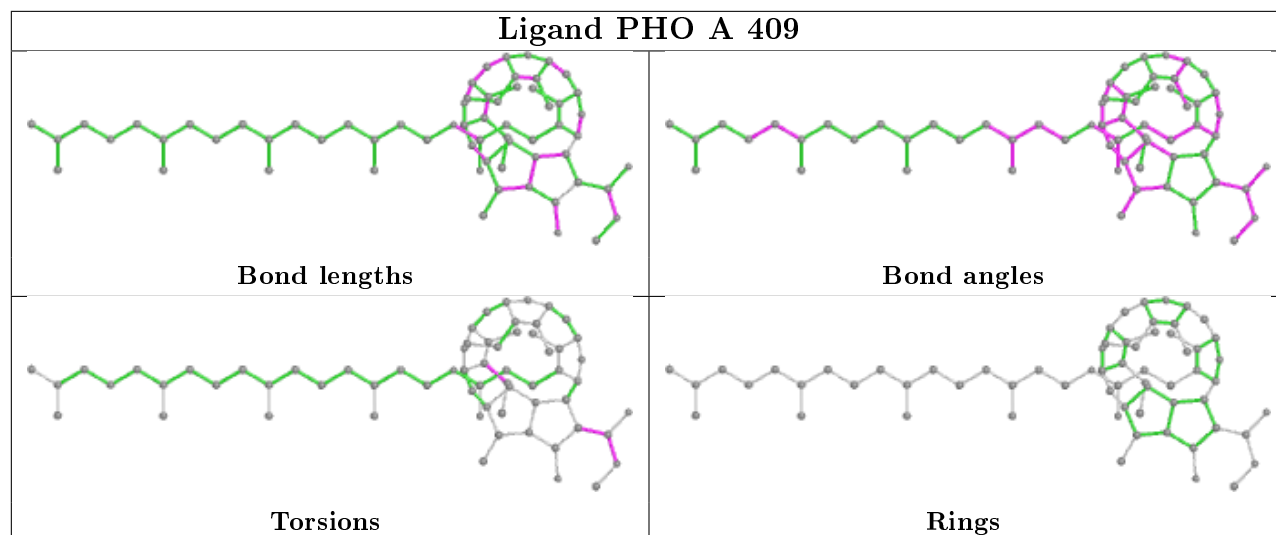
## Ligand HTG C 522

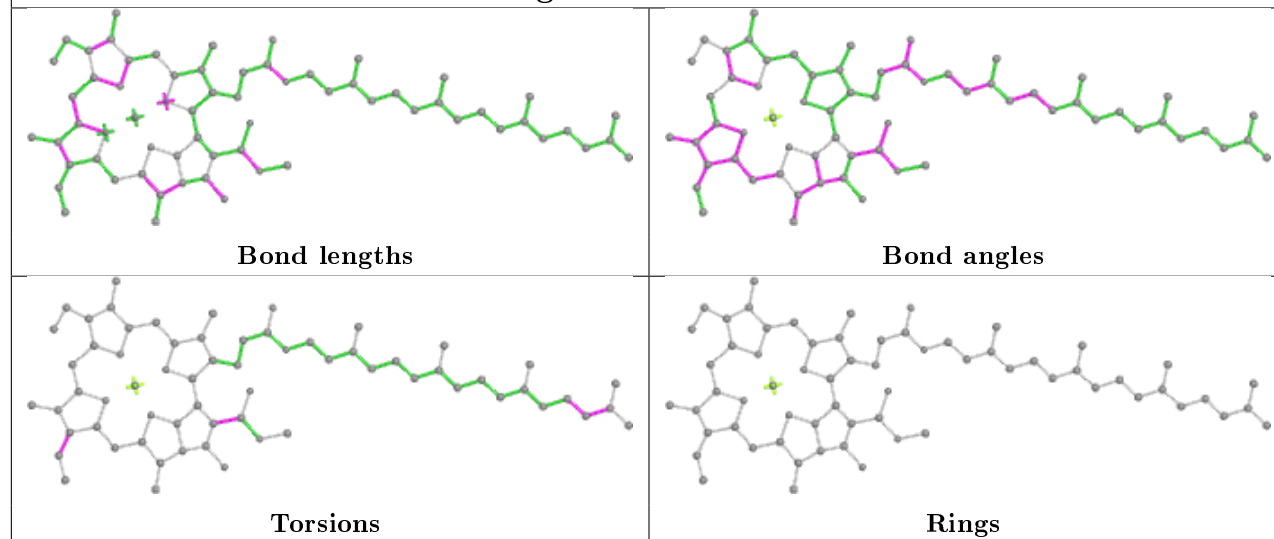
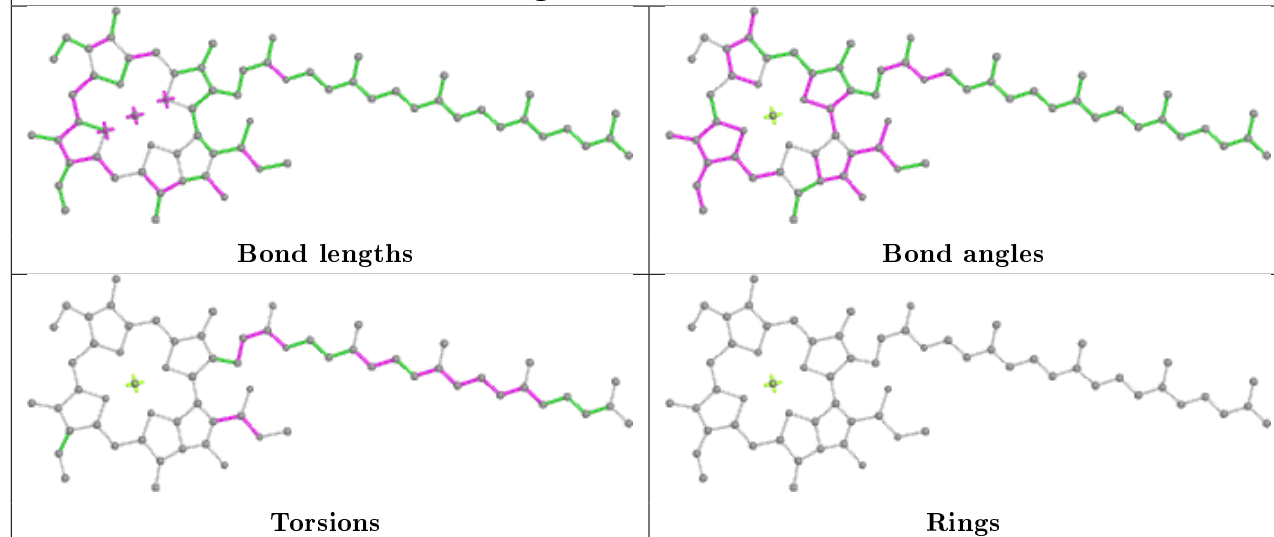
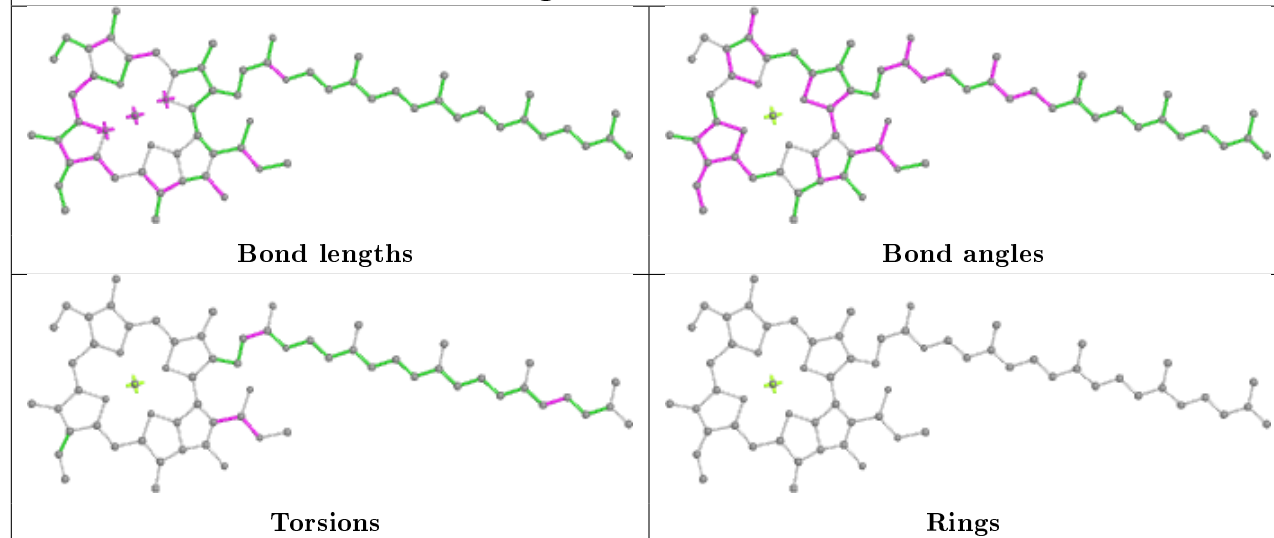




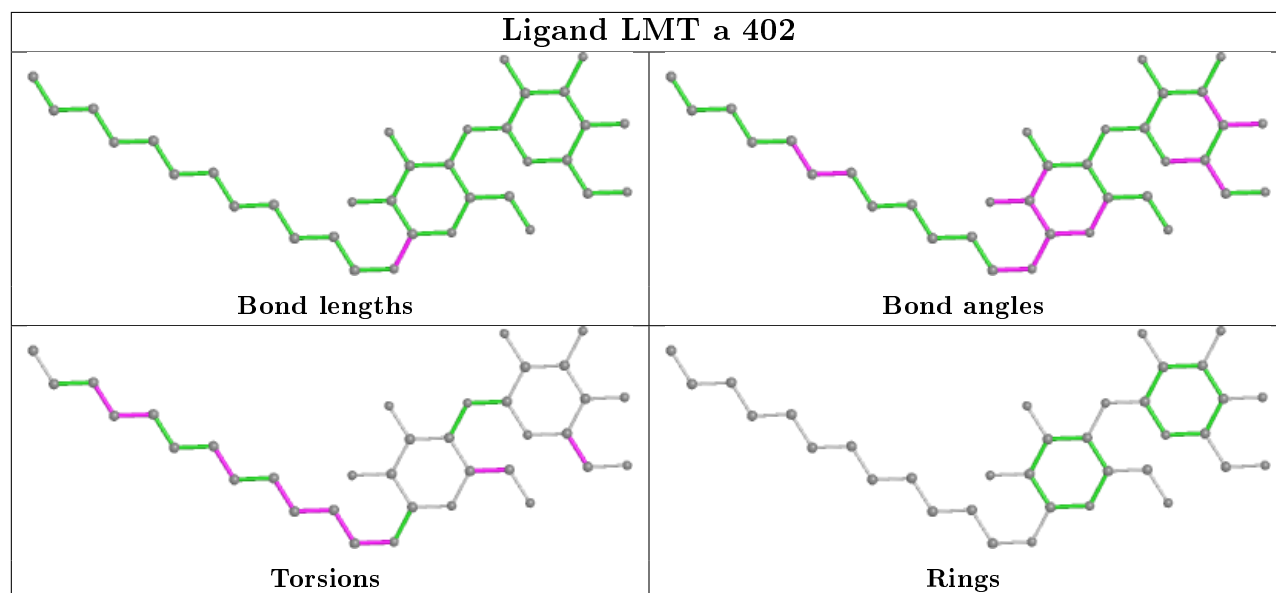
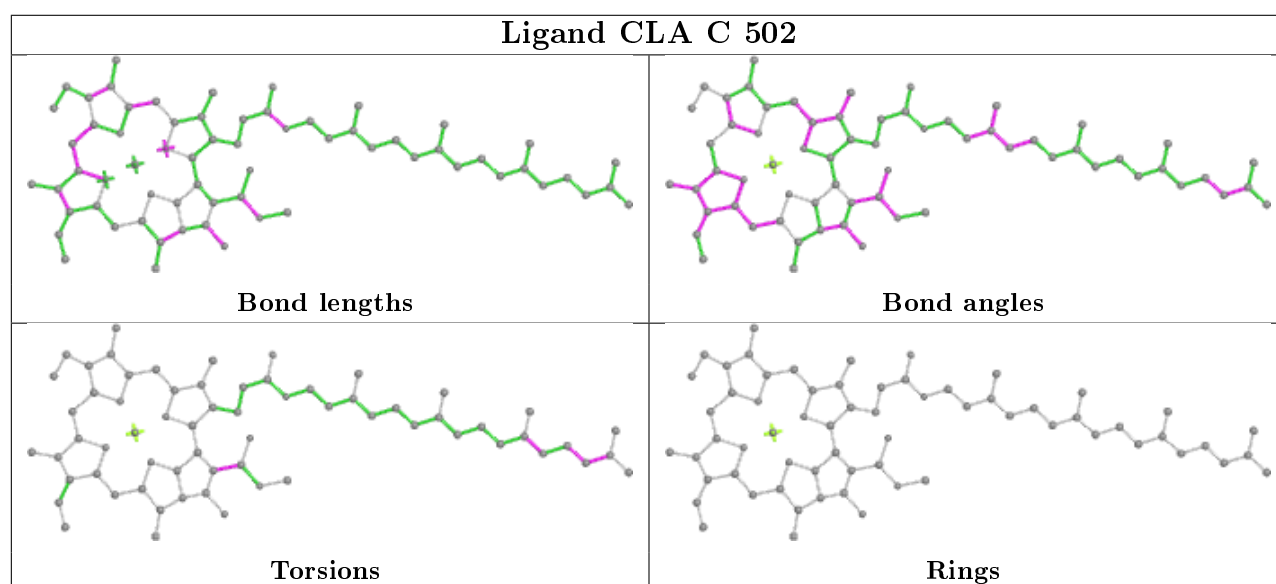
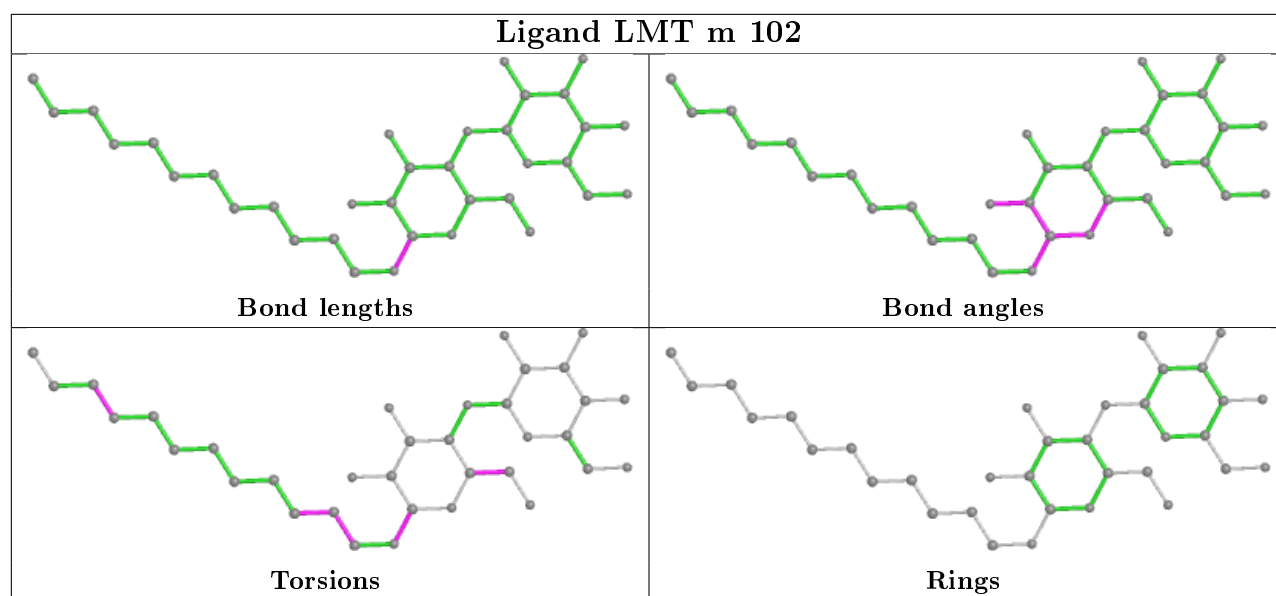


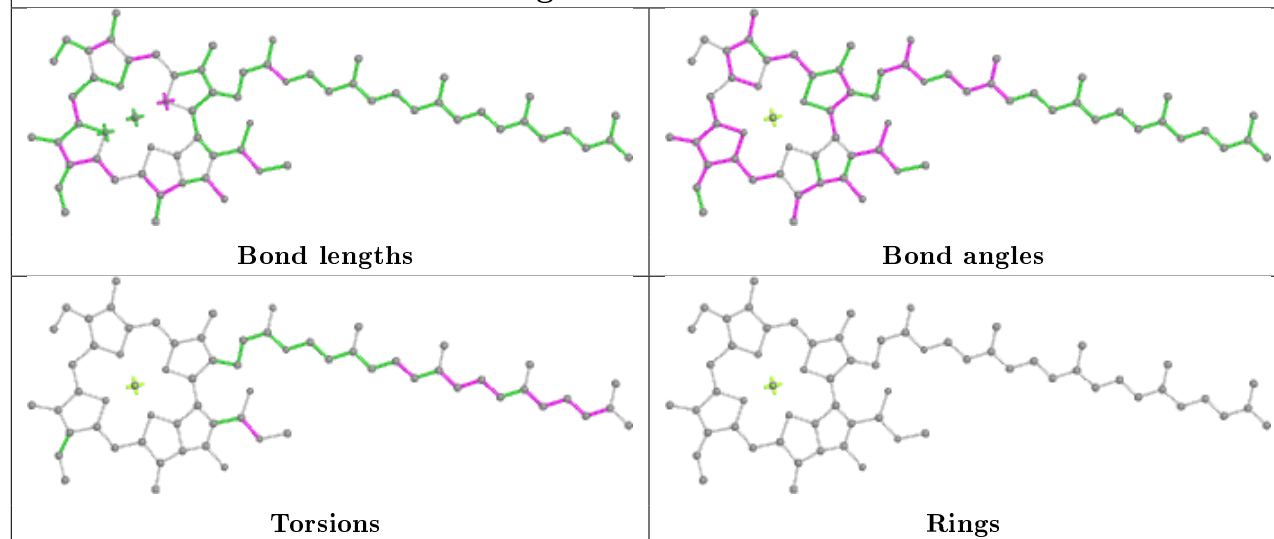
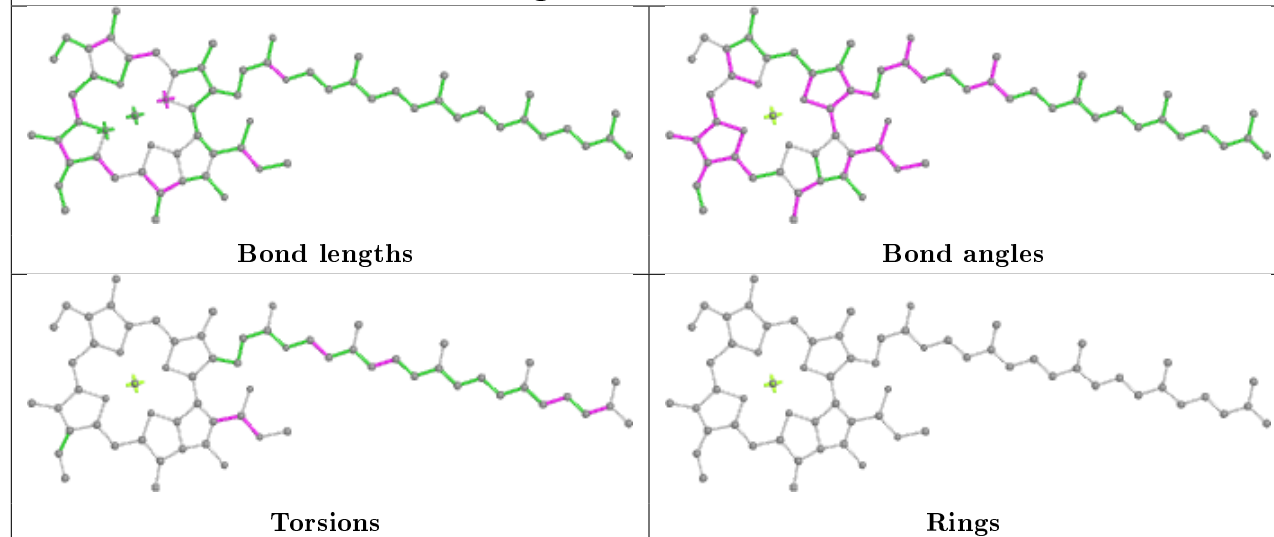


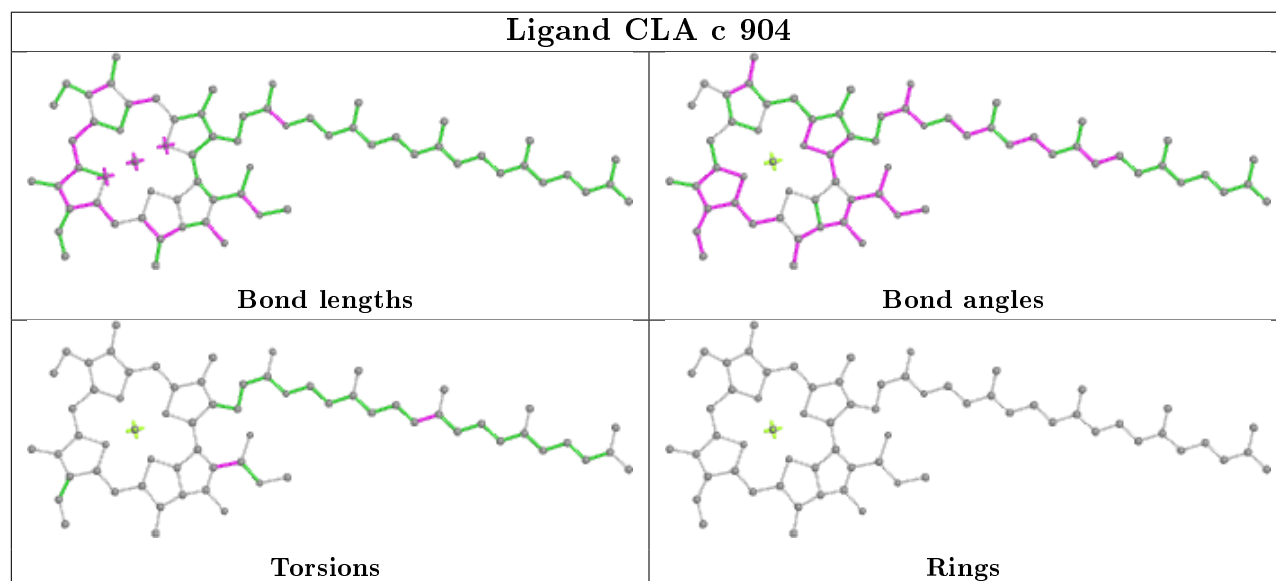
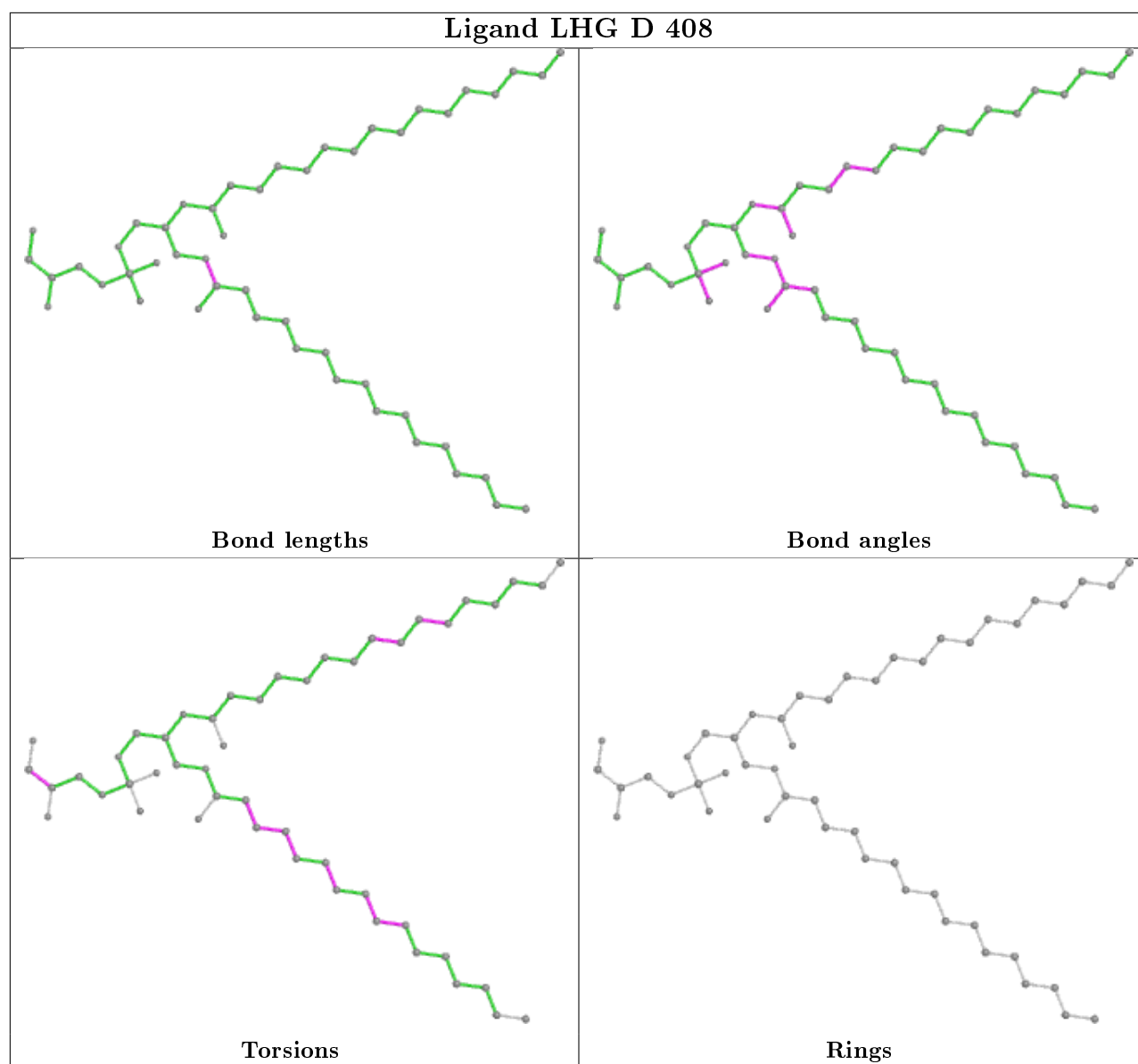


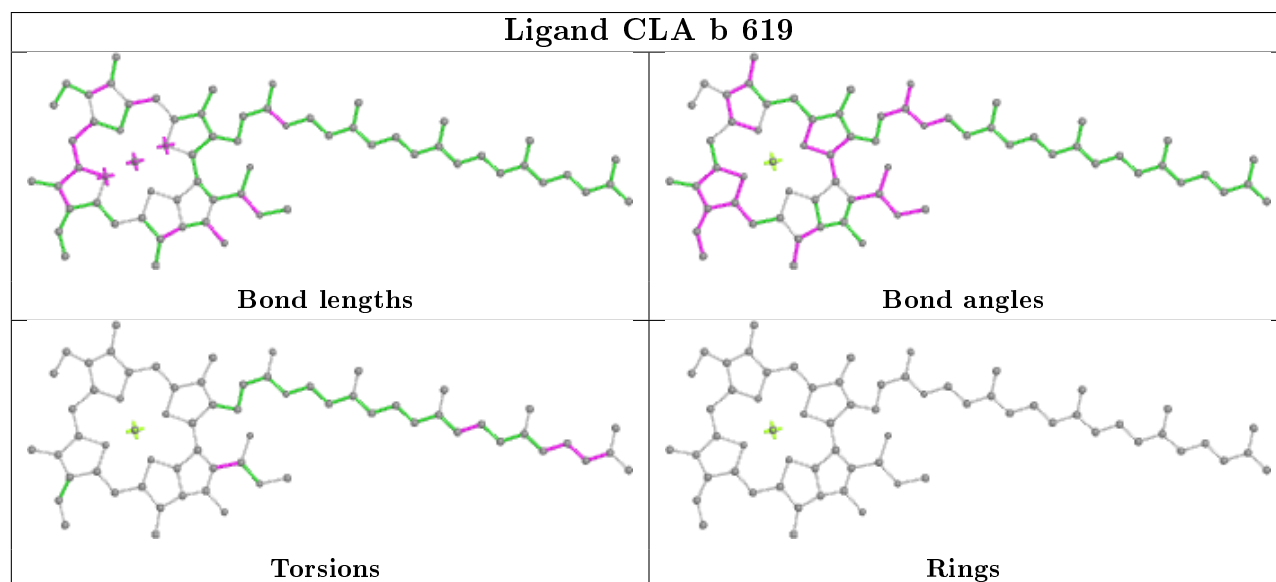
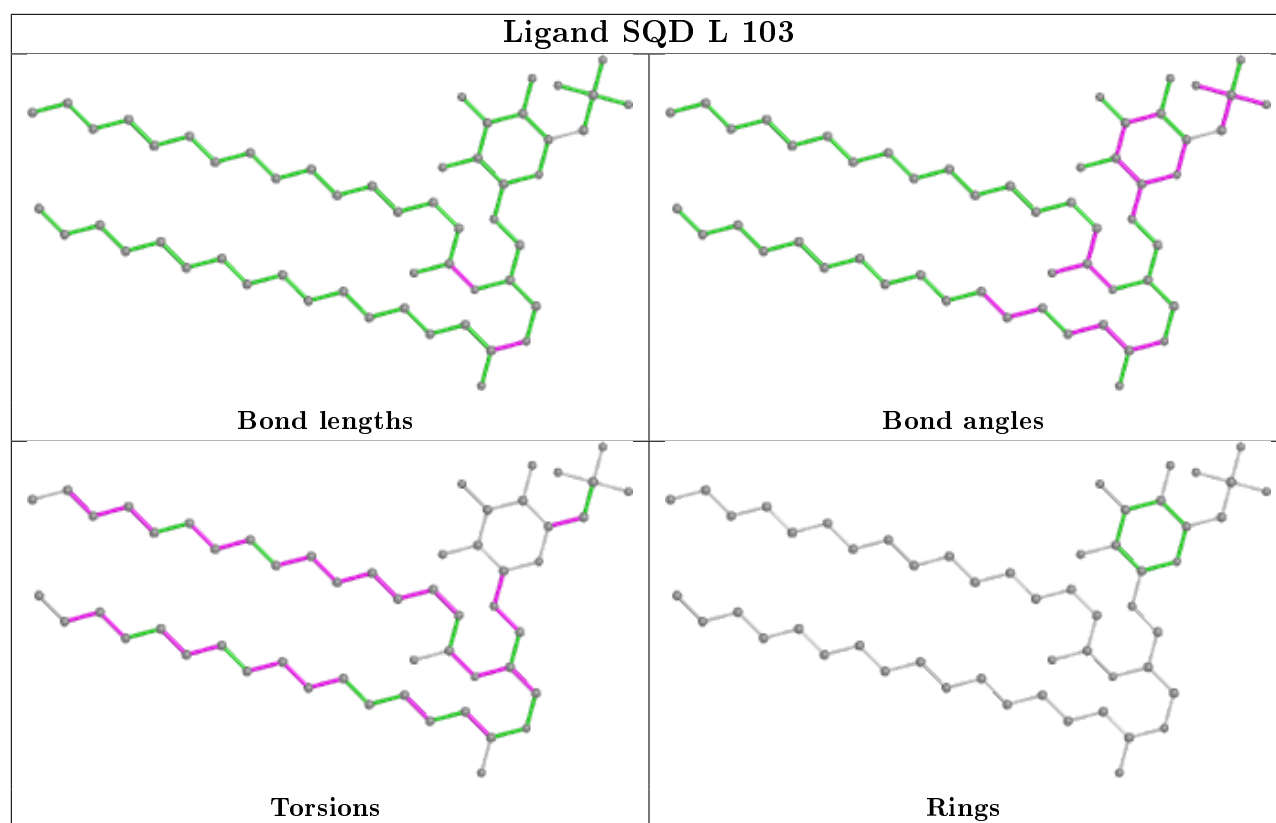
**Ligand CLA a 409****Ligand CLA B 602****Ligand CLA c 902**



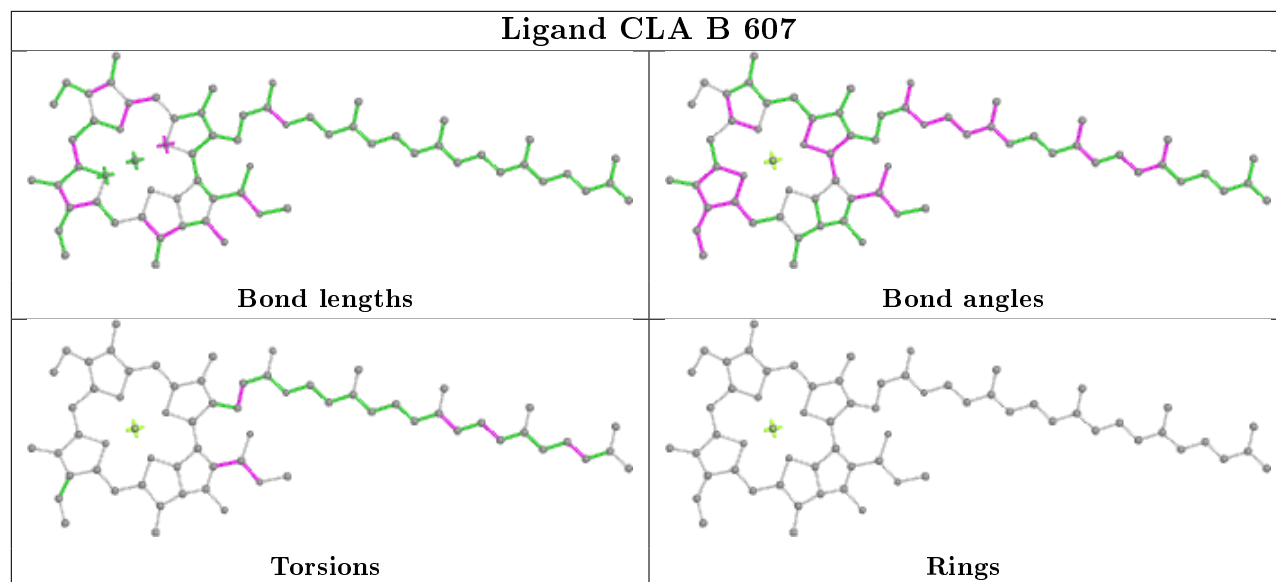


**Ligand CLA a 414****Ligand CLA B 605**

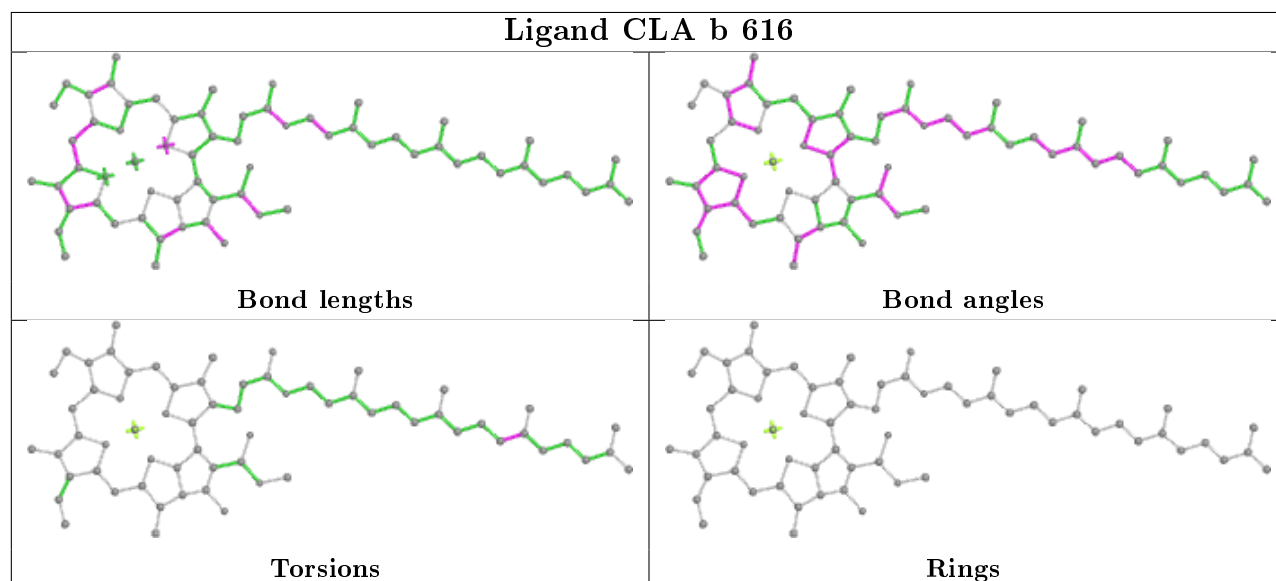




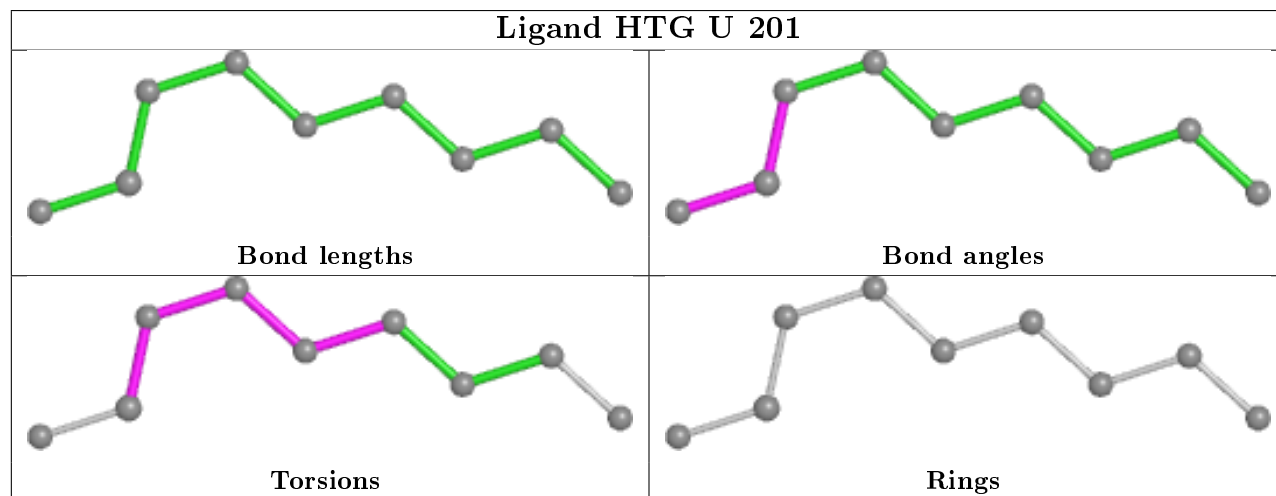
## Ligand CLA B 607



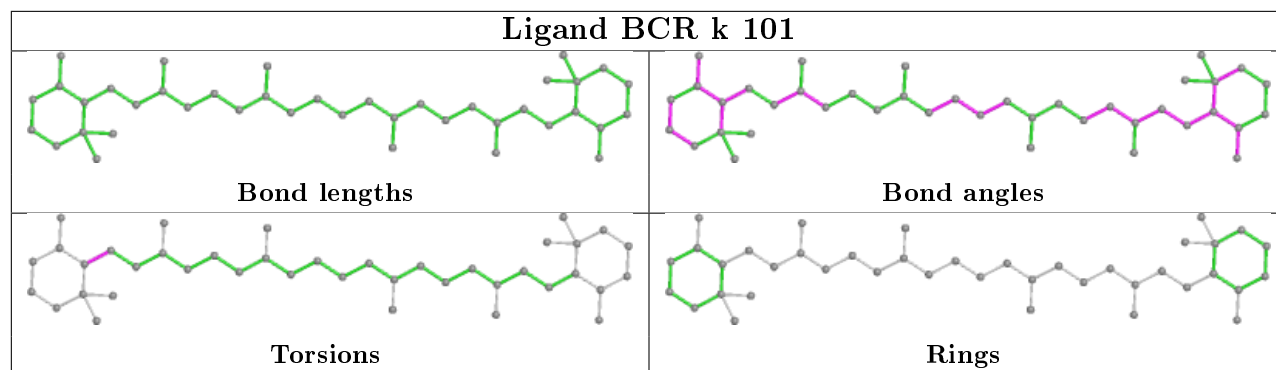
## Ligand CLA b 616



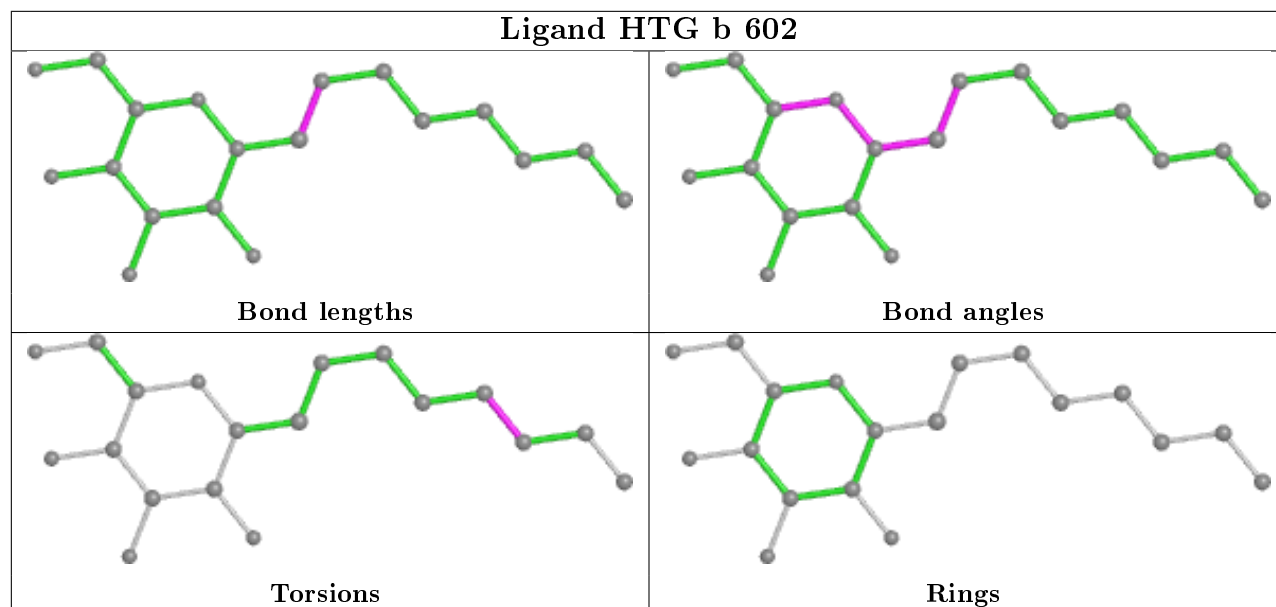
## Ligand HTG U 201



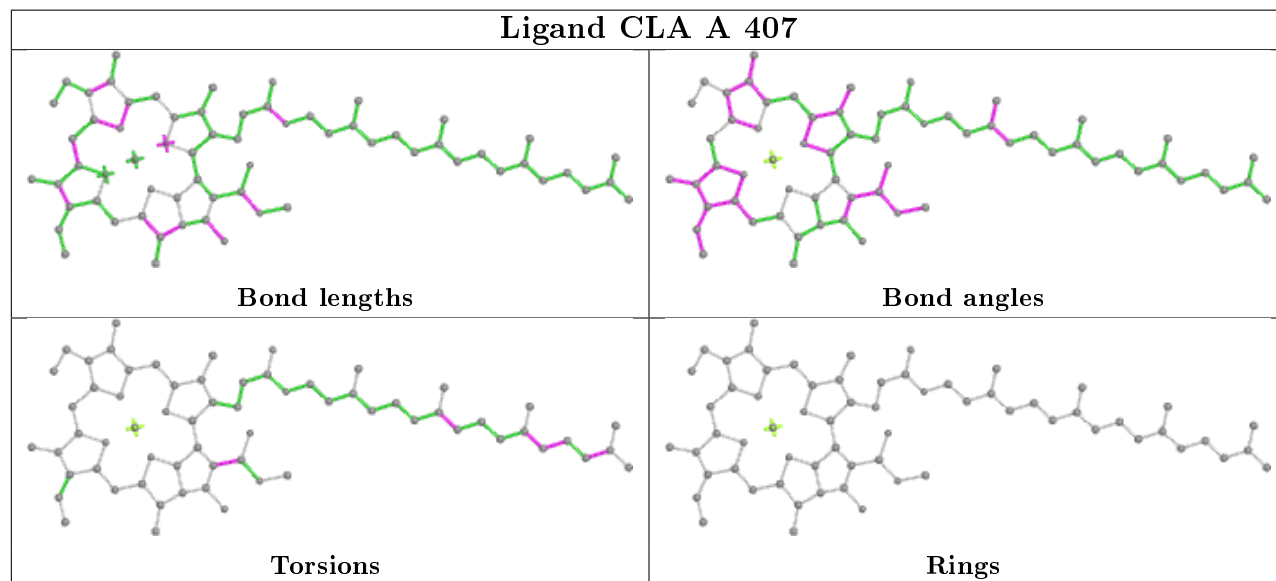
## Ligand BCR k 101

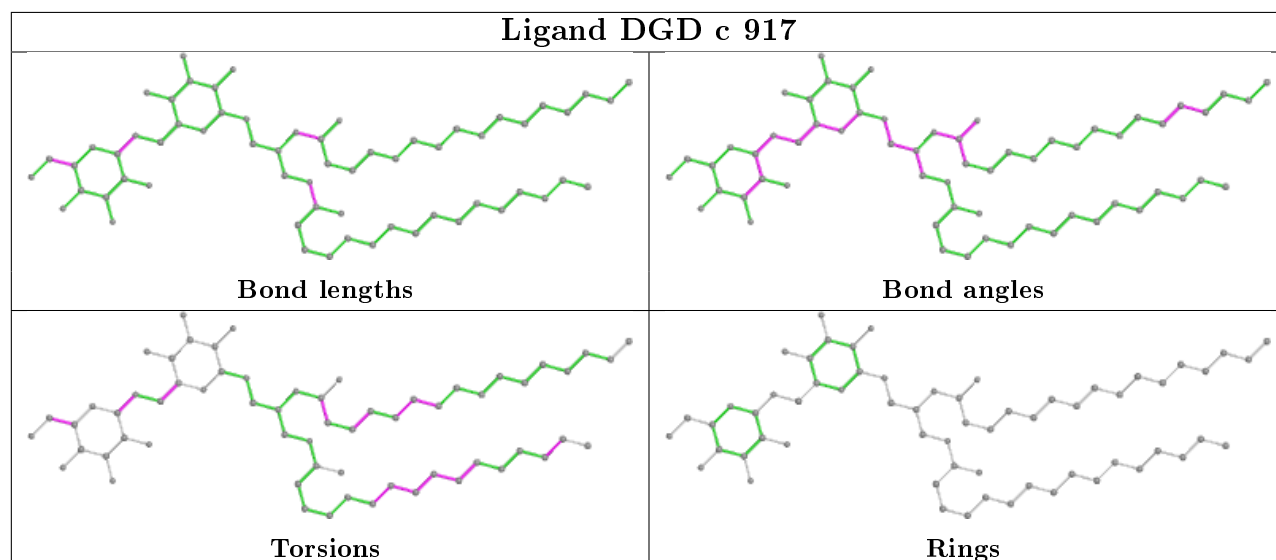
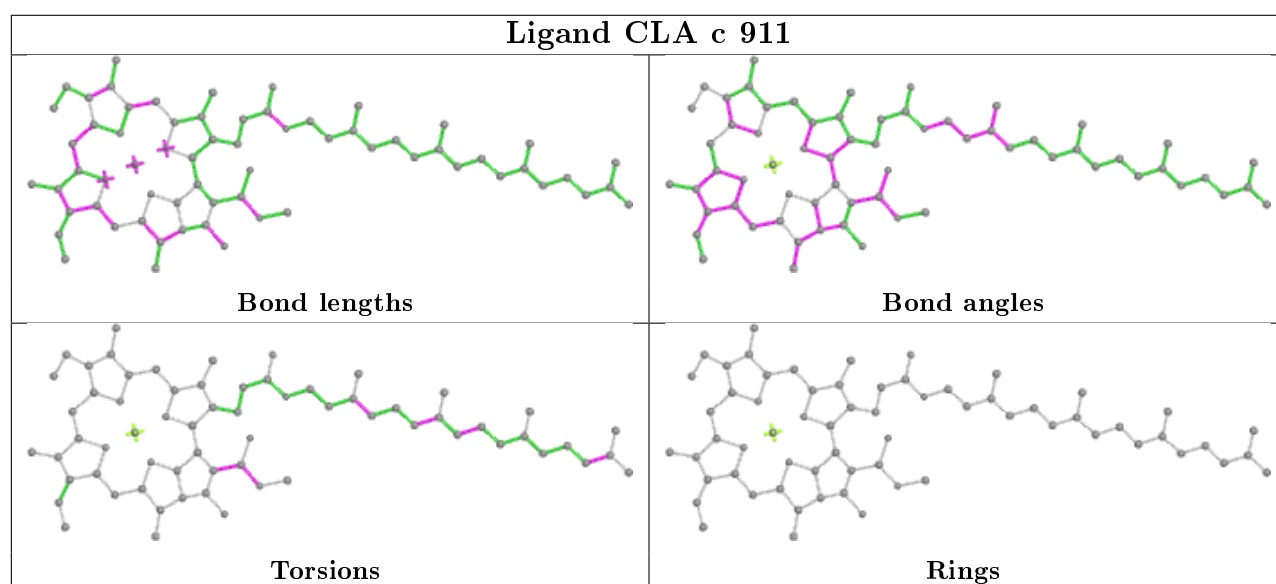
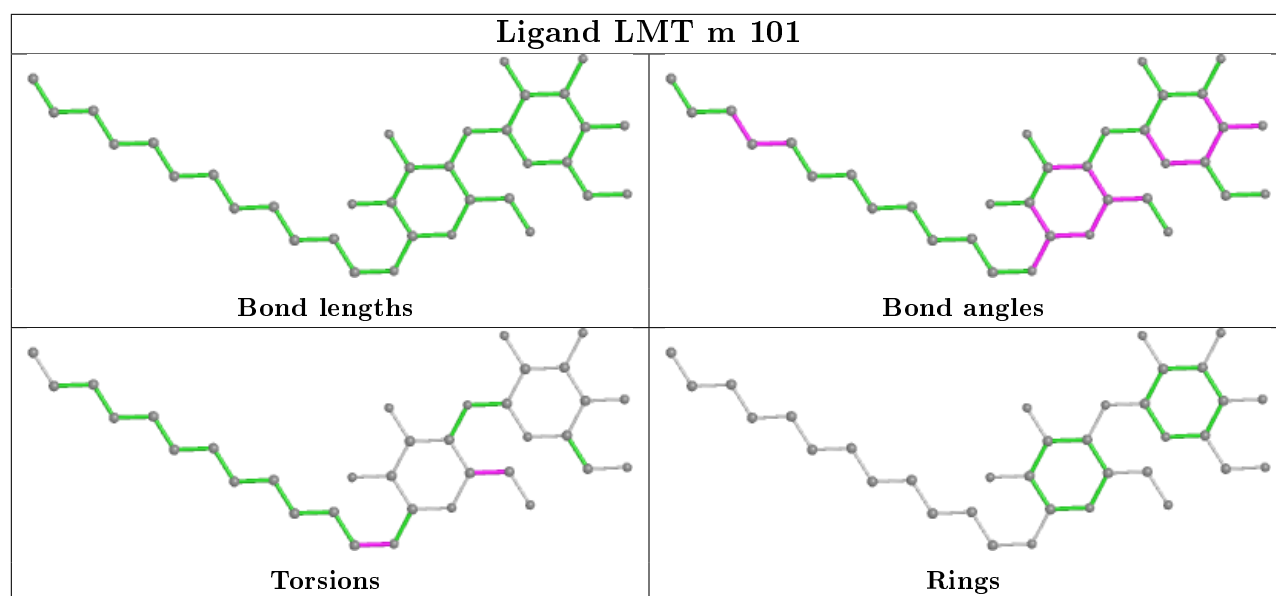


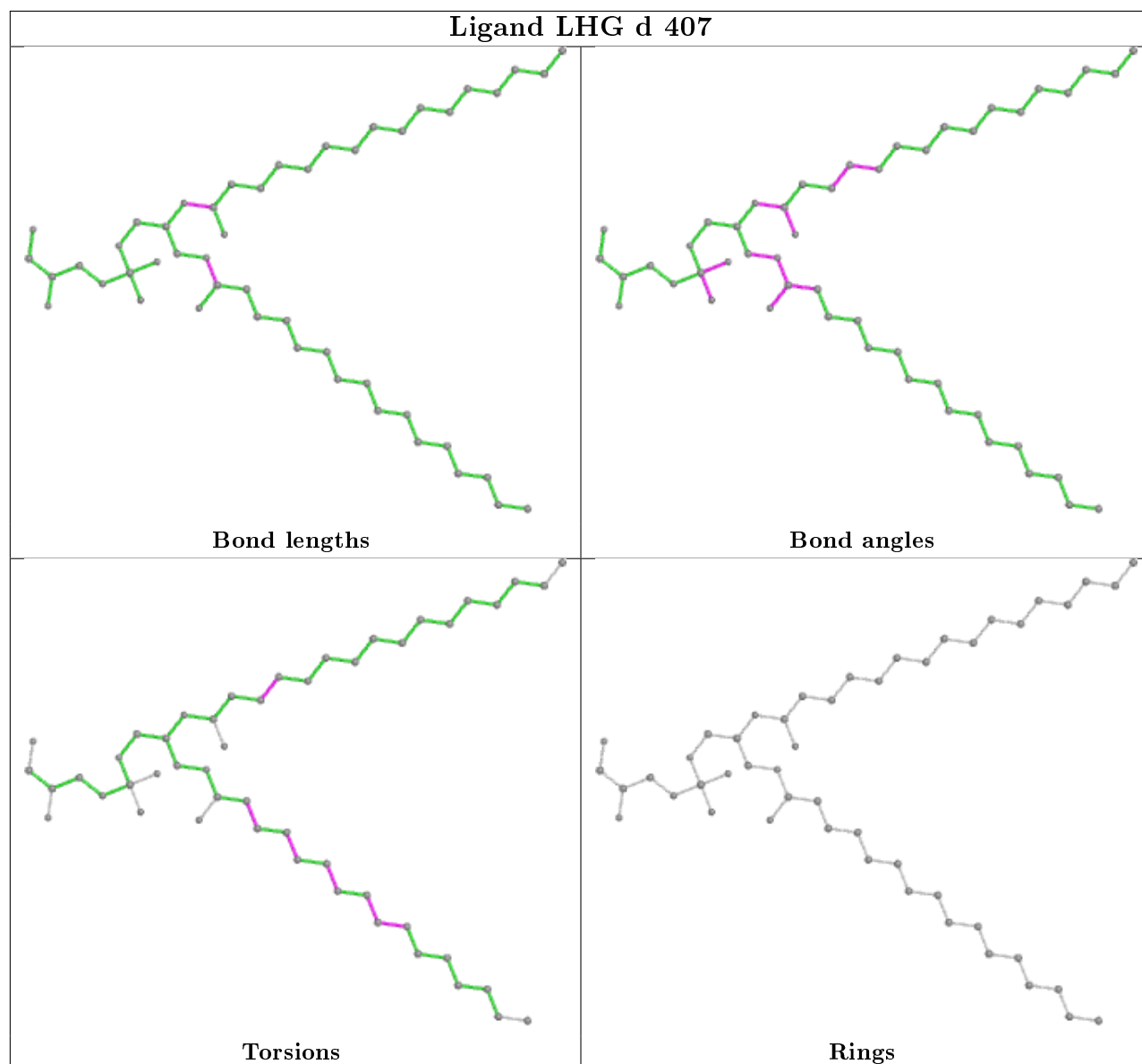
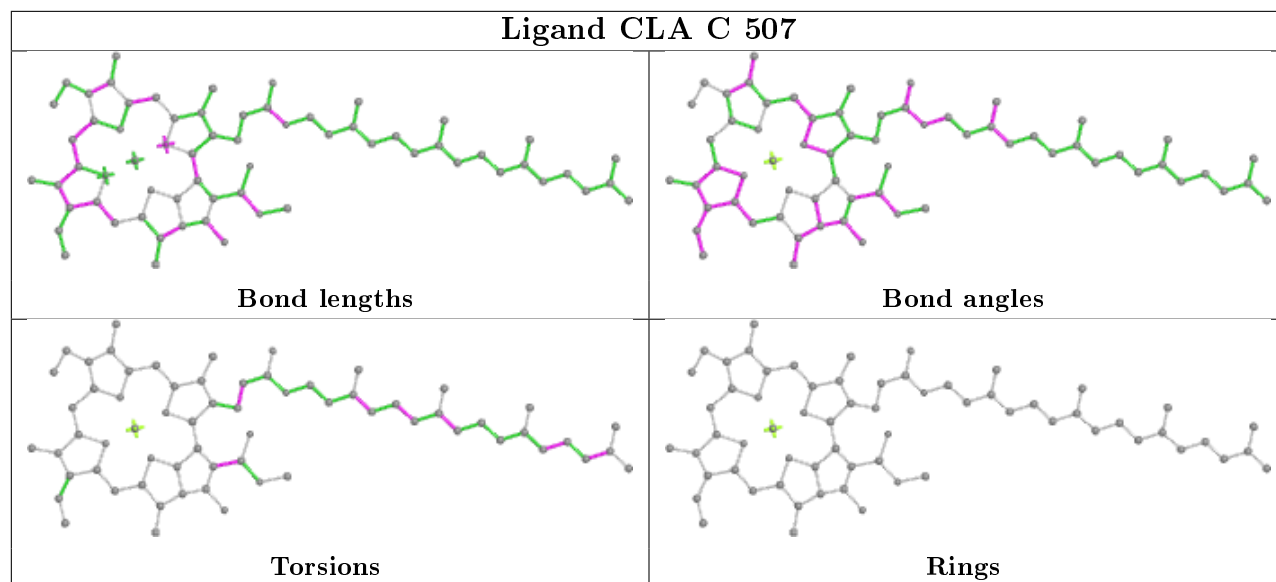
## Ligand HTG b 602



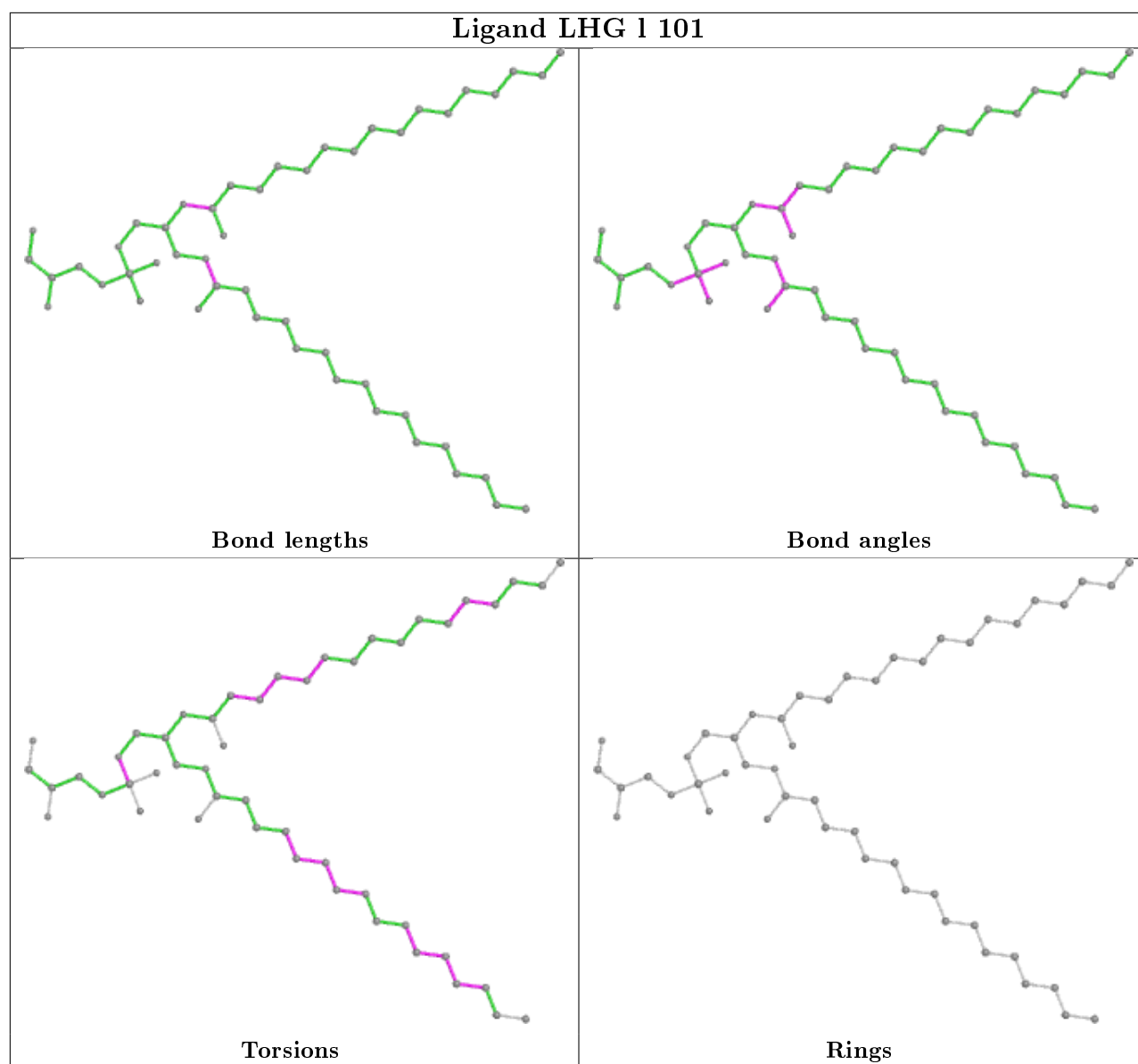
## Ligand CLA A 407

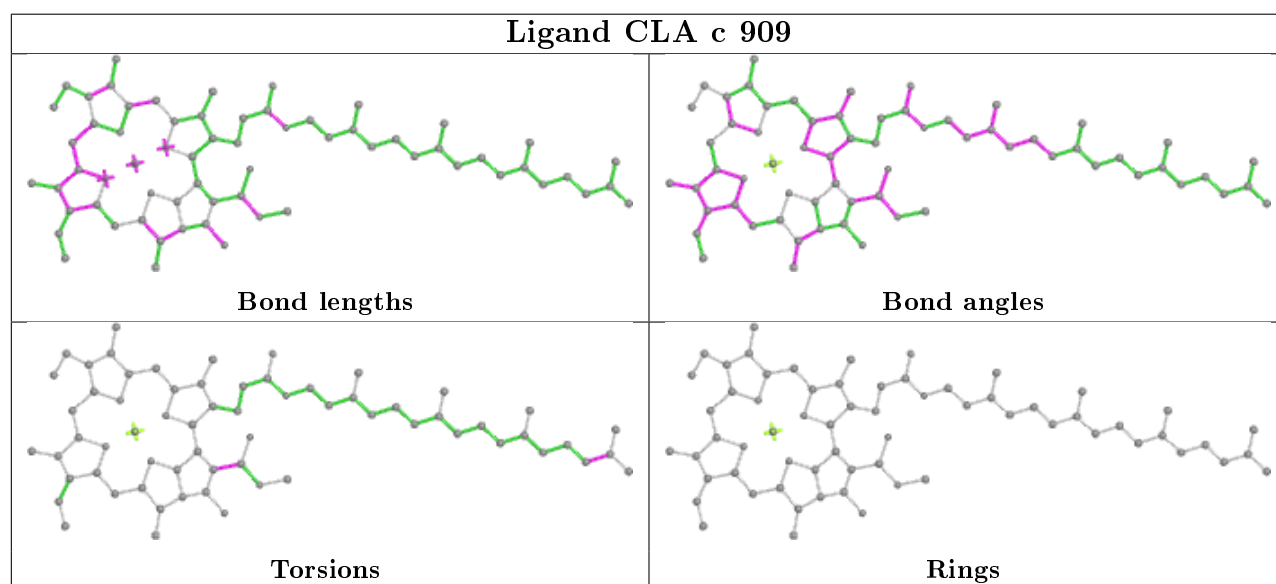
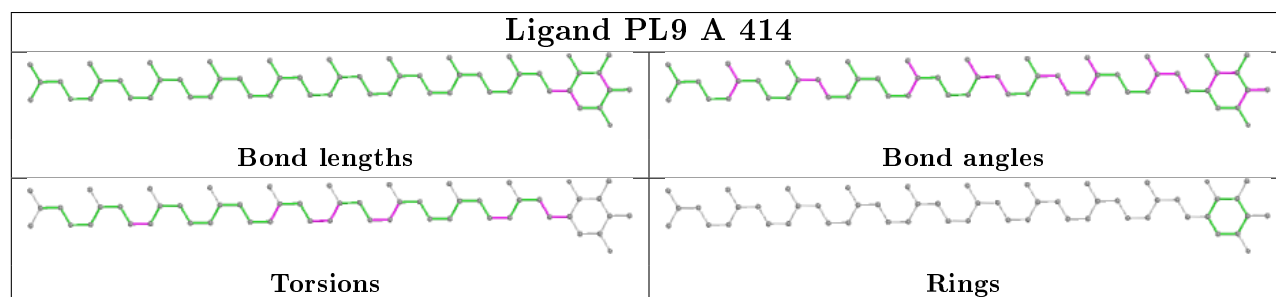
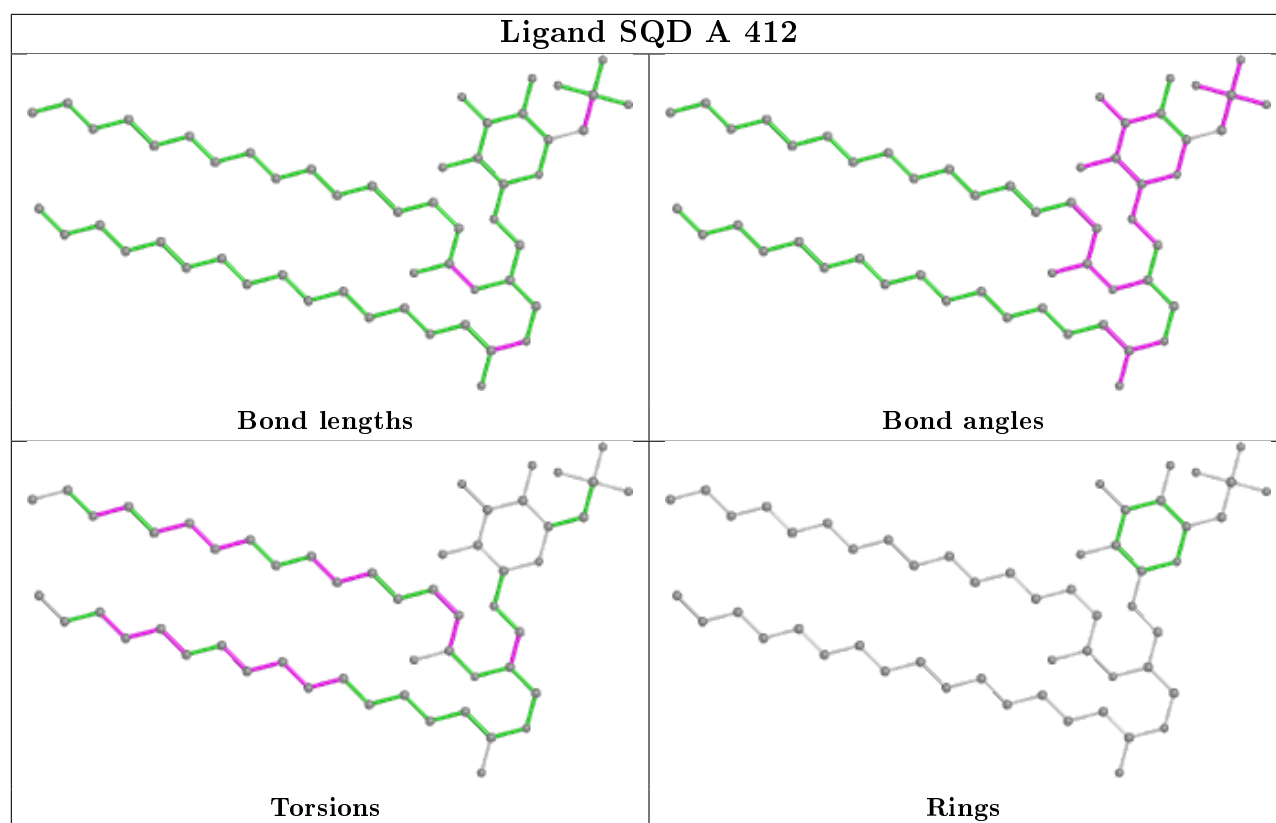


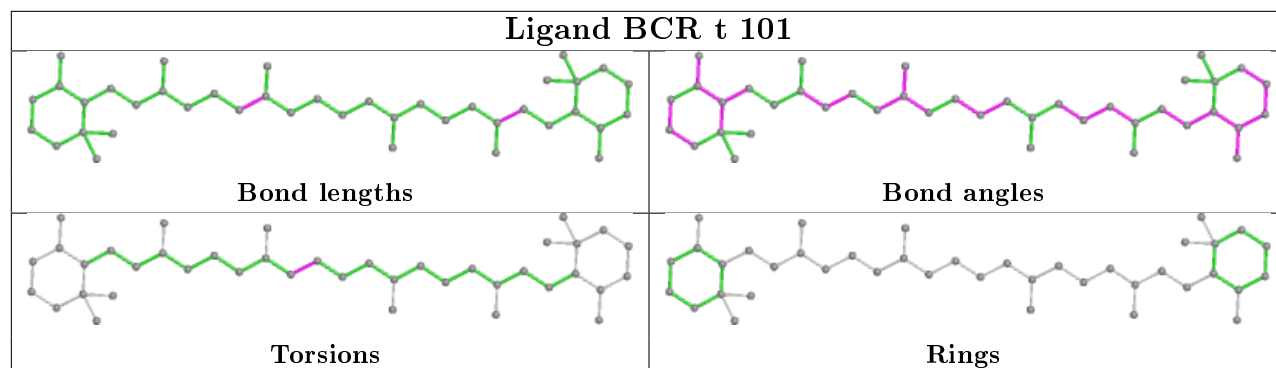
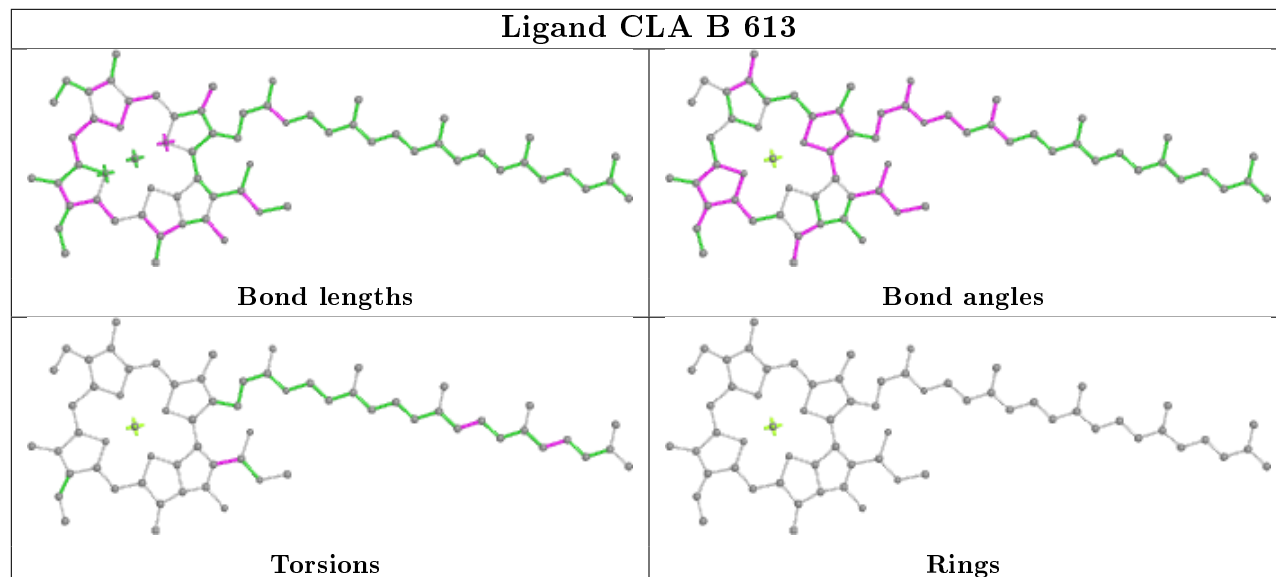
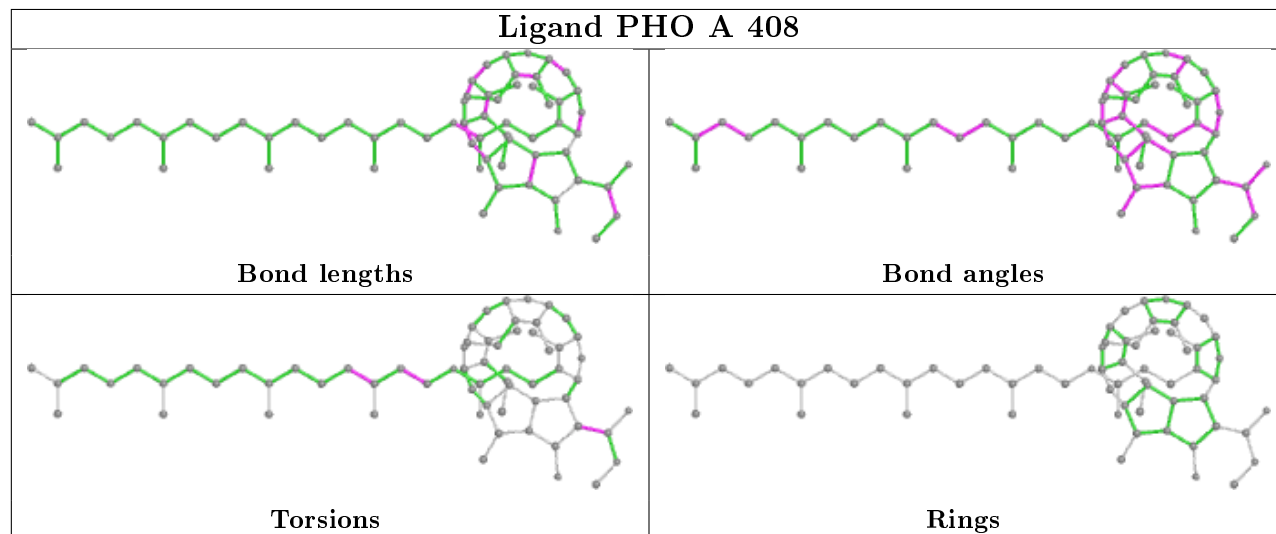




