



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:31 AM BST

PDB ID : 6JLM  
Title : XFEL structure of cyanobacterial photosystem II (dark state, dataset2)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

---

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

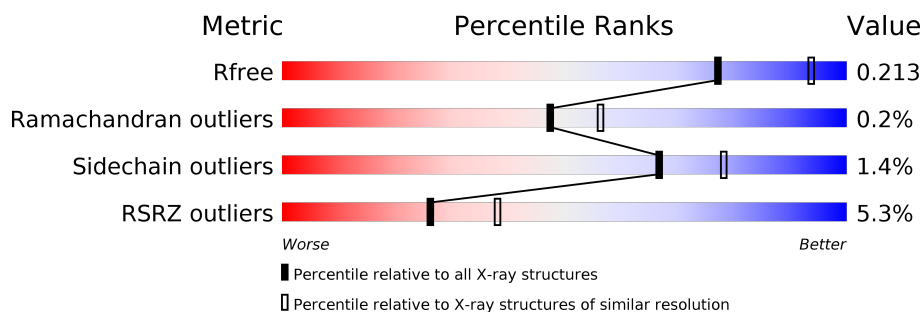
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

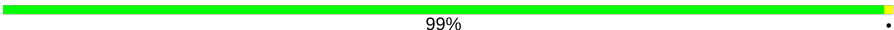

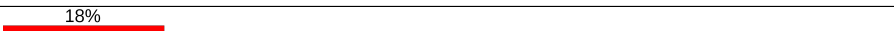
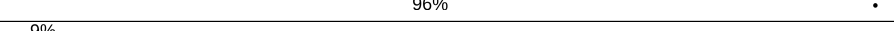



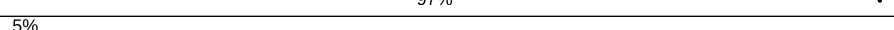
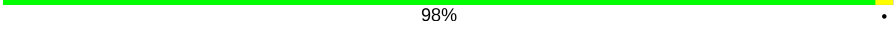



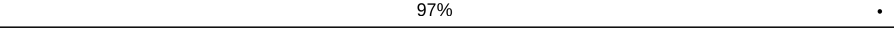
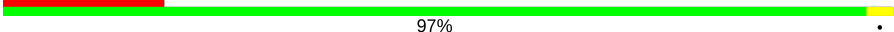


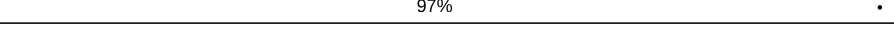
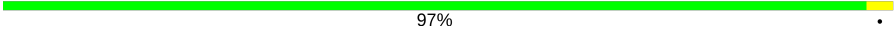
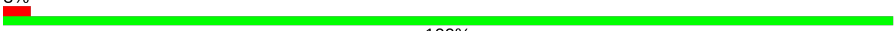


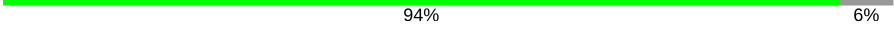


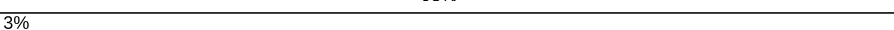
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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>%</div> <div>97%</div> <div>..</div> </div>
1	a	344	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>3%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>6%</div> <div>99%</div> </div>
3	C	455	<div> <div>4%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div>%</div> <div>99%</div> <div>.</div> </div>

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	407	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	d	406	X	-	-	-
28	GOL	V	204	-	-	-	X
29	LMT	F	101	-	-	-	X
37	DGD	e	101	-	-	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 54101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	See sequence details	UNP D0VWR7
C	20	SER	-	See sequence details	UNP D0VWR7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	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	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	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	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	S	98	0	0
			239	163	41	35				

- 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	d	1	Total	Fe	0	0
			1	1		

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

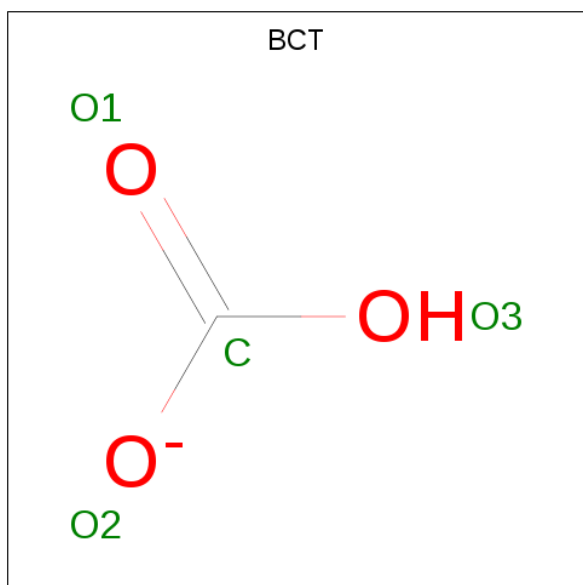
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

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



*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

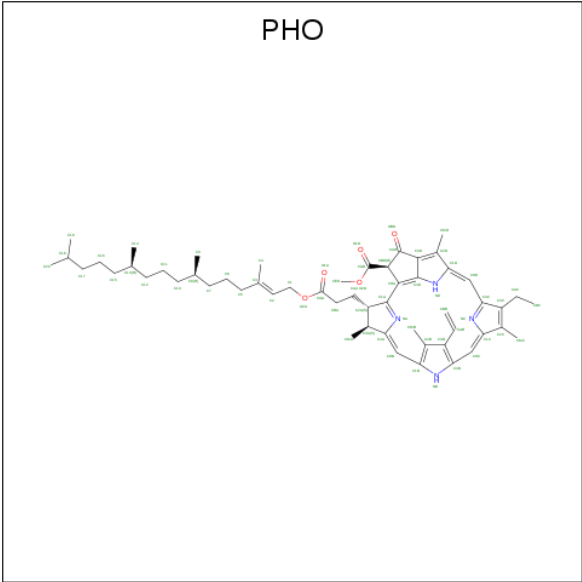
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

*Continued on next page...*

*Continued from previous page...*

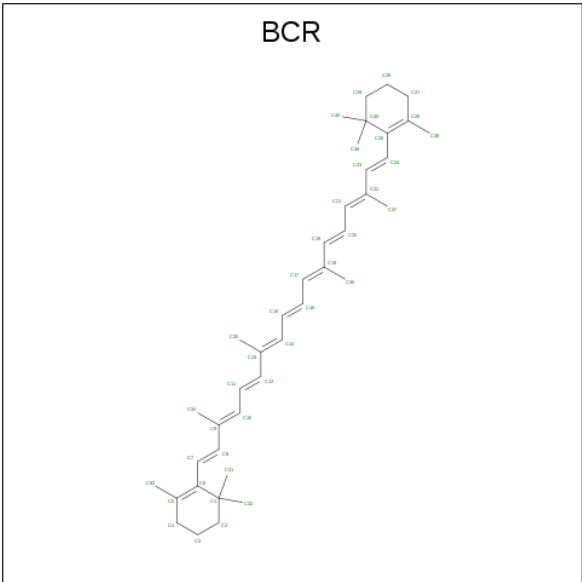
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



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

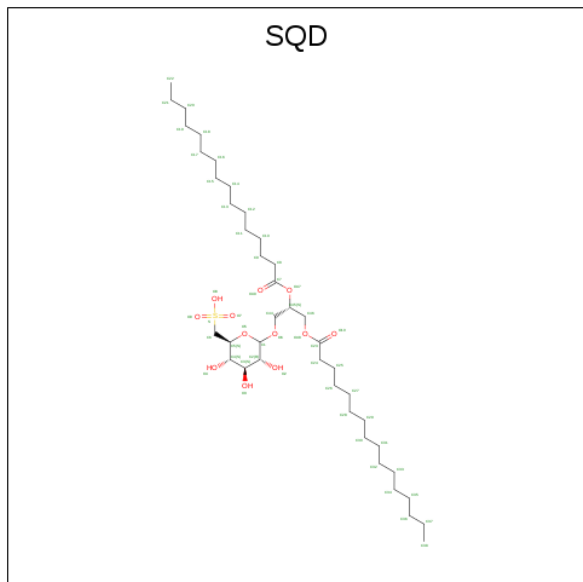
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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



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



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

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



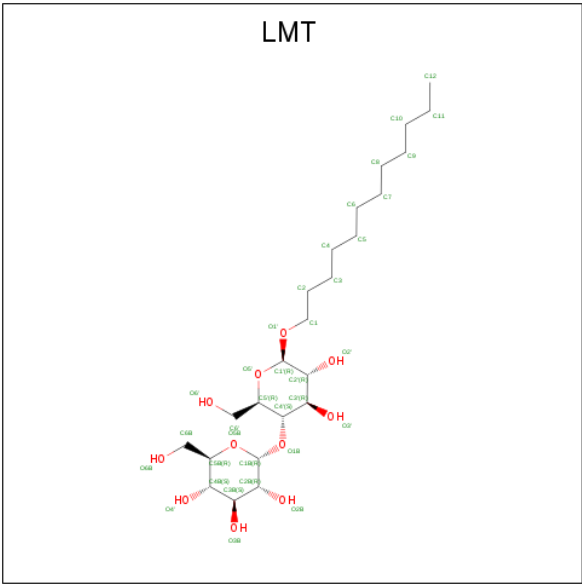
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



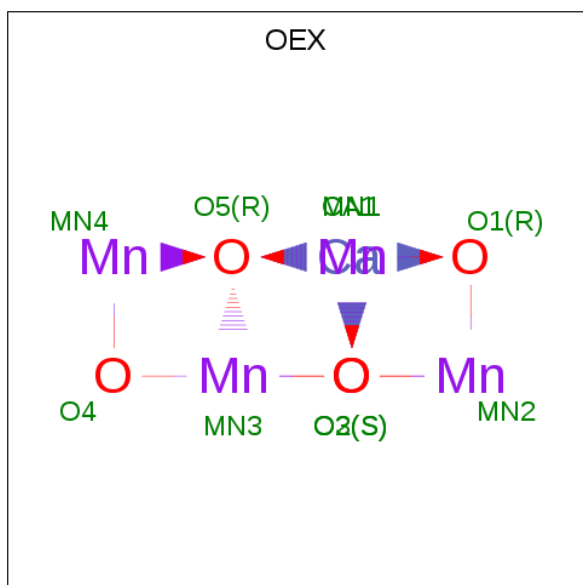
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	b	1	Total	C	O	0	0
			25	19	6		
29	e	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

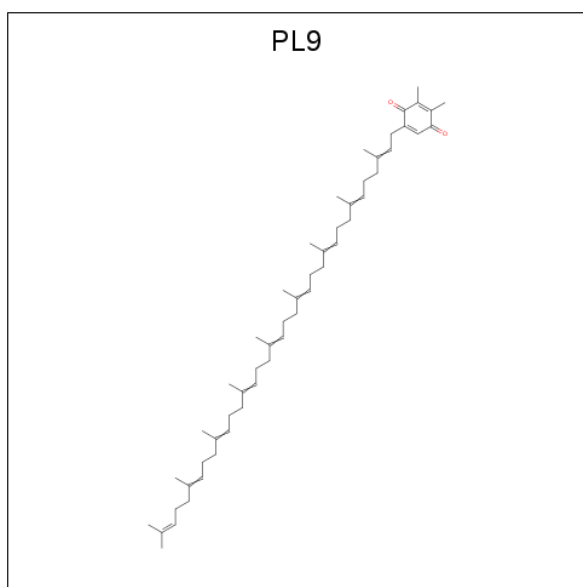
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	t	1	Total	C	O	0	0
			25	19	6		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

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



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

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

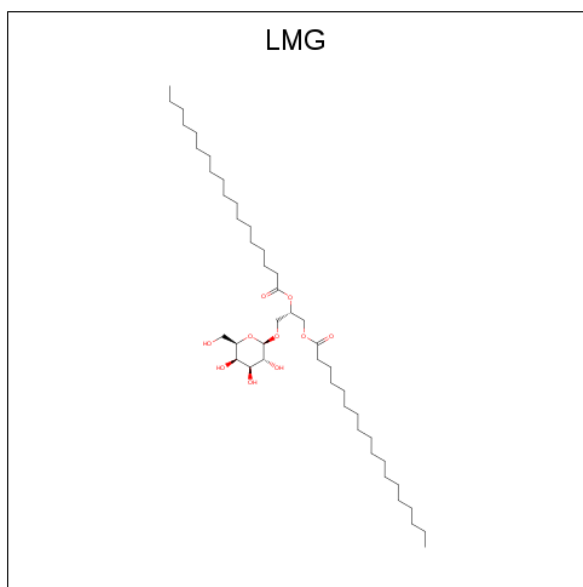
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	a	1	Total	C	O	0	0
			30	25	5		
32	c	1	Total	C	O	0	0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	x	1	Total C O 18 16 2	0	0
32	A	1	Total C O 28 23 5	0	0
32	j	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	d	2	Total C O 53 47 6	0	0
32	m	1	Total C 10 10	0	0
32	b	1	Total C O 33 28 5	0	0
32	M	1	Total C 10 10	0	0

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



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

*Continued on next page...*

*Continued from previous page...*

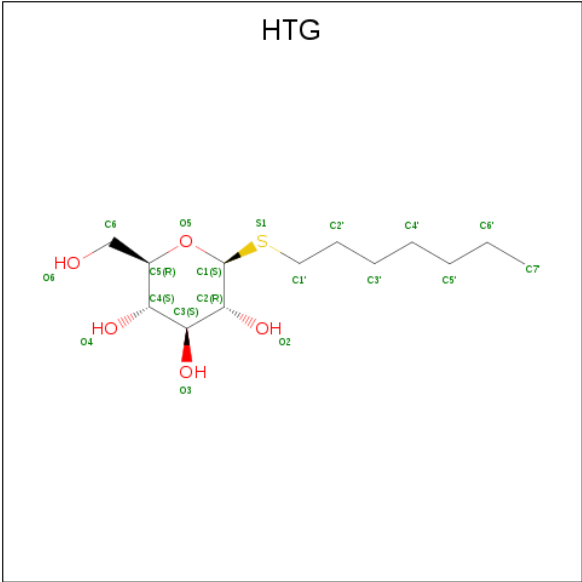
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	J	1	Total	C	O	0	0
			51	41	10		
33	Y	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total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

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	1	Total	Ca	0	0
			1	1		
34	C	1	Total	Ca	0	0
			1	1		
34	c	2	Total	Ca	0	0
			2	2		
34	f	1	Total	Ca	0	0
			1	1		
34	o	1	Total	Ca	0	0
			1	1		
34	O	1	Total	Ca	0	0
			1	1		
34	b	1	Total	Ca	0	0
			1	1		
34	F	1	Total	Ca	0	0
			1	1		

- Molecule 35 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).





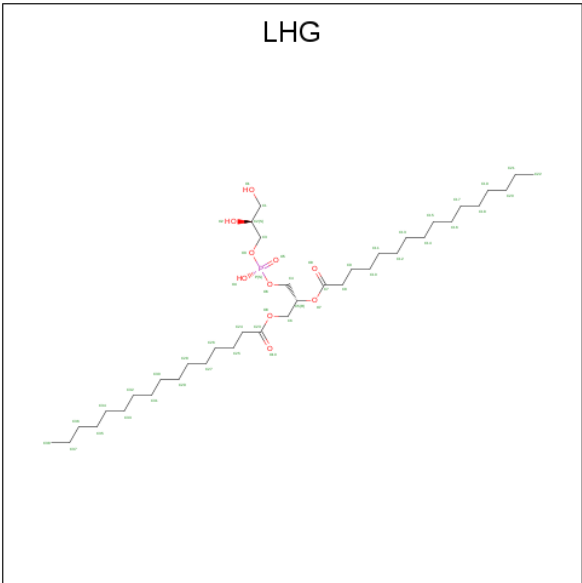
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

Continued on next page...

Continued from previous page...

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

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



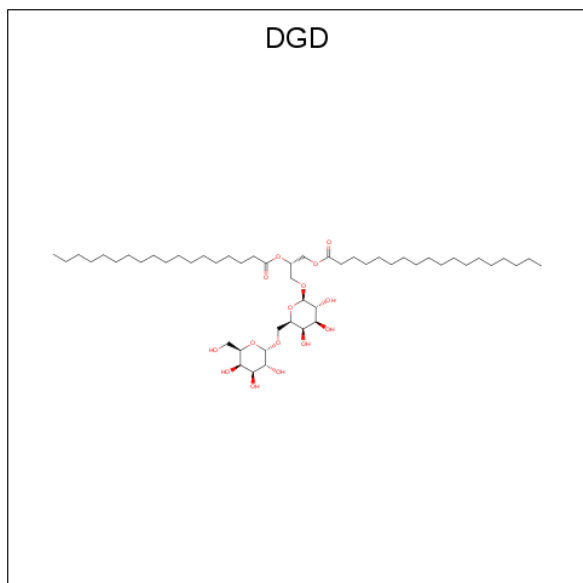
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			42	31	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			42	31	10	1		
36	b	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		

Continued on next page...

*Continued from previous page...*

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		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	e	1	Total	C	O	0	0
			62	47	15		

*Continued on next page...*

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

- # HEM

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

- 
- WORLD WIDE  
**PDB**  
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	164	Total O 167 167	0	3
40	B	295	Total O 299 299	0	4
40	C	232	Total O 234 234	0	2
40	D	140	Total O 144 144	0	4
40	E	30	Total O 31 31	0	1
40	F	10	Total O 10 10	0	0
40	H	48	Total O 48 48	0	0
40	I	6	Total O 6 6	0	0
40	J	12	Total O 12 12	0	0
40	K	7	Total O 7 7	0	0
40	L	14	Total O 15 15	0	1
40	M	13	Total O 13 13	0	0
40	O	179	Total O 181 181	0	2
40	T	16	Total O 17 17	0	1
40	U	80	Total O 80 80	0	0
40	V	114	Total O 116 116	0	2
40	Y	4	Total O 4 4	0	0
40	X	9	Total O 9 9	0	0
40	Z	1	Total O 1 1	0	0
40	a	158	Total O 159 159	0	1
40	b	262	Total O 265 265	0	3
40	c	207	Total O 210 210	0	3

Continued on next page...

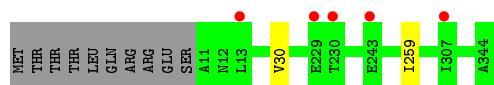
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	d	129	Total 132	O 132	0	3
40	e	19	Total 19	O 19	0	0
40	f	6	Total 6	O 6	0	0
40	h	40	Total 40	O 40	0	0
40	i	4	Total 4	O 4	0	0
40	j	6	Total 6	O 6	0	0
40	k	7	Total 7	O 7	0	0
40	l	10	Total 10	O 10	0	0
40	m	15	Total 15	O 15	0	0
40	o	155	Total 155	O 155	0	0
40	t	11	Total 11	O 11	0	0
40	u	97	Total 97	O 97	0	0
40	v	77	Total 78	O 78	0	1
40	y	2	Total 2	O 2	0	0
40	x	6	Total 6	O 6	0	0

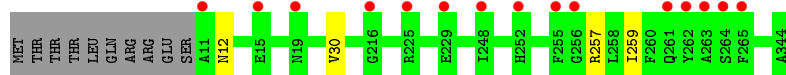
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1



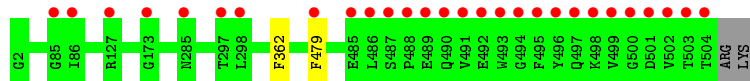
- Molecule 1: Photosystem II protein D1



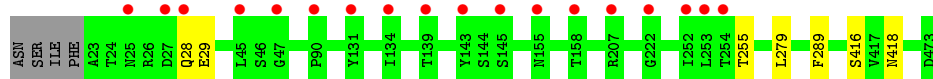
- Molecule 2: Photosystem II CP47 reaction center protein



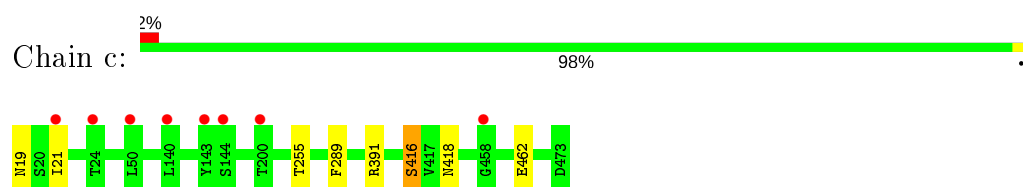
- Molecule 2: Photosystem II CP47 reaction center protein



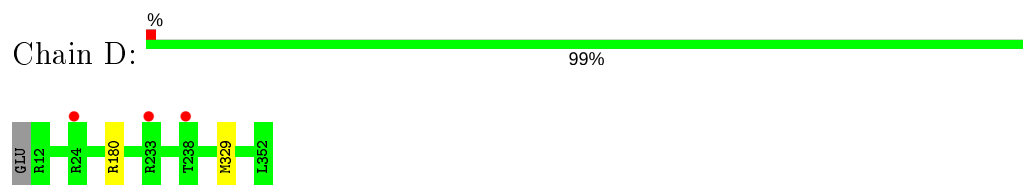
- Molecule 3: Photosystem II CP43 reaction center protein



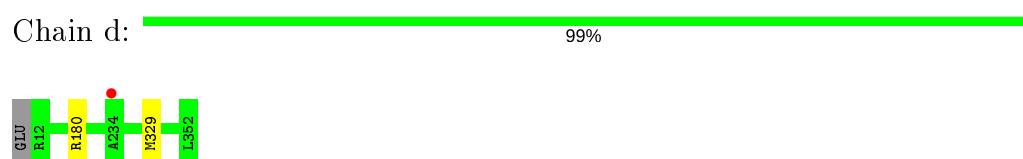
- Molecule 3: Photosystem II CP43 reaction center protein



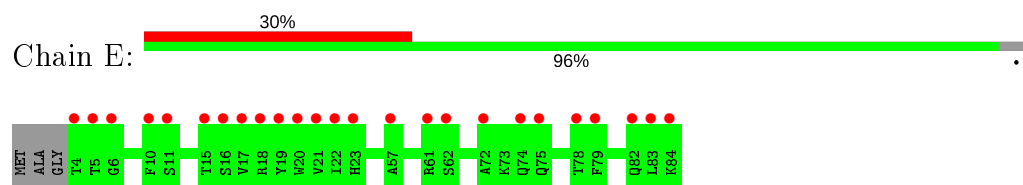
- Molecule 4: Photosystem II D2 protein



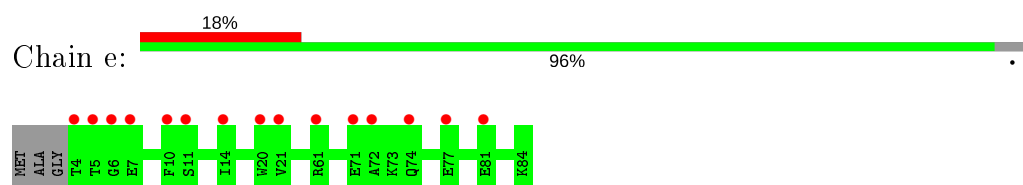
- Molecule 4: Photosystem II D2 protein



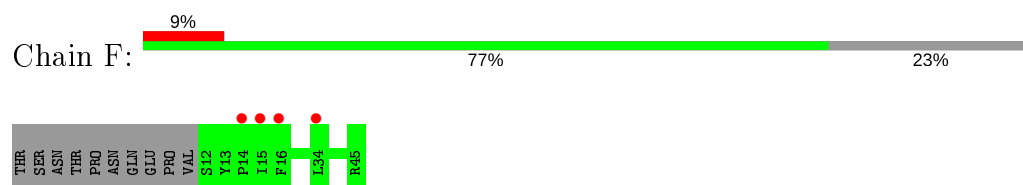
- Molecule 5: Cytochrome b559 subunit alpha



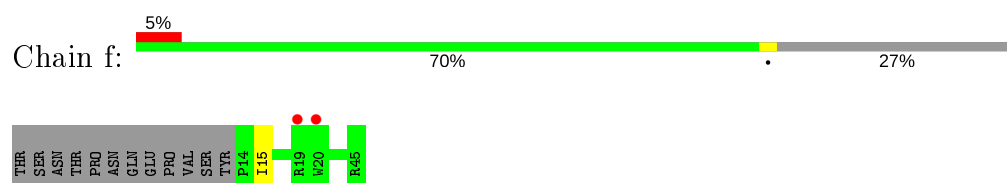
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

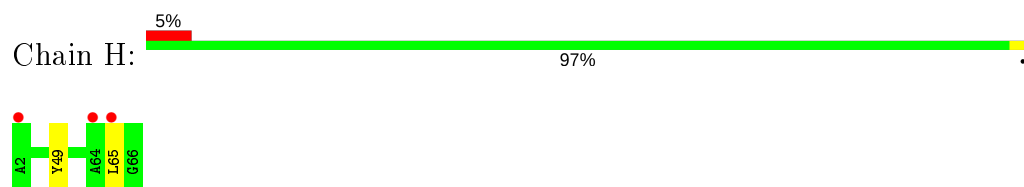


- Molecule 6: Cytochrome b559 subunit beta

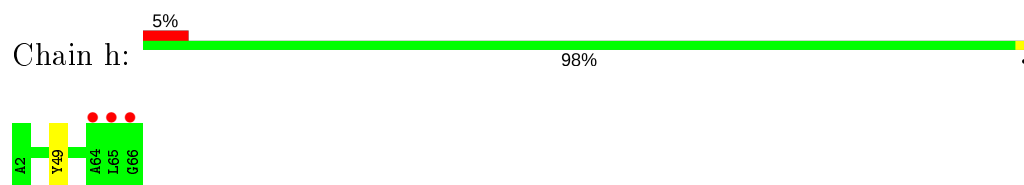




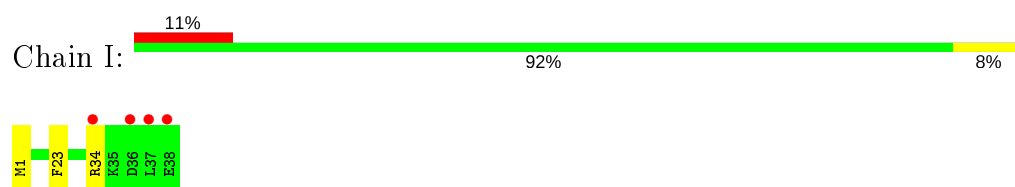
- Molecule 7: Photosystem II reaction center protein H



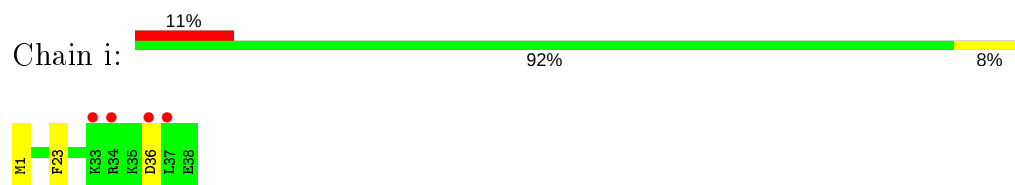
- Molecule 7: Photosystem II reaction center protein H



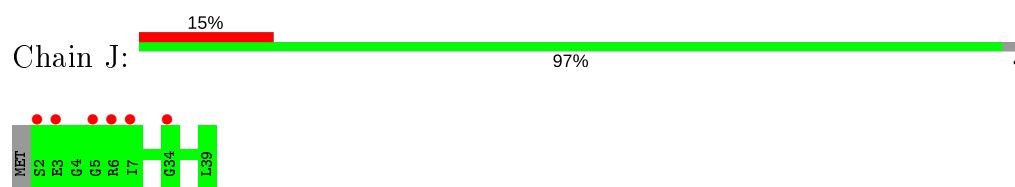
- Molecule 8: Photosystem II reaction center protein I



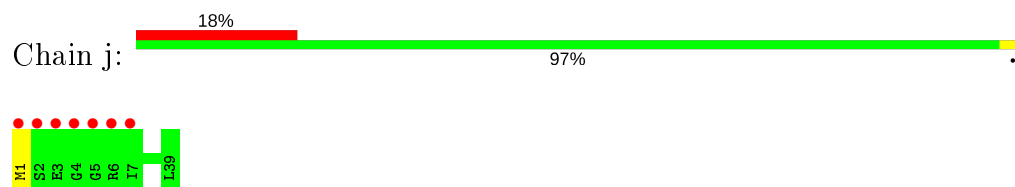
- Molecule 8: Photosystem II reaction center protein I



- 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

Chain k: 97%



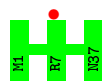
- Molecule 11: Photosystem II reaction center protein L

Chain L: 97%



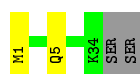
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%



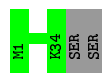
- Molecule 12: Photosystem II reaction center protein M

Chain M: 89% 6% 6%



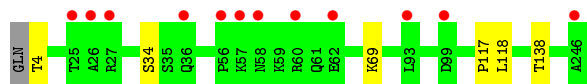
- Molecule 12: Photosystem II reaction center protein M

Chain m: 94% 6%



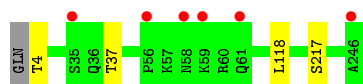
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 97%

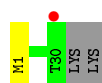
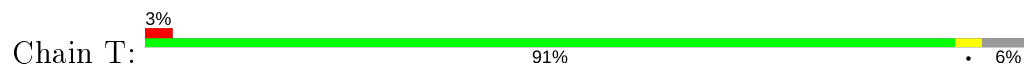


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

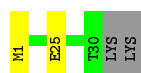
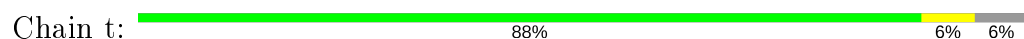
Chain o: 98%



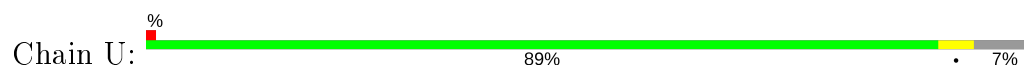
- Molecule 14: Photosystem II reaction center protein T



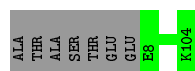
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



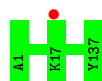
- Molecule 15: Photosystem II 12 kDa extrinsic protein



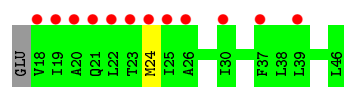
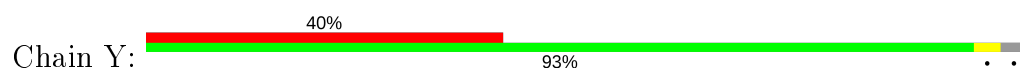
- Molecule 16: Cytochrome c-550



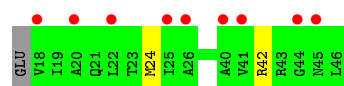
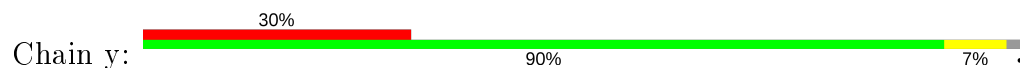
- Molecule 16: Cytochrome c-550



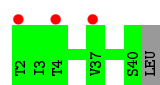
- Molecule 17: Photosystem II reaction center protein Ycf12



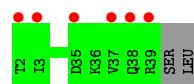
- Molecule 17: Photosystem II reaction center protein Ycf12



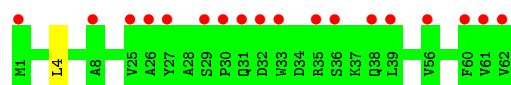
- Molecule 18: Photosystem II reaction center protein X



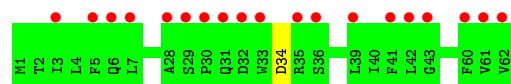
- Molecule 18: Photosystem II reaction center protein X



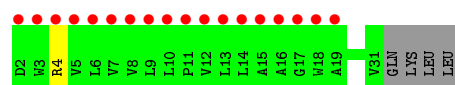
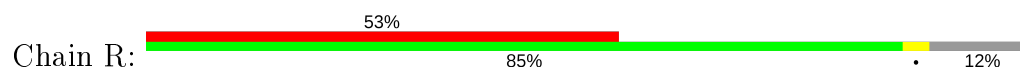
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.35 121.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.35) 99.9 (121.57-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.153 , 0.209 0.160 , 0.213	Depositor DCC
$R_{free}$ test set	17809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 83.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, HTG, BCR, 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	0.46	0/2728	0.56	0/3719
1	a	0.47	0/2748	0.57	0/3746
2	B	0.44	0/4191	0.54	0/5709
2	b	0.44	0/4198	0.54	0/5720
3	C	0.40	0/3626	0.52	0/4936
3	c	0.39	0/3676	0.52	0/5004
4	D	0.48	0/2818	0.56	0/3840
4	d	0.47	0/2818	0.56	0/3840
5	E	0.37	0/693	0.51	0/944
5	e	0.36	0/695	0.52	0/948
6	F	0.44	0/284	0.53	0/387
6	f	0.44	0/265	0.54	0/360
7	H	0.38	0/535	0.57	0/728
7	h	0.37	0/524	0.51	0/713
8	I	0.37	0/311	0.51	0/419
8	i	0.40	0/311	0.49	0/419
9	J	0.37	0/278	0.43	0/376
9	j	0.37	0/286	0.46	0/386
10	K	0.36	0/303	0.54	0/416
10	k	0.37	0/303	0.50	0/416
11	L	0.41	0/319	0.51	0/433
11	l	0.45	0/319	0.48	0/433
12	M	0.52	0/270	0.69	0/368
12	m	0.49	0/262	0.62	0/357
13	O	0.39	0/1958	0.56	0/2654
13	o	0.39	0/1937	0.57	0/2625
14	T	0.45	0/266	0.54	0/362
14	t	0.53	0/266	0.52	0/362
15	U	0.41	0/785	0.56	0/1064
15	u	0.41	0/785	0.56	0/1064
16	V	0.38	0/1096	0.52	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1085	0.54	0/1473
17	Y	0.36	0/216	0.50	0/289
17	y	0.33	0/216	0.46	0/289
18	X	0.35	0/290	0.47	0/392
18	x	0.34	0/284	0.47	0/384
19	Z	0.32	0/490	0.48	0/669
19	z	0.29	0/490	0.50	0/669
20	R	0.24	0/245	0.39	0/338
All	All	0.42	0/43170	0.54	0/58738

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	5 (2%)	2 (1%)	25	27
1	a	338/344 (98%)	331 (98%)	5 (2%)	2 (1%)	25	27
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	442 (98%)	9 (2%)	2 (0%)	34	38
3	c	459/455 (101%)	448 (98%)	9 (2%)	2 (0%)	34	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	2
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	242 (97%)	6 (2%)	1 (0%)	34	38
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5282/5384 (98%)	5151 (98%)	121 (2%)	10 (0%)	47	56

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	I	34	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	273 (99%)	2 (1%)	84	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	82
2	b	413/403 (102%)	411 (100%)	2 (0%)	88	94
3	C	356/356 (100%)	350 (98%)	6 (2%)	60	72
3	c	362/356 (102%)	352 (97%)	10 (3%)	43	53
4	D	277/277 (100%)	275 (99%)	2 (1%)	84	91
4	d	277/277 (100%)	275 (99%)	2 (1%)	84	91
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	74 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	41
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	43
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	52
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	42
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	46
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	46
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	53
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	30 (97%)	1 (3%)	39	47
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	61
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	59
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	14
15	U	84/89 (94%)	81 (96%)	3 (4%)	35	43
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	89
16	v	117/117 (100%)	117 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	33
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	8
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	68
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	68
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	39
All	All	4387/4403 (100%)	4324 (99%)	63 (1%)	67	78

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Y	24	MET
3	c	19	ASN
14	t	25[A]	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	Z	4	LEU
1	a	12	ASN

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

Mol	Chain	Res	Type
19	Z	58	ASN
2	b	53	ASN
16	v	86	GLN
2	b	14	ASN
2	b	331	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.44	1 (14%)
12	FME	m	1	12	8,9,10	0.67	0	7,9,11	1.08	0
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.26	1 (14%)
14	FME	t	1	14	8,9,10	0.80	0	7,9,11	2.51	5 (71%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.23	1 (14%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.16	1 (14%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.15	116.44	122.82
14	t	1	FME	C-CA-N	3.05	115.23	109.73
14	T	1	FME	O-C-CA	-2.50	118.21	124.78
14	t	1	FME	O-C-CA	-2.47	118.31	124.78
14	t	1	FME	CE-SD-CG	-2.19	92.88	100.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 18 are unknown and 19 are monoatomic - leaving 214 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.37	0
31	PL9	A	417	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	23 (33%)
27	SQD	A	414	-	53,54,54	1.03	3 (5%)	62,65,65	1.12	6 (9%)
26	BCR	c	927	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)
30	OEX	A	416	1,3,40	0,15,15	0.00	-	-	-	-
24	CLA	B	614	-	59,73,73	2.06	13 (22%)	67,113,113	2.16	25 (37%)
24	CLA	B	606	-	59,73,73	1.98	12 (20%)	67,113,113	2.24	20 (29%)
31	PL9	d	408	-	55,55,55	0.67	2 (3%)	68,69,69	1.69	16 (23%)
26	BCR	b	624	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
38	HEM	f	101	5,6	27,50,50	0.82	1 (3%)	17,82,82	2.15	3 (17%)
24	CLA	C	510	-	59,73,73	2.06	13 (22%)	67,113,113	2.18	21 (31%)
24	CLA	b	608	-	59,73,73	1.98	14 (23%)	67,113,113	2.29	21 (31%)
24	CLA	b	607	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	24 (35%)
36	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
26	BCR	b	623	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
35	HTG	B	625	-	19,19,19	1.05	2 (10%)	23,24,24	1.64	2 (8%)
24	CLA	B	605	-	59,73,73	1.89	13 (22%)	67,113,113	2.20	22 (32%)
24	CLA	d	406	-	59,73,73	2.02	12 (20%)	67,113,113	2.14	20 (29%)
36	LHG	d	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
29	LMT	C	520	-	36,36,36	0.48	0	47,47,47	1.17	4 (8%)
24	CLA	b	610	-	59,73,73	1.97	13 (22%)	67,113,113	2.22	18 (26%)
24	CLA	a	405	-	59,73,73	2.00	13 (22%)	67,113,113	2.21	24 (35%)
28	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.35	0
26	BCR	A	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.11	4 (7%)
24	CLA	A	409	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	23 (34%)
33	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
24	CLA	b	615	40	59,73,73	2.05	13 (22%)	67,113,113	2.17	24 (35%)
23	BCT	A	404	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
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.41	9 (16%)
28	GOL	V	206	-	5,5,5	0.43	0	5,5,5	0.32	0
24	CLA	B	602	40	59,73,73	2.03	14 (23%)	67,113,113	2.13	17 (25%)
28	GOL	v	205	-	5,5,5	0.33	0	5,5,5	0.47	0
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
37	DGD	c	917	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	613	-	59,73,73	2.05	13 (22%)	67,113,113	2.24	25 (37%)
26	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	10 (17%)
24	CLA	c	913	-	59,73,73	2.03	12 (20%)	67,113,113	2.28	22 (32%)
29	LMT	a	401	-	36,36,36	0.51	1 (2%)	47,47,47	1.15	3 (6%)
36	LHG	a	418	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
25	PHO	A	408	-	67,69,69	2.16	17 (25%)	85,99,99	1.83	20 (23%)
24	CLA	c	904	-	59,73,73	1.99	12 (20%)	67,113,113	2.06	19 (28%)
23	BCT	d	402	21	0,3,3	0.00	-	0,3,3	0.00	-
29	LMT	m	103	-	36,36,36	0.49	0	47,47,47	1.08	3 (6%)
24	CLA	b	611	-	59,73,73	1.99	13 (22%)	67,113,113	2.22	21 (31%)
24	CLA	C	512	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	23 (34%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	11 (17%)
24	CLA	b	614	-	59,73,73	1.99	12 (20%)	67,113,113	2.20	21 (31%)
24	CLA	b	620	-	59,73,73	2.02	13 (22%)	67,113,113	2.20	24 (35%)
35	HTG	B	633	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
24	CLA	A	406	40	59,73,73	2.07	13 (22%)	67,113,113	2.30	24 (35%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	13 (23%)
24	CLA	B	617	-	59,73,73	1.99	12 (20%)	67,113,113	2.19	21 (31%)
26	BCR	D	406	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	10 (17%)
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	4 (5%)
24	CLA	b	616	-	59,73,73	1.95	13 (22%)	67,113,113	2.24	22 (32%)
24	CLA	B	612	-	59,73,73	1.94	13 (22%)	67,113,113	2.30	23 (34%)
29	LMT	M	101	-	36,36,36	0.46	0	47,47,47	0.92	0
24	CLA	B	611	40	59,73,73	2.00	14 (23%)	67,113,113	2.16	24 (35%)
24	CLA	c	910	-	59,73,73	2.10	13 (22%)	67,113,113	2.28	22 (32%)
37	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.04	5 (6%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	15 (26%)
27	SQD	a	402	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	6 (9%)
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PHO	a	407	-	67,69,69	2.11	17 (25%)	85,99,99	1.91	26 (30%)
29	LMT	a	417	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
38	HEM	F	102	5,6	27,50,50	0.90	2 (7%)	17,82,82	2.32	3 (17%)
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	6 (11%)
24	CLA	D	405	-	59,73,73	1.94	14 (23%)	67,113,113	2.17	22 (32%)
27	SQD	F	103	-	42,43,54	1.17	3 (7%)	51,54,65	1.58	9 (17%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.49	0
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.64	11 (17%)
26	BCR	b	622	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	9 (16%)
28	GOL	c	928	-	5,5,5	0.41	0	5,5,5	0.25	0
24	CLA	b	619	-	59,73,73	2.03	13 (22%)	67,113,113	2.25	27 (40%)
36	LHG	D	409	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	3 (5%)
24	CLA	B	608	40	59,73,73	1.99	14 (23%)	67,113,113	2.11	21 (31%)
24	CLA	b	609	-	59,73,73	2.00	15 (25%)	67,113,113	2.25	19 (28%)
28	GOL	B	626	-	5,5,5	0.41	0	5,5,5	0.34	0
24	CLA	B	607	-	59,73,73	2.00	13 (22%)	67,113,113	2.25	23 (34%)
35	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	1 (4%)
24	CLA	d	404	40	59,73,73	2.04	12 (20%)	67,113,113	2.30	24 (35%)
24	CLA	C	509	-	59,73,73	2.09	13 (22%)	67,113,113	2.25	23 (34%)
24	CLA	d	405	-	59,73,73	1.98	14 (23%)	67,113,113	2.29	21 (31%)
28	GOL	v	203	-	5,5,5	0.35	0	5,5,5	0.27	0
27	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.45	6 (11%)
24	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	22 (32%)
29	LMT	t	101	-	25,25,36	0.50	0	30,30,47	0.77	1 (3%)
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.74	4 (17%)
28	GOL	T	101	-	5,5,5	0.38	0	5,5,5	0.22	0
24	CLA	C	508	-	59,73,73	2.05	13 (22%)	67,113,113	2.19	21 (31%)
24	CLA	C	507	40	59,73,73	1.97	13 (22%)	67,113,113	2.15	21 (31%)
28	GOL	b	631	-	5,5,5	0.32	0	5,5,5	0.26	0
35	HTG	B	623	-	19,19,19	1.20	1 (5%)	23,24,24	1.28	1 (4%)
37	DGD	D	408	-	52,52,67	1.04	3 (5%)	60,60,81	1.17	5 (8%)
28	GOL	B	631	-	5,5,5	0.33	0	5,5,5	0.43	0
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.53	10 (17%)
36	LHG	B	635	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
24	CLA	B	615	-	59,73,73	2.07	13 (22%)	67,113,113	2.13	22 (32%)
28	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	GOL	v	204	-	5,5,5	0.36	0	5,5,5	0.34	0
35	HTG	c	921	-	19,19,19	1.00	2 (10%)	23,24,24	1.56	1 (4%)
24	CLA	c	914	-	59,73,73	2.02	13 (22%)	67,113,113	2.12	21 (31%)
30	OEX	a	416	1,3,40	0,15,15	0.00	-	-	-	-
24	CLA	b	606	40	59,73,73	2.06	12 (20%)	67,113,113	2.23	18 (26%)
29	LMT	D	403	-	36,36,36	0.47	0	47,47,47	1.04	3 (6%)
28	GOL	V	201	34	5,5,5	0.34	0	5,5,5	0.26	0
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.49	0
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.85	1 (2%)
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.97	3 (5%)
36	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	C	501	-	59,73,73	2.02	13 (22%)	67,113,113	2.20	22 (32%)
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	8 (13%)
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.61	0
28	GOL	A	413	-	5,5,5	0.38	0	5,5,5	0.22	0
35	HTG	d	414	-	16,16,19	1.14	2 (12%)	20,21,24	1.76	1 (5%)
38	HEM	V	202	16	27,50,50	0.84	1 (3%)	17,82,82	1.49	4 (23%)
33	LMG	A	419	-	51,51,55	0.96	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	B	603	-	59,73,73	1.99	13 (22%)	67,113,113	2.31	23 (34%)
24	CLA	c	907	-	59,73,73	1.97	14 (23%)	67,113,113	2.19	23 (34%)
35	HTG	V	203	-	19,19,19	1.02	2 (10%)	23,24,24	1.31	3 (13%)
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
29	LMT	F	101	-	36,36,36	0.46	0	47,47,47	0.90	1 (2%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
26	BCR	Y	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.67	11 (19%)
24	CLA	c	912	3	59,73,73	2.00	12 (20%)	67,113,113	2.03	19 (28%)
26	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	14 (25%)
26	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	8 (14%)
25	PHO	d	403	-	67,69,69	2.16	17 (25%)	85,99,99	2.05	23 (27%)
24	CLA	C	505	-	59,73,73	1.92	13 (22%)	67,113,113	2.18	20 (29%)
31	PL9	a	415	-	55,55,55	0.64	2 (3%)	68,69,69	1.88	21 (30%)
28	GOL	l	101	-	5,5,5	0.47	0	5,5,5	0.24	0
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.12	6 (7%)
35	HTG	b	627	-	19,19,19	0.81	1 (5%)	23,24,24	1.54	3 (13%)
28	GOL	b	632	-	5,5,5	0.38	0	5,5,5	0.33	0
35	HTG	D	413	-	16,16,19	1.07	2 (12%)	20,21,24	1.52	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	GOL	T	103	-	5,5,5	0.40	0	5,5,5	0.30	0
28	GOL	A	412	-	5,5,5	0.39	0	5,5,5	0.29	0
36	LHG	b	635	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
28	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.47	0
33	LMG	a	411	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	5 (8%)
24	CLA	c	908	40	59,73,73	1.99	13 (22%)	67,113,113	2.20	20 (29%)
24	CLA	C	506	-	59,73,73	2.00	13 (22%)	67,113,113	2.22	24 (35%)
24	CLA	B	610	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	22 (32%)
35	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.76	3 (13%)
33	LMG	b	625	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	5 (8%)
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.30	0
24	CLA	a	408	-	59,73,73	2.00	13 (22%)	67,113,113	2.23	25 (37%)
28	GOL	a	412	-	5,5,5	0.39	0	5,5,5	0.53	0
38	HEM	v	202	16	27,50,50	0.87	1 (3%)	17,82,82	1.39	2 (11%)
25	PHO	D	401	-	67,69,69	2.17	18 (26%)	85,99,99	1.95	21 (24%)
36	LHG	L	101	-	48,48,48	0.95	3 (6%)	51,54,54	1.13	5 (9%)
29	LMT	M	103	-	36,36,36	0.59	1 (2%)	47,47,47	1.08	4 (8%)
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.44	8 (12%)
24	CLA	c	902	-	59,73,73	2.00	13 (22%)	67,113,113	2.17	24 (35%)
31	PL9	D	407	-	55,55,55	0.64	2 (3%)	68,69,69	1.89	22 (32%)
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.37	2 (8%)
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	4 (17%)
24	CLA	c	905	40	59,73,73	2.00	13 (22%)	67,113,113	2.21	25 (37%)
24	CLA	C	511	3	59,73,73	2.05	13 (22%)	67,113,113	2.12	21 (31%)
24	CLA	a	406	40	59,73,73	2.00	12 (20%)	67,113,113	2.18	22 (32%)
26	BCR	T	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	17 (30%)
29	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.86	1 (2%)
26	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
28	GOL	B	629	-	5,5,5	0.35	0	5,5,5	0.31	0
24	CLA	B	616	-	59,73,73	2.00	13 (22%)	67,113,113	2.12	20 (29%)
24	CLA	A	405	-	59,73,73	2.05	13 (22%)	67,113,113	2.17	23 (34%)
24	CLA	b	621	-	59,73,73	2.03	13 (22%)	67,113,113	2.24	24 (35%)
24	CLA	D	404	-	59,73,73	1.97	14 (23%)	67,113,113	2.21	26 (38%)
28	GOL	c	923	-	5,5,5	0.37	0	5,5,5	0.22	0
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.39	0
35	HTG	b	628	-	19,19,19	1.21	2 (10%)	23,24,24	1.69	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	604	-	59,73,73	2.05	13 (22%)	67,113,113	2.25	20 (29%)
29	LMT	b	626	-	25,25,36	0.47	0	30,30,47	0.58	0
37	DGD	c	916	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	7 (9%)
28	GOL	B	630	-	5,5,5	0.39	0	5,5,5	0.21	0
35	HTG	b	603	-	19,19,19	1.00	2 (10%)	23,24,24	1.55	4 (17%)
28	GOL	a	413	-	5,5,5	0.41	0	5,5,5	0.26	0
26	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	9 (16%)
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
35	HTG	c	922	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	3 (13%)
24	CLA	C	504	40	59,73,73	2.06	13 (22%)	67,113,113	2.31	23 (34%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.41	0
26	BCR	a	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.28	2 (3%)
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.47	12 (21%)
28	GOL	C	524	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	C	503	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	19 (28%)
24	CLA	A	407	40	59,73,73	1.99	13 (22%)	67,113,113	2.15	23 (34%)
28	GOL	a	419	34	5,5,5	0.31	0	5,5,5	0.40	0
24	CLA	b	617	-	59,73,73	2.02	12 (20%)	67,113,113	2.25	25 (37%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	B	609	-	59,73,73	2.06	13 (22%)	67,113,113	2.10	21 (31%)
24	CLA	b	618	-	59,73,73	2.01	12 (20%)	67,113,113	2.25	21 (31%)
24	CLA	b	612	40	59,73,73	1.94	12 (20%)	67,113,113	2.15	22 (32%)
26	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	9 (16%)
24	CLA	C	513	-	59,73,73	1.99	12 (20%)	67,113,113	2.13	22 (32%)
36	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.20	4 (7%)
29	LMT	A	415	-	36,36,36	0.67	1 (2%)	47,47,47	1.43	5 (10%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.47	0
24	CLA	c	911	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	22 (32%)
37	DGD	C	517	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	7 (9%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.57	0
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
29	LMT	b	602	-	25,25,36	0.57	1 (4%)	30,30,47	1.12	2 (6%)
24	CLA	c	906	-	59,73,73	1.96	13 (22%)	67,113,113	2.19	19 (28%)
26	BCR	c	915	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	10 (17%)
24	CLA	B	613	-	59,73,73	2.00	13 (22%)	67,113,113	2.18	20 (29%)
24	CLA	c	909	-	59,73,73	2.04	13 (22%)	67,113,113	2.29	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	903	-	59,73,73	2.04	13 (22%)	67,113,113	2.14	19 (28%)
33	LMG	Y	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.00	4 (6%)
35	HTG	b	604	-	19,19,19	0.99	2 (10%)	23,24,24	1.11	1 (4%)
28	GOL	b	630	-	5,5,5	0.40	0	5,5,5	0.14	0
33	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.30	7 (11%)
33	LMG	c	919	-	51,51,55	0.88	2 (3%)	59,59,63	1.18	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	V	204	-	-	2/4/4/4	-
31	PL9	A	417	-	-	13/53/73/73	0/1/1/1
27	SQD	A	414	-	-	13/49/69/69	0/1/1/1
24	CLA	c	913	-	3/3/20/25	12/37/135/135	-
24	CLA	B	614	-	3/3/20/25	8/37/135/135	-
24	CLA	B	606	-	3/3/20/25	6/37/135/135	-
31	PL9	d	408	-	-	3/53/73/73	0/1/1/1
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
38	HEM	f	101	5,6	-	1/6/54/54	-
24	CLA	C	510	-	3/3/20/25	8/37/135/135	-
24	CLA	b	608	-	2/2/20/25	5/37/135/135	-
24	CLA	b	607	-	2/2/20/25	5/37/135/135	-
36	LHG	E	101	-	-	19/46/46/53	-
26	BCR	b	623	-	-	1/29/63/63	0/2/2/2
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
24	CLA	B	605	-	3/3/20/25	4/37/135/135	-
24	CLA	d	406	-	3/3/20/25	6/37/135/135	-
36	LHG	d	411	-	-	12/53/53/53	-
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1
29	LMT	C	520	-	-	6/21/61/61	0/2/2/2
24	CLA	b	610	-	3/3/20/25	4/37/135/135	-
24	CLA	a	405	-	3/3/20/25	4/37/135/135	-
28	GOL	D	402	-	-	4/4/4/4	-
26	BCR	A	410	-	-	4/29/63/63	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	409	-	3/3/20/25	10/37/135/135	-
33	LMG	B	622	-	-	8/46/66/70	0/1/1/1
24	CLA	b	615	40	3/3/20/25	5/37/135/135	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
28	GOL	V	206	-	-	2/4/4/4	-
24	CLA	B	602	40	3/3/20/25	14/37/135/135	-
28	GOL	v	205	-	-	2/4/4/4	-
33	LMG	z	101	-	-	11/34/54/70	0/1/1/1
37	DGD	c	917	-	-	18/51/91/95	0/2/2/2
24	CLA	b	613	-	2/2/20/25	1/37/135/135	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	BCR	c	927	-	-	0/29/63/63	0/2/2/2
29	LMT	a	401	-	-	7/21/61/61	0/2/2/2
36	LHG	a	418	-	-	15/46/46/53	-
25	PHO	A	408	-	-	2/53/103/103	0/5/6/6
24	CLA	c	904	-	3/3/20/25	6/37/135/135	-
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
24	CLA	b	611	-	3/3/20/25	14/37/135/135	-
24	CLA	C	512	-	3/3/20/25	9/37/135/135	-
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
24	CLA	b	614	-	2/2/20/25	3/37/135/135	-
24	CLA	b	620	-	3/3/20/25	7/37/135/135	-
24	CLA	c	910	-	3/3/20/25	15/37/135/135	-
24	CLA	A	406	40	3/3/20/25	4/37/135/135	-
26	BCR	t	102	-	-	5/29/63/63	0/2/2/2
24	CLA	B	617	-	3/3/20/25	8/37/135/135	-
26	BCR	D	406	-	-	8/29/63/63	0/2/2/2
37	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	b	616	-	3/3/20/25	3/37/135/135	-
24	CLA	B	612	-	3/3/20/25	1/37/135/135	-
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
24	CLA	B	611	40	3/3/20/25	4/37/135/135	-
37	DGD	c	918	-	-	13/51/91/95	0/2/2/2
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
27	SQD	a	402	-	-	10/49/69/69	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
25	PHO	a	407	-	-	5/53/103/103	0/5/6/6
29	LMT	a	417	-	-	4/21/61/61	0/2/2/2
38	HEM	F	102	5,6	-	0/6/54/54	-
36	LHG	d	409	-	-	18/53/53/53	-
24	CLA	D	405	-	3/3/20/25	4/37/135/135	-
27	SQD	F	103	-	-	15/38/58/69	0/1/1/1
28	GOL	B	627	-	-	2/4/4/4	-
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
28	GOL	c	928	-	-	2/4/4/4	-
24	CLA	b	619	-	3/3/20/25	20/37/135/135	-
24	CLA	B	608	40	3/3/20/25	4/37/135/135	-
24	CLA	b	609	-	3/3/20/25	3/37/135/135	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	B	607	-	3/3/20/25	5/37/135/135	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	d	404	40	3/3/20/25	6/37/135/135	-
24	CLA	C	509	-	3/3/20/25	14/37/135/135	-
24	CLA	d	405	-	1/1/20/25	5/37/135/135	-
28	GOL	v	203	-	-	2/4/4/4	-
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
24	CLA	C	502	-	3/3/20/25	8/37/135/135	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	C	508	-	3/3/20/25	5/37/135/135	-
24	CLA	C	507	40	3/3/20/25	3/37/135/135	-
28	GOL	b	631	-	-	4/4/4/4	-
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
37	DGD	D	408	-	-	18/47/67/95	0/1/1/2
28	GOL	B	631	-	-	1/4/4/4	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	B	635	-	-	13/53/53/53	-
24	CLA	B	615	-	3/3/20/25	18/37/135/135	-
28	GOL	C	523	-	-	2/4/4/4	-
28	GOL	v	204	-	-	2/4/4/4	-
35	HTG	c	921	-	-	4/10/30/30	0/1/1/1
24	CLA	b	606	40	3/3/20/25	16/37/135/135	-
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
28	GOL	V	201	34	-	2/4/4/4	-
28	GOL	b	629	-	-	0/4/4/4	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
33	LMG	J	101	39	-	11/46/66/70	0/1/1/1
36	LHG	d	410	-	-	9/53/53/53	-
24	CLA	C	501	-	3/3/20/25	7/37/135/135	-
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
28	GOL	c	924	-	-	2/4/4/4	-
28	GOL	A	413	-	-	2/4/4/4	-
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
38	HEM	V	202	16	-	0/6/54/54	-
33	LMG	A	419	-	-	21/46/66/70	0/1/1/1
24	CLA	B	603	-	2/2/20/25	3/37/135/135	-
24	CLA	c	907	-	3/3/20/25	13/37/135/135	-
35	HTG	V	203	-	-	5/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMT	F	101	-	-	6/21/61/61	0/2/2/2
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	Y	102	-	-	4/29/63/63	0/2/2/2
24	CLA	c	912	3	3/3/20/25	6/37/135/135	-
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
25	PHO	d	403	-	-	4/53/103/103	0/5/6/6
24	CLA	C	505	-	1/1/20/25	6/37/135/135	-
31	PL9	a	415	-	-	15/53/73/73	0/1/1/1
28	GOL	l	101	-	-	0/4/4/4	-
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
35	HTG	b	627	-	-	2/10/30/30	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	b	632	-	-	2/4/4/4	-
35	HTG	D	413	-	-	0/7/27/30	0/1/1/1
28	GOL	T	103	-	-	2/4/4/4	-
28	GOL	A	412	-	-	0/4/4/4	-
36	LHG	b	635	-	-	20/53/53/53	-
28	GOL	B	628	-	-	2/4/4/4	-
33	LMG	a	411	-	-	14/46/66/70	0/1/1/1
24	CLA	c	908	40	3/3/20/25	4/37/135/135	-
24	CLA	C	506	-	3/3/20/25	6/37/135/135	-
24	CLA	B	610	-	2/2/20/25	3/37/135/135	-
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
33	LMG	b	625	-	-	8/46/66/70	0/1/1/1
28	GOL	V	207	-	-	4/4/4/4	-
24	CLA	a	408	-	3/3/20/25	10/37/135/135	-
28	GOL	a	412	-	-	4/4/4/4	-
38	HEM	v	202	16	-	0/6/54/54	-
25	PHO	D	401	-	-	5/53/103/103	0/5/6/6
24	CLA	c	914	-	2/2/20/25	5/37/135/135	-
29	LMT	M	103	-	-	11/21/61/61	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	c	902	-	3/3/20/25	5/37/135/135	-
31	PL9	D	407	-	-	9/53/73/73	0/1/1/1
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1
35	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	c	905	40	3/3/20/25	4/37/135/135	-
24	CLA	C	511	3	3/3/20/25	4/37/135/135	-
24	CLA	a	406	40	2/2/20/25	11/37/135/135	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
29	LMT	e	102	-	-	9/21/61/61	0/2/2/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	B	629	-	-	3/4/4/4	-
24	CLA	B	616	-	3/3/20/25	11/37/135/135	-
24	CLA	A	405	-	3/3/20/25	4/37/135/135	-
24	CLA	b	621	-	3/3/20/25	9/37/135/135	-
24	CLA	D	404	-	1/1/20/25	0/37/135/135	-
28	GOL	c	923	-	-	0/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	O	302	-	-	0/4/4/4	-
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	B	604	-	3/3/20/25	4/37/135/135	-
29	LMT	b	626	-	-	5/17/37/61	0/1/1/2
24	CLA	A	407	40	2/2/20/25	6/37/135/135	-
28	GOL	B	630	-	-	4/4/4/4	-
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
28	GOL	a	413	-	-	2/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
36	LHG	L	101	-	-	16/53/53/53	-
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
24	CLA	C	504	40	3/3/20/25	7/37/135/135	-
28	GOL	b	633	-	-	2/4/4/4	-
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	C	503	-	3/3/20/25	2/37/135/135	-
37	DGD	c	916	-	-	12/51/91/95	0/2/2/2
28	GOL	a	419	34	-	3/4/4/4	-
24	CLA	b	617	-	3/3/20/25	4/37/135/135	-
37	DGD	H	102	-	-	9/51/91/95	0/2/2/2
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-
24	CLA	b	618	-	3/3/20/25	3/37/135/135	-
24	CLA	b	612	40	3/3/20/25	1/37/135/135	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
36	LHG	D	409	-	-	11/53/53/53	-
36	LHG	D	410	-	-	18/53/53/53	-
29	LMT	A	415	-	-	5/21/61/61	0/2/2/2
28	GOL	B	636	-	-	2/4/4/4	-
24	CLA	c	911	-	3/3/20/25	7/37/135/135	-
37	DGD	C	517	-	-	19/51/91/95	0/2/2/2
28	GOL	V	205	-	-	0/4/4/4	-
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
29	LMT	b	602	-	-	7/17/37/61	0/1/1/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	906	-	2/2/20/25	8/37/135/135	-
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
24	CLA	B	613	-	3/3/20/25	5/37/135/135	-
24	CLA	c	909	-	3/3/20/25	7/37/135/135	-
24	CLA	c	903	-	2/2/20/25	5/37/135/135	-
33	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
24	CLA	C	513	-	3/3/20/25	8/37/135/135	-
28	GOL	b	630	-	-	0/4/4/4	-
33	LMG	c	920	-	-	5/46/66/70	0/1/1/1
33	LMG	c	919	-	-	12/46/66/70	0/1/1/1

The worst 5 of 1137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	910	CLA	C3B-C2B	6.68	1.49	1.40
24	A	406	CLA	C3B-C2B	6.68	1.49	1.40
24	c	912	CLA	C3B-C2B	6.65	1.49	1.40
25	d	403	PHO	C3C-C2C	6.64	1.50	1.36
24	C	509	CLA	C3B-C2B	6.59	1.49	1.40

The worst 5 of 2222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	405	CLA	C4A-NA-C1A	-7.75	103.22	106.71
25	d	403	PHO	CMD-C2D-C1D	7.30	136.30	125.06
24	b	608	CLA	C4A-NA-C1A	-7.14	103.50	106.71
24	B	606	CLA	CHD-C4C-C3C	-7.13	114.36	124.84
24	B	607	CLA	C4A-NA-C1A	-7.03	103.54	106.71

5 of 192 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND

5 of 1314 torsion outliers are listed below:

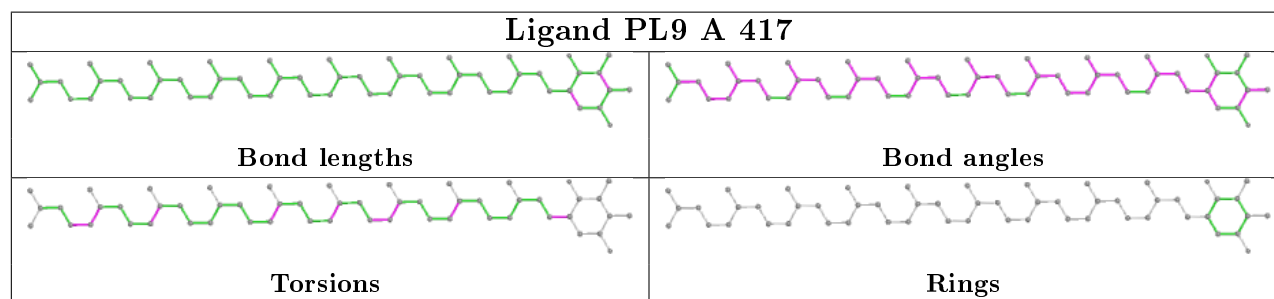
Mol	Chain	Res	Type	Atoms
28	V	204	GOL	C1-C2-C3-O3
27	A	414	SQD	O6-C44-C45-O47
27	A	414	SQD	O5-C5-C6-S
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6

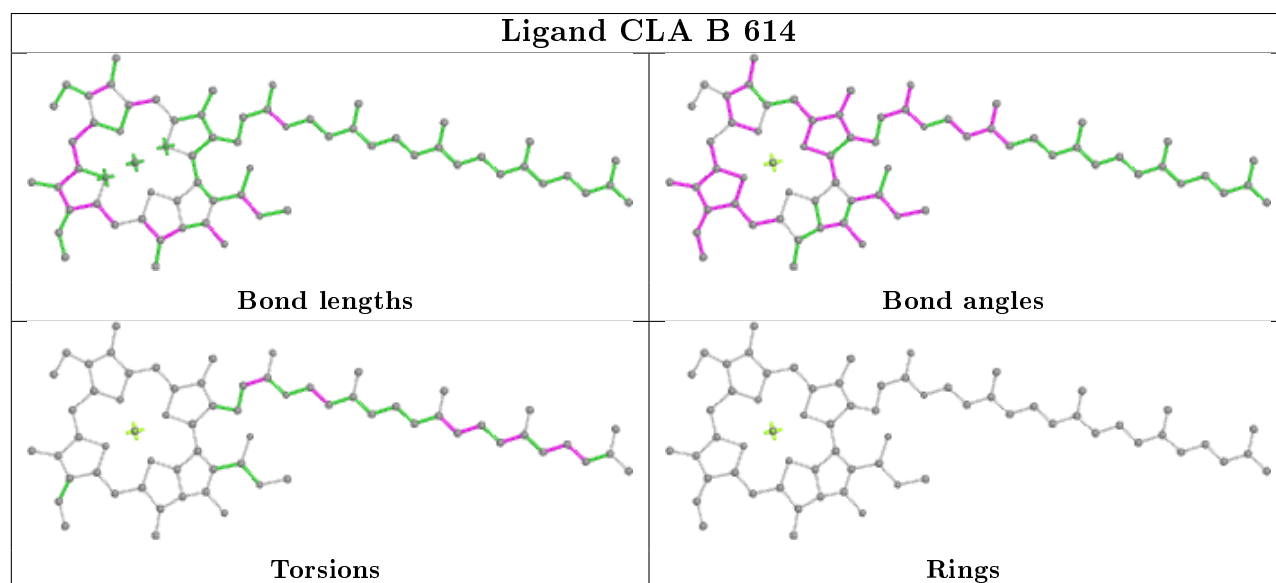
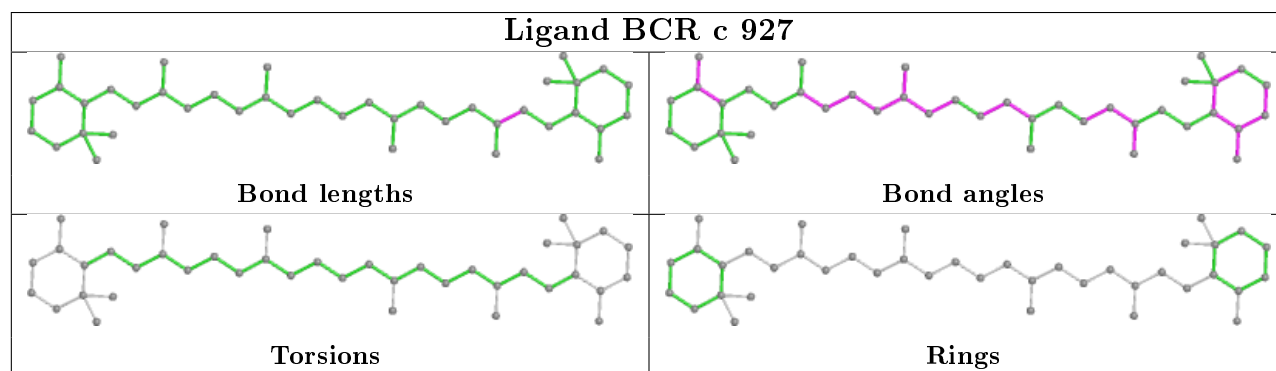
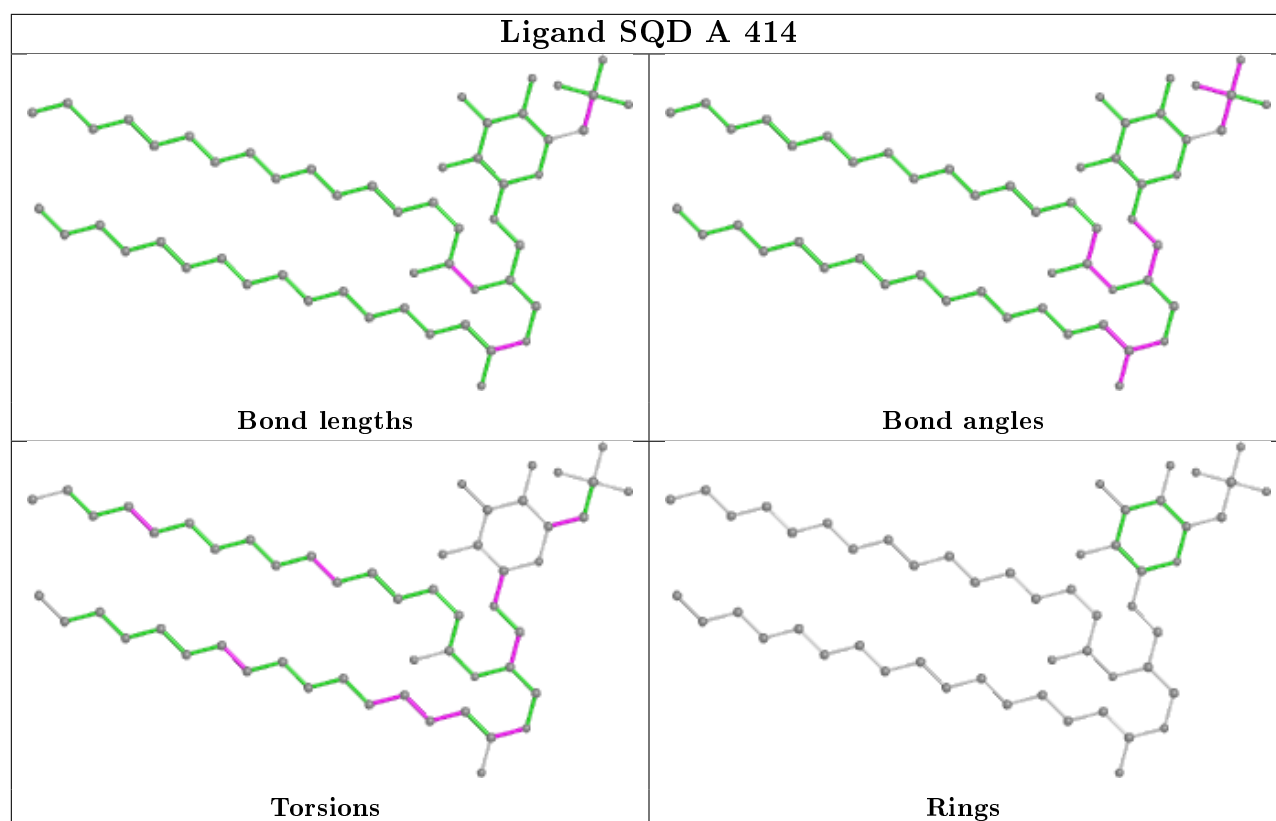
There are no ring outliers.

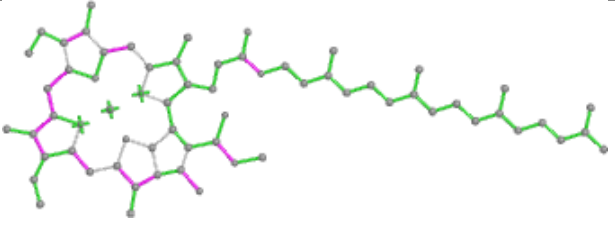
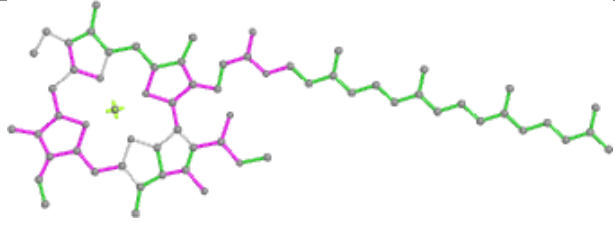
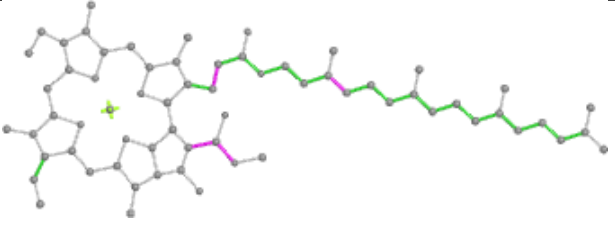
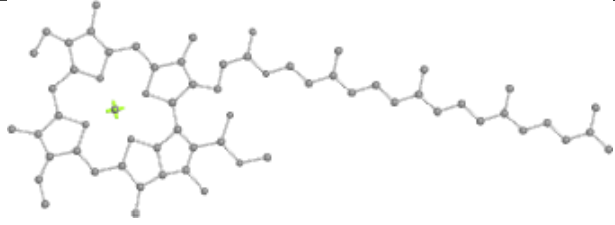
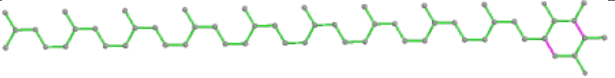
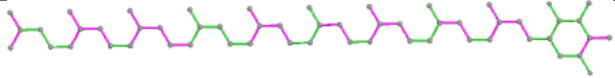
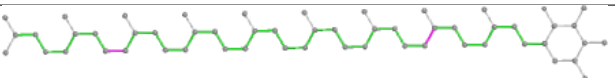
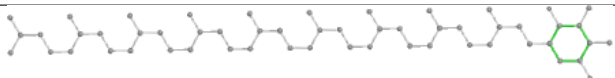
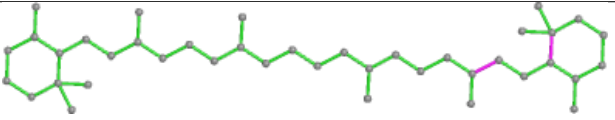
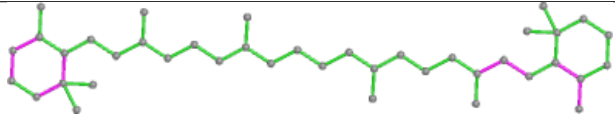
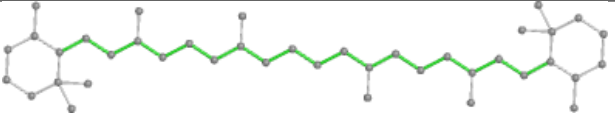
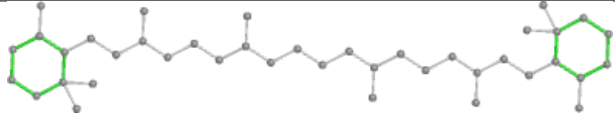
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	f	102	SQD	0	1

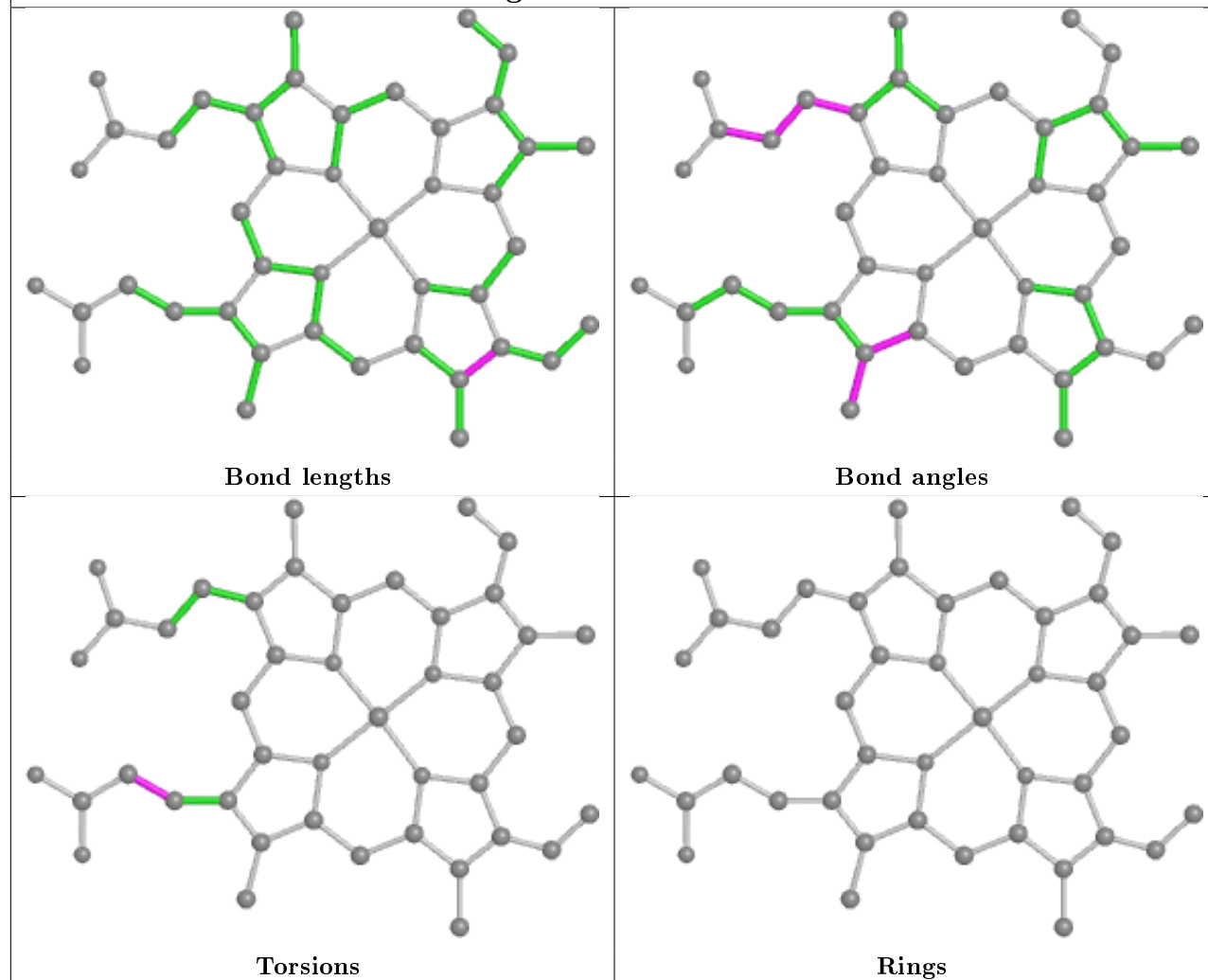
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



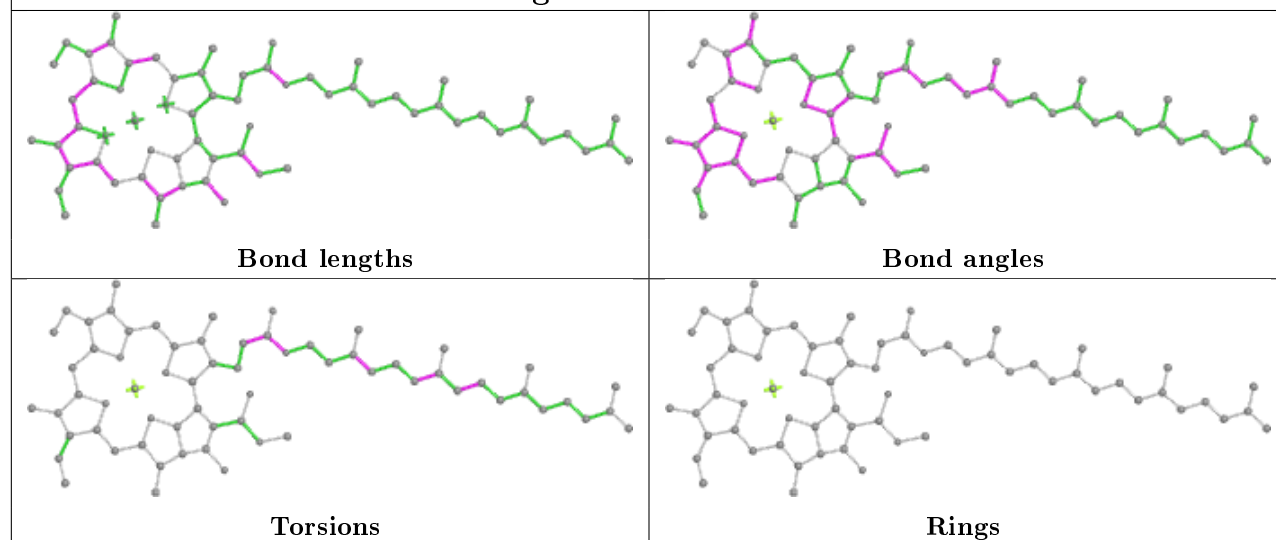


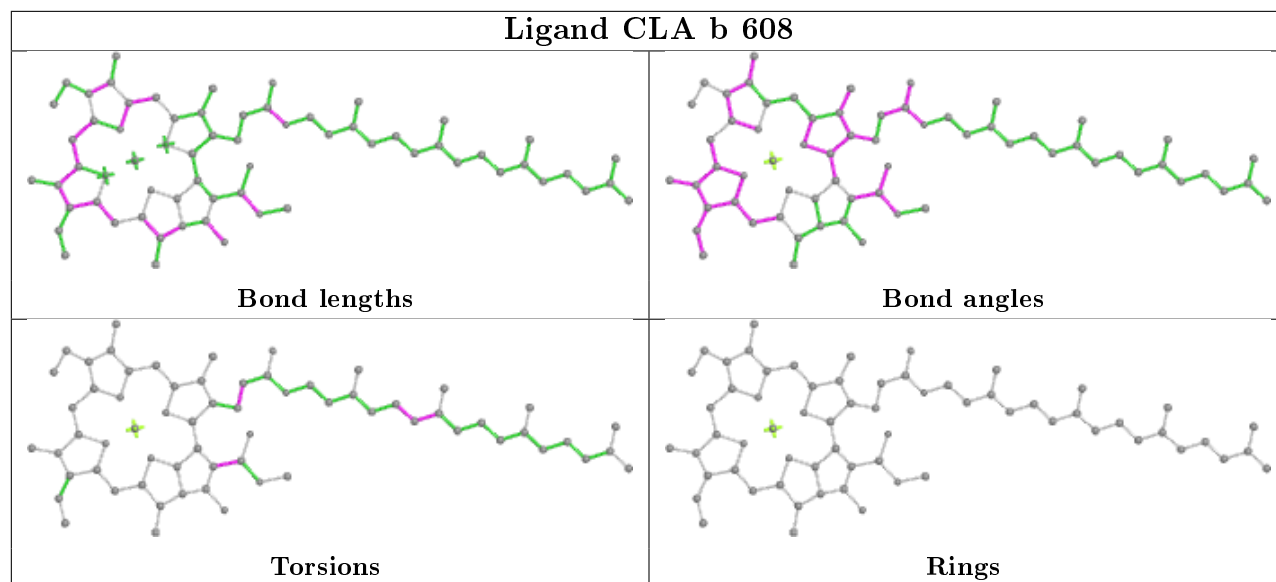
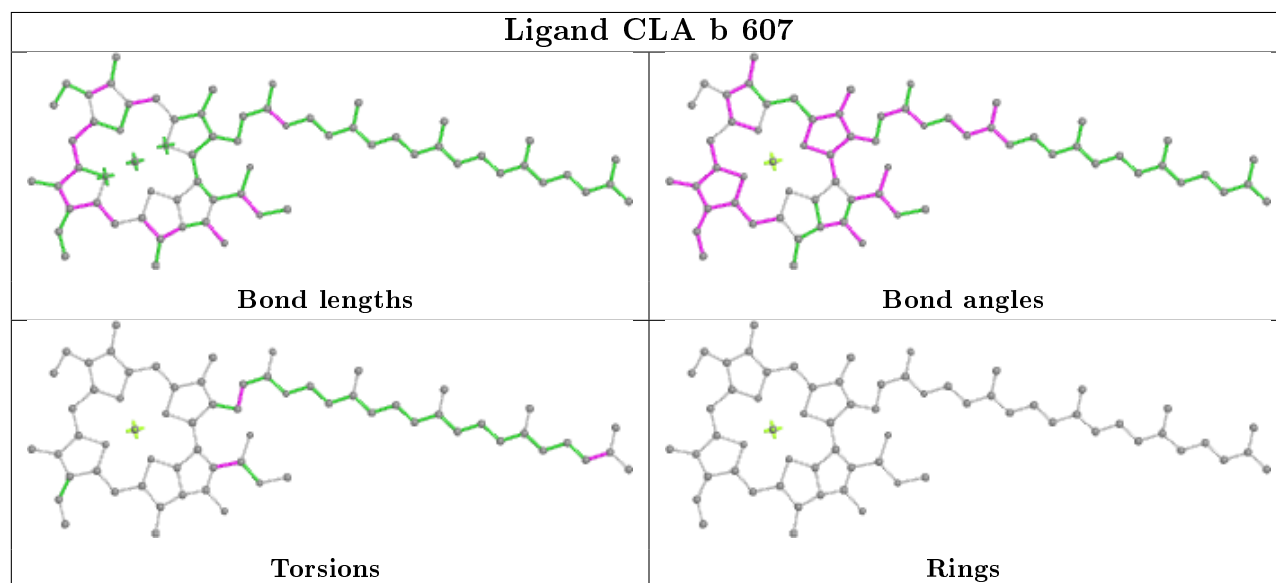
Ligand CLA B 606	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 408	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 624	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

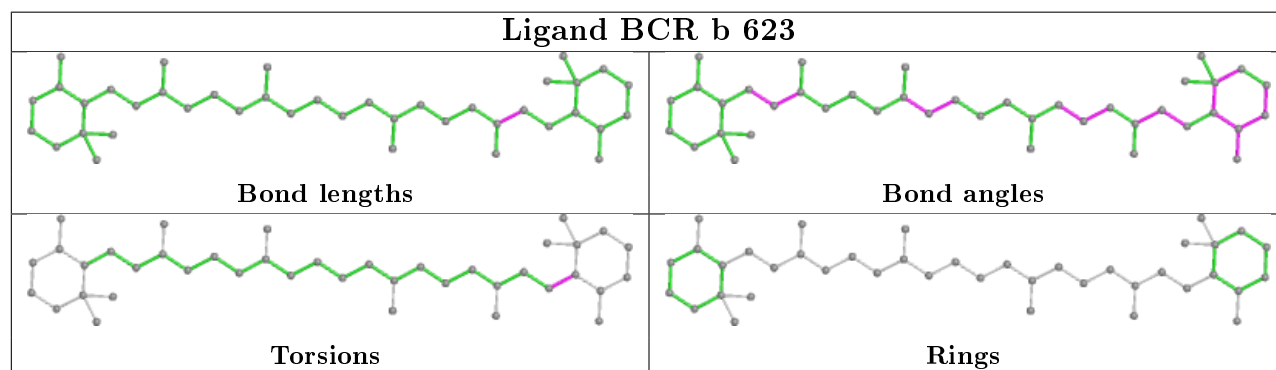
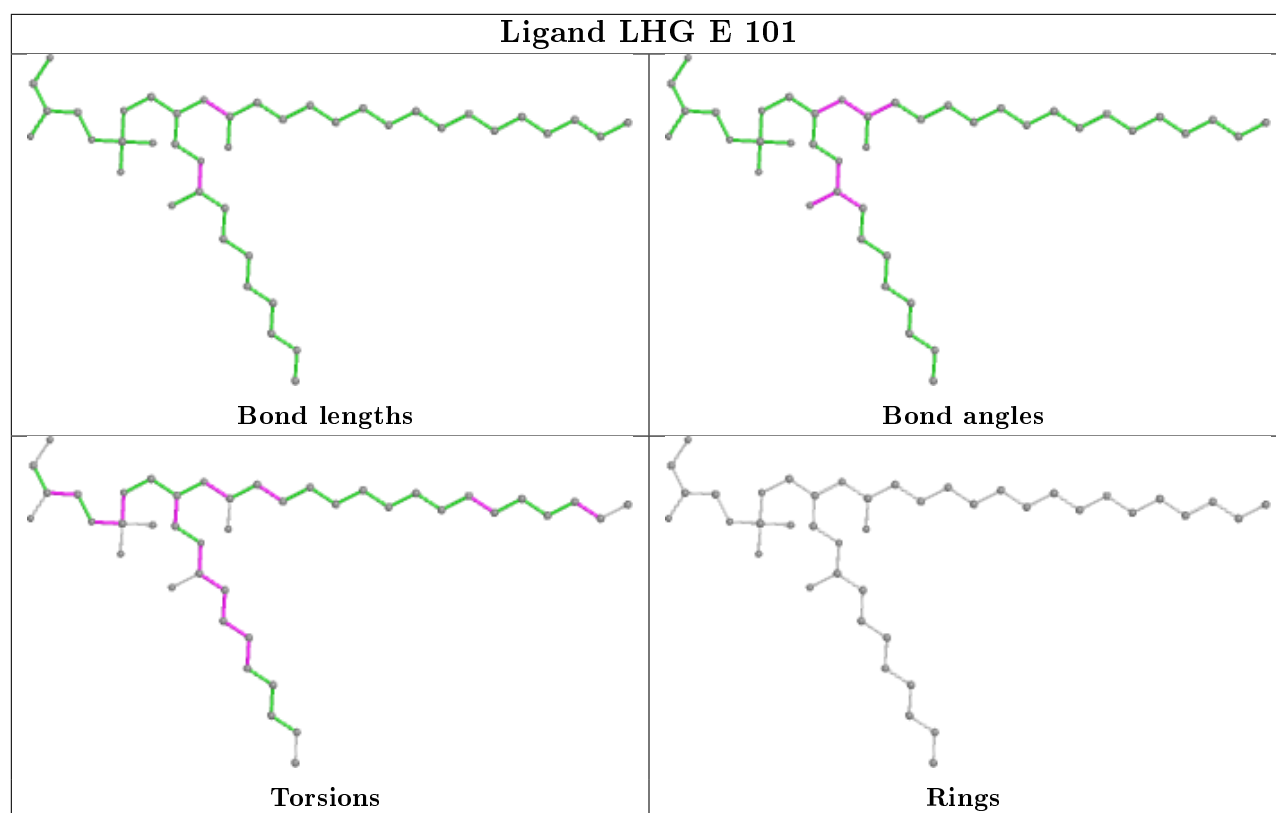
## Ligand HEM f 101

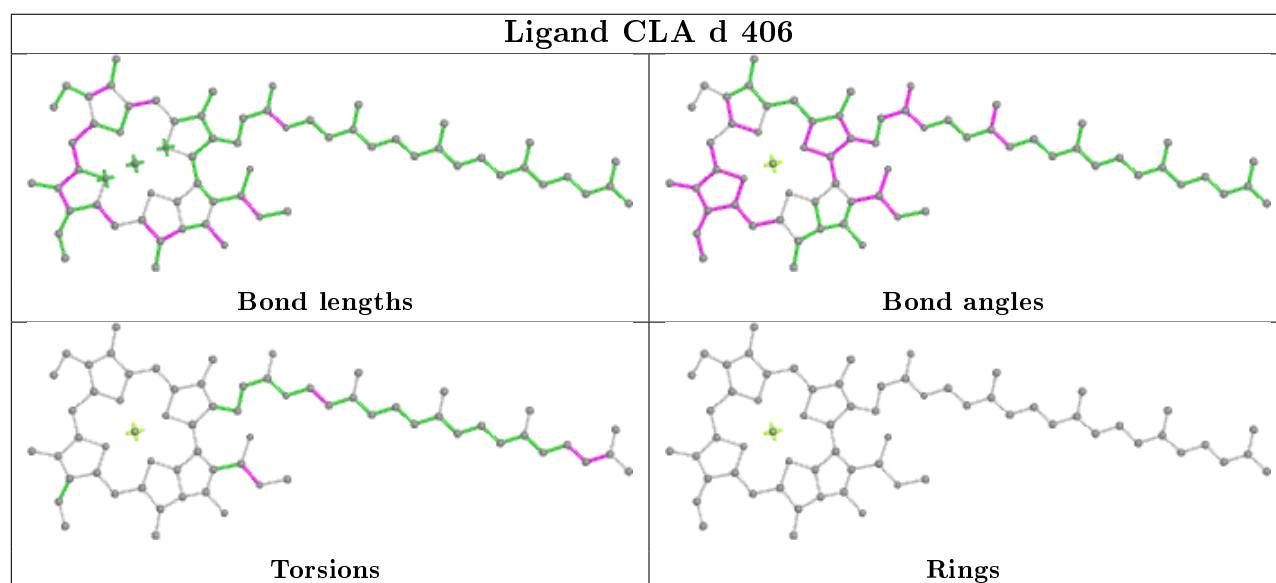
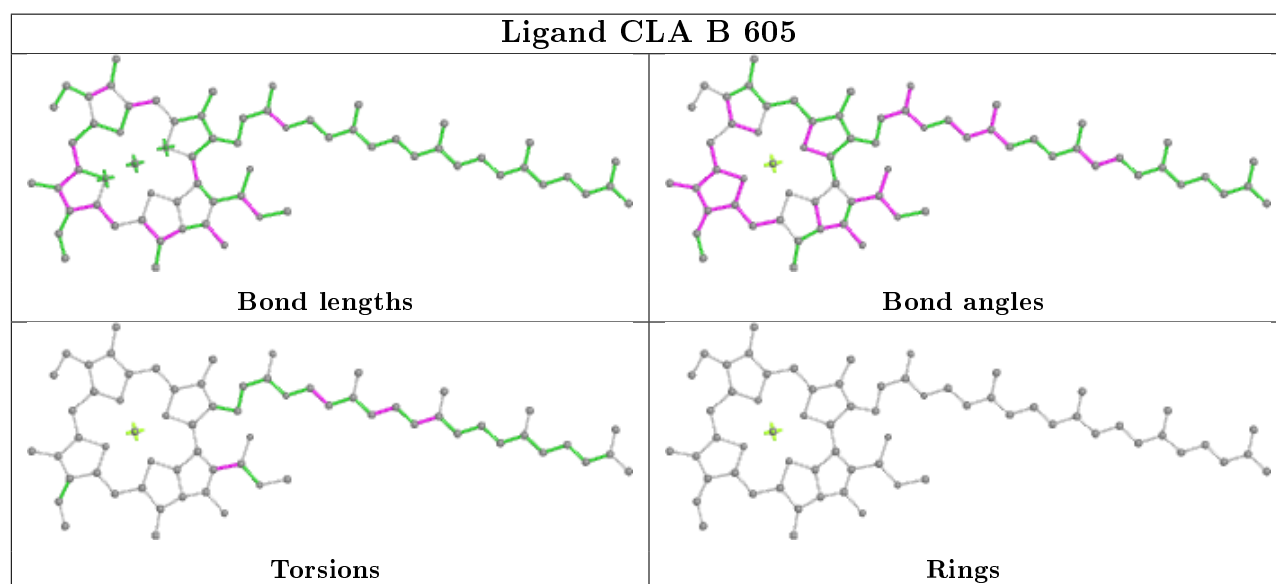
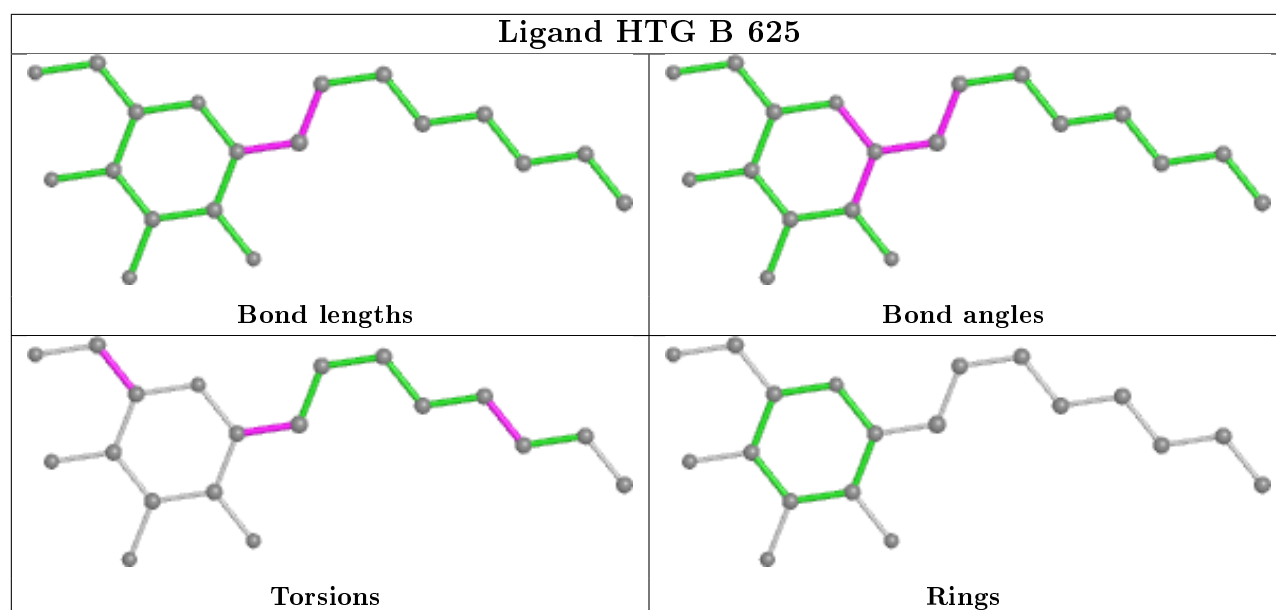


## Ligand CLA C 510

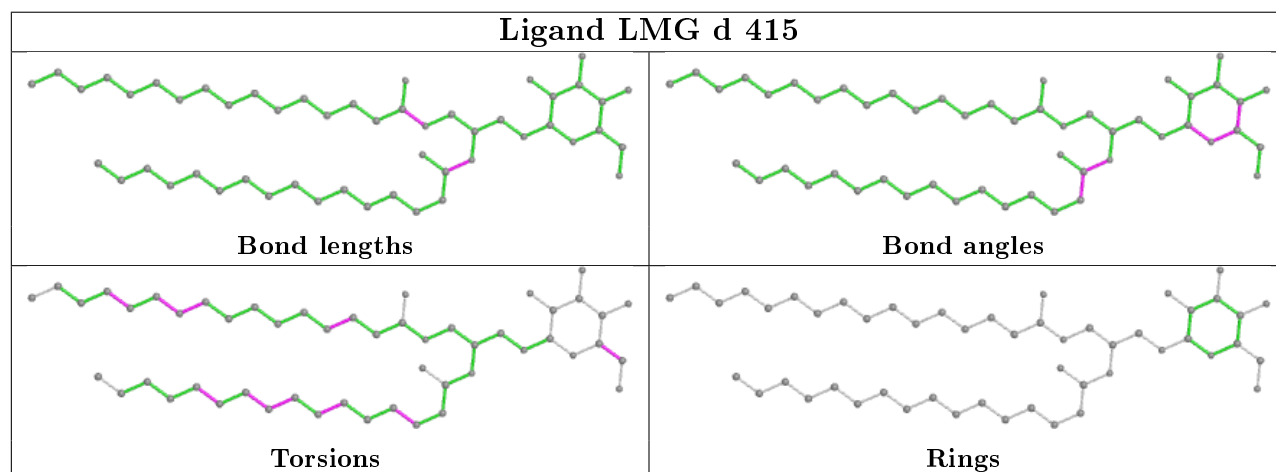
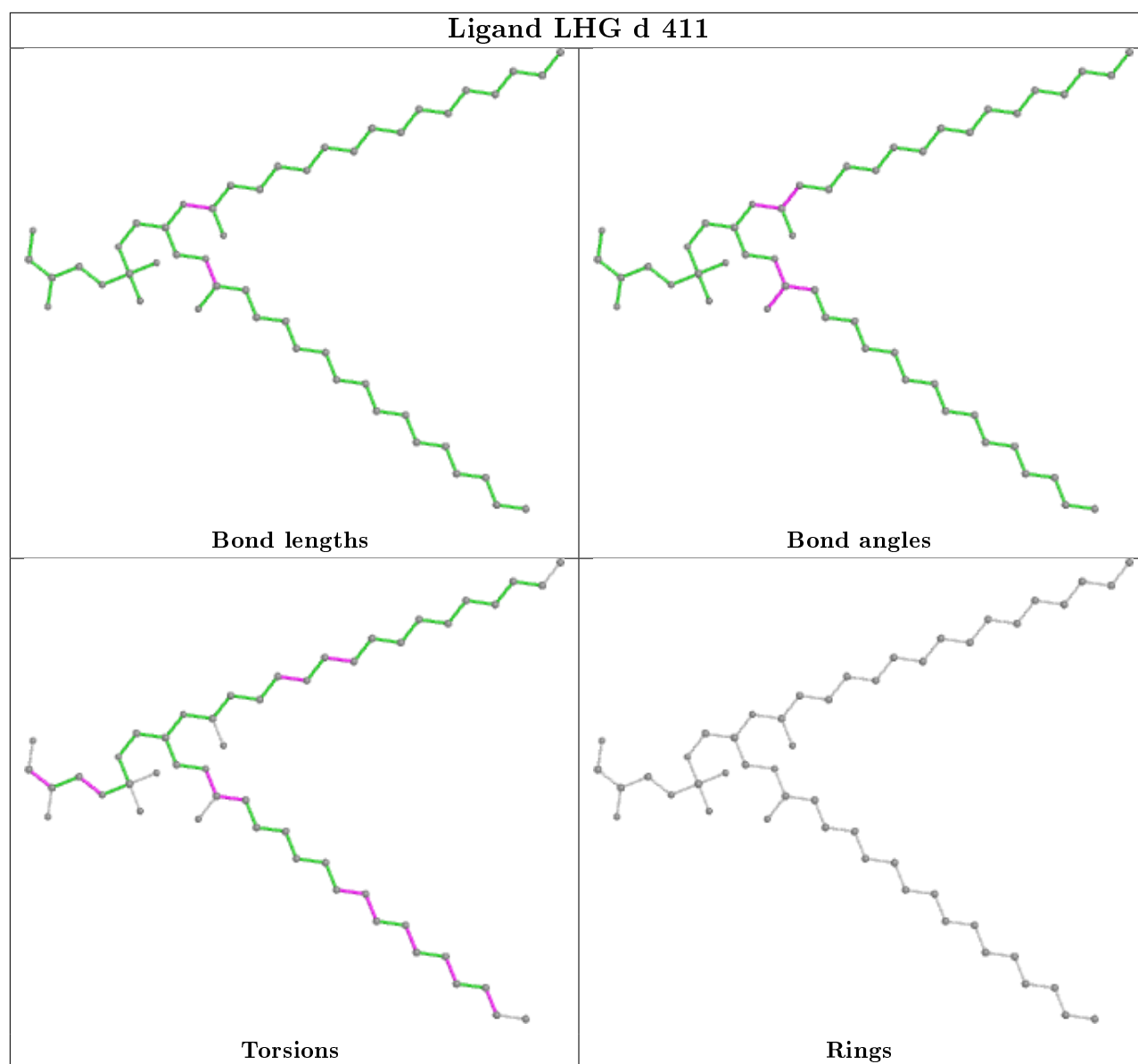