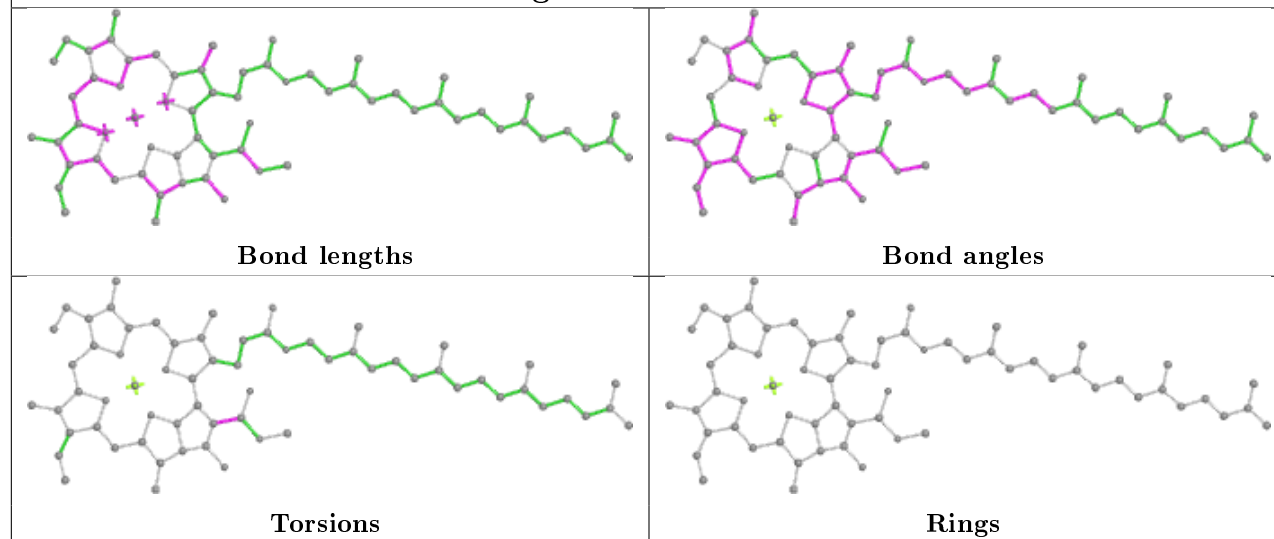




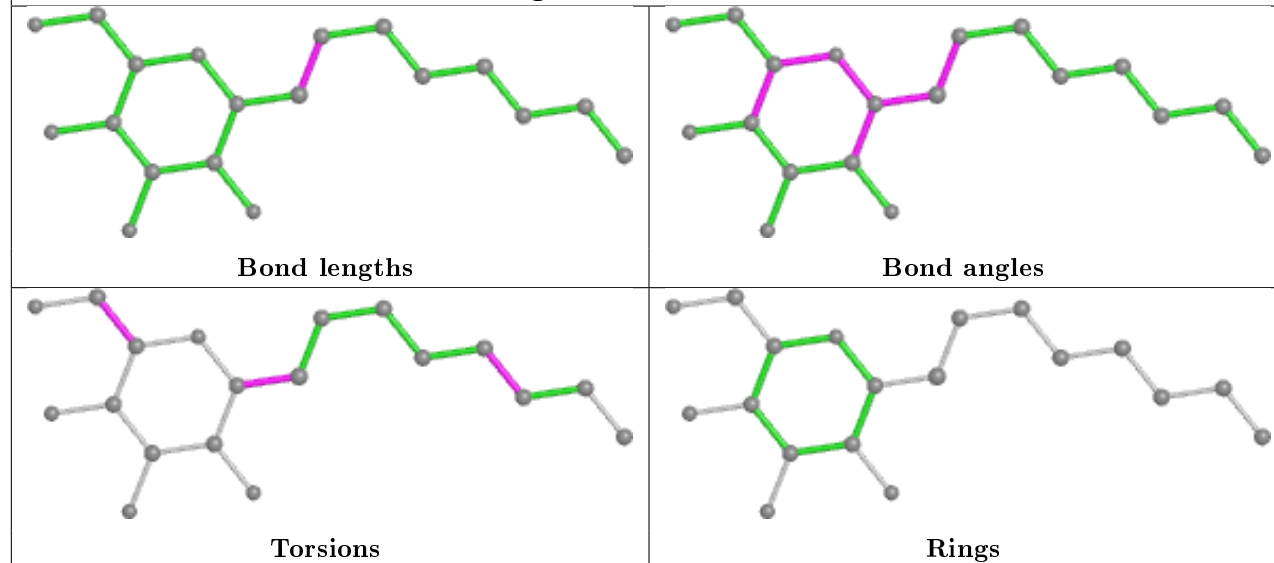


**Ligand BCR t 101****Ligand CLA B 613****Ligand PHO A 408**

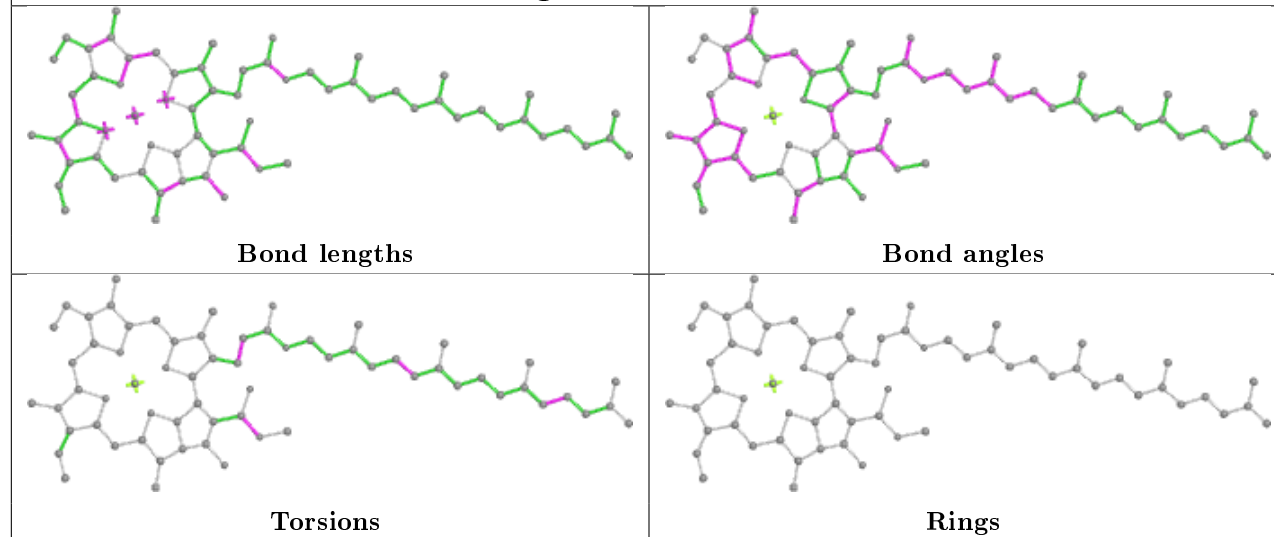
## Ligand CLA B 608

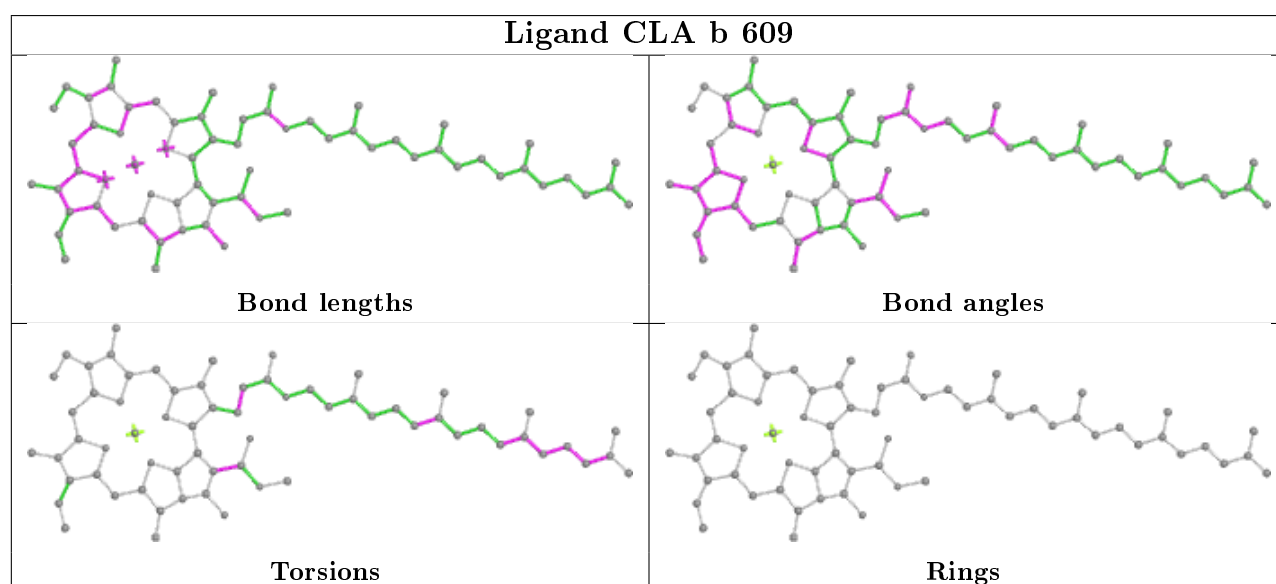
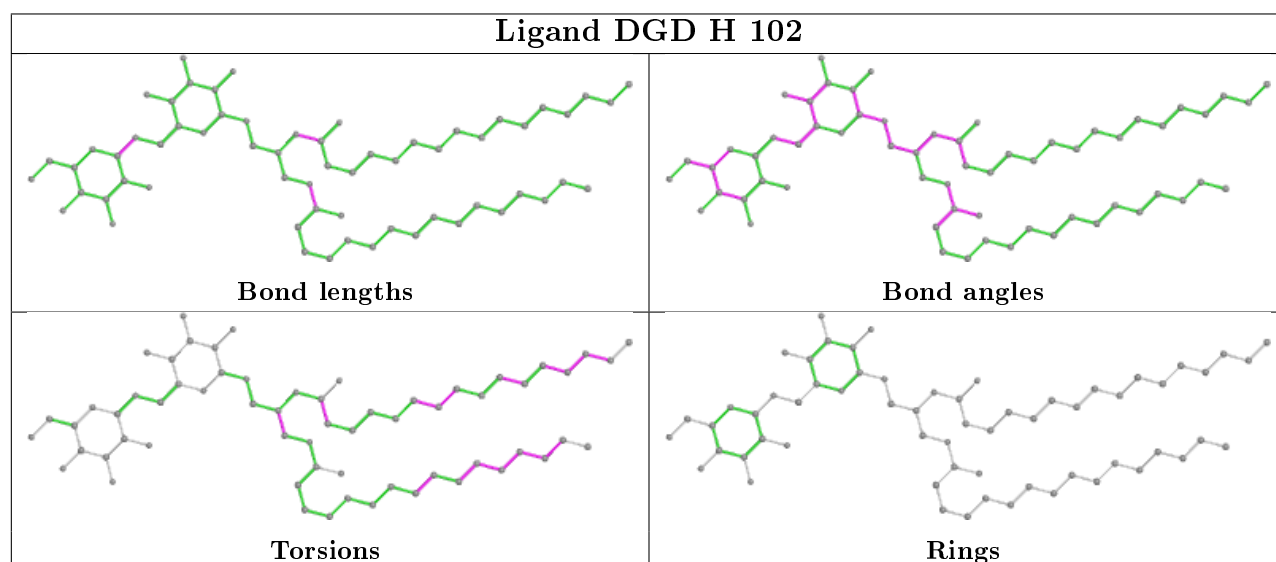
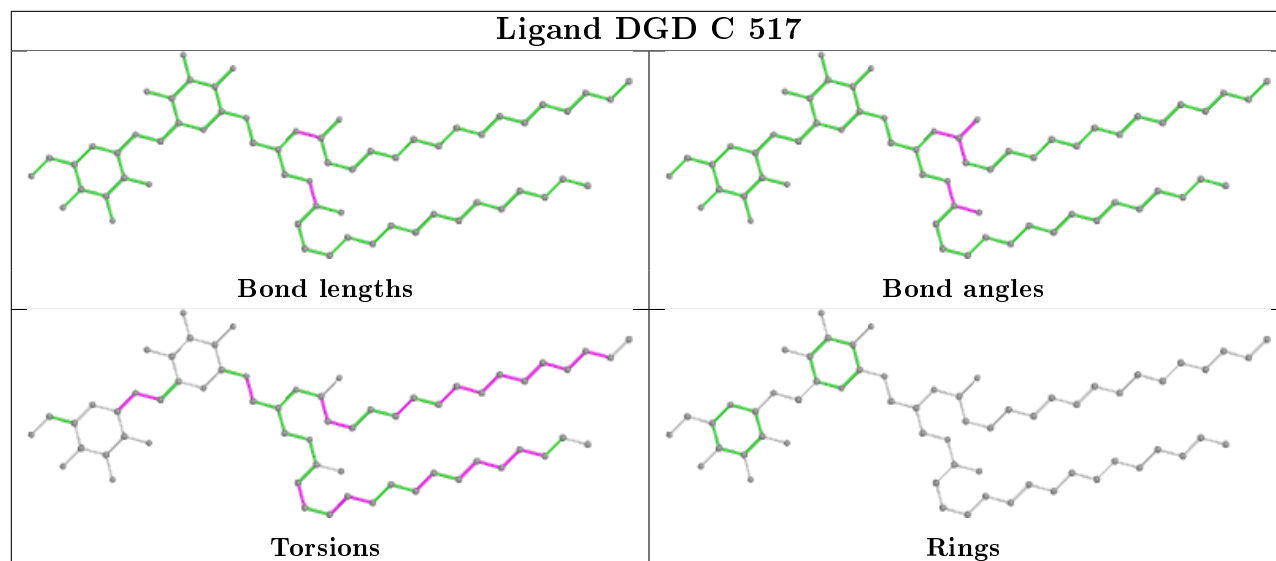


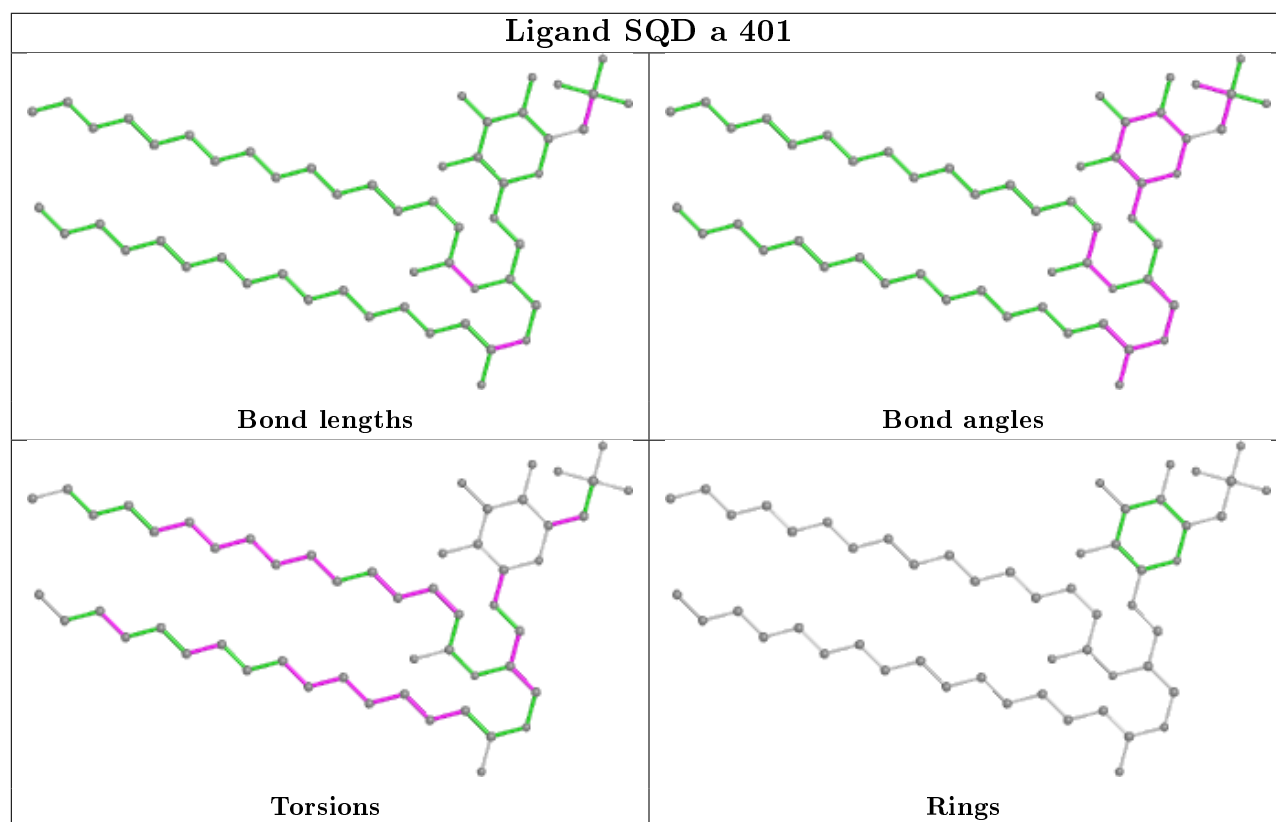
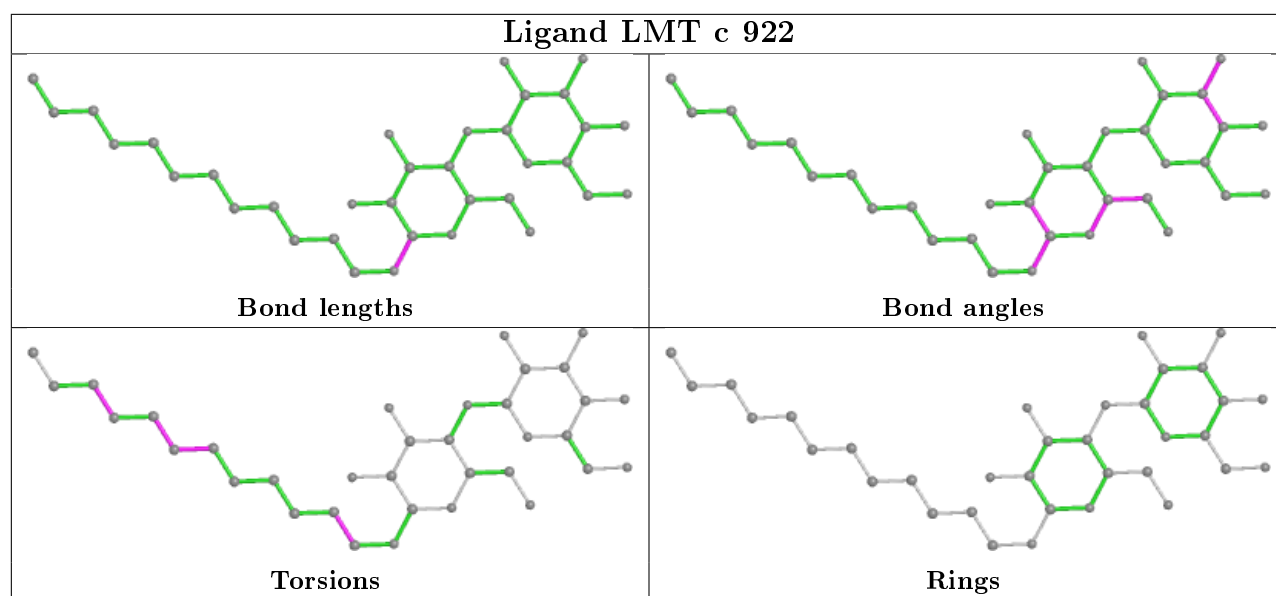
## Ligand HTG B 626

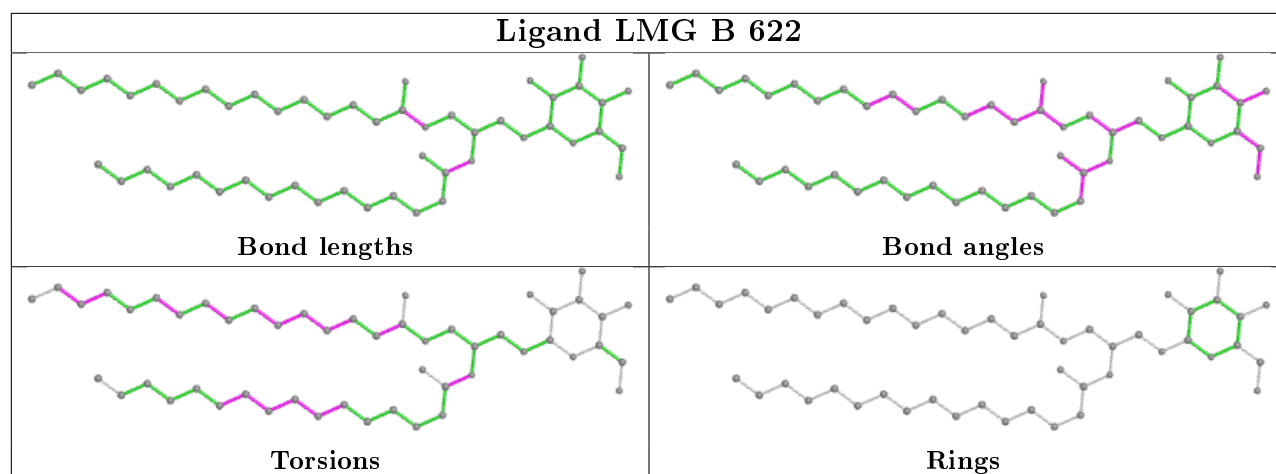
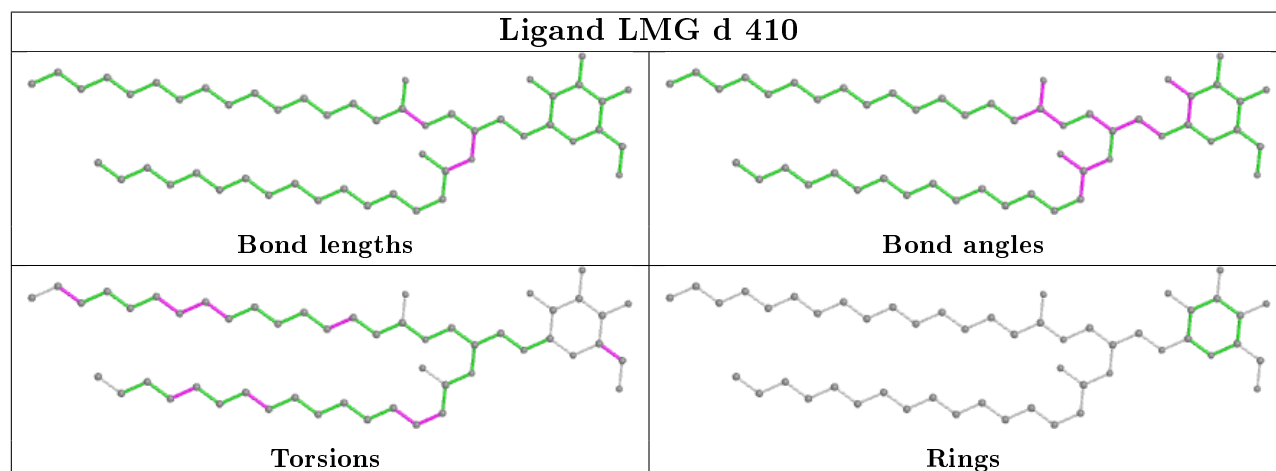
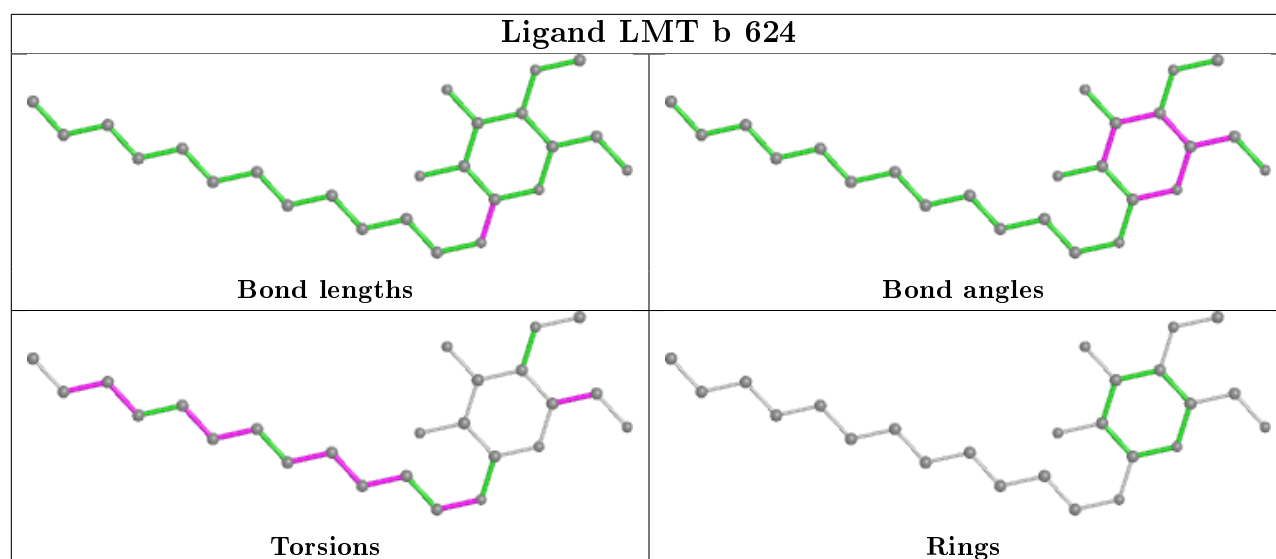


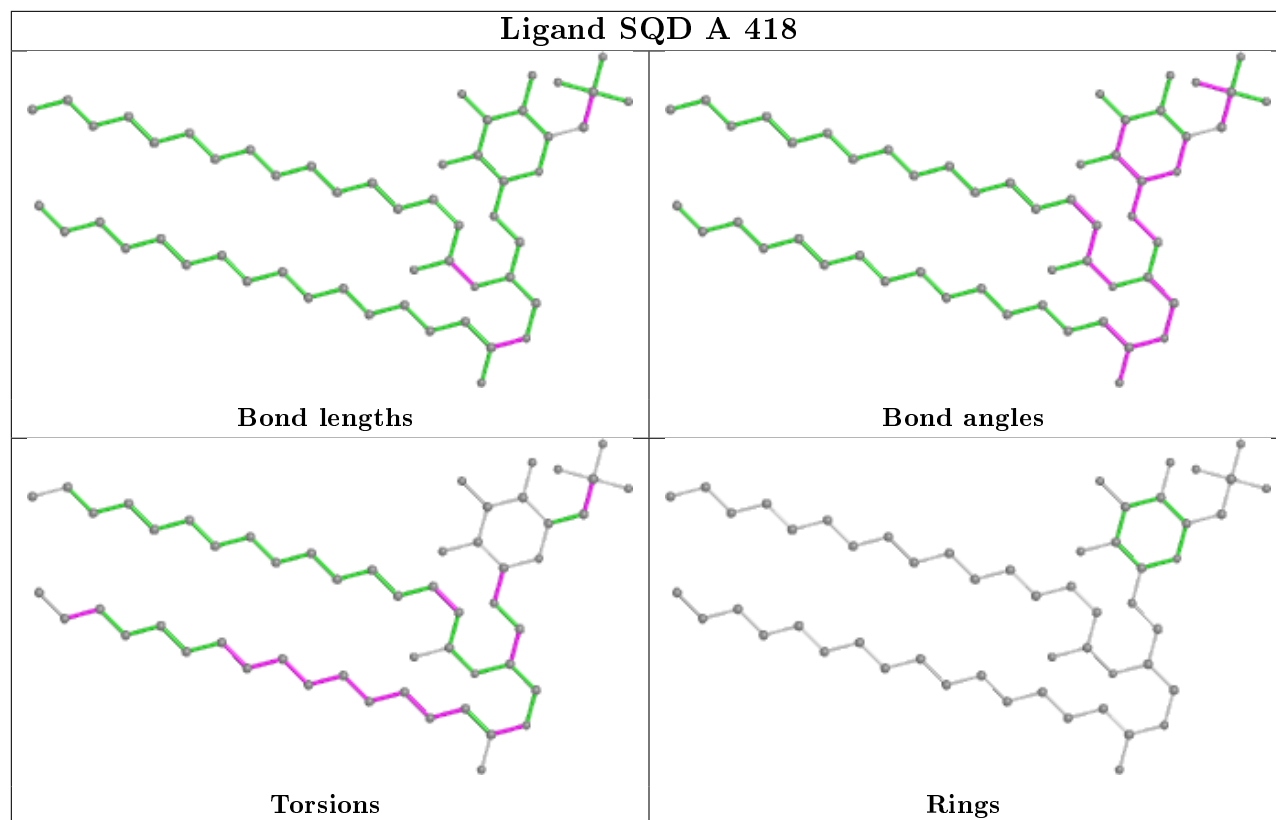
## Ligand CLA b 606



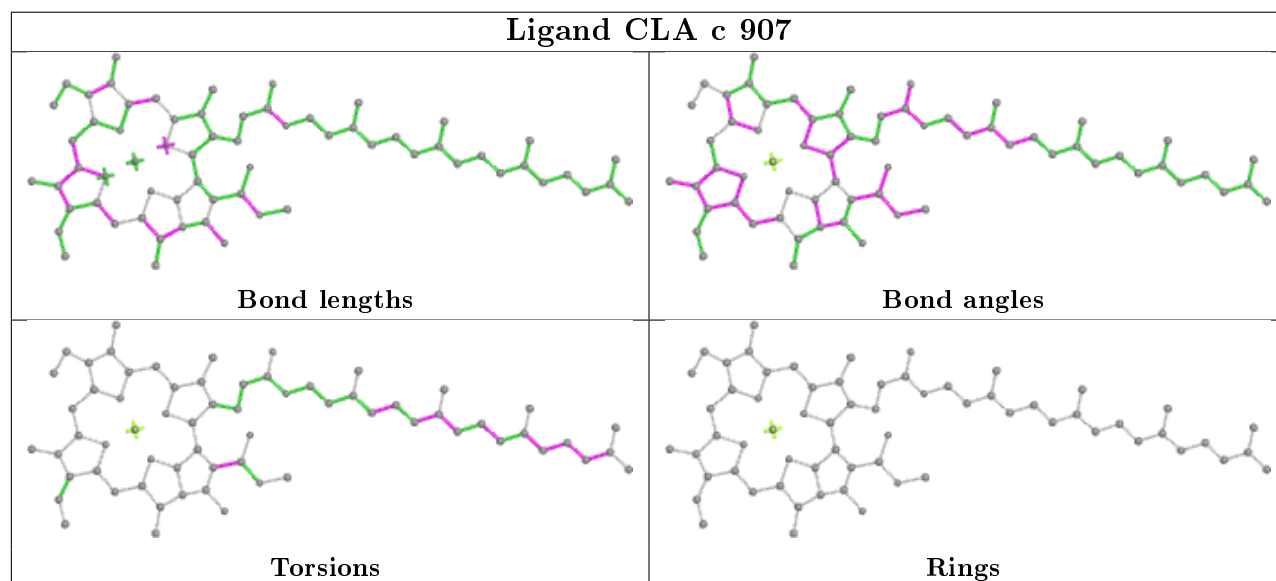
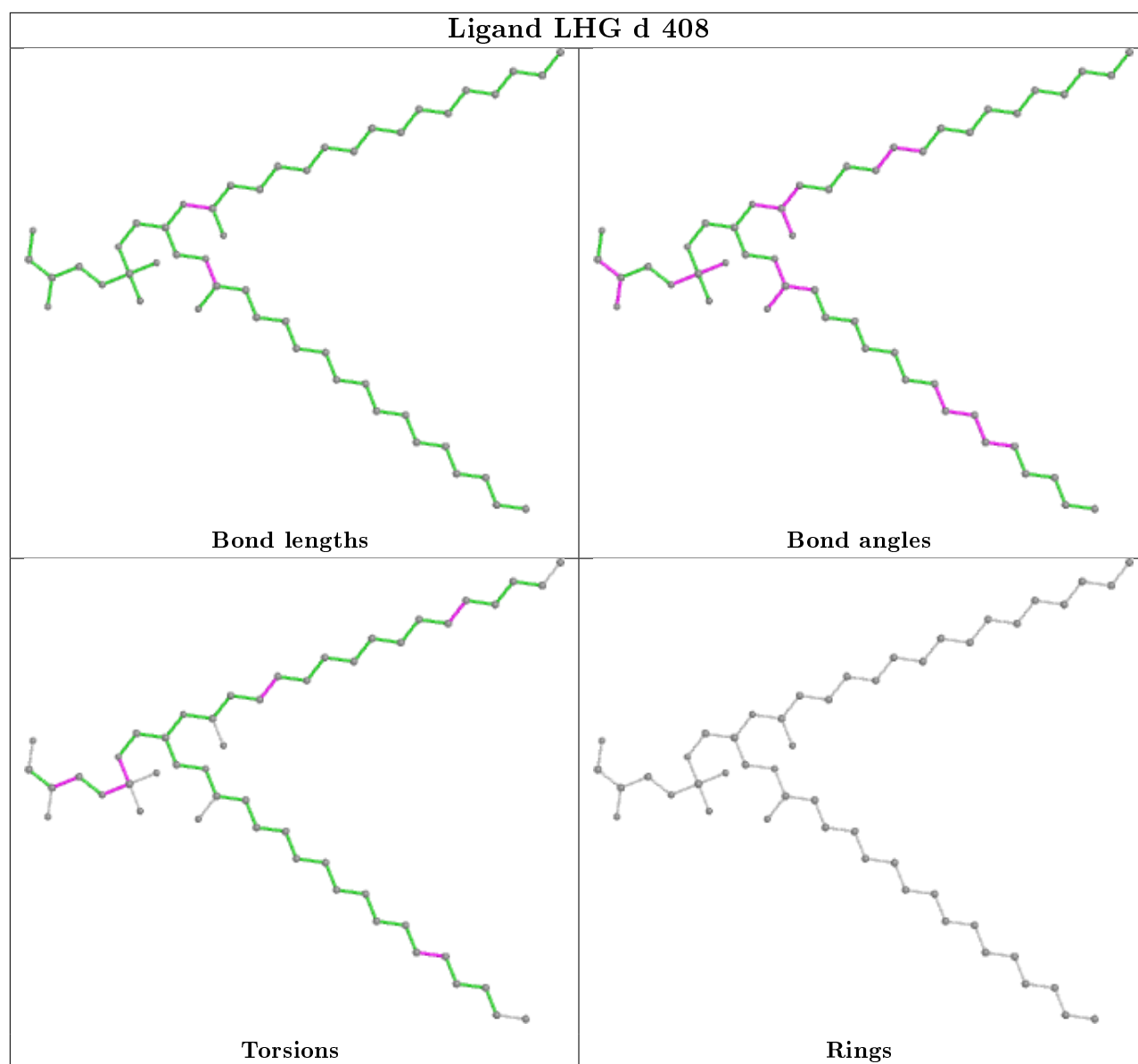


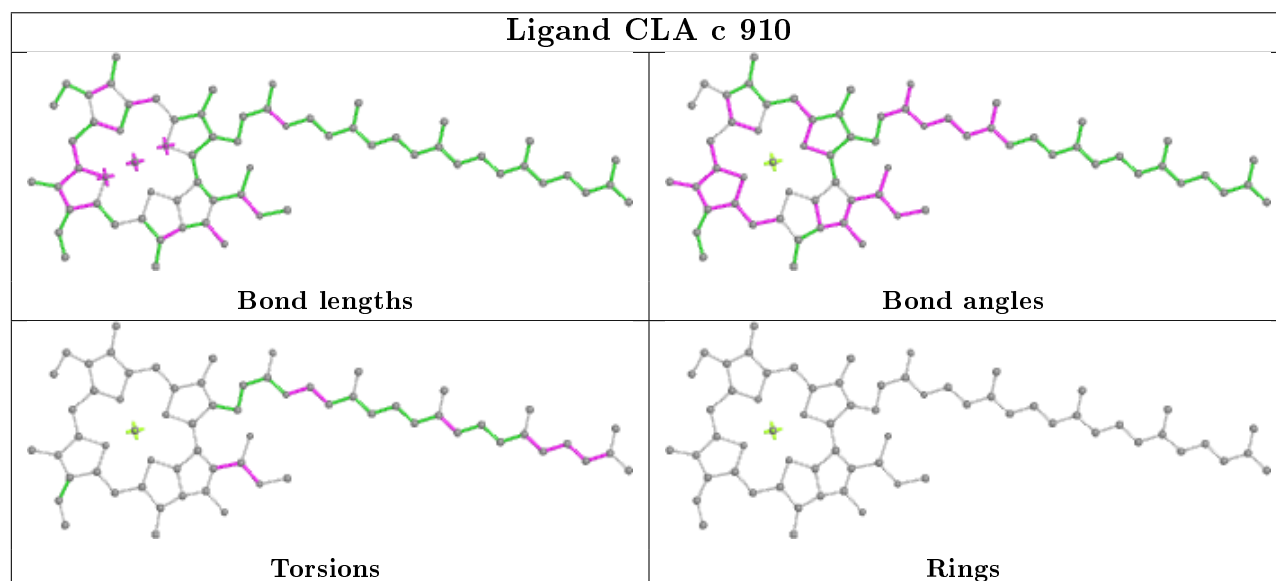
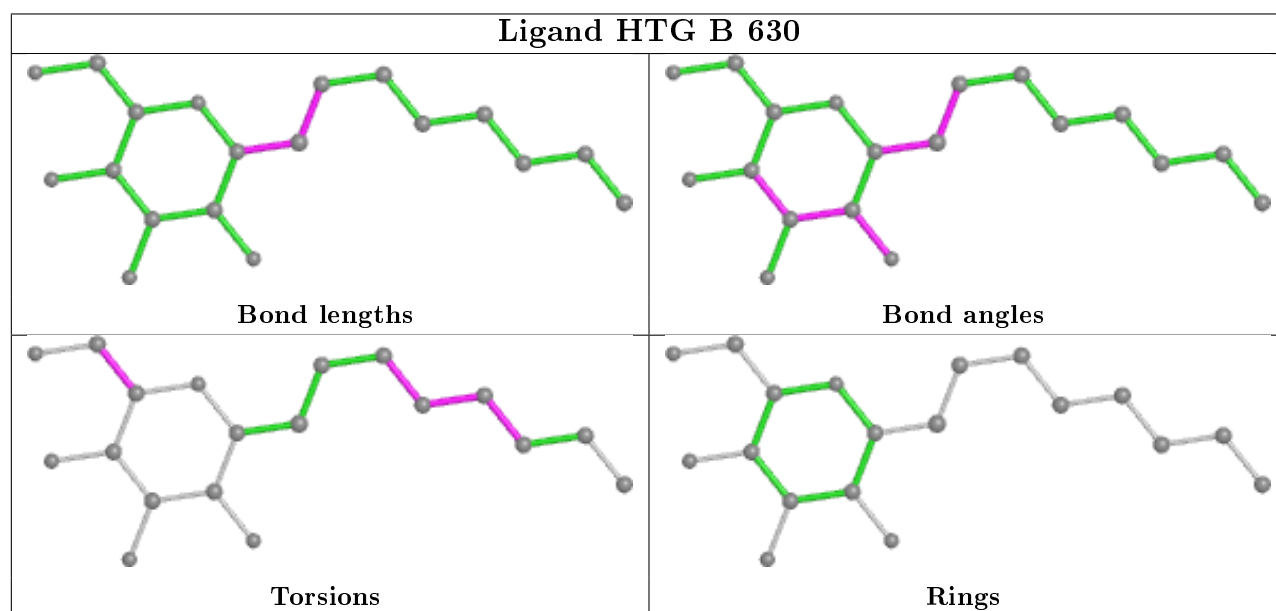
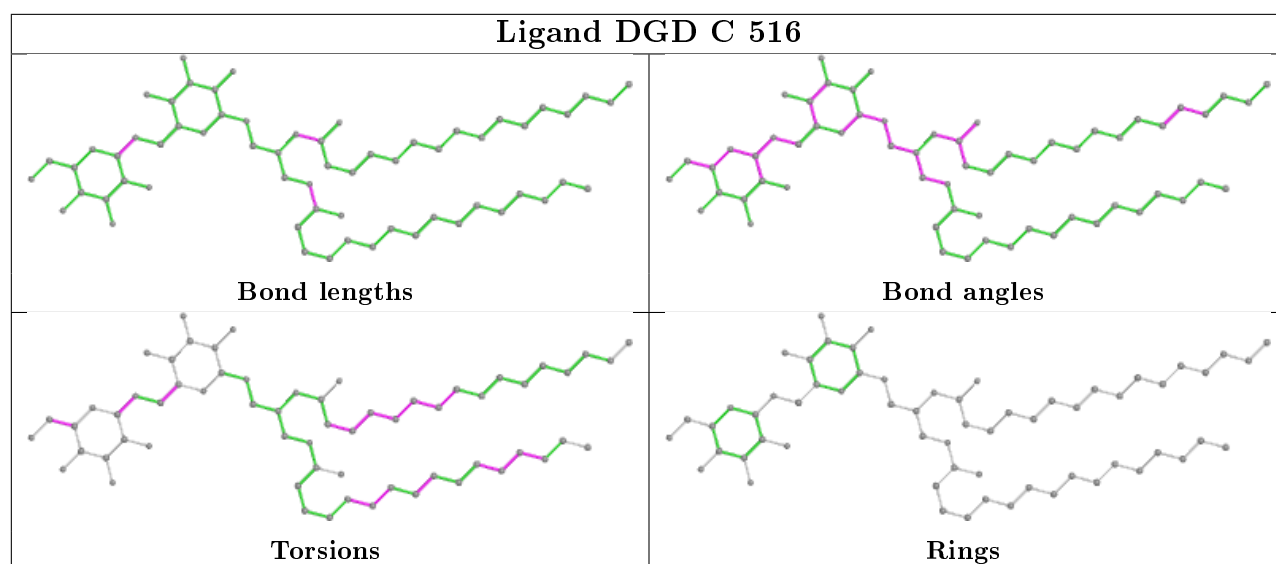


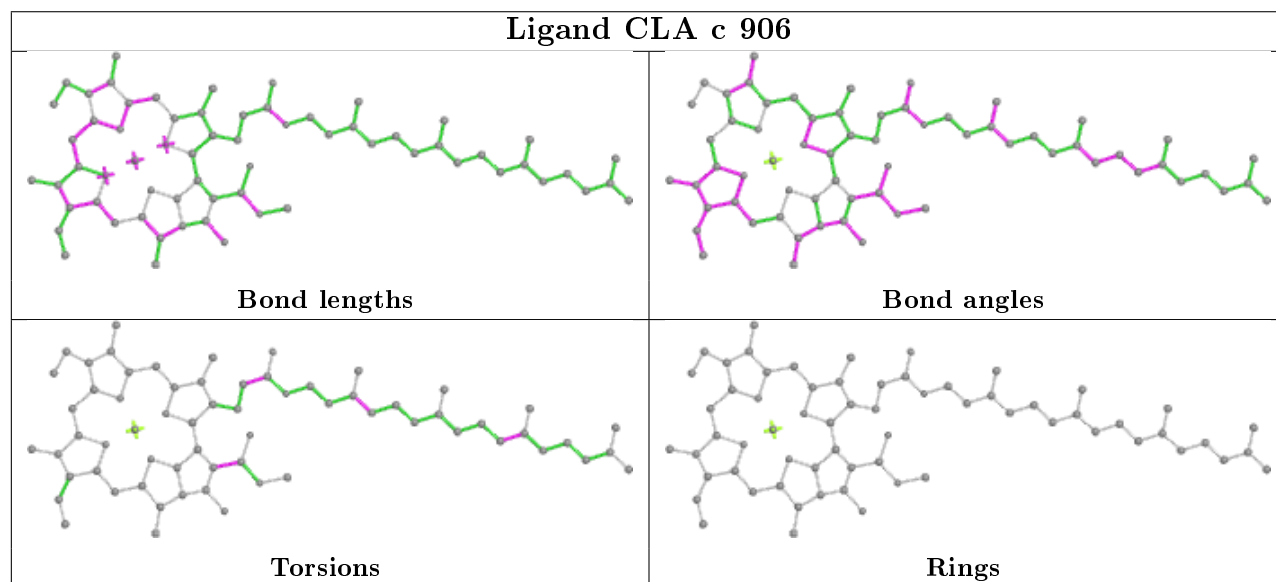
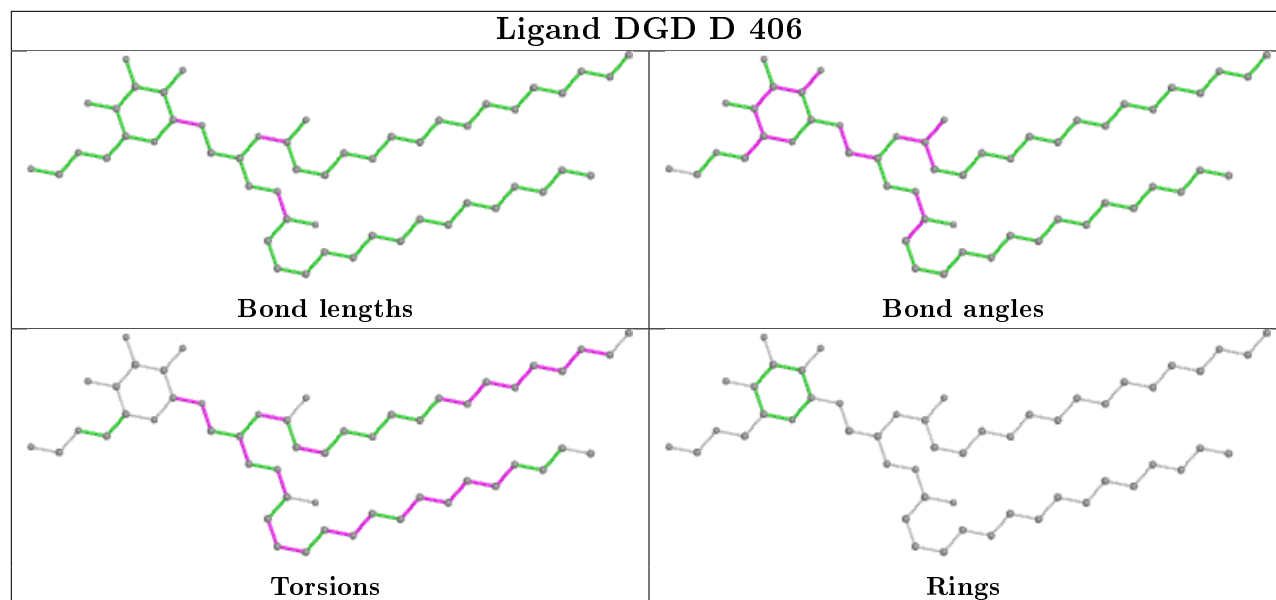
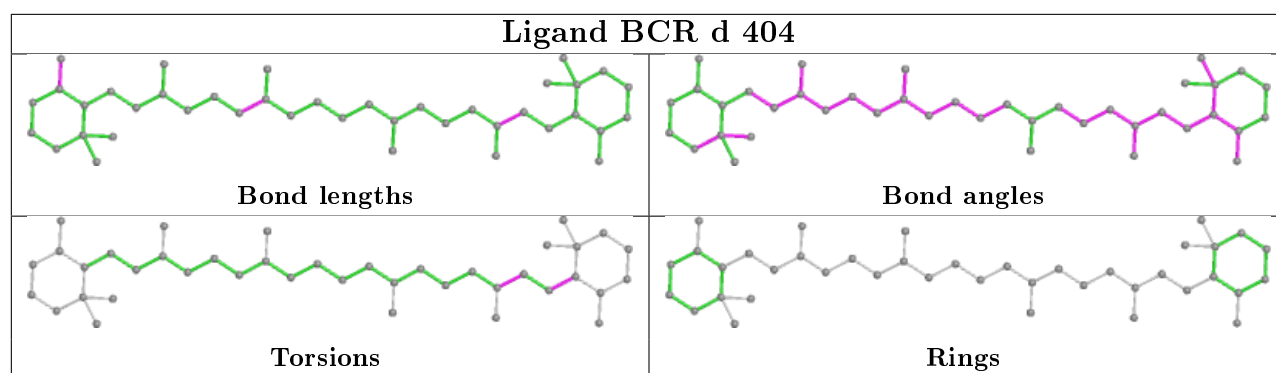




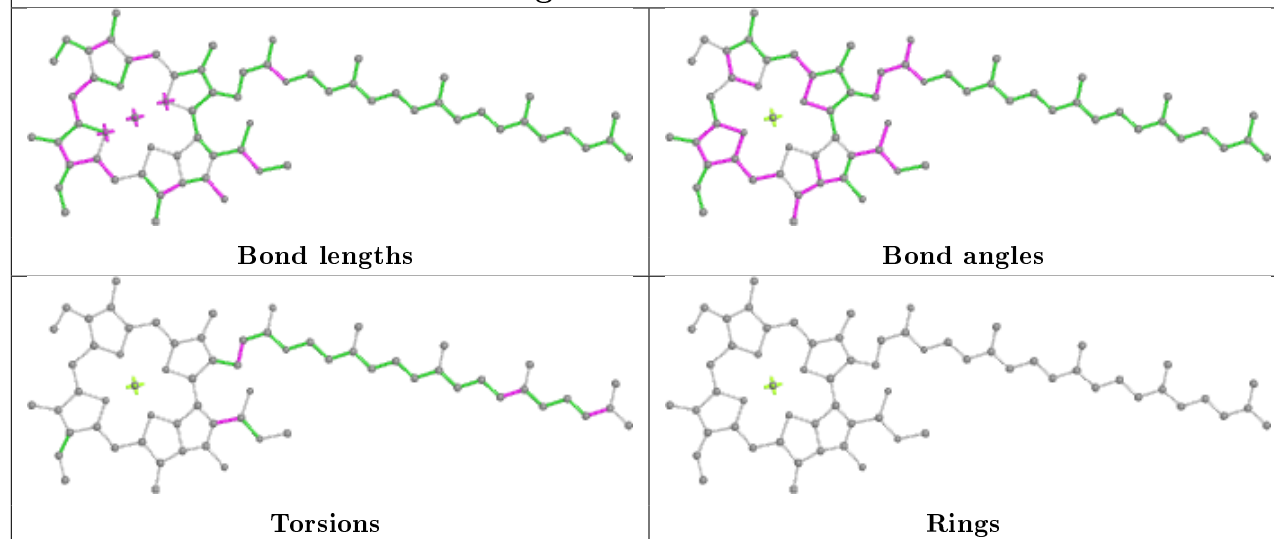




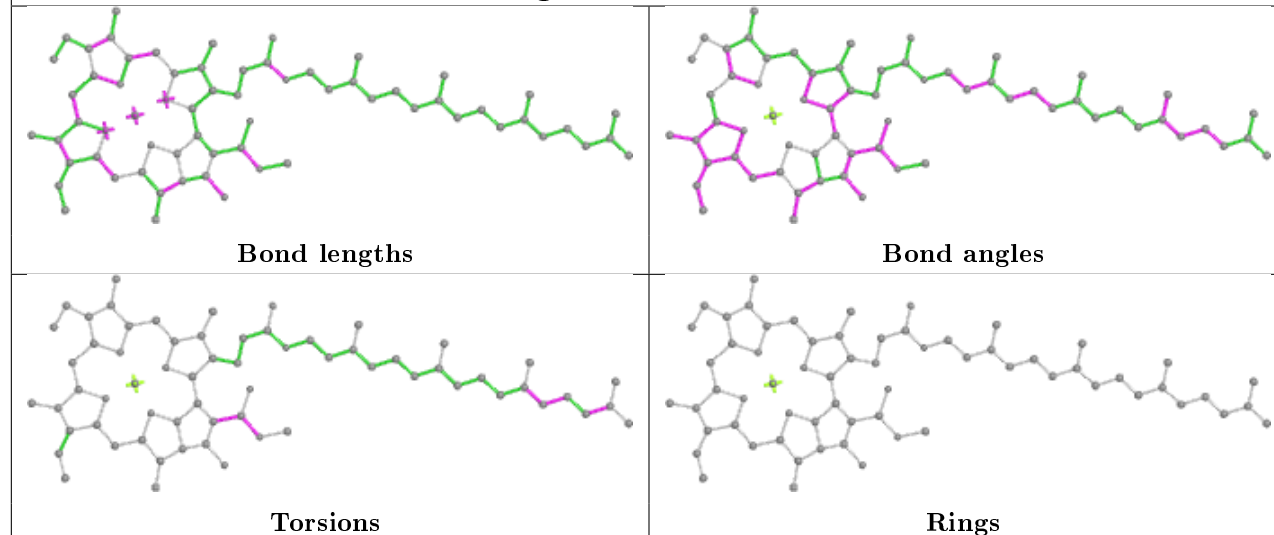




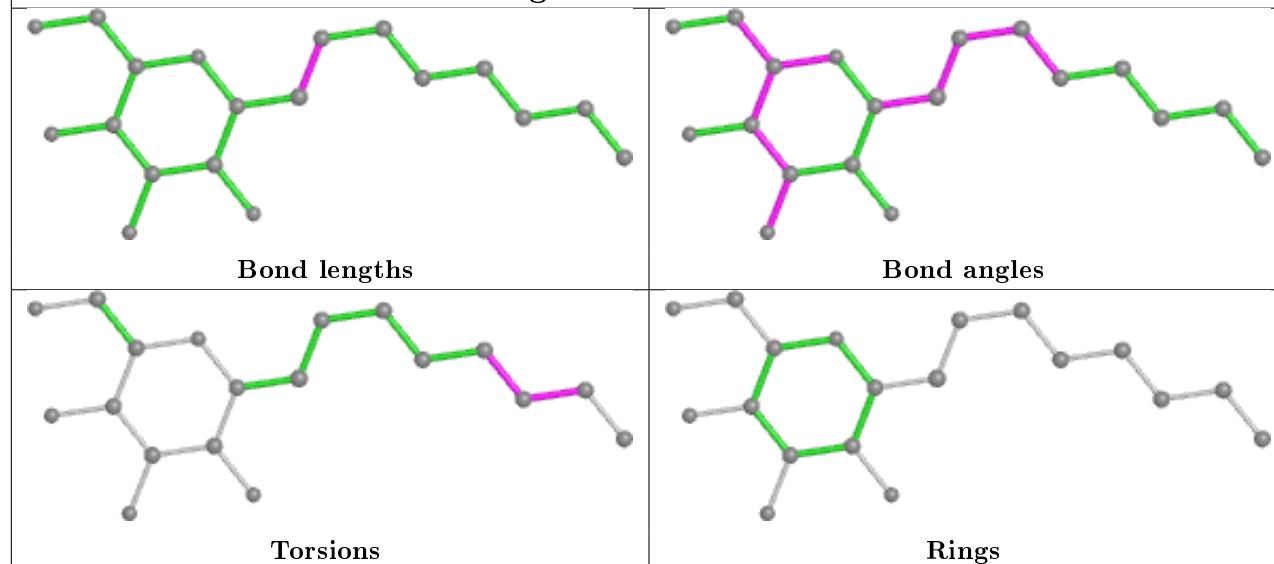
## Ligand CLA b 613

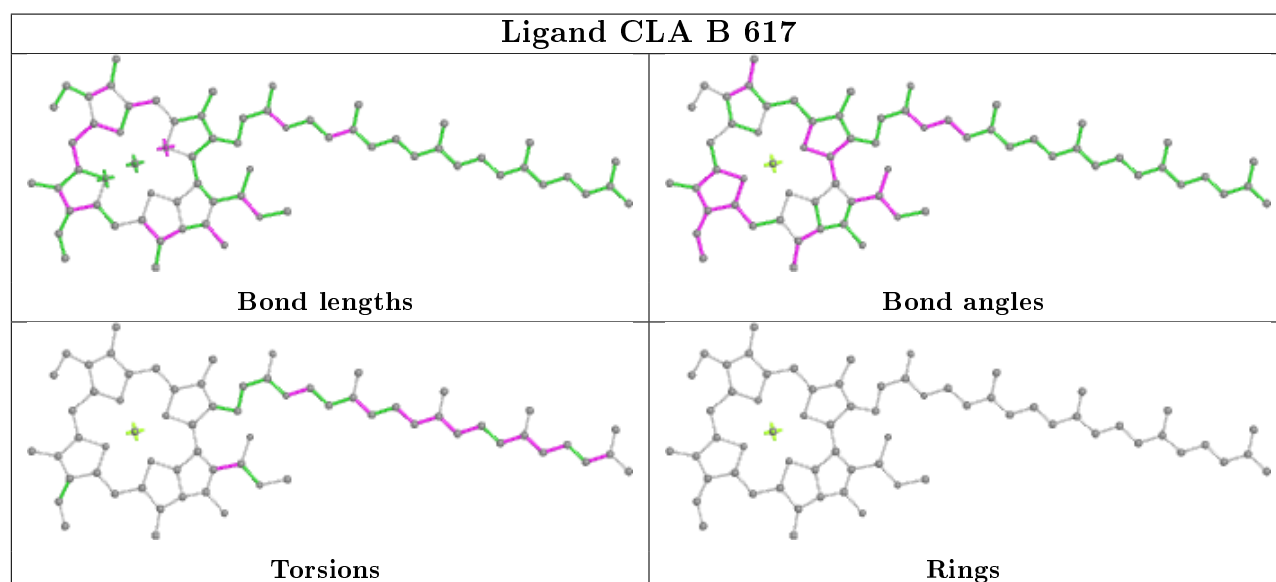
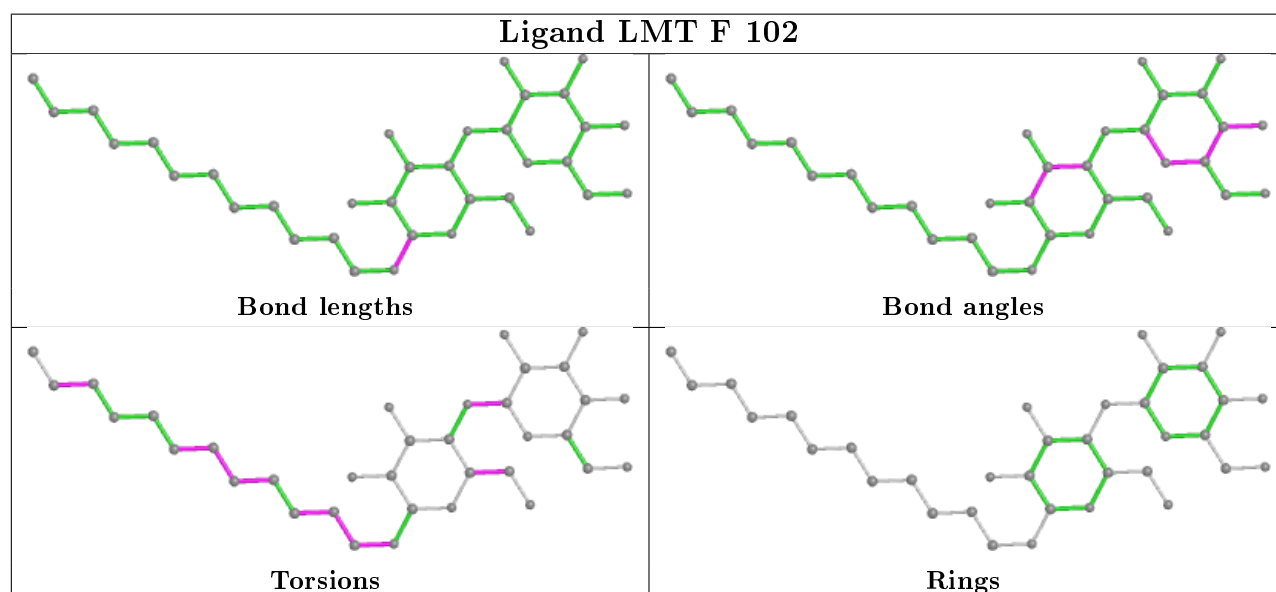
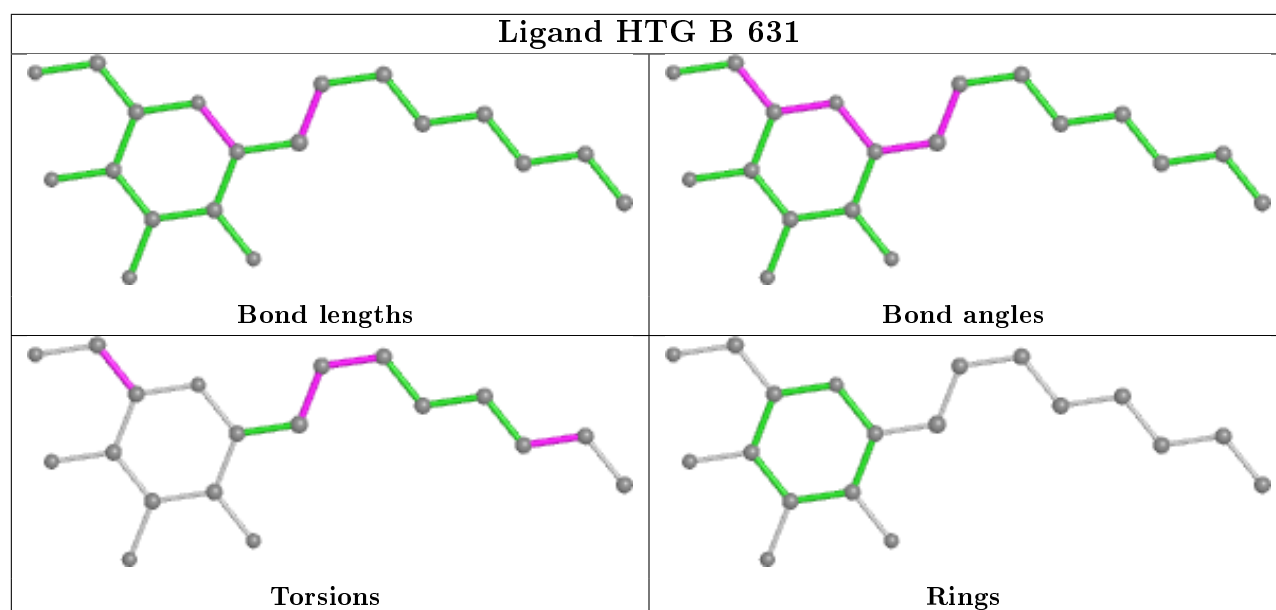


## Ligand CLA b 614

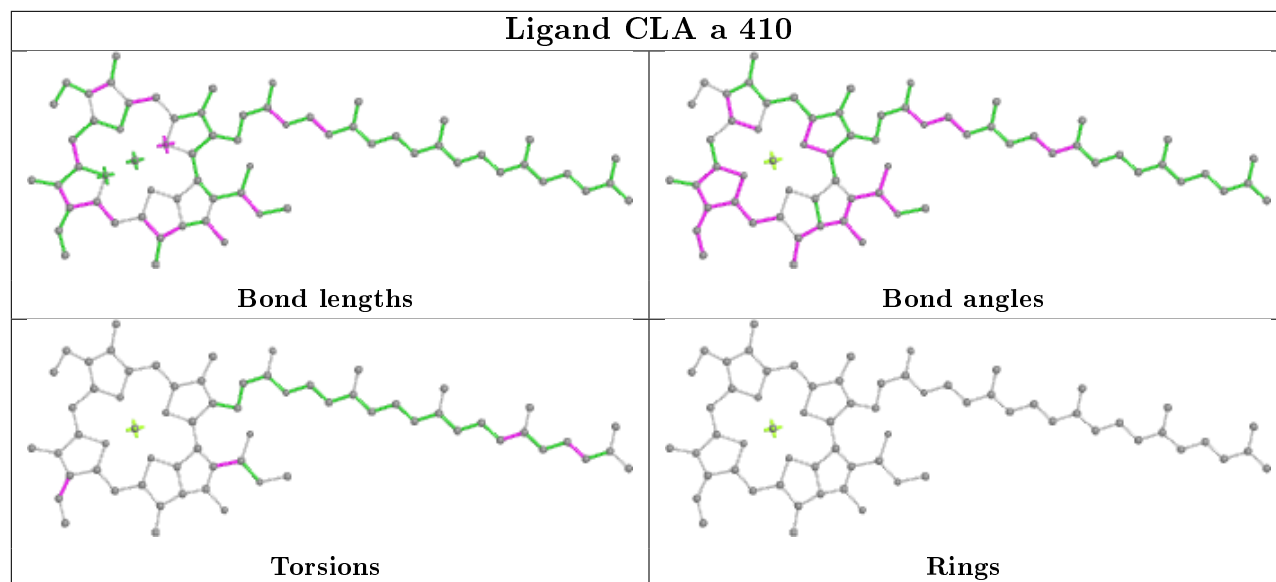


## Ligand HTG B 624

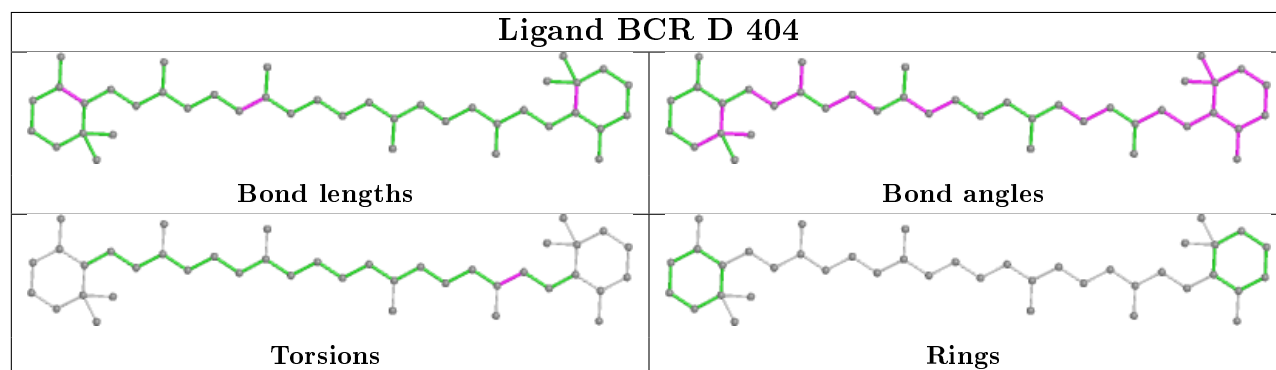




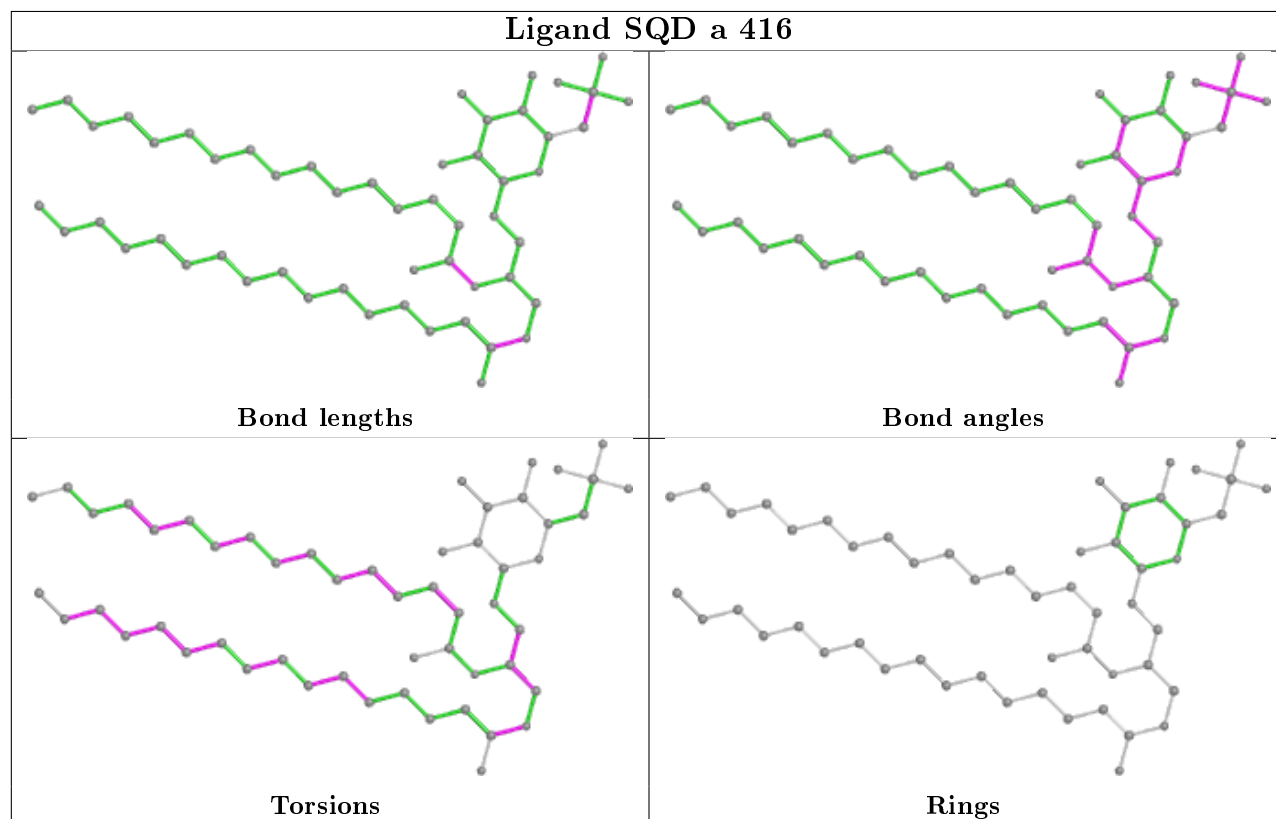
## Ligand CLA a 410

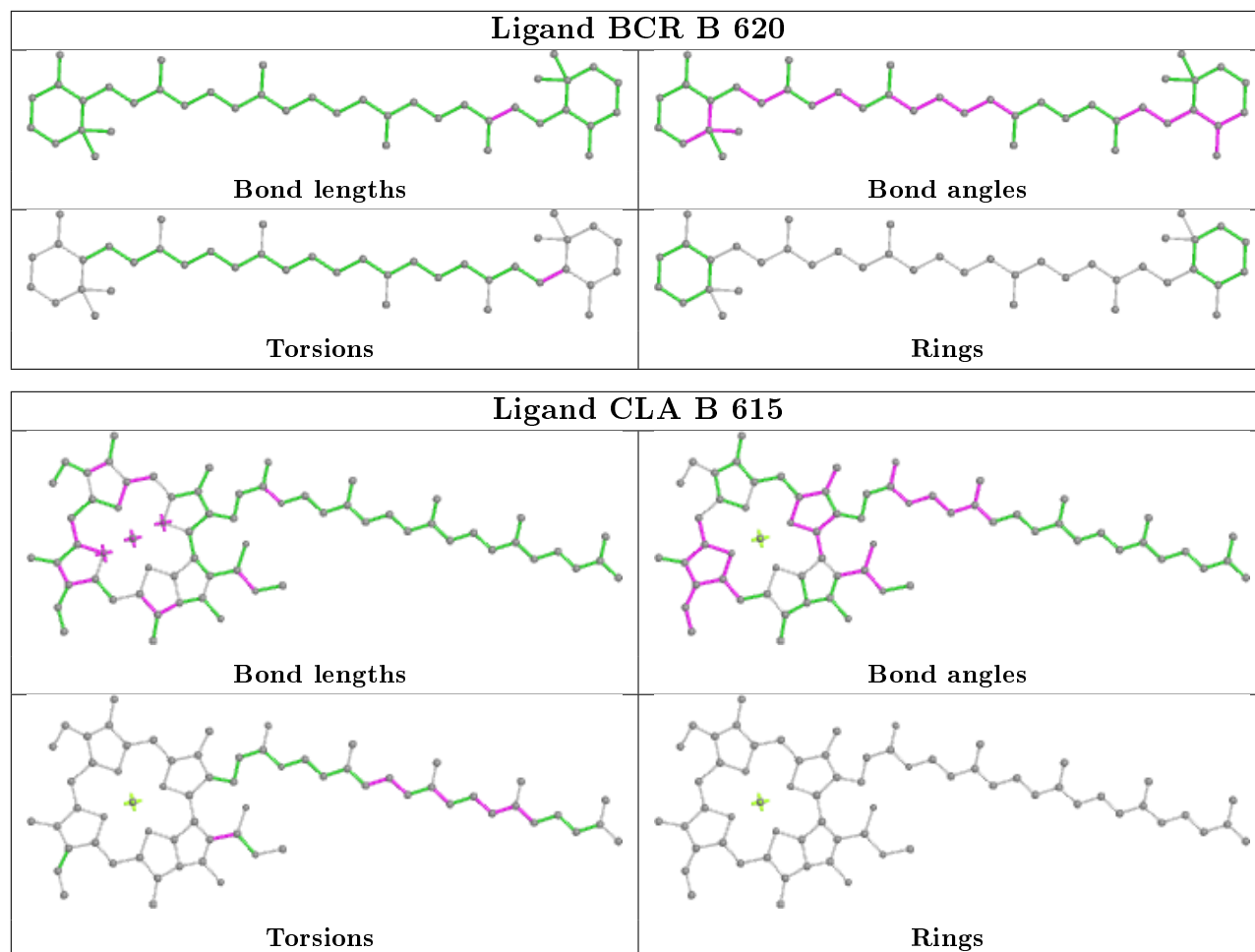


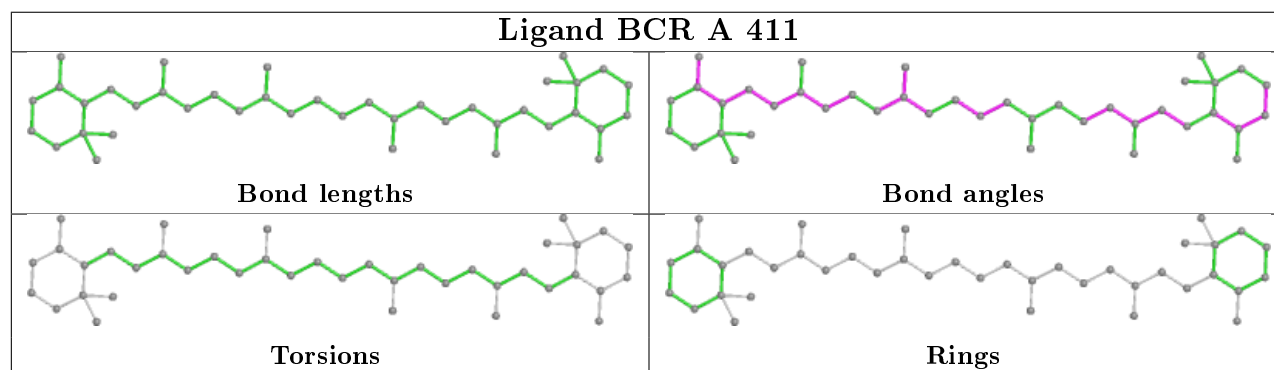
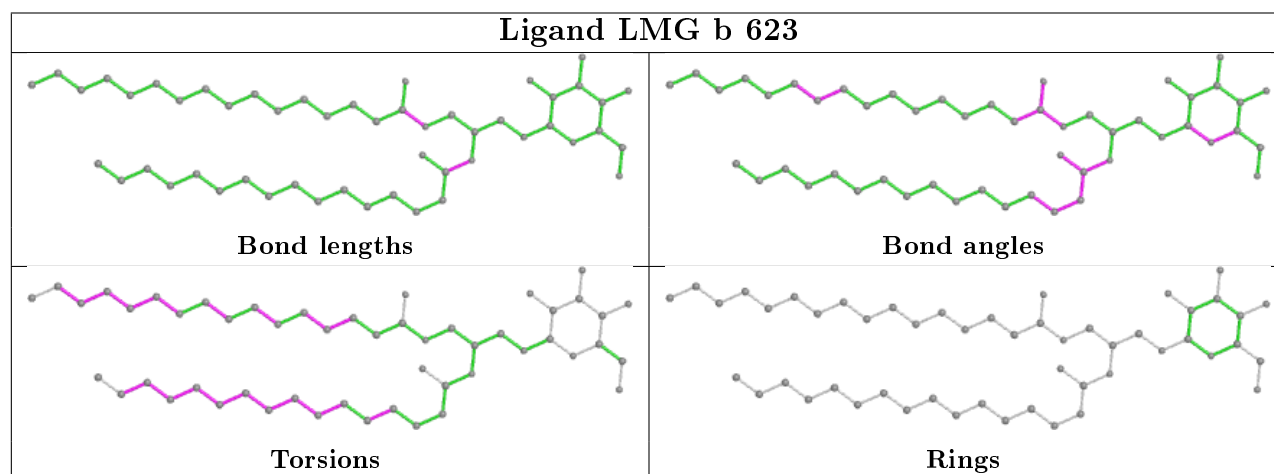
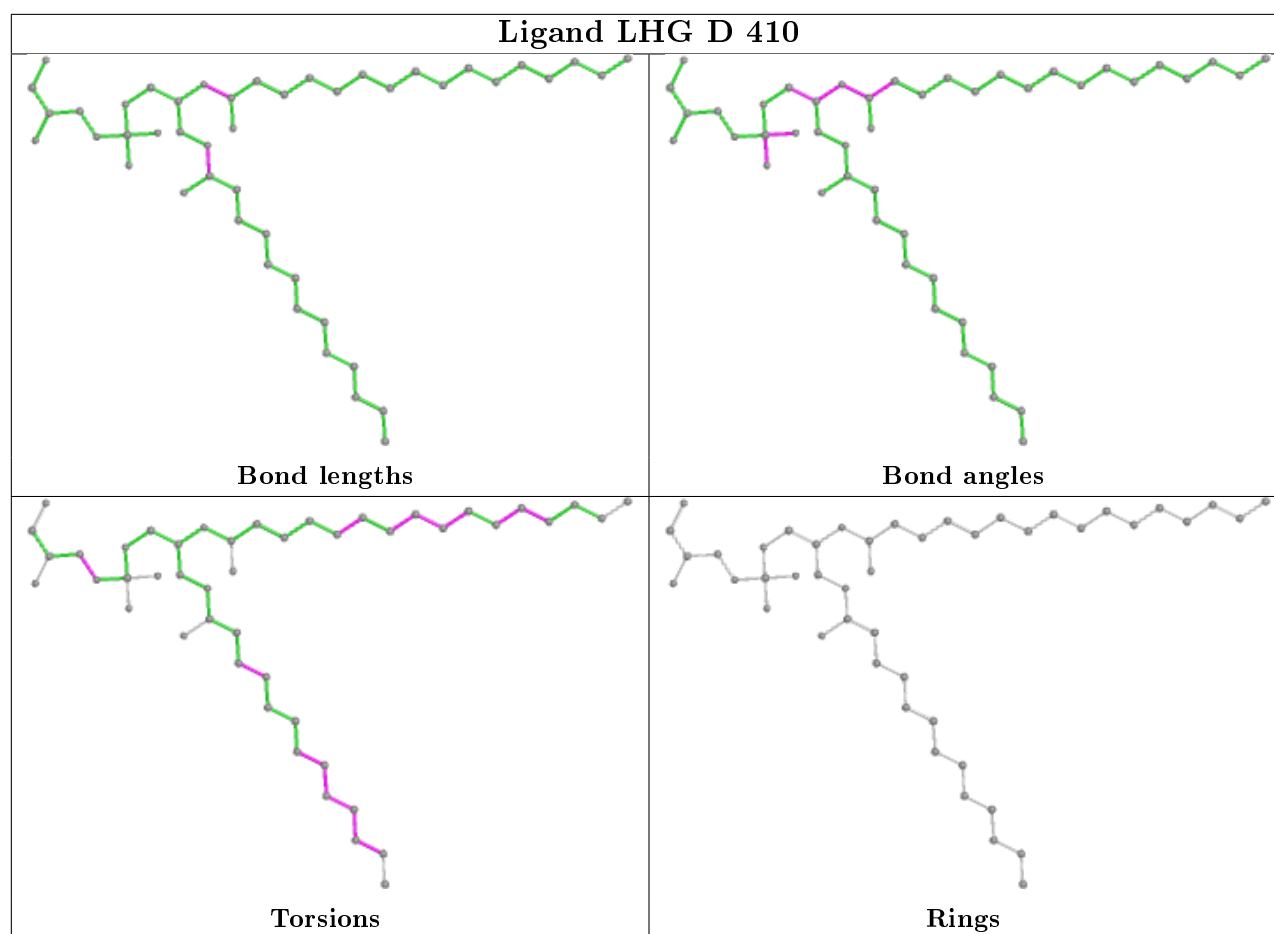
## Ligand BCR D 404



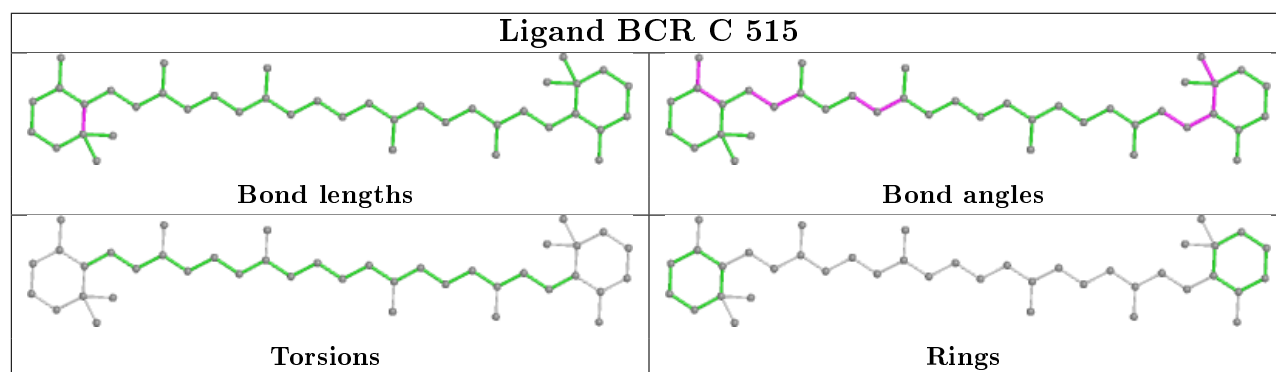
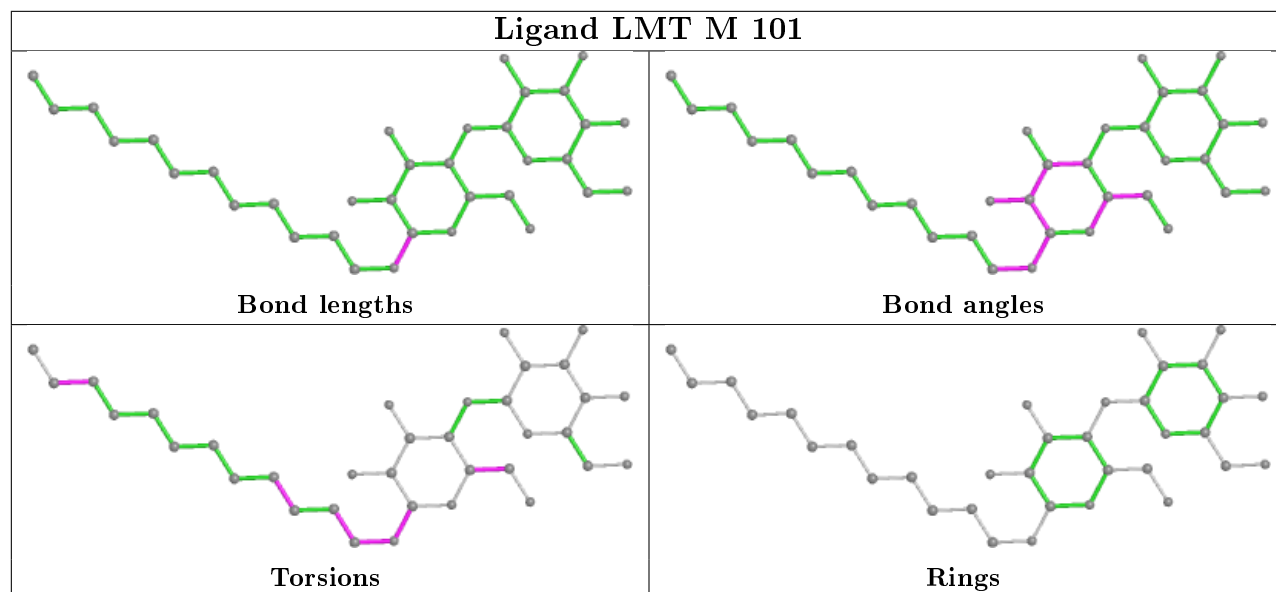
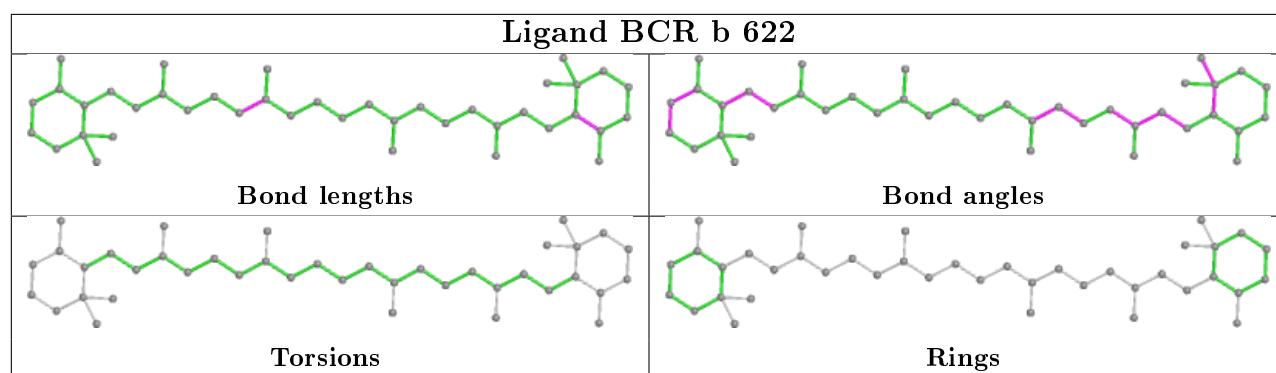
## Ligand SQD a 416



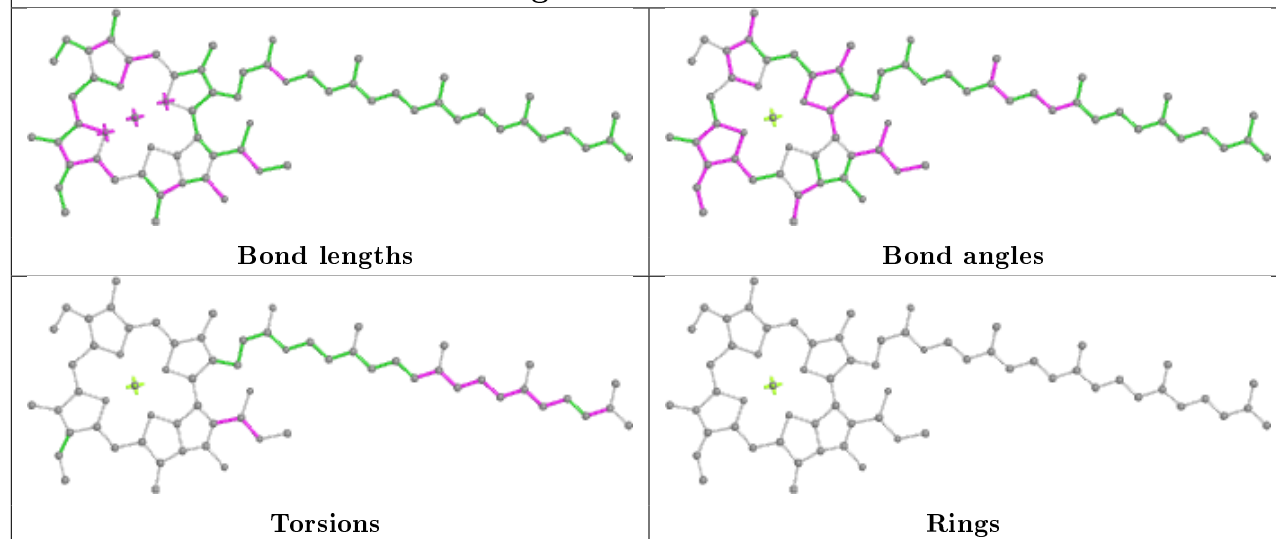




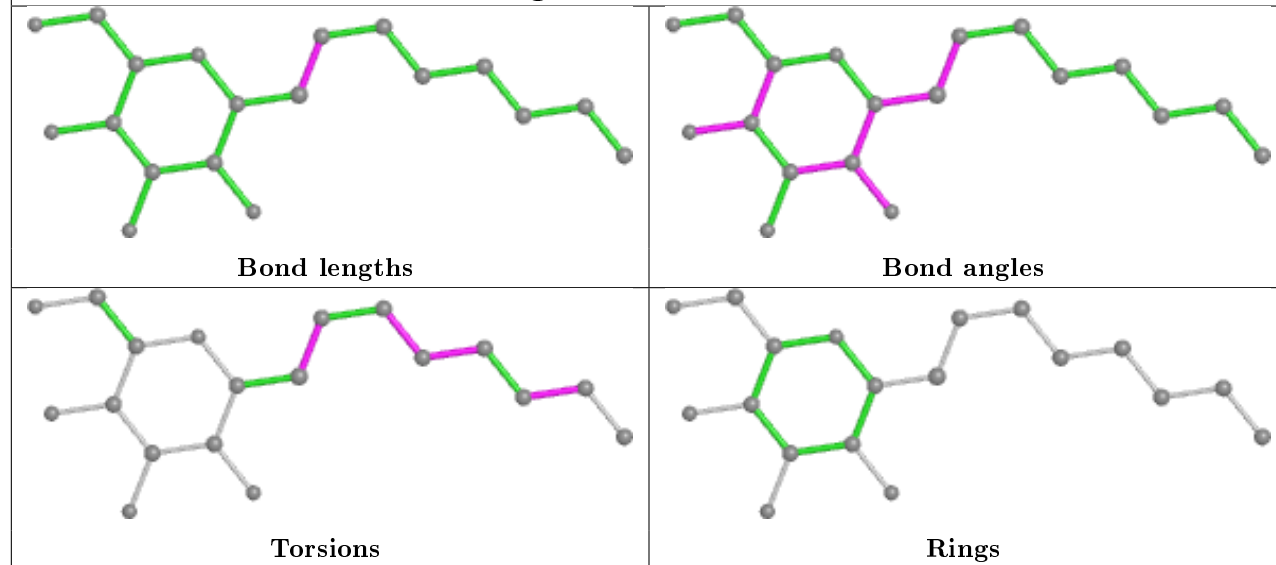


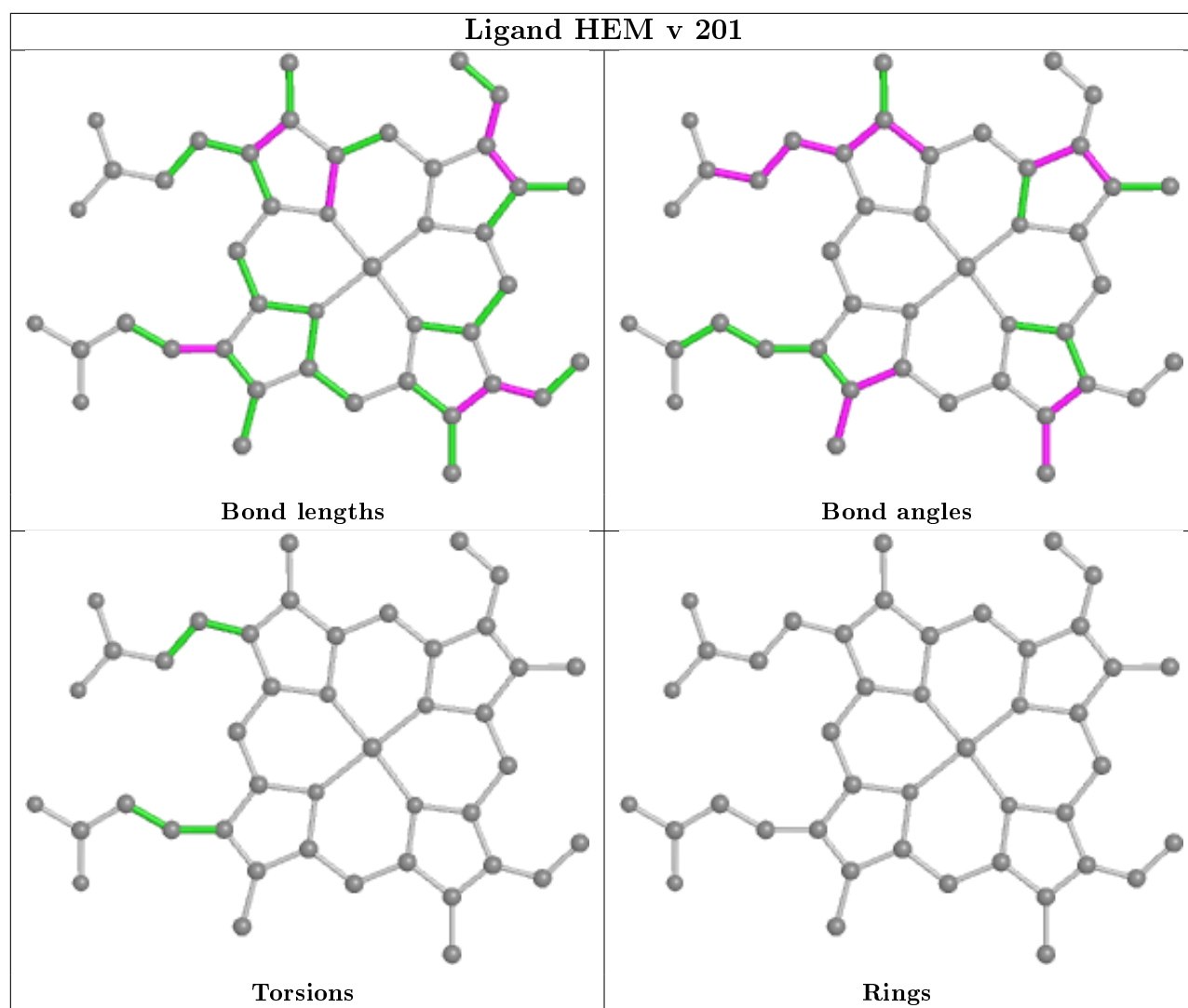


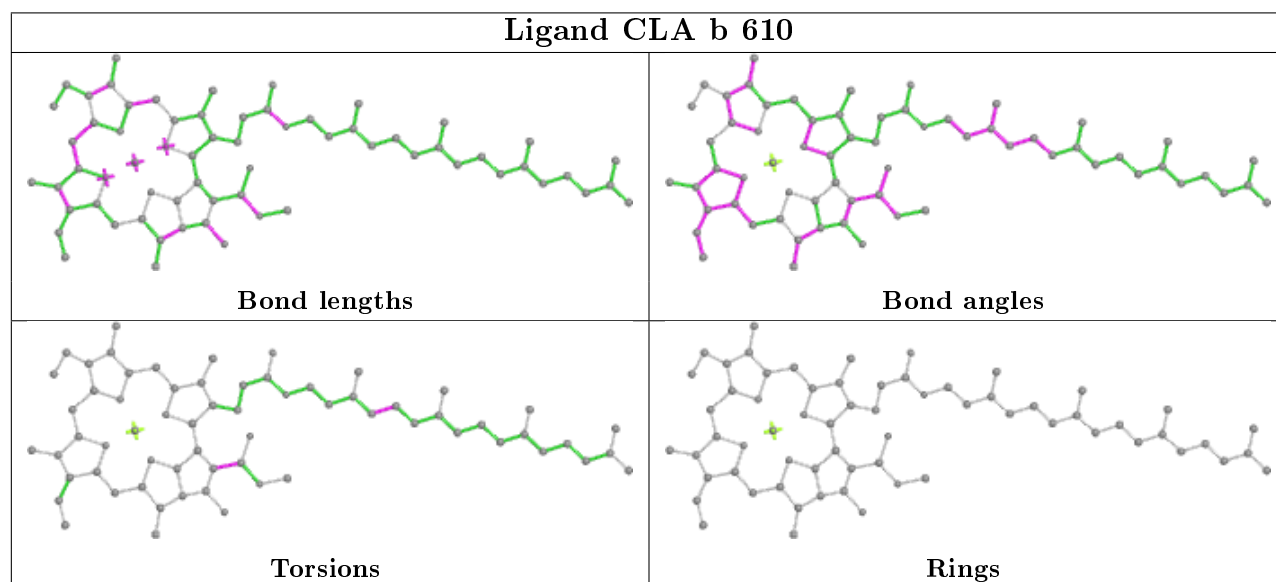
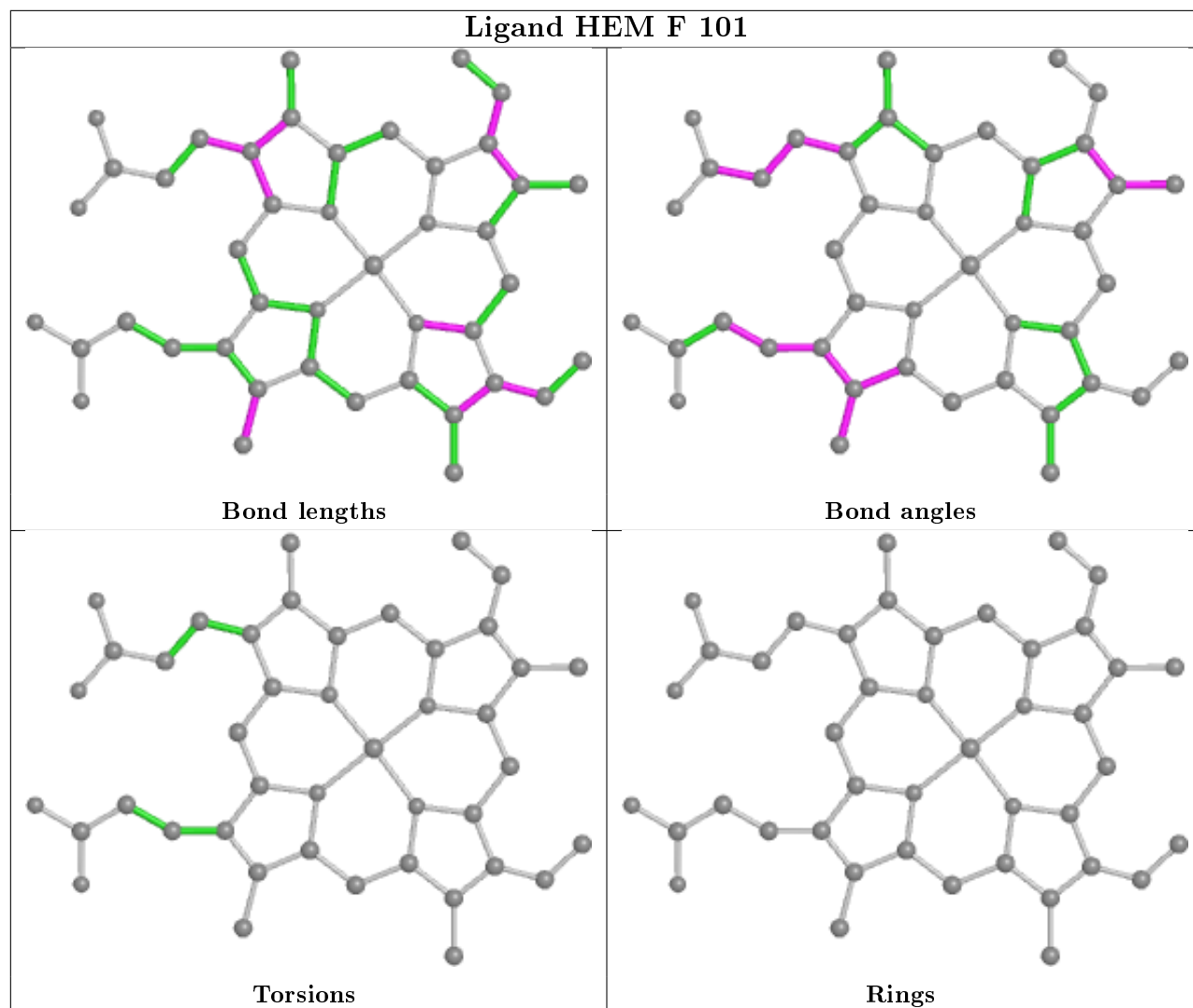
## Ligand CLA D 403

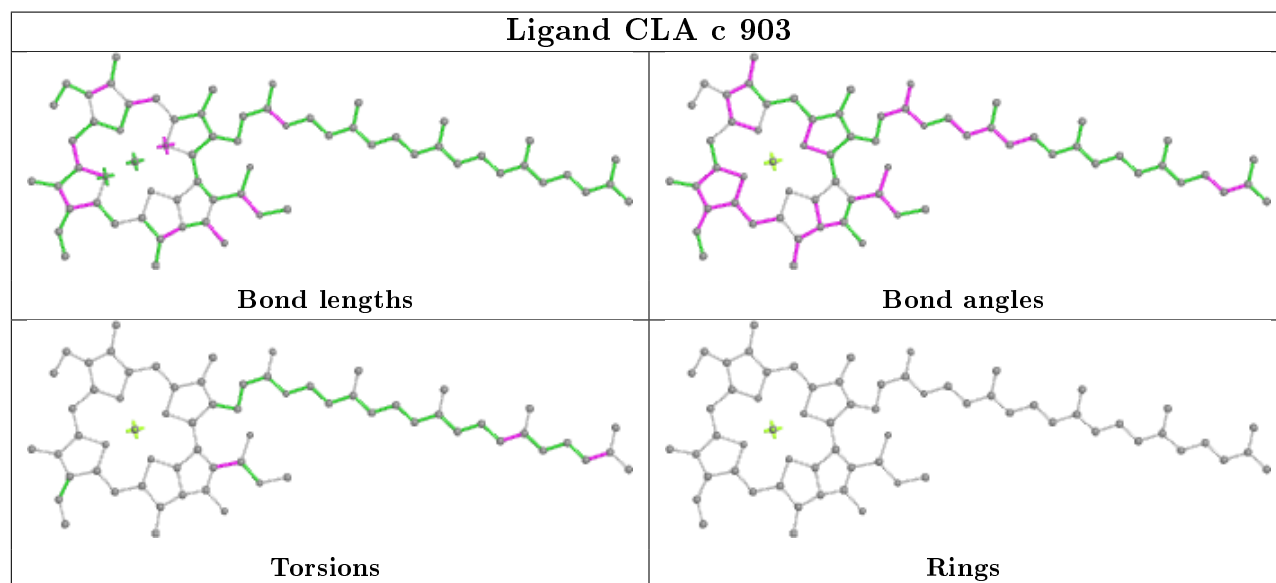
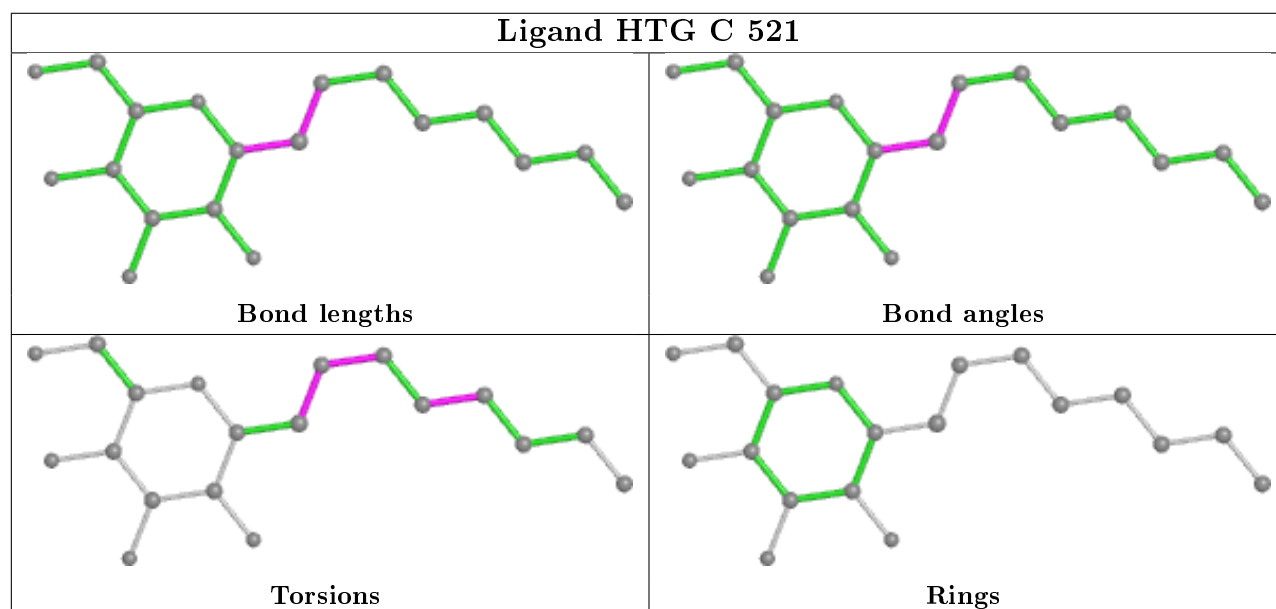
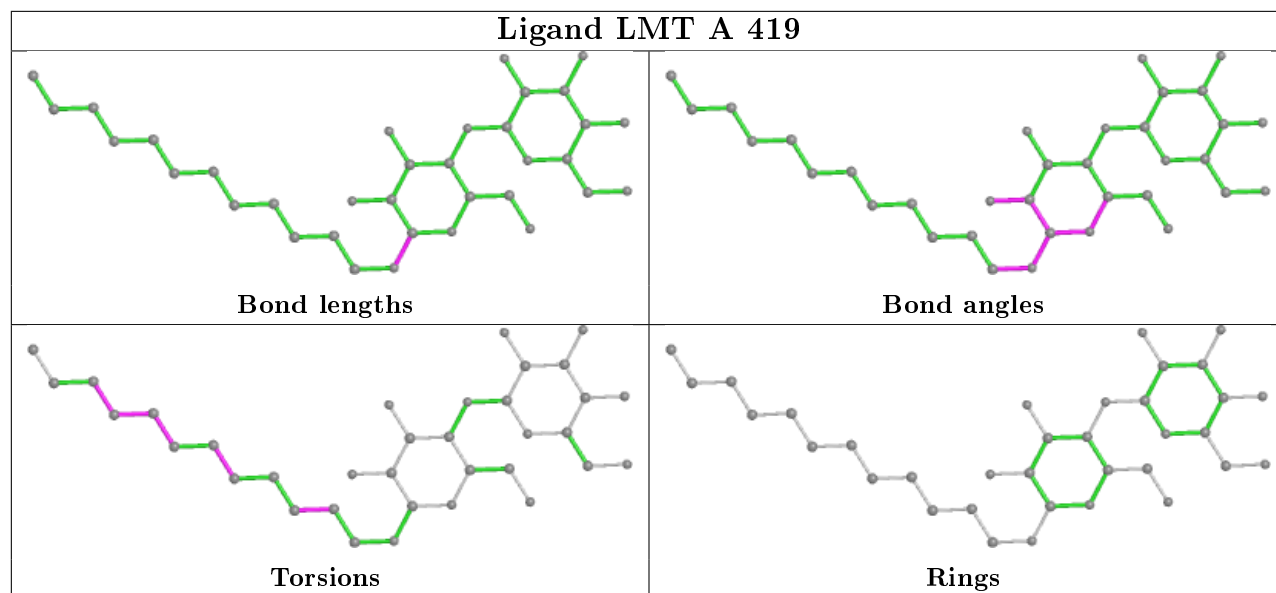


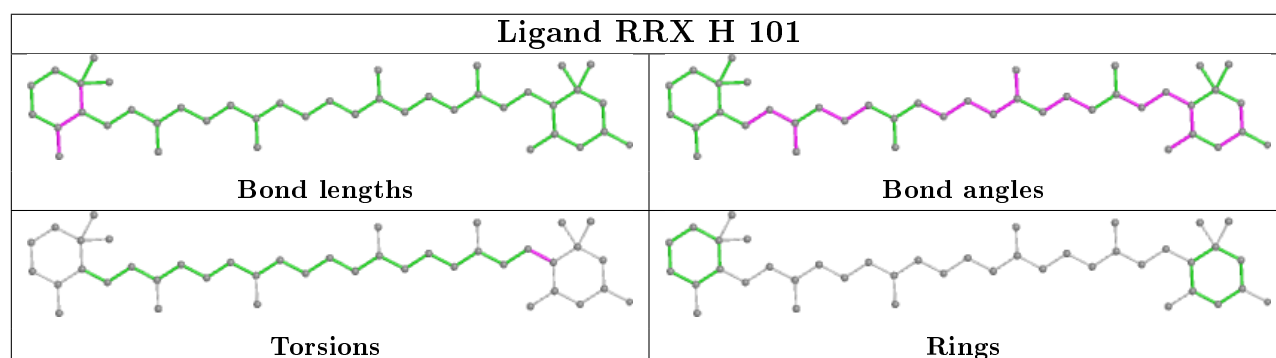
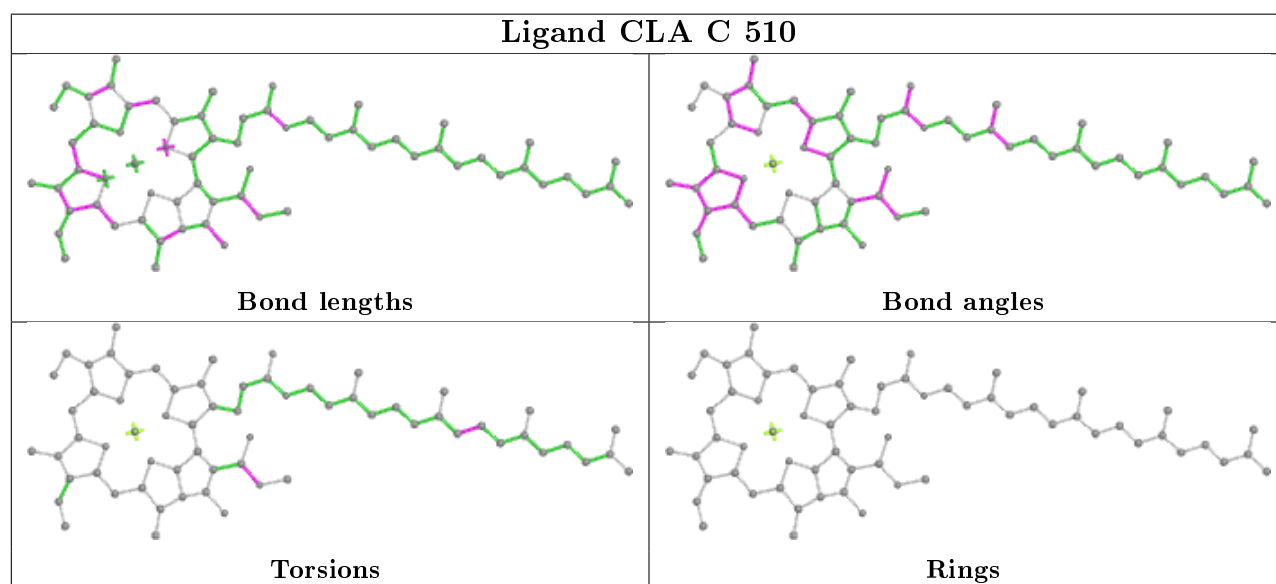
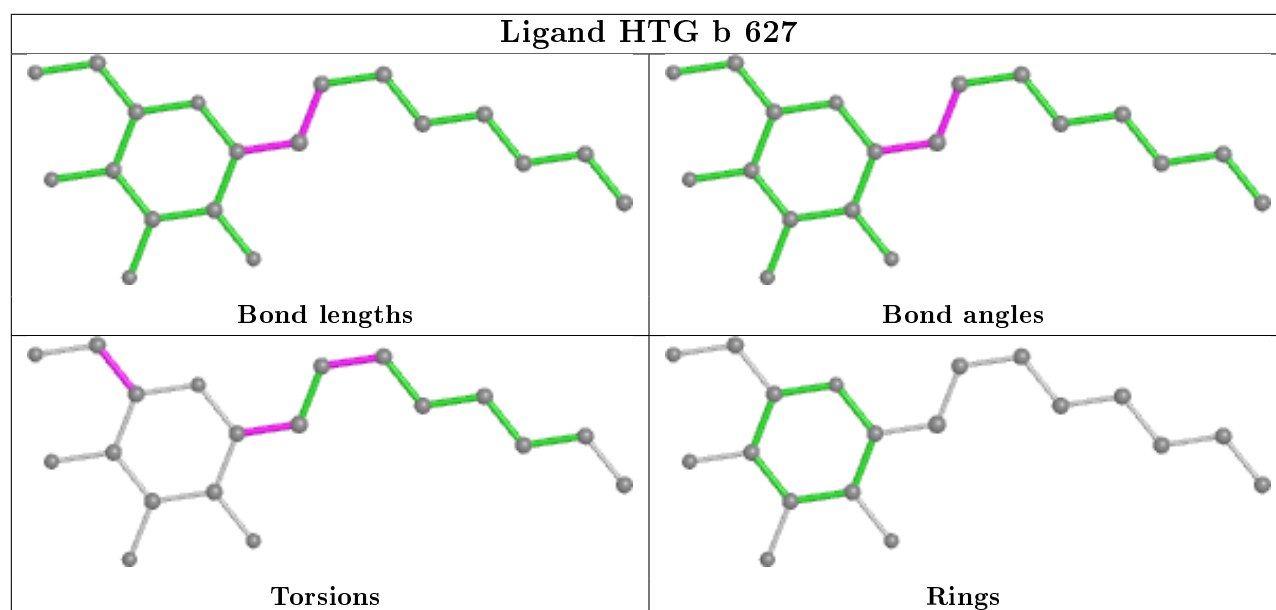
## Ligand HTG B 625

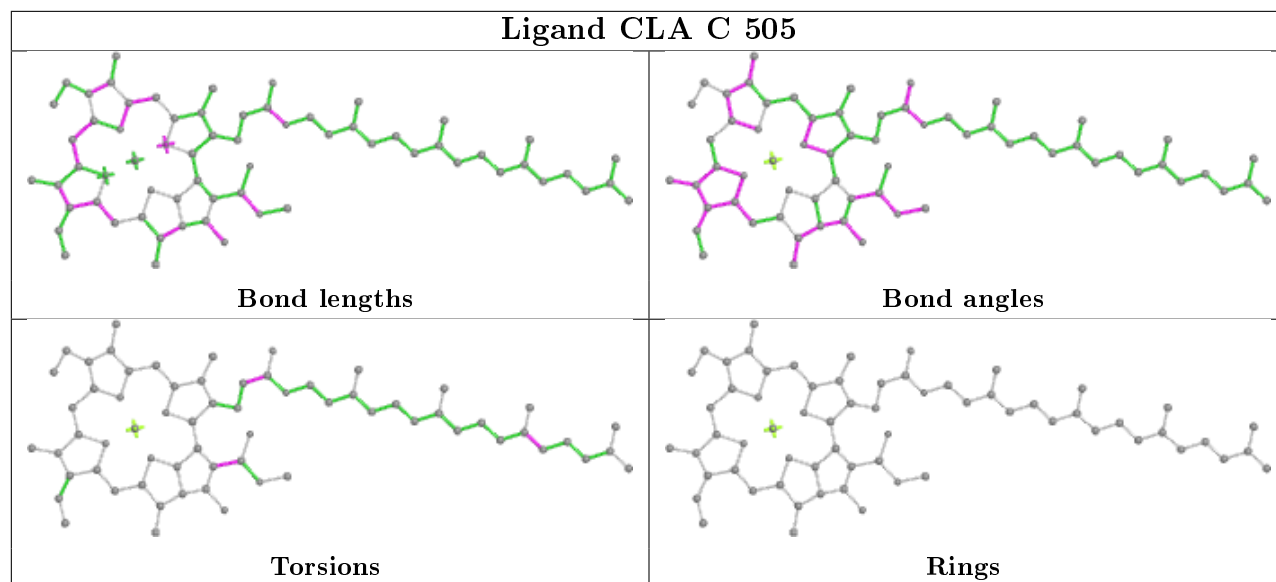
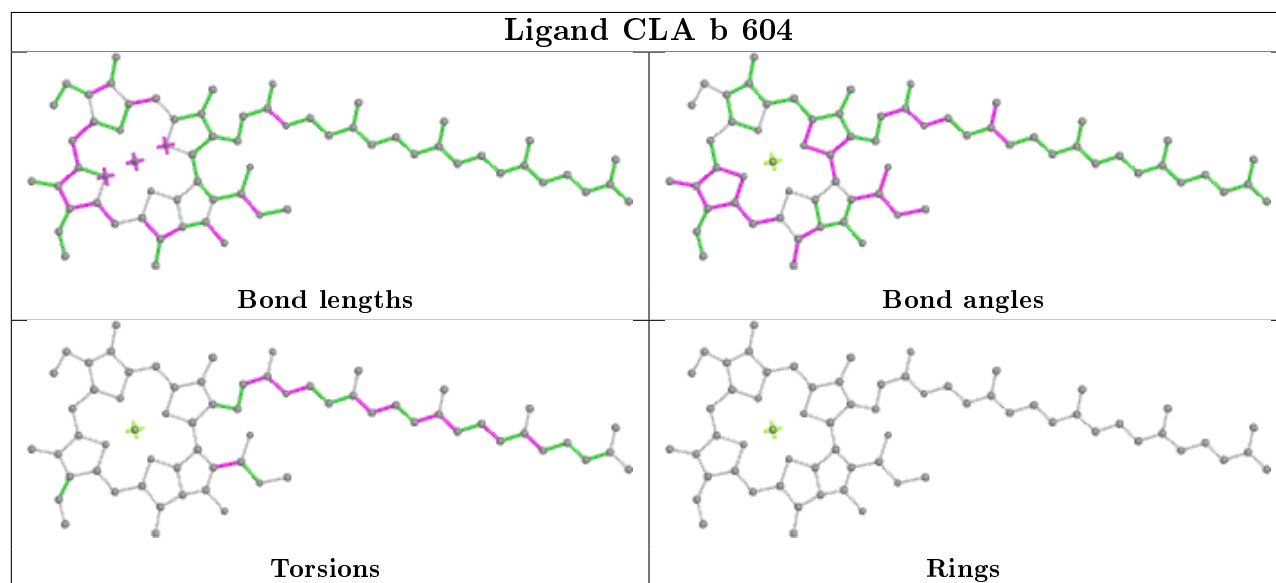


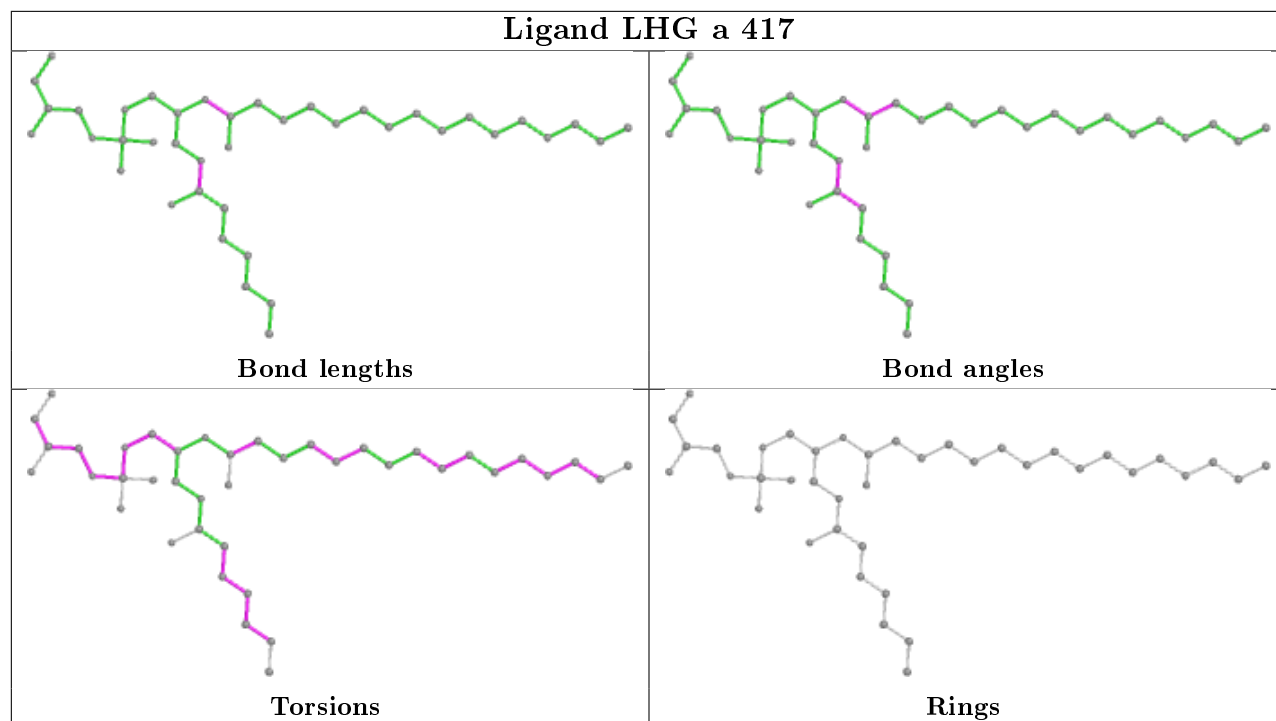
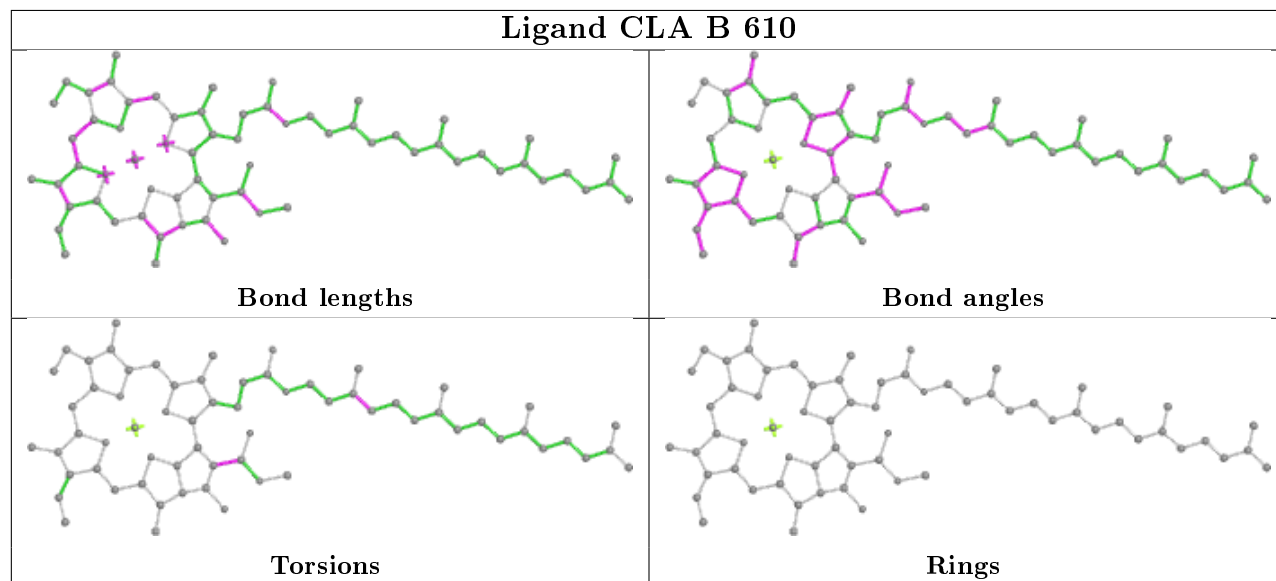




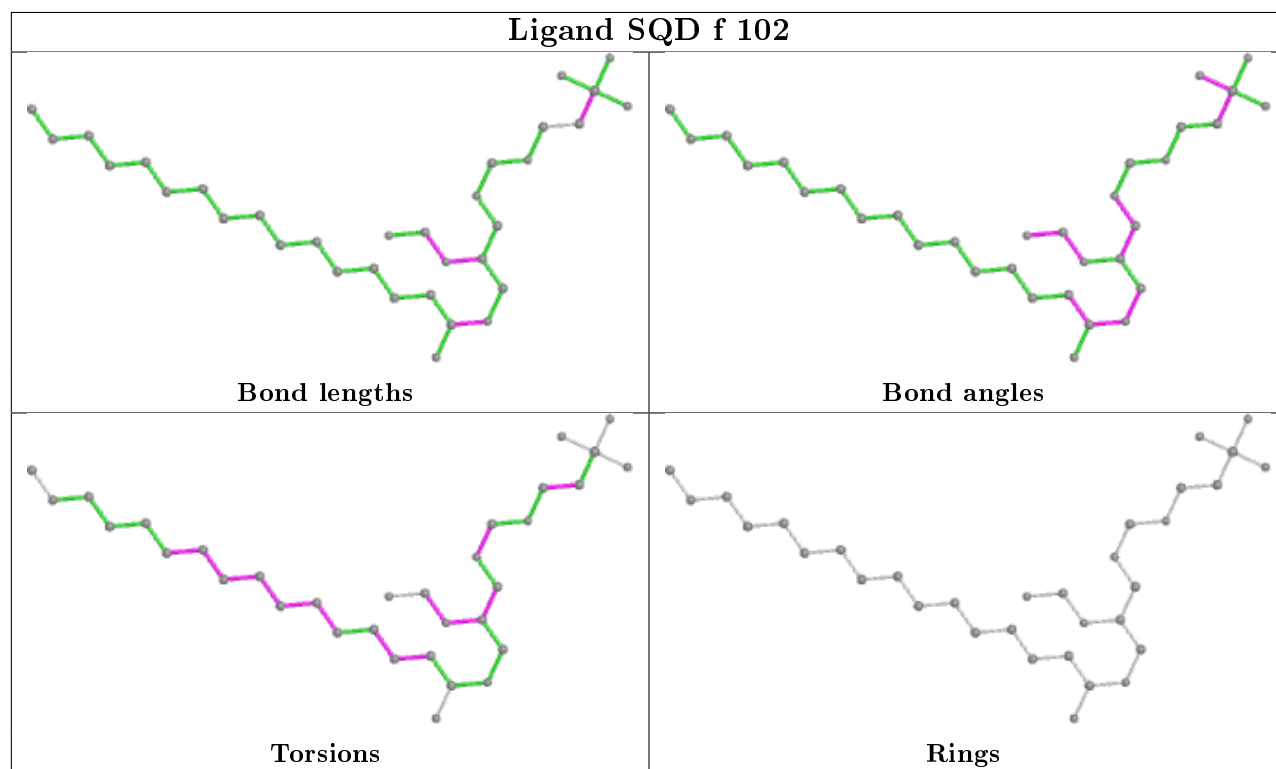
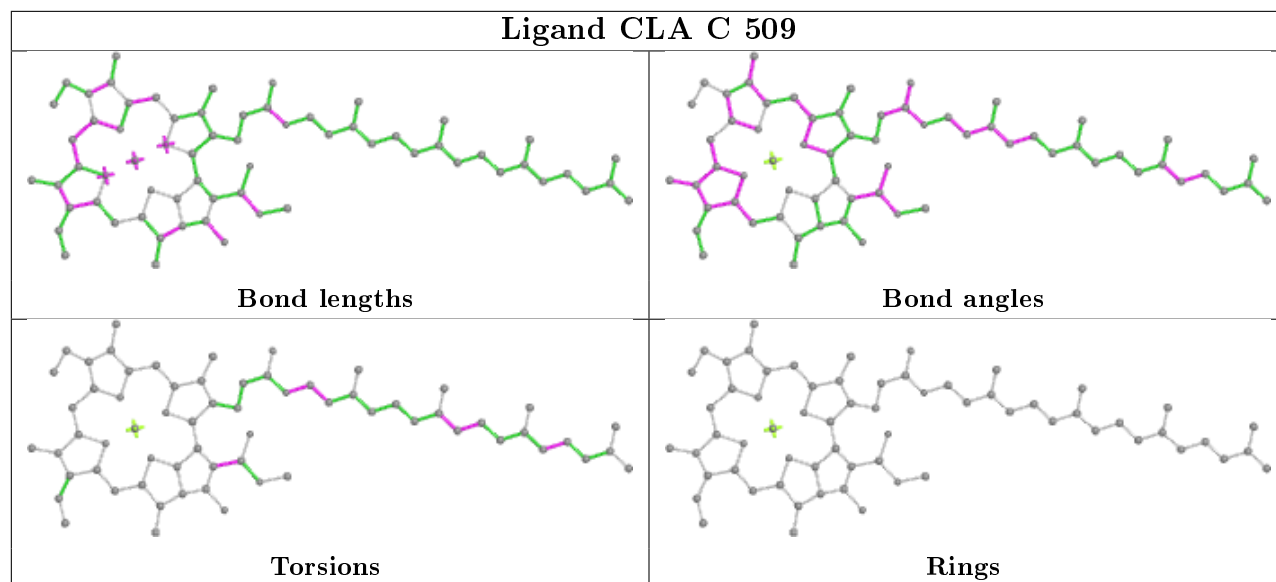


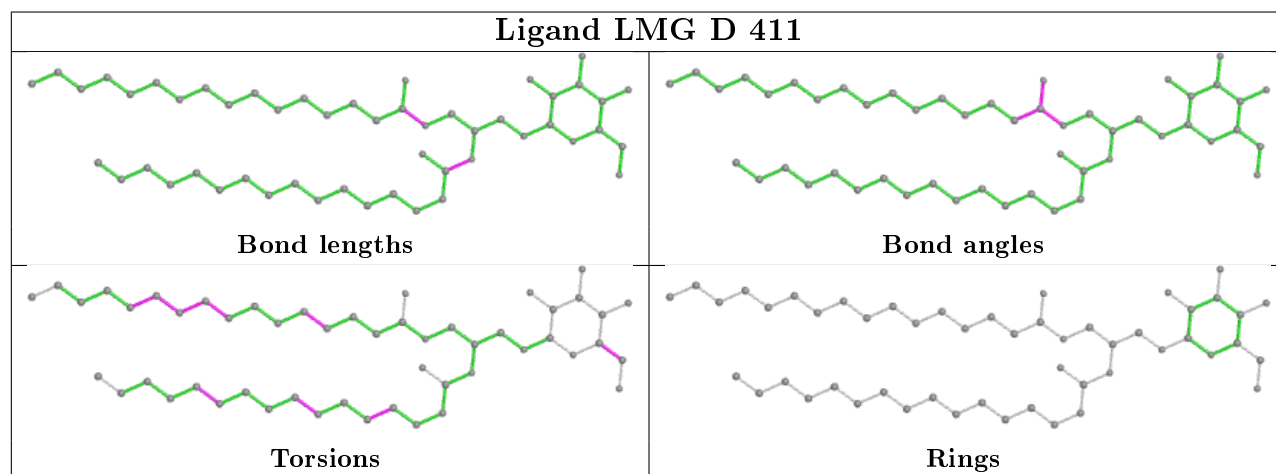
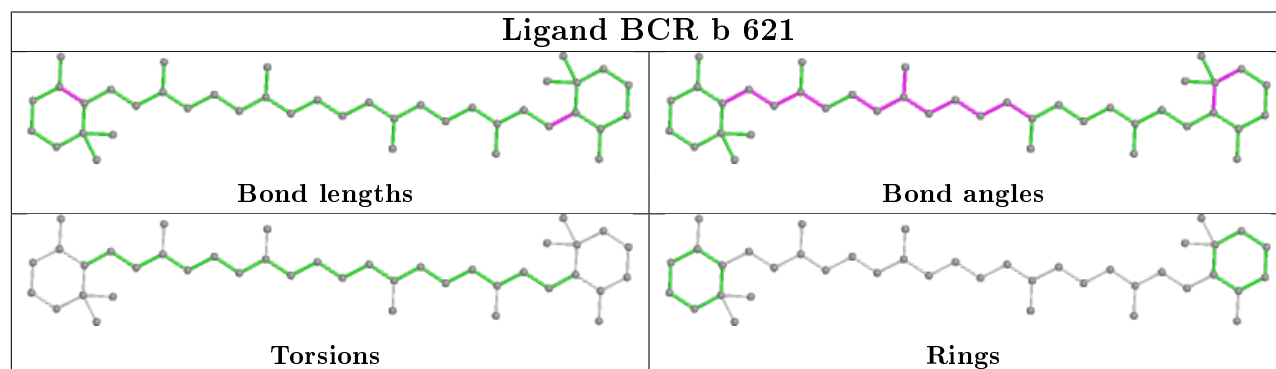
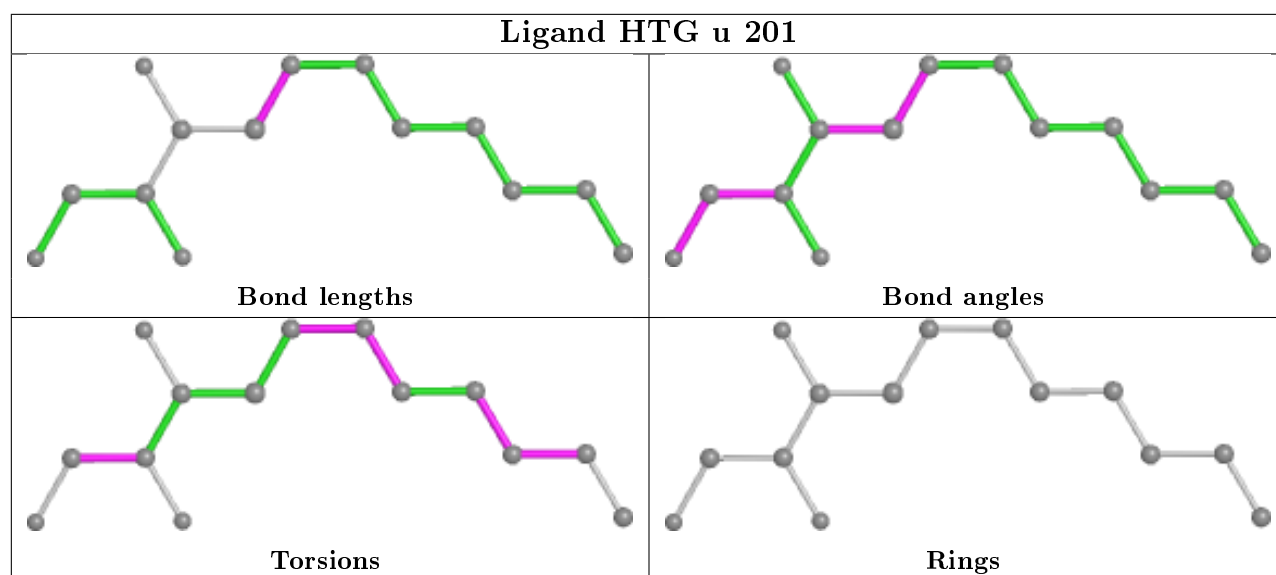


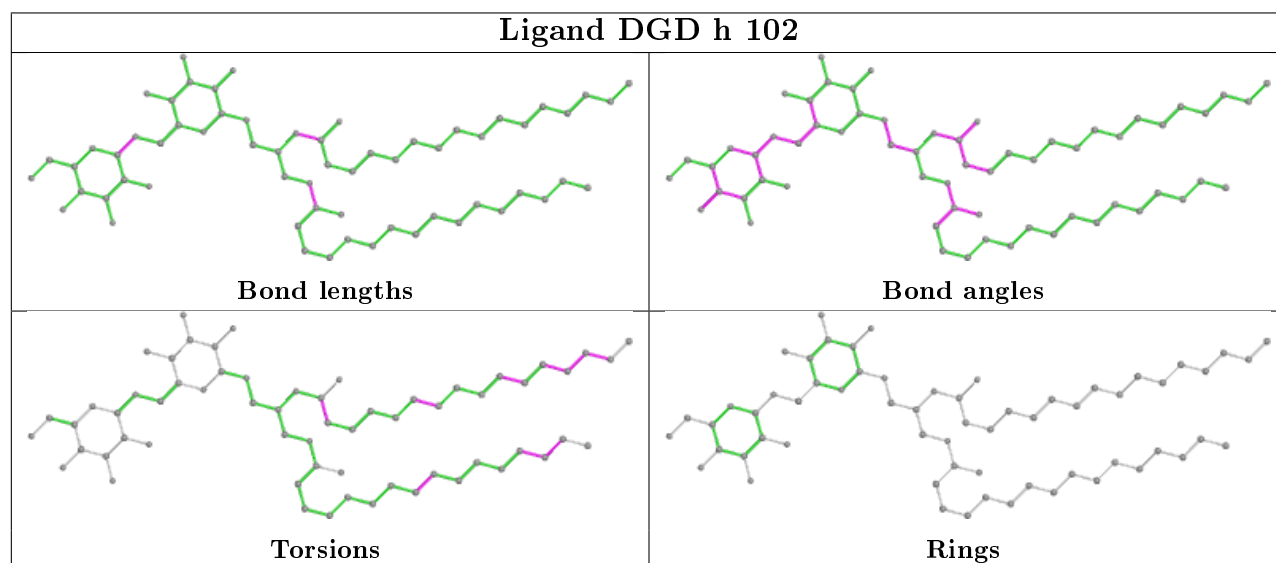
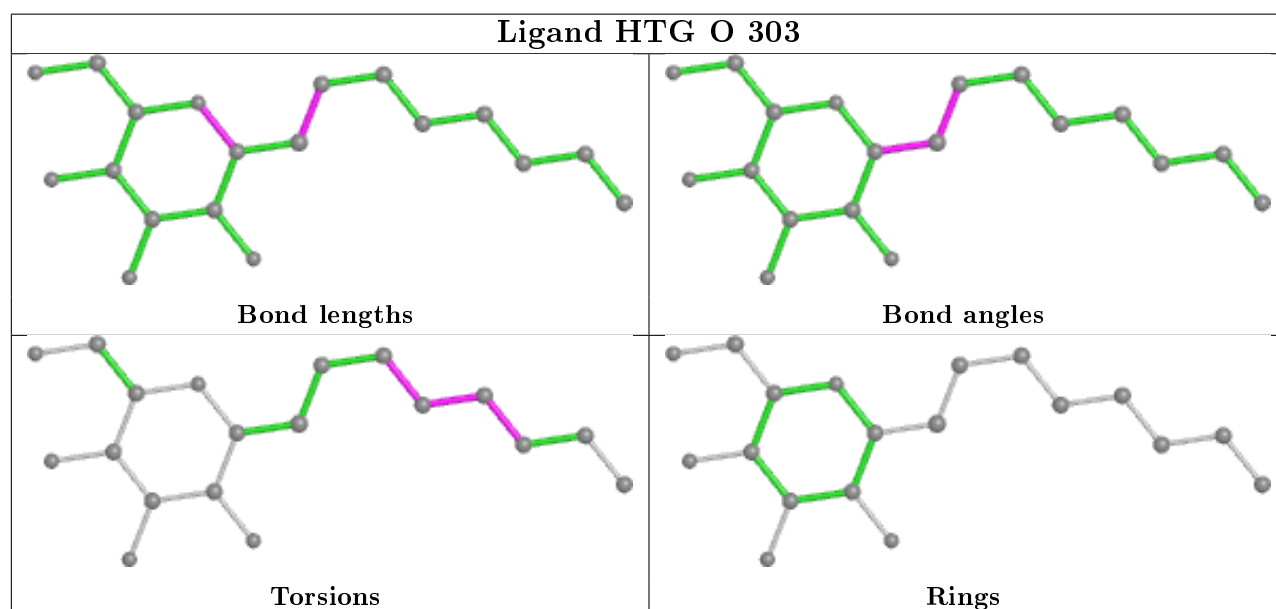
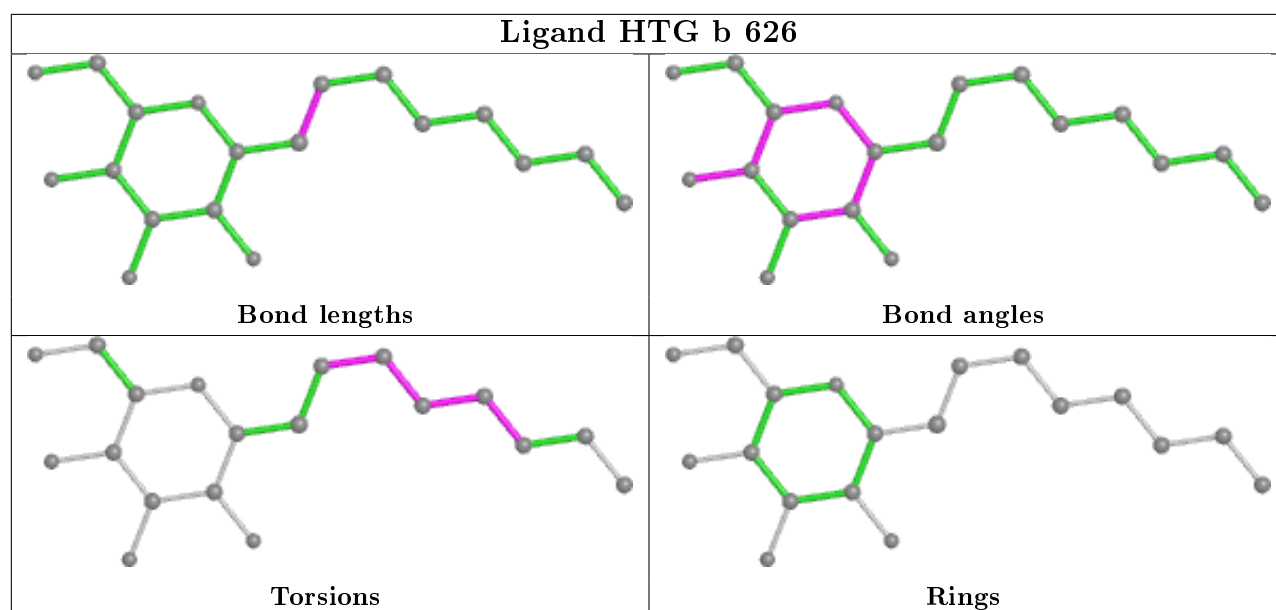
**Ligand CLA C 505****Ligand CLA b 604**

**Ligand LHG a 417****Ligand CLA B 610**

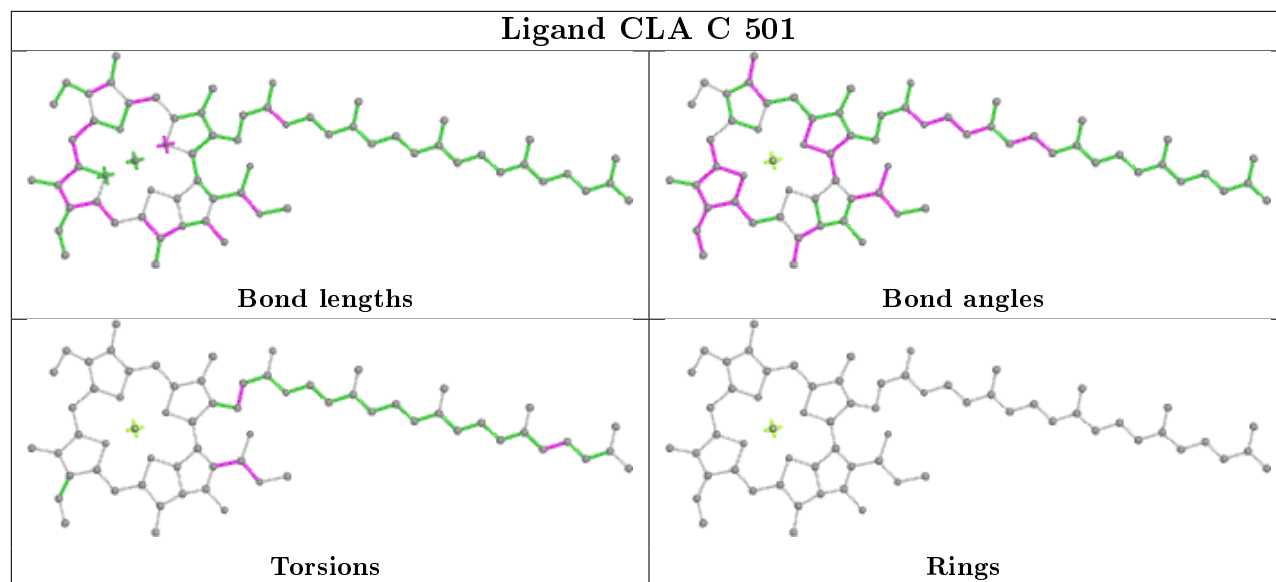




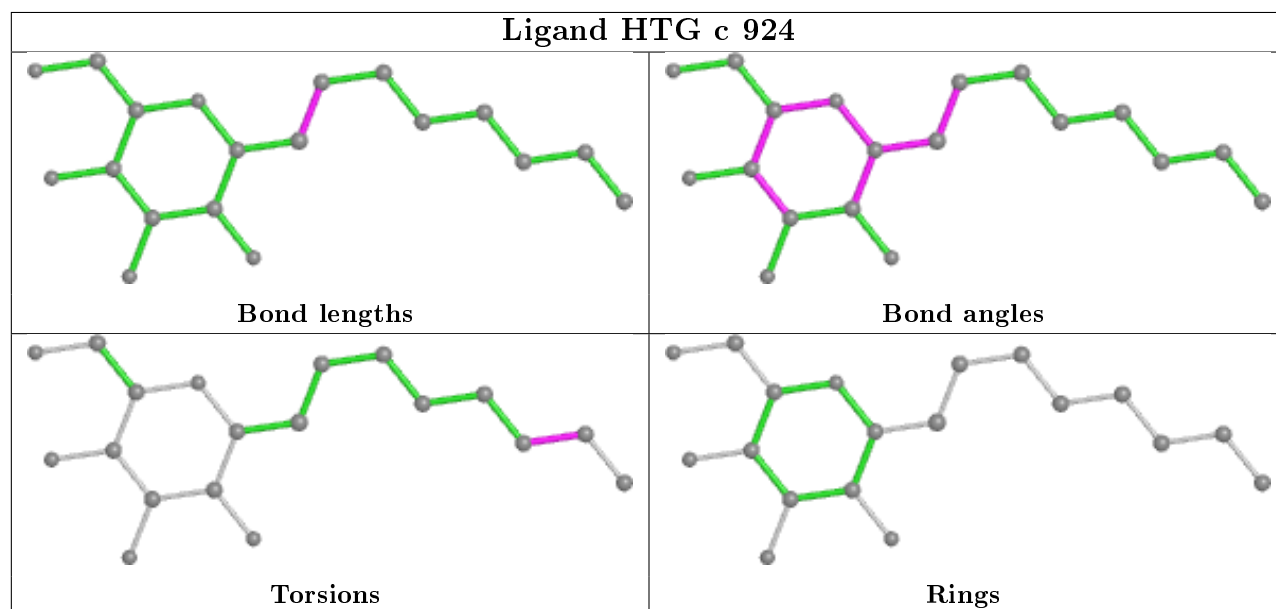




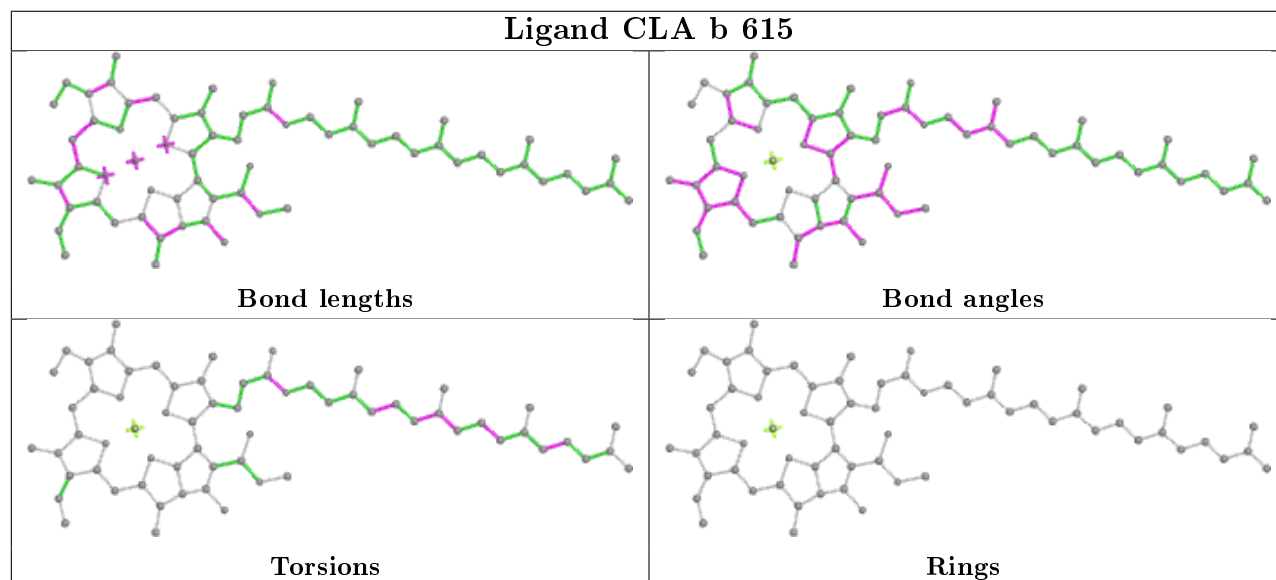
## Ligand CLA C 501

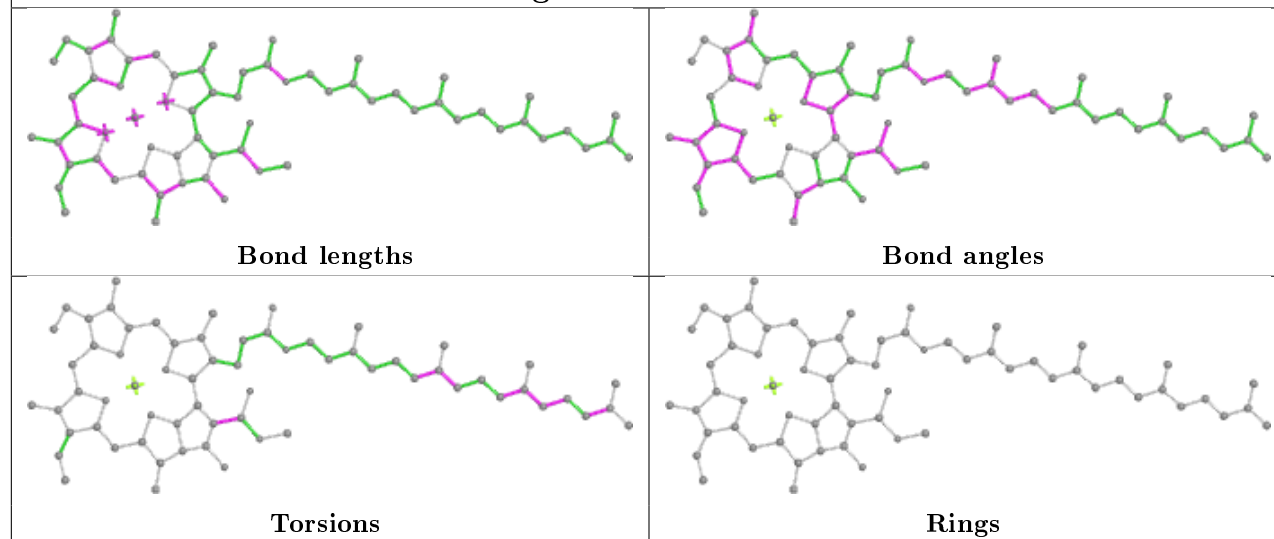
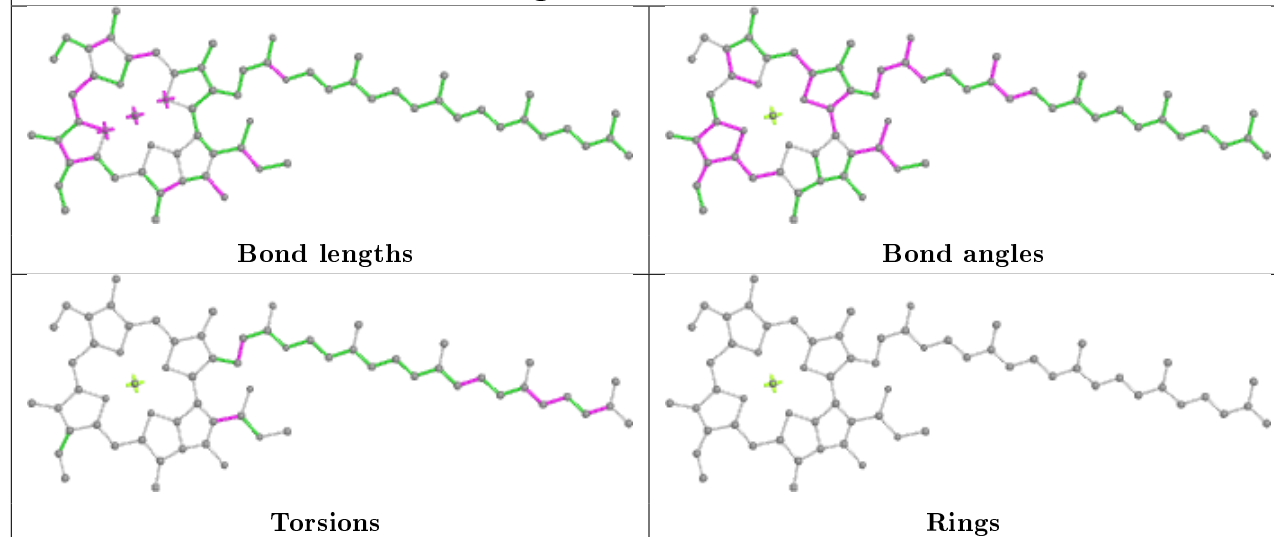
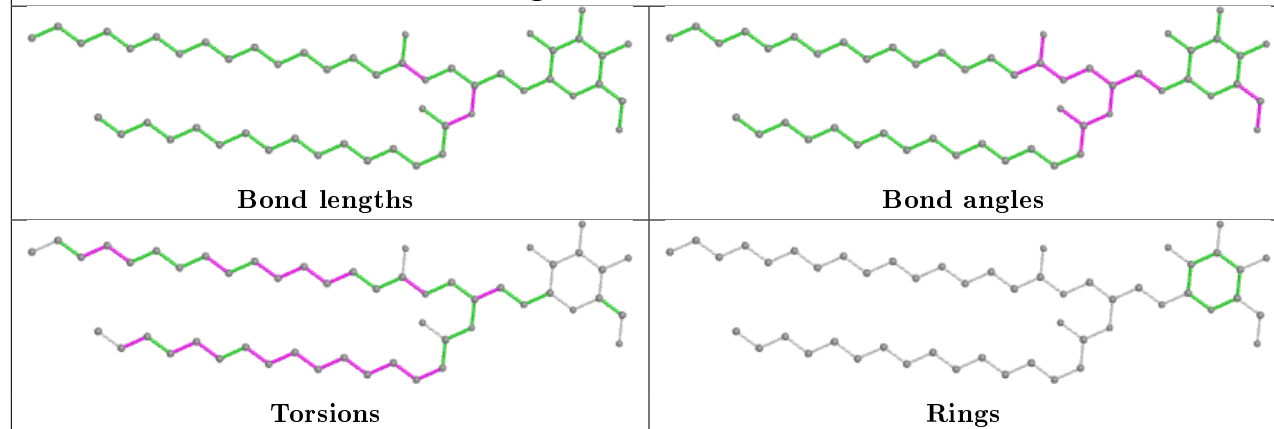