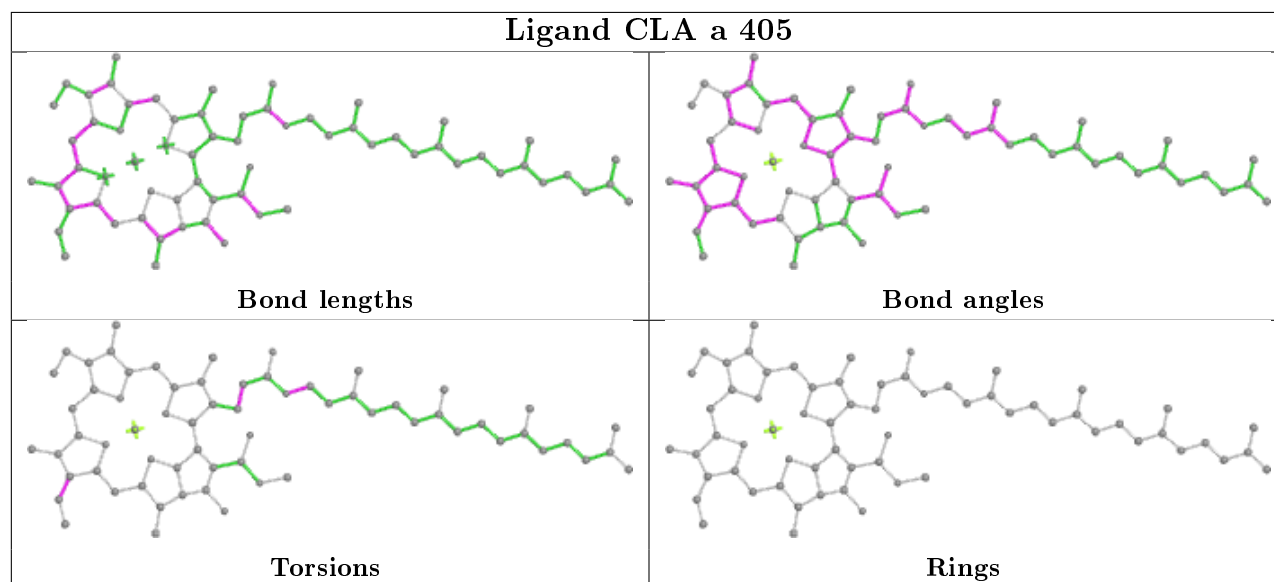
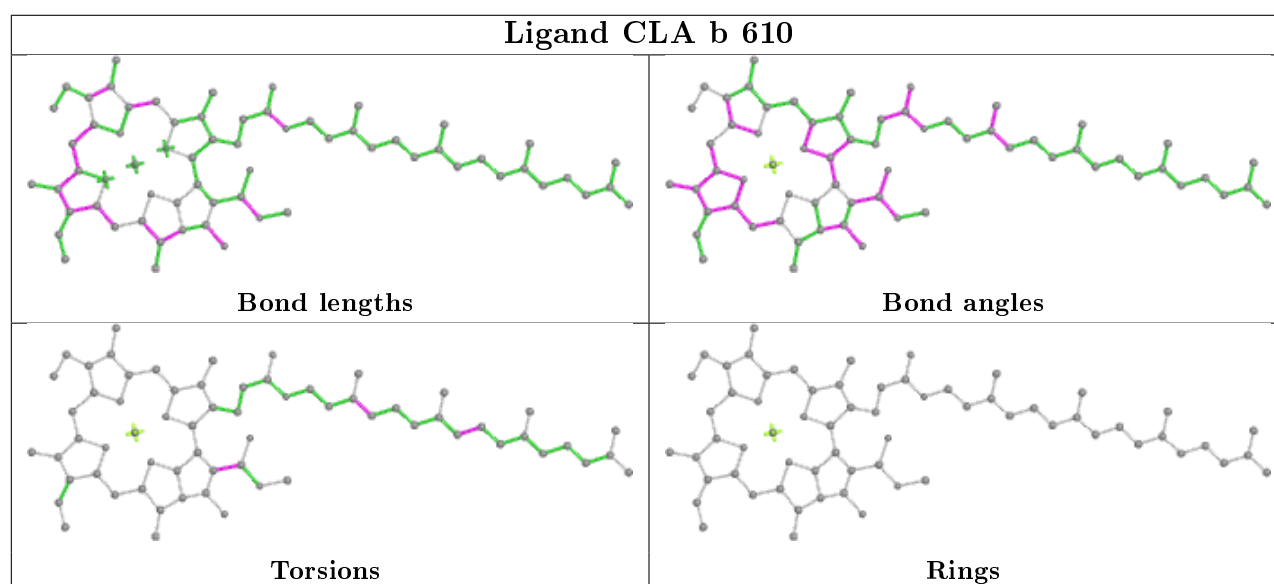
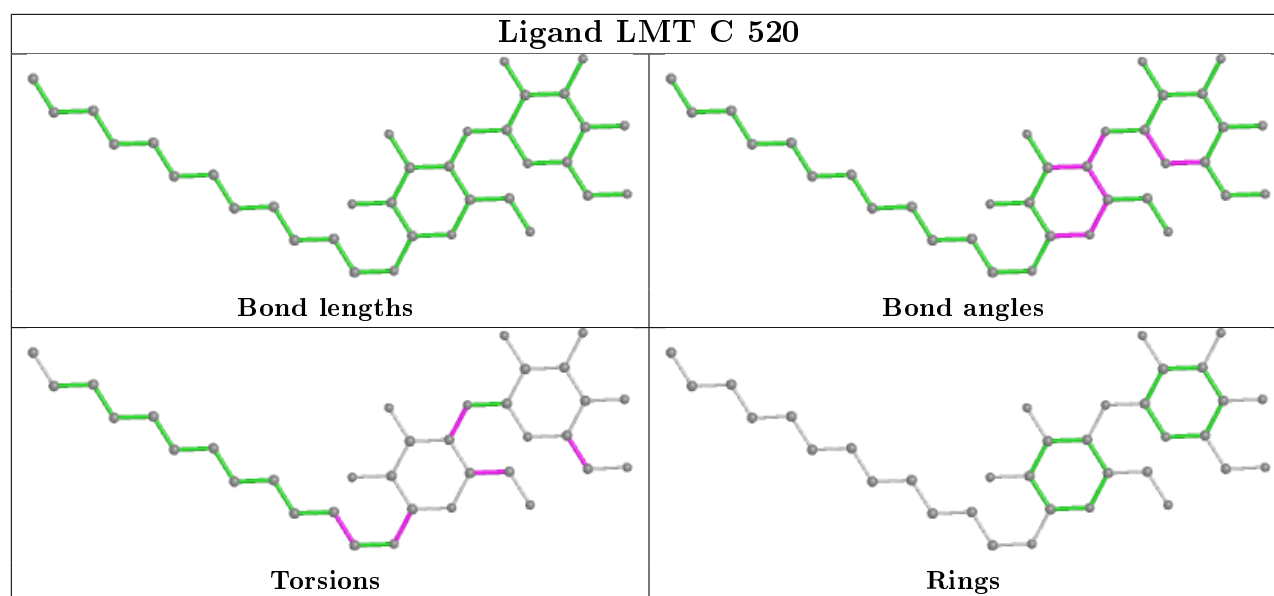
**Ligand CLA b 608****Ligand CLA b 607**

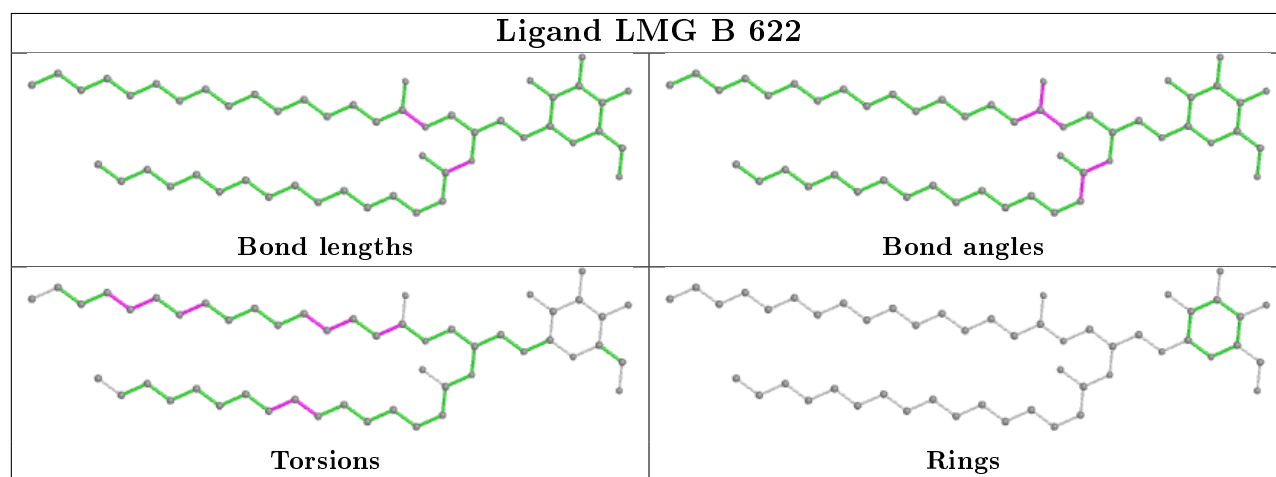
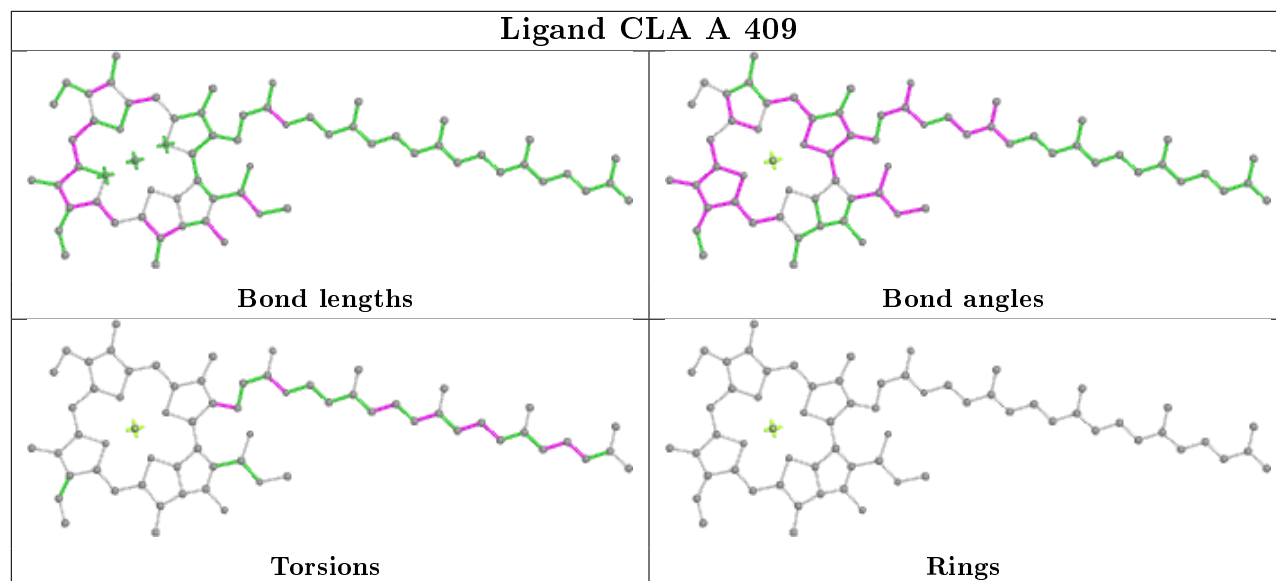
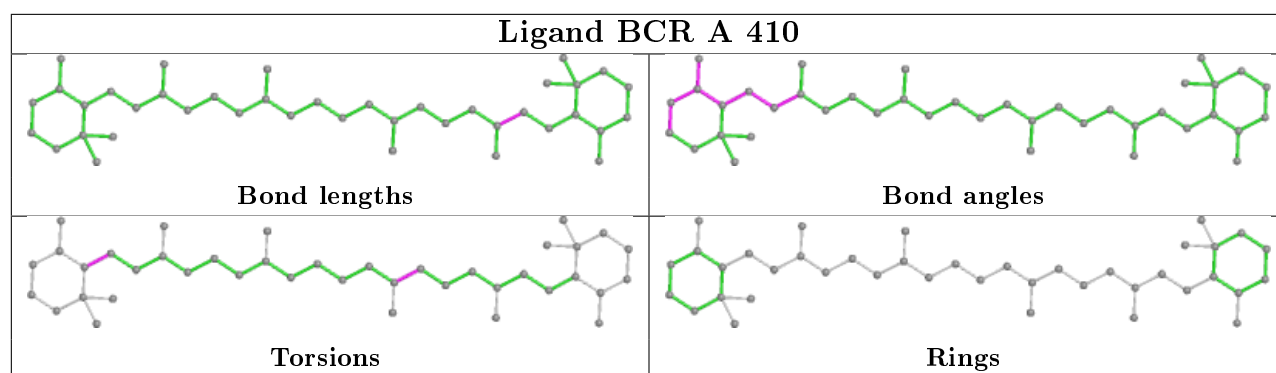


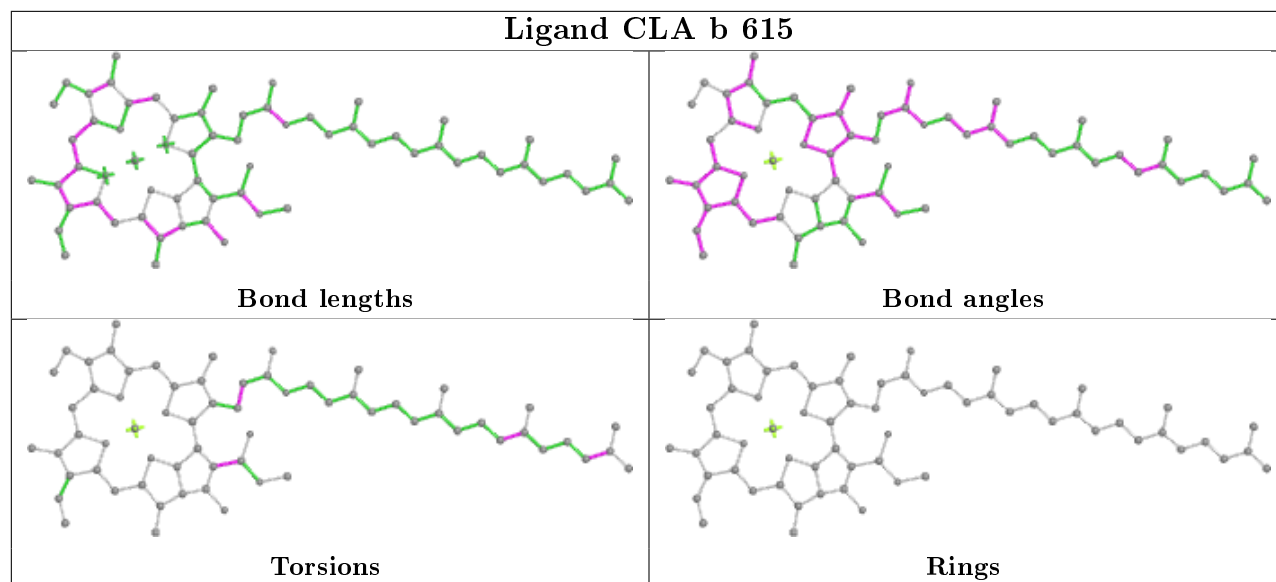
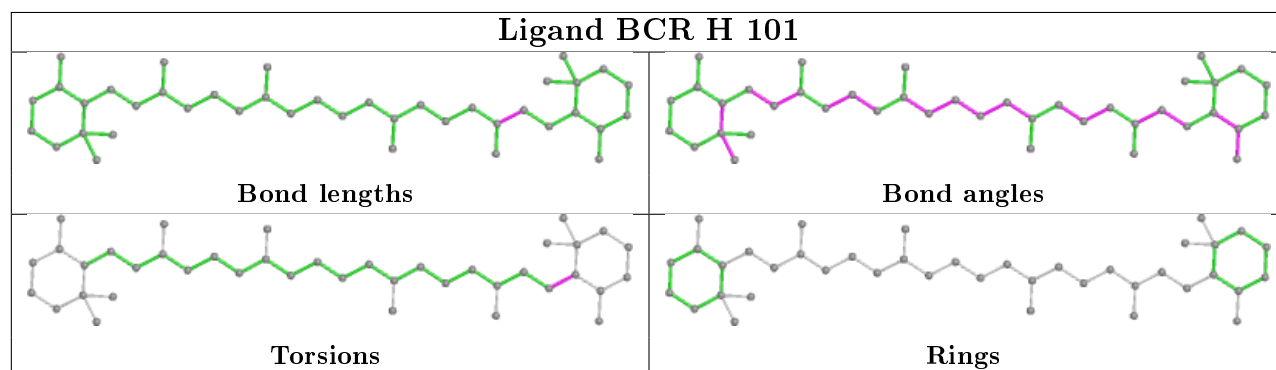
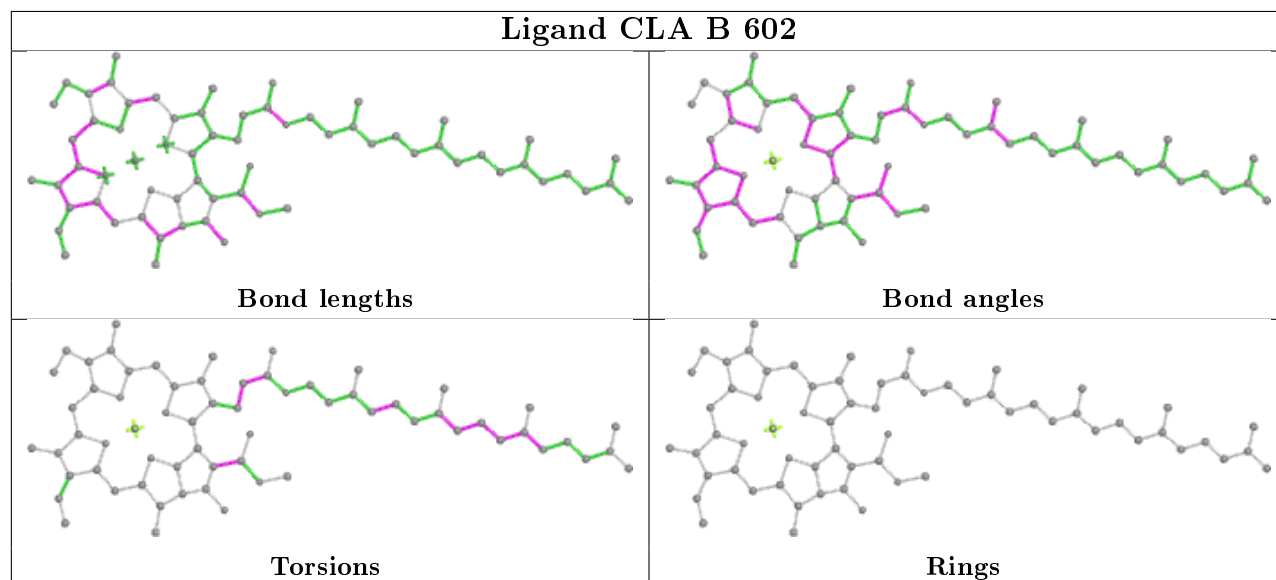


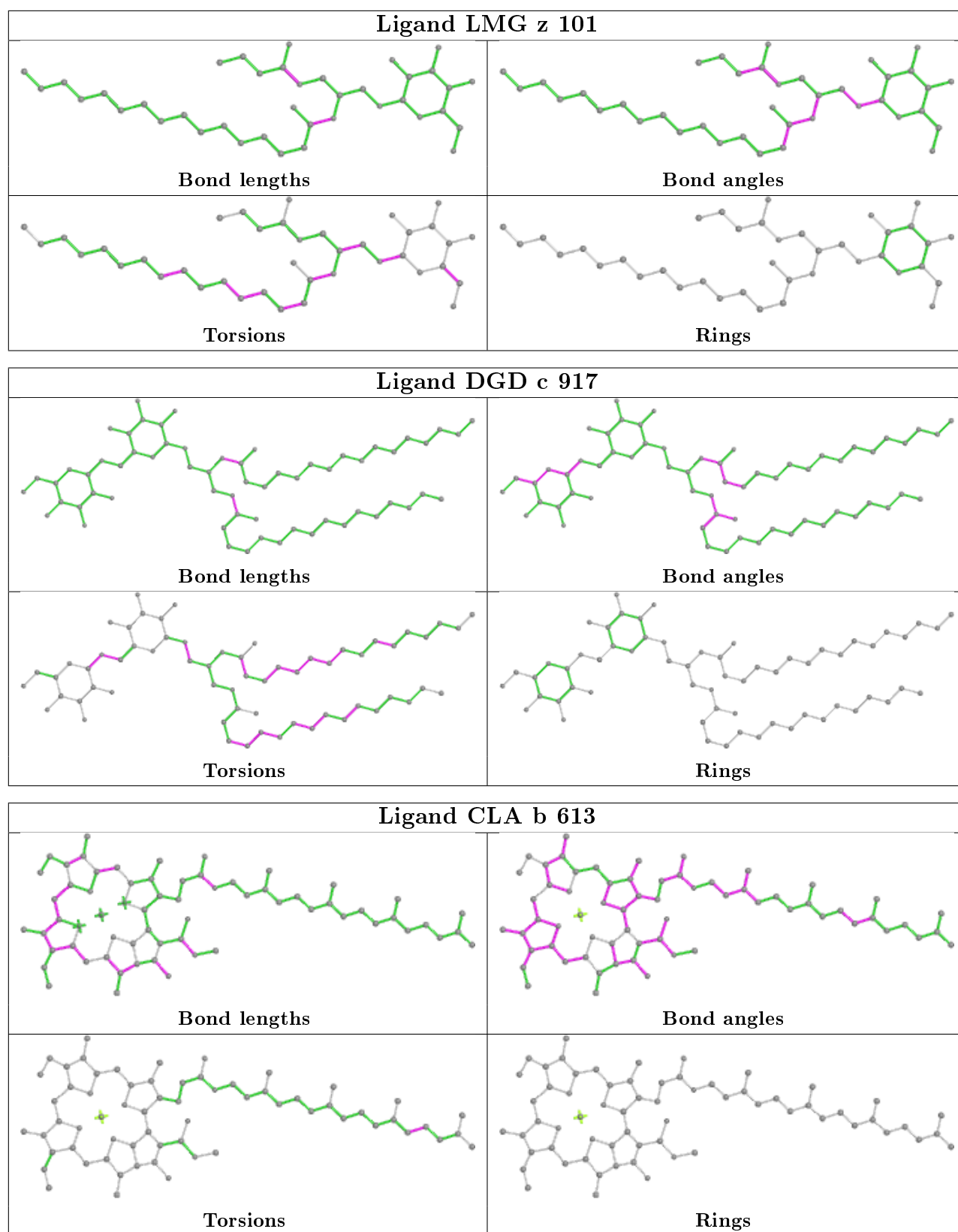


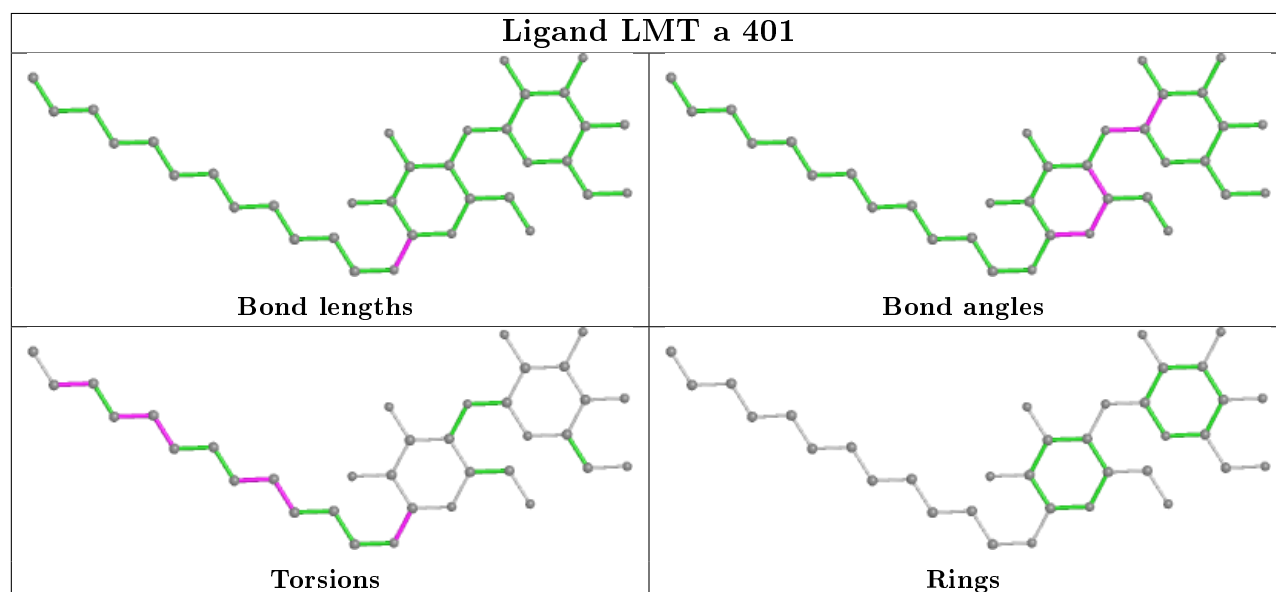
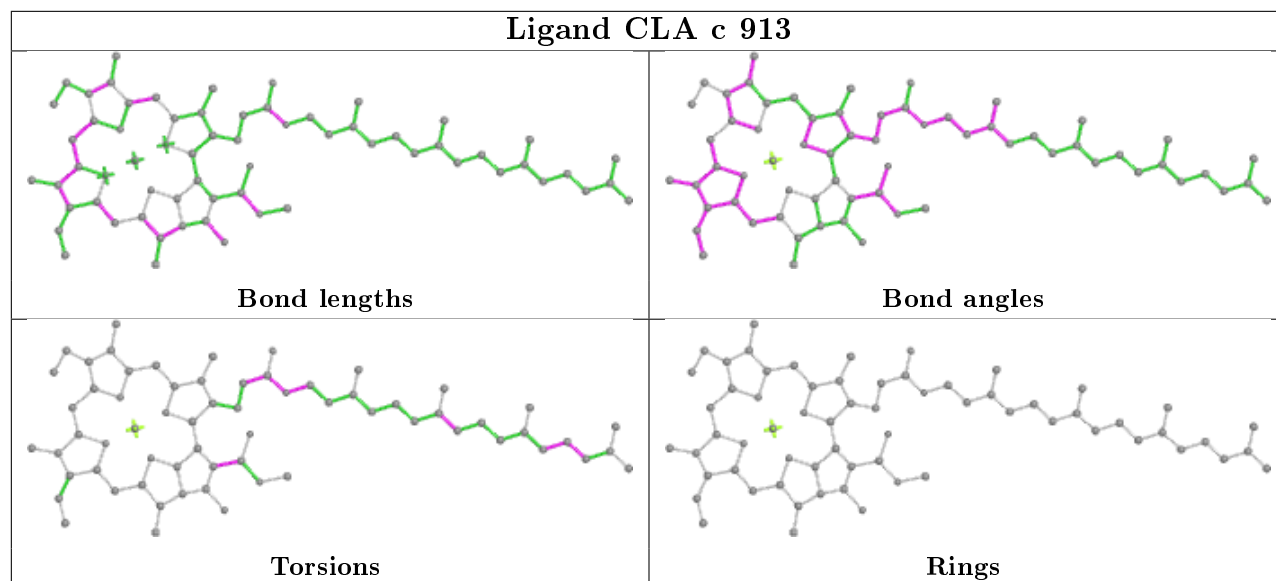
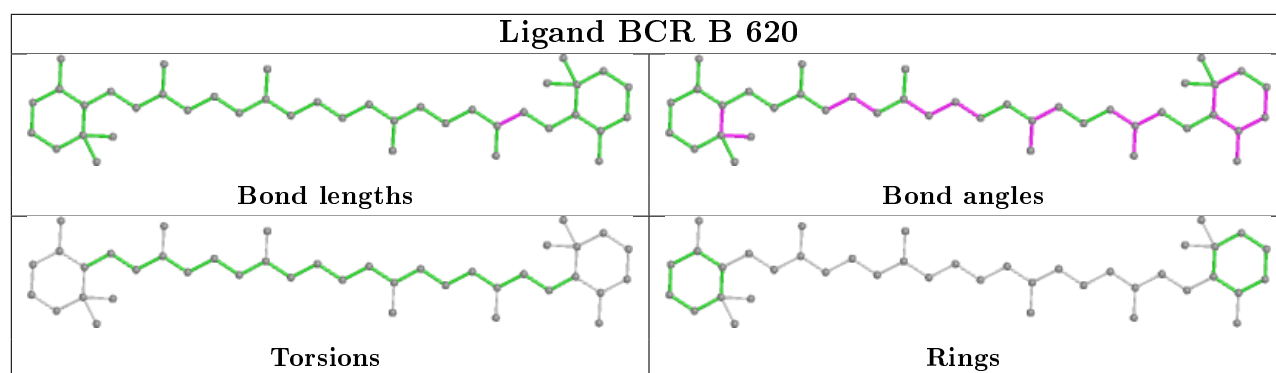


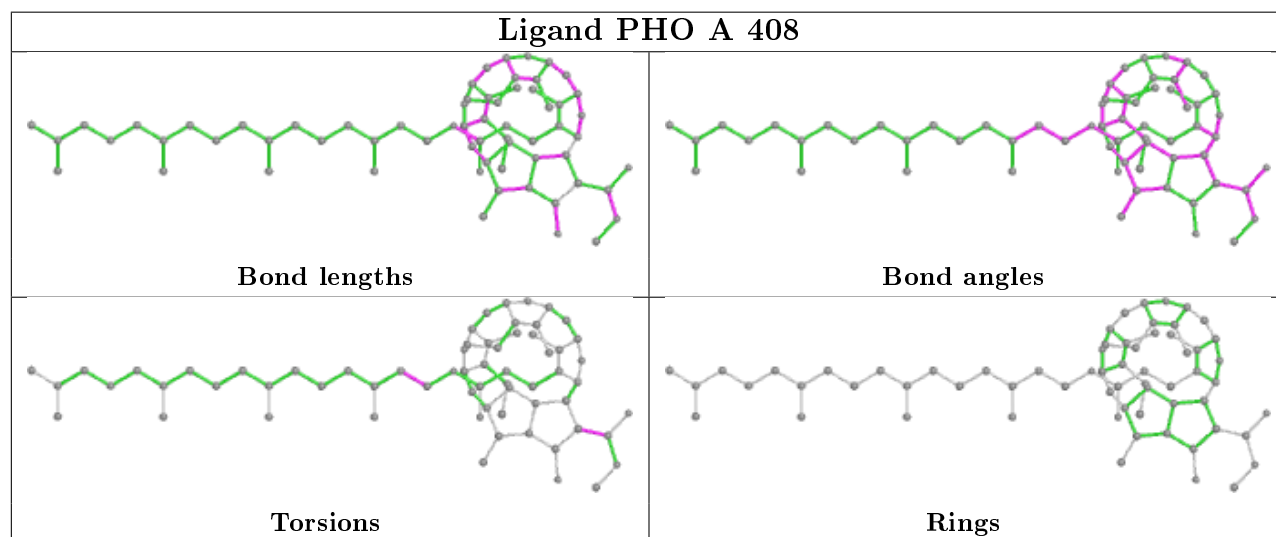
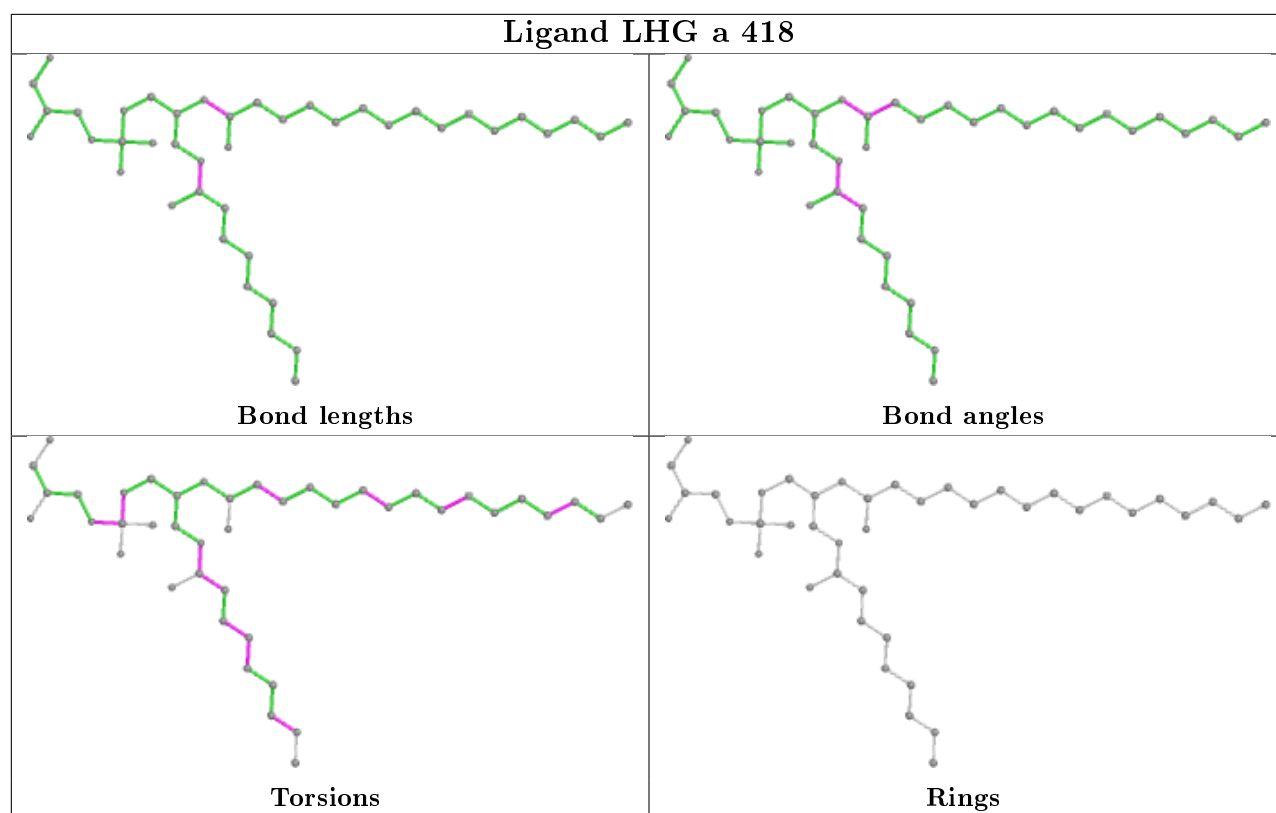




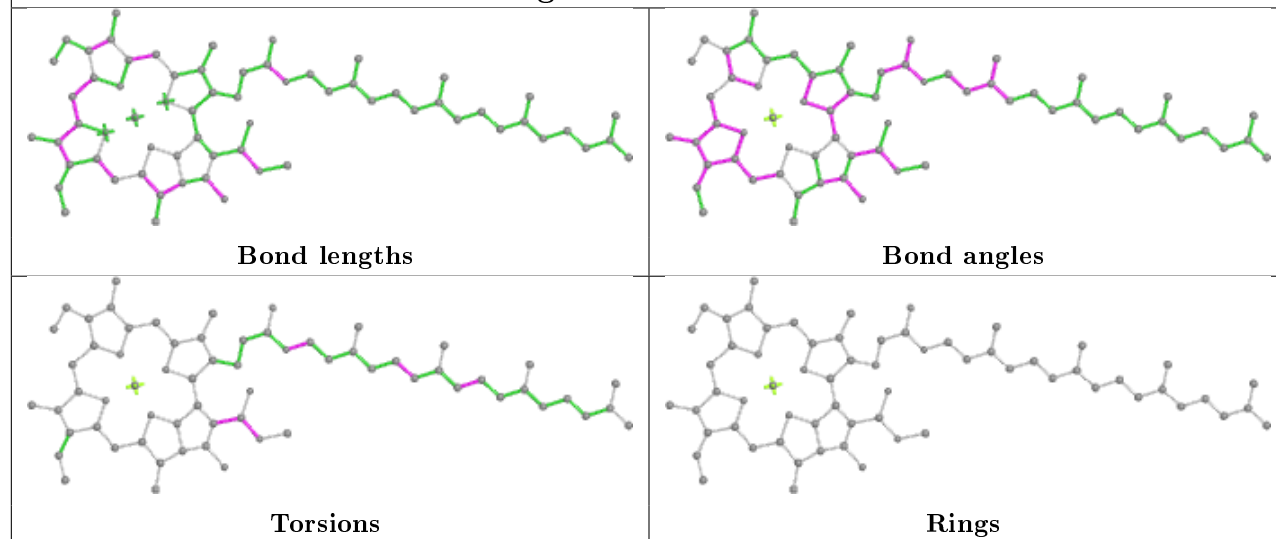
**Ligand CLA b 615****Ligand BCR H 101****Ligand CLA B 602**



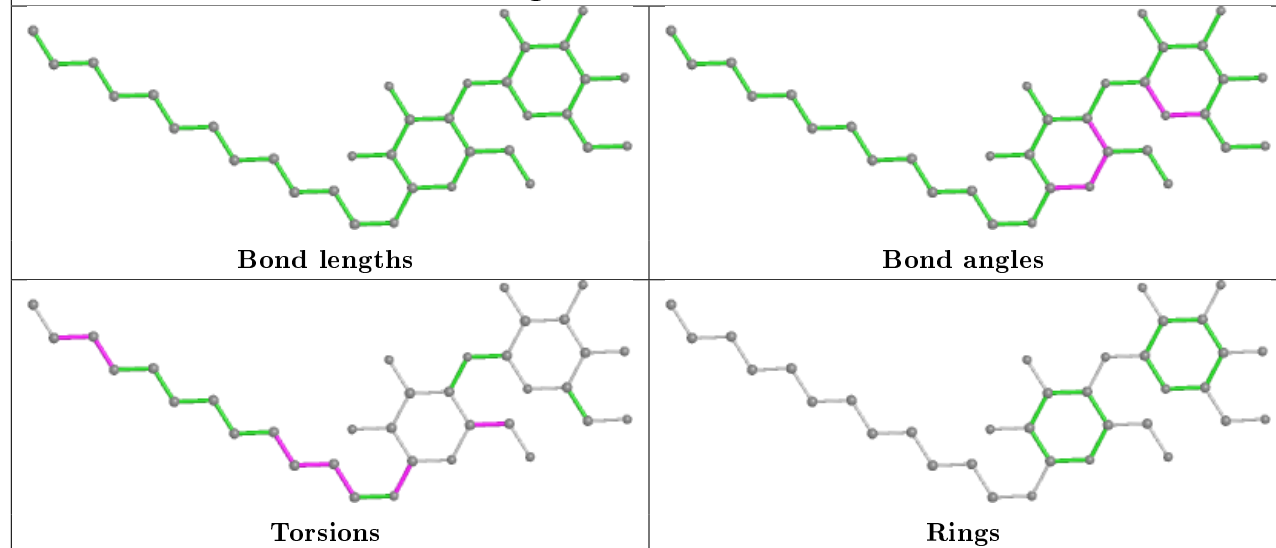




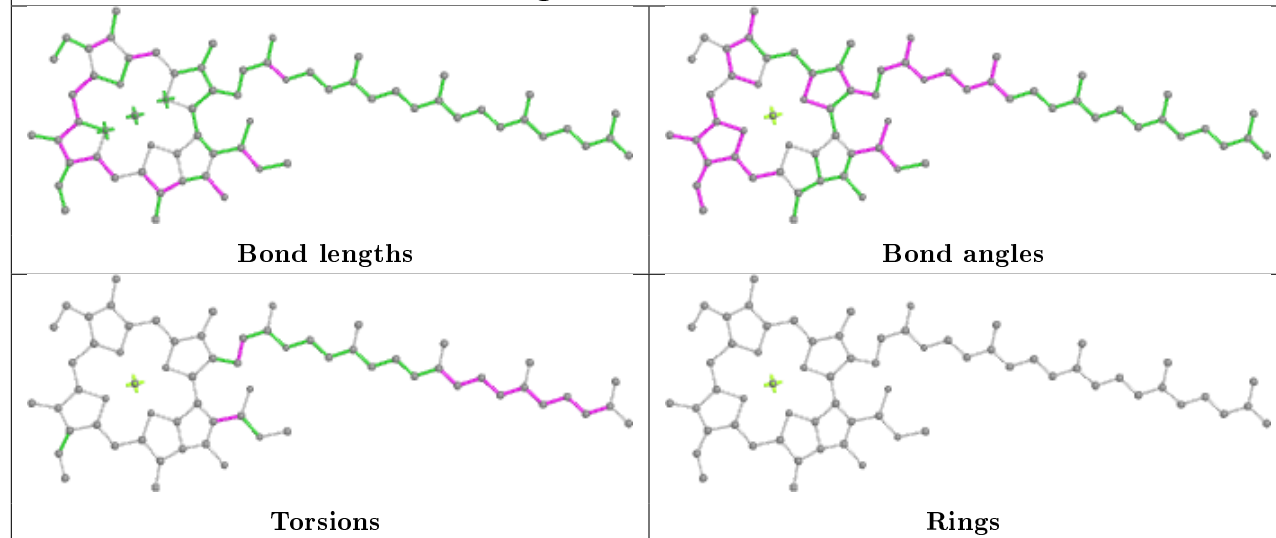
## Ligand CLA c 904



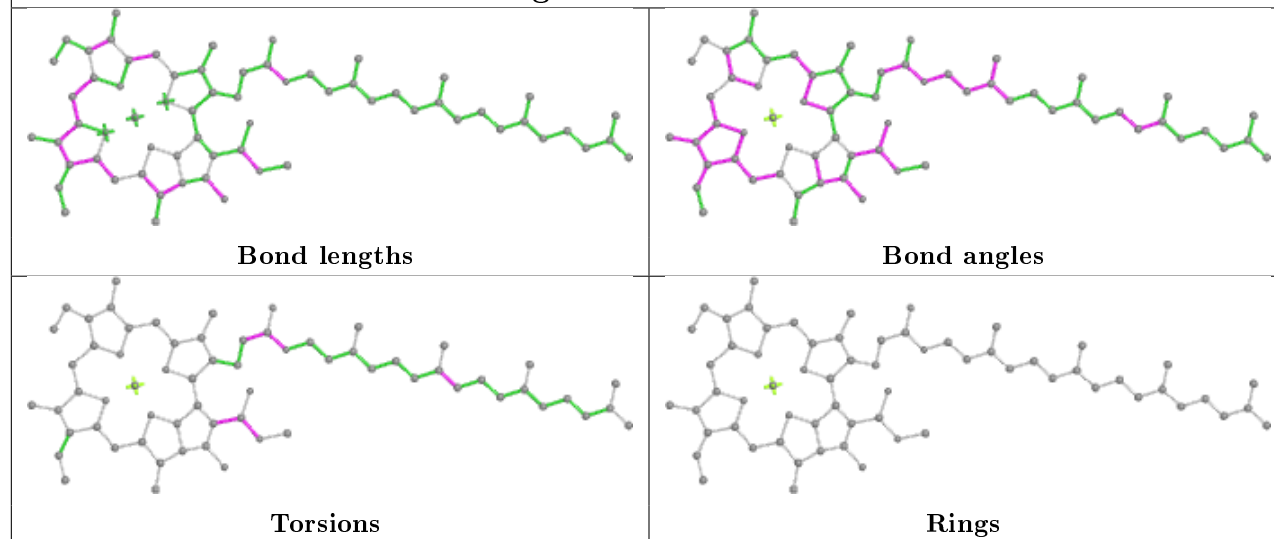
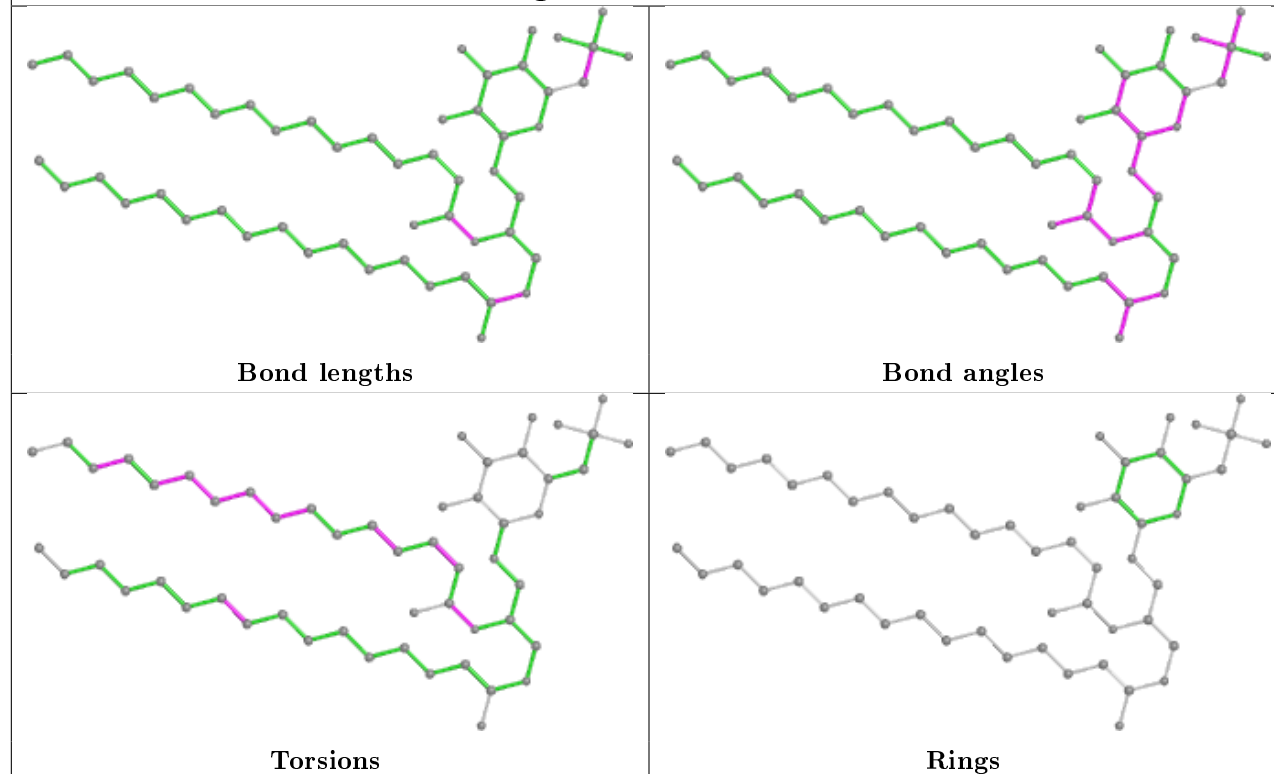
## Ligand LMT m 103



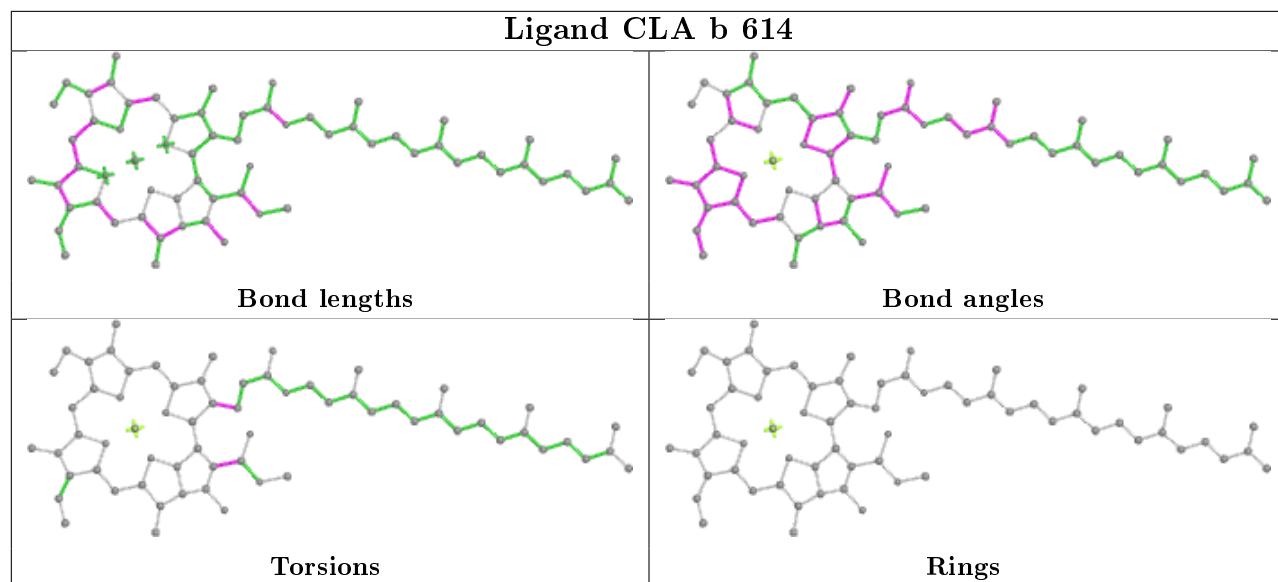
## Ligand CLA b 611



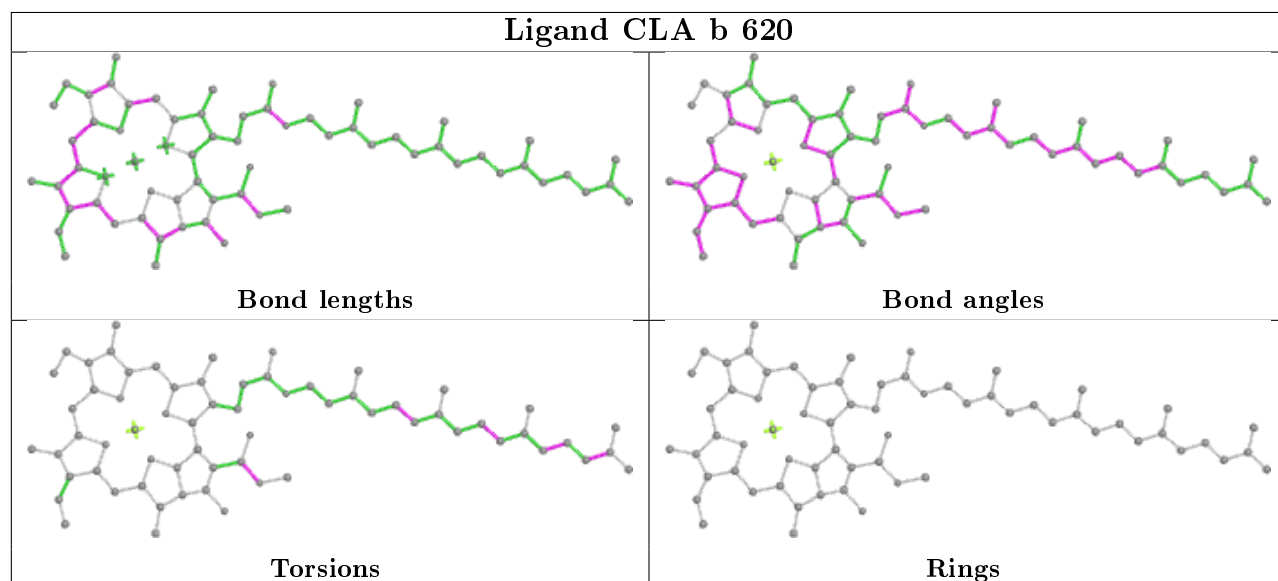


**Ligand CLA C 512****Ligand SQD A 411**

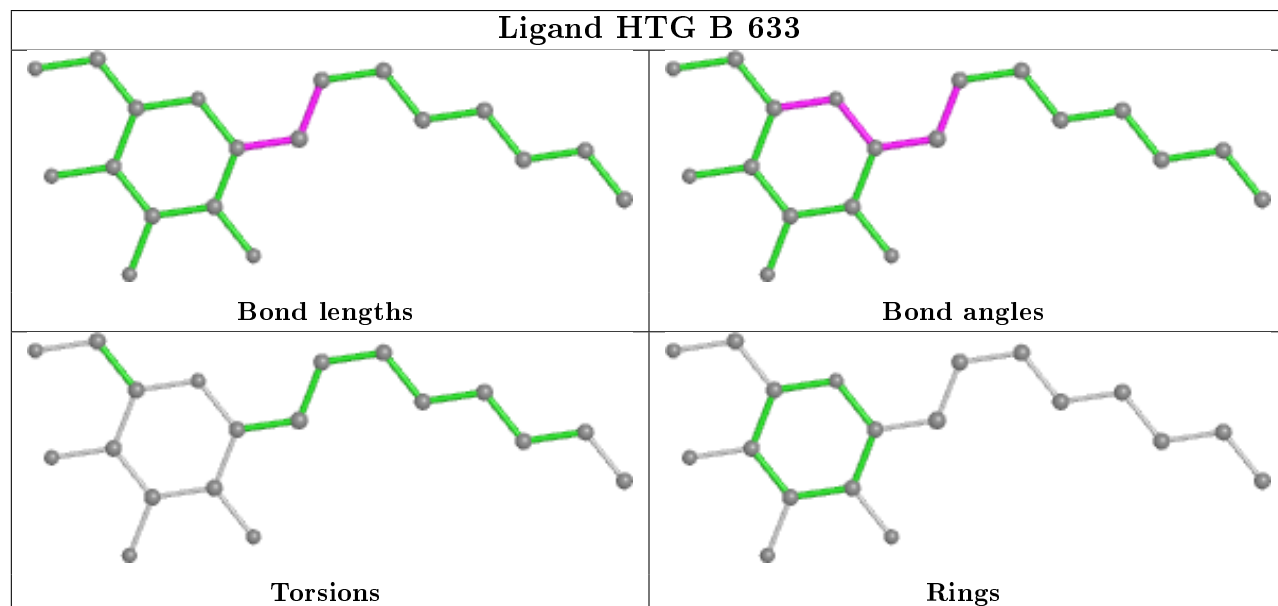
## Ligand CLA b 614

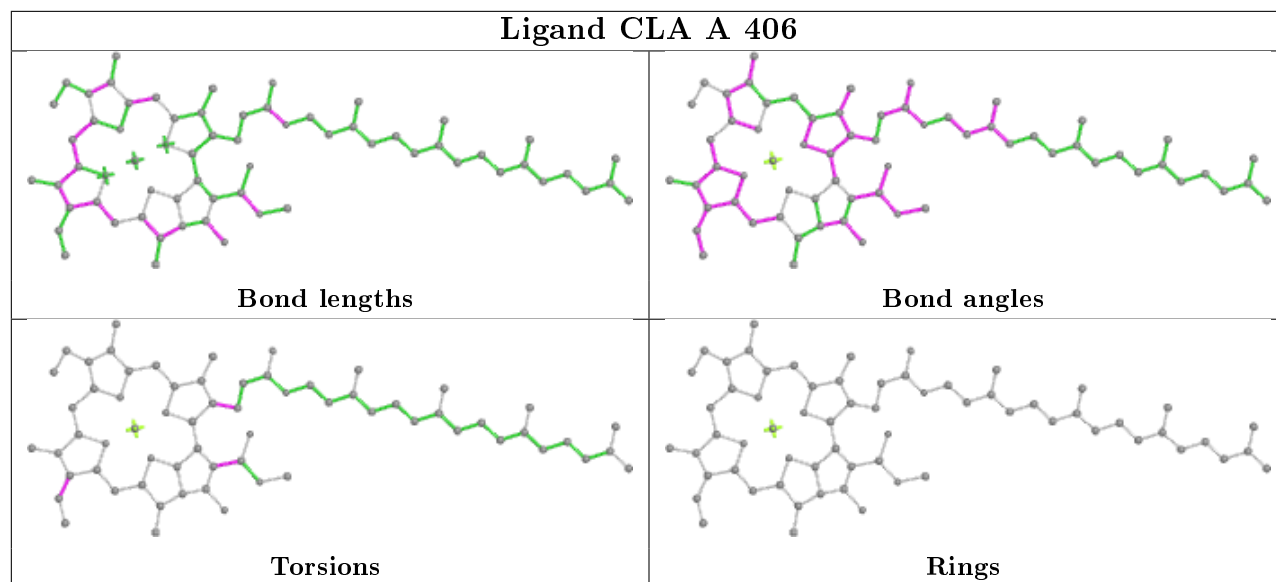
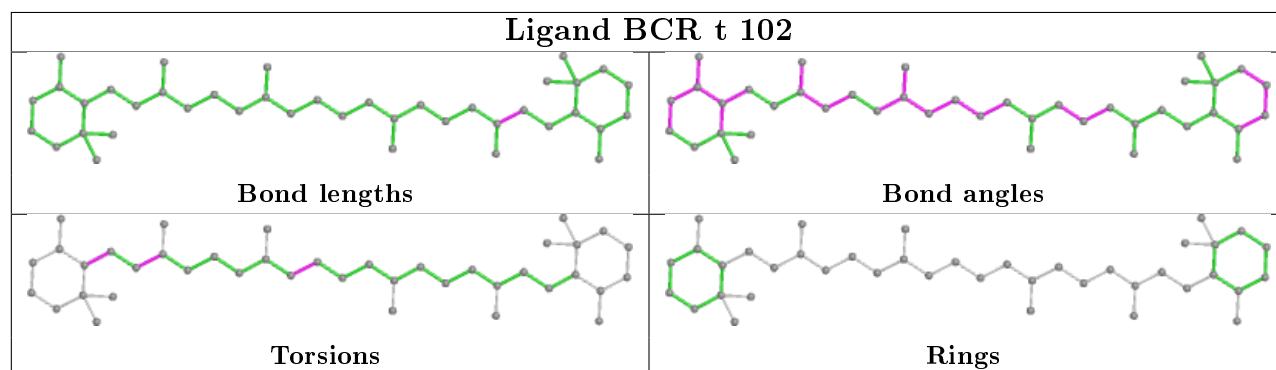
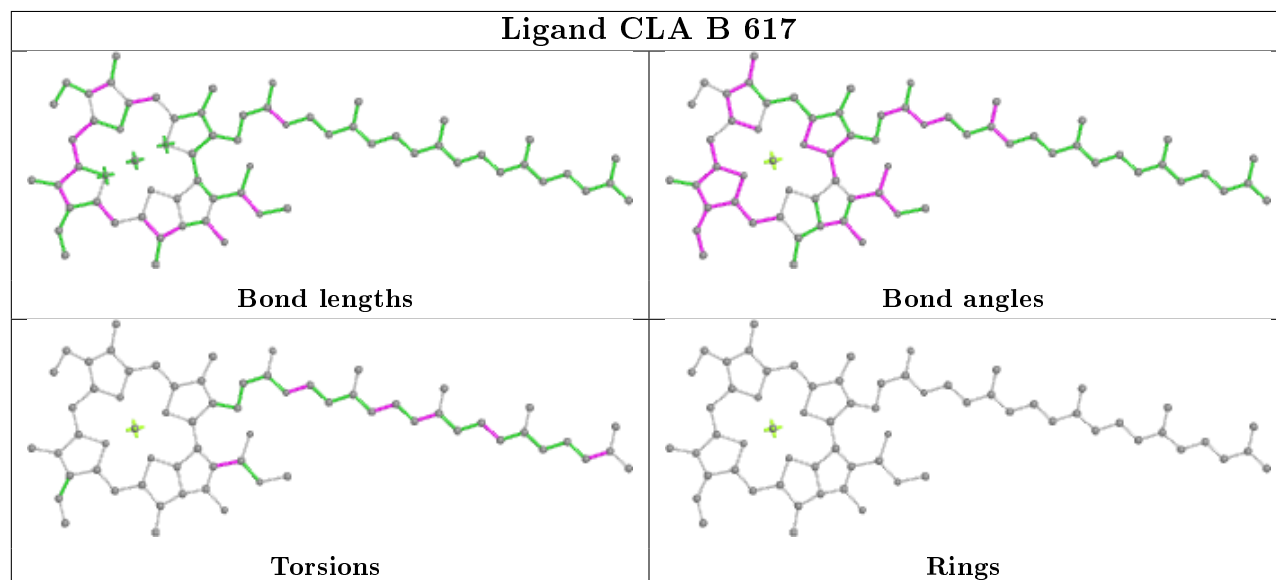


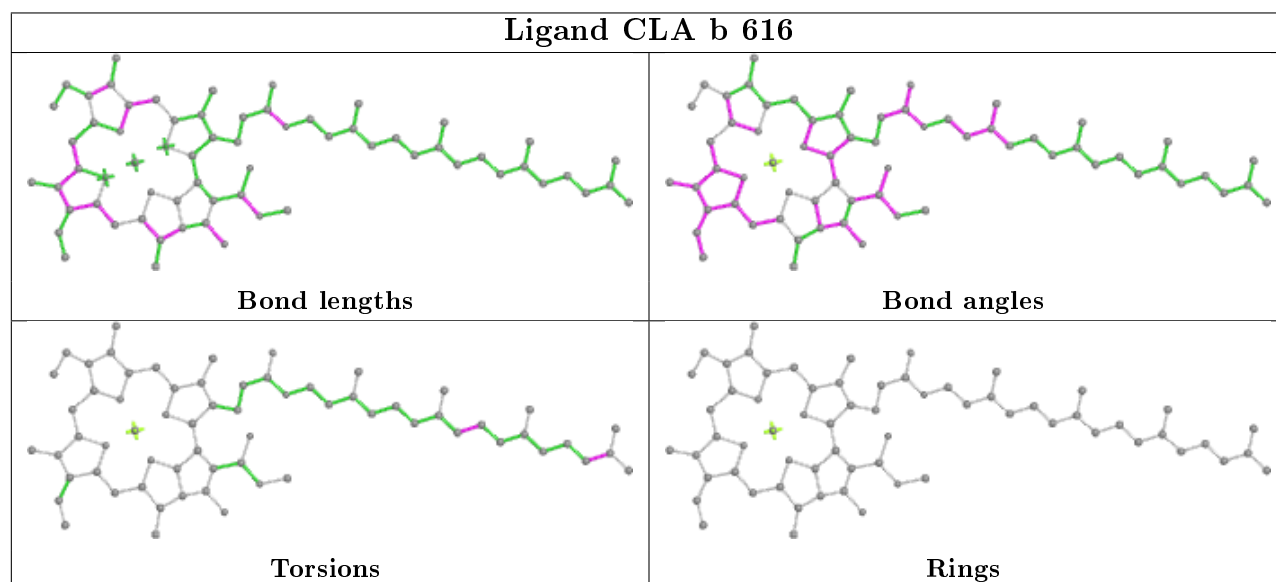
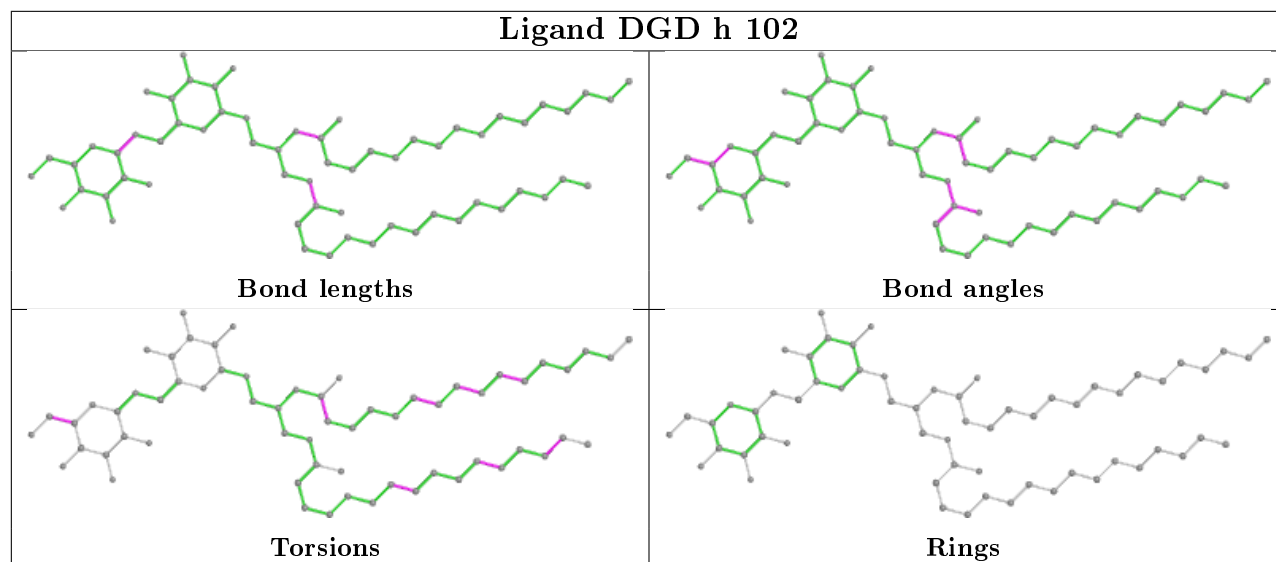
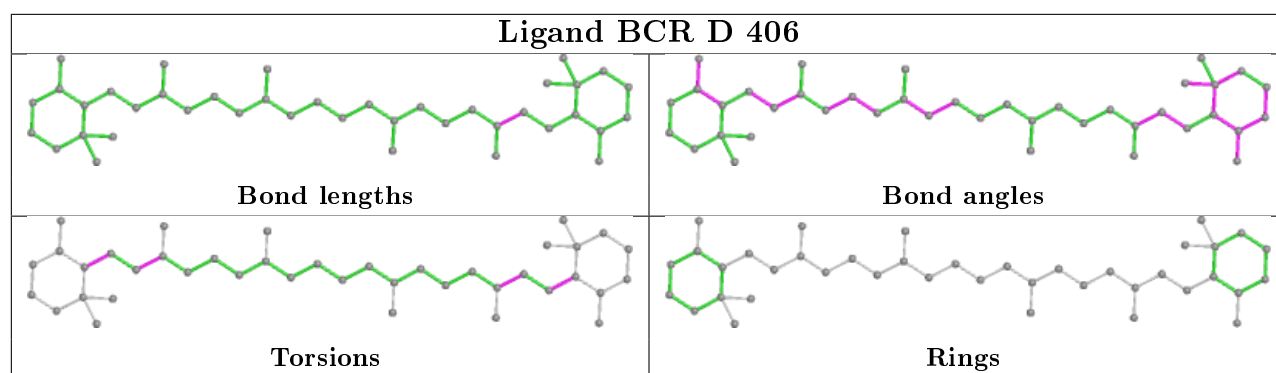
## Ligand CLA b 620



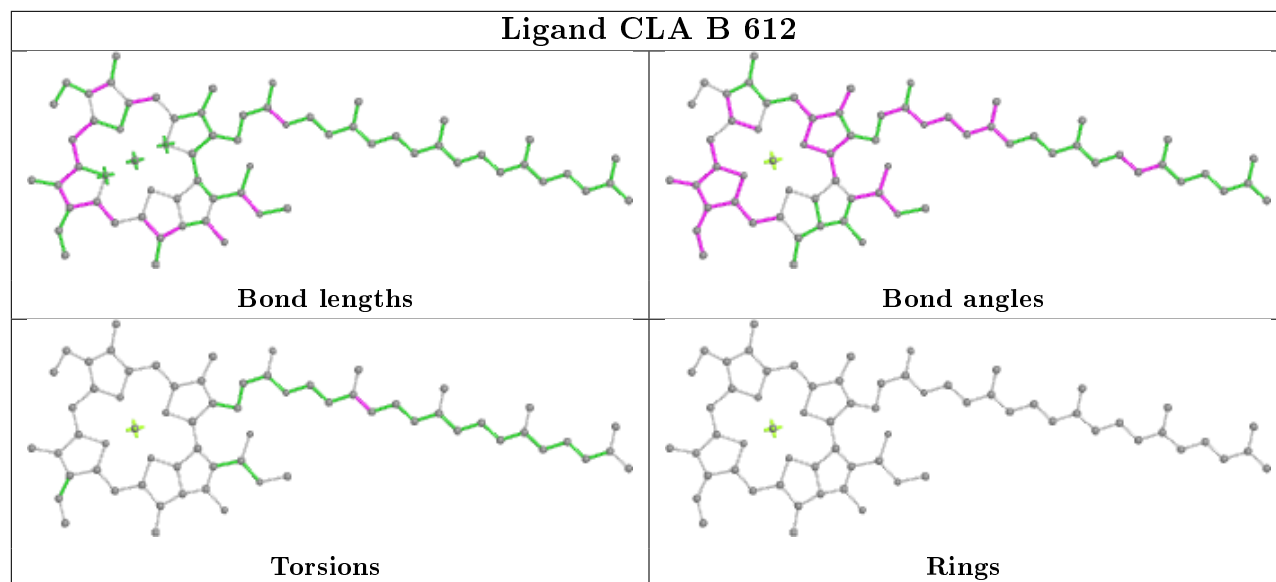
## Ligand HTG B 633



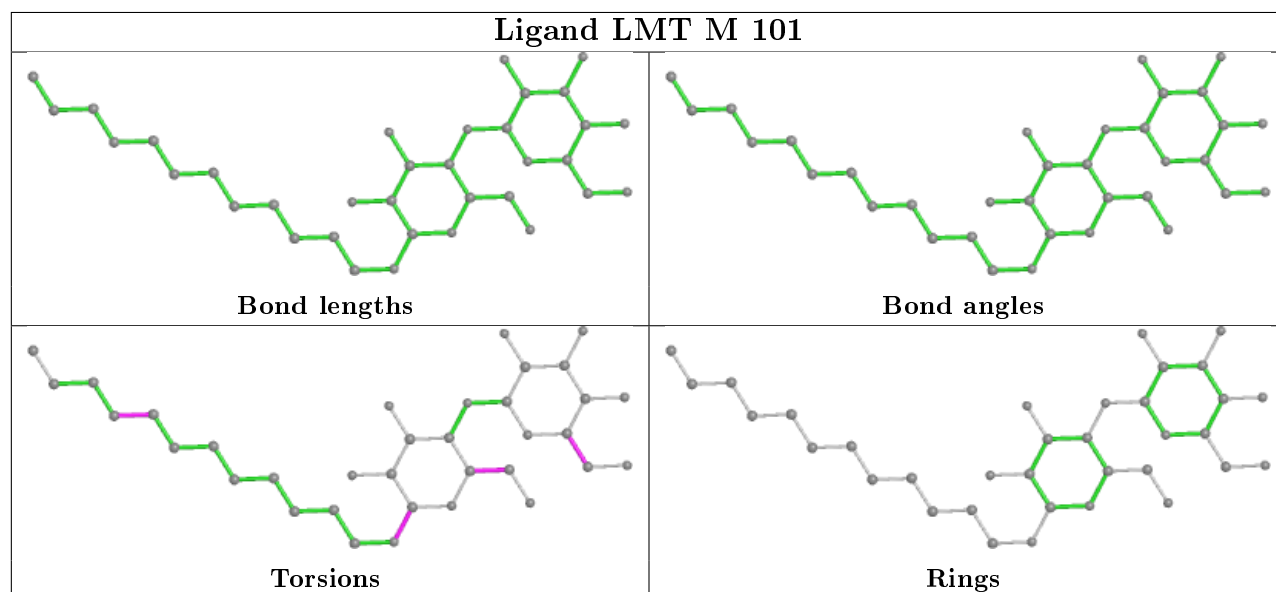
**Ligand CLA A 406****Ligand BCR t 102****Ligand CLA B 617**



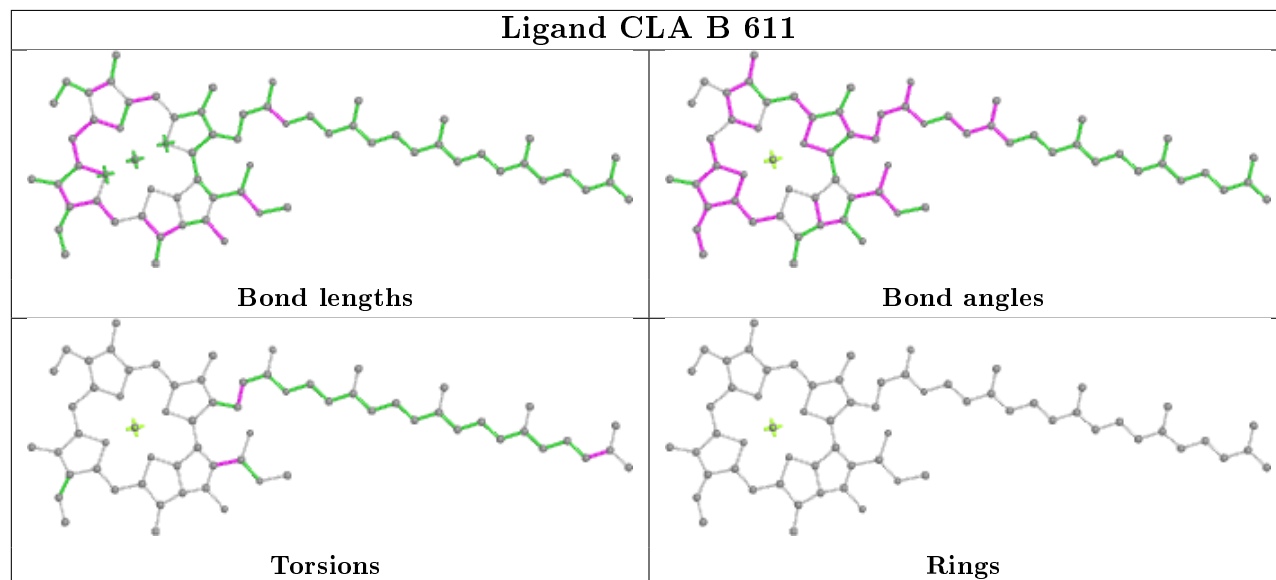
## Ligand CLA B 612

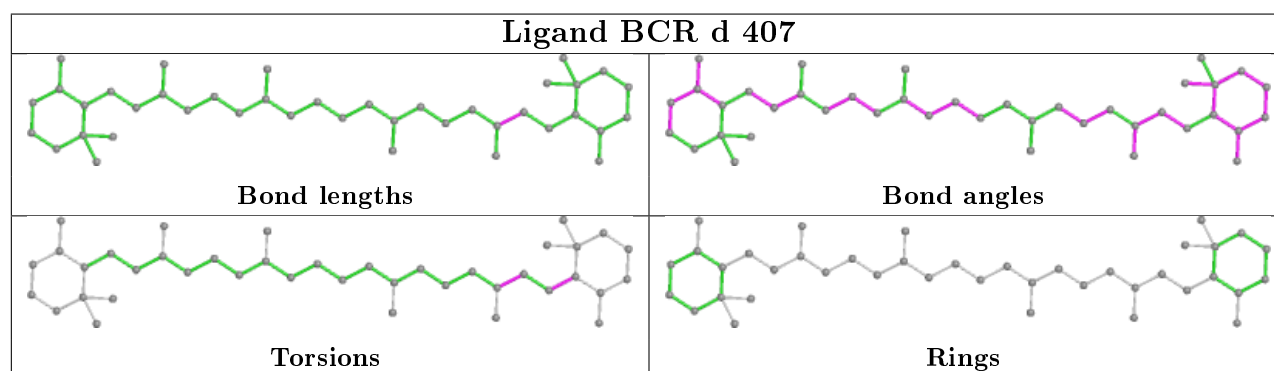
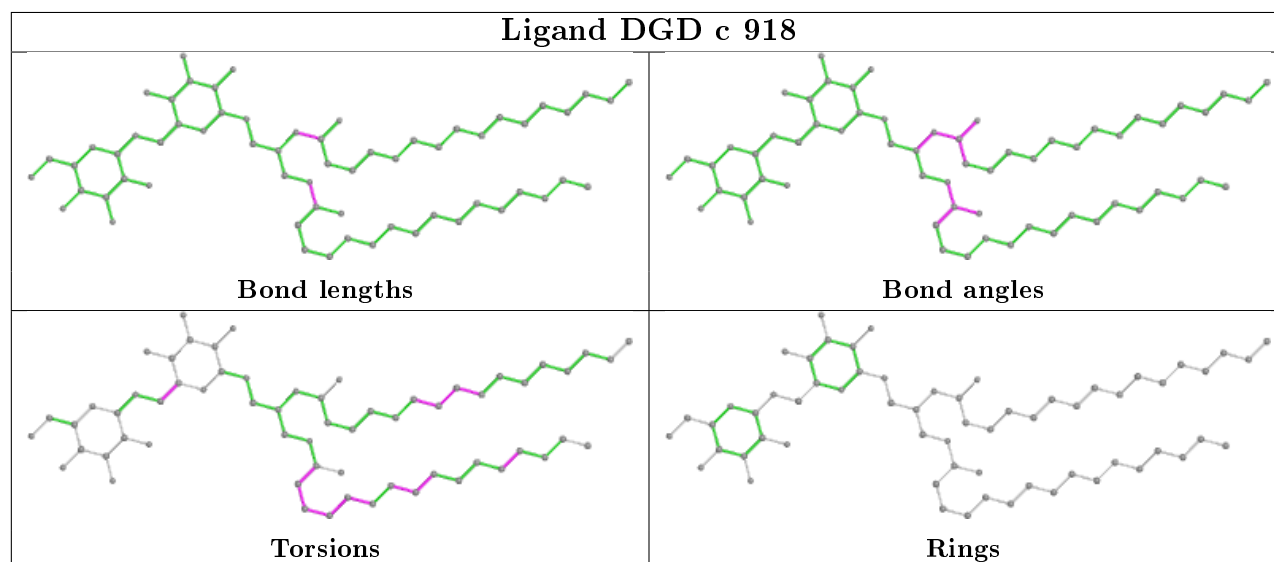
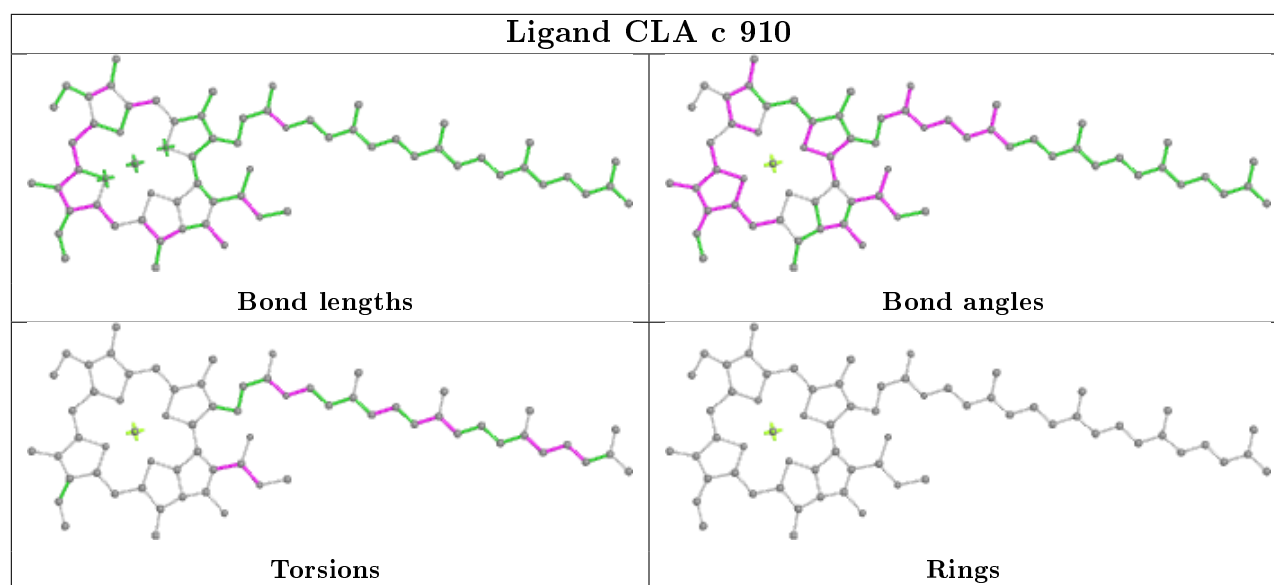


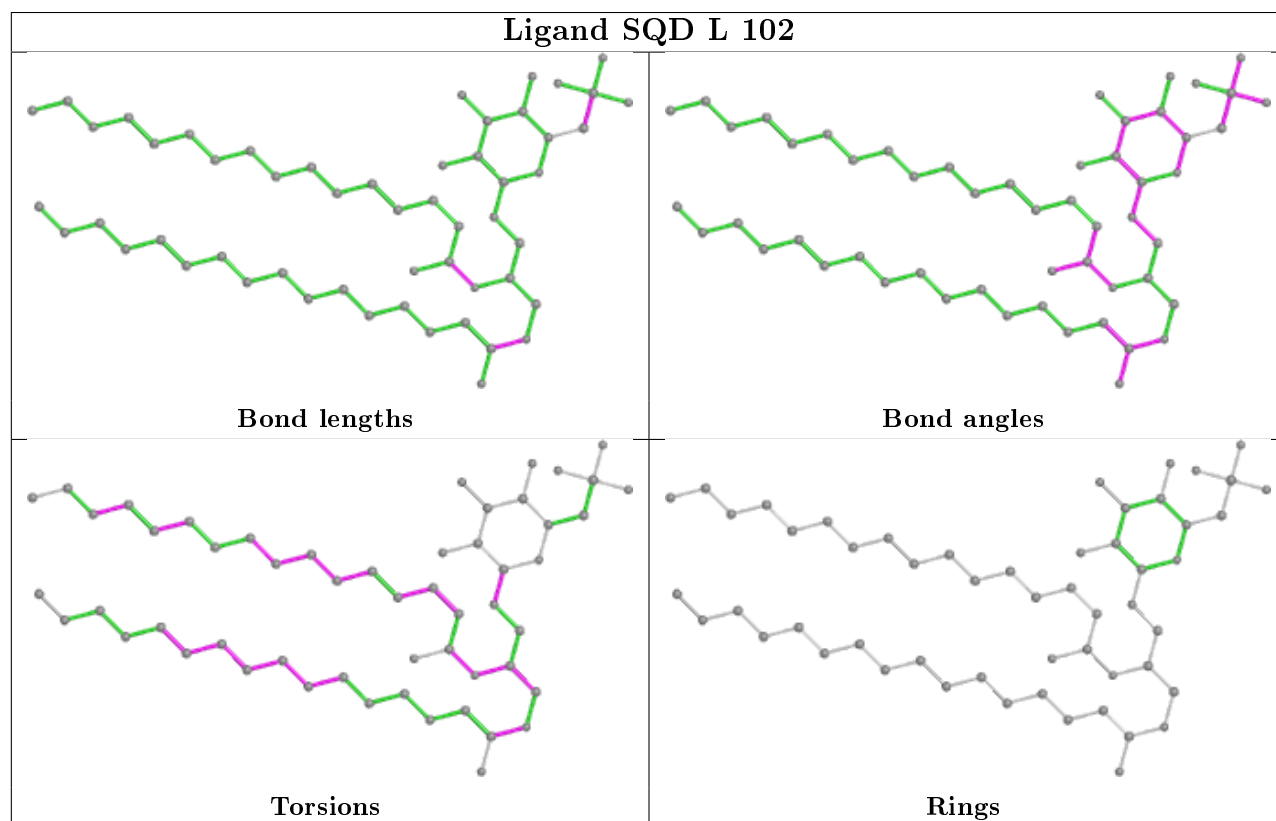
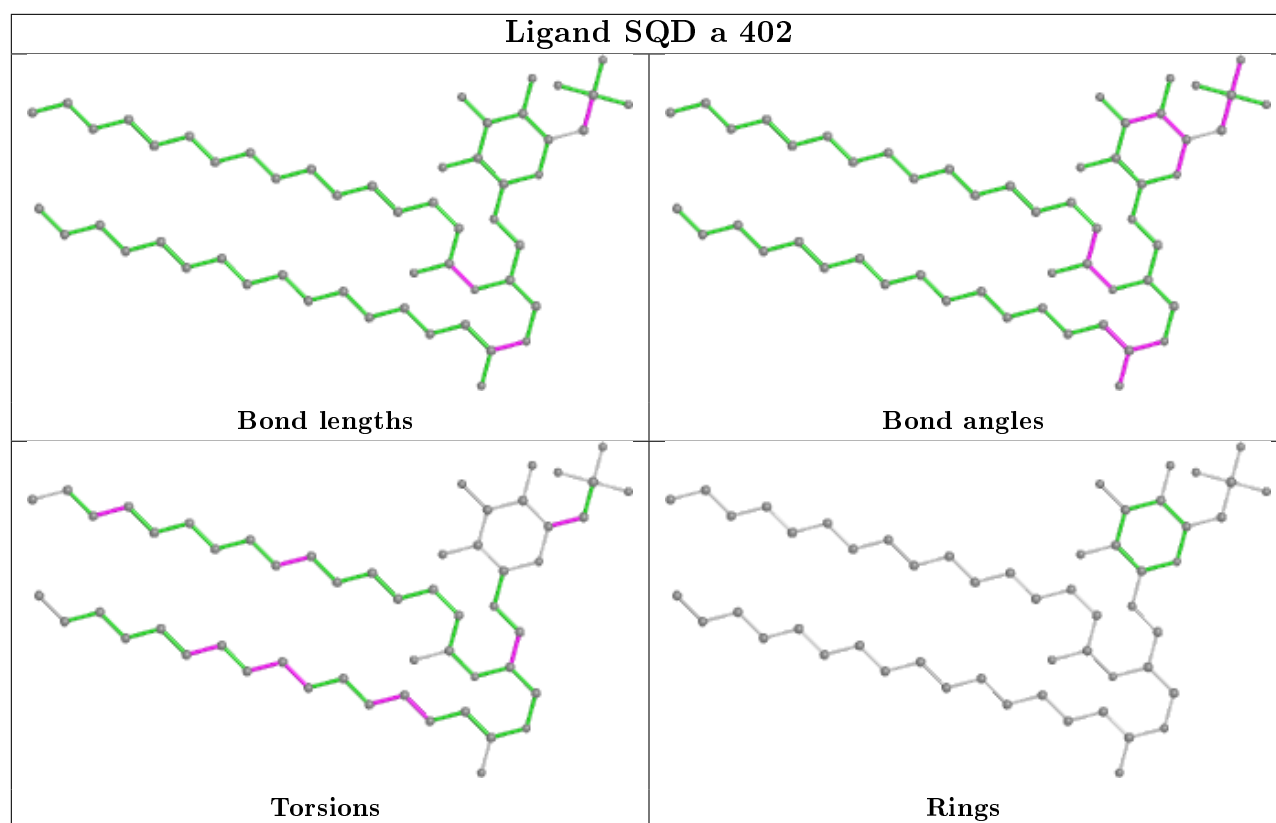
## Ligand LMT M 101

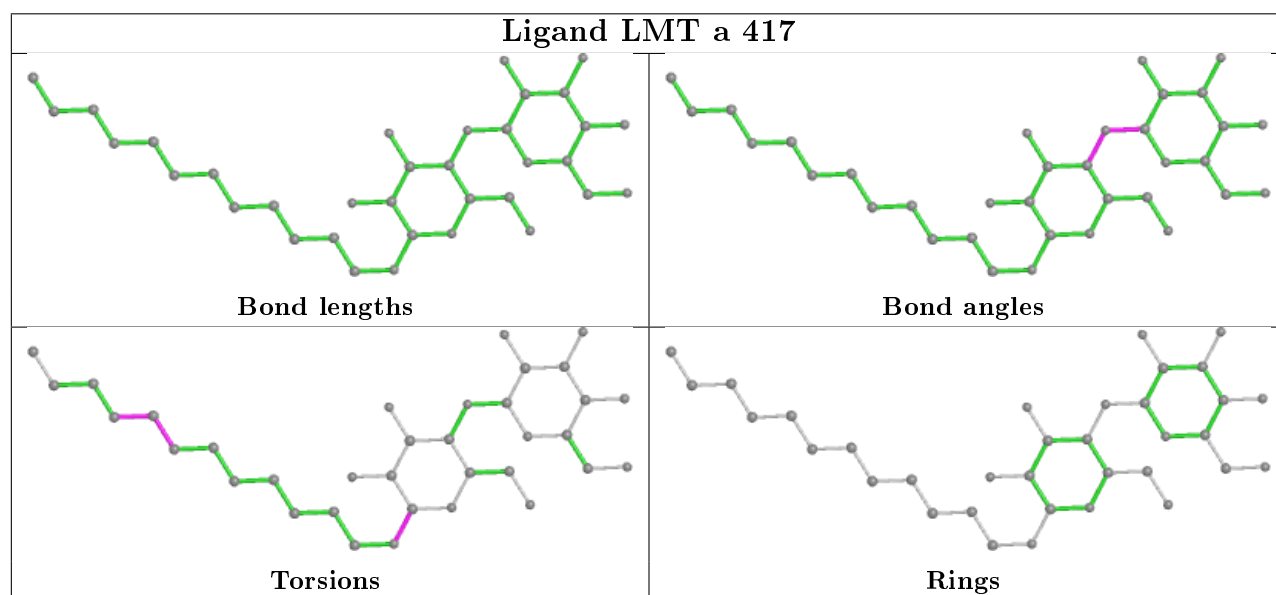
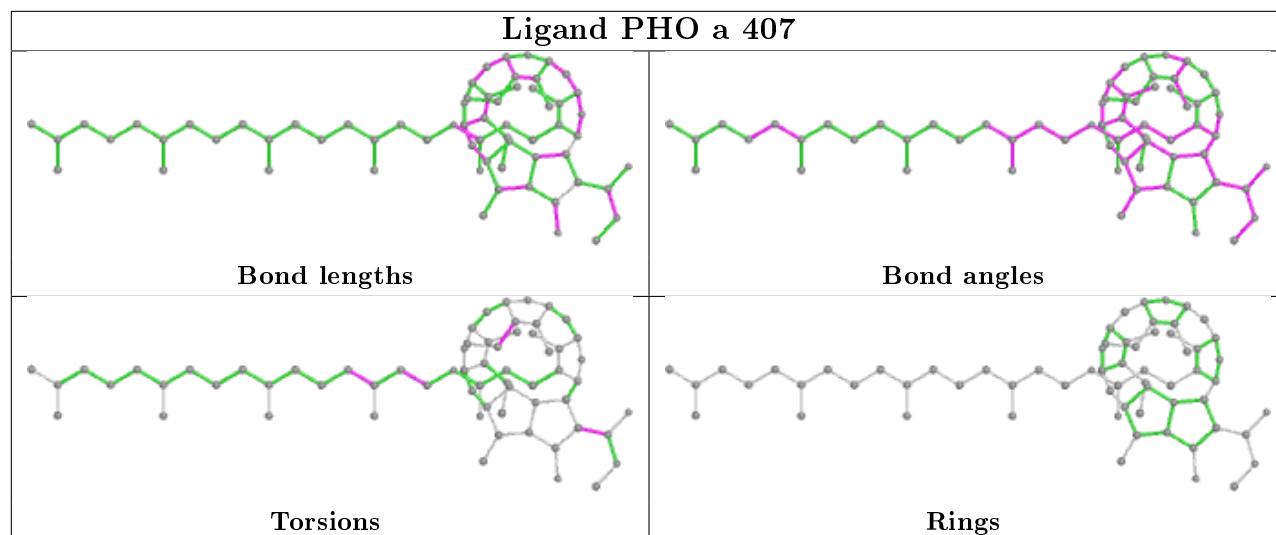


## Ligand CLA B 611

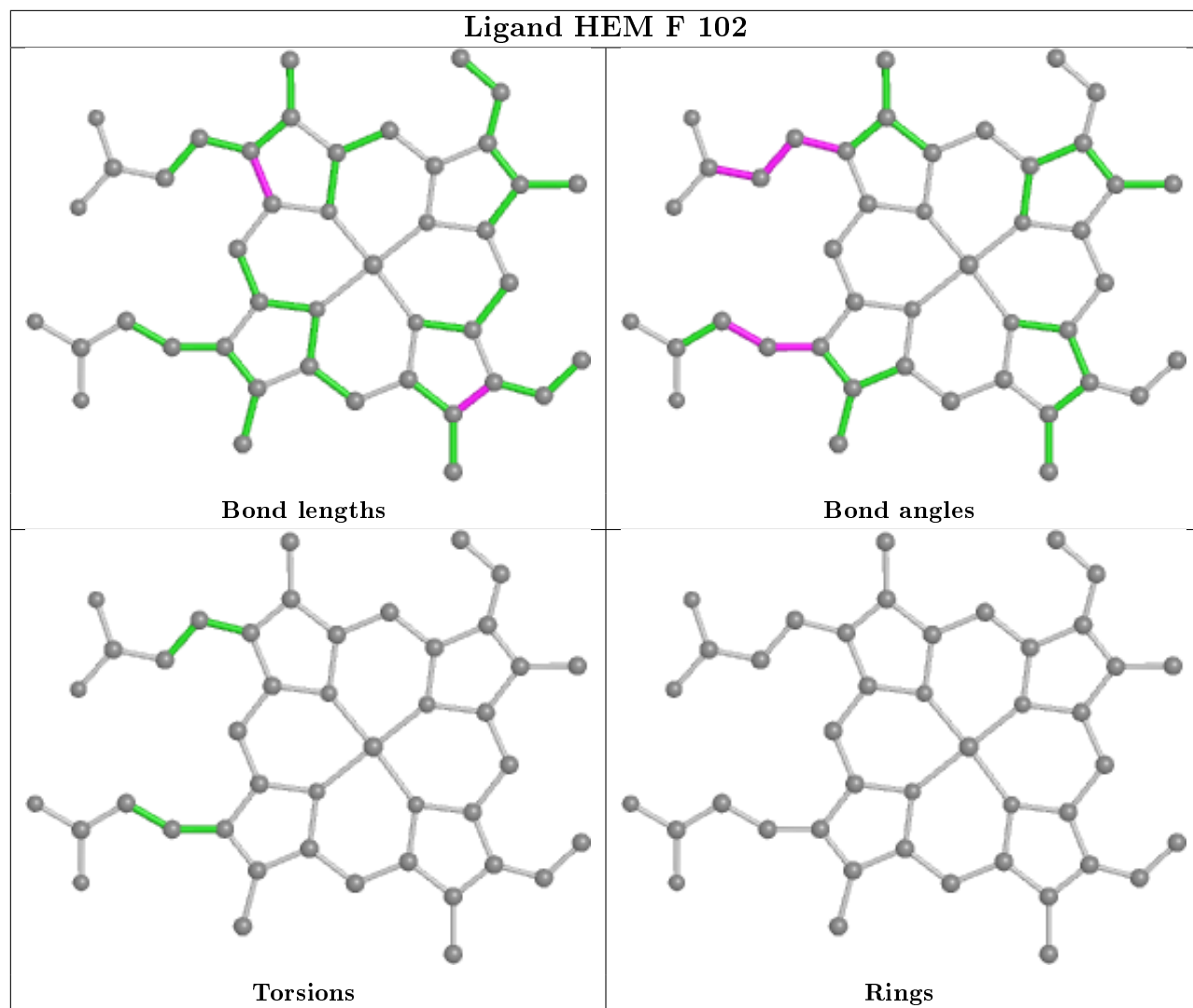


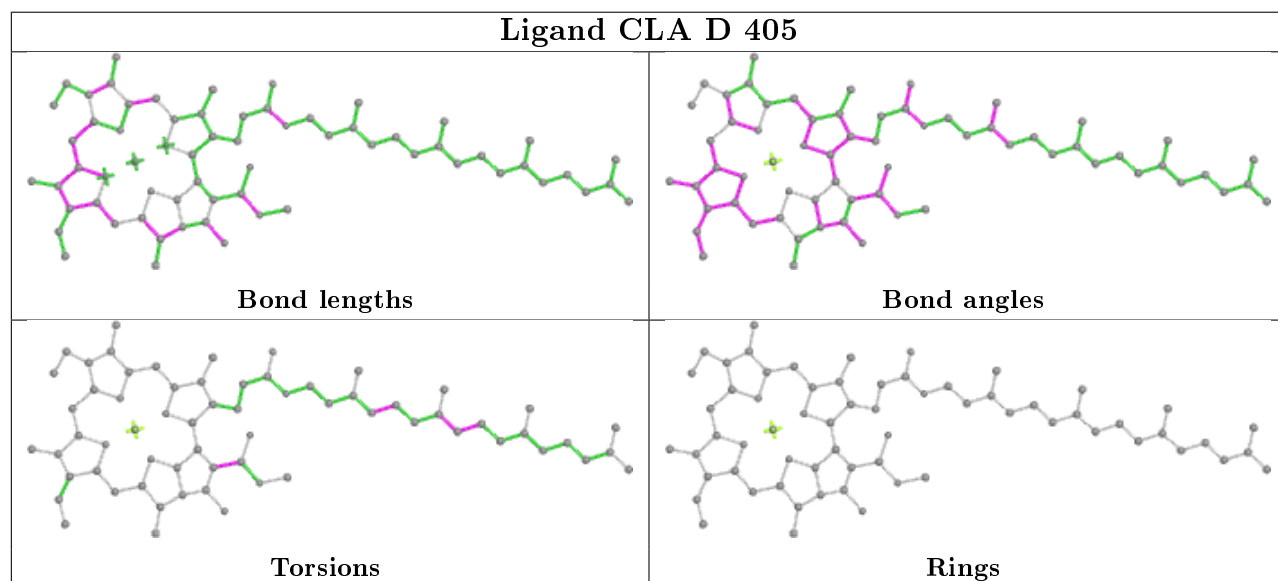
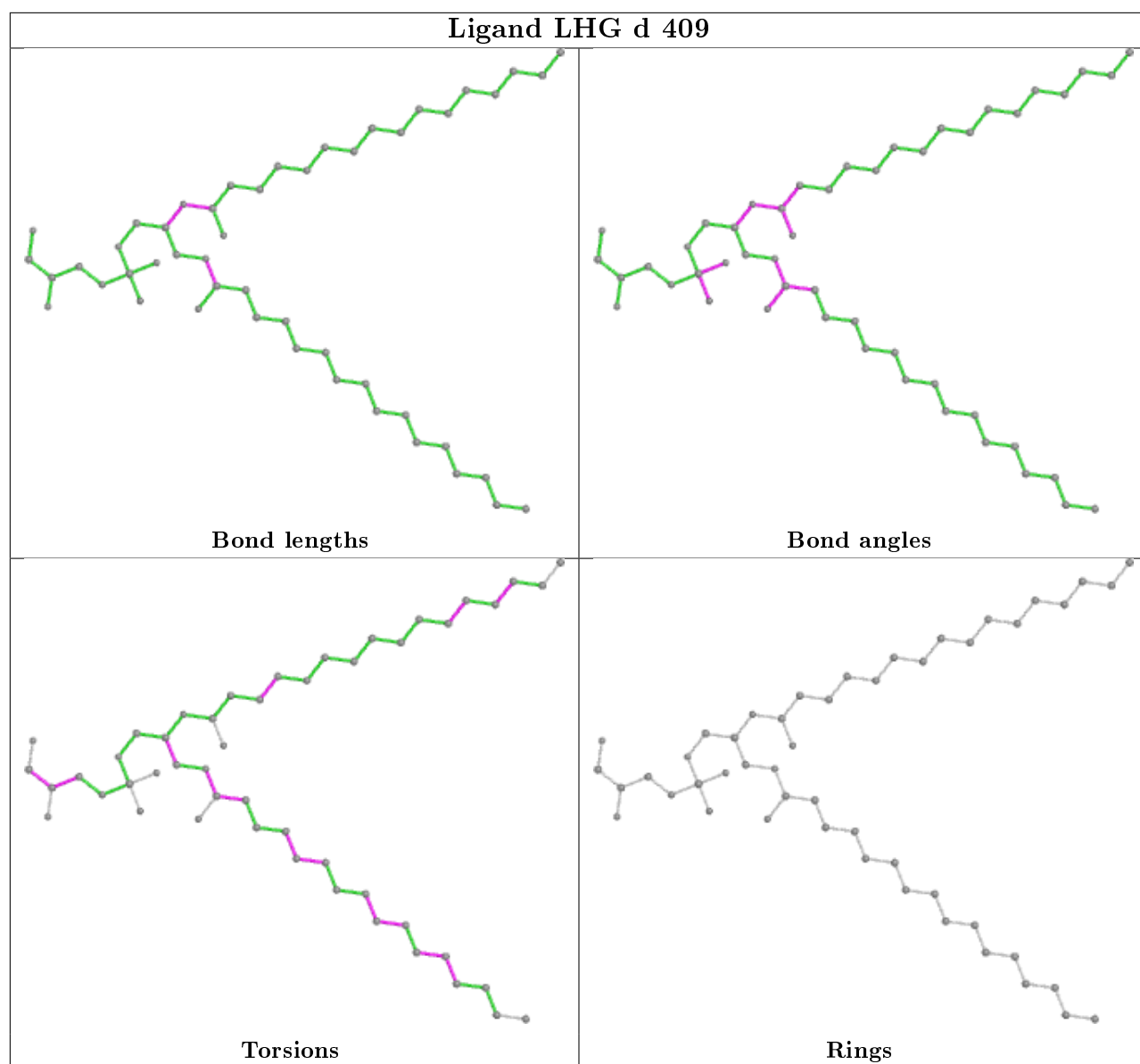