## Ligand HTG c 924

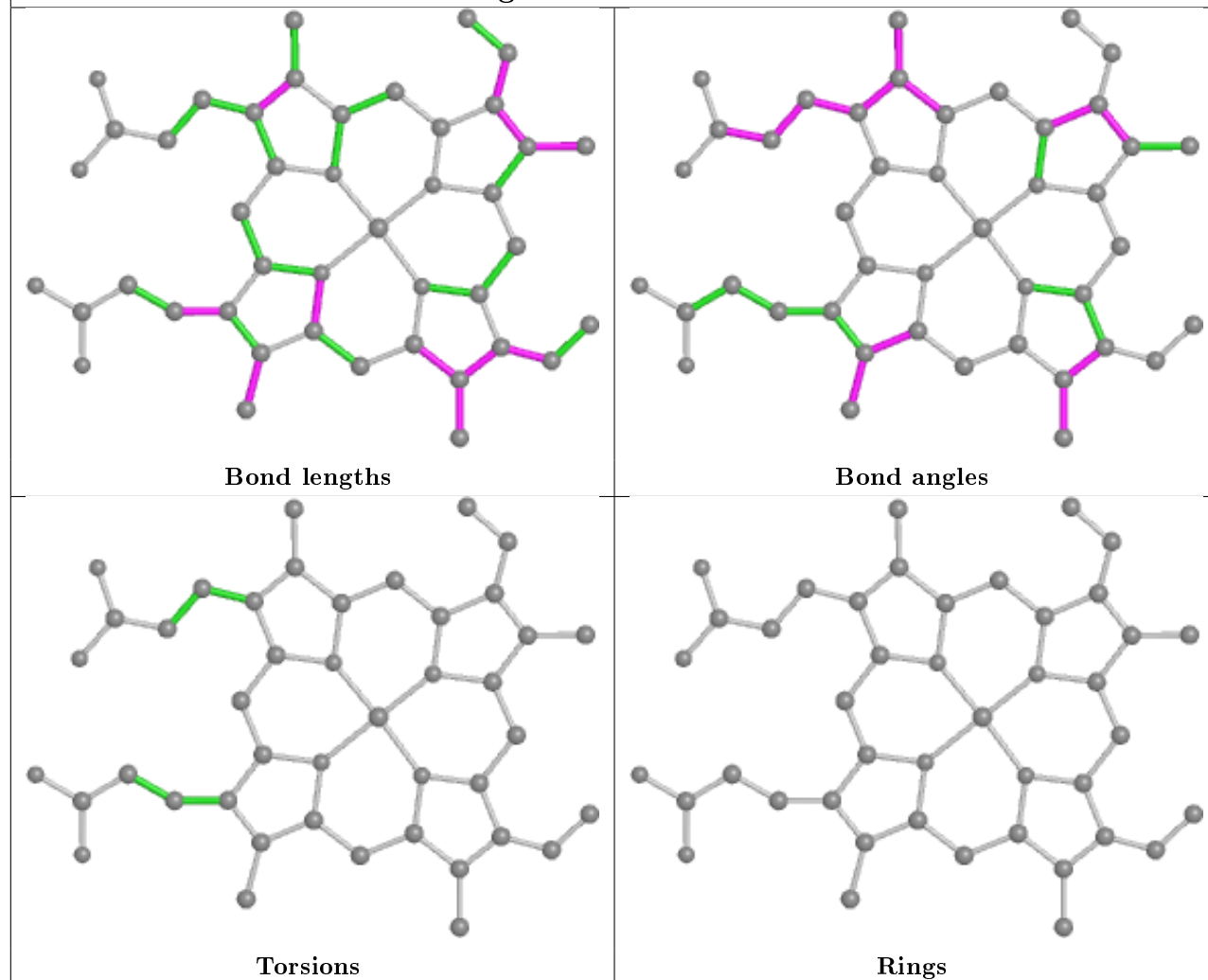


## Ligand CLA b 615

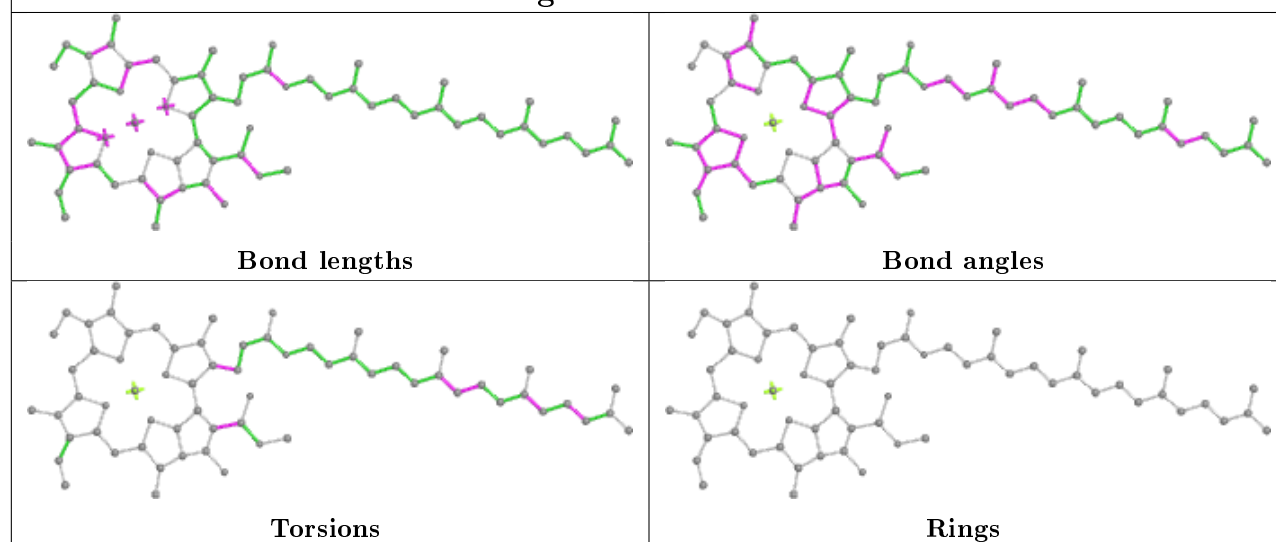


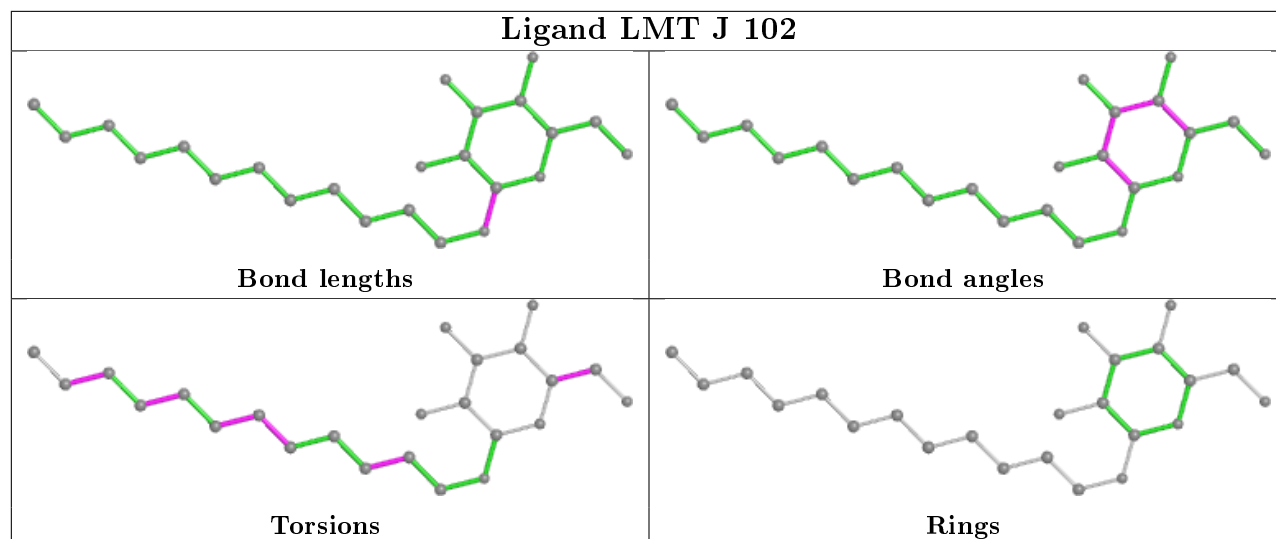
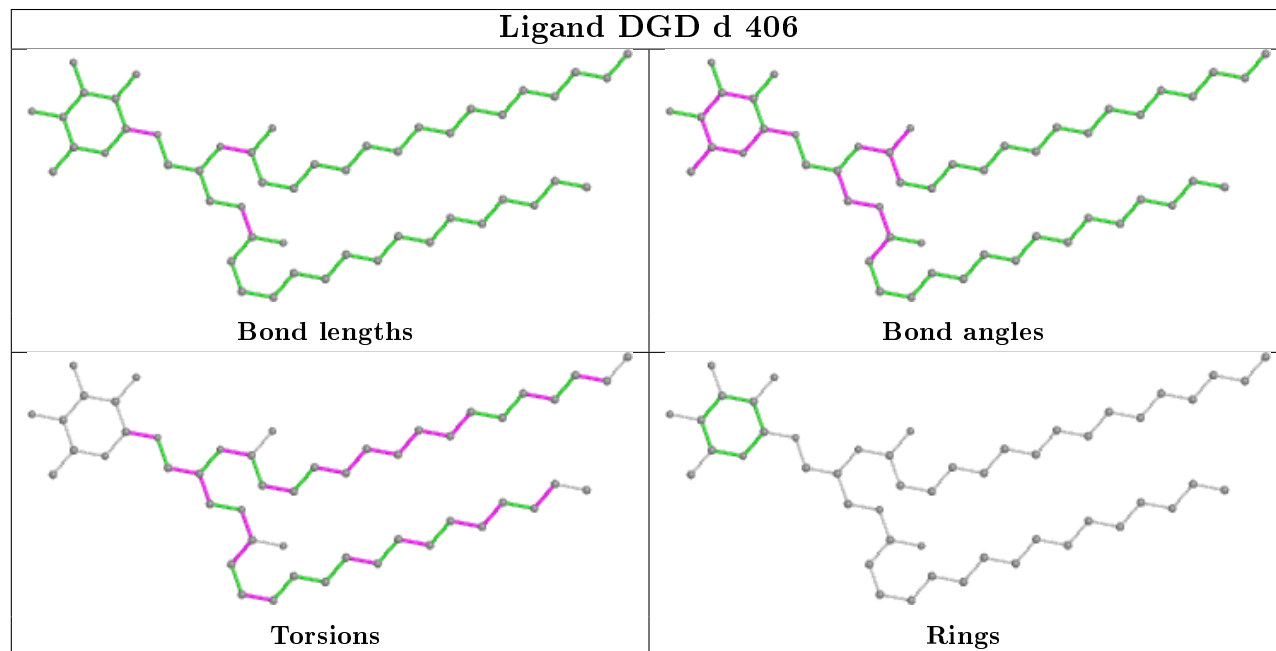
**Ligand CLA C 504****Ligand CLA B 611****Ligand LMG C 519**

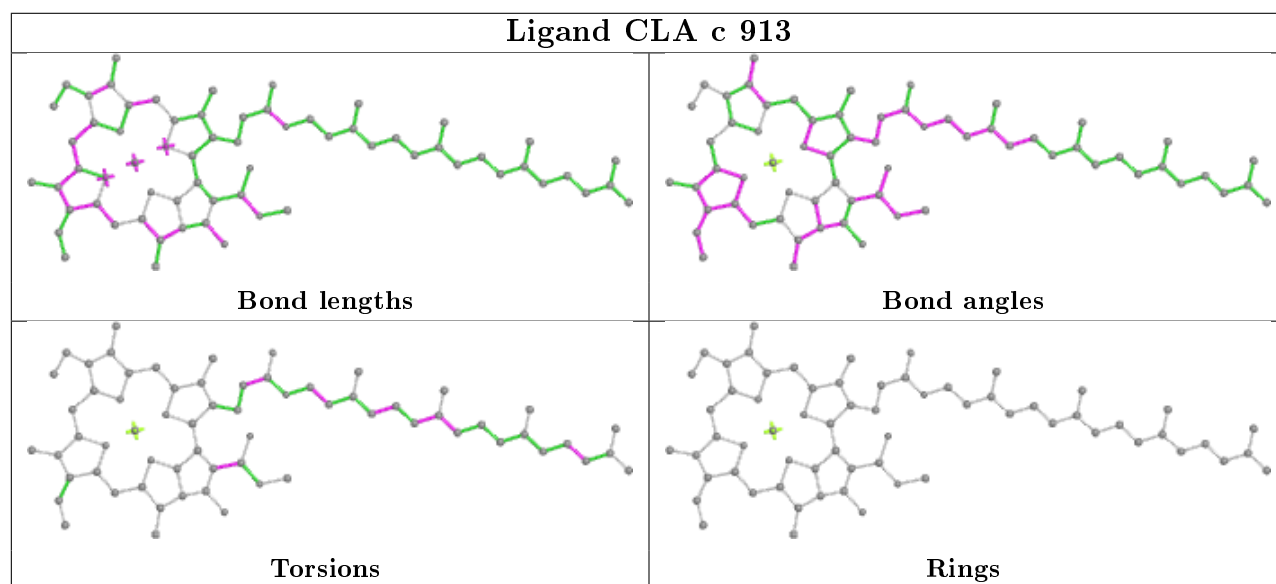
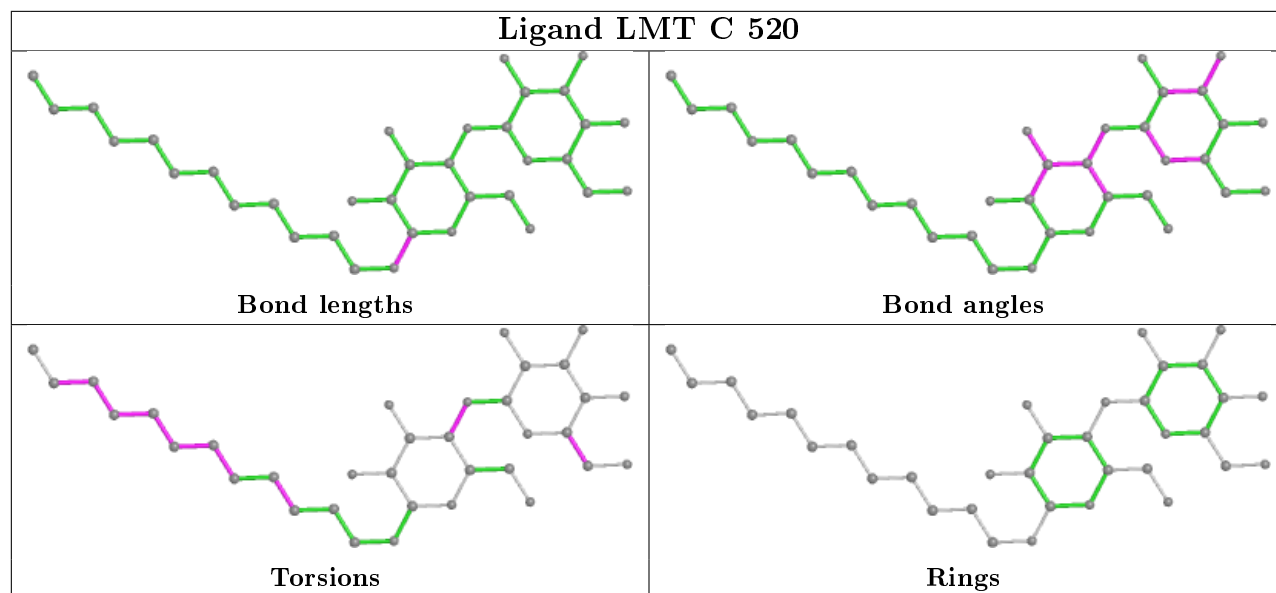
## Ligand HEM V 201



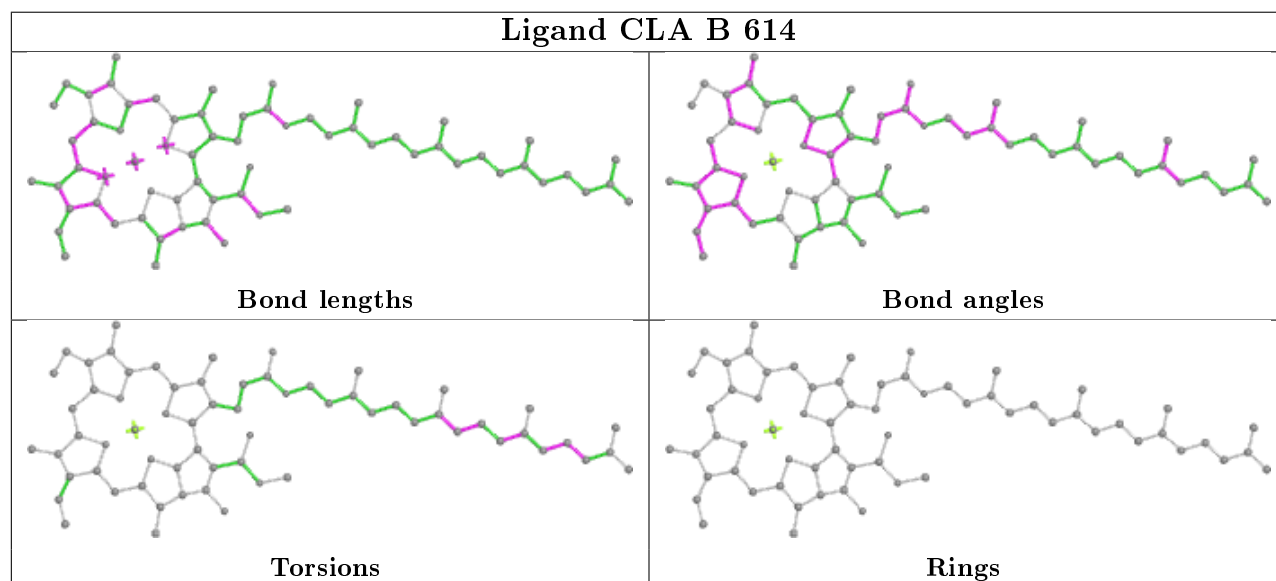
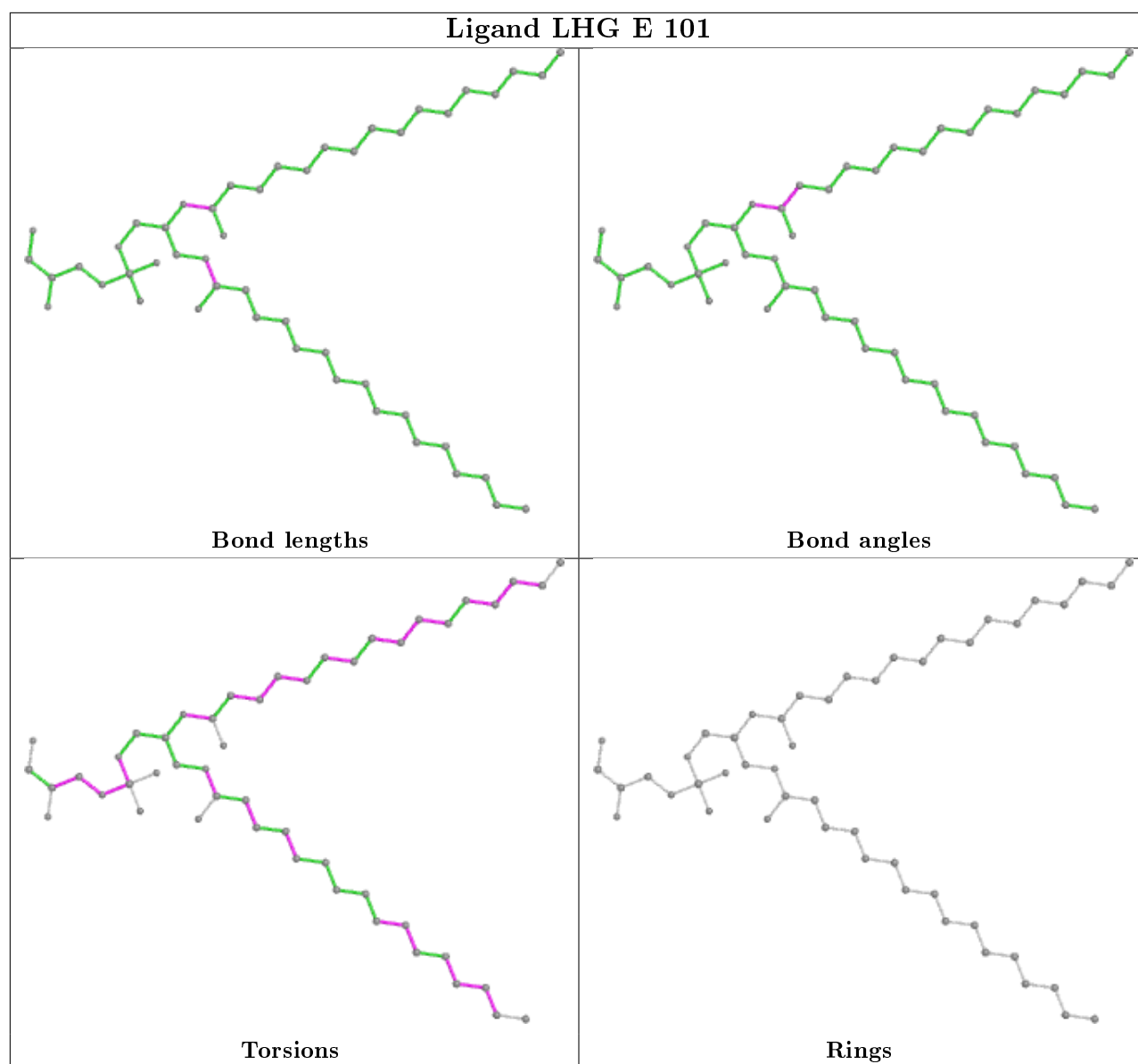
## Ligand CLA c 905

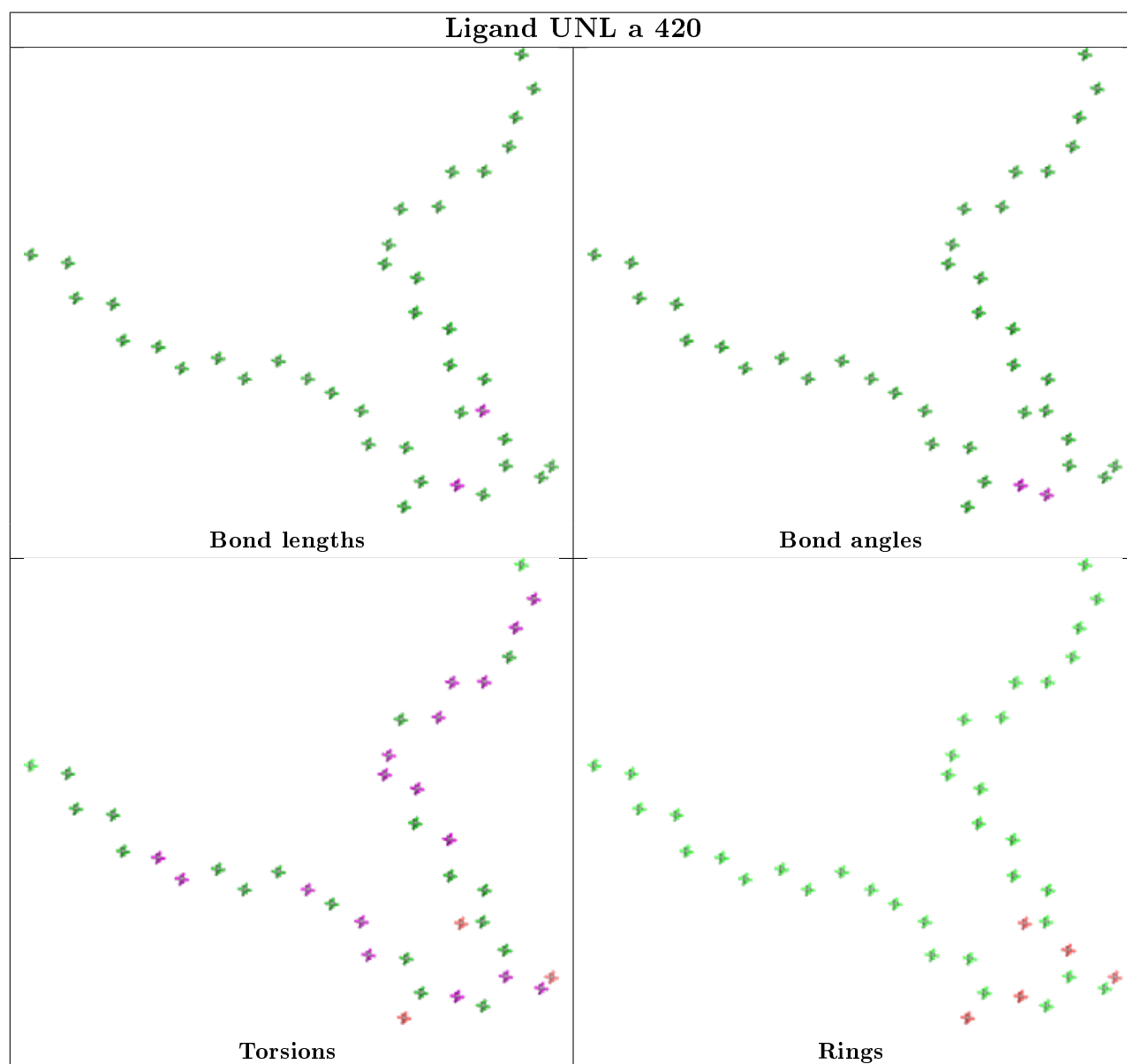
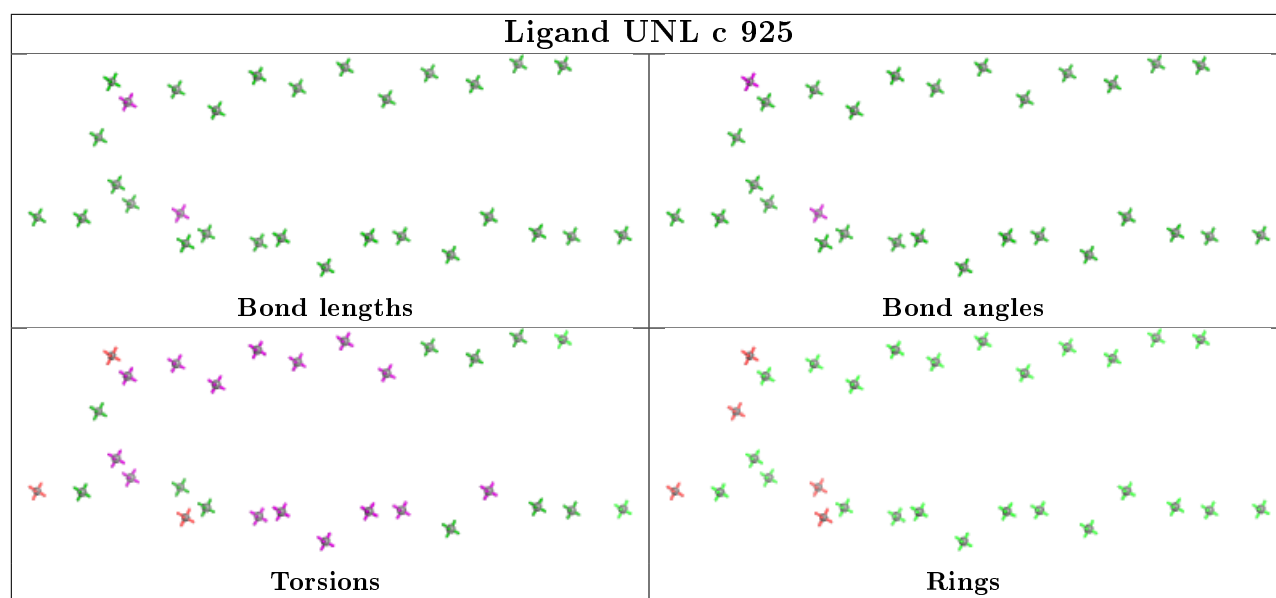


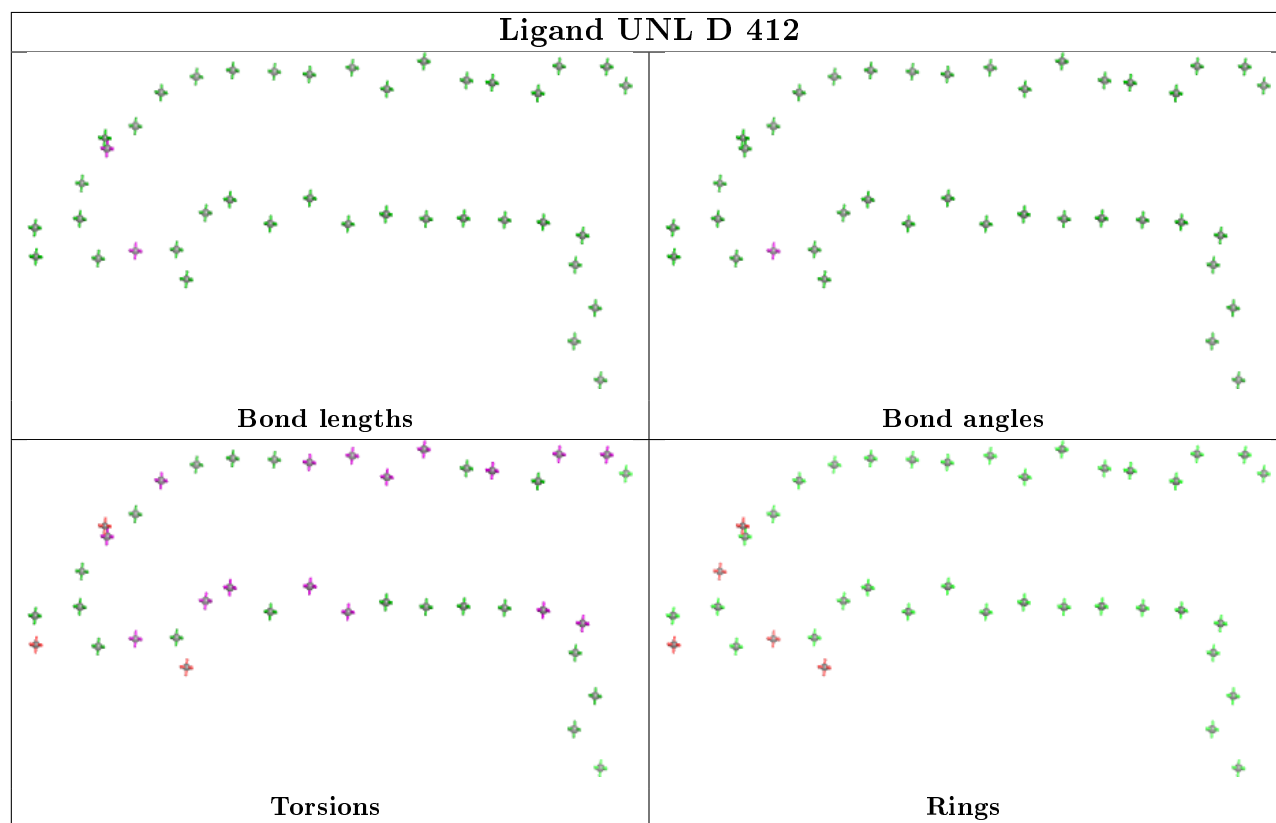
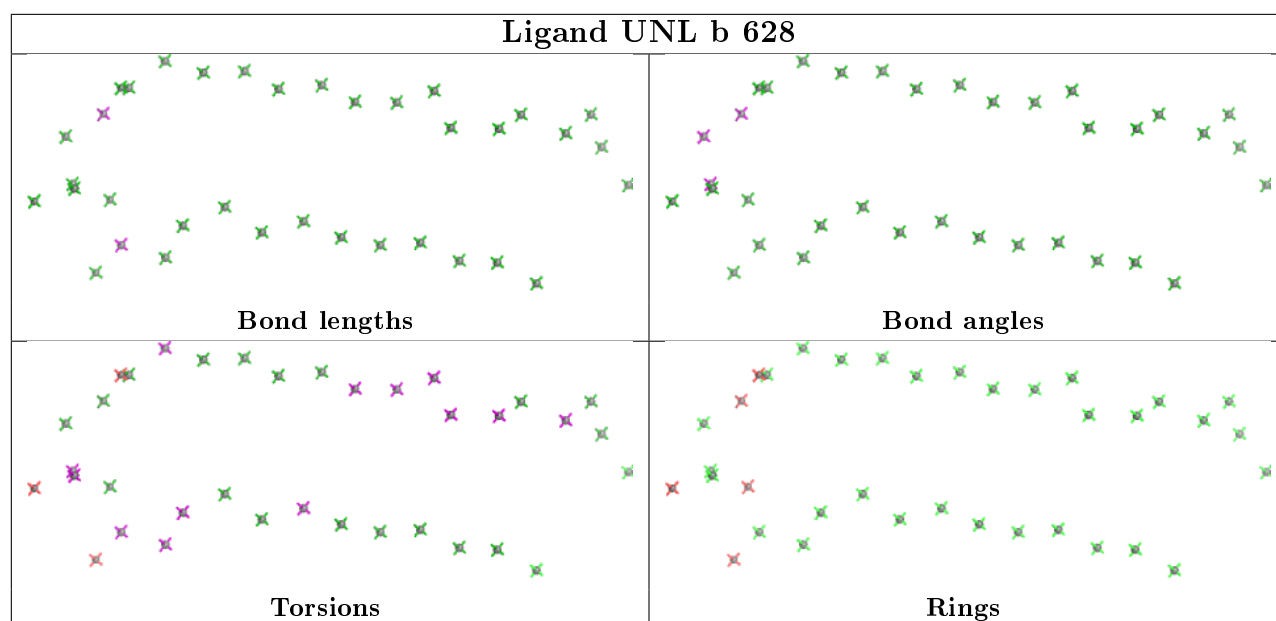
**Ligand LMT J 102****Ligand DGD d 406**

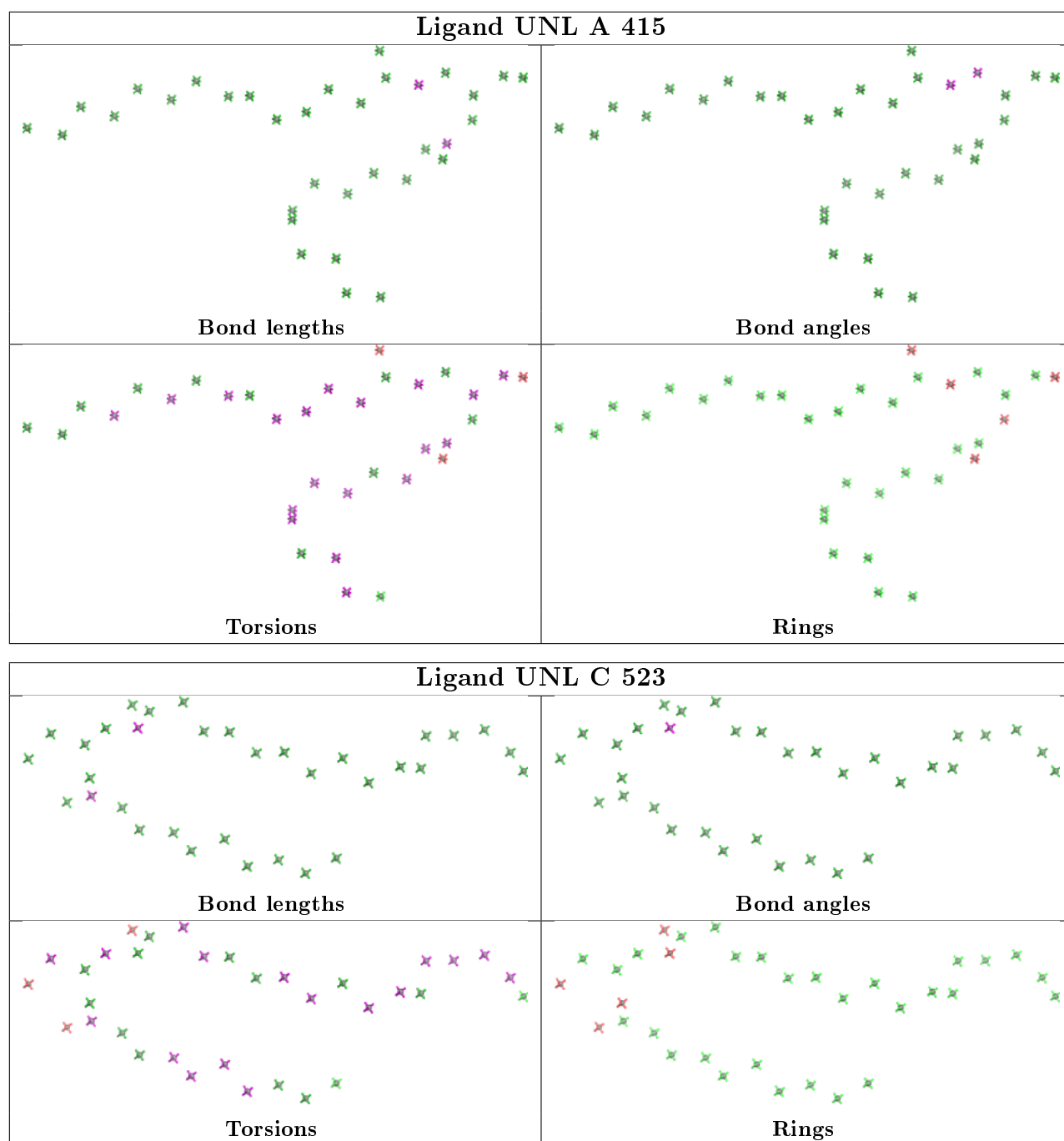












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.18	4 (1%) 79 81	16, 23, 46, 69	0
1	a	334/344 (97%)	-0.00	13 (3%) 39 42	19, 24, 50, 76	0
2	B	504/504 (100%)	0.07	39 (7%) 13 15	18, 27, 54, 88	0
2	b	501/504 (99%)	0.10	43 (8%) 10 12	20, 29, 58, 119	0
3	C	451/455 (99%)	-0.11	14 (3%) 49 51	21, 31, 46, 81	0
3	c	455/455 (100%)	0.14	25 (5%) 25 28	23, 34, 48, 79	0
4	D	340/342 (99%)	-0.23	7 (2%) 63 66	17, 24, 40, 70	0
4	d	340/342 (99%)	-0.19	6 (1%) 68 71	19, 26, 45, 80	0
5	E	81/83 (97%)	0.92	17 (20%) 1 1	27, 40, 62, 82	0
5	e	79/83 (95%)	1.19	23 (29%) 0 0	32, 44, 72, 82	0
6	F	34/44 (77%)	0.20	5 (14%) 2 2	26, 34, 63, 74	0
6	f	32/44 (72%)	0.35	3 (9%) 8 9	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.08	1 (1%) 72 74	24, 33, 43, 70	0
7	h	63/63 (100%)	0.37	5 (7%) 12 14	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.11	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	0.21	2 (5%) 25 29	26, 34, 71, 83	0
9	J	36/40 (90%)	0.14	4 (11%) 5 6	26, 38, 65, 79	0
9	j	39/40 (97%)	0.59	8 (20%) 1 1	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.17	0 100 100	32, 38, 47, 63	0
10	k	37/37 (100%)	0.30	3 (8%) 12 13	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.14	3 (8%) 12 13	17, 22, 65, 75	0
11	l	37/37 (100%)	0.13	2 (5%) 25 29	19, 23, 64, 95	0
12	M	32/36 (88%)	-0.17	1 (3%) 49 51	21, 24, 40, 56	0
12	m	33/36 (91%)	-0.01	2 (6%) 21 24	20, 25, 48, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	0.31	34 (13%) 2 3	18, 33, 66, 120	0
13	o	241/244 (98%)	0.38	39 (16%) 1 1	20, 35, 71, 87	0
14	T	29/32 (90%)	-0.01	1 (3%) 45 48	19, 23, 49, 85	0
14	t	29/32 (90%)	-0.01	1 (3%) 45 48	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.13	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.36	1 (1%) 82 84	24, 30, 40, 66	0
16	V	137/137 (100%)	-0.37	0 100 100	22, 28, 43, 51	0
16	v	137/137 (100%)	0.44	13 (9%) 8 9	26, 37, 52, 72	0
17	Y	27/30 (90%)	1.04	4 (14%) 2 2	37, 47, 70, 77	0
17	y	28/30 (93%)	1.15	7 (25%) 0 0	45, 55, 73, 77	0
18	X	38/40 (95%)	0.69	7 (18%) 1 1	32, 39, 65, 69	0
18	x	38/40 (95%)	0.94	9 (23%) 0 0	34, 42, 83, 94	0
19	Z	62/62 (100%)	1.46	19 (30%) 0 0	37, 46, 75, 92	0
19	z	60/62 (96%)	1.96	25 (41%) 0 0	47, 57, 88, 95	0
All	All	5235/5344 (97%)	0.11	390 (7%) 14 16	16, 30, 59, 120	0

The worst 5 of 390 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	8.3
2	b	496	TYR	8.1
18	x	37	VAL	7.9
13	o	246	ALA	7.4
13	O	60	ARG	7.4

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
12	FME	m	1	10/11	0.92	0.12	31,38,54,60	0
14	FME	t	1	10/11	0.95	0.09	20,23,41,50	0
12	FME	M	1	10/11	0.96	0.11	27,34,51,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HSK	d	336[A]	10/12	0.96	0.10	30,33,40,44	7
4	HSK	d	336[B]	11/12	0.96	0.10	30,31,37,38	8
8	FME	I	1	10/11	0.97	0.13	27,34,38,39	0
14	FME	T	1	10/11	0.97	0.08	24,27,43,50	0
8	FME	i	1	10/11	0.98	0.11	30,32,37,39	0
4	HSK	D	336[A]	10/12	0.98	0.10	26,28,31,34	7
4	HSK	D	336[B]	11/12	0.98	0.10	23,26,27,29	8

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	DGD	D	406	53/66	0.54	0.29	53,77,92,103	0
29	UNL	a	420	40/-	0.56	0.33	53,72,88,94	0
31	GOL	h	103	6/6	0.56	0.28	78,83,83,84	0
33	HTG	d	401	19/19	0.57	0.30	55,101,111,114	0
29	UNL	E	103	12/-	0.59	0.29	65,73,83,88	0
29	UNL	A	415	36/-	0.60	0.25	58,67,75,79	0
34	DGD	d	406	50/66	0.62	0.26	56,75,94,97	0
26	SQD	B	621	54/54	0.63	0.27	48,65,108,109	0
30	LMT	M	102	35/35	0.63	0.24	35,52,60,63	0
29	UNL	E	102	15/-	0.63	0.23	57,64,83,83	0
29	UNL	i	103	13/-	0.65	0.29	58,65,76,78	0
29	UNL	B	629	14/-	0.66	0.27	61,70,89,90	0
33	HTG	b	602	19/19	0.67	0.28	50,93,111,117	0
33	HTG	B	631	19/19	0.68	0.26	49,111,120,125	0
30	LMT	M	101	35/35	0.68	0.24	43,61,77,90	0
36	LHG	a	417	40/49	0.69	0.26	60,109,148,151	0
29	UNL	C	523	34/-	0.69	0.28	52,77,88,93	0
30	LMT	F	102	35/35	0.70	0.36	53,84,91,96	0
30	LMT	b	624	25/35	0.70	0.21	51,71,94,98	0
26	SQD	L	103	54/54	0.71	0.24	43,64,89,96	0
29	UNL	t	103	16/-	0.71	0.46	63,74,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	j	103	12/-	0.71	0.25	55,65,70,71	0
33	HTG	D	414	19/19	0.71	0.31	66,93,106,107	0
29	UNL	b	631	16/-	0.72	0.23	59,66,77,79	0
30	LMT	m	101	35/35	0.73	0.22	32,51,61,62	0
27	LMG	Z	101	51/55	0.73	0.27	41,76,102,113	0
27	LMG	c	921	51/55	0.74	0.27	38,80,95,111	0
33	HTG	b	627	19/19	0.74	0.34	53,94,104,105	0
30	LMT	B	623	35/35	0.74	0.24	43,79,117,129	0
29	UNL	c	925	30/-	0.74	0.18	59,72,89,95	0
33	HTG	B	626	19/19	0.74	0.42	48,87,92,93	0
29	UNL	Z	103	16/-	0.74	0.21	48,63,81,81	0
29	UNL	H	103	10/-	0.75	0.23	60,69,74,76	0
29	UNL	c	926	10/-	0.75	0.17	65,67,71,72	0
29	UNL	b	630	16/-	0.75	0.39	51,62,73,74	0
28	PL9	a	419	55/55	0.75	0.23	52,74,98,109	0
27	LMG	a	418	51/55	0.75	0.22	43,60,68,73	0
26	SQD	a	401	54/54	0.75	0.18	45,59,85,90	0
33	HTG	C	522	19/19	0.75	0.34	50,79,92,94	0
30	LMT	J	102	24/35	0.75	0.19	45,55,79,83	0
29	UNL	i	104	10/-	0.75	0.28	67,72,77,78	0
29	UNL	e	800	11/-	0.76	0.29	53,60,68,68	0
30	LMT	m	102	35/35	0.76	0.19	41,54,72,84	0
28	PL9	A	414	55/55	0.76	0.26	47,66,93,96	0
29	UNL	J	103	14/-	0.77	0.16	61,66,73,76	0
29	UNL	z	102	16/-	0.77	0.22	51,70,89,92	0
29	UNL	I	101	13/-	0.77	0.22	44,53,61,63	0
30	LMT	b	625	24/35	0.78	0.25	35,61,99,100	0
29	UNL	T	102	13/-	0.78	0.54	66,70,83,87	0
29	UNL	B	632	16/-	0.78	0.31	50,59,73,73	0
33	HTG	c	924	19/19	0.78	0.41	53,85,97,100	0
30	LMT	c	922	35/35	0.78	0.32	61,73,85,90	0
30	LMT	Z	102	35/35	0.78	0.27	41,87,102,107	0
30	LMT	t	102	24/35	0.78	0.26	33,55,94,95	0
30	LMT	z	101	32/35	0.79	0.24	46,85,90,100	0
29	UNL	i	102	16/-	0.79	0.23	54,65,83,84	0
27	LMG	A	413	51/55	0.79	0.24	42,57,76,78	0
33	HTG	U	201	9/19	0.79	0.23	54,59,82,98	0
29	UNL	D	412	40/-	0.79	0.20	39,60,96,99	0
29	UNL	j	102	16/-	0.80	0.17	52,61,69,69	0
31	GOL	O	304	6/6	0.80	0.17	52,60,61,63	0
29	UNL	A	417	13/-	0.81	0.35	56,59,66,66	0
26	SQD	f	102	33/54	0.81	0.21	63,73,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	GOL	b	635	6/6	0.81	0.14	40,43,46,48	0
26	SQD	A	418	54/54	0.81	0.19	42,59,81,86	0
32	CA	B	601	1/1	0.82	0.09	81,81,81,81	0
29	UNL	b	628	36/-	0.82	0.26	44,65,101,106	0
40	SO4	O	302	5/5	0.82	0.29	78,87,95,105	0
26	SQD	D	407	45/54	0.82	0.28	50,78,94,101	0
27	LMG	c	920	51/55	0.82	0.23	30,65,100,104	0
36	LHG	E	101	49/49	0.82	0.21	50,80,94,97	0
30	LMT	C	520	35/35	0.83	0.31	52,71,83,89	0
29	UNL	B	627	16/-	0.83	0.14	43,47,69,69	0
33	HTG	u	201	14/19	0.83	0.25	46,64,90,96	0
30	LMT	a	402	35/35	0.84	0.17	37,54,69,80	0
29	UNL	I	102	11/-	0.84	0.22	62,65,66,68	0
33	HTG	B	630	19/19	0.84	0.15	39,52,66,79	0
31	GOL	a	424	6/6	0.85	0.20	42,56,59,74	0
29	UNL	M	103	16/-	0.85	0.23	49,58,77,79	0
33	HTG	c	923	19/19	0.85	0.24	64,75,82,83	0
31	GOL	c	927	6/6	0.86	0.13	43,53,60,68	0
29	UNL	J	104	12/-	0.86	0.17	53,65,72,74	0
29	UNL	d	411	16/-	0.86	0.32	39,49,63,66	0
29	UNL	B	628	10/-	0.86	0.27	52,56,70,74	0
27	LMG	C	519	51/55	0.86	0.19	29,59,97,105	0
31	GOL	b	636	6/6	0.87	0.12	45,56,58,60	0
30	LMT	A	419	35/35	0.87	0.15	37,56,73,94	0
33	HTG	b	601	19/19	0.87	0.15	43,51,62,68	0
27	LMG	B	622	51/55	0.87	0.18	28,37,53,63	0
34	DGD	h	102	62/66	0.88	0.18	27,35,45,52	0
38	RRX	h	101	41/41	0.88	0.12	27,35,49,54	0
27	LMG	b	623	51/55	0.88	0.19	30,39,52,63	0
38	RRX	H	101	41/41	0.88	0.14	25,30,44,47	0
23	CLA	B	610	65/65	0.88	0.13	23,28,33,35	0
23	CLA	b	612	65/65	0.89	0.13	26,30,36,38	0
31	GOL	C	526	6/6	0.89	0.14	38,43,51,57	0
29	UNL	a	421	10/-	0.89	0.29	53,57,61,64	0
25	BCR	k	102	40/40	0.89	0.13	29,41,48,50	0
31	GOL	A	422	6/6	0.89	0.13	42,55,58,67	0
31	GOL	l	102	6/6	0.89	0.38	37,55,57,57	0
29	UNL	b	629	16/-	0.89	0.11	43,48,56,60	0
29	UNL	L	102	14/-	0.89	0.22	52,58,66,69	0
29	UNL	D	413	16/-	0.89	0.26	39,47,65,65	0
23	CLA	C	506	65/65	0.90	0.13	25,38,94,97	0
23	CLA	c	914	65/65	0.90	0.15	38,53,90,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	CA	b	603	1/1	0.90	0.09	82,82,82,82	0
29	UNL	A	416	16/-	0.90	0.14	41,46,73,73	0
31	GOL	L	104	6/6	0.91	0.26	44,52,54,55	0
26	SQD	a	416	54/54	0.91	0.17	37,55,88,90	0
34	DGD	H	102	62/66	0.91	0.20	24,31,40,45	0
31	GOL	f	104	6/6	0.91	0.33	46,51,51,54	0
29	UNL	X	101	16/-	0.91	0.12	34,39,58,60	0
31	GOL	C	524	6/6	0.91	0.17	36,45,47,53	0
29	UNL	x	101	16/-	0.91	0.15	36,45,70,73	0
34	DGD	c	919	62/66	0.91	0.14	25,35,60,71	0
34	DGD	c	918	62/66	0.92	0.15	27,35,79,91	0
23	CLA	B	603	65/65	0.92	0.14	23,26,34,37	0
33	HTG	V	202	13/19	0.92	0.26	43,48,76,84	0
27	LMG	d	410	51/55	0.92	0.12	29,36,80,91	0
29	UNL	a	403	6/-	0.92	0.42	57,62,66,66	0
25	BCR	c	915	40/40	0.92	0.10	44,51,59,60	0
23	CLA	B	602	65/65	0.92	0.18	29,41,78,95	0
33	HTG	C	521	19/19	0.92	0.18	56,63,76,80	0
29	UNL	i	101	16/-	0.92	0.13	40,46,56,62	0
23	CLA	b	609	65/65	0.92	0.11	23,31,57,63	0
36	LHG	l	101	49/49	0.92	0.17	22,31,47,57	0
31	GOL	B	638	6/6	0.93	0.10	35,47,49,53	0
23	CLA	C	513	65/65	0.93	0.13	35,46,78,83	0
27	LMG	D	411	51/55	0.93	0.17	23,35,91,99	0
23	CLA	b	604	65/65	0.93	0.16	34,47,73,81	0
31	GOL	B	637	6/6	0.93	0.13	36,38,45,54	0
23	CLA	b	605	65/65	0.93	0.12	24,29,36,39	0
23	CLA	c	913	65/65	0.93	0.12	33,45,67,72	0
29	UNL	A	420	4/-	0.93	0.54	64,66,66,66	0
31	GOL	b	633	6/6	0.93	0.23	41,46,49,52	0
34	DGD	C	517	62/66	0.94	0.14	22,31,78,92	0
23	CLA	C	512	65/65	0.94	0.10	34,41,69,74	0
36	LHG	D	408	49/49	0.94	0.16	26,35,45,45	0
25	BCR	k	101	40/40	0.94	0.09	33,39,47,49	0
23	CLA	c	902	65/65	0.94	0.13	27,34,46,50	0
34	DGD	c	917	62/66	0.94	0.16	24,33,77,80	0
36	LHG	L	101	49/49	0.94	0.14	22,31,44,49	0
31	GOL	B	635	6/6	0.94	0.12	38,47,49,50	0
36	LHG	d	407	49/49	0.94	0.23	27,36,46,49	0
33	HTG	B	625	19/19	0.94	0.15	31,38,71,75	0
23	CLA	c	907	65/65	0.94	0.09	28,36,76,80	0
34	DGD	C	516	62/66	0.94	0.20	22,32,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	GOL	c	928	6/6	0.94	0.22	42,51,54,54	0
25	BCR	d	404	40/40	0.94	0.10	25,33,56,58	0
23	CLA	c	905	65/65	0.94	0.18	24,31,64,66	0
26	SQD	A	412	54/54	0.94	0.14	35,54,71,74	0
23	CLA	B	607	65/65	0.94	0.10	21,27,55,61	0
23	CLA	c	904	65/65	0.94	0.15	24,37,42,42	0
31	GOL	a	422	6/6	0.94	0.10	30,38,44,45	0
25	BCR	c	916	40/40	0.94	0.10	28,36,45,47	0
23	CLA	c	908	65/65	0.94	0.12	26,32,52,55	0
25	BCR	B	620	40/40	0.95	0.09	22,31,41,44	0
25	BCR	C	514	40/40	0.95	0.07	33,42,46,46	0
25	BCR	K	101	40/40	0.95	0.10	30,35,40,43	0
31	GOL	v	203	6/6	0.95	0.15	31,35,41,43	0
25	BCR	B	619	40/40	0.95	0.19	19,26,42,45	0
25	BCR	b	622	40/40	0.95	0.10	25,33,43,45	0
23	CLA	C	511	65/65	0.95	0.09	27,34,40,42	0
36	LHG	d	408	49/49	0.95	0.14	22,27,42,47	0
32	CA	o	301	1/1	0.95	0.11	51,51,51,51	0
31	GOL	V	203	6/6	0.95	0.15	26,32,36,38	0
25	BCR	t	101	40/40	0.95	0.14	23,30,42,44	0
28	PL9	d	405	55/55	0.95	0.16	19,25,30,34	0
31	GOL	V	204	6/6	0.95	0.26	39,52,59,59	0
32	CA	O	301	1/1	0.95	0.14	49,49,49,49	0
31	GOL	v	204	6/6	0.95	0.25	46,50,61,62	0
23	CLA	c	903	65/65	0.95	0.19	22,29,42,55	0
31	GOL	b	632	6/6	0.95	0.11	35,42,46,47	0
31	GOL	B	636	6/6	0.95	0.14	33,43,47,56	0
23	CLA	b	618	65/65	0.95	0.08	24,30,49,53	0
23	CLA	c	912	65/65	0.95	0.09	29,37,45,50	0
31	GOL	B	633	6/6	0.95	0.13	34,39,47,52	0
23	CLA	C	507	65/65	0.95	0.10	26,33,56,61	0
31	GOL	c	930	6/6	0.95	0.21	49,54,57,59	0
31	GOL	a	423	6/6	0.96	0.14	33,34,35,45	0
36	LHG	d	409	49/49	0.96	0.16	27,32,85,91	0
31	GOL	A	421	6/6	0.96	0.13	30,37,38,41	0
23	CLA	b	613	65/65	0.96	0.13	24,28,35,40	0
23	CLA	C	503	65/65	0.96	0.12	26,31,38,39	0
23	CLA	C	510	65/65	0.96	0.15	22,28,38,41	0
36	LHG	D	409	49/49	0.96	0.12	22,28,40,44	0
23	CLA	b	607	65/65	0.96	0.16	20,25,54,59	0
25	BCR	a	415	40/40	0.96	0.07	21,25,30,31	0
25	BCR	T	101	40/40	0.96	0.16	24,32,47,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	c	906	65/65	0.96	0.10	26,31,46,50	0
23	CLA	B	611	65/65	0.96	0.14	19,25,34,39	0
23	CLA	D	402	65/65	0.96	0.11	13,18,36,39	0
33	HTG	B	624	19/19	0.96	0.09	27,33,41,51	0
23	CLA	C	509	65/65	0.96	0.13	27,31,47,51	0
32	CA	c	901	1/1	0.96	0.07	46,46,46,46	0
23	CLA	B	612	65/65	0.96	0.13	18,21,34,37	0
23	CLA	B	617	65/65	0.96	0.10	20,28,79,83	0
25	BCR	D	404	40/40	0.96	0.16	24,29,55,57	0
25	BCR	b	621	40/40	0.96	0.20	21,28,43,46	0
31	GOL	B	634	6/6	0.96	0.10	29,29,34,37	0
31	GOL	D	415	6/6	0.96	0.20	35,36,42,46	0
33	HTG	b	626	19/19	0.96	0.17	29,40,73,75	0
35	BCT	a	408	4/4	0.96	0.09	30,32,37,46	0
23	CLA	b	619	65/65	0.96	0.12	25,32,89,97	0
23	CLA	C	505	65/65	0.96	0.14	26,31,47,51	0
23	CLA	B	615	65/65	0.96	0.11	19,24,67,74	0
23	CLA	C	501	65/65	0.96	0.14	25,32,46,53	0
23	CLA	b	606	65/65	0.96	0.12	20,26,37,42	0
23	CLA	b	615	65/65	0.96	0.14	19,27,33,38	0
23	CLA	C	504	65/65	0.96	0.15	23,28,62,68	0
23	CLA	C	508	65/65	0.96	0.14	24,29,73,81	0
23	CLA	b	617	65/65	0.96	0.14	20,25,71,83	0
32	CA	F	103	1/1	0.96	0.15	55,55,55,55	0
34	DGD	C	518	62/66	0.96	0.15	20,30,68,75	0
25	BCR	C	515	40/40	0.96	0.14	28,34,41,44	0
31	GOL	v	202	6/6	0.96	0.10	35,36,40,41	0
23	CLA	A	410	65/65	0.96	0.11	20,24,99,105	0
31	GOL	b	634	6/6	0.96	0.12	32,39,44,46	0
23	CLA	D	403	65/65	0.96	0.11	22,28,73,79	0
25	BCR	K	102	40/40	0.96	0.08	28,31,39,42	0
25	BCR	B	618	40/40	0.96	0.15	20,26,29,30	0
23	CLA	c	910	65/65	0.97	0.18	25,31,49,52	0
23	CLA	B	613	65/65	0.97	0.14	19,24,31,34	0
23	CLA	B	608	65/65	0.97	0.14	17,20,34,37	0
23	CLA	C	502	65/65	0.97	0.14	21,26,39,48	0
23	CLA	A	405	65/65	0.97	0.10	14,19,25,42	0
31	GOL	V	205	6/6	0.97	0.23	33,36,37,41	0
32	CA	f	103	1/1	0.97	0.18	56,56,56,56	0
25	BCR	b	620	40/40	0.97	0.16	23,27,33,33	0
33	HTG	O	303	19/19	0.97	0.09	27,32,50,52	0
23	CLA	b	614	65/65	0.97	0.17	20,24,36,45	0

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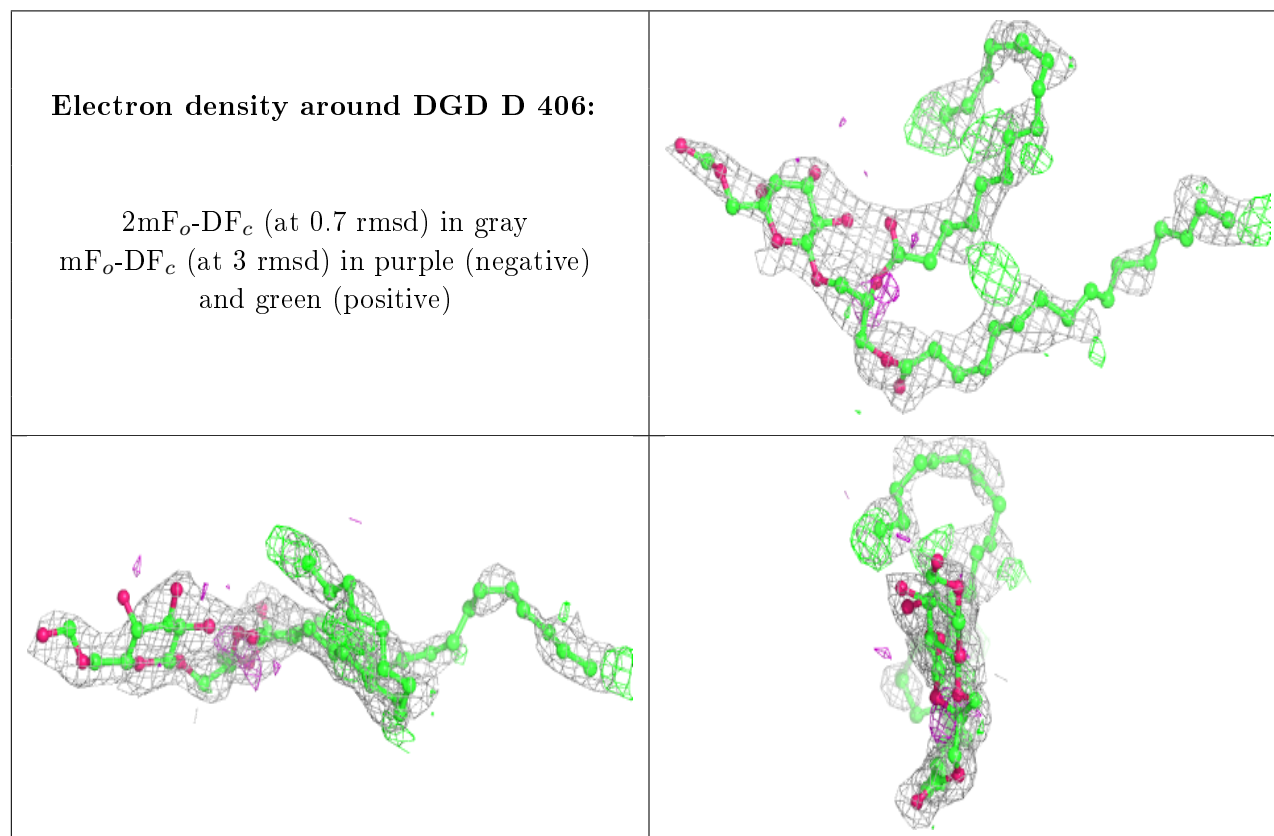
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	HEM	F	101	43/43	0.97	0.12	36,42,49,52	0
23	CLA	A	407	65/65	0.97	0.16	18,21,80,92	0
23	CLA	b	610	65/65	0.97	0.15	18,23,32,35	0
23	CLA	a	414	65/65	0.97	0.09	19,25,99,104	0
23	CLA	B	605	65/65	0.97	0.18	19,22,53,55	0
23	CLA	d	403	65/65	0.97	0.08	25,32,83,90	0
23	CLA	B	609	65/65	0.97	0.16	18,24,31,34	0
23	CLA	A	406	65/65	0.97	0.09	13,18,29,39	0
23	CLA	B	606	65/65	0.97	0.15	17,23,35,40	0
24	PHO	a	413	64/64	0.97	0.13	19,25,30,35	0
23	CLA	B	604	65/65	0.97	0.14	17,22,34,41	0
23	CLA	B	616	65/65	0.97	0.10	23,28,48,50	0
28	PL9	D	405	55/55	0.97	0.10	18,23,31,38	0
36	LHG	D	410	46/49	0.97	0.14	24,32,82,87	0
23	CLA	c	911	65/65	0.97	0.22	24,30,41,45	0
23	CLA	c	909	65/65	0.97	0.18	25,30,82,98	0
24	PHO	A	409	64/64	0.97	0.14	19,22,29,37	0
25	BCR	A	411	40/40	0.97	0.12	21,26,33,36	0
23	CLA	B	614	65/65	0.97	0.17	18,23,48,54	0
23	CLA	d	402	65/65	0.98	0.12	18,21,39,44	0
37	HEM	f	101	43/43	0.98	0.19	39,47,61,77	0
35	BCT	D	401	4/4	0.98	0.08	32,35,41,51	0
31	GOL	C	525	6/6	0.98	0.15	26,26,27,29	0
23	CLA	b	611	65/65	0.98	0.18	22,27,39,43	0
23	CLA	b	608	65/65	0.98	0.11	20,24,33,34	0
24	PHO	A	408	64/64	0.98	0.11	16,21,25,27	0
37	HEM	v	201	43/43	0.98	0.08	25,31,35,38	0
23	CLA	a	409	65/65	0.98	0.12	18,21,31,43	0
23	CLA	a	410	65/65	0.98	0.13	17,20,28,34	0
24	PHO	a	412	64/64	0.98	0.12	17,22,26,27	0
23	CLA	b	616	65/65	0.98	0.20	20,24,46,50	0
23	CLA	a	411	65/65	0.98	0.14	18,23,106,117	0
31	GOL	A	423	6/6	0.98	0.25	39,43,45,53	0
39	MG	j	101	1/1	0.99	0.17	35,35,35,35	0
21	FE2	a	405	1/1	0.99	0.06	27,27,27,27	0
22	CL	a	407	1/1	0.99	0.12	27,27,27,27	0
22	CL	A	403	1/1	0.99	0.06	25,25,25,25	0
22	CL	A	404	1/1	0.99	0.13	22,22,22,22	0
39	MG	J	101	1/1	0.99	0.09	28,28,28,28	0
37	HEM	V	201	43/43	0.99	0.07	22,24,28,33	0
31	GOL	c	929	6/6	0.99	0.15	25,27,30,30	0
22	CL	a	406	1/1	1.00	0.04	29,29,29,29	0

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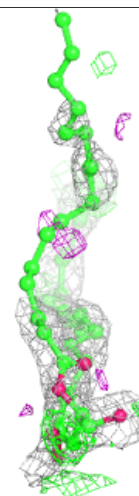
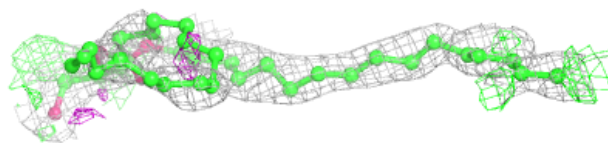
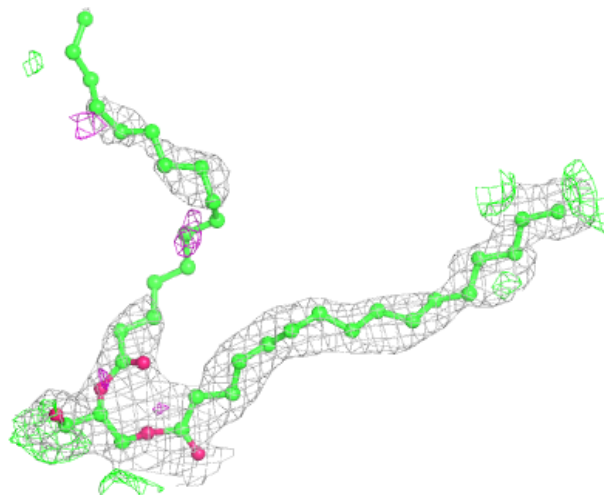
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	OEX	A	401	10/10	1.00	0.07	21,23,27,28	0
20	OEX	a	404	10/10	1.00	0.07	22,26,28,29	0
21	FE2	A	402	1/1	1.00	0.05	26,26,26,26	0

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.



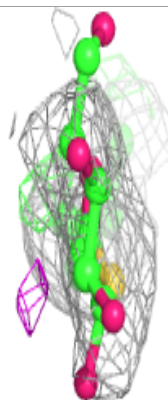
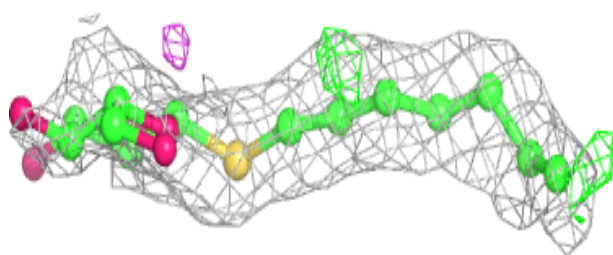
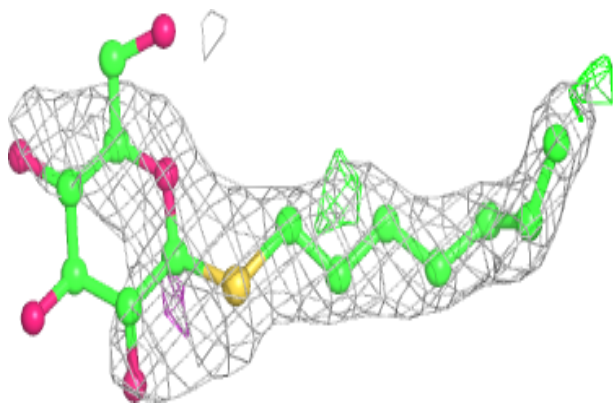
**Electron density around UNL a 420:**

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

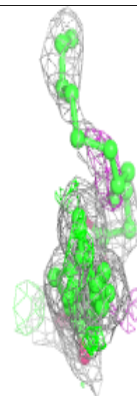
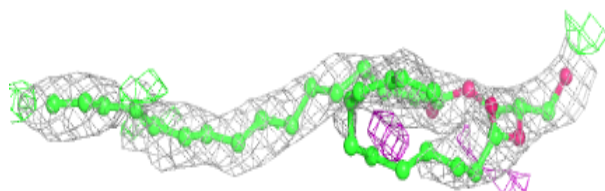
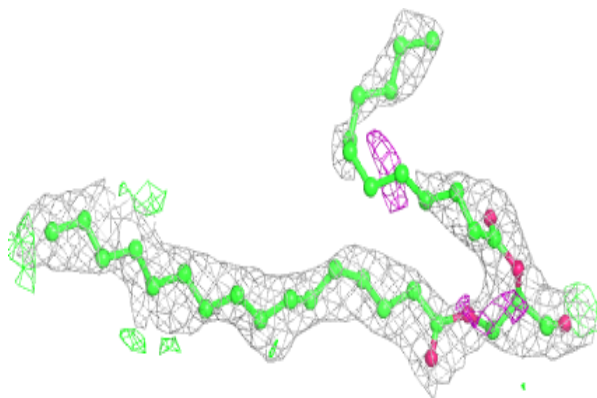


**Electron density around HTG d 401:**

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

**Electron density around UNL A 415:**

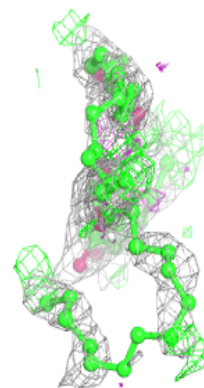
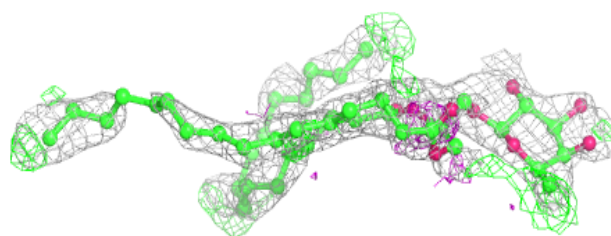
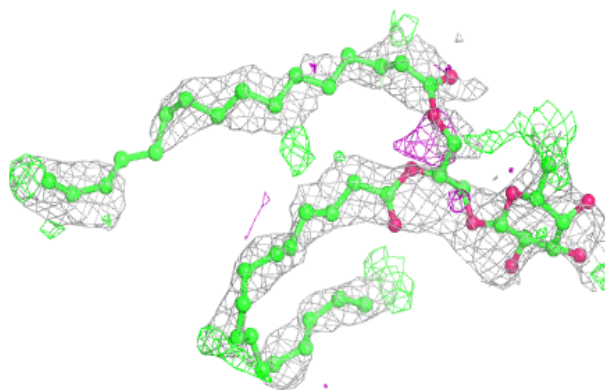
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



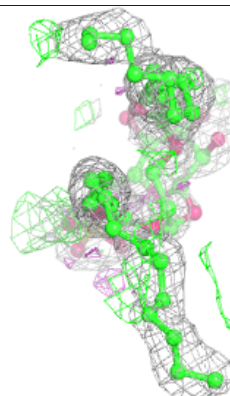
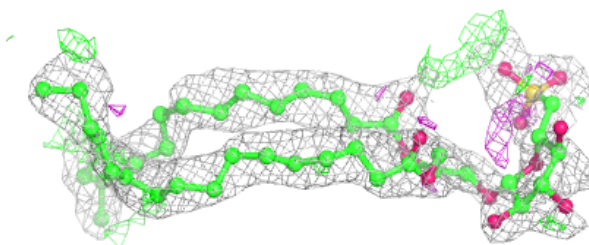
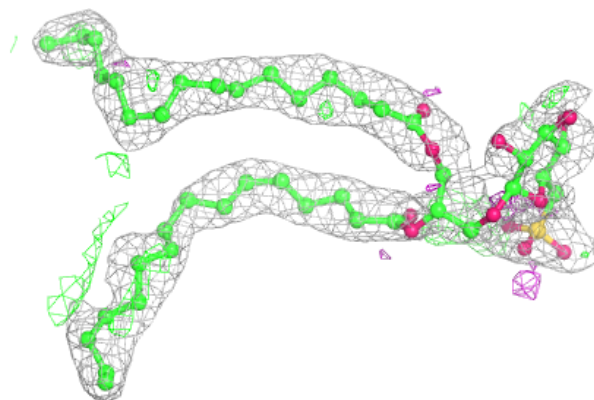


**Electron density around DGD d 406:**

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

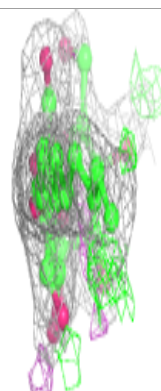
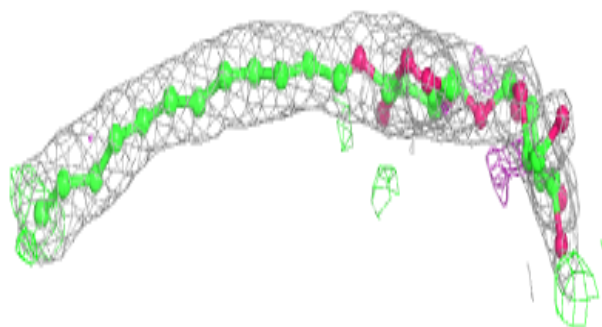
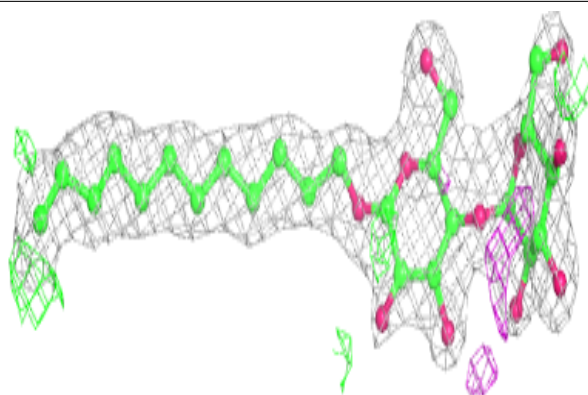
**Electron density around SQD B 621:**

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

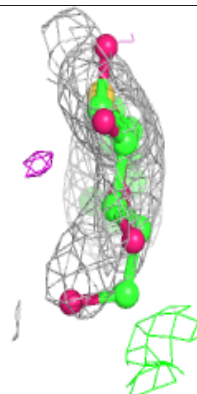
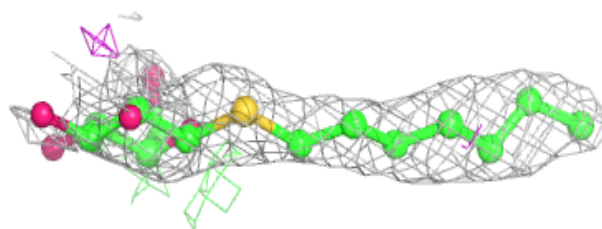
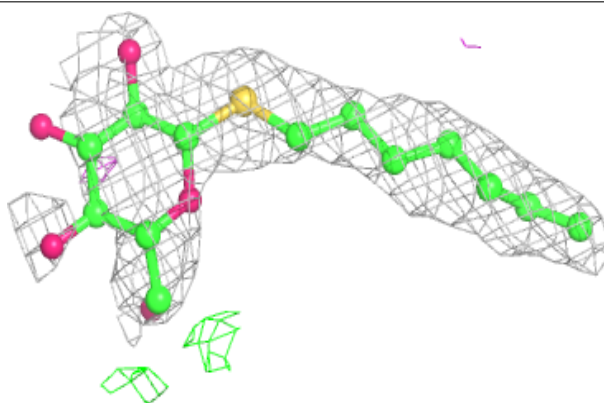


**Electron density around LMT M 102:**

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

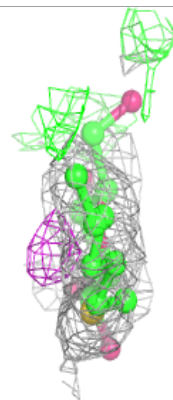
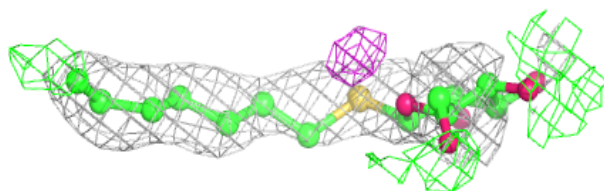
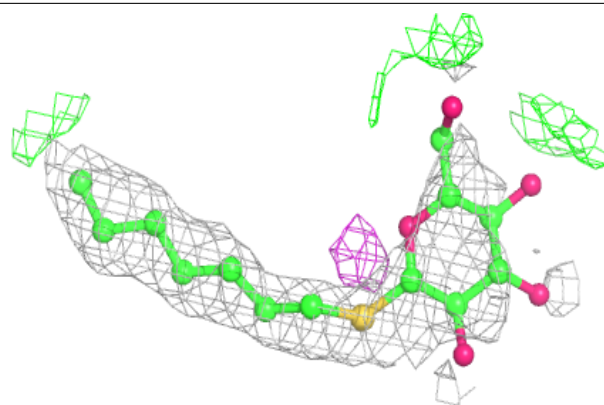
**Electron density around HTG b 602:**

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

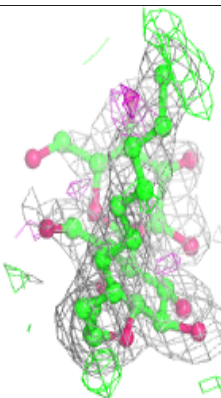
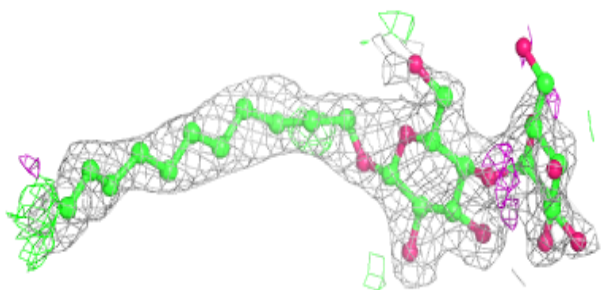
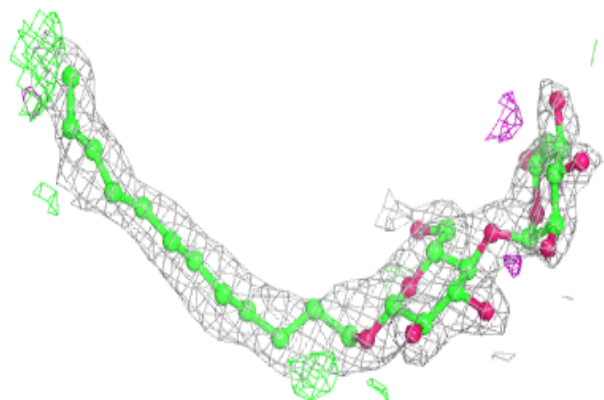


**Electron density around HTG B 631:**

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

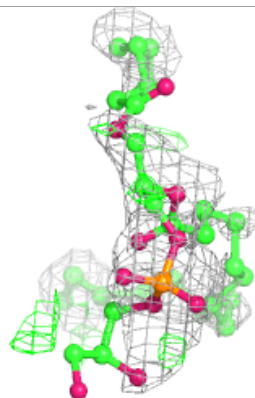
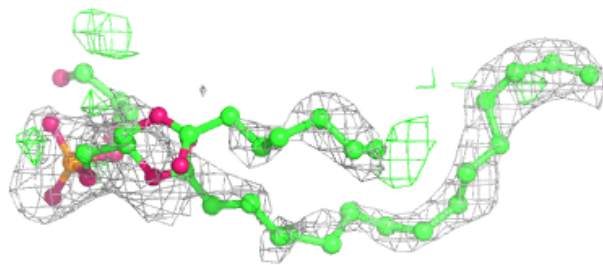
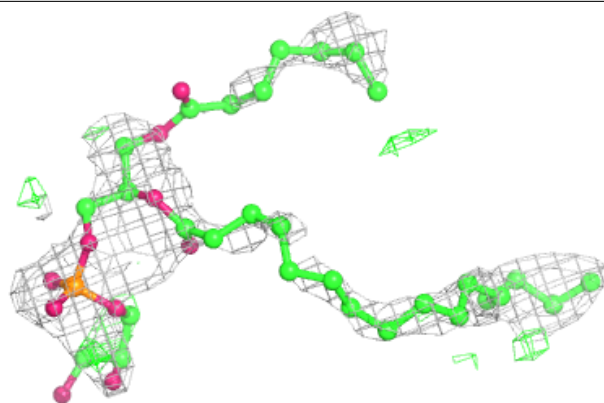
**Electron density around LMT M 101:**