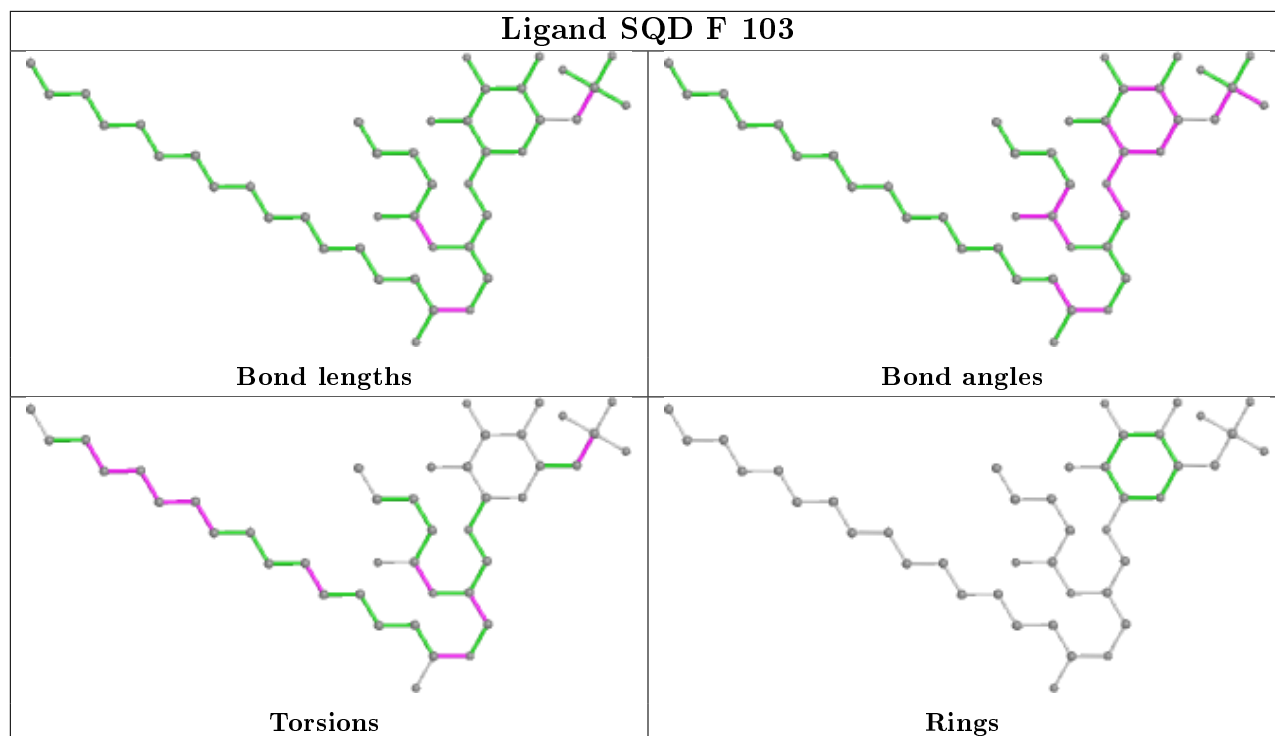




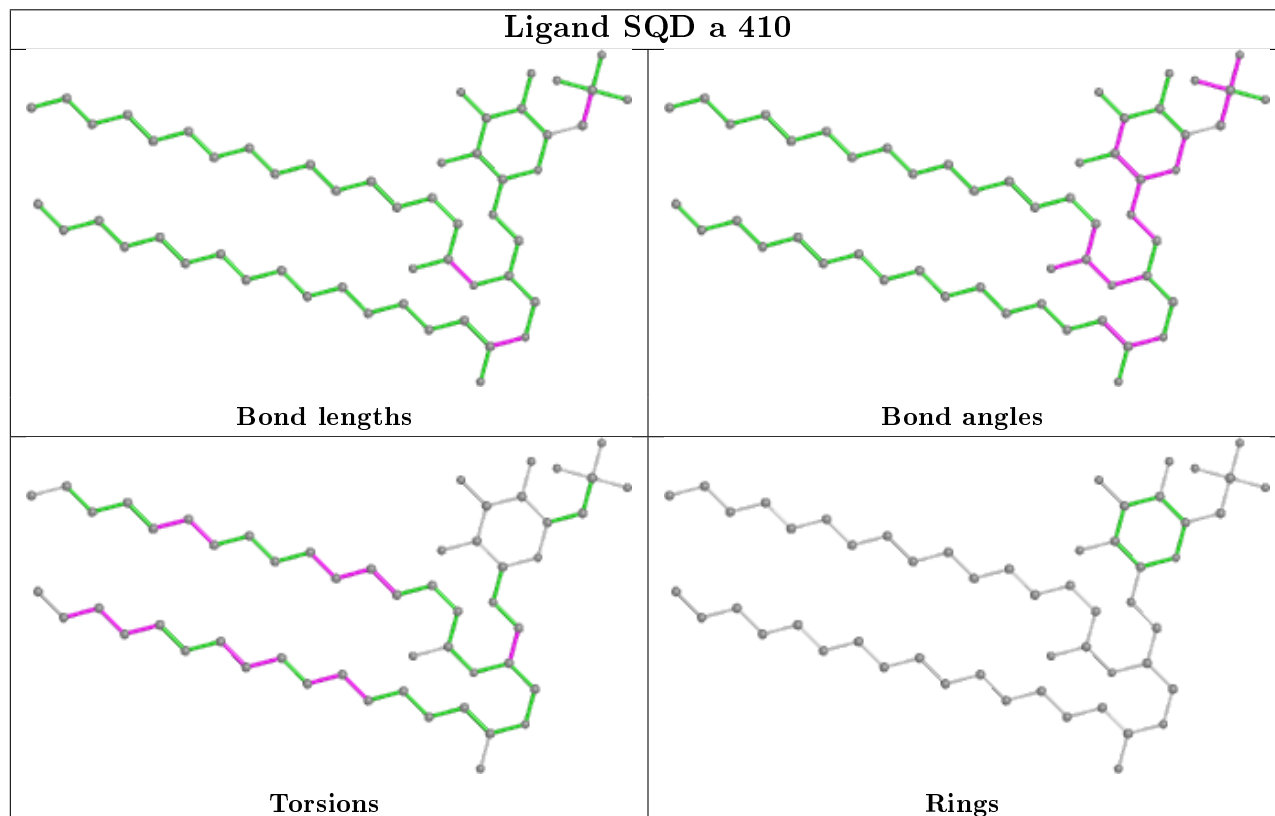


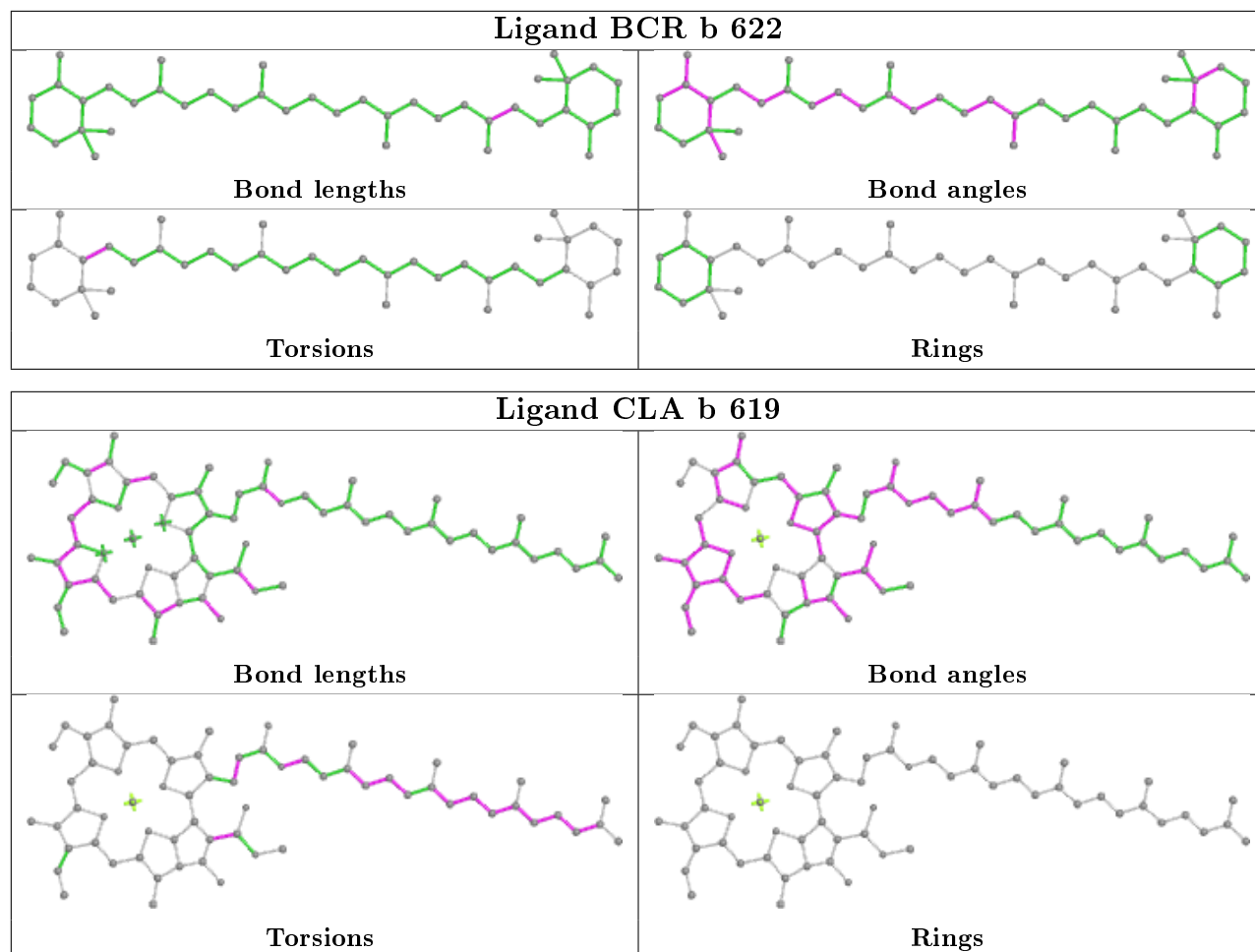


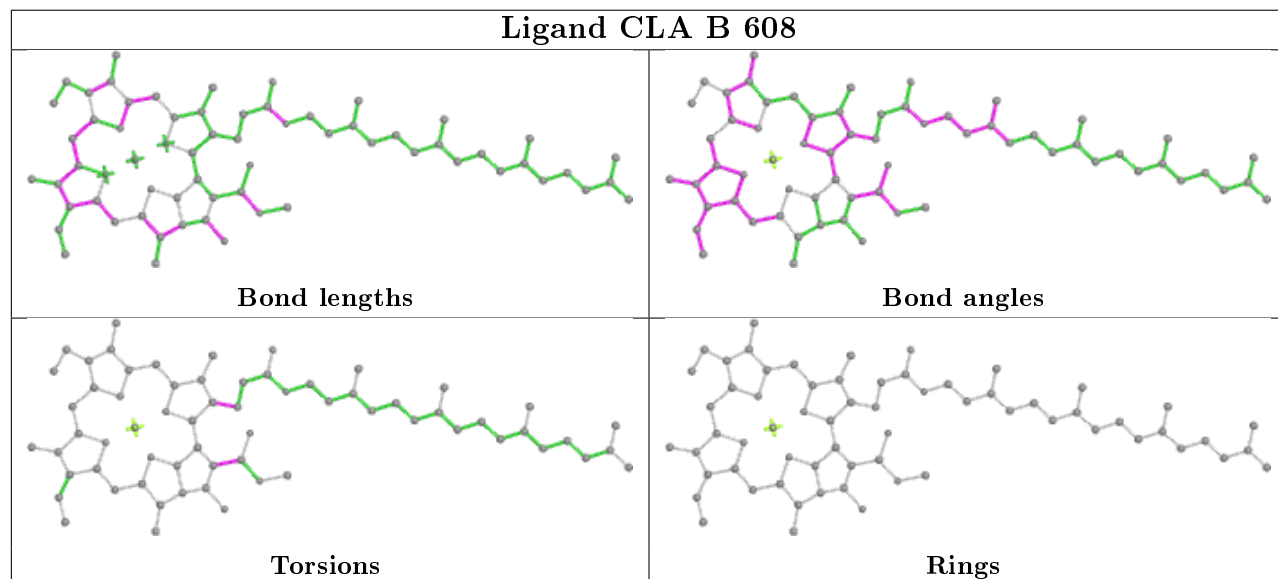
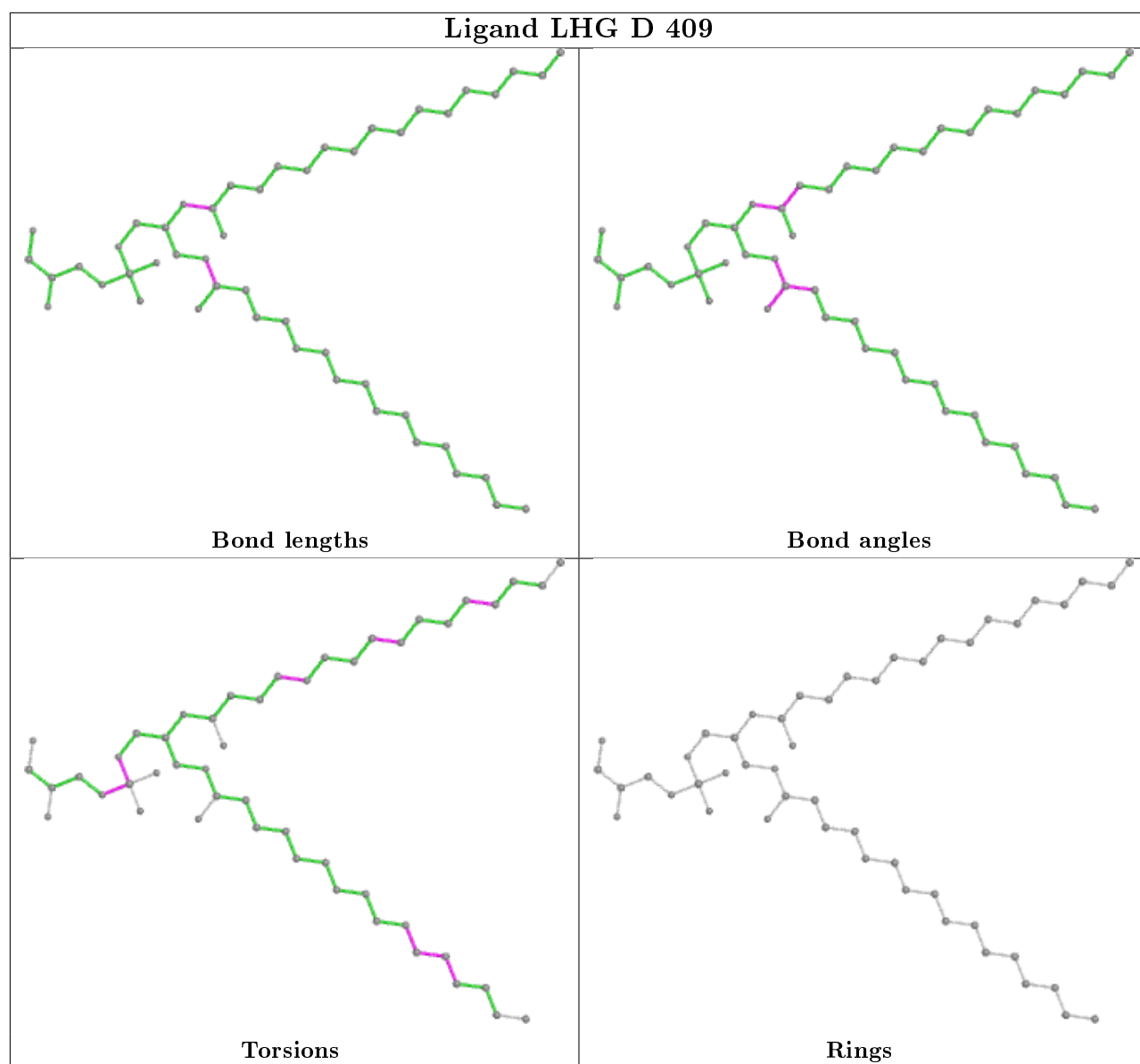
## Ligand SQD F 103



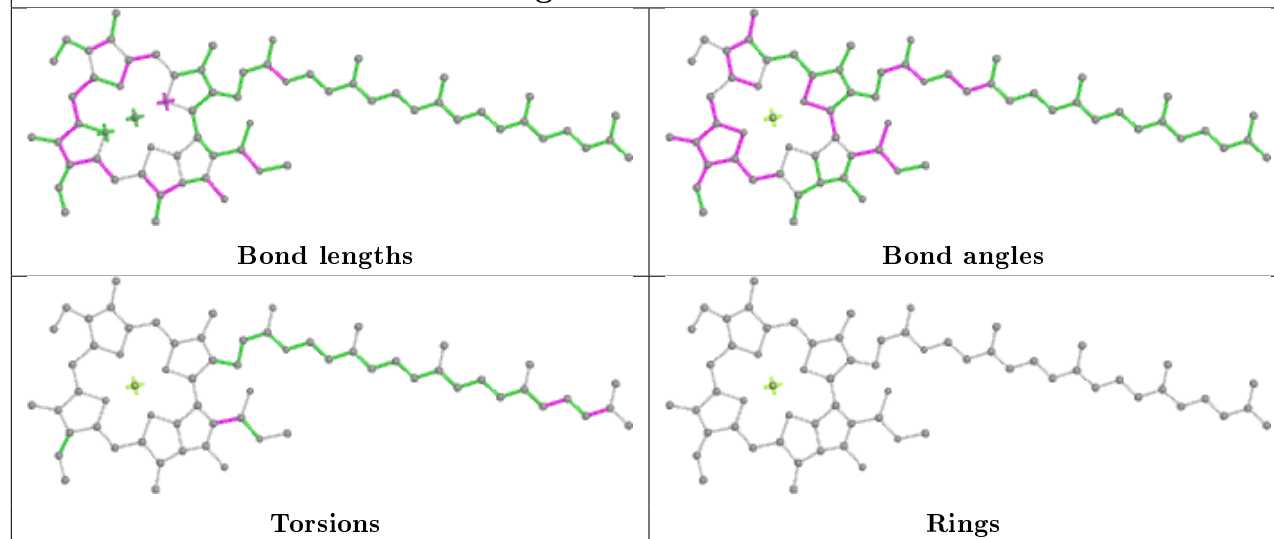
## Ligand SQD a 410



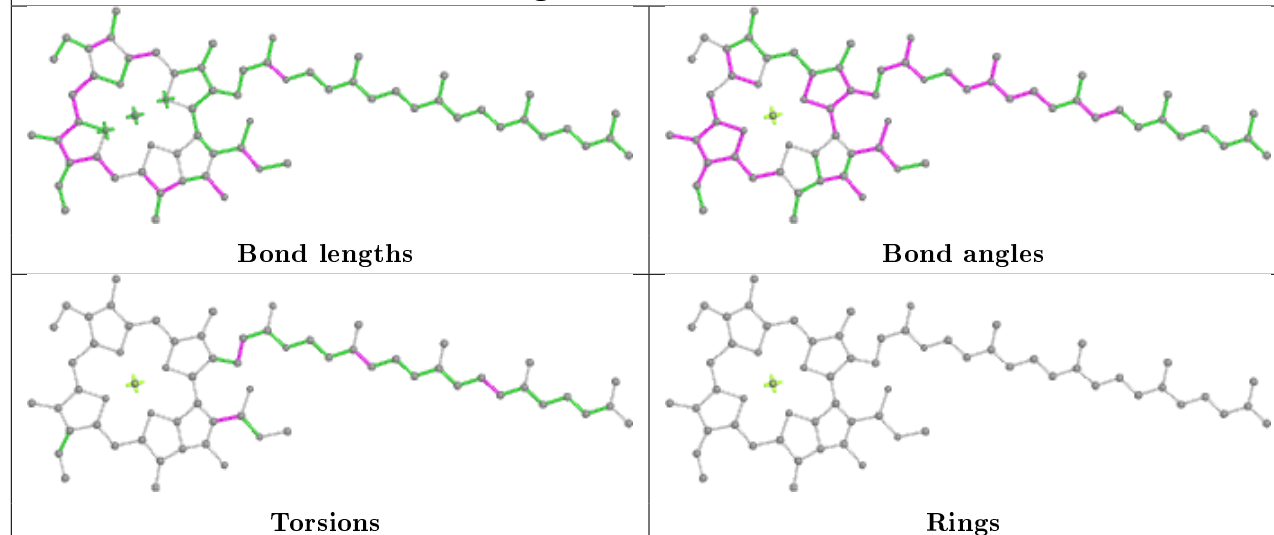




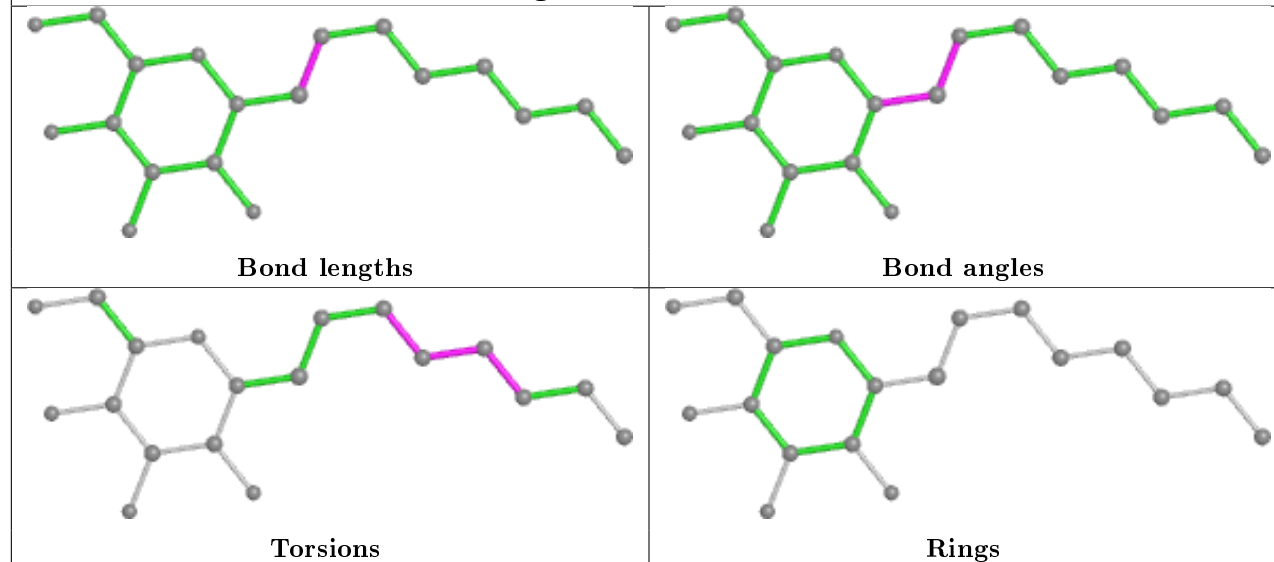
## Ligand CLA b 609



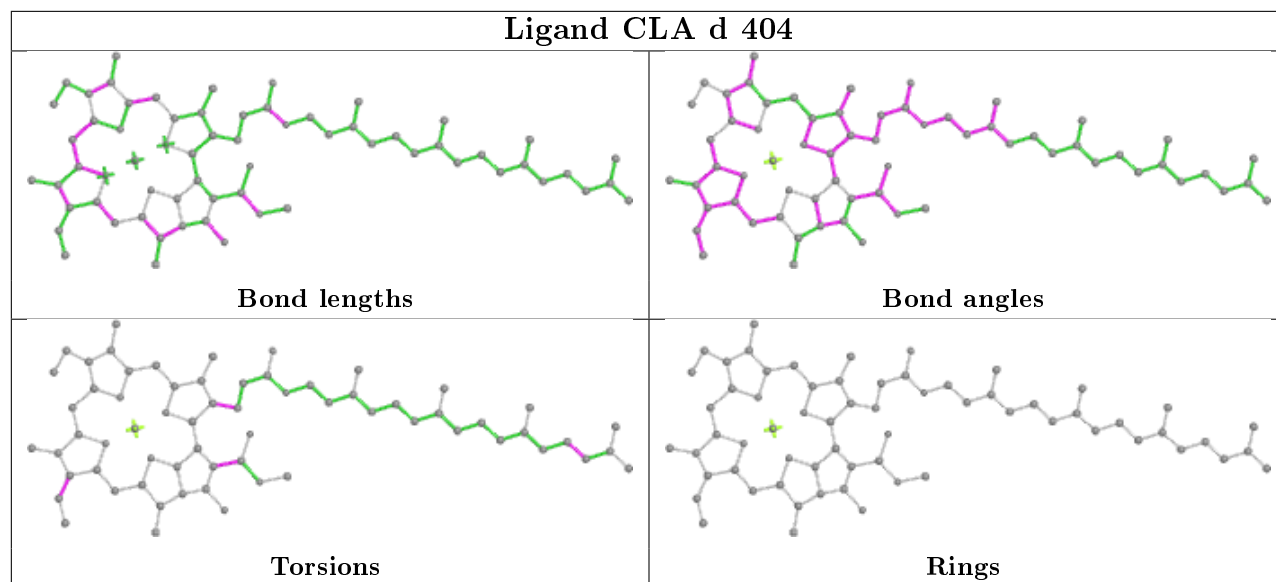
## Ligand CLA B 607



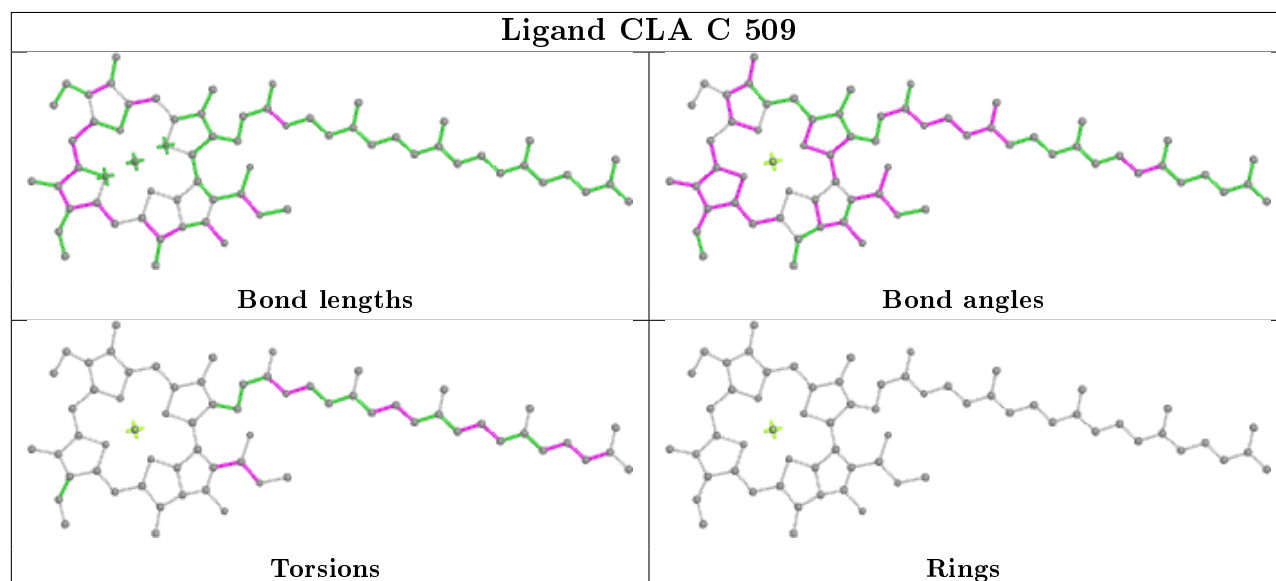
## Ligand HTG b 601



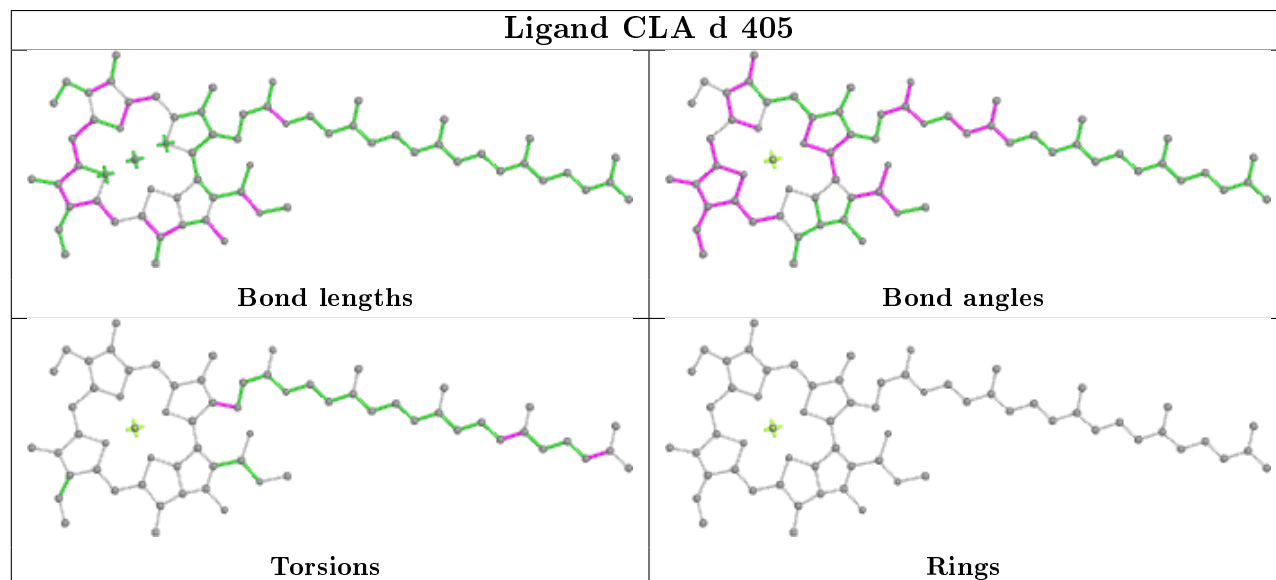
## Ligand CLA d 404

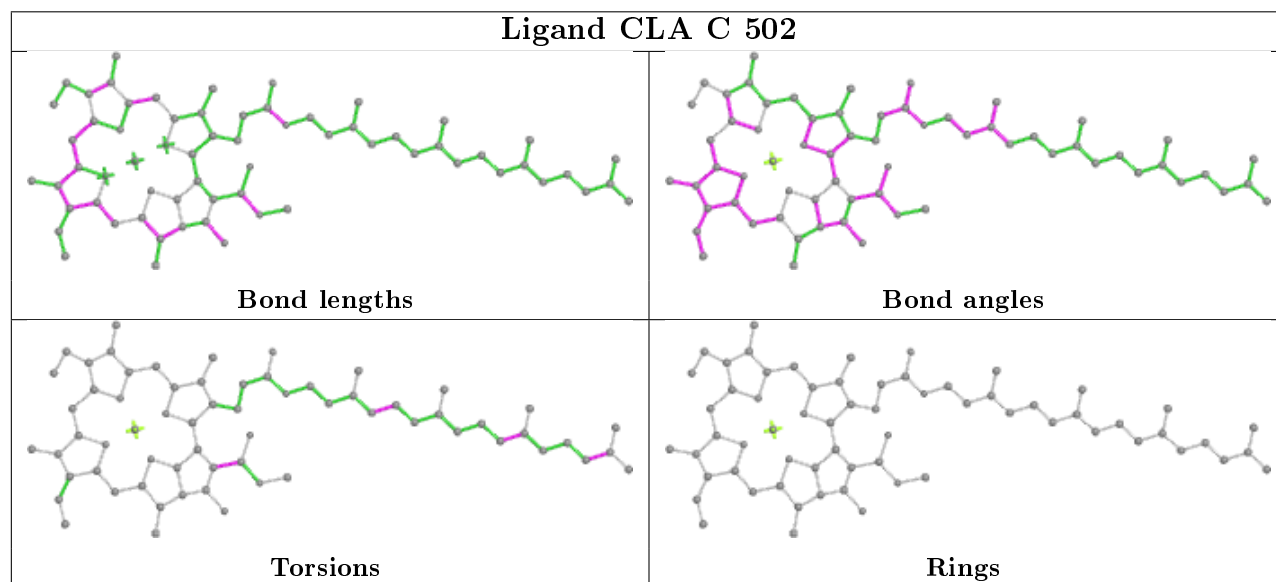
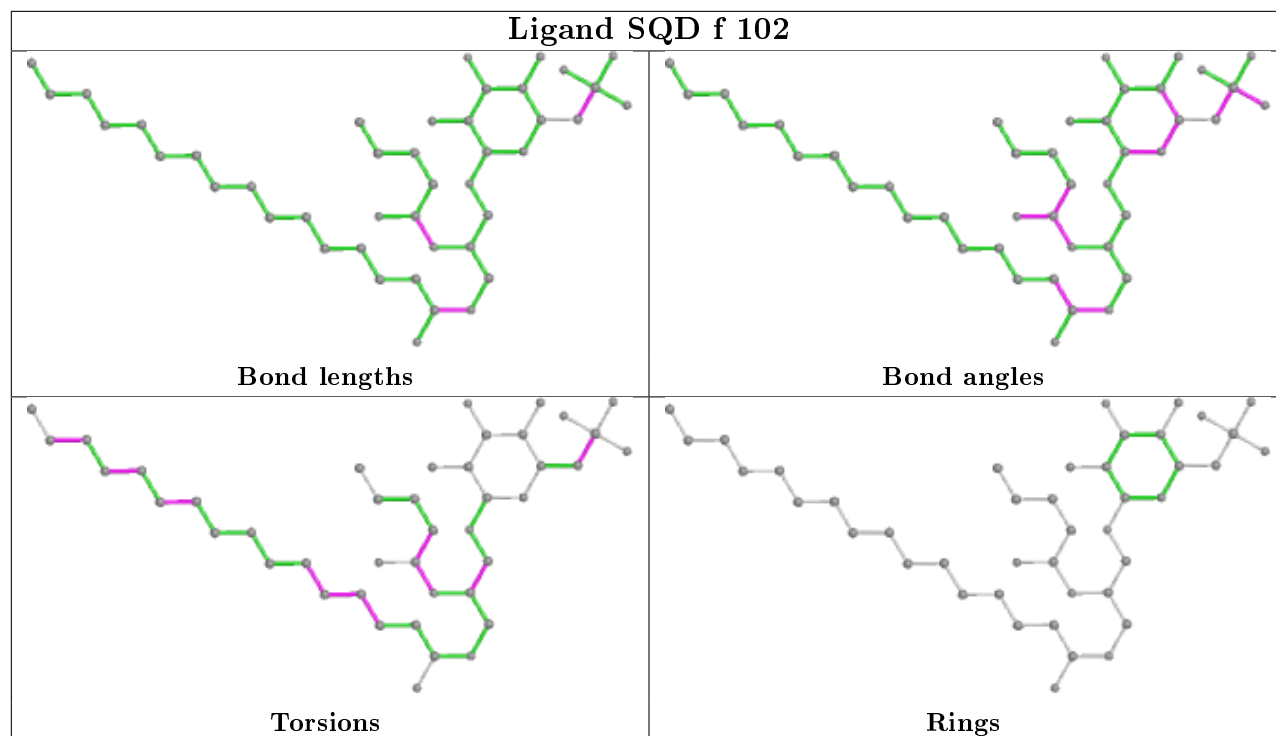


## Ligand CLA C 509

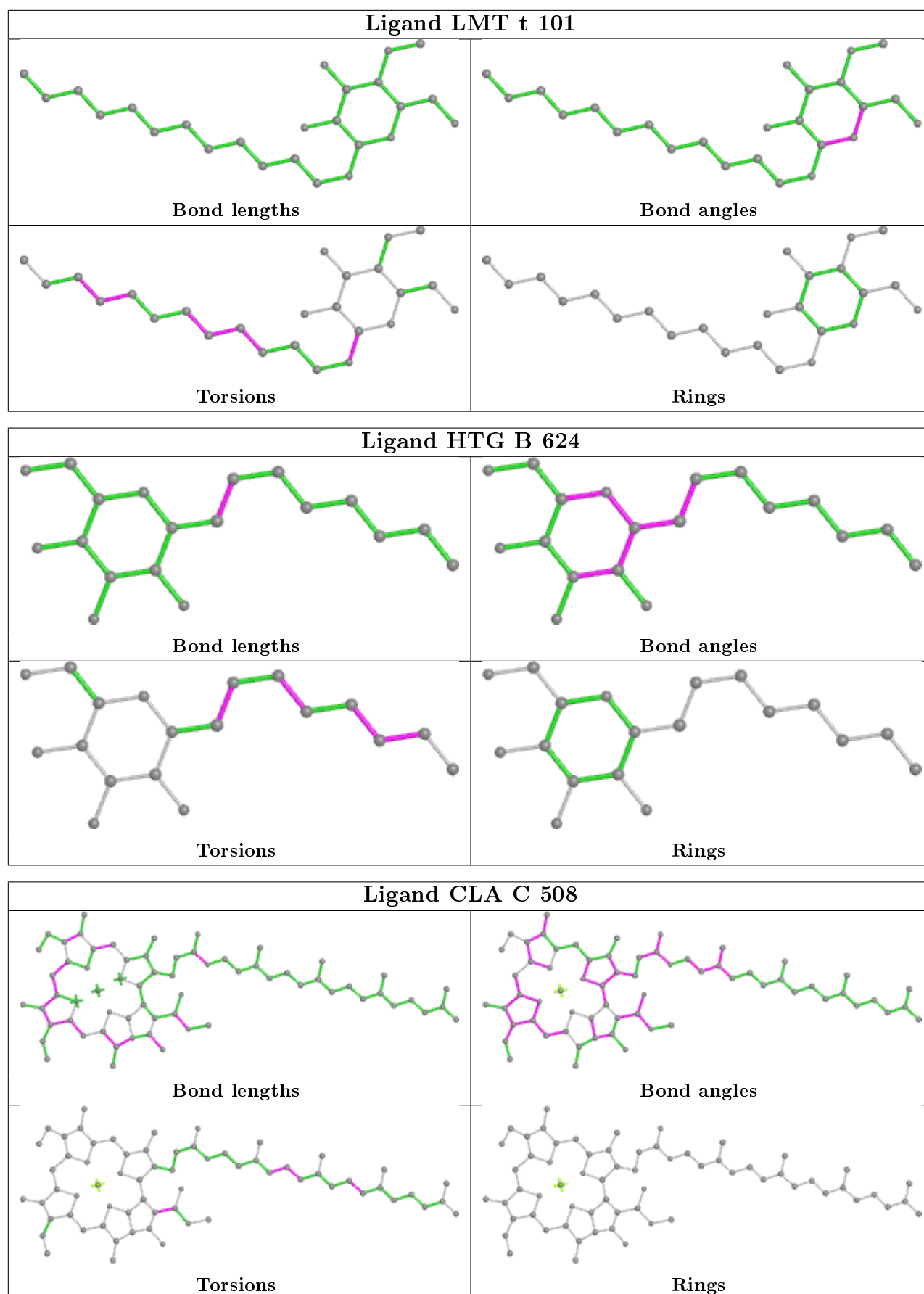


## Ligand CLA d 405

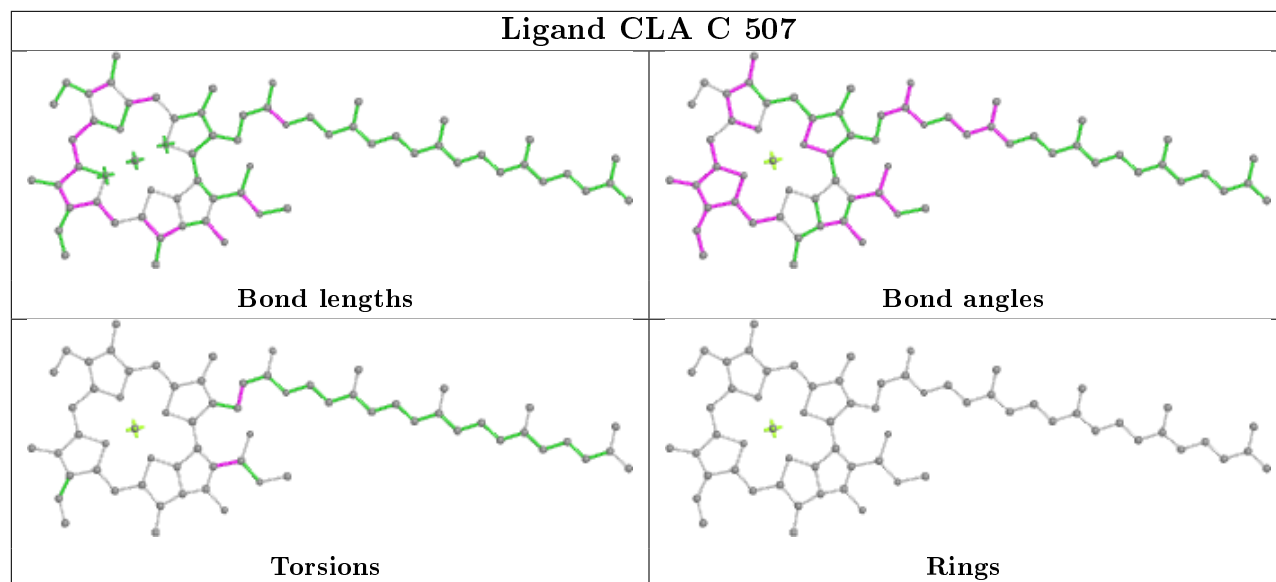




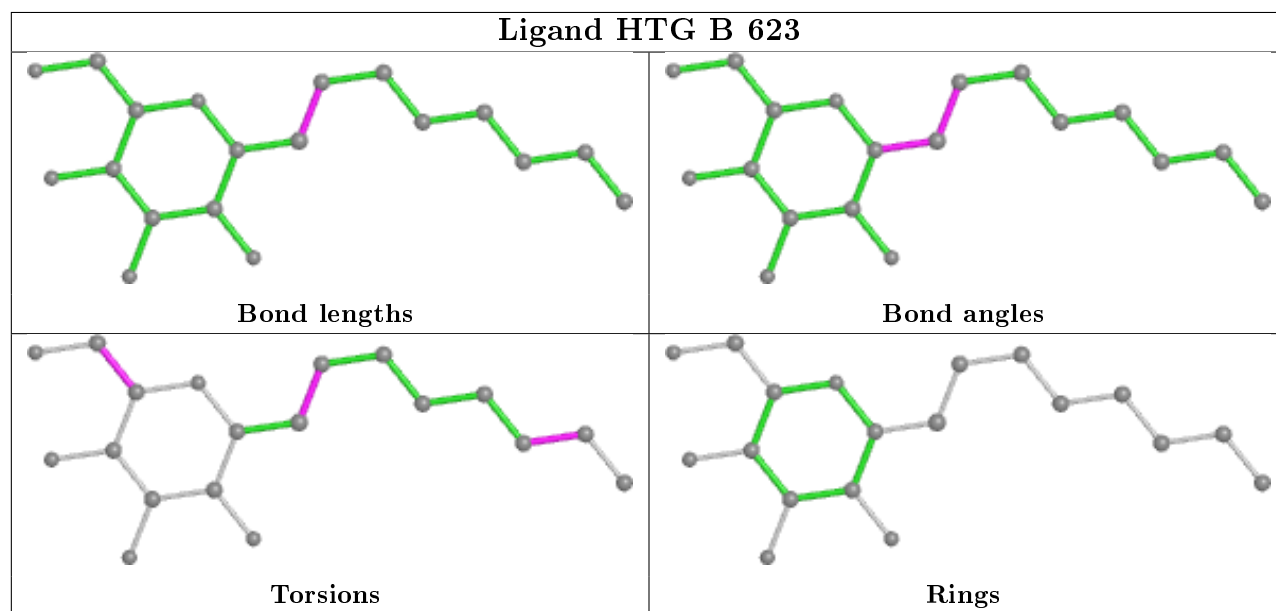


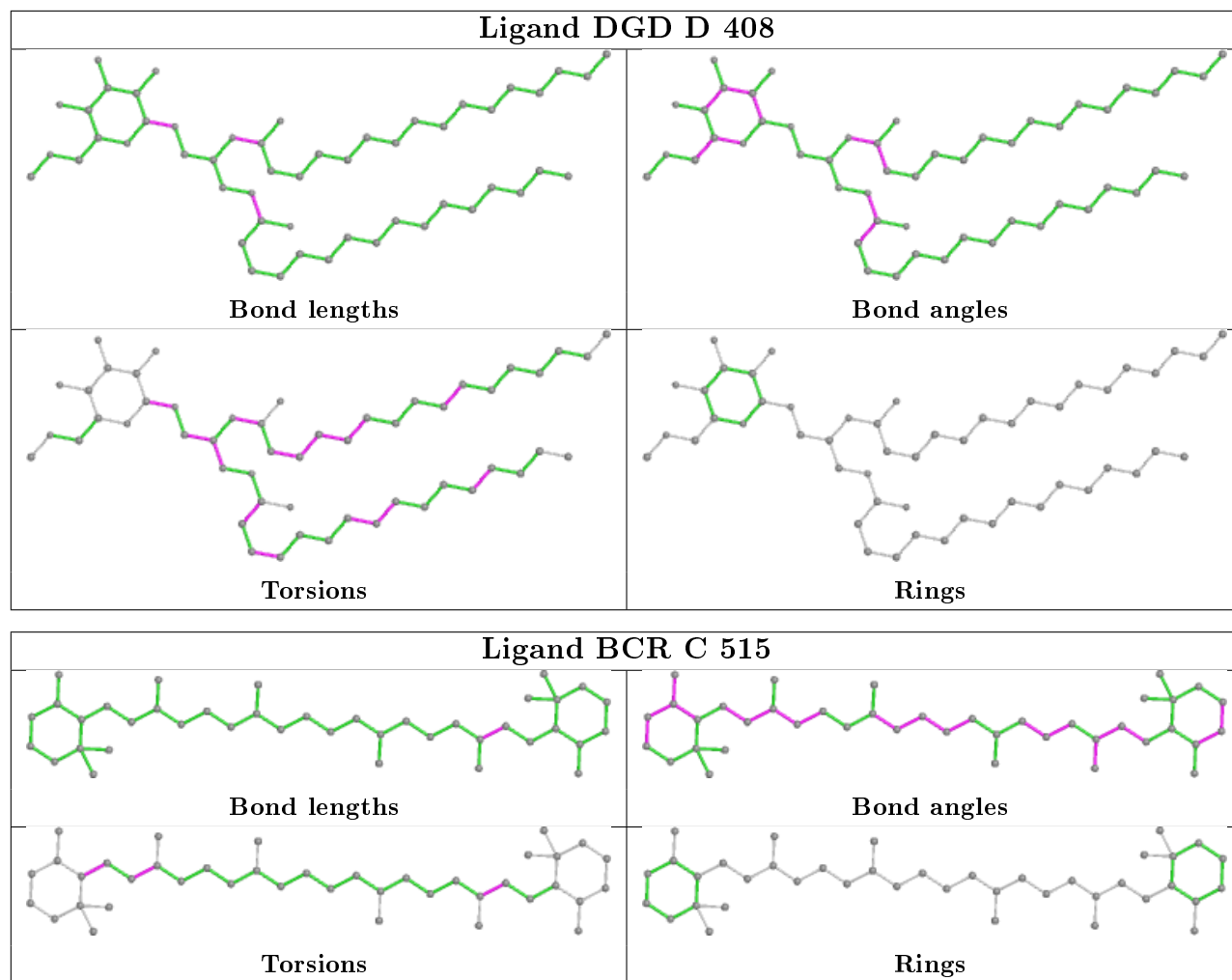


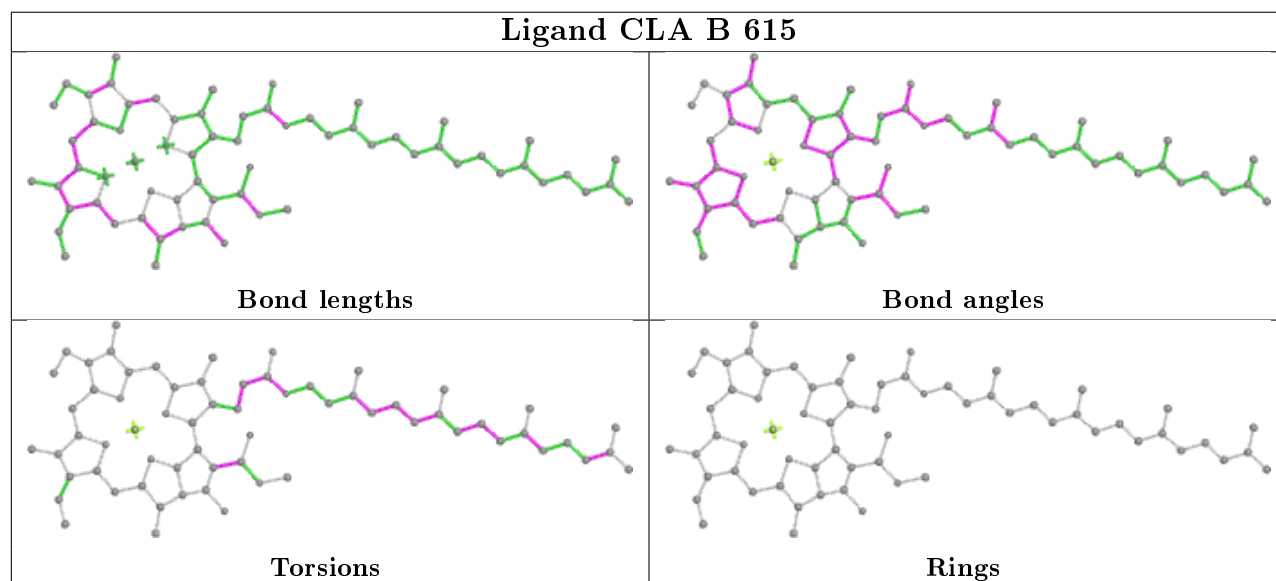
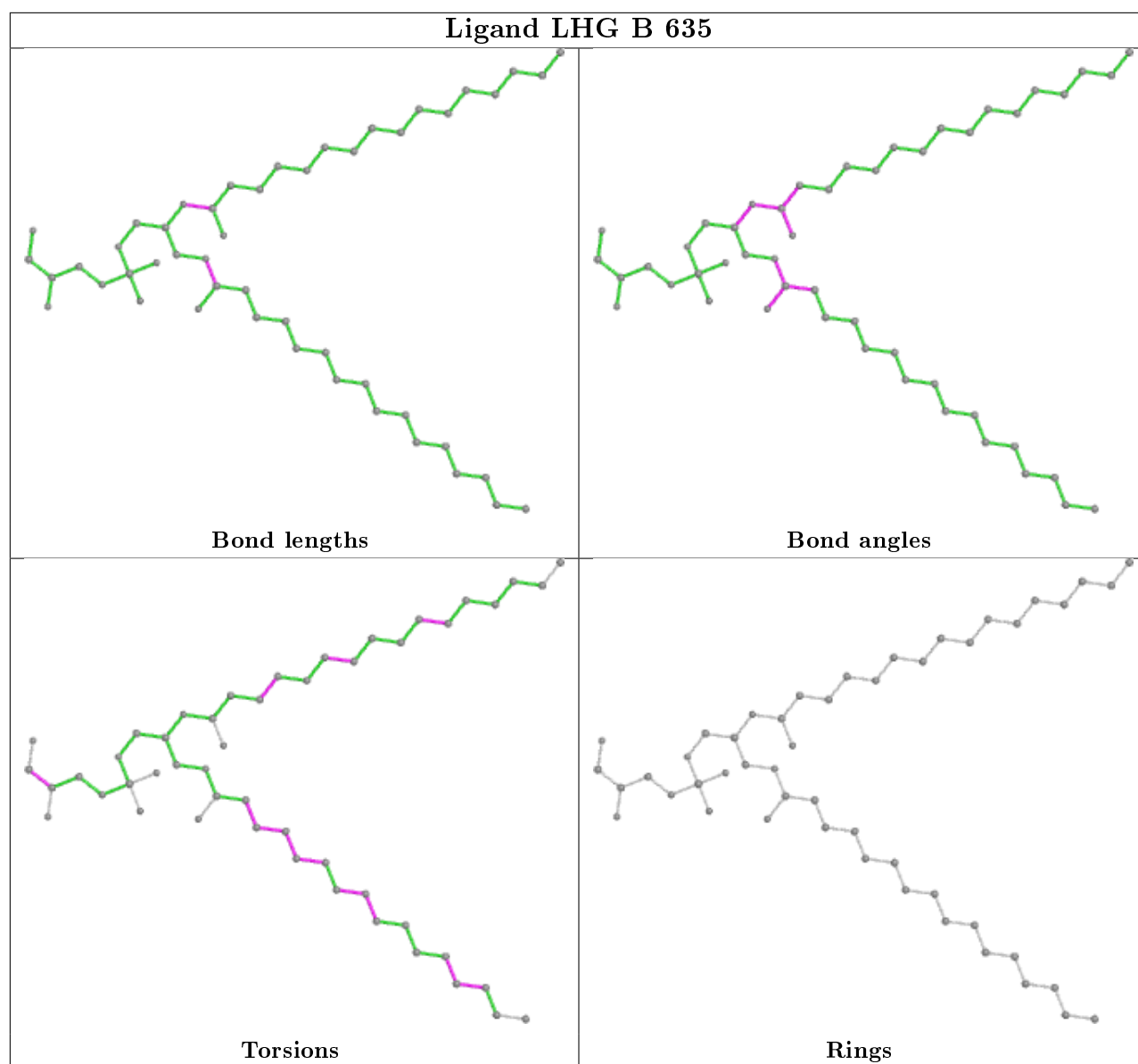
## Ligand CLA C 507

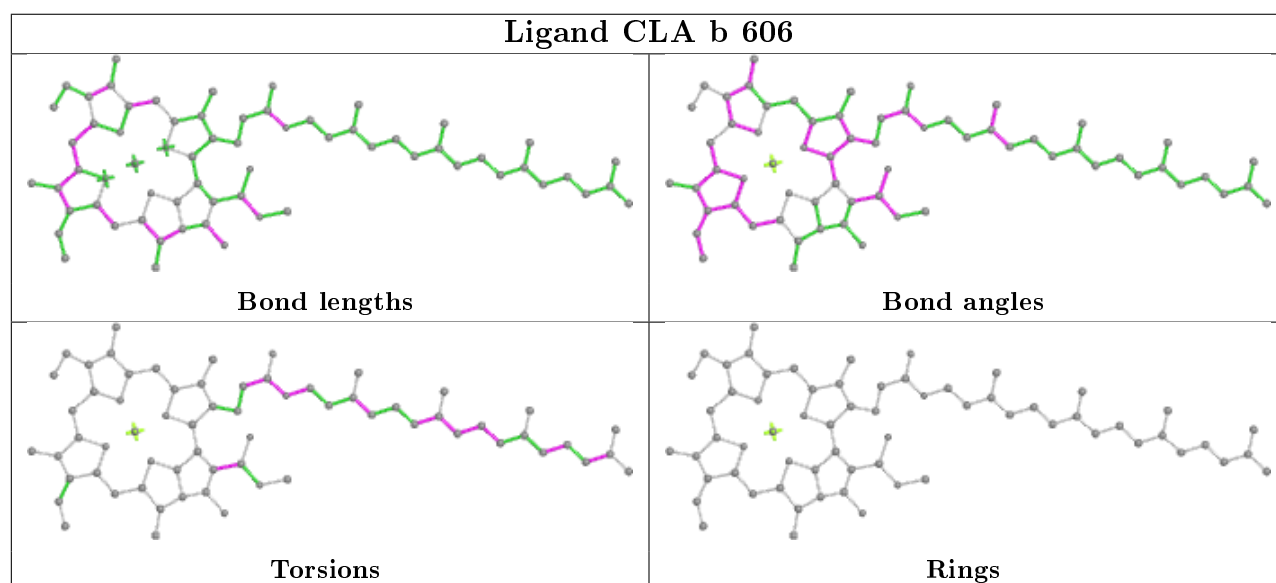
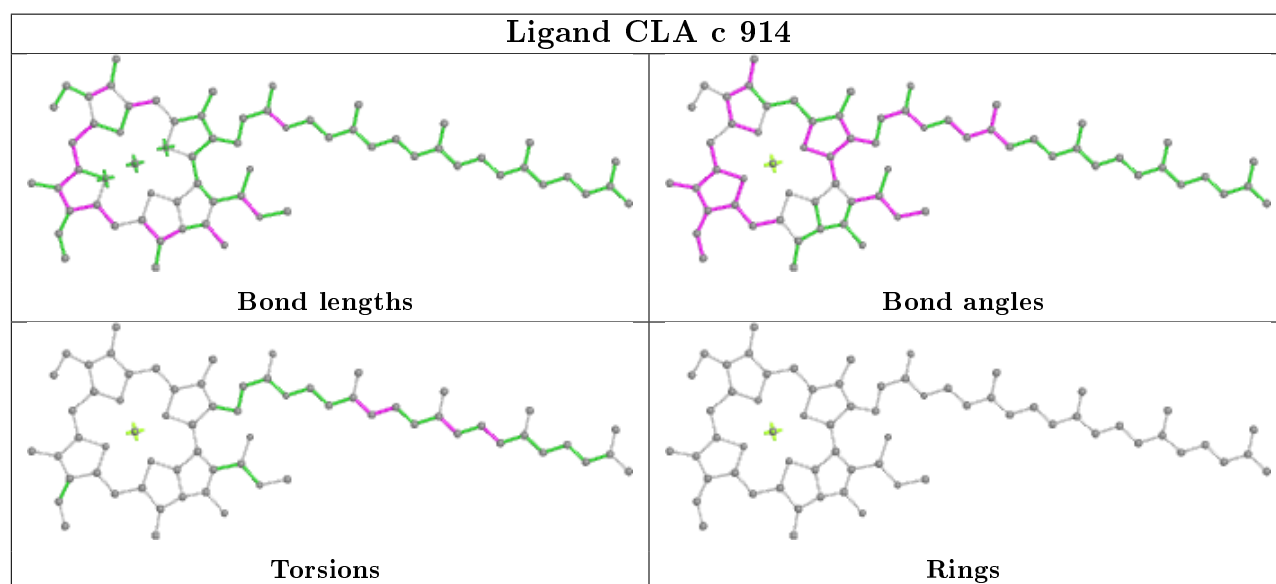
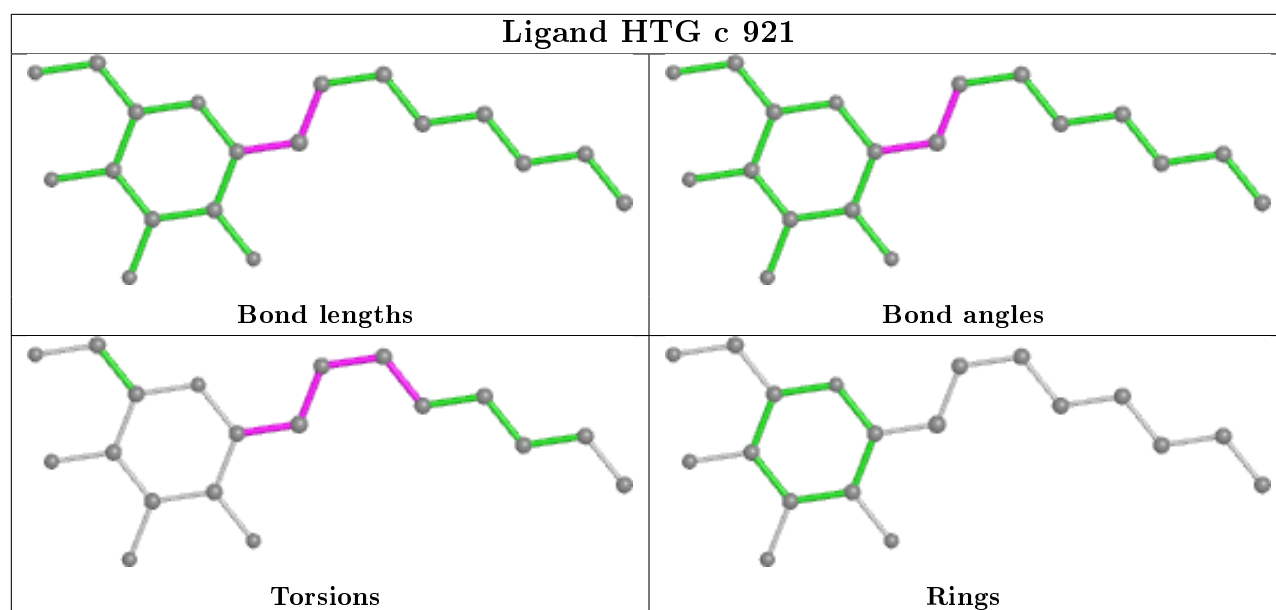


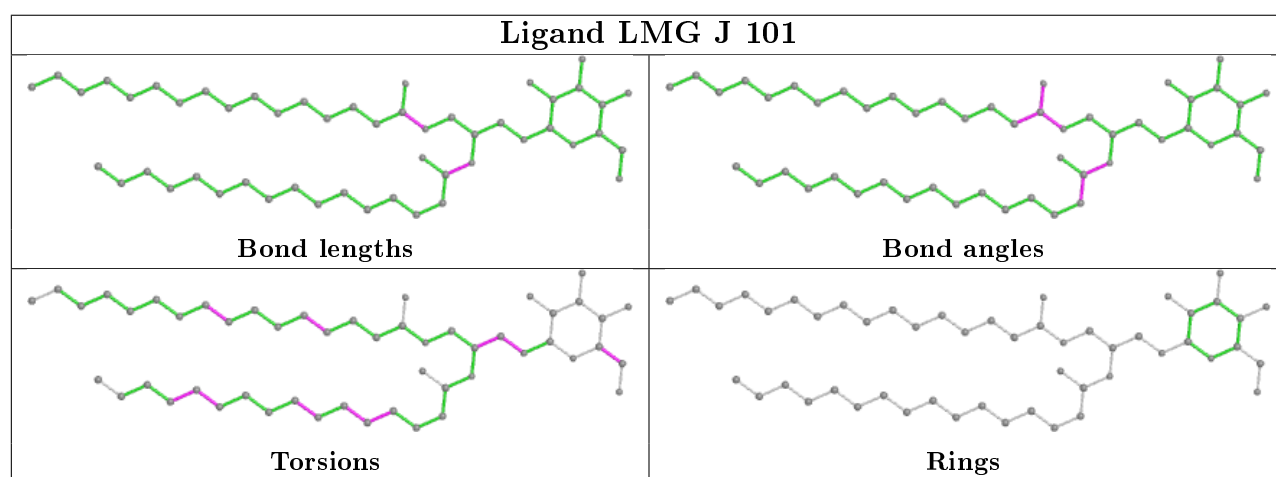
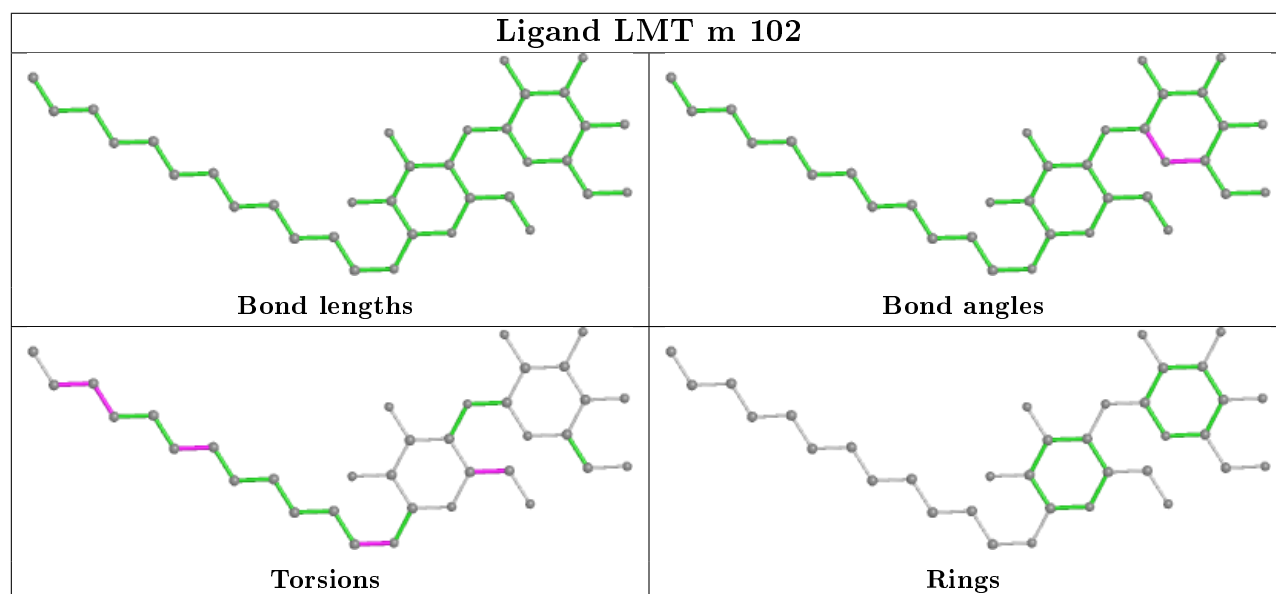
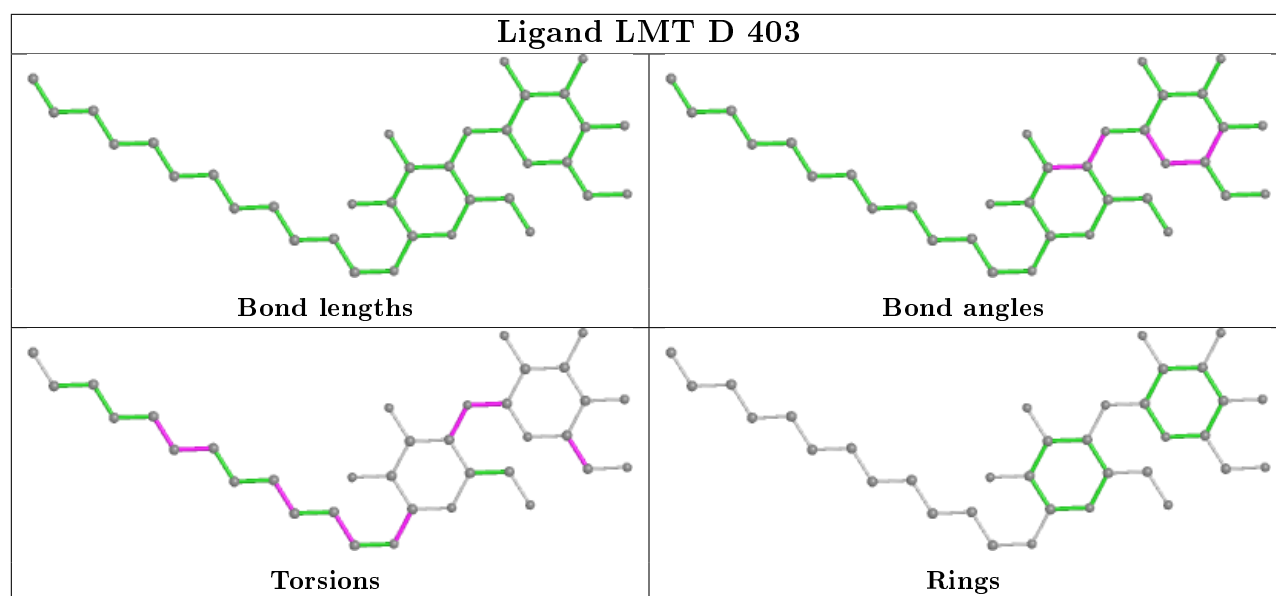
## Ligand HTG B 623

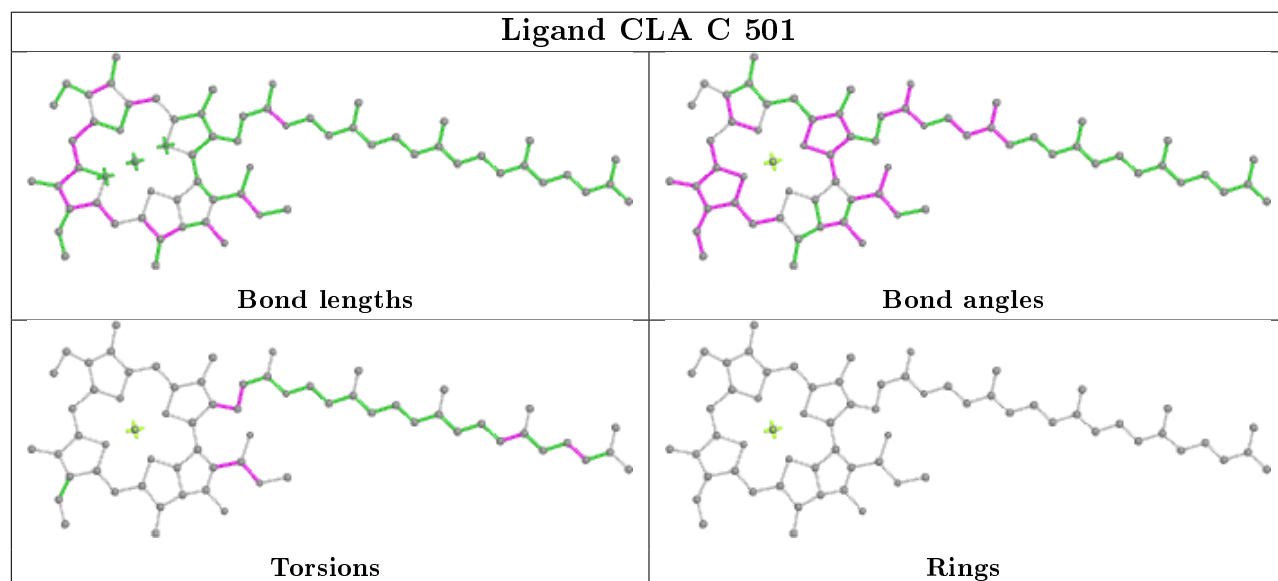
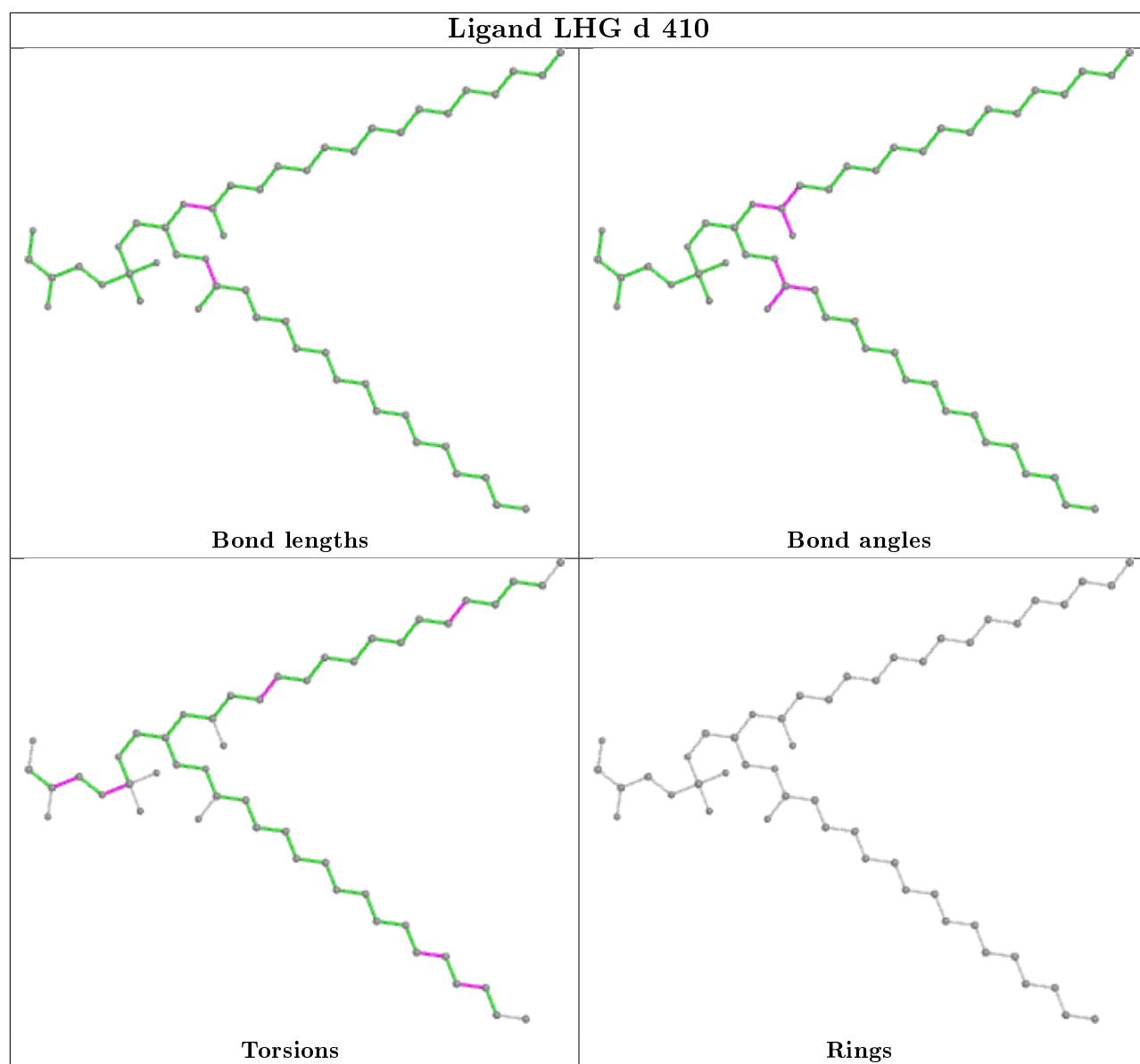


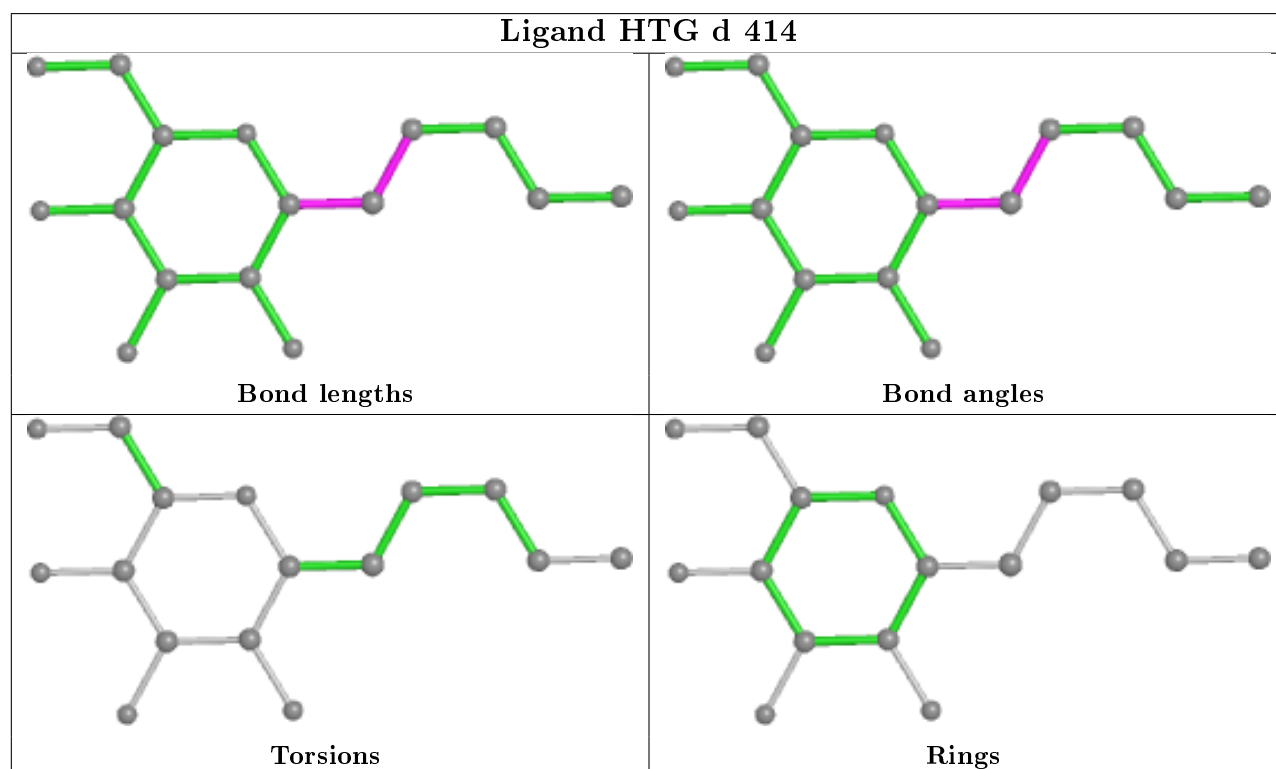
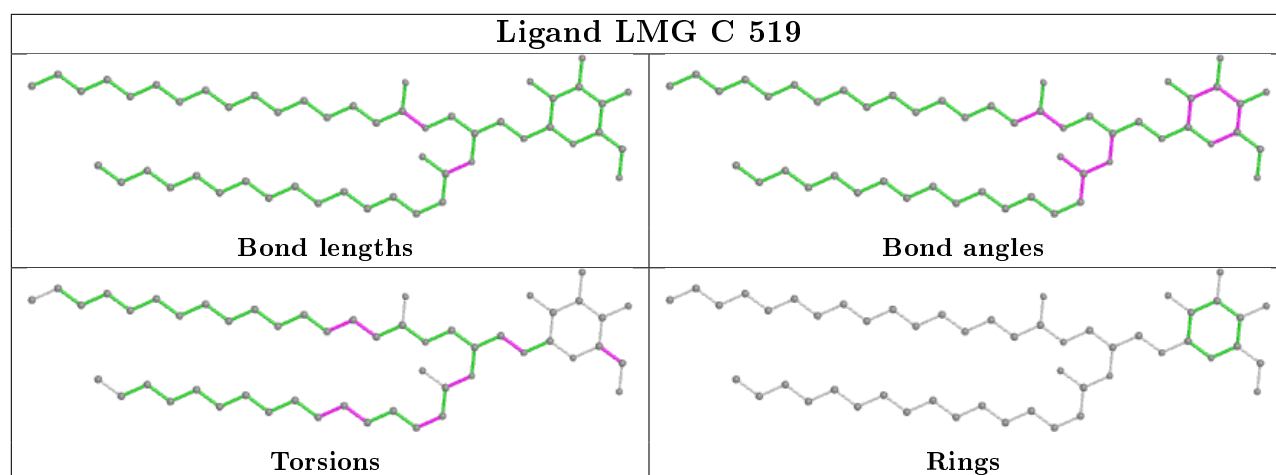




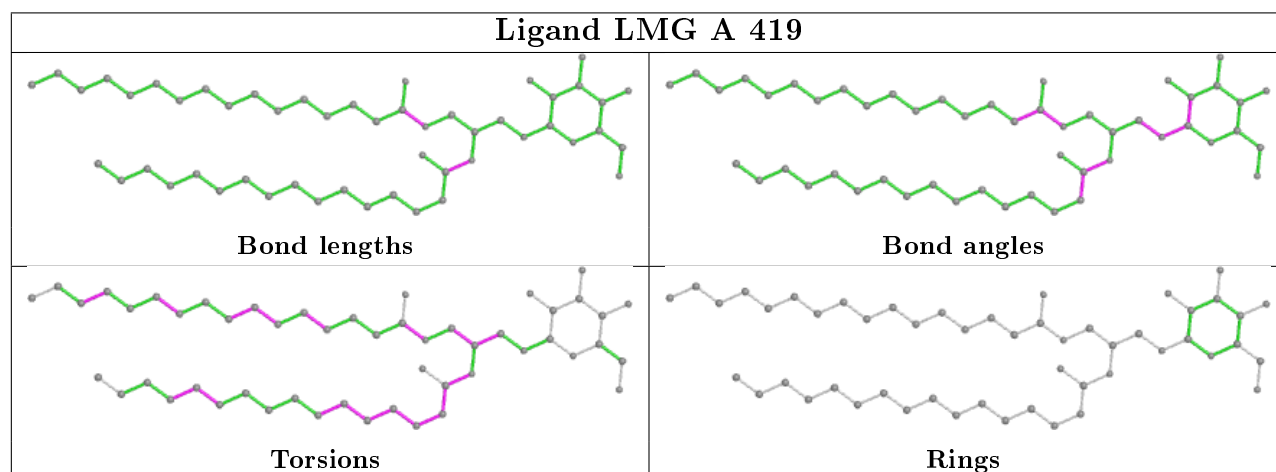
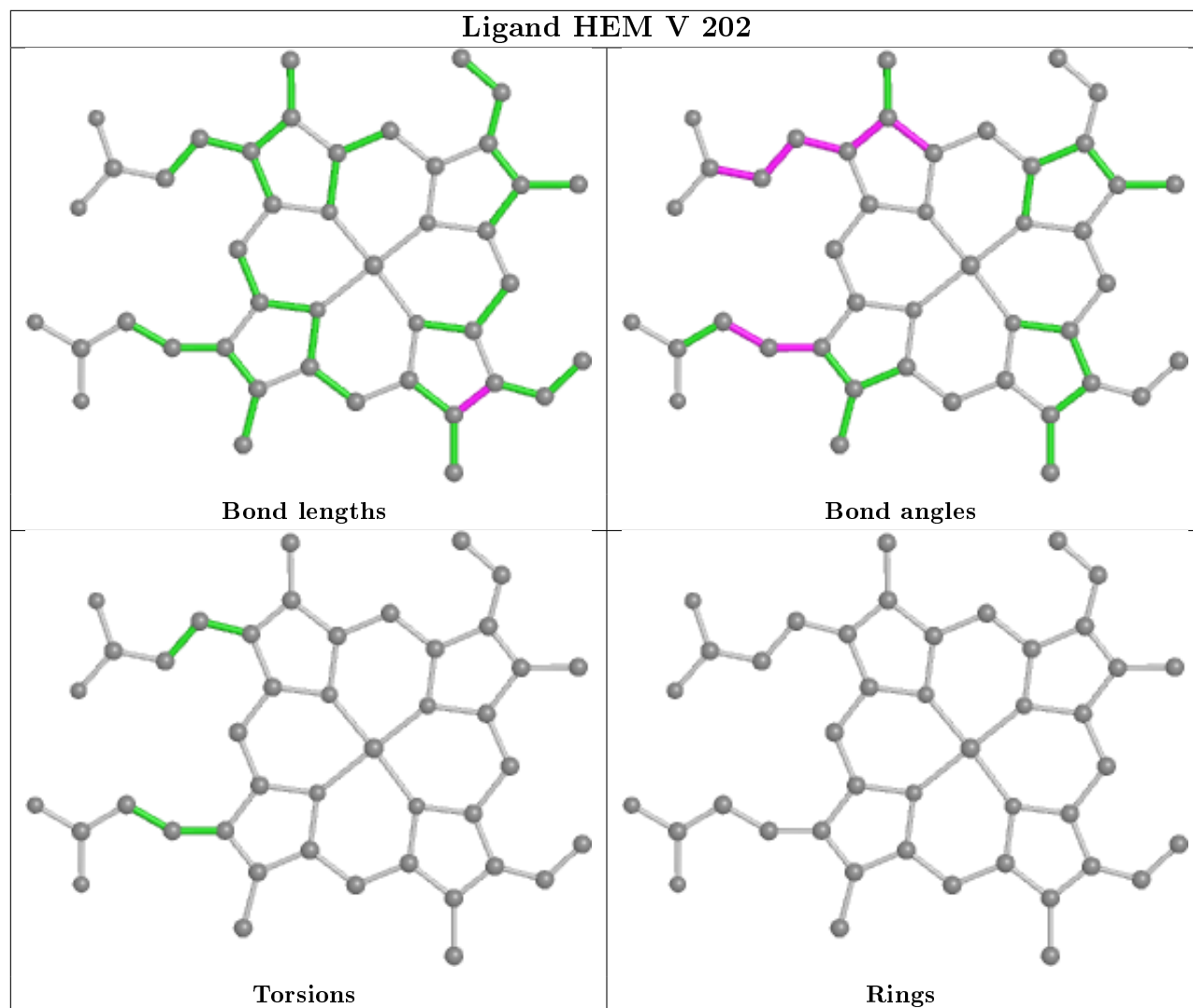


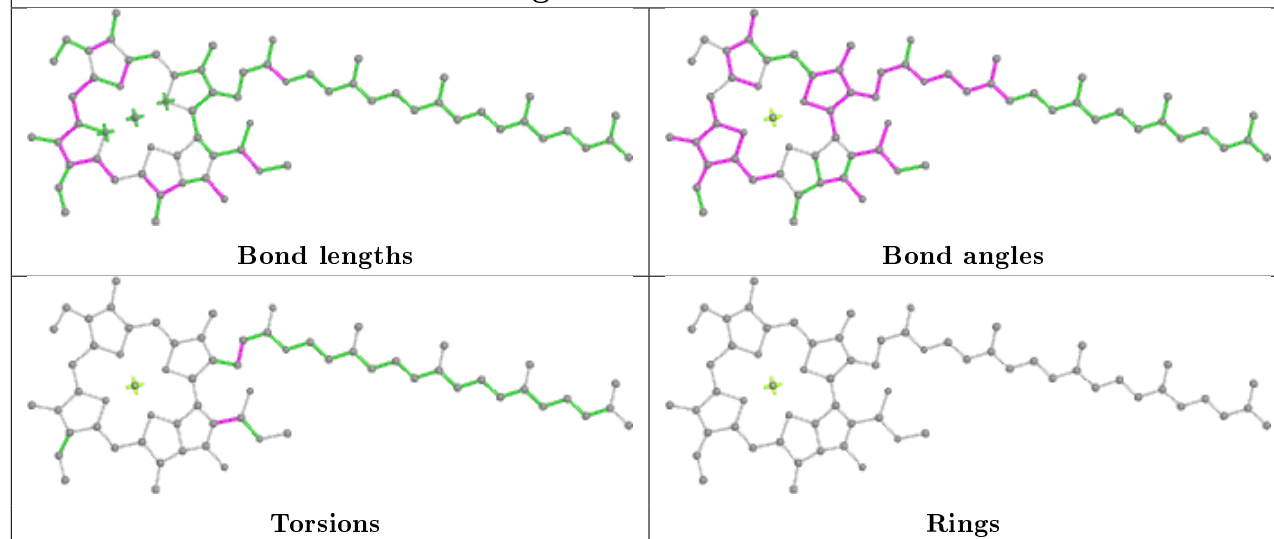
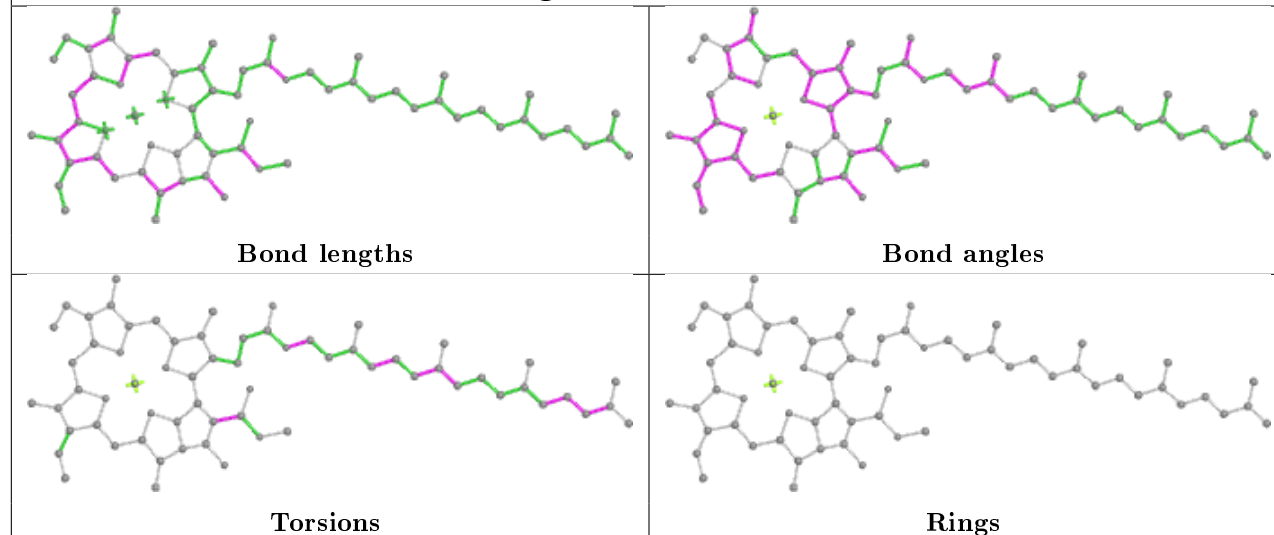
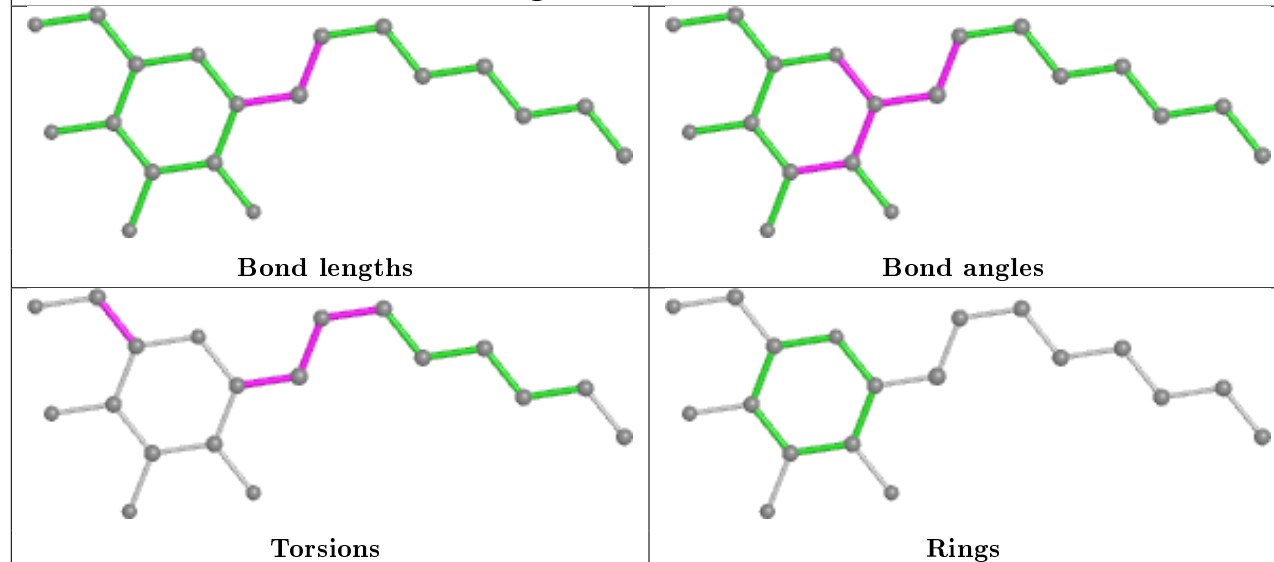


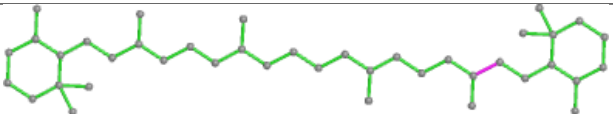
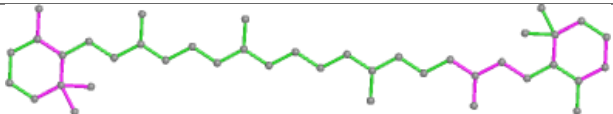
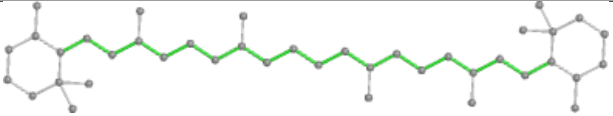
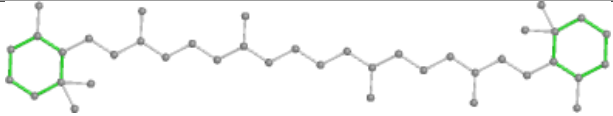


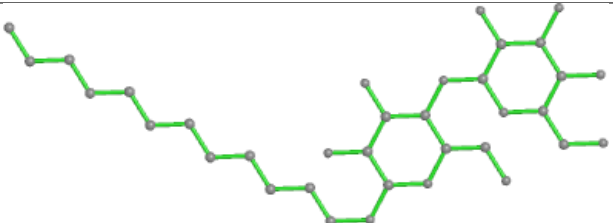
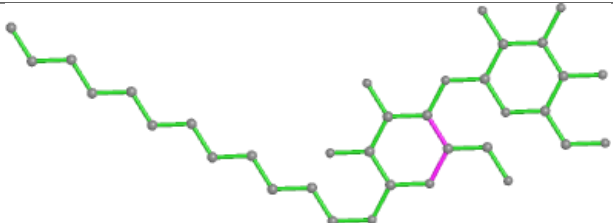
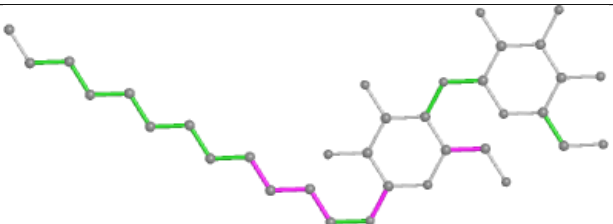
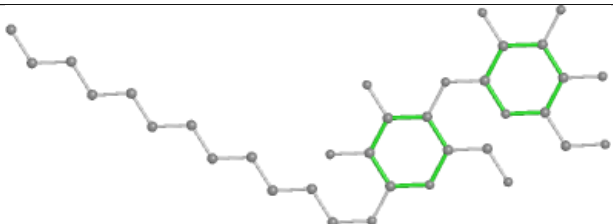


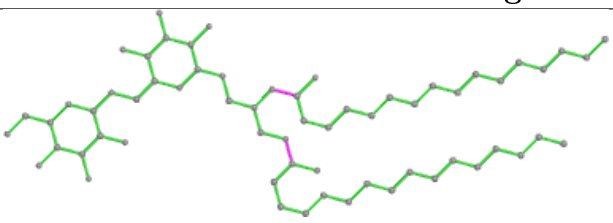
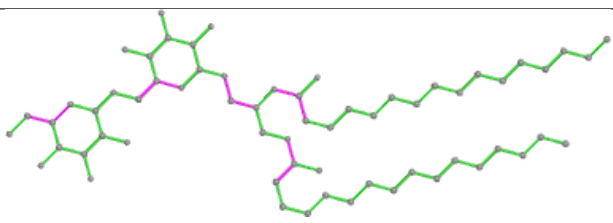
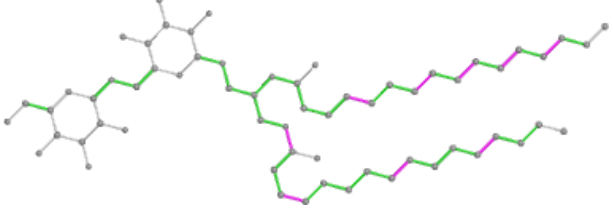
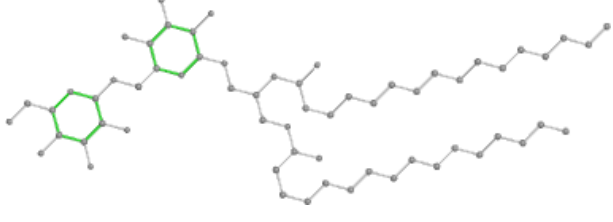


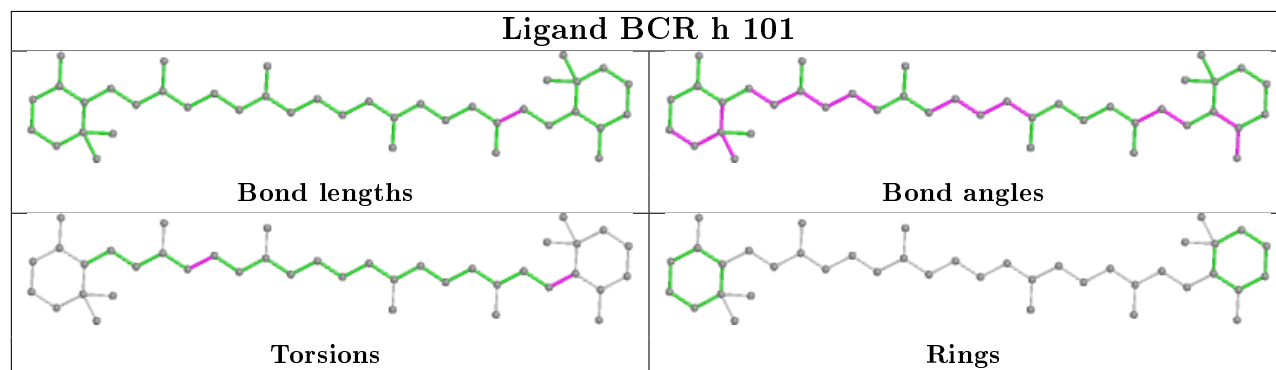
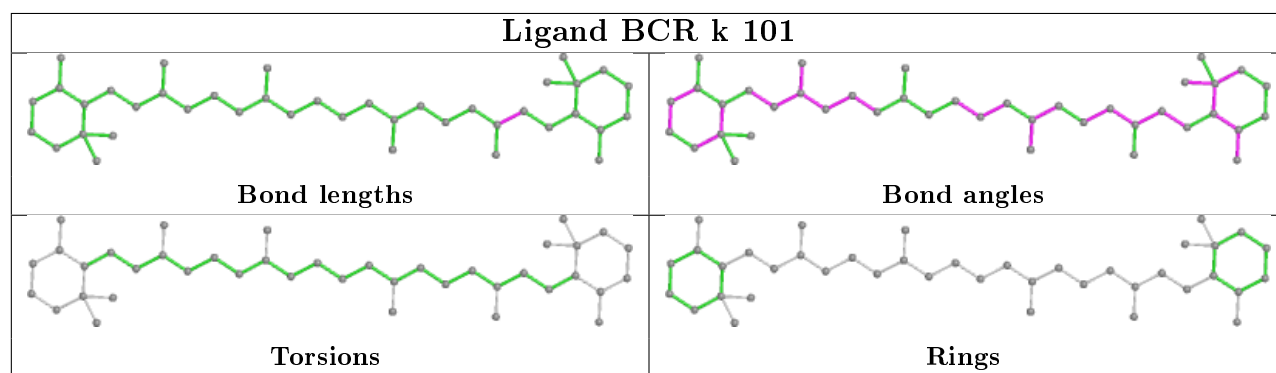
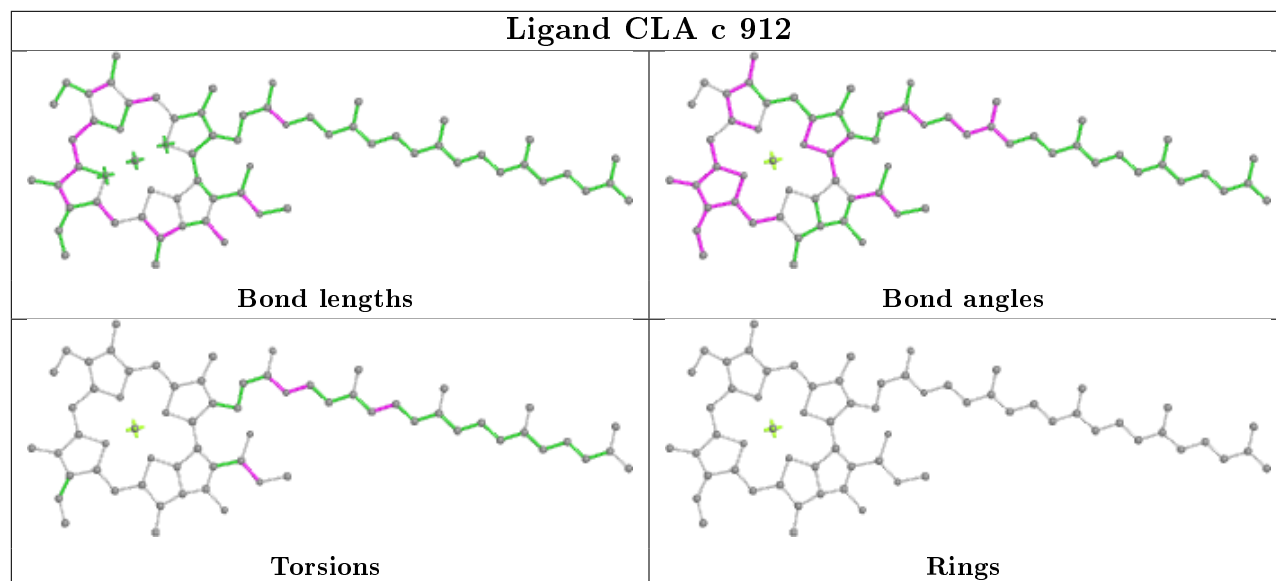
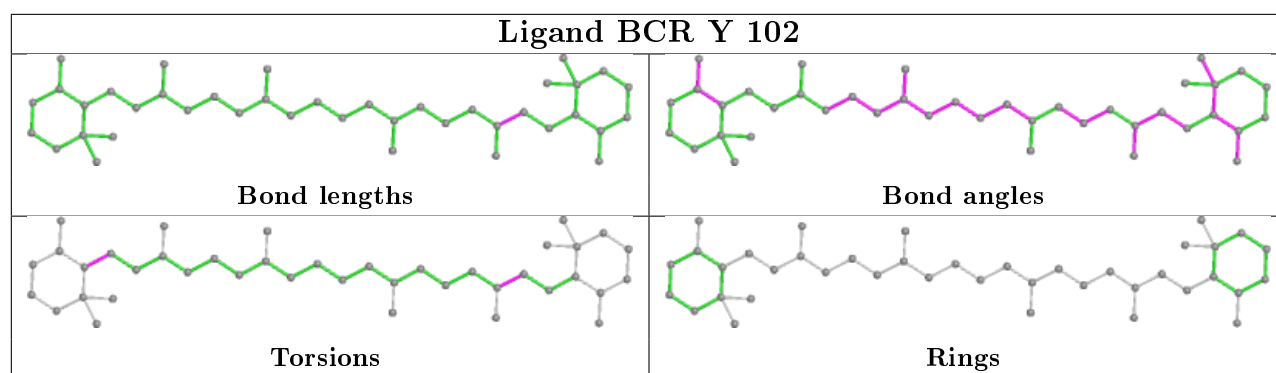


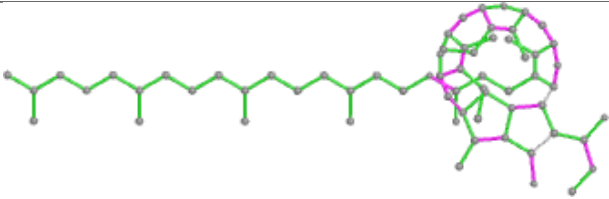
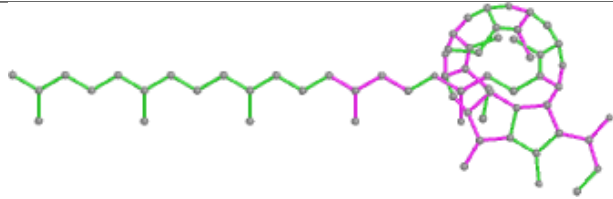
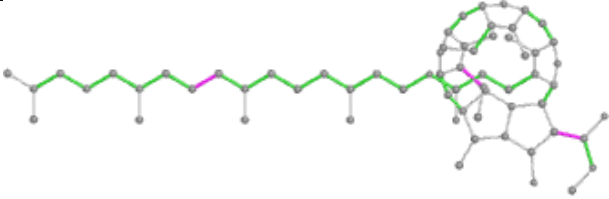
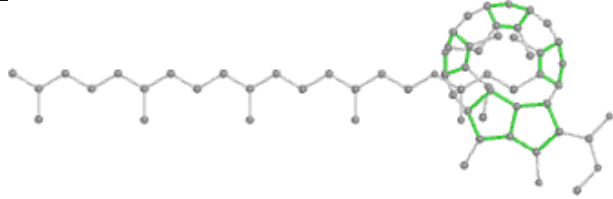
**Ligand CLA B 603****Ligand CLA c 907****Ligand HTG V 203**

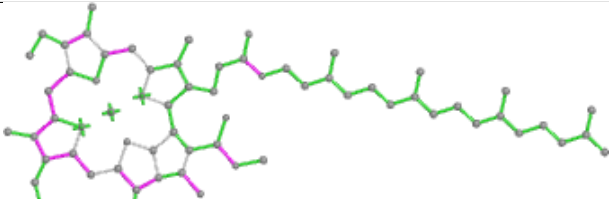
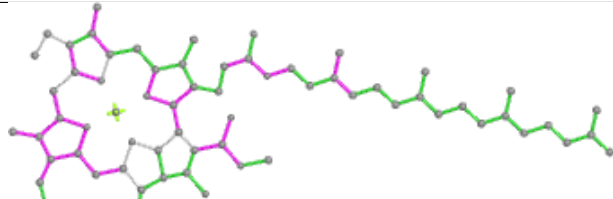
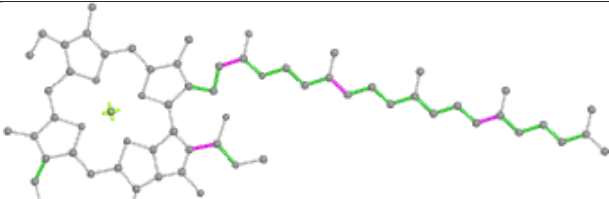
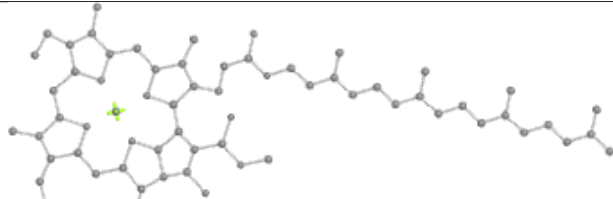
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

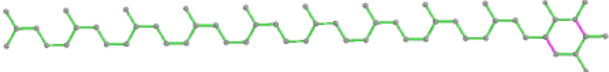
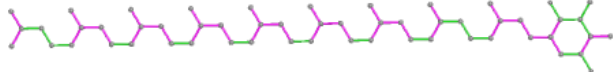
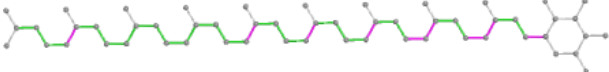
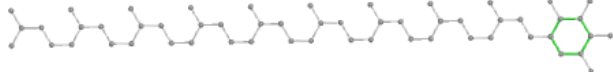
Ligand LMT F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

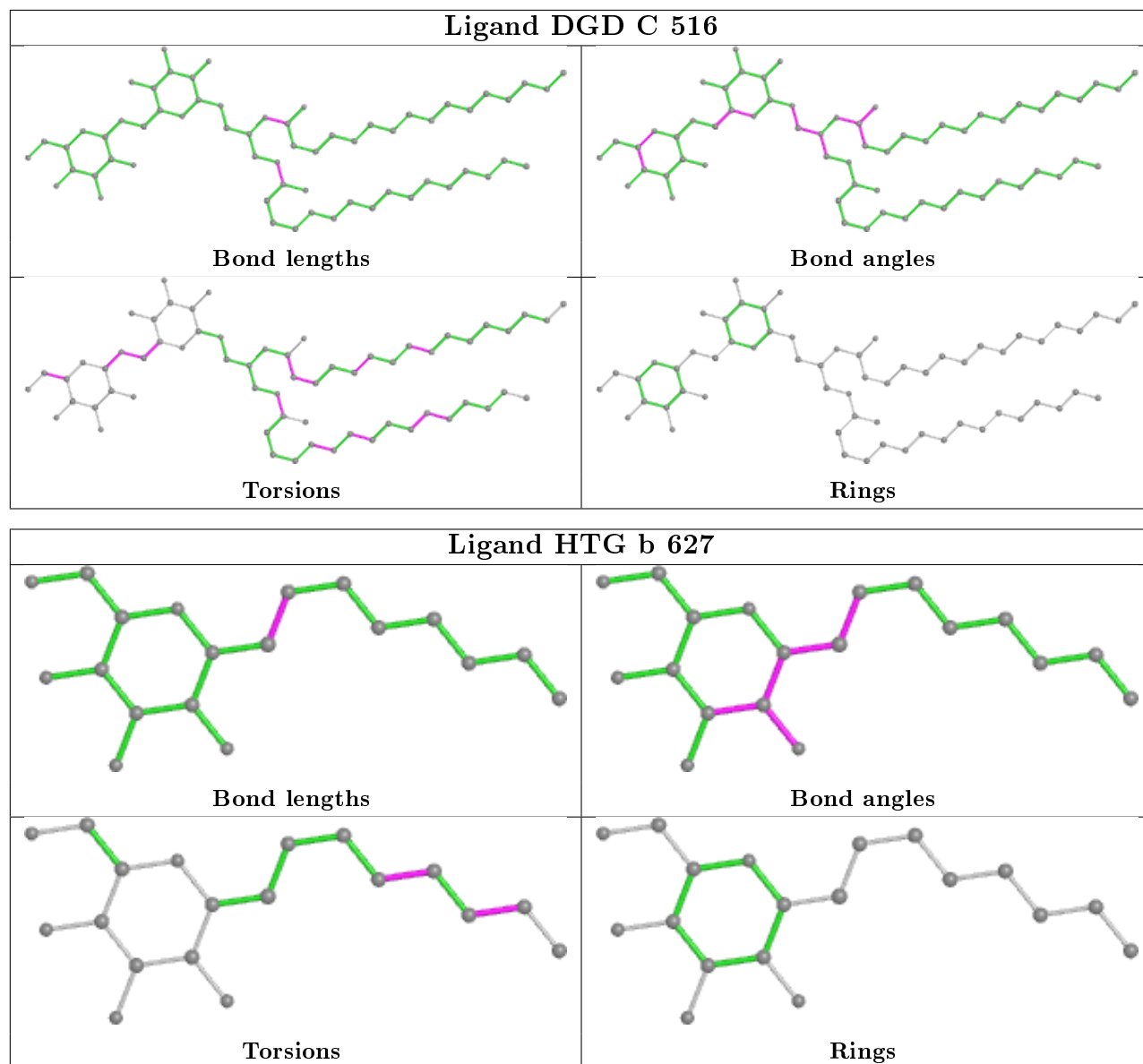
Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

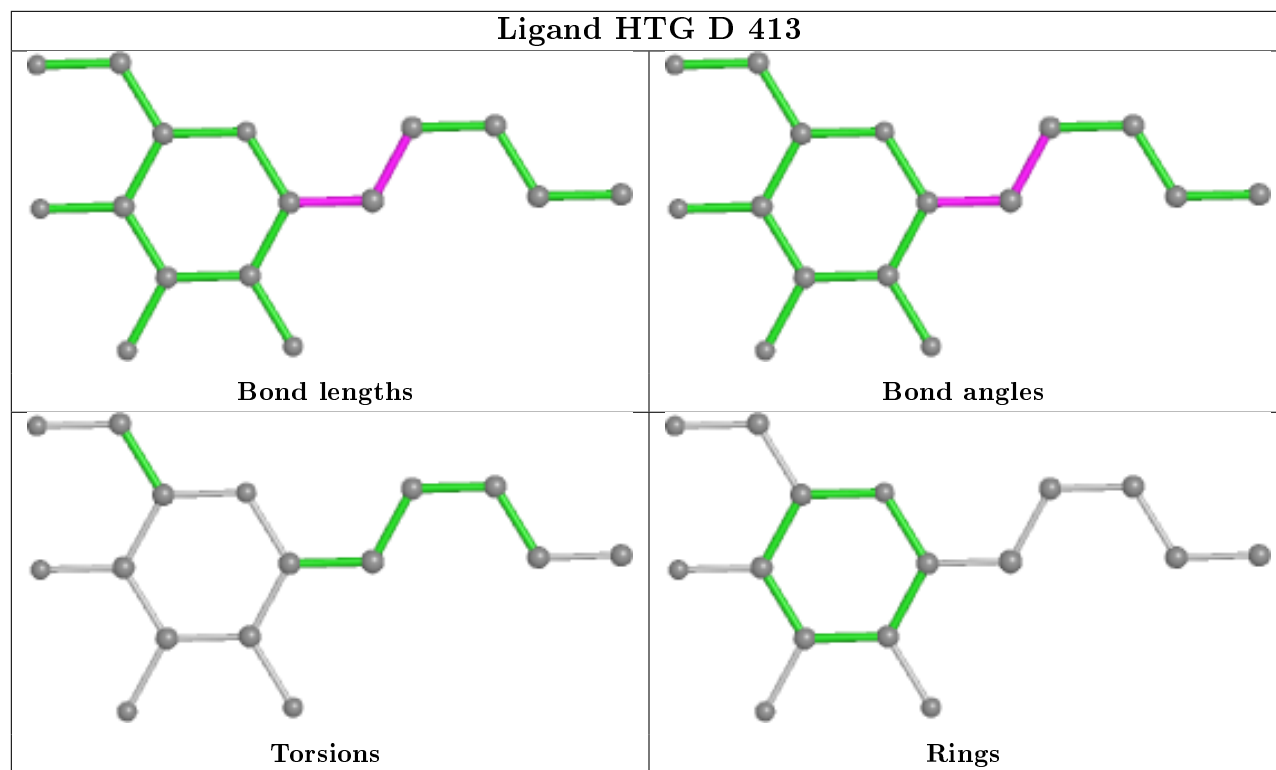


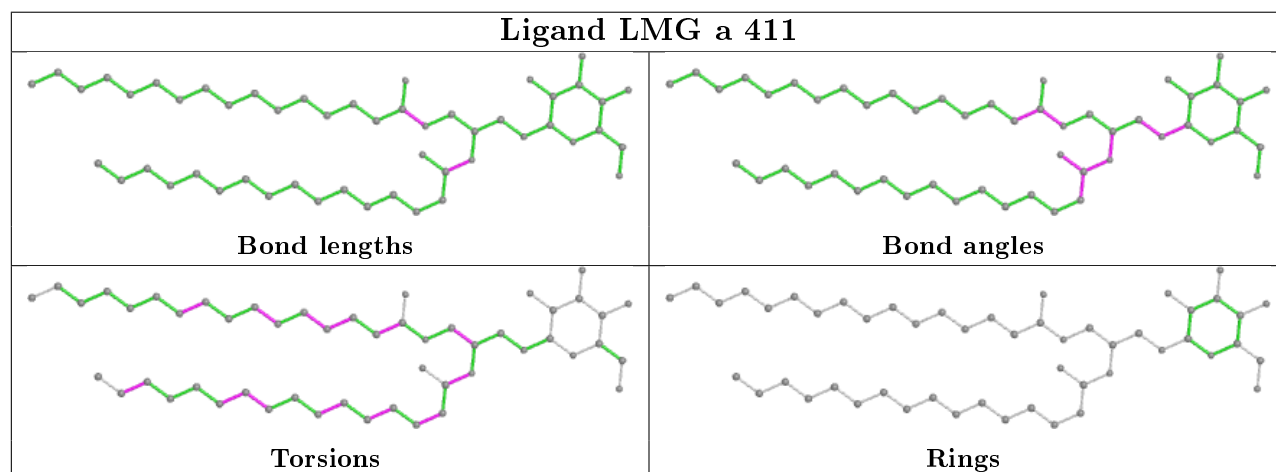
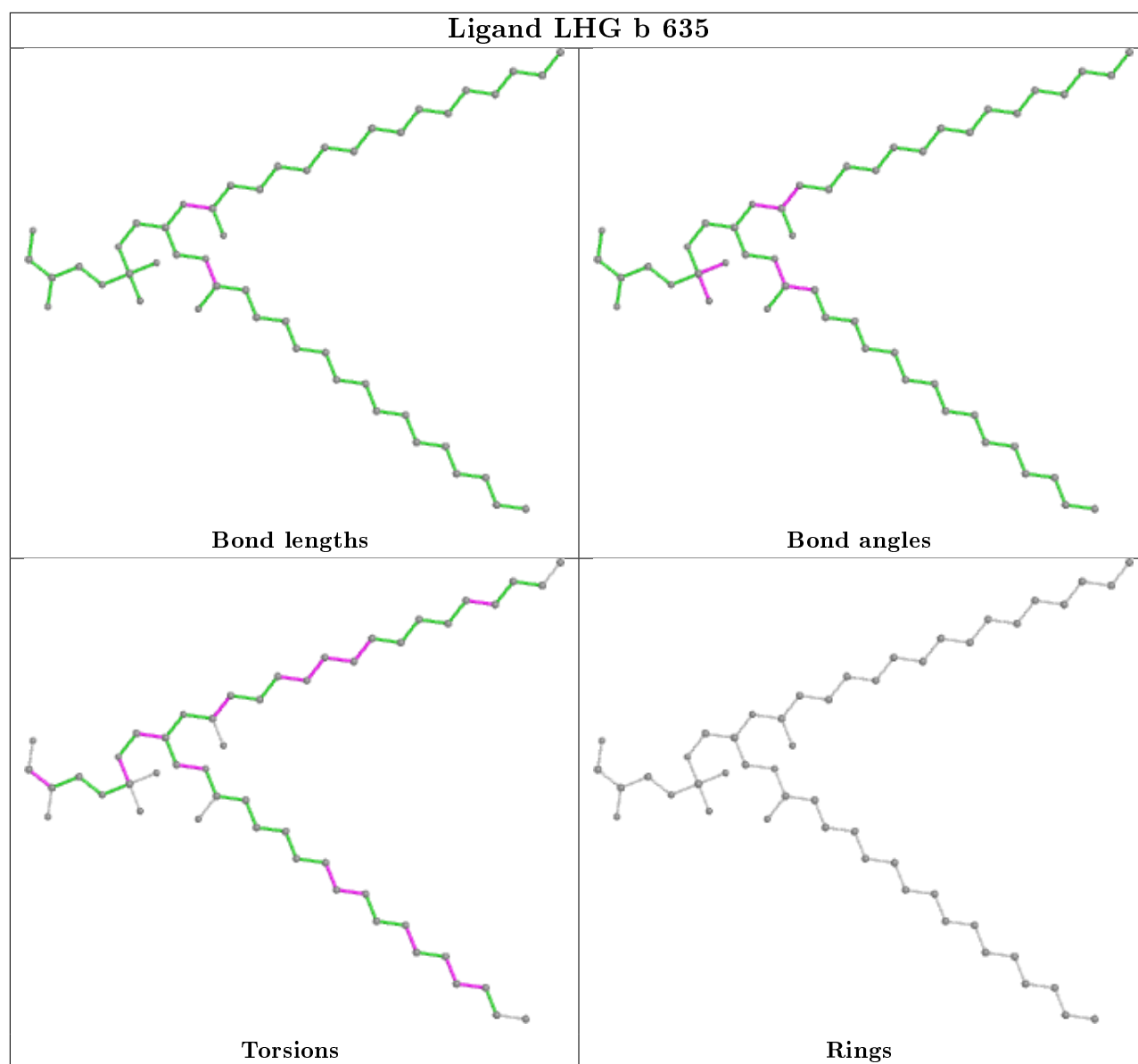
Ligand PHO d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

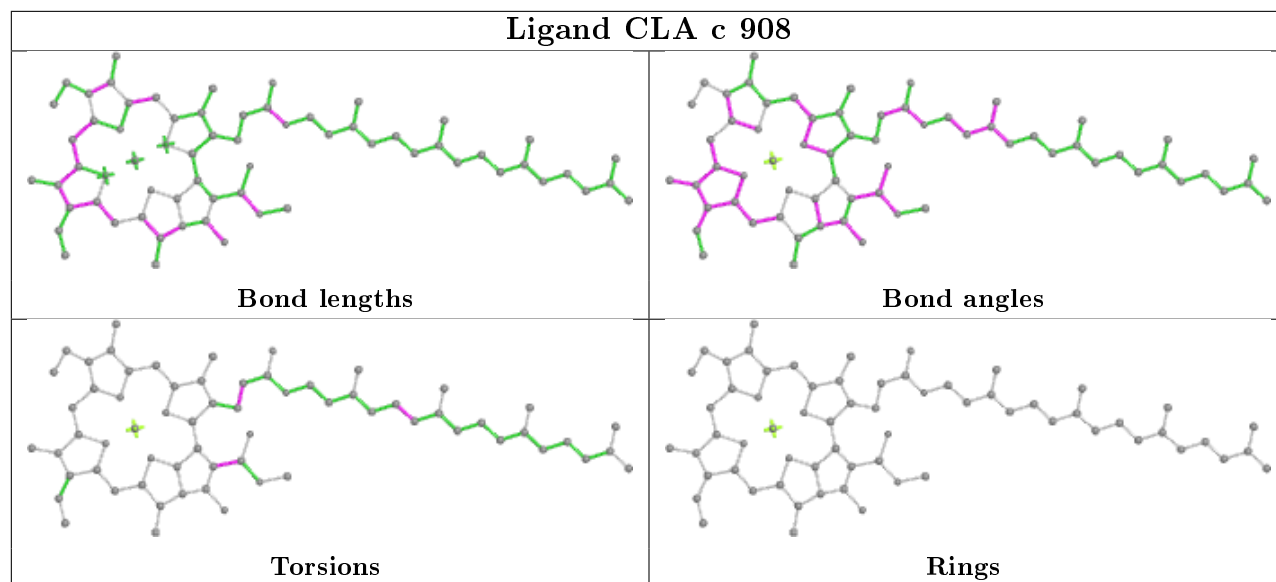




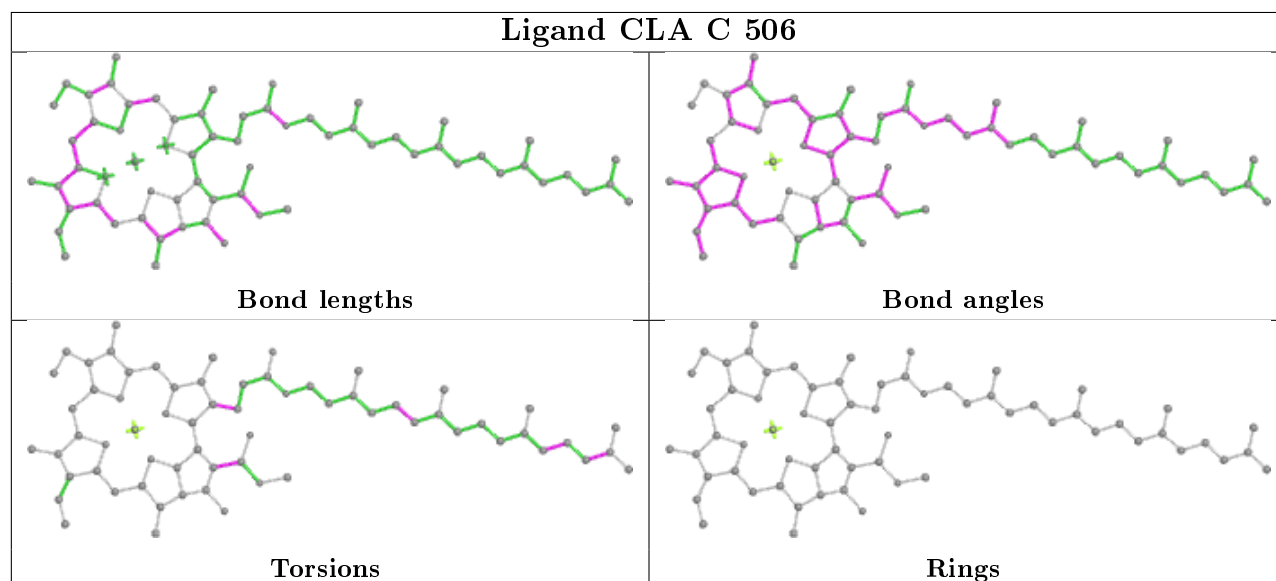




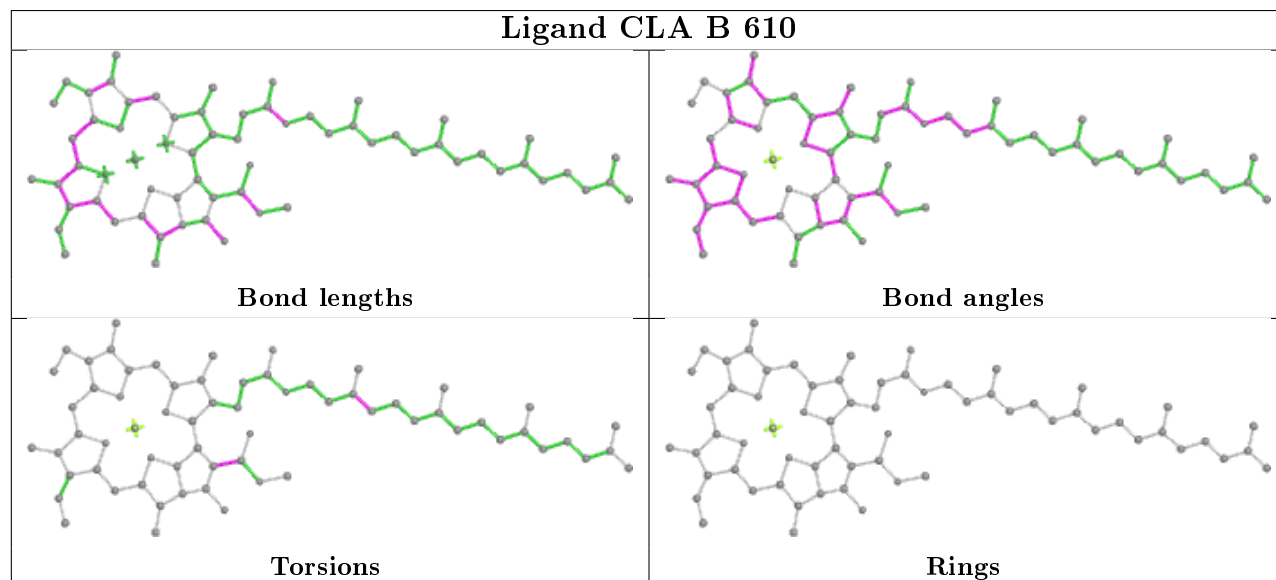
## Ligand CLA c 908

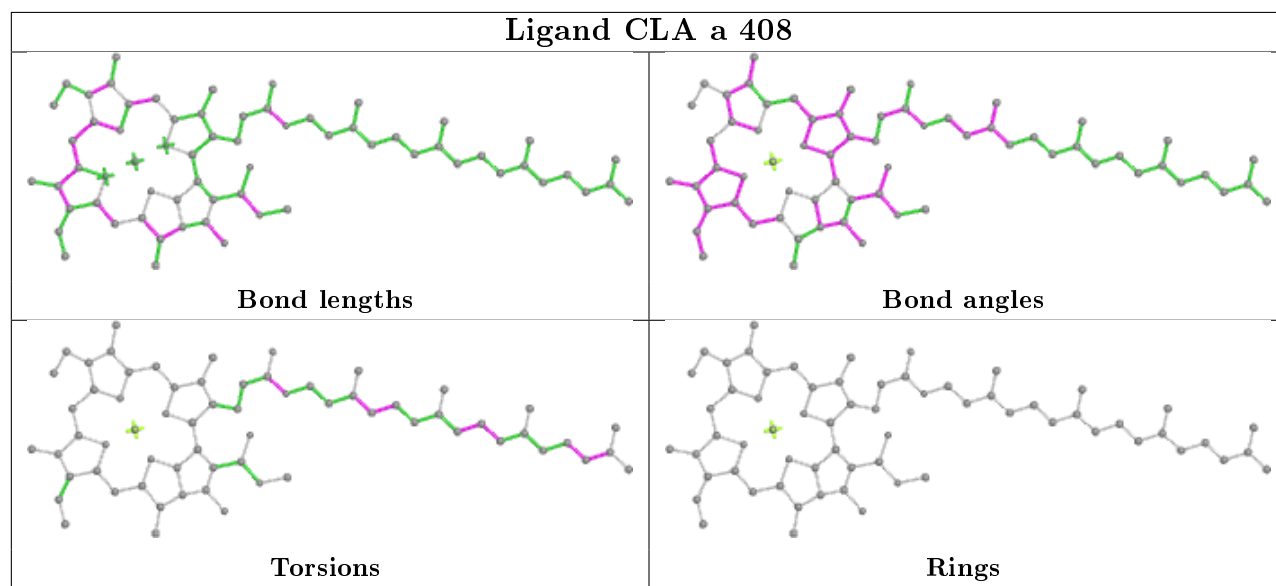
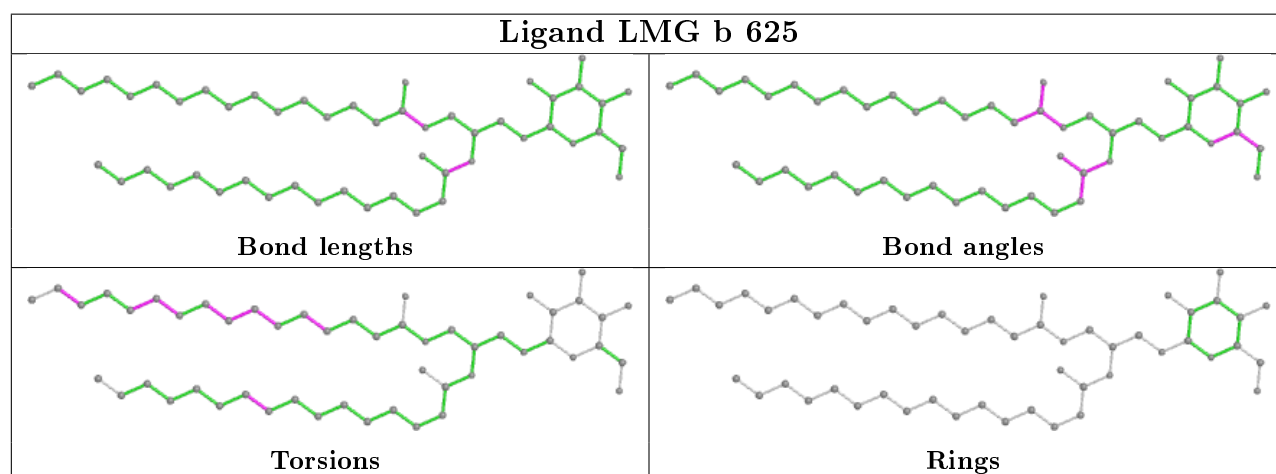
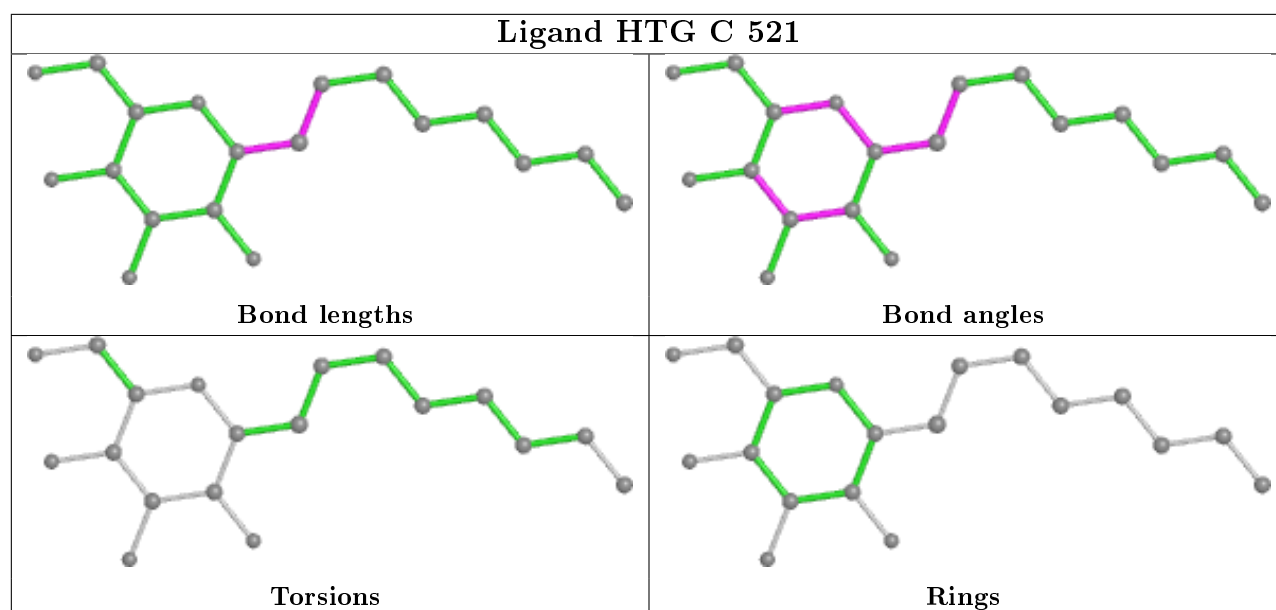


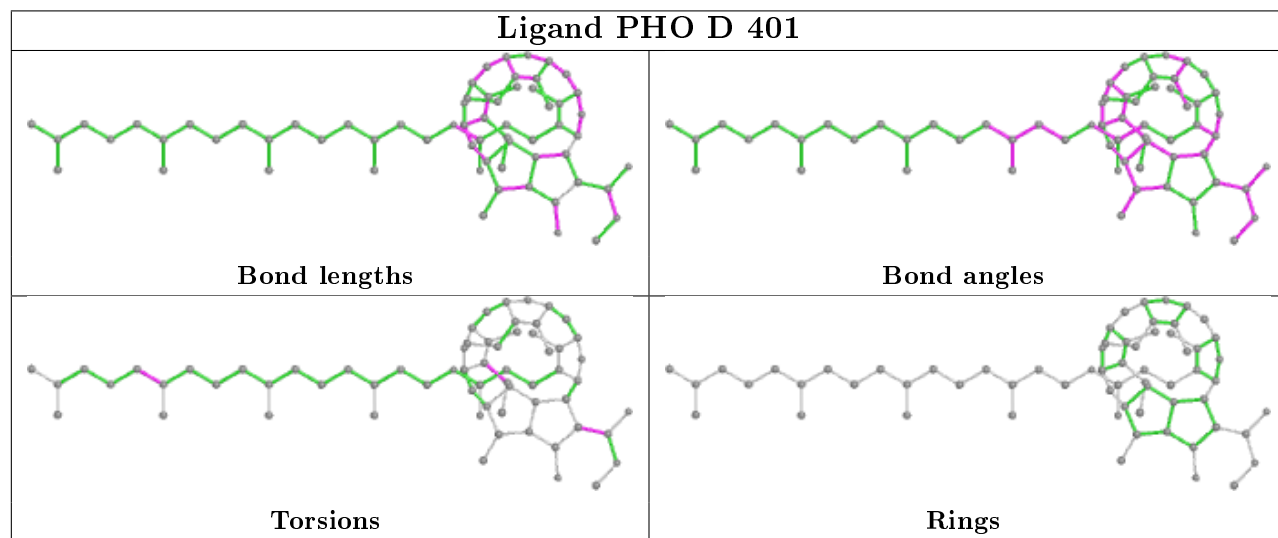
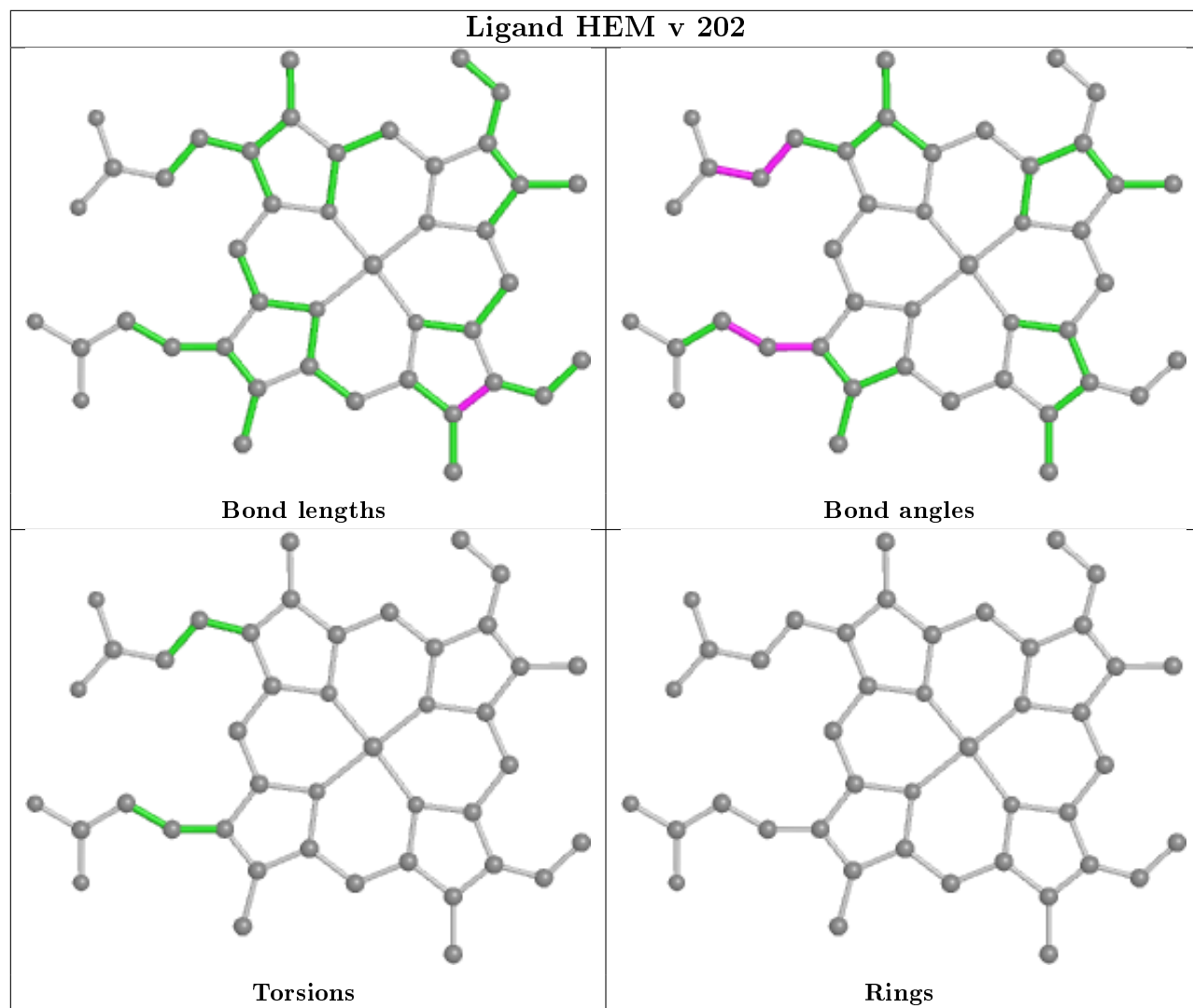
## Ligand CLA C 506

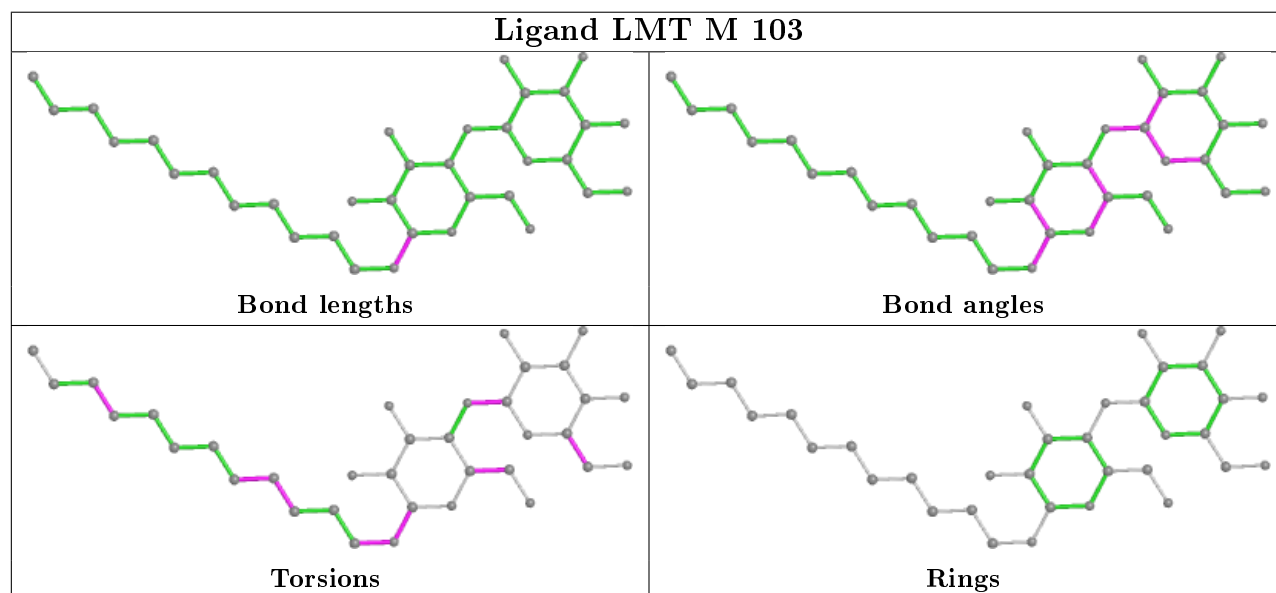
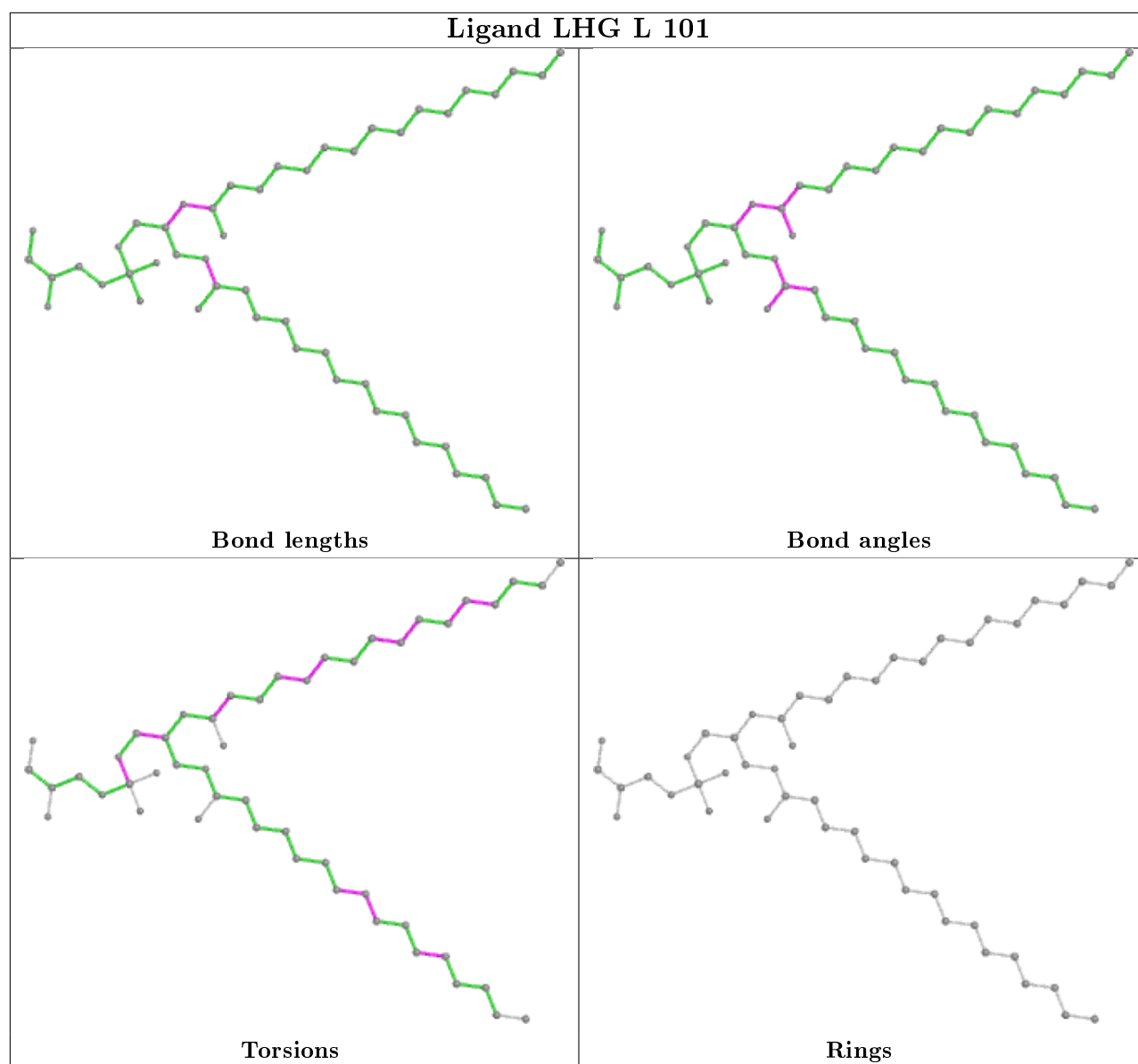


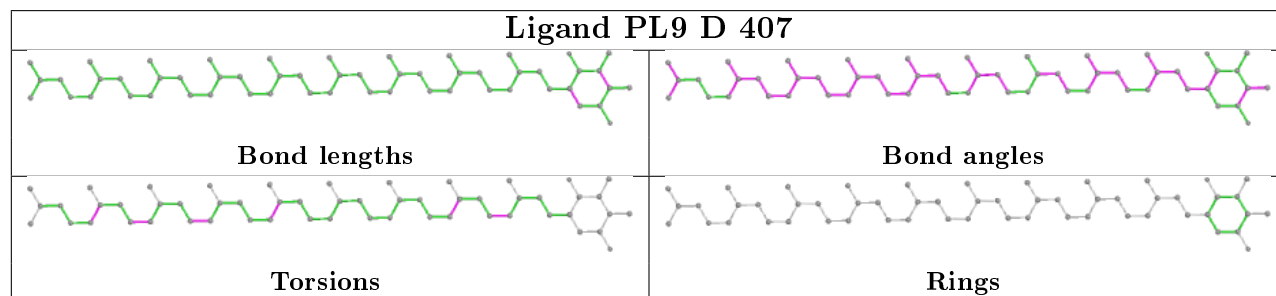
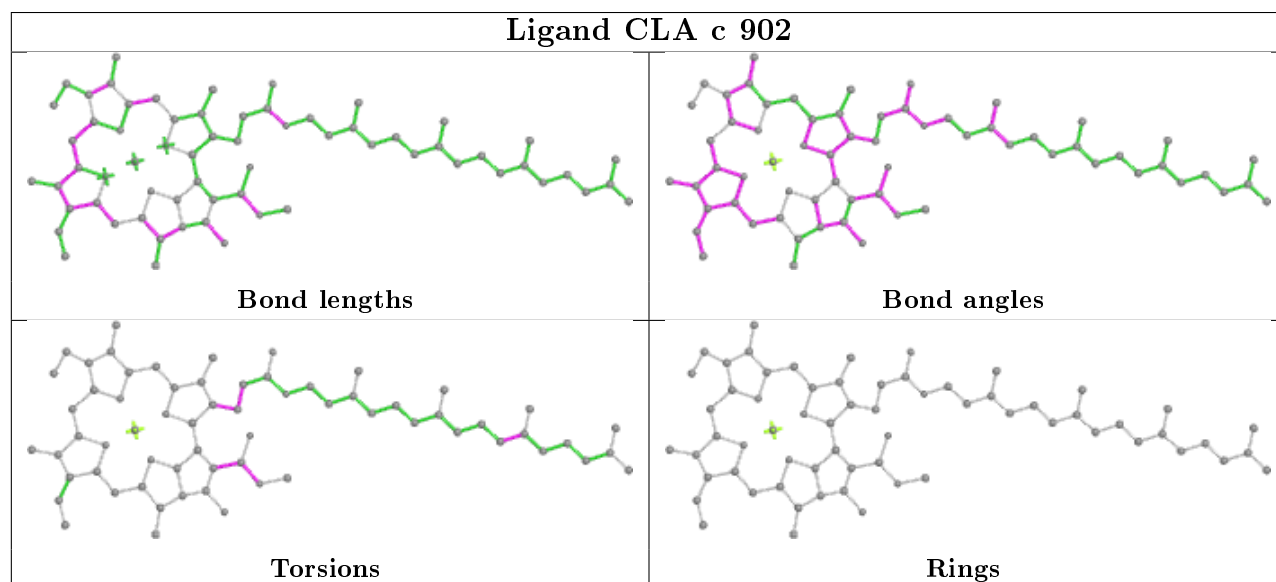
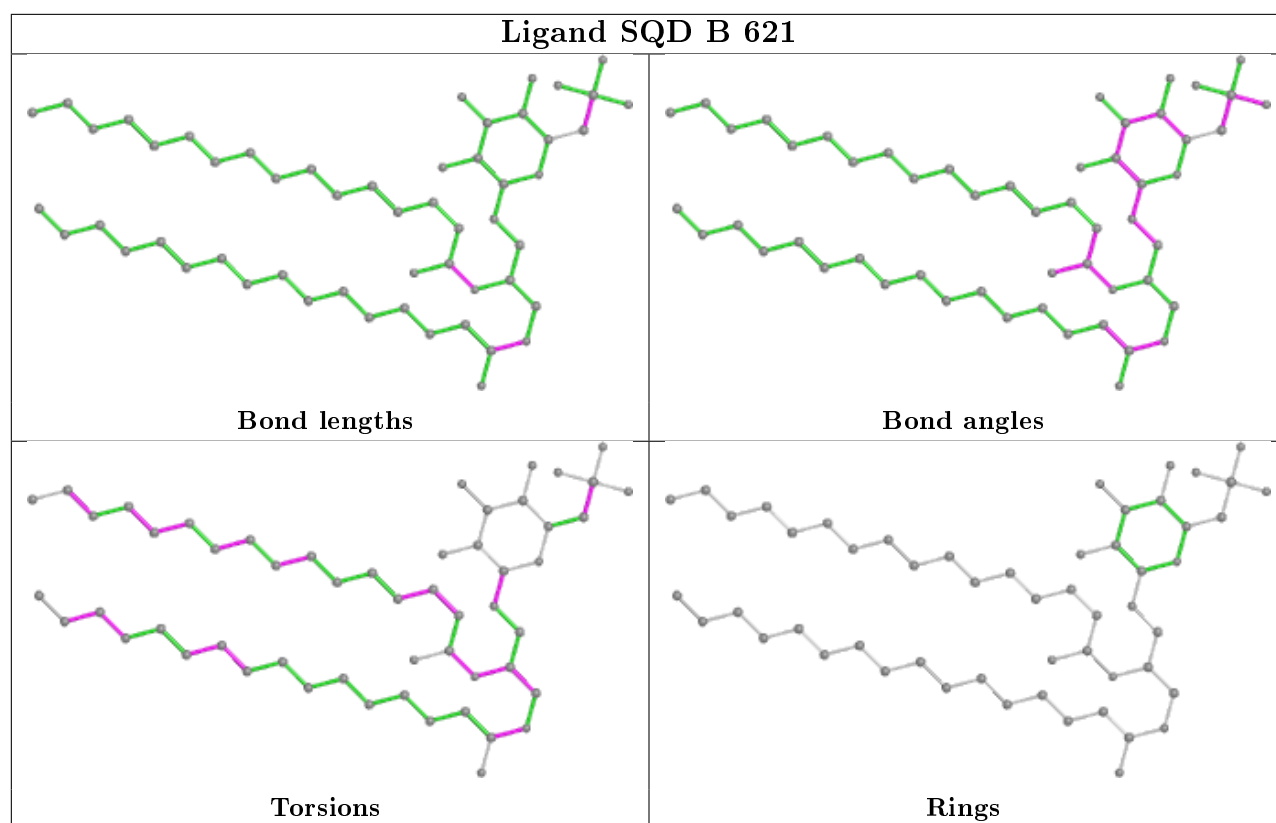
## Ligand CLA B 610

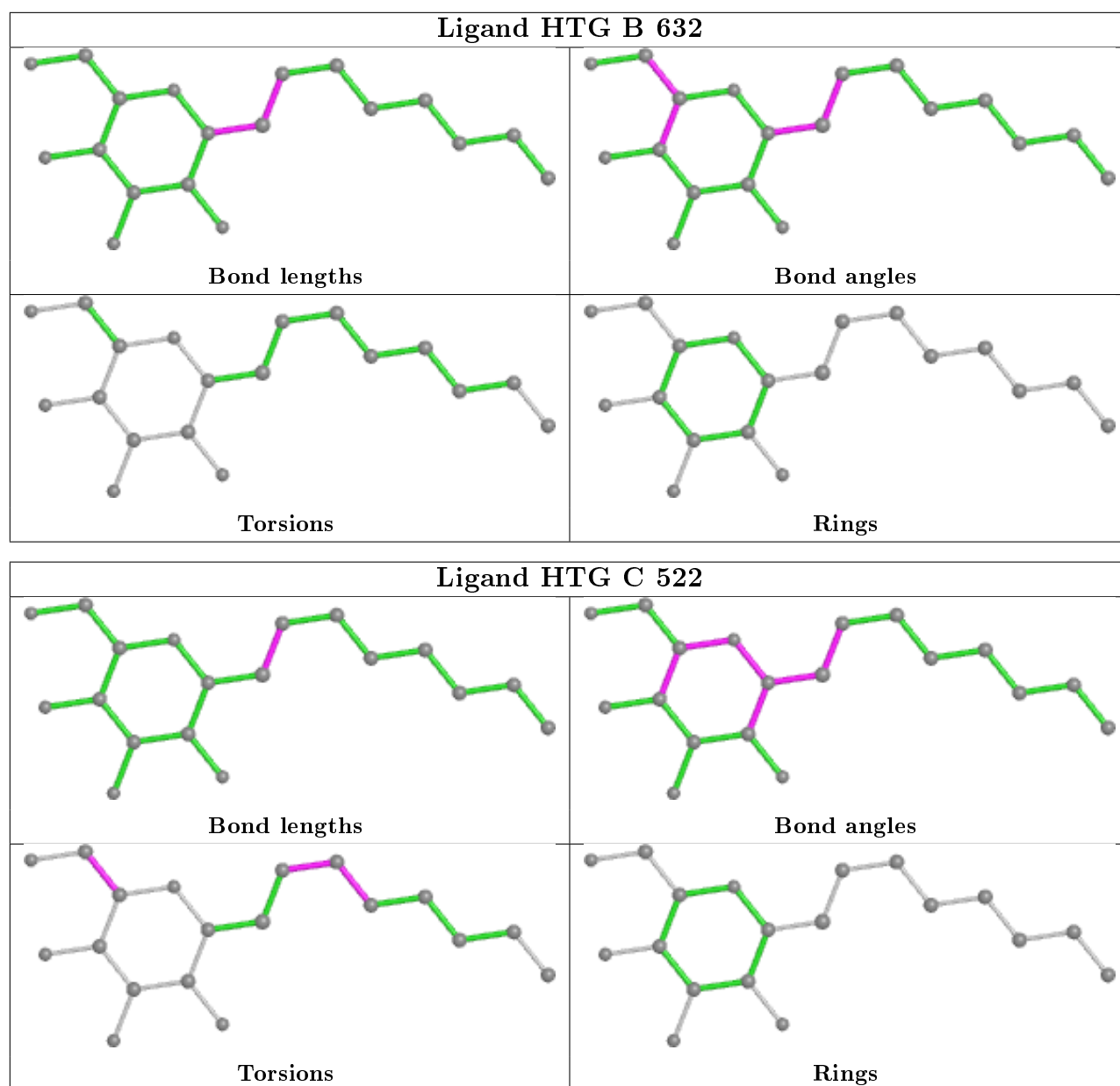




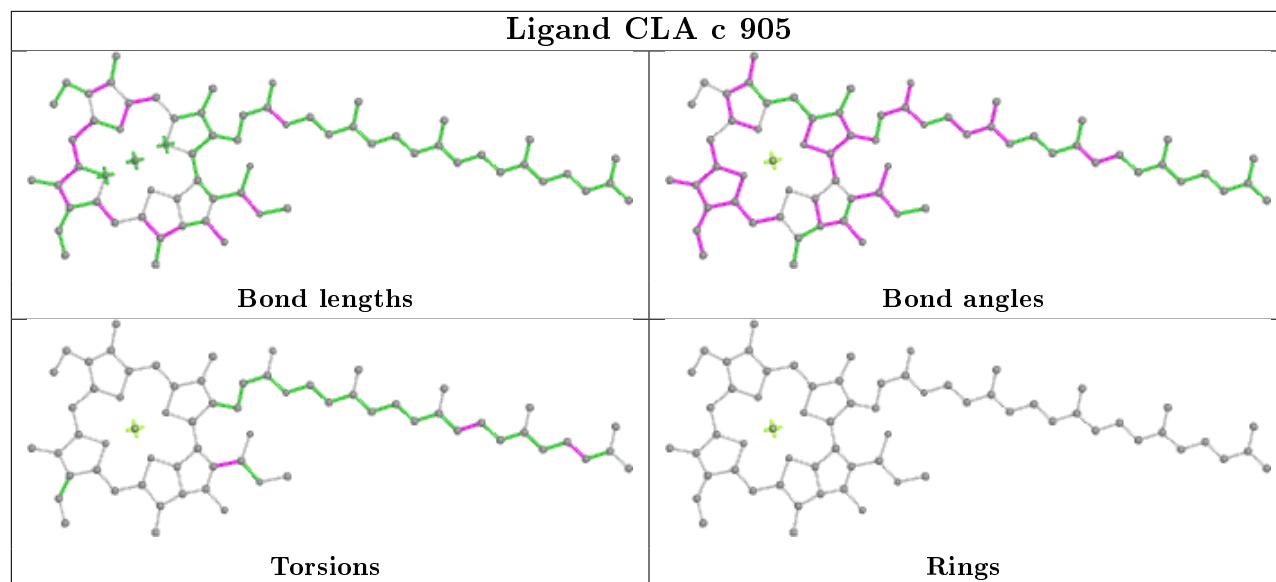




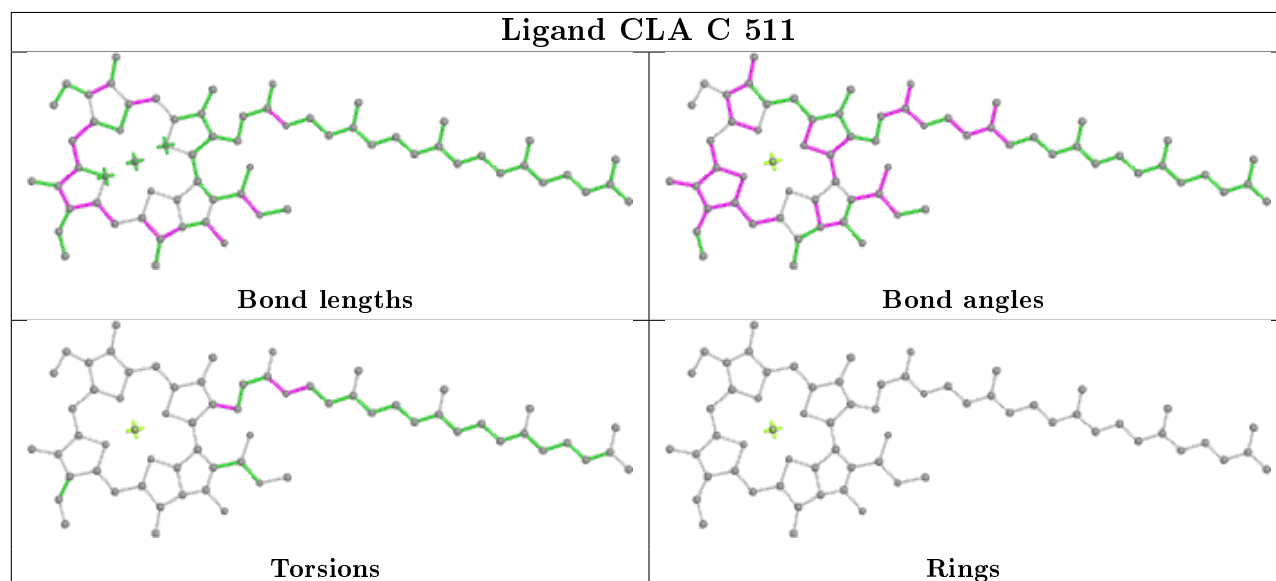




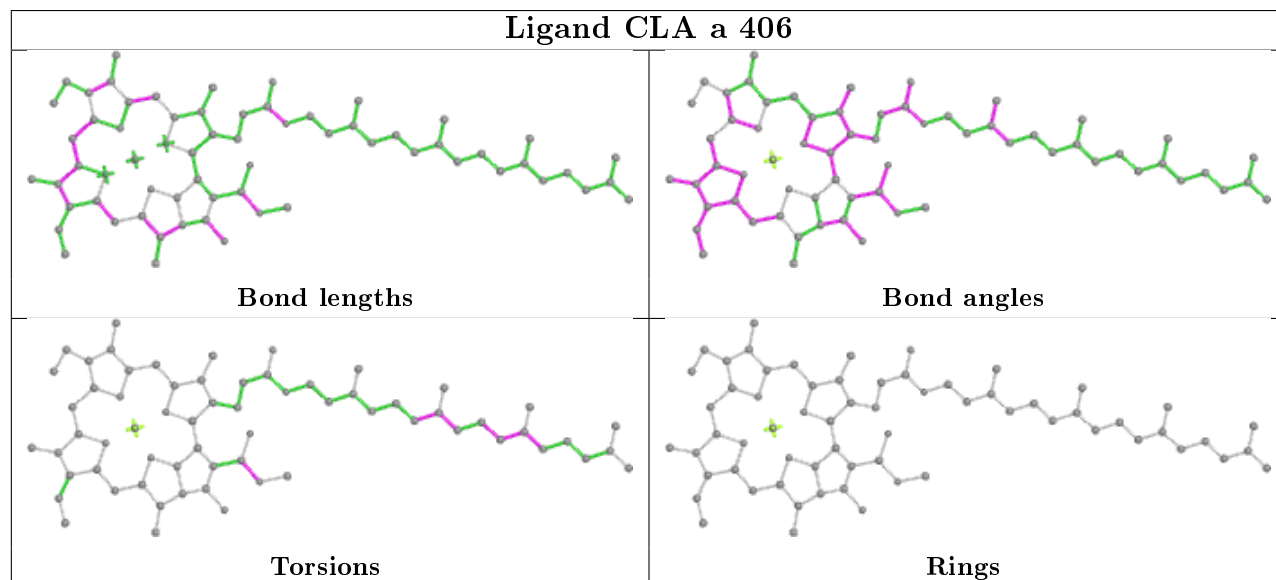
## Ligand CLA c 905

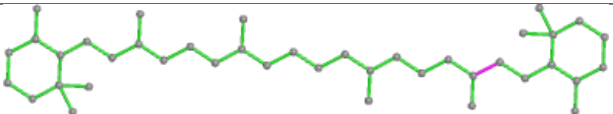
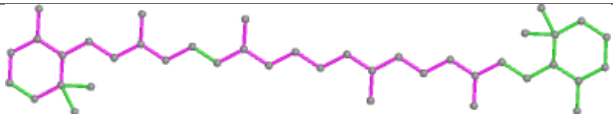
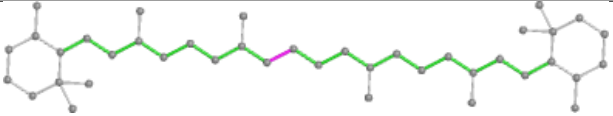
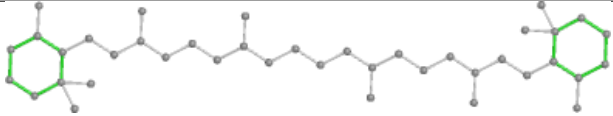


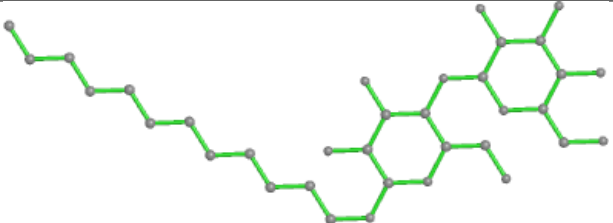
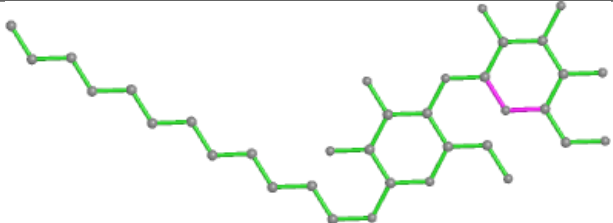
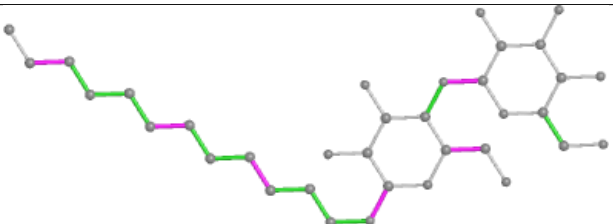
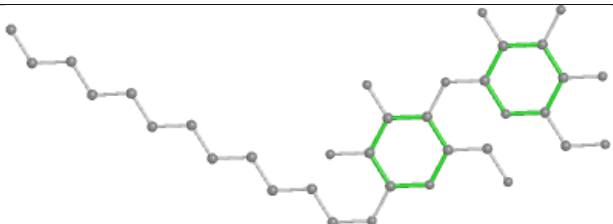
## Ligand CLA C 511

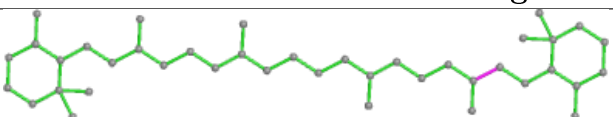
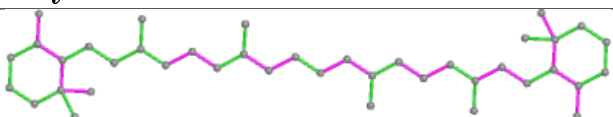
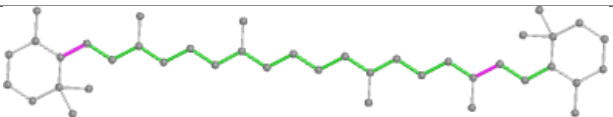
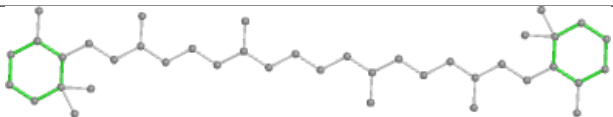


## Ligand CLA a 406

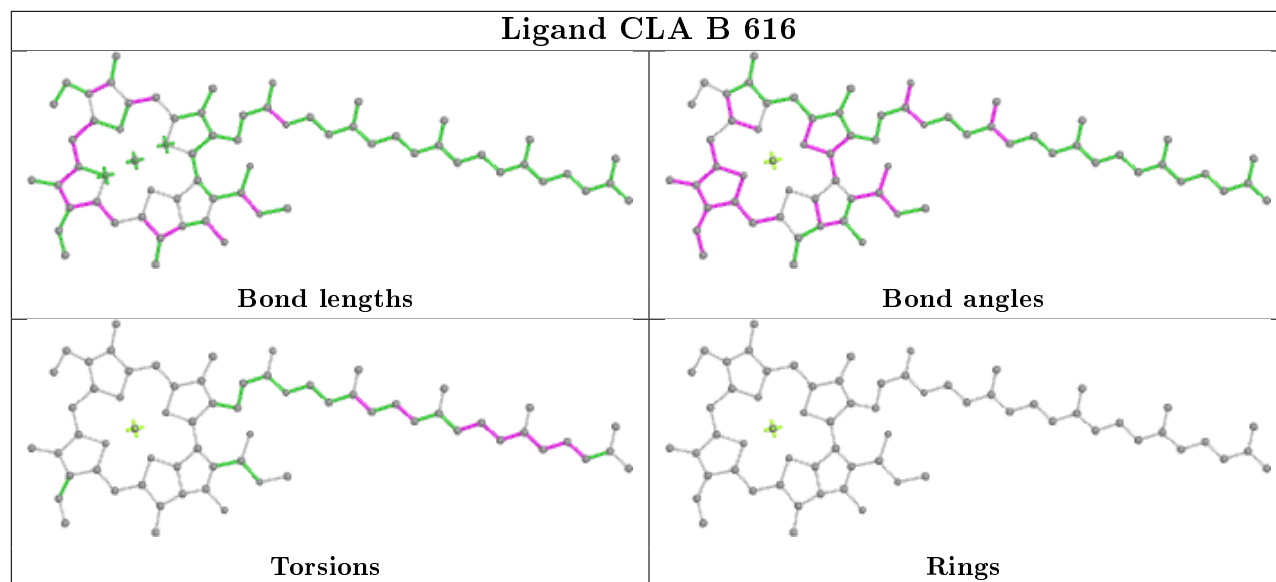
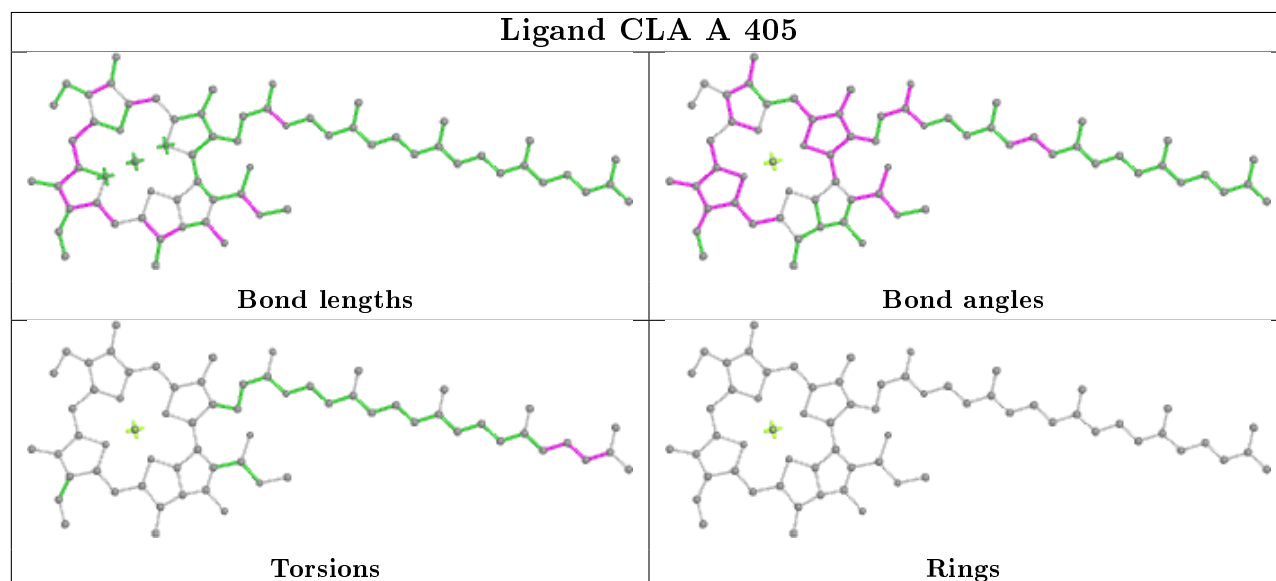
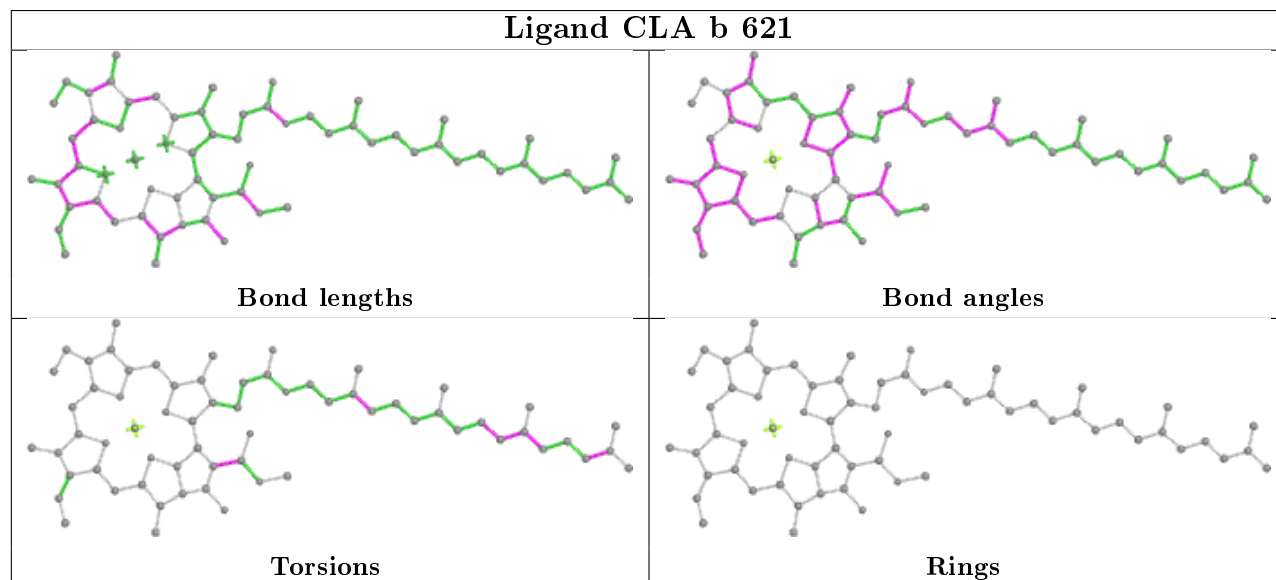


Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

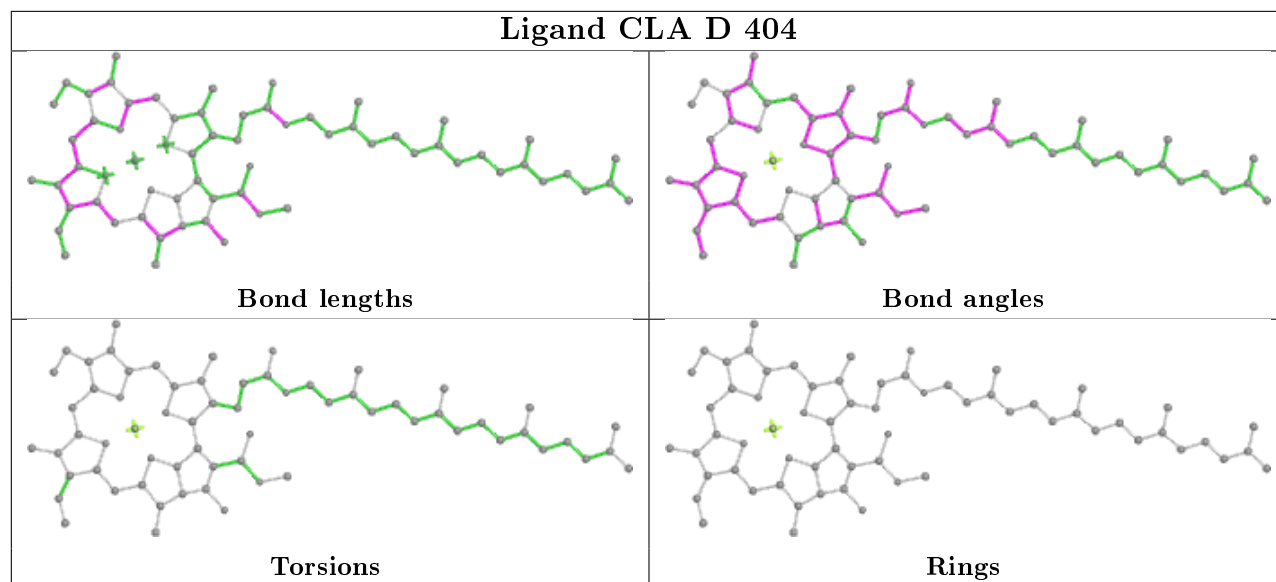
Ligand LMT e 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

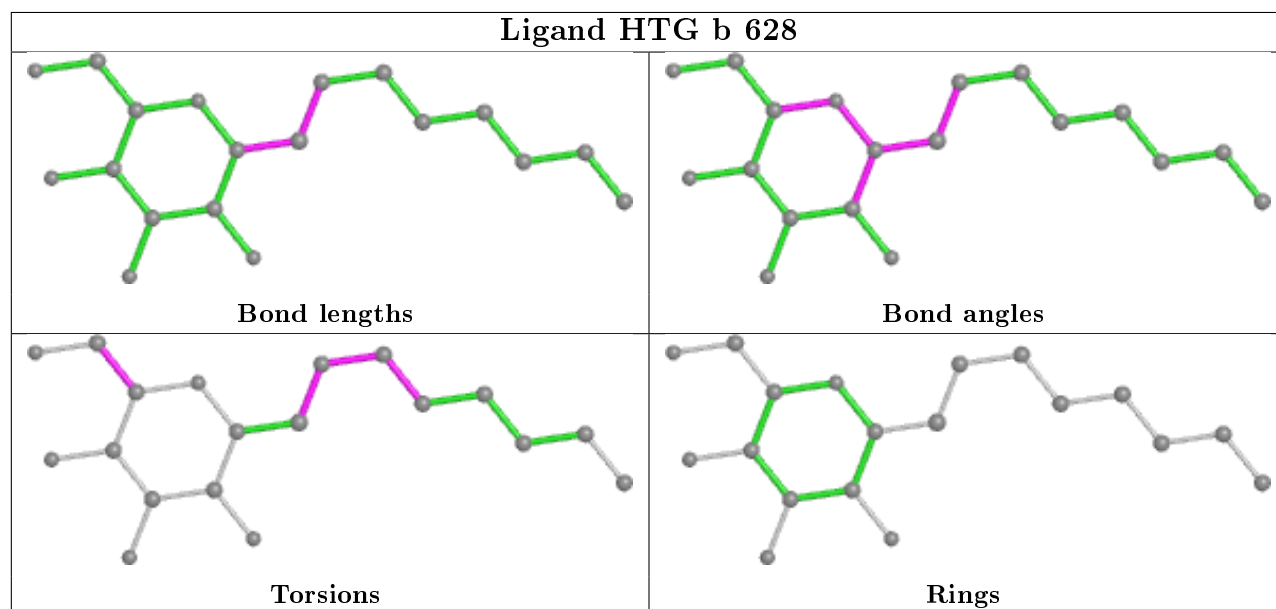


**Ligand CLA B 616****Ligand CLA A 405****Ligand CLA b 621**

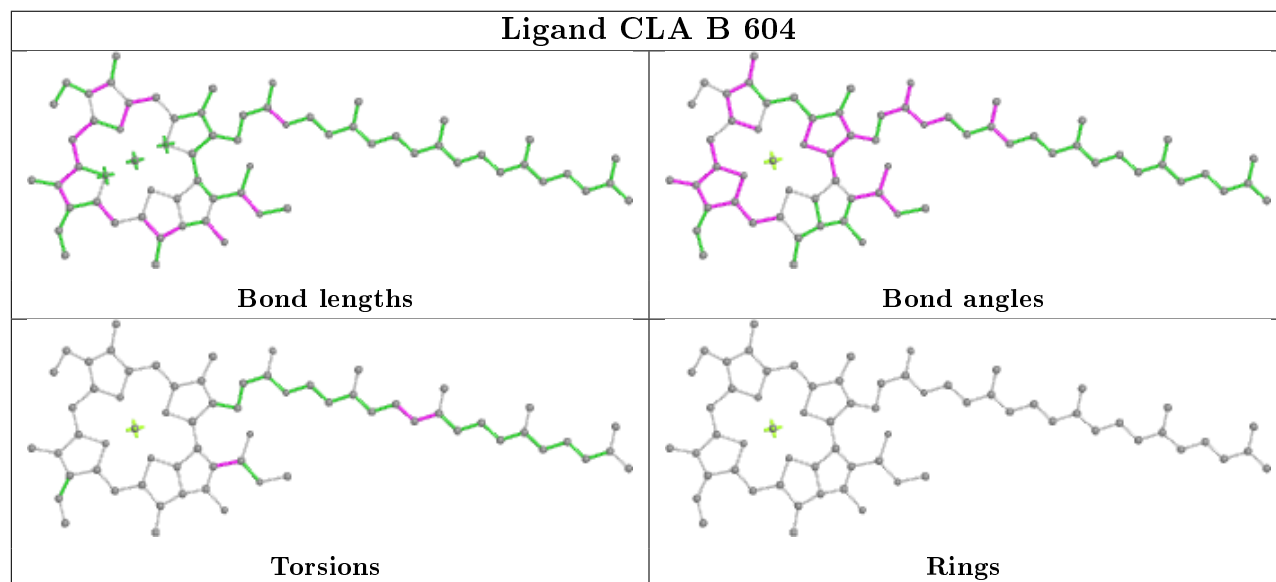
## Ligand CLA D 404

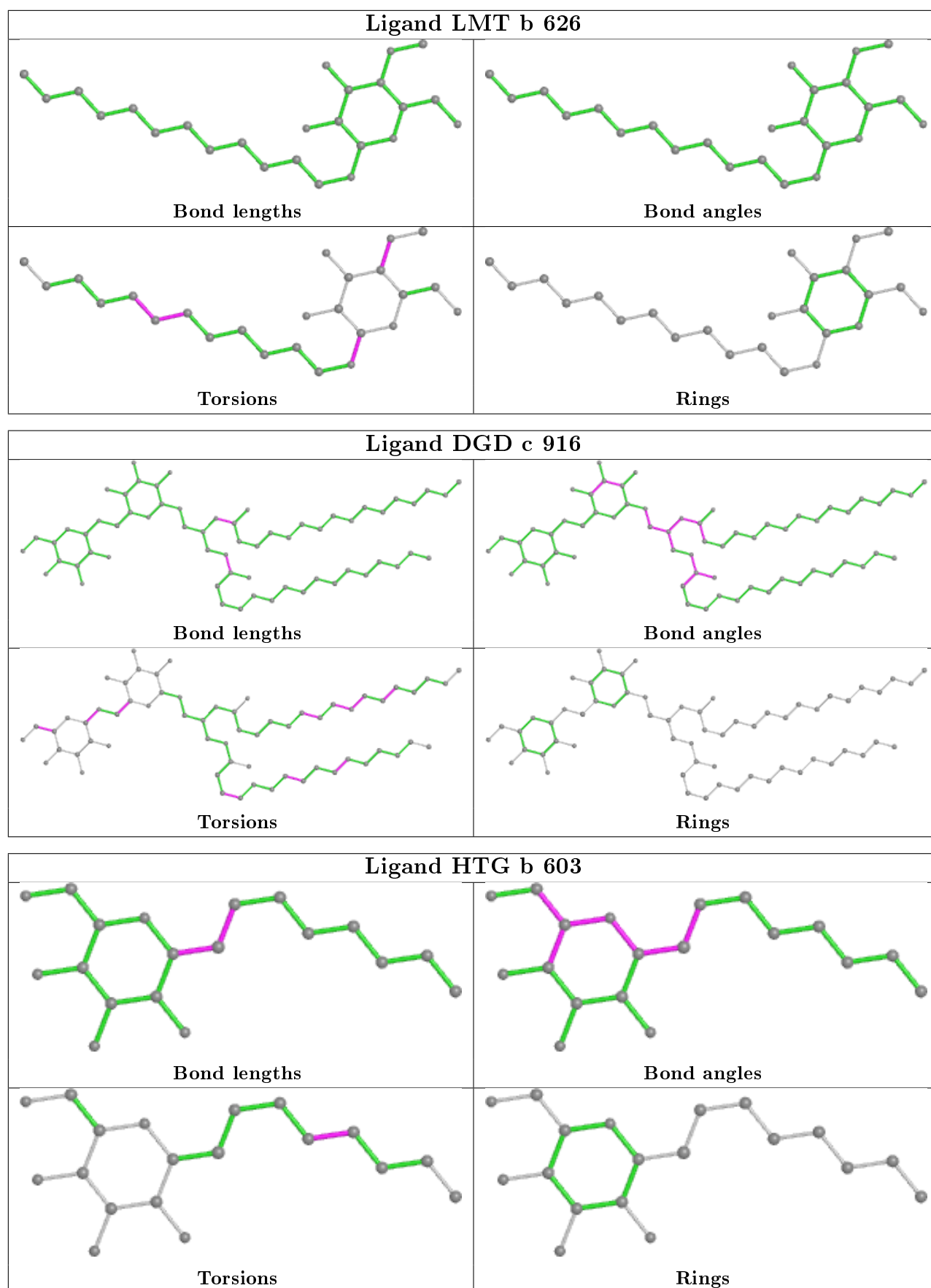


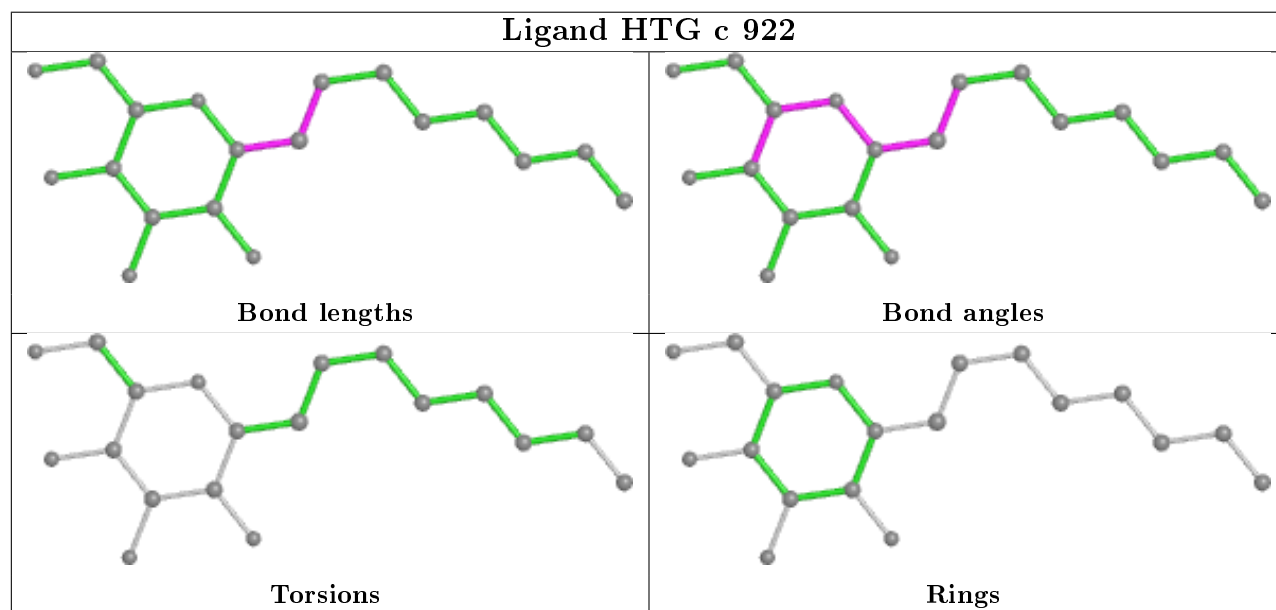
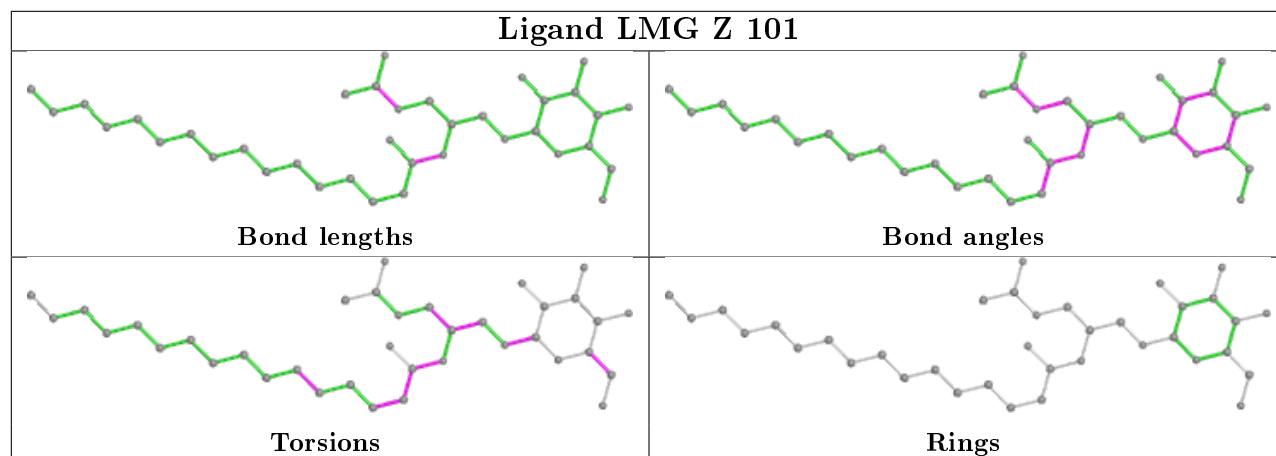
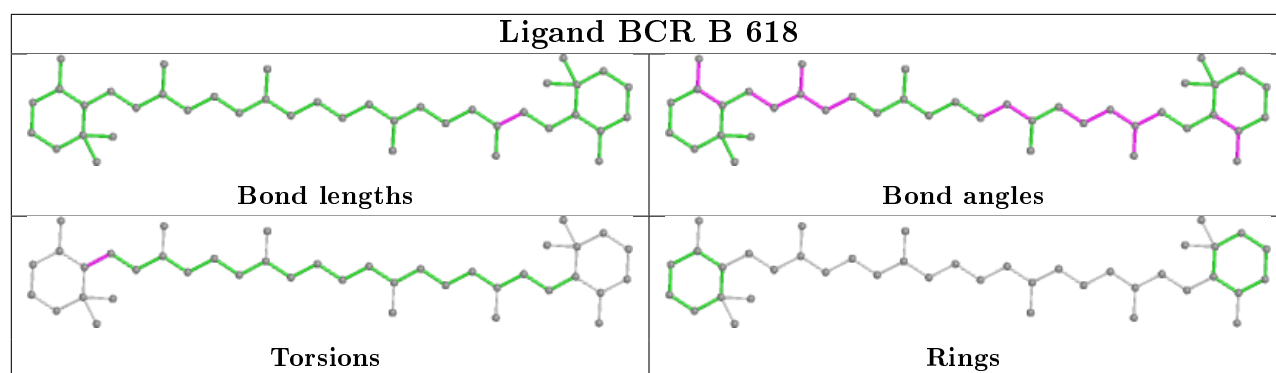
## Ligand HTG b 628

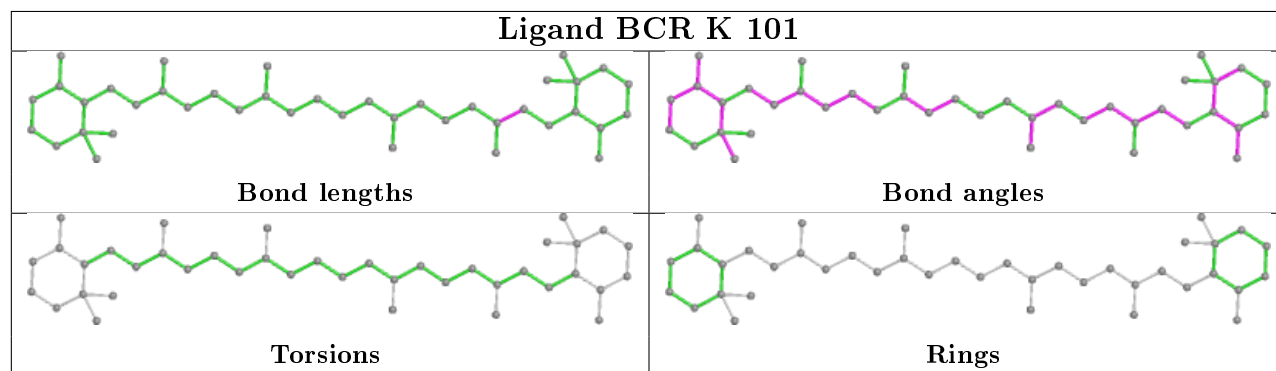
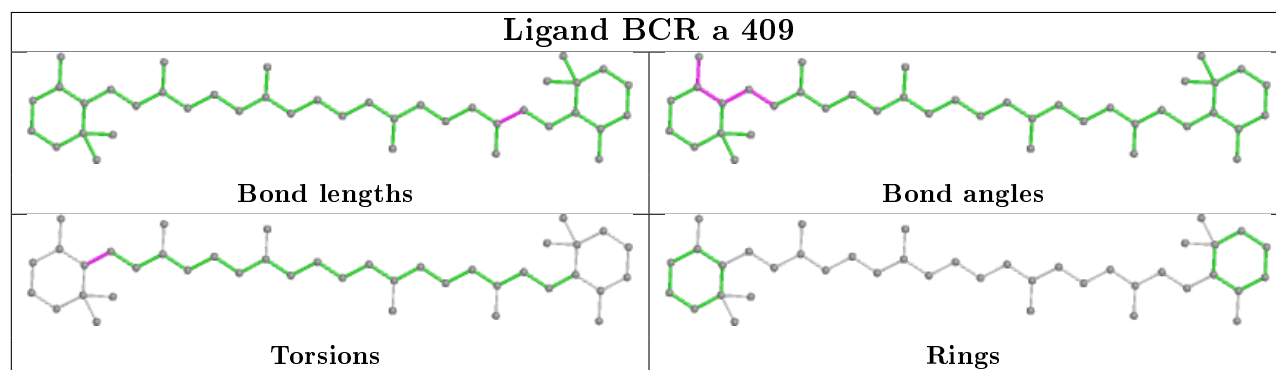
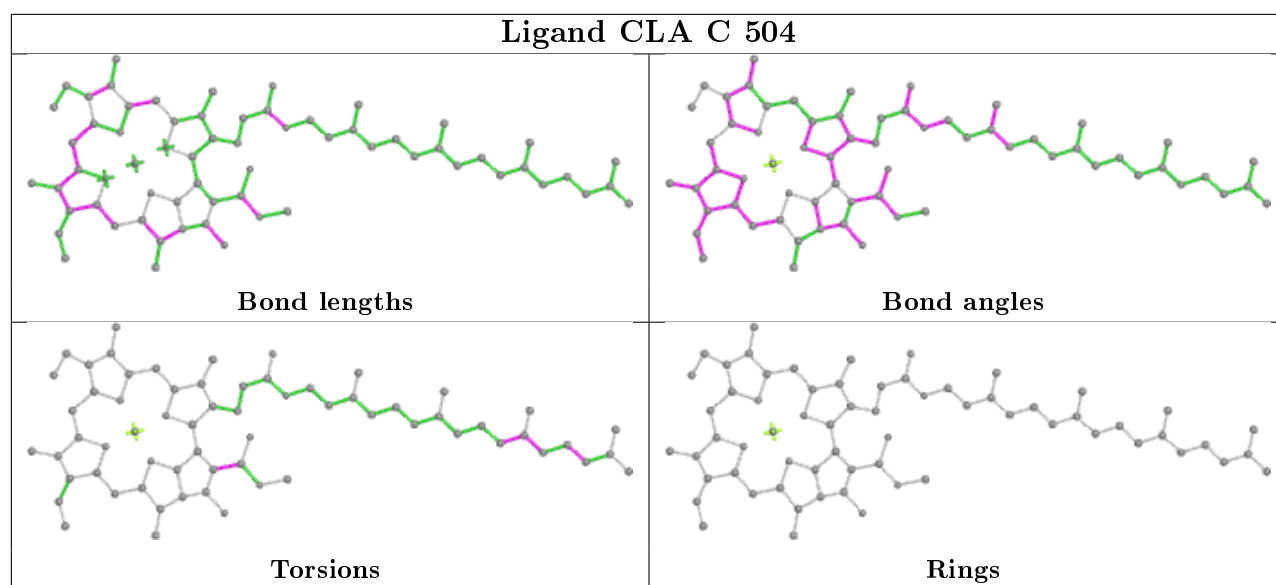


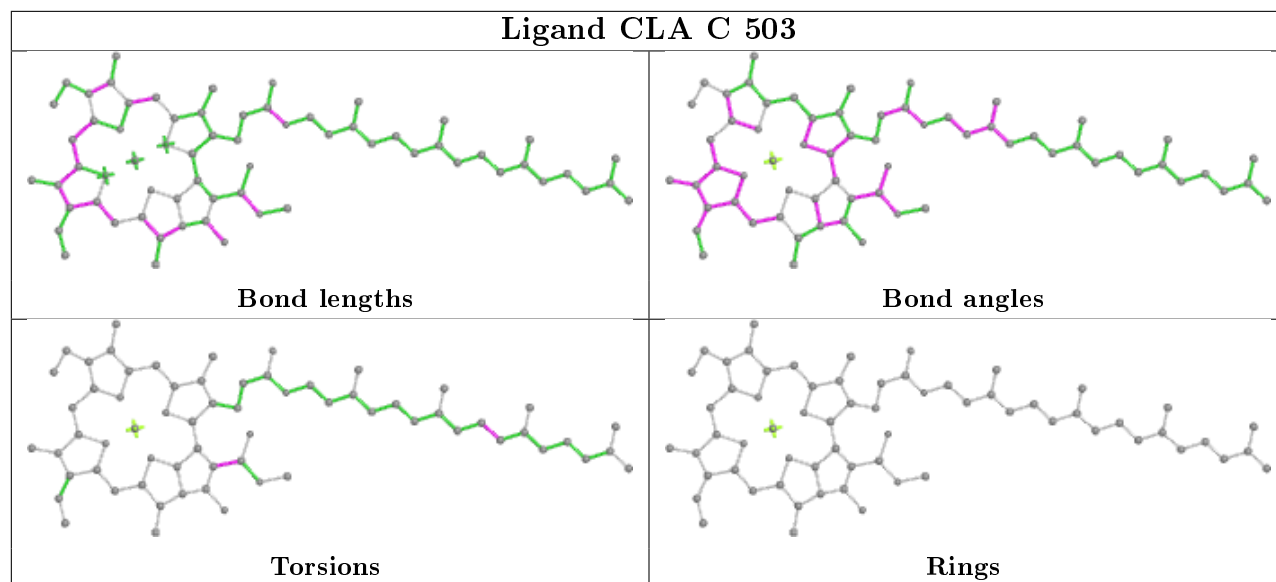
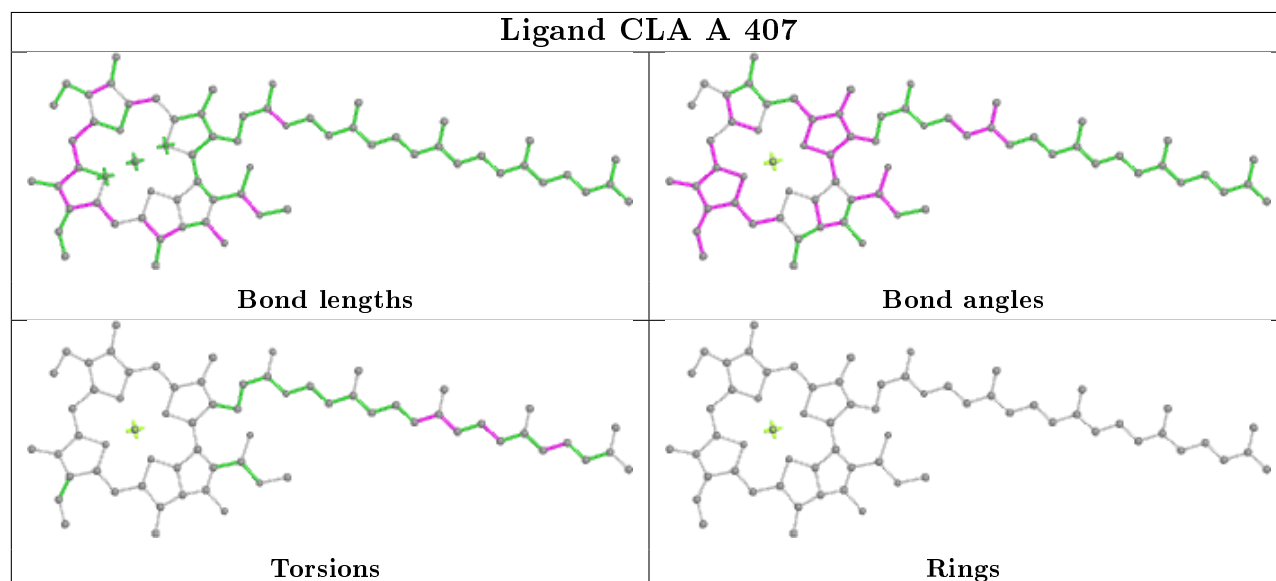
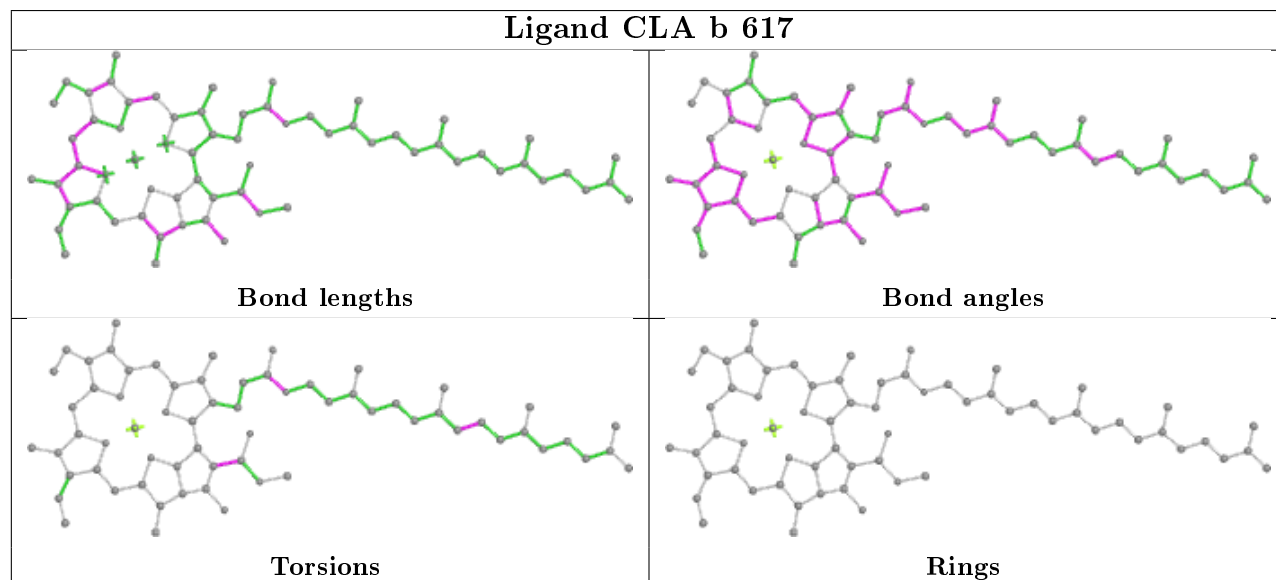
## Ligand CLA B 604

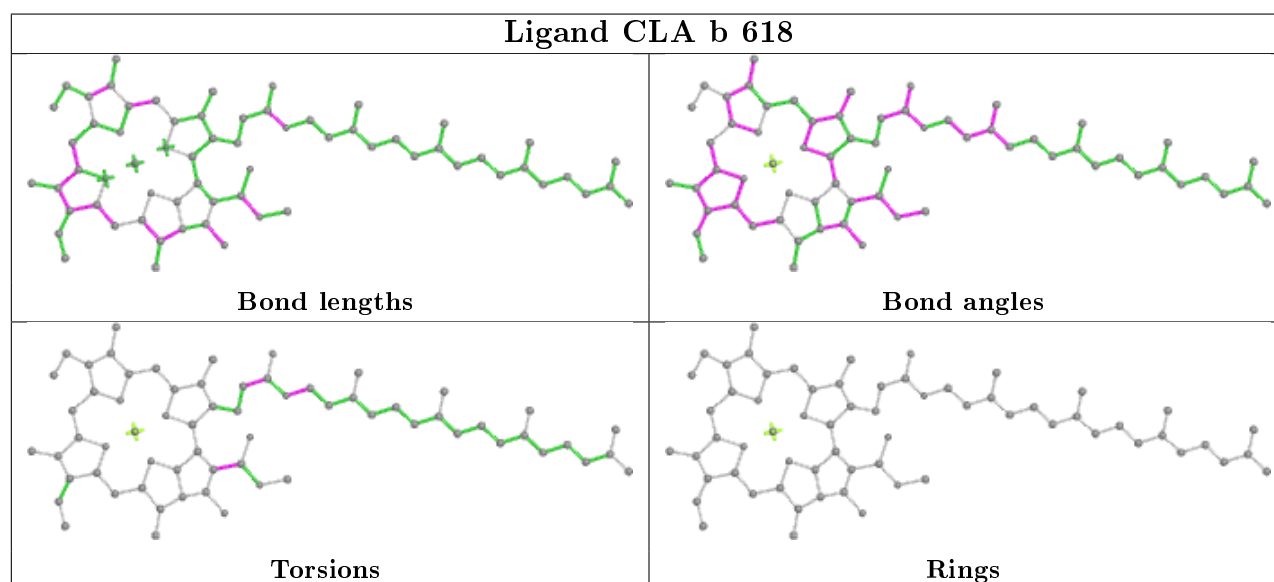
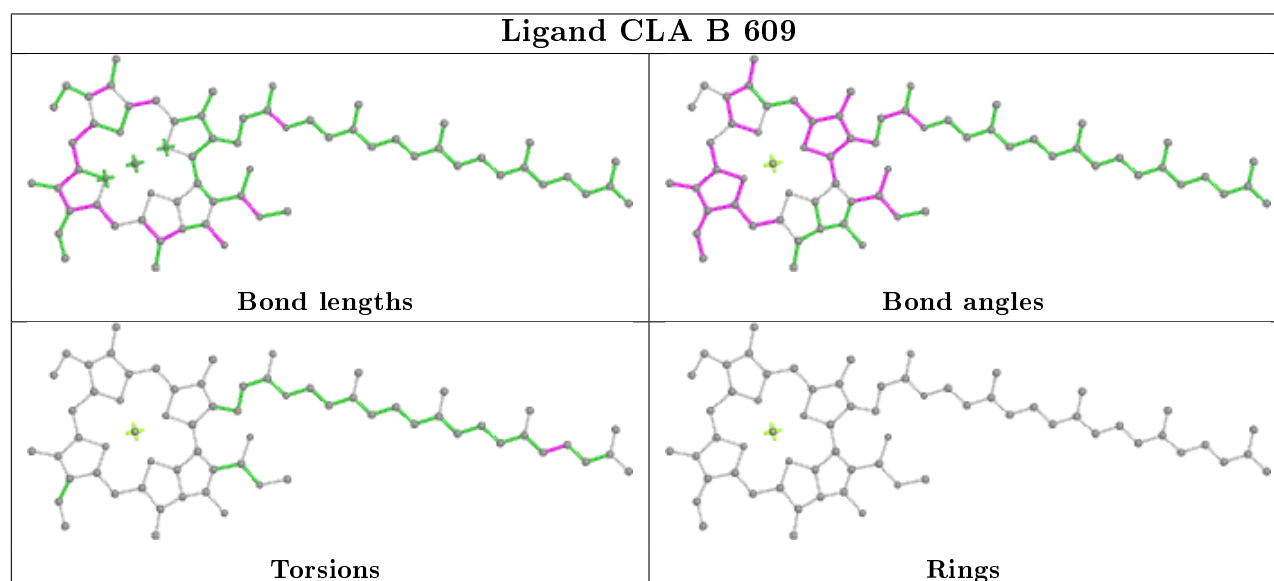
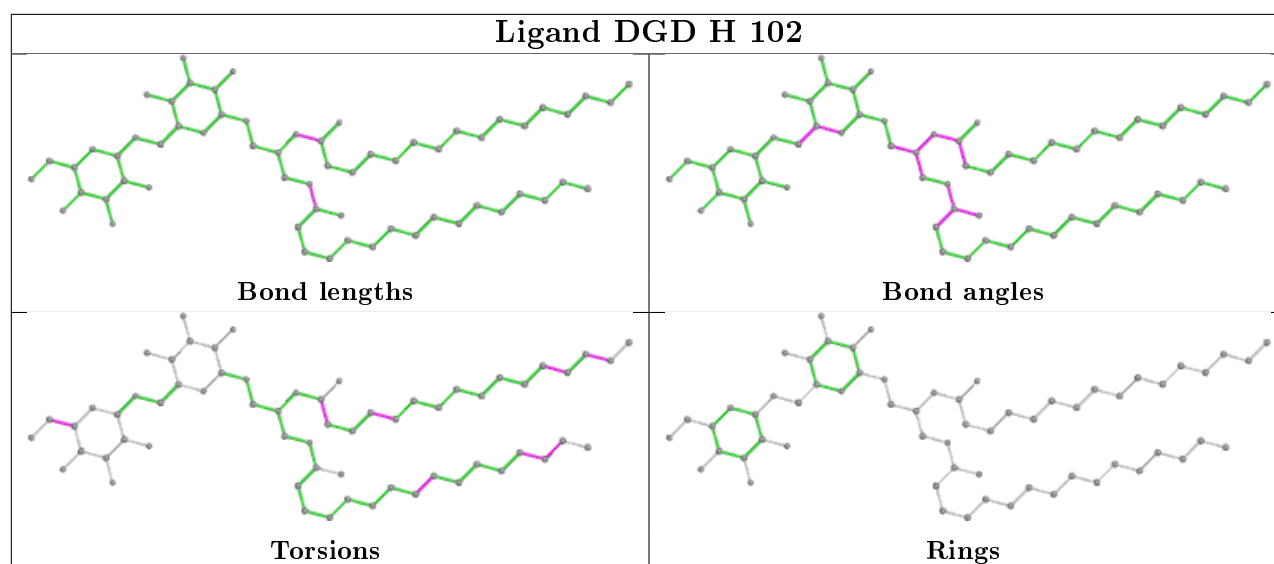