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

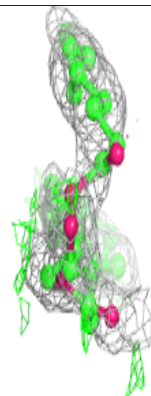
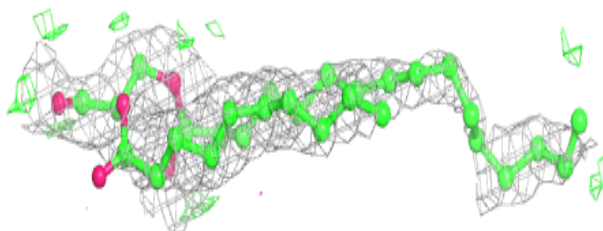
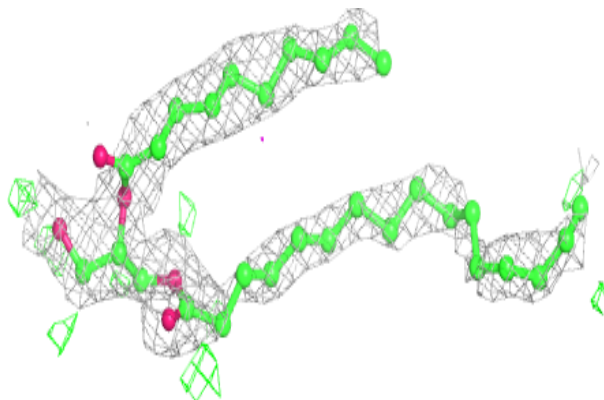


**Electron density around LHG a 417:**

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

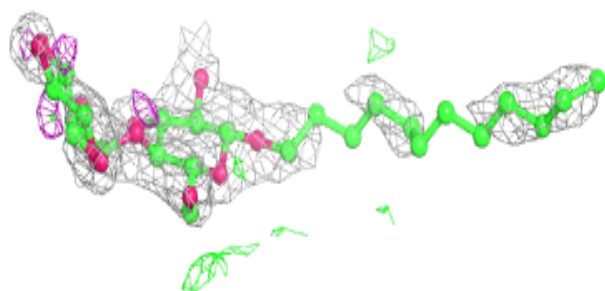
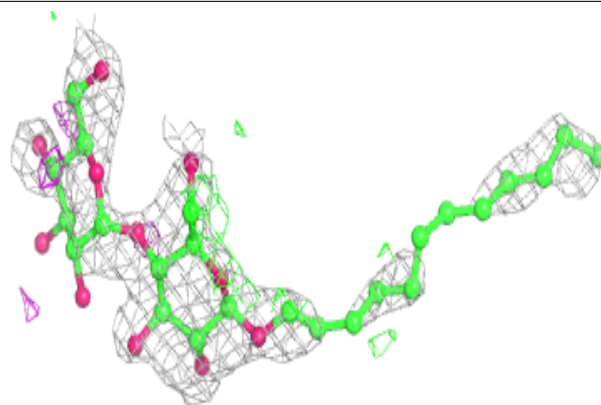
**Electron density around UNL C 523:**

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

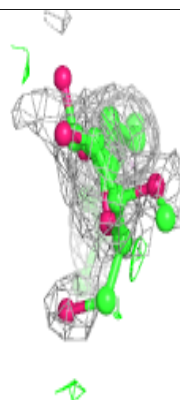
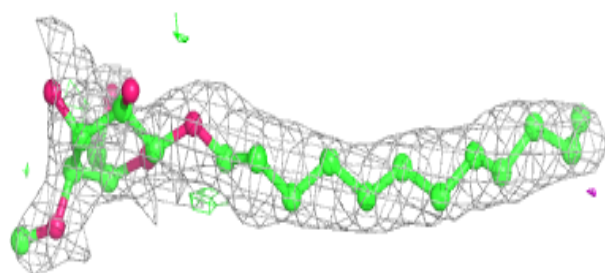
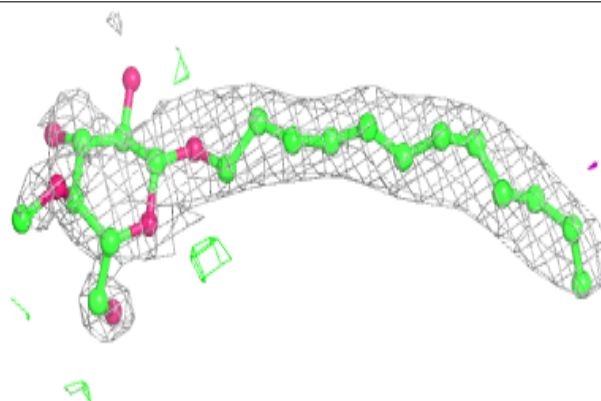


**Electron density around LMT F 102:**

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

**Electron density around LMT b 624:**

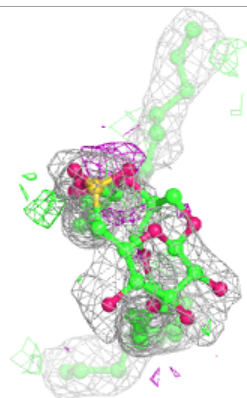
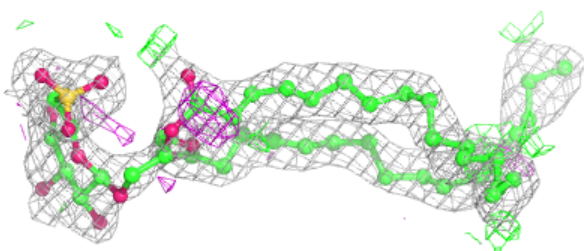
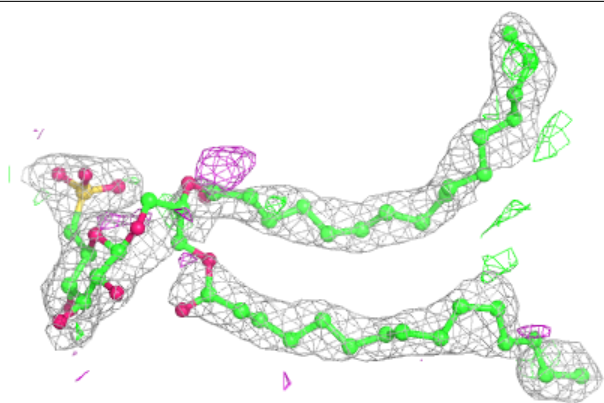
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



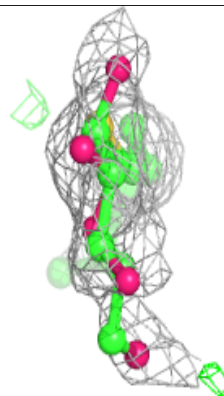
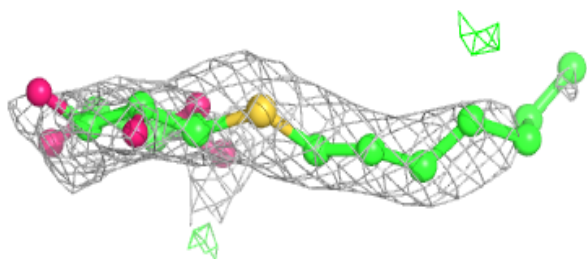
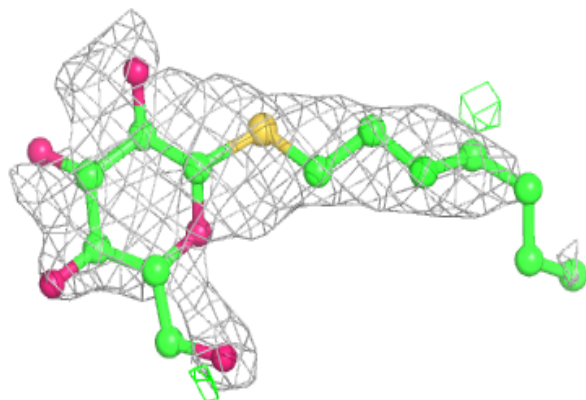


**Electron density around SQD L 103:**

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

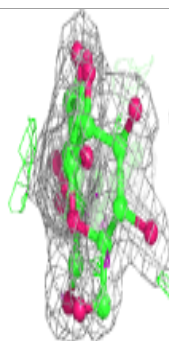
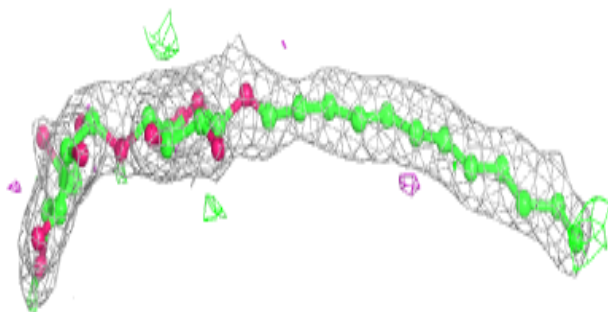
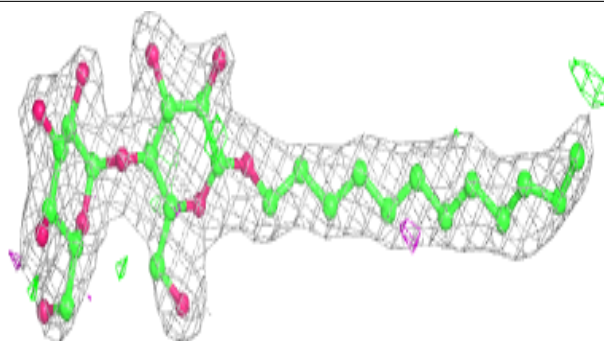
**Electron density around HTG D 414:**

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

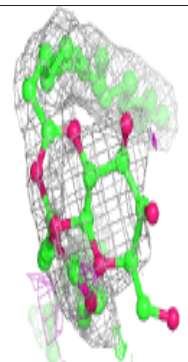
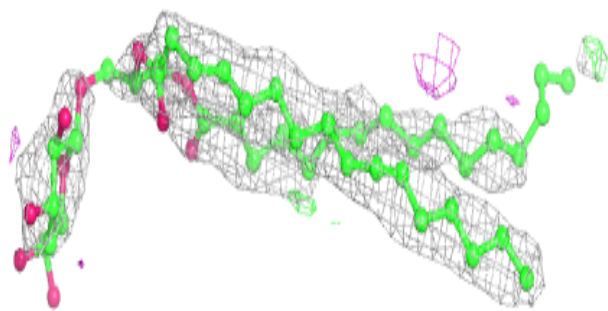
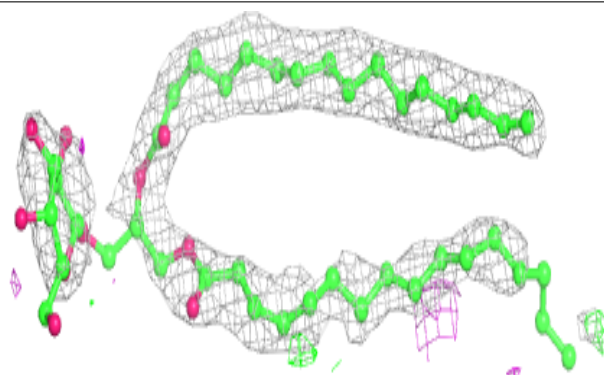


**Electron density around LMT m 101:**

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

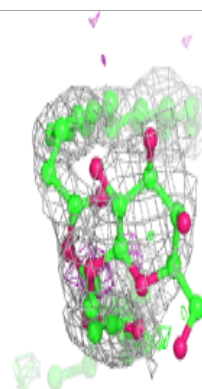
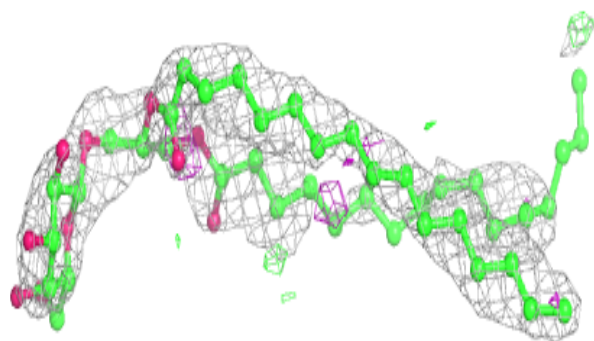
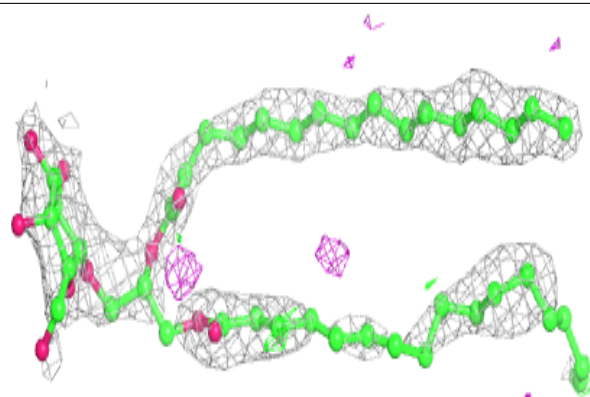
**Electron density around LMG Z 101:**

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

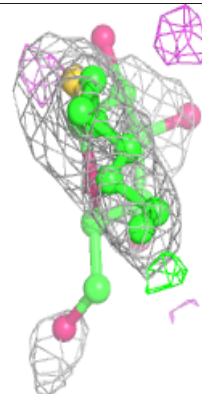
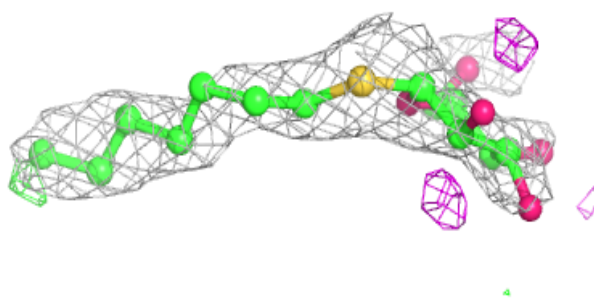
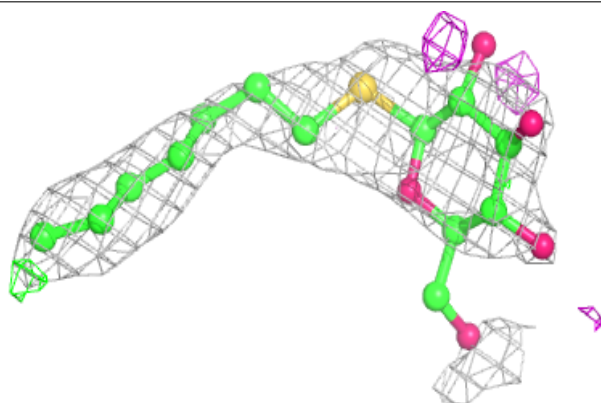


**Electron density around LMG c 921:**

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

**Electron density around HTG b 627:**

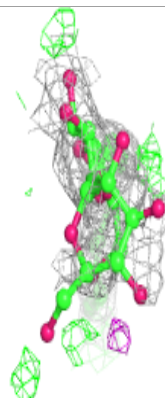
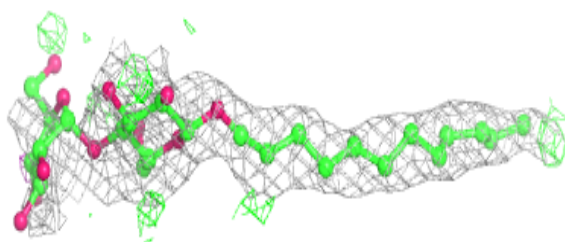
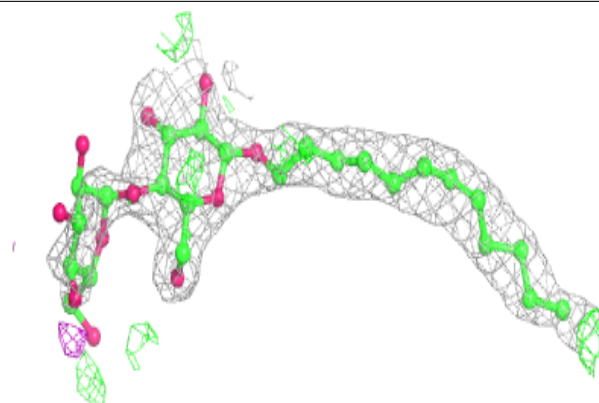
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



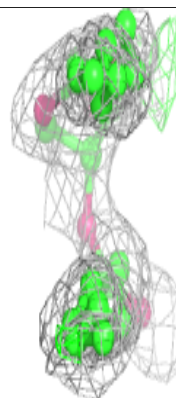
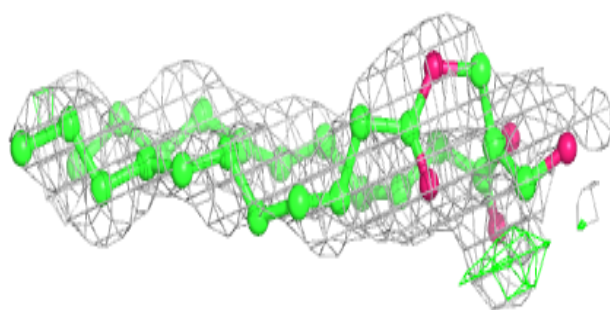
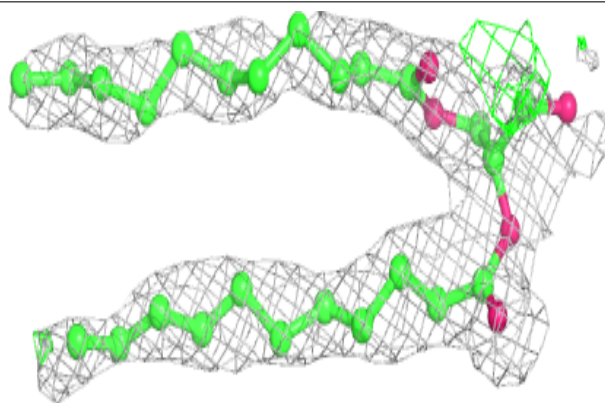


**Electron density around LMT B 623:**

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

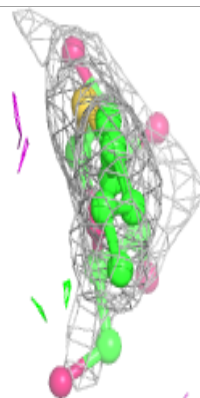
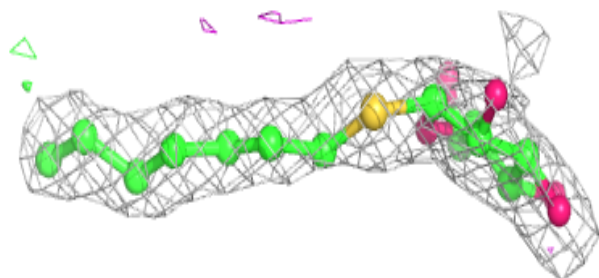
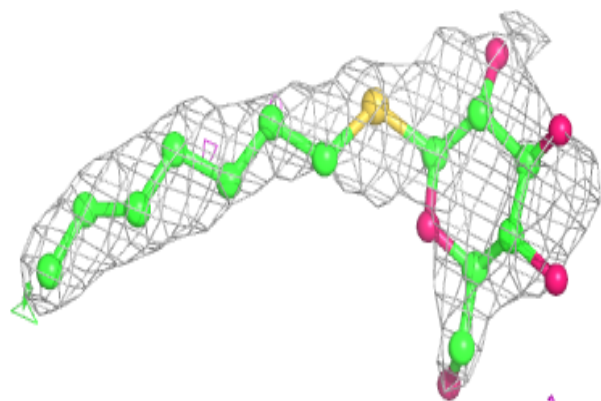
**Electron density around UNL c 925:**

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

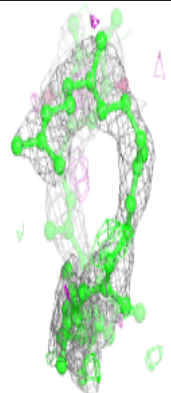
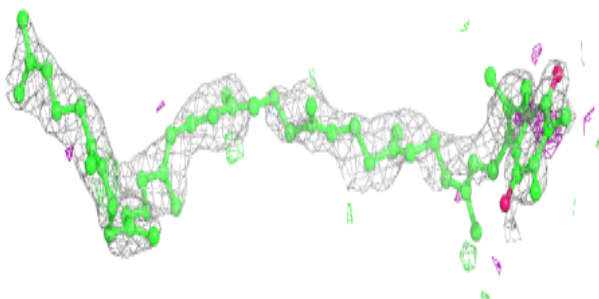
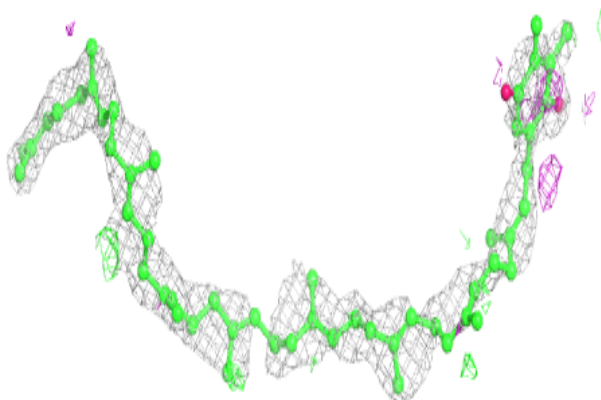


**Electron density around HTG B 626:**

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

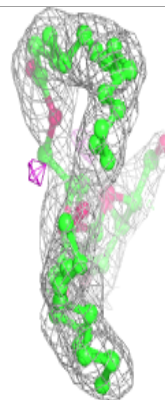
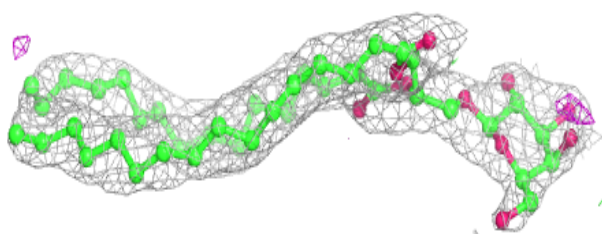
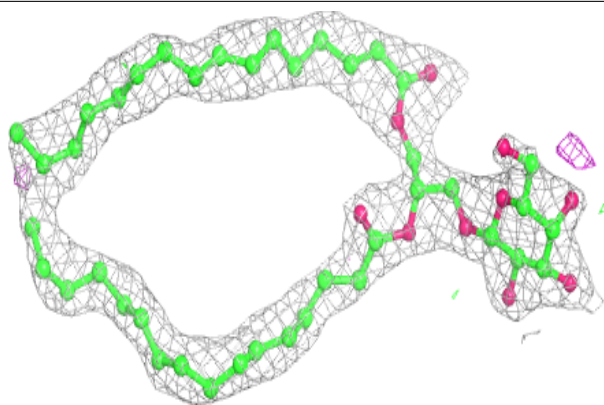
**Electron density around PL9 a 419:**

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

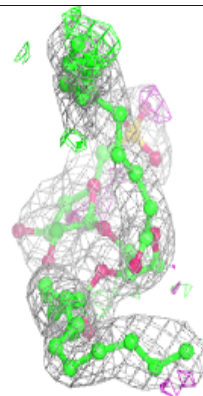
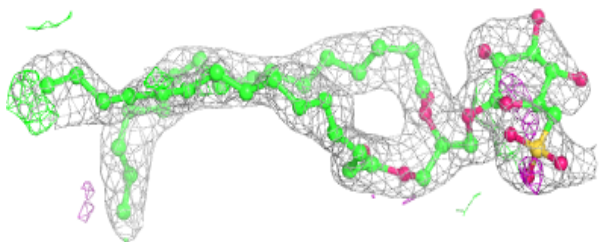
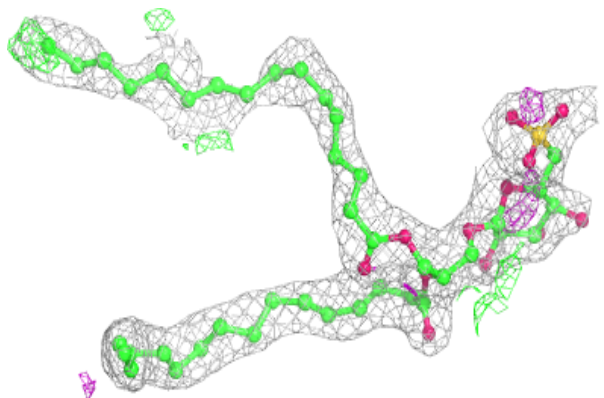


**Electron density around LMG a 418:**

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

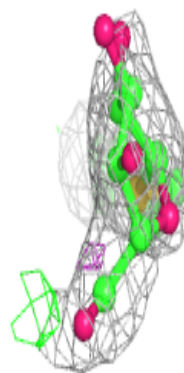
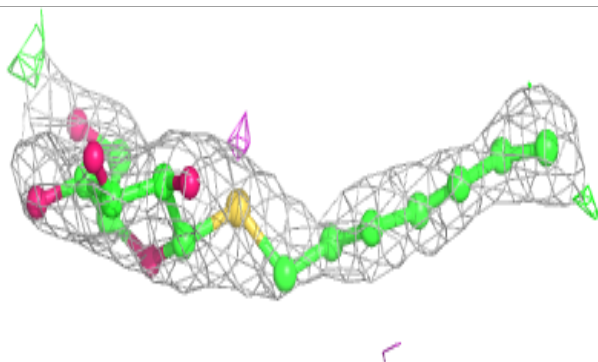
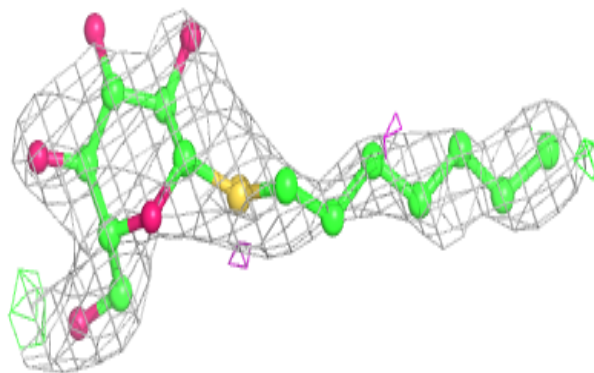
**Electron density around SQD a 401:**

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

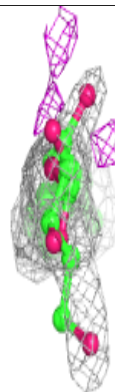
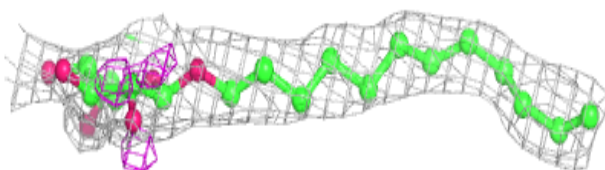
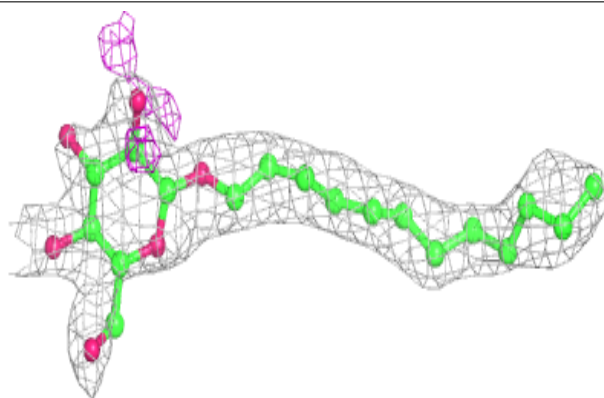


**Electron density around HTG C 522:**

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

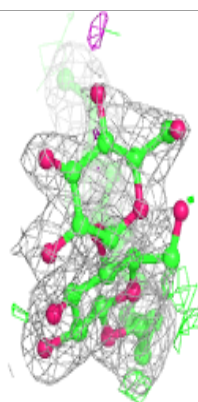
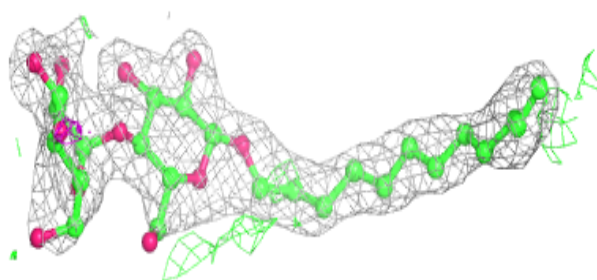
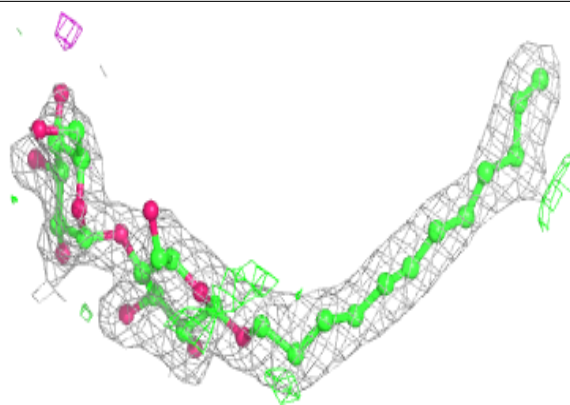
**Electron density around LMT J 102:**

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

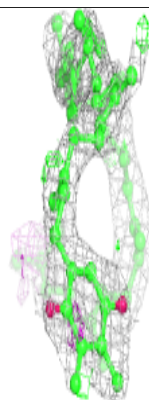
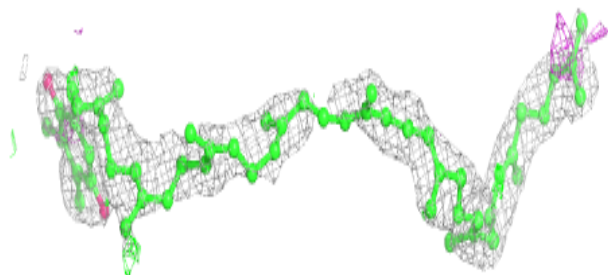
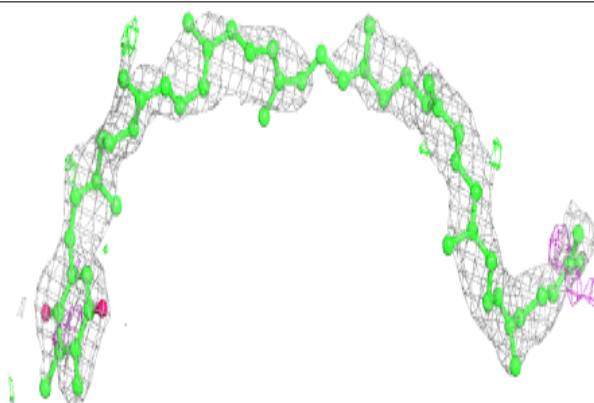


**Electron density around LMT m 102:**

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

**Electron density around PL9 A 414:**

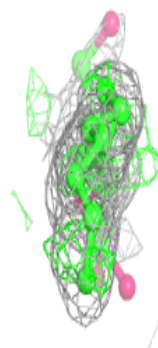
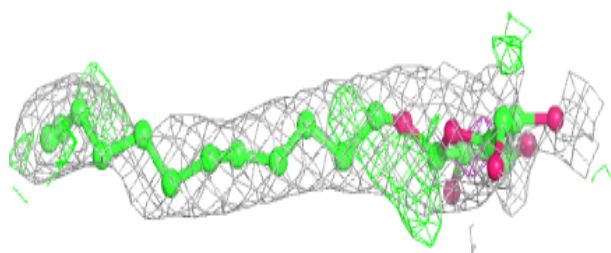
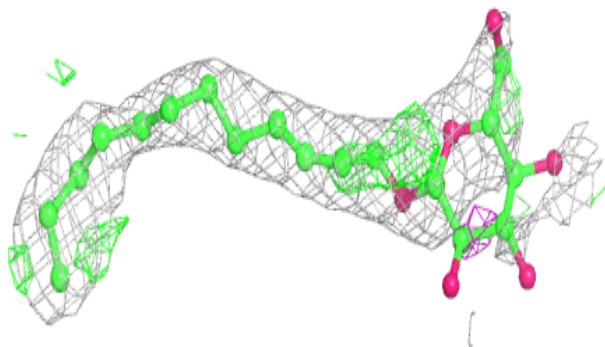
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



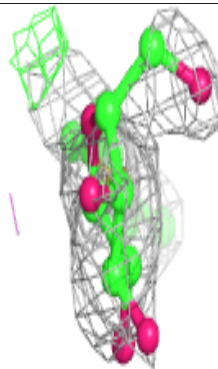
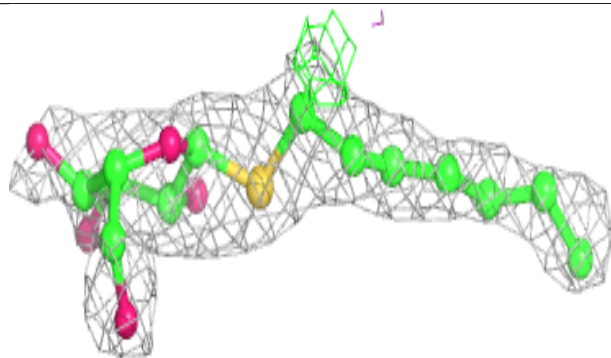
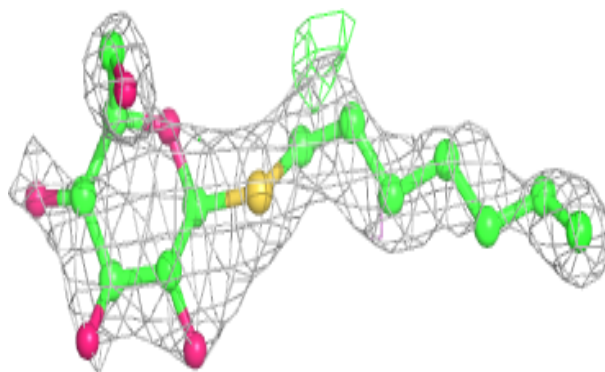


**Electron density around LMT b 625:**

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

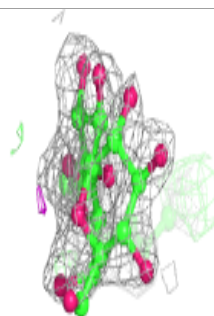
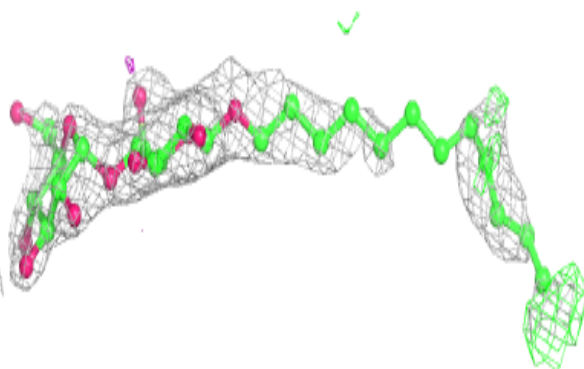
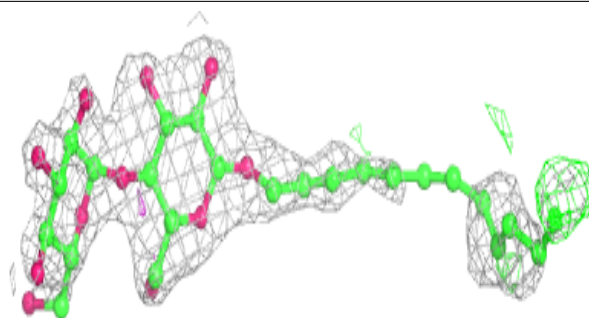
**Electron density around HTG c 924:**

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

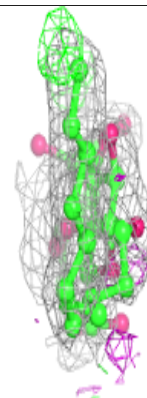
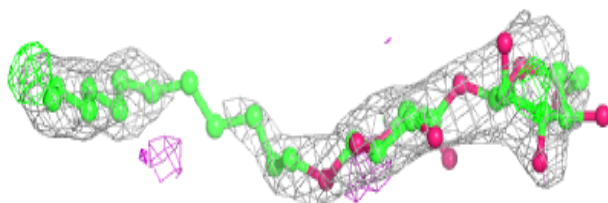
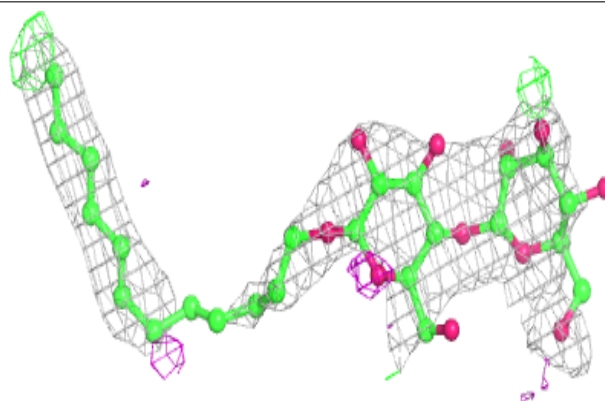


**Electron density around LMT c 922:**

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

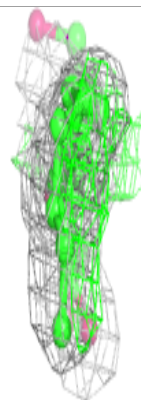
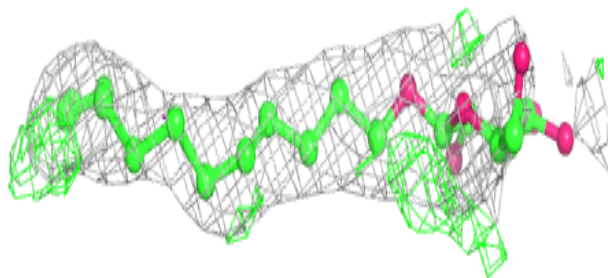
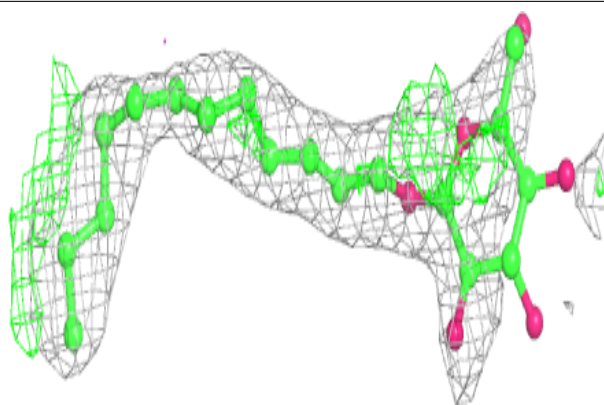
**Electron density around LMT Z 102:**

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

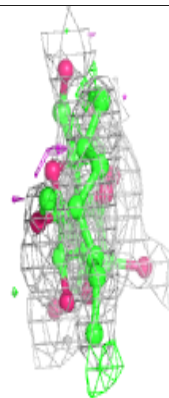
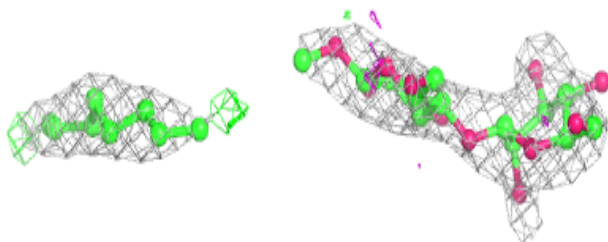
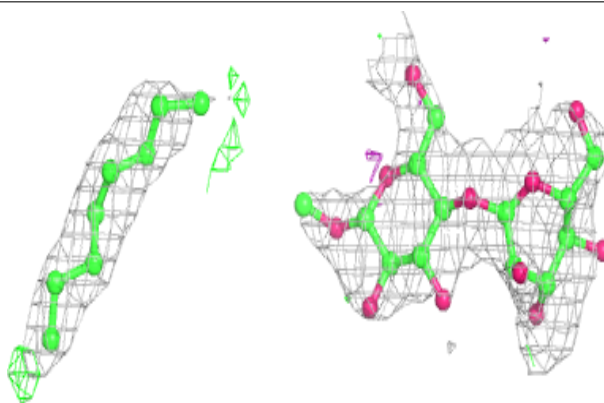


**Electron density around LMT t 102:**

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

**Electron density around LMT z 101:**

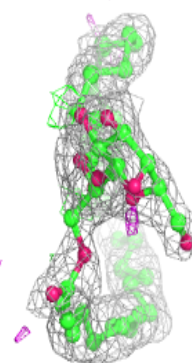
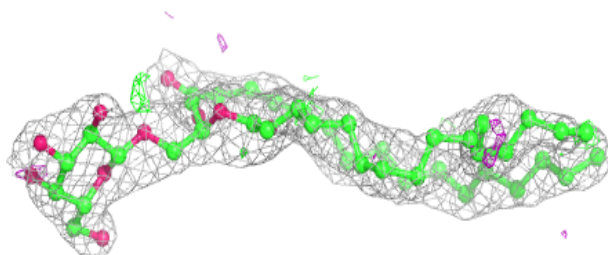
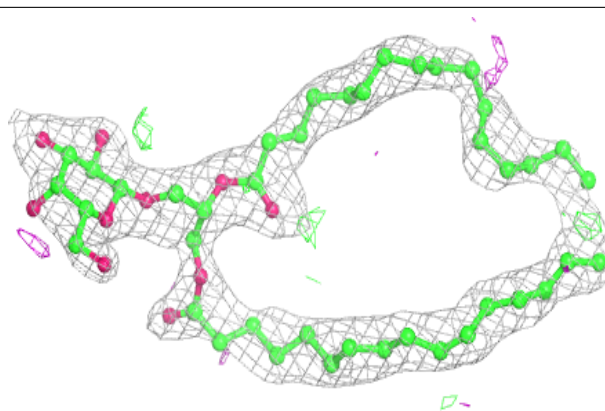
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



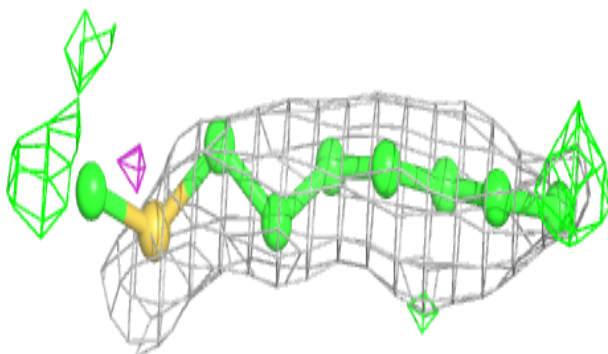
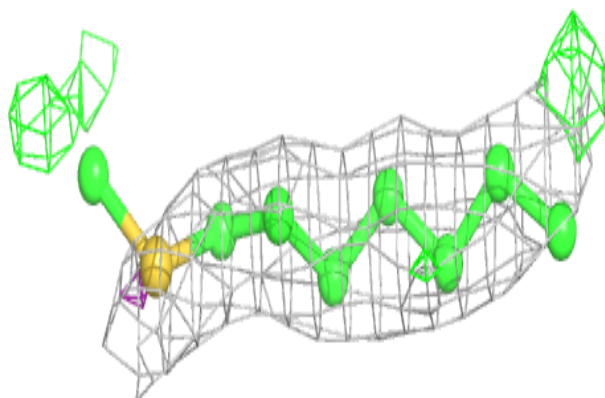


**Electron density around LMG A 413:**

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

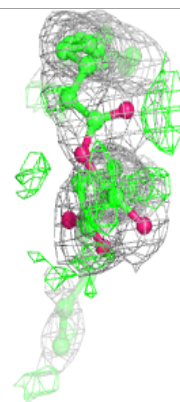
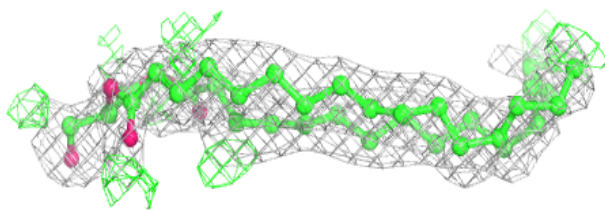
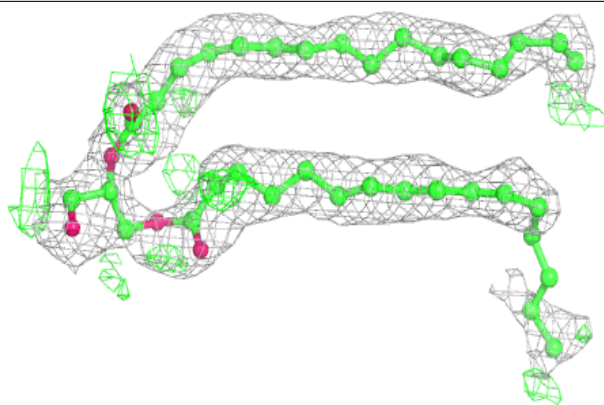
**Electron density around HTG U 201:**

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

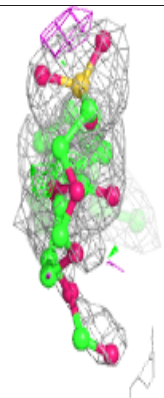
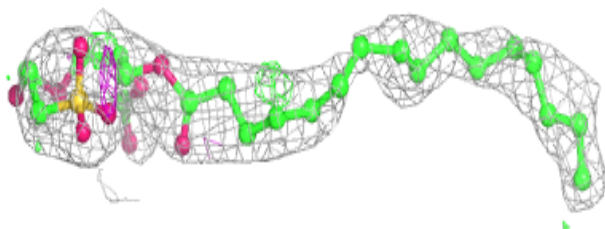
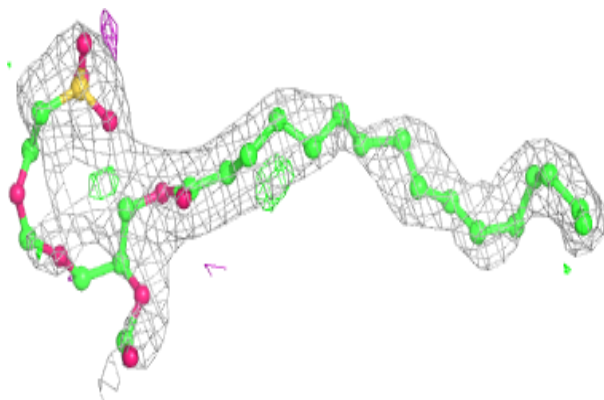


**Electron density around UNL D 412:**

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

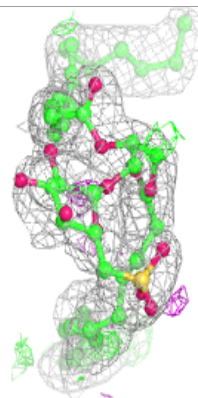
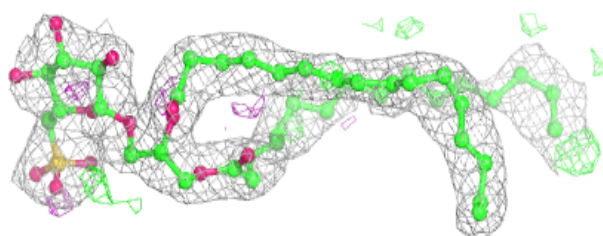
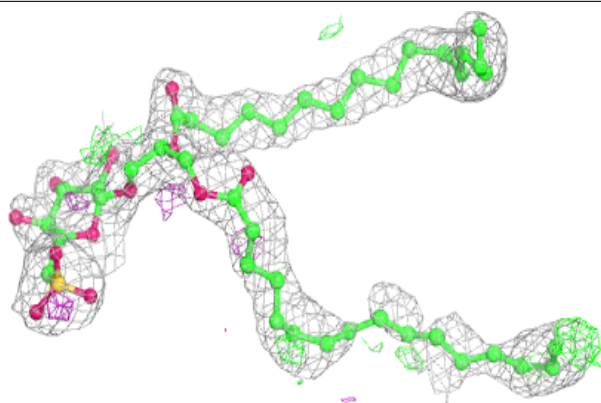
**Electron density around SQD f 102:**

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

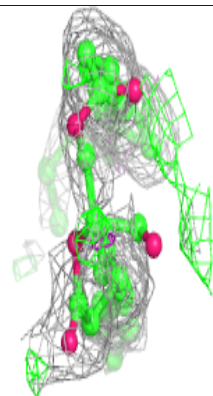
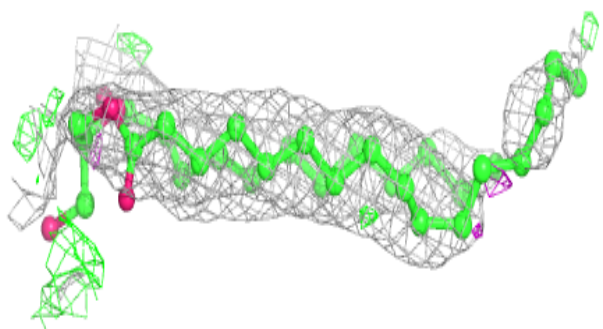
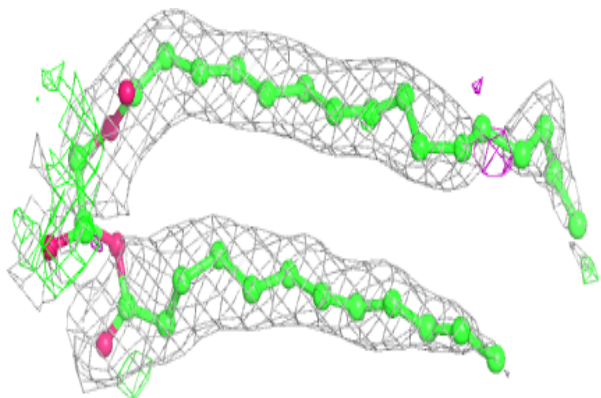


**Electron density around SQD A 418:**

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

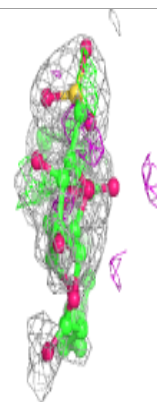
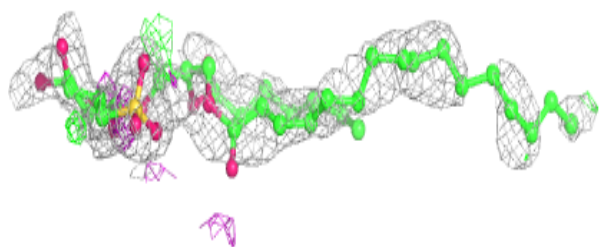
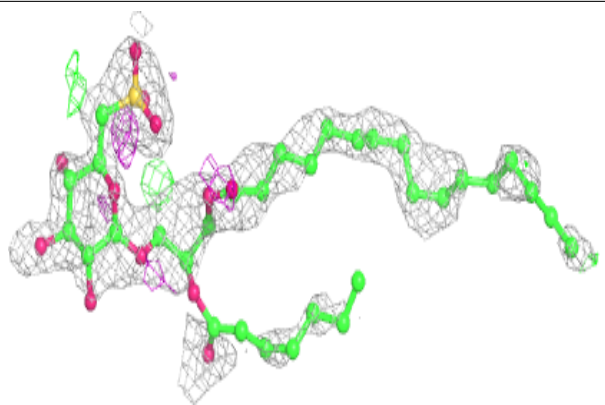
**Electron density around UNL b 628:**

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

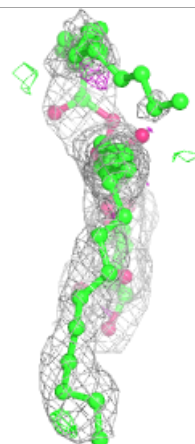
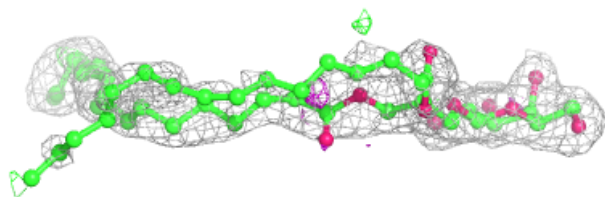
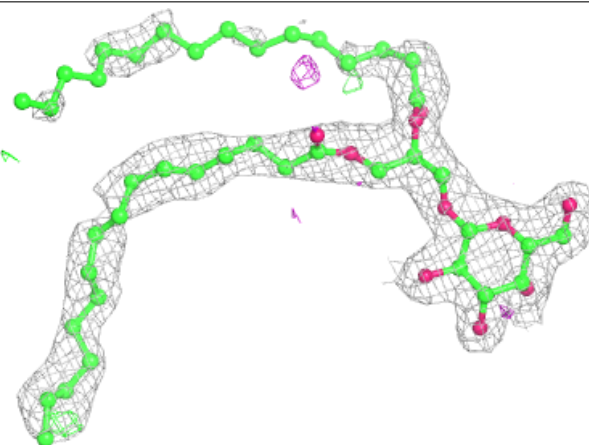


**Electron density around SQD D 407:**

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

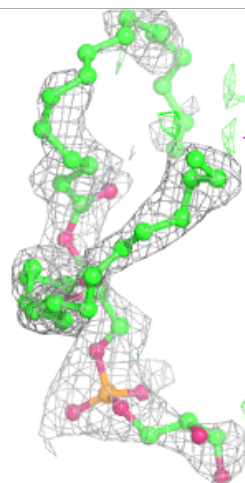
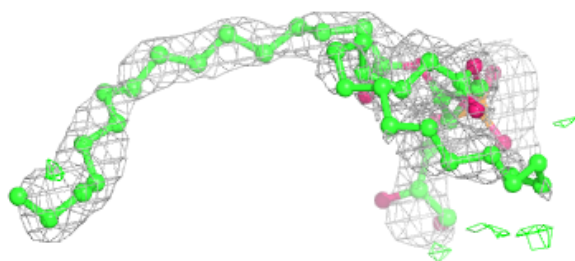
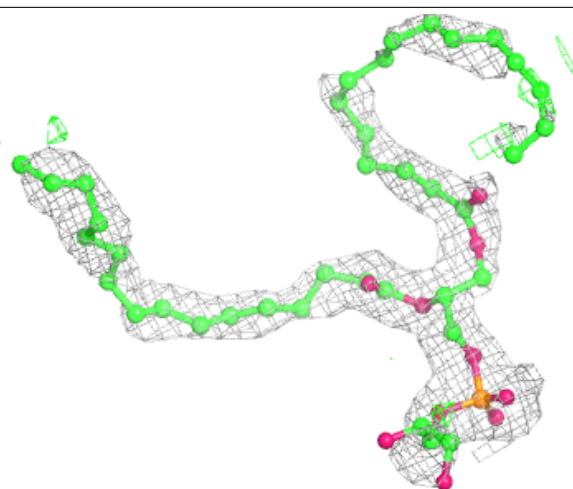
**Electron density around LMG c 920:**

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



**Electron density around LHG E 101:**

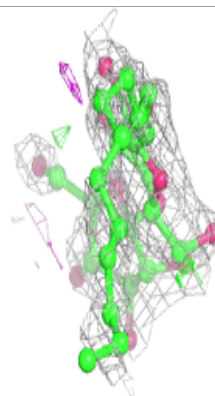
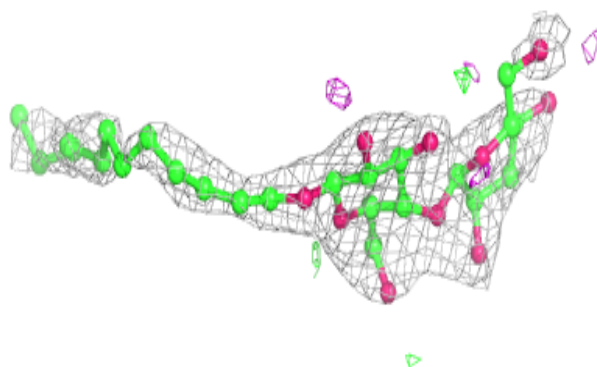
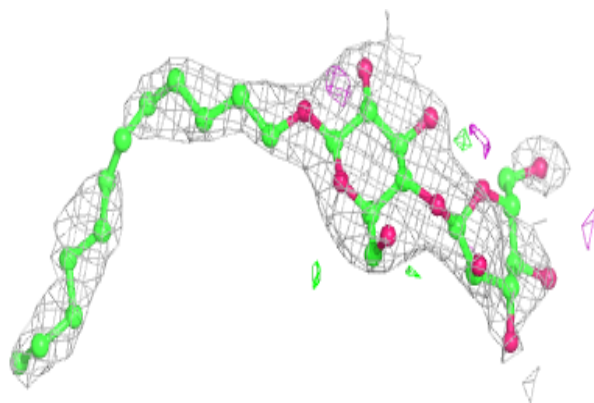
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



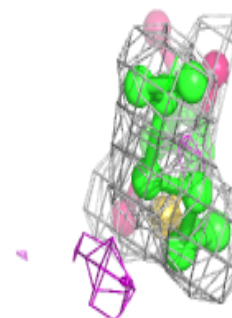
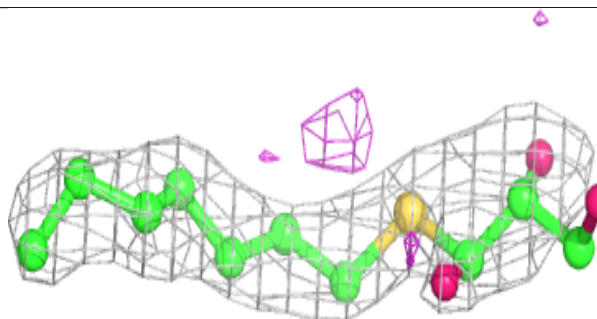
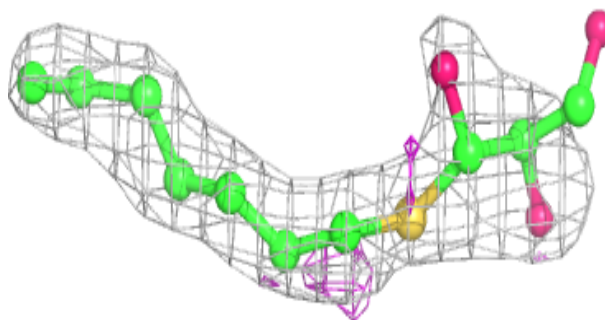


**Electron density around LMT C 520:**

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

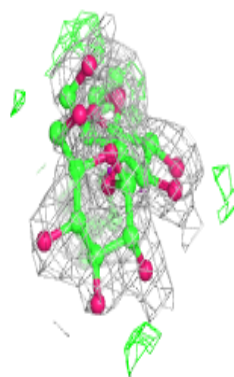
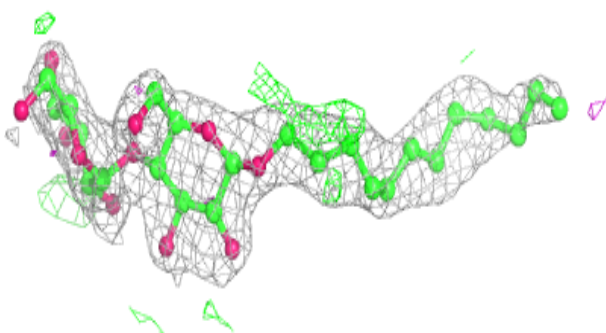
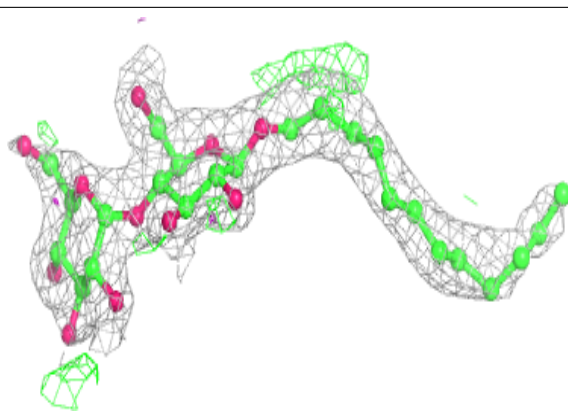
**Electron density around HTG u 201:**

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

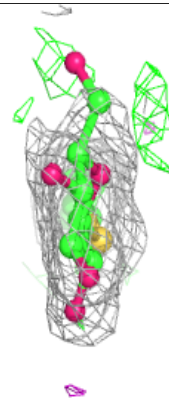
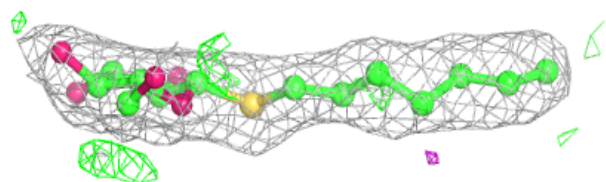
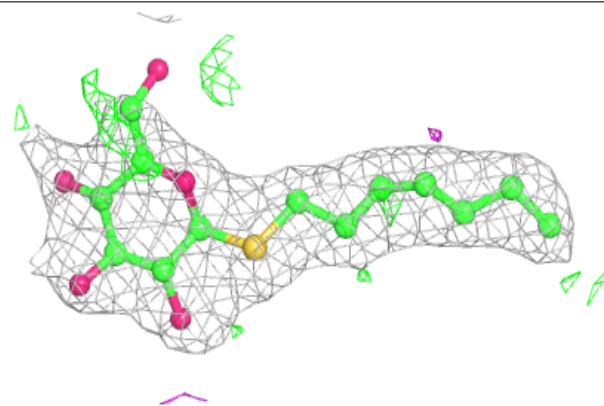


**Electron density around LMT a 402:**

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

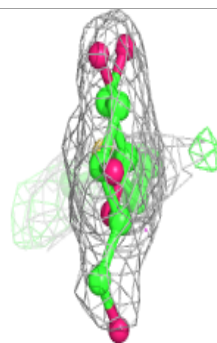
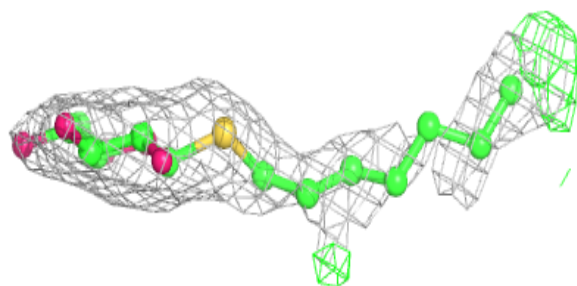
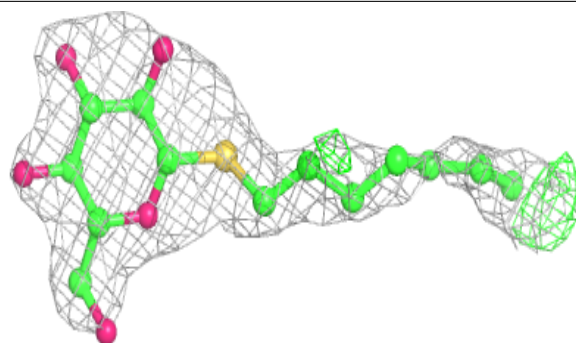
**Electron density around HTG B 630:**

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

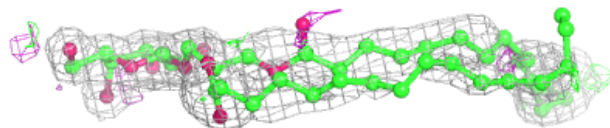
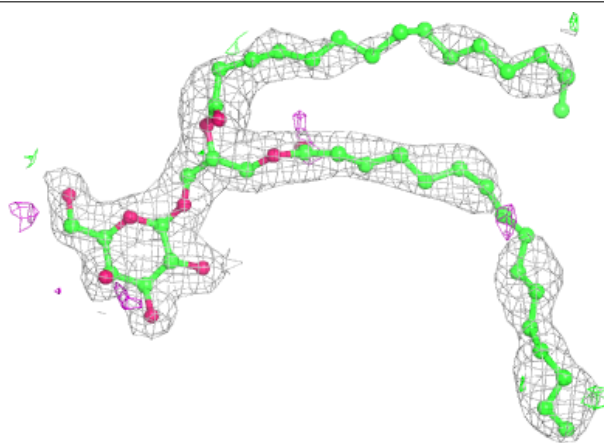


**Electron density around HTG c 923:**

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

**Electron density around LMG C 519:**

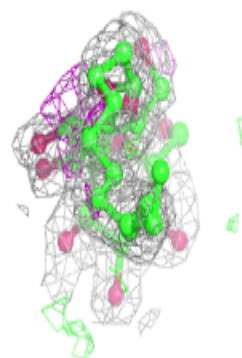
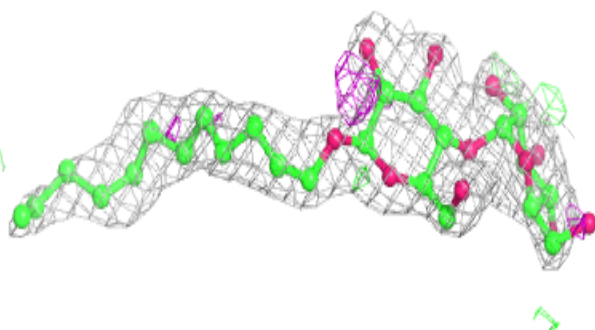
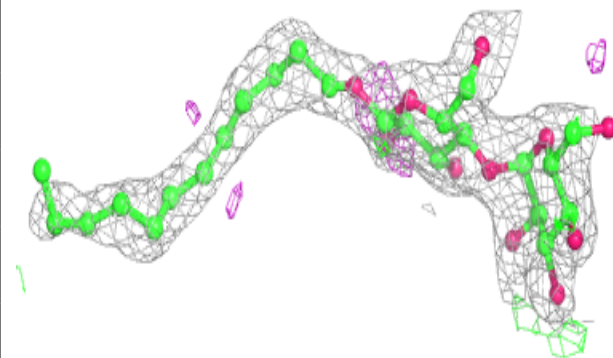
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



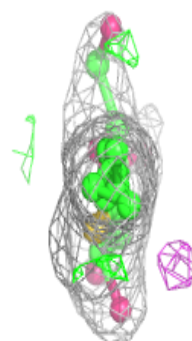
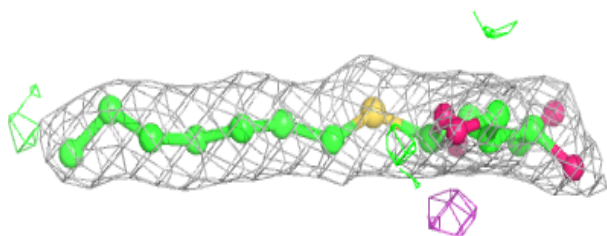
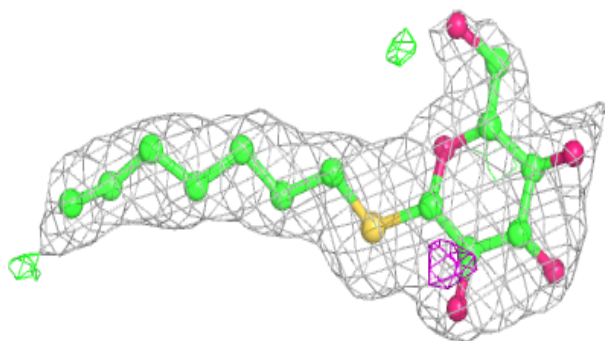


**Electron density around LMT A 419:**

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

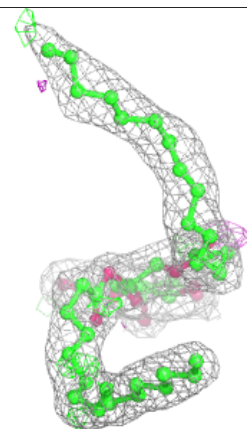
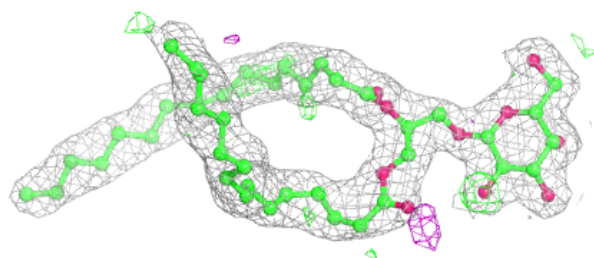
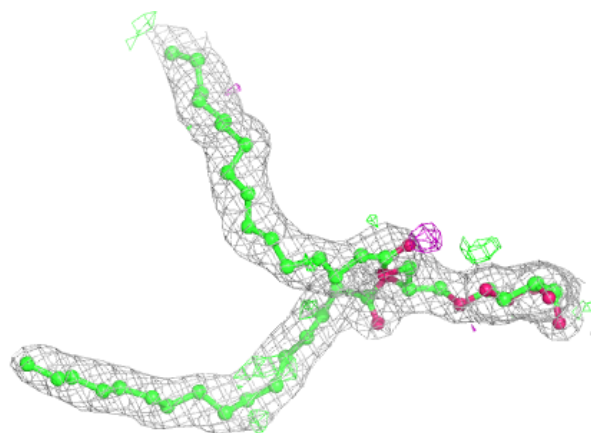
**Electron density around HTG b 601:**

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

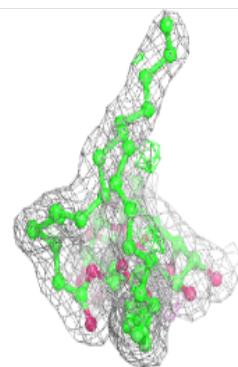
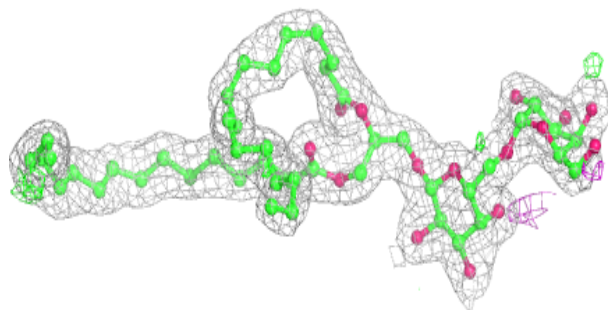
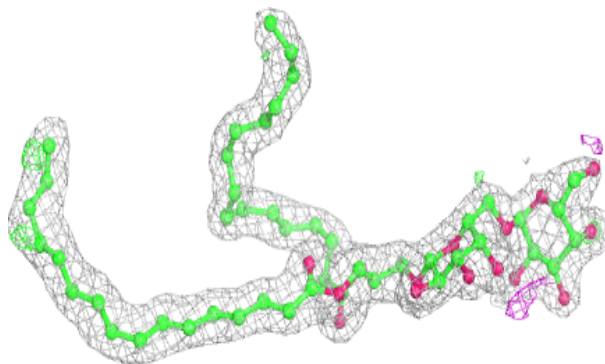


**Electron density around LMG B 622:**

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

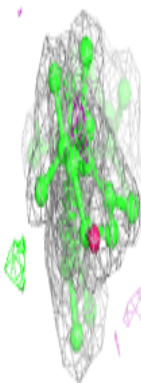
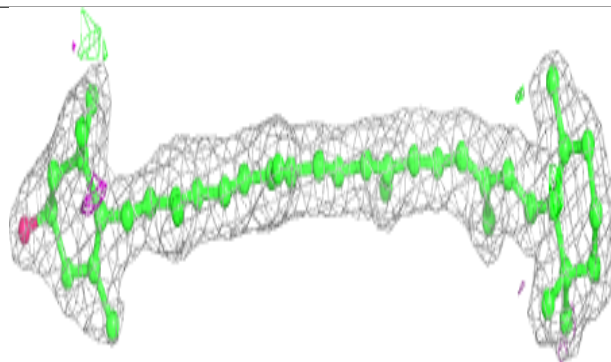
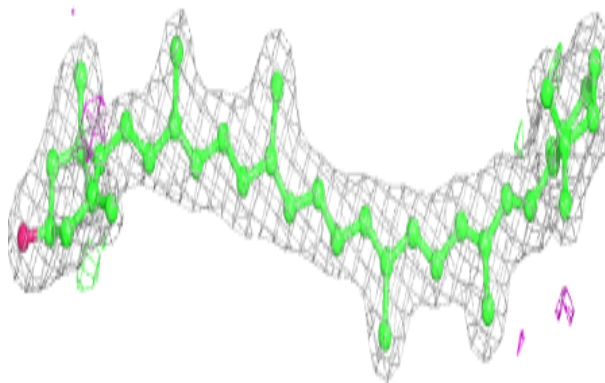
**Electron density around DGD h 102:**

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

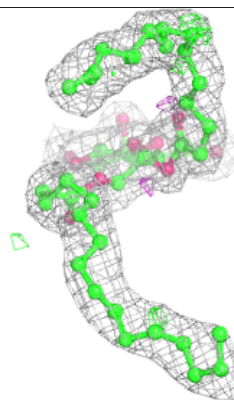
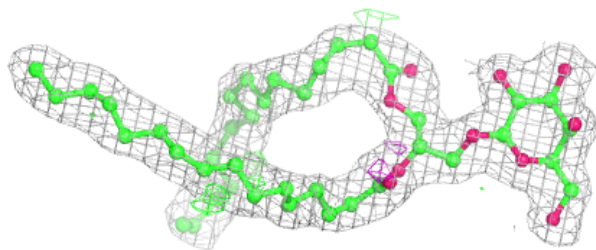
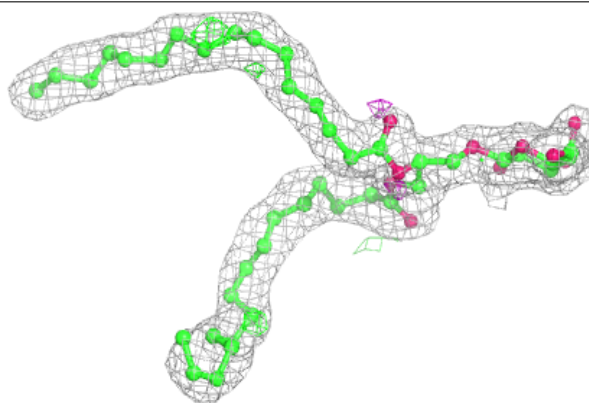


**Electron density around RRX h 101:**

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

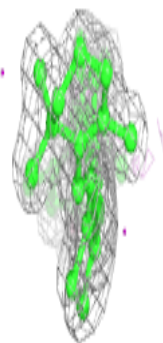
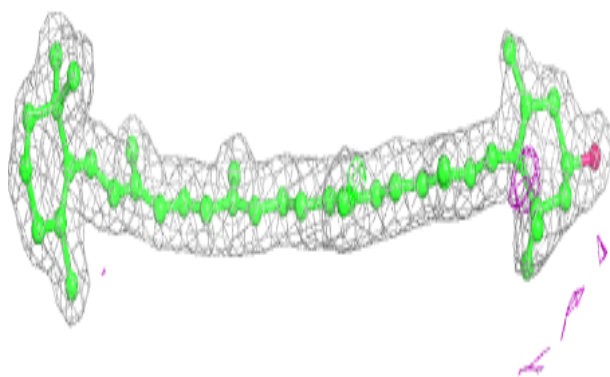
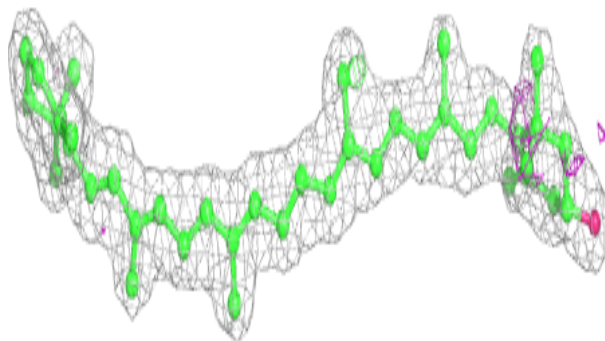
**Electron density around LMG b 623:**

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

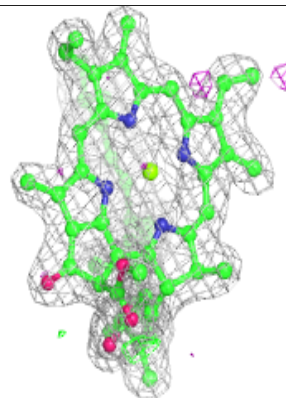
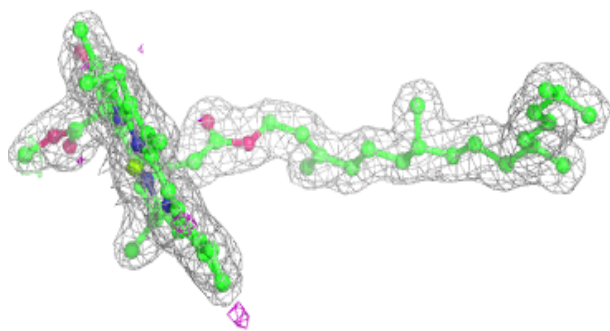
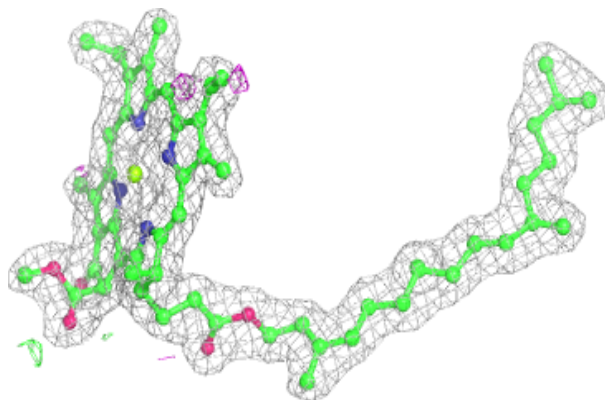