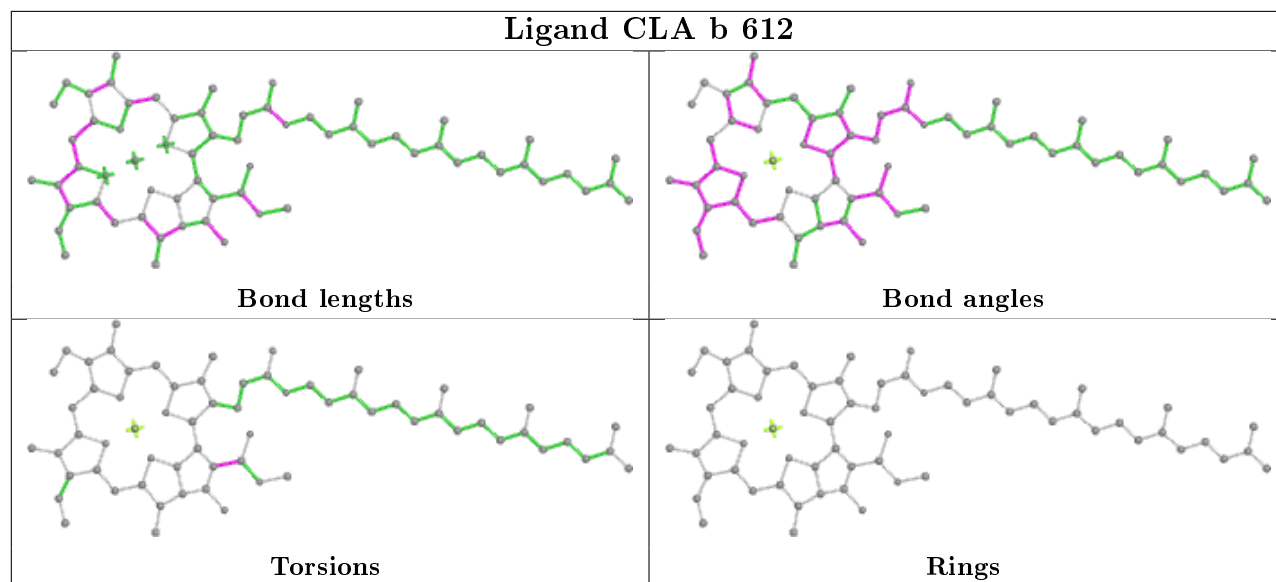
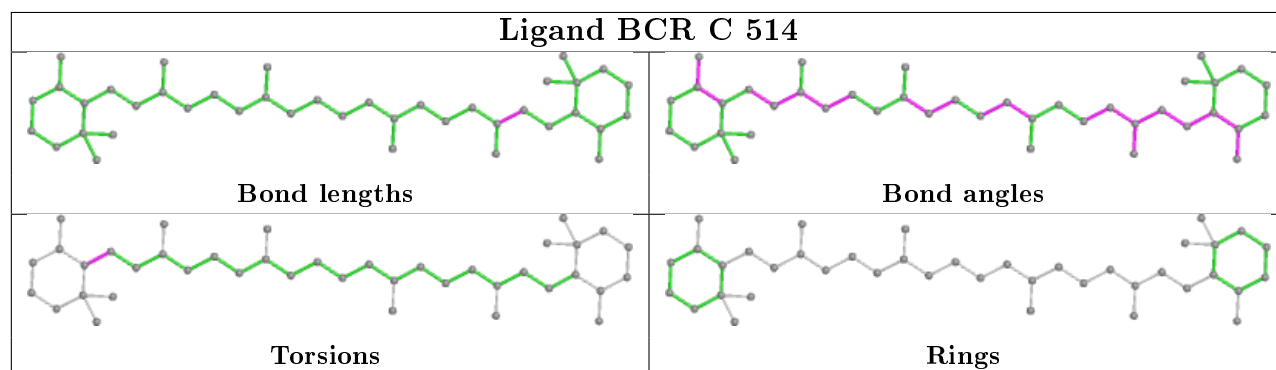
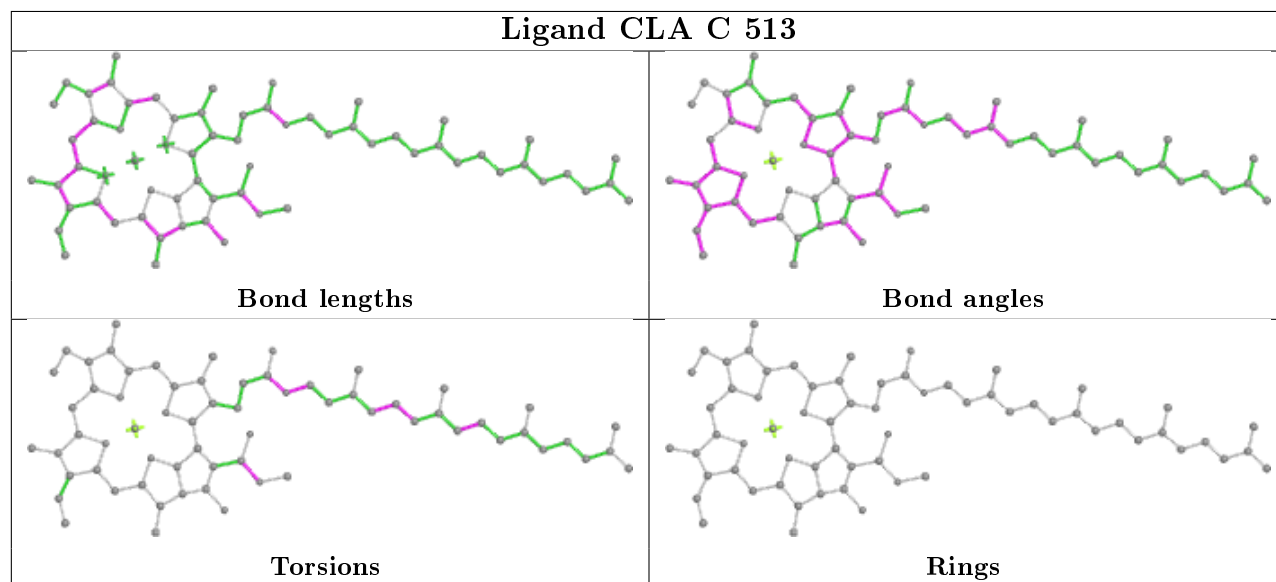




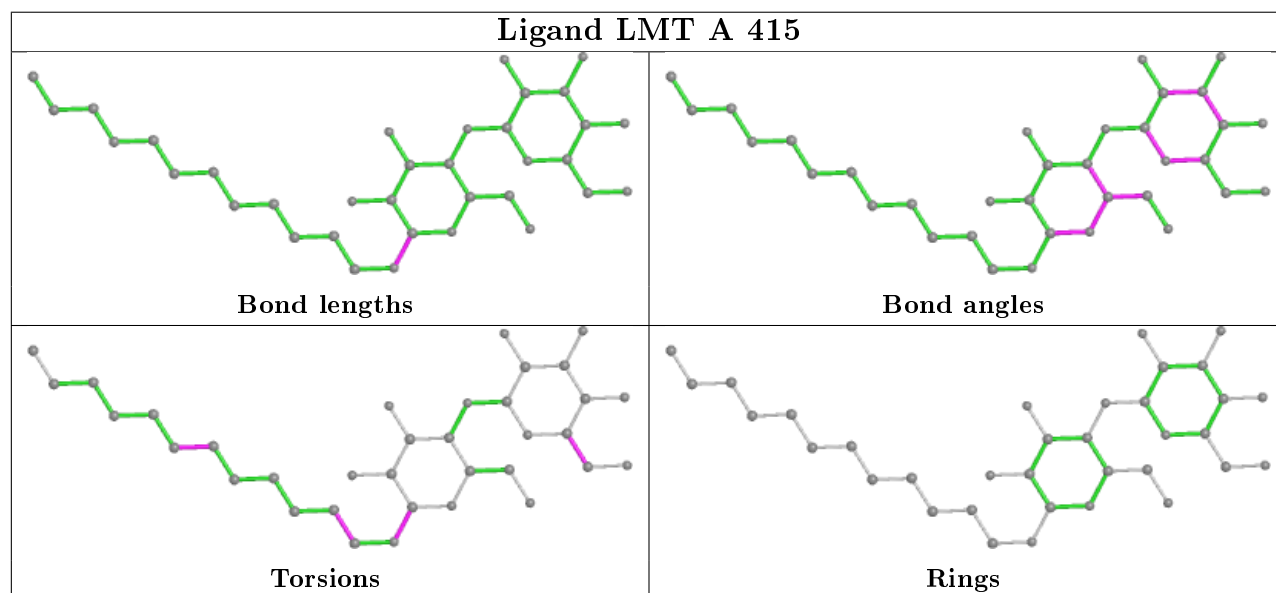
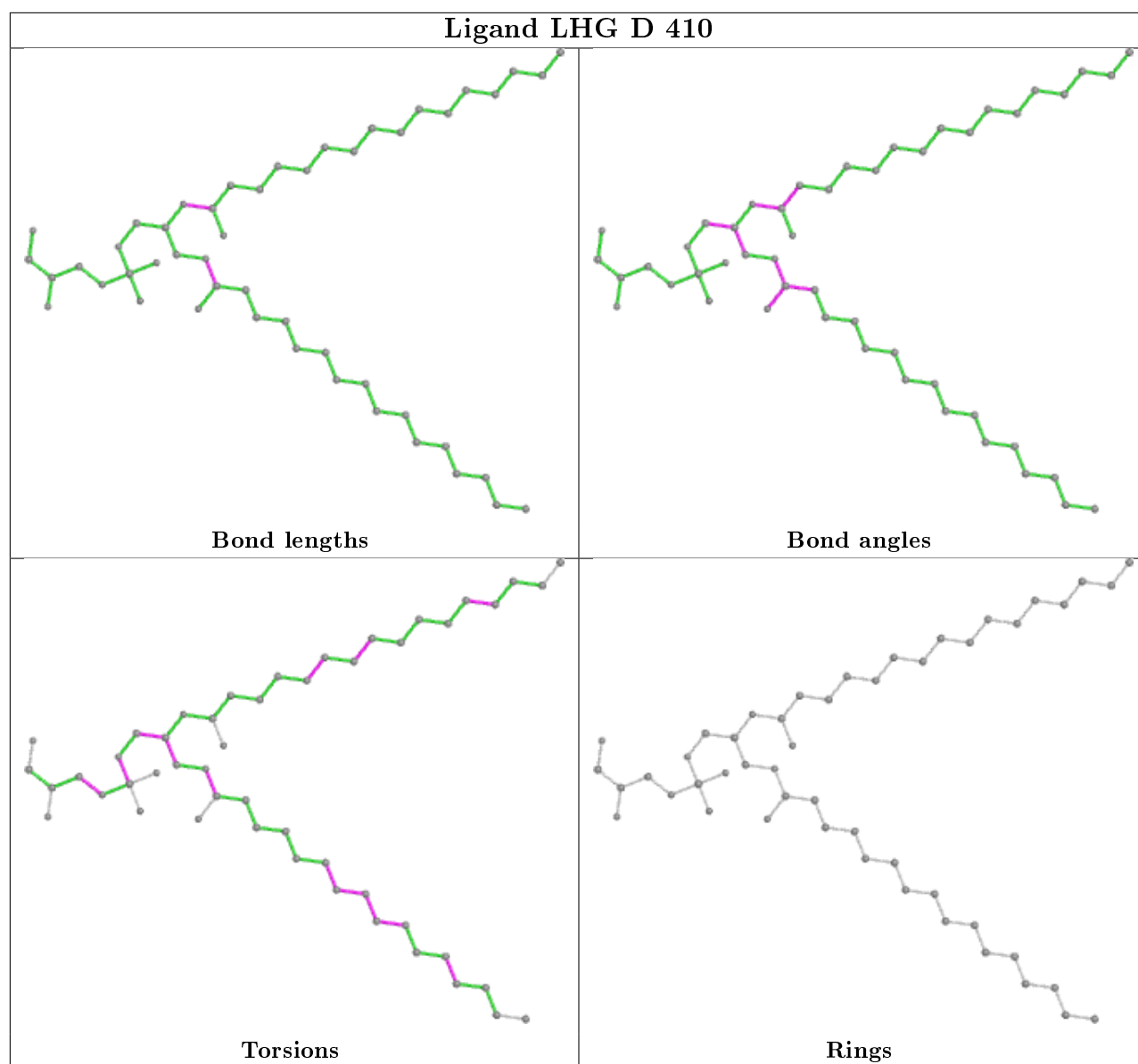


**Ligand CLA C 503****Ligand CLA A 407****Ligand CLA b 617**

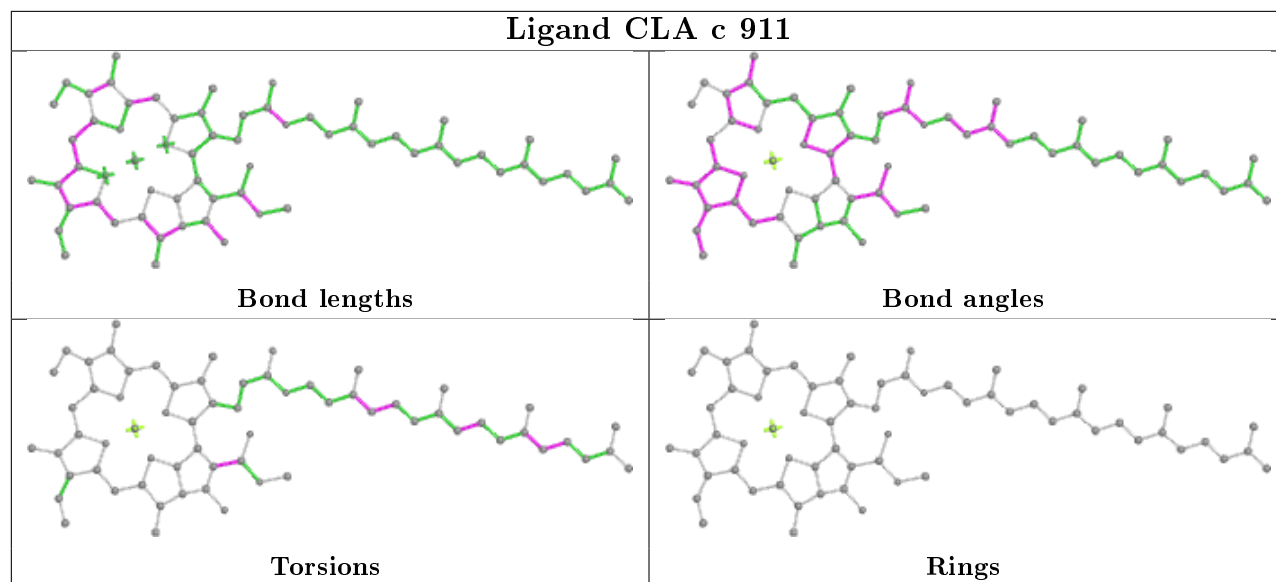


**Ligand CLA b 612****Ligand BCR C 514****Ligand CLA C 513**

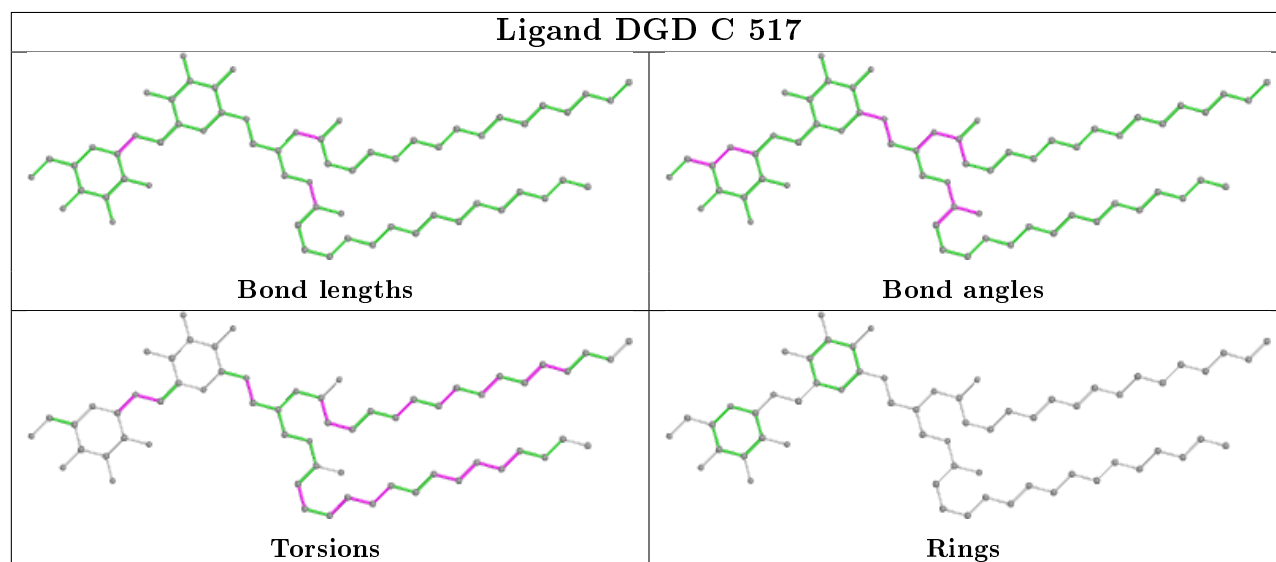




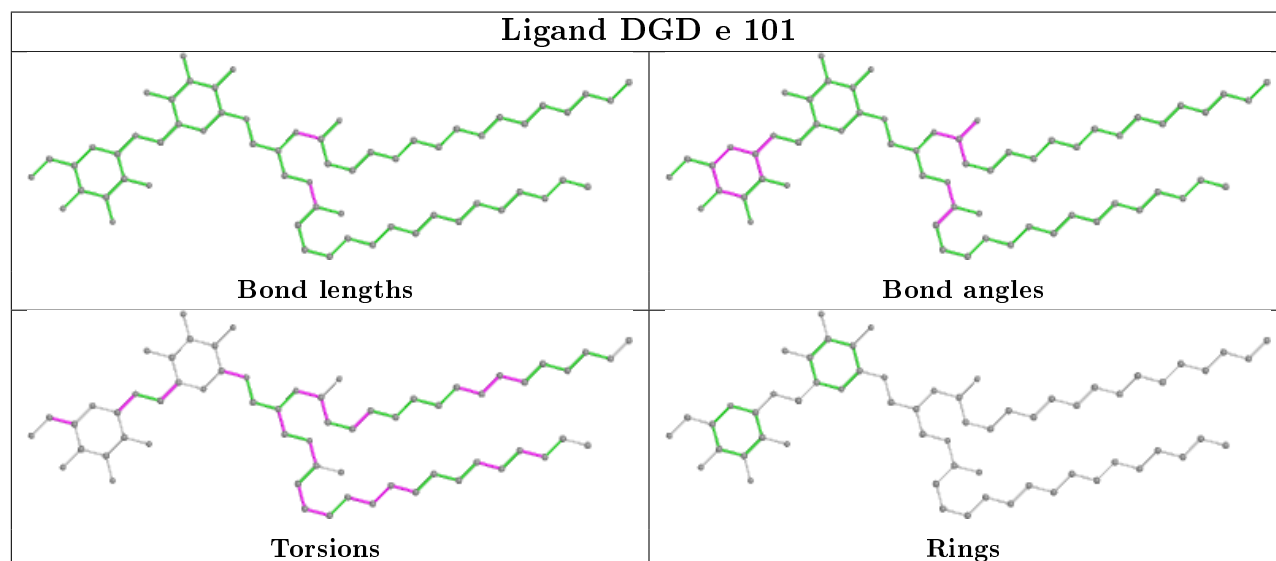
## Ligand CLA c 911

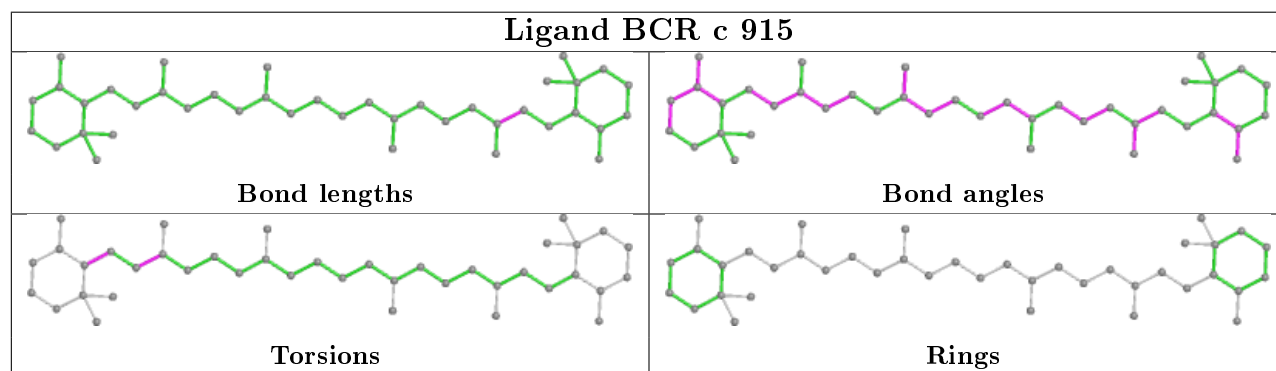
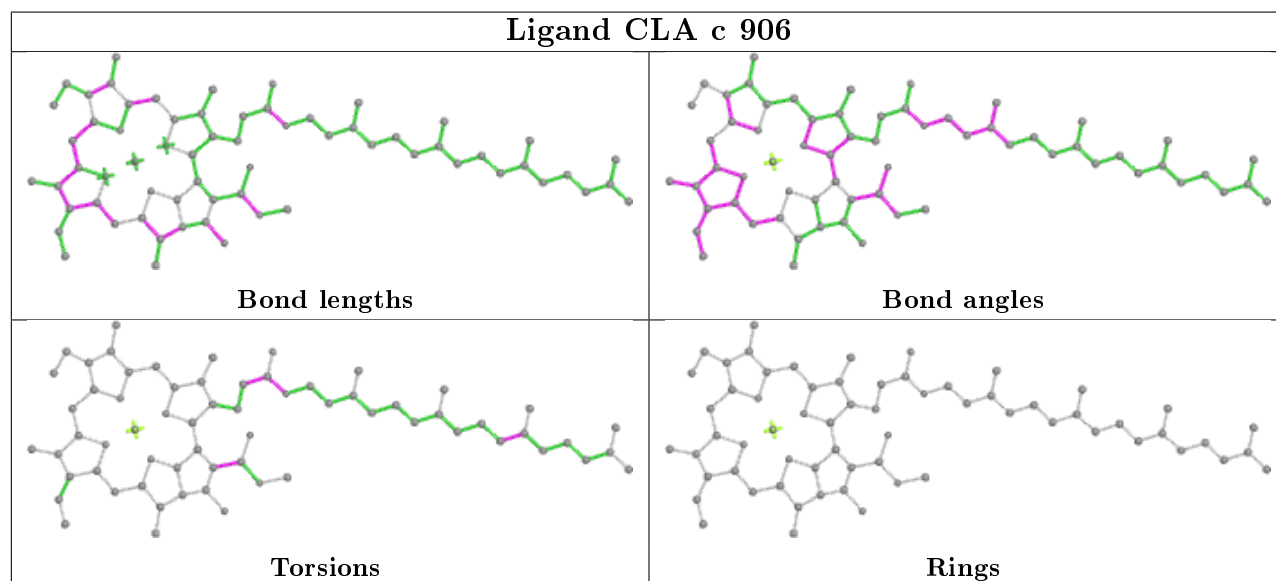
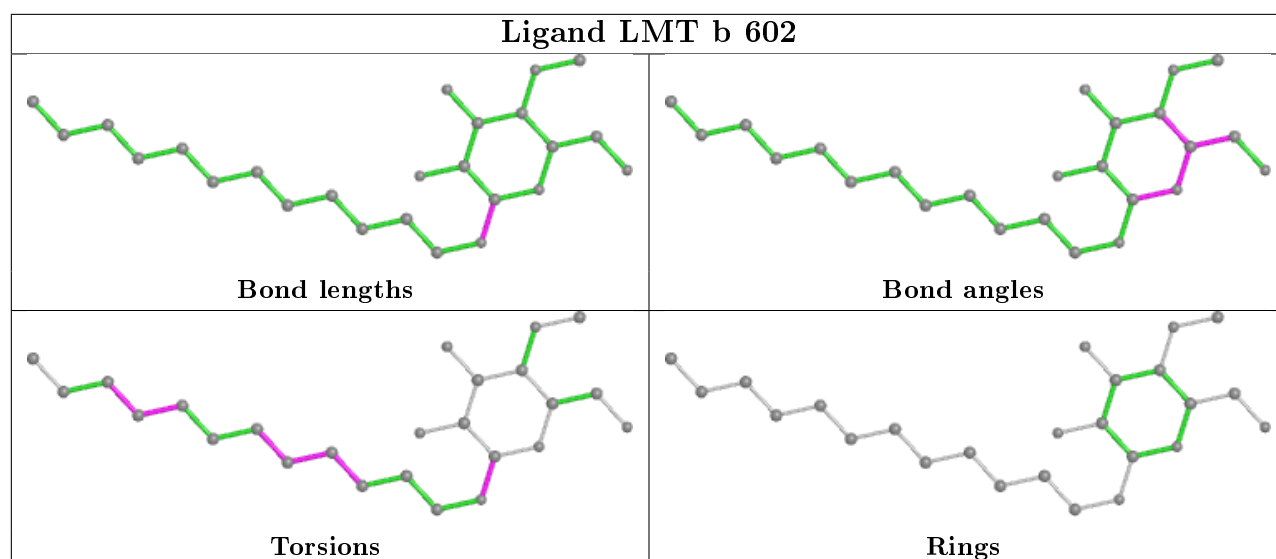


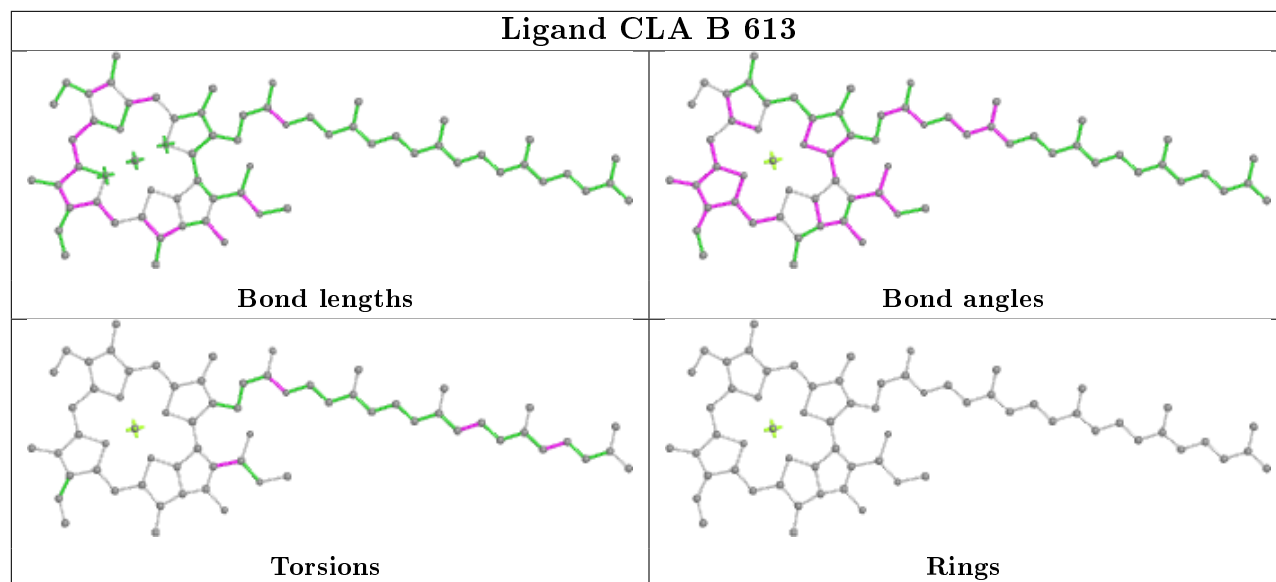
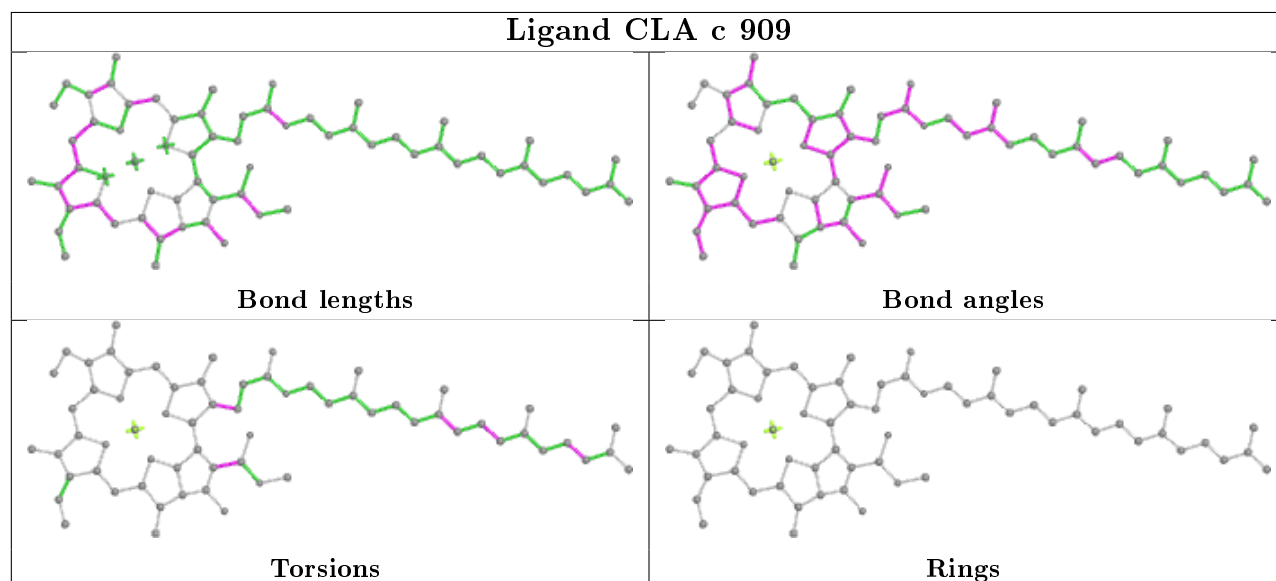
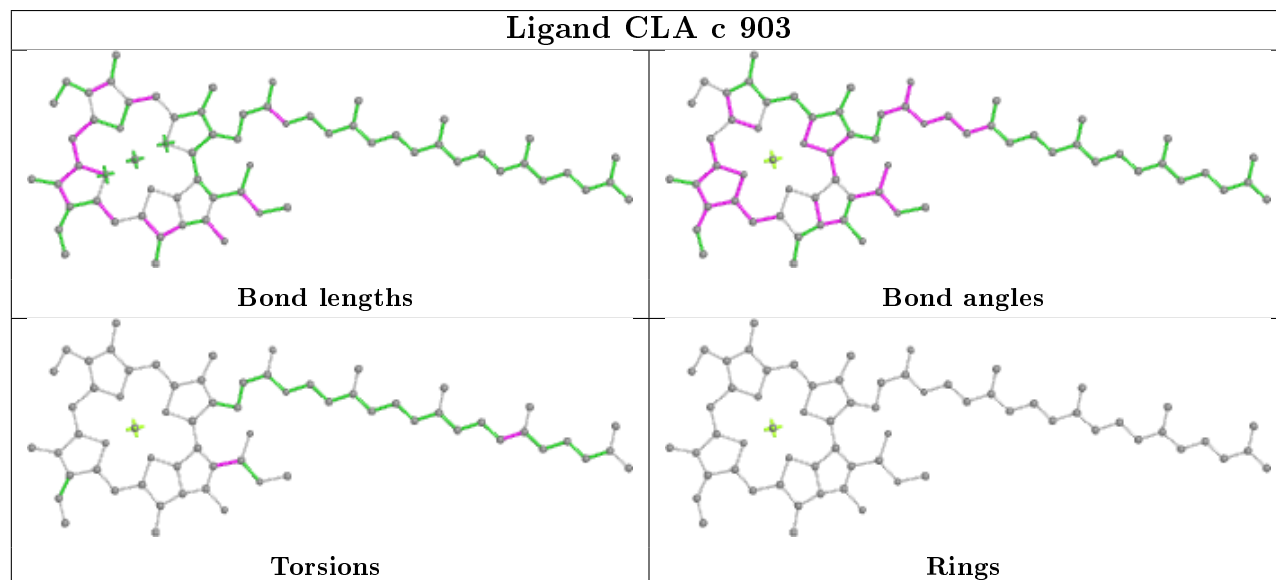
## Ligand DGD C 517

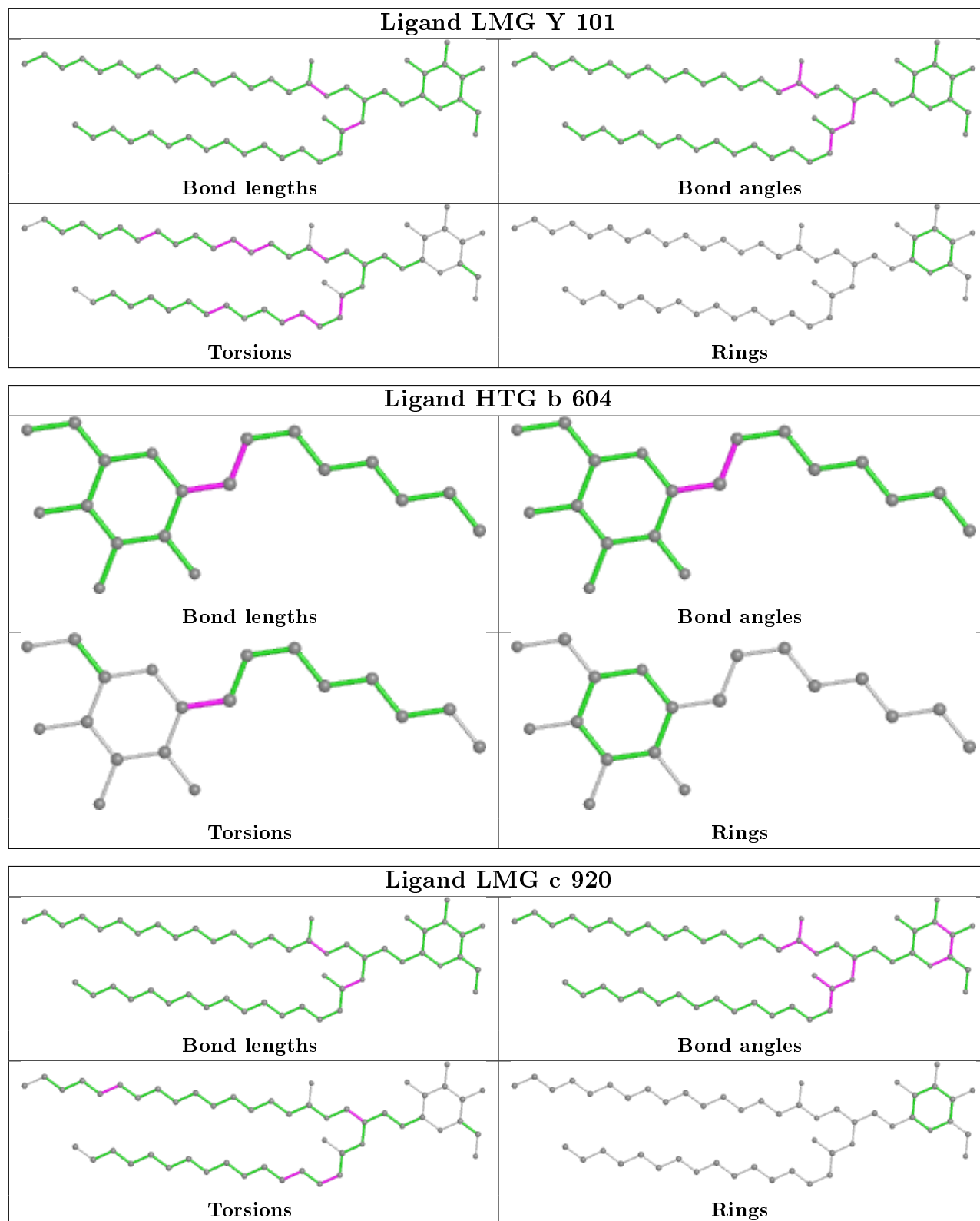


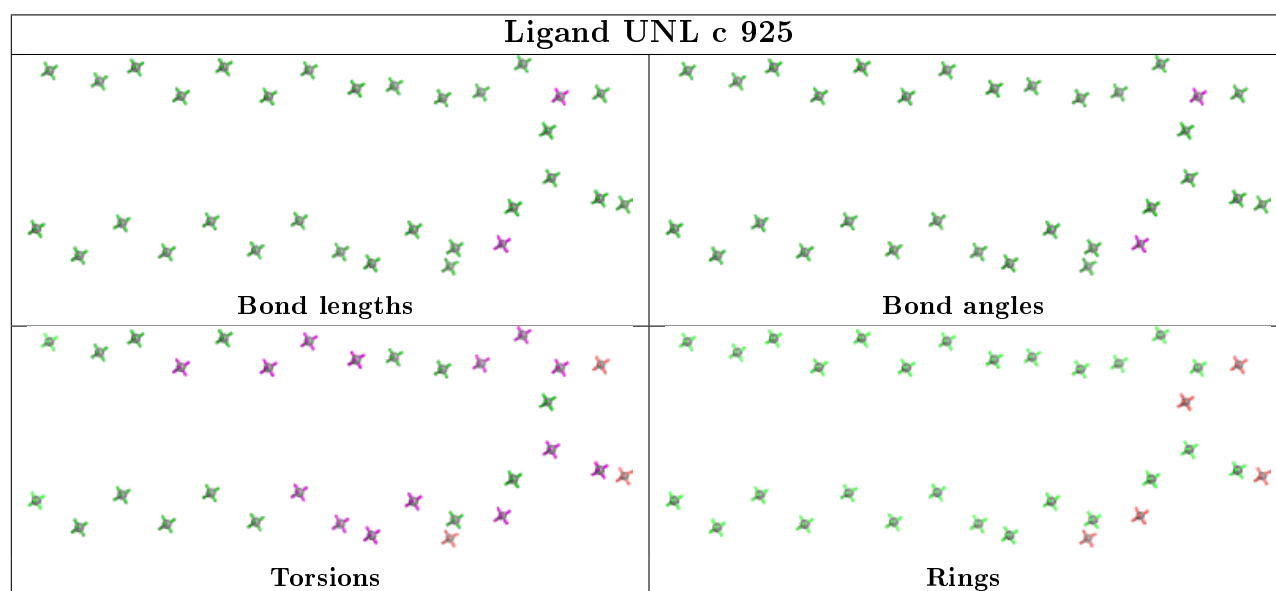
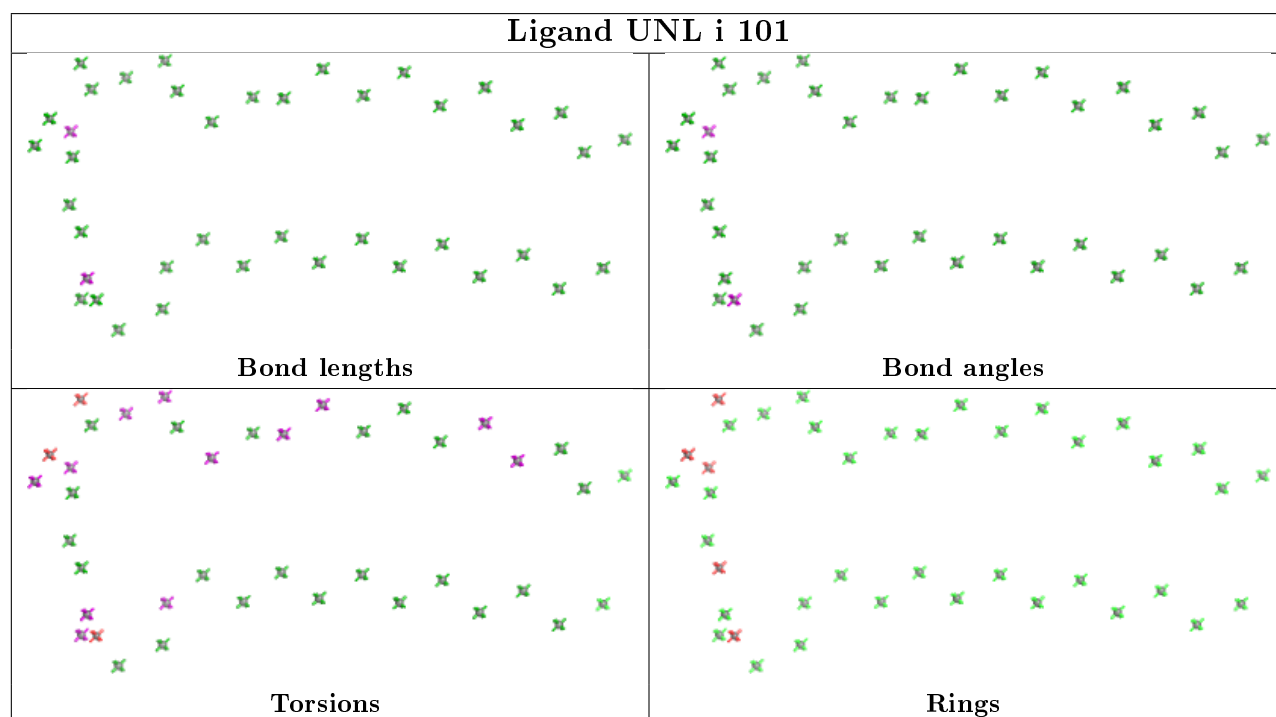
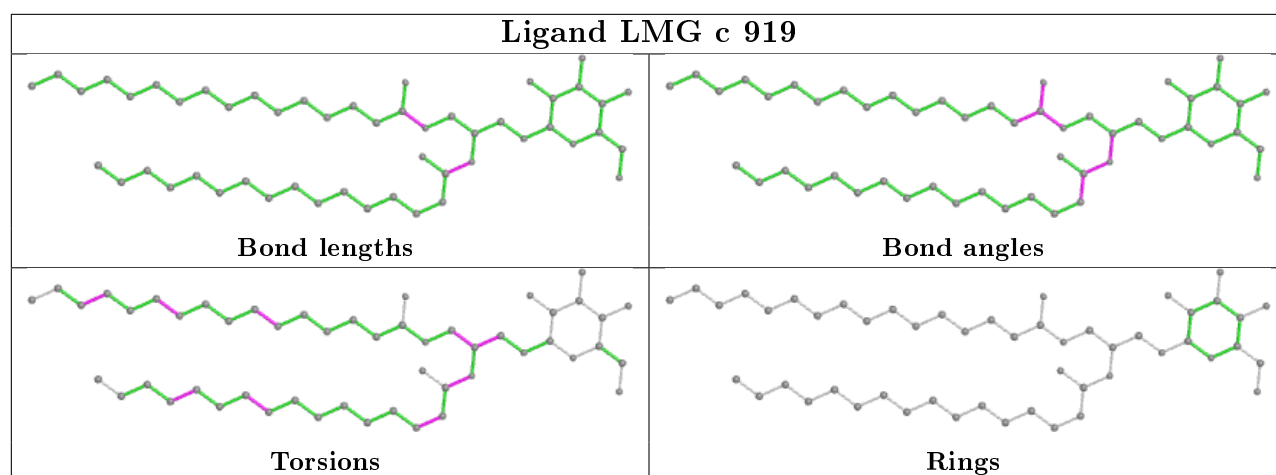
## Ligand DGD e 101

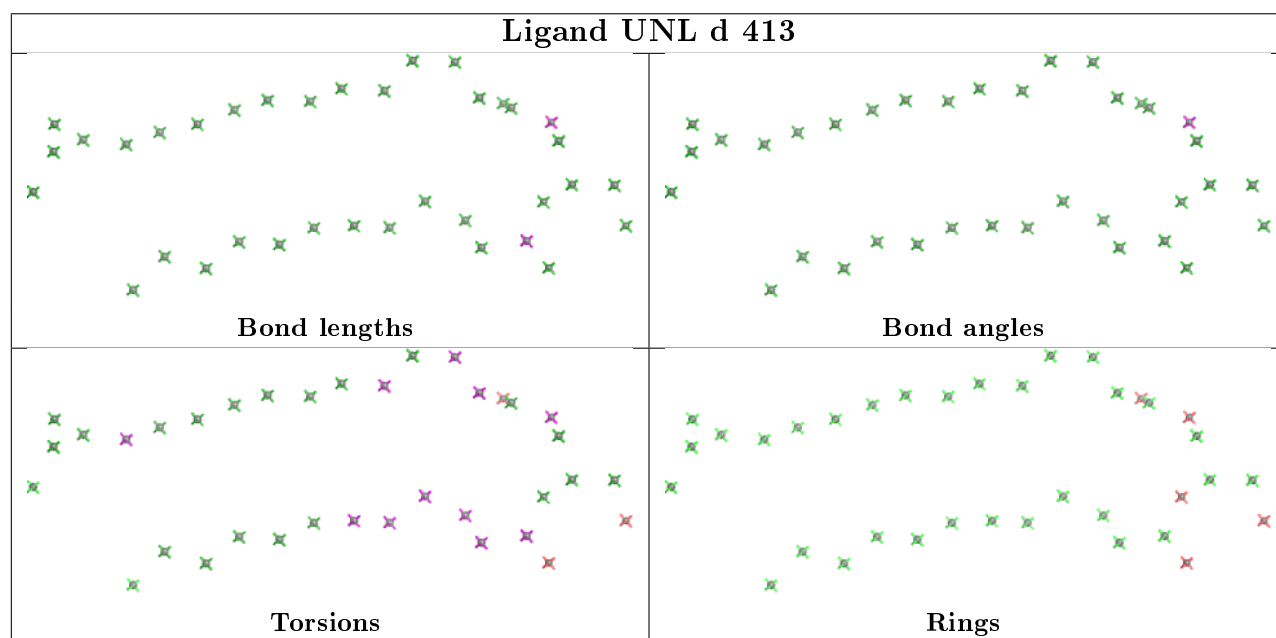
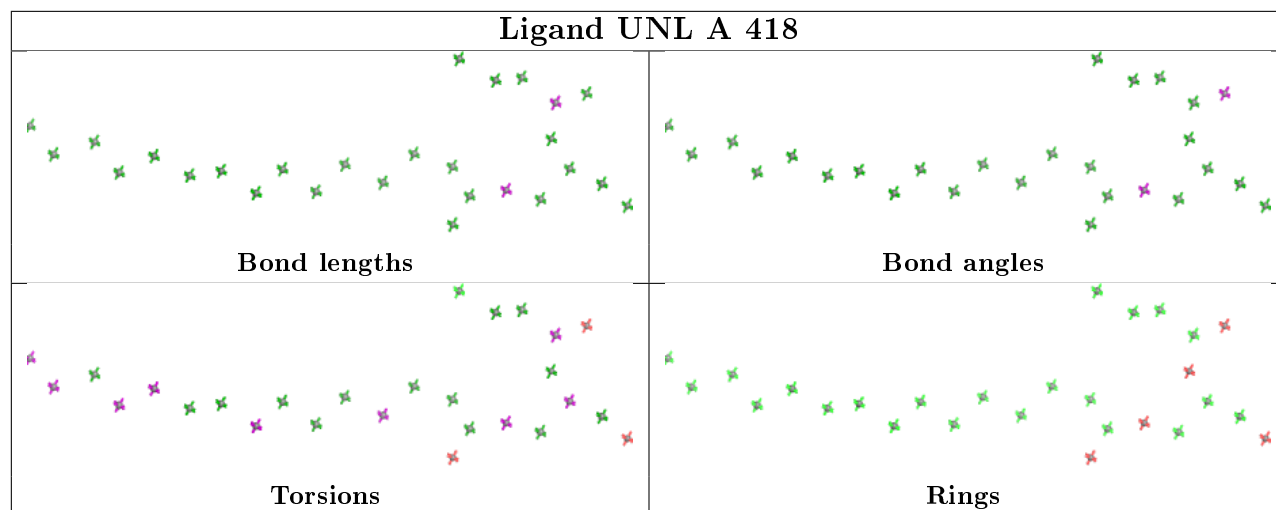


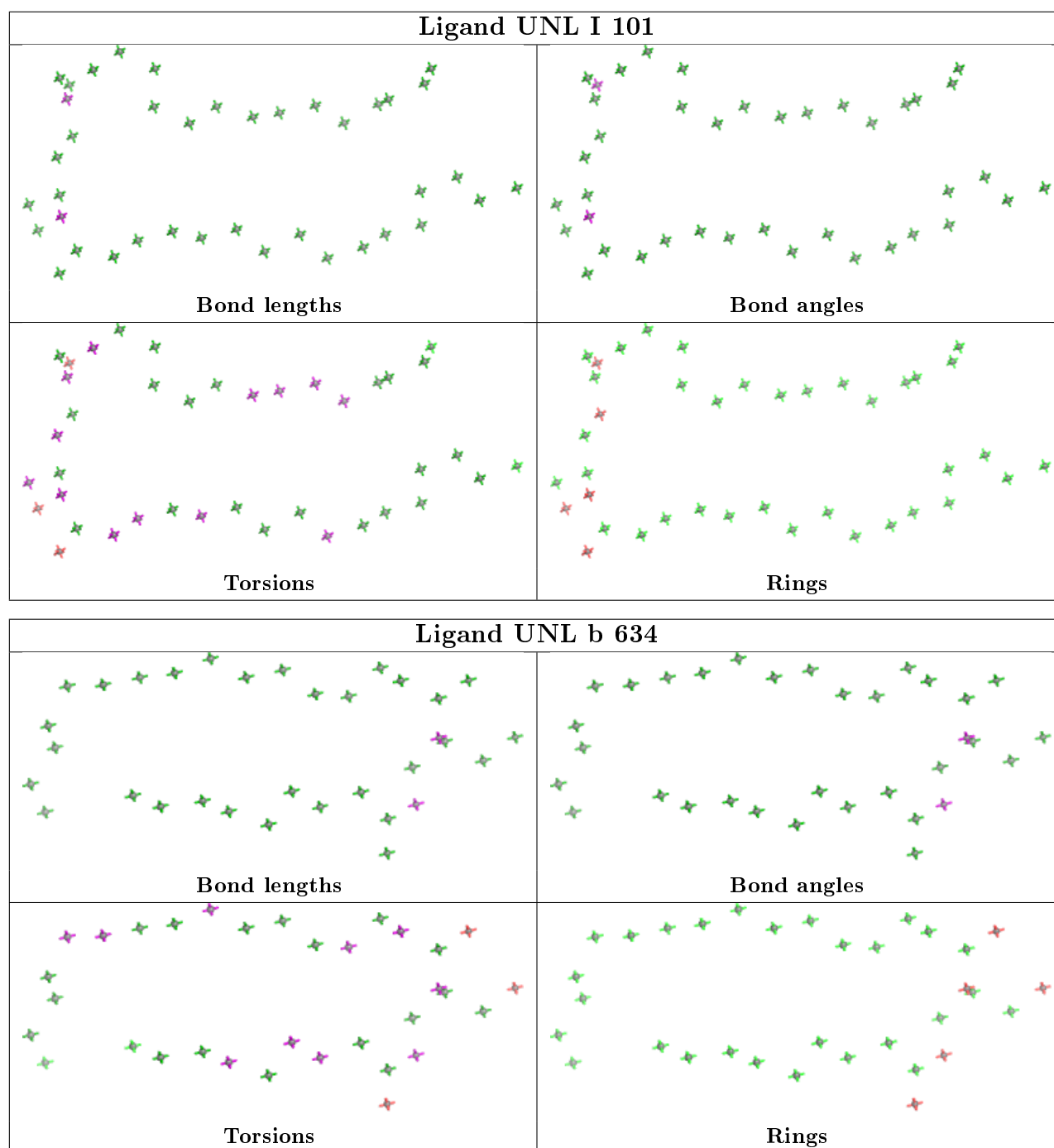


**Ligand CLA B 613****Ligand CLA c 909****Ligand CLA c 903**

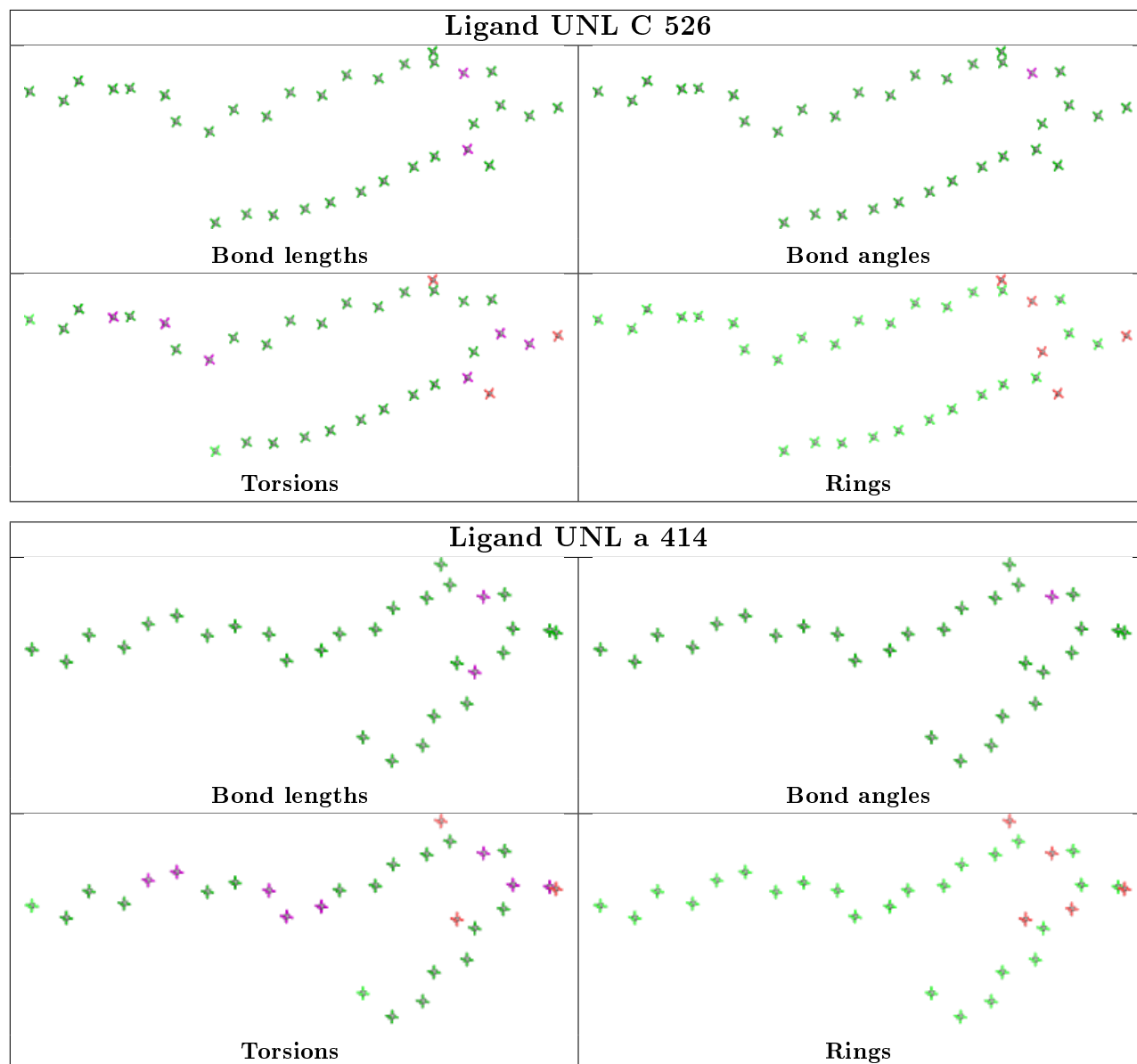


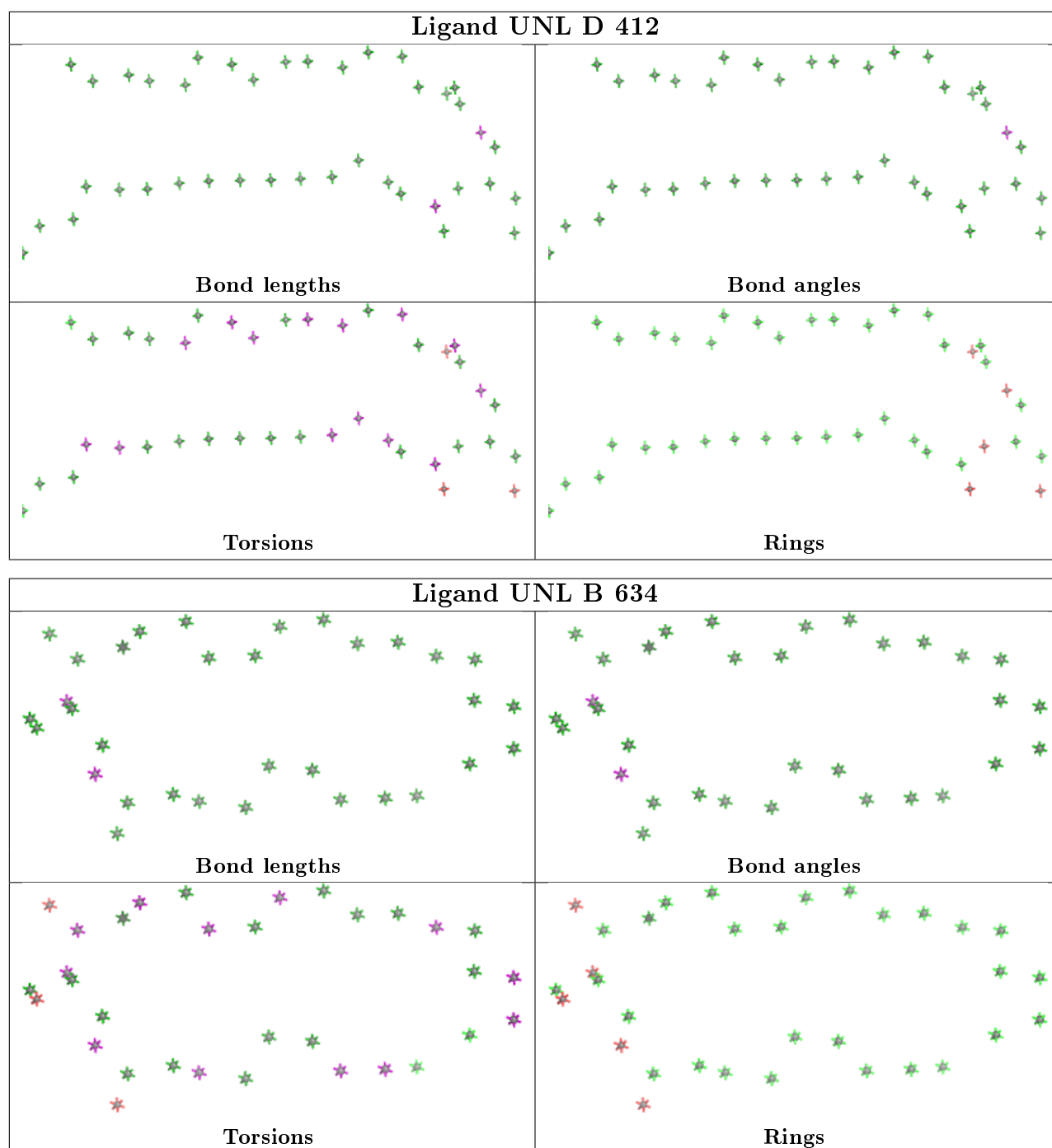












## 5.7 Other polymers [i](#)

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%)	0.28	5 (1%) 73 81	33, 43, 75, 139	0
1	a	334/344 (97%)	0.48	15 (4%) 33 46	31, 44, 84, 146	0
2	B	504/505 (99%)	0.38	14 (2%) 53 64	34, 48, 86, 137	0
2	b	503/505 (99%)	0.50	28 (5%) 24 35	34, 48, 93, 193	0
3	C	451/455 (99%)	0.42	18 (3%) 38 51	37, 56, 82, 134	0
3	c	455/455 (100%)	0.27	8 (1%) 68 77	39, 58, 83, 118	0
4	D	341/342 (99%)	0.29	3 (0%) 84 90	32, 45, 70, 129	0
4	d	341/342 (99%)	0.35	1 (0%) 94 97	34, 45, 69, 115	0
5	E	81/84 (96%)	1.37	25 (30%) 0 0	50, 73, 116, 150	0
5	e	81/84 (96%)	0.84	15 (18%) 1 2	51, 71, 125, 201	0
6	F	34/44 (77%)	0.48	4 (11%) 4 7	51, 62, 103, 104	0
6	f	32/44 (72%)	0.31	2 (6%) 20 29	50, 62, 118, 148	0
7	H	65/65 (100%)	0.30	3 (4%) 32 45	47, 57, 83, 145	0
7	h	65/65 (100%)	0.36	3 (4%) 32 45	47, 60, 83, 167	0
8	I	37/38 (97%)	0.57	4 (10%) 5 9	45, 58, 123, 187	0
8	i	37/38 (97%)	0.64	4 (10%) 5 9	44, 57, 116, 159	0
9	J	38/39 (97%)	0.99	6 (15%) 2 3	52, 68, 151, 185	0
9	j	39/39 (100%)	0.75	7 (17%) 1 2	52, 68, 140, 190	0
10	K	37/37 (100%)	0.71	4 (10%) 5 9	60, 68, 88, 112	0
10	k	37/37 (100%)	0.42	0 100 100	59, 67, 88, 112	0
11	L	37/37 (100%)	0.40	0 100 100	34, 39, 101, 132	0
11	l	37/37 (100%)	0.51	1 (2%) 54 64	34, 40, 105, 130	0
12	M	33/36 (91%)	0.64	0 100 100	29, 41, 75, 126	0
12	m	33/36 (91%)	0.55	0 100 100	35, 42, 78, 126	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.42	12 (4%) 29 42	36, 54, 102, 146	0
13	o	243/244 (99%)	0.31	6 (2%) 57 67	36, 56, 112, 179	0
14	T	29/32 (90%)	0.57	1 (3%) 45 57	35, 40, 70, 142	0
14	t	29/32 (90%)	0.45	0 100 100	35, 39, 68, 141	0
15	U	97/104 (93%)	0.20	1 (1%) 82 88	39, 51, 82, 128	0
15	u	97/104 (93%)	0.17	0 100 100	42, 52, 76, 126	0
16	V	137/137 (100%)	0.36	1 (0%) 87 92	41, 54, 88, 123	0
16	v	137/137 (100%)	0.21	1 (0%) 87 92	43, 58, 89, 121	0
17	Y	29/30 (96%)	3.31	12 (41%) 0 0	73, 85, 162, 203	0
17	y	29/30 (96%)	1.50	9 (31%) 0 0	75, 85, 164, 202	0
18	X	39/40 (97%)	0.57	3 (7%) 13 20	52, 67, 135, 143	0
18	x	38/40 (95%)	0.94	6 (15%) 2 3	55, 67, 130, 140	0
19	Z	62/62 (100%)	1.44	18 (29%) 0 0	75, 89, 144, 191	0
19	z	62/62 (100%)	1.64	19 (30%) 0 0	75, 90, 144, 188	0
20	R	18/34 (52%)	5.55	18 (100%) 0 0	102, 135, 170, 172	0
All	All	5275/5384 (97%)	0.48	277 (5%) 26 38	29, 52, 103, 203	0

The worst 5 of 277 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	14.8
17	Y	20	ALA	13.7
2	b	494	GLY	12.3
17	Y	19	ILE	11.9
20	R	6	LEU	10.3

## 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
14	FME	T	1	10/11	0.94	0.14	30,49,67,82	0
14	FME	t	1	10/11	0.94	0.14	26,36,47,88	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FME	M	1	10/11	0.95	0.18	30,50,87,93	0
8	FME	i	1	10/11	0.95	0.15	43,60,73,75	0
12	FME	m	1	10/11	0.95	0.16	31,50,100,103	0
8	FME	I	1	10/11	0.96	0.12	28,49,62,64	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
29	LMT	F	101	35/35	0.33	0.53	102,149,179,184	0
37	DGD	e	101	62/66	0.41	0.43	72,118,208,212	0
35	HTG	d	414	16/19	0.47	0.25	68,115,134,134	0
32	UNL	j	101	10/-	0.50	0.28	56,83,95,98	0
29	LMT	a	417	35/35	0.53	0.38	95,123,147,148	0
37	DGD	D	408	52/66	0.54	0.36	58,108,151,171	0
28	GOL	V	204	6/6	0.55	0.60	75,90,97,100	0
36	LHG	a	418	42/49	0.55	0.32	69,131,187,193	0
32	UNL	C	526	34/-	0.58	0.24	76,120,132,136	0
22	CL	v	201	1/1	0.58	0.10	124,124,124,124	0
29	LMT	a	401	35/35	0.59	0.32	52,87,118,142	0
29	LMT	b	626	25/35	0.59	0.39	71,102,168,175	0
32	UNL	J	102	10/-	0.60	0.24	50,85,104,107	0
29	LMT	e	102	35/35	0.60	0.31	83,129,164,170	0
29	LMT	m	103	35/35	0.60	0.31	42,109,140,144	0
33	LMG	Z	101	37/55	0.62	0.31	55,121,146,154	0
29	LMT	C	520	35/35	0.62	0.36	88,135,162,175	0
29	LMT	A	415	35/35	0.65	0.25	41,84,115,119	0
27	SQD	f	102	43/54	0.67	0.29	97,116,175,182	0
33	LMG	Y	101	51/55	0.67	0.25	60,93,118,127	0
29	LMT	M	103	35/35	0.68	0.28	47,99,150,158	0
32	UNL	a	414	30/-	0.68	0.26	64,85,117,134	0
35	HTG	B	633	19/19	0.68	0.24	53,103,141,160	0
35	HTG	c	922	19/19	0.69	0.29	73,114,134,192	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UNL	c	925	32/-	0.69	0.25	66,101,138,147	0
36	LHG	E	101	42/49	0.70	0.26	59,115,138,140	0
32	UNL	A	418	28/-	0.70	0.26	59,88,108,111	0
29	LMT	b	602	25/35	0.71	0.28	41,91,134,149	0
35	HTG	b	604	19/19	0.71	0.19	51,112,150,150	0
32	UNL	b	634	33/-	0.72	0.26	47,86,155,158	0
29	LMT	D	403	35/35	0.72	0.27	58,132,172,179	0
35	HTG	D	413	16/19	0.72	0.27	76,142,160,166	0
33	LMG	z	101	39/55	0.73	0.28	65,124,153,161	0
35	HTG	B	625	19/19	0.73	0.23	75,132,140,190	0
28	GOL	O	302	6/6	0.73	0.17	68,79,84,89	0
29	LMT	M	101	35/35	0.74	0.23	45,93,118,133	0
37	DGD	C	517	62/66	0.74	0.23	48,65,94,116	0
35	HTG	C	522	19/19	0.75	0.31	81,112,138,140	0
32	UNL	B	634	33/-	0.75	0.29	54,73,126,134	0
27	SQD	L	102	54/54	0.76	0.23	48,79,126,149	0
29	LMT	m	102	35/35	0.76	0.26	42,90,122,128	0
29	LMT	t	101	25/35	0.76	0.31	43,92,140,150	0
35	HTG	b	628	19/19	0.77	0.22	72,130,158,159	0
33	LMG	C	519	51/55	0.77	0.25	53,121,145,151	0
31	PL9	A	417	55/55	0.77	0.25	61,98,125,131	0
33	LMG	b	625	51/55	0.78	0.23	40,54,73,98	0
32	UNL	M	102	10/-	0.78	0.31	50,55,74,86	0
33	LMG	c	920	51/55	0.78	0.24	50,111,142,145	0
28	GOL	l	101	6/6	0.79	0.39	48,92,98,103	0
35	HTG	c	921	19/19	0.79	0.18	93,101,107,111	0
34	CA	f	103	1/1	0.79	0.09	126,126,126,126	0
27	SQD	a	402	54/54	0.79	0.22	45,75,125,133	0
27	SQD	F	103	43/54	0.80	0.25	77,120,145,149	0
27	SQD	B	621	54/54	0.80	0.25	53,88,137,156	0
22	CL	U	201	1/1	0.80	0.08	117,117,117,117	0
24	CLA	C	513	65/65	0.80	0.28	53,84,113,119	0
33	LMG	B	622	51/55	0.80	0.22	38,53,78,91	0
32	UNL	d	413	36/-	0.81	0.25	60,85,140,142	0
28	GOL	T	101	6/6	0.81	0.33	60,77,82,83	0
31	PL9	a	415	55/55	0.81	0.24	65,110,127,130	0
28	GOL	b	633	6/6	0.81	0.20	68,74,80,88	0
34	CA	B	601	1/1	0.81	0.06	138,138,138,138	0
35	HTG	b	601	19/19	0.81	0.20	42,57,82,87	0
35	HTG	b	603	19/19	0.81	0.19	47,75,92,93	0
32	UNL	D	412	40/-	0.82	0.20	51,88,141,144	0
32	UNL	m	101	10/-	0.82	0.34	58,66,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	HTG	b	627	19/19	0.82	0.25	55,73,94,109	0
24	CLA	C	504	65/65	0.82	0.20	36,57,79,95	0
37	DGD	h	102	62/66	0.82	0.21	34,52,71,82	0
28	GOL	V	207	6/6	0.82	0.18	81,86,89,98	0
28	GOL	v	204	6/6	0.82	0.22	84,87,94,112	0
33	LMG	c	919	51/55	0.82	0.20	51,89,123,128	0
33	LMG	A	419	51/55	0.83	0.19	54,88,107,128	0
35	HTG	B	632	19/19	0.83	0.17	48,84,110,115	0
37	DGD	H	102	62/66	0.83	0.21	31,51,88,102	0
28	GOL	v	203	6/6	0.83	0.21	72,88,91,94	0
37	DGD	C	518	62/66	0.83	0.18	39,58,92,100	0
27	SQD	A	414	54/54	0.83	0.22	49,75,134,141	0
27	SQD	a	410	54/54	0.84	0.18	51,81,110,114	0
32	UNL	i	101	40/-	0.84	0.24	48,77,140,147	0
35	HTG	V	203	19/19	0.84	0.33	73,95,125,231	0
32	UNL	I	101	40/-	0.84	0.24	42,88,155,156	0
35	HTG	B	624	19/19	0.84	0.23	50,73,82,92	0
33	LMG	a	411	51/55	0.84	0.22	51,84,96,105	0
32	UNL	X	101	18/-	0.85	0.17	53,73,112,114	0
28	GOL	C	523	6/6	0.85	0.34	74,80,89,92	0
28	GOL	T	103	6/6	0.85	0.47	103,108,112,114	0
28	GOL	a	419	6/6	0.85	0.17	73,85,94,95	0
37	DGD	c	917	62/66	0.85	0.20	35,60,112,137	0
28	GOL	c	924	6/6	0.85	0.34	81,87,97,102	0
24	CLA	c	914	65/65	0.85	0.20	68,84,105,115	0
27	SQD	A	411	54/54	0.86	0.20	43,87,114,116	0
24	CLA	B	602	65/65	0.87	0.19	43,67,119,143	0
37	DGD	c	918	62/66	0.87	0.19	41,56,90,110	0
24	CLA	b	607	65/65	0.87	0.20	30,50,60,63	0
34	CA	F	104	1/1	0.87	0.06	107,107,107,107	0
24	CLA	b	612	65/65	0.87	0.20	27,38,48,58	0
24	CLA	B	607	65/65	0.87	0.19	31,52,95,99	0
24	CLA	c	907	65/65	0.87	0.17	44,65,104,111	0
33	LMG	d	415	51/55	0.88	0.20	38,61,112,126	0
24	CLA	c	908	65/65	0.88	0.17	45,63,74,84	0
24	CLA	b	614	65/65	0.88	0.18	39,51,61,72	0
24	CLA	c	904	65/65	0.88	0.17	41,60,73,84	0
33	LMG	J	101	51/55	0.88	0.20	44,65,120,137	0
28	GOL	V	201	6/6	0.89	0.23	88,99,104,109	0
24	CLA	C	511	65/65	0.89	0.16	48,67,85,109	0
28	GOL	b	632	6/6	0.89	0.24	77,78,102,105	0
24	CLA	B	614	65/65	0.89	0.19	29,41,64,93	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	c	906	65/65	0.89	0.17	36,51,70,76	0
36	LHG	B	635	49/49	0.89	0.26	30,52,68,77	0
24	CLA	b	606	65/65	0.89	0.20	39,67,123,145	0
28	GOL	a	413	6/6	0.89	0.20	73,83,95,97	0
32	UNL	x	101	18/-	0.89	0.22	51,71,116,116	0
24	CLA	C	512	65/65	0.90	0.15	49,76,99,106	0
24	CLA	c	905	65/65	0.90	0.16	31,57,74,85	0
28	GOL	c	928	6/6	0.90	0.14	75,83,90,98	0
24	CLA	c	910	65/65	0.90	0.16	43,58,77,81	0
24	CLA	d	404	65/65	0.90	0.18	29,39,48,56	0
36	LHG	D	410	49/49	0.90	0.23	47,67,121,138	0
24	CLA	c	912	65/65	0.90	0.16	43,63,83,99	0
28	GOL	B	630	6/6	0.90	0.21	51,59,70,81	0
26	BCR	C	514	40/40	0.90	0.17	50,72,86,87	0
35	HTG	B	623	19/19	0.90	0.18	38,56,78,93	0
24	CLA	C	501	65/65	0.90	0.15	39,57,85,91	0
24	CLA	c	909	65/65	0.90	0.15	38,54,125,137	0
37	DGD	c	916	62/66	0.90	0.18	38,56,100,114	0
24	CLA	C	506	65/65	0.90	0.15	41,70,114,128	0
24	CLA	B	610	65/65	0.90	0.18	36,52,65,82	0
35	HTG	C	521	19/19	0.90	0.19	70,99,121,123	0
36	LHG	b	635	49/49	0.91	0.22	30,48,61,64	0
24	CLA	b	619	65/65	0.91	0.18	25,43,86,108	0
24	CLA	B	616	65/65	0.91	0.17	37,50,65,77	0
24	CLA	A	405	65/65	0.91	0.17	24,37,51,66	0
24	CLA	c	911	65/65	0.91	0.15	43,55,69,81	0
36	LHG	d	411	49/49	0.91	0.20	37,53,112,120	0
24	CLA	b	620	65/65	0.91	0.17	36,50,64,69	0
24	CLA	C	503	65/65	0.91	0.18	36,59,72,85	0
28	GOL	B	636	6/6	0.91	0.18	49,56,64,65	0
24	CLA	b	611	65/65	0.91	0.17	37,51,97,108	0
28	GOL	D	402	6/6	0.91	0.31	52,57,83,90	0
24	CLA	B	605	65/65	0.91	0.17	28,41,72,78	0
28	GOL	A	412	6/6	0.91	0.18	49,55,57,69	0
37	DGD	C	516	62/66	0.92	0.18	32,50,88,97	0
36	LHG	d	410	49/49	0.92	0.23	29,44,63,98	0
24	CLA	C	508	65/65	0.92	0.15	35,61,138,148	0
24	CLA	b	616	65/65	0.92	0.17	29,41,54,66	0
24	CLA	C	510	65/65	0.92	0.15	40,60,77,92	0
36	LHG	d	409	49/49	0.92	0.23	40,52,66,70	0
28	GOL	A	413	6/6	0.92	0.17	61,79,84,86	0
24	CLA	B	615	65/65	0.92	0.19	26,43,97,103	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	C	509	65/65	0.92	0.15	53,65,82,93	0
24	CLA	B	603	65/65	0.92	0.16	38,50,57,66	0
24	CLA	D	405	65/65	0.92	0.15	39,55,106,121	0
24	CLA	b	621	65/65	0.92	0.17	33,53,103,118	0
24	CLA	D	404	65/65	0.92	0.16	24,37,58,69	0
24	CLA	B	612	65/65	0.92	0.20	24,40,56,63	0
26	BCR	c	927	40/40	0.92	0.15	54,77,91,100	0
24	CLA	b	613	65/65	0.92	0.17	36,49,59,62	0
24	CLA	c	913	65/65	0.92	0.16	47,74,93,99	0
26	BCR	b	623	40/40	0.92	0.19	29,46,66,68	0
26	BCR	k	101	40/40	0.92	0.14	51,64,75,80	0
34	CA	o	301	1/1	0.92	0.05	97,97,97,97	0
24	CLA	a	405	65/65	0.92	0.19	24,38,53,67	0
26	BCR	H	101	40/40	0.92	0.17	33,57,78,85	0
24	CLA	d	406	65/65	0.93	0.19	40,54,106,124	0
24	CLA	d	405	65/65	0.93	0.17	24,40,55,69	0
32	UNL	D	411	17/-	0.93	0.22	40,71,92,94	0
24	CLA	b	615	65/65	0.93	0.18	35,47,61,67	0
24	CLA	C	507	65/65	0.93	0.16	41,66,77,86	0
24	CLA	B	608	65/65	0.93	0.17	25,41,51,61	0
24	CLA	a	408	65/65	0.93	0.20	32,53,122,130	0
26	BCR	y	101	40/40	0.93	0.15	47,63,74,82	0
28	GOL	B	626	6/6	0.93	0.19	44,53,66,87	0
34	CA	b	605	1/1	0.93	0.06	124,124,124,124	0
28	GOL	B	628	6/6	0.93	0.22	62,80,83,84	0
26	BCR	h	101	40/40	0.93	0.18	36,60,79,81	0
24	CLA	B	613	65/65	0.93	0.16	26,42,50,53	0
26	BCR	d	407	40/40	0.93	0.19	39,54,85,88	0
26	BCR	D	406	40/40	0.93	0.15	39,58,89,104	0
24	CLA	b	608	65/65	0.93	0.17	38,48,58,66	0
24	CLA	b	617	65/65	0.93	0.17	25,42,53,65	0
24	CLA	B	604	65/65	0.93	0.18	35,48,60,63	0
24	CLA	b	618	65/65	0.94	0.20	24,44,60,67	0
28	GOL	V	206	6/6	0.94	0.31	52,60,67,71	0
24	CLA	A	406	65/65	0.94	0.16	23,36,45,55	0
32	UNL	d	412	17/-	0.94	0.25	47,62,95,102	0
24	CLA	B	617	65/65	0.94	0.20	34,54,130,139	0
36	LHG	D	409	49/49	0.94	0.22	31,46,67,79	0
31	PL9	d	408	55/55	0.94	0.21	22,39,53,73	0
26	BCR	Y	102	40/40	0.94	0.14	51,71,90,107	0
36	LHG	L	101	49/49	0.94	0.22	36,47,56,62	0
25	PHO	A	408	64/64	0.94	0.16	26,39,46,54	0

*Continued on next page...*

*Continued from previous page...*

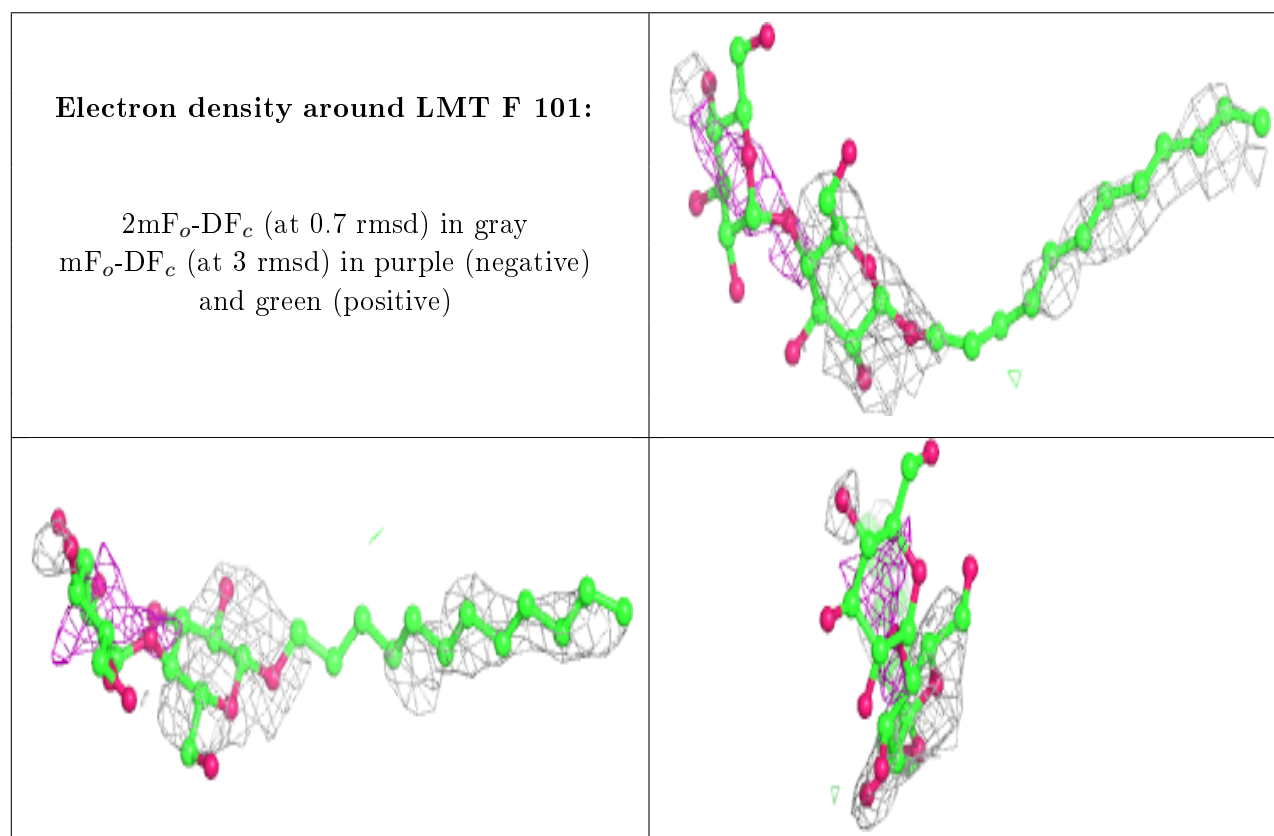
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	PHO	d	403	64/64	0.94	0.17	27,44,54,62	0
24	CLA	C	505	65/65	0.94	0.15	41,54,71,89	0
26	BCR	K	101	40/40	0.94	0.15	43,63,79,82	0
24	CLA	B	606	65/65	0.94	0.16	28,40,55,57	0
28	GOL	B	627	6/6	0.94	0.25	54,64,88,102	0
24	CLA	c	902	65/65	0.94	0.16	44,60,72,81	0
24	CLA	c	903	65/65	0.94	0.15	39,52,76,80	0
31	PL9	D	407	55/55	0.94	0.21	29,42,52,60	0
24	CLA	b	610	65/65	0.94	0.17	31,43,53,61	0
28	GOL	b	630	6/6	0.94	0.17	50,82,94,95	0
24	CLA	A	407	65/65	0.94	0.15	28,43,106,119	0
24	CLA	B	609	65/65	0.94	0.18	32,46,59,67	0
28	GOL	v	205	6/6	0.95	0.21	48,59,69,78	0
26	BCR	A	410	40/40	0.95	0.18	32,42,54,54	0
28	GOL	b	631	6/6	0.95	0.19	58,70,81,100	0
24	CLA	C	502	65/65	0.95	0.14	42,56,69,85	0
28	GOL	V	205	6/6	0.95	0.17	45,51,58,72	0
26	BCR	b	622	40/40	0.95	0.18	32,44,56,60	0
34	CA	c	901	1/1	0.95	0.08	74,74,74,74	0
28	GOL	b	629	6/6	0.95	0.21	57,62,67,81	0
26	BCR	c	915	40/40	0.95	0.18	32,56,67,75	0
24	CLA	a	406	65/65	0.95	0.19	31,44,118,125	0
26	BCR	T	102	40/40	0.95	0.17	29,46,64,65	0
25	PHO	D	401	64/64	0.95	0.17	31,46,58,60	0
26	BCR	C	515	40/40	0.95	0.18	38,55,68,78	0
28	GOL	B	629	6/6	0.95	0.28	56,60,69,95	0
24	CLA	b	609	65/65	0.95	0.17	27,42,74,77	0
24	CLA	A	409	65/65	0.95	0.16	33,50,116,132	0
24	CLA	B	611	65/65	0.95	0.20	31,50,62,66	0
26	BCR	b	624	40/40	0.96	0.19	39,50,61,65	0
23	BCT	d	402	4/4	0.96	0.23	70,72,76,97	0
26	BCR	B	619	40/40	0.96	0.20	31,42,60,66	0
25	PHO	a	407	64/64	0.96	0.18	28,40,48,54	0
26	BCR	B	620	40/40	0.96	0.20	36,52,64,67	0
34	CA	O	301	1/1	0.96	0.06	89,89,89,89	0
38	HEM	f	101	43/43	0.96	0.16	51,85,128,152	0
26	BCR	B	618	40/40	0.96	0.21	29,40,51,54	0
22	CL	A	403	1/1	0.96	0.09	38,38,38,38	0
39	MG	j	102	1/1	0.96	0.13	61,61,61,61	0
38	HEM	V	202	43/43	0.96	0.14	31,45,54,59	0
26	BCR	a	409	40/40	0.96	0.19	28,43,54,59	0
23	BCT	A	404	4/4	0.96	0.21	59,62,74,108	0

*Continued on next page...*

Continued from previous page...

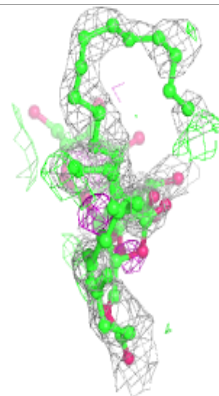
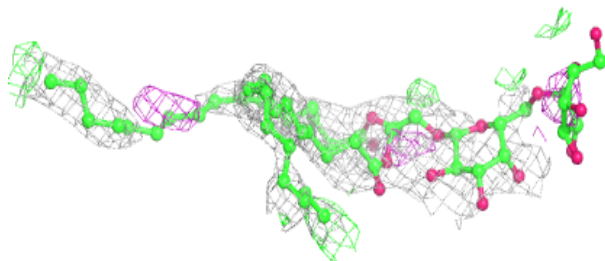
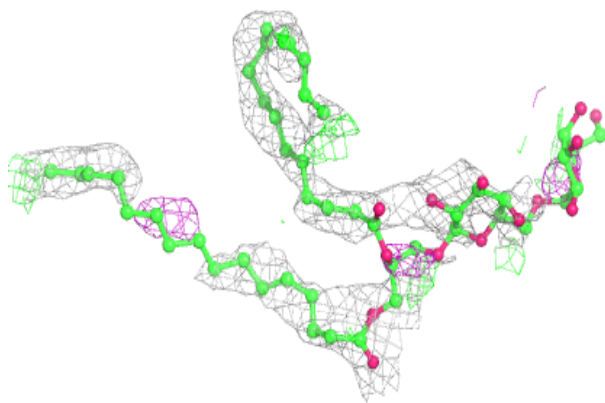
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	GOL	a	412	6/6	0.96	0.24	54,61,67,72	0
26	BCR	t	102	40/40	0.96	0.19	33,46,62,64	0
38	HEM	v	202	43/43	0.97	0.14	46,58,65,70	0
34	CA	C	525	1/1	0.97	0.16	79,79,79,79	0
28	GOL	B	631	6/6	0.97	0.31	40,78,87,93	0
38	HEM	F	102	43/43	0.97	0.16	53,74,105,111	0
28	GOL	c	923	6/6	0.98	0.19	41,51,54,57	0
34	CA	c	926	1/1	0.98	0.11	77,77,77,77	0
39	MG	J	103	1/1	0.98	0.12	54,54,54,54	0
30	OEX	a	416	10/10	0.98	0.15	35,45,63,74	0
28	GOL	C	524	6/6	0.98	0.17	39,44,53,61	0
21	FE2	d	401	1/1	0.99	0.20	55,55,55,55	0
22	CL	a	403	1/1	0.99	0.17	37,37,37,37	0
21	FE2	A	401	1/1	0.99	0.16	56,56,56,56	0
30	OEX	A	416	10/10	0.99	0.14	39,45,61,77	0
22	CL	a	404	1/1	1.00	0.14	42,42,42,42	0
22	CL	A	402	1/1	1.00	0.16	35,35,35,35	0

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

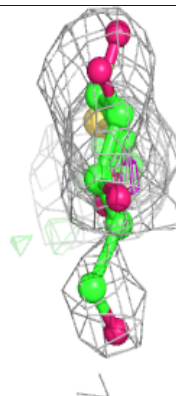
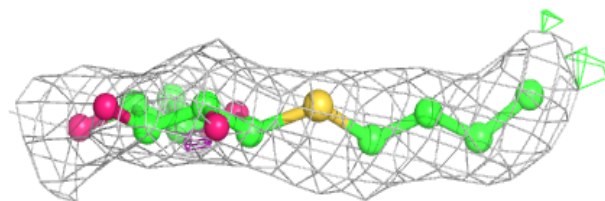
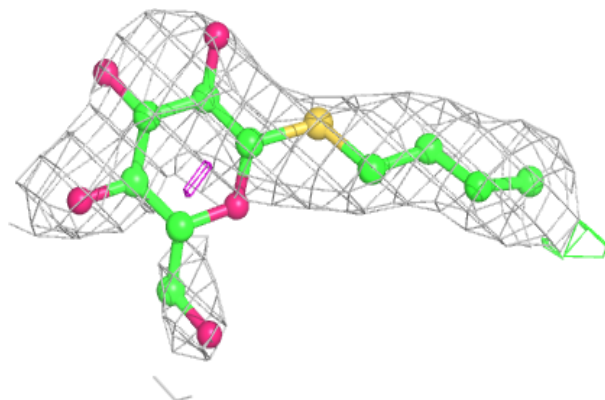


**Electron density around DGD e 101:**

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

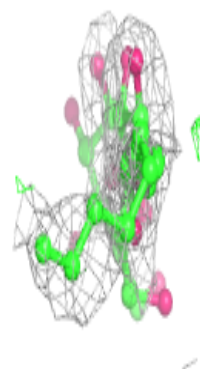
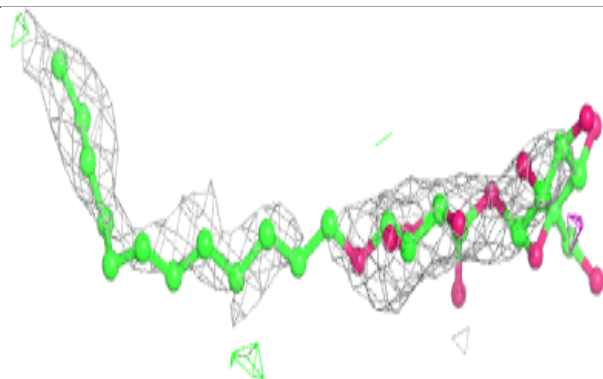
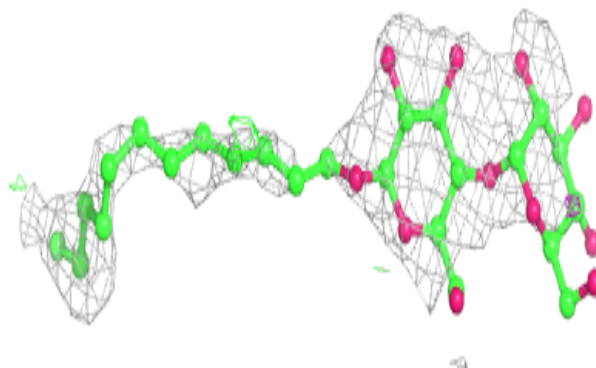
**Electron density around HTG d 414:**

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

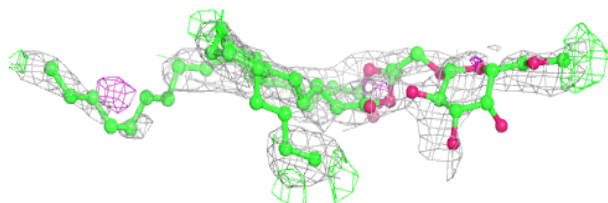
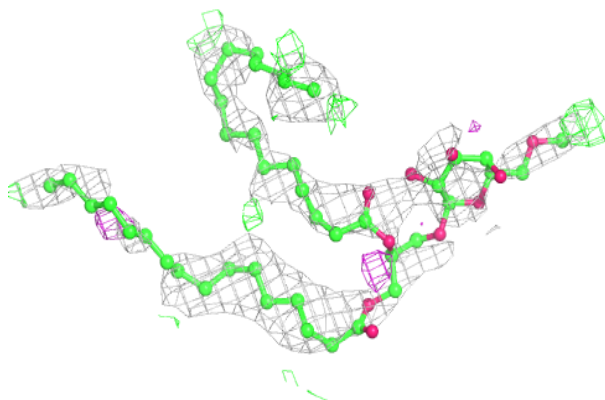


**Electron density around LMT a 417:**

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

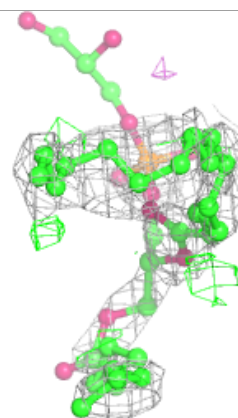
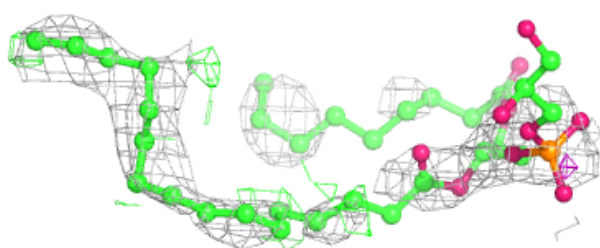
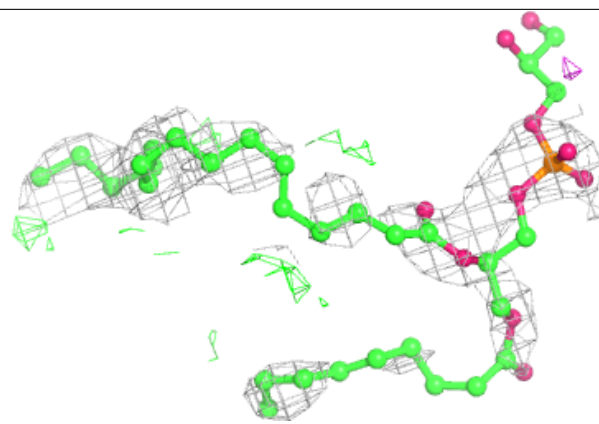
**Electron density around DGD D 408:**

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

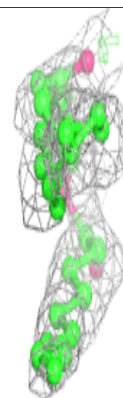
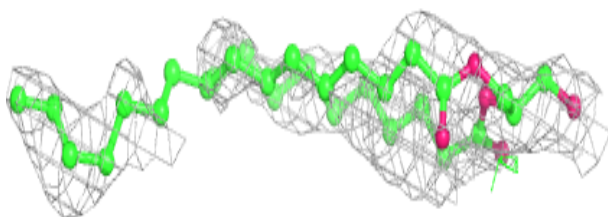
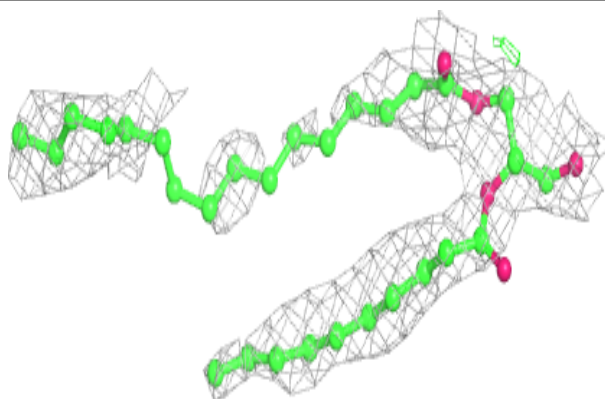


**Electron density around LHG a 418:**

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

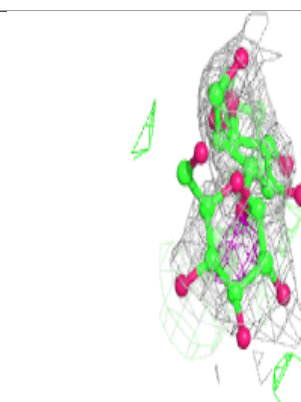
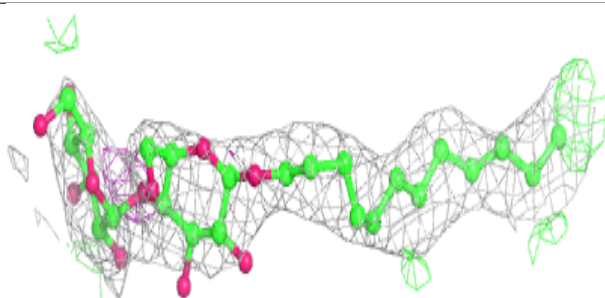
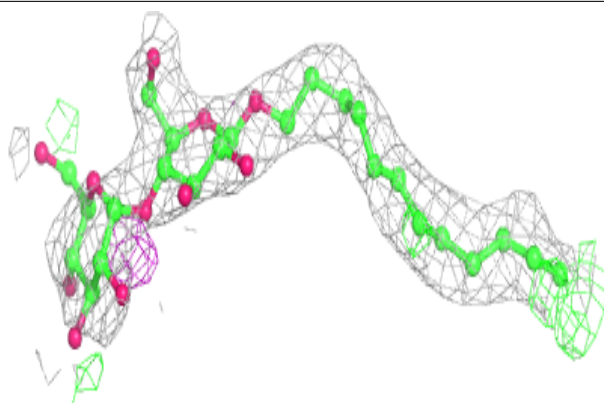
**Electron density around UNL C 526:**

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

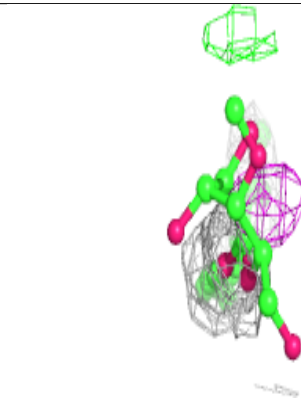
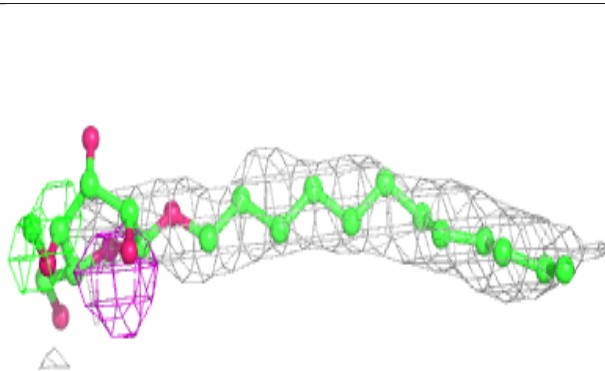
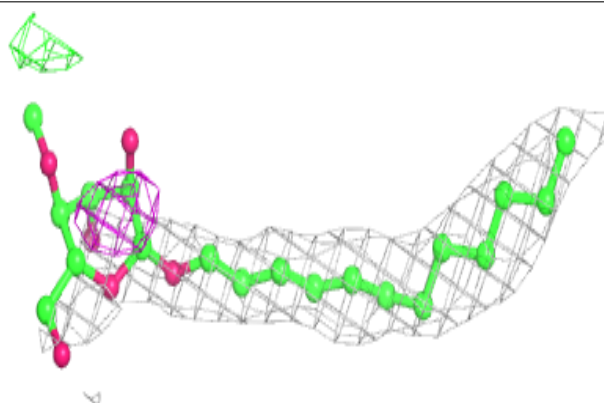


**Electron density around LMT a 401:**

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

**Electron density around LMT b 626:**

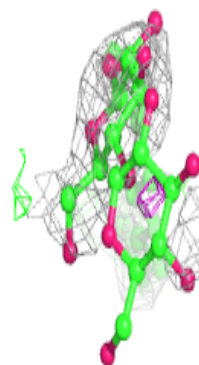
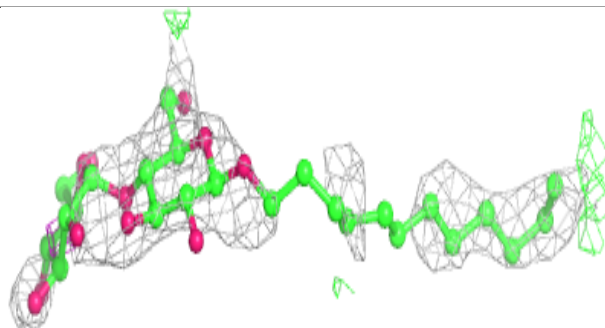
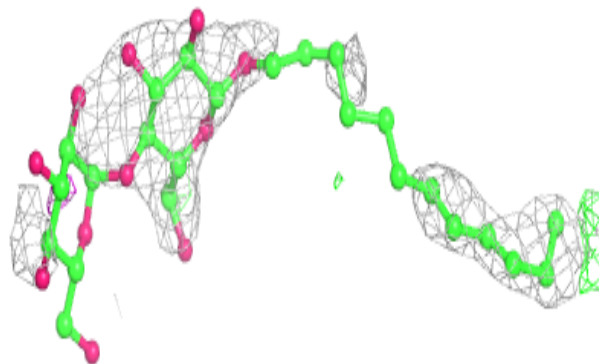
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



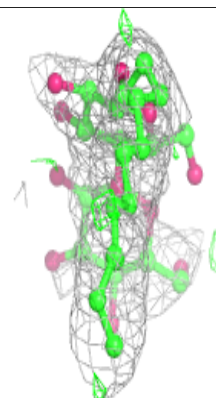
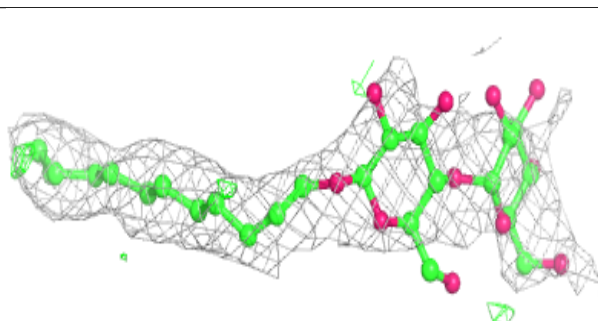
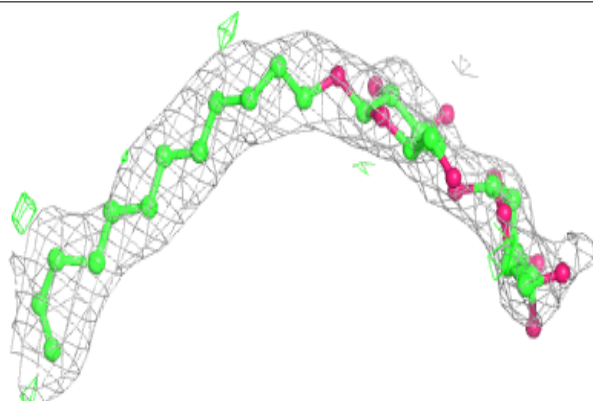


**Electron density around LMT e 102:**

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

**Electron density around LMT m 103:**

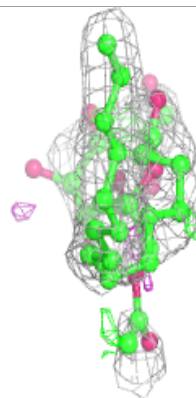
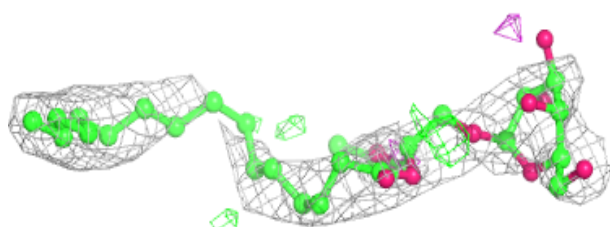
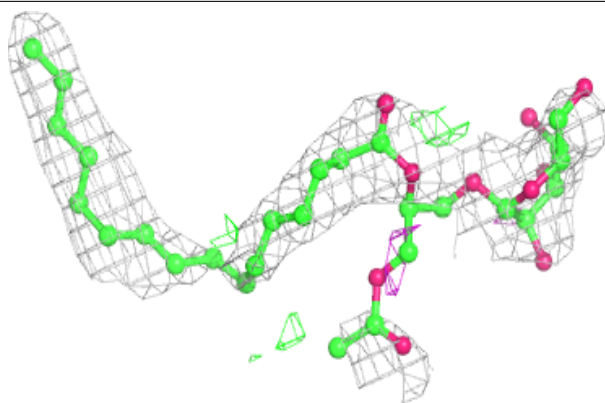
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



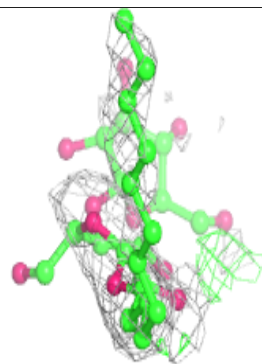
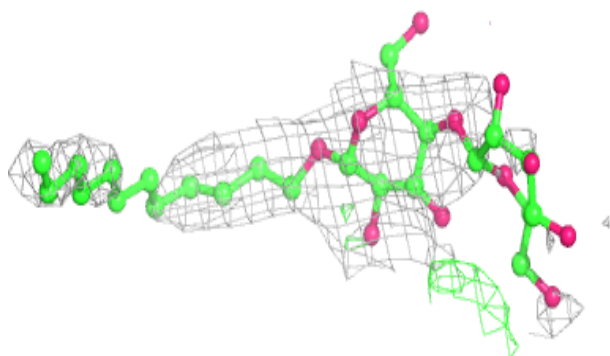
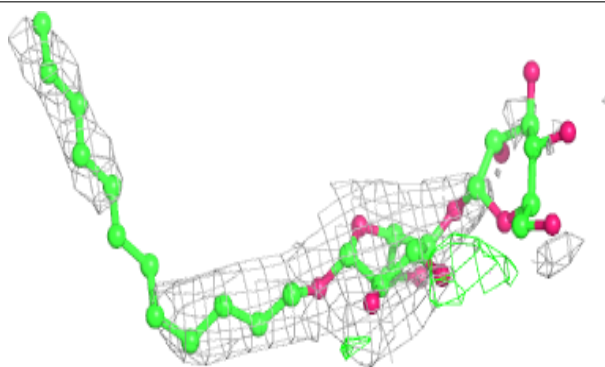


**Electron density around LMG Z 101:**

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

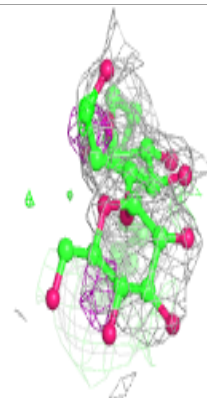
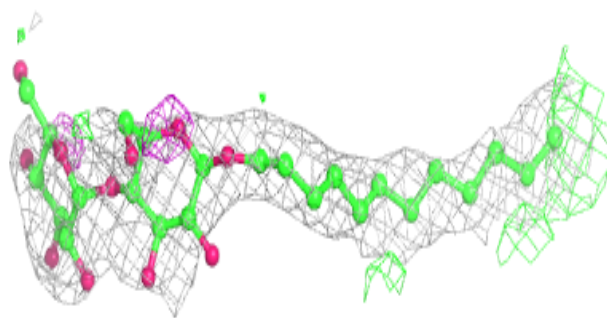
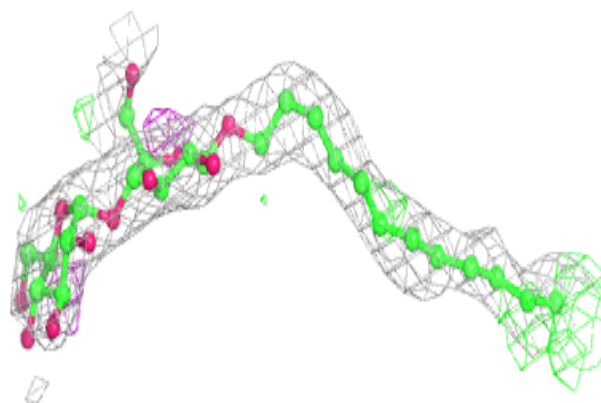
**Electron density around LMT C 520:**

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

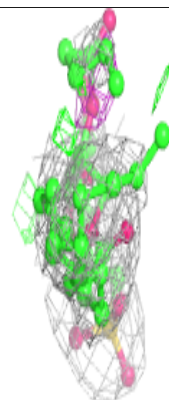
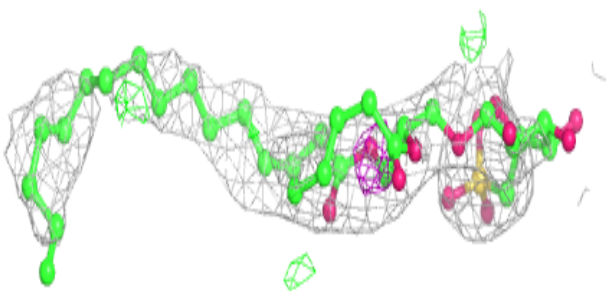
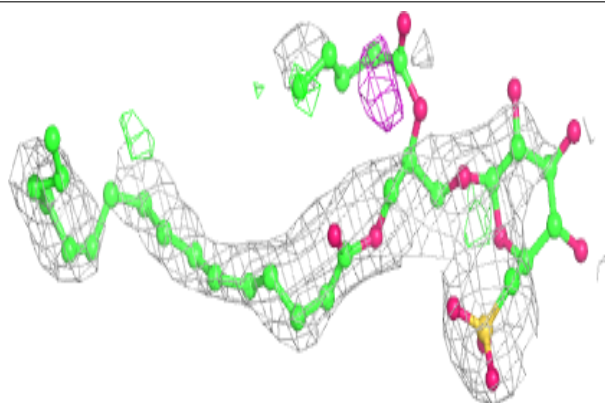


**Electron density around LMT A 415:**

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

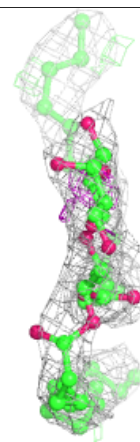
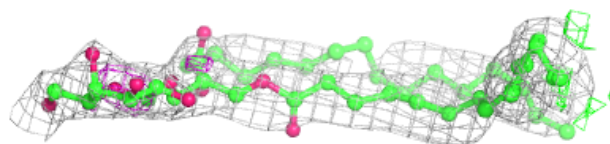
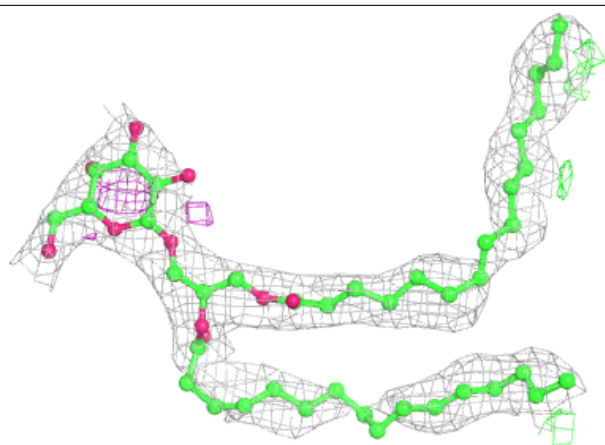
**Electron density around SQD f 102:**

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

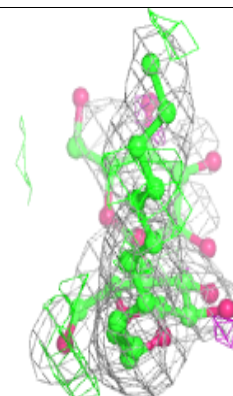
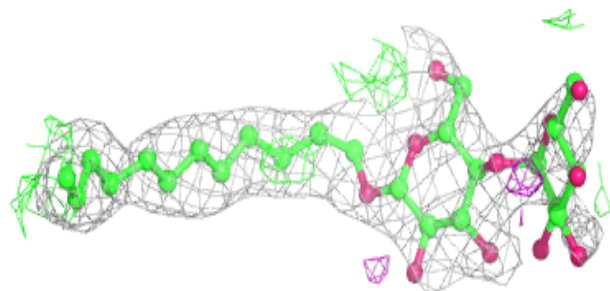
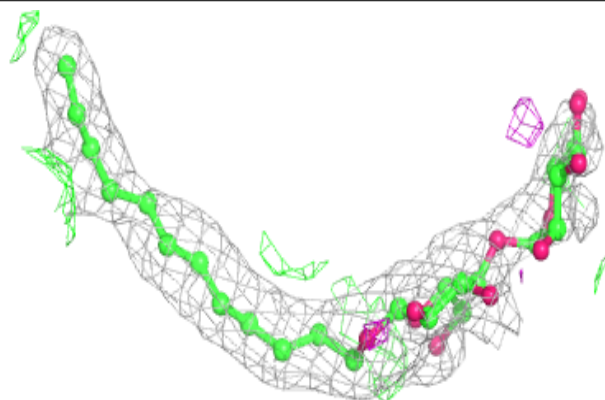


**Electron density around LMG Y 101:**

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

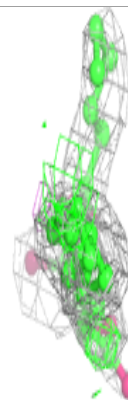
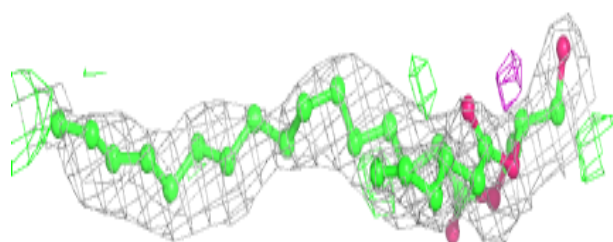
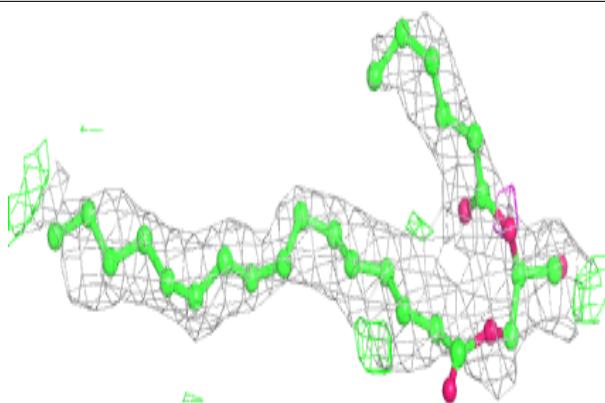
**Electron density around LMT M 103:**

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

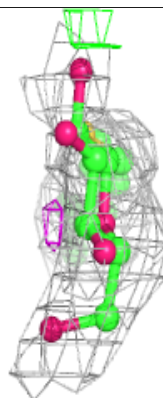
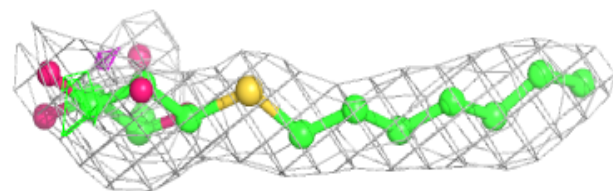
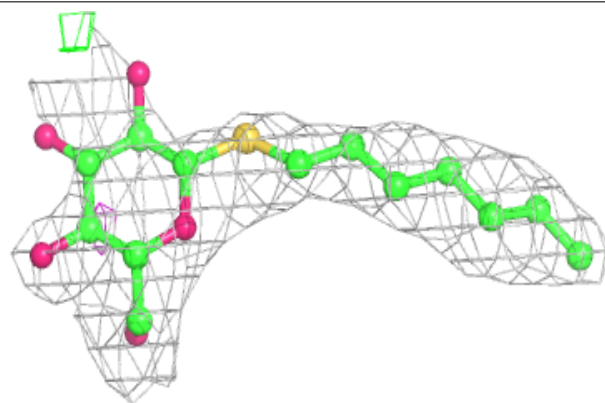


**Electron density around UNL a 414:**

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

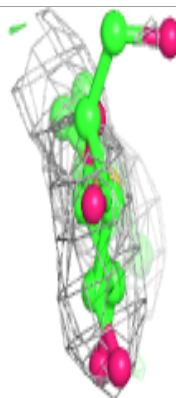
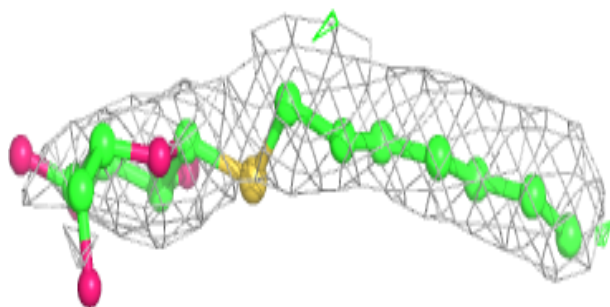
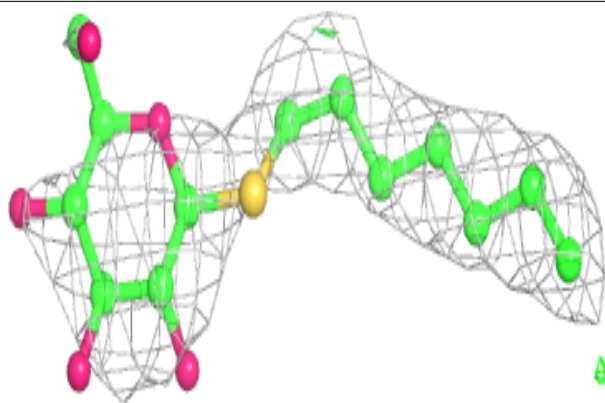
**Electron density around HTG B 633:**

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

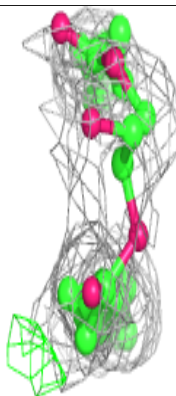
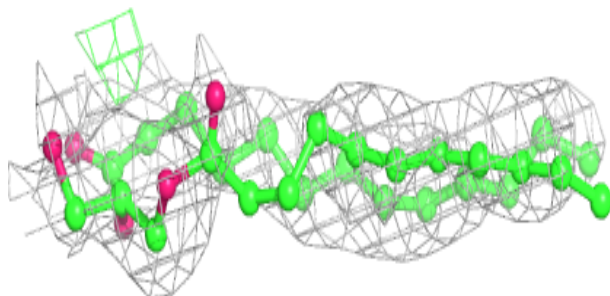
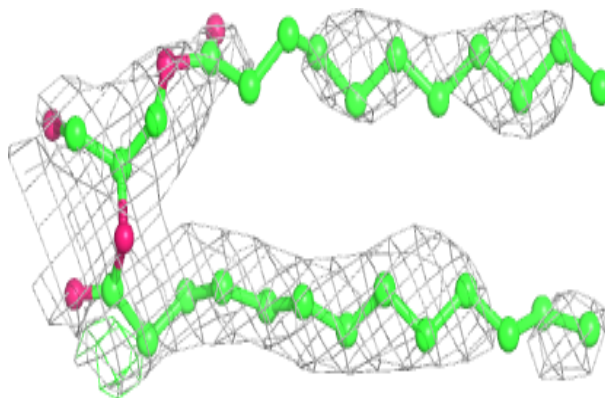


**Electron density around HTG c 922:**

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

**Electron density around UNL c 925:**

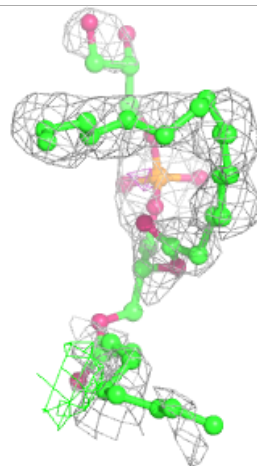
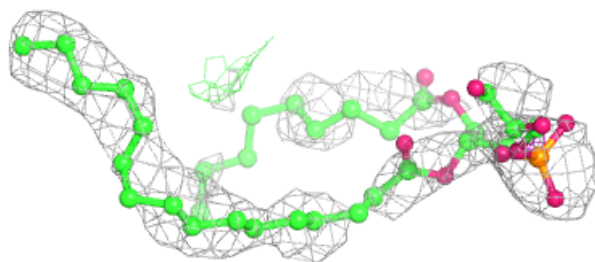
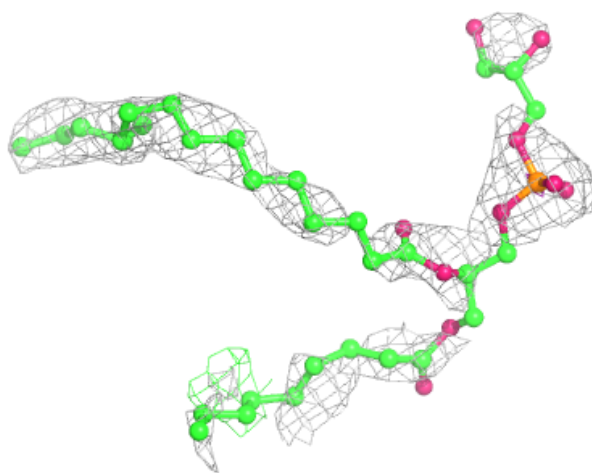
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





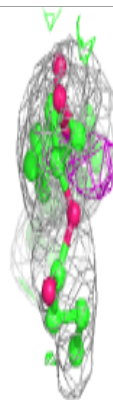
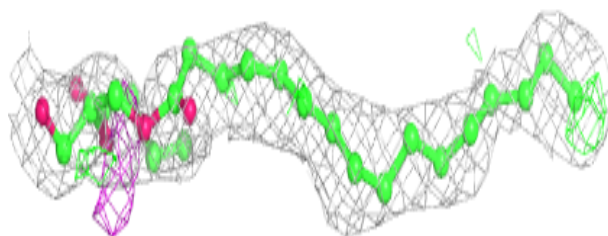
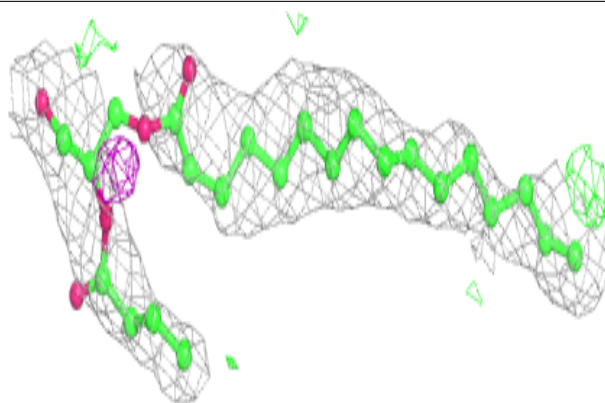
**Electron density around LHG E 101:**

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

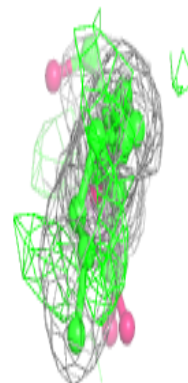
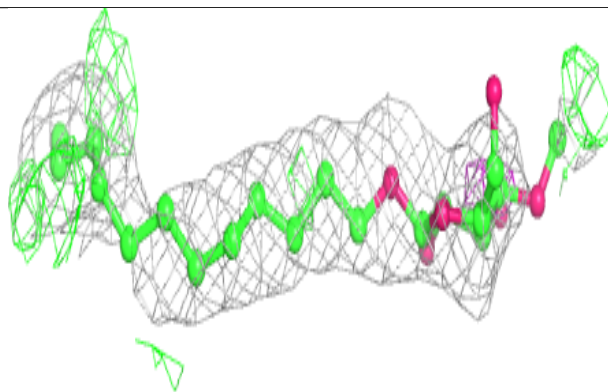
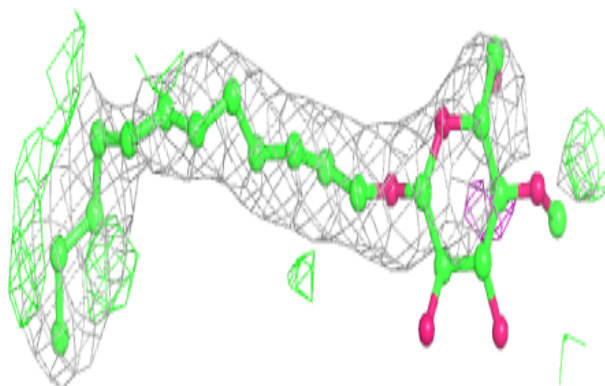


**Electron density around UNL A 418:**

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

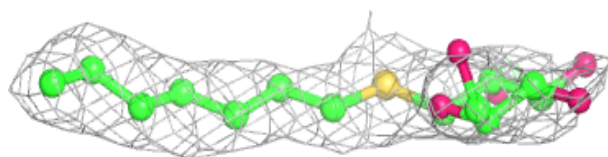
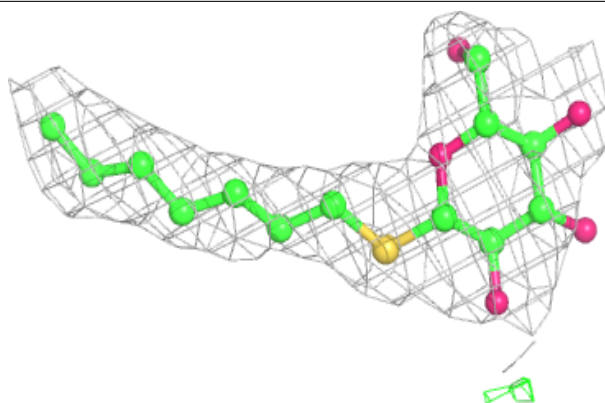
**Electron density around LMT b 602:**

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

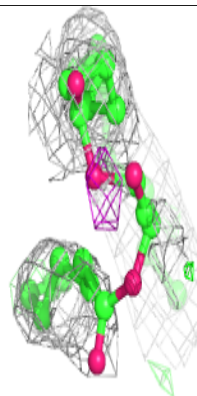
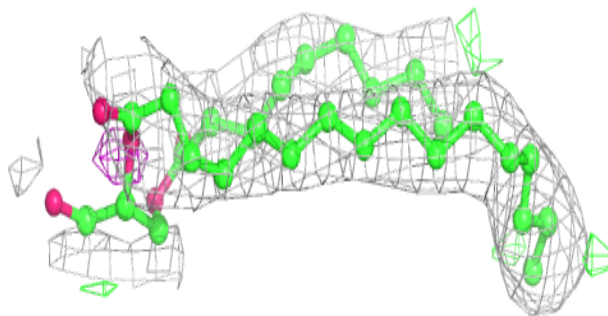
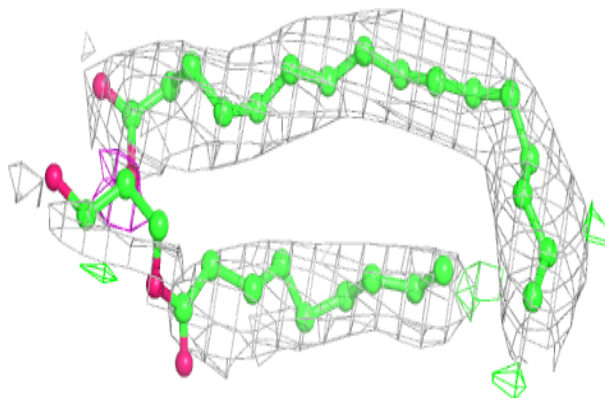


**Electron density around HTG b 604:**

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

**Electron density around UNL b 634:**

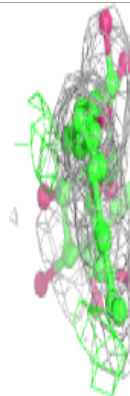
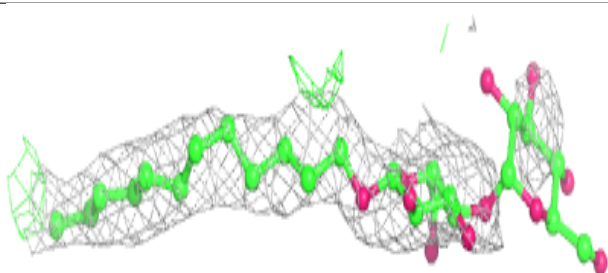
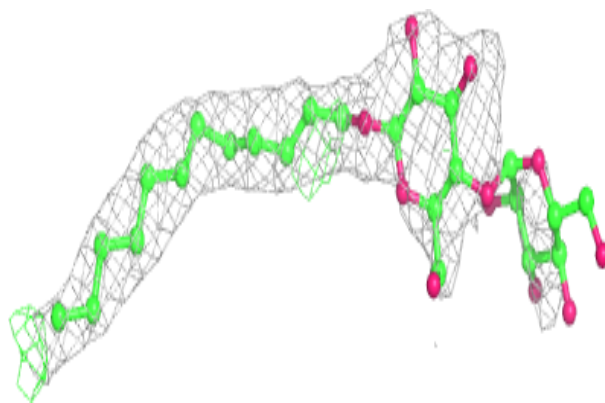
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



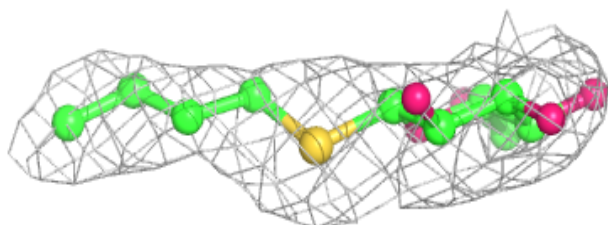
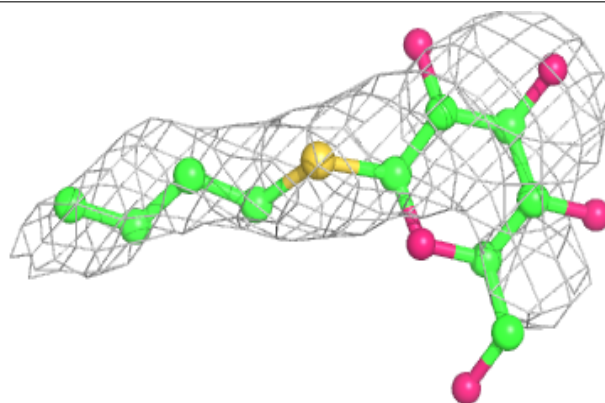


**Electron density around LMT D 403:**

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

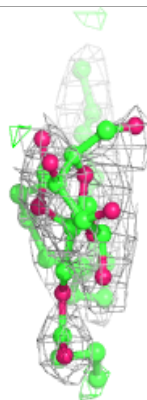
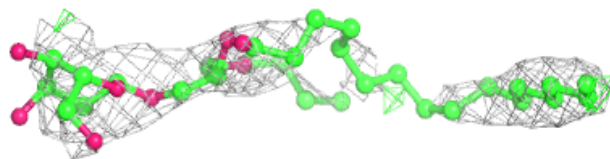
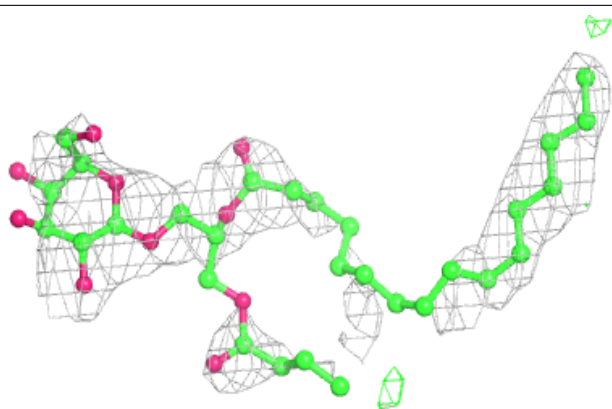
**Electron density around HTG D 413:**

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

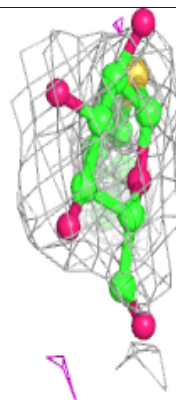
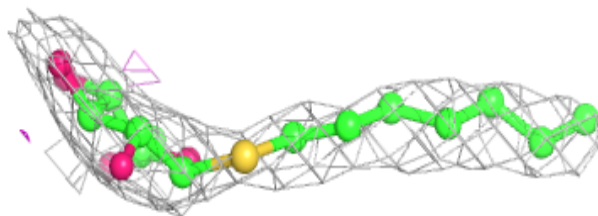
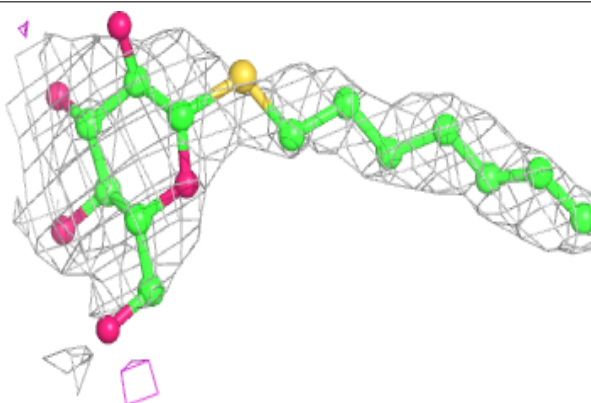


**Electron density around LMG z 101:**

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

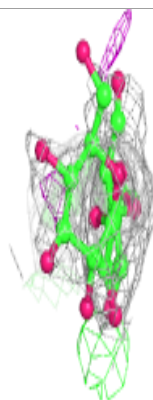
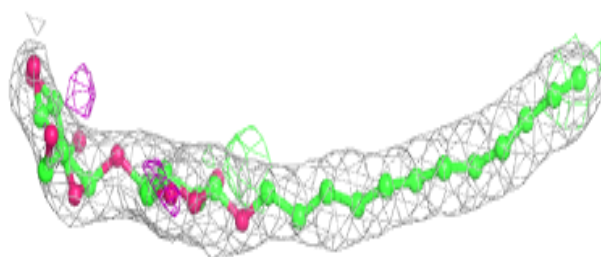
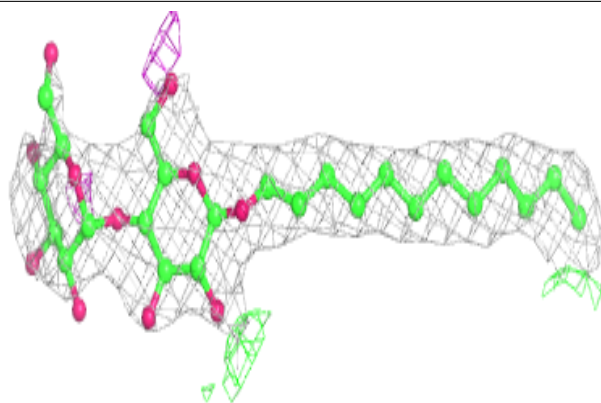
**Electron density around HTG B 625:**

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

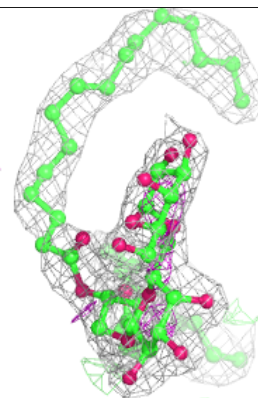
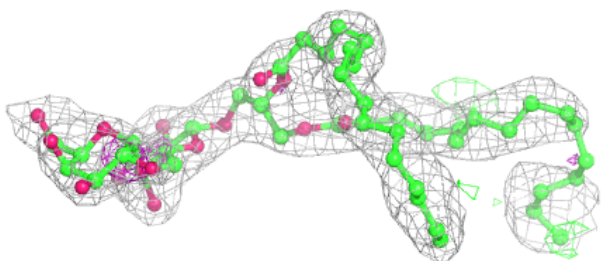
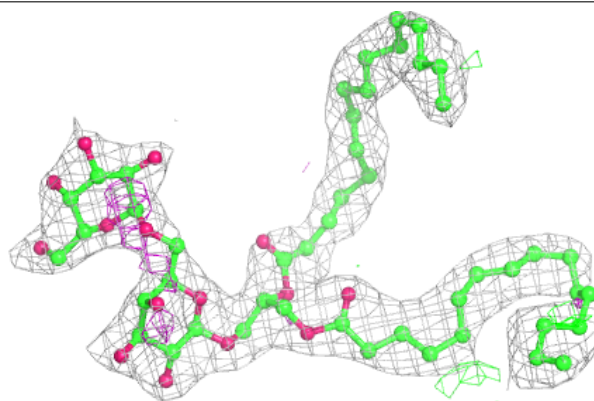


**Electron density around LMT M 101:**

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

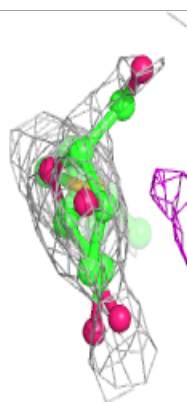
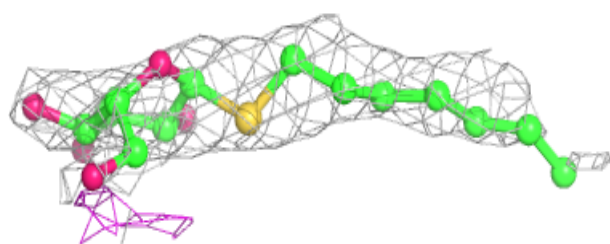
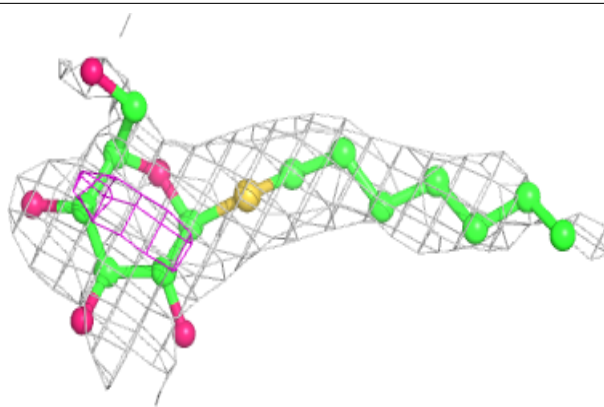
**Electron density around DGD C 517:**

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

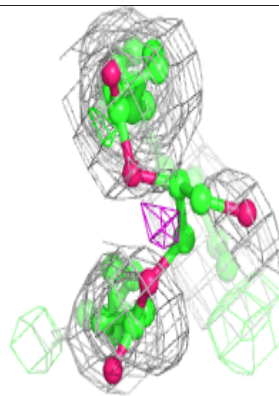
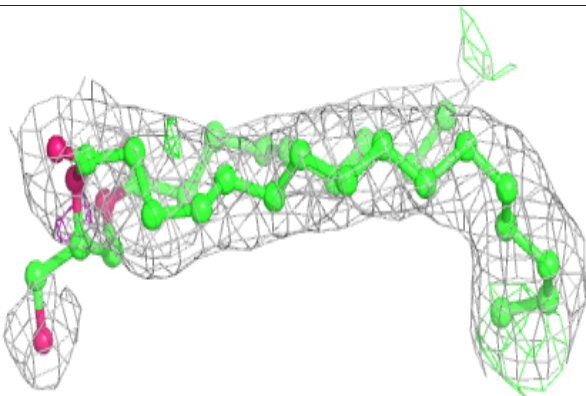
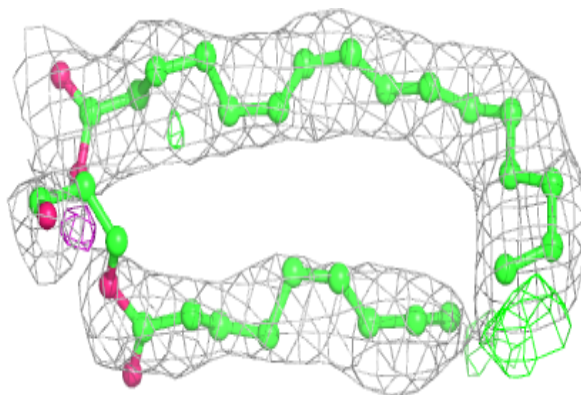


**Electron density around HTG C 522:**

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

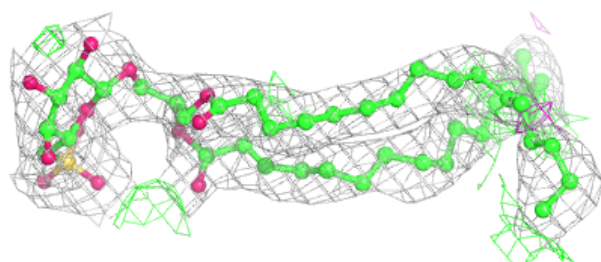
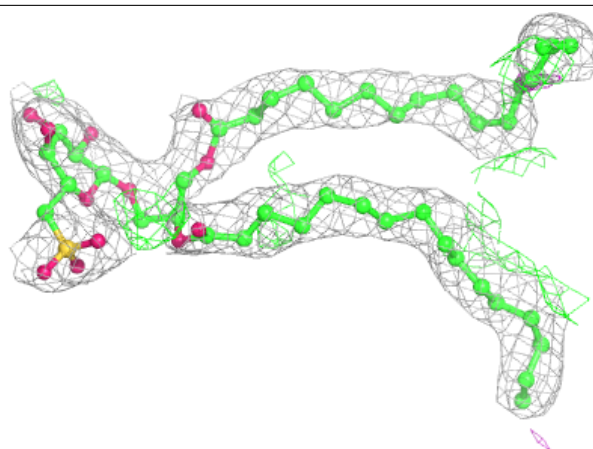
**Electron density around UNL B 634:**

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

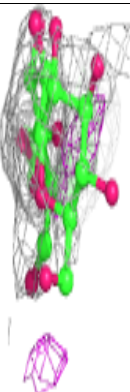
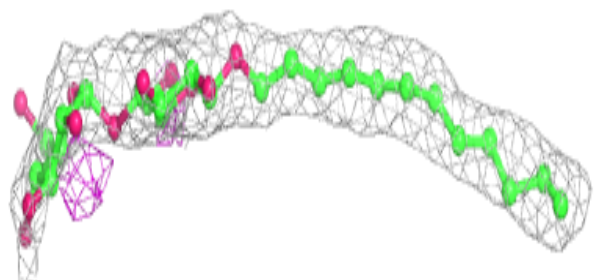
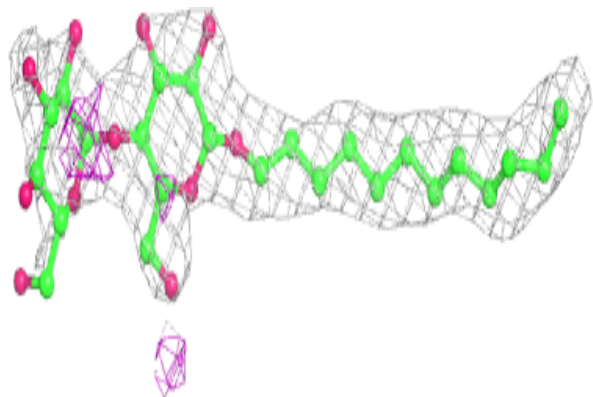


**Electron density around SQD L 102:**

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

**Electron density around LMT m 102:**

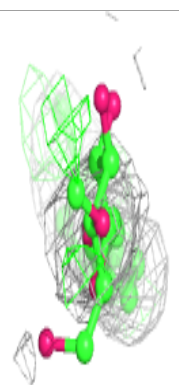
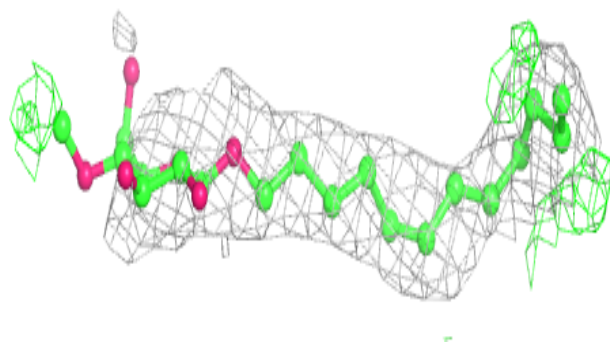
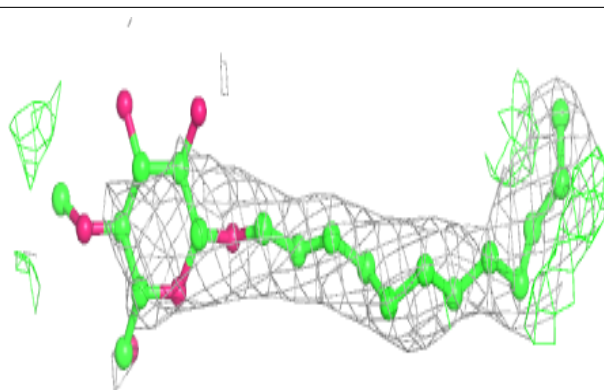
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



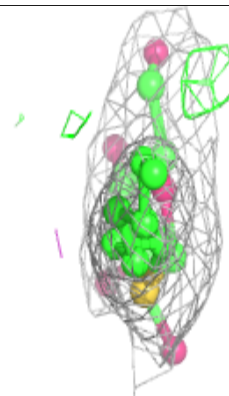
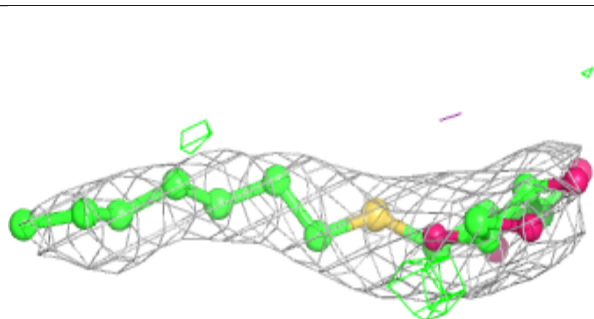
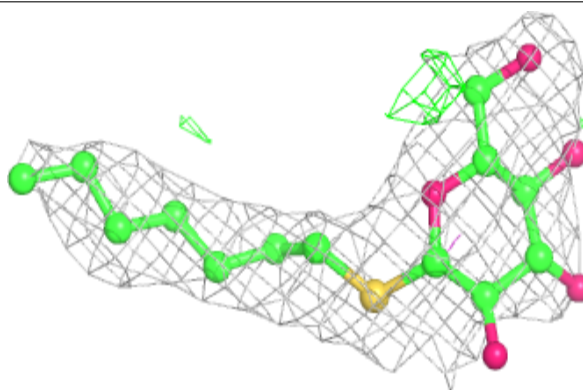


**Electron density around LMT t 101:**

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

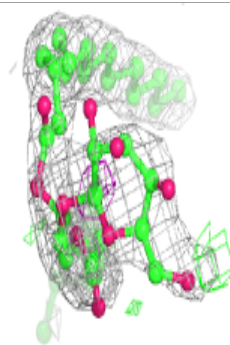
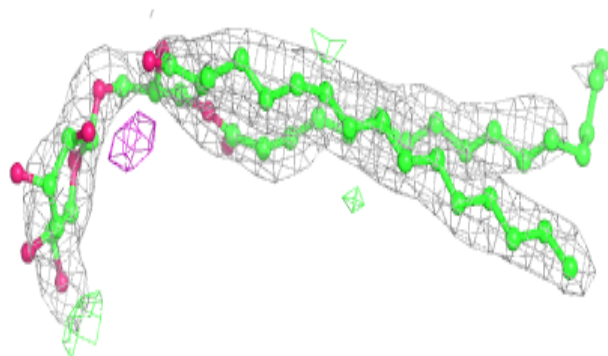
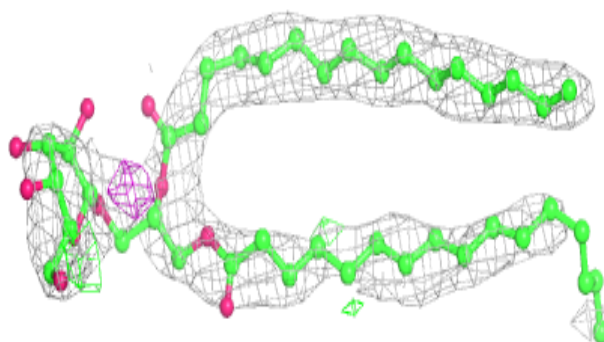
**Electron density around HTG b 628:**

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

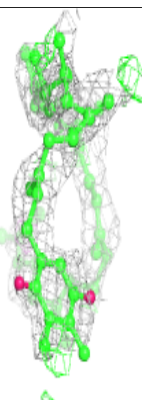
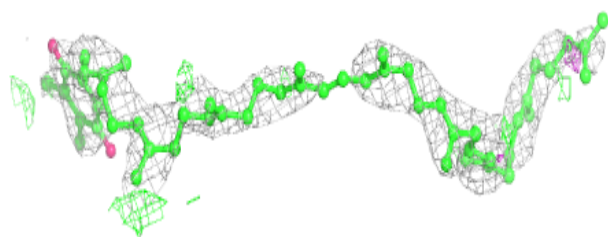
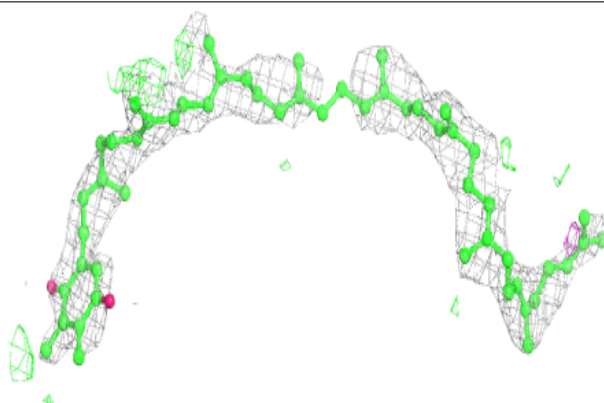


**Electron density around LMG C 519:**

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

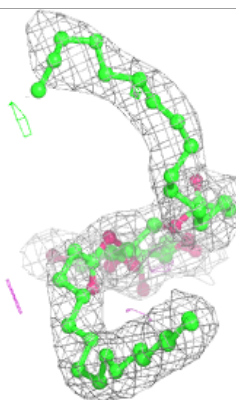
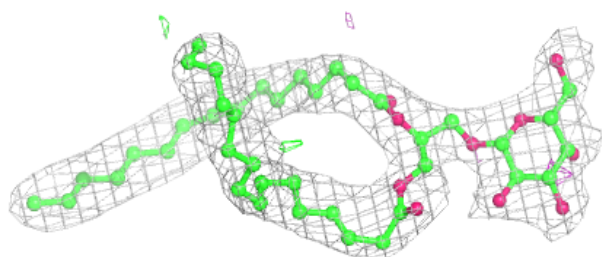
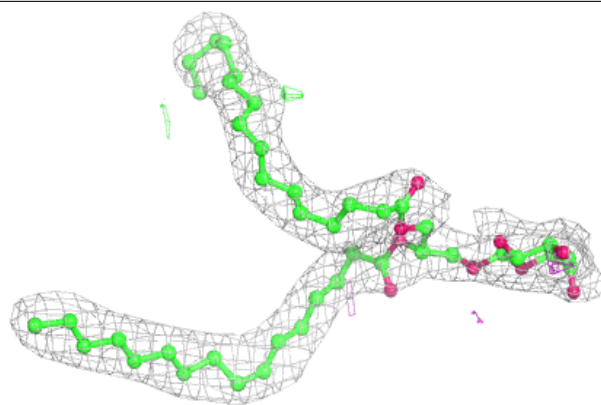
**Electron density around PL9 A 417:**

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

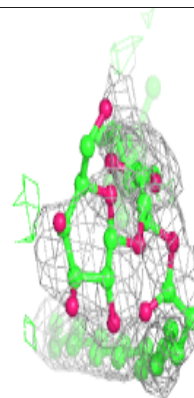
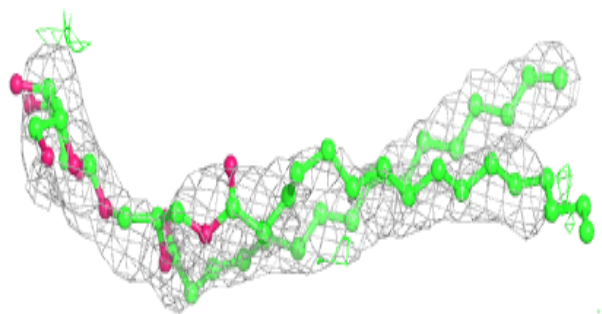
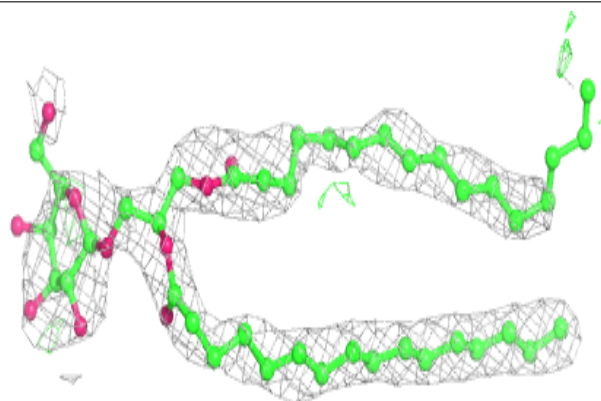


**Electron density around LMG b 625:**

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

**Electron density around LMG c 920:**

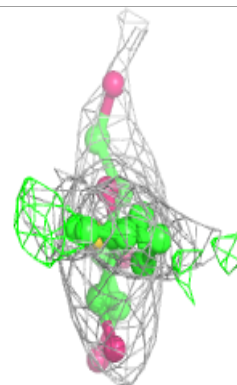
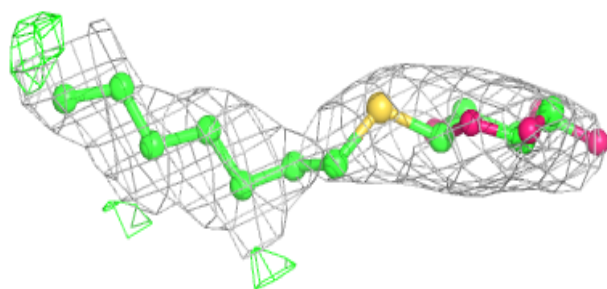
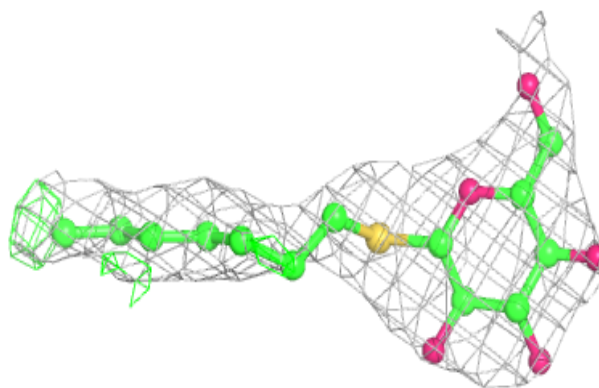
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



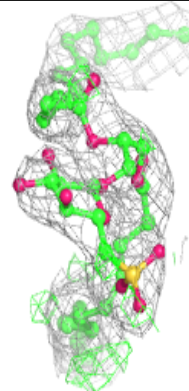
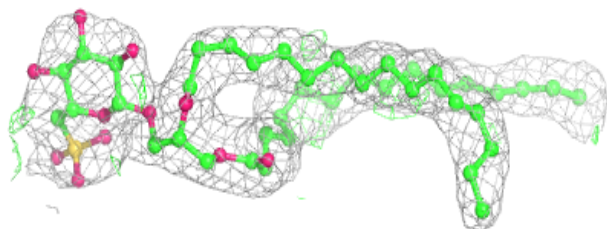
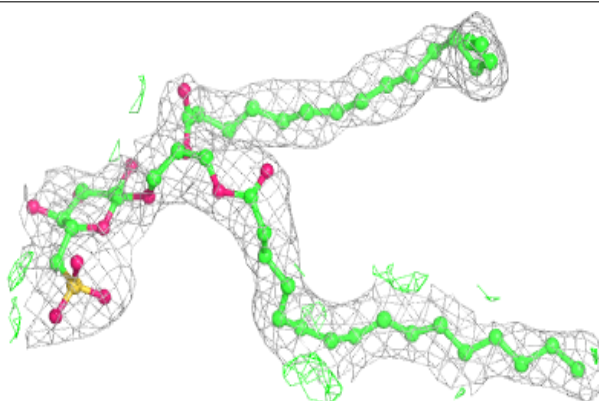


**Electron density around HTG c 921:**

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

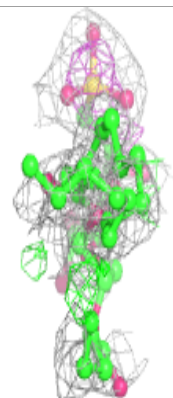
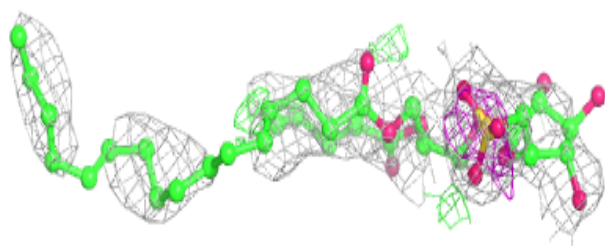
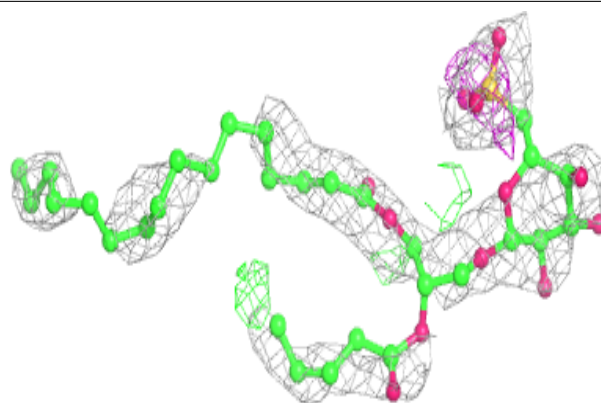
**Electron density around SQD a 402:**

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

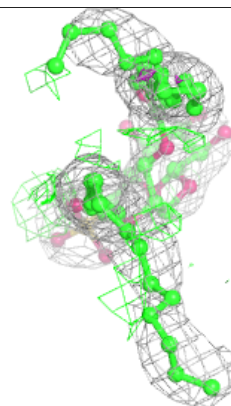
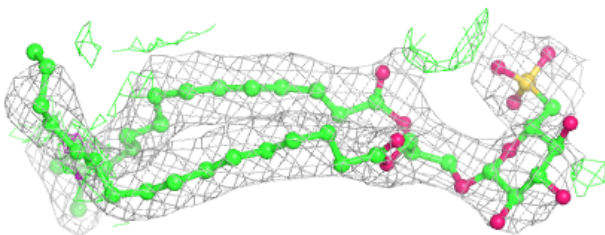
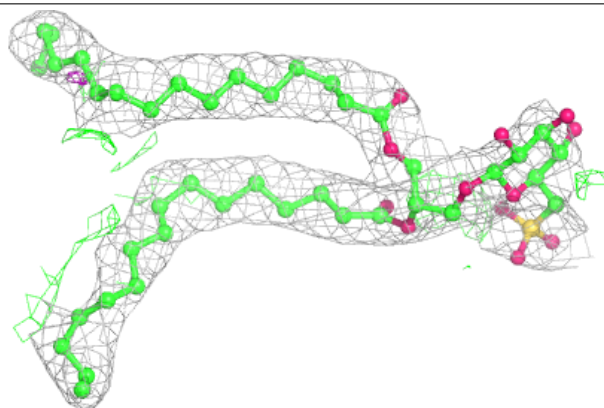


**Electron density around SQD F 103:**

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

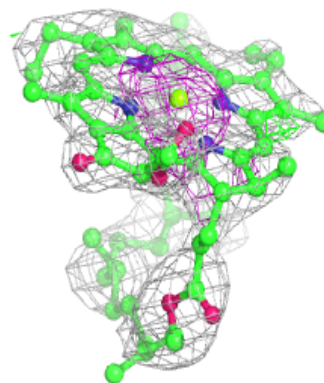
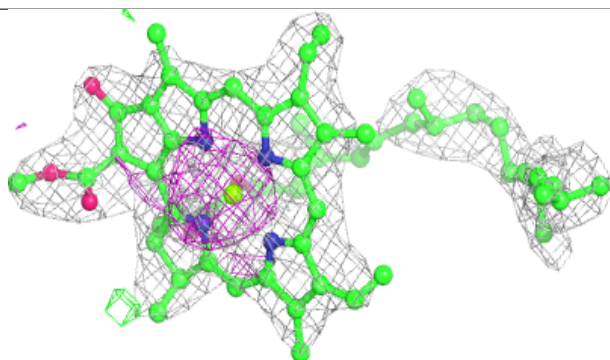
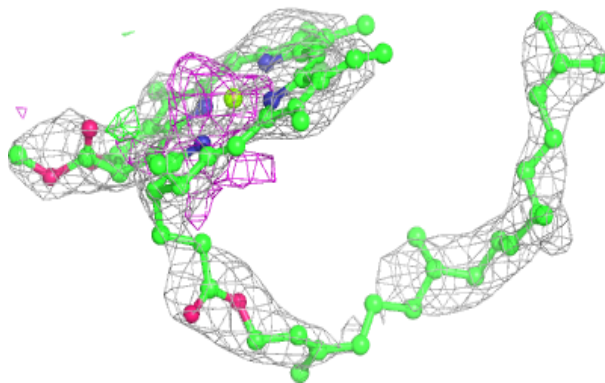
**Electron density around SQD B 621:**

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

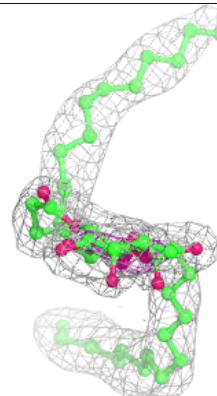
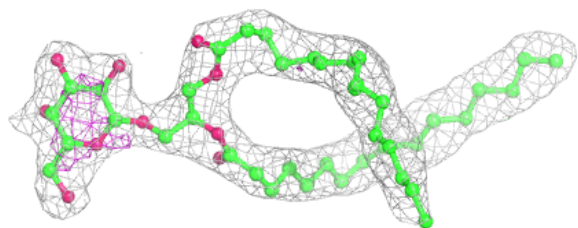
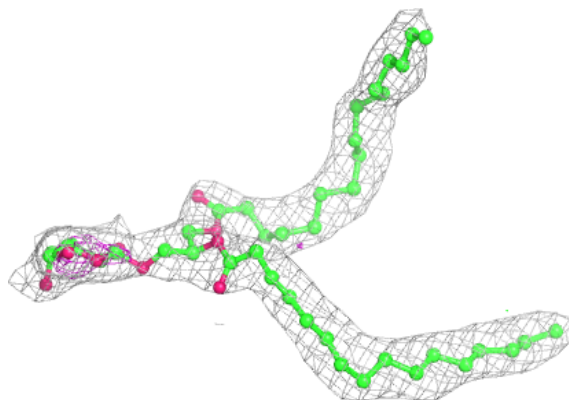


**Electron density around CLA C 513:**

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

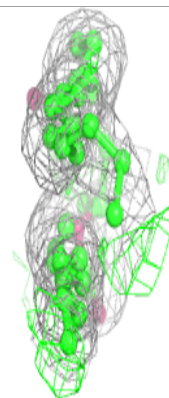
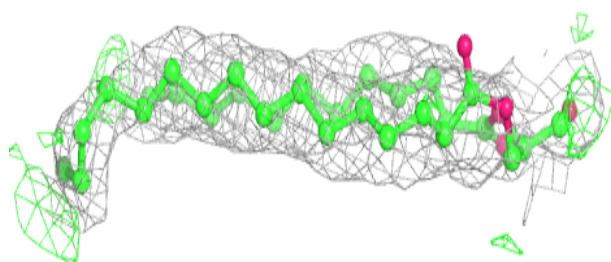
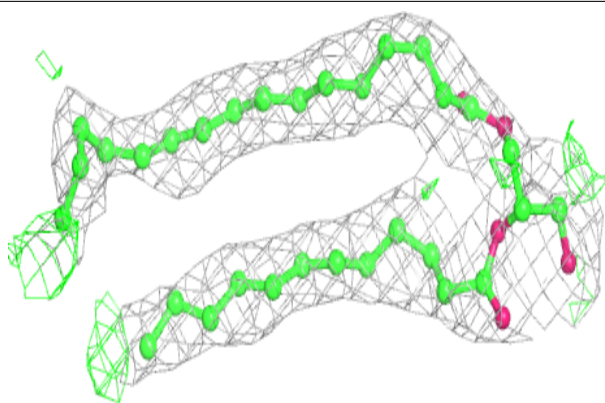
**Electron density around LMG B 622:**

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

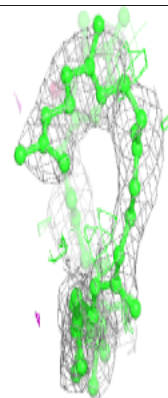
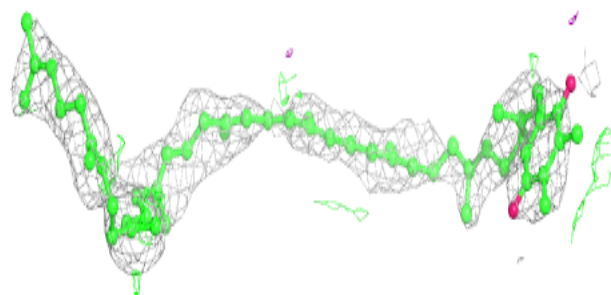
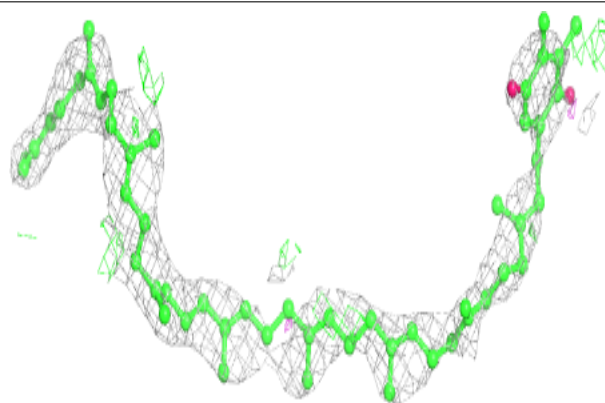


**Electron density around UNL d 413:**

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

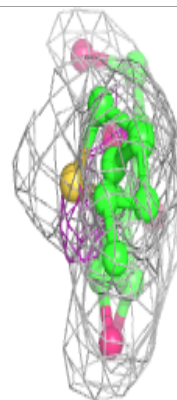
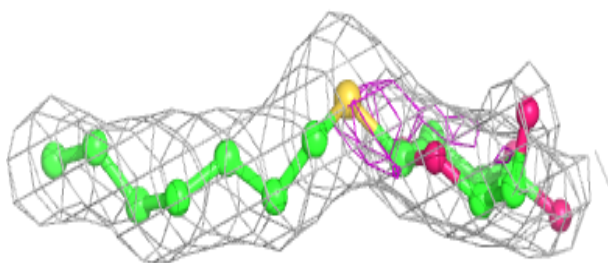
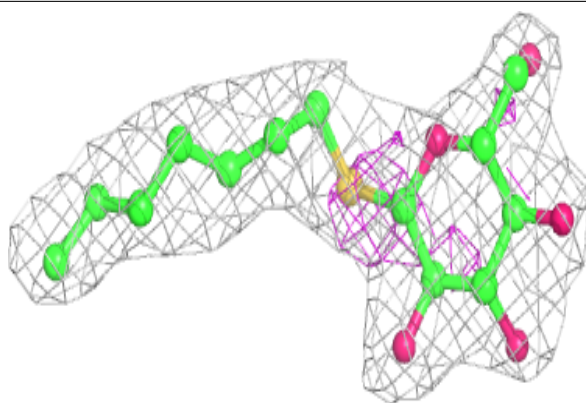
**Electron density around PL9 a 415:**

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

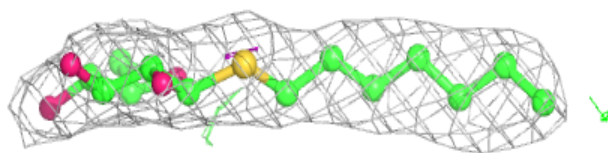
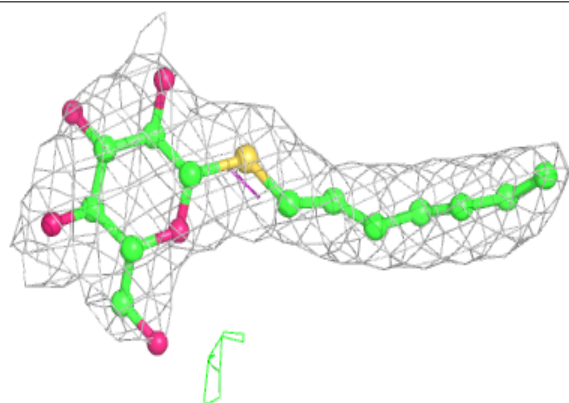


**Electron density around HTG b 601:**

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

**Electron density around HTG b 603:**

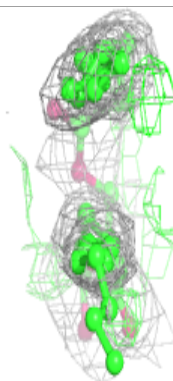
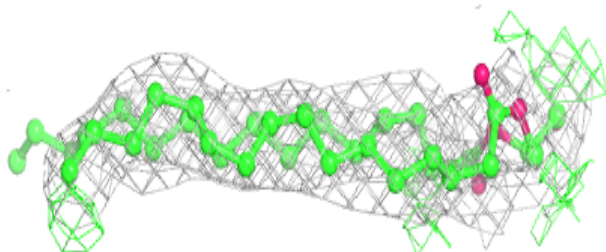
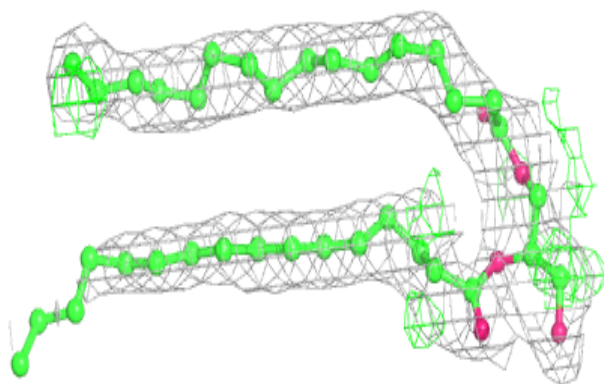
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



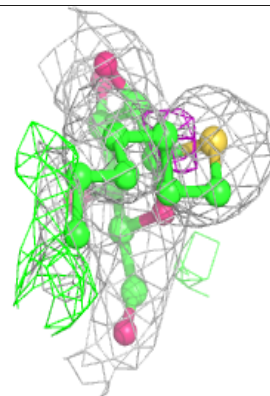
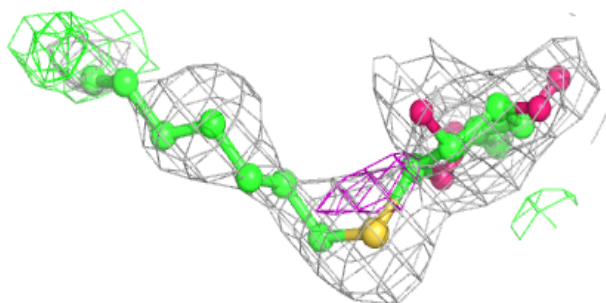
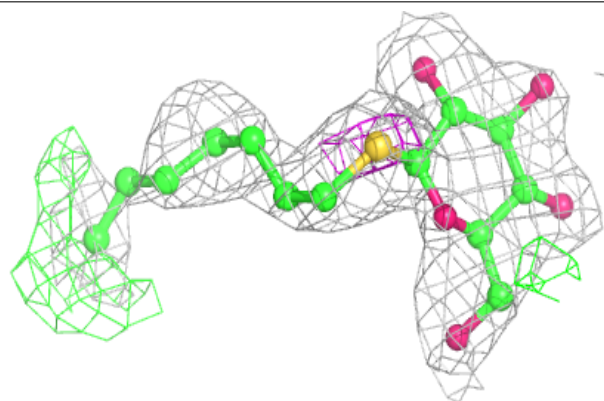


**Electron density around UNL D 412:**

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

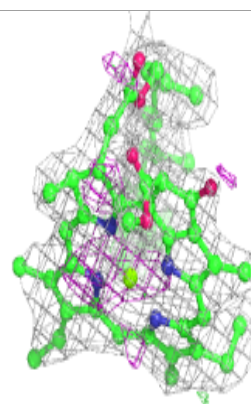
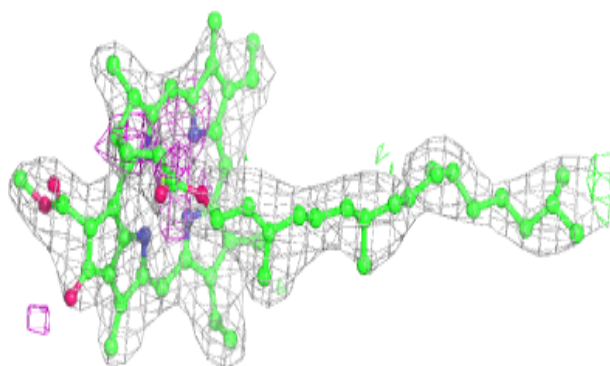
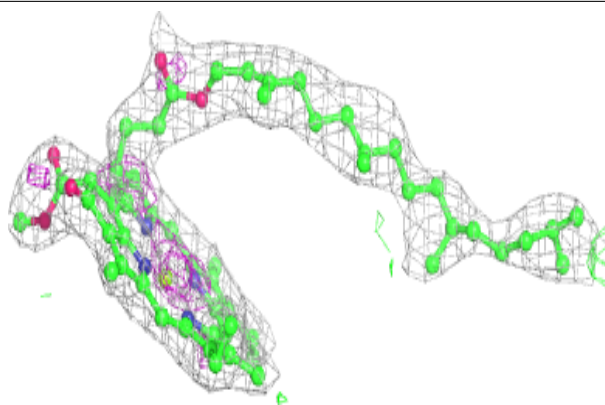
**Electron density around HTG b 627:**

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

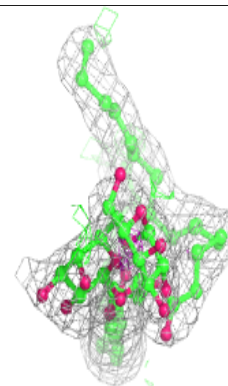
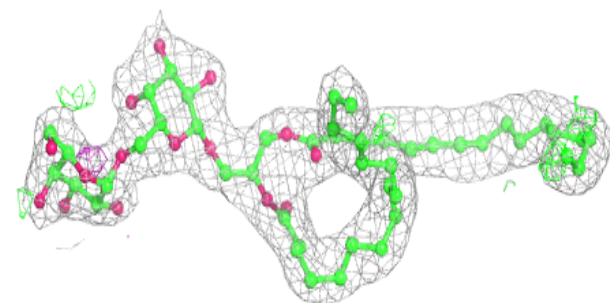
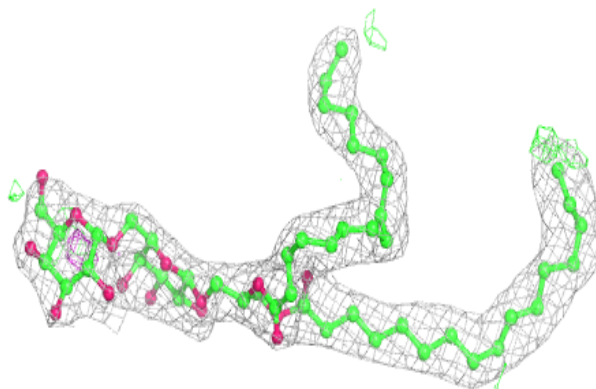


**Electron density around CLA C 504:**

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

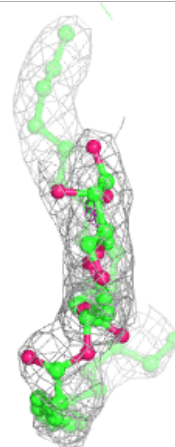
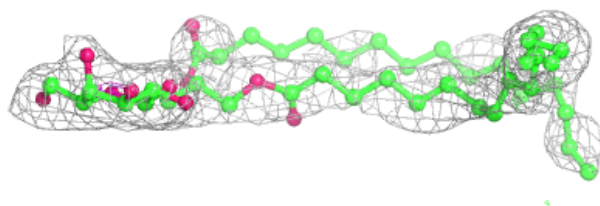
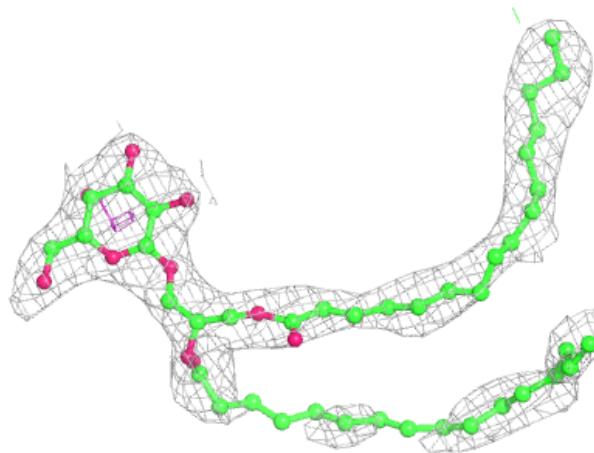
**Electron density around DGD h 102:**

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



**Electron density around LMG c 919:**

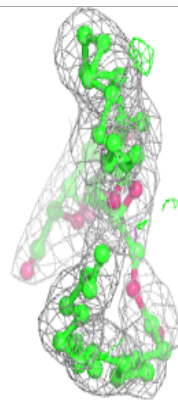
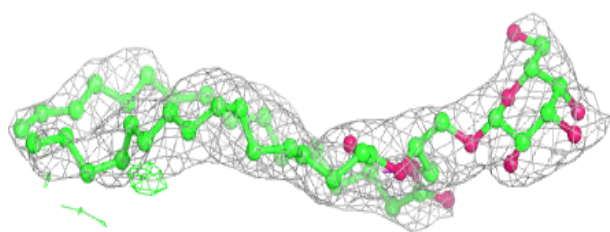
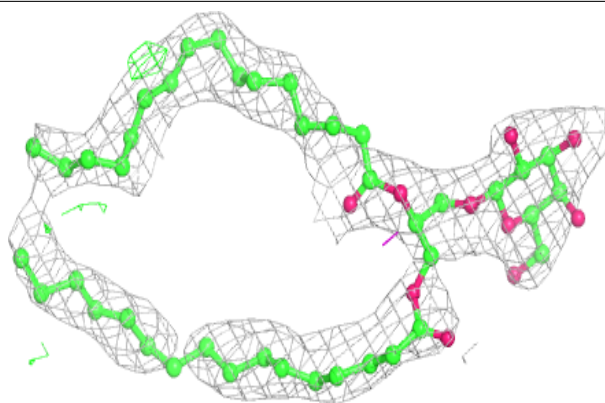
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



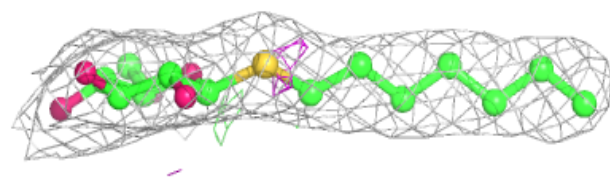
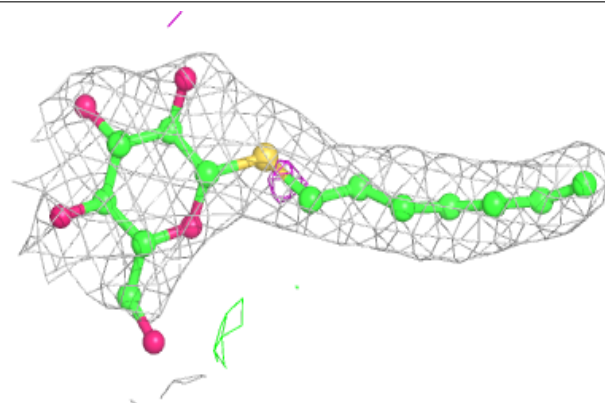


**Electron density around LMG A 419:**

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

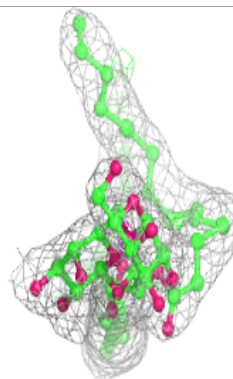
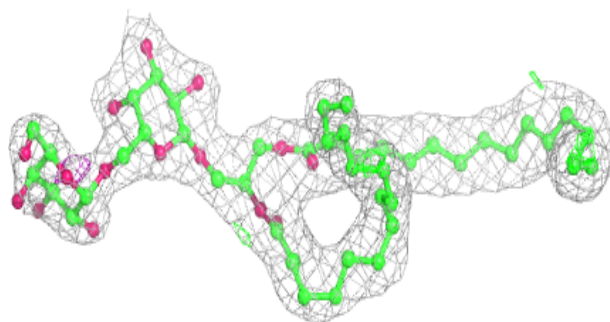
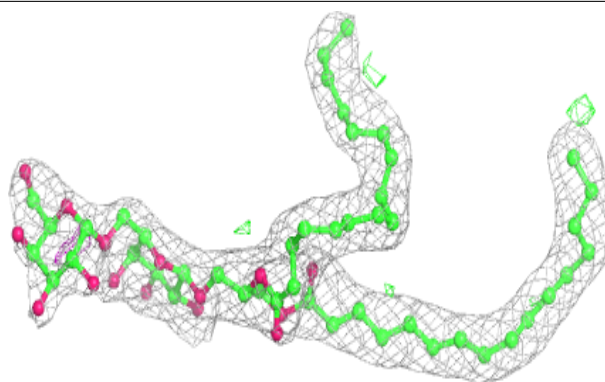
**Electron density around HTG B 632:**

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

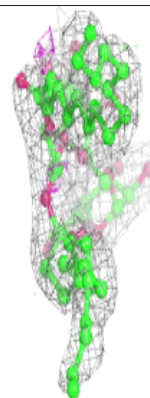
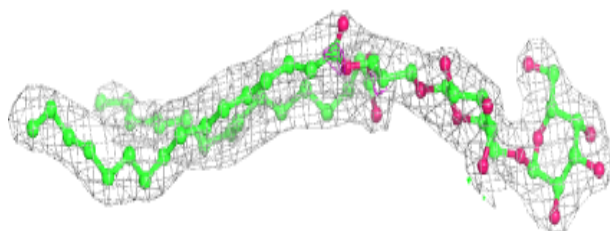
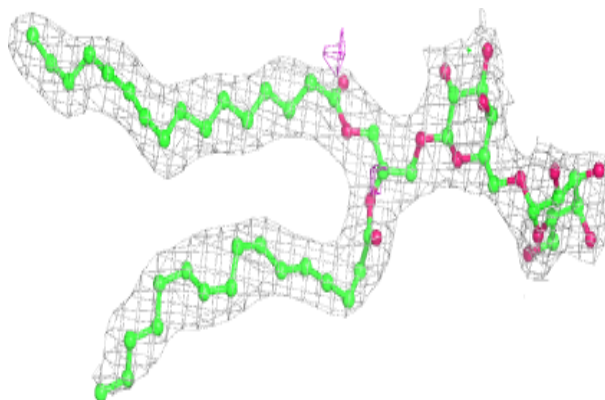


**Electron density around DGD H 102:**

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

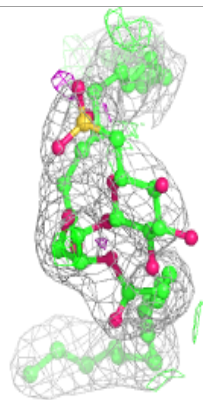
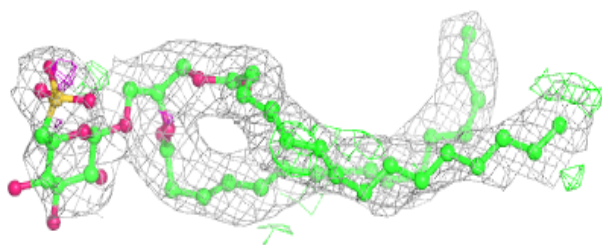
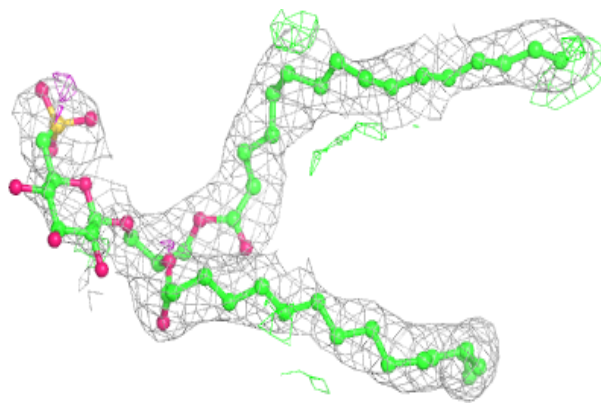
**Electron density around DGD C 518:**

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



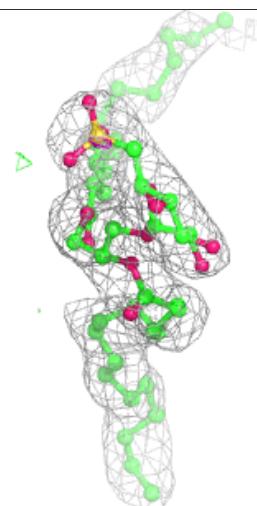
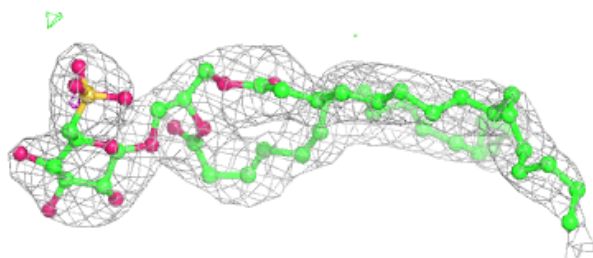
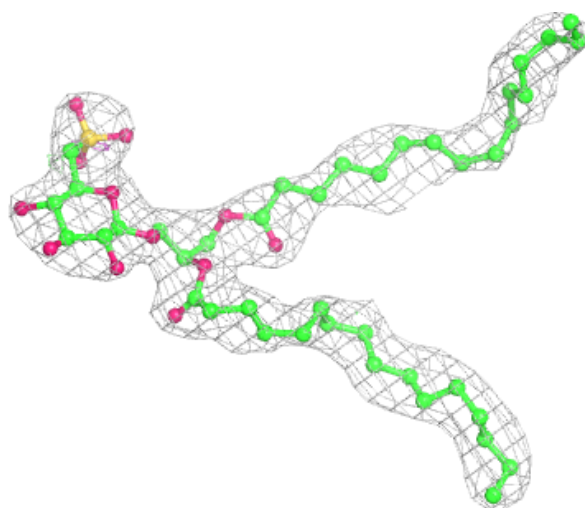
**Electron density around SQD A 414:**

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



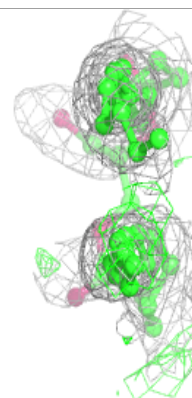
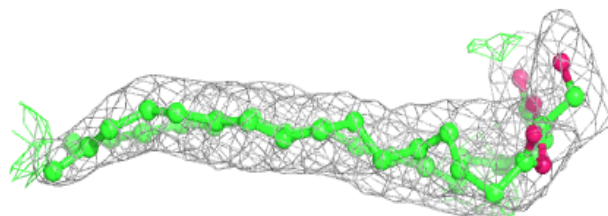
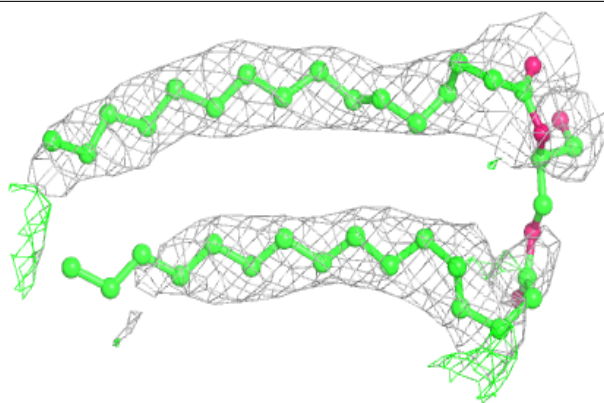
**Electron density around SQD a 410:**

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

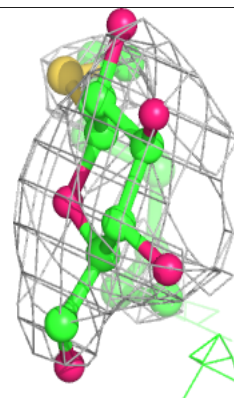
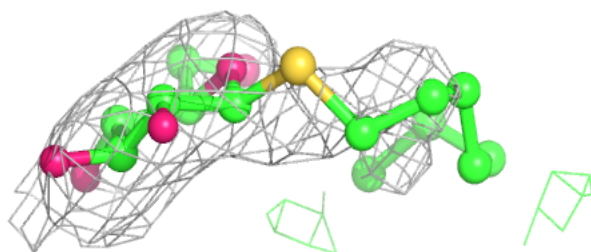
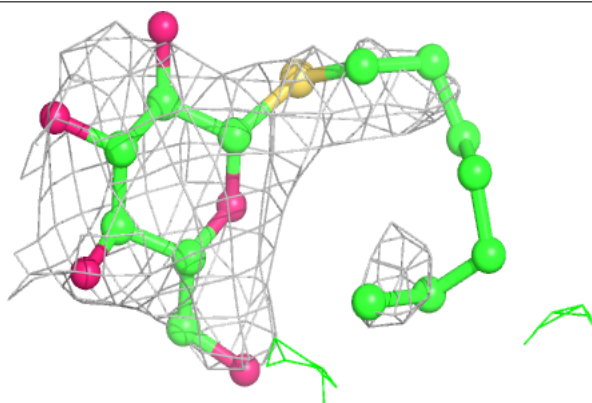


**Electron density around UNL i 101:**

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

**Electron density around HTG V 203:**

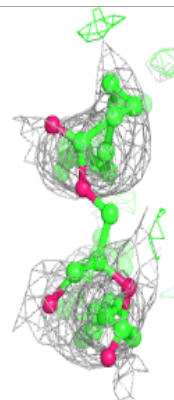
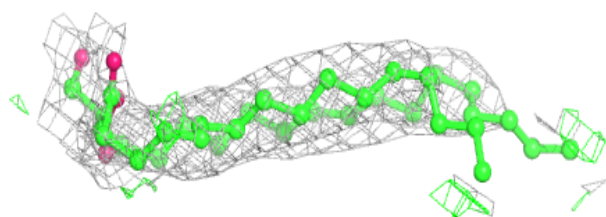
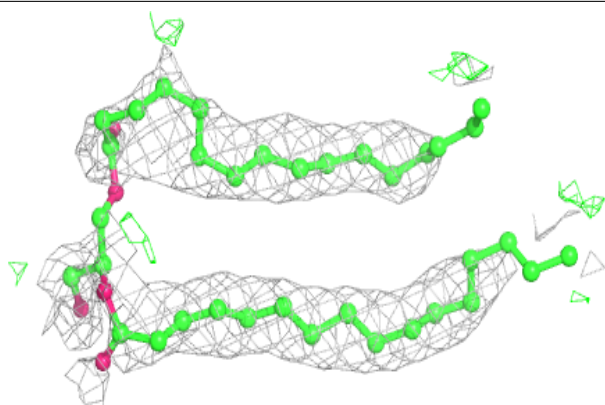
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



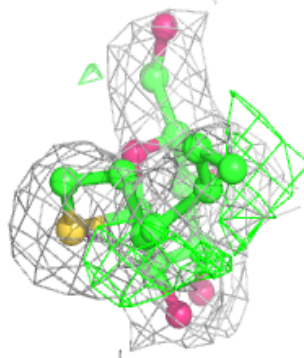
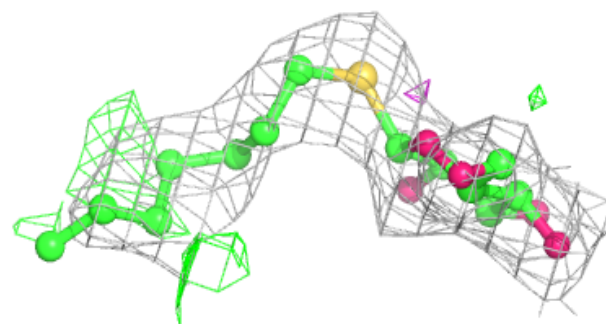
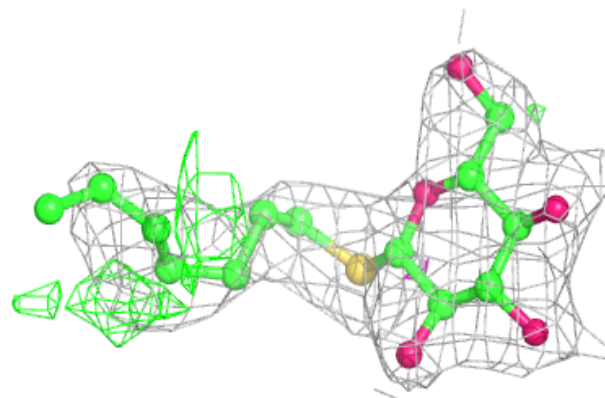


**Electron density around UNL I 101:**

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

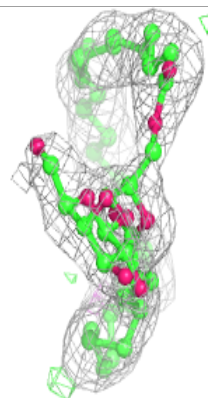
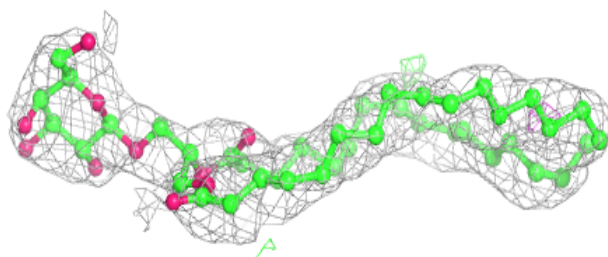
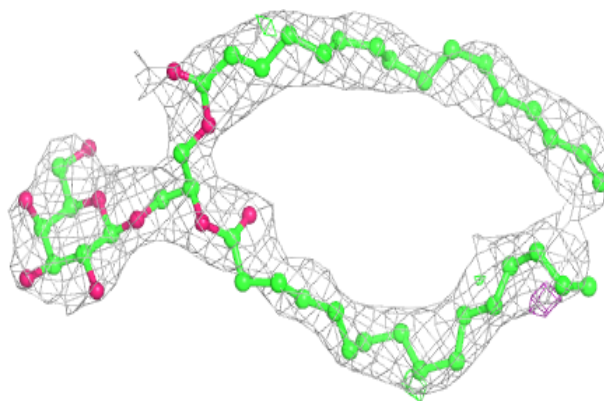
**Electron density around HTG B 624:**

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

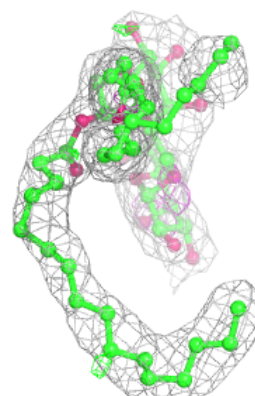
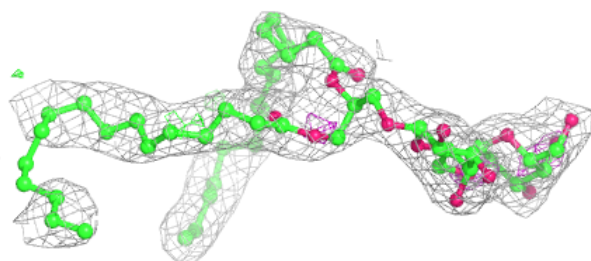
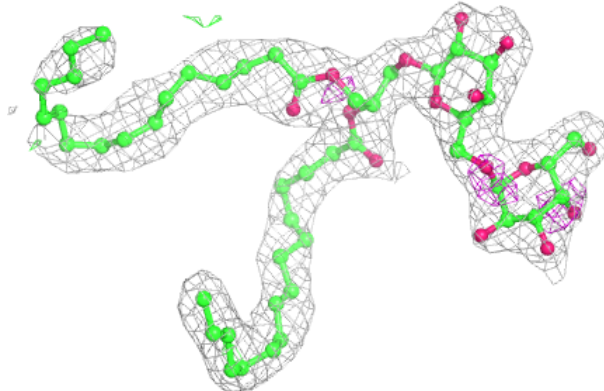


**Electron density around LMG a 411:**

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

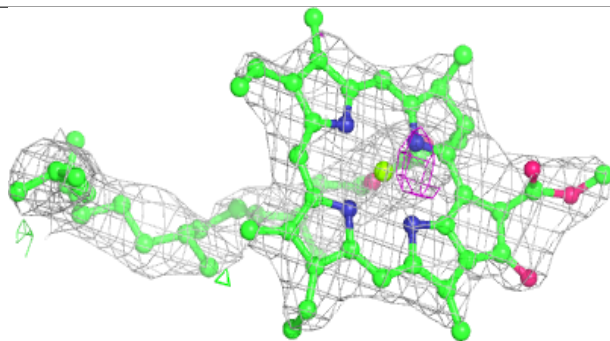
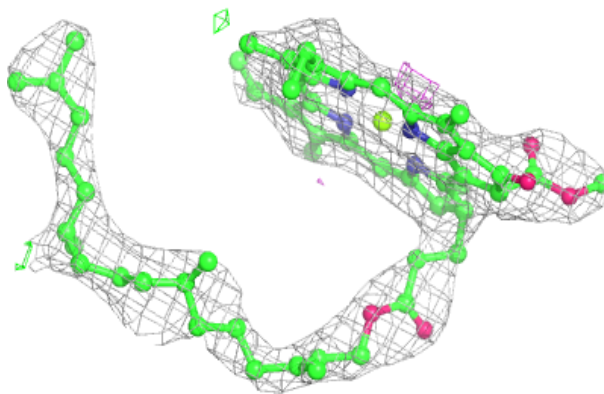
**Electron density around DGD c 917:**

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



**Electron density around CLA c 914:**

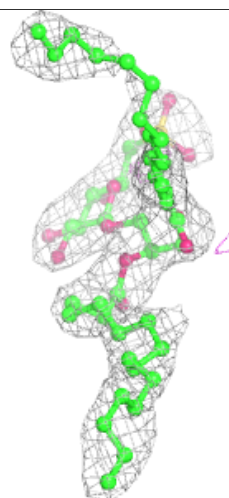
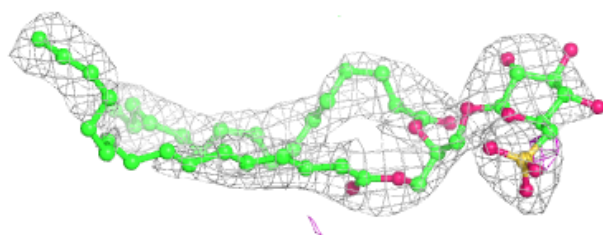
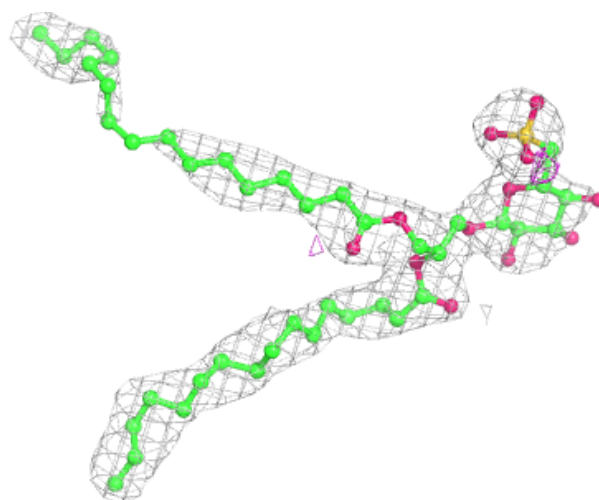
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





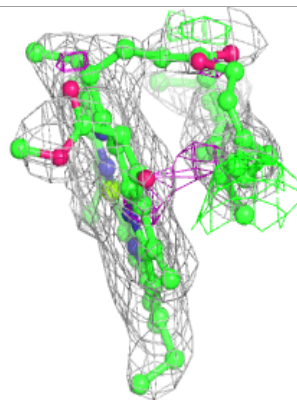
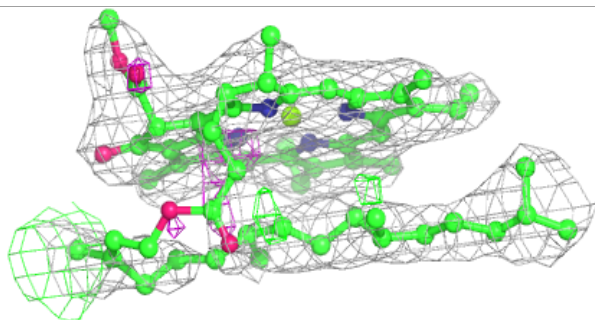
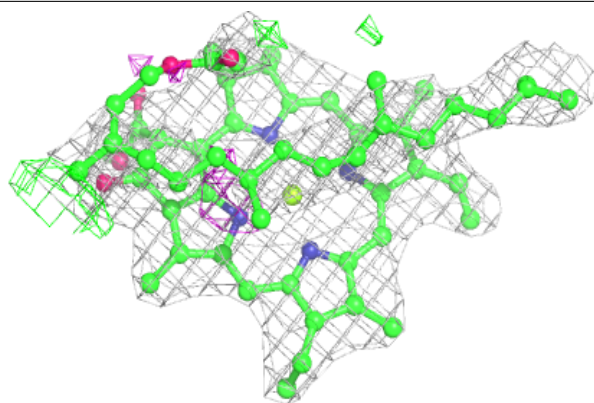
**Electron density around SQD A 411:**

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

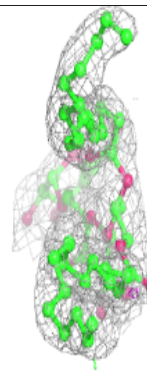
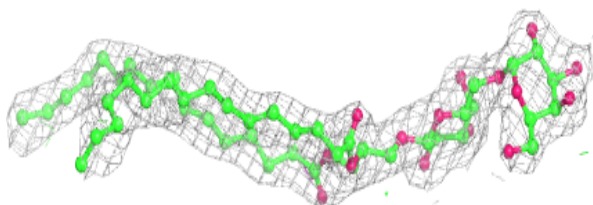
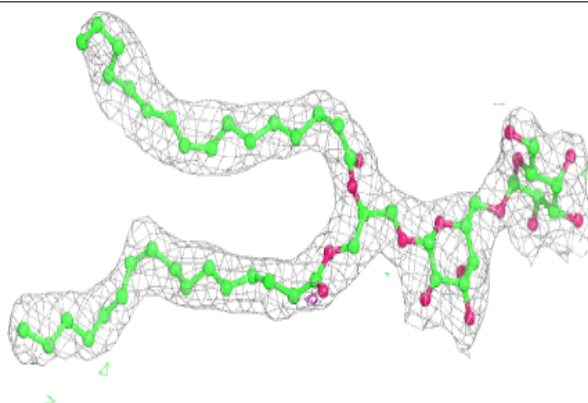