**Electron density around RRX H 101:**

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

**Electron density around CLA B 610:**

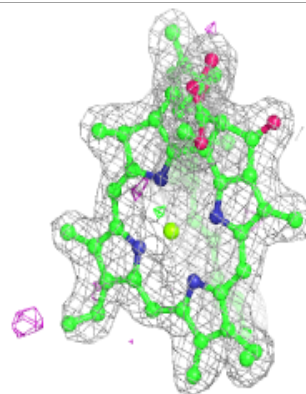
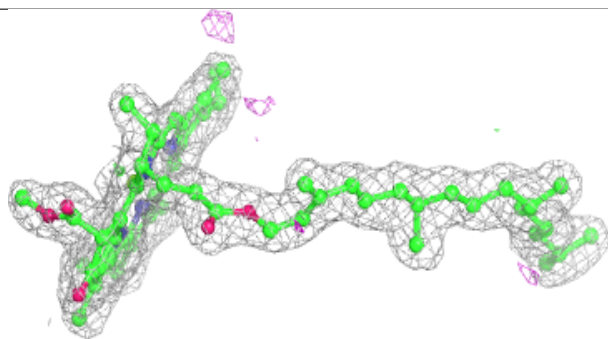
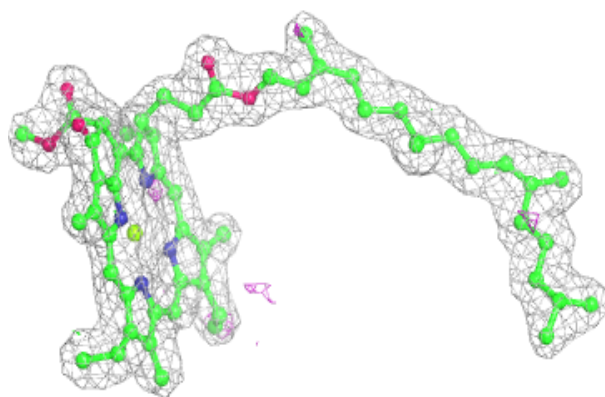
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



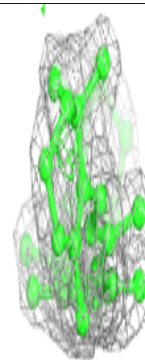
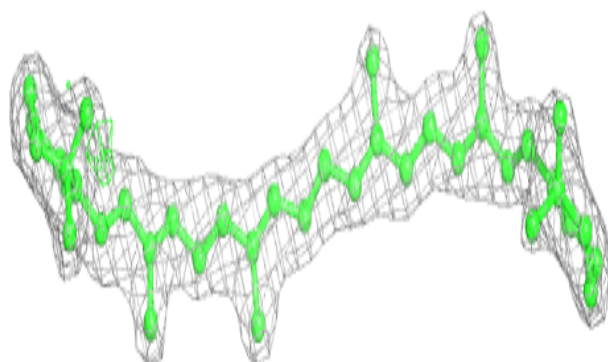
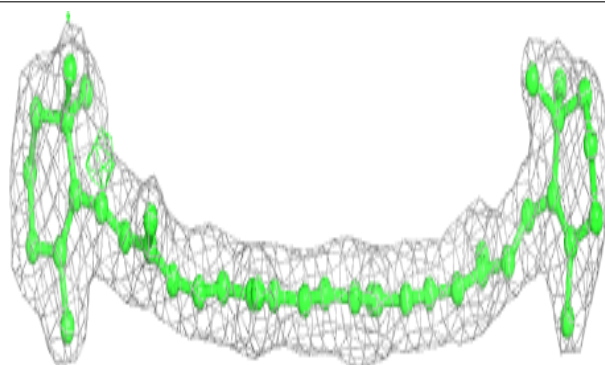


**Electron density around CLA b 612:**

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

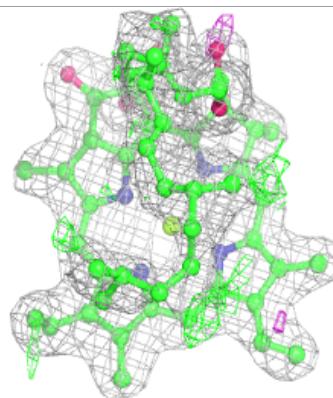
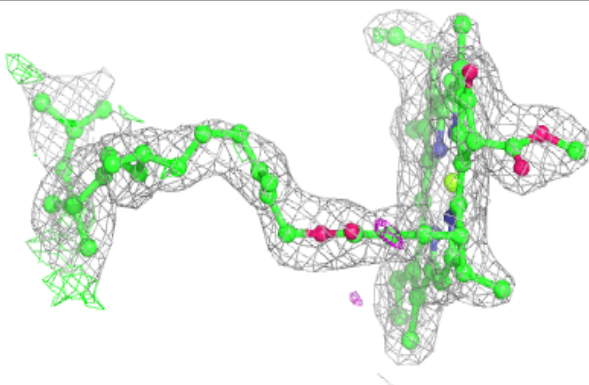
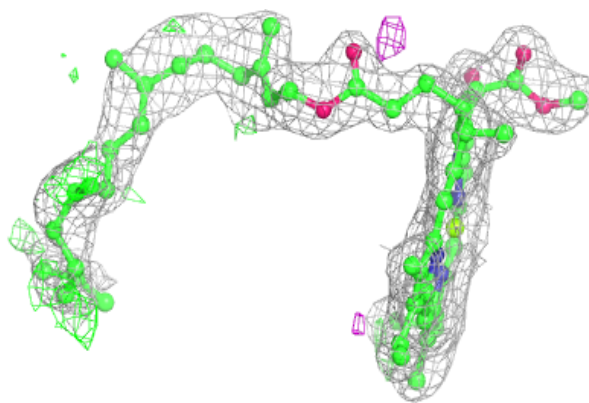
**Electron density around BCR k 102:**

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

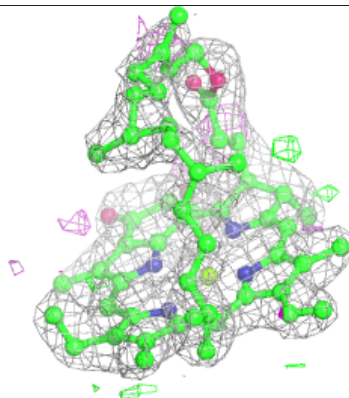
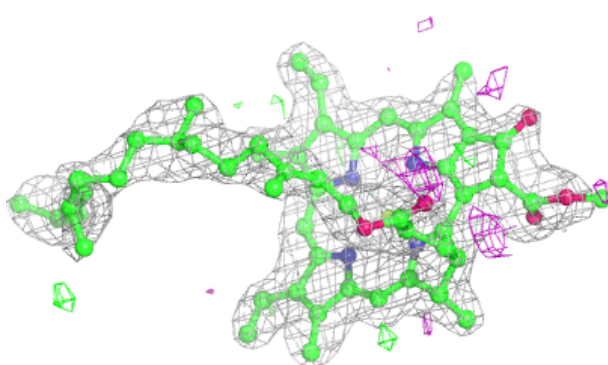
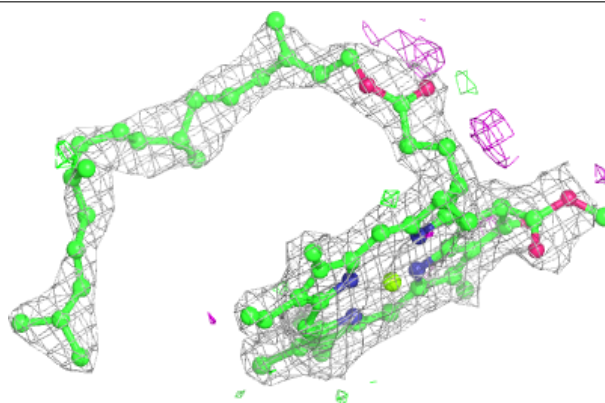


**Electron density around CLA C 506:**

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

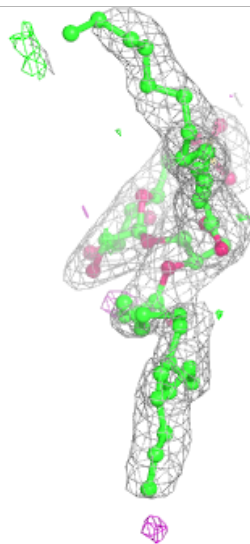
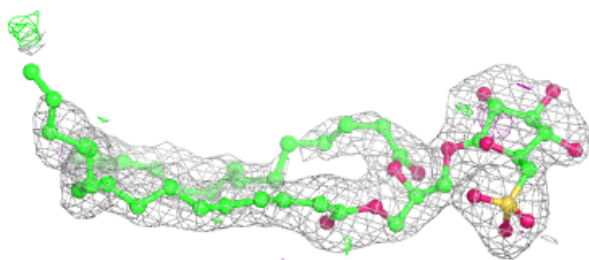
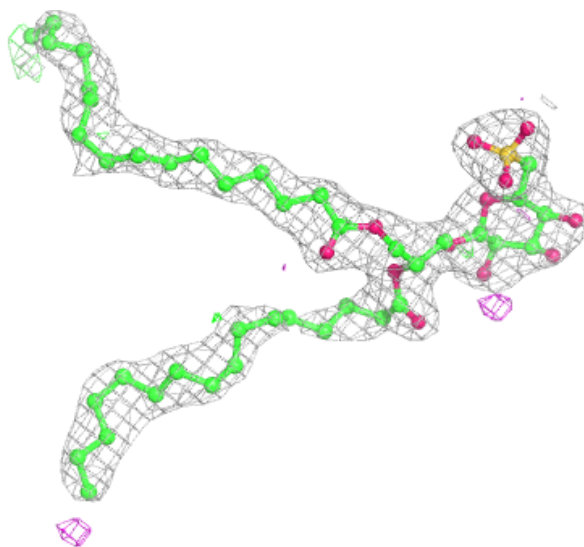
**Electron density around CLA c 914:**

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



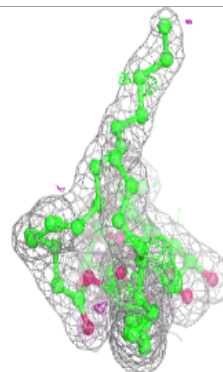
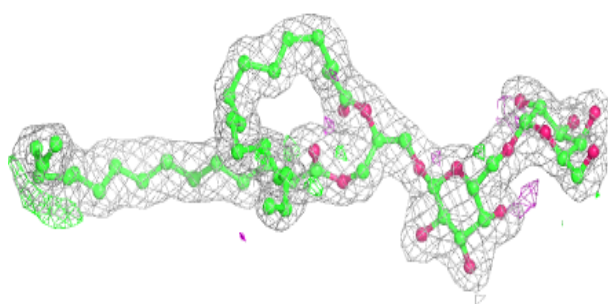
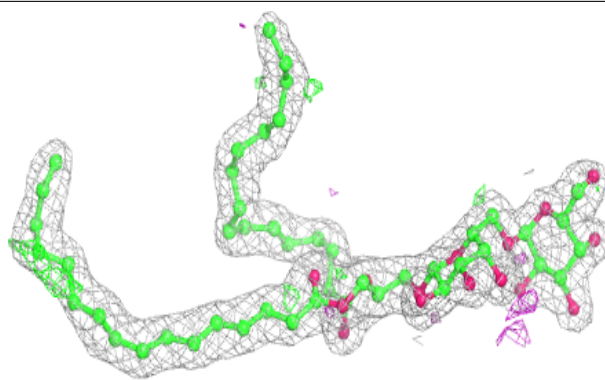
**Electron density around SQD a 416:**

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

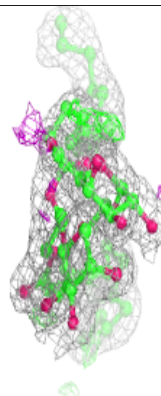
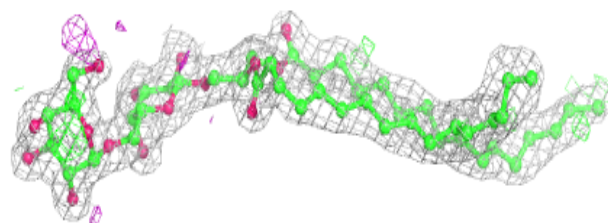
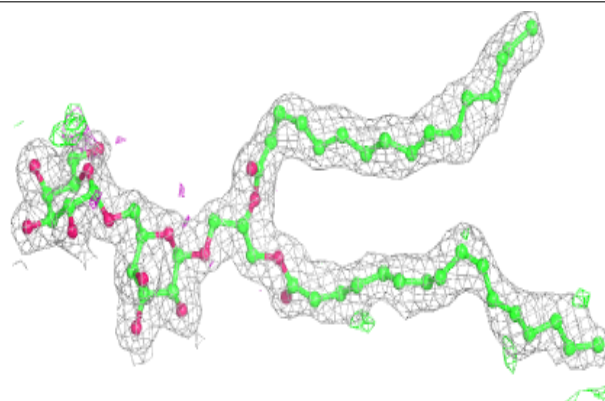


**Electron density around DGD H 102:**

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

**Electron density around DGD c 919:**

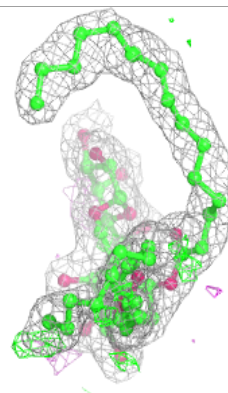
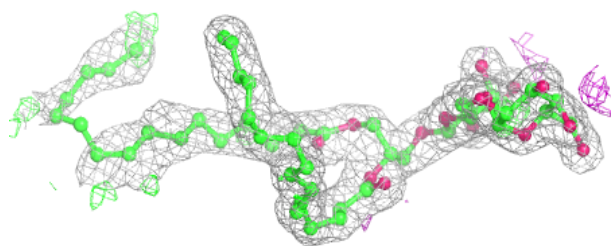
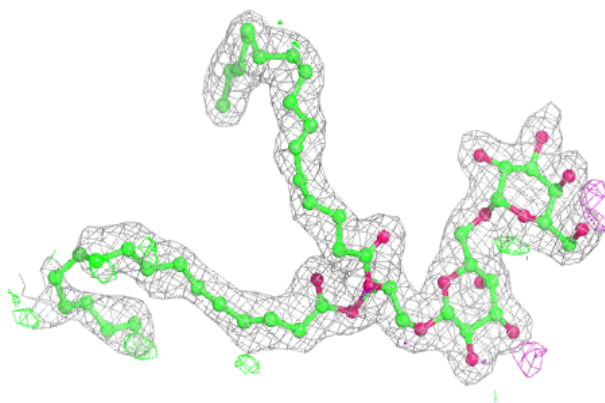
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



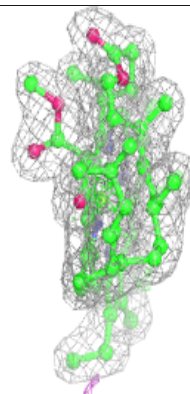
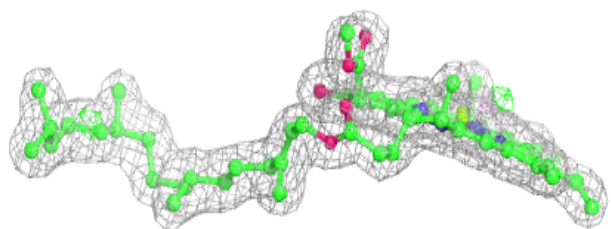
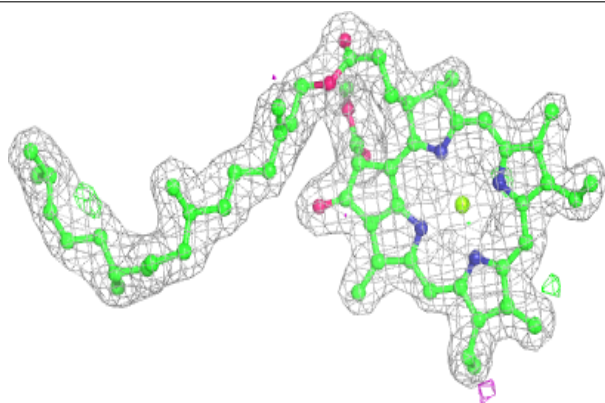


**Electron density around DGD c 918:**

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

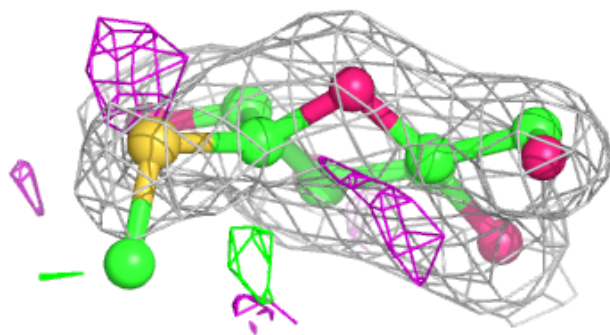
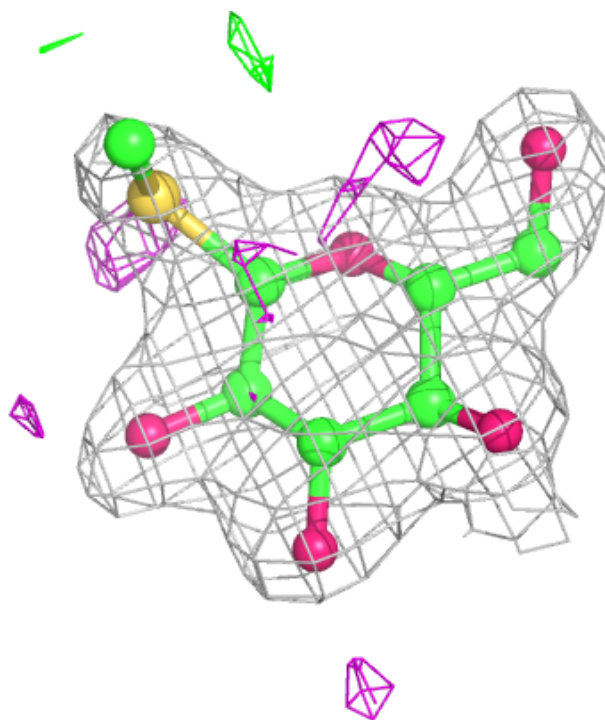
**Electron density around CLA B 603:**

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



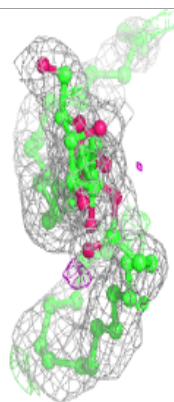
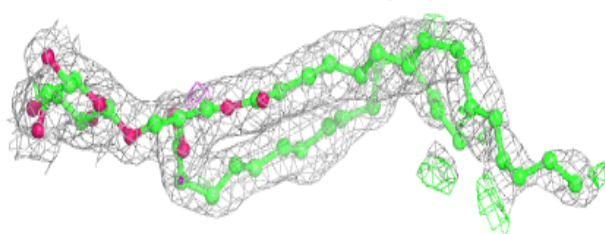
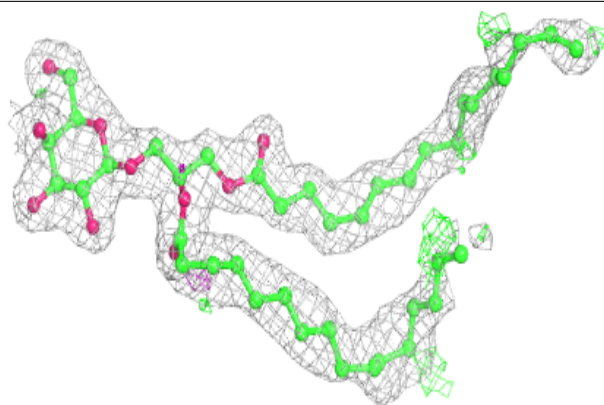
**Electron density around HTG V 202:**

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

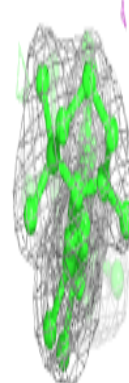
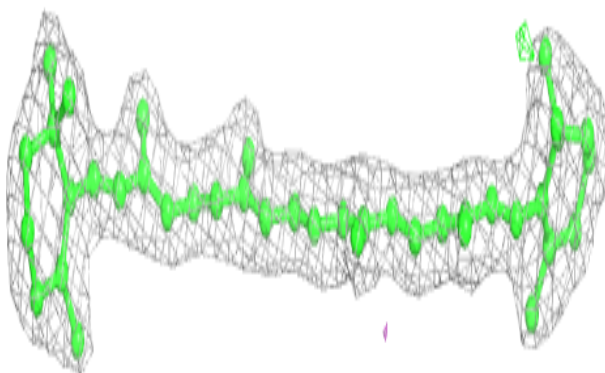
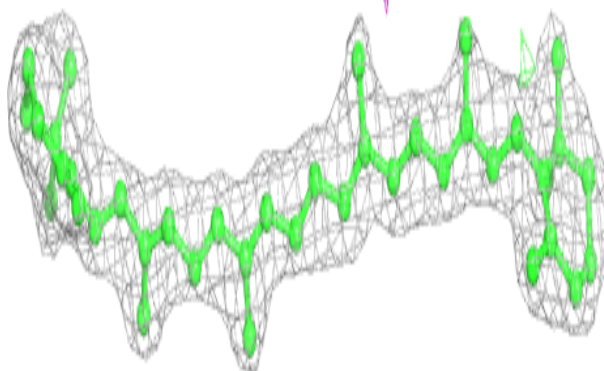


**Electron density around LMG d 410:**

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

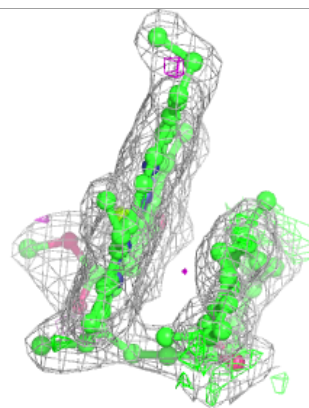
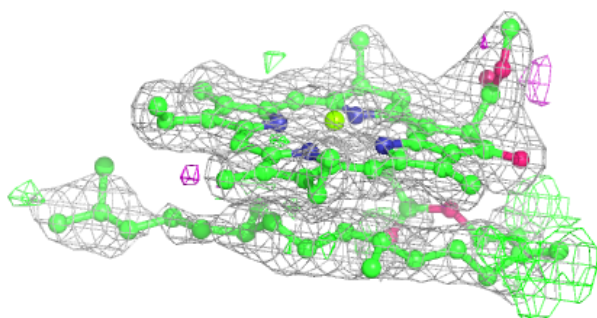
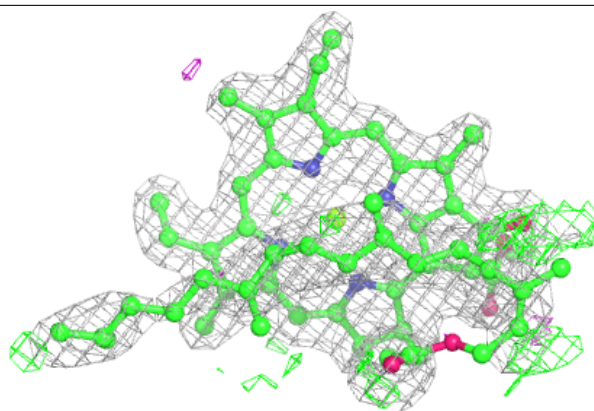
**Electron density around BCR c 915:**

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

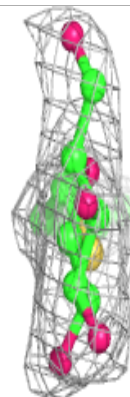
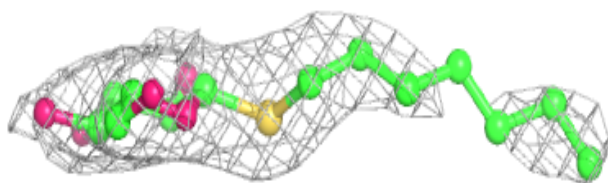
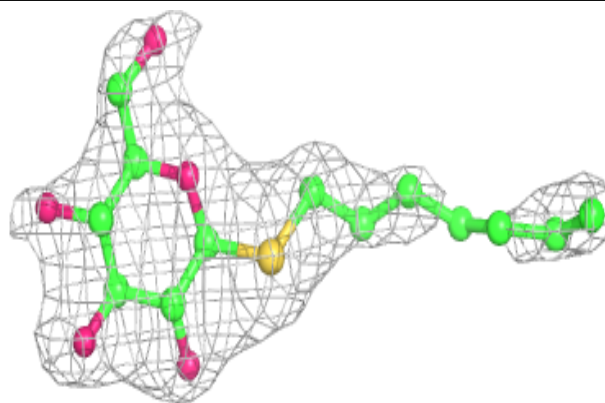


**Electron density around CLA B 602:**

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

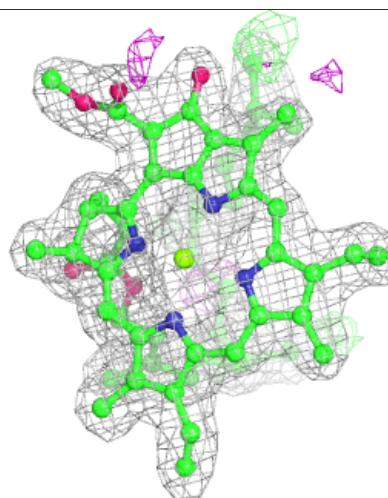
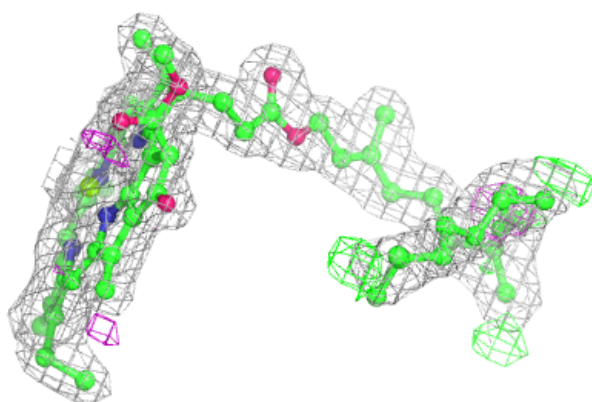
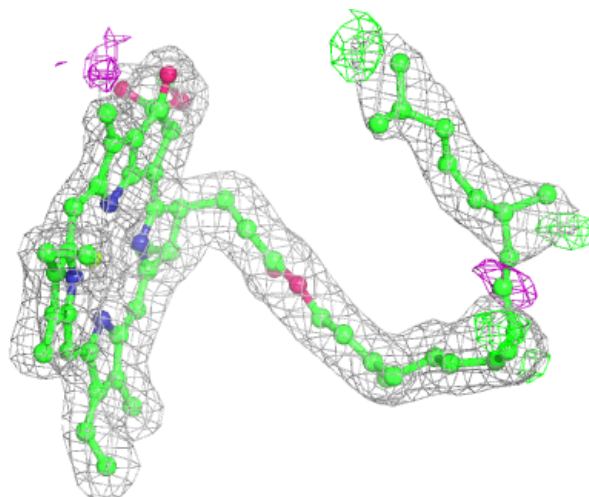
**Electron density around HTG C 521:**

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



**Electron density around CLA b 609:**

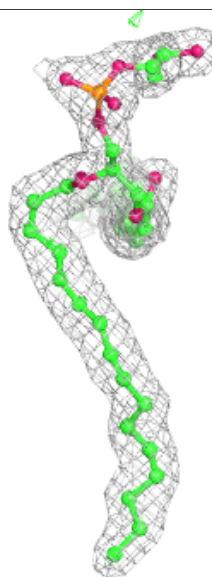
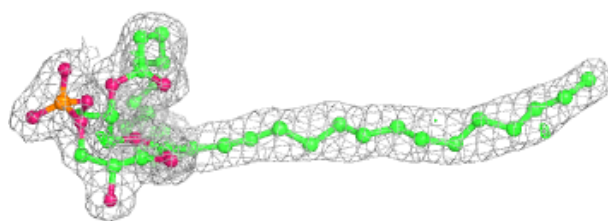
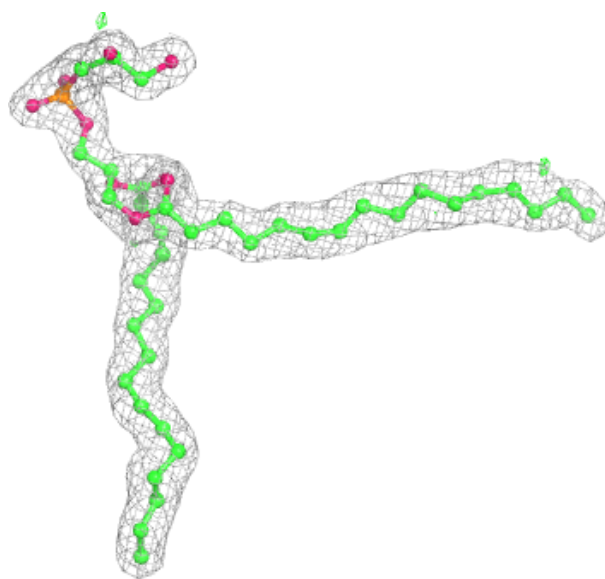
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





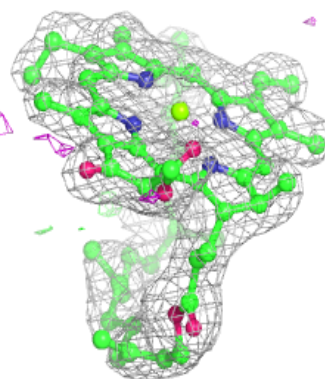
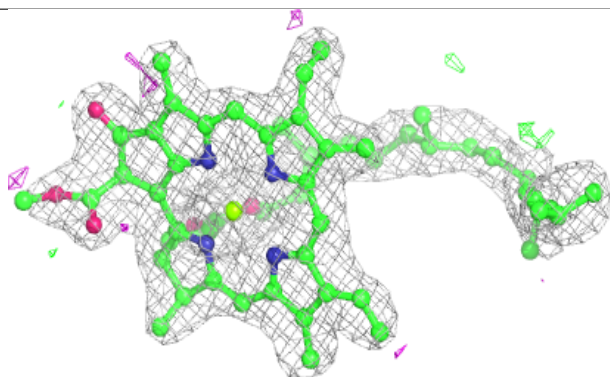
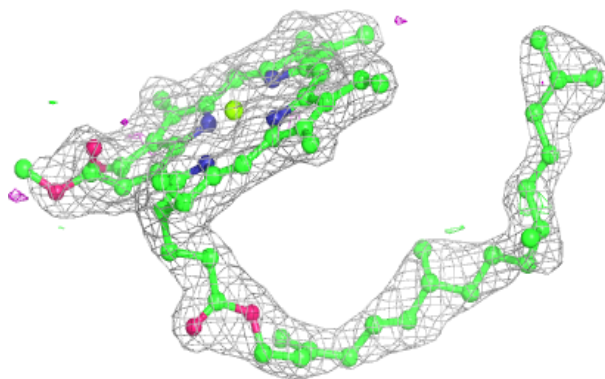
**Electron density around LHG 1 101:**

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

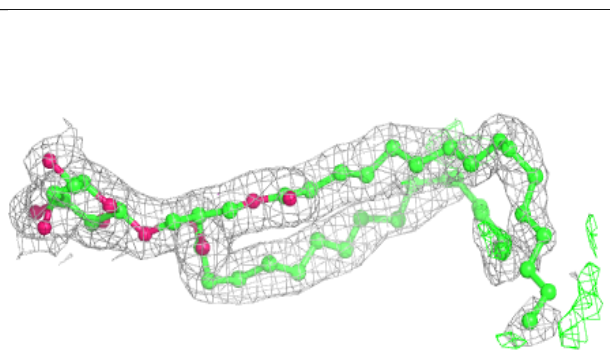
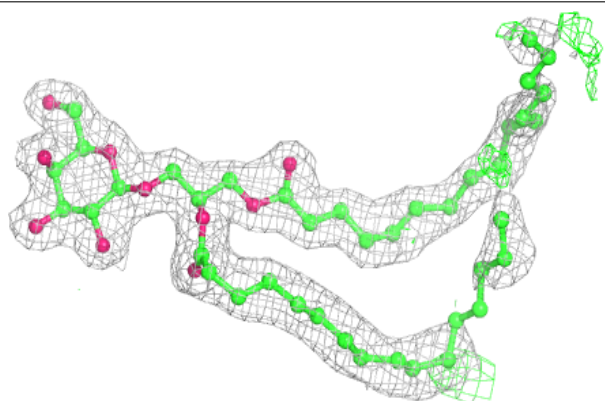


**Electron density around CLA C 513:**

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

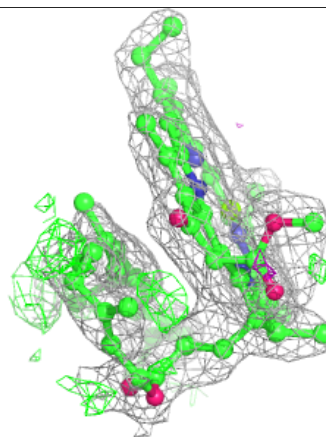
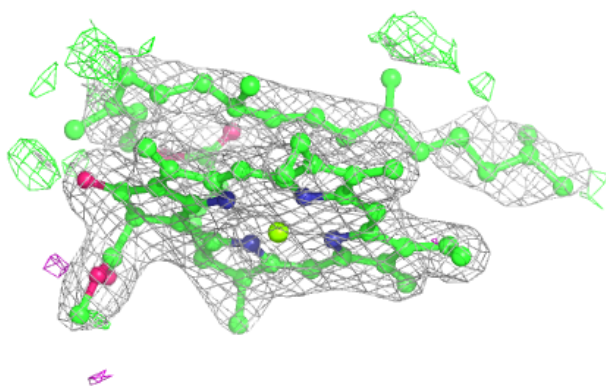
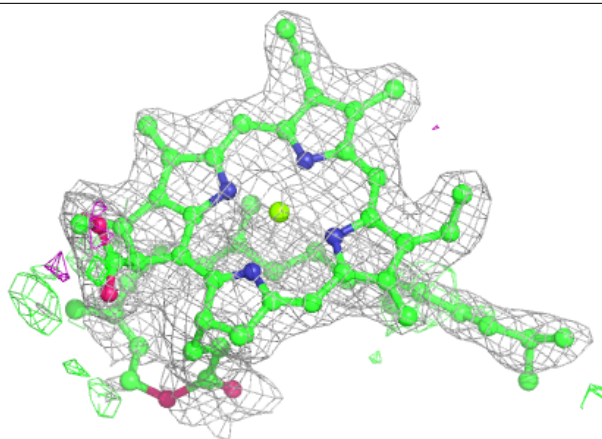
**Electron density around LMG D 411:**

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

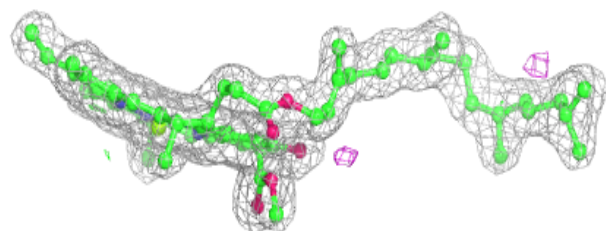
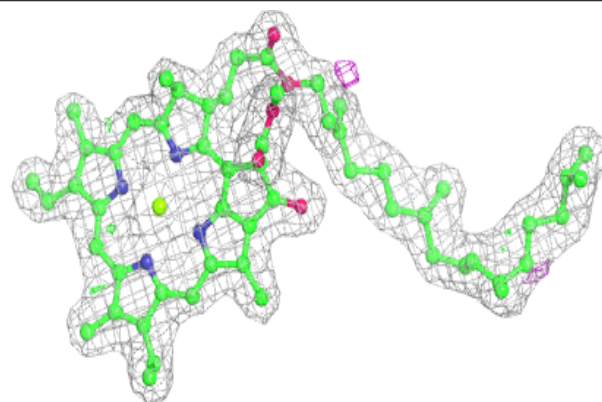


**Electron density around CLA b 604:**

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

**Electron density around CLA b 605:**

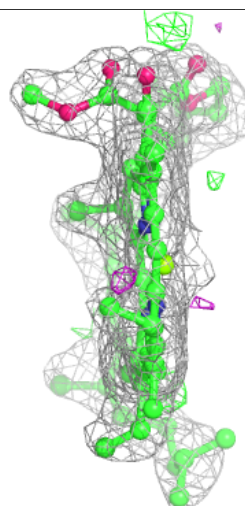
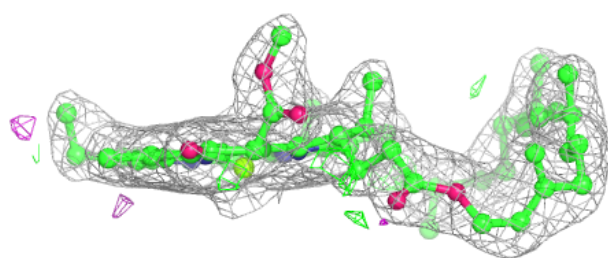
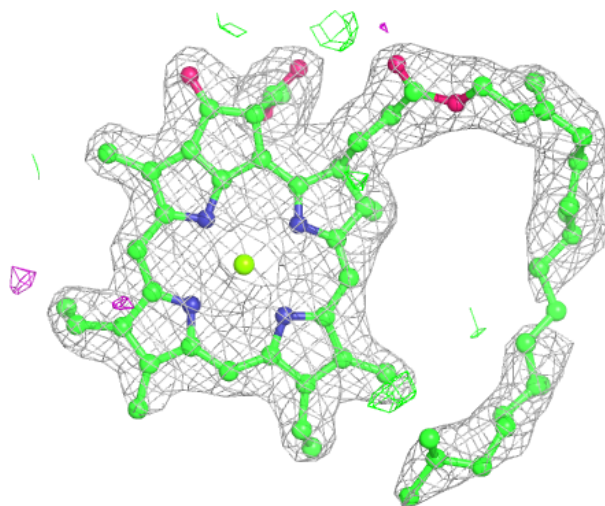
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





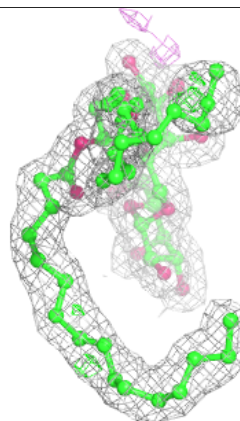
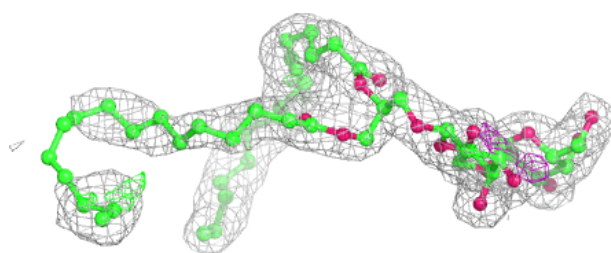
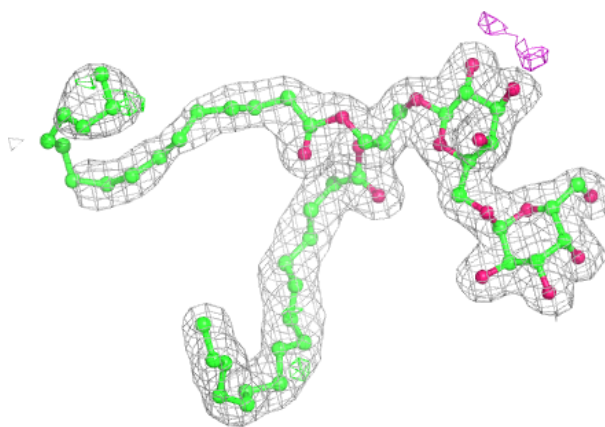
**Electron density around CLA c 913:**

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



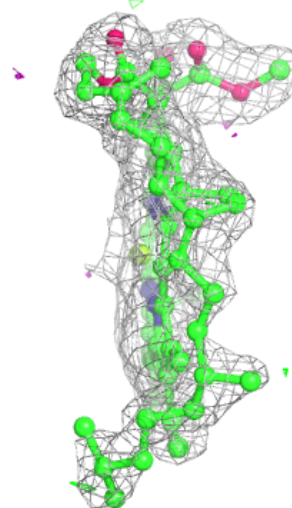
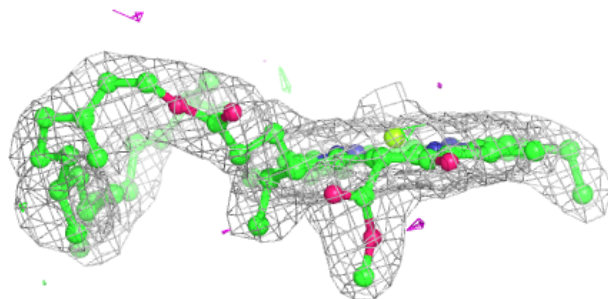
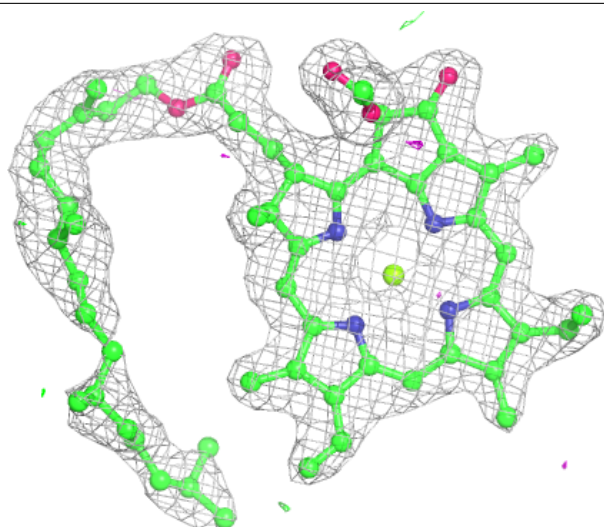
**Electron density around DGD C 517:**

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



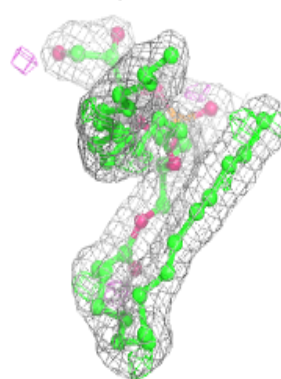
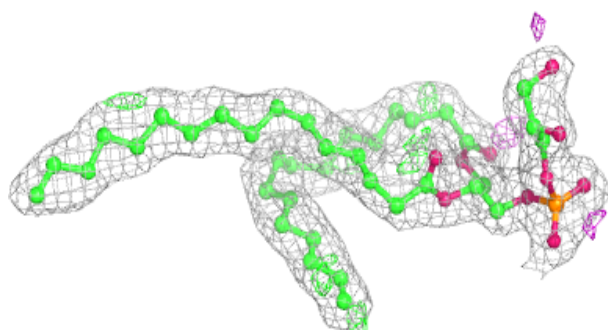
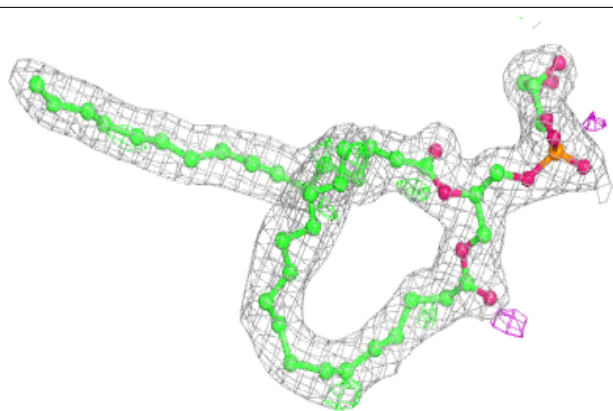
**Electron density around CLA C 512:**

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

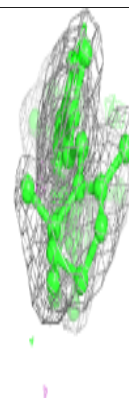
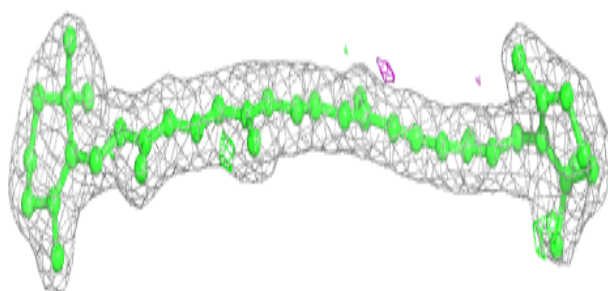
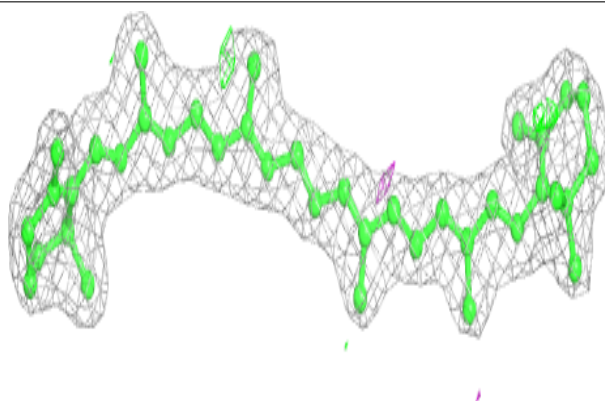


**Electron density around LHG D 408:**

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

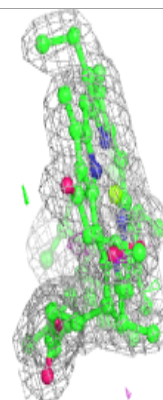
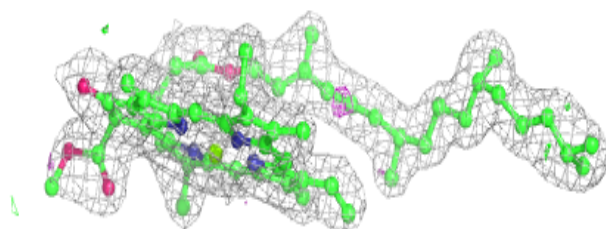
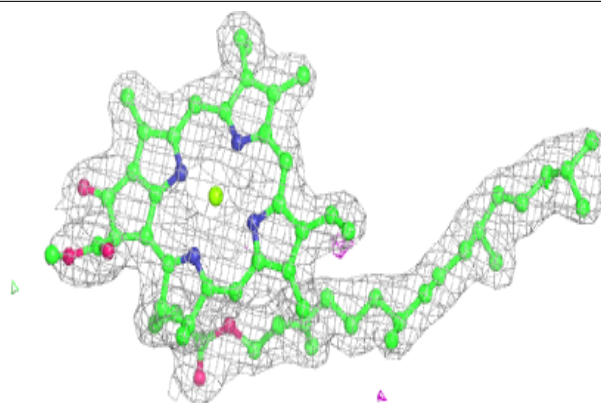
**Electron density around BCR k 101:**

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

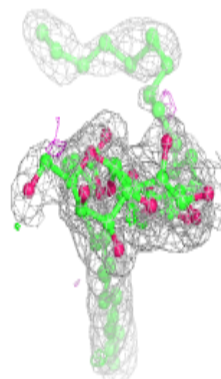
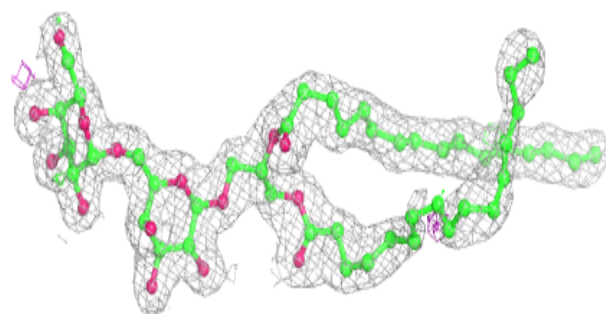
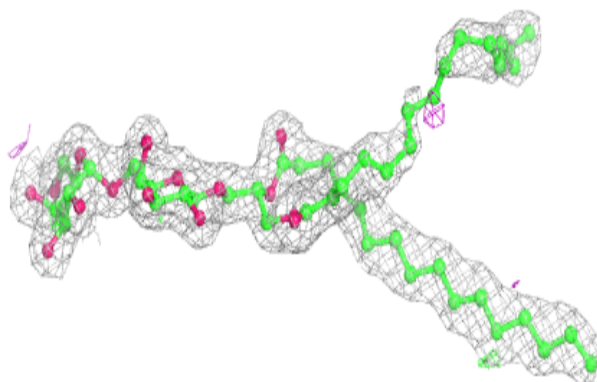


**Electron density around CLA c 902:**

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

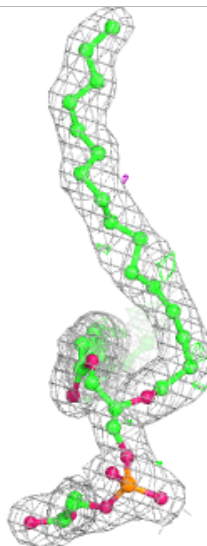
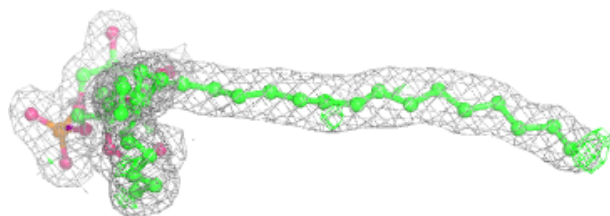
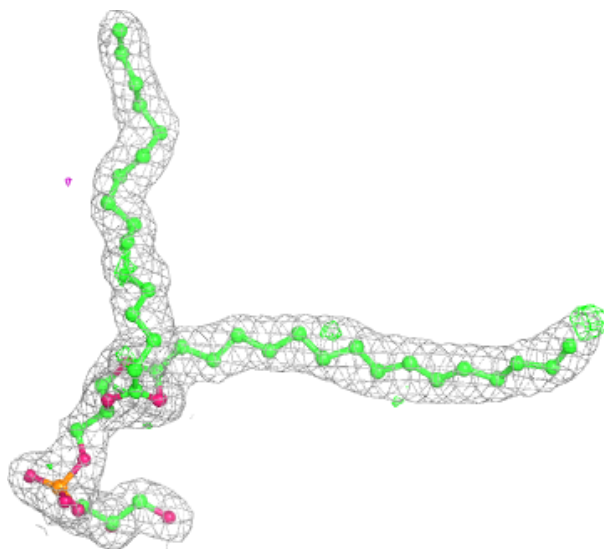
**Electron density around DGD c 917:**

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



**Electron density around LHG L 101:**

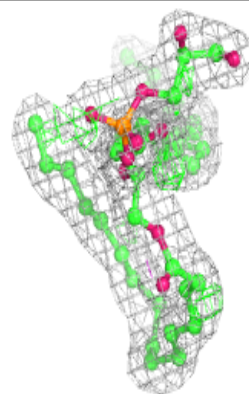
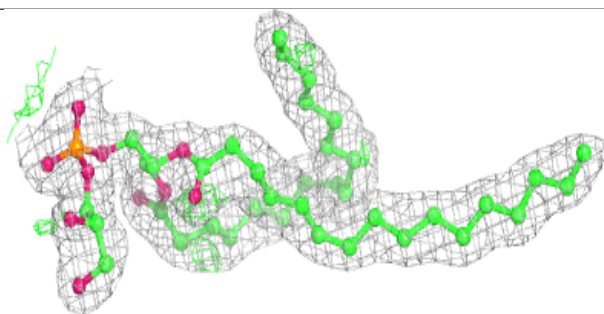
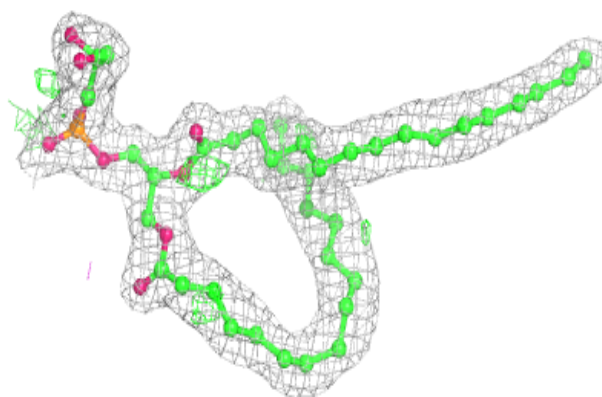
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



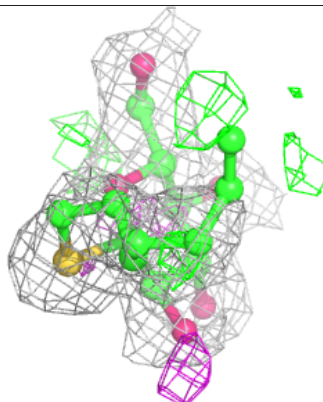
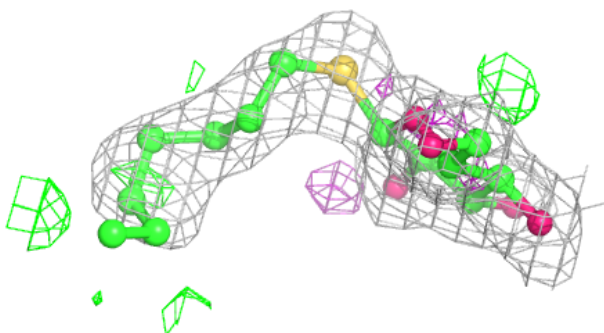
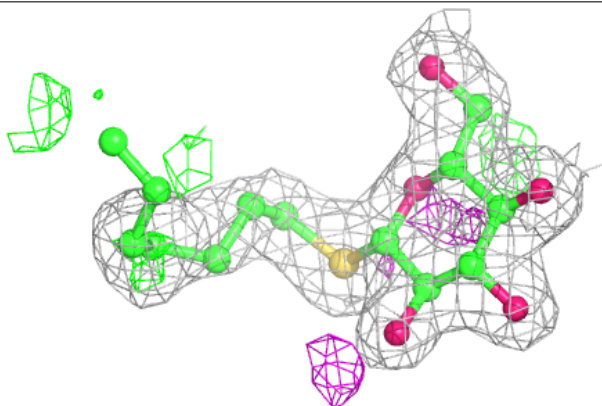


**Electron density around LHG d 407:**

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

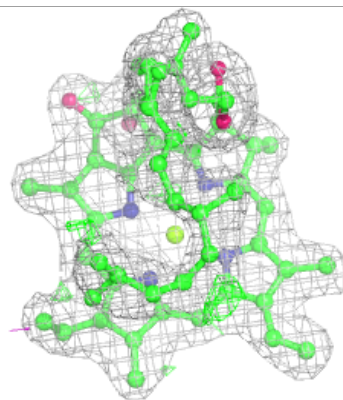
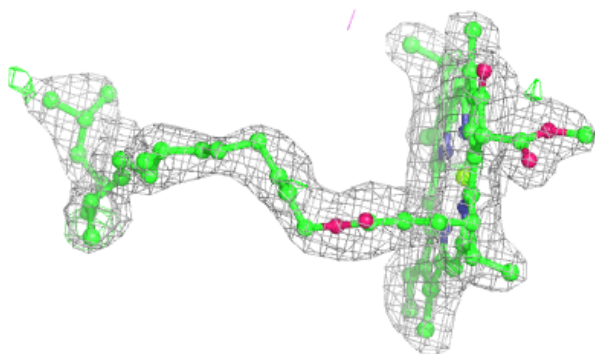
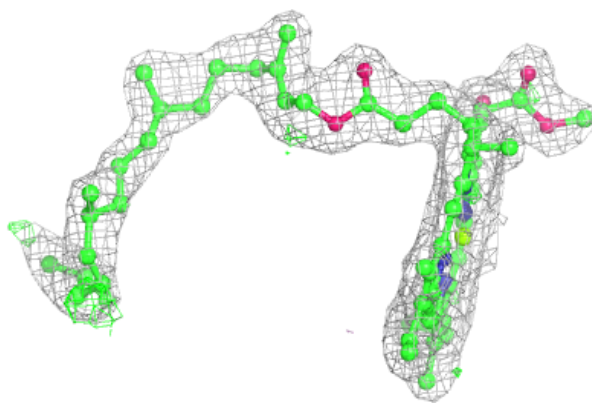
**Electron density around HTG B 625:**

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

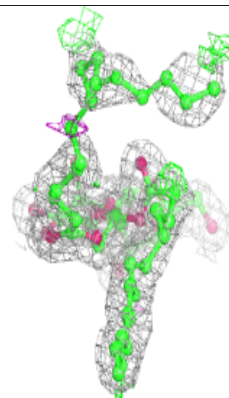
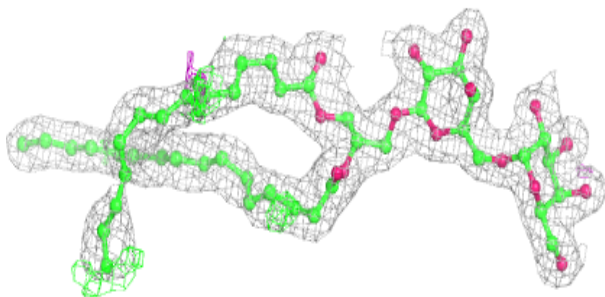
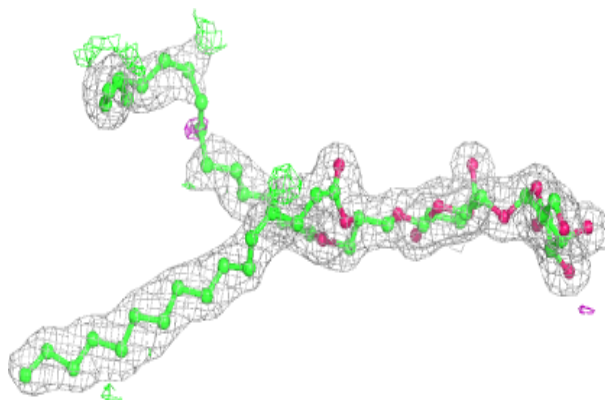


**Electron density around CLA c 907:**

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

**Electron density around DGD C 516:**

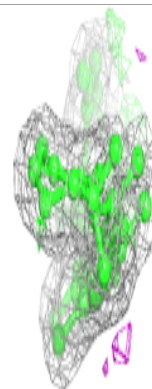
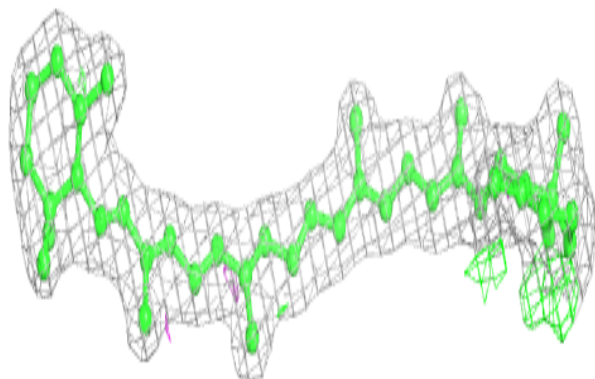
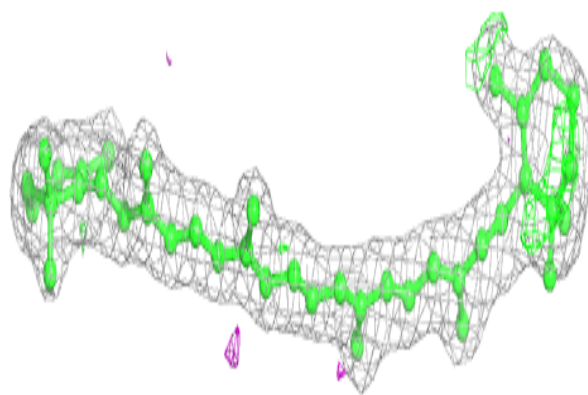
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



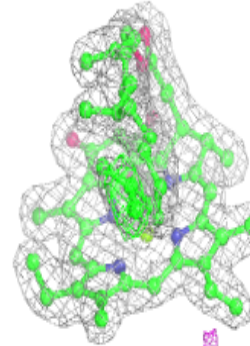
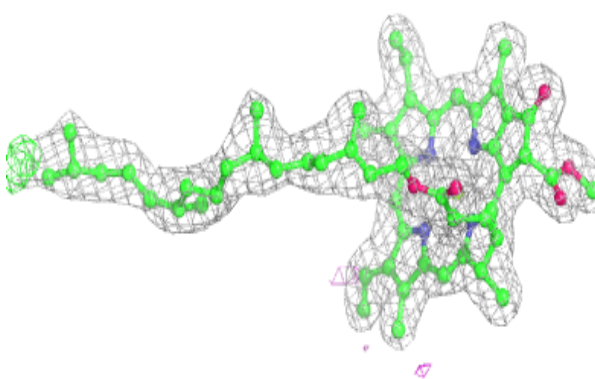
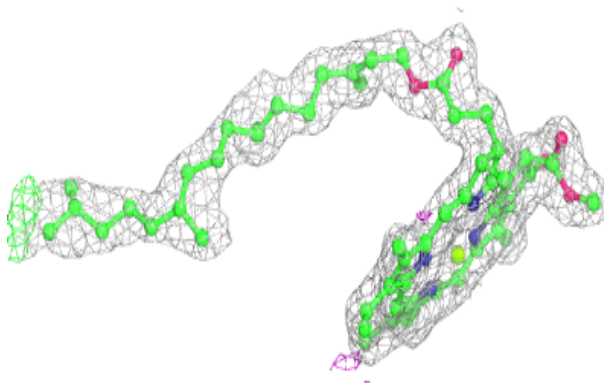


**Electron density around BCR d 404:**

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

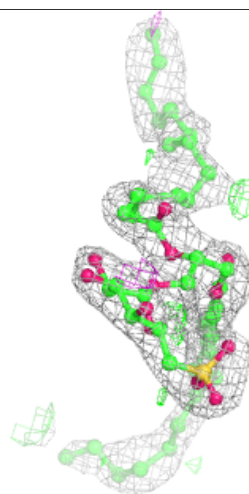
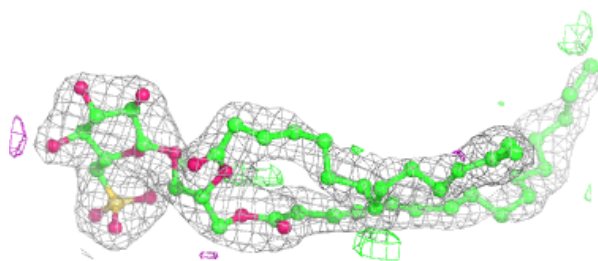
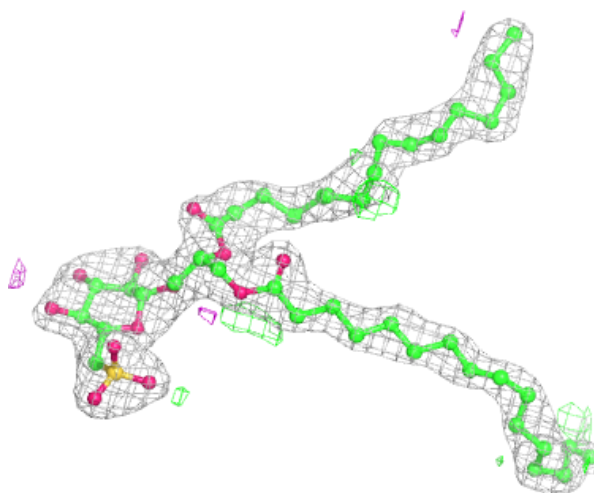
**Electron density around CLA c 905:**

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



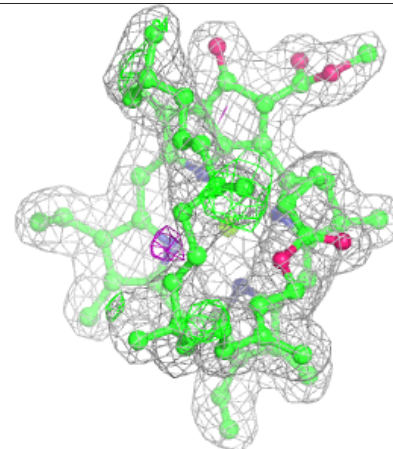
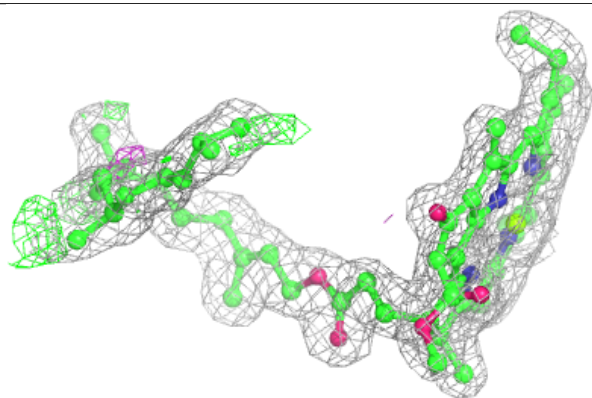
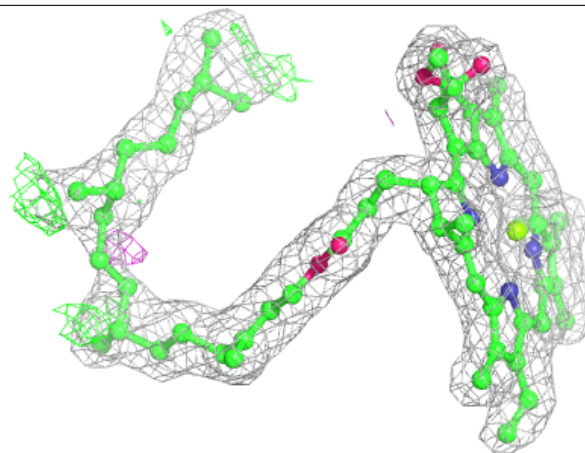
**Electron density around SQD A 412:**

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

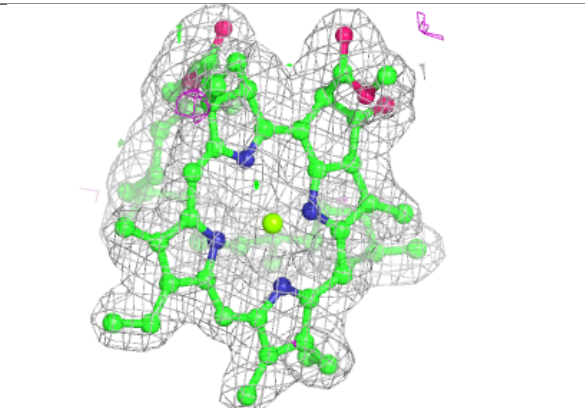
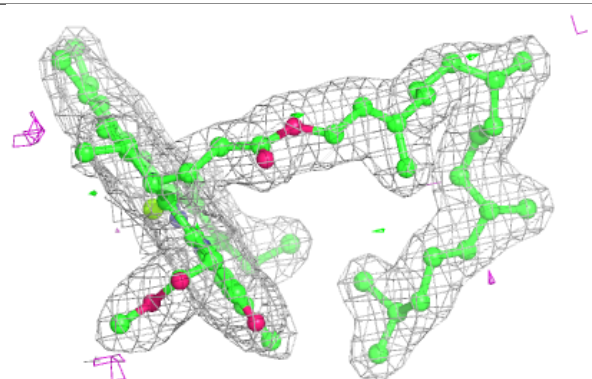
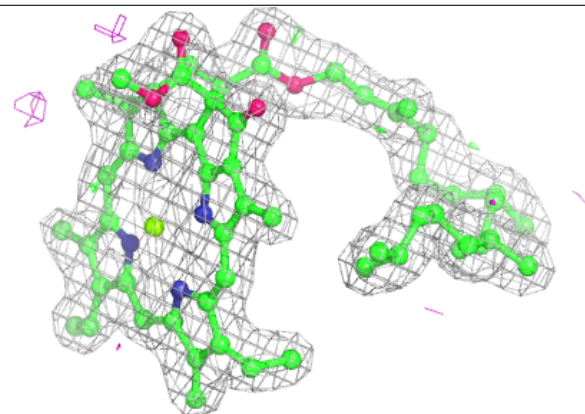


**Electron density around CLA B 607:**

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

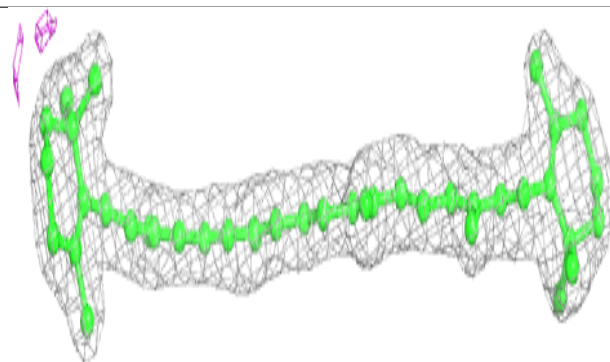
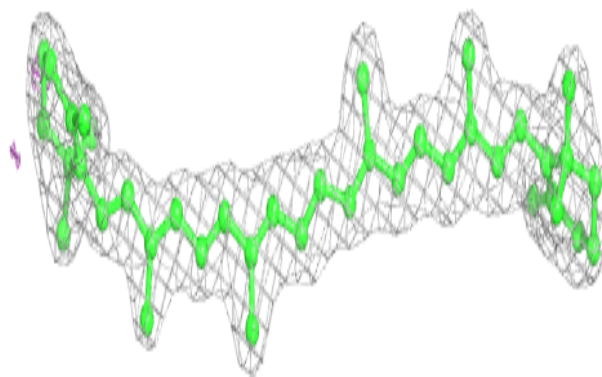
**Electron density around CLA c 904:**

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



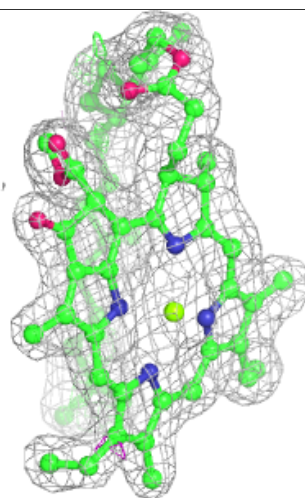
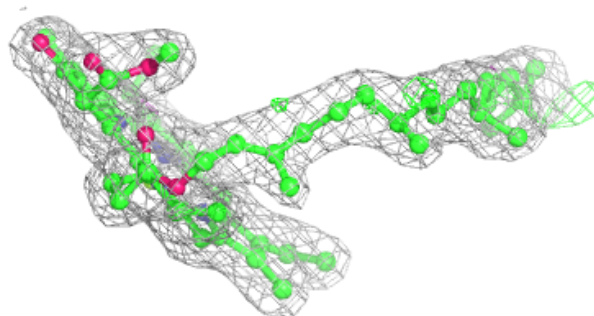
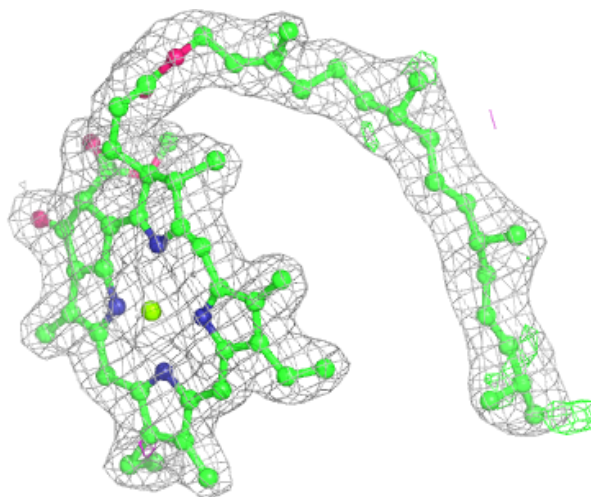
**Electron density around BCR c 916:**

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



**Electron density around CLA c 908:**

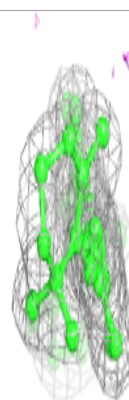
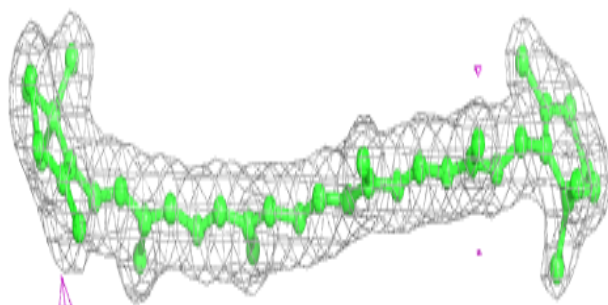
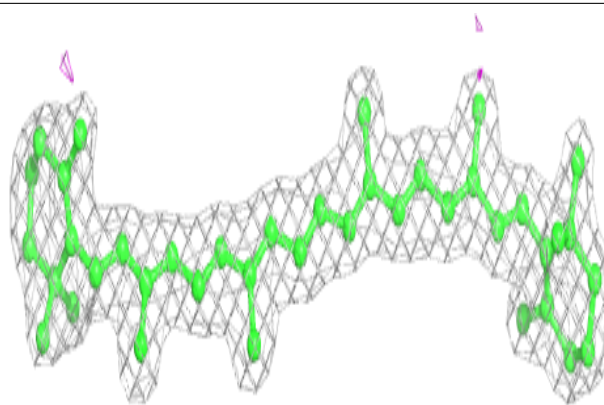
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



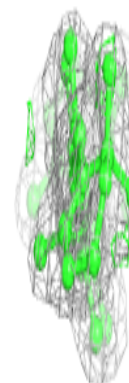
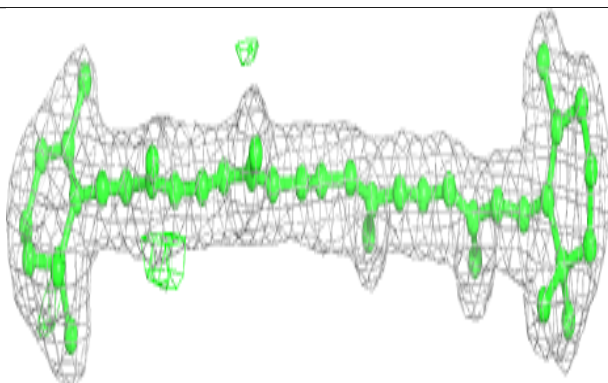
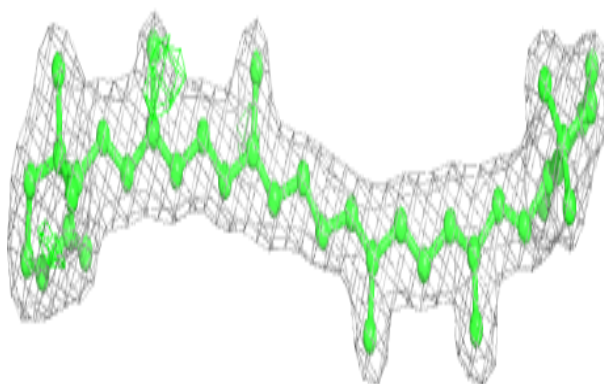


**Electron density around BCR B 620:**

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

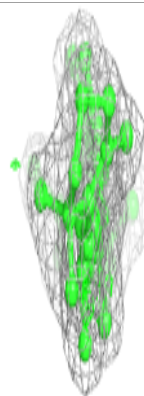
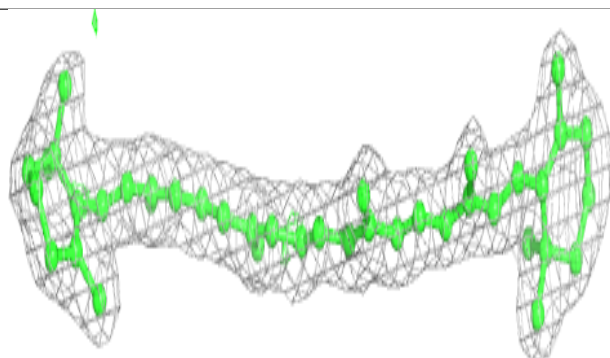
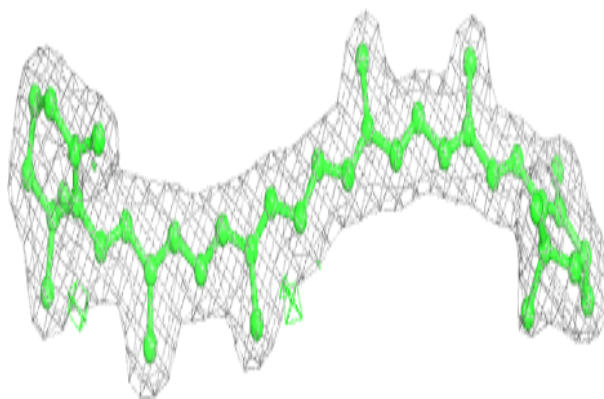
**Electron density around BCR C 514:**

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

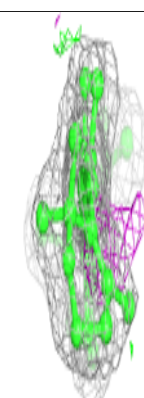
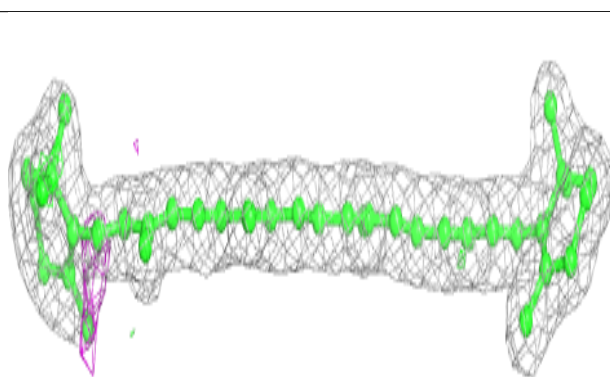
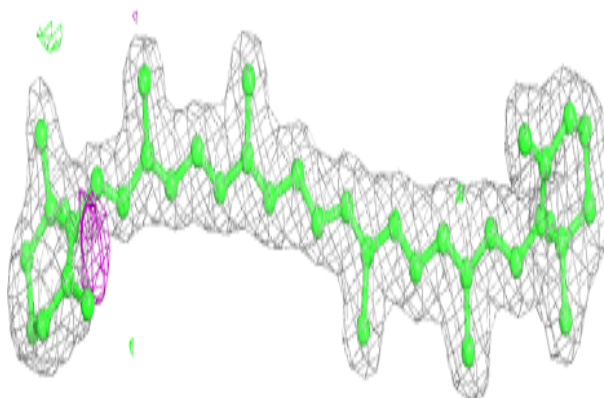


**Electron density around BCR K 101:**

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

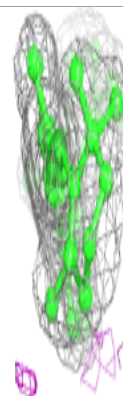
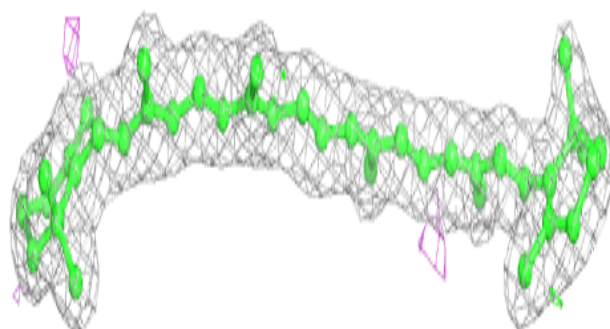
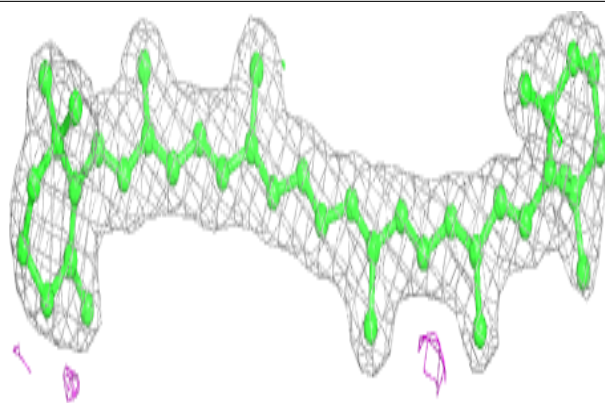
**Electron density around BCR B 619:**

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

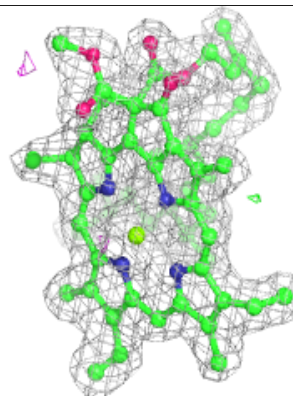
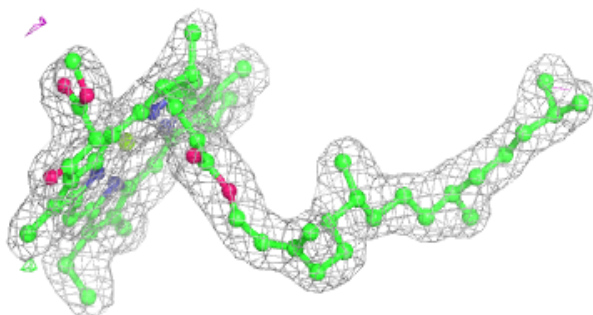
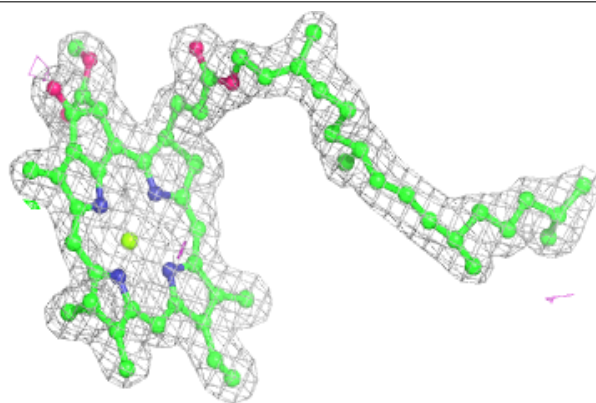


**Electron density around BCR b 622:**

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

**Electron density around CLA C 511:**

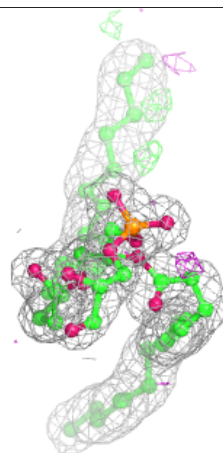
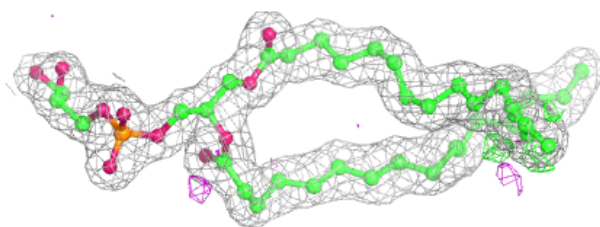
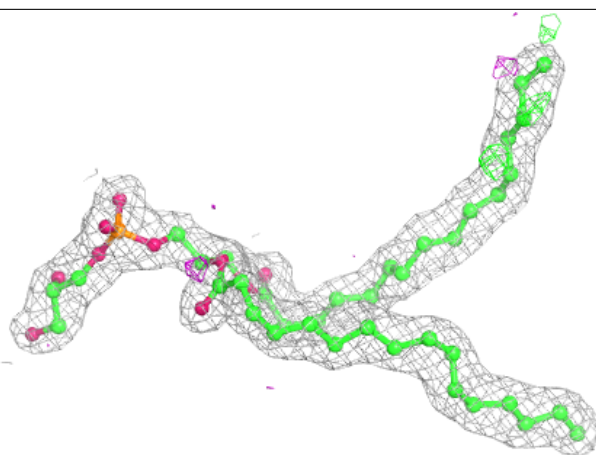
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



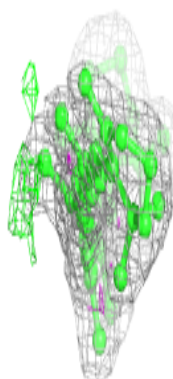
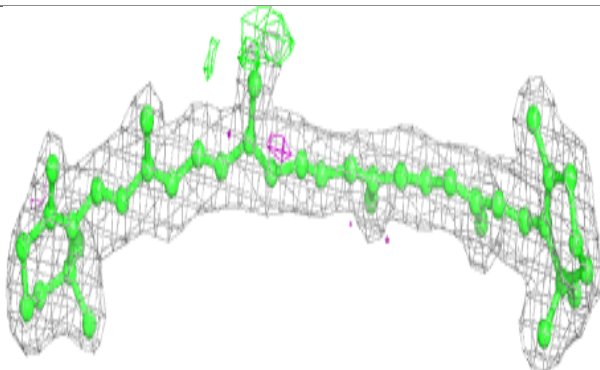
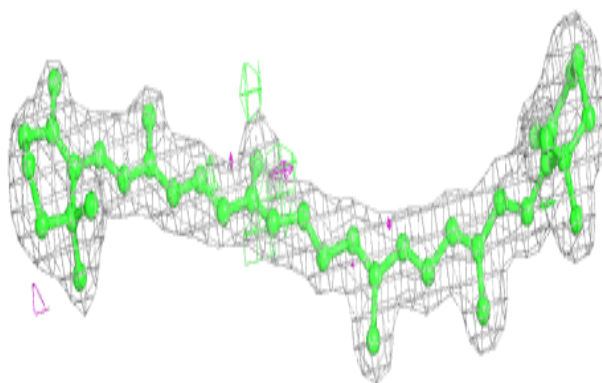


**Electron density around LHG d 408:**

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

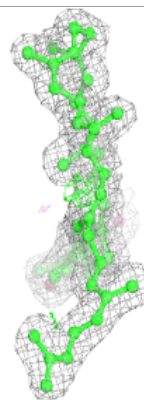
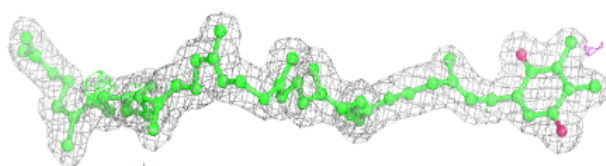
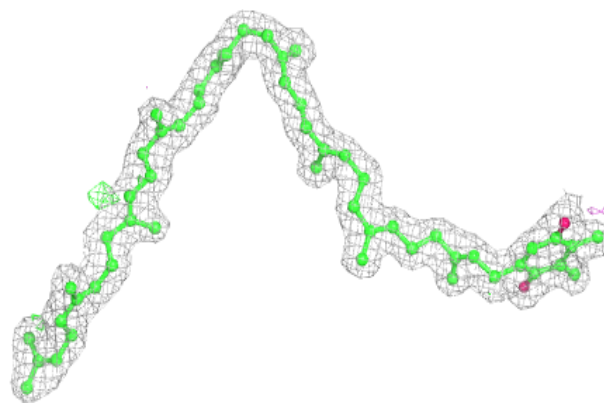
**Electron density around BCR t 101:**

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

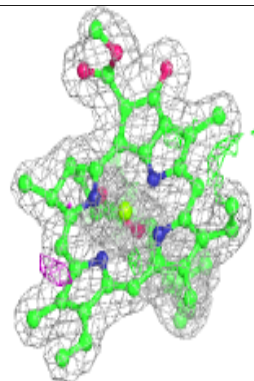
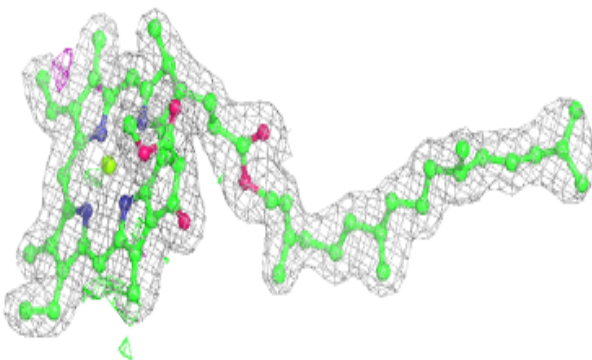
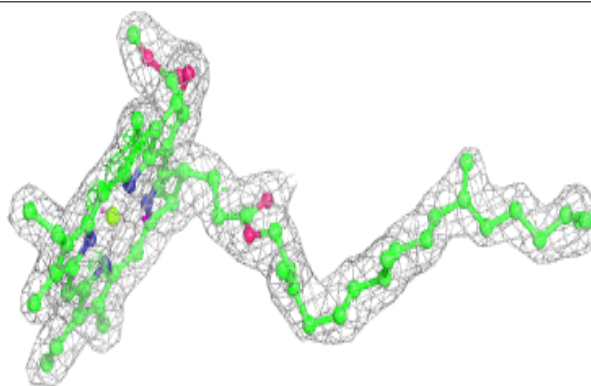


**Electron density around PL9 d 405:**

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

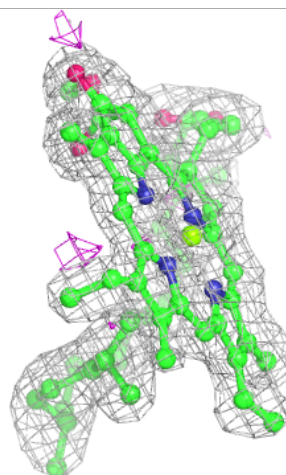
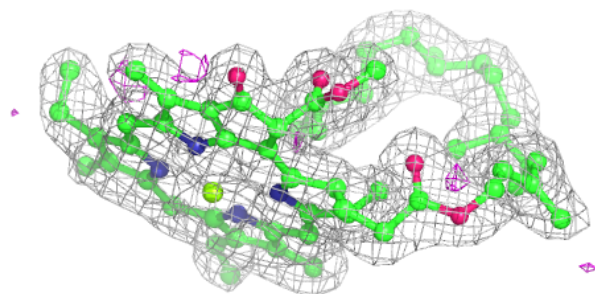
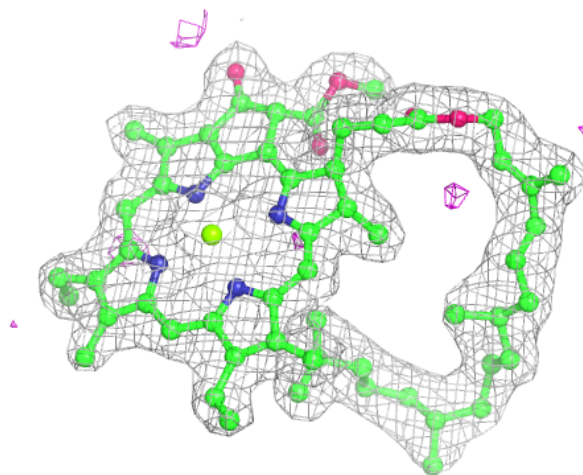
**Electron density around CLA c 903:**

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



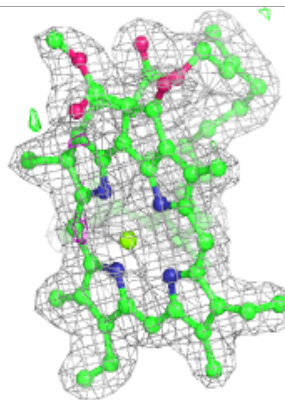
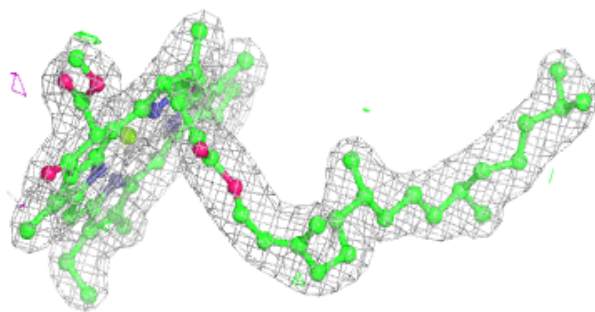
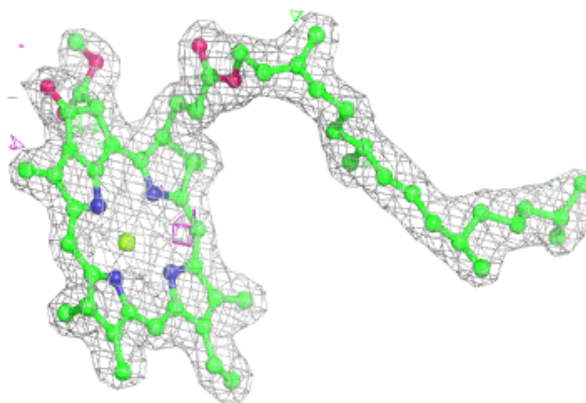
**Electron density around CLA b 618:**

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



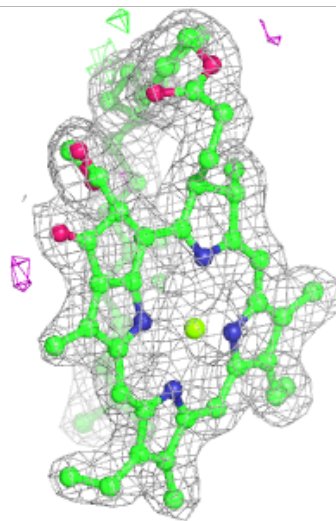
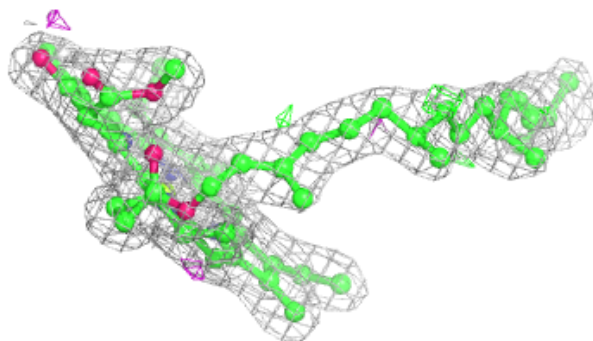
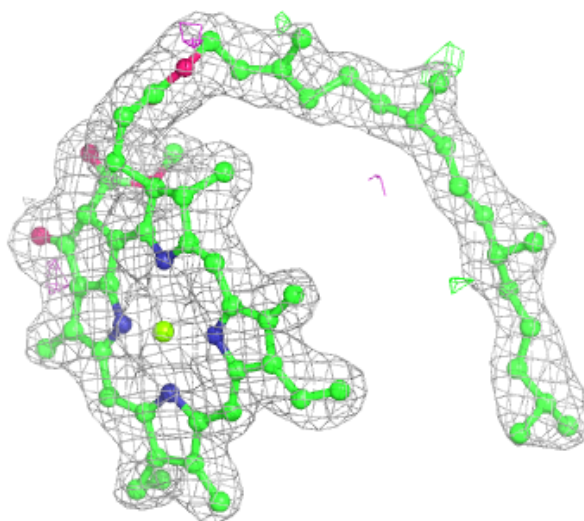
**Electron density around CLA c 912:**

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



**Electron density around CLA C 507:**

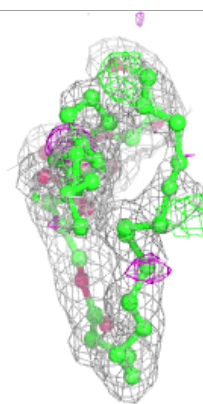
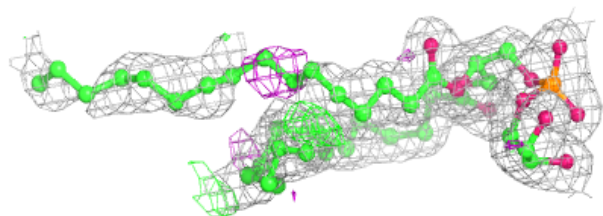
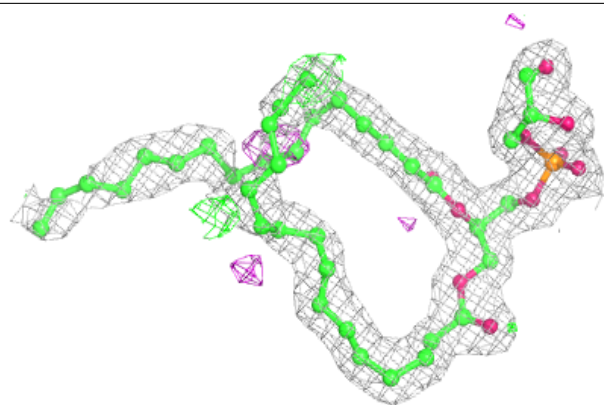
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



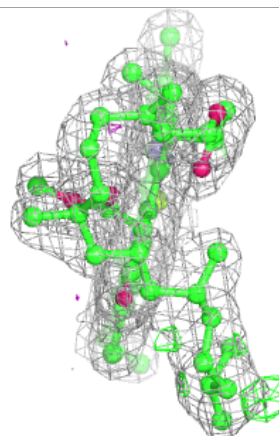
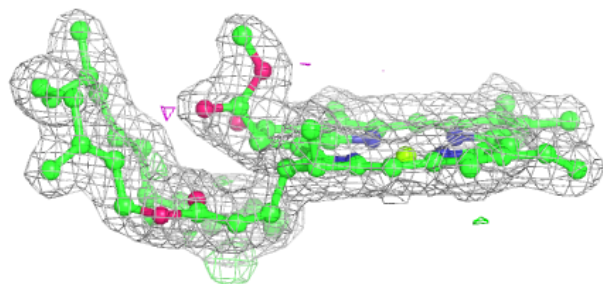
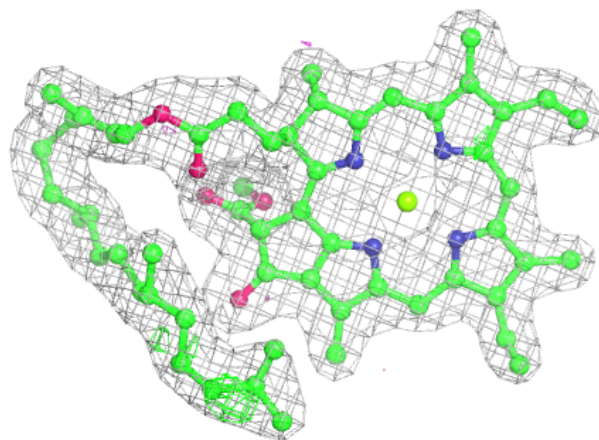


**Electron density around LHG d 409:**

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

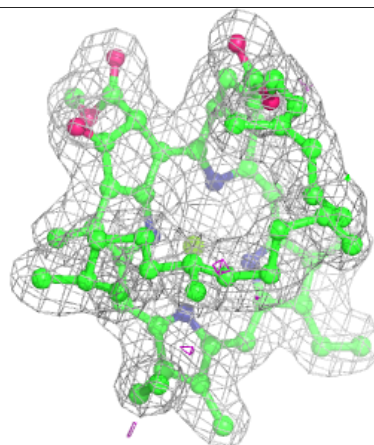
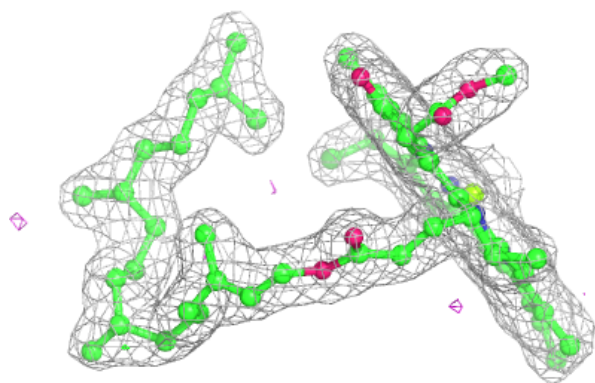
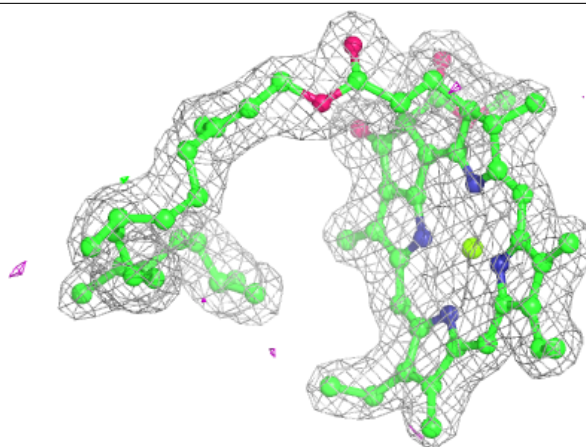
**Electron density around CLA b 613:**

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



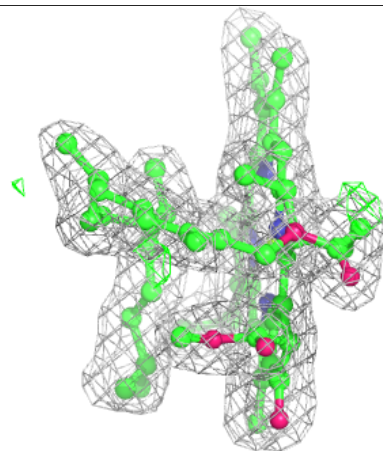
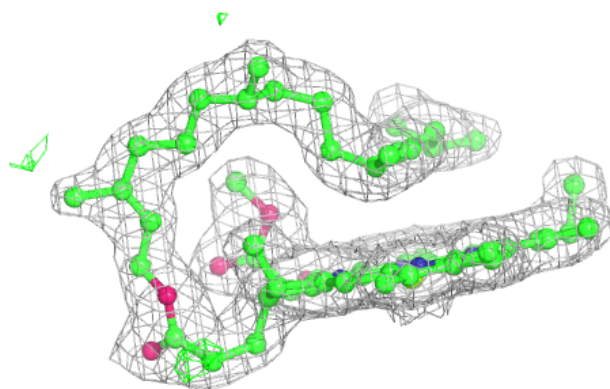
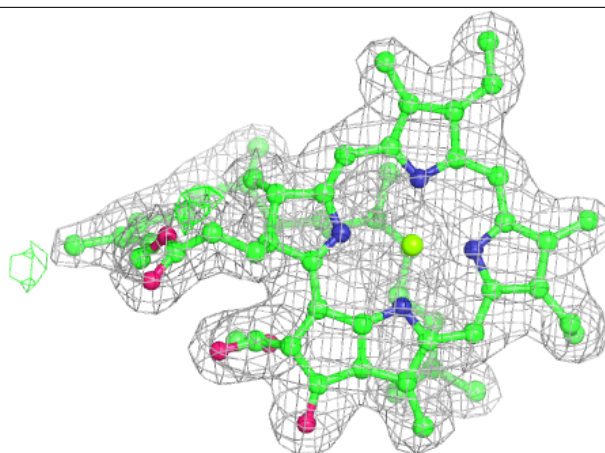
**Electron density around CLA C 503:**

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



**Electron density around CLA C 510:**

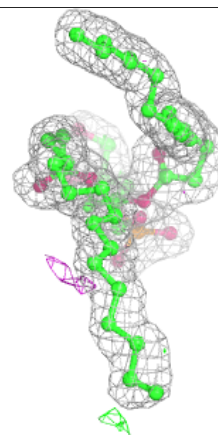
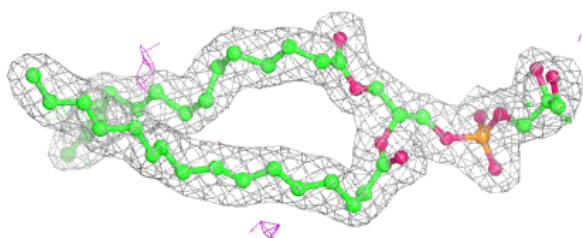
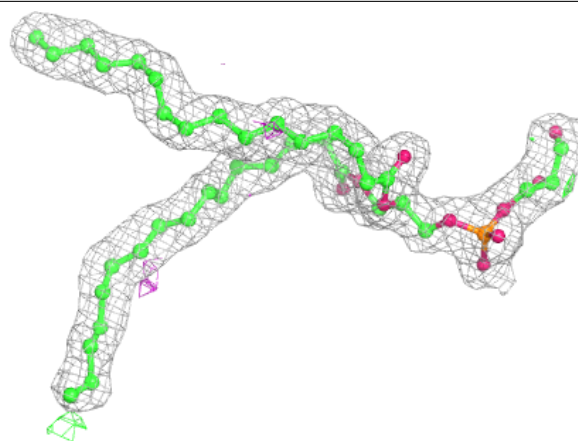
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



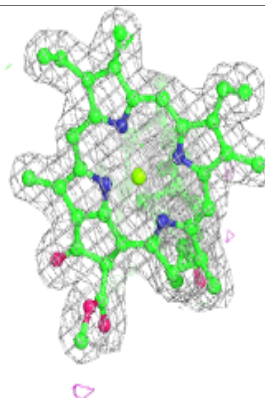
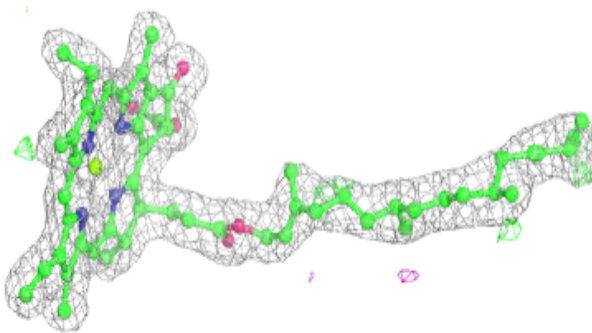
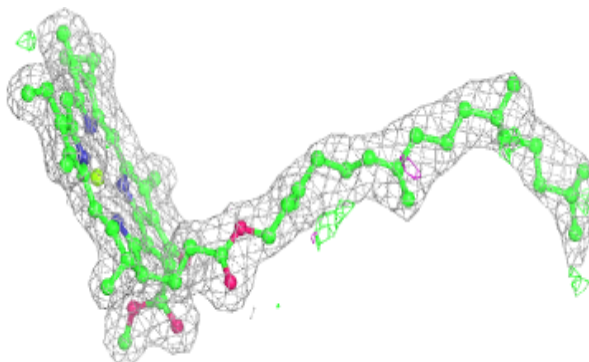


**Electron density around LHG D 409:**

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

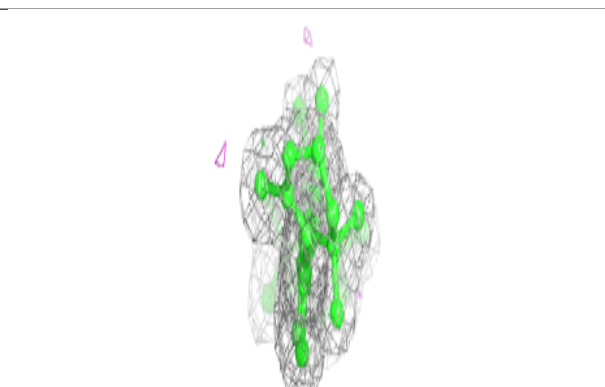
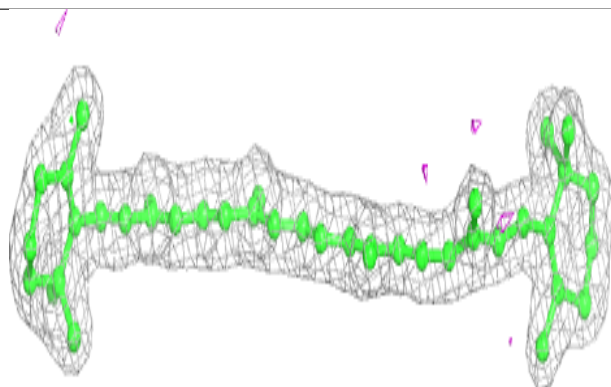
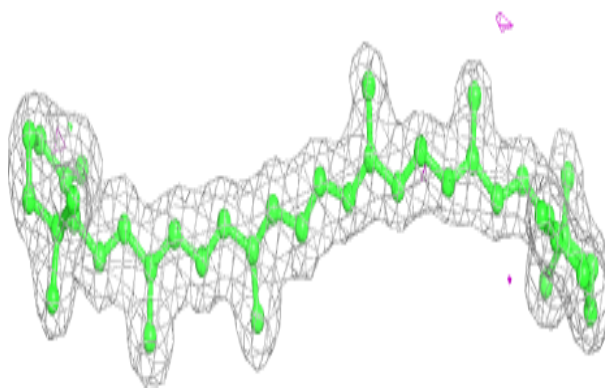
**Electron density around CLA b 607:**

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

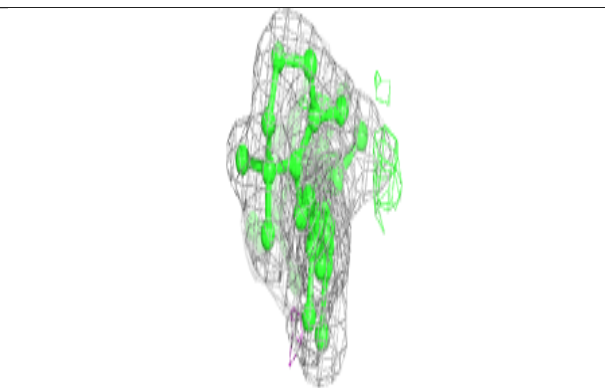
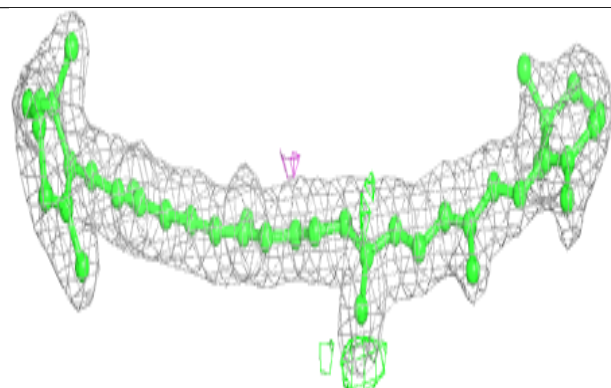
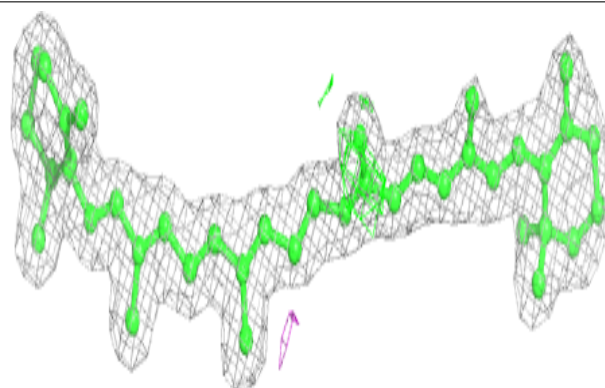


**Electron density around BCR a 415:**

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

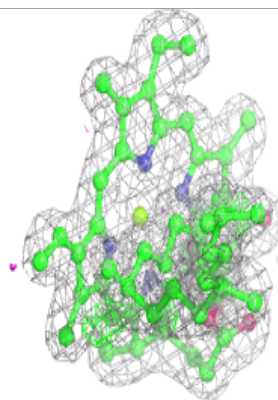
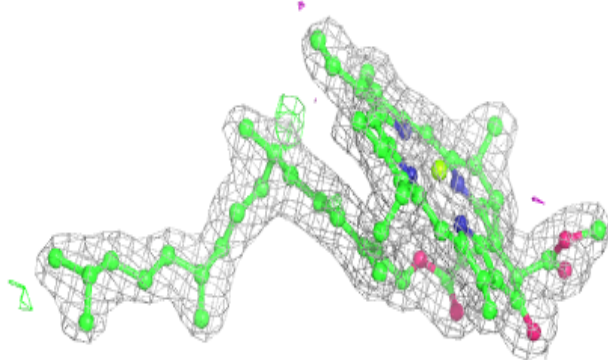
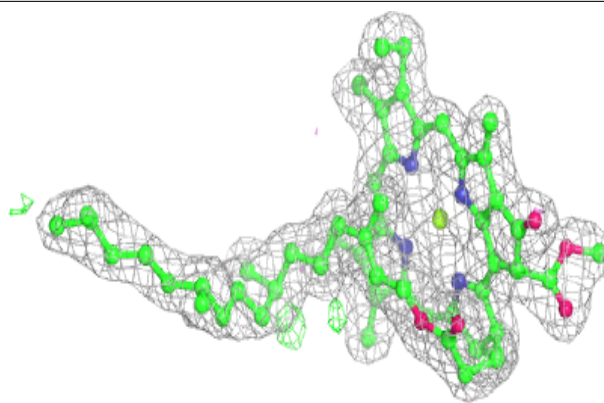
**Electron density around BCR T 101:**

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

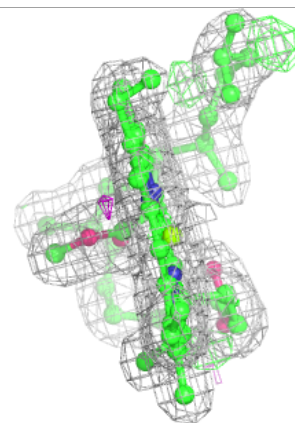
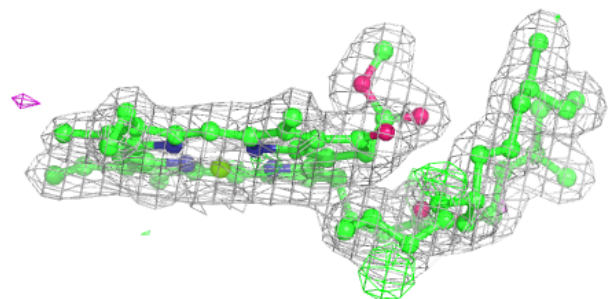
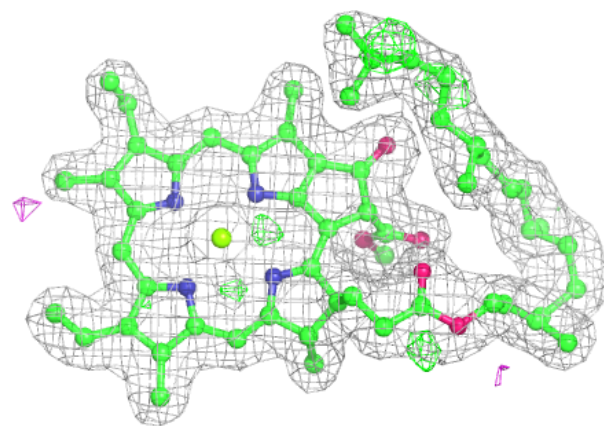


**Electron density around CLA c 906:**

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

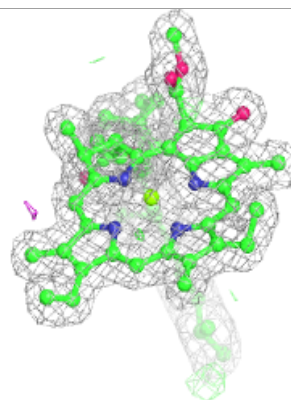
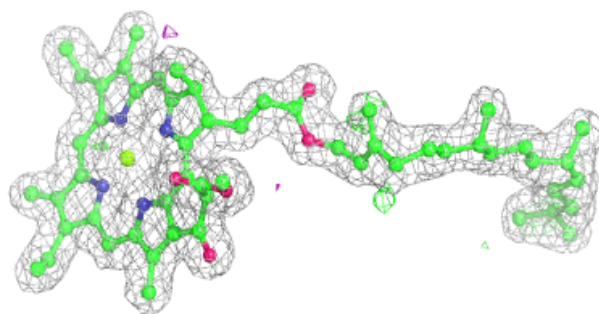
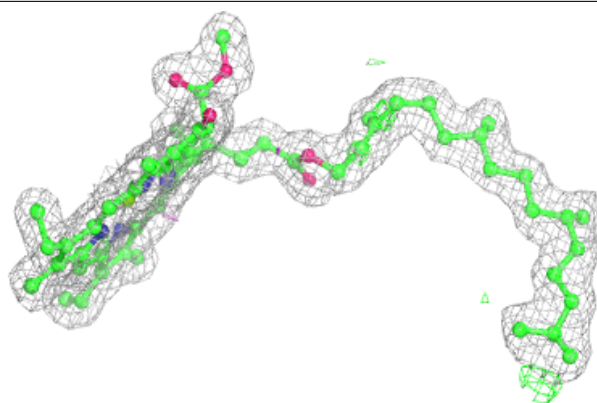
**Electron density around CLA B 611:**

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

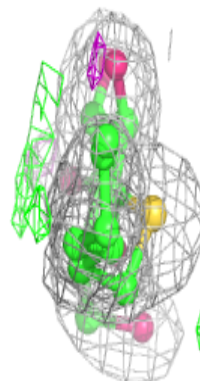
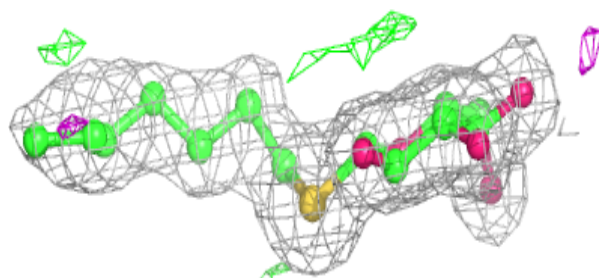
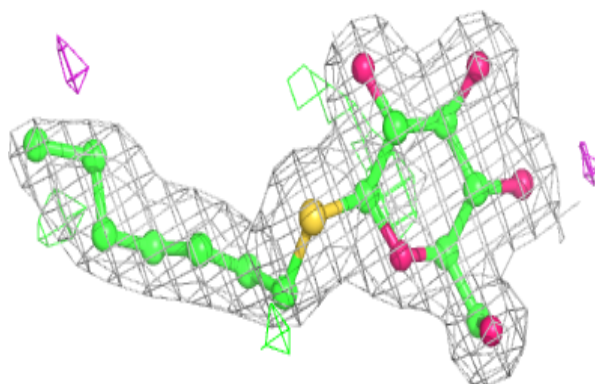


**Electron density around CLA D 402:**

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

**Electron density around HTG B 624:**

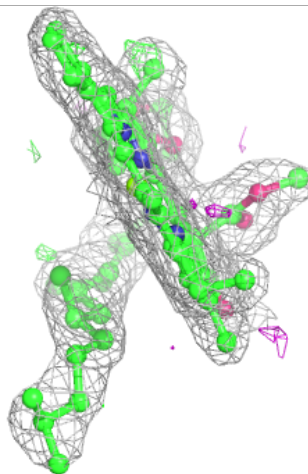
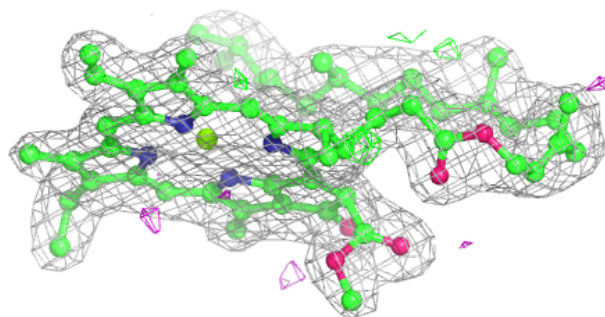
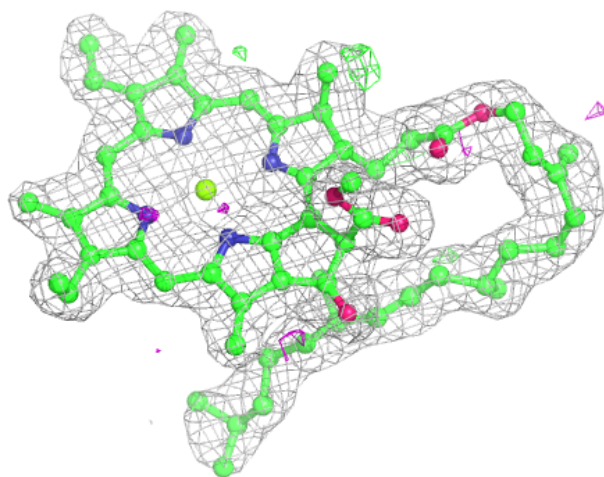
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





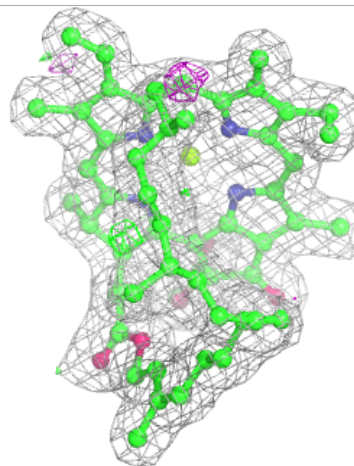
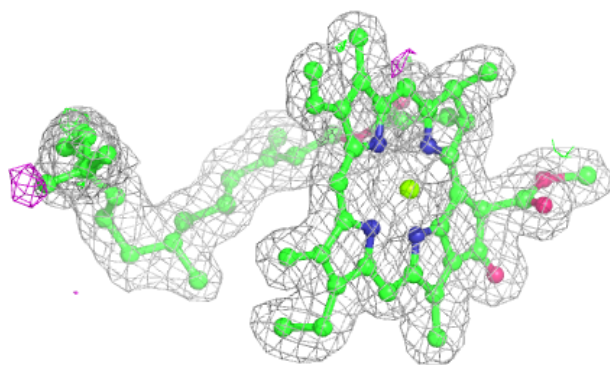
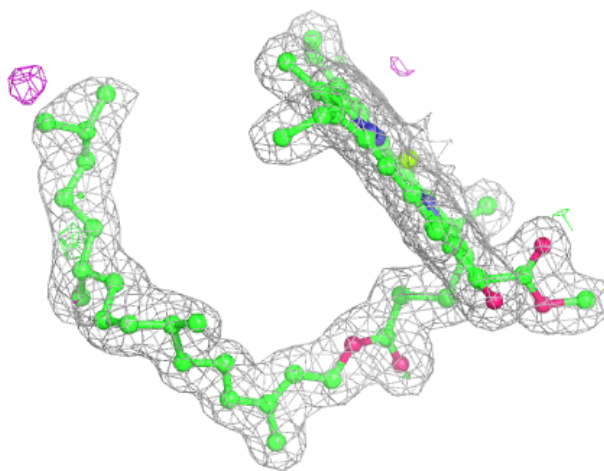
**Electron density around CLA C 509:**

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



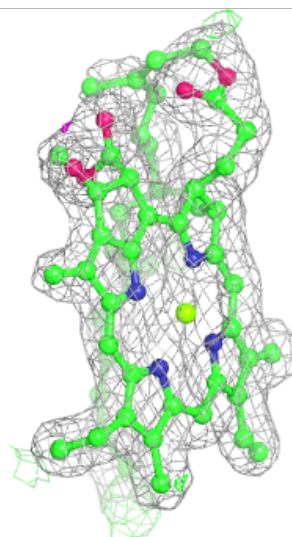
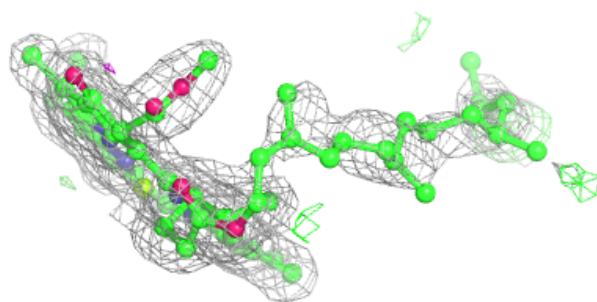
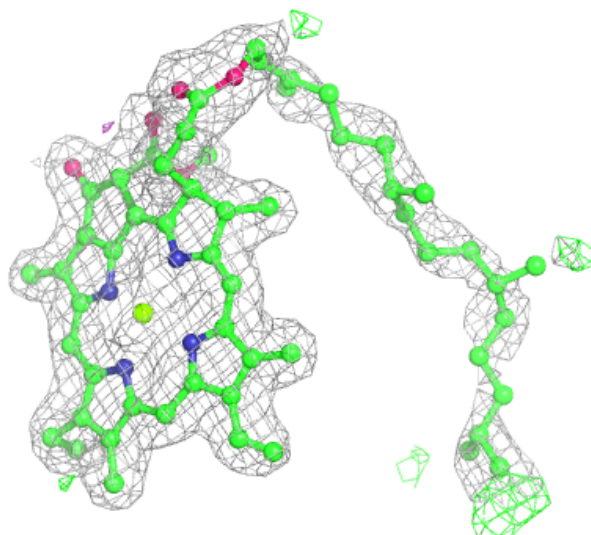
**Electron density around CLA B 612:**

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



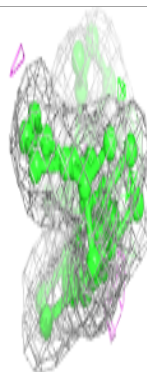
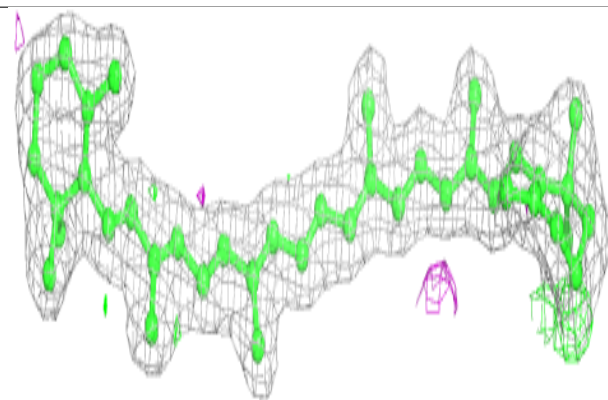
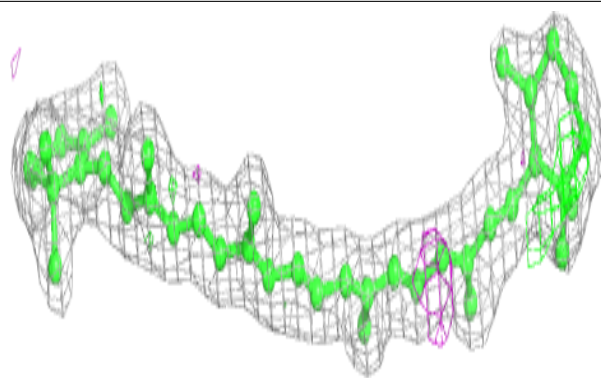
**Electron density around CLA B 617:**

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

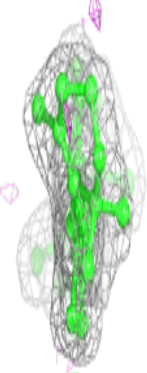
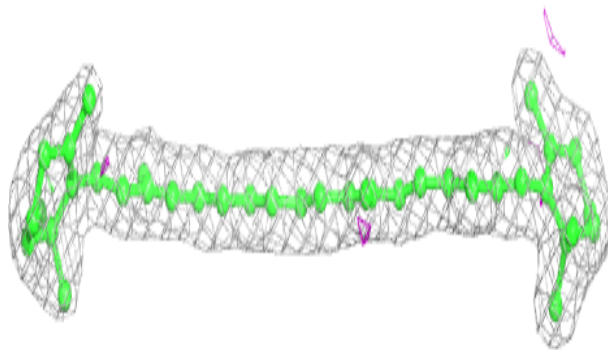
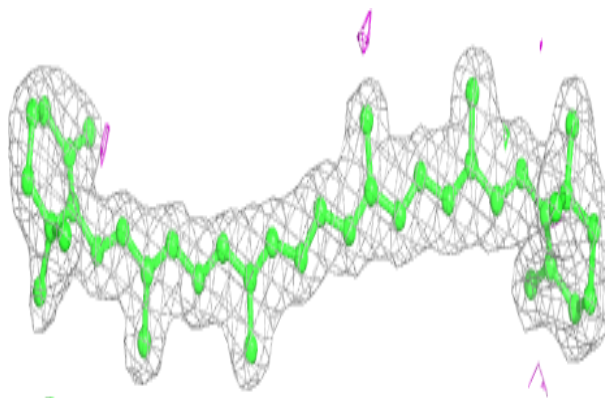


**Electron density around BCR D 404:**

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

**Electron density around BCR b 621:**

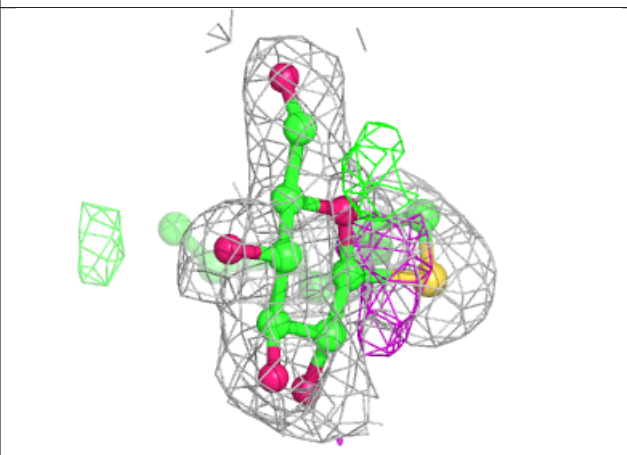
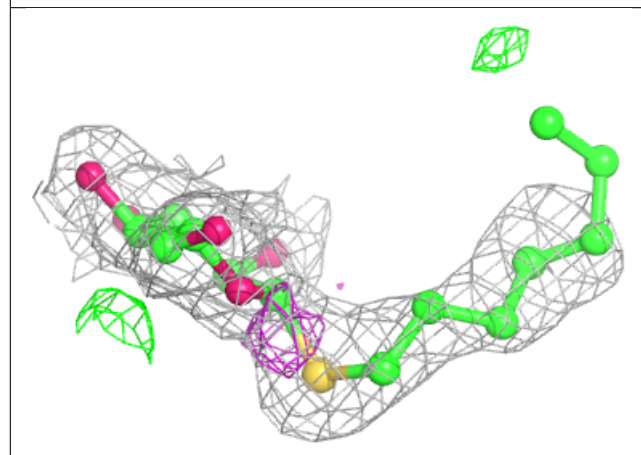
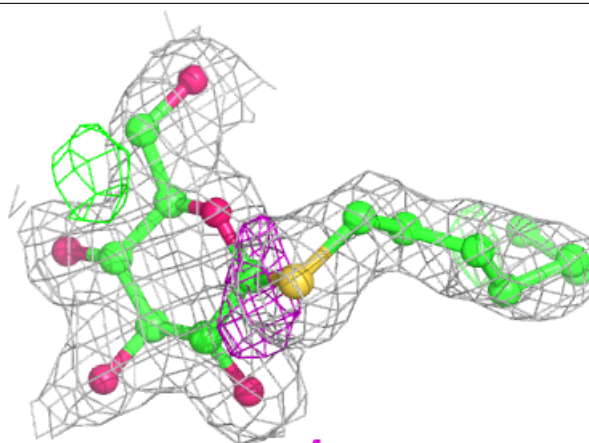
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





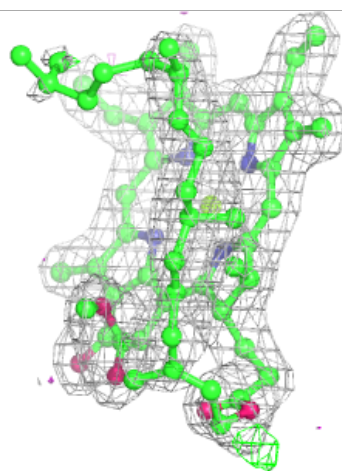
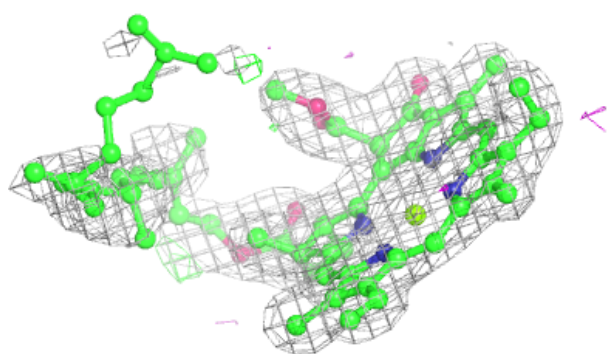
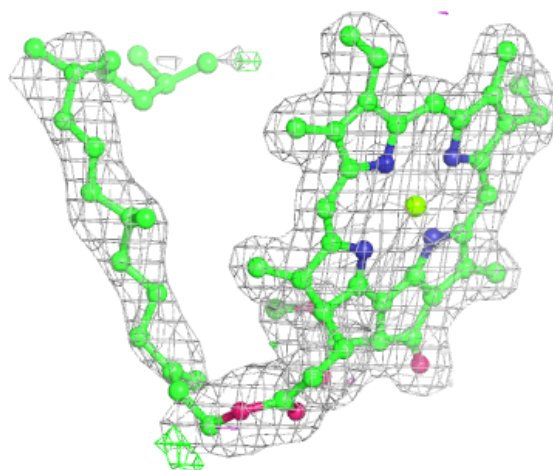
**Electron density around HTG b 626:**

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



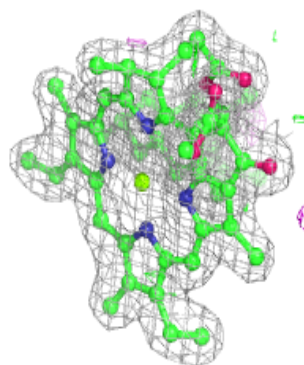
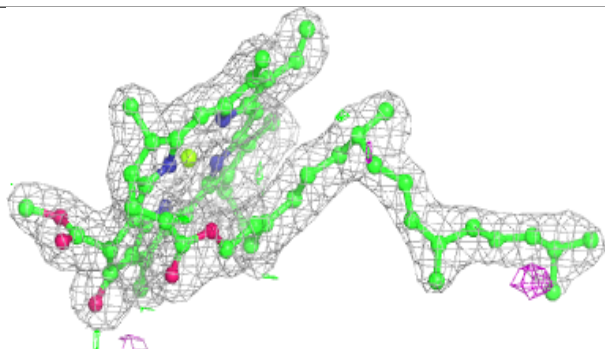
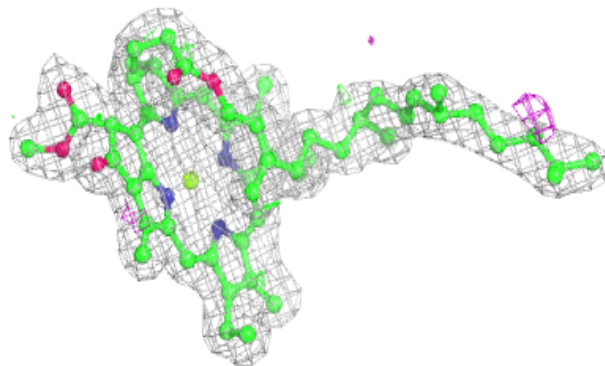
**Electron density around CLA b 619:**

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

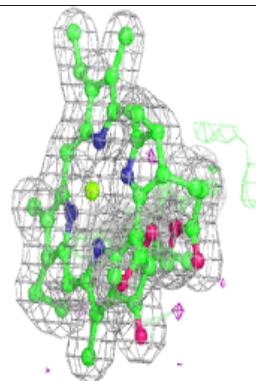
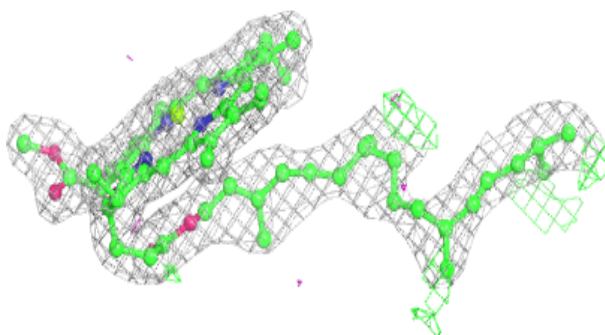
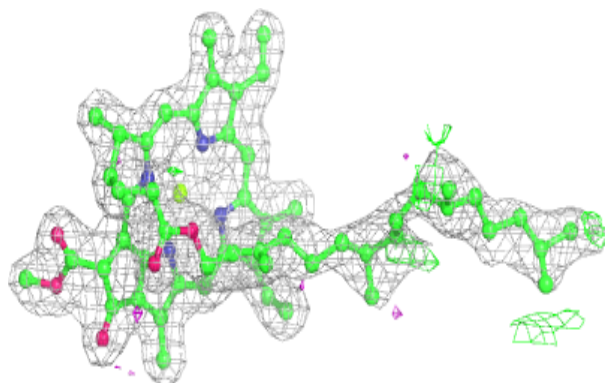


**Electron density around CLA C 505:**

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

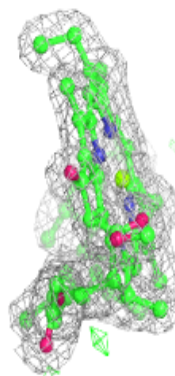
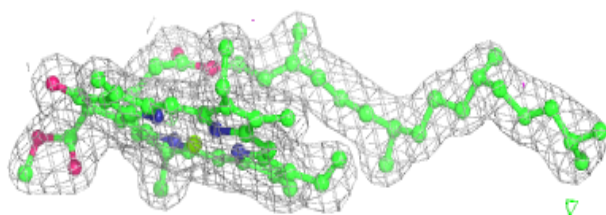
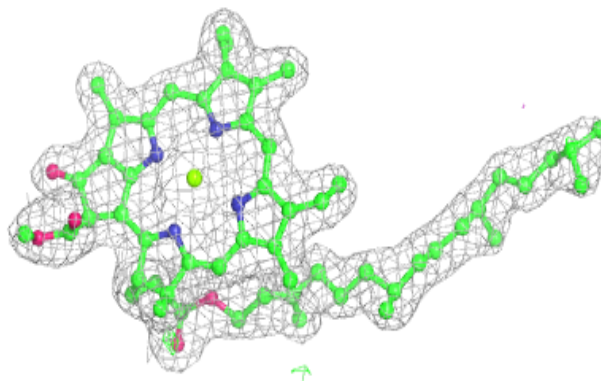
**Electron density around CLA B 615:**

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

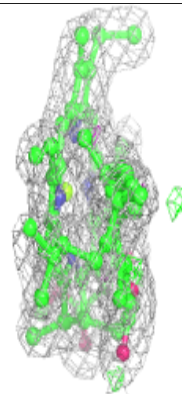
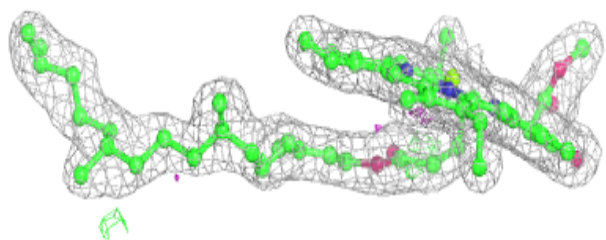
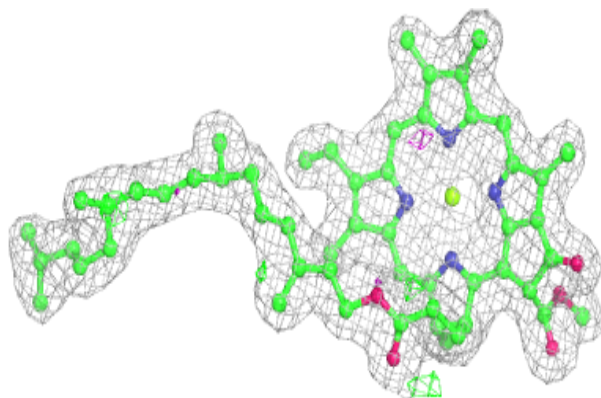


**Electron density around CLA C 501:**

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

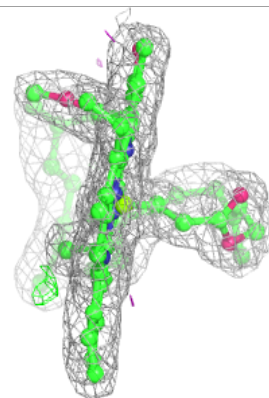
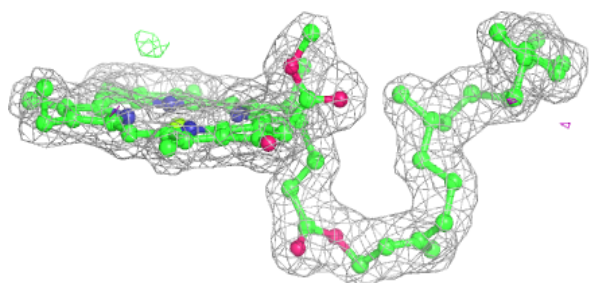
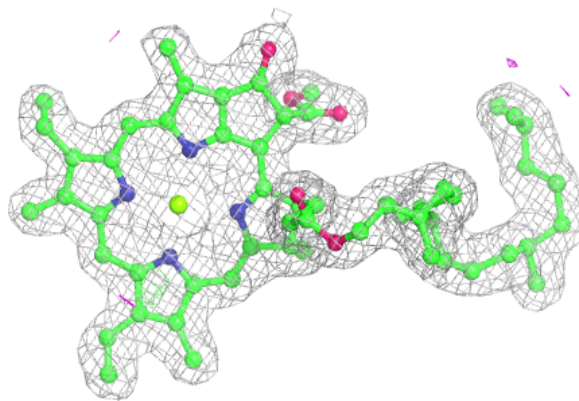
**Electron density around CLA b 606:**

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

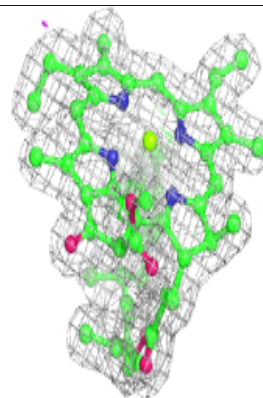
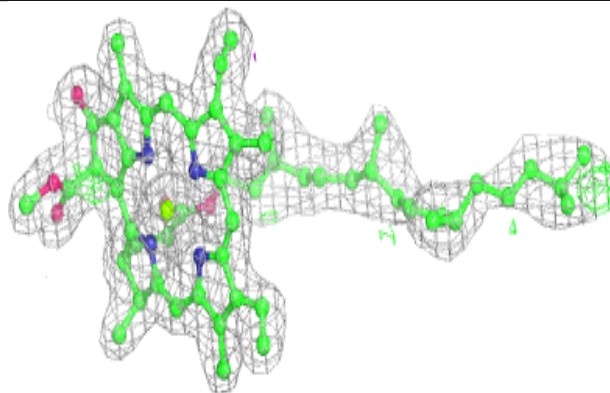
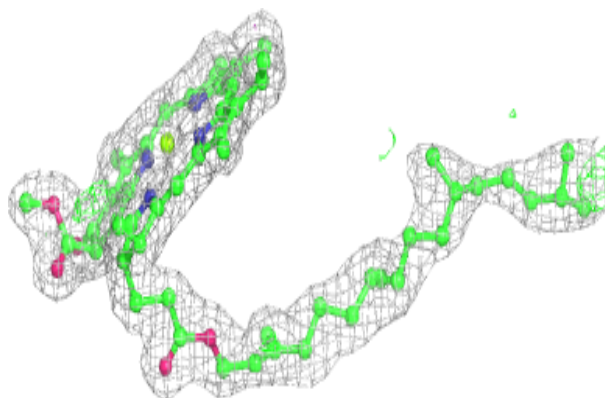


**Electron density around CLA b 615:**

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

**Electron density around CLA C 504:**

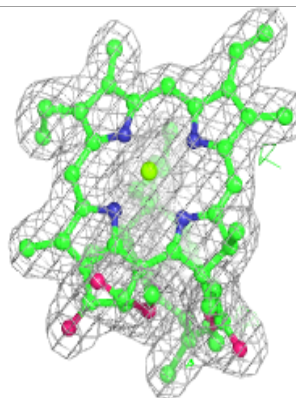
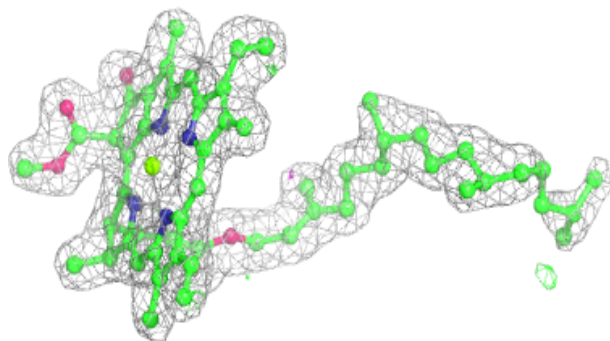
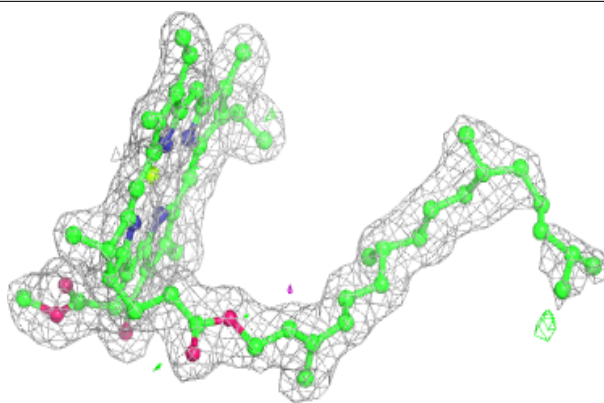
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



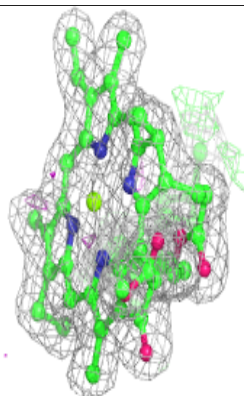
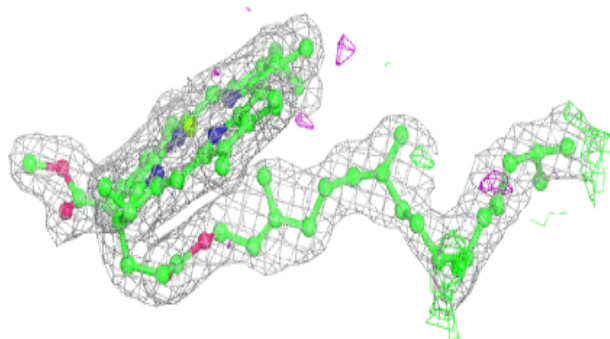
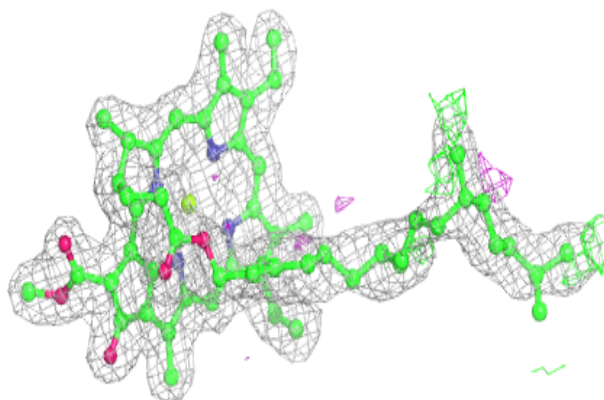


**Electron density around CLA C 508:**

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

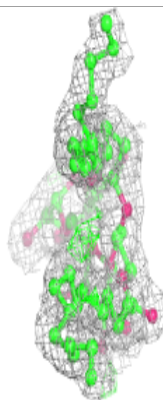
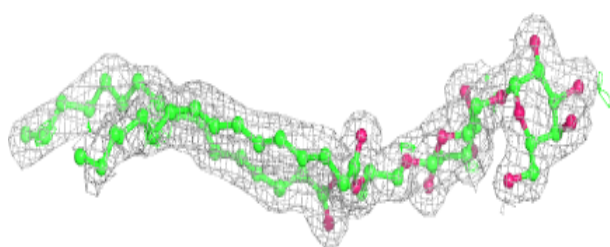
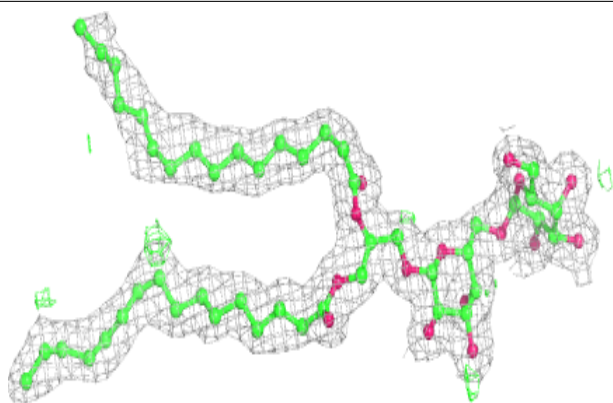
**Electron density around CLA b 617:**

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

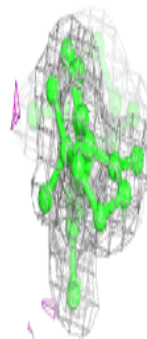
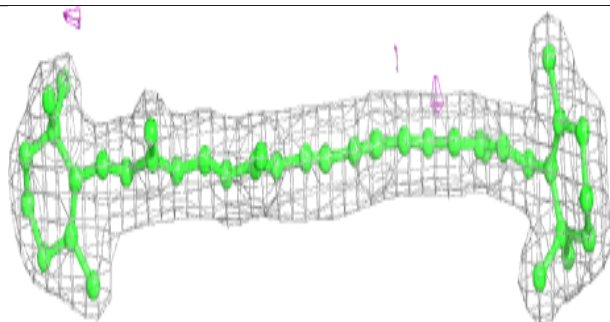
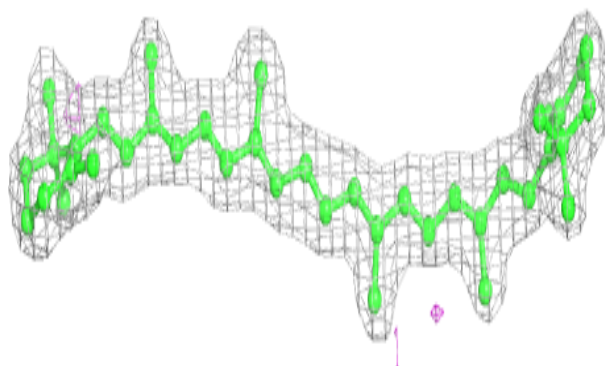


**Electron density around DGD C 518:**

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

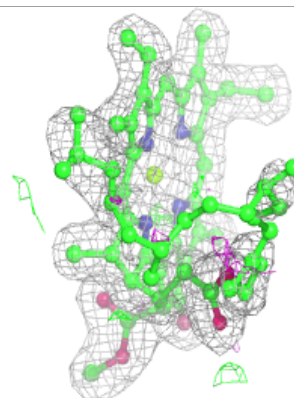
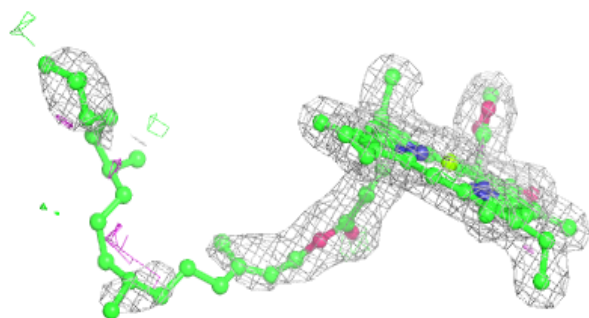
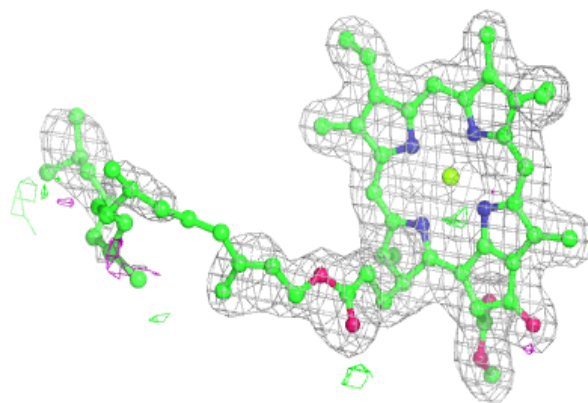
**Electron density around BCR C 515:**

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

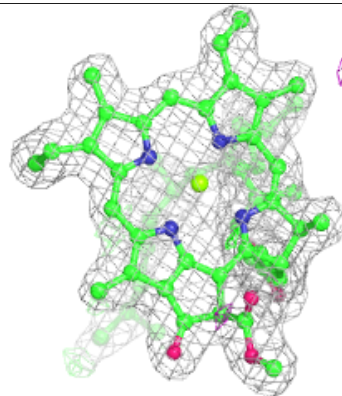
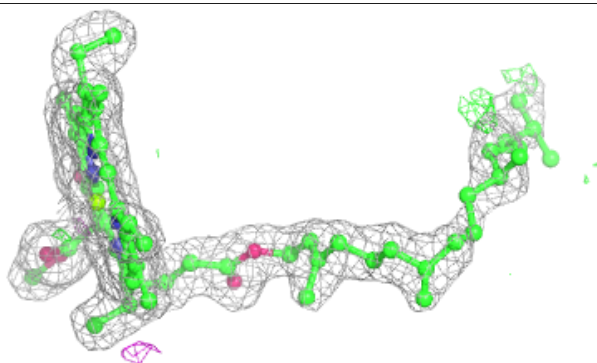
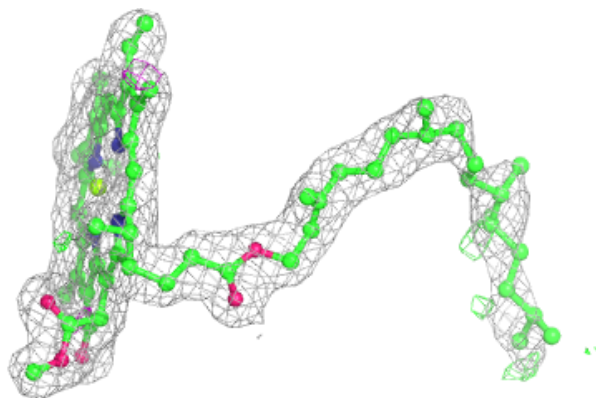


**Electron density around CLA A 410:**

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

**Electron density around CLA D 403:**

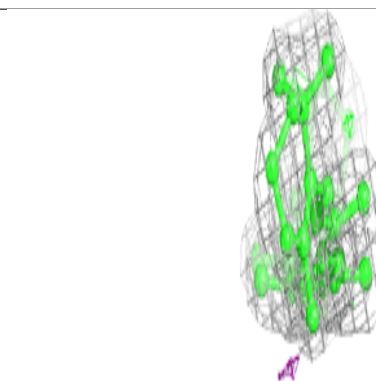
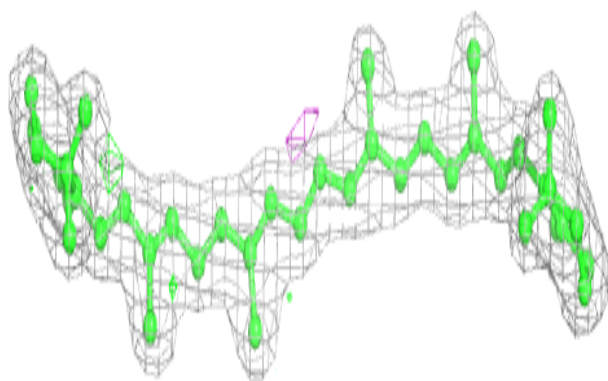
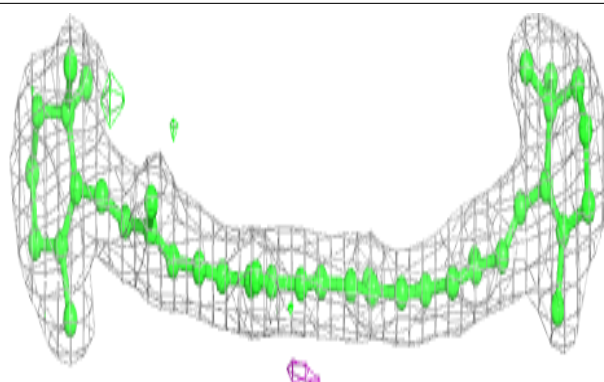
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