**Electron density around CLA B 602:**

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

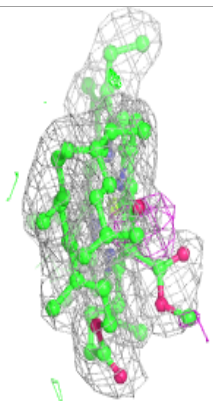
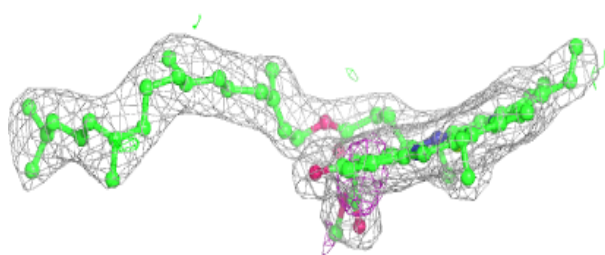
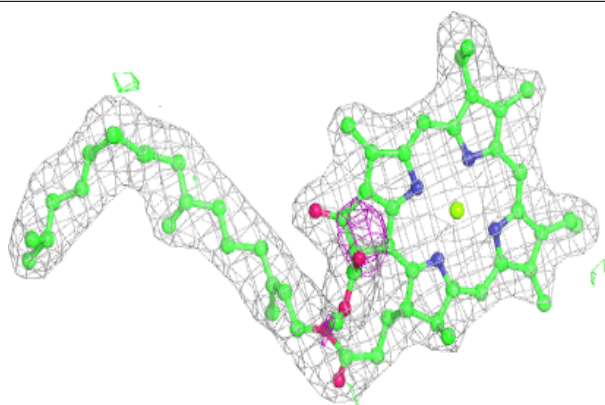
**Electron density around DGD c 918:**

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

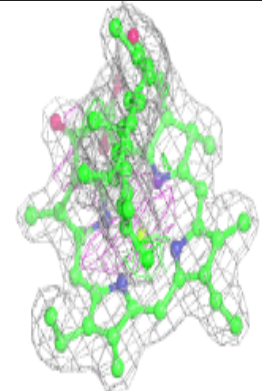
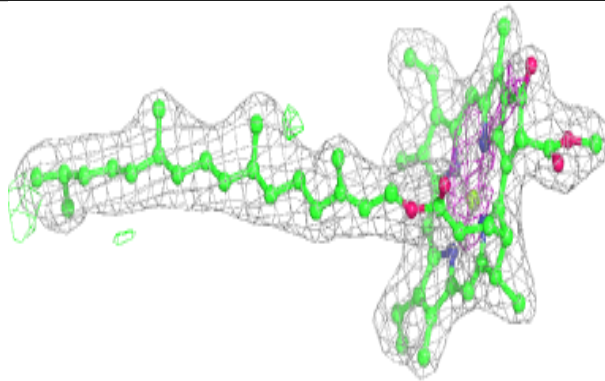
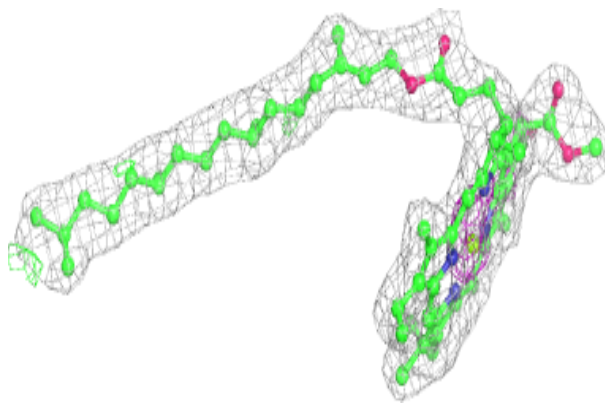


**Electron density around CLA b 607:**

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

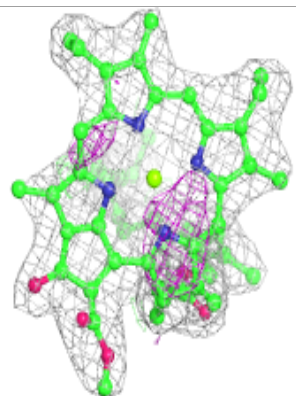
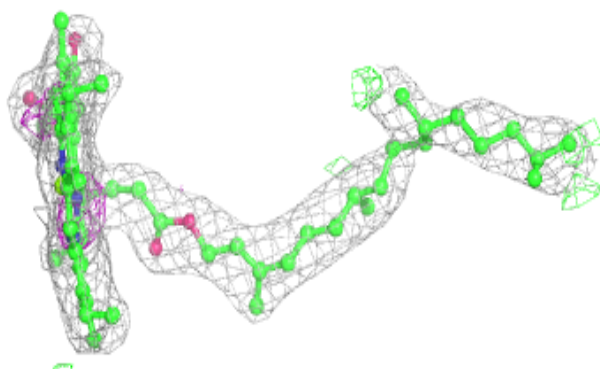
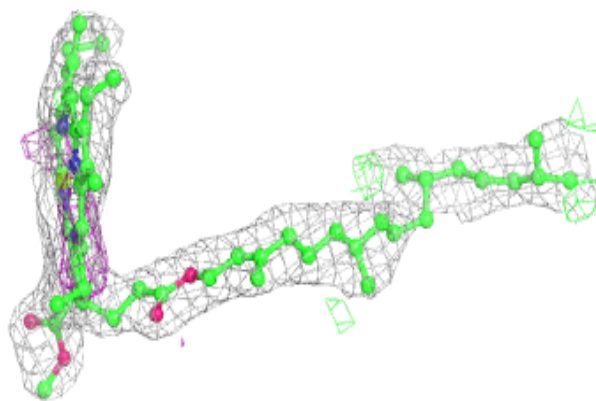
**Electron density around CLA b 612:**

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

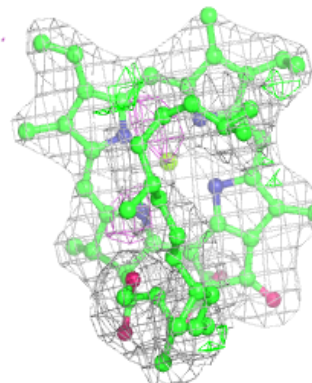
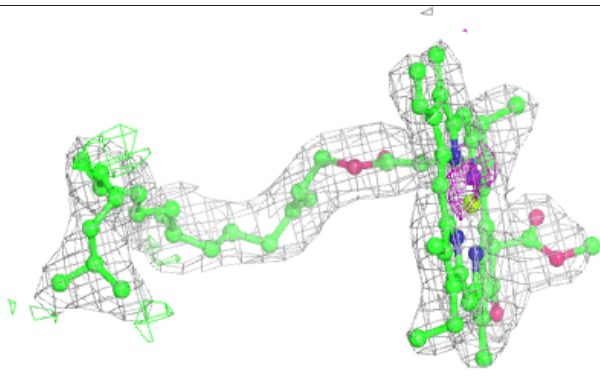
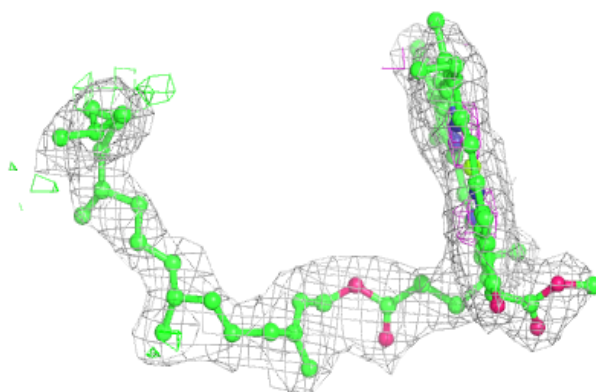


**Electron density around CLA B 607:**

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

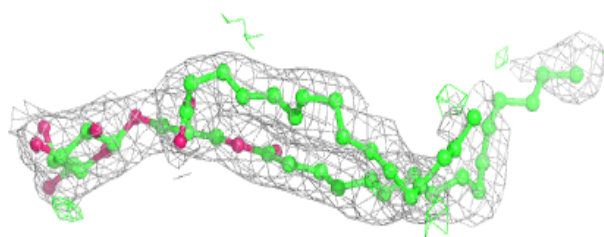
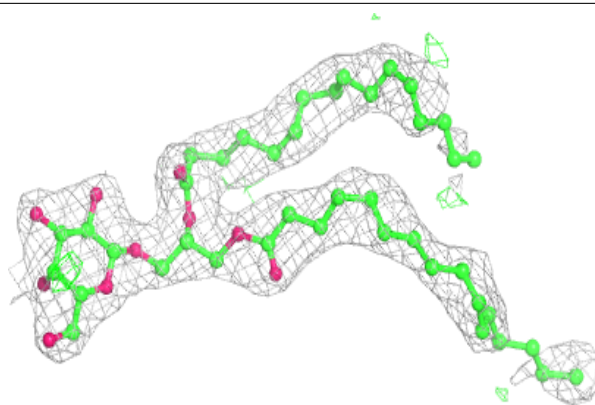
**Electron density around CLA c 907:**

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



**Electron density around LMG d 415:**

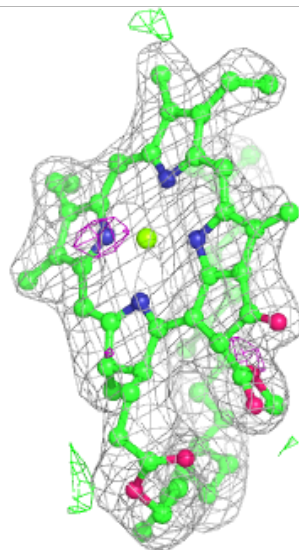
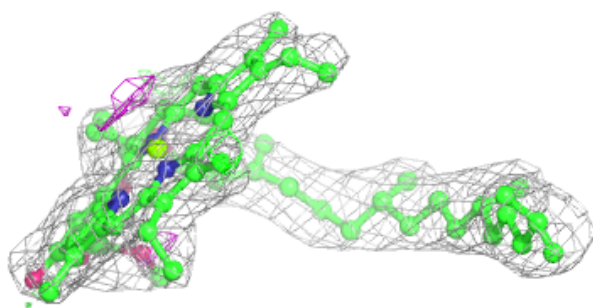
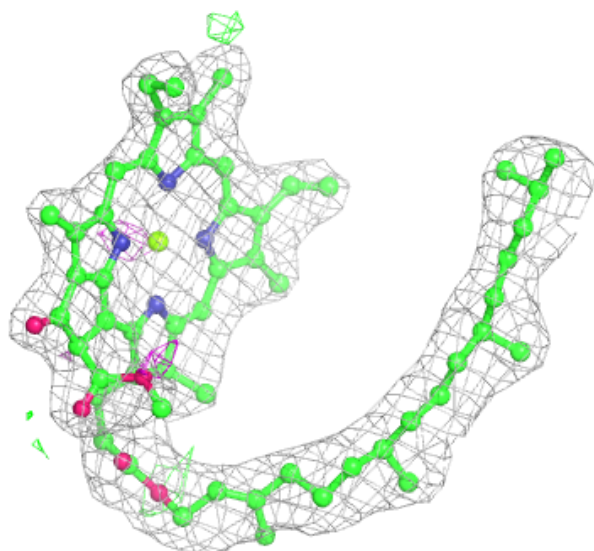
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





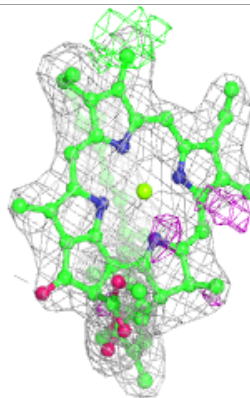
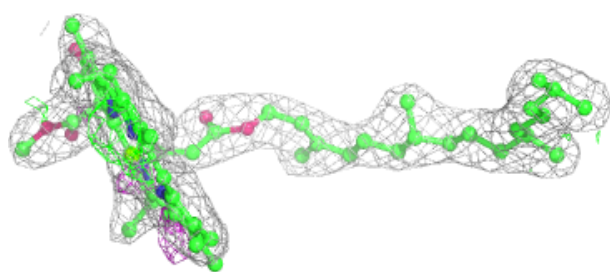
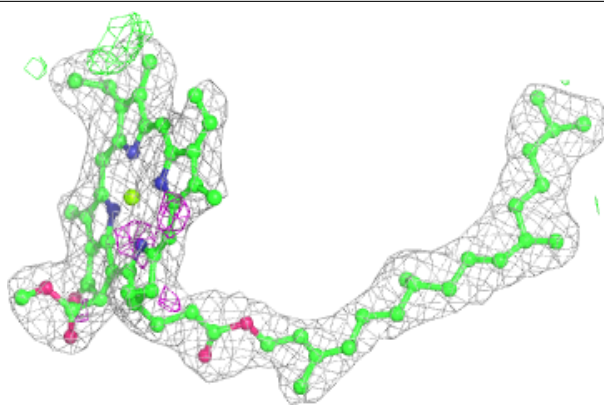
**Electron density around CLA c 908:**

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



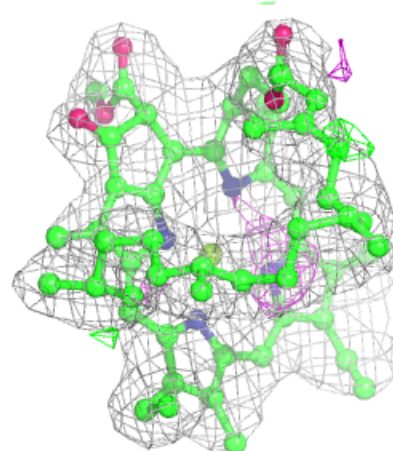
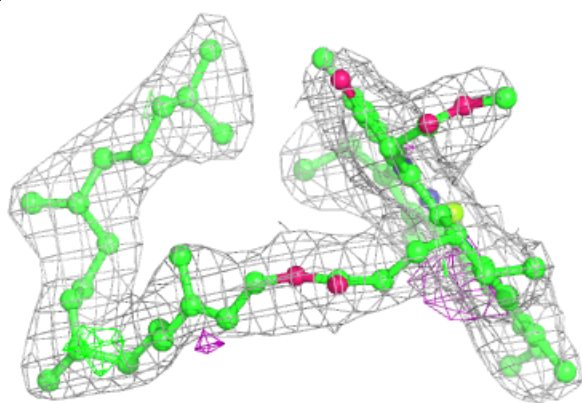
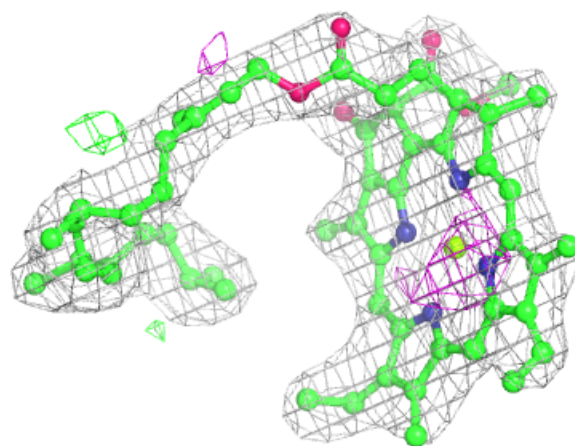
**Electron density around CLA b 614:**

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



**Electron density around CLA c 904:**

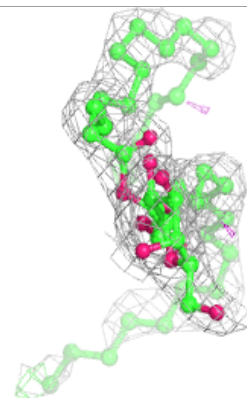
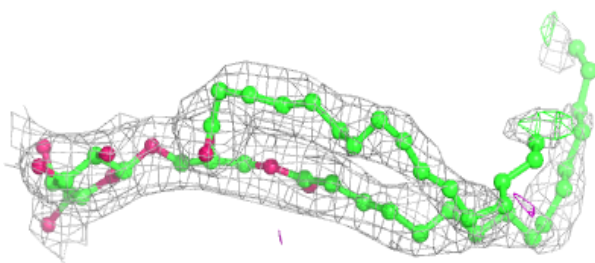
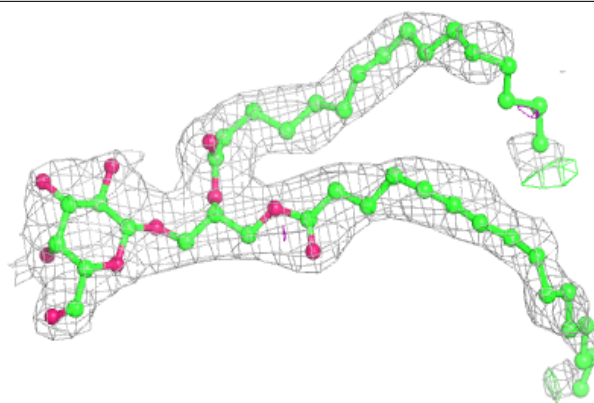
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



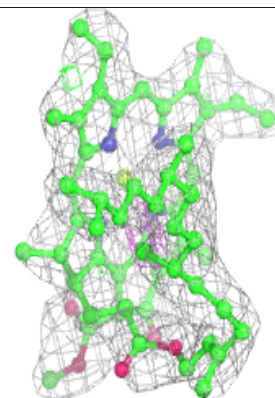
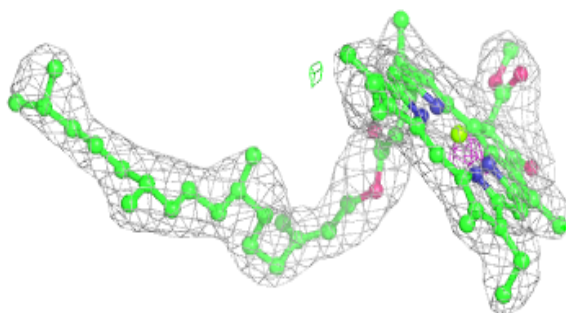
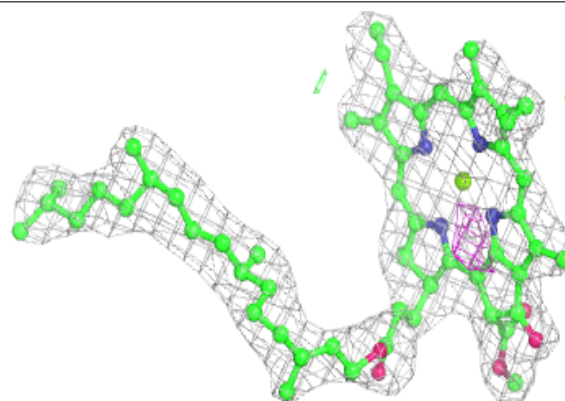


**Electron density around LMG J 101:**

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

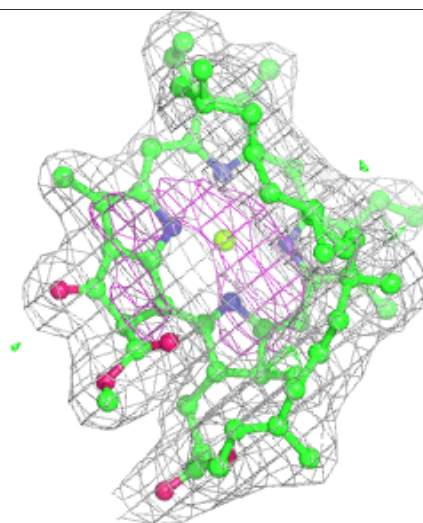
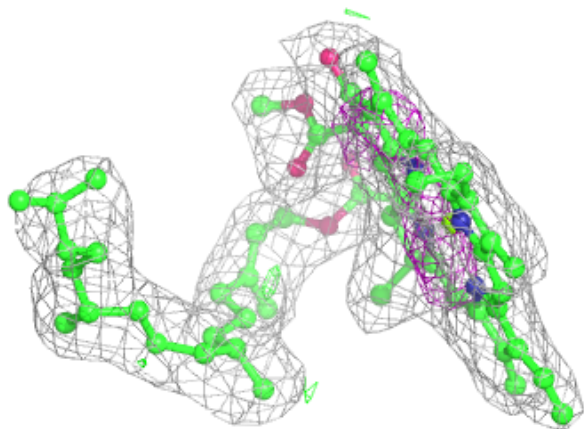
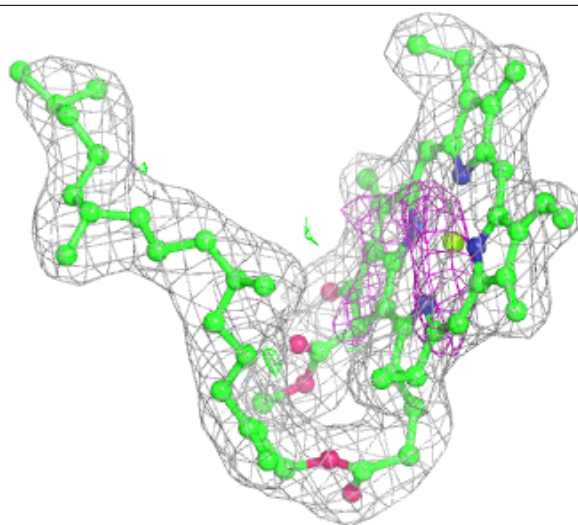
**Electron density around CLA C 511:**

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



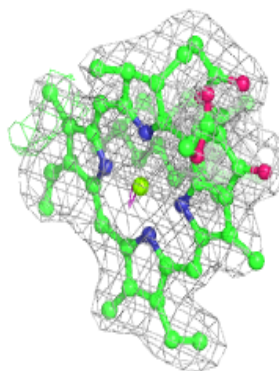
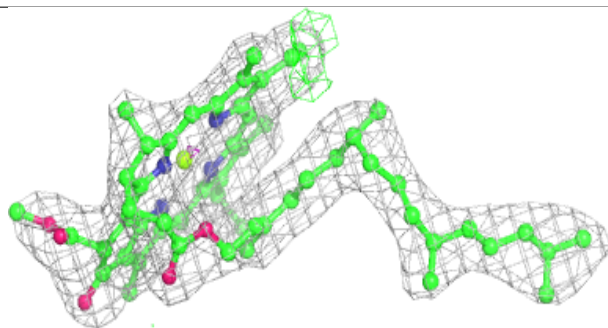
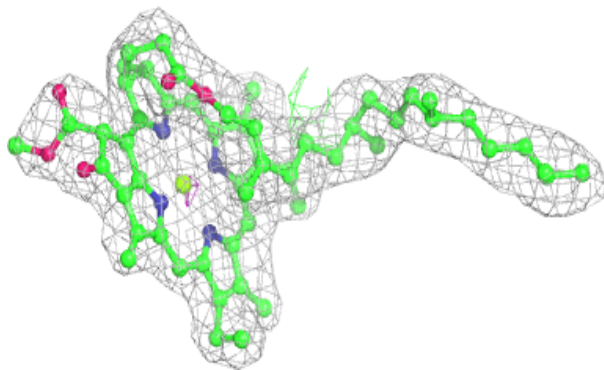
**Electron density around CLA B 614:**

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

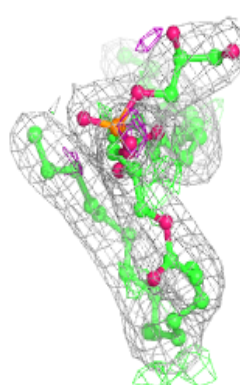
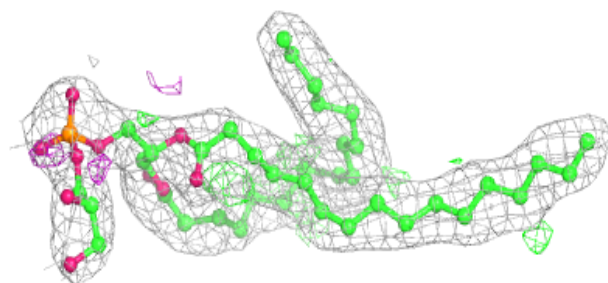
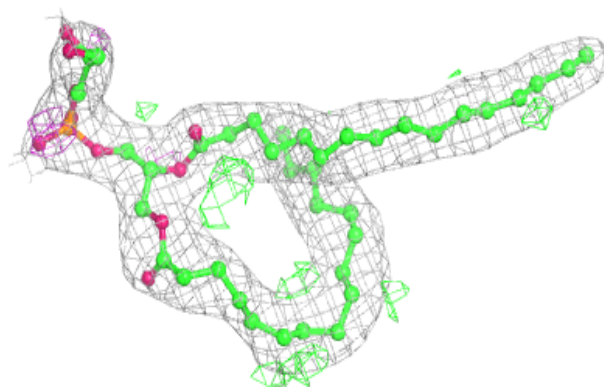


**Electron density around CLA c 906:**

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

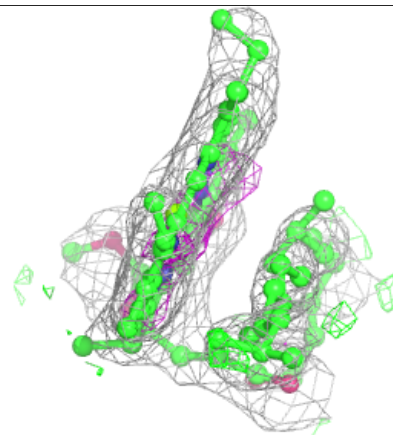
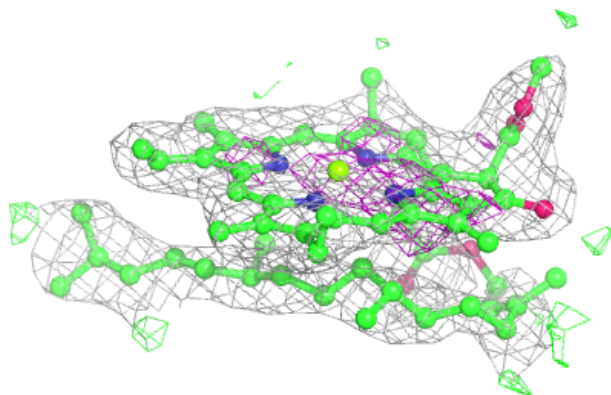
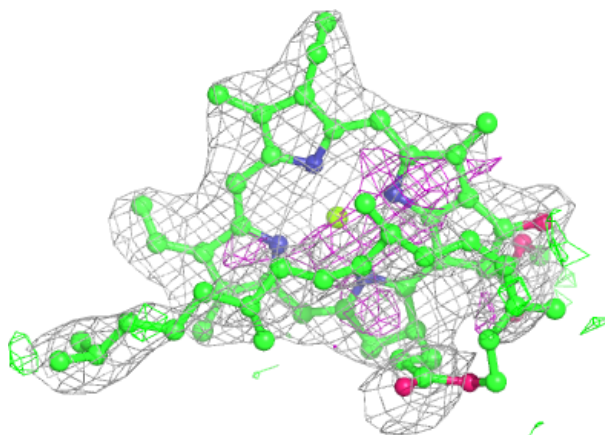
**Electron density around LHG B 635:**

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



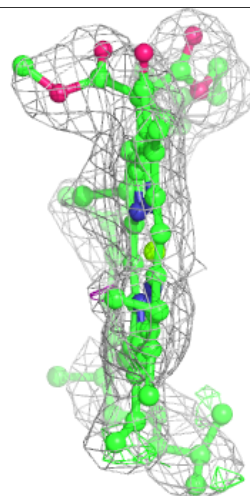
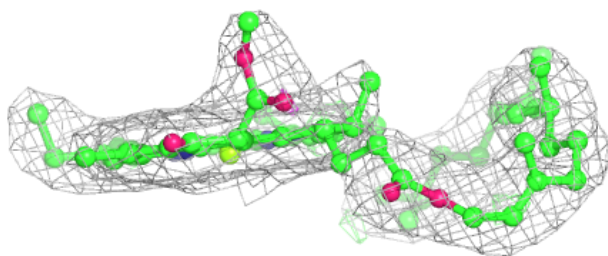
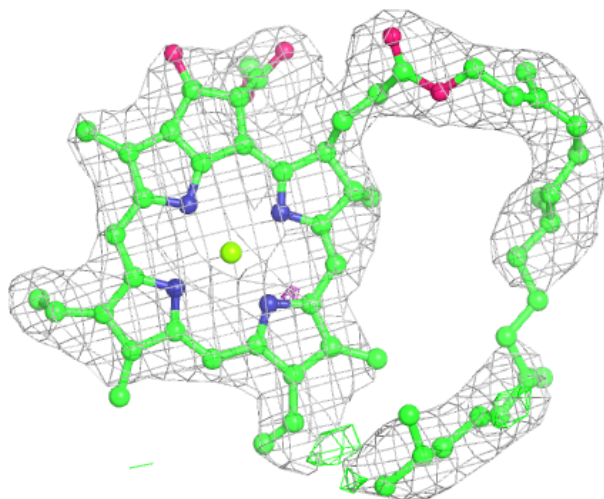
**Electron density around CLA b 606:**

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



**Electron density around CLA C 512:**

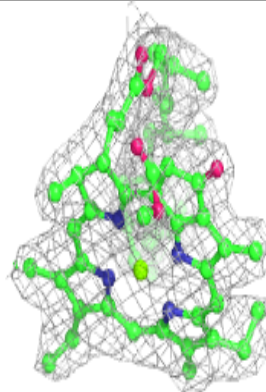
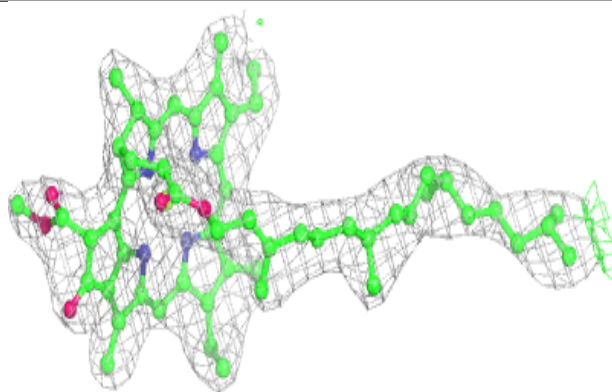
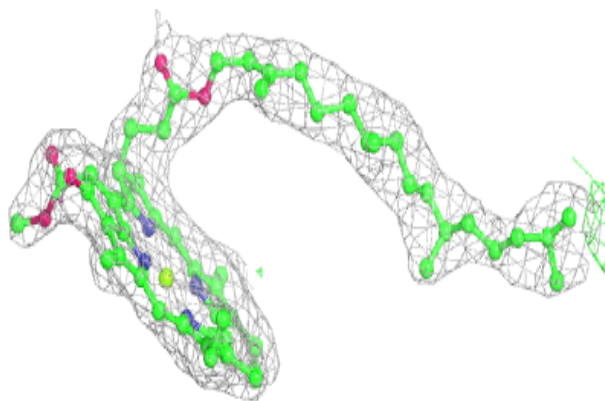
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





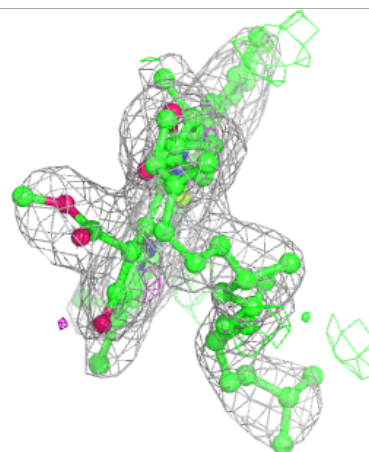
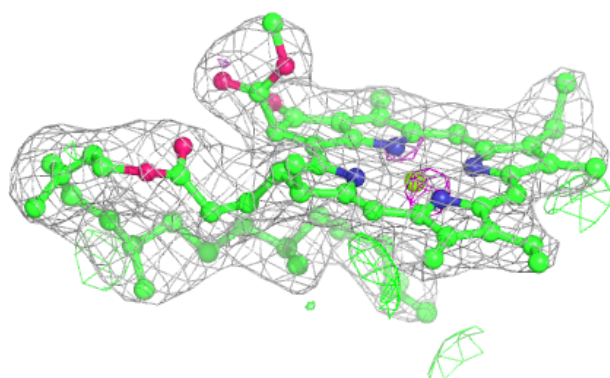
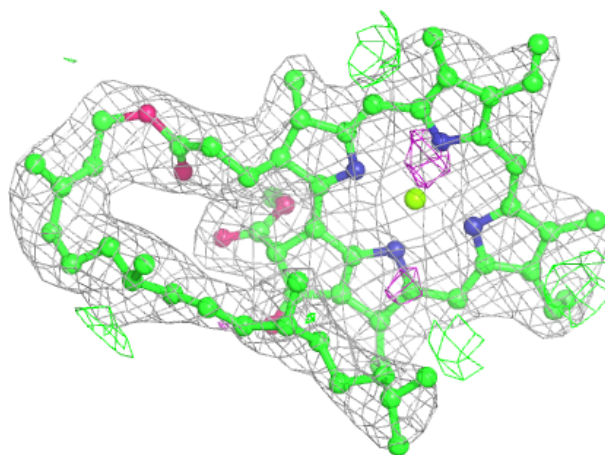
**Electron density around CLA c 905:**

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



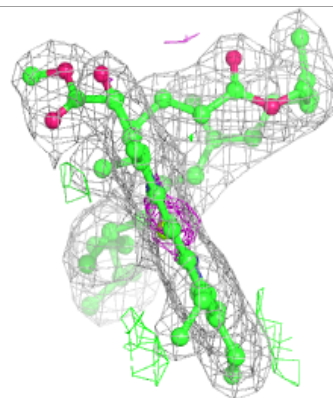
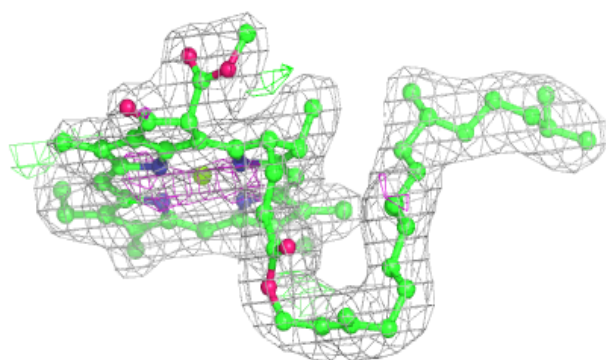
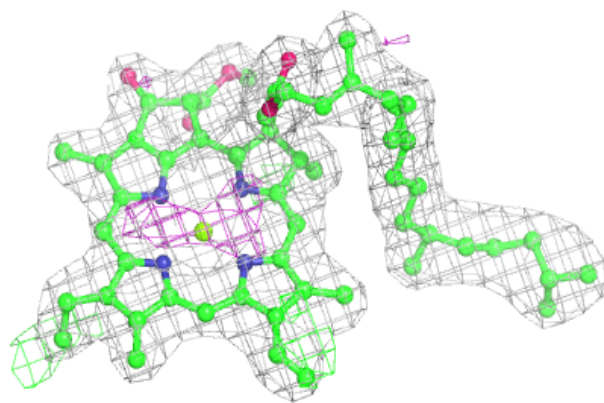
**Electron density around CLA c 910:**

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

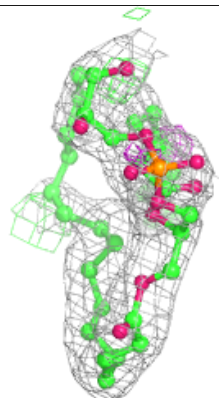
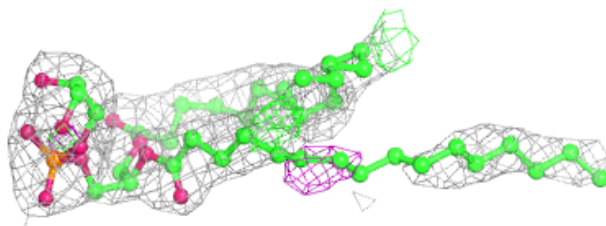
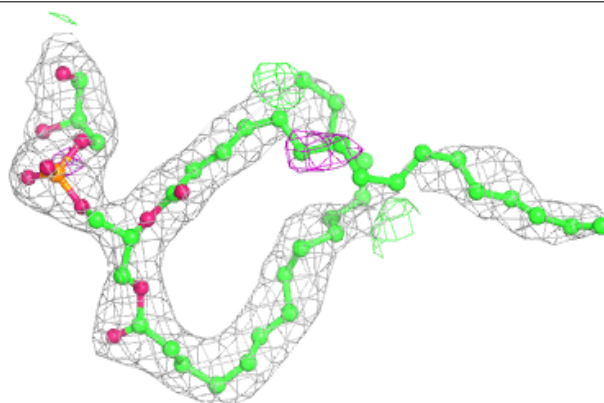


**Electron density around CLA d 404:**

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

**Electron density around LHG D 410:**

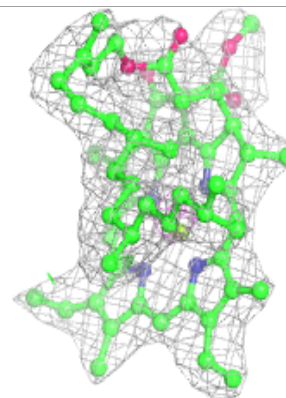
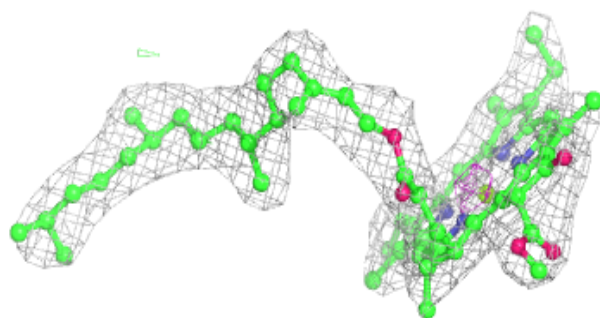
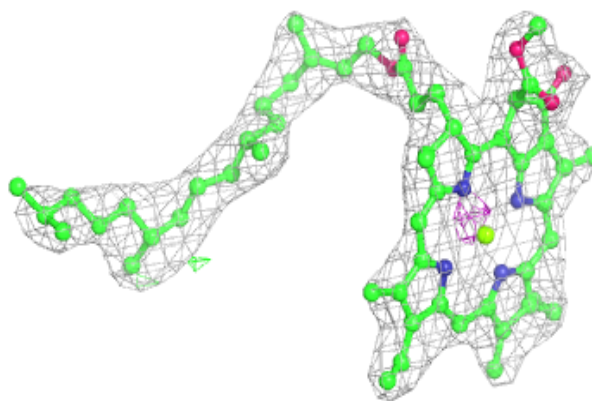
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



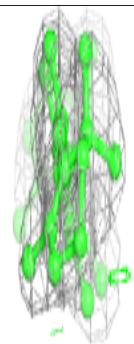
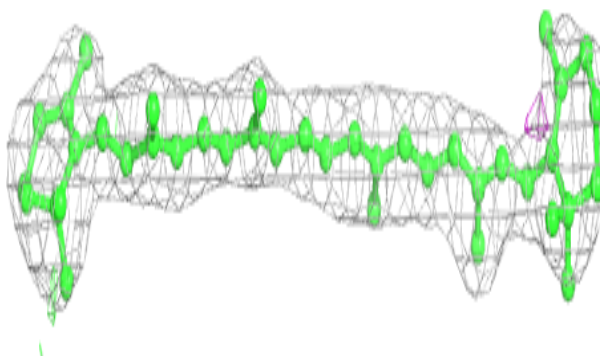
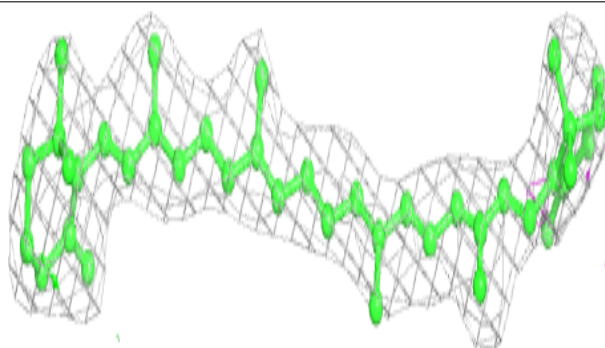


**Electron density around CLA c 912:**

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

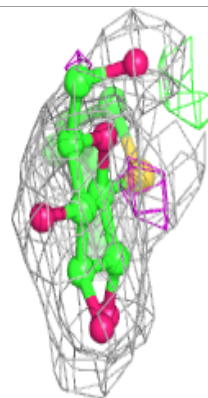
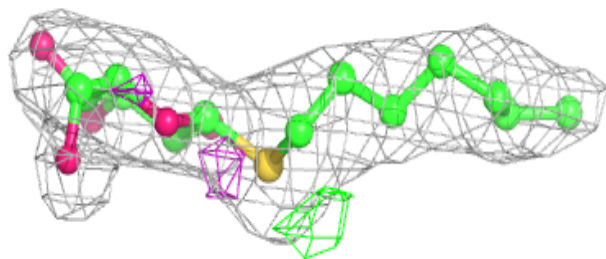
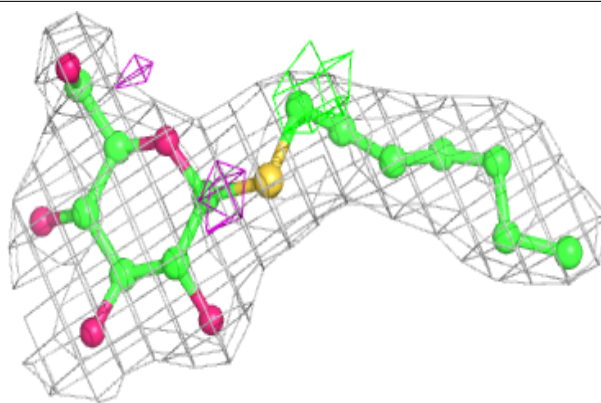
**Electron density around BCR C 514:**

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

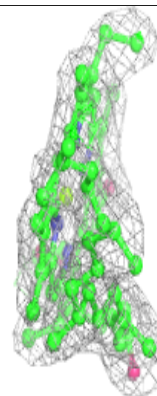
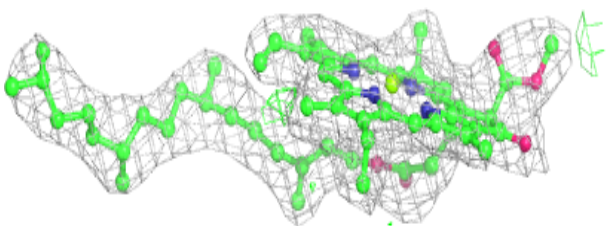
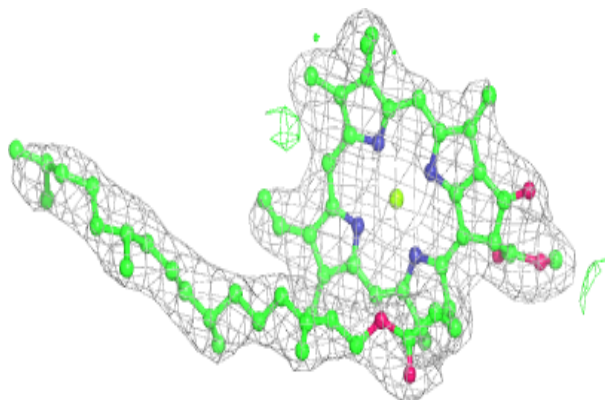


**Electron density around HTG B 623:**

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

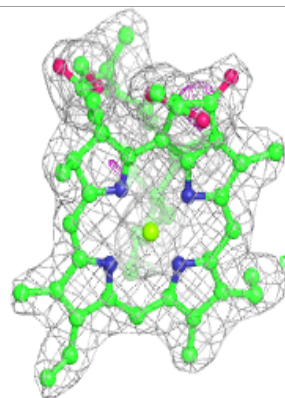
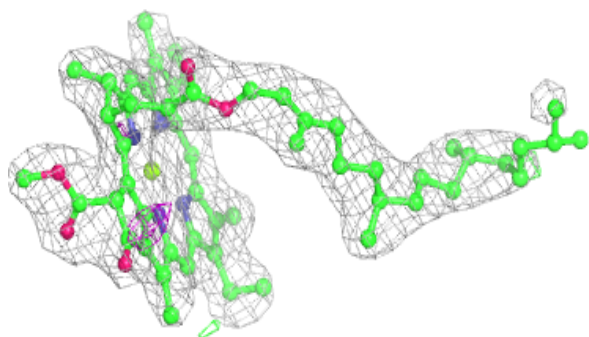
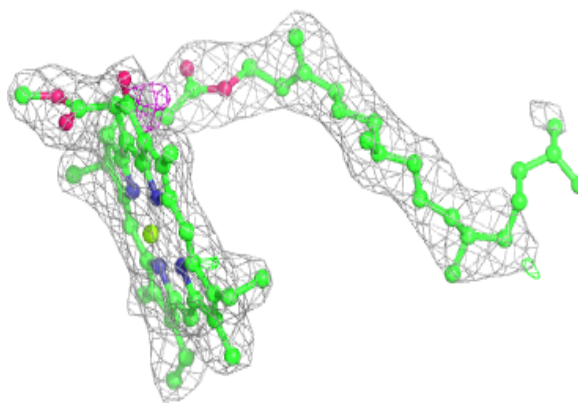
**Electron density around CLA C 501:**

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

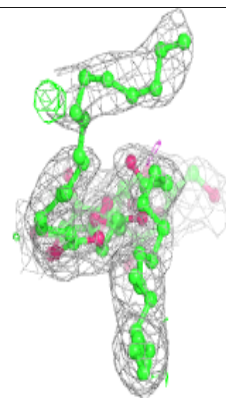
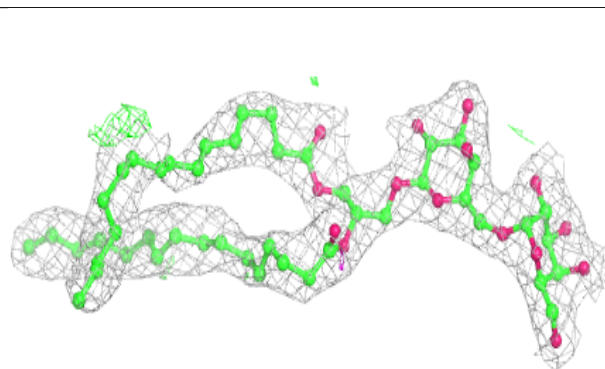
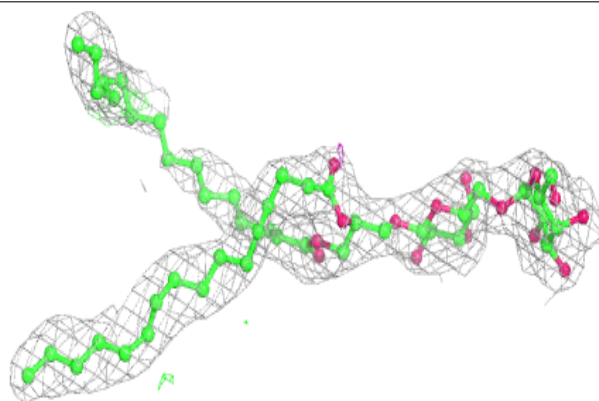


**Electron density around CLA c 909:**

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

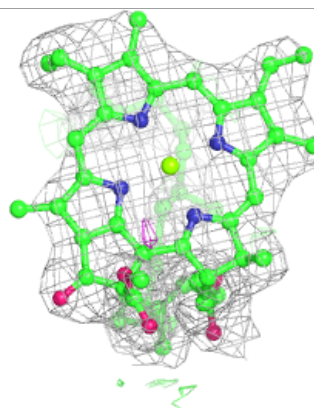
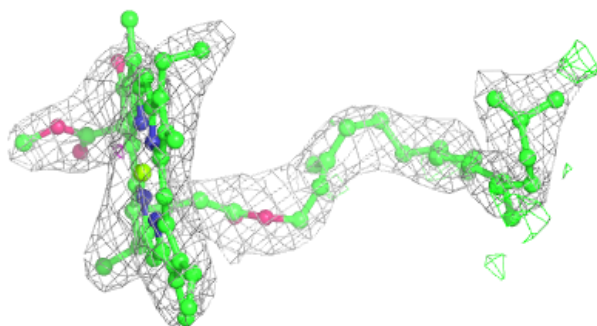
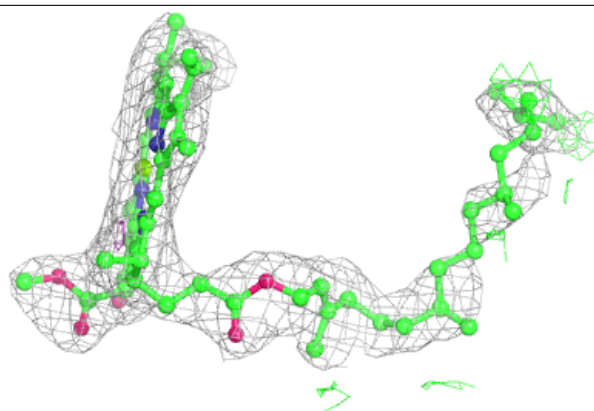
**Electron density around DGD c 916:**

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

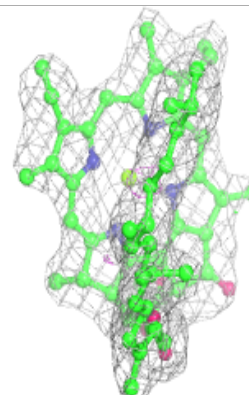
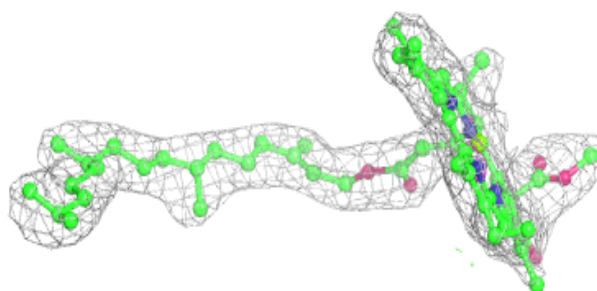
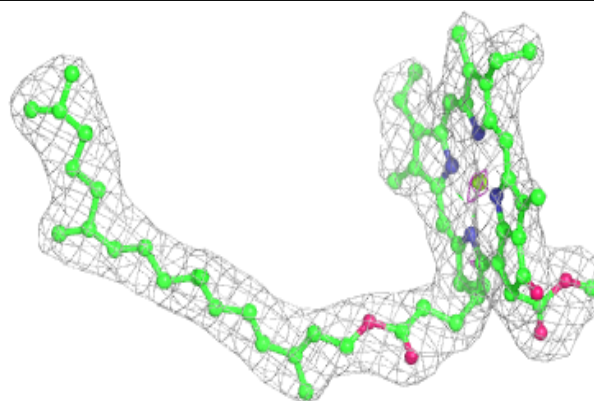


**Electron density around CLA C 506:**

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

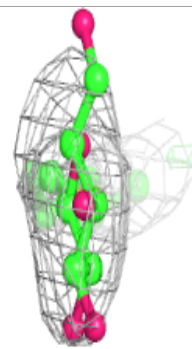
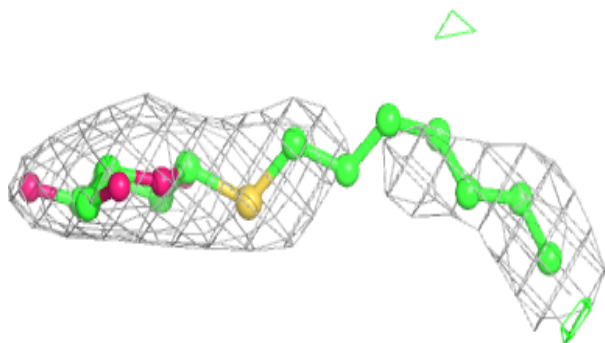
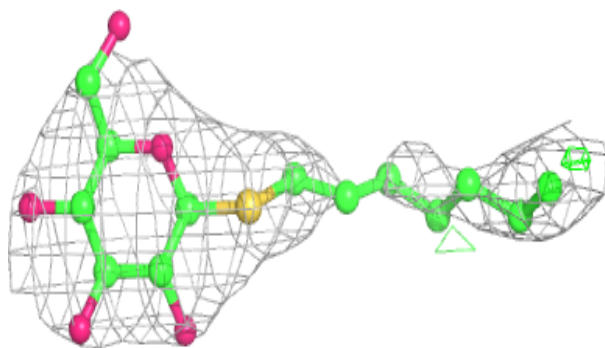
**Electron density around CLA B 610:**

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



**Electron density around HTG C 521:**

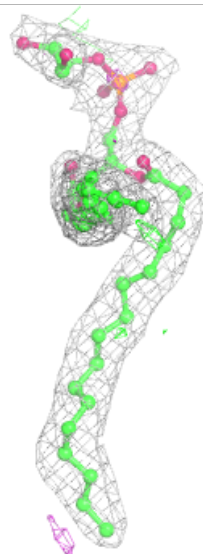
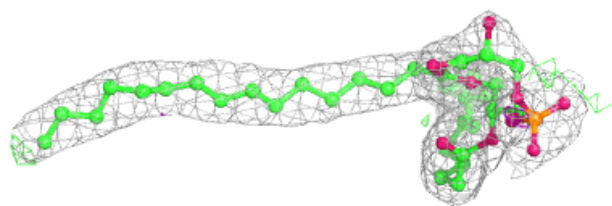
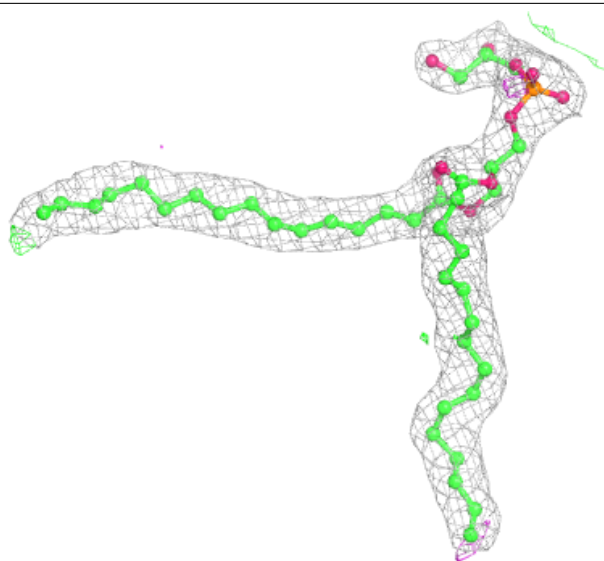
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





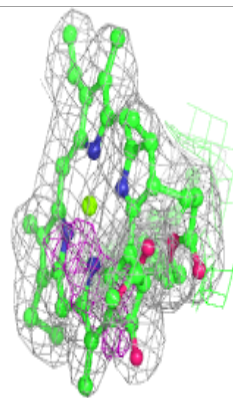
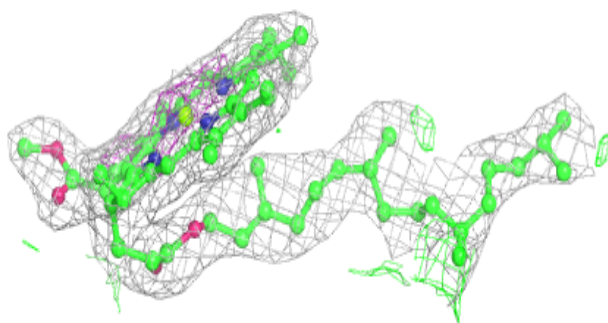
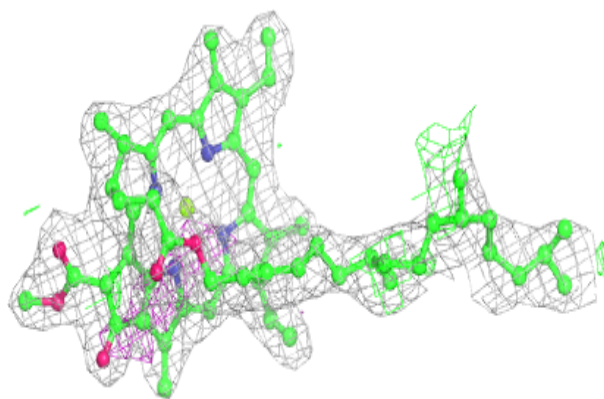
**Electron density around LHG b 635:**

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



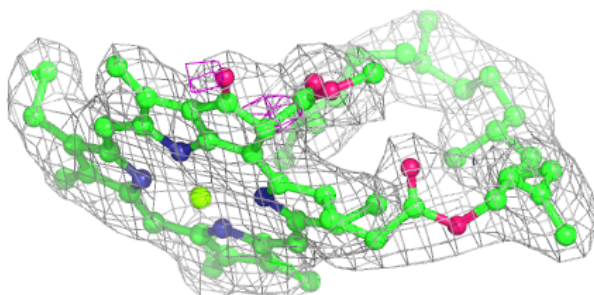
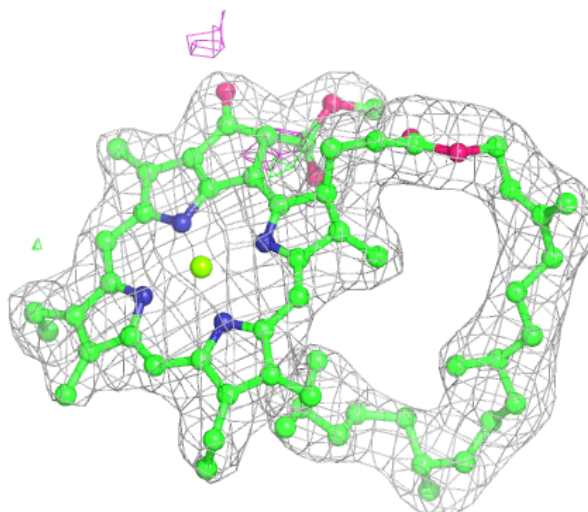
**Electron density around CLA b 619:**

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



**Electron density around CLA B 616:**

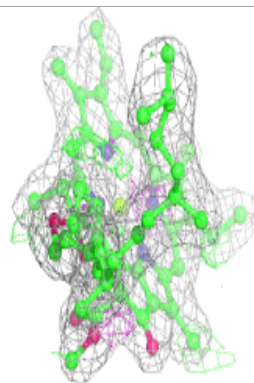
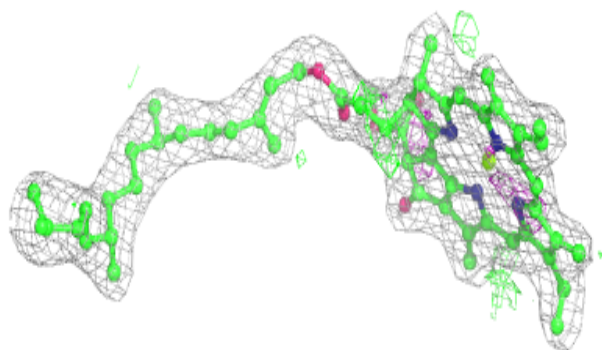
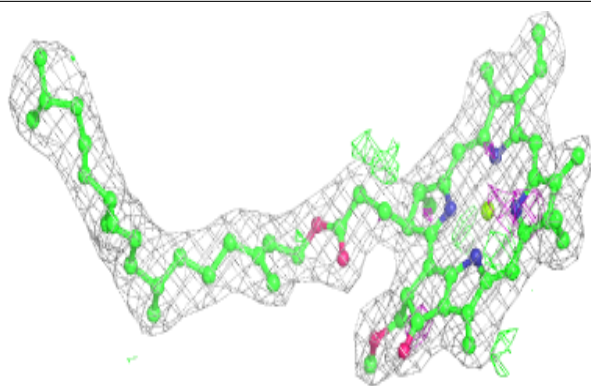
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





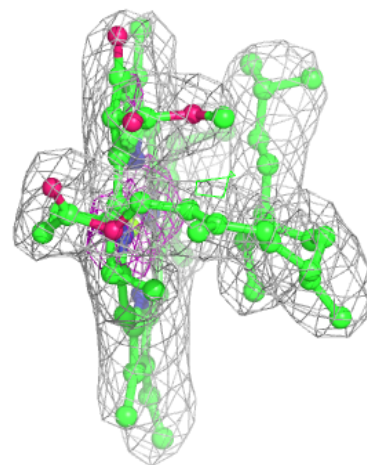
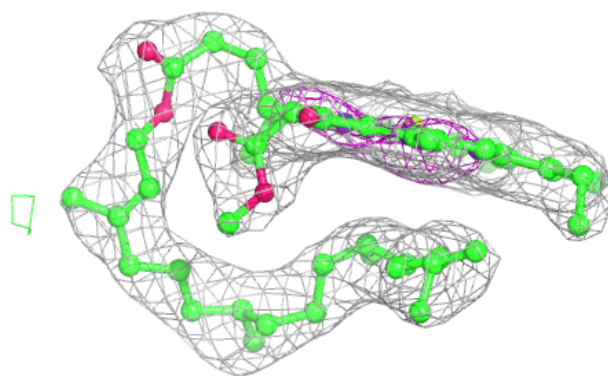
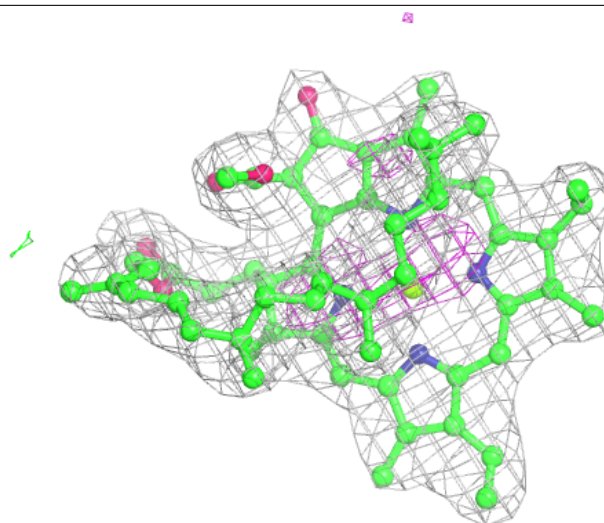
**Electron density around CLA A 405:**

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



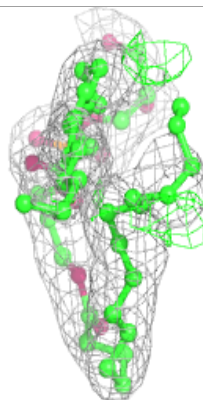
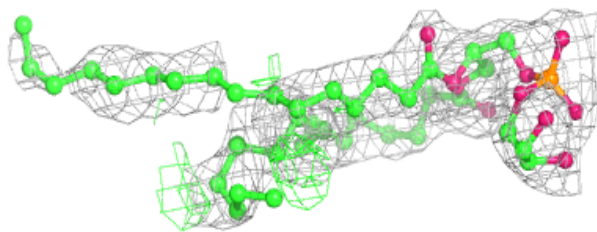
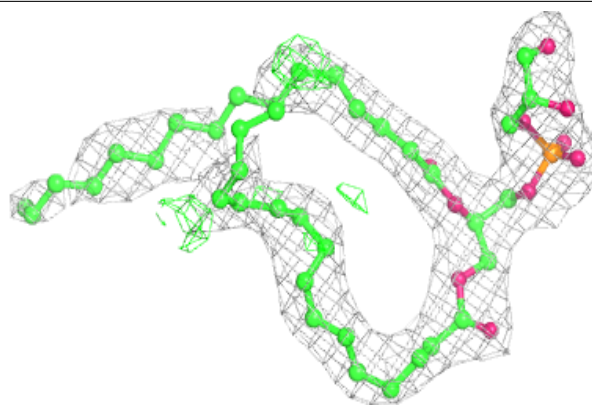
**Electron density around CLA c 911:**

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

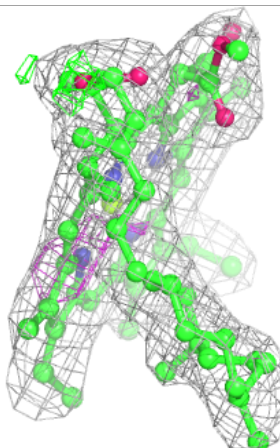
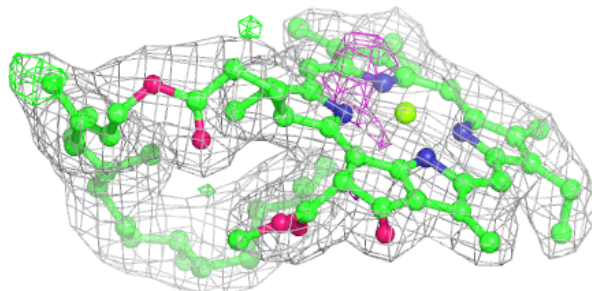
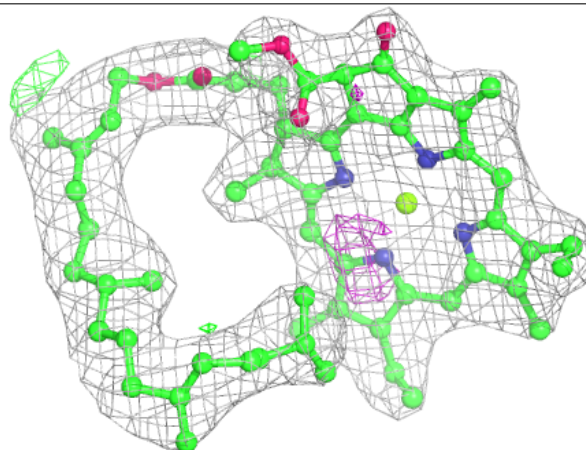


**Electron density around LHG d 411:**

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

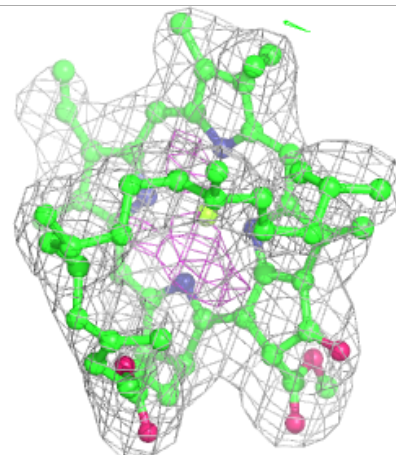
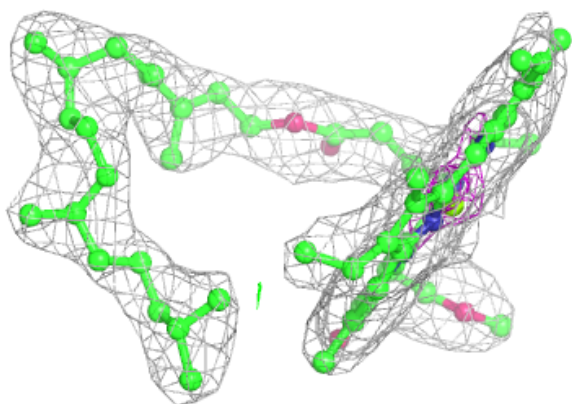
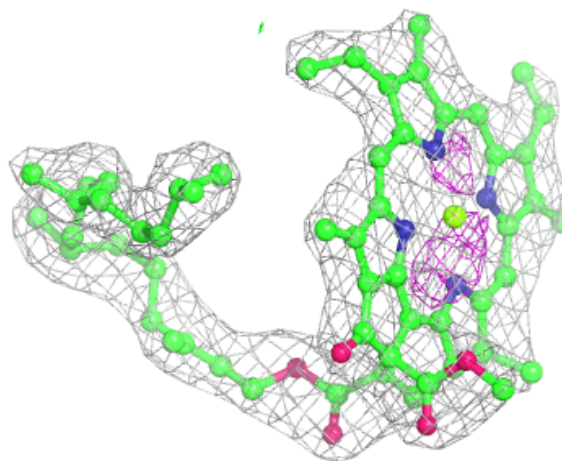
**Electron density around CLA b 620:**

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



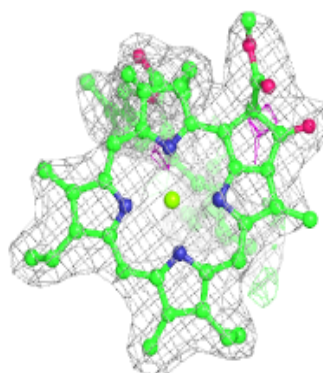
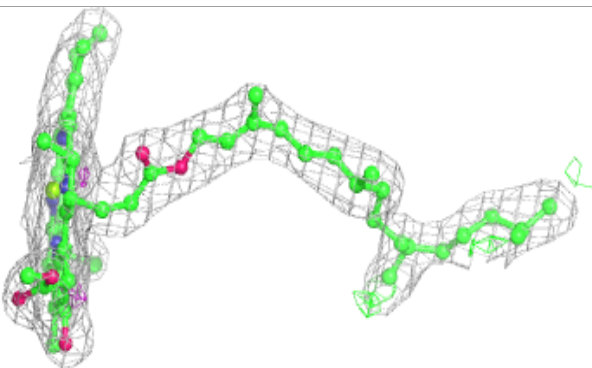
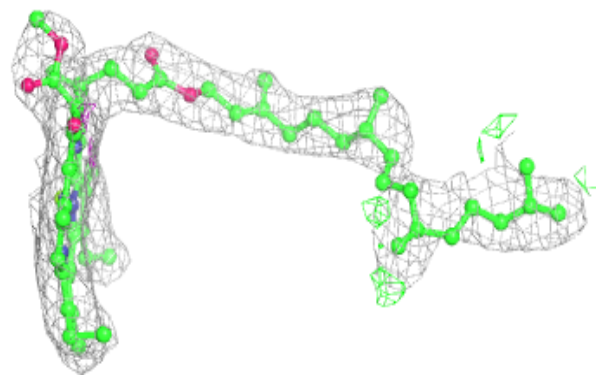
**Electron density around CLA C 503:**

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

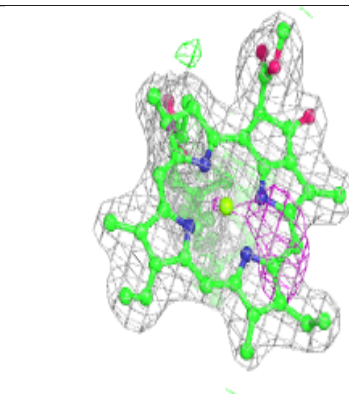
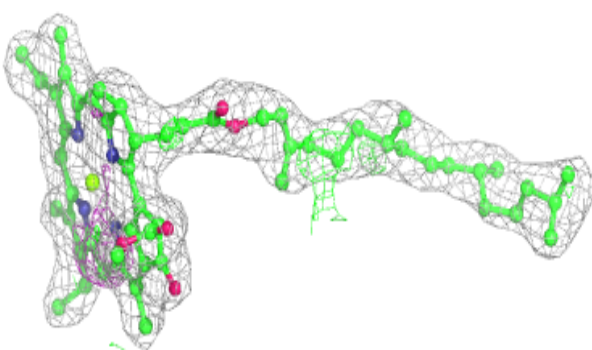
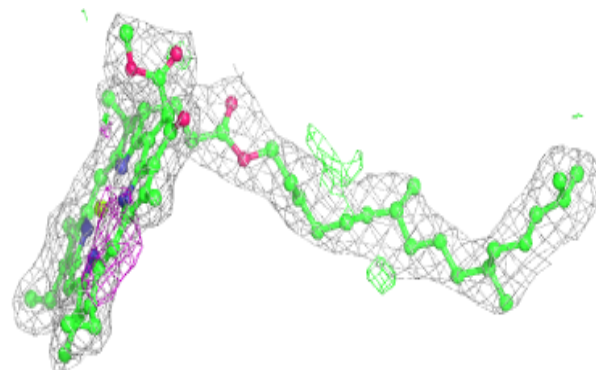


**Electron density around CLA b 611:**

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

**Electron density around CLA B 605:**

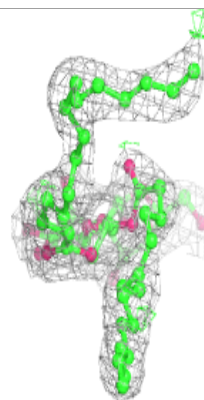
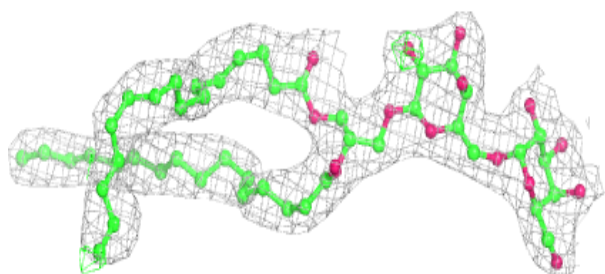
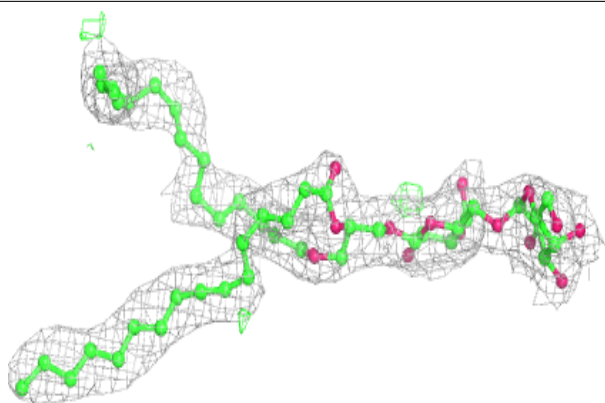
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



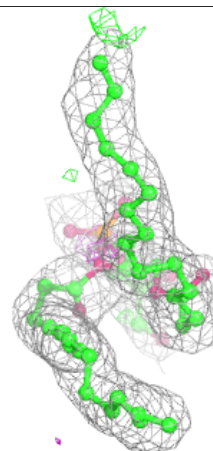
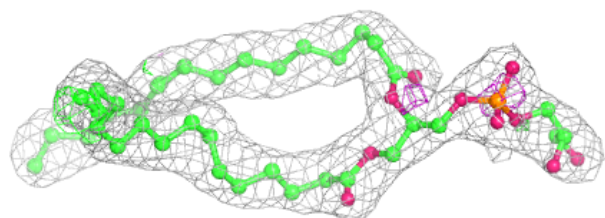
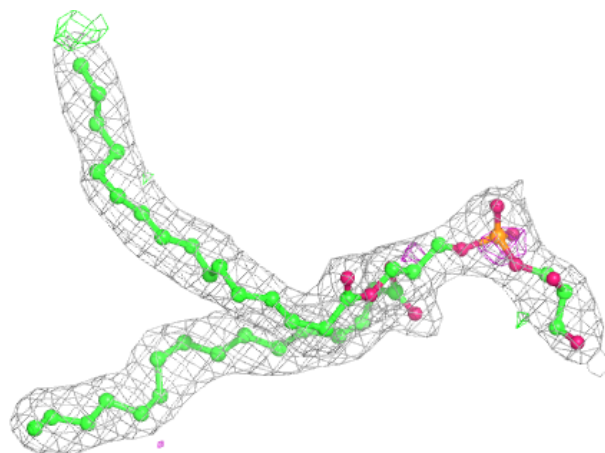


**Electron density around DGD C 516:**

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

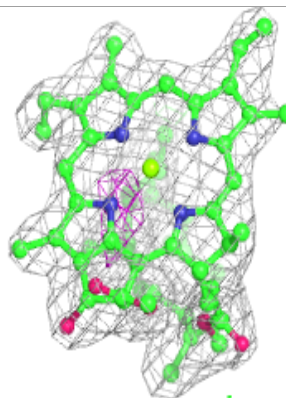
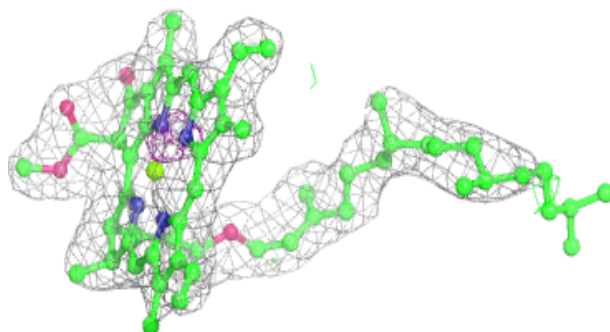
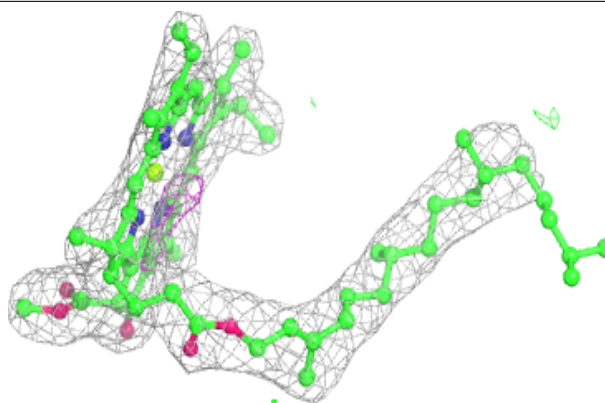
**Electron density around LHG d 410:**

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

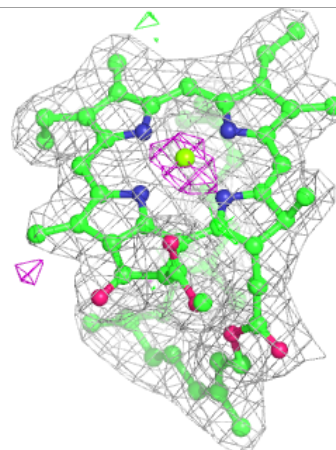
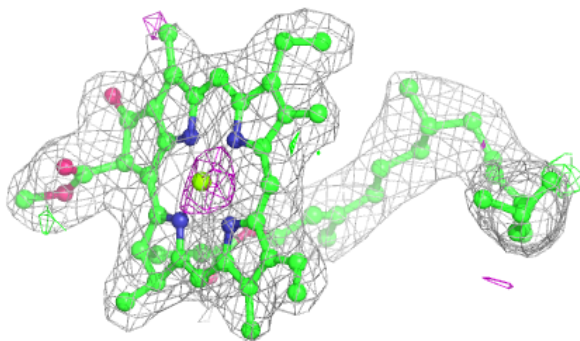
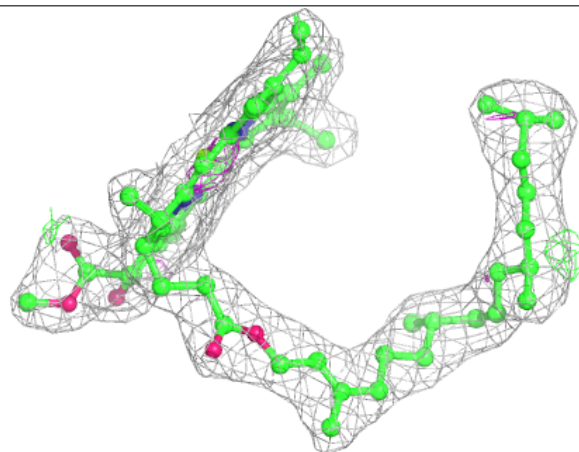


**Electron density around CLA C 508:**

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

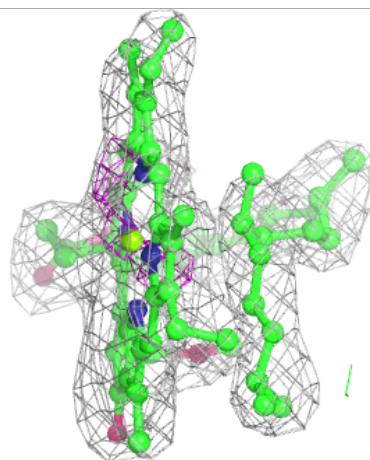
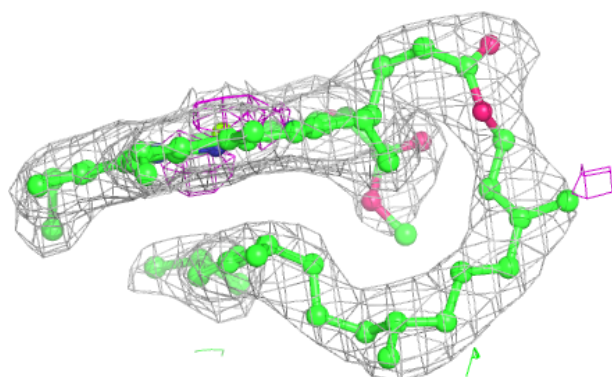
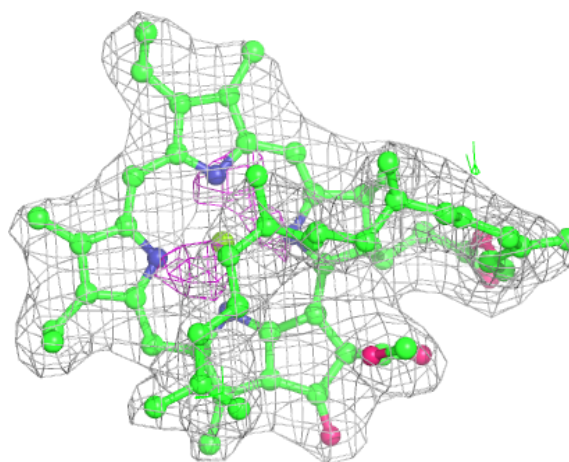
**Electron density around CLA b 616:**

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



**Electron density around CLA C 510:**

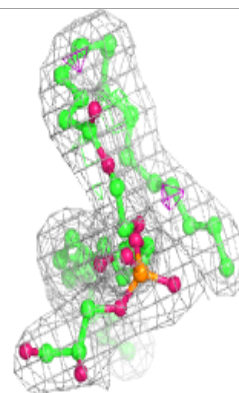
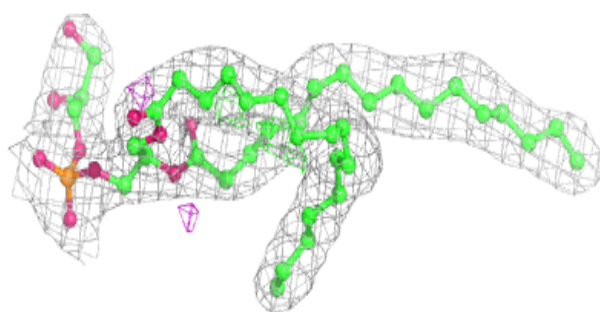
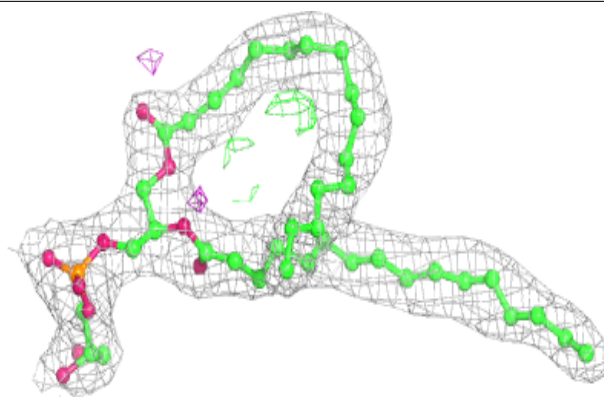
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



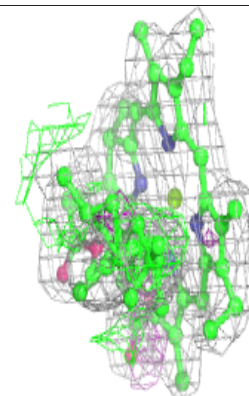
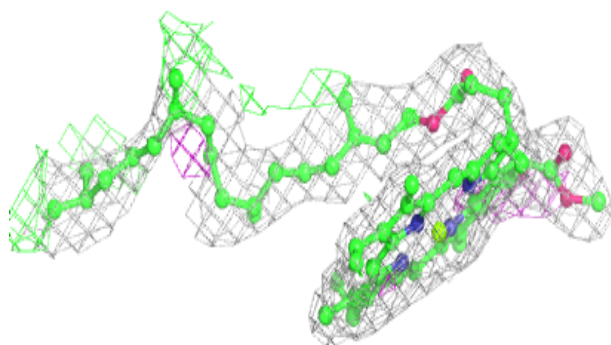
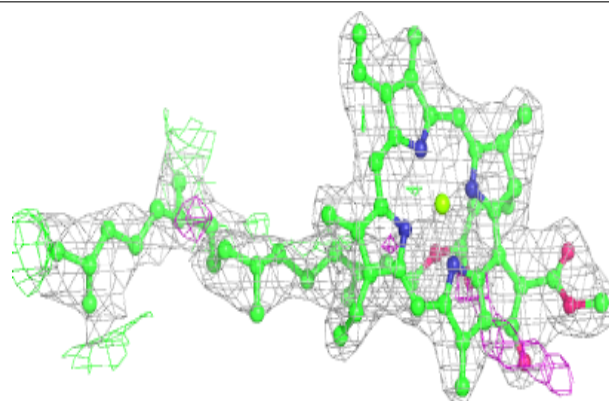


**Electron density around LHG d 409:**

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

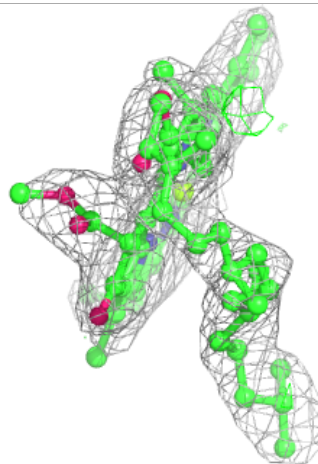
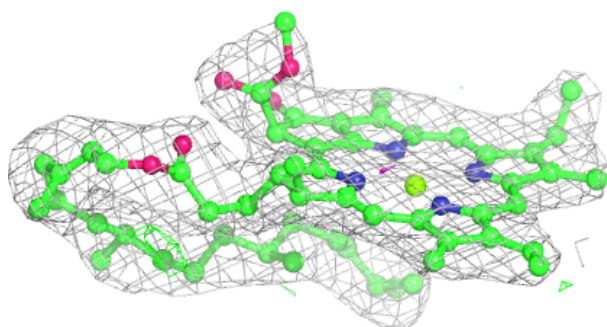
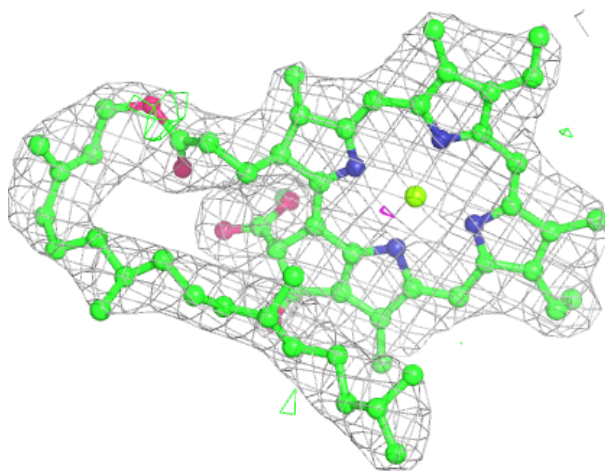
**Electron density around CLA B 615:**

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



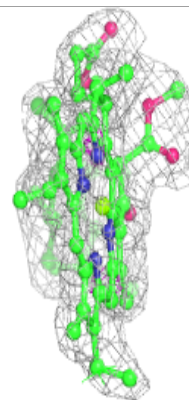
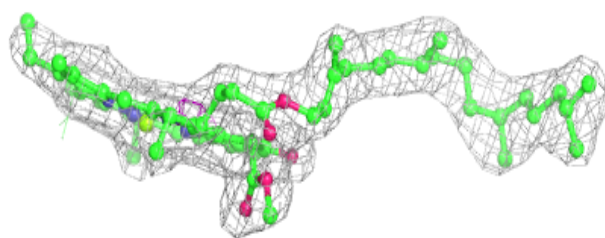
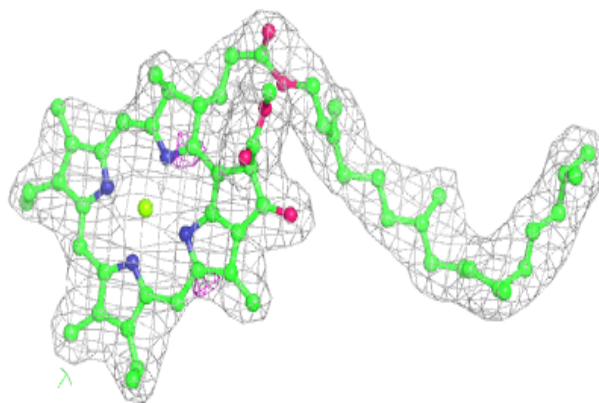
**Electron density around CLA C 509:**

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

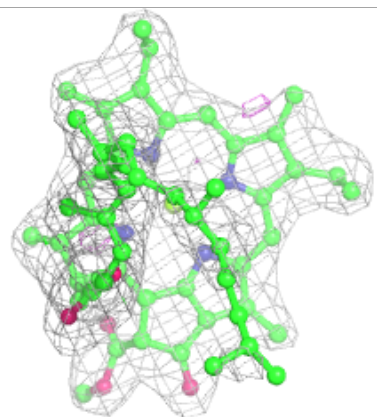
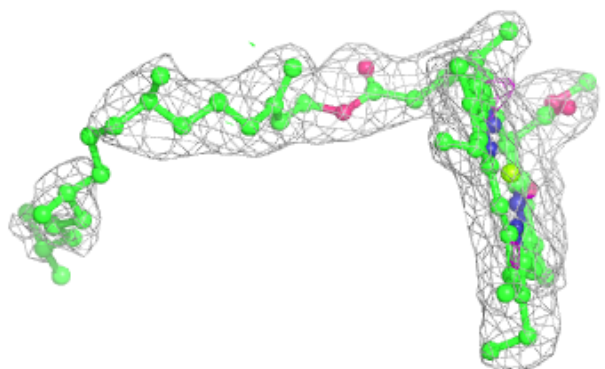
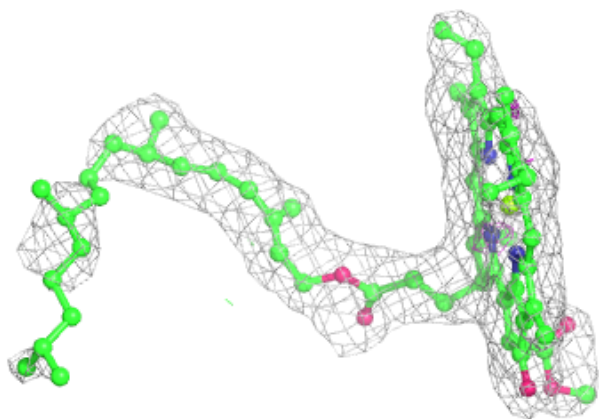


**Electron density around CLA B 603:**

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

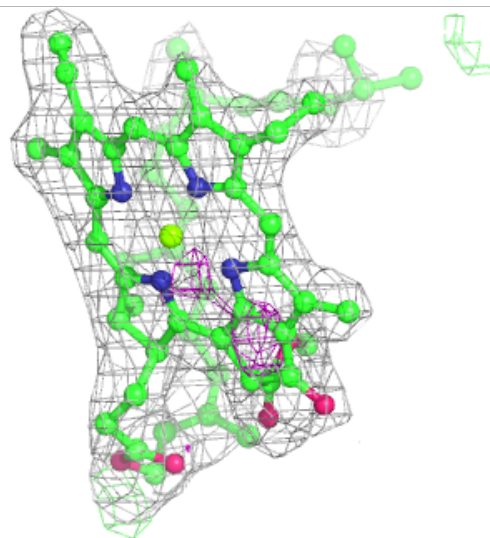
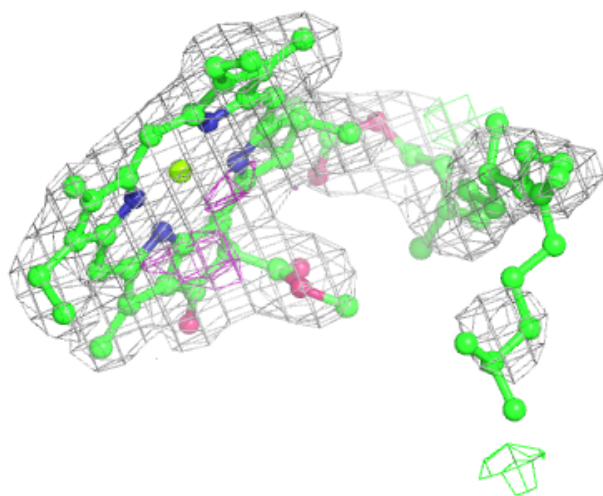
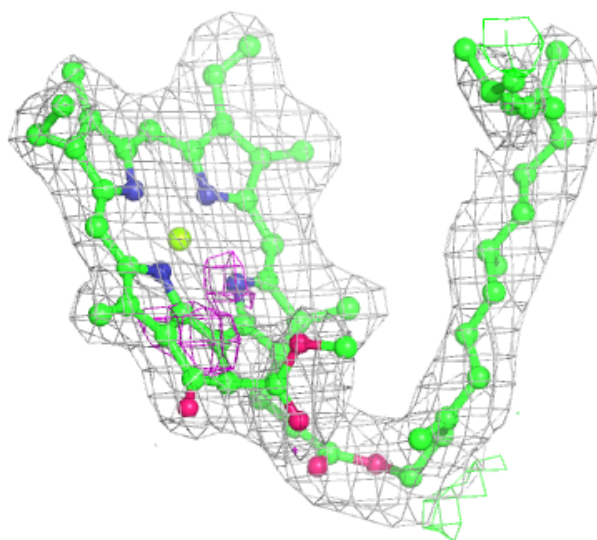
**Electron density around CLA D 405:**

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



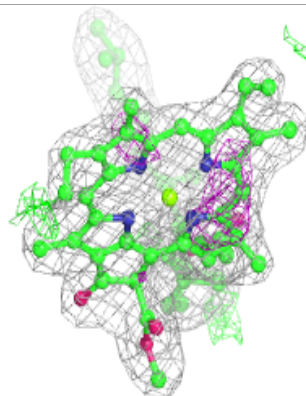
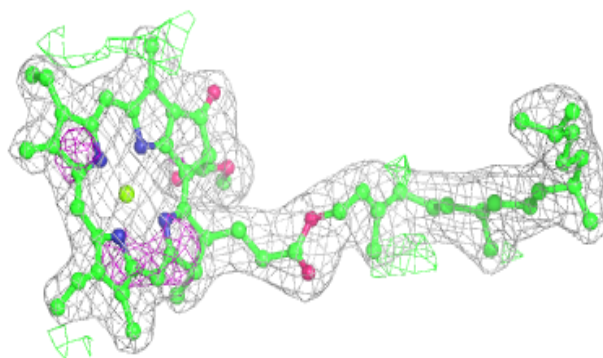
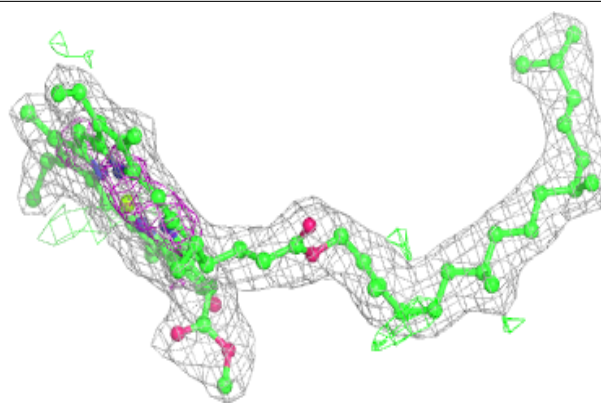
**Electron density around CLA b 621:**

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



**Electron density around CLA D 404:**

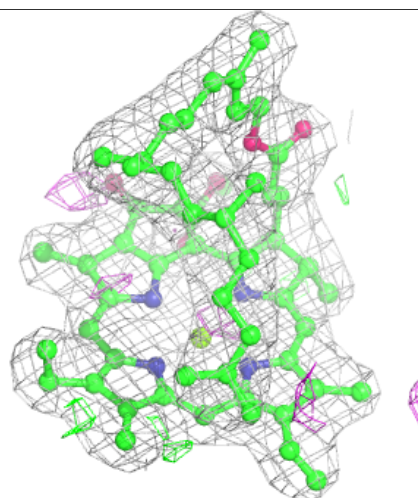
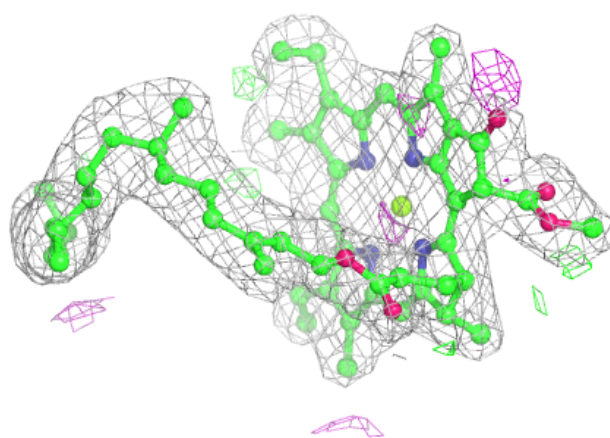
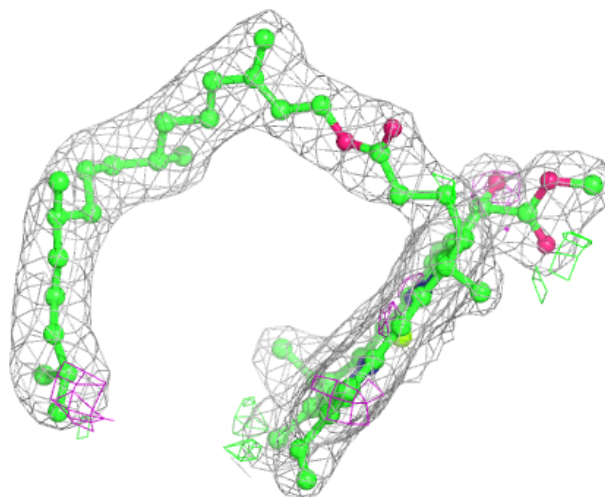
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





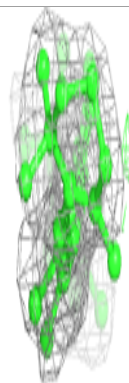
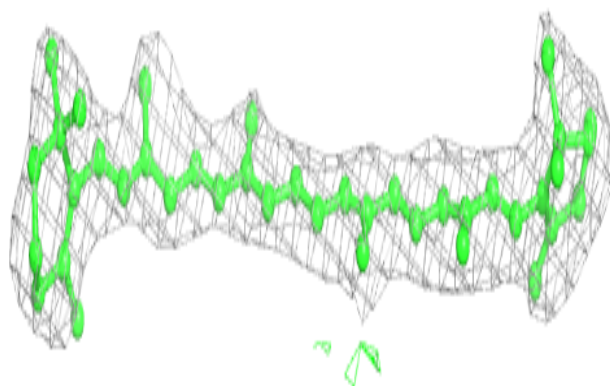
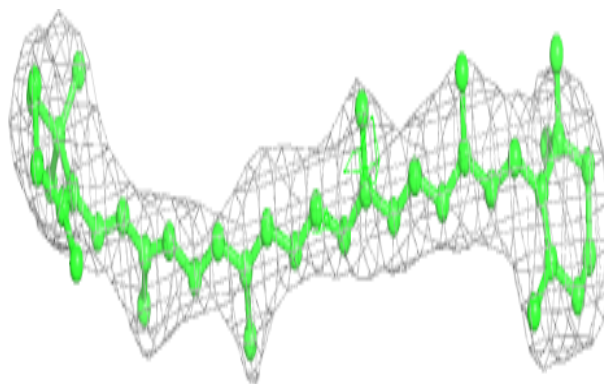
**Electron density around CLA B 612:**

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

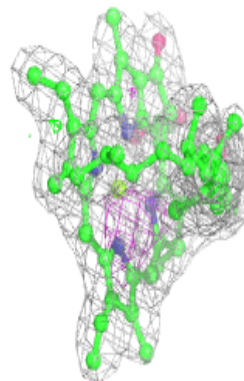
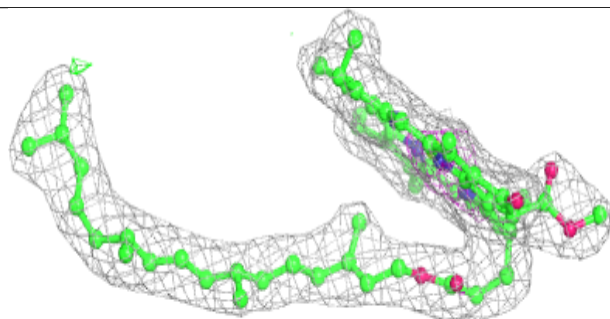
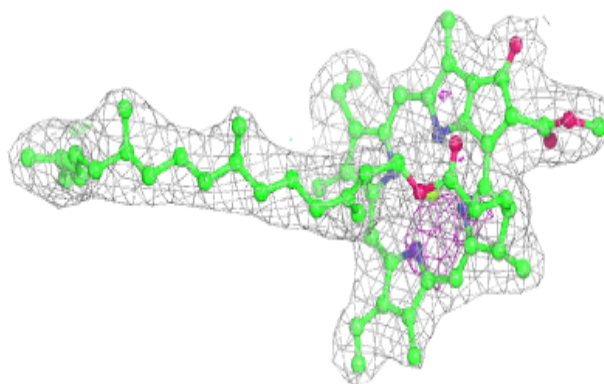


**Electron density around BCR c 927:**

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

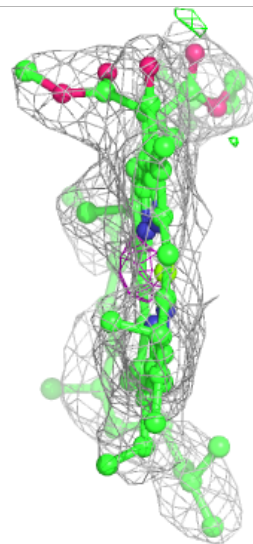
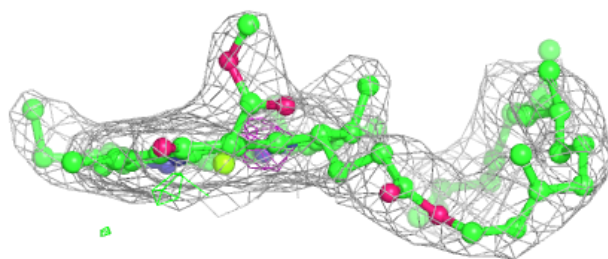
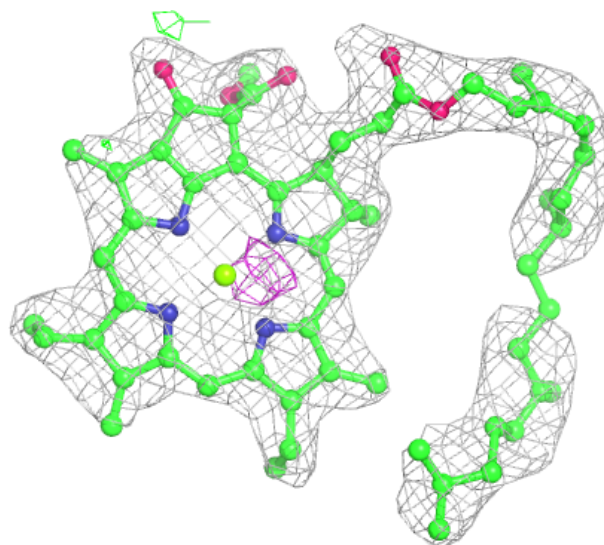
**Electron density around CLA b 613:**