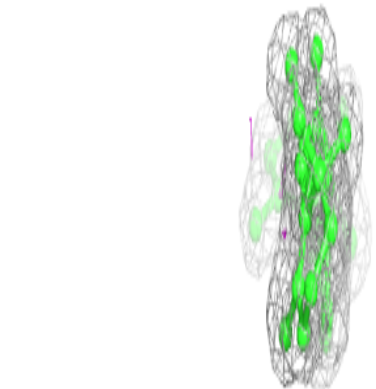
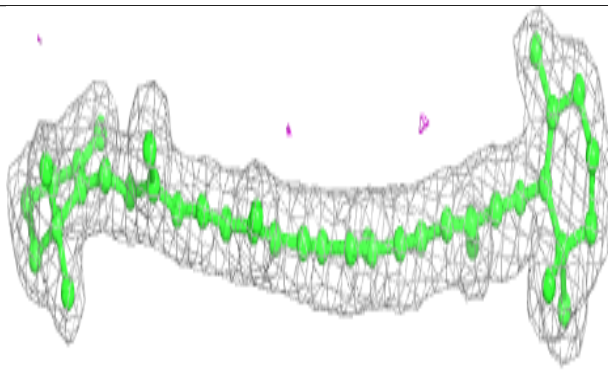
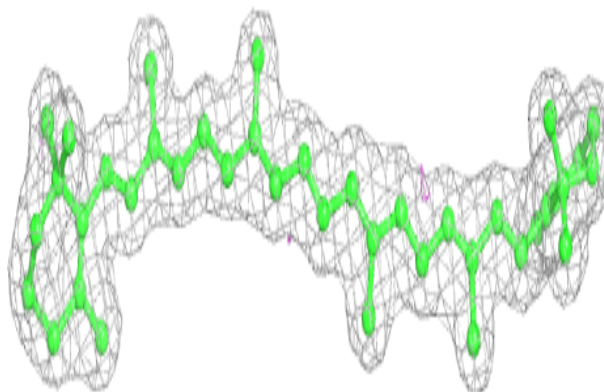


**Electron density around BCR K 102:**

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

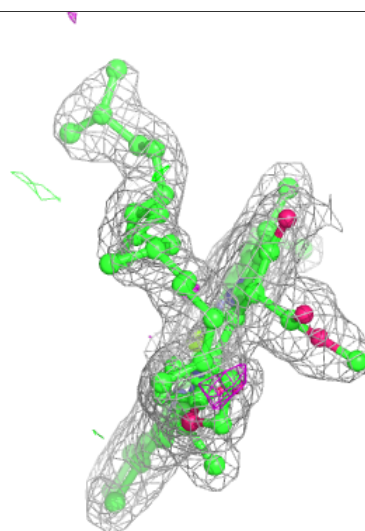
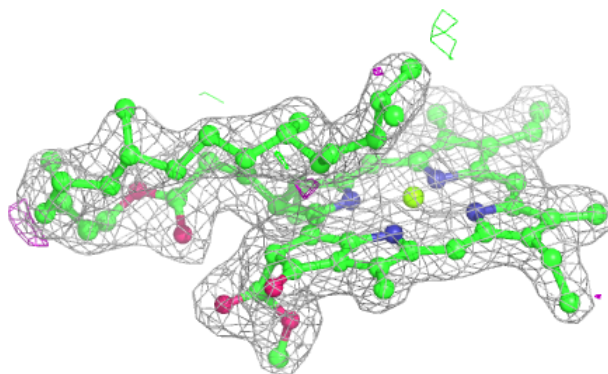
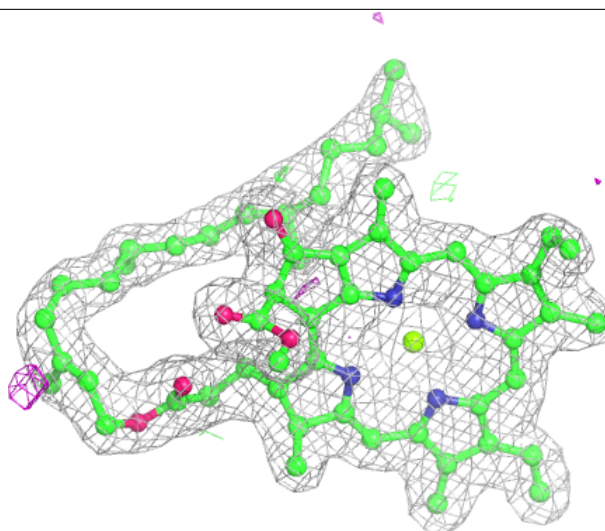
**Electron density around BCR B 618:**

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



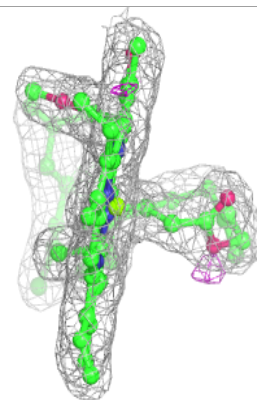
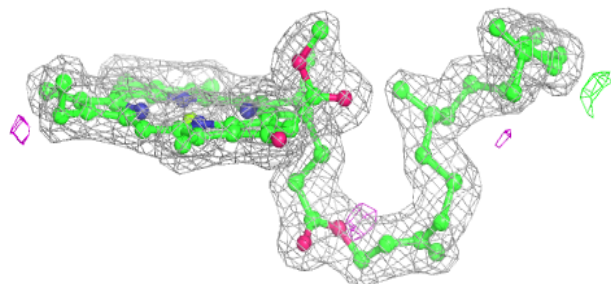
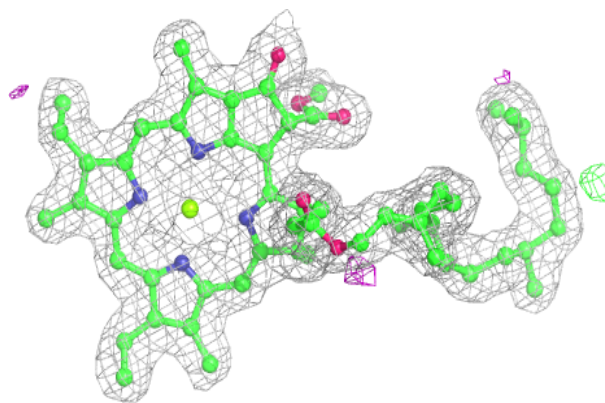
**Electron density around CLA c 910:**

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

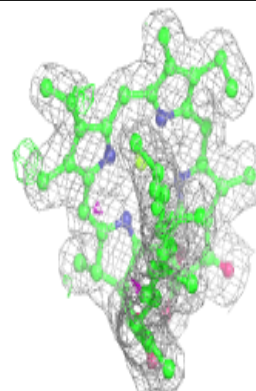
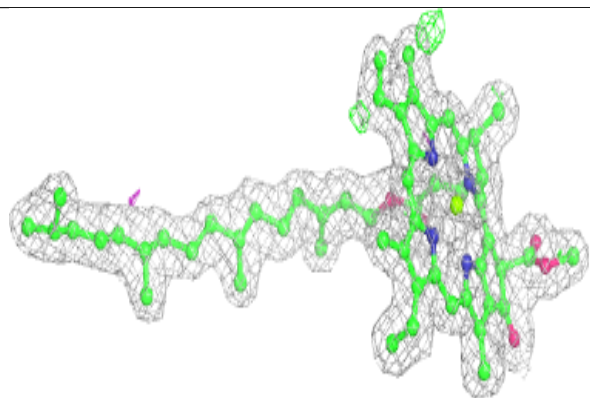
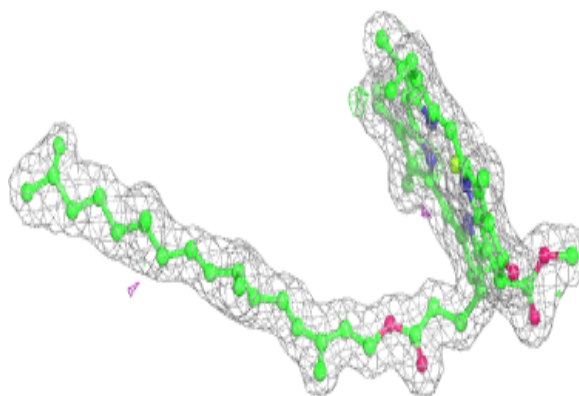


**Electron density around CLA B 613:**

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

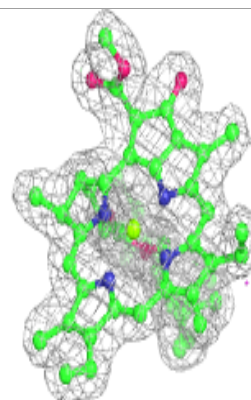
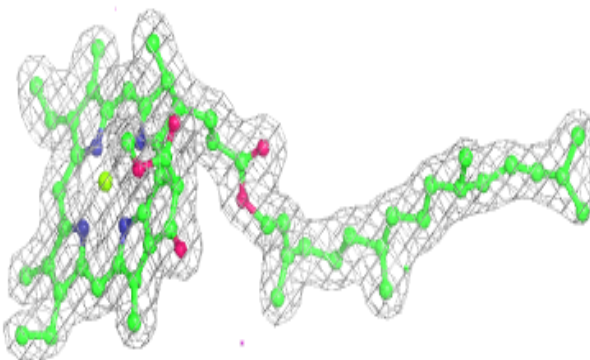
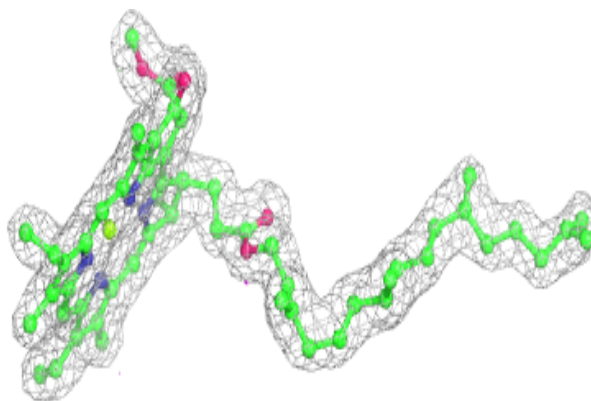
**Electron density around CLA B 608:**

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

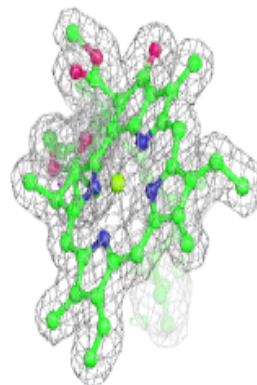
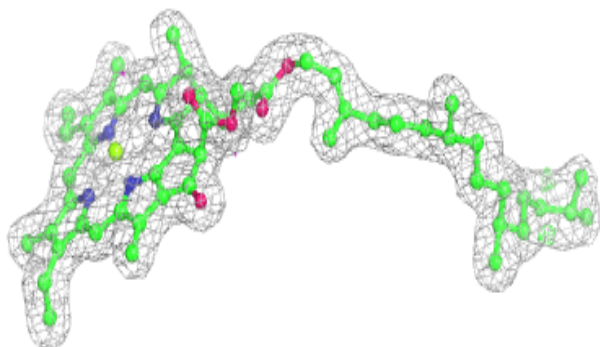
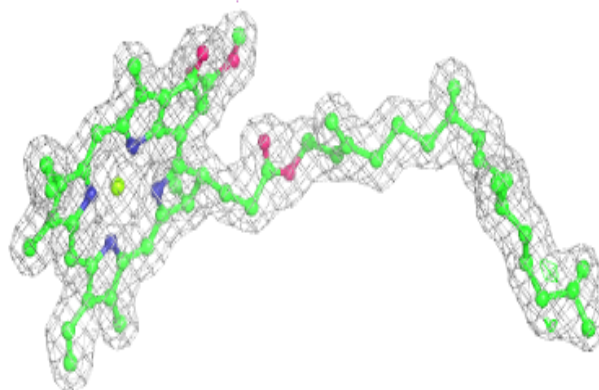


**Electron density around CLA C 502:**

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

**Electron density around CLA A 405:**

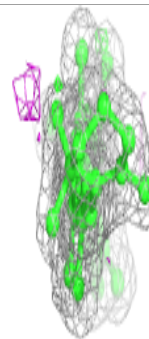
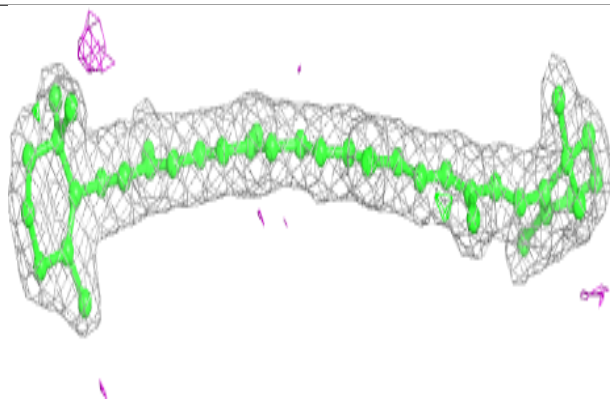
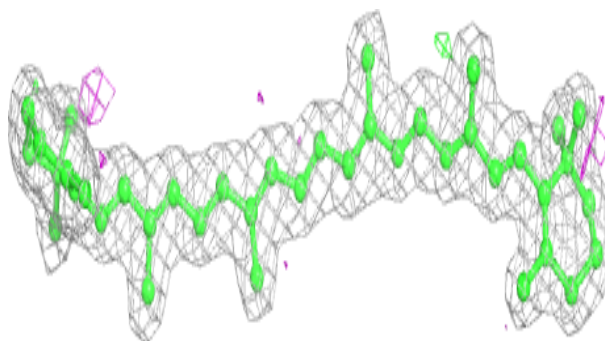
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



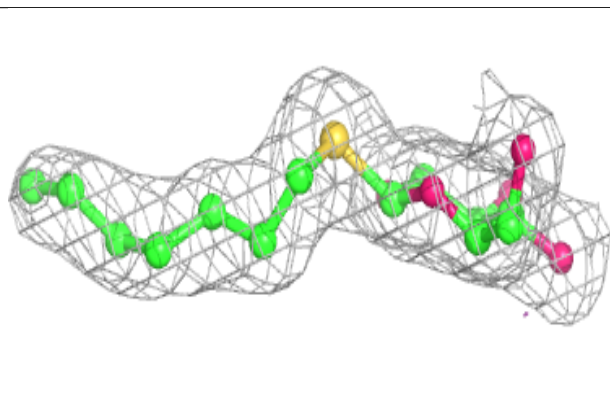
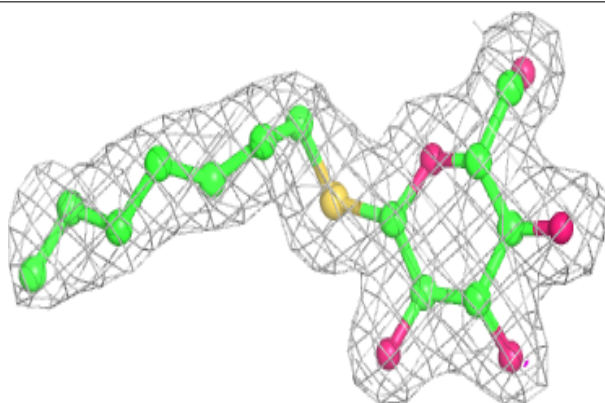


**Electron density around BCR b 620:**

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

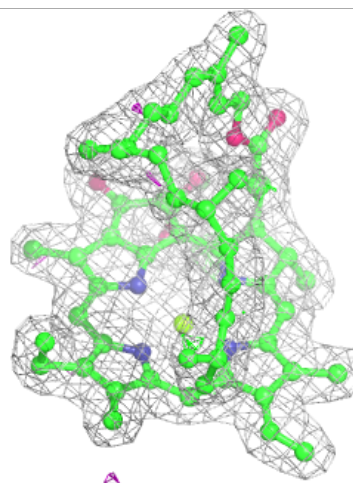
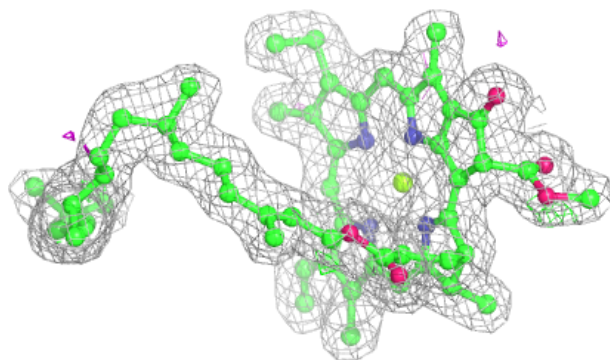
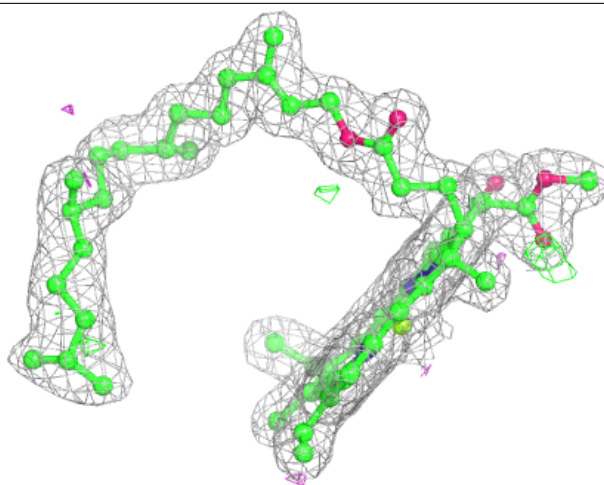
**Electron density around HTG O 303:**

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



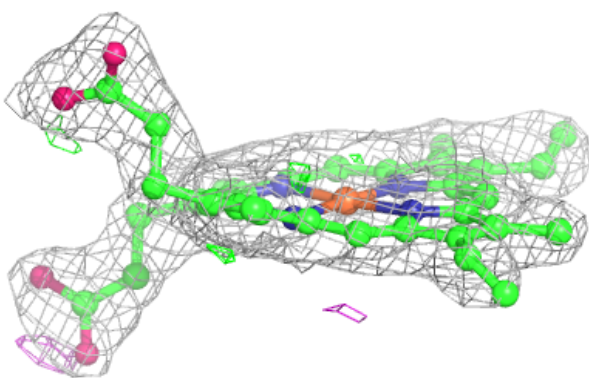
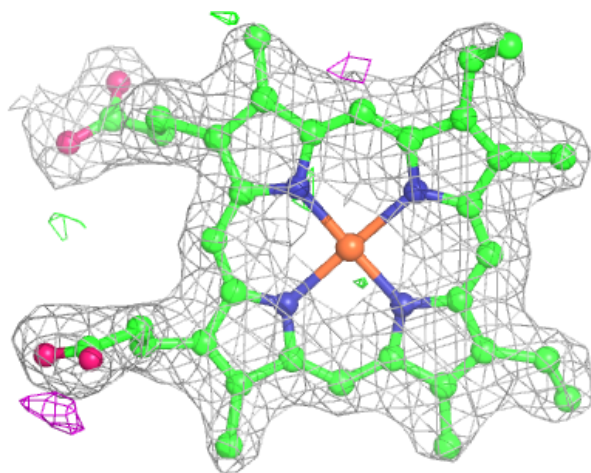
**Electron density around CLA b 614:**

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



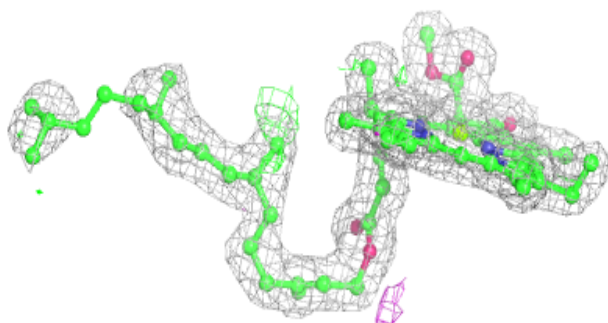
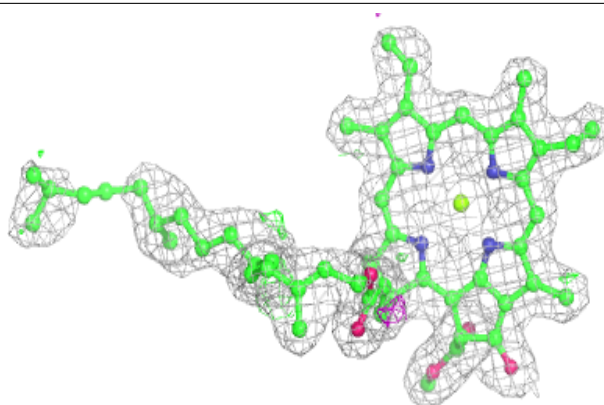
**Electron density around HEM F 101:**

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

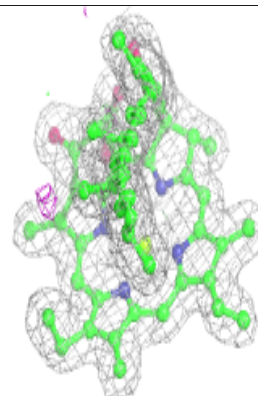
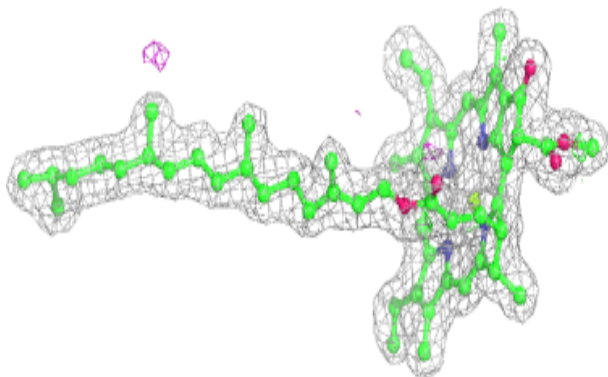
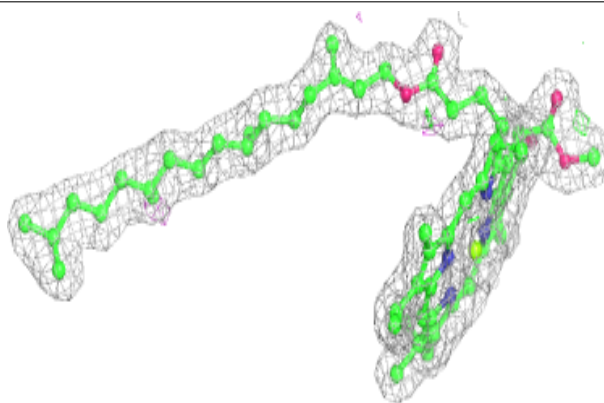


**Electron density around CLA A 407:**

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

**Electron density around CLA b 610:**

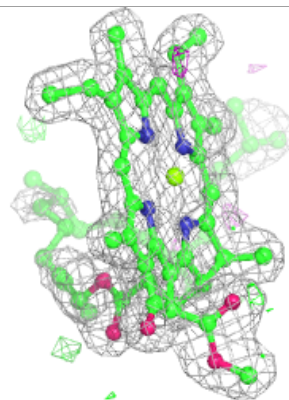
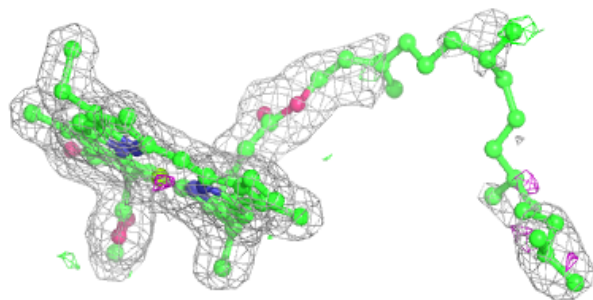
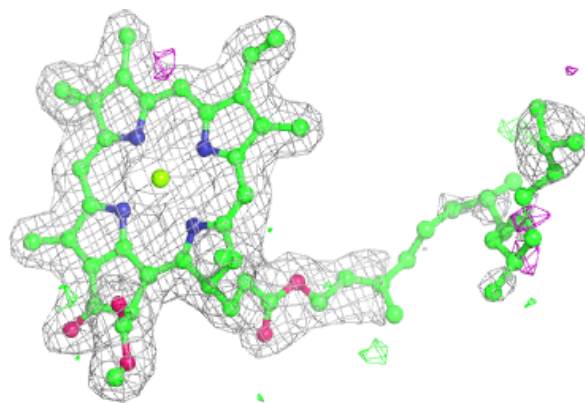
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



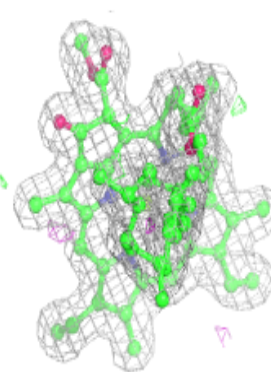
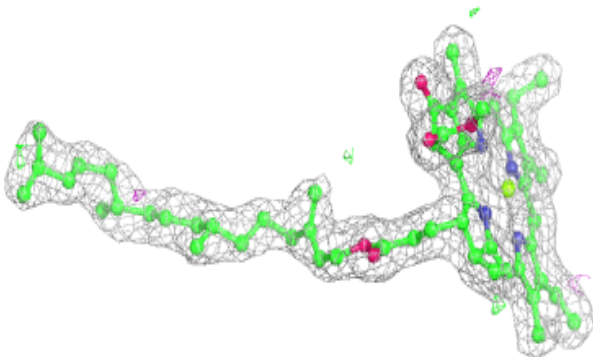
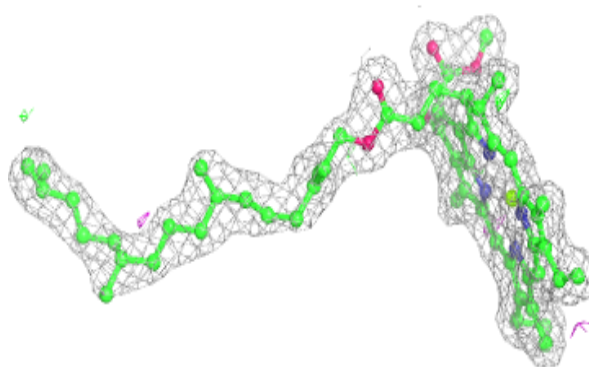


**Electron density around CLA a 414:**

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

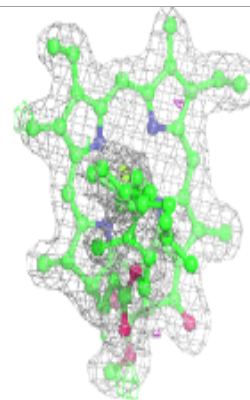
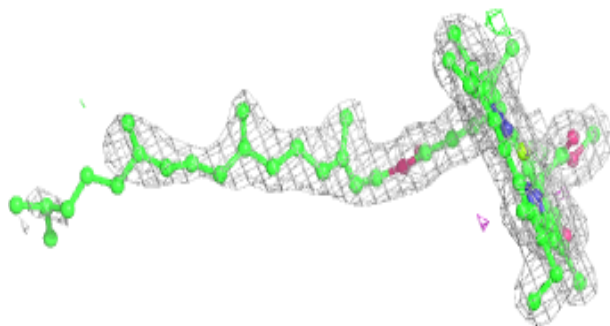
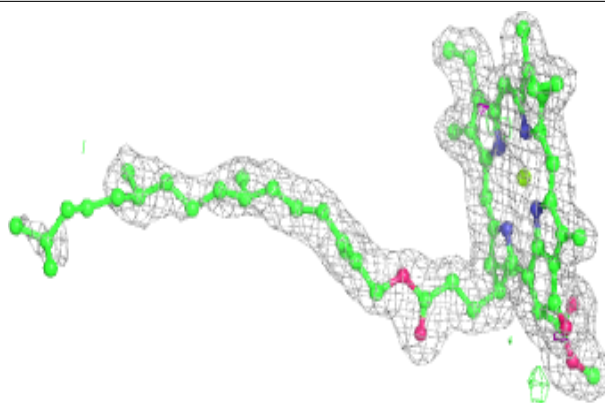
**Electron density around CLA B 605:**

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

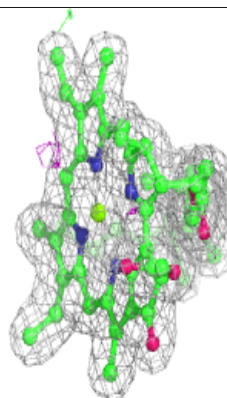
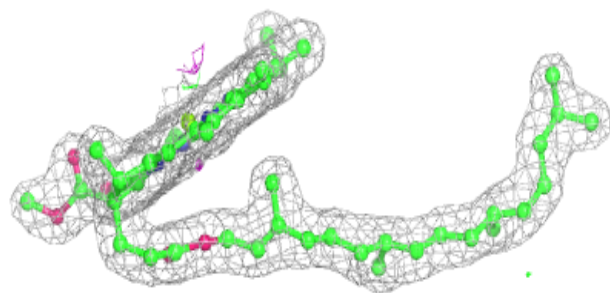
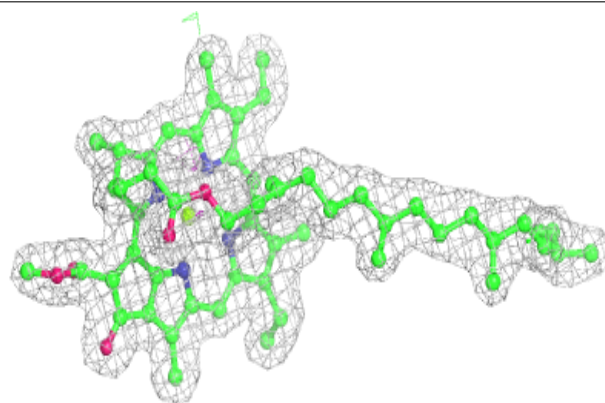


**Electron density around CLA d 403:**

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

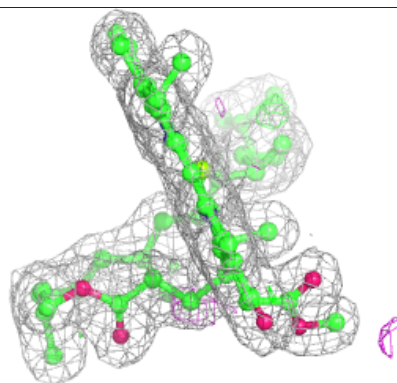
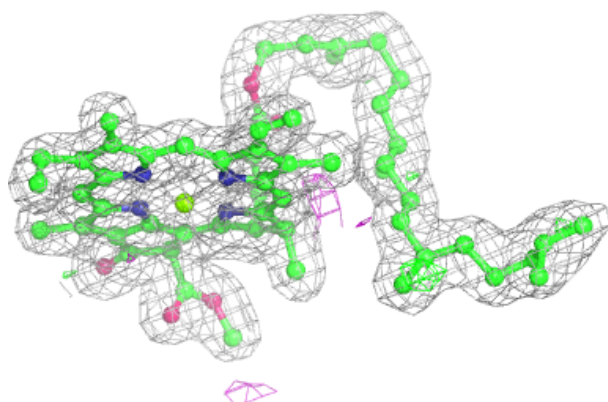
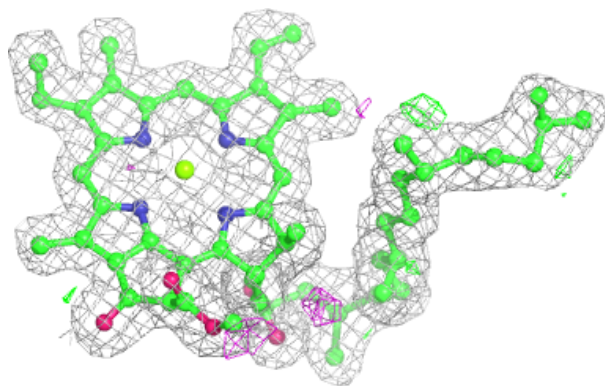
**Electron density around CLA B 609:**

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

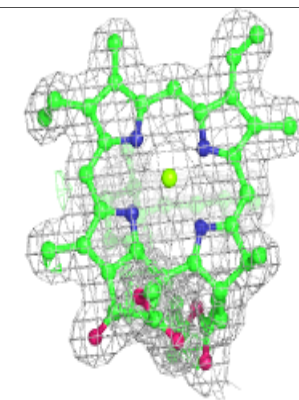
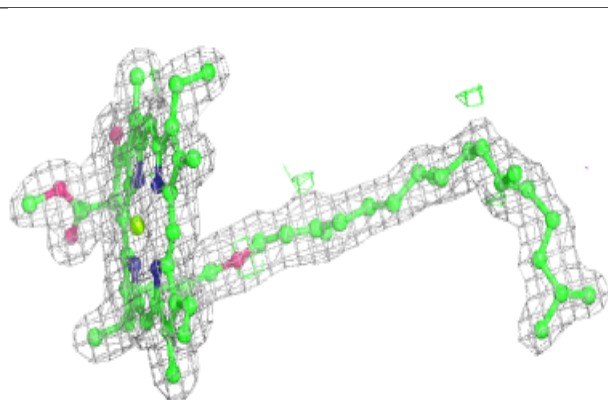
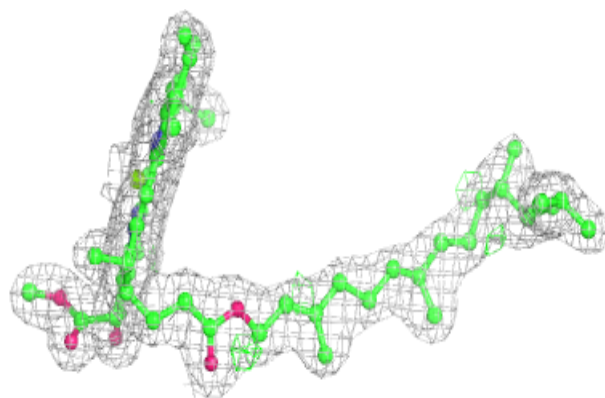


**Electron density around CLA A 406:**

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

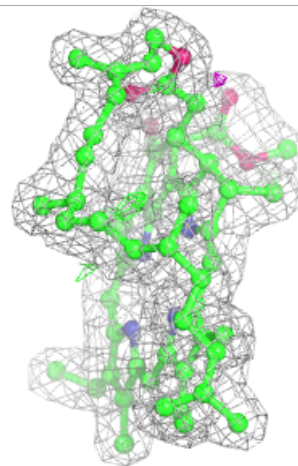
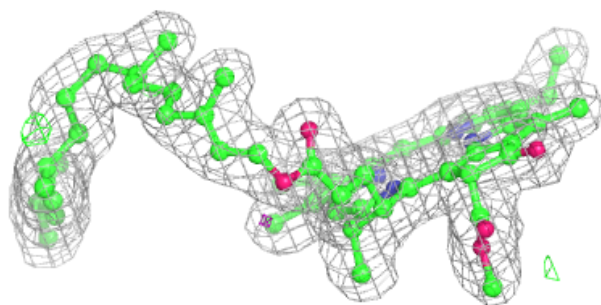
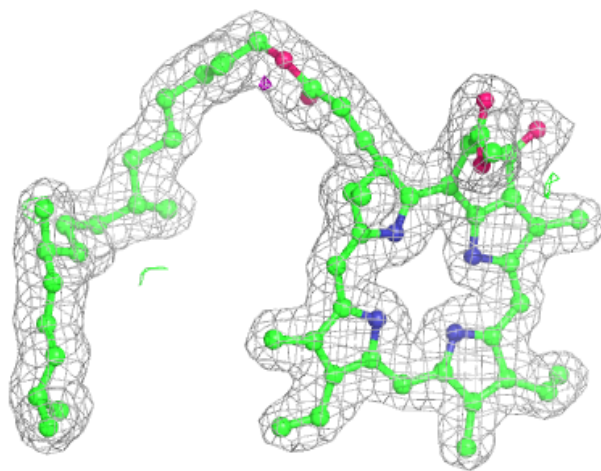
**Electron density around CLA B 606:**

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



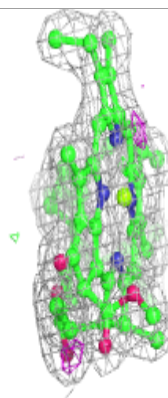
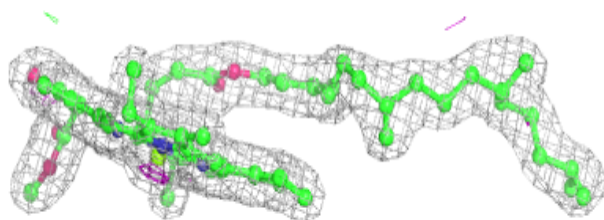
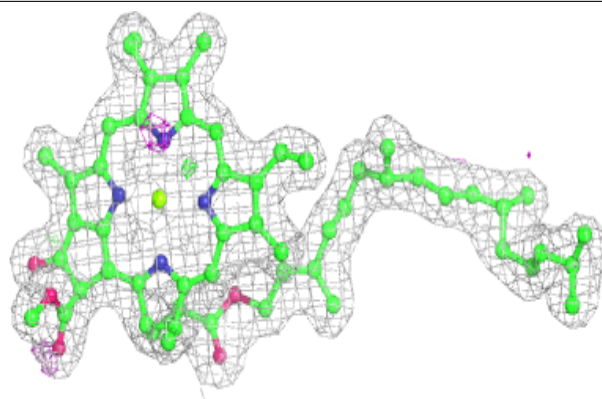
**Electron density around PHO a 413:**

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



**Electron density around CLA B 604:**

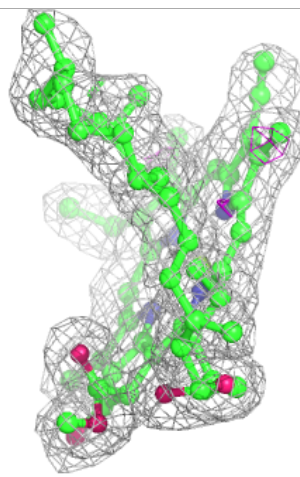
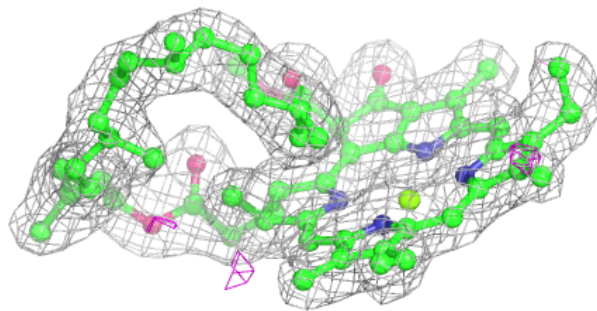
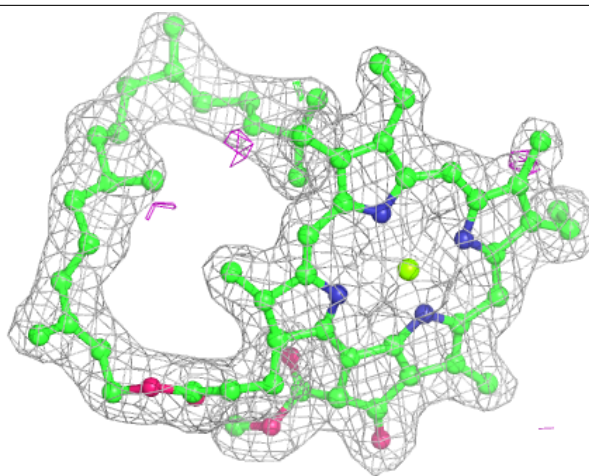
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





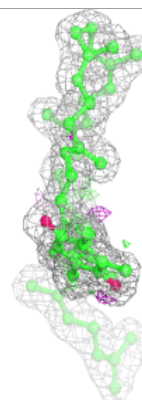
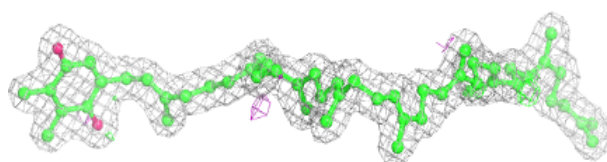
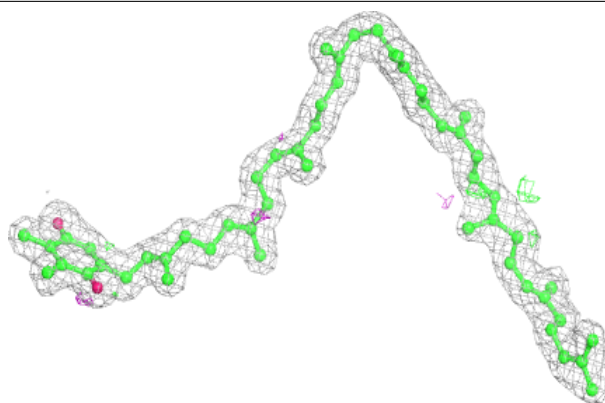
**Electron density around CLA B 616:**

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

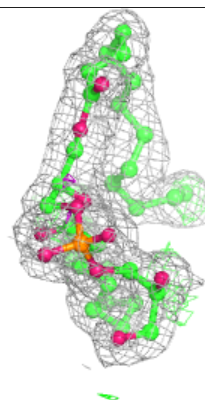
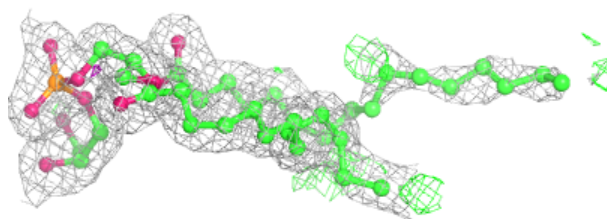
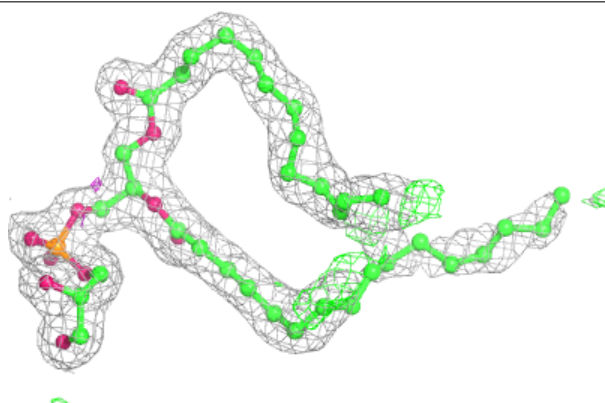


**Electron density around PL9 D 405:**

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

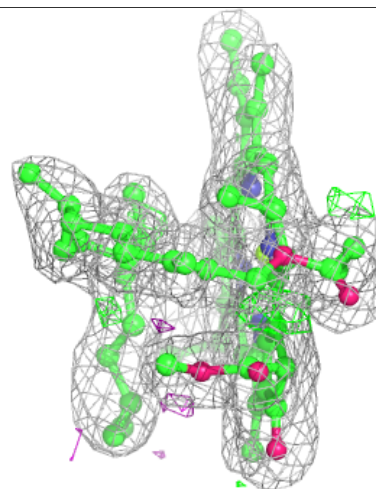
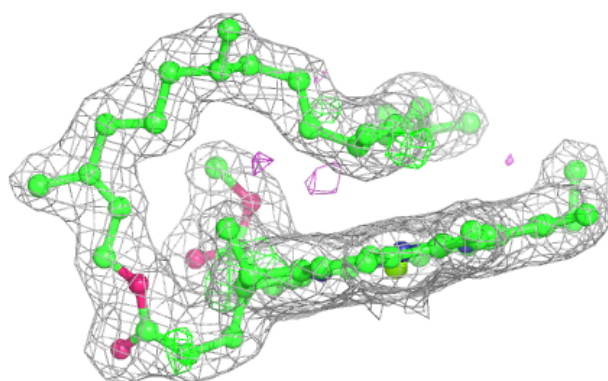
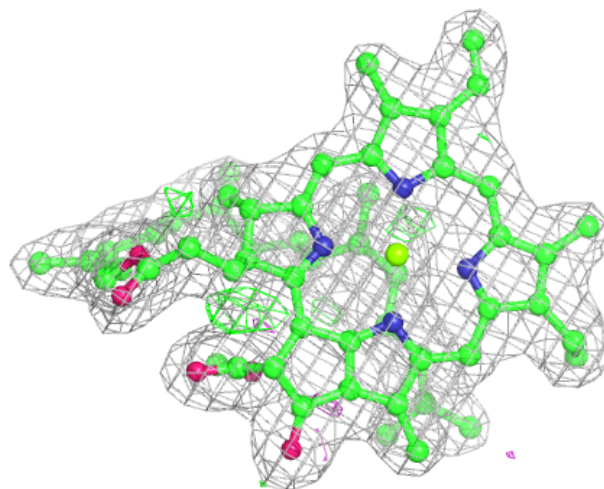
**Electron density around LHG D 410:**

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



**Electron density around CLA c 911:**

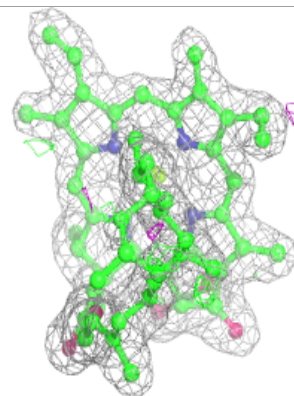
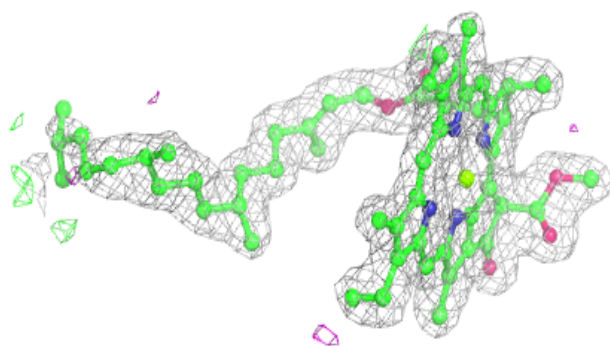
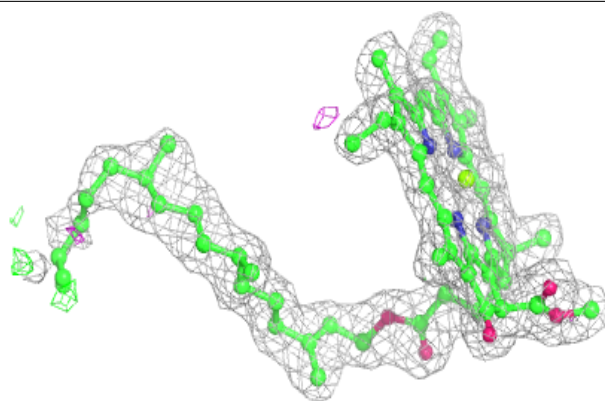
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





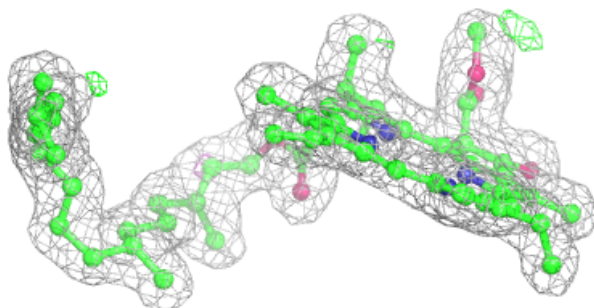
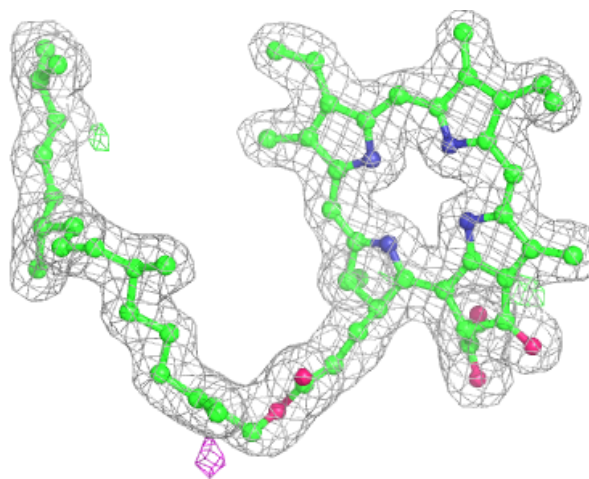
**Electron density around CLA c 909:**

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



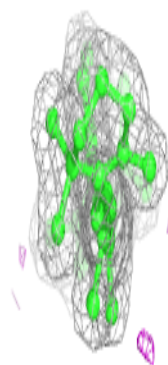
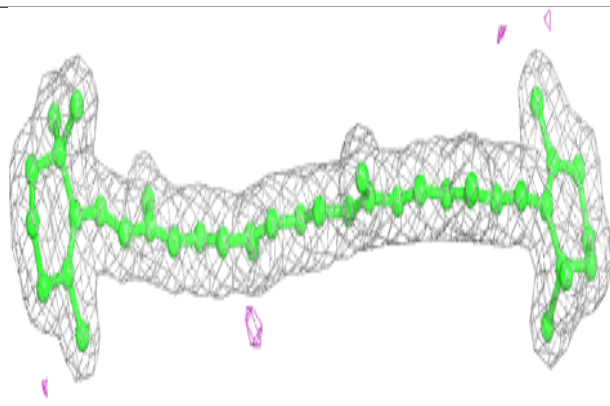
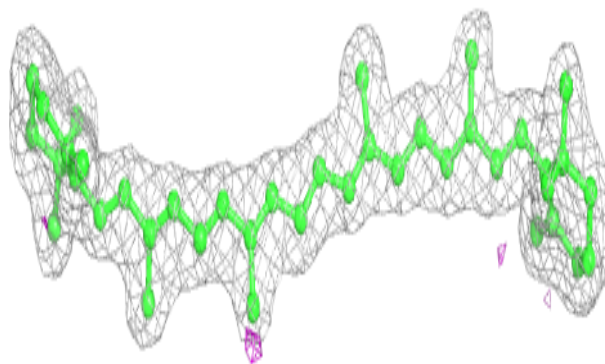
**Electron density around PHO A 409:**

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



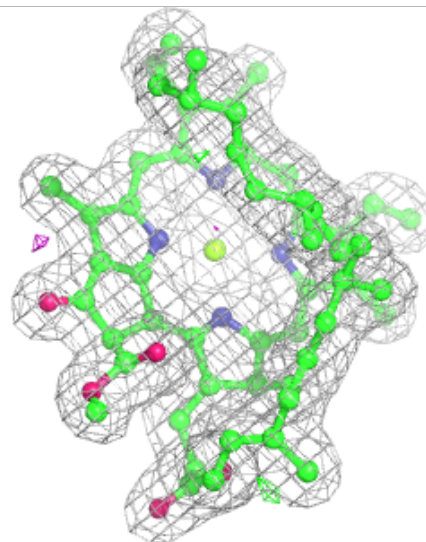
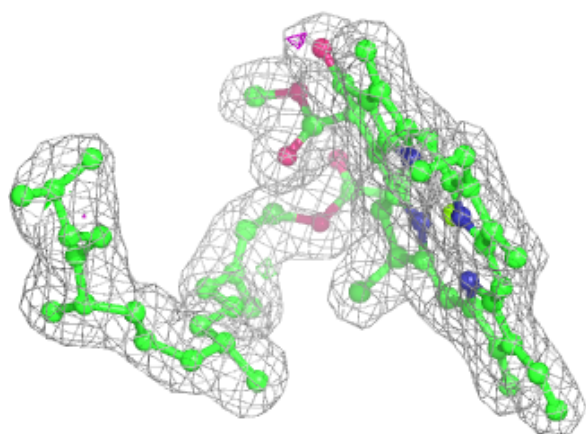
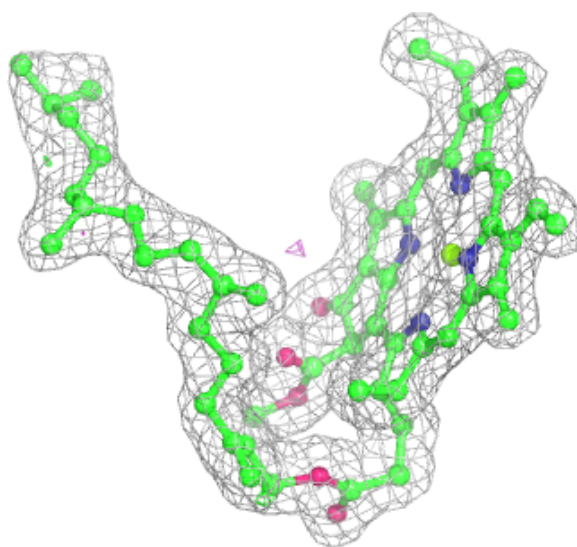
**Electron density around BCR A 411:**

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



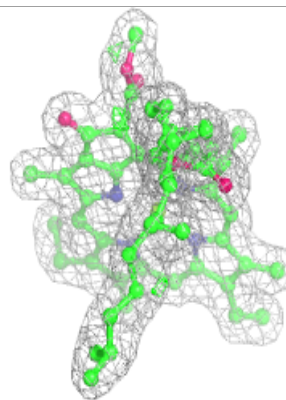
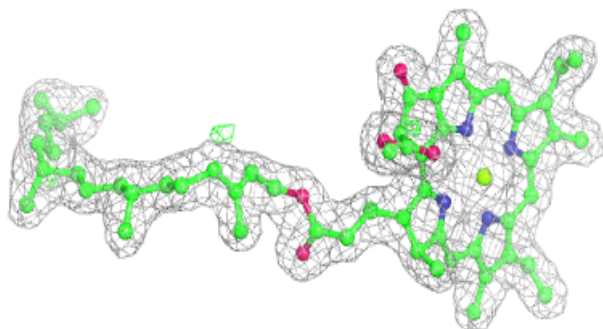
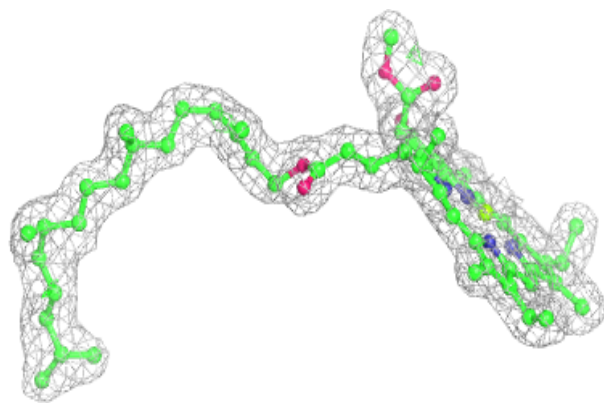
**Electron density around CLA B 614:**

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



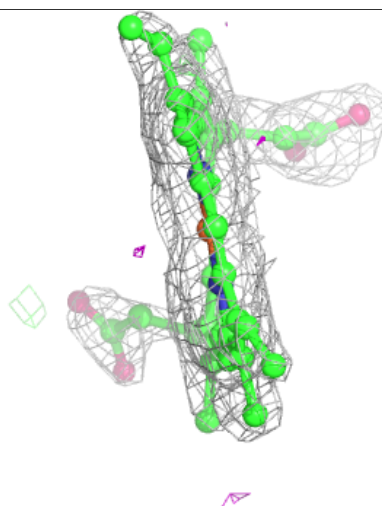
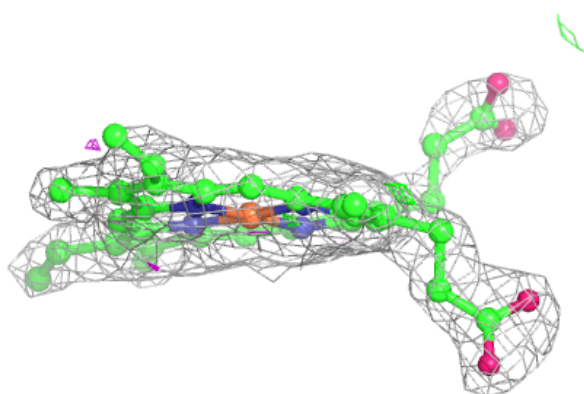
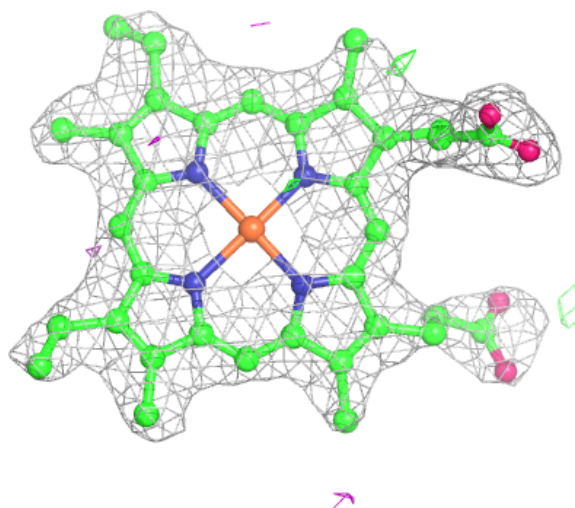
**Electron density around CLA d 402:**

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



**Electron density around HEM f 101:**

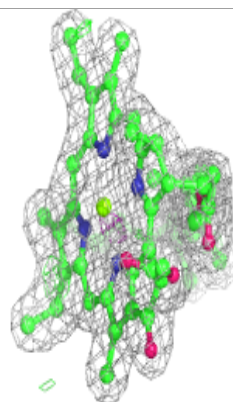
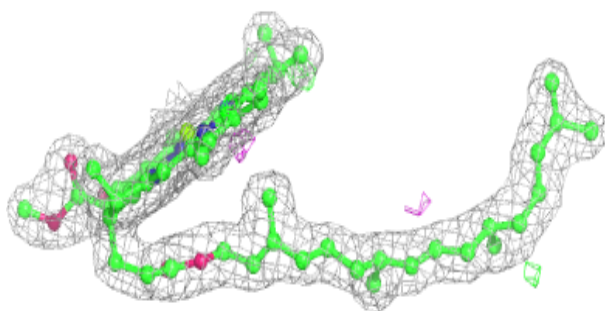
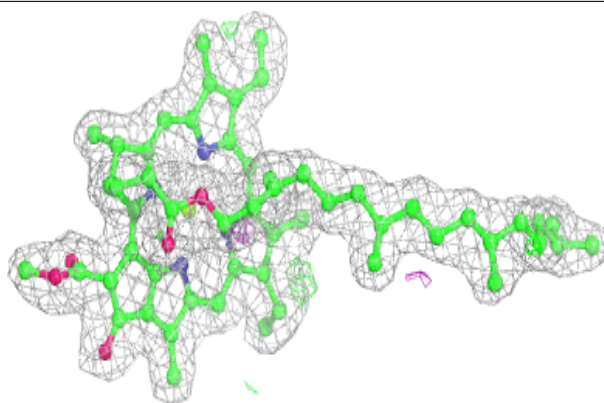
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



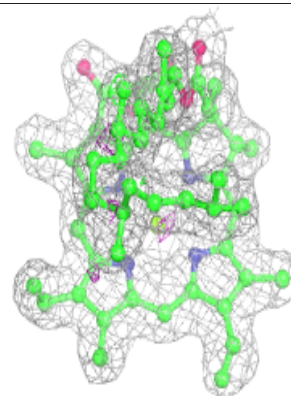
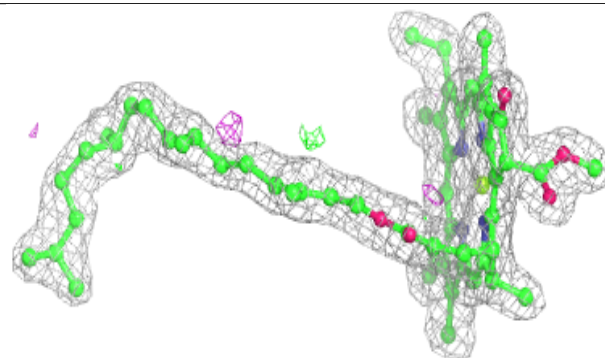
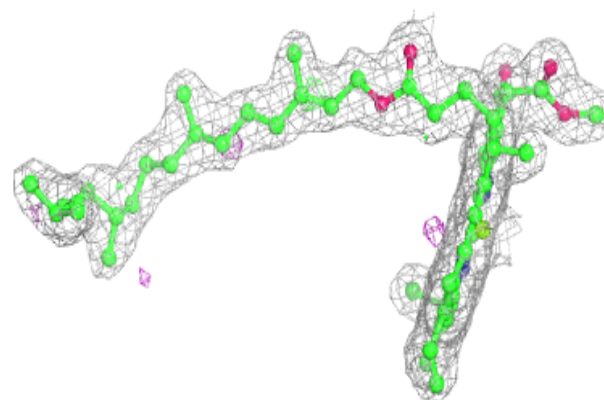


**Electron density around CLA b 611:**

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

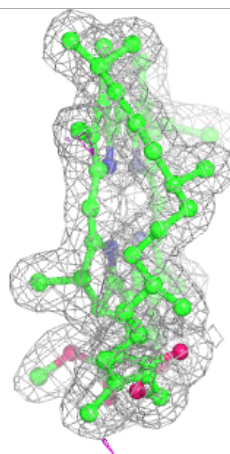
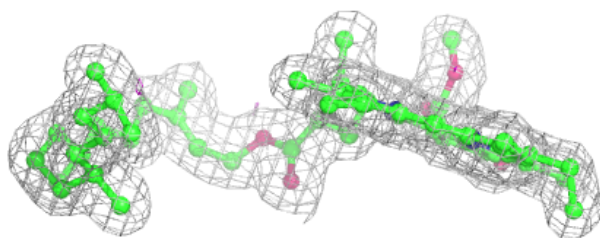
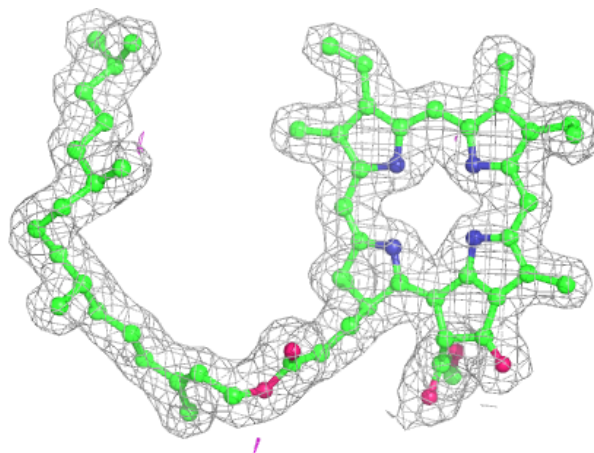
**Electron density around CLA b 608:**

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



**Electron density around PHO A 408:**

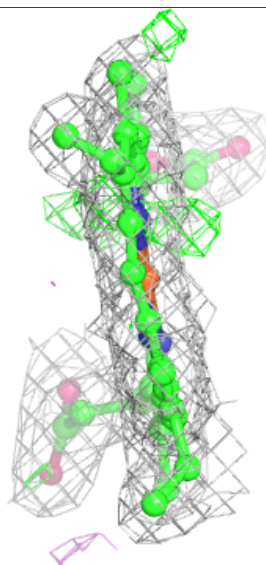
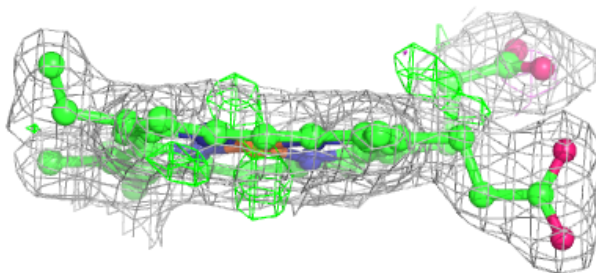
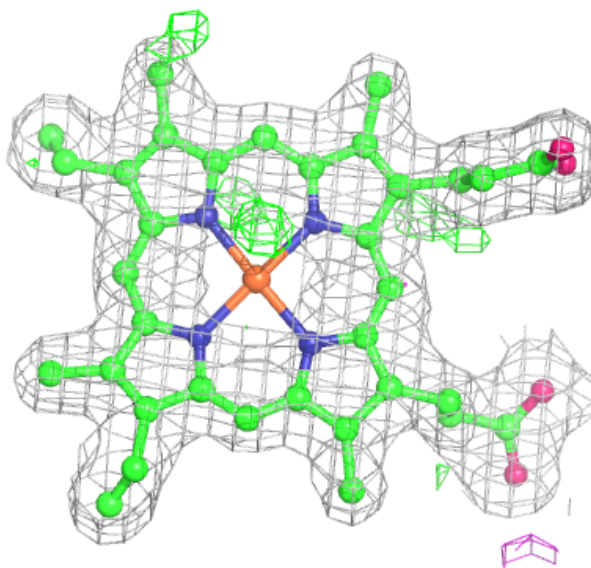
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





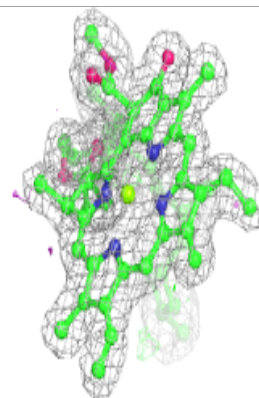
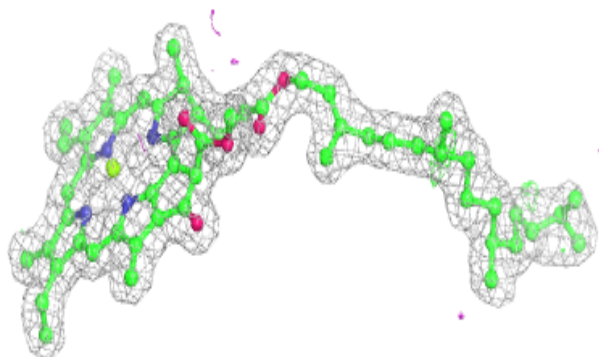
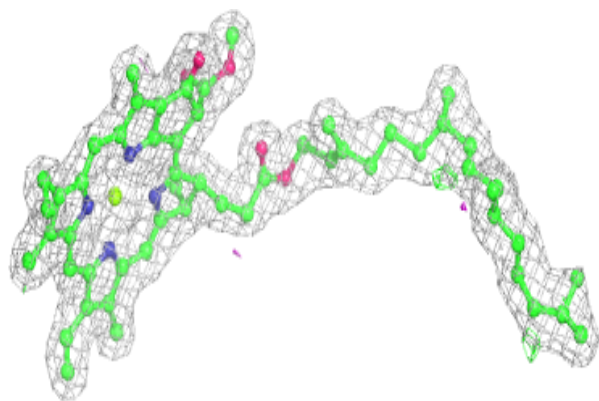
**Electron density around HEM v 201:**

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

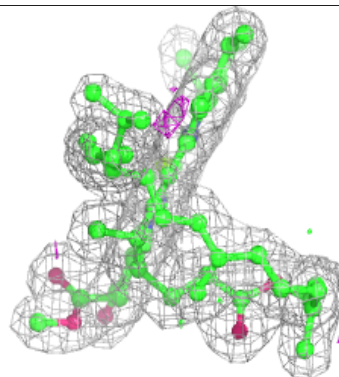
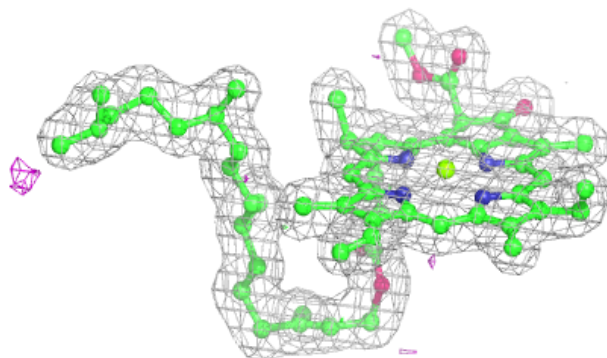
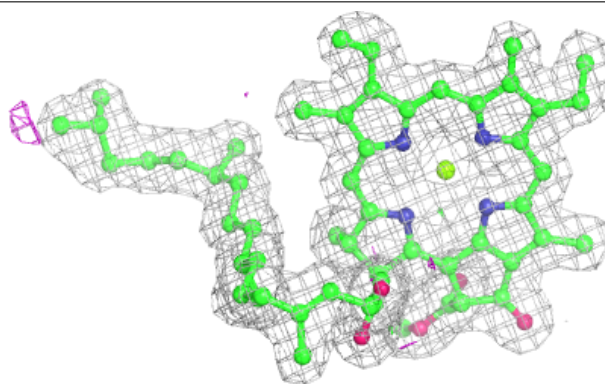


**Electron density around CLA a 409:**

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

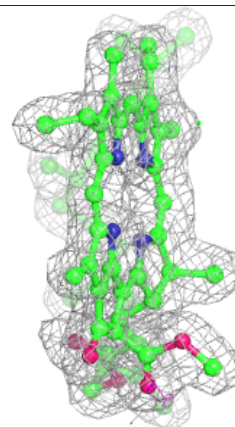
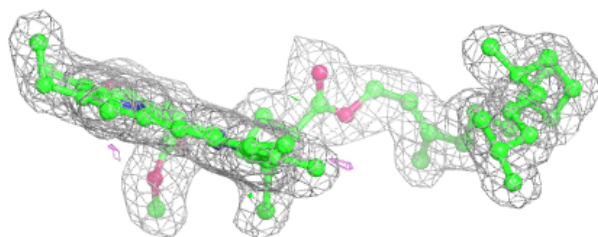
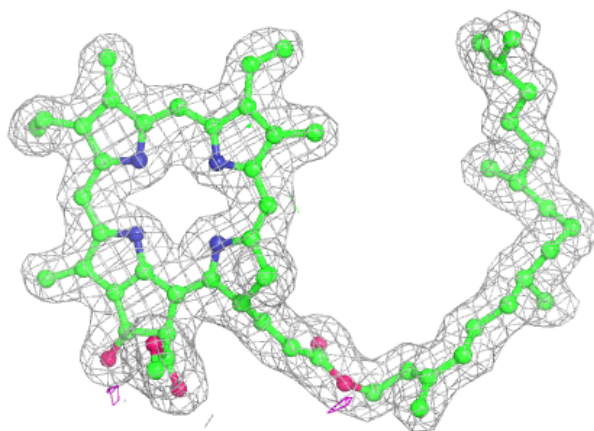
**Electron density around CLA a 410:**

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



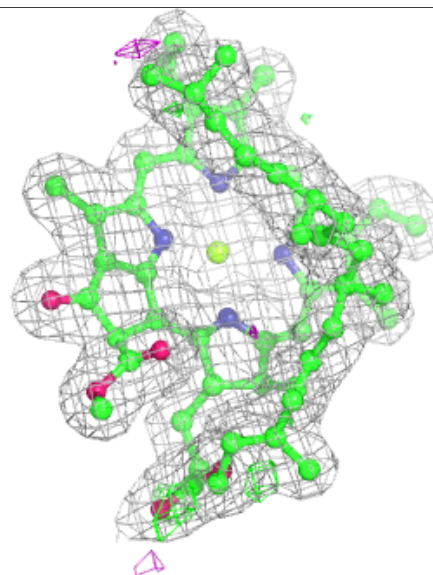
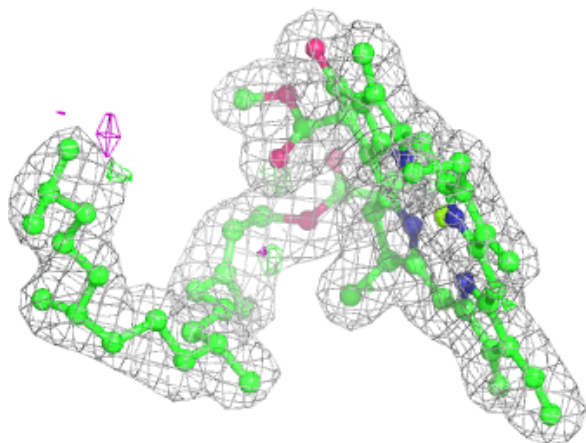
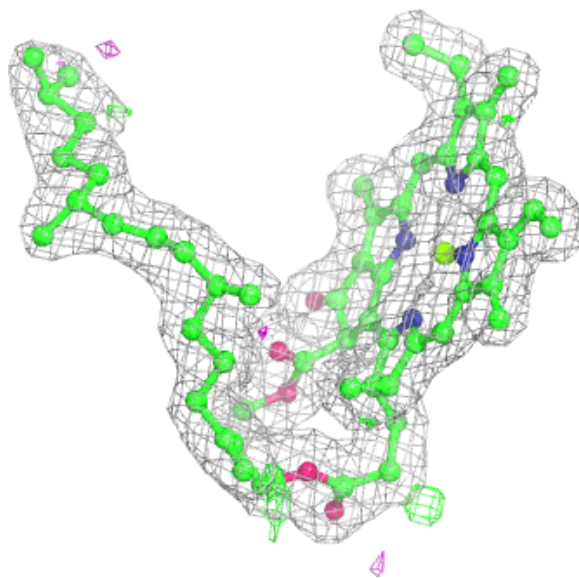
**Electron density around PHO a 412:**

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



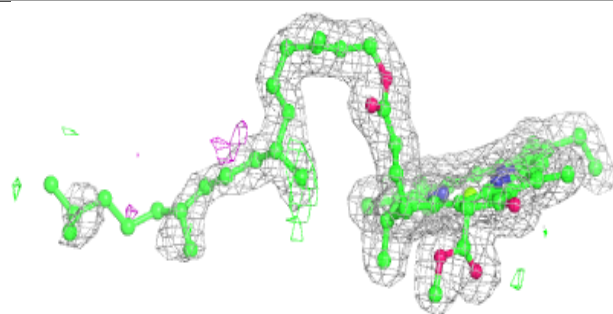
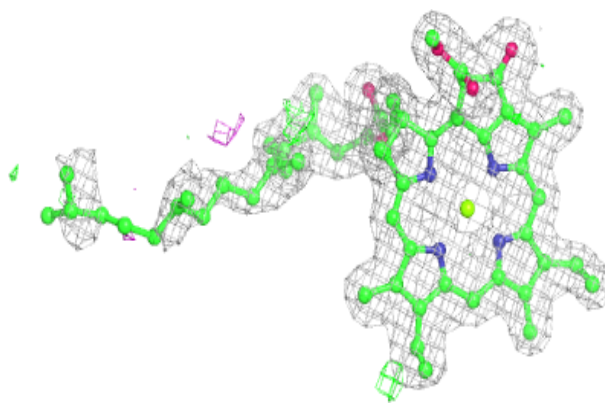
**Electron density around CLA b 616:**

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

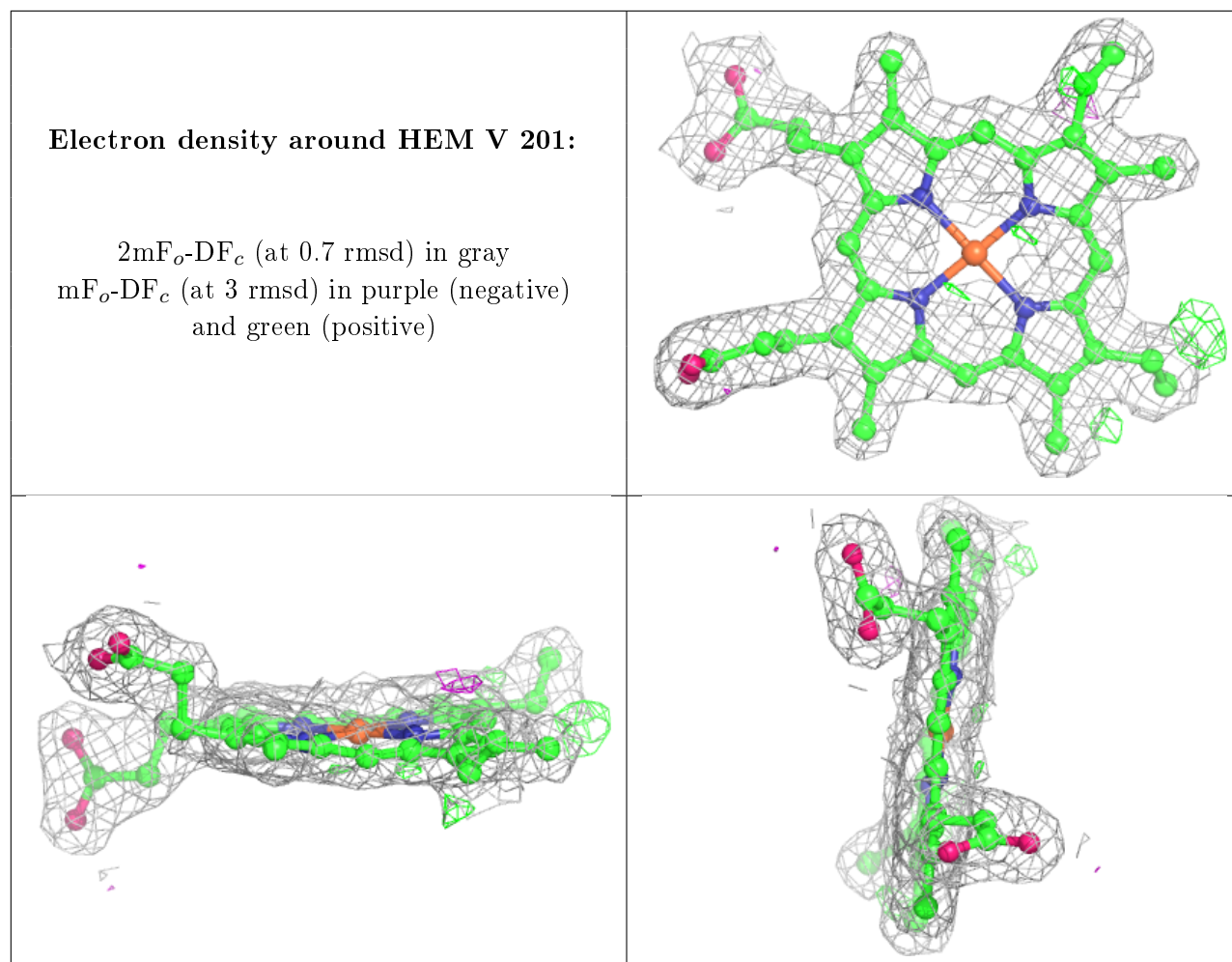


**Electron density around CLA a 411:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.