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



**Electron density around CLA c 913:**

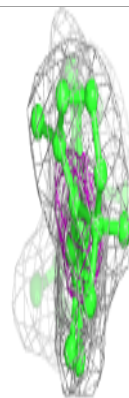
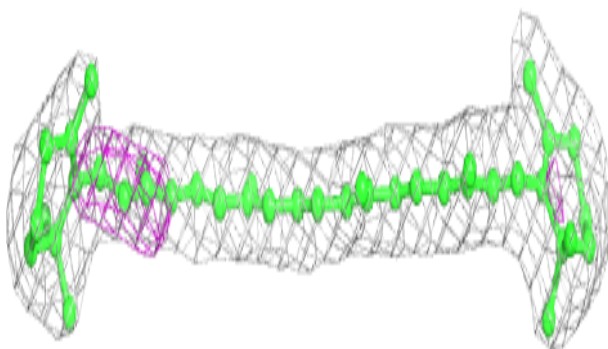
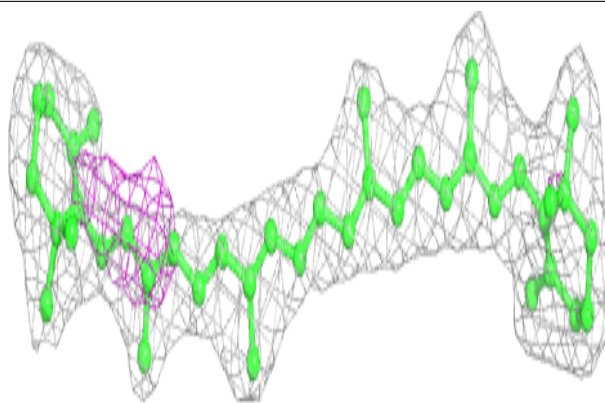
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



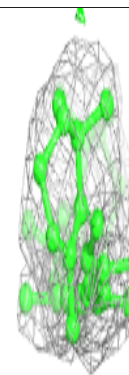
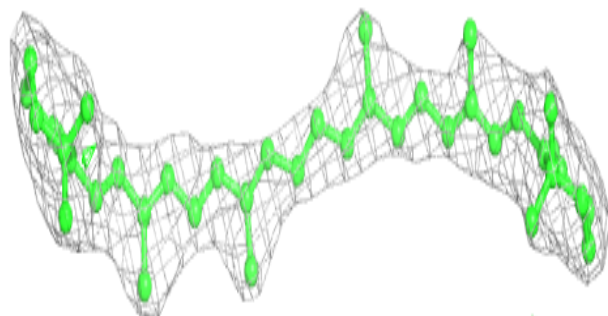
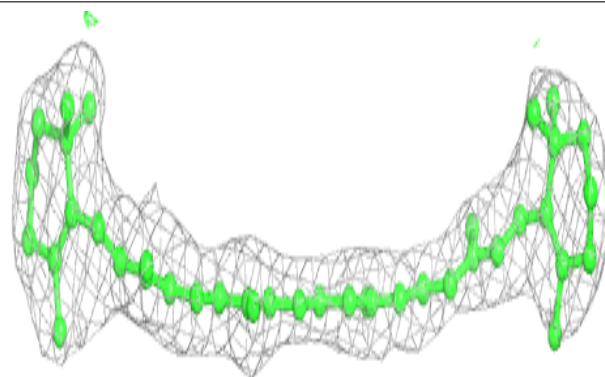


**Electron density around BCR b 623:**

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

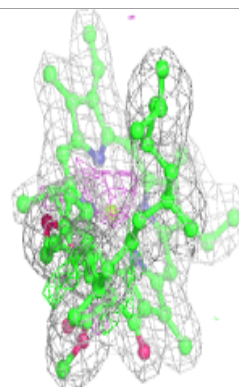
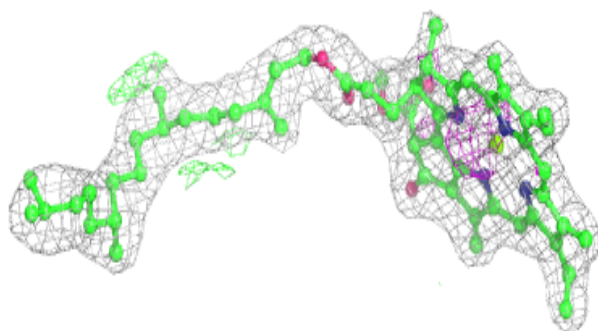
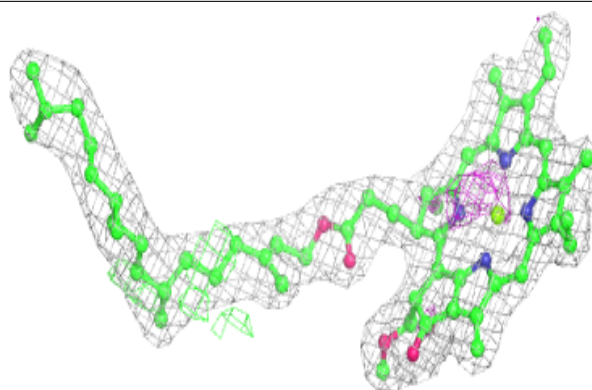
**Electron density around BCR k 101:**

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

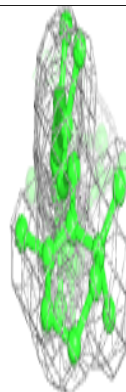
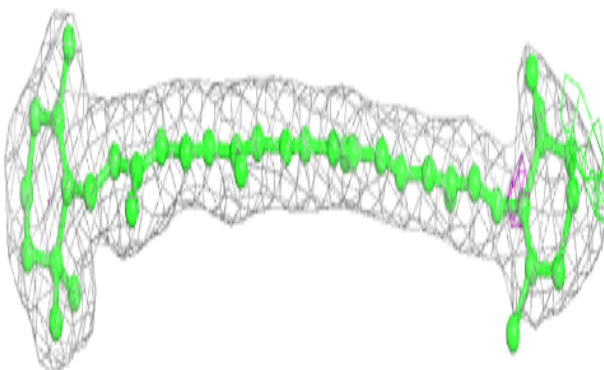
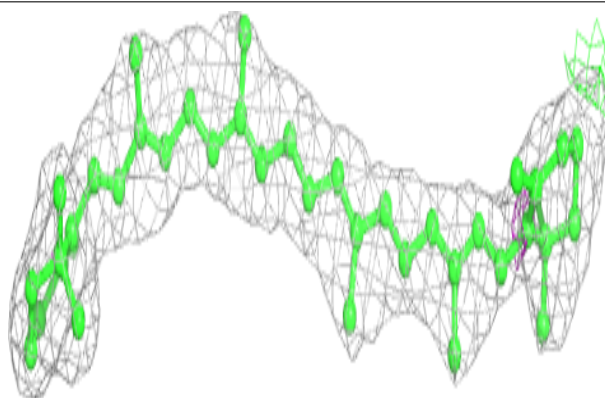


**Electron density around CLA a 405:**

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

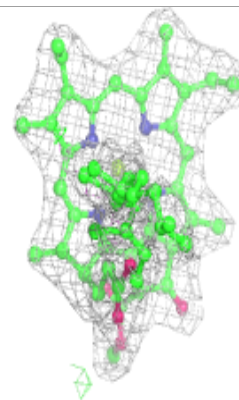
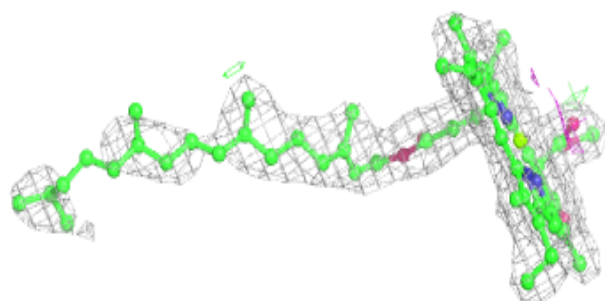
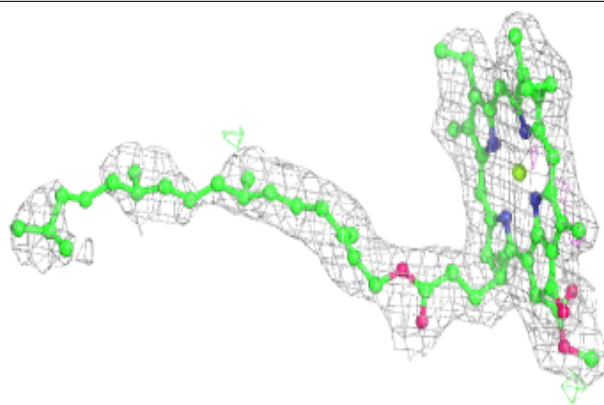
**Electron density around BCR H 101:**

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

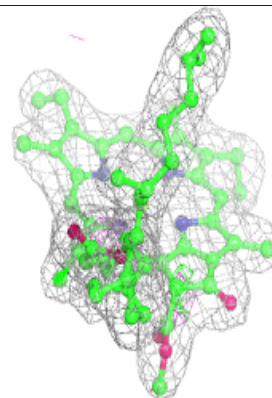
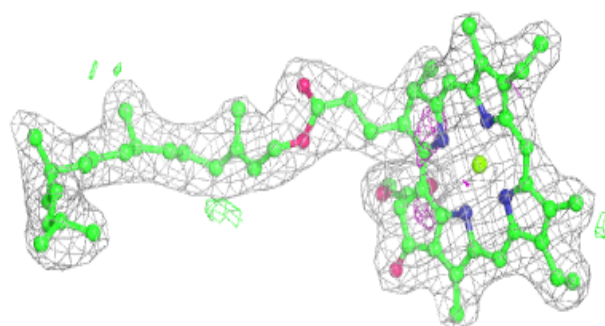
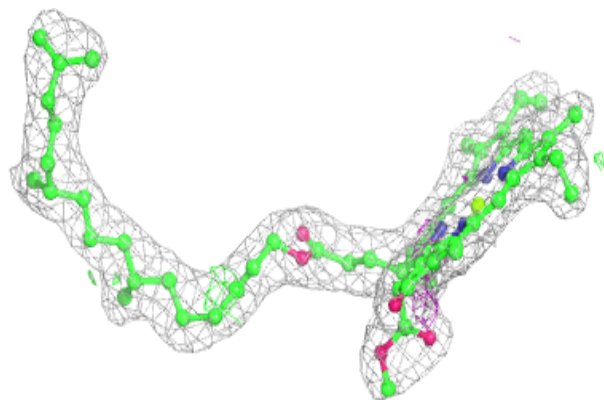


**Electron density around CLA d 406:**

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

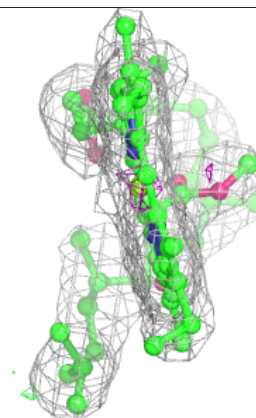
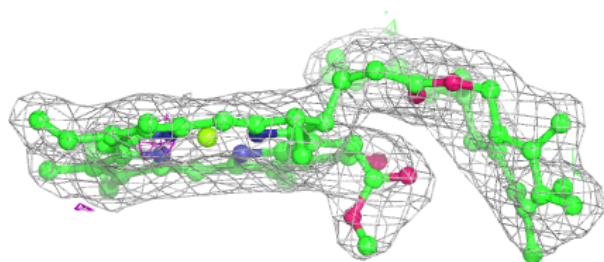
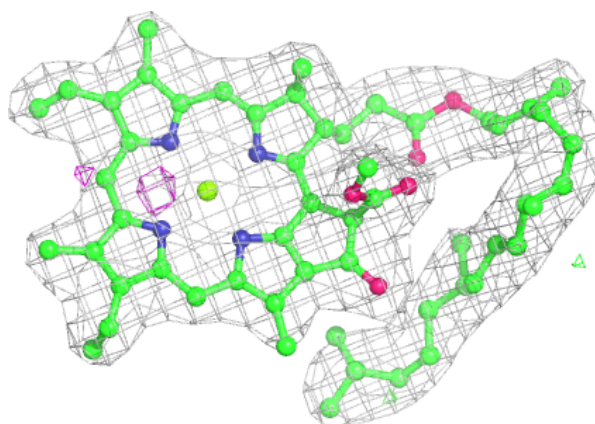
**Electron density around CLA d 405:**

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



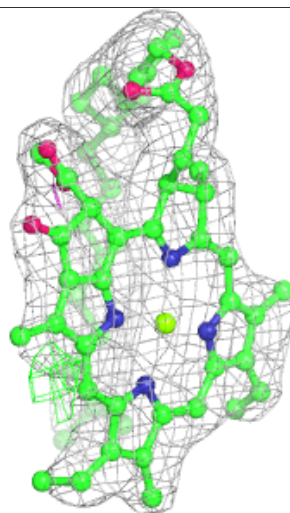
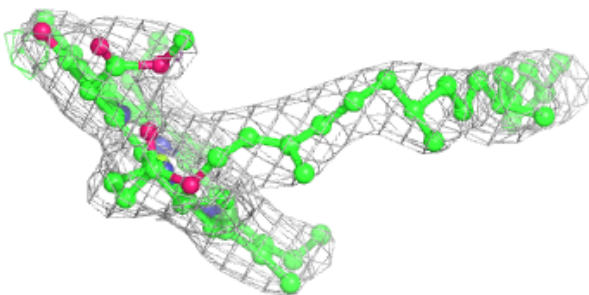
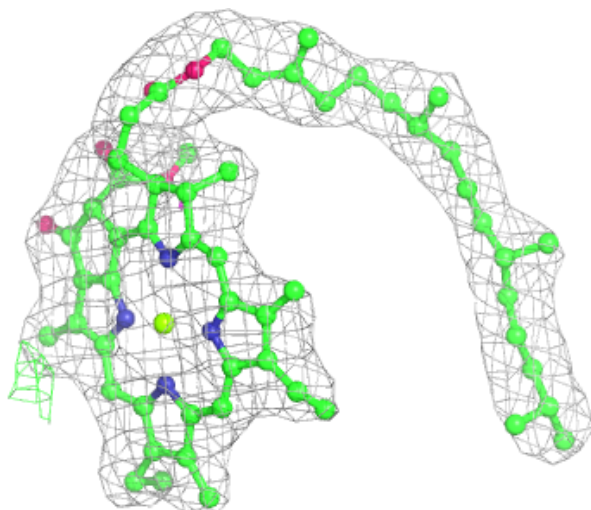
**Electron density around CLA b 615:**

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



**Electron density around CLA C 507:**

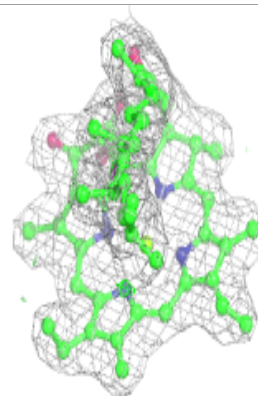
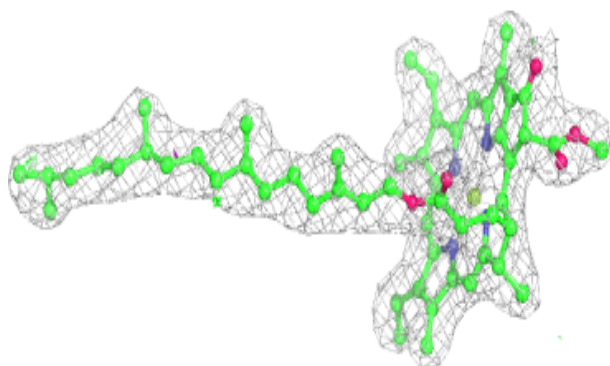
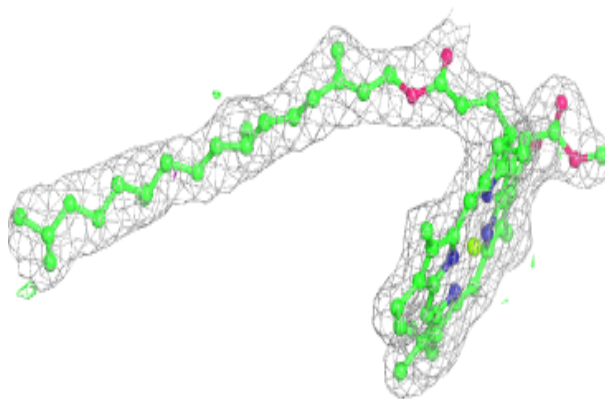
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



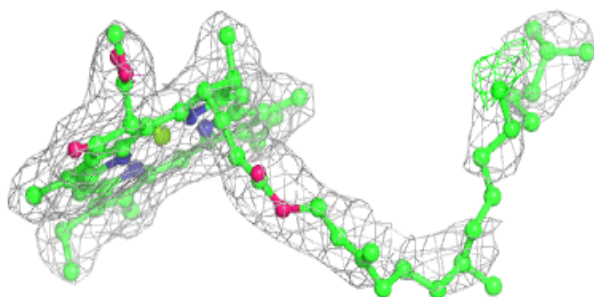
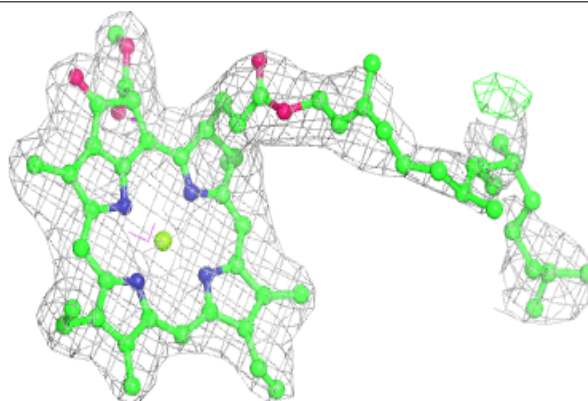


**Electron density around CLA B 608:**

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

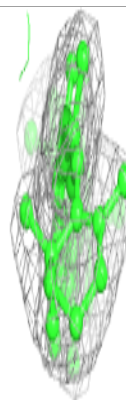
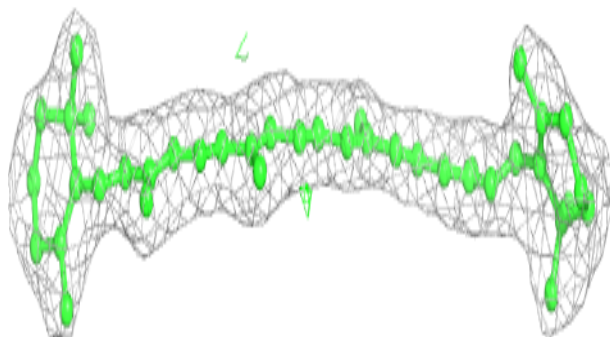
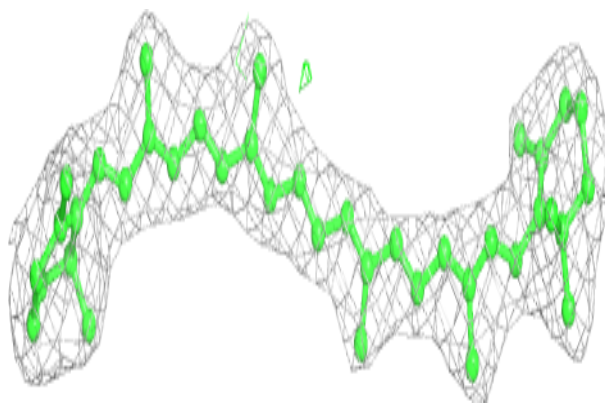
**Electron density around CLA a 408:**

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

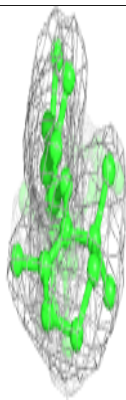
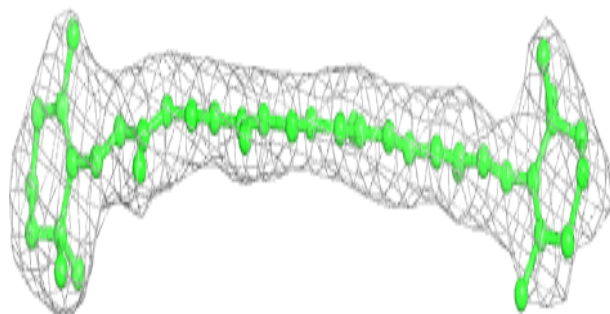
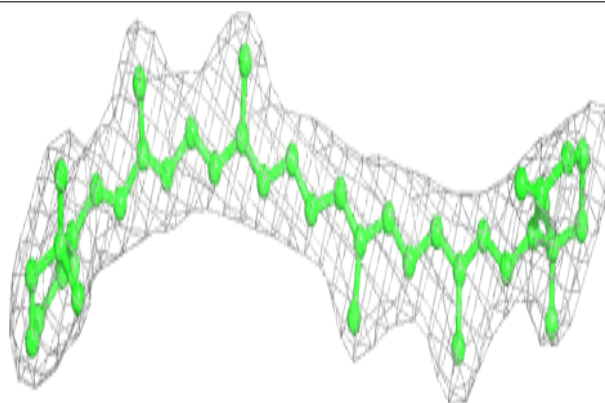


**Electron density around BCR y 101:**

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

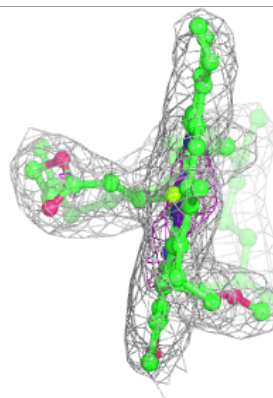
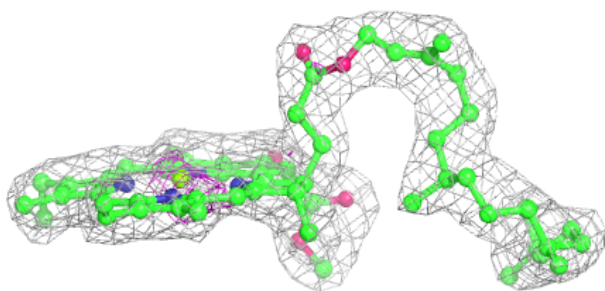
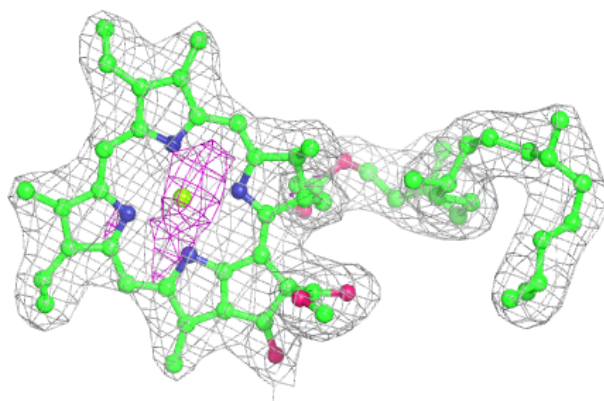
**Electron density around BCR h 101:**

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

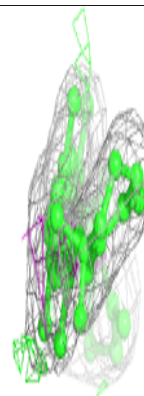
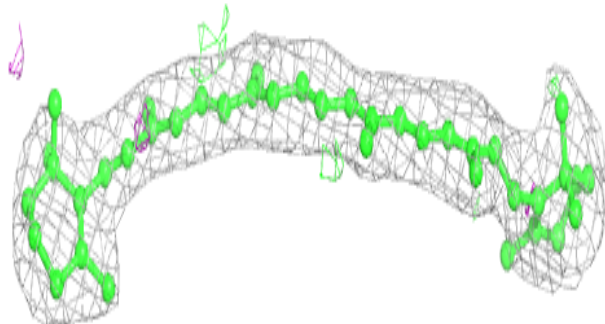
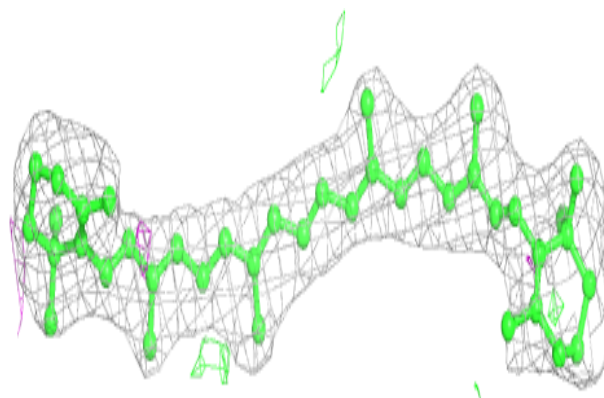


**Electron density around CLA B 613:**

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

**Electron density around BCR d 407:**

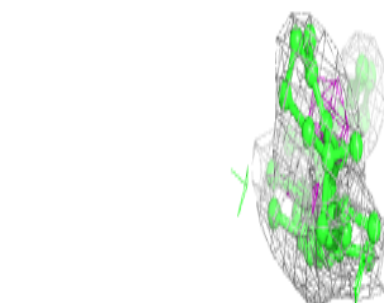
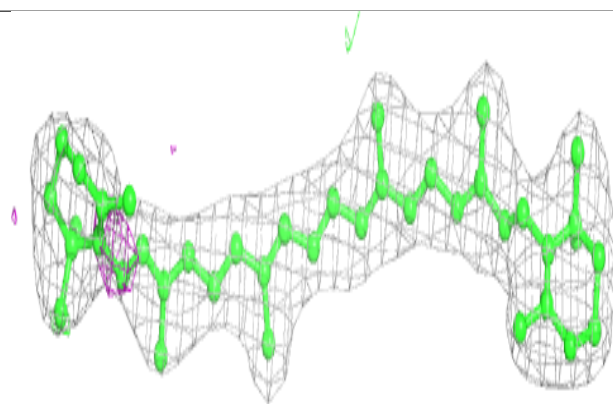
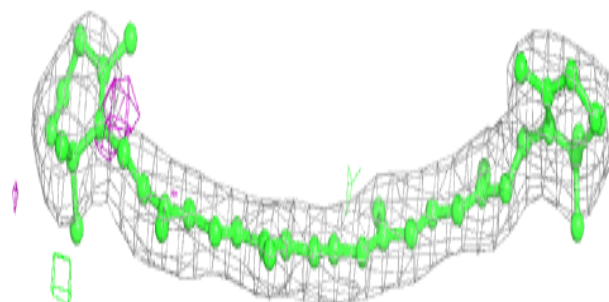
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



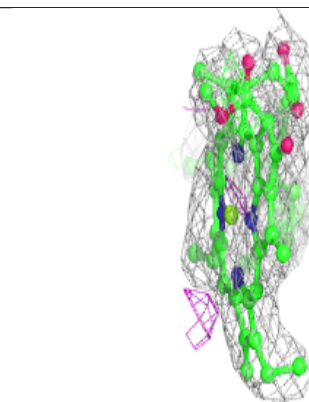
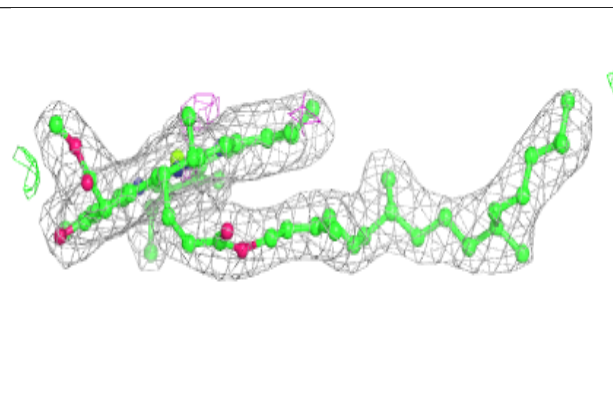
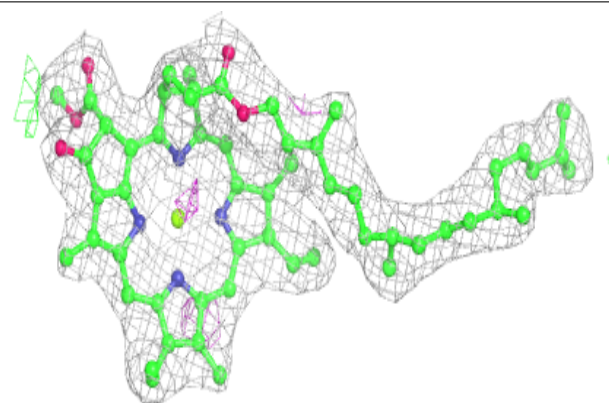


**Electron density around BCR D 406:**

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

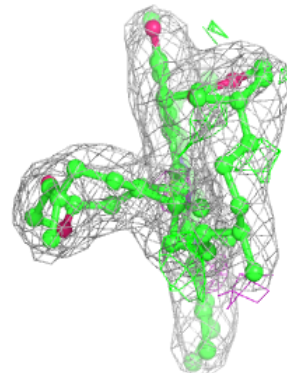
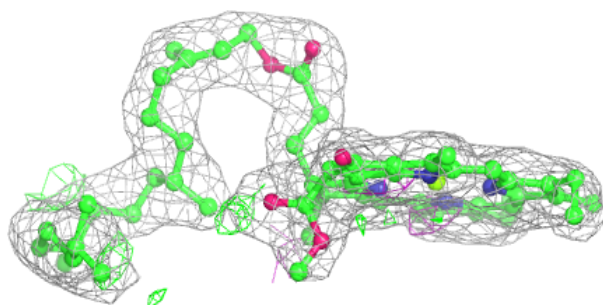
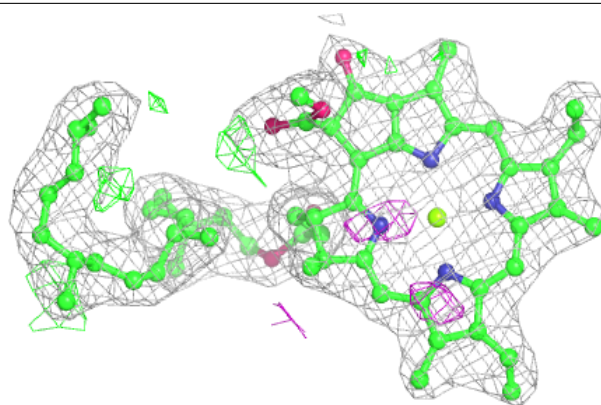
**Electron density around CLA b 608:**

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

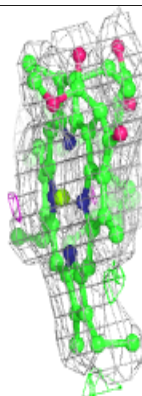
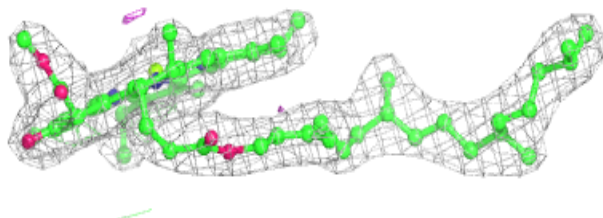
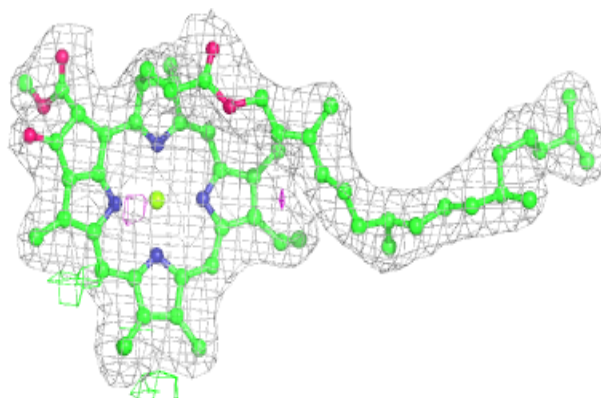


**Electron density around CLA b 617:**

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

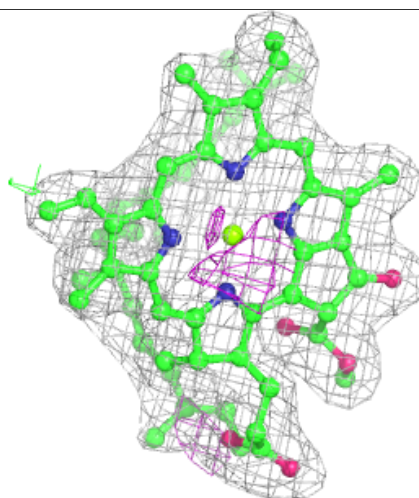
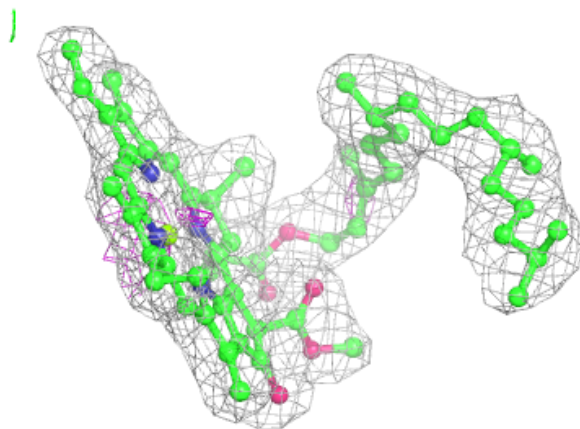
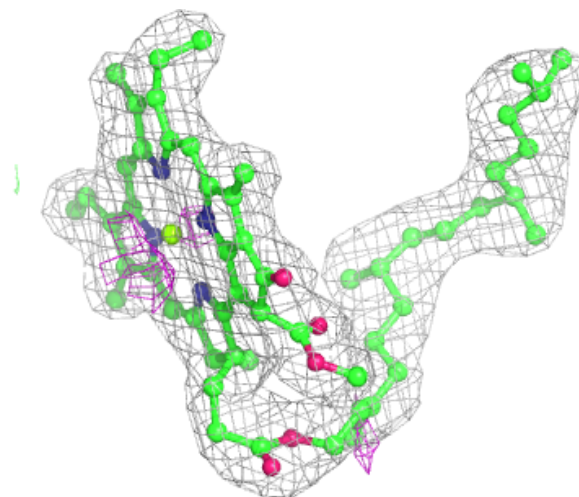
**Electron density around CLA B 604:**

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



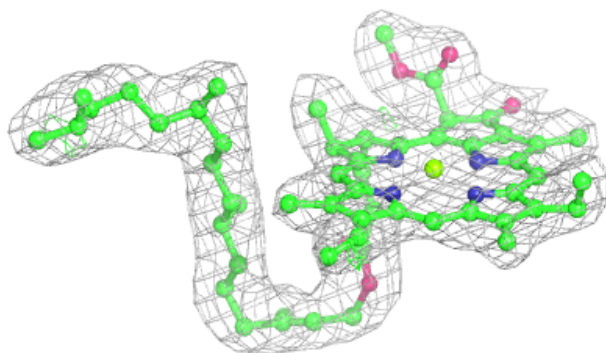
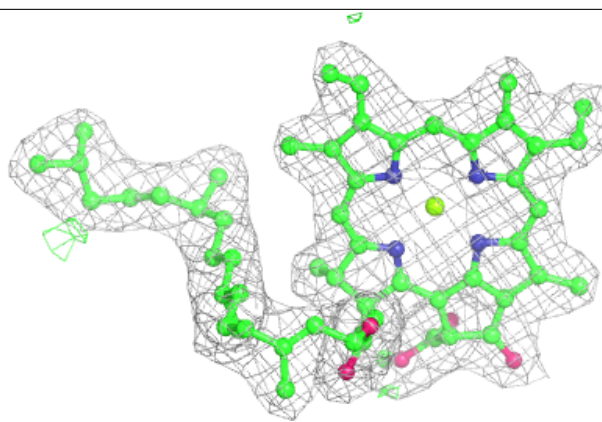
**Electron density around CLA b 618:**

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



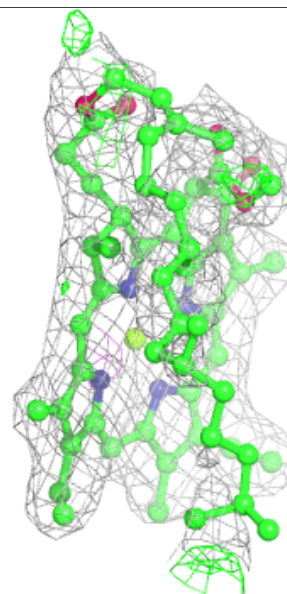
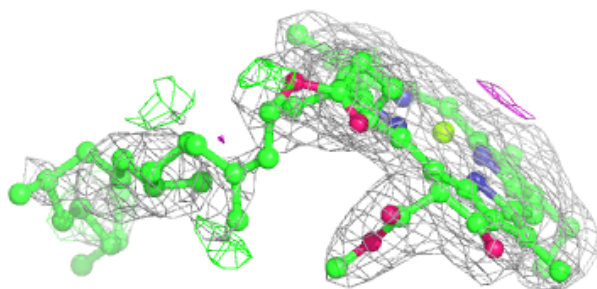
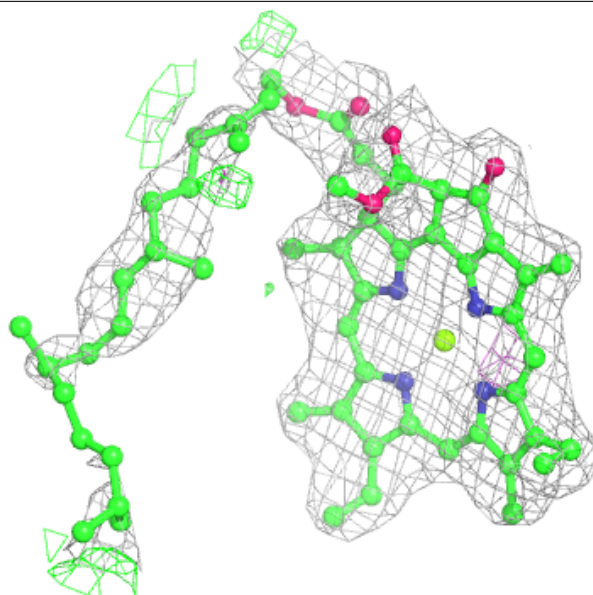
**Electron density around CLA A 406:**

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



**Electron density around CLA B 617:**

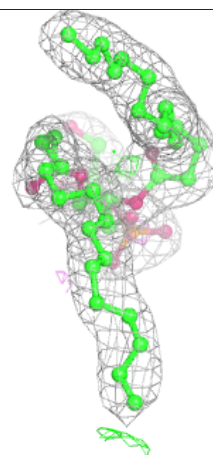
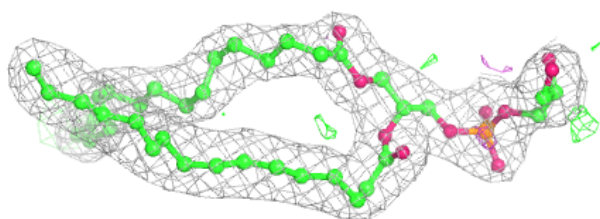
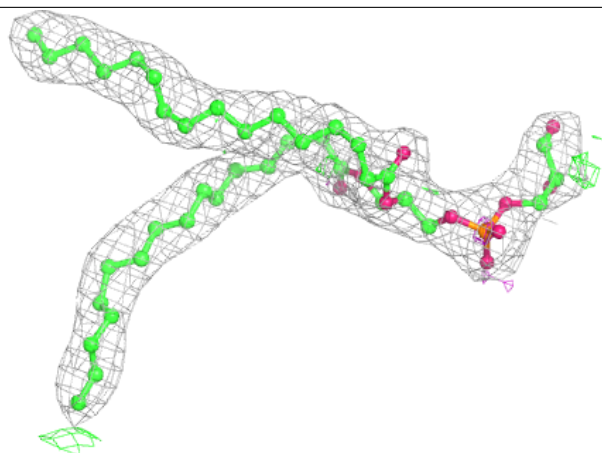
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



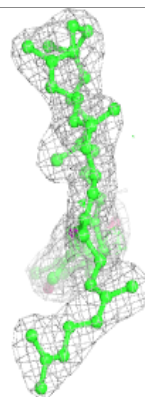
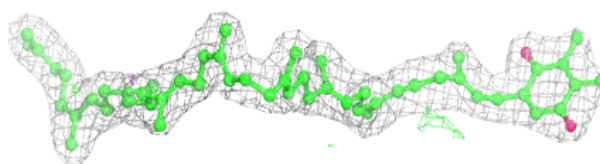
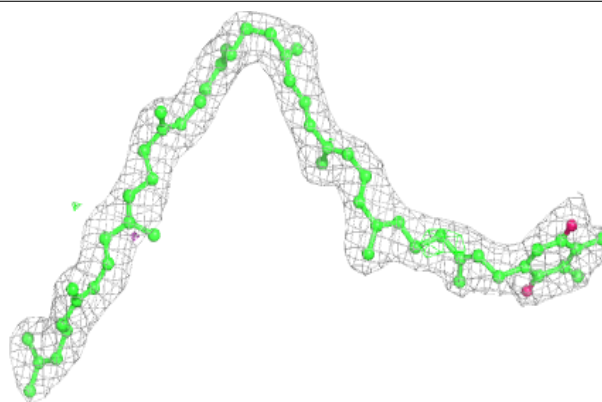


**Electron density around LHG D 409:**

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

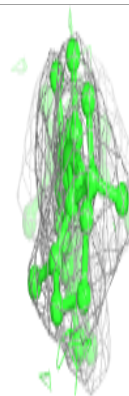
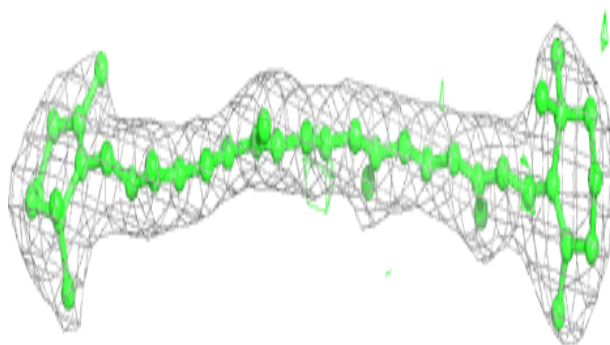
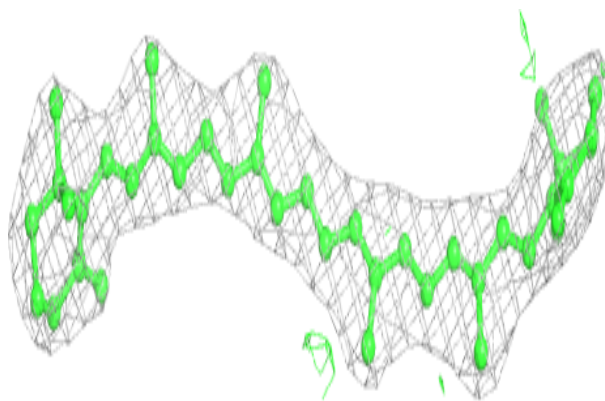
**Electron density around PL9 d 408:**

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



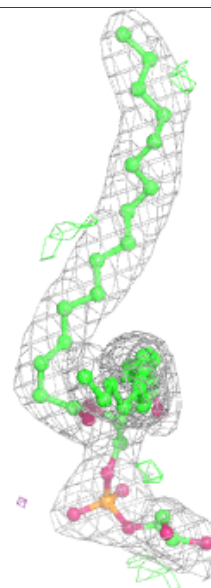
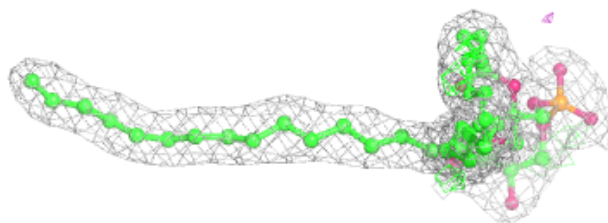
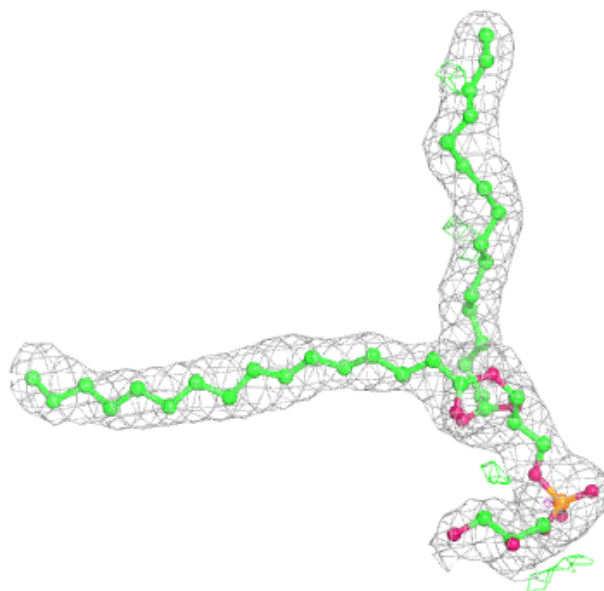
**Electron density around BCR Y 102:**

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



**Electron density around LHG L 101:**

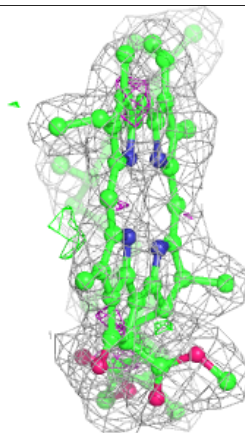
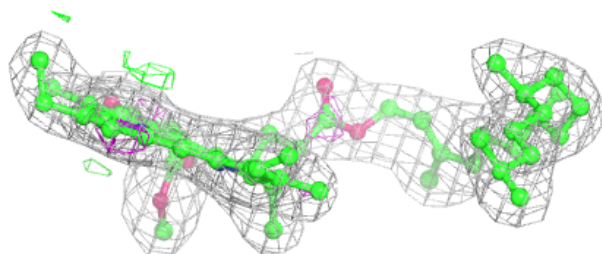
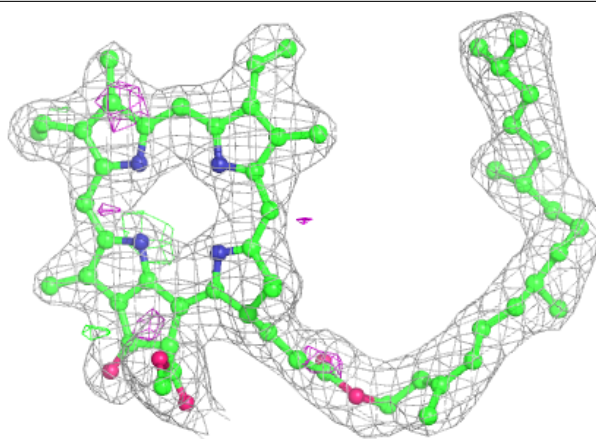
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





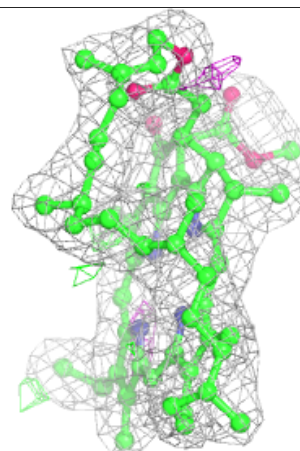
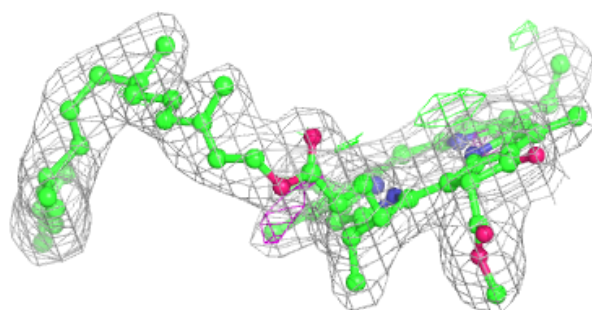
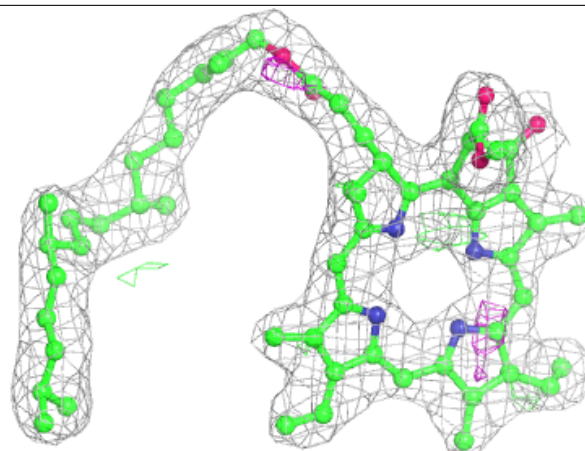
**Electron density around PHO A 408:**

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

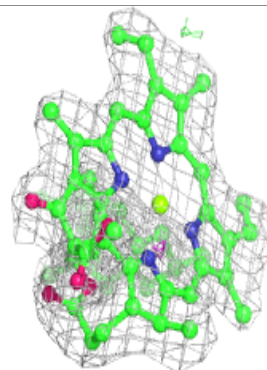
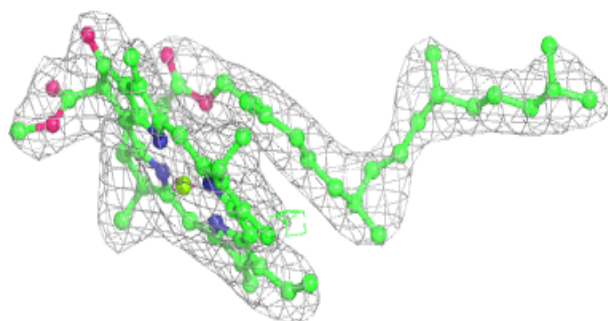
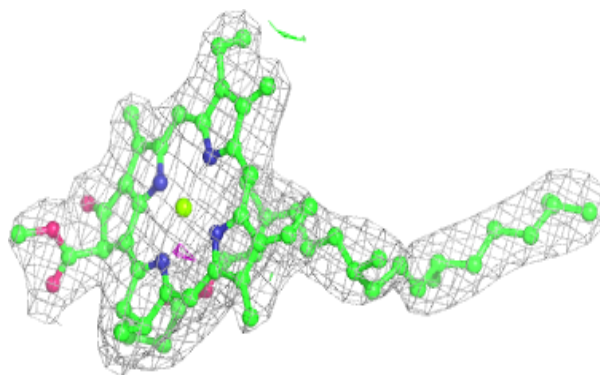


**Electron density around PHO d 403:**

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

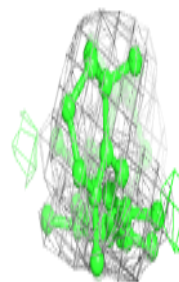
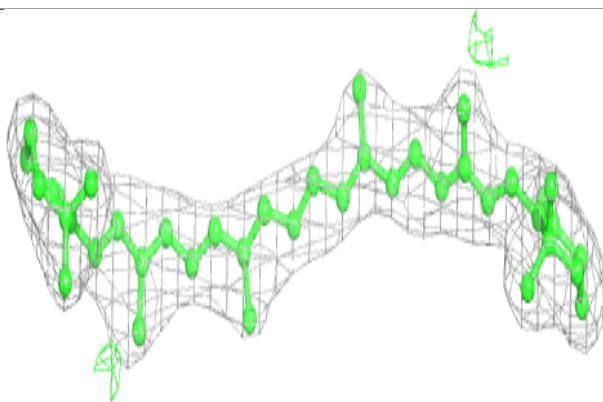
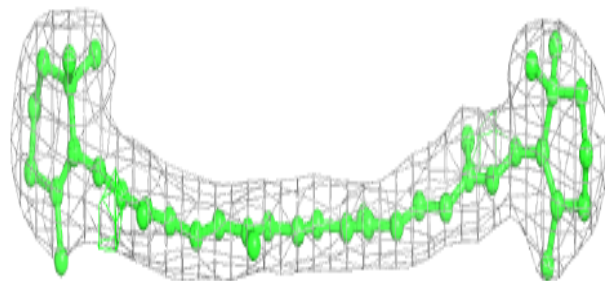
**Electron density around CLA C 505:**

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

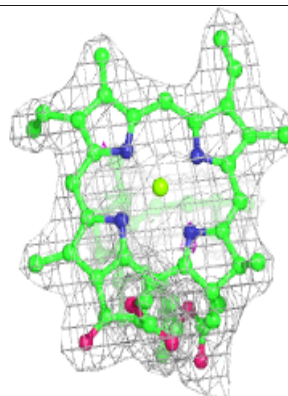
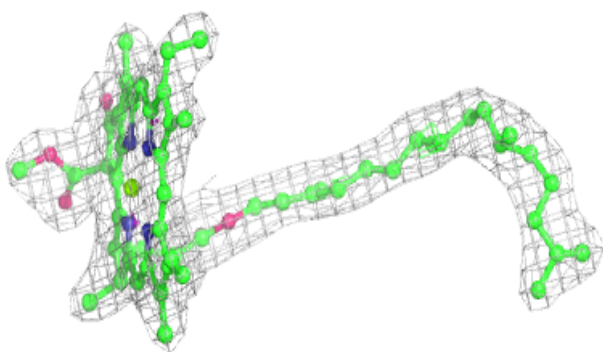
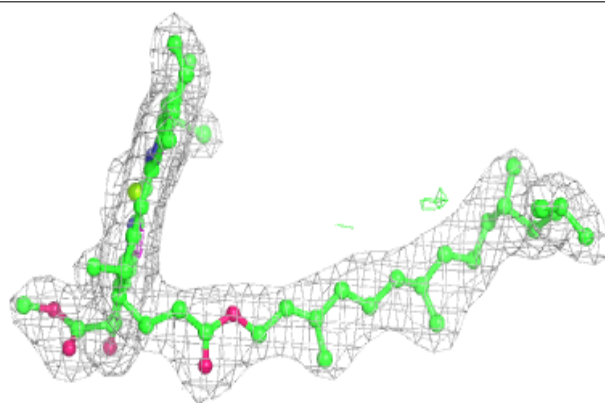


**Electron density around BCR K 101:**

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

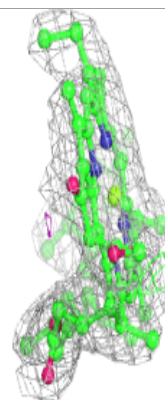
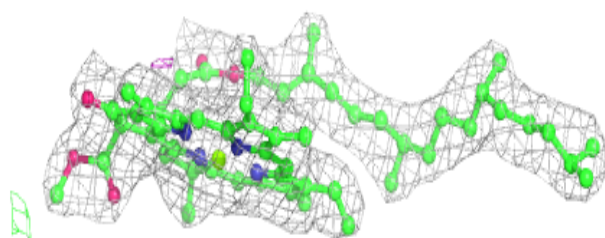
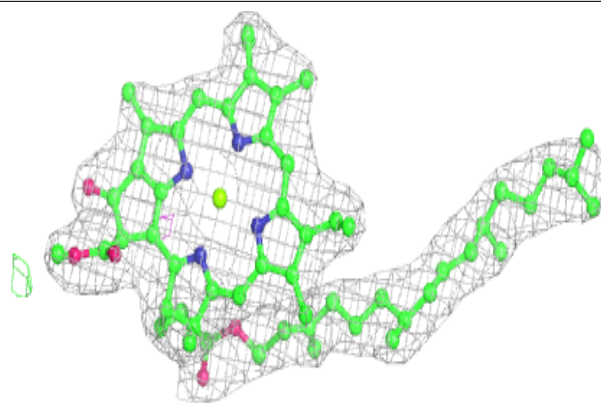
**Electron density around CLA B 606:**

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

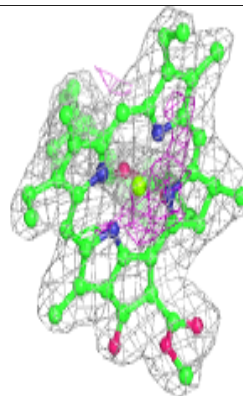
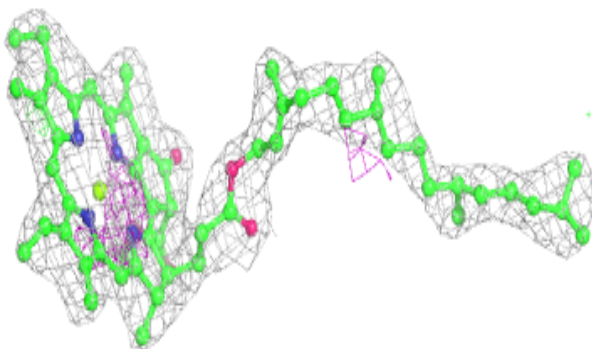
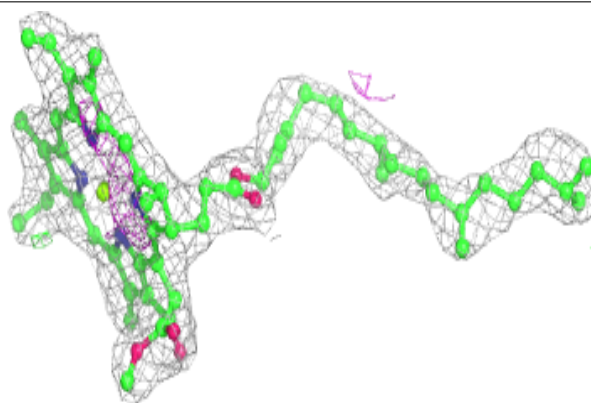


**Electron density around CLA c 902:**

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

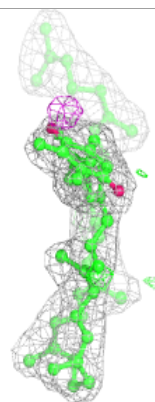
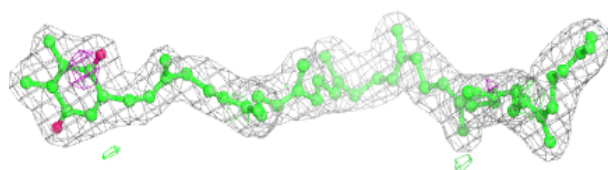
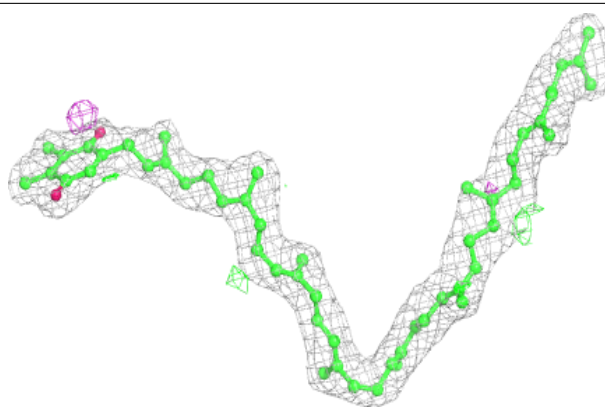
**Electron density around CLA c 903:**

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

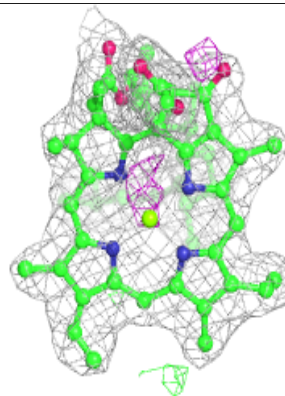
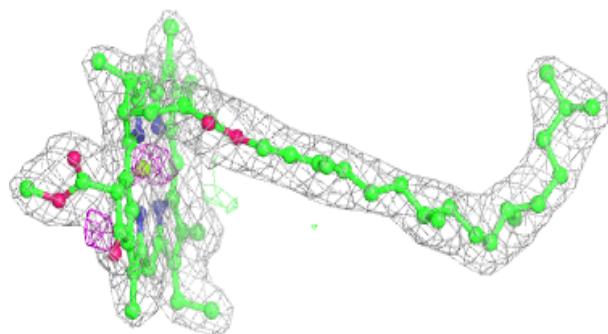
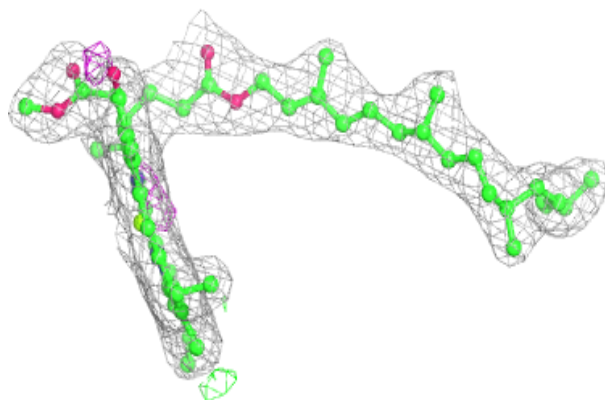


**Electron density around PL9 D 407:**

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

**Electron density around CLA b 610:**

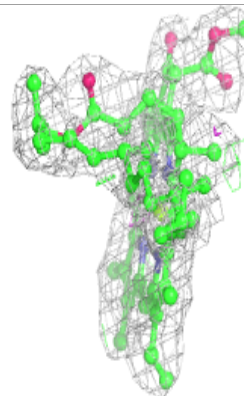
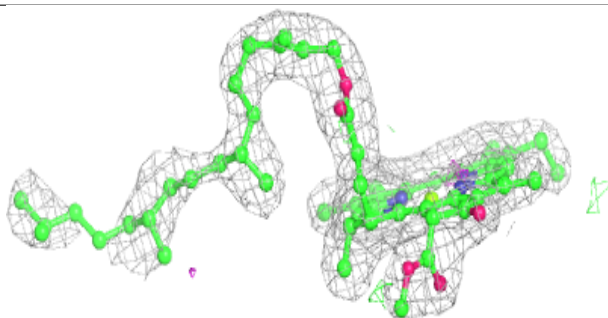
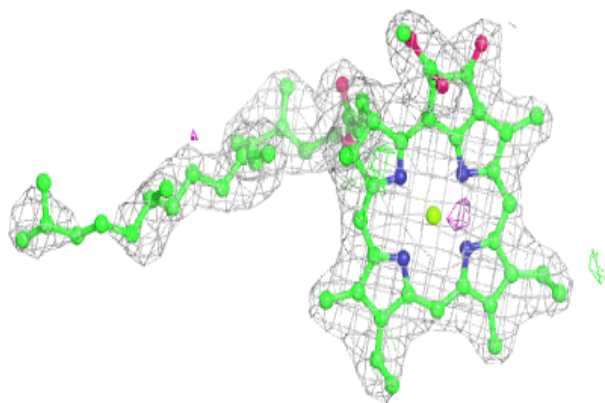
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



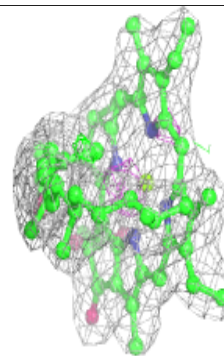
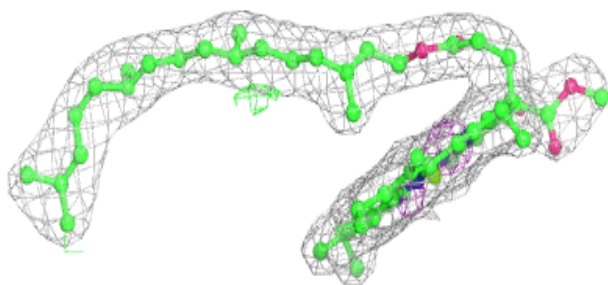
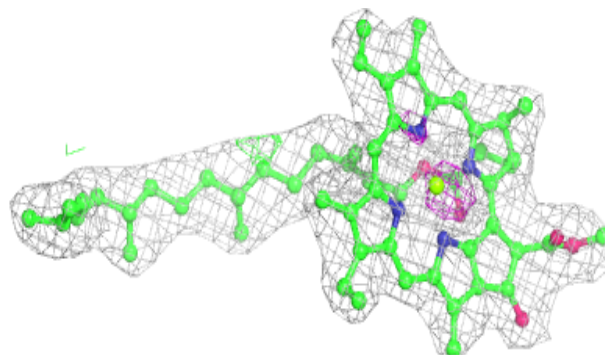


**Electron density around CLA A 407:**

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

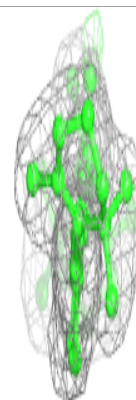
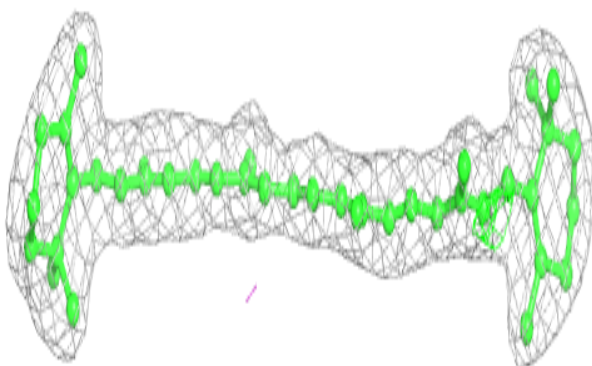
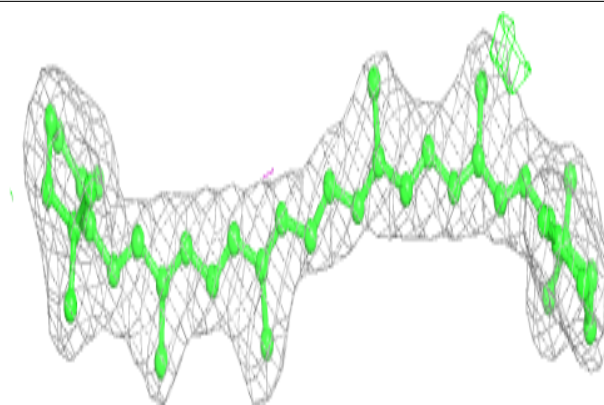
**Electron density around CLA B 609:**

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

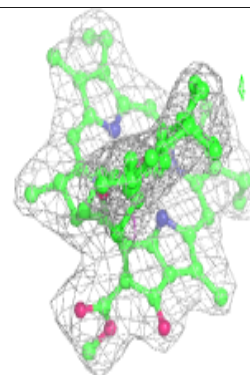
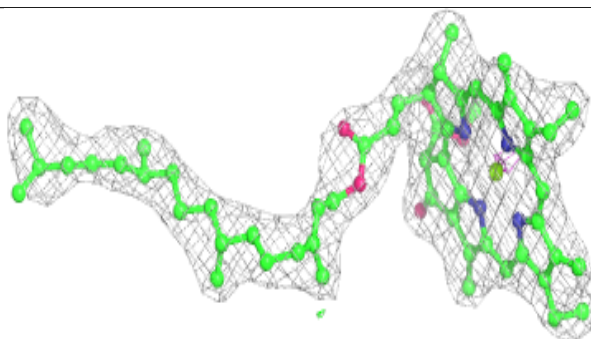
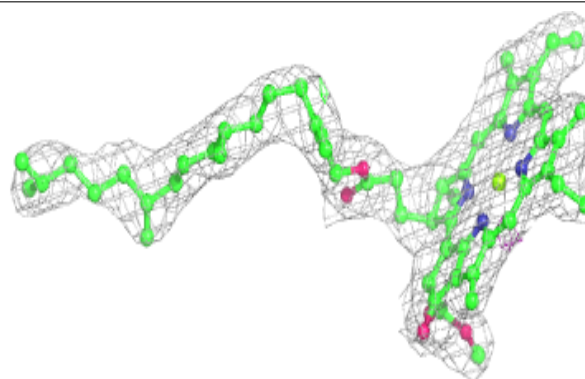


**Electron density around BCR A 410:**

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

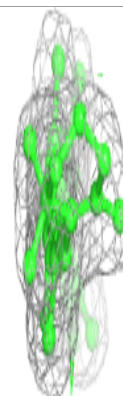
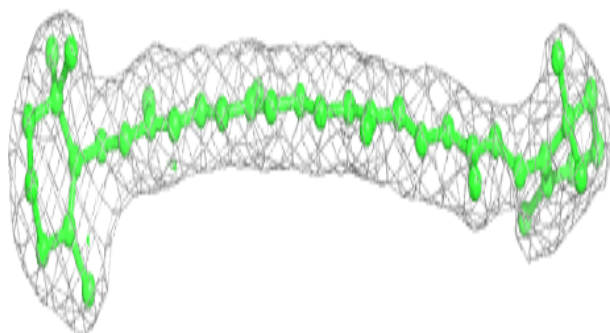
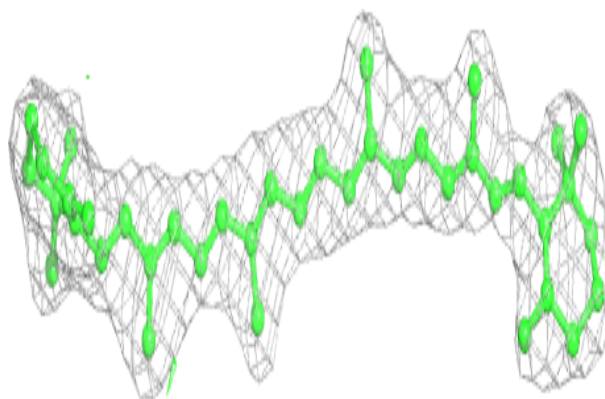
**Electron density around CLA C 502:**

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

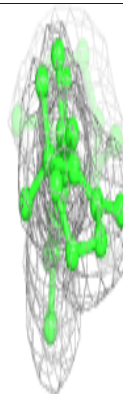
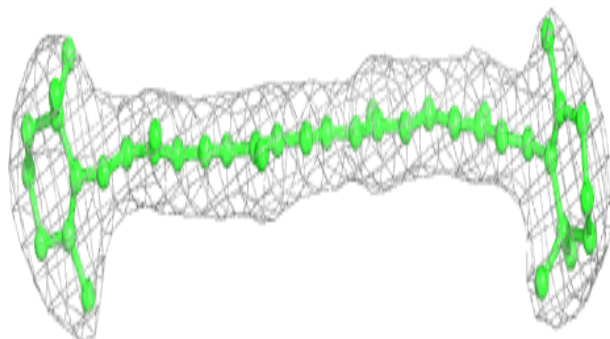
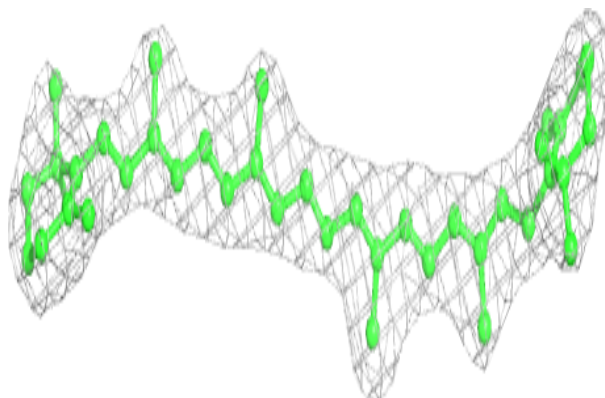


**Electron density around BCR b 622:**

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

**Electron density around BCR c 915:**

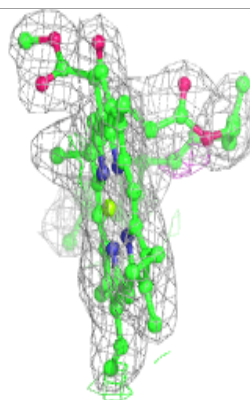
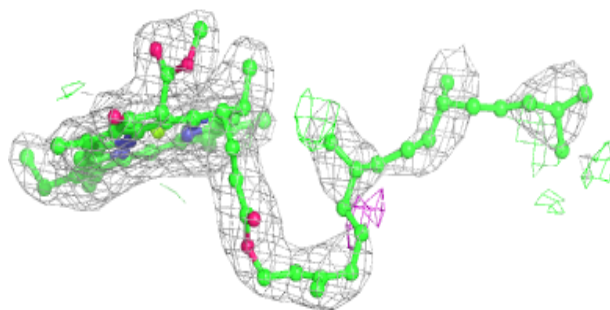
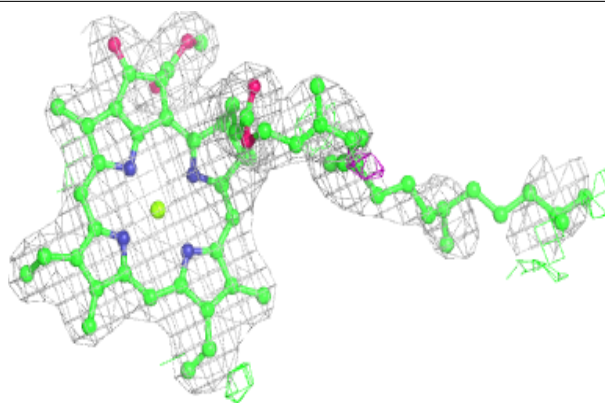
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



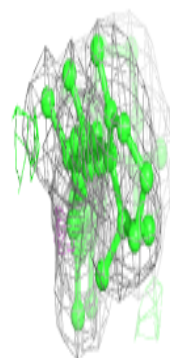
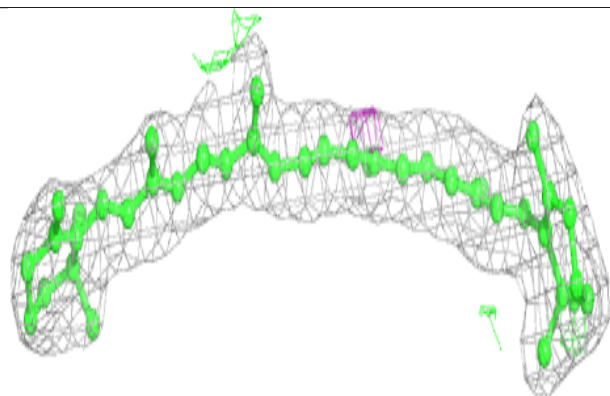
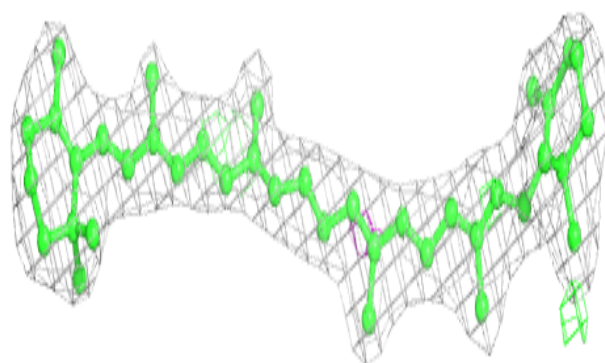


**Electron density around CLA a 406:**

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

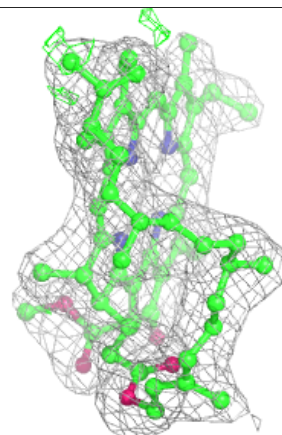
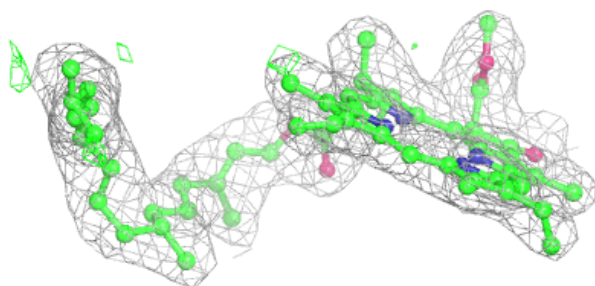
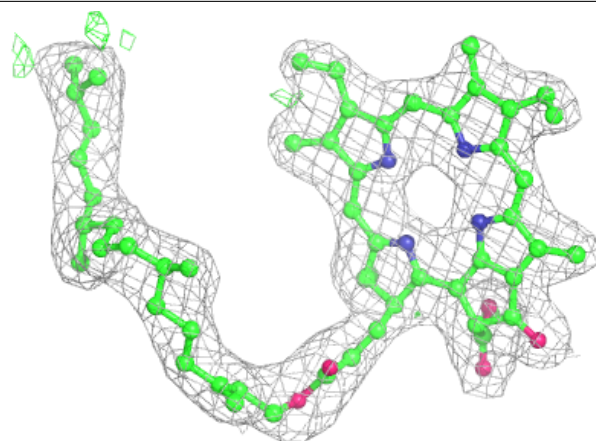
**Electron density around BCR T 102:**

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

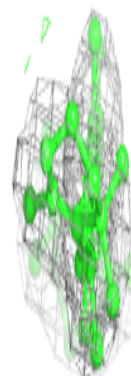
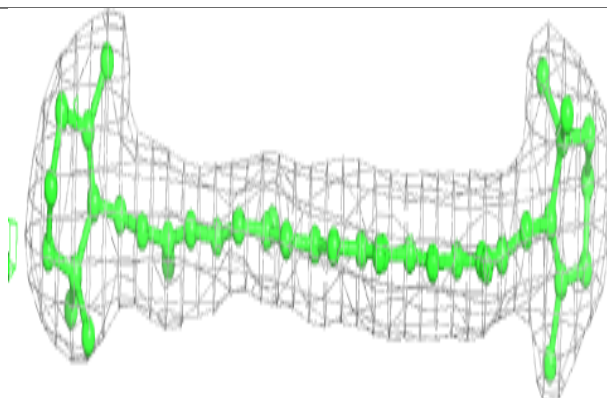
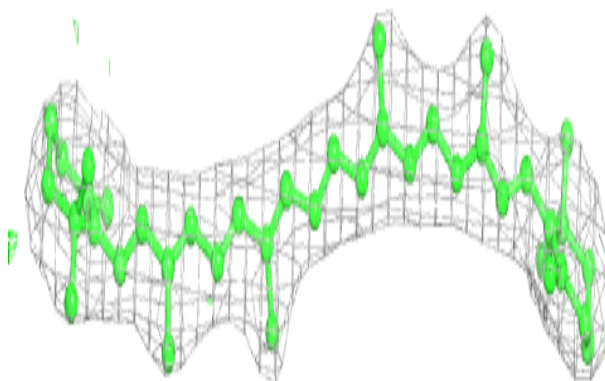


**Electron density around PHO D 401:**

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

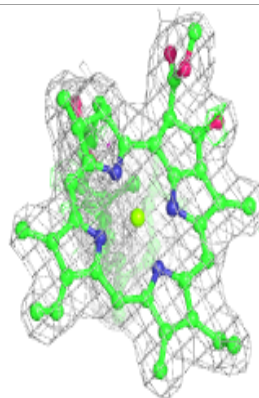
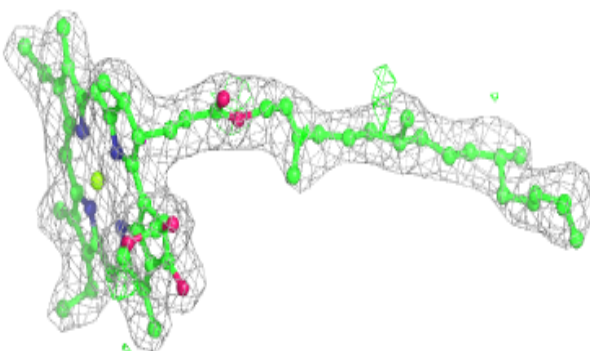
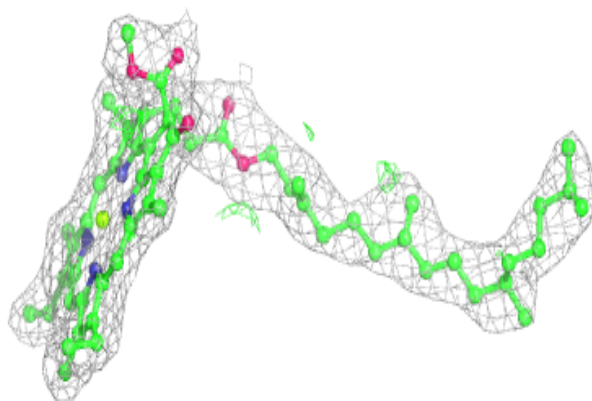
**Electron density around BCR C 515:**

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

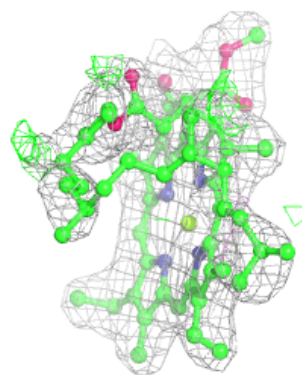
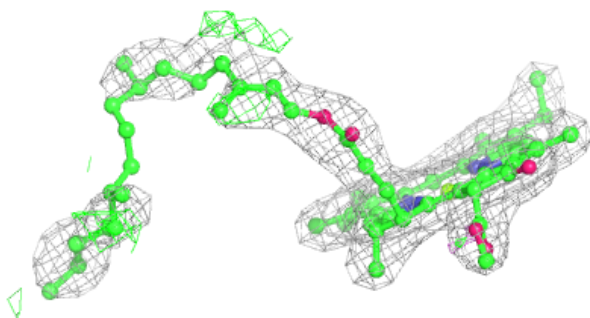
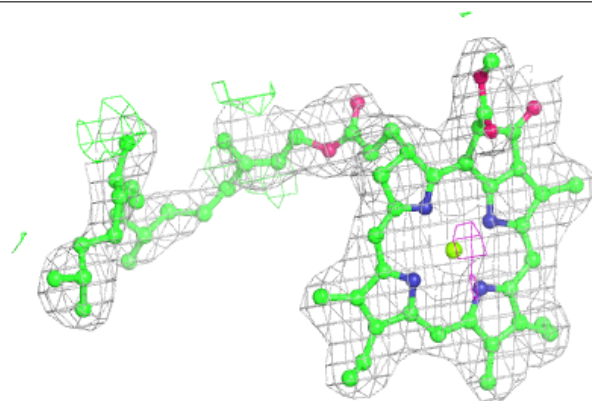


**Electron density around CLA b 609:**

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

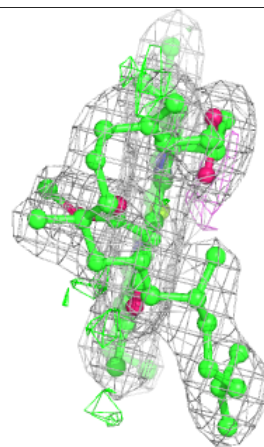
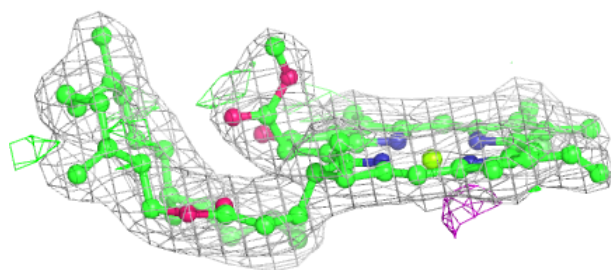
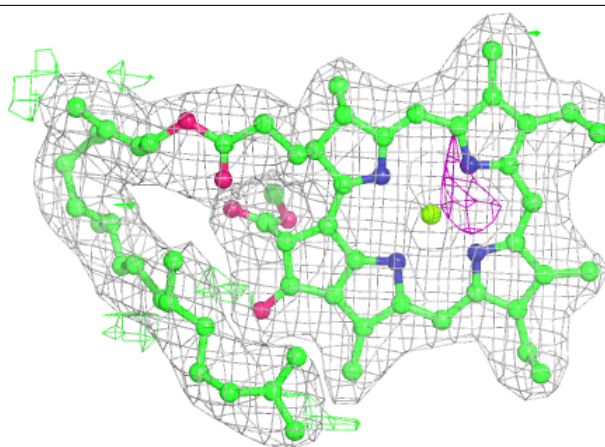
**Electron density around CLA A 409:**

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

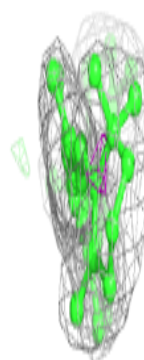
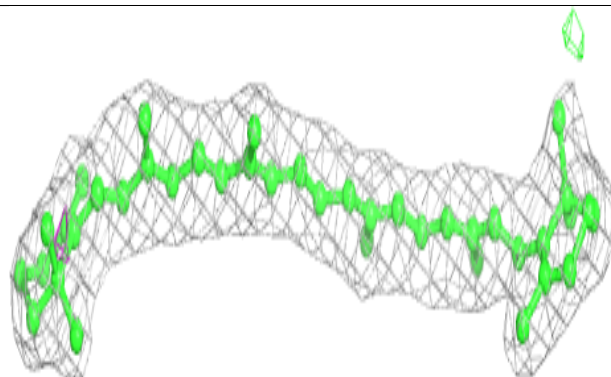
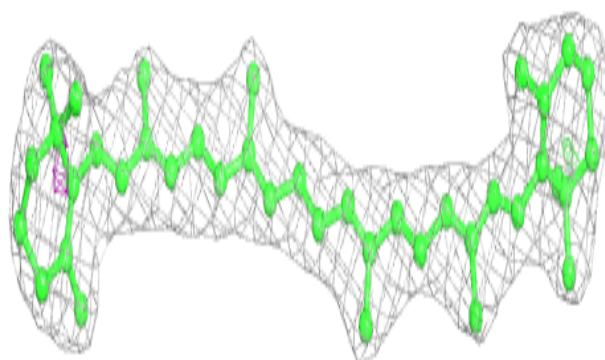


**Electron density around CLA B 611:**

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

**Electron density around BCR b 624:**

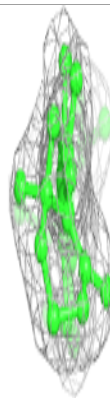
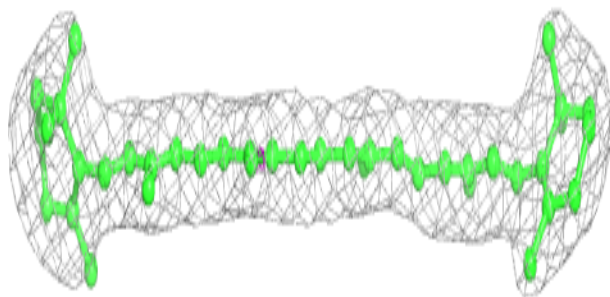
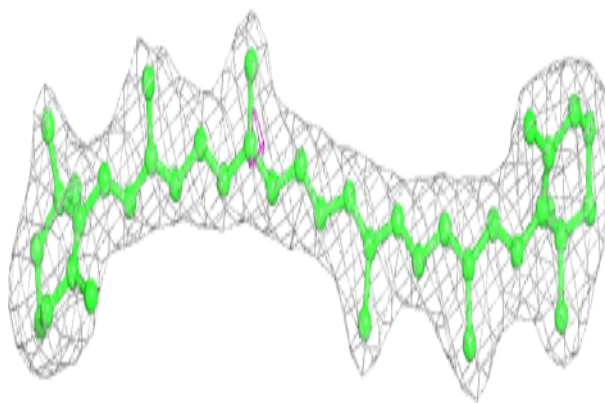
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





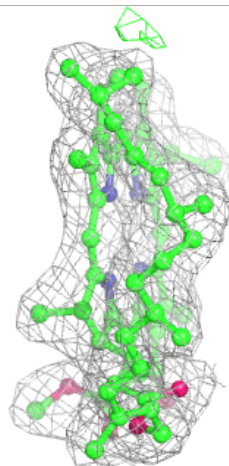
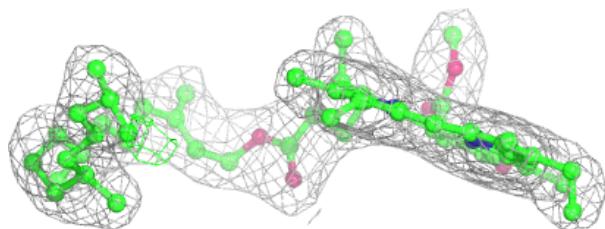
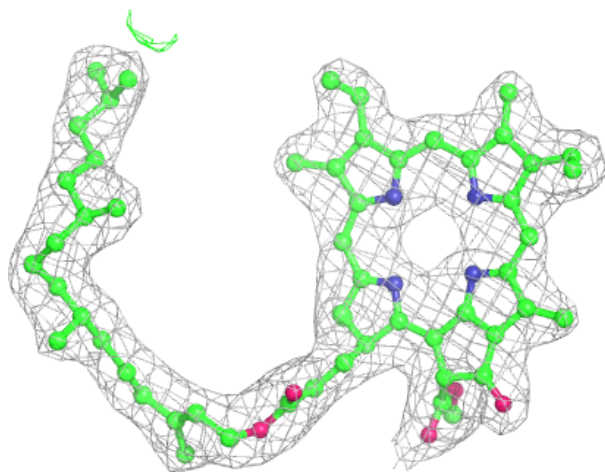
**Electron density around BCR B 619:**

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



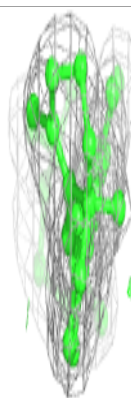
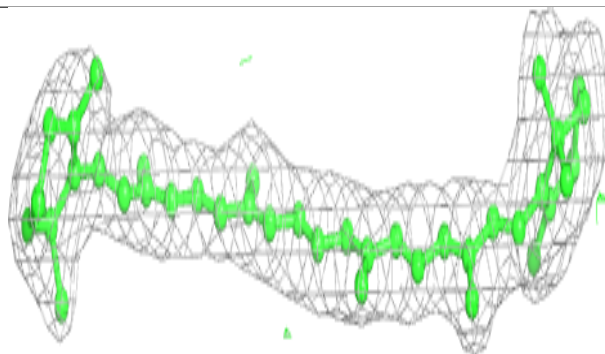
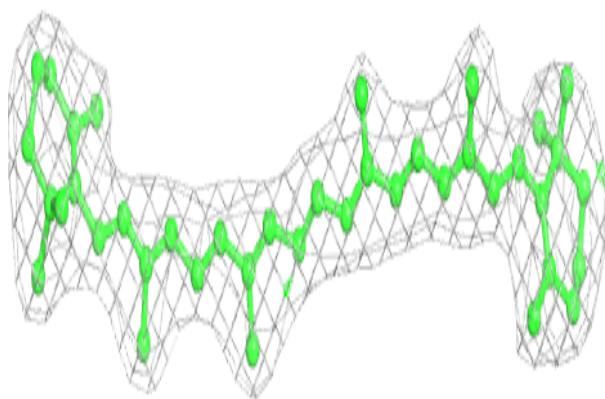
**Electron density around PHO a 407:**

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



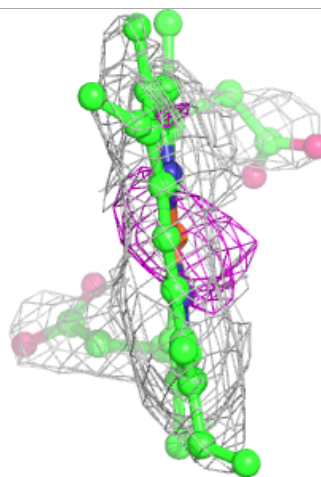
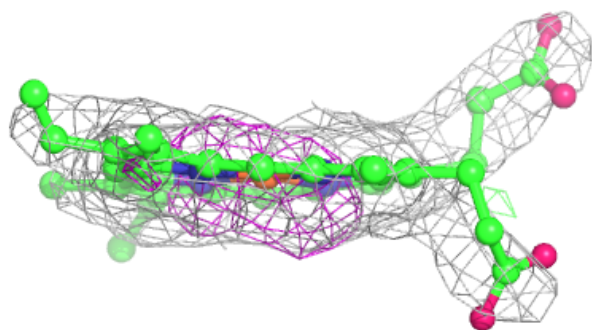
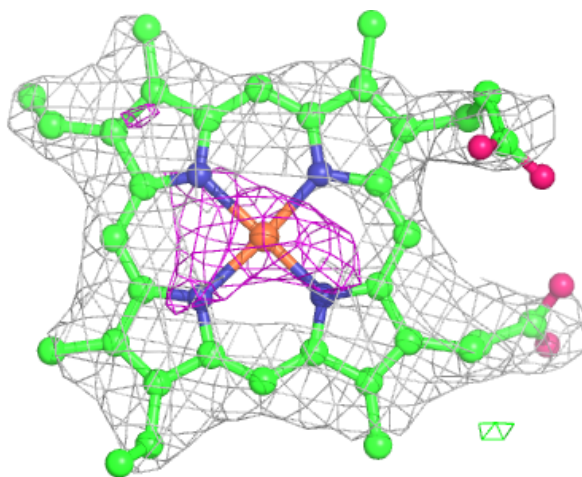
**Electron density around BCR B 620:**

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



**Electron density around HEM f 101:**

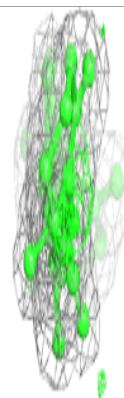
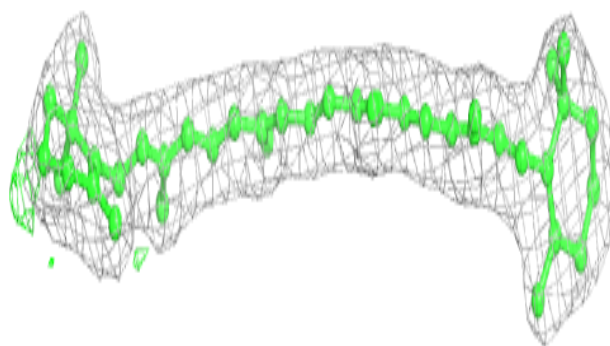
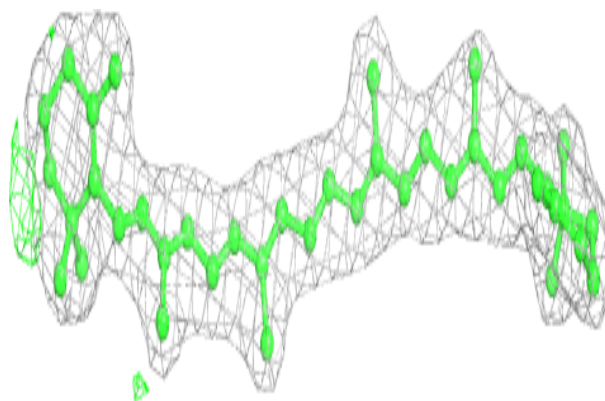
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





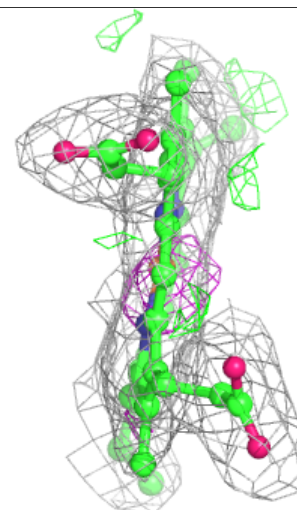
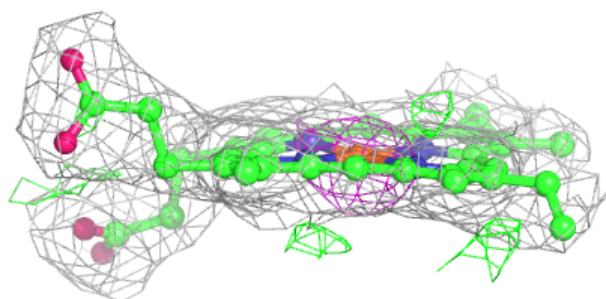
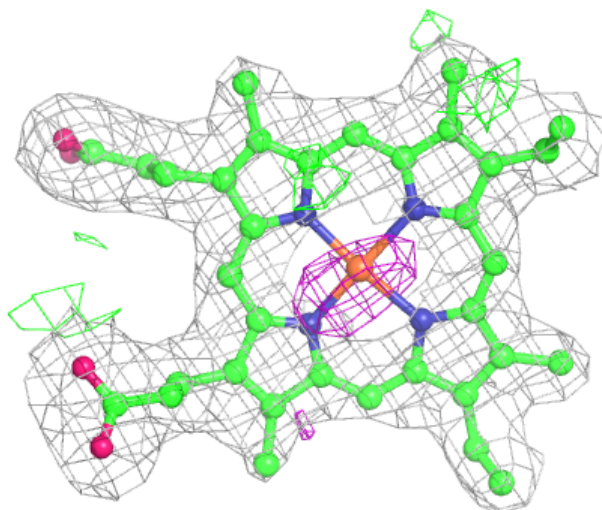
**Electron density around BCR B 618:**

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



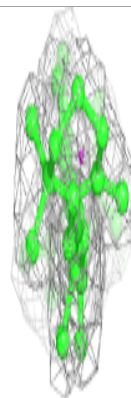
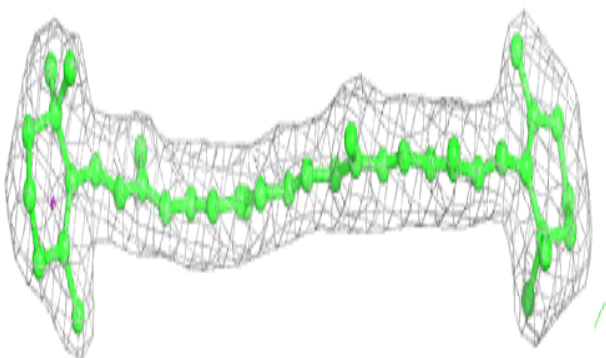
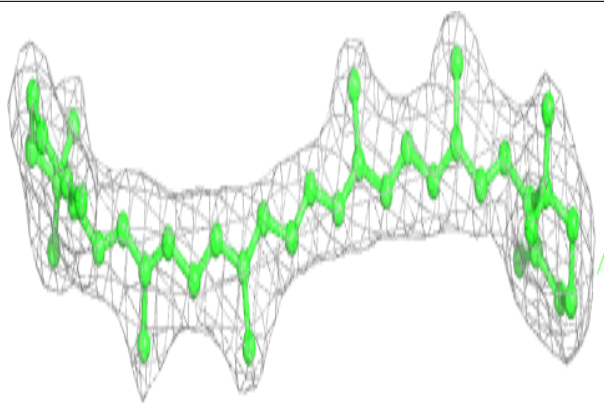
**Electron density around HEM V 202:**

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

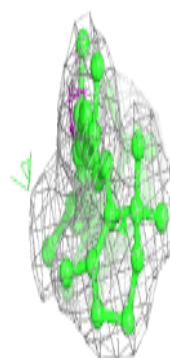
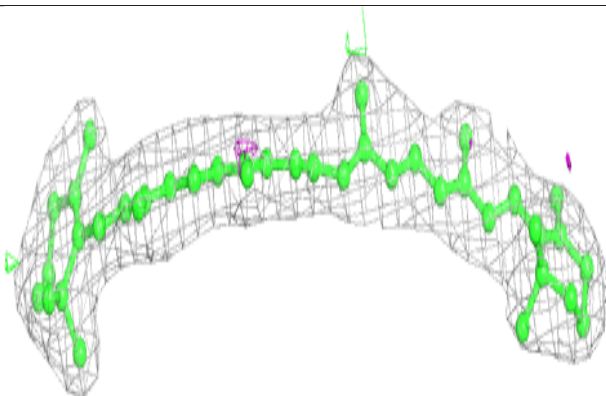
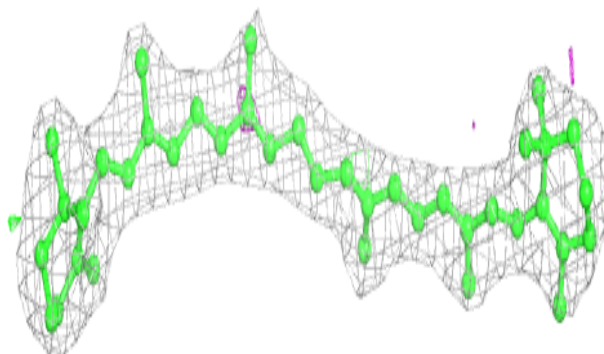


**Electron density around BCR a 409:**

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

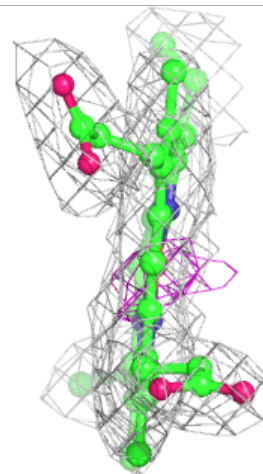
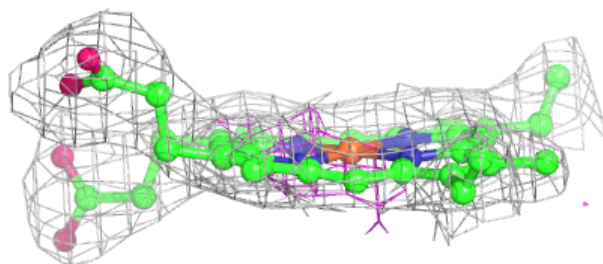
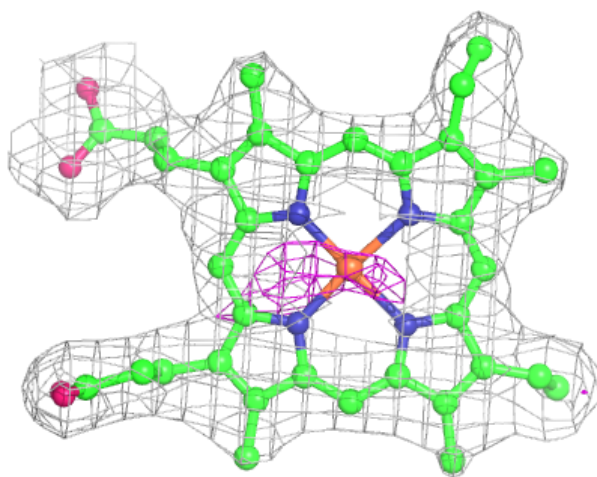
**Electron density around BCR t 102:**

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



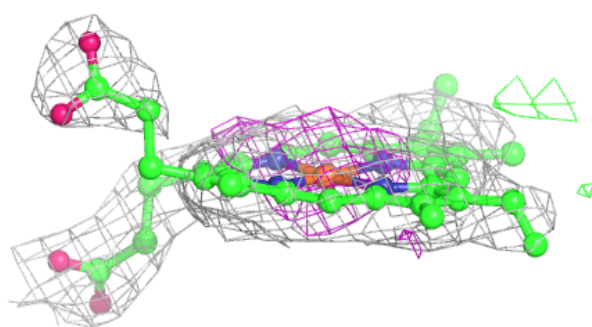
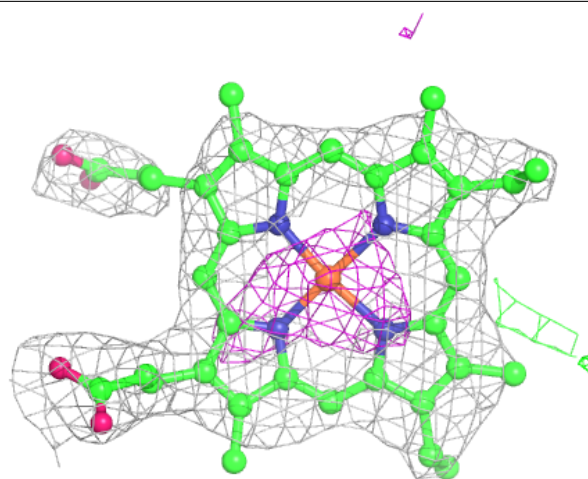
**Electron density around HEM v 202:**

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



**Electron density around HEM 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